Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 06:56 PM JST

PDB ID	:	6IGZ / pdb_00006igz
EMDB ID	:	EMD-9670
Title	:	Structure of PSI-LHCI
Authors	:	Xiong, P.; Xiaochun, Q.
Deposited on	:	2018-09-27
Resolution	:	3.49 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

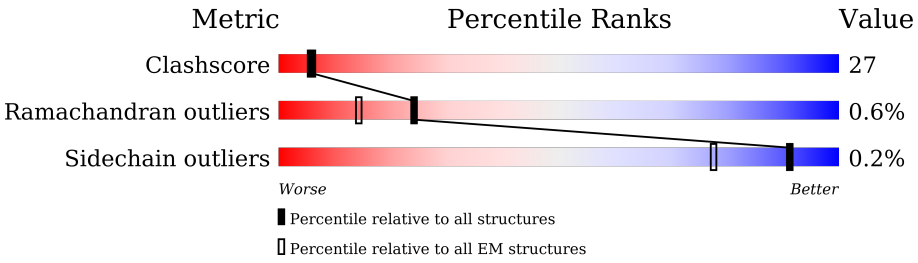
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	7% 58% 40% ··
2	B	734	8% 56% 43%
3	C	81	11% 51% 47% ··
4	D	198	16% 44% 27% ·· 28%
5	E	91	18% 46% 21% 33%
6	F	236	15% 41% 28% 31%
7	G	167	54% 30% 25% 45%
8	H	133	66% 35% 28% · 34%

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Mol	Chain	Length	Quality of chain
9	I	36	33% 56% 33% 11%
10	J	41	24% 71% 29%
11	K	123	28% 37% 26% 35%
12	L	204	59% 47% 27% 24%
13	1	226	22% 48% 37% 15%
13	5	226	35% 48% 37% 14%
14	2	256	6% 51% 32% 17%
15	3	281	6% 51% 28% 20%
16	4	248	15% 50% 34% 17%
16	8	248	21% 44% 38% 17%
17	6	267	13% 47% 39% 14%
18	7	264	12% 47% 39% 14%
19	9	222	38% 49% 33% 18%
20	0	245	68% 47% 35% 18%
21	M	32	28% 75% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	0	302	X	-	-	-
22	CLA	0	303	X	-	-	-
22	CLA	0	304	X	-	-	-
22	CLA	0	305	X	-	-	-
22	CLA	0	307	X	-	-	-
22	CLA	0	308	X	-	-	-
22	CLA	0	309	X	-	-	-
22	CLA	0	310	X	-	-	-
22	CLA	0	311	X	-	-	-
22	CLA	0	312	X	-	-	-
22	CLA	1	301	X	-	-	-
22	CLA	1	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	303	X	-	-	-
22	CLA	1	304	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	307	X	-	-	-
22	CLA	1	308	X	-	-	-
22	CLA	1	309	X	-	-	-
22	CLA	1	310	X	-	-	-
22	CLA	1	311	X	-	-	-
22	CLA	1	312	X	-	-	-
22	CLA	1	313	X	-	-	-
22	CLA	2	302	X	-	-	-
22	CLA	2	303	X	-	-	-
22	CLA	2	304	X	-	-	-
22	CLA	2	308	X	-	-	-
22	CLA	2	309	X	-	-	-
22	CLA	2	310	X	-	-	-
22	CLA	2	311	X	-	-	-
22	CLA	2	312	X	-	-	-
22	CLA	2	313	X	-	-	-
22	CLA	2	314	X	-	-	-
22	CLA	2	319	X	-	-	-
22	CLA	3	301	X	-	-	-
22	CLA	3	302	X	-	-	-
22	CLA	3	303	X	-	-	-
22	CLA	3	304	X	-	-	-
22	CLA	3	305	X	-	-	-
22	CLA	3	307	X	-	-	-
22	CLA	3	308	X	-	-	-
22	CLA	3	309	X	-	-	-
22	CLA	3	310	X	-	-	-
22	CLA	3	311	X	-	-	-
22	CLA	3	312	X	-	-	-
22	CLA	3	313	X	-	-	-
22	CLA	3	319	X	-	-	-
22	CLA	4	302	X	-	-	-
22	CLA	4	303	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	4	308	X	-	-	-
22	CLA	4	309	X	-	-	-
22	CLA	4	310	X	-	-	-
22	CLA	4	311	X	-	-	-
22	CLA	4	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	4	313	X	-	-	-
22	CLA	4	314	X	-	-	-
22	CLA	5	302	X	-	-	-
22	CLA	5	304	X	-	-	-
22	CLA	5	305	X	-	-	-
22	CLA	5	307	X	-	-	-
22	CLA	5	308	X	-	-	-
22	CLA	5	309	X	-	-	-
22	CLA	5	310	X	-	-	-
22	CLA	5	311	X	-	-	-
22	CLA	5	312	X	-	-	-
22	CLA	5	313	X	-	-	-
22	CLA	5	314	X	-	-	-
22	CLA	6	301	X	-	-	-
22	CLA	6	303	X	-	-	-
22	CLA	6	304	X	-	-	-
22	CLA	6	305	X	-	-	-
22	CLA	6	309	X	-	-	-
22	CLA	6	310	X	-	-	-
22	CLA	6	311	X	-	-	-
22	CLA	6	312	X	-	-	-
22	CLA	6	313	X	-	-	-
22	CLA	6	314	X	-	-	-
22	CLA	6	315	X	-	-	-
22	CLA	6	317	X	-	-	-
22	CLA	6	318	X	-	-	-
22	CLA	6	323	X	-	-	-
22	CLA	7	302	X	-	-	-
22	CLA	7	303	X	-	-	-
22	CLA	7	304	X	-	-	-
22	CLA	7	305	X	-	-	-
22	CLA	7	306	X	-	-	-
22	CLA	7	307	X	-	-	-
22	CLA	7	309	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	313	X	-	-	-
22	CLA	7	314	X	-	-	-
22	CLA	7	315	X	-	-	-
22	CLA	7	316	X	-	-	-
22	CLA	7	317	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	7	318	X	-	-	-
22	CLA	8	302	X	-	-	-
22	CLA	8	303	X	-	-	-
22	CLA	8	304	X	-	-	-
22	CLA	8	308	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-
22	CLA	8	312	X	-	-	-
22	CLA	8	313	X	-	-	-
22	CLA	8	315	X	-	-	-
22	CLA	9	301	X	-	-	-
22	CLA	9	303	X	-	-	-
22	CLA	9	304	X	-	-	-
22	CLA	9	305	X	-	-	-
22	CLA	9	306	X	-	-	-
22	CLA	9	308	X	-	-	-
22	CLA	9	309	X	-	-	-
22	CLA	9	310	X	-	-	-
22	CLA	9	311	X	-	-	-
22	CLA	9	312	X	-	-	-
22	CLA	9	313	X	-	-	-
22	CLA	A	801	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	852	X	-	-	-
22	CLA	A	853	X	-	-	-
22	CLA	B	801	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	B	850	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	G	101	X	-	-	-
22	CLA	G	102	X	-	-	-
22	CLA	G	103	X	-	-	-
22	CLA	H	201	X	-	-	-
22	CLA	J	103	X	-	-	-
22	CLA	K	101	X	-	-	-
22	CLA	K	102	X	-	-	-
22	CLA	K	104	X	-	-	-
22	CLA	K	105	X	-	-	-
22	CLA	L	201	X	-	-	-
22	CLA	L	202	X	-	-	-
22	CLA	L	203	X	-	-	-
22	CLA	L	204	X	-	-	-
25	8CT	7	323	-	-	X	-
29	CHL	0	301	X	-	-	-
29	CHL	0	306	X	-	-	-
29	CHL	1	305	X	-	-	-
29	CHL	2	301	X	-	-	-
29	CHL	2	305	X	-	-	-
29	CHL	2	306	X	-	-	-
29	CHL	2	307	X	-	-	-
29	CHL	3	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CHL	4	301	X	-	-	-
29	CHL	4	305	X	-	-	-
29	CHL	4	306	X	-	-	-
29	CHL	4	307	X	-	-	-
29	CHL	5	301	X	-	-	-
29	CHL	5	306	X	-	-	-
29	CHL	6	302	X	-	-	-
29	CHL	6	306	X	-	-	-
29	CHL	6	307	X	-	-	-
29	CHL	6	308	X	-	-	-
29	CHL	6	316	X	-	-	-
29	CHL	7	308	X	-	-	-
29	CHL	8	305	X	-	-	-
29	CHL	8	306	X	-	-	-
29	CHL	8	307	X	-	-	-
29	CHL	8	314	X	-	-	-
29	CHL	9	302	X	-	-	-
29	CHL	9	307	X	-	-	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 51585 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	740	5819	3803	988	1006	22	0	0

- Molecule 2 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5824	3824	979	1002	19	0	0

- Molecule 3 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	602	370	105	116	11	0	0

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	142	1109	709	193	202	5	0	0

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	61	488	308	87	92	1	0	0

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	163	1257	799	219	233	6	0	0

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	92	Total	C	N	O	0	0
			714	462	118	134		

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	88	Total	C	N	O	S	0	0
			677	426	119	131	1		

- Molecule 9 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	32	Total	C	N	O	S	0	0
			243	168	34	39	2		

- Molecule 10 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			336	232	49	54	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	80	Total	C	N	O	S	0	0
			558	363	92	100	3		

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	155	Total	C	N	O	S	0	0
			1139	736	187	212	4		

- Molecule 13 is a protein called Lhca-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	193	Total	C	N	O	S	0	0
			1466	942	241	271	12		
13	5	195	Total	C	N	O	S	0	0
			1484	956	243	273	12		

- Molecule 14 is a protein called Lhca-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	212	Total	C	N	O	S	0	0
			1641	1066	265	298	12		

- Molecule 15 is a protein called Lhca-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	226	Total	C	N	O	S	0	0
			1751	1132	283	326	10		

- Molecule 16 is a protein called Lhca-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	207	Total	C	N	O	S	0	0
			1589	1046	258	276	9		
16	8	205	Total	C	N	O	S	0	0
			1574	1035	256	274	9		

- Molecule 17 is a protein called Lhca-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	229	Total	C	N	O	S	0	0
			1797	1182	292	313	10		

- Molecule 18 is a protein called Lhca-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	7	228	Total	C	N	O	S	0	0
			1758	1137	291	319	11		

- Molecule 19 is a protein called Lhca-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	9	183	Total	C	N	O	S	0	0
			1416	913	235	259	9		

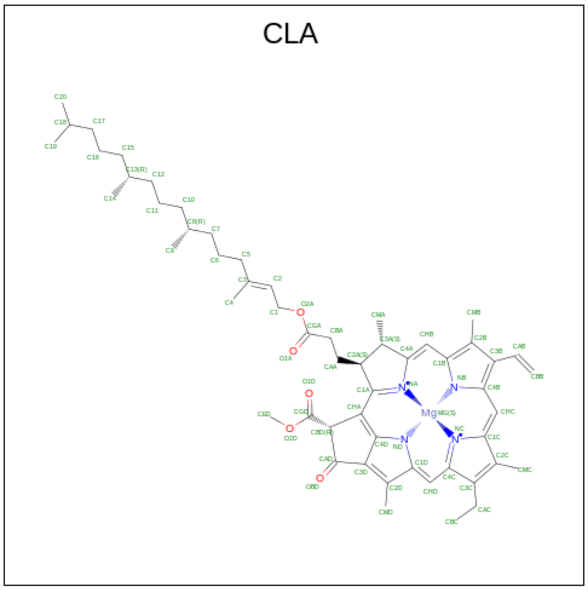
- Molecule 20 is a protein called Lhca-j.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	0	202	Total	C	N	O	S	0	0
			1560	1014	255	280	11		

- Molecule 21 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	M	31	238	158	37	43	0	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	A	1	65	55	1	4	5	0
22	A	1	65	55	1	4	5	0
22	A	1	65	55	1	4	5	0
22	A	1	55	45	1	4	5	0
22	A	1	65	55	1	4	5	0
22	A	1	65	55	1	4	5	0
22	A	1	65	55	1	4	5	0
22	A	1	65	55	1	4	5	0
22	A	1	65	55	1	4	5	0
22	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
22	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	7	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
22	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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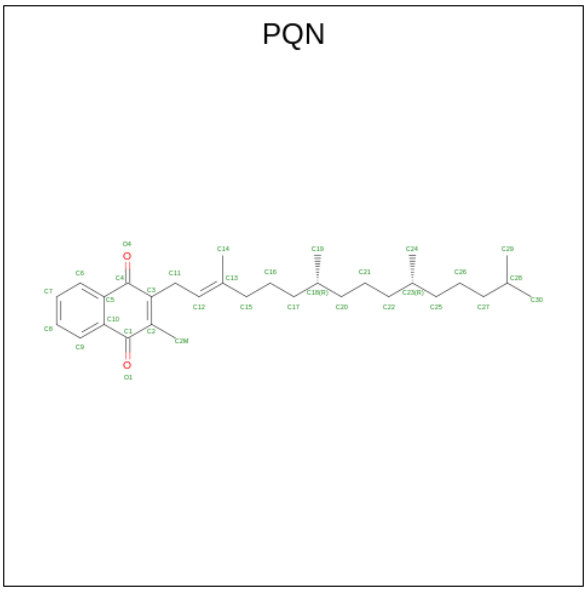
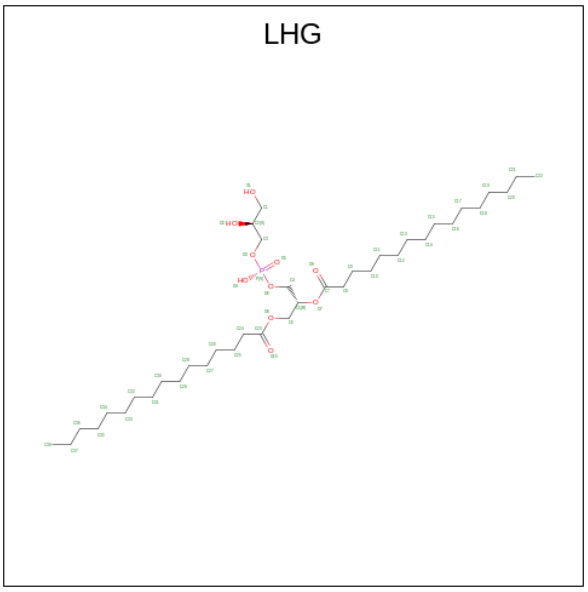
Mol	Chain	Residues	Atoms					AltConf
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	0	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			33	31	2	
23	B	1	Total	C	O	0
			33	31	2	

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			49	38	10	1	

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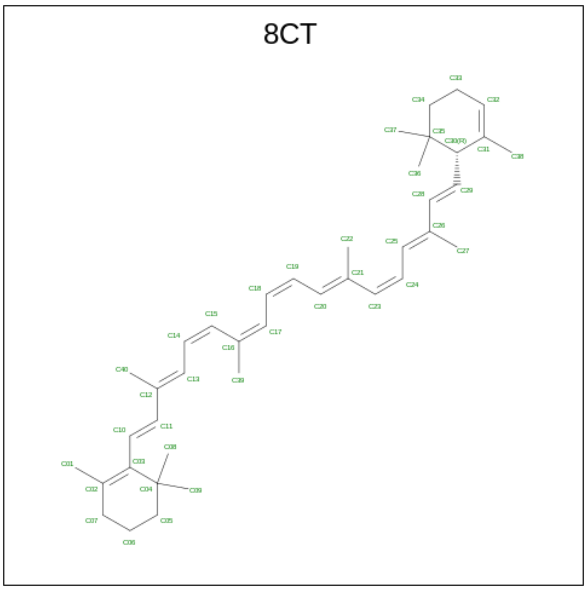
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C O P 27 16 10 1	0
24	B	1	Total C O P 23 12 10 1	0
24	1	1	Total C O P 49 38 10 1	0
24	2	1	Total C O P 32 21 10 1	0
24	3	1	Total C O P 20 10 9 1	0
24	6	1	Total C O P 37 26 10 1	0
24	5	1	Total C O P 49 38 10 1	0
24	7	1	Total C O P 20 10 9 1	0
24	9	1	Total C O P 49 38 10 1	0
24	0	1	Total C O P 49 38 10 1	0

- Molecule 25 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0

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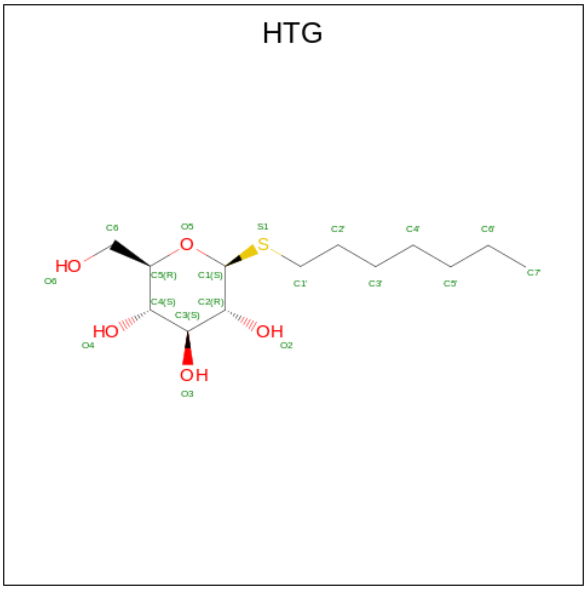
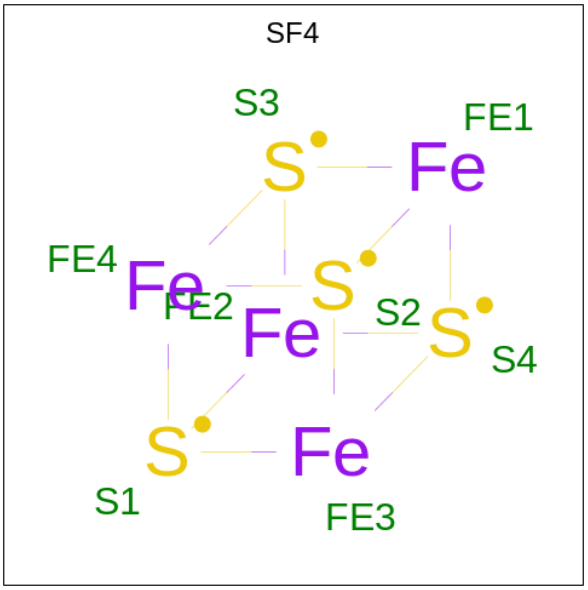
Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	5	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	8	1	Total C 40 40	0
25	8	1	Total C 40 40	0

- Molecule 26 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



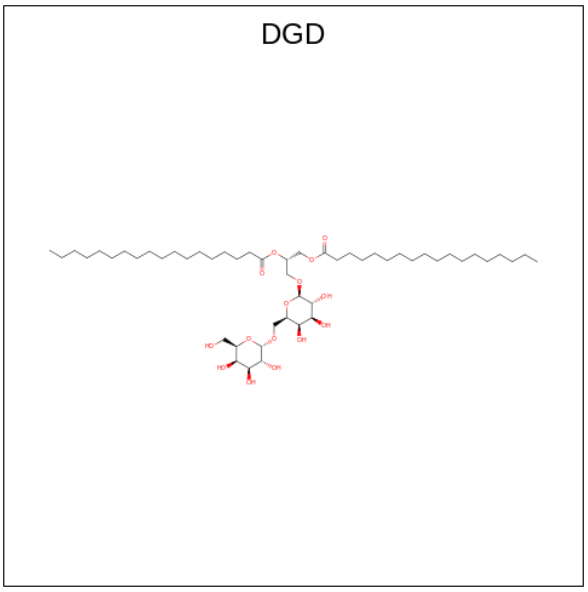
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			19	13	5	1	
26	J	1	Total	C	O	S	0
			19	13	5	1	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



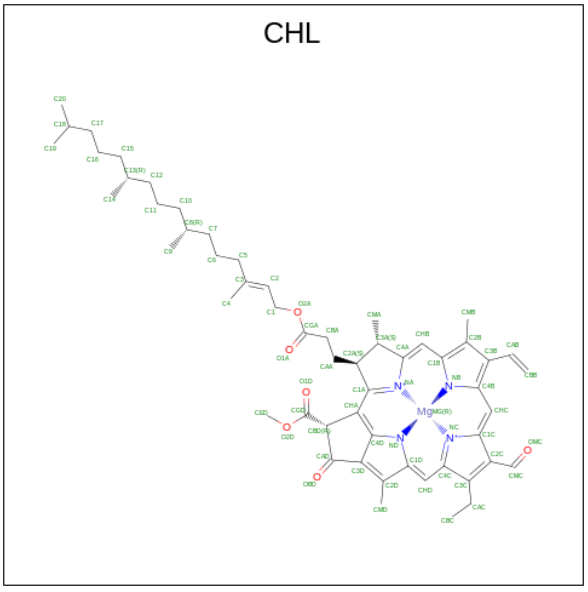
Mol	Chain	Residues	Atoms				AltConf
27	B	1	Total	Fe	S		0
			8	4	4		
27	C	1	Total	Fe	S		0
			8	4	4		
27	C	1	Total	Fe	S		0
			8	4	4		

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			66	51	15	

- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
29	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	5	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	5	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
29	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	9	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

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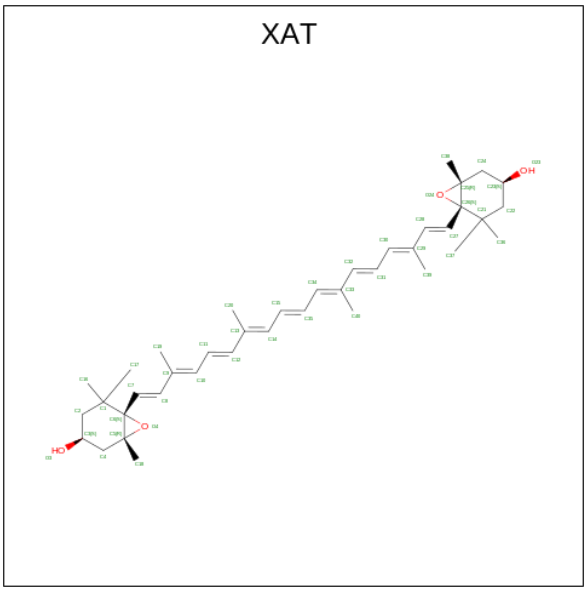
Mol	Chain	Residues	Atoms					AltConf
29	0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	0	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

- Molecule 30 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			44	40	4	
30	1	1	Total	C	O	0
			44	40	4	
30	2	1	Total	C	O	0
			44	40	4	
30	2	1	Total	C	O	0
			44	40	4	
30	3	1	Total	C	O	0
			44	40	4	
30	3	1	Total	C	O	0
			44	40	4	
30	4	1	Total	C	O	0
			44	40	4	
30	4	1	Total	C	O	0
			44	40	4	
30	6	1	Total	C	O	0
			44	40	4	

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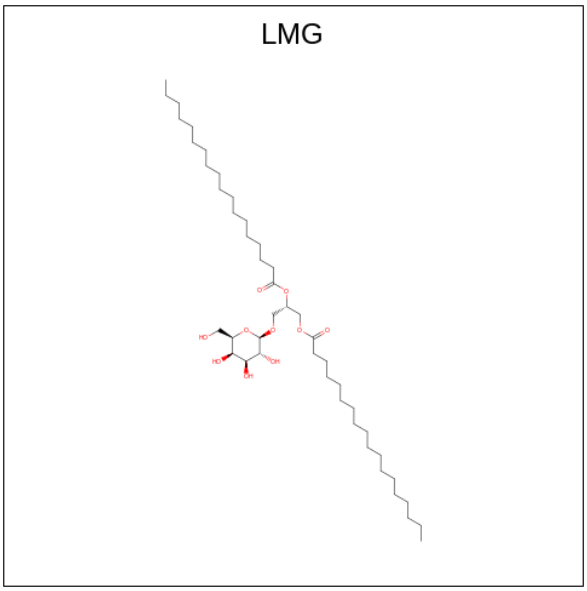
Mol	Chain	Residues	Atoms	AltConf
30	6	1	Total C O 44 40 4	0
30	5	1	Total C O 44 40 4	0
30	5	1	Total C O 44 40 4	0
30	7	1	Total C O 44 40 4	0
30	7	1	Total C O 44 40 4	0
30	8	1	Total C O 44 40 4	0
30	8	1	Total C O 44 40 4	0
30	9	1	Total C O 44 40 4	0
30	9	1	Total C O 44 40 4	0
30	0	1	Total C O 44 40 4	0
30	0	1	Total C O 44 40 4	0

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



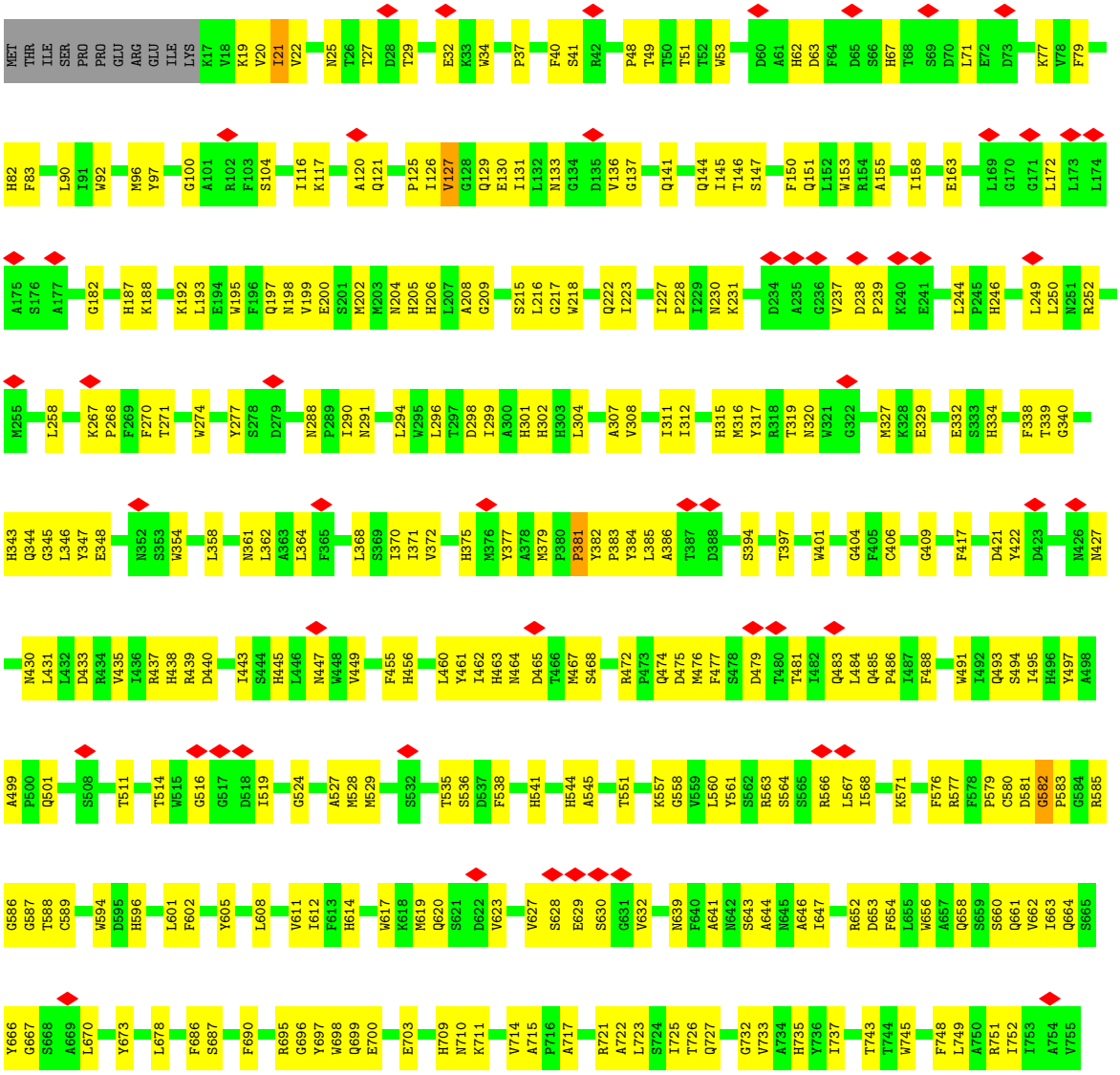
Mol	Chain	Residues	Atoms			AltConf
31	4	1	Total	C	O	0
			44	34	10	
31	5	1	Total	C	O	0
			44	34	10	
31	8	1	Total	C	O	0
			44	34	10	

3 Residue-property plots (i)

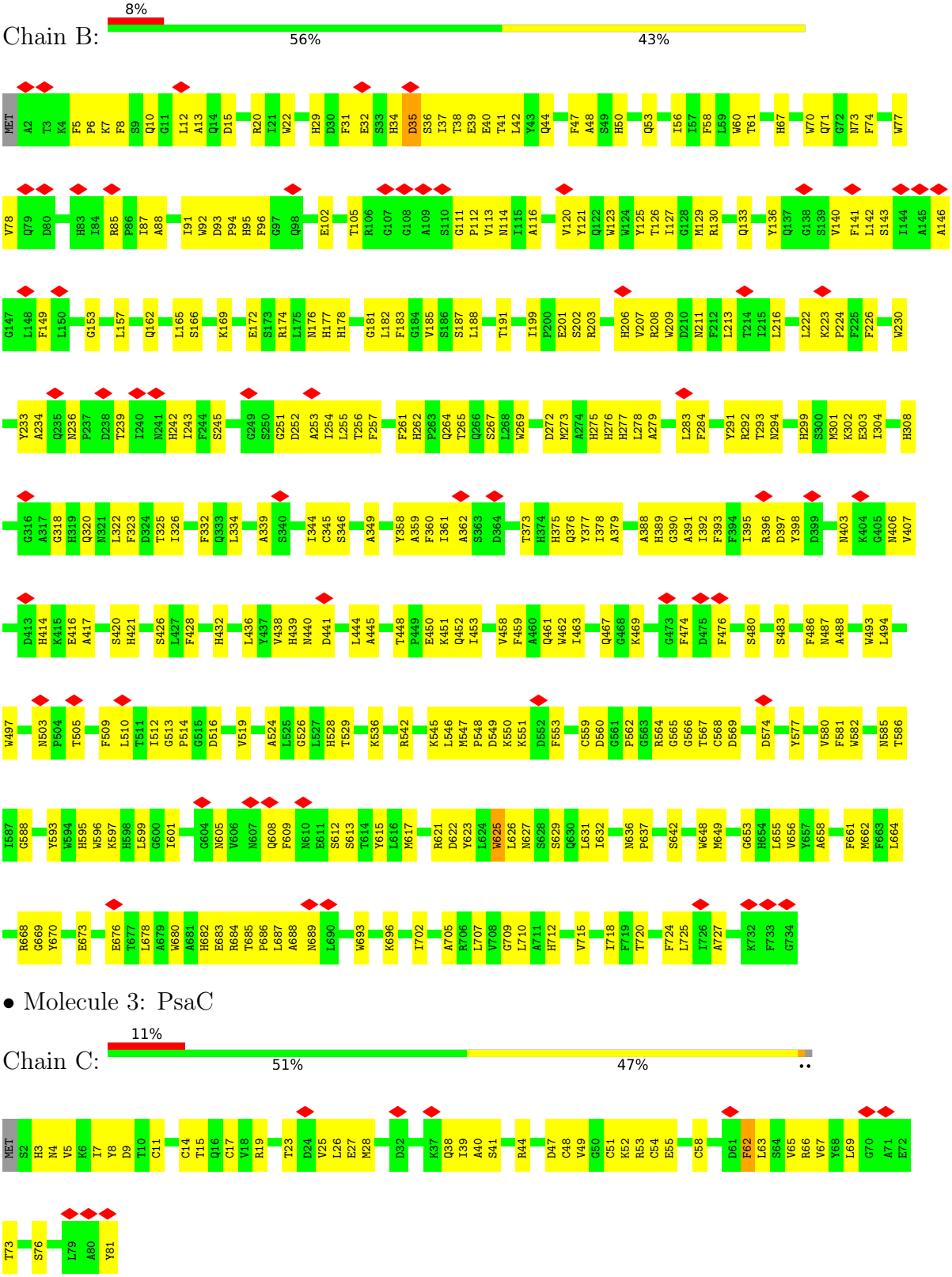
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PsaA

Chain A:



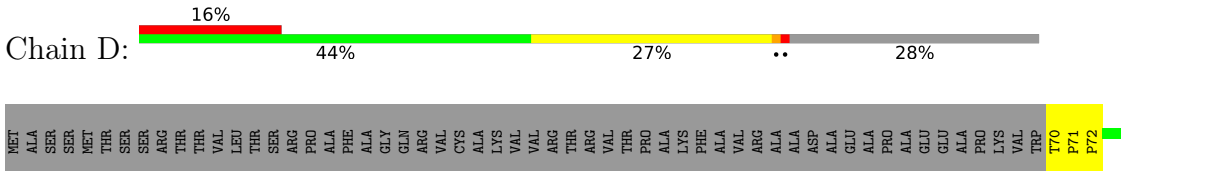
• Molecule 2: PsaB

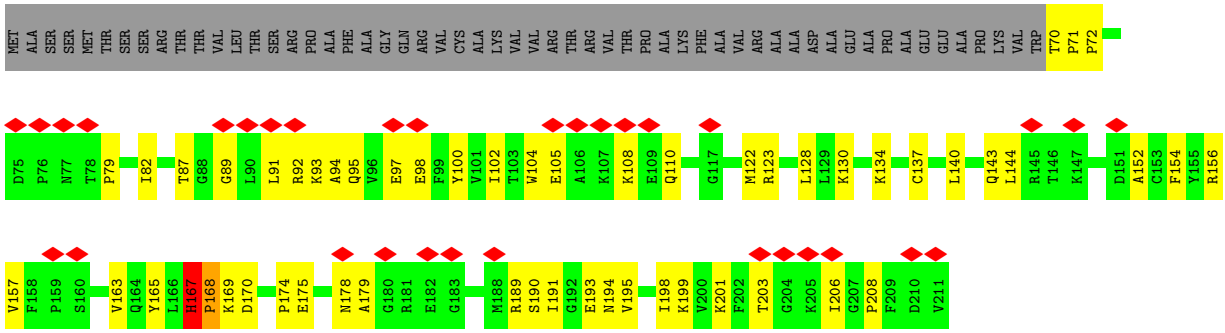


• Molecule 3: PsaC

• Molecule 4: PsaD

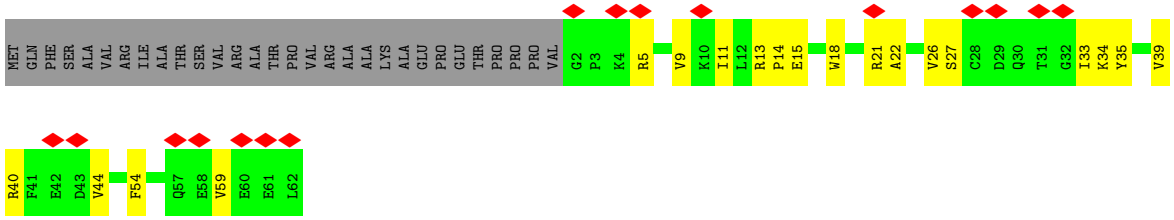
Chain D:





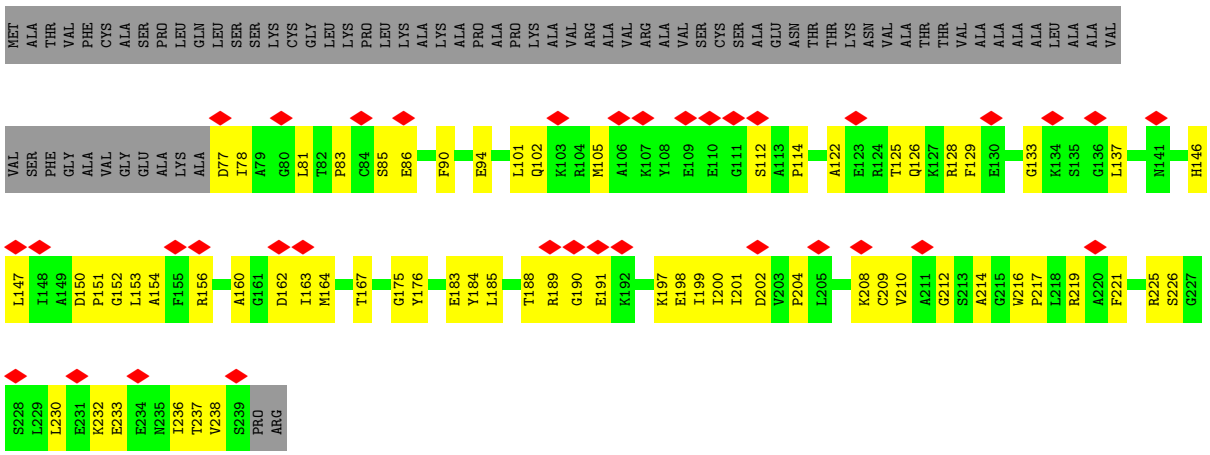
• Molecule 5: PsaE

Chain E:



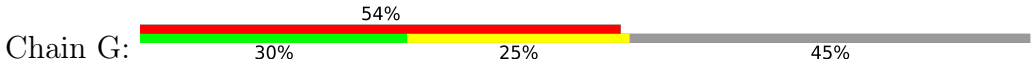
• Molecule 6: PsaF

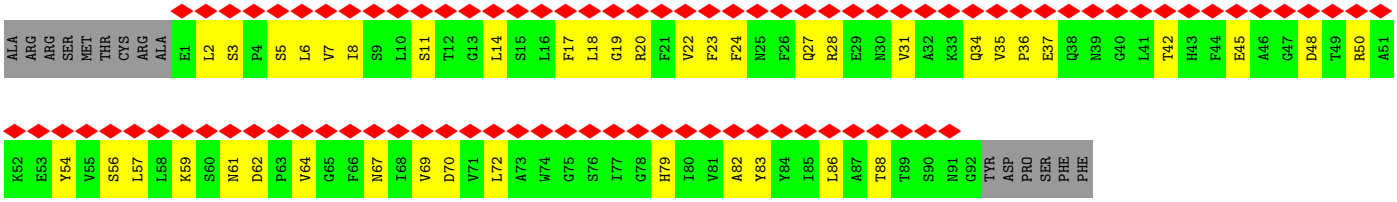
Chain F:



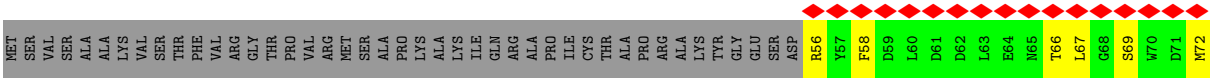
• Molecule 7: PsaG

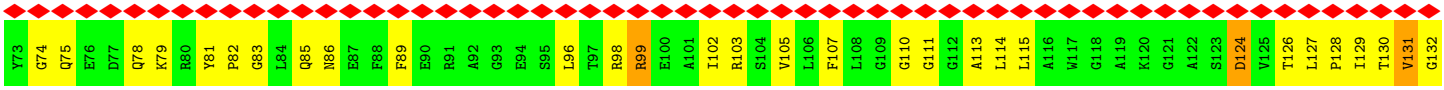
Chain G:



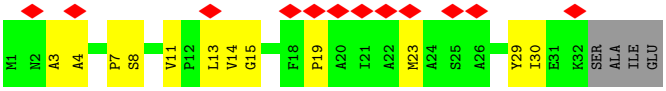


• Molecule 8: PsaH

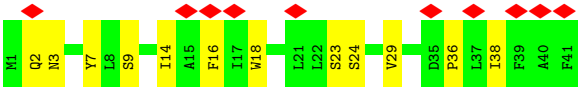




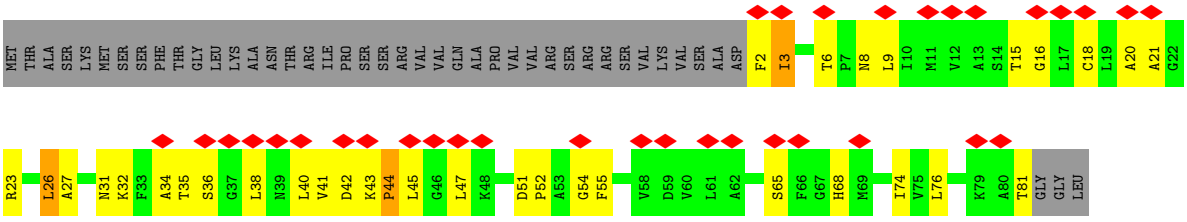
• Molecule 9: PsaI



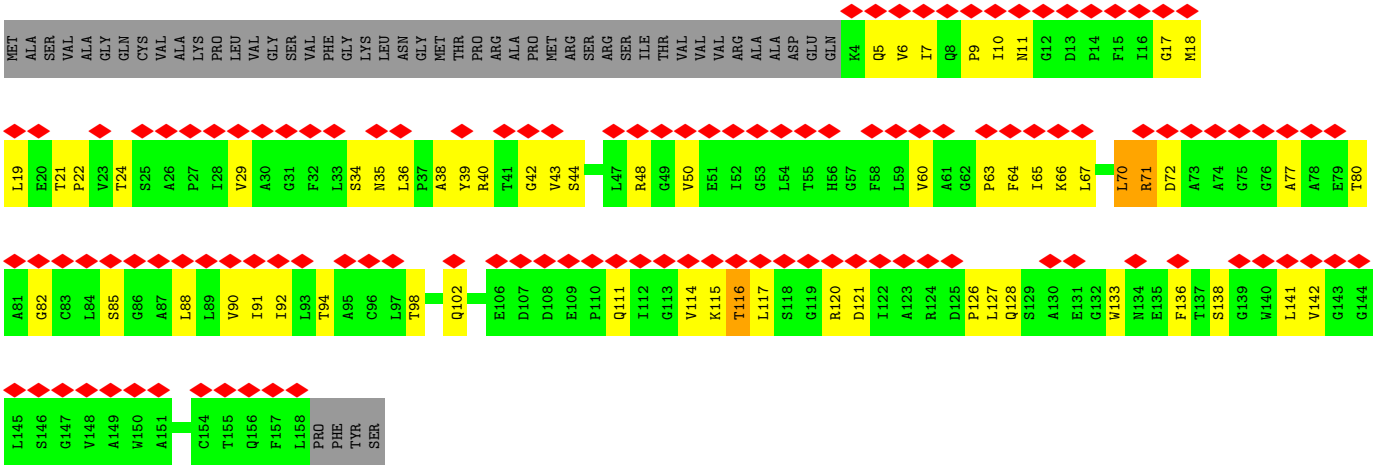
• Molecule 10: PsaJ



• Molecule 11: PsaK

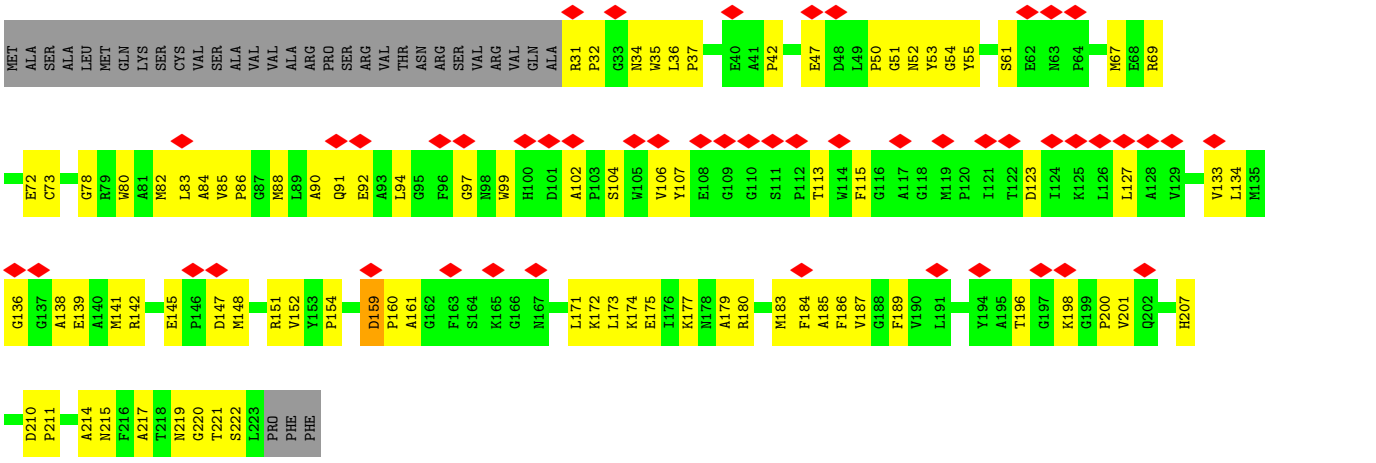


• Molecule 12: PsaL



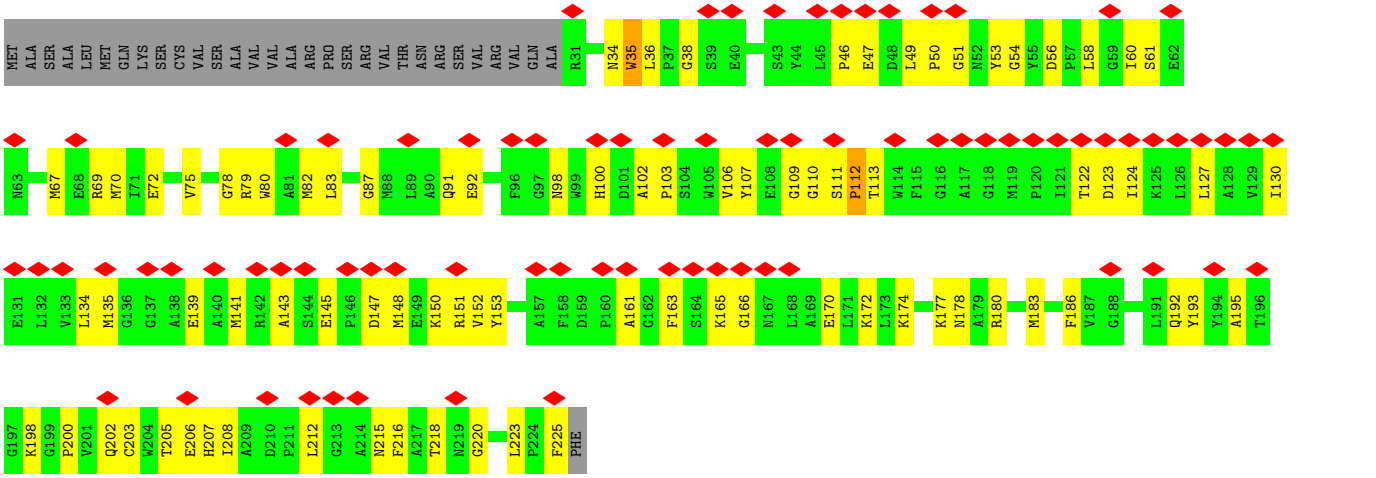
• Molecule 13: Lhca-a

Chain 1:



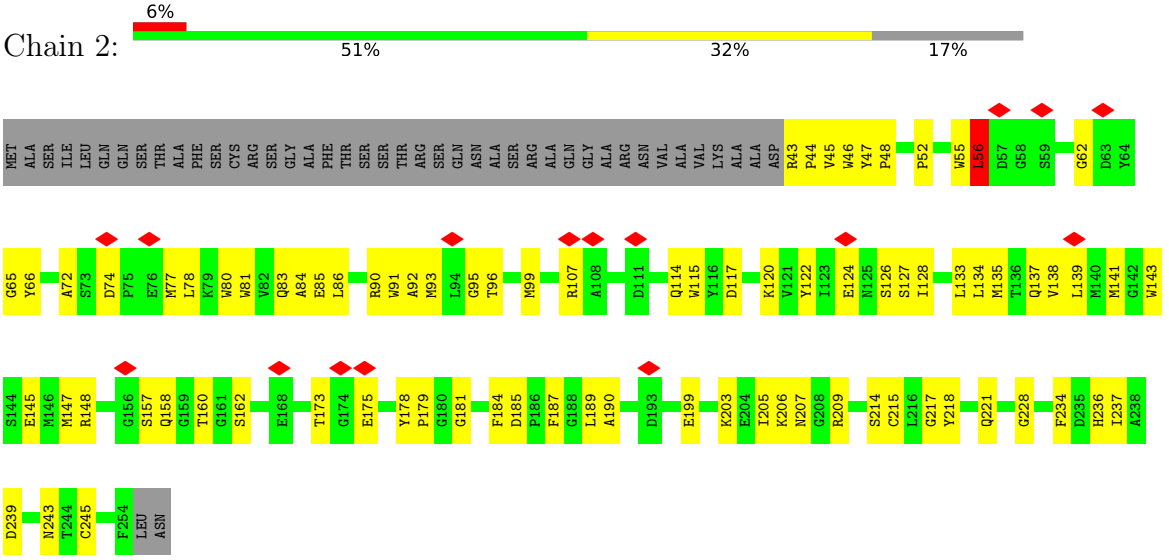
• Molecule 13: Lhca-a

Chain 5:



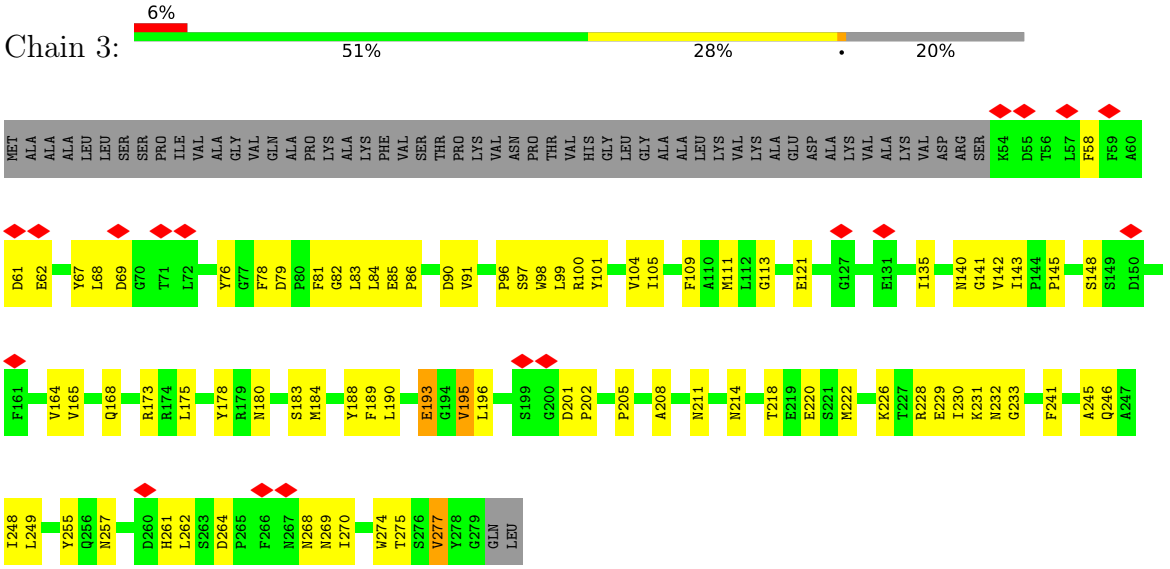
• Molecule 14: Lhca-c

Chain 2:



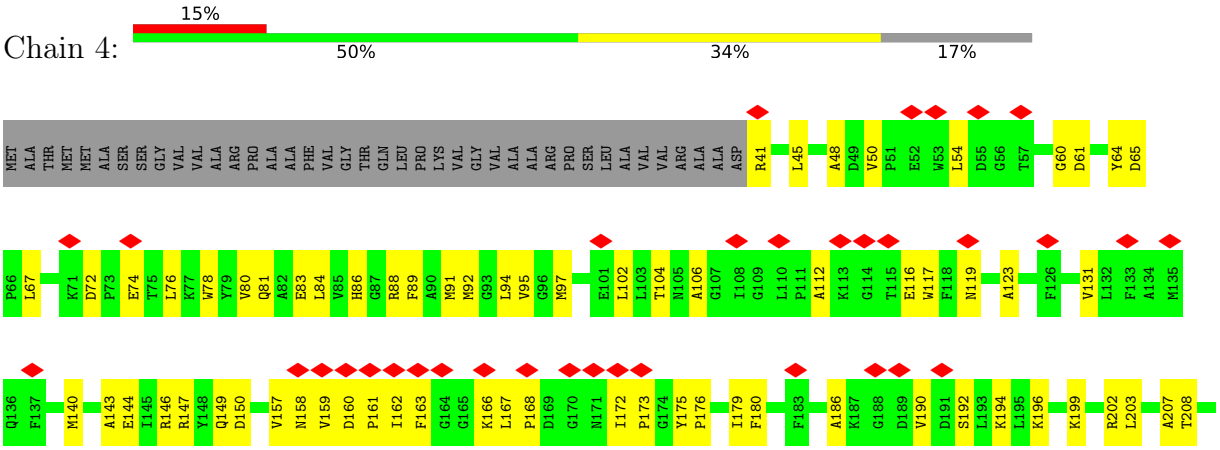
• Molecule 15: Lhca-d

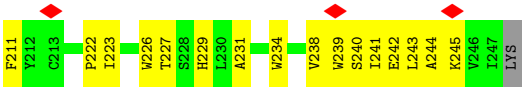
Chain 3:



• Molecule 16: Lhca-b

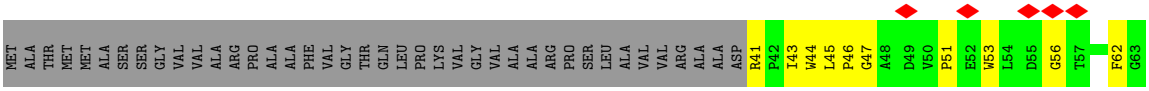
Chain 4:

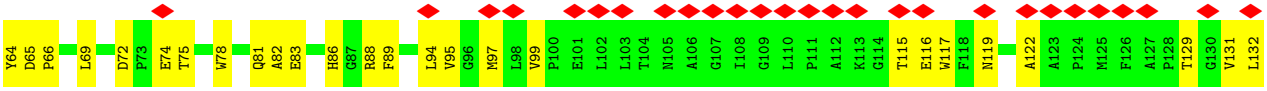


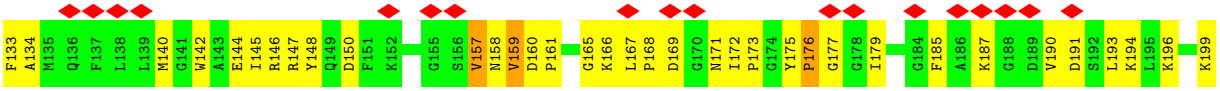


• Molecule 16: Lhca-b

Chain 8:

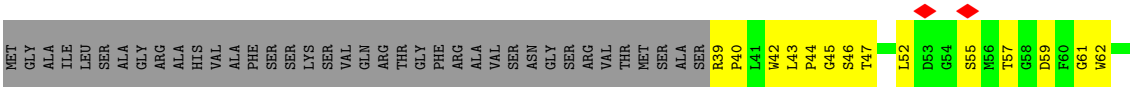


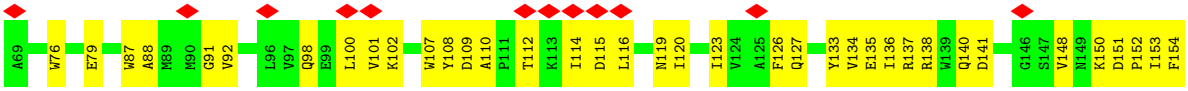


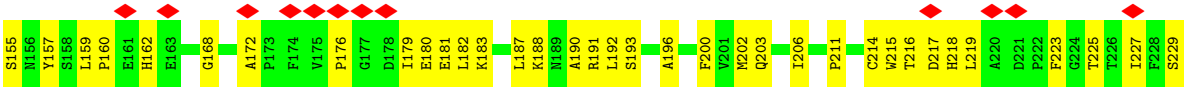


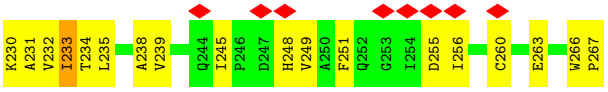
• Molecule 17: Lhca-g

Chain 6:



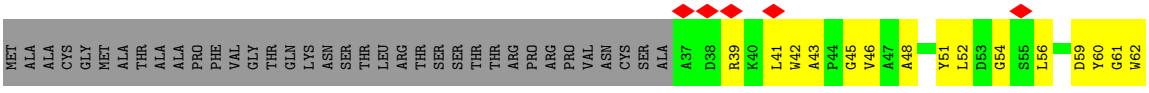


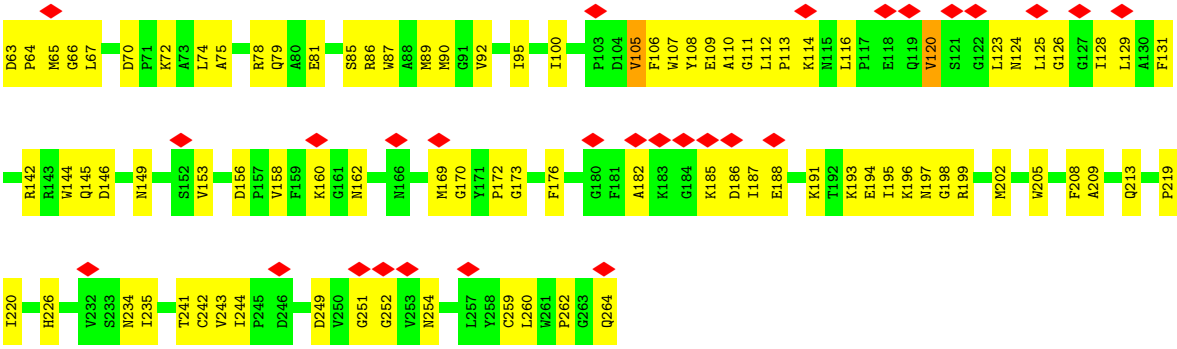




• Molecule 18: Lhca-h

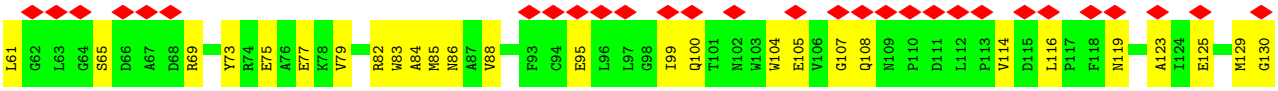
Chain 7:

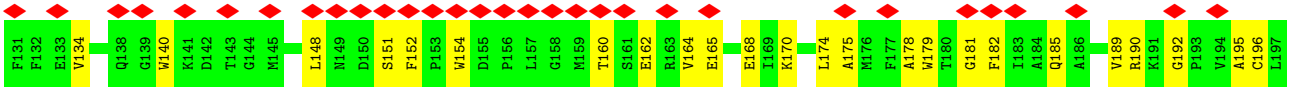


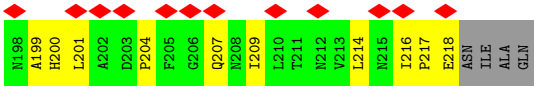


• Molecule 19: Lhca-i

Chain 9:

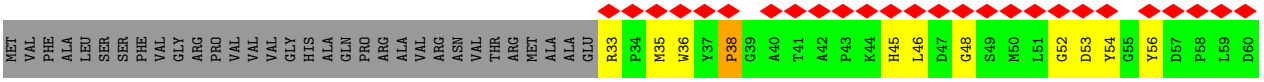


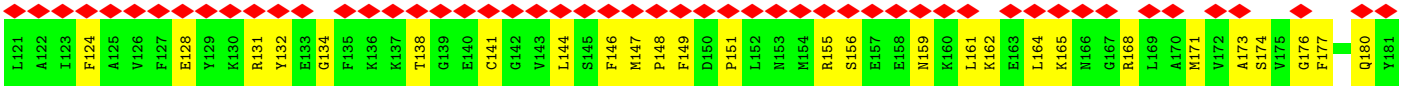


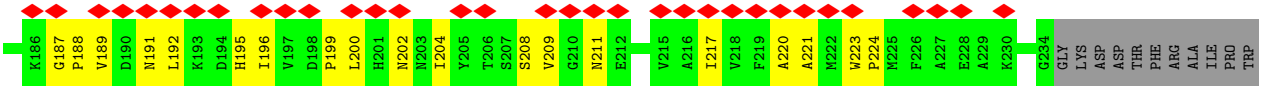


• Molecule 20: Lhca-j

Chain 0:

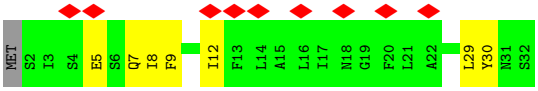






• Molecule 21: Photosystem I reaction center subunit XII

Chain M:


MET
S2
I3
S4
E5
S6
Q7
I8
F9
I12
F13
L14
A15
L16
I17
N18
G19
F20
L21
A22
L29
Y30
N31
S32

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59525	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.852	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.187	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.034	Depositor
Map size (Å)	401.442, 401.442, 401.442	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8727, 0.8727, 0.8727	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LMG, CHL, SF4, XAT, DGD, LHG, PQN, HTG, 8CT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.51	0/6015	0.53	0/8196
2	B	0.50	0/6034	0.54	0/8239
3	C	0.55	0/612	0.58	0/830
4	D	0.44	0/1135	0.59	0/1533
5	E	0.46	0/498	0.50	0/673
6	F	0.44	0/1281	0.56	0/1724
7	G	0.32	0/730	0.53	0/992
8	H	0.34	0/691	0.52	0/929
9	I	0.45	0/250	0.48	0/341
10	J	0.48	0/346	0.60	0/472
11	K	0.34	0/567	0.68	1/769 (0.1%)
12	L	0.33	0/1165	0.54	0/1591
13	1	0.41	0/1510	0.50	0/2054
13	5	0.40	0/1530	0.56	1/2082 (0.0%)
14	2	0.53	0/1701	0.56	1/2315 (0.0%)
15	3	0.49	0/1801	0.55	0/2444
16	4	0.49	0/1642	0.58	0/2238
16	8	0.43	0/1627	0.56	0/2217
17	6	0.43	0/1862	0.56	0/2542
18	7	0.46	0/1812	0.53	0/2468
19	9	0.39	0/1456	0.58	0/1986
20	0	0.33	0/1603	0.53	0/2174
21	M	0.41	0/241	0.43	0/325
All	All	0.46	0/36109	0.55	3/49134 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	1
4	D	0	1
11	K	0	1
13	1	0	1
14	2	0	2
16	4	0	1
17	6	0	3
20	0	0	3
All	All	0	14

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	5	35	TRP	C-N-CA	-5.90	106.96	121.70
11	K	26	LEU	CA-CB-CG	5.33	127.57	115.30
14	2	56	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	0	156	SER	Peptide
20	0	38	PRO	Peptide
20	0	97	LEU	Peptide
13	1	159	ASP	Peptide
14	2	162	SER	Peptide
14	2	56	LEU	Peptide
16	4	123	ALA	Peptide
17	6	107	TRP	Peptide
17	6	109	ASP	Peptide
17	6	155	SER	Peptide
1	A	582	GLY	Peptide
3	C	62	PHE	Peptide
4	D	167	HIS	Peptide
11	K	41	VAL	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5819	0	5659	288	0
2	B	5824	0	5604	363	0
3	C	602	0	591	42	0
4	D	1109	0	1124	51	0
5	E	488	0	480	16	0
6	F	1257	0	1274	60	0
7	G	714	0	708	39	0
8	H	677	0	654	60	0
9	I	243	0	258	10	0
10	J	336	0	355	15	0
11	K	558	0	591	38	0
12	L	1139	0	1147	72	0
13	1	1466	0	1411	83	0
13	5	1484	0	1427	78	0
14	2	1641	0	1537	81	0
15	3	1751	0	1684	91	0
16	4	1589	0	1570	98	0
16	8	1574	0	1550	139	0
17	6	1797	0	1752	116	0
18	7	1758	0	1701	113	0
19	9	1416	0	1367	76	0
20	0	1560	0	1540	91	0
21	M	238	0	248	8	0
22	0	572	0	542	53	0
22	1	683	0	657	79	0
22	2	596	0	548	37	0
22	3	644	0	529	48	0
22	4	539	0	476	38	0
22	5	653	0	599	62	0
22	6	785	0	741	71	0
22	7	817	0	694	80	0
22	8	539	0	477	47	0
22	9	595	0	534	47	0
22	A	2628	0	2677	218	0
22	B	2420	0	2485	239	0
22	F	45	0	33	5	0
22	G	141	0	105	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	H	65	0	72	18	0
22	J	42	0	31	1	0
22	K	187	0	138	29	0
22	L	245	0	255	26	0
22	M	46	0	33	5	0
23	A	33	0	46	3	0
23	B	33	0	46	3	0
24	0	49	0	72	12	0
24	1	49	0	74	3	0
24	2	32	0	34	3	0
24	3	20	0	14	4	0
24	5	49	0	72	8	0
24	6	37	0	44	4	0
24	7	20	0	13	2	0
24	9	49	0	74	8	0
24	A	76	0	98	5	0
24	B	23	0	16	1	0
25	1	40	0	0	13	0
25	2	40	0	0	13	0
25	3	80	0	0	10	0
25	4	40	0	0	12	0
25	5	40	0	0	6	0
25	6	40	0	0	14	0
25	7	120	0	0	36	0
25	8	80	0	0	13	0
25	A	240	0	0	32	0
25	B	320	0	0	40	0
25	F	40	0	0	0	0
25	G	40	0	0	20	0
25	I	40	0	0	0	0
25	J	80	0	0	25	0
25	K	40	0	0	14	0
25	L	80	0	0	0	0
26	A	19	0	26	0	0
26	J	19	0	26	1	0
27	B	8	0	0	1	0
27	C	16	0	0	1	0
28	B	66	0	96	11	0
29	0	109	0	87	18	0
29	1	48	0	33	3	0
29	2	203	0	154	16	0
29	3	47	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	4	219	0	176	30	0
29	5	109	0	90	17	0
29	6	241	0	181	22	0
29	7	47	0	31	11	0
29	8	201	0	148	27	0
29	9	109	0	90	6	0
30	0	88	0	104	19	0
30	1	88	0	109	15	0
30	2	88	0	112	14	0
30	3	88	0	110	17	0
30	4	88	0	109	16	0
30	5	88	0	107	13	0
30	6	88	0	111	14	0
30	7	88	0	109	15	0
30	8	88	0	109	21	0
30	9	88	0	109	13	0
31	4	44	0	61	1	0
31	5	44	0	61	5	0
31	8	44	0	60	6	0
All	All	51585	0	48901	2693	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (2693) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:832:CLA:H43	25:B:848:8CT:C27	1.26	1.58
22:1:304:CLA:H3A	25:1:316:8CT:C27	1.31	1.57
22:B:840:CLA:C1C	25:B:848:8CT:C22	1.82	1.57
18:7:251:GLY:HA3	25:7:323:8CT:C01	1.35	1.54
15:3:195:VAL:CG2	15:3:208:ALA:HB3	1.44	1.48
25:A:846:8CT:C40	25:A:854:8CT:C01	1.98	1.39
22:1:304:CLA:HAA1	25:1:316:8CT:C27	1.52	1.39
15:3:189:PHE:CE1	25:3:316:8CT:C27	2.07	1.38
18:7:124:ASN:OD1	25:7:323:8CT:C08	1.71	1.37
18:7:251:GLY:CA	25:7:323:8CT:C01	2.02	1.36
25:B:843:8CT:C18	25:G:104:8CT:C08	2.00	1.36
22:G:103:CLA:C4B	25:G:104:8CT:C37	2.05	1.34
22:A:808:CLA:C2	25:J:104:8CT:C40	2.07	1.32
15:3:189:PHE:CZ	25:3:316:8CT:C27	2.11	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:809:CLA:CBB	25:J:104:8CT:C38	2.08	1.30
22:B:840:CLA:CHC	25:B:848:8CT:C22	2.08	1.29
22:7:307:CLA:C1B	25:7:323:8CT:C27	2.09	1.28
7:G:83:TYR:CD2	25:G:104:8CT:C01	2.16	1.27
16:8:179:ILE:CD1	29:8:314:CHL:HHB	1.64	1.26
29:3:306:CHL:HMB1	25:3:316:8CT:C22	1.67	1.22
22:7:307:CLA:C2B	25:7:323:8CT:C27	2.17	1.22
22:A:808:CLA:H12	25:J:104:8CT:C40	1.70	1.21
22:B:840:CLA:C2C	25:B:848:8CT:C22	2.19	1.21
22:A:808:CLA:C1	25:J:104:8CT:C40	2.17	1.20
22:A:832:CLA:C4	25:B:848:8CT:C27	2.20	1.20
22:1:304:CLA:C3A	25:1:316:8CT:C27	2.19	1.20
22:A:808:CLA:H2	25:J:104:8CT:C40	1.70	1.19
1:A:745:TRP:CG	25:A:850:8CT:C38	2.28	1.16
15:3:195:VAL:HG22	15:3:208:ALA:HB3	1.26	1.16
22:B:826:CLA:C2B	25:B:847:8CT:C22	2.24	1.14
8:H:124:ASP:HB3	8:H:127:LEU:HD12	1.16	1.13
22:G:103:CLA:CHC	25:G:104:8CT:C37	2.26	1.12
1:A:663:ILE:CG2	2:B:621:ARG:HG3	1.80	1.11
1:A:663:ILE:HG22	2:B:621:ARG:HG3	1.32	1.11
11:K:68:HIS:CE1	25:K:103:8CT:C15	2.34	1.09
1:A:745:TRP:CD1	25:A:850:8CT:C38	2.35	1.09
16:8:166:LYS:HE3	16:8:179:ILE:HG13	1.30	1.08
14:2:143:TRP:CH2	25:2:317:8CT:C09	2.36	1.08
29:4:305:CHL:NB	25:4:317:8CT:C38	2.17	1.07
22:G:103:CLA:NB	25:G:104:8CT:C37	2.17	1.07
8:H:124:ASP:CB	8:H:127:LEU:HD12	1.83	1.06
22:6:305:CLA:C4B	25:6:321:8CT:C33	2.33	1.06
17:6:133:TYR:CE2	25:6:321:8CT:C40	2.40	1.05
22:7:306:CLA:H3A	25:7:321:8CT:C25	1.85	1.05
29:4:305:CHL:C1B	25:4:317:8CT:C38	2.36	1.03
22:A:809:CLA:CAB	25:J:104:8CT:C38	2.37	1.02
22:B:826:CLA:C3B	25:B:847:8CT:C22	2.37	1.02
16:8:179:ILE:HD12	29:8:314:CHL:CHB	1.91	1.01
15:3:195:VAL:CG2	15:3:208:ALA:CB	2.39	1.00
22:1:304:CLA:CAA	25:1:316:8CT:C27	2.38	1.00
2:B:595:HIS:CD2	2:B:623:TYR:OH	2.15	0.99
29:6:307:CHL:HMA1	25:8:301:8CT:C38	1.91	0.99
25:A:850:8CT:C05	22:B:832:CLA:HMB3	1.93	0.99
22:G:102:CLA:HBB1	25:G:104:8CT:C39	1.92	0.99
15:3:195:VAL:HG23	15:3:208:ALA:HB3	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:134:LEU:HD11	25:1:316:8CT:C19	1.89	0.98
22:A:809:CLA:HBB2	25:J:104:8CT:C38	1.93	0.98
2:B:627:ASN:HB2	2:B:724:PHE:HE1	1.25	0.97
16:8:179:ILE:CD1	29:8:314:CHL:CHB	2.42	0.96
2:B:627:ASN:HD22	2:B:724:PHE:HZ	0.98	0.96
7:G:83:TYR:HD2	25:G:104:8CT:C01	1.64	0.96
19:9:39:LEU:HD12	19:9:40:VAL:H	1.28	0.96
24:6:322:LHG:HC81	25:7:321:8CT:C08	1.95	0.96
29:2:305:CHL:CHB	25:2:317:8CT:C27	2.43	0.95
22:B:850:CLA:HMA2	22:B:850:CLA:H2	1.48	0.95
25:K:103:8CT:C38	22:K:104:CLA:C2B	2.44	0.95
15:3:189:PHE:HZ	25:3:316:8CT:C27	1.69	0.95
25:J:101:8CT:C39	25:J:104:8CT:C39	2.45	0.95
18:7:251:GLY:HA2	25:7:323:8CT:C01	1.97	0.95
2:B:631:LEU:HD11	2:B:724:PHE:HA	1.48	0.94
22:A:809:CLA:H11	25:J:104:8CT:C39	1.95	0.94
16:8:172:ILE:H	16:8:172:ILE:HD12	1.28	0.94
19:9:37:MET:SD	19:9:42:ALA:O	2.26	0.93
22:7:306:CLA:CBA	25:7:321:8CT:C25	2.46	0.93
16:8:179:ILE:HD12	29:8:314:CHL:HHB	0.95	0.93
8:H:124:ASP:HB3	8:H:127:LEU:CD1	1.99	0.92
2:B:623:TYR:O	2:B:627:ASN:ND2	2.01	0.92
17:6:133:TYR:CD2	25:6:321:8CT:C40	2.51	0.92
16:8:166:LYS:HE2	16:8:168:PRO:HG3	1.51	0.92
2:B:395:ILE:HG23	2:B:396:ARG:HG3	1.51	0.92
15:3:189:PHE:HE1	25:3:316:8CT:C27	1.62	0.91
22:B:826:CLA:C1B	25:B:847:8CT:C22	2.48	0.91
22:B:841:CLA:HMA3	25:B:846:8CT:C40	2.02	0.90
29:7:308:CHL:HMB3	25:7:321:8CT:C19	2.02	0.90
19:9:85:MET:HE2	30:9:314:XAT:H14	1.50	0.90
8:H:82:PRO:HD3	22:L:202:CLA:HMD1	1.53	0.90
29:4:305:CHL:CHB	25:4:317:8CT:C38	2.50	0.89
1:A:660:SER:HB3	2:B:625:TRP:CZ2	2.08	0.88
2:B:73:ASN:O	2:B:121:TYR:OH	1.90	0.88
2:B:627:ASN:HB2	2:B:724:PHE:CE1	2.09	0.88
1:A:479:ASP:O	1:A:483:GLN:NE2	2.07	0.87
22:G:102:CLA:CBB	25:G:104:8CT:C39	2.52	0.87
25:K:103:8CT:C38	22:K:104:CLA:C3B	2.53	0.87
29:6:307:CHL:CMA	25:8:301:8CT:C38	2.53	0.87
17:6:133:TYR:CZ	25:6:321:8CT:C40	2.58	0.86
22:7:307:CLA:CHB	25:7:323:8CT:C27	2.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:40:ARG:O	12:L:48:ARG:NH2	2.09	0.85
16:4:150:ASP:HB2	16:4:157:VAL:HG22	1.58	0.85
16:8:176:PRO:O	22:8:309:CLA:OBD	1.95	0.84
15:3:270:ILE:HD11	22:3:311:CLA:H12	1.57	0.84
2:B:595:HIS:HD2	2:B:623:TYR:OH	1.59	0.84
20:0:124:PHE:HZ	22:0:305:CLA:HHD	1.42	0.84
14:2:141:MET:HA	25:2:317:8CT:C22	2.07	0.84
22:B:824:CLA:HBC3	25:B:846:8CT:C27	2.08	0.83
2:B:684:ARG:HD3	12:L:18:MET:HB2	1.60	0.83
22:G:103:CLA:C1C	25:G:104:8CT:C37	2.55	0.83
15:3:262:LEU:HD21	22:3:312:CLA:HMC3	1.61	0.83
2:B:595:HIS:HD2	2:B:623:TYR:CE1	1.97	0.83
18:7:86:ARG:NH1	18:7:194:GLU:OE2	2.12	0.83
22:A:810:CLA:HBB2	22:A:813:CLA:HMA3	1.61	0.82
17:6:134:VAL:HG23	25:6:321:8CT:C39	2.10	0.82
1:A:151:GLN:NE2	1:A:384:TYR:O	2.13	0.82
18:7:60:TYR:OH	24:7:322:LHG:O5	1.97	0.82
29:2:305:CHL:HHB	25:2:317:8CT:C27	2.09	0.82
29:0:301:CHL:HAC2	24:0:315:LHG:HC41	1.62	0.81
2:B:631:LEU:HD21	2:B:727:ALA:HB3	1.60	0.81
29:6:307:CHL:H3A	25:8:301:8CT:C38	2.10	0.81
22:1:312:CLA:H93	29:4:301:CHL:H51	1.62	0.81
16:8:166:LYS:CE	16:8:179:ILE:HG13	2.11	0.81
1:A:745:TRP:CD2	25:A:850:8CT:C38	2.63	0.81
2:B:48:ALA:HB2	2:B:157:LEU:HD11	1.62	0.80
25:A:850:8CT:C22	22:B:803:CLA:H161	2.10	0.80
22:B:829:CLA:HBB1	22:B:829:CLA:HHC	1.64	0.80
14:2:145:GLU:OE1	14:2:148:ARG:NH2	2.14	0.80
16:8:166:LYS:CE	16:8:179:ILE:H	1.94	0.80
7:G:8:ILE:HD12	7:G:82:ALA:HB1	1.64	0.80
17:6:91:GLY:HA3	30:6:320:XAT:H193	1.64	0.80
16:4:146:ARG:HH12	16:4:158:ASN:HB2	1.47	0.80
16:8:166:LYS:NZ	16:8:179:ILE:H	1.79	0.80
18:7:199:ARG:HH22	22:7:303:CLA:HED2	1.45	0.80
2:B:707:LEU:HD11	28:B:849:DGD:HB41	1.64	0.79
18:7:262:PRO:HD2	22:7:317:CLA:HAA1	1.63	0.79
2:B:120:VAL:HG22	22:B:829:CLA:HAA2	1.65	0.79
14:2:114:GLN:HE21	14:2:228:GLY:HA3	1.47	0.79
15:3:188:TYR:HA	15:3:193:GLU:OE1	1.82	0.79
2:B:516:ASP:OD1	2:B:593:TYR:OH	2.00	0.78
22:3:301:CLA:HAB	30:3:315:XAT:H32	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:9:58:TYR:HE2	30:9:315:XAT:H383	1.49	0.78
2:B:390:GLY:CA	25:B:847:8CT:C32	2.62	0.78
22:G:102:CLA:HBB1	25:G:104:8CT:C16	2.12	0.78
3:C:7:ILE:HG12	3:C:65:VAL:HG12	1.65	0.78
12:L:71:ARG:O	12:L:72:ASP:OD1	2.01	0.78
2:B:595:HIS:HD2	2:B:623:TYR:CZ	2.01	0.78
29:6:307:CHL:C3A	25:8:301:8CT:C38	2.62	0.78
22:6:310:CLA:H52	30:6:319:XAT:H30	1.66	0.78
2:B:294:ASN:HD22	22:B:813:CLA:HMA2	1.47	0.77
4:D:94:ALA:HB1	8:H:67:LEU:HD22	1.67	0.77
8:H:98:ARG:H	8:H:102:ILE:HD12	1.49	0.77
13:1:113:THR:HG22	13:1:115:PHE:H	1.49	0.77
25:K:103:8CT:C38	22:K:104:CLA:C1B	2.61	0.77
13:1:91:GLN:O	13:1:97:GLY:N	2.15	0.77
29:3:306:CHL:CMB	25:3:316:8CT:C22	2.58	0.77
17:6:232:VAL:HG12	17:6:239:VAL:HG22	1.65	0.77
29:8:305:CHL:HHC	29:8:305:CHL:HBB1	1.66	0.77
19:9:160:THR:HG22	19:9:162:GLU:H	1.49	0.77
22:B:824:CLA:CBC	25:B:846:8CT:C27	2.63	0.76
29:4:305:CHL:O2A	25:4:317:8CT:C22	2.34	0.76
1:A:121:GLN:NE2	22:A:809:CLA:OBD	2.17	0.76
2:B:562:PRO:HA	2:B:566:GLY:HA2	1.66	0.76
1:A:147:SER:OG	22:A:808:CLA:OBD	2.03	0.76
16:8:176:PRO:HD2	22:8:309:CLA:OBD	1.84	0.76
12:L:70:LEU:H	12:L:70:LEU:HD12	1.49	0.76
17:6:140:GLN:NE2	16:8:46:PRO:O	2.19	0.75
2:B:177:HIS:CD2	22:B:814:CLA:HMC2	2.20	0.75
2:B:390:GLY:HA2	25:B:847:8CT:C32	2.17	0.75
22:0:309:CLA:HBC3	24:0:315:LHG:HC62	1.66	0.75
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.68	0.75
19:9:75:GLU:OE1	19:9:140:TRP:NE1	2.17	0.75
20:0:162:LYS:HD3	22:0:310:CLA:HBD	1.69	0.75
1:A:666:TYR:HD1	2:B:445:ALA:HA	1.52	0.75
22:B:813:CLA:H11	22:B:813:CLA:H92	1.67	0.75
22:5:309:CLA:HBB1	30:5:315:XAT:H10	1.67	0.75
17:6:225:THR:HA	17:6:230:LYS:HD2	1.69	0.74
19:9:38:TRP:CD1	19:9:43:SER:HB3	2.22	0.74
22:B:826:CLA:C4B	25:B:847:8CT:C22	2.65	0.74
1:A:77:LYS:NZ	22:A:811:CLA:OBD	2.21	0.74
18:7:205:TRP:CE2	30:7:320:XAT:H10	2.23	0.74
14:2:141:MET:HG2	22:2:308:CLA:HMC3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:0:301:CHL:HHC	29:0:301:CHL:HBB1	1.69	0.74
16:4:158:ASN:ND2	16:4:163:PHE:HB3	2.03	0.74
13:5:106:VAL:O	13:5:110:GLY:N	2.18	0.74
2:B:339:ALA:HB2	25:B:847:8CT:C27	2.17	0.74
2:B:560:ASP:OD2	2:B:564:ARG:NH2	2.16	0.74
13:1:55:TYR:HE2	30:1:315:XAT:H383	1.51	0.74
16:8:172:ILE:HD12	16:8:172:ILE:N	2.01	0.74
16:8:196:LYS:O	16:8:200:ASN:ND2	2.19	0.74
29:5:301:CHL:HHC	29:5:301:CHL:HBB1	1.70	0.73
2:B:585:ASN:HD21	22:B:803:CLA:HBC2	1.53	0.73
16:8:175:TYR:HB3	22:8:309:CLA:O1D	1.87	0.73
2:B:35:ASP:OD1	2:B:36:SER:N	2.19	0.73
6:F:191:GLU:OE2	6:F:197:LYS:NZ	2.21	0.73
13:1:73:CYS:SG	22:1:302:CLA:HAA2	2.28	0.73
16:8:86:HIS:HE1	30:8:317:XAT:H15	1.54	0.73
9:I:29:TYR:OH	21:M:30:TYR:OH	2.05	0.73
20:0:36:TRP:HA	29:0:301:CHL:C4C	2.18	0.73
15:3:173:ARG:HG2	29:3:306:CHL:HBB1	1.71	0.73
16:8:179:ILE:HD11	29:8:314:CHL:H3A	1.71	0.73
1:A:21:ILE:HG22	1:A:192:LYS:HD2	1.71	0.73
13:5:46:PRO:HG2	13:5:49:LEU:HB2	1.69	0.72
18:7:173:GLY:HA2	18:7:176:PHE:HB2	1.70	0.72
1:A:577:ARG:NH1	24:A:844:LHG:O10	2.21	0.72
11:K:21:ALA:HB3	11:K:26:LEU:HD23	1.70	0.72
1:A:695:ARG:NE	2:B:565:GLY:O	2.22	0.72
2:B:627:ASN:ND2	2:B:724:PHE:HZ	1.82	0.72
2:B:627:ASN:CB	2:B:724:PHE:CE1	2.73	0.72
13:1:134:LEU:CD1	25:1:316:8CT:C19	2.65	0.72
16:4:104:THR:HG1	16:4:112:ALA:H	1.37	0.72
16:4:223:ILE:HA	16:4:226:TRP:HB3	1.72	0.72
12:L:114:VAL:HG12	12:L:115:LYS:H	1.52	0.72
14:2:62:GLY:O	14:2:209:ARG:NH1	2.22	0.72
22:5:303:CLA:H102	22:5:303:CLA:H41	1.71	0.72
20:0:155:ARG:HH22	20:0:162:LYS:HD2	1.55	0.72
1:A:127:VAL:HG11	22:A:809:CLA:HAB	1.72	0.72
20:0:141:CYS:HB3	20:0:144:LEU:HB2	1.71	0.72
22:H:201:CLA:H72	12:L:88:LEU:HD11	1.71	0.71
19:9:185:GLN:NE2	19:9:196:CYS:SG	2.63	0.71
14:2:143:TRP:HH2	25:2:317:8CT:C09	2.01	0.71
29:7:308:CHL:HMB3	25:7:321:8CT:C18	2.19	0.71
13:1:174:LYS:HD3	22:1:310:CLA:HBA1	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:801:CLA:CGA	22:B:801:CLA:H3A	2.21	0.71
14:2:115:TRP:HB2	30:2:316:XAT:H21	1.71	0.71
18:7:113:PRO:HA	18:7:116:LEU:HD13	1.72	0.71
1:A:656:TRP:HZ2	2:B:629:SER:HG	1.39	0.71
2:B:683:GLU:HG2	4:D:92:ARG:HH11	1.55	0.71
2:B:720:THR:OG1	22:B:805:CLA:O1D	2.08	0.71
12:L:63:PRO:HG3	22:L:204:CLA:HAB	1.73	0.71
14:2:128:ILE:HD11	14:2:133:LEU:HD12	1.73	0.71
15:3:195:VAL:HG21	15:3:208:ALA:HB3	1.65	0.71
17:6:227:ILE:HD12	22:6:313:CLA:HMD1	1.73	0.71
16:8:86:HIS:CE1	30:8:317:XAT:H15	2.25	0.71
1:A:587:GLY:O	2:B:668:ARG:NH1	2.24	0.70
22:B:841:CLA:HBB2	22:1:301:CLA:H41	1.73	0.70
29:2:305:CHL:HHC	29:2:305:CHL:HBB1	1.72	0.70
17:6:135:GLU:HA	17:6:138:ARG:HG2	1.73	0.70
1:A:404:GLY:HA3	1:A:608:LEU:HD11	1.73	0.70
2:B:546:LEU:HD21	2:B:567:THR:HG22	1.72	0.70
22:7:318:CLA:H43	22:7:318:CLA:H121	1.72	0.70
20:0:54:TYR:HE2	20:0:165:LYS:HZ3	1.37	0.70
1:A:100:GLY:O	1:A:104:SER:OG	2.08	0.70
1:A:268:PRO:HA	1:A:271:THR:HG22	1.72	0.70
22:A:810:CLA:H43	22:A:812:CLA:H43	1.73	0.70
4:D:100:TYR:OH	4:D:156:ARG:NH1	2.25	0.70
14:2:135:MET:HB3	16:4:239:TRP:HE3	1.56	0.70
15:3:81:PHE:HD2	30:3:315:XAT:H221	1.55	0.70
18:7:67:LEU:HD23	22:7:303:CLA:H43	1.73	0.70
22:7:318:CLA:HMA3	22:7:318:CLA:H42	1.73	0.70
1:A:567:LEU:HD23	1:A:568:ILE:HG13	1.73	0.70
22:A:812:CLA:HMB2	15:3:81:PHE:HE1	1.56	0.70
22:6:305:CLA:NB	25:6:321:8CT:C33	2.53	0.70
22:A:807:CLA:HMB3	22:A:808:CLA:H3A	1.74	0.70
25:A:850:8CT:C09	22:B:833:CLA:HMC2	2.22	0.70
16:8:199:LYS:NZ	22:8:310:CLA:O1D	2.24	0.70
2:B:85:ARG:HH22	8:H:142:LYS:HB3	1.55	0.70
7:G:17:PHE:HD2	7:G:18:LEU:HD12	1.56	0.70
13:1:134:LEU:HD23	22:1:304:CLA:HMA2	1.73	0.70
1:A:639:ASN:HB2	1:A:643:SER:HB2	1.74	0.70
7:G:50:ARG:NH1	19:9:65:SER:OG	2.25	0.70
1:A:126:ILE:HG12	1:A:127:VAL:HG23	1.74	0.70
22:B:820:CLA:HMB2	22:B:825:CLA:HMA3	1.74	0.70
2:B:39:GLU:OE2	2:B:169:LYS:NZ	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:8:166:LYS:HZ1	16:8:179:ILE:H	1.37	0.69
22:A:801:CLA:HBB1	22:B:803:CLA:HED1	1.74	0.69
13:5:198:LYS:NZ	13:5:206:GLU:OE1	2.24	0.69
1:A:752:ILE:O	1:A:756:GLY:N	2.25	0.69
4:D:190:SER:OG	5:E:13:ARG:NH1	2.25	0.69
6:F:221:PHE:HB3	6:F:225:ARG:HH12	1.57	0.69
22:6:314:CLA:HAA2	18:7:131:PHE:HA	1.73	0.69
2:B:129:MET:O	2:B:208:ARG:NH2	2.26	0.69
22:6:309:CLA:HBB1	22:6:315:CLA:HAA1	1.75	0.69
18:7:124:ASN:CG	25:7:323:8CT:C08	2.60	0.69
22:6:304:CLA:H141	22:6:315:CLA:H161	1.74	0.69
22:7:303:CLA:H62	22:7:304:CLA:H3A	1.74	0.69
7:G:20:ARG:NH1	7:G:62:ASP:OD2	2.24	0.69
7:G:28:ARG:NH2	7:G:70:ASP:OD2	2.25	0.69
22:B:833:CLA:HAA2	10:J:36:PRO:HG2	1.74	0.69
13:1:219:ASN:HB3	13:1:221:THR:HG22	1.73	0.69
17:6:98:GLN:HA	17:6:102:LYS:HD3	1.74	0.69
13:5:80:TRP:CE3	22:5:308:CLA:H2A	2.28	0.69
13:5:215:ASN:ND2	22:5:313:CLA:O1D	2.26	0.69
20:0:70:TRP:HZ2	22:0:307:CLA:HBA1	1.57	0.69
22:B:820:CLA:HBC2	22:B:824:CLA:H72	1.73	0.69
16:4:157:VAL:HG21	29:4:307:CHL:HMC	1.73	0.69
16:4:229:HIS:CG	22:4:312:CLA:HAA2	2.28	0.69
16:8:150:ASP:HB2	16:8:158:ASN:HD22	1.58	0.69
1:A:660:SER:HB3	2:B:625:TRP:HZ2	1.56	0.68
22:B:810:CLA:HBC1	21:M:12:ILE:HA	1.75	0.68
18:7:42:TRP:CD1	18:7:62:TRP:HB2	2.28	0.68
1:A:252:ARG:NH1	15:3:275:THR:O	2.22	0.68
1:A:620:GLN:OE1	1:A:658:GLN:NE2	2.25	0.68
14:2:66:TYR:HE2	30:2:316:XAT:H383	1.58	0.68
29:5:306:CHL:HHC	29:5:306:CHL:HBB1	1.75	0.68
13:1:69:ARG:NH1	22:1:302:CLA:O1A	2.27	0.68
16:8:83:GLU:OE2	16:8:202:ARG:NE	2.23	0.68
2:B:542:ARG:HD3	2:B:551:LYS:HB3	1.76	0.68
22:A:828:CLA:H42	25:A:850:8CT:C36	2.23	0.68
16:8:166:LYS:HG2	16:8:168:PRO:HD3	1.76	0.68
22:B:832:CLA:HAB	22:B:833:CLA:HMB2	1.74	0.68
12:L:40:ARG:HB2	12:L:48:ARG:HH22	1.59	0.68
29:4:307:CHL:HMB3	25:4:317:8CT:C20	2.24	0.68
16:8:190:VAL:O	16:8:194:LYS:N	2.24	0.68
6:F:221:PHE:HB3	6:F:225:ARG:NH1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:8:172:ILE:H	16:8:172:ILE:CD1	2.04	0.68
2:B:174:ARG:HG3	22:B:814:CLA:HBC2	1.76	0.68
2:B:693:TRP:HE1	2:B:696:LYS:HG2	1.59	0.68
6:F:237:THR:HG22	6:F:238:VAL:H	1.59	0.68
22:7:307:CLA:CMB	25:7:323:8CT:C27	2.71	0.68
11:K:23:ARG:HH11	11:K:52:PRO:HG2	1.58	0.67
14:2:141:MET:SD	25:2:317:8CT:C22	2.82	0.67
22:A:804:CLA:HMA2	22:A:811:CLA:HMD2	1.77	0.67
6:F:214:ALA:HB3	16:4:67:LEU:HD22	1.75	0.67
1:A:270:PHE:HD1	22:K:102:CLA:HBC2	1.59	0.67
22:A:803:CLA:HBB1	25:J:101:8CT:C07	2.25	0.67
16:4:83:GLU:OE2	16:4:202:ARG:NE	2.19	0.67
29:2:305:CHL:NA	25:2:317:8CT:C38	2.58	0.67
17:6:137:ARG:NH1	22:6:323:CLA:OBD	2.28	0.67
13:5:80:TRP:CZ3	22:5:308:CLA:H2A	2.29	0.67
24:0:315:LHG:H311	24:0:315:LHG:H191	1.75	0.67
14:2:203:LYS:HD3	22:2:311:CLA:HAA2	1.76	0.67
16:4:158:ASN:ND2	16:4:162:ILE:O	2.18	0.67
22:8:310:CLA:H2	22:8:311:CLA:CAD	2.24	0.67
19:9:114:VAL:HB	22:9:306:CLA:HMD1	1.76	0.67
6:F:101:LEU:HD22	6:F:122:ALA:HB2	1.77	0.67
12:L:116:THR:OG1	12:L:120:ARG:O	2.10	0.67
16:8:81:GLN:NE2	16:8:173:PRO:HB2	2.10	0.67
22:L:202:CLA:H12	22:L:202:CLA:H3A	1.76	0.67
16:4:226:TRP:HZ3	22:4:313:CLA:HAC1	1.58	0.67
13:5:83:LEU:HB3	22:5:304:CLA:HBB2	1.75	0.67
20:0:171:MET:O	20:0:174:SER:OG	2.13	0.67
1:A:460:LEU:O	1:A:464:ASN:ND2	2.27	0.67
2:B:93:ASP:HB2	2:B:96:PHE:CE2	2.29	0.67
15:3:195:VAL:HG22	15:3:208:ALA:CB	2.16	0.67
29:5:301:CHL:HBA2	24:5:318:LHG:H162	1.76	0.67
22:7:303:CLA:HMB2	22:7:303:CLA:H2	1.76	0.66
20:0:56:TYR:N	22:0:302:CLA:OBD	2.29	0.66
2:B:582:TRP:CH2	22:B:803:CLA:HAB	2.30	0.66
20:0:195:HIS:HB2	20:0:202:ASN:HD22	1.60	0.66
2:B:631:LEU:HD21	2:B:727:ALA:CB	2.26	0.66
15:3:195:VAL:HG23	15:3:208:ALA:CB	2.15	0.66
19:9:47:TYR:OH	19:9:59:ASP:OD2	2.13	0.66
4:D:87:THR:HA	12:L:17:GLY:O	1.95	0.66
22:7:306:CLA:HBB1	22:7:306:CLA:HMB1	1.78	0.66
16:8:211:PHE:CZ	30:8:316:XAT:H363	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:79:LYS:HG2	12:L:43:VAL:HG23	1.78	0.66
25:A:850:8CT:C40	22:B:833:CLA:HMC1	2.26	0.66
22:8:309:CLA:H41	22:8:311:CLA:H2	1.75	0.66
19:9:45:PRO:CG	19:9:48:LEU:HG	2.26	0.66
6:F:176:TYR:CE2	22:F:301:CLA:HBD	2.31	0.66
22:4:308:CLA:HMB1	22:4:308:CLA:HBB1	1.78	0.66
17:6:219:LEU:HD11	22:6:314:CLA:HMC3	1.76	0.66
1:A:422:TYR:HE1	1:A:427:ASN:HD21	1.44	0.66
11:K:23:ARG:NH1	11:K:52:PRO:HG2	2.10	0.66
19:9:119:ASN:ND2	20:0:211:ASN:OD1	2.28	0.66
22:A:809:CLA:H91	25:J:101:8CT:C40	2.26	0.66
2:B:140:VAL:O	2:B:143:SER:OG	2.11	0.66
22:B:839:CLA:H122	22:B:840:CLA:H112	1.78	0.66
29:7:308:CHL:CMB	25:7:321:8CT:C18	2.74	0.66
13:1:171:LEU:HD23	13:1:174:LYS:HD2	1.77	0.66
15:3:140:ASN:ND2	30:3:315:XAT:O3	2.28	0.66
2:B:693:TRP:HE3	22:B:839:CLA:HMD3	1.61	0.65
17:6:100:LEU:HD12	17:6:101:VAL:HG23	1.78	0.65
17:6:229:SER:O	25:7:323:8CT:C09	2.45	0.65
13:5:202:GLN:O	13:5:206:GLU:N	2.25	0.65
16:8:144:GLU:OE1	16:8:147:ARG:NH2	2.29	0.65
14:2:85:GLU:OE2	14:2:209:ARG:NH2	2.29	0.65
22:2:309:CLA:H121	30:2:315:XAT:H193	1.77	0.65
13:5:147:ASP:HB3	13:5:150:LYS:HB3	1.79	0.65
22:0:302:CLA:HBB1	30:0:314:XAT:H31	1.79	0.65
22:B:850:CLA:H93	6:F:153:LEU:HD22	1.78	0.65
4:D:130:LYS:NZ	8:H:66:THR:O	2.27	0.65
22:6:305:CLA:C3B	25:6:321:8CT:C33	2.75	0.65
22:A:809:CLA:H122	25:J:104:8CT:C07	2.27	0.65
11:K:45:LEU:HD23	11:K:47:LEU:H	1.62	0.65
1:A:133:ASN:HB3	1:A:141:GLN:HB3	1.78	0.65
13:1:207:HIS:CG	22:1:311:CLA:HAA2	2.32	0.65
18:7:106:PHE:CE2	18:7:108:TYR:HB3	2.31	0.65
22:A:841:CLA:HBB1	22:A:841:CLA:H92	1.78	0.65
2:B:174:ARG:NH1	22:B:808:CLA:H162	2.12	0.65
1:A:386:ALA:HB1	1:A:527:ALA:HA	1.77	0.65
16:4:175:TYR:HE2	16:4:194:LYS:HE2	1.61	0.65
17:6:92:VAL:HG23	17:6:200:PHE:CE2	2.31	0.65
1:A:96:MET:HE2	22:A:828:CLA:HED1	1.79	0.64
1:A:205:HIS:CD2	22:A:813:CLA:HMC2	2.33	0.64
8:H:75:GLN:HG3	12:L:34:SER:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:THR:HA	2:B:112:PRO:HA	1.77	0.64
13:1:159:ASP:O	13:1:161:ALA:N	2.30	0.64
14:2:138:VAL:HA	22:2:308:CLA:HBB2	1.79	0.64
13:5:91:GLN:HE22	22:5:304:CLA:CGD	2.11	0.64
13:1:219:ASN:OD1	13:1:220:GLY:N	2.29	0.64
16:8:166:LYS:HE3	16:8:179:ILE:H	1.60	0.64
25:K:103:8CT:C38	22:K:104:CLA:C4B	2.76	0.64
14:2:147:MET:HG3	14:2:158:GLN:NE2	2.12	0.64
16:8:140:MET:HG2	22:8:308:CLA:HMC3	1.78	0.64
22:B:803:CLA:HHB	22:B:805:CLA:H202	1.80	0.64
15:3:135:ILE:HD12	15:3:140:ASN:HA	1.80	0.64
16:8:237:ASN:O	16:8:241:ILE:HG12	1.98	0.64
1:A:199:VAL:HG11	22:A:825:CLA:HAC2	1.79	0.64
22:B:806:CLA:H3A	22:B:806:CLA:CGA	2.27	0.64
22:B:837:CLA:HMB1	22:B:837:CLA:HBB1	1.79	0.64
22:2:304:CLA:HMD2	22:6:301:CLA:HBC3	1.78	0.64
1:A:401:TRP:HB3	22:A:828:CLA:HMC3	1.80	0.64
13:1:139:GLU:OE1	13:1:142:ARG:NH2	2.22	0.64
22:5:309:CLA:H13	30:5:315:XAT:H203	1.78	0.64
16:8:210:GLY:O	16:8:214:GLN:N	2.22	0.64
29:5:301:CHL:HED1	16:8:146:ARG:HA	1.80	0.64
18:7:39:ARG:NH1	18:7:59:ASP:O	2.31	0.64
18:7:234:ASN:OD1	18:7:235:ILE:N	2.31	0.64
29:7:308:CHL:HBB2	22:7:316:CLA:HMC3	1.78	0.64
1:A:308:VAL:O	1:A:312:ILE:HG12	1.98	0.64
4:D:130:LYS:NZ	8:H:66:THR:OG1	2.20	0.64
17:6:133:TYR:CG	25:6:321:8CT:C40	2.80	0.64
2:B:397:ASP:HA	4:D:198:ILE:HD11	1.80	0.63
13:1:36:LEU:HD12	29:4:301:CHL:HMA3	1.79	0.63
29:4:307:CHL:HMB3	25:4:317:8CT:C18	2.28	0.63
1:A:71:LEU:HB2	1:A:193:LEU:HD12	1.79	0.63
1:A:629:GLU:HG3	1:A:630:SER:H	1.63	0.63
22:G:102:CLA:HBB1	25:G:104:8CT:C15	2.29	0.63
1:A:544:HIS:HE1	1:A:611:VAL:HA	1.64	0.63
2:B:545:LYS:HE2	6:F:236:ILE:HG12	1.79	0.63
22:G:102:CLA:HMB2	25:G:104:8CT:C19	2.27	0.63
13:5:47:GLU:N	13:5:47:GLU:OE1	2.30	0.63
14:2:206:LYS:NZ	24:2:318:LHG:O5	2.23	0.63
1:A:205:HIS:O	1:A:209:GLY:N	2.27	0.63
19:9:209:ILE:N	22:9:312:CLA:O1A	2.32	0.63
7:G:7:VAL:O	7:G:11:SER:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:8:179:ILE:HD11	29:8:314:CHL:C3A	2.27	0.63
20:0:72:ARG:HH21	20:0:164:LEU:HD11	1.63	0.63
1:A:601:LEU:HB3	1:A:737:ILE:HD11	1.80	0.63
6:F:154:ALA:HB1	6:F:160:ALA:HA	1.81	0.63
8:H:99:ARG:HH21	12:L:102:GLN:HG2	1.63	0.63
29:7:308:CHL:CBB	22:7:316:CLA:HMC3	2.29	0.63
16:8:199:LYS:NZ	31:8:319:LMG:O5	2.29	0.63
11:K:32:LYS:HB3	11:K:43:LYS:HG3	1.80	0.63
13:1:78:GLY:HA3	13:1:179:ALA:HB1	1.81	0.63
16:4:92:MET:HG2	22:4:309:CLA:HMC1	1.81	0.63
17:6:134:VAL:CG2	25:6:321:8CT:C39	2.77	0.63
18:7:62:TRP:CZ3	30:7:320:XAT:H383	2.34	0.63
16:8:166:LYS:HZ1	16:8:179:ILE:N	1.96	0.63
20:0:93:ASN:HD22	20:0:188:PRO:HD2	1.63	0.63
2:B:582:TRP:HH2	22:B:803:CLA:HAB	1.64	0.62
2:B:687:LEU:N	12:L:39:TYR:OH	2.32	0.62
7:G:79:HIS:CG	25:G:104:8CT:C40	2.82	0.62
1:A:695:ARG:NH1	1:A:722:ALA:O	2.25	0.62
4:D:167:HIS:O	4:D:169:LYS:N	2.32	0.62
8:H:83:GLY:HA2	8:H:86:ASN:HB2	1.81	0.62
8:H:103:ARG:NH2	12:L:98:THR:O	2.32	0.62
22:4:311:CLA:H2A	22:4:311:CLA:O2A	1.98	0.62
16:8:89:PHE:CZ	22:8:308:CLA:HBC1	2.34	0.62
1:A:223:ILE:HA	1:A:227:ILE:HD12	1.81	0.62
1:A:491:TRP:O	1:A:494:SER:OG	2.14	0.62
16:4:238:VAL:HB	16:4:239:TRP:CD1	2.33	0.62
2:B:31:PHE:HD2	22:B:808:CLA:HMC2	1.64	0.62
13:1:186:PHE:HA	13:1:189:PHE:HD2	1.65	0.62
29:0:301:CHL:H72	22:0:312:CLA:H93	1.81	0.62
1:A:304:LEU:HD12	22:A:815:CLA:HMC1	1.80	0.62
2:B:398:TYR:HD2	2:B:542:ARG:HH22	1.45	0.62
2:B:595:HIS:CD2	2:B:623:TYR:CE1	2.85	0.62
22:B:806:CLA:H162	25:B:848:8CT:C18	2.29	0.62
4:D:178:ASN:OD1	4:D:179:ALA:N	2.29	0.62
22:1:303:CLA:NB	25:1:316:8CT:C36	2.63	0.62
15:3:81:PHE:CD2	30:3:315:XAT:H221	2.33	0.62
18:7:226:HIS:CG	22:7:313:CLA:HAA2	2.34	0.62
16:8:176:PRO:HD2	22:8:309:CLA:CAD	2.29	0.62
2:B:339:ALA:CB	25:B:847:8CT:C27	2.78	0.62
14:2:215:CYS:SG	30:2:316:XAT:H12	2.39	0.62
15:3:261:HIS:CG	22:3:311:CLA:HAA2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:159:LEU:HD22	17:6:168:GLY:HA3	1.80	0.62
19:9:174:LEU:HD21	30:9:314:XAT:H391	1.79	0.62
22:A:821:CLA:HMB2	22:A:825:CLA:HMA3	1.81	0.62
22:A:840:CLA:H202	22:F:301:CLA:HBB1	1.81	0.62
2:B:676:GLU:O	3:C:81:TYR:OH	2.11	0.62
24:5:318:LHG:H282	24:5:318:LHG:HC82	1.82	0.62
22:A:826:CLA:H92	25:A:849:8CT:C40	2.30	0.62
22:B:840:CLA:NC	25:B:848:8CT:C22	2.57	0.62
11:K:65:SER:N	25:K:103:8CT:C39	2.63	0.62
13:1:55:TYR:CE2	30:1:315:XAT:H383	2.35	0.62
18:7:109:GLU:O	18:7:111:GLY:N	2.31	0.62
29:8:314:CHL:HHC	29:8:314:CHL:HBB1	1.80	0.62
19:9:45:PRO:HG2	19:9:48:LEU:HG	1.82	0.62
19:9:86:ASN:HD21	22:9:309:CLA:HAC1	1.64	0.62
1:A:125:PRO:HA	1:A:130:GLU:HB2	1.82	0.62
2:B:92:TRP:NE1	8:H:129:ILE:HG12	2.15	0.62
3:C:7:ILE:HD12	3:C:41:SER:HA	1.81	0.62
22:4:302:CLA:H2	30:4:316:XAT:O24	1.99	0.62
13:5:207:HIS:CG	22:5:312:CLA:HAA2	2.35	0.62
1:A:666:TYR:CE2	2:B:617:MET:HG2	2.35	0.61
17:6:116:LEU:HD21	17:6:120:ILE:HD11	1.82	0.61
18:7:90:MET:HB3	22:7:305:CLA:HBB2	1.82	0.61
20:0:147:MET:HG2	20:0:148:PRO:HD3	1.82	0.61
2:B:133:GLN:HE22	21:M:7:GLN:HE22	1.48	0.61
13:1:104:SER:HB2	29:1:305:CHL:C2D	2.30	0.61
18:7:78:ARG:HH22	22:7:303:CLA:HED3	1.65	0.61
22:9:303:CLA:H3A	22:9:303:CLA:CGA	2.30	0.61
20:0:75:GLU:OE2	20:0:168:ARG:NH1	2.27	0.61
1:A:274:TRP:CD1	22:A:817:CLA:HMB2	2.36	0.61
2:B:223:LYS:HA	19:9:214:LEU:HG	1.82	0.61
14:2:114:GLN:NE2	14:2:228:GLY:HA3	2.16	0.61
14:2:237:ILE:HD13	22:2:313:CLA:HMC3	1.82	0.61
17:6:223:PHE:HD2	18:7:123:LEU:HD22	1.65	0.61
22:A:802:CLA:HBB1	22:A:802:CLA:HMB1	1.83	0.61
4:D:167:HIS:CG	4:D:168:PRO:HD3	2.36	0.61
6:F:77:ASP:N	6:F:81:LEU:O	2.33	0.61
22:3:308:CLA:HMB1	22:3:308:CLA:HBB1	1.83	0.61
22:3:310:CLA:HMB2	30:3:314:XAT:H402	1.81	0.61
29:6:302:CHL:HBB2	22:6:303:CLA:HBC2	1.83	0.61
20:0:83:MET:HB2	30:0:313:XAT:H15	1.82	0.61
1:A:90:LEU:HD21	22:A:805:CLA:H91	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:THR:HB	1:A:431:LEU:HD21	1.81	0.61
2:B:302:LYS:NZ	7:G:37:GLU:HG3	2.15	0.61
22:B:850:CLA:H2A	22:B:850:CLA:H12	1.82	0.61
11:K:38:LEU:HA	22:K:105:CLA:H42	1.82	0.61
13:1:53:TYR:OH	13:1:177:LYS:NZ	2.25	0.61
22:1:303:CLA:H2	25:1:316:8CT:C34	2.30	0.61
22:1:304:CLA:C2A	25:1:316:8CT:C27	2.79	0.61
14:2:48:PRO:HB2	15:3:184:MET:HE1	1.81	0.61
14:2:66:TYR:CE2	30:2:316:XAT:H383	2.34	0.61
22:6:305:CLA:C3B	30:6:320:XAT:H163	2.30	0.61
8:H:124:ASP:CG	8:H:127:LEU:HD12	2.21	0.61
22:1:304:CLA:H2A	22:1:304:CLA:O1A	1.99	0.61
22:1:310:CLA:HMC2	30:1:314:XAT:H203	1.83	0.61
20:0:128:GLU:HA	20:0:131:ARG:HG2	1.81	0.61
2:B:92:TRP:CZ2	9:I:8:SER:HA	2.36	0.61
22:8:310:CLA:HBC3	31:8:319:LMG:HC92	1.82	0.61
1:A:208:ALA:HB1	22:A:820:CLA:HBC3	1.81	0.60
22:A:814:CLA:HAC2	22:A:815:CLA:HMB3	1.83	0.60
2:B:375:HIS:HA	2:B:378:ILE:HG22	1.83	0.60
16:4:208:THR:HG21	30:4:316:XAT:H12	1.83	0.60
16:8:161:PRO:HB3	29:8:314:CHL:C3B	2.31	0.60
19:9:47:TYR:HE1	19:9:48:LEU:HD23	1.66	0.60
2:B:191:THR:HG23	2:B:277:HIS:HB2	1.83	0.60
2:B:326:ILE:HD12	2:B:332:PHE:CE1	2.37	0.60
16:8:179:ILE:CD1	29:8:314:CHL:C4A	2.79	0.60
2:B:303:GLU:OE1	7:G:34:GLN:HA	1.99	0.60
2:B:580:VAL:HB	2:B:710:LEU:HD11	1.83	0.60
22:B:840:CLA:CMC	25:B:848:8CT:C22	2.78	0.60
19:9:69:ARG:HH12	22:9:301:CLA:CGD	2.14	0.60
2:B:361:ILE:HG22	2:B:362:ALA:H	1.65	0.60
12:L:21:THR:H	12:L:24:THR:HG1	1.46	0.60
12:L:111:GLN:HG2	12:L:128:GLN:HB2	1.83	0.60
14:2:96:THR:HG21	30:2:315:XAT:H32	1.84	0.60
16:4:161:PRO:HG2	16:4:162:ILE:HD12	1.83	0.60
16:8:190:VAL:HG23	16:8:191:ASP:H	1.66	0.60
19:9:59:ASP:OD1	30:9:315:XAT:O23	2.15	0.60
29:2:306:CHL:HHC	29:2:306:CHL:HBB1	1.83	0.60
18:7:105:VAL:HG11	22:7:305:CLA:HED1	1.81	0.60
13:5:50:PRO:HB3	13:5:172:LYS:HG2	1.83	0.60
2:B:56:ILE:HG21	22:B:809:CLA:HMD2	1.82	0.60
2:B:61:THR:HG21	22:B:829:CLA:H42	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:PHE:HA	2:B:121:TYR:OH	2.02	0.60
2:B:292:ARG:HD2	7:G:36:PRO:HD3	1.84	0.60
12:L:77:ALA:HA	12:L:80:THR:HG22	1.83	0.60
29:2:305:CHL:C4A	25:2:317:8CT:C38	2.80	0.60
22:4:313:CLA:O1D	22:4:313:CLA:H2A	2.01	0.60
17:6:120:ILE:HD13	25:8:301:8CT:C40	2.31	0.60
1:A:430:ASN:H	1:A:433:ASP:HB3	1.67	0.60
22:A:837:CLA:HBB1	22:A:837:CLA:HMB1	1.83	0.60
22:2:319:CLA:HBB1	31:4:318:LMG:H162	1.84	0.60
15:3:61:ASP:OD1	15:3:62:GLU:N	2.34	0.60
17:6:62:TRP:CD1	30:6:320:XAT:H383	2.36	0.60
19:9:58:TYR:CE2	30:9:315:XAT:H383	2.33	0.60
20:0:109:VAL:HG11	22:0:305:CLA:HBA2	1.84	0.60
1:A:307:ALA:O	1:A:311:ILE:HD12	2.02	0.60
22:A:819:CLA:HMB1	22:A:819:CLA:HBB1	1.82	0.60
14:2:203:LYS:O	14:2:207:ASN:ND2	2.30	0.60
15:3:190:LEU:HD13	25:3:316:8CT:C38	2.31	0.60
17:6:153:ILE:HG22	22:8:310:CLA:HAB	1.83	0.60
13:5:78:GLY:O	13:5:82:MET:N	2.27	0.60
19:9:39:LEU:CD1	19:9:40:VAL:H	2.09	0.60
1:A:725:ILE:HD11	2:B:566:GLY:HA3	1.83	0.59
16:4:159:VAL:HG13	16:4:161:PRO:HD2	1.84	0.59
29:5:301:CHL:H11	16:8:142:TRP:HE3	1.67	0.59
18:7:234:ASN:ND2	22:7:314:CLA:O1D	2.34	0.59
22:A:826:CLA:HBB1	22:A:838:CLA:HMA1	1.83	0.59
2:B:623:TYR:O	2:B:627:ASN:CG	2.39	0.59
2:B:627:ASN:CB	2:B:724:PHE:HE1	2.04	0.59
6:F:176:TYR:OH	6:F:210:VAL:O	2.13	0.59
11:K:15:THR:HG21	11:K:68:HIS:CE1	2.37	0.59
13:1:175:GLU:HB3	22:1:308:CLA:C1B	2.33	0.59
1:A:544:HIS:CE1	1:A:611:VAL:HA	2.36	0.59
2:B:302:LYS:HZ2	7:G:37:GLU:HG3	1.67	0.59
6:F:232:LYS:HG2	6:F:233:GLU:H	1.66	0.59
17:6:108:TYR:HE2	17:6:245:ILE:HG21	1.66	0.59
17:6:119:ASN:HD21	16:8:235:ALA:HB2	1.68	0.59
17:6:140:GLN:NE2	16:8:47:GLY:O	2.36	0.59
22:A:815:CLA:HBD	15:3:277:VAL:HG11	1.85	0.59
22:A:826:CLA:HAA2	22:A:827:CLA:OBD	2.02	0.59
5:E:18:TRP:HD1	5:E:21:ARG:HD2	1.66	0.59
6:F:176:TYR:CD2	22:F:301:CLA:HBD	2.37	0.59
14:2:147:MET:HG3	14:2:158:GLN:HE21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:7:307:CLA:C4D	25:7:323:8CT:C22	2.80	0.59
19:9:170:LYS:NZ	22:9:310:CLA:O1D	2.26	0.59
10:J:16:PHE:HE1	25:J:101:8CT:C17	2.16	0.59
17:6:133:TYR:CE1	25:6:321:8CT:C40	2.86	0.59
22:7:310:CLA:HMB1	22:7:310:CLA:HBB1	1.85	0.59
3:C:63:LEU:HD12	3:C:66:ARG:HH21	1.67	0.59
7:G:2:LEU:HD23	7:G:3:SER:H	1.66	0.59
8:H:111:GLY:HA2	22:H:201:CLA:H13	1.84	0.59
12:L:21:THR:HB	12:L:22:PRO:HD2	1.84	0.59
20:0:84:LEU:HD23	22:0:308:CLA:HMC1	1.83	0.59
2:B:548:PRO:HD2	3:C:62:PHE:CE1	2.37	0.59
16:4:175:TYR:CE2	16:4:194:LYS:HE2	2.37	0.59
2:B:390:GLY:HA3	25:B:847:8CT:C32	2.32	0.59
3:C:47:ASP:OD2	4:D:134:LYS:NZ	2.30	0.59
19:9:79:VAL:O	19:9:83:TRP:N	2.35	0.59
1:A:238:ASP:HB2	1:A:239:PRO:HD2	1.83	0.59
8:H:99:ARG:HB3	12:L:102:GLN:HE21	1.68	0.59
11:K:31:ASN:ND2	11:K:54:GLY:O	2.36	0.59
11:K:34:ALA:HA	22:K:105:CLA:H41	1.85	0.59
4:D:170:ASP:OD2	4:D:178:ASN:ND2	2.36	0.59
16:4:166:LYS:H	22:5:303:CLA:C3	2.16	0.59
22:7:307:CLA:HMB2	25:7:323:8CT:C27	2.32	0.59
20:0:128:GLU:HB3	20:0:132:TYR:CE2	2.38	0.59
1:A:199:VAL:HG13	22:A:825:CLA:HMD3	1.84	0.58
22:A:843:CLA:HMB3	24:A:845:LHG:HC62	1.84	0.58
2:B:94:PRO:HG2	22:H:201:CLA:HMB2	1.84	0.58
4:D:71:PRO:HG2	4:D:72:PRO:HD3	1.85	0.58
6:F:183:GLU:HB2	6:F:209:CYS:SG	2.43	0.58
15:3:58:PHE:HD2	15:3:76:TYR:HB3	1.67	0.58
15:3:241:PHE:HD2	22:3:311:CLA:HMC1	1.68	0.58
16:4:168:PRO:HB3	13:5:60:ILE:HG23	1.85	0.58
20:0:187:GLY:O	20:0:191:ASN:ND2	2.36	0.58
2:B:234:ALA:HA	2:B:256:THR:HG22	1.85	0.58
14:2:234:PHE:HA	14:2:237:ILE:HG22	1.84	0.58
17:6:43:LEU:HB3	17:6:46:SER:HB2	1.85	0.58
2:B:580:VAL:HG11	2:B:710:LEU:HD21	1.85	0.58
2:B:682:HIS:CE1	2:B:688:ALA:HB1	2.38	0.58
18:7:129:LEU:HD22	25:7:323:8CT:C39	2.33	0.58
22:8:312:CLA:HMD2	22:8:315:CLA:HBC3	1.84	0.58
22:6:318:CLA:CMA	25:7:323:8CT:C39	2.81	0.58
8:H:96:LEU:HB3	8:H:102:ILE:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:166:LYS:H	22:5:303:CLA:C2	2.17	0.58
1:A:364:LEU:HD12	22:A:825:CLA:HHB	1.85	0.58
8:H:96:LEU:HD22	8:H:102:ILE:HG12	1.85	0.58
22:0:308:CLA:H61	30:0:313:XAT:H11	1.84	0.58
2:B:463:ILE:O	2:B:467:GLN:HG2	2.03	0.58
22:K:105:CLA:HMA2	22:K:105:CLA:H2	1.86	0.58
29:6:306:CHL:HMB1	22:6:309:CLA:HBC2	1.86	0.58
22:5:303:CLA:CHD	22:5:308:CLA:HAA1	2.33	0.58
19:9:99:ILE:HG12	19:9:100:GLN:H	1.69	0.58
2:B:292:ARG:NH1	7:G:34:GLN:O	2.34	0.58
3:C:5:VAL:HG22	3:C:67:VAL:HG22	1.85	0.58
16:4:160:ASP:OD1	16:4:160:ASP:N	2.36	0.58
17:6:229:SER:HA	18:7:126:GLY:HA3	1.86	0.58
22:A:816:CLA:HMD2	15:3:145:PRO:HG3	1.86	0.58
13:1:99:TRP:HD1	13:1:200:PRO:HD3	1.68	0.58
17:6:231:ALA:HA	17:6:239:VAL:HG23	1.86	0.58
25:A:850:8CT:C40	2:B:438:VAL:HG11	2.33	0.58
2:B:91:ILE:HD12	22:B:812:CLA:HMD1	1.85	0.58
22:B:834:CLA:HBC2	22:B:835:CLA:HAB	1.86	0.58
22:B:850:CLA:O1A	22:B:850:CLA:H3A	2.04	0.58
1:A:465:ASP:OD1	1:A:646:ALA:HB1	2.04	0.57
1:A:690:PHE:HZ	22:A:840:CLA:HBC3	1.69	0.57
22:A:826:CLA:HMA1	25:A:849:8CT:C22	2.34	0.57
2:B:322:LEU:O	2:B:326:ILE:HG12	2.04	0.57
8:H:127:LEU:HD13	8:H:129:ILE:HD12	1.86	0.57
16:4:95:VAL:HG21	30:4:315:XAT:H401	1.86	0.57
16:8:185:PHE:HA	16:8:187:LYS:HG3	1.86	0.57
22:9:303:CLA:HBC1	24:9:316:LHG:H262	1.86	0.57
1:A:329:GLU:OE1	1:A:329:GLU:N	2.36	0.57
13:1:141:MET:HG3	22:1:306:CLA:HMC3	1.85	0.57
29:2:301:CHL:H42	15:3:165:VAL:HG22	1.86	0.57
13:5:46:PRO:O	13:5:49:LEU:N	2.31	0.57
20:0:46:LEU:HD13	22:0:302:CLA:HBD	1.85	0.57
2:B:213:LEU:HD13	19:9:190:ARG:HH11	1.69	0.57
22:B:826:CLA:HMA1	25:B:847:8CT:C17	2.35	0.57
12:L:115:LYS:HB3	12:L:121:ASP:HA	1.85	0.57
17:6:153:ILE:HG13	17:6:154:PHE:H	1.68	0.57
13:5:195:ALA:HB2	22:5:314:CLA:HED3	1.87	0.57
22:9:304:CLA:HMD2	22:9:308:CLA:C1D	2.35	0.57
6:F:102:GLN:HA	6:F:105:MET:HG2	1.85	0.57
22:2:304:CLA:HMB3	30:2:316:XAT:H182	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:314:XAT:H30	30:3:314:XAT:H403	1.86	0.57
18:7:199:ARG:NH2	22:7:303:CLA:HED2	2.17	0.57
19:9:116:LEU:HD23	20:0:200:LEU:HG	1.86	0.57
13:1:217:ALA:HB3	16:4:131:VAL:HG22	1.86	0.57
17:6:227:ILE:HA	17:6:230:LYS:HB2	1.85	0.57
16:8:158:ASN:HD22	29:8:307:CHL:HAC1	1.68	0.57
24:9:316:LHG:H341	24:9:316:LHG:H171	1.86	0.57
20:0:68:LEU:O	20:0:71:PHE:N	2.37	0.57
1:A:120:ALA:CB	1:A:145:ILE:HD11	2.35	0.57
22:A:805:CLA:H51	22:A:813:CLA:H12	1.86	0.57
22:B:807:CLA:O2D	22:B:807:CLA:H2A	2.03	0.57
22:B:828:CLA:HBC3	28:B:849:DGD:HBV1	1.86	0.57
7:G:42:THR:N	7:G:45:GLU:OE2	2.38	0.57
18:7:125:LEU:HD23	18:7:128:ILE:HD12	1.86	0.57
16:8:81:GLN:HE22	16:8:173:PRO:HB2	1.69	0.57
1:A:40:PHE:HB2	1:A:67:HIS:CD2	2.39	0.57
1:A:92:TRP:O	1:A:96:MET:HG2	2.05	0.57
1:A:215:SER:HB3	1:A:307:ALA:HB2	1.87	0.57
1:A:687:SER:OG	1:A:732:GLY:O	2.22	0.57
2:B:102:GLU:O	2:B:105:THR:HG22	2.05	0.57
2:B:596:TRP:HB2	2:B:623:TYR:CD1	2.39	0.57
22:6:310:CLA:O1D	22:6:310:CLA:H2A	2.05	0.57
13:5:174:LYS:NZ	22:5:311:CLA:OBD	2.34	0.57
22:5:304:CLA:C2B	25:5:317:8CT:C38	2.83	0.57
1:A:97:TYR:HE1	1:A:153:TRP:HE1	1.53	0.57
1:A:151:GLN:OE1	1:A:385:LEU:HD23	2.05	0.57
22:B:850:CLA:OBD	6:F:156:ARG:NH2	2.37	0.57
11:K:68:HIS:HE1	25:K:103:8CT:C15	2.13	0.57
13:1:145:GLU:HB2	13:1:151:ARG:HD2	1.85	0.57
14:2:179:PRO:HD3	29:2:307:CHL:HMD2	1.86	0.57
15:3:231:LYS:NZ	24:3:317:LHG:O5	2.38	0.57
22:A:804:CLA:H43	22:A:811:CLA:H92	1.86	0.57
2:B:392:ILE:HA	2:B:395:ILE:HG22	1.85	0.57
14:2:55:TRP:HE1	14:2:72:ALA:HB3	1.68	0.57
14:2:236:HIS:CG	22:2:312:CLA:HAA2	2.40	0.57
17:6:179:ILE:HG22	17:6:181:GLU:H	1.70	0.57
13:5:165:LYS:HG2	13:5:166:GLY:H	1.70	0.57
18:7:185:LYS:HG2	18:7:186:ASP:H	1.69	0.57
1:A:497:TYR:HB2	1:A:516:GLY:H	1.70	0.57
1:A:726:THR:OG1	24:A:844:LHG:O4	2.22	0.57
4:D:93:LYS:NZ	4:D:97:GLU:HG2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:141:GLY:HA2	15:3:148:SER:HA	1.87	0.57
15:3:246:GLN:HG2	15:3:257:ASN:HD22	1.70	0.57
17:6:136:ILE:HD11	22:6:323:CLA:H2A	1.86	0.57
1:A:274:TRP:CZ3	11:K:76:LEU:HD11	2.40	0.56
2:B:474:PHE:CG	22:B:850:CLA:H52	2.40	0.56
13:1:90:ALA:O	13:1:94:LEU:N	2.37	0.56
13:1:183:MET:SD	22:1:301:CLA:HBB1	2.45	0.56
22:3:304:CLA:HBB1	22:3:307:CLA:HMC1	1.86	0.56
17:6:92:VAL:HG23	17:6:200:PHE:HE2	1.70	0.56
22:8:308:CLA:HBB1	22:8:308:CLA:HHC	1.85	0.56
2:B:631:LEU:CD1	2:B:724:PHE:HA	2.30	0.56
22:B:838:CLA:HMB1	22:B:838:CLA:HBB1	1.86	0.56
8:H:81:TYR:HD1	22:L:202:CLA:HMD3	1.68	0.56
16:4:104:THR:OG1	16:4:112:ALA:N	2.23	0.56
19:9:201:LEU:HD11	22:9:313:CLA:HMC3	1.85	0.56
1:A:63:ASP:O	1:A:67:HIS:ND1	2.37	0.56
1:A:455:PHE:HB3	22:A:833:CLA:HBB2	1.87	0.56
2:B:10:GLN:HA	2:B:13:ALA:HB3	1.86	0.56
2:B:275:HIS:HD2	22:B:818:CLA:HMB1	1.70	0.56
2:B:631:LEU:CD2	2:B:727:ALA:HB3	2.32	0.56
22:B:809:CLA:H42	22:B:809:CLA:HMA2	1.86	0.56
8:H:74:GLY:HA2	12:L:39:TYR:HB3	1.88	0.56
8:H:103:ARG:HH22	12:L:102:GLN:HG3	1.70	0.56
16:4:157:VAL:HG21	29:4:307:CHL:HAC1	1.87	0.56
13:5:103:PRO:O	13:5:107:TYR:N	2.37	0.56
13:5:130:ILE:HG23	13:5:134:LEU:HD12	1.88	0.56
22:5:304:CLA:HBB1	25:5:317:8CT:C37	2.35	0.56
18:7:95:ILE:HG12	18:7:107:TRP:NE1	2.20	0.56
29:9:307:CHL:HHC	29:9:307:CHL:HBB1	1.87	0.56
1:A:19:LYS:HE3	1:A:21:ILE:HD11	1.87	0.56
2:B:349:ALA:HB2	2:B:375:HIS:HB2	1.87	0.56
6:F:175:GLY:HA3	6:F:216:TRP:CZ2	2.40	0.56
12:L:70:LEU:HD12	12:L:70:LEU:N	2.20	0.56
16:4:94:LEU:HD22	30:4:315:XAT:H12	1.86	0.56
16:4:176:PRO:HB2	16:4:180:PHE:CD2	2.40	0.56
22:5:305:CLA:H3A	25:5:317:8CT:C26	2.36	0.56
1:A:580:CYS:HB3	1:A:589:CYS:HA	1.88	0.56
2:B:37:ILE:HD12	2:B:41:THR:HG23	1.88	0.56
2:B:398:TYR:HD2	2:B:542:ARG:NH2	2.04	0.56
22:B:850:CLA:H71	6:F:153:LEU:HD13	1.88	0.56
18:7:59:ASP:OD1	18:7:61:GLY:N	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:GLY:HA2	1:A:348:GLU:OE2	2.05	0.56
22:K:102:CLA:HMB1	22:K:102:CLA:HBB1	1.87	0.56
22:2:304:CLA:HBC2	22:6:301:CLA:HBC1	1.87	0.56
22:3:309:CLA:HBB1	22:3:309:CLA:HMB1	1.87	0.56
20:0:36:TRP:H	29:0:301:CHL:HBC3	1.71	0.56
1:A:117:LYS:HB2	1:A:136:VAL:HG13	1.86	0.56
2:B:436:LEU:O	2:B:440:ASN:ND2	2.39	0.56
12:L:66:LYS:O	12:L:71:ARG:HG2	2.06	0.56
13:1:215:ASN:HD21	22:1:312:CLA:HED2	1.69	0.56
14:2:66:TYR:HB3	22:2:302:CLA:CAD	2.35	0.56
22:3:319:CLA:HED3	18:7:264:GLN:HE22	1.70	0.56
22:6:318:CLA:HMA2	25:7:323:8CT:C39	2.36	0.56
18:7:107:TRP:HE1	30:7:320:XAT:H3	1.71	0.56
1:A:230:ASN:HD22	1:A:296:LEU:HD13	1.70	0.56
1:A:249:LEU:HD12	1:A:250:LEU:HG	1.88	0.56
1:A:304:LEU:HD21	22:A:817:CLA:C3B	2.35	0.56
15:3:195:VAL:HB	18:7:66:GLY:HA3	1.87	0.56
29:4:307:CHL:CMB	25:4:317:8CT:C18	2.83	0.56
17:6:115:ASP:OD1	17:6:116:LEU:N	2.38	0.56
2:B:141:PHE:CZ	22:B:815:CLA:H12	2.40	0.56
2:B:349:ALA:HB3	2:B:376:GLN:HE21	1.69	0.56
4:D:191:ILE:O	4:D:194:ASN:ND2	2.38	0.56
7:G:56:SER:O	19:9:42:ALA:HB1	2.06	0.56
13:1:184:PHE:CE2	22:1:311:CLA:HAB	2.41	0.56
13:1:185:ALA:HB2	30:1:314:XAT:H192	1.88	0.56
13:5:49:LEU:HD12	13:5:50:PRO:HD2	1.87	0.56
20:0:134:GLY:O	20:0:138:THR:N	2.24	0.56
1:A:664:GLN:N	1:A:664:GLN:OE1	2.39	0.56
3:C:19:ARG:NE	4:D:175:GLU:OE2	2.39	0.56
16:4:226:TRP:CZ3	22:4:313:CLA:HAC1	2.41	0.56
17:6:79:GLU:OE2	17:6:138:ARG:NH2	2.37	0.56
22:5:312:CLA:H2A	22:5:312:CLA:O1D	2.06	0.56
1:A:361:ASN:ND2	22:A:805:CLA:OBD	2.39	0.55
2:B:224:PRO:HG2	2:B:233:TYR:OH	2.06	0.55
1:A:619:MET:HE3	1:A:623:VAL:HG11	1.87	0.55
1:A:743:THR:OG1	22:A:801:CLA:O1D	2.24	0.55
22:A:853:CLA:H121	10:J:18:TRP:HD1	1.72	0.55
22:B:830:CLA:H101	28:B:849:DGD:HAG1	1.87	0.55
13:5:223:LEU:HD11	16:8:134:ALA:HB2	1.88	0.55
18:7:193:LYS:HD3	22:7:312:CLA:HBD	1.87	0.55
22:7:307:CLA:C1D	25:7:323:8CT:C22	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:0:36:TRP:CH2	20:0:38:PRO:HB3	2.42	0.55
1:A:206:HIS:HE1	22:A:813:CLA:NA	2.04	0.55
1:A:745:TRP:CE2	25:A:850:8CT:C38	2.89	0.55
31:5:319:LMG:H112	29:8:306:CHL:HBB1	1.88	0.55
29:7:308:CHL:CMB	25:7:321:8CT:C19	2.81	0.55
16:8:64:TYR:HE2	30:8:317:XAT:H383	1.71	0.55
16:8:158:ASN:HB3	29:8:307:CHL:HMC	1.87	0.55
2:B:88:ALA:HB2	2:B:116:ALA:HB2	1.88	0.55
2:B:469:LYS:NZ	2:B:509:PHE:O	2.40	0.55
22:B:806:CLA:HBC2	22:B:806:CLA:HHD	1.88	0.55
3:C:15:THR:HG22	3:C:28:MET:HG3	1.88	0.55
7:G:37:GLU:HA	7:G:42:THR:HA	1.88	0.55
13:1:80:TRP:CD1	22:1:307:CLA:HMD3	2.41	0.55
16:4:84:LEU:HB3	16:4:88:ARG:NH1	2.22	0.55
20:0:53:ASP:HA	22:0:302:CLA:O2D	2.06	0.55
22:0:305:CLA:HED3	22:0:305:CLA:H2	1.86	0.55
2:B:414:HIS:ND1	2:B:414:HIS:O	2.39	0.55
4:D:93:LYS:O	4:D:97:GLU:N	2.36	0.55
22:6:310:CLA:H2	30:6:319:XAT:H28	1.88	0.55
16:8:161:PRO:HD2	16:8:165:GLY:HA2	1.89	0.55
29:0:306:CHL:HHC	29:0:306:CHL:HBB1	1.88	0.55
22:B:830:CLA:HBB1	22:B:830:CLA:HMB1	1.88	0.55
8:H:113:ALA:HB3	22:H:201:CLA:H121	1.87	0.55
17:6:206:ILE:HD11	17:6:227:ILE:HD13	1.89	0.55
16:8:78:TRP:HZ2	22:8:308:CLA:HAA2	1.72	0.55
22:9:311:CLA:H11	22:9:311:CLA:HMA2	1.86	0.55
2:B:44:GLN:HG3	2:B:162:GLN:HE21	1.70	0.55
8:H:81:TYR:CE2	12:L:43:VAL:HG21	2.41	0.55
13:5:141:MET:HB3	22:5:307:CLA:HMC3	1.88	0.55
13:5:212:LEU:HD22	16:8:131:VAL:HG11	1.87	0.55
22:8:310:CLA:C4C	31:8:319:LMG:HC71	2.36	0.55
1:A:120:ALA:HB2	1:A:145:ILE:HD11	1.89	0.55
22:B:826:CLA:HMB1	22:B:826:CLA:HBB1	1.88	0.55
8:H:99:ARG:HE	12:L:102:GLN:HG2	1.72	0.55
8:H:133:PRO:O	8:H:135:LYS:N	2.40	0.55
12:L:35:ASN:O	12:L:40:ARG:NH2	2.38	0.55
15:3:189:PHE:CD1	25:3:316:8CT:C38	2.89	0.55
16:4:186:ALA:HA	16:4:190:VAL:HG22	1.87	0.55
20:0:72:ARG:HH12	22:0:302:CLA:HED3	1.70	0.55
1:A:206:HIS:HE1	22:A:813:CLA:C1A	2.20	0.55
2:B:85:ARG:NH2	8:H:142:LYS:HB3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:809:CLA:HMB2	22:B:830:CLA:HBB2	1.88	0.55
13:1:196:THR:HG22	13:1:198:LYS:H	1.71	0.55
17:6:248:HIS:ND1	17:6:255:ASP:OD1	2.36	0.55
22:A:821:CLA:HMB1	22:A:821:CLA:HBB1	1.89	0.55
25:B:846:8CT:C39	25:B:846:8CT:C13	2.85	0.55
22:H:201:CLA:HMB1	22:H:201:CLA:HBB1	1.89	0.55
16:4:239:TRP:CD1	16:4:243:LEU:HD11	2.42	0.55
17:6:57:THR:HG21	17:6:183:LYS:HG2	1.88	0.55
16:8:142:TRP:O	16:8:146:ARG:HG2	2.07	0.55
22:A:839:CLA:HBC3	22:A:853:CLA:NC	2.22	0.54
2:B:216:LEU:HD21	19:9:216:ILE:HG12	1.88	0.54
22:3:319:CLA:H51	22:3:319:CLA:H121	1.88	0.54
16:4:172:ILE:HD11	16:4:175:TYR:HB2	1.88	0.54
1:A:745:TRP:NE1	22:A:828:CLA:O1A	2.41	0.54
25:B:847:8CT:C27	25:B:847:8CT:C23	2.85	0.54
3:C:51:CYS:HB3	3:C:53:ARG:HG3	1.89	0.54
25:J:104:8CT:C38	25:J:104:8CT:C28	2.86	0.54
16:8:72:ASP:OD1	16:8:75:THR:OG1	2.24	0.54
25:A:850:8CT:C09	25:A:850:8CT:C11	2.85	0.54
2:B:476:PHE:CE2	22:B:850:CLA:H11	2.42	0.54
2:B:503:ASN:O	2:B:505:THR:N	2.35	0.54
25:G:104:8CT:C15	25:G:104:8CT:C40	2.86	0.54
25:K:103:8CT:C39	25:K:103:8CT:C13	2.85	0.54
13:1:134:LEU:HD22	22:1:304:CLA:H2	1.88	0.54
22:2:302:CLA:HMB1	22:2:302:CLA:HBB1	1.89	0.54
22:6:301:CLA:HED2	22:6:301:CLA:H12	1.89	0.54
22:6:305:CLA:CHC	25:6:321:8CT:C33	2.84	0.54
16:8:221:GLY:H	16:8:224:ALA:HB3	1.72	0.54
1:A:687:SER:HB2	1:A:735:HIS:HB2	1.89	0.54
22:A:817:CLA:HBB1	22:A:817:CLA:HMB1	1.88	0.54
25:A:850:8CT:C36	25:A:850:8CT:C28	2.85	0.54
25:B:843:8CT:C19	25:G:104:8CT:C08	2.77	0.54
22:2:302:CLA:O1A	22:2:302:CLA:H3A	2.07	0.54
15:3:264:ASP:HB3	15:3:268:ASN:HD22	1.73	0.54
25:8:301:8CT:C11	25:8:301:8CT:C09	2.86	0.54
2:B:358:TYR:HB2	2:B:361:ILE:HD12	1.88	0.54
2:B:685:THR:O	2:B:689:ASN:ND2	2.41	0.54
22:G:103:CLA:NC	25:G:104:8CT:C37	2.70	0.54
25:J:101:8CT:C37	25:J:101:8CT:C28	2.86	0.54
15:3:175:LEU:O	15:3:178:TYR:N	2.40	0.54
25:3:316:8CT:C19	25:3:316:8CT:C39	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:7:264:GLN:OE1	18:7:264:GLN:N	2.36	0.54
22:9:312:CLA:H93	24:9:316:LHG:H172	1.90	0.54
20:0:146:PHE:HB2	20:0:149:PHE:O	2.08	0.54
1:A:581:ASP:OD2	3:C:53:ARG:NH2	2.24	0.54
22:A:813:CLA:HBB1	22:A:813:CLA:HMB1	1.89	0.54
2:B:439:HIS:CD2	2:B:453:ILE:HG12	2.43	0.54
12:L:114:VAL:HG12	12:L:115:LYS:N	2.22	0.54
17:6:227:ILE:CD1	22:6:313:CLA:HMD1	2.36	0.54
13:5:153:TYR:HB3	22:5:309:CLA:HED2	1.89	0.54
18:7:75:ALA:O	18:7:79:GLN:HG2	2.07	0.54
25:7:323:8CT:C22	25:7:323:8CT:C18	2.85	0.54
25:7:323:8CT:C39	25:7:323:8CT:C19	2.85	0.54
16:8:144:GLU:HG3	22:8:308:CLA:C4B	2.38	0.54
29:8:307:CHL:O1A	22:8:309:CLA:HHD	2.08	0.54
1:A:566:ARG:NE	2:B:676:GLU:OE2	2.30	0.54
1:A:709:HIS:HE1	22:A:839:CLA:NA	2.06	0.54
25:B:846:8CT:C37	25:B:846:8CT:C28	2.85	0.54
5:E:9:VAL:CG1	5:E:59:VAL:HG13	2.38	0.54
13:1:72:GLU:HG3	13:1:152:VAL:HG22	1.88	0.54
13:1:92:GLU:OE1	13:1:201:VAL:HB	2.07	0.54
15:3:241:PHE:HD1	22:3:302:CLA:HBB2	1.72	0.54
22:A:819:CLA:O1A	22:A:829:CLA:HMD1	2.07	0.54
25:A:849:8CT:C22	25:A:849:8CT:C18	2.86	0.54
2:B:308:HIS:HA	22:B:841:CLA:HMD1	1.89	0.54
22:B:807:CLA:H3A	21:M:29:LEU:HD22	1.90	0.54
22:1:311:CLA:H71	22:1:312:CLA:H91	1.89	0.54
25:1:316:8CT:C40	25:1:316:8CT:C15	2.86	0.54
15:3:69:ASP:OD1	15:3:69:ASP:N	2.38	0.54
13:5:111:SER:O	13:5:113:THR:N	2.37	0.54
18:7:170:GLY:HA2	29:7:308:CHL:HMD2	1.88	0.54
1:A:663:ILE:CG2	2:B:621:ARG:CG	2.71	0.54
22:B:810:CLA:CGA	9:I:14:VAL:HG11	2.37	0.54
4:D:82:ILE:HG13	4:D:123:ARG:HE	1.73	0.54
7:G:79:HIS:CB	25:G:104:8CT:C40	2.86	0.54
8:H:98:ARG:H	8:H:102:ILE:CD1	2.21	0.54
25:J:101:8CT:C40	25:J:101:8CT:C15	2.85	0.54
13:1:134:LEU:O	13:1:138:ALA:N	2.36	0.54
17:6:176:PRO:HD2	22:6:310:CLA:O1A	2.07	0.54
22:5:307:CLA:O1D	22:5:307:CLA:H2A	2.08	0.54
18:7:162:ASN:N	18:7:162:ASN:OD1	2.41	0.54
25:8:318:8CT:C38	25:8:318:8CT:C28	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:849:8CT:C40	25:A:849:8CT:C15	2.85	0.54
25:1:316:8CT:C28	25:1:316:8CT:C38	2.86	0.54
22:5:310:CLA:HBC3	24:5:318:LHG:HC62	1.90	0.54
16:8:238:VAL:HG13	16:8:239:TRP:CD1	2.43	0.54
1:A:711:LYS:HE2	6:F:230:LEU:HD23	1.89	0.53
2:B:636:ASN:OD1	2:B:637:PRO:HD2	2.08	0.53
22:B:816:CLA:O1D	22:B:816:CLA:H2A	2.08	0.53
17:6:263:GLU:HG3	17:6:266:TRP:CE3	2.43	0.53
16:8:78:TRP:CZ2	22:8:308:CLA:HAA2	2.44	0.53
19:9:209:ILE:HB	22:9:312:CLA:H12	1.90	0.53
1:A:695:ARG:O	1:A:698:TRP:N	2.38	0.53
22:A:802:CLA:O1A	22:A:802:CLA:H3A	2.07	0.53
17:6:42:TRP:NE1	17:6:61:GLY:O	2.42	0.53
17:6:116:LEU:HD11	17:6:120:ILE:HG13	1.90	0.53
22:5:311:CLA:HMB1	22:5:311:CLA:HBB1	1.89	0.53
19:9:38:TRP:NE1	19:9:43:SER:HB3	2.22	0.53
1:A:299:ILE:O	1:A:302:HIS:HB3	2.08	0.53
1:A:433:ASP:OD1	1:A:437:ARG:HD2	2.08	0.53
2:B:206:HIS:O	2:B:211:ASN:ND2	2.39	0.53
2:B:377:TYR:HB3	22:B:828:CLA:HMC3	1.90	0.53
2:B:685:THR:HG23	2:B:688:ALA:HB3	1.89	0.53
2:B:705:ALA:O	2:B:709:GLY:N	2.35	0.53
3:C:73:THR:H	3:C:76:SER:HG	1.57	0.53
5:E:26:VAL:HG11	5:E:40:ARG:HE	1.73	0.53
25:2:317:8CT:C09	25:2:317:8CT:C11	2.86	0.53
17:6:191:ARG:HH21	22:6:303:CLA:HMD3	1.73	0.53
22:6:303:CLA:HBA1	22:6:303:CLA:C4A	2.37	0.53
20:0:204:ILE:HD11	20:0:209:VAL:HG23	1.90	0.53
25:A:854:8CT:C36	25:A:854:8CT:C28	2.86	0.53
2:B:627:ASN:ND2	2:B:724:PHE:CZ	2.65	0.53
3:C:28:MET:HE3	3:C:38:GLN:HG2	1.91	0.53
25:2:317:8CT:C27	25:2:317:8CT:C38	2.85	0.53
22:3:311:CLA:C2B	30:3:314:XAT:H183	2.38	0.53
19:9:181:GLY:O	19:9:185:GLN:HG2	2.09	0.53
20:0:73:GLU:O	20:0:77:MET:N	2.36	0.53
29:0:301:CHL:HAA1	24:0:315:LHG:H151	1.90	0.53
22:A:820:CLA:HMB1	25:K:103:8CT:C40	2.39	0.53
25:B:843:8CT:C17	25:G:104:8CT:C08	2.84	0.53
22:1:309:CLA:C1D	22:1:310:CLA:HMD2	2.39	0.53
16:4:60:GLY:O	16:4:202:ARG:NH2	2.39	0.53
13:5:53:TYR:OH	13:5:177:LYS:NZ	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:7:146:ASP:OD2	29:7:308:CHL:HAC1	2.08	0.53
25:7:321:8CT:C37	25:7:321:8CT:C28	2.87	0.53
22:8:310:CLA:C1D	22:8:311:CLA:HMD2	2.39	0.53
20:0:209:VAL:HG21	22:M:101:CLA:HMD3	1.91	0.53
4:D:128:LEU:HD13	8:H:58:PHE:CE1	2.44	0.53
6:F:112:SER:HB3	6:F:114:PRO:HD2	1.90	0.53
14:2:46:TRP:NE1	14:2:65:GLY:O	2.36	0.53
2:B:459:PHE:CD1	22:B:850:CLA:HMB3	2.43	0.53
25:J:101:8CT:C28	25:J:101:8CT:C36	2.86	0.53
19:9:195:ALA:O	19:9:199:ALA:N	2.41	0.53
20:0:174:SER:HA	20:0:177:PHE:HD2	1.74	0.53
2:B:513:GLY:H	2:B:516:ASP:HB3	1.74	0.53
6:F:137:LEU:HD21	10:J:38:ILE:HG21	1.91	0.53
15:3:85:GLU:HB2	15:3:86:PRO:HD2	1.90	0.53
19:9:104:TRP:CD1	19:9:105:GLU:HG3	2.44	0.53
1:A:364:LEU:HD12	22:A:825:CLA:HMA1	1.91	0.53
22:H:201:CLA:HBB2	9:I:15:GLY:HA3	1.91	0.53
11:K:52:PRO:HD3	22:K:104:CLA:C1D	2.39	0.53
15:3:109:PHE:O	15:3:113:GLY:N	2.34	0.53
18:7:195:ILE:O	18:7:198:GLY:N	2.42	0.53
16:8:115:THR:N	16:8:119:ASN:OD1	2.42	0.53
2:B:299:HIS:HB3	2:B:304:ILE:HD11	1.91	0.53
22:B:826:CLA:NB	25:B:847:8CT:C22	2.72	0.53
6:F:150:ASP:HB2	6:F:153:LEU:HD12	1.91	0.53
22:7:306:CLA:HMC3	22:7:307:CLA:C1C	2.39	0.53
2:B:707:LEU:HD22	28:B:849:DGD:HA22	1.90	0.52
22:1:302:CLA:HBB1	22:1:307:CLA:H151	1.92	0.52
14:2:157:SER:HA	14:2:160:THR:HG23	1.91	0.52
15:3:269:ASN:OD1	15:3:270:ILE:HD12	2.09	0.52
18:7:42:TRP:CE2	18:7:62:TRP:HD1	2.27	0.52
16:8:226:TRP:CD1	30:8:316:XAT:H241	2.44	0.52
13:1:88:MET:HG2	13:1:99:TRP:HB2	1.91	0.52
1:A:126:ILE:O	1:A:129:GLN:HG2	2.10	0.52
1:A:386:ALA:CB	1:A:527:ALA:HA	2.40	0.52
25:A:850:8CT:C22	22:B:803:CLA:C16	2.85	0.52
2:B:166:SER:OG	7:G:48:ASP:N	2.42	0.52
22:B:825:CLA:H2A	22:B:825:CLA:O1A	2.08	0.52
7:G:28:ARG:HH22	7:G:67:ASN:ND2	2.07	0.52
18:7:144:TRP:CE2	22:7:315:CLA:HBC1	2.45	0.52
25:7:321:8CT:C40	25:7:321:8CT:C15	2.87	0.52
16:8:115:THR:H	16:8:119:ASN:ND2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:9:204:PRO:HB2	22:9:313:CLA:HMA1	1.91	0.52
1:A:216:LEU:HG	1:A:307:ALA:HB1	1.92	0.52
2:B:126:THR:HG21	2:B:358:TYR:CD1	2.44	0.52
2:B:547:MET:HB2	2:B:564:ARG:HH21	1.74	0.52
4:D:140:LEU:O	4:D:143:GLN:HB3	2.09	0.52
8:H:114:LEU:HG	22:H:201:CLA:H112	1.90	0.52
10:J:9:SER:HA	10:J:14:ILE:HD11	1.91	0.52
14:2:56:LEU:HD12	14:2:56:LEU:O	2.09	0.52
16:4:116:GLU:HB2	16:4:119:ASN:HD22	1.75	0.52
25:7:323:8CT:C09	25:7:323:8CT:C11	2.86	0.52
16:8:215:ALA:O	16:8:219:GLY:N	2.43	0.52
19:9:73:TYR:HE1	22:9:304:CLA:H2	1.73	0.52
1:A:643:SER:OG	1:A:653:ASP:OD2	2.16	0.52
22:B:827:CLA:H171	25:B:846:8CT:C37	2.39	0.52
22:B:830:CLA:H72	28:B:849:DGD:HAV1	1.92	0.52
5:E:15:GLU:O	5:E:15:GLU:HG2	2.09	0.52
11:K:51:ASP:CG	11:K:52:PRO:HD2	2.30	0.52
16:8:169:ASP:O	16:8:171:ASN:OD1	2.27	0.52
1:A:200:GLU:HB3	1:A:317:TYR:HB3	1.92	0.52
1:A:268:PRO:HG2	1:A:277:TYR:OH	2.10	0.52
1:A:585:ARG:HG3	3:C:49:VAL:CG1	2.40	0.52
13:5:79:ARG:O	13:5:83:LEU:N	2.37	0.52
13:5:87:GLY:O	13:5:91:GLN:HG2	2.09	0.52
1:A:117:LYS:HD3	1:A:144:GLN:HE22	1.74	0.52
1:A:146:THR:HG21	1:A:749:LEU:HD22	1.92	0.52
1:A:663:ILE:HG22	2:B:621:ARG:CG	2.22	0.52
22:B:803:CLA:H112	22:B:833:CLA:HBC1	1.91	0.52
15:3:245:ALA:HA	15:3:248:ILE:HG22	1.91	0.52
16:4:86:HIS:CD2	22:4:308:CLA:HMD1	2.44	0.52
18:7:235:ILE:H	18:7:235:ILE:HD12	1.75	0.52
16:8:150:ASP:HB2	16:8:158:ASN:ND2	2.24	0.52
19:9:130:GLY:HA2	22:9:308:CLA:HAB	1.92	0.52
1:A:250:LEU:HD11	22:A:816:CLA:HAC2	1.92	0.52
2:B:451:LYS:HE3	6:F:128:ARG:NH1	2.24	0.52
2:B:585:ASN:O	2:B:588:GLY:N	2.43	0.52
14:2:91:TRP:CE2	29:2:307:CHL:HED2	2.44	0.52
22:3:319:CLA:H18	18:7:264:GLN:HB2	1.91	0.52
22:8:312:CLA:CHB	22:8:313:CLA:HMD3	2.40	0.52
1:A:541:HIS:HA	1:A:544:HIS:HD2	1.75	0.52
22:B:824:CLA:HMA1	22:B:841:CLA:CGD	2.40	0.52
17:6:151:ASP:HB3	17:6:154:PHE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:8:316:XAT:H371	30:8:316:XAT:H28	1.91	0.52
19:9:47:TYR:CE1	19:9:48:LEU:HD23	2.44	0.52
1:A:104:SER:HB2	1:A:150:PHE:HZ	1.75	0.52
2:B:292:ARG:NH1	7:G:35:VAL:HA	2.24	0.52
3:C:39:ILE:HG22	3:C:40:ALA:O	2.09	0.52
3:C:58:CYS:SG	3:C:65:VAL:HG22	2.50	0.52
13:1:50:PRO:HG3	13:1:172:LYS:HE3	1.91	0.52
29:6:302:CHL:H41	22:6:313:CLA:H161	1.91	0.52
2:B:39:GLU:HG2	2:B:165:LEU:HD11	1.92	0.51
22:1:303:CLA:C2B	30:1:315:XAT:H183	2.40	0.51
13:5:174:LYS:HE2	22:5:311:CLA:CGD	2.40	0.51
18:7:89:MET:HE3	22:7:310:CLA:HMC3	1.91	0.51
2:B:474:PHE:CZ	22:B:850:CLA:H72	2.45	0.51
3:C:17:CYS:HB3	3:C:26:LEU:HD12	1.91	0.51
10:J:24:SER:OG	22:J:103:CLA:HAB	2.10	0.51
14:2:245:CYS:SG	22:2:314:CLA:HMD3	2.50	0.51
22:3:308:CLA:HAB	30:3:314:XAT:H403	1.92	0.51
18:7:213:GLN:HE21	18:7:259:CYS:HB2	1.74	0.51
16:8:172:ILE:HG21	16:8:175:TYR:HD1	1.75	0.51
19:9:154:TRP:HB2	22:9:309:CLA:OBD	2.10	0.51
20:0:35:MET:HA	20:0:54:TYR:HB3	1.92	0.51
1:A:27:THR:OG1	1:A:187:HIS:ND1	2.39	0.51
22:A:801:CLA:HMB3	22:B:803:CLA:HMD1	1.93	0.51
2:B:526:GLY:HA3	2:B:586:THR:HB	1.92	0.51
22:2:302:CLA:HMB2	22:2:302:CLA:H2	1.91	0.51
16:4:45:LEU:HD11	16:4:48:ALA:HB2	1.92	0.51
29:4:305:CHL:CBA	25:4:317:8CT:C22	2.89	0.51
18:7:205:TRP:CD2	30:7:320:XAT:H12	2.46	0.51
16:8:175:TYR:HB3	22:8:309:CLA:CGD	2.41	0.51
2:B:149:PHE:O	2:B:153:GLY:N	2.25	0.51
8:H:105:VAL:HG22	22:0:303:CLA:H42	1.91	0.51
22:1:302:CLA:HMD2	22:1:307:CLA:C1D	2.40	0.51
14:2:135:MET:HB3	16:4:239:TRP:CE3	2.40	0.51
15:3:78:PHE:HE2	30:3:315:XAT:H383	1.76	0.51
25:7:321:8CT:C32	25:7:321:8CT:C36	2.86	0.51
20:0:174:SER:HB2	30:0:314:XAT:H203	1.92	0.51
25:B:846:8CT:C22	25:B:846:8CT:C25	2.88	0.51
7:G:19:GLY:O	7:G:24:PHE:N	2.43	0.51
13:1:173:LEU:HD23	22:1:309:CLA:HED2	1.93	0.51
13:5:208:ILE:HD11	22:5:313:CLA:HBB1	1.91	0.51
20:0:76:LEU:O	20:0:80:ARG:N	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:313:XAT:H381	30:0:313:XAT:H28	1.92	0.51
1:A:49:THR:HB	5:E:44:VAL:HG21	1.91	0.51
1:A:83:PHE:HD2	1:A:182:GLY:HA2	1.75	0.51
1:A:290:ILE:HG23	1:A:291:ASN:H	1.75	0.51
2:B:712:HIS:HE1	22:B:840:CLA:NA	2.09	0.51
22:B:819:CLA:HBB1	22:B:819:CLA:HMB1	1.91	0.51
22:B:824:CLA:HBC2	25:B:846:8CT:C27	2.39	0.51
6:F:146:HIS:O	6:F:147:LEU:HD23	2.09	0.51
22:H:201:CLA:H102	12:L:88:LEU:HD21	1.91	0.51
22:6:317:CLA:HBC3	22:6:318:CLA:C1C	2.40	0.51
1:A:663:ILE:HG21	2:B:621:ARG:HG3	1.82	0.51
2:B:595:HIS:CD2	2:B:623:TYR:HE1	2.26	0.51
22:B:841:CLA:CMA	25:B:846:8CT:C40	2.84	0.51
12:L:21:THR:N	12:L:24:THR:OG1	2.29	0.51
15:3:79:ASP:OD2	15:3:82:GLY:HA2	2.10	0.51
13:5:102:ALA:O	13:5:106:VAL:HG22	2.10	0.51
22:5:313:CLA:HBA2	22:5:313:CLA:H42	1.92	0.51
18:7:85:SER:HB2	18:7:198:GLY:HA3	1.93	0.51
19:9:107:GLY:O	29:9:307:CHL:HMD3	2.11	0.51
20:0:35:MET:O	20:0:38:PRO:HD3	2.10	0.51
2:B:686:PRO:HD3	22:L:201:CLA:HBA1	1.92	0.51
22:K:105:CLA:H2	22:K:105:CLA:H2A	1.92	0.51
17:6:112:THR:OG1	17:6:115:ASP:O	2.28	0.51
29:6:308:CHL:H2A	29:6:308:CHL:HED3	1.93	0.51
13:5:127:LEU:HD11	22:5:305:CLA:HMD3	1.91	0.51
29:5:301:CHL:H11	16:8:142:TRP:CE3	2.46	0.51
1:A:493:GLN:NE2	22:A:836:CLA:OBD	2.36	0.51
3:C:4:ASN:ND2	4:D:206:ILE:HG21	2.26	0.51
7:G:5:SER:HA	22:G:102:CLA:OBD	2.10	0.51
22:L:202:CLA:HBB1	22:L:202:CLA:HMB1	1.92	0.51
17:6:43:LEU:HD23	17:6:45:GLY:H	1.76	0.51
18:7:65:MET:HG3	30:7:320:XAT:H372	1.93	0.51
18:7:109:GLU:C	18:7:111:GLY:H	2.13	0.51
22:7:304:CLA:HBC1	22:7:309:CLA:HAC1	1.93	0.51
2:B:676:GLU:HG2	3:C:81:TYR:CE2	2.46	0.51
14:2:181:GLY:O	14:2:185:ASP:HB3	2.11	0.51
14:2:199:GLU:OE2	14:2:203:LYS:HE2	2.10	0.51
15:3:205:PRO:HD2	22:3:308:CLA:OBD	2.10	0.51
18:7:60:TYR:OH	18:7:196:LYS:HE2	2.11	0.51
1:A:370:ILE:HD13	22:A:826:CLA:HMD3	1.93	0.50
25:A:850:8CT:C37	25:A:850:8CT:C32	2.86	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:103:ARG:NH1	12:L:102:GLN:OE1	2.45	0.50
14:2:178:TYR:HB3	22:2:309:CLA:HED2	1.92	0.50
15:3:111:MET:SD	22:3:308:CLA:HMC3	2.52	0.50
16:8:243:LEU:HD22	25:8:301:8CT:C07	2.40	0.50
19:9:216:ILE:O	19:9:218:GLU:N	2.44	0.50
2:B:302:LYS:HG3	2:B:303:GLU:HG3	1.93	0.50
22:B:827:CLA:O1D	22:B:827:CLA:H2A	2.11	0.50
3:C:14:CYS:O	3:C:15:THR:OG1	2.22	0.50
17:6:92:VAL:HG11	17:6:193:SER:HB2	1.92	0.50
22:0:302:CLA:CGA	22:0:302:CLA:H3A	2.41	0.50
1:A:32:GLU:HA	10:J:3:ASN:ND2	2.26	0.50
1:A:334:HIS:HE1	22:A:824:CLA:HED3	1.76	0.50
2:B:174:ARG:HH11	22:B:808:CLA:H141	1.75	0.50
13:1:107:TYR:HE2	22:1:304:CLA:HAC1	1.76	0.50
22:1:303:CLA:HBA1	22:1:304:CLA:CHD	2.41	0.50
22:2:312:CLA:HMB1	22:2:312:CLA:HBB1	1.94	0.50
22:6:313:CLA:C2B	30:6:319:XAT:H183	2.41	0.50
13:5:91:GLN:NE2	22:5:304:CLA:O1D	2.43	0.50
19:9:88:VAL:HG13	19:9:182:PHE:CZ	2.46	0.50
1:A:456:HIS:O	1:A:460:LEU:HG	2.12	0.50
1:A:551:THR:HG21	22:A:826:CLA:HBC3	1.93	0.50
1:A:602:PHE:CZ	1:A:733:VAL:HG22	2.46	0.50
2:B:29:HIS:HE1	22:B:807:CLA:NB	2.09	0.50
2:B:35:ASP:CG	2:B:36:SER:H	2.14	0.50
5:E:14:PRO:HG2	5:E:15:GLU:OE1	2.11	0.50
12:L:88:LEU:O	12:L:92:ILE:HD12	2.11	0.50
16:8:95:VAL:O	16:8:99:VAL:HG23	2.11	0.50
16:8:179:ILE:HD11	29:8:314:CHL:C4A	2.41	0.50
22:8:304:CLA:H12	29:8:305:CHL:C3D	2.40	0.50
1:A:343:HIS:HB3	1:A:346:LEU:HD12	1.94	0.50
1:A:583:PRO:HB3	2:B:559:CYS:SG	2.51	0.50
1:A:703:GLU:CD	2:B:545:LYS:HB2	2.32	0.50
2:B:275:HIS:HE1	22:B:817:CLA:NA	2.10	0.50
2:B:617:MET:HG3	2:B:621:ARG:HB2	1.94	0.50
2:B:676:GLU:HG2	3:C:81:TYR:HE2	1.76	0.50
2:B:693:TRP:CD1	2:B:696:LYS:HA	2.46	0.50
6:F:94:GLU:HB3	6:F:129:PHE:CD2	2.47	0.50
6:F:125:THR:O	6:F:128:ARG:HG2	2.11	0.50
6:F:201:ILE:O	10:J:9:SER:HB3	2.11	0.50
22:H:201:CLA:H162	12:L:92:ILE:HD11	1.94	0.50
13:1:31:ARG:N	13:1:47:GLU:OE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:301:CHL:HED3	16:8:145:ILE:HG22	1.93	0.50
16:8:95:VAL:HG21	30:8:316:XAT:H14	1.94	0.50
1:A:51:THR:CG2	1:A:721:ARG:H	2.25	0.50
2:B:239:THR:HG23	2:B:242:HIS:N	2.26	0.50
2:B:325:THR:HG21	2:B:403:ASN:HD21	1.76	0.50
2:B:631:LEU:CD2	2:B:727:ALA:CB	2.90	0.50
29:2:305:CHL:CHB	25:2:317:8CT:C38	2.90	0.50
15:3:96:PRO:O	15:3:100:ARG:NE	2.43	0.50
20:0:161:LEU:O	20:0:165:LYS:N	2.43	0.50
22:0:308:CLA:H102	30:0:313:XAT:C11	2.42	0.50
1:A:316:MET:HB3	22:A:822:CLA:HAC2	1.93	0.50
22:A:841:CLA:HAA2	22:L:201:CLA:HMB1	1.94	0.50
6:F:212:GLY:O	6:F:219:ARG:NH2	2.42	0.50
7:G:56:SER:O	19:9:43:SER:N	2.44	0.50
13:1:184:PHE:HE2	22:1:311:CLA:HAB	1.76	0.50
18:7:70:ASP:O	18:7:72:LYS:N	2.45	0.50
22:A:808:CLA:HHC	22:A:828:CLA:H142	1.94	0.50
22:A:839:CLA:H2A	22:A:839:CLA:HED3	1.94	0.50
2:B:183:PHE:CE1	22:B:814:CLA:H72	2.47	0.50
2:B:648:TRP:HZ3	25:B:848:8CT:C07	2.25	0.50
15:3:111:MET:HB3	30:3:314:XAT:C34	2.42	0.50
15:3:189:PHE:N	15:3:193:GLU:OE1	2.41	0.50
24:3:317:LHG:O3	24:3:317:LHG:O1	2.15	0.50
22:5:312:CLA:H18	22:5:312:CLA:HMB1	1.94	0.50
18:7:62:TRP:CD1	18:7:64:PRO:HD3	2.47	0.50
18:7:242:CYS:O	18:7:244:ILE:HG12	2.12	0.50
25:A:850:8CT:C06	22:B:832:CLA:HMB3	2.40	0.50
2:B:403:ASN:HA	2:B:406:ASN:ND2	2.27	0.50
2:B:416:GLU:O	2:B:420:SER:N	2.31	0.50
22:B:805:CLA:O1D	22:B:805:CLA:H2A	2.11	0.50
13:1:31:ARG:HH22	13:1:42:PRO:HD2	1.76	0.50
13:1:211:PRO:HG3	22:1:312:CLA:HMB3	1.93	0.50
22:6:303:CLA:H93	22:6:304:CLA:HMA1	1.94	0.50
16:8:146:ARG:O	16:8:158:ASN:ND2	2.39	0.50
22:A:831:CLA:HAA1	12:L:7:ILE:HD13	1.93	0.49
6:F:216:TRP:CG	6:F:217:PRO:HD3	2.47	0.49
14:2:173:THR:HG23	14:2:175:GLU:OE1	2.12	0.49
16:8:43:ILE:HG22	16:8:44:TRP:N	2.25	0.49
16:8:190:VAL:O	16:8:194:LYS:HG2	2.12	0.49
20:0:67:SER:HB3	22:0:307:CLA:H111	1.94	0.49
20:0:171:MET:HG2	22:0:302:CLA:HMC3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:0:301:CHL:HAA1	24:0:315:LHG:H132	1.93	0.49
1:A:218:TRP:HE1	1:A:222:GLN:NE2	2.10	0.49
1:A:358:LEU:HB2	22:A:805:CLA:HMD3	1.93	0.49
3:C:8:TYR:CE2	4:D:191:ILE:HG12	2.47	0.49
22:G:103:CLA:HED2	25:G:104:8CT:C38	2.41	0.49
10:J:23:SER:HB3	25:J:104:8CT:C24	2.42	0.49
11:K:40:LEU:O	11:K:40:LEU:HD23	2.12	0.49
14:2:115:TRP:CE3	30:2:316:XAT:H172	2.47	0.49
15:3:201:ASP:HB2	15:3:202:PRO:HD2	1.94	0.49
16:4:238:VAL:HG13	22:4:312:CLA:O1A	2.11	0.49
17:6:229:SER:HB2	18:7:124:ASN:HD21	1.76	0.49
13:5:109:GLY:O	13:5:112:PRO:HD2	2.12	0.49
18:7:65:MET:HG2	30:7:320:XAT:H221	1.94	0.49
22:A:819:CLA:H13	22:A:819:CLA:HBB2	1.94	0.49
2:B:358:TYR:OH	22:B:829:CLA:OBD	2.18	0.49
2:B:553:PHE:HZ	3:C:52:LYS:HZ3	1.60	0.49
6:F:94:GLU:HA	6:F:94:GLU:OE1	2.12	0.49
12:L:67:LEU:HA	12:L:71:ARG:HD3	1.93	0.49
22:L:202:CLA:HBD	22:L:202:CLA:H193	1.94	0.49
14:2:84:ALA:HB2	22:2:308:CLA:HED1	1.95	0.49
22:2:312:CLA:C2B	30:2:315:XAT:H383	2.42	0.49
17:6:151:ASP:OD1	17:6:152:PRO:HD2	2.12	0.49
17:6:231:ALA:HB1	17:6:267:PRO:O	2.12	0.49
13:5:215:ASN:OD1	16:8:131:VAL:HG22	2.12	0.49
1:A:332:GLU:HG2	1:A:344:GLN:HA	1.93	0.49
22:A:803:CLA:H91	10:J:16:PHE:HB2	1.94	0.49
25:A:850:8CT:C05	22:B:832:CLA:CMB	2.81	0.49
2:B:130:ARG:HH11	2:B:245:SER:HB3	1.78	0.49
2:B:549:ASP:OD2	3:C:66:ARG:NH1	2.46	0.49
12:L:88:LEU:O	12:L:91:ILE:N	2.46	0.49
14:2:134:LEU:O	14:2:137:GLN:HB3	2.13	0.49
16:4:176:PRO:HD3	29:4:307:CHL:HMD2	1.95	0.49
20:0:72:ARG:O	20:0:76:LEU:N	2.38	0.49
1:A:354:TRP:CE2	22:A:825:CLA:H18	2.47	0.49
22:A:831:CLA:HMA2	12:L:21:THR:HG21	1.92	0.49
2:B:31:PHE:CD2	22:B:808:CLA:HMC2	2.45	0.49
2:B:53:GLN:HG2	22:B:808:CLA:HMA1	1.94	0.49
2:B:174:ARG:NH1	22:B:808:CLA:H141	2.27	0.49
2:B:174:ARG:HH12	22:B:808:CLA:H162	1.76	0.49
22:2:303:CLA:HMD2	22:2:308:CLA:CHD	2.43	0.49
22:3:303:CLA:O2A	22:7:317:CLA:H11	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:133:TYR:CD1	25:6:321:8CT:C40	2.95	0.49
29:5:301:CHL:H51	22:5:313:CLA:H62	1.95	0.49
22:5:302:CLA:HMB2	22:5:303:CLA:HBA2	1.95	0.49
16:8:133:PHE:HB2	29:8:306:CHL:HBC1	1.93	0.49
16:8:211:PHE:CE1	30:8:316:XAT:H363	2.47	0.49
25:A:850:8CT:C28	25:A:850:8CT:C34	2.87	0.49
2:B:165:LEU:HD21	2:B:169:LYS:HZ2	1.77	0.49
2:B:334:LEU:HD22	2:B:389:HIS:CD2	2.48	0.49
22:B:813:CLA:HHC	22:B:813:CLA:HBB1	1.94	0.49
4:D:79:PRO:HB3	8:H:56:ARG:HB3	1.94	0.49
8:H:79:LYS:HE3	12:L:44:SER:H	1.76	0.49
11:K:40:LEU:HB2	22:K:105:CLA:C2	2.43	0.49
16:4:64:TYR:HE2	30:4:316:XAT:H383	1.78	0.49
17:6:202:MET:HB3	22:6:317:CLA:HED1	1.94	0.49
22:8:309:CLA:HAB	30:8:316:XAT:H203	1.95	0.49
19:9:200:HIS:CG	22:9:312:CLA:HAA2	2.47	0.49
2:B:70:TRP:CE3	2:B:71:GLN:HG3	2.47	0.49
2:B:497:TRP:CZ3	22:B:834:CLA:HED2	2.48	0.49
3:C:51:CYS:N	27:C:101:SF4:S2	2.86	0.49
5:E:9:VAL:HG13	5:E:59:VAL:HG13	1.94	0.49
17:6:172:ALA:HB2	22:6:310:CLA:HBD	1.93	0.49
13:5:102:ALA:HB3	13:5:103:PRO:HD3	1.94	0.49
18:7:156:ASP:O	18:7:160:LYS:HA	2.11	0.49
22:7:312:CLA:C3B	30:7:319:XAT:H35	2.42	0.49
22:9:308:CLA:H72	22:9:308:CLA:H142	1.95	0.49
22:A:838:CLA:H71	25:A:849:8CT:C40	2.43	0.49
2:B:136:TYR:CZ	21:M:7:GLN:HB3	2.48	0.49
6:F:232:LYS:HG2	6:F:233:GLU:N	2.28	0.49
22:H:201:CLA:H143	12:L:88:LEU:HD22	1.95	0.49
13:1:36:LEU:HD21	16:4:149:GLN:HG3	1.95	0.49
22:4:304:CLA:HBB1	22:4:304:CLA:HMB1	1.95	0.49
30:4:315:XAT:H401	30:4:315:XAT:H35	1.50	0.49
20:0:132:TYR:CG	22:0:307:CLA:HMA3	2.48	0.49
22:0:307:CLA:H92	22:0:307:CLA:H2	1.94	0.49
1:A:666:TYR:CD1	2:B:445:ALA:HA	2.40	0.49
1:A:714:VAL:O	1:A:714:VAL:HG12	2.13	0.49
17:6:203:GLN:HE21	22:6:313:CLA:C4D	2.26	0.49
13:5:100:HIS:NE2	29:5:306:CHL:HMA3	2.28	0.49
18:7:100:ILE:HD11	18:7:220:ILE:HG21	1.94	0.49
19:9:73:TYR:CE1	22:9:304:CLA:H2	2.46	0.49
22:9:301:CLA:H11	22:9:301:CLA:CHA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:0:159:ASN:O	20:0:162:LYS:N	2.35	0.49
1:A:483:GLN:OE1	1:A:485:GLN:NE2	2.46	0.49
25:B:848:8CT:C32	25:B:848:8CT:C36	2.90	0.49
4:D:108:LYS:HG3	4:D:110:GLN:OE1	2.12	0.49
4:D:157:VAL:HG22	4:D:163:VAL:HG22	1.94	0.49
13:1:32:PRO:O	13:1:53:TYR:HE1	1.96	0.49
20:0:46:LEU:HB3	20:0:53:ASP:OD1	2.13	0.49
1:A:116:ILE:HG23	1:A:137:GLY:HA3	1.95	0.48
1:A:382:TYR:HB2	1:A:385:LEU:HG	1.95	0.48
1:A:745:TRP:NE1	25:A:850:8CT:C38	2.73	0.48
22:A:829:CLA:H2	25:A:847:8CT:C28	2.43	0.48
2:B:519:VAL:HG11	2:B:593:TYR:CG	2.47	0.48
25:B:847:8CT:C40	25:B:847:8CT:C15	2.90	0.48
22:K:105:CLA:HMA2	22:K:105:CLA:C2	2.43	0.48
22:1:303:CLA:H12	22:1:304:CLA:CAD	2.43	0.48
14:2:189:LEU:HD23	14:2:190:ALA:N	2.28	0.48
17:6:43:LEU:HD21	18:7:145:GLN:HG2	1.95	0.48
22:5:304:CLA:NB	25:5:317:8CT:C32	2.75	0.48
16:8:229:HIS:CG	22:8:312:CLA:HAA2	2.47	0.48
1:A:440:ASP:OD2	1:A:566:ARG:NH2	2.38	0.48
1:A:566:ARG:HH12	4:D:89:GLY:H	1.60	0.48
2:B:318:GLY:O	2:B:407:VAL:HG23	2.13	0.48
4:D:195:VAL:CG1	4:D:199:LYS:HB3	2.44	0.48
5:E:33:ILE:HG22	5:E:35:TYR:H	1.78	0.48
15:3:274:TRP:O	15:3:277:VAL:HG23	2.13	0.48
30:5:315:XAT:H391	30:5:315:XAT:H31	1.48	0.48
18:7:45:GLY:O	18:7:46:VAL:HG13	2.14	0.48
18:7:78:ARG:NH2	22:7:303:CLA:HED3	2.27	0.48
18:7:144:TRP:HB2	22:7:309:CLA:HMA1	1.95	0.48
18:7:205:TRP:NE1	30:7:320:XAT:H10	2.29	0.48
30:0:313:XAT:H391	30:0:313:XAT:H31	1.59	0.48
2:B:176:ASN:HD22	2:B:293:THR:HG23	1.78	0.48
2:B:176:ASN:ND2	2:B:291:TYR:O	2.29	0.48
7:G:2:LEU:HD23	7:G:3:SER:N	2.29	0.48
20:0:46:LEU:HD11	22:0:302:CLA:HAA1	1.95	0.48
1:A:472:ARG:HD3	1:A:475:ASP:OD2	2.13	0.48
22:A:840:CLA:H11	22:A:840:CLA:C4D	2.44	0.48
13:5:69:ARG:O	13:5:72:GLU:HG2	2.13	0.48
13:5:186:PHE:CE1	30:5:316:XAT:H10	2.47	0.48
22:7:318:CLA:H122	22:7:318:CLA:H162	1.66	0.48
1:A:127:VAL:HG12	1:A:127:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ILE:HB	1:A:228:PRO:HD3	1.96	0.48
1:A:486:PRO:HD3	1:A:538:PHE:HB2	1.95	0.48
2:B:524:ALA:O	2:B:528:HIS:HD2	1.95	0.48
2:B:661:PHE:HB2	22:B:806:CLA:HMC3	1.96	0.48
22:B:833:CLA:H52	10:J:29:VAL:HG11	1.95	0.48
3:C:54:CYS:HB3	3:C:65:VAL:HG21	1.94	0.48
24:1:317:LHG:H291	24:1:317:LHG:H102	1.95	0.48
14:2:107:ARG:HD2	14:2:234:PHE:CE2	2.49	0.48
22:4:312:CLA:O1D	22:4:312:CLA:H2A	2.13	0.48
2:B:174:ARG:HB3	2:B:178:HIS:HD2	1.78	0.48
2:B:216:LEU:HA	22:B:816:CLA:HED1	1.94	0.48
2:B:254:ILE:HG13	2:B:255:LEU:H	1.78	0.48
25:B:848:8CT:C40	25:B:848:8CT:C15	2.91	0.48
12:L:115:LYS:HD3	12:L:121:ASP:HB3	1.96	0.48
13:1:185:ALA:HB2	30:1:314:XAT:C19	2.43	0.48
15:3:98:TRP:O	15:3:101:TYR:N	2.43	0.48
15:3:228:ARG:O	15:3:232:ASN:ND2	2.37	0.48
16:4:239:TRP:CD1	16:4:239:TRP:N	2.80	0.48
17:6:260:CYS:SG	17:6:263:GLU:HB2	2.53	0.48
18:7:202:MET:HE3	22:7:303:CLA:HMC3	1.95	0.48
22:7:309:CLA:HMB2	22:7:315:CLA:C1C	2.43	0.48
22:7:316:CLA:H122	22:7:316:CLA:H162	1.38	0.48
22:8:302:CLA:O1A	22:8:302:CLA:H3A	2.12	0.48
1:A:340:GLY:HA2	12:L:5:GLN:HE21	1.78	0.48
1:A:362:LEU:HD13	1:A:409:GLY:HA3	1.96	0.48
1:A:443:ILE:HD11	1:A:560:LEU:HD12	1.95	0.48
1:A:488:PHE:HE2	22:A:837:CLA:H42	1.78	0.48
22:A:839:CLA:HBC3	22:A:853:CLA:C1C	2.43	0.48
3:C:4:ASN:HD21	4:D:206:ILE:HG21	1.79	0.48
22:2:308:CLA:HHC	22:2:308:CLA:HBB1	1.94	0.48
15:3:173:ARG:HD3	15:3:184:MET:HE2	1.96	0.48
22:4:309:CLA:CHC	30:4:315:XAT:H30	2.43	0.48
16:8:41:ARG:NH1	16:8:56:GLY:H	2.12	0.48
16:8:64:TYR:CE2	30:8:317:XAT:H383	2.48	0.48
16:8:65:ASP:OD2	16:8:69:LEU:N	2.46	0.48
1:A:195:TRP:CZ2	22:A:813:CLA:HAC2	2.48	0.48
1:A:252:ARG:NH2	15:3:277:VAL:HB	2.29	0.48
1:A:696:GLY:N	2:B:568:CYS:O	2.47	0.48
22:A:839:CLA:HBC2	22:A:839:CLA:HMC1	1.96	0.48
2:B:112:PRO:HG3	8:H:128:PRO:HB3	1.96	0.48
22:B:801:CLA:H3A	22:B:801:CLA:O2A	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:840:CLA:HMC2	25:B:848:8CT:C22	2.43	0.48
30:1:314:XAT:H373	30:1:314:XAT:H23	1.70	0.48
17:6:87:TRP:CE2	29:6:308:CHL:HED2	2.48	0.48
24:6:322:LHG:H101	25:7:321:8CT:C08	2.43	0.48
13:5:70:MET:O	22:5:302:CLA:HMA1	2.14	0.48
18:7:51:TYR:OH	18:7:63:ASP:OD2	2.26	0.48
22:7:307:CLA:C3B	25:7:323:8CT:C27	2.87	0.48
19:9:179:TRP:CD1	30:9:315:XAT:H14	2.48	0.48
22:0:302:CLA:HHC	30:0:314:XAT:H403	1.95	0.48
1:A:338:PHE:HE1	12:L:6:VAL:HG11	1.79	0.48
1:A:476:MET:O	1:A:481:THR:OG1	2.17	0.48
2:B:474:PHE:CD2	22:B:850:CLA:H52	2.49	0.48
9:I:4:ALA:O	9:I:7:PRO:HD2	2.14	0.48
14:2:45:VAL:HG11	14:2:52:PRO:HG3	1.96	0.48
14:2:126:SER:O	14:2:127:SER:OG	2.21	0.48
15:3:67:TYR:OH	15:3:79:ASP:OD2	2.32	0.48
22:4:311:CLA:HMC2	30:4:315:XAT:C10	2.44	0.48
16:8:243:LEU:CD2	25:8:301:8CT:C07	2.92	0.48
20:0:192:LEU:O	20:0:196:ILE:HG12	2.14	0.48
21:M:5:GLU:HG2	21:M:9:PHE:HE2	1.78	0.48
22:A:835:CLA:O2D	22:A:835:CLA:H2A	2.14	0.48
22:B:831:CLA:HBA2	22:B:831:CLA:H3A	1.45	0.48
3:C:27:GLU:HG2	4:D:174:PRO:HB3	1.96	0.48
13:1:85:VAL:HG13	13:1:189:PHE:CZ	2.49	0.48
16:4:229:HIS:CD2	22:4:312:CLA:HAA2	2.48	0.48
16:4:238:VAL:HG12	22:4:312:CLA:C3D	2.44	0.48
22:6:304:CLA:H92	22:6:304:CLA:H61	1.72	0.48
22:6:311:CLA:C2	22:6:311:CLA:HMA2	2.44	0.48
18:7:41:LEU:HD21	18:7:48:ALA:HB2	1.95	0.48
16:8:238:VAL:O	16:8:242:GLU:HB3	2.13	0.48
19:9:125:GLU:HA	22:9:306:CLA:HMA3	1.96	0.48
1:A:62:HIS:ND1	22:A:805:CLA:HBB2	2.29	0.47
2:B:5:PHE:HB3	2:B:20:ARG:NH1	2.29	0.47
2:B:207:VAL:HA	2:B:211:ASN:HD21	1.77	0.47
6:F:160:ALA:HB1	6:F:164:MET:HB2	1.96	0.47
13:1:142:ARG:HD3	22:1:306:CLA:C1D	2.44	0.47
22:4:309:CLA:CGA	22:4:309:CLA:C4A	2.92	0.47
13:5:145:GLU:HB2	13:5:151:ARG:HB3	1.96	0.47
13:5:225:PHE:HD1	31:5:319:LMG:H212	1.78	0.47
22:5:309:CLA:H61	30:5:315:XAT:H161	1.96	0.47
16:8:211:PHE:HZ	30:8:316:XAT:H363	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:SER:HB2	1:A:476:MET:SD	2.54	0.47
1:A:558:GLY:HA2	1:A:596:HIS:CD2	2.49	0.47
22:B:830:CLA:H61	22:B:830:CLA:H41	1.54	0.47
3:C:25:VAL:HG11	3:C:48:CYS:SG	2.53	0.47
11:K:26:LEU:HD22	22:K:105:CLA:C1C	2.44	0.47
29:4:305:CHL:H41	29:4:305:CHL:H61	1.71	0.47
25:4:317:8CT:C39	25:4:317:8CT:C19	2.92	0.47
17:6:232:VAL:HB	25:7:323:8CT:C40	2.44	0.47
16:8:166:LYS:HZ2	16:8:179:ILE:HB	1.78	0.47
1:A:717:ALA:N	6:F:198:GLU:OE2	2.28	0.47
22:A:821:CLA:H2	22:A:821:CLA:H62	1.72	0.47
22:A:833:CLA:HAA2	12:L:67:LEU:O	2.14	0.47
2:B:642:SER:OG	8:H:138:GLU:OE1	2.32	0.47
2:B:680:TRP:CD1	4:D:91:LEU:HD21	2.49	0.47
6:F:226:SER:OG	16:4:74:GLU:OE2	2.22	0.47
16:4:72:ASP:N	16:4:72:ASP:OD1	2.47	0.47
17:6:44:PRO:HD2	29:6:302:CHL:O2D	2.14	0.47
22:8:302:CLA:H102	22:8:303:CLA:HMB3	1.96	0.47
1:A:206:HIS:CE1	22:A:813:CLA:NA	2.83	0.47
1:A:697:TYR:CE1	2:B:536:LYS:HD3	2.49	0.47
22:A:803:CLA:CBB	25:J:101:8CT:C07	2.92	0.47
2:B:344:ILE:HD12	22:B:819:CLA:H71	1.96	0.47
12:L:90:VAL:O	12:L:94:THR:HG23	2.14	0.47
13:1:187:VAL:HG12	22:1:311:CLA:HAC1	1.96	0.47
20:0:99:ASN:O	20:0:103:ALA:N	2.47	0.47
20:0:147:MET:CG	20:0:148:PRO:HD3	2.44	0.47
20:0:176:GLY:O	20:0:180:GLN:HG2	2.14	0.47
1:A:339:THR:HG1	24:A:845:LHG:H02	1.58	0.47
1:A:499:ALA:O	1:A:501:GLN:N	2.40	0.47
1:A:511:THR:HG21	22:A:827:CLA:HAB	1.96	0.47
1:A:524:GLY:O	1:A:627:VAL:N	2.36	0.47
22:A:833:CLA:H2A	22:A:833:CLA:O2D	2.15	0.47
2:B:12:LEU:HG	28:B:849:DGD:HE2	1.97	0.47
2:B:58:PHE:HB2	2:B:146:ALA:HB2	1.96	0.47
2:B:476:PHE:HE2	22:B:850:CLA:H11	1.79	0.47
2:B:514:PRO:HG3	6:F:146:HIS:CD2	2.49	0.47
2:B:715:VAL:HG22	28:B:849:DGD:HBS2	1.95	0.47
22:B:801:CLA:HMC2	22:B:803:CLA:HAC1	1.97	0.47
7:G:59:LYS:HB2	19:9:42:ALA:HB2	1.96	0.47
8:H:75:GLN:CG	12:L:34:SER:HB2	2.44	0.47
22:2:302:CLA:H92	22:2:302:CLA:H61	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:89:PHE:CE2	29:4:307:CHL:HED2	2.49	0.47
16:4:159:VAL:HG22	16:4:160:ASP:OD1	2.14	0.47
16:4:211:PHE:CE1	16:4:222:PRO:HB3	2.50	0.47
29:4:306:CHL:HBB1	29:4:306:CHL:HHC	1.96	0.47
16:8:230:LEU:HD21	22:8:313:CLA:HMC3	1.95	0.47
19:9:38:TRP:CD1	19:9:58:TYR:HA	2.50	0.47
1:A:301:HIS:HD2	22:A:818:CLA:HMB1	1.79	0.47
22:A:830:CLA:HMB1	22:A:830:CLA:HBB1	1.96	0.47
2:B:656:VAL:HG22	22:B:840:CLA:HMB3	1.97	0.47
22:B:811:CLA:H142	22:B:811:CLA:H112	1.68	0.47
7:G:54:TYR:CE2	7:G:57:LEU:HB2	2.49	0.47
7:G:79:HIS:CE1	25:G:104:8CT:C17	2.98	0.47
15:3:231:LYS:HZ1	24:3:317:LHG:HC62	1.80	0.47
19:9:152:PHE:O	19:9:154:TRP:HE3	1.98	0.47
1:A:117:LYS:HB3	1:A:144:GLN:OE1	2.15	0.47
1:A:204:ASN:OD1	1:A:317:TYR:HB2	2.14	0.47
1:A:315:HIS:CD2	25:A:854:8CT:C24	2.97	0.47
1:A:567:LEU:HB3	2:B:673:GLU:OE2	2.15	0.47
2:B:123:TRP:HA	2:B:126:THR:HG22	1.96	0.47
2:B:444:LEU:HD13	2:B:615:TYR:CD1	2.50	0.47
22:B:803:CLA:H2A	22:B:803:CLA:O1D	2.15	0.47
22:B:850:CLA:HMA3	6:F:153:LEU:HD11	1.96	0.47
22:1:310:CLA:HBB1	30:1:314:XAT:C14	2.43	0.47
14:2:120:LYS:O	14:2:124:GLU:HG2	2.14	0.47
15:3:109:PHE:CE1	22:3:307:CLA:HBC3	2.50	0.47
15:3:142:VAL:HG13	15:3:143:ILE:HG13	1.95	0.47
17:6:62:TRP:NE1	30:6:320:XAT:H383	2.30	0.47
17:6:154:PHE:HZ	29:6:316:CHL:HAA1	1.79	0.47
13:5:100:HIS:ND1	13:5:193:TYR:HE2	2.12	0.47
22:5:303:CLA:H2A	22:5:303:CLA:H43	1.95	0.47
22:5:303:CLA:HHD	22:5:308:CLA:HAA1	1.96	0.47
22:5:304:CLA:C4A	22:5:304:CLA:HBA2	2.44	0.47
29:5:306:CHL:HBA1	29:5:306:CHL:H3A	1.66	0.47
30:5:316:XAT:H35	30:5:316:XAT:H401	1.55	0.47
18:7:43:ALA:HB3	18:7:46:VAL:HG13	1.96	0.47
18:7:112:LEU:O	18:7:114:LYS:N	2.39	0.47
18:7:123:LEU:HB2	18:7:128:ILE:HD11	1.97	0.47
18:7:187:ILE:HG23	18:7:188:GLU:H	1.79	0.47
1:A:62:HIS:HD1	22:A:805:CLA:HBB2	1.79	0.47
1:A:244:LEU:HD13	1:A:246:HIS:HE1	1.79	0.47
2:B:191:THR:CG2	2:B:277:HIS:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:808:CLA:H3A	22:B:808:CLA:HBA1	1.44	0.47
22:1:311:CLA:NC	22:1:311:CLA:H43	2.30	0.47
29:4:301:CHL:H62	29:4:301:CHL:H41	1.62	0.47
22:6:317:CLA:HBC2	22:6:317:CLA:HMC1	1.97	0.47
22:7:316:CLA:CBB	25:7:321:8CT:C13	2.92	0.47
22:7:317:CLA:H12	22:7:317:CLA:HBA2	1.55	0.47
16:8:89:PHE:CE1	22:8:308:CLA:HBC1	2.49	0.47
19:9:148:LEU:HD13	19:9:151:SER:O	2.15	0.47
22:9:312:CLA:H2	22:9:313:CLA:HMD1	1.97	0.47
20:0:83:MET:CB	30:0:313:XAT:H15	2.45	0.47
22:0:312:CLA:H91	22:0:312:CLA:CAD	2.45	0.47
1:A:298:ASP:O	1:A:302:HIS:N	2.48	0.47
1:A:362:LEU:HB3	1:A:406:CYS:O	2.15	0.47
2:B:451:LYS:HE3	6:F:128:ARG:HH12	1.78	0.47
22:B:819:CLA:HBA2	22:B:819:CLA:H3A	1.46	0.47
3:C:73:THR:N	3:C:76:SER:OG	2.38	0.47
17:6:52:LEU:HD22	17:6:61:GLY:HA2	1.95	0.47
17:6:215:TRP:HD1	17:6:216:THR:HG23	1.80	0.47
17:6:227:ILE:H	17:6:230:LYS:HD3	1.80	0.47
13:5:56:ASP:OD1	22:5:302:CLA:HBA2	2.14	0.47
13:5:147:ASP:OD1	13:5:148:MET:N	2.48	0.47
18:7:262:PRO:CD	22:7:317:CLA:HAA1	2.39	0.47
16:8:44:TRP:CE2	16:8:64:TYR:HD1	2.33	0.47
16:8:214:GLN:O	16:8:218:THR:OG1	2.23	0.47
20:0:128:GLU:HB3	20:0:132:TYR:CD2	2.50	0.47
1:A:294:LEU:HD12	1:A:381:PRO:HB3	1.97	0.47
1:A:445:HIS:O	1:A:449:VAL:HG23	2.15	0.47
1:A:663:ILE:HD11	22:A:801:CLA:CBC	2.45	0.47
2:B:279:ALA:HA	22:B:817:CLA:HMC3	1.97	0.47
22:B:829:CLA:C4A	22:B:829:CLA:HBA2	2.44	0.47
22:1:303:CLA:C4B	25:1:316:8CT:C36	2.93	0.47
14:2:187:PHE:HD2	30:2:315:XAT:H21	1.80	0.47
16:4:78:TRP:NE1	22:4:303:CLA:O1A	2.38	0.47
17:6:150:LYS:HA	17:6:157:TYR:HD1	1.80	0.47
17:6:234:THR:HG23	17:6:235:LEU:O	2.14	0.47
16:8:208:THR:HG21	30:8:317:XAT:H12	1.97	0.47
22:9:303:CLA:H93	22:9:304:CLA:HMA1	1.97	0.47
20:0:86:VAL:HG12	20:0:90:ALA:HB2	1.96	0.47
20:0:221:ALA:O	20:0:224:PRO:HD2	2.15	0.47
1:A:417:PHE:CD1	1:A:421:ASP:HB2	2.49	0.46
2:B:585:ASN:HD21	22:B:803:CLA:CBC	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:810:CLA:HHB	22:B:811:CLA:HMB3	1.97	0.46
22:B:815:CLA:H2A	22:B:815:CLA:O2D	2.15	0.46
22:B:825:CLA:H111	22:B:825:CLA:H72	1.50	0.46
5:E:5:ARG:HG2	5:E:27:SER:HA	1.97	0.46
11:K:81:THR:HG23	22:K:101:CLA:HMA1	1.97	0.46
12:L:10:ILE:HG23	12:L:11:ASN:HD22	1.80	0.46
15:3:270:ILE:HD11	22:3:311:CLA:C1	2.39	0.46
16:4:64:TYR:CE2	30:4:316:XAT:H383	2.49	0.46
22:6:312:CLA:H61	22:6:312:CLA:H41	1.54	0.46
16:8:159:VAL:CG1	16:8:167:LEU:HA	2.45	0.46
1:A:661:GLN:HG3	1:A:751:ARG:HD2	1.96	0.46
1:A:686:PHE:CE2	1:A:690:PHE:HE2	2.33	0.46
22:A:833:CLA:H3A	22:A:833:CLA:HBA2	1.48	0.46
22:A:852:CLA:C2D	22:B:831:CLA:HMB2	2.46	0.46
2:B:20:ARG:HH22	9:I:30:ILE:HG22	1.80	0.46
2:B:78:VAL:HG13	2:B:125:TYR:CE1	2.50	0.46
2:B:474:PHE:CD1	22:B:850:CLA:H52	2.49	0.46
2:B:487:ASN:OD1	2:B:488:ALA:N	2.49	0.46
2:B:510:LEU:HD22	2:B:601:ILE:HD13	1.96	0.46
22:B:820:CLA:H91	22:B:820:CLA:H111	1.60	0.46
6:F:122:ALA:O	6:F:125:THR:HG22	2.16	0.46
15:3:218:THR:C	15:3:220:GLU:H	2.17	0.46
30:3:314:XAT:H401	30:3:314:XAT:H35	1.49	0.46
30:6:319:XAT:H402	30:6:319:XAT:H31	1.79	0.46
13:5:163:PHE:HB2	22:5:309:CLA:O1A	2.15	0.46
24:5:318:LHG:H192	24:5:318:LHG:H372	1.97	0.46
25:8:301:8CT:C23	25:8:301:8CT:C27	2.93	0.46
22:8:309:CLA:H52	30:8:316:XAT:H192	1.98	0.46
22:A:822:CLA:H2A	22:A:822:CLA:O2D	2.16	0.46
2:B:111:GLY:HA2	8:H:133:PRO:HG2	1.98	0.46
2:B:172:GLU:HG2	2:B:301:MET:HG2	1.95	0.46
2:B:191:THR:HG21	2:B:278:LEU:HB2	1.97	0.46
2:B:242:HIS:HD2	2:B:262:HIS:CE1	2.33	0.46
6:F:85:SER:HB3	6:F:133:GLY:O	2.15	0.46
8:H:129:ILE:HG22	8:H:130:THR:HG23	1.96	0.46
22:L:203:CLA:H141	22:L:203:CLA:H162	1.62	0.46
14:2:93:MET:HB2	22:2:309:CLA:HMC3	1.97	0.46
16:4:157:VAL:CG2	29:4:307:CHL:HAC1	2.45	0.46
22:5:303:CLA:HBB1	30:5:316:XAT:H35	1.97	0.46
18:7:260:LEU:HD11	22:7:317:CLA:C1C	2.45	0.46
22:7:314:CLA:O1D	22:7:314:CLA:H2A	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:0:93:ASN:OD1	20:0:94:ALA:N	2.48	0.46
20:0:111:ILE:O	20:0:115:VAL:HB	2.16	0.46
2:B:569:ASP:HA	2:B:574:ASP:OD2	2.16	0.46
22:B:810:CLA:H3A	22:B:811:CLA:HMB3	1.96	0.46
22:B:820:CLA:H112	22:B:820:CLA:H152	1.72	0.46
22:B:841:CLA:H3A	22:B:841:CLA:HBA1	1.50	0.46
22:L:201:CLA:H41	22:L:201:CLA:H61	1.59	0.46
22:1:311:CLA:H121	29:4:301:CHL:H92	1.97	0.46
22:1:311:CLA:O1D	22:1:311:CLA:H2A	2.15	0.46
31:5:319:LMG:H201	16:8:129:THR:HG21	1.97	0.46
25:8:301:8CT:C40	25:8:301:8CT:C15	2.94	0.46
19:9:95:GLU:OE2	19:9:192:GLY:HA3	2.16	0.46
1:A:116:ILE:HD12	1:A:137:GLY:HA3	1.98	0.46
22:A:840:CLA:H161	25:A:850:8CT:C01	2.45	0.46
3:C:3:HIS:CE1	3:C:69:LEU:HD22	2.50	0.46
11:K:26:LEU:HD12	11:K:27:ALA:N	2.30	0.46
13:1:51:GLY:O	13:1:180:ARG:NH1	2.34	0.46
14:2:143:TRP:CZ3	25:2:317:8CT:C09	2.96	0.46
22:3:303:CLA:HMB3	30:3:315:XAT:H162	1.97	0.46
17:6:190:ALA:O	17:6:193:SER:N	2.49	0.46
22:6:315:CLA:H152	22:6:315:CLA:H112	1.62	0.46
22:6:315:CLA:HMC2	22:6:323:CLA:HMA1	1.98	0.46
13:5:100:HIS:HE2	29:5:306:CHL:HMA3	1.81	0.46
16:8:82:ALA:O	16:8:86:HIS:N	2.35	0.46
16:8:211:PHE:CE1	30:8:316:XAT:H372	2.51	0.46
20:0:220:ALA:O	29:0:301:CHL:HMA2	2.15	0.46
21:M:5:GLU:HA	21:M:8:ILE:HD12	1.98	0.46
1:A:158:ILE:HG23	1:A:163:GLU:HB2	1.97	0.46
1:A:379:MET:CE	22:A:827:CLA:HMC2	2.46	0.46
1:A:587:GLY:HA3	2:B:702:ILE:HD11	1.97	0.46
1:A:605:TYR:OH	22:A:801:CLA:HED3	2.15	0.46
22:A:826:CLA:CAD	22:A:836:CLA:HBB1	2.46	0.46
22:A:832:CLA:C3B	22:A:833:CLA:HMB2	2.46	0.46
22:A:835:CLA:HBB1	22:A:835:CLA:HMB1	1.97	0.46
2:B:31:PHE:HA	2:B:34:HIS:NE2	2.30	0.46
4:D:144:LEU:HD11	4:D:152:ALA:HB2	1.97	0.46
11:K:51:ASP:OD2	11:K:55:PHE:HB3	2.16	0.46
12:L:138:SER:O	12:L:142:VAL:HG23	2.15	0.46
14:2:175:GLU:OE1	14:2:175:GLU:N	2.48	0.46
22:4:309:CLA:H62	22:4:309:CLA:H41	1.55	0.46
18:7:75:ALA:HB1	18:7:169:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:8:311:CLA:HMB2	30:8:316:XAT:H202	1.98	0.46
24:0:315:LHG:H292	24:0:315:LHG:H171	1.97	0.46
1:A:62:HIS:HD2	22:A:830:CLA:H12	1.80	0.46
1:A:401:TRP:CB	22:A:828:CLA:HMC3	2.45	0.46
1:A:628:SER:O	1:A:629:GLU:HG2	2.16	0.46
22:A:816:CLA:HHC	22:A:816:CLA:HBB1	1.97	0.46
2:B:395:ILE:HD11	2:B:550:LYS:O	2.16	0.46
2:B:680:TRP:HD1	4:D:91:LEU:HD21	1.80	0.46
22:B:828:CLA:CGA	22:B:828:CLA:H3A	2.44	0.46
22:B:837:CLA:H61	22:B:837:CLA:H41	1.49	0.46
3:C:62:PHE:CD2	4:D:191:ILE:HD12	2.51	0.46
14:2:80:TRP:CZ2	22:2:308:CLA:HED3	2.51	0.46
22:6:317:CLA:HMD3	22:6:318:CLA:CBB	2.44	0.46
25:6:321:8CT:C36	25:6:321:8CT:C32	2.93	0.46
22:5:311:CLA:HBB2	30:5:315:XAT:H393	1.96	0.46
18:7:162:ASN:HD22	22:7:316:CLA:CAD	2.29	0.46
22:8:309:CLA:H51	22:8:311:CLA:H3A	1.98	0.46
19:9:83:TRP:CZ2	22:9:308:CLA:HAC2	2.51	0.46
19:9:123:ALA:HB1	20:0:217:ILE:HG21	1.97	0.46
19:9:174:LEU:HD21	30:9:314:XAT:H30	1.97	0.46
20:0:61:LEU:HD13	22:0:302:CLA:H42	1.97	0.46
29:0:301:CHL:H52	22:0:311:CLA:H121	1.98	0.46
1:A:218:TRP:N	22:A:814:CLA:HAB	2.31	0.46
1:A:617:TRP:HB2	1:A:654:PHE:CE1	2.51	0.46
1:A:710:ASN:OD1	1:A:715:ALA:HB2	2.16	0.46
22:A:826:CLA:HBA1	22:A:826:CLA:H3A	1.64	0.46
2:B:459:PHE:HD2	22:B:837:CLA:C3D	2.29	0.46
13:1:161:ALA:HB3	22:1:308:CLA:HBA2	1.97	0.46
30:1:314:XAT:H171	30:1:314:XAT:H7	1.29	0.46
15:3:140:ASN:ND2	30:3:315:XAT:HO3	2.13	0.46
15:3:249:LEU:HD22	22:3:311:CLA:HMD1	1.97	0.46
22:3:319:CLA:HED1	22:3:319:CLA:H42	1.98	0.46
16:4:242:GLU:OE1	16:4:243:LEU:HB3	2.16	0.46
16:4:242:GLU:H	16:4:245:LYS:HE3	1.80	0.46
13:5:122:THR:HG23	13:5:127:LEU:HD12	1.96	0.46
13:5:139:GLU:HG3	22:5:308:CLA:C1D	2.46	0.46
22:7:310:CLA:HMC2	30:7:319:XAT:H202	1.98	0.46
22:9:309:CLA:CBB	22:9:311:CLA:H3A	2.46	0.46
20:0:45:HIS:CD2	20:0:63:ALA:HA	2.50	0.46
21:M:9:PHE:O	22:M:101:CLA:HBB1	2.16	0.46
1:A:155:ALA:HB1	22:A:819:CLA:HED1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:813:CLA:C2	19:9:61:LEU:HD13	2.46	0.46
4:D:102:ILE:O	4:D:128:LEU:HA	2.16	0.46
6:F:162:ASP:OD1	6:F:163:ILE:N	2.47	0.46
22:L:202:CLA:H3A	22:L:202:CLA:HBA2	1.55	0.46
22:1:312:CLA:H3A	22:1:312:CLA:HBA1	1.32	0.46
14:2:120:LYS:C	14:2:124:GLU:HG2	2.36	0.46
15:3:190:LEU:CD1	25:3:316:8CT:C38	2.94	0.46
22:4:312:CLA:H2	22:4:313:CLA:HMD1	1.98	0.46
17:6:218:HIS:HE1	22:6:314:CLA:NB	2.14	0.46
18:7:249:ASP:HB3	18:7:254:ASN:H	1.80	0.46
20:0:208:SER:OG	20:0:209:VAL:N	2.49	0.46
1:A:585:ARG:O	2:B:668:ARG:NH1	2.49	0.46
22:A:828:CLA:H203	25:J:104:8CT:C22	2.46	0.46
5:E:11:ILE:HG12	5:E:54:PHE:CE2	2.50	0.46
7:G:20:ARG:NH1	7:G:64:VAL:HG22	2.31	0.46
16:4:146:ARG:NH1	16:4:158:ASN:HB2	2.25	0.46
13:5:145:GLU:CB	13:5:151:ARG:HB3	2.46	0.46
22:7:307:CLA:ND	25:7:323:8CT:C22	2.79	0.46
1:A:362:LEU:HD23	22:A:805:CLA:HED1	1.97	0.45
22:A:828:CLA:H2A	22:A:828:CLA:O1D	2.15	0.45
2:B:254:ILE:HG13	2:B:255:LEU:N	2.31	0.45
22:B:809:CLA:H71	22:B:809:CLA:H111	1.61	0.45
22:B:813:CLA:H91	22:B:813:CLA:C1D	2.46	0.45
22:B:814:CLA:H71	22:B:814:CLA:H111	1.46	0.45
8:H:85:GLN:HE22	22:L:202:CLA:H192	1.81	0.45
22:L:202:CLA:C2D	22:L:202:CLA:H121	2.47	0.45
22:1:312:CLA:O1D	22:1:312:CLA:H2A	2.16	0.45
17:6:102:LYS:HB3	17:6:102:LYS:HE3	1.73	0.45
20:0:195:HIS:CG	22:0:311:CLA:HAA2	2.51	0.45
1:A:21:ILE:CG2	1:A:192:LYS:HD2	2.45	0.45
1:A:200:GLU:OE2	1:A:327:MET:N	2.48	0.45
1:A:519:ILE:HG22	1:A:529:MET:HB2	1.98	0.45
22:A:808:CLA:HMC3	22:A:809:CLA:HMD2	1.98	0.45
2:B:361:ILE:HG22	2:B:362:ALA:N	2.31	0.45
2:B:622:ASP:O	2:B:626:LEU:HG	2.15	0.45
4:D:95:GLN:HE21	8:H:69:SER:HB2	1.82	0.45
25:J:104:8CT:C01	25:J:104:8CT:C11	2.94	0.45
22:K:105:CLA:H3A	22:K:105:CLA:HBA1	1.58	0.45
15:3:231:LYS:NZ	24:3:317:LHG:HC62	2.30	0.45
22:3:311:CLA:H2A	22:3:311:CLA:O1D	2.16	0.45
17:6:227:ILE:O	17:6:227:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:6:301:CLA:H3A	22:6:301:CLA:HBA1	1.53	0.45
13:5:92:GLU:OE1	13:5:200:PRO:HD2	2.16	0.45
16:8:44:TRP:CD1	16:8:64:TYR:HB2	2.51	0.45
16:8:74:GLU:HG2	16:8:75:THR:N	2.32	0.45
16:8:199:LYS:HD2	22:8:310:CLA:C3D	2.46	0.45
22:0:308:CLA:H2	22:0:308:CLA:CHB	2.46	0.45
1:A:34:TRP:CH2	22:A:804:CLA:H2	2.51	0.45
1:A:34:TRP:HE1	22:A:811:CLA:HBA1	1.81	0.45
2:B:230:TRP:O	22:B:817:CLA:H3A	2.15	0.45
2:B:444:LEU:HD13	2:B:615:TYR:CE1	2.51	0.45
6:F:163:ILE:O	6:F:167:THR:N	2.37	0.45
25:J:104:8CT:C22	25:J:104:8CT:C25	2.95	0.45
22:L:204:CLA:HBA1	22:L:204:CLA:H3A	1.70	0.45
14:2:122:TYR:O	14:2:126:SER:N	2.45	0.45
29:2:305:CHL:HED3	16:4:234:TRP:HH2	1.81	0.45
24:2:318:LHG:H272	24:2:318:LHG:H242	1.63	0.45
16:4:65:ASP:OD1	30:4:316:XAT:O23	2.21	0.45
16:4:238:VAL:C	16:4:240:SER:H	2.17	0.45
13:5:51:GLY:O	13:5:180:ARG:NH2	2.44	0.45
16:8:190:VAL:HB	16:8:194:LYS:HE2	1.99	0.45
30:0:314:XAT:H191	30:0:314:XAT:H11	1.65	0.45
1:A:270:PHE:CD1	22:K:102:CLA:HBC2	2.46	0.45
1:A:464:ASN:HB3	1:A:646:ALA:HB2	1.96	0.45
22:A:804:CLA:H61	22:A:809:CLA:H202	1.99	0.45
22:A:839:CLA:C4A	22:A:839:CLA:HBA2	2.45	0.45
25:A:850:8CT:C06	22:B:832:CLA:CMB	2.95	0.45
2:B:509:PHE:CE1	22:B:827:CLA:HBC2	2.51	0.45
22:B:812:CLA:HED3	22:B:812:CLA:HBD	1.72	0.45
6:F:176:TYR:HE2	22:F:301:CLA:HBD	1.77	0.45
22:L:204:CLA:HBA1	22:L:204:CLA:H11	1.81	0.45
13:1:99:TRP:CD1	13:1:200:PRO:HD3	2.50	0.45
15:3:81:PHE:HB2	15:3:83:LEU:HD13	1.98	0.45
16:4:227:THR:O	16:4:231:ALA:N	2.39	0.45
13:5:75:VAL:HG11	13:5:152:VAL:HG21	1.98	0.45
22:7:305:CLA:C4A	22:7:305:CLA:HBA2	2.47	0.45
30:0:313:XAT:H30	30:0:313:XAT:H403	1.99	0.45
22:A:823:CLA:H12	22:A:823:CLA:CHB	2.46	0.45
2:B:595:HIS:CG	2:B:623:TYR:OH	2.66	0.45
2:B:617:MET:O	2:B:621:ARG:N	2.32	0.45
22:B:828:CLA:H3A	22:B:828:CLA:HBA2	1.62	0.45
5:E:39:VAL:HG12	5:E:40:ARG:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:78:GLN:HA	12:L:42:GLY:HA3	1.99	0.45
8:H:113:ALA:HB3	22:H:201:CLA:C12	2.47	0.45
22:H:201:CLA:H151	12:L:88:LEU:HD13	1.99	0.45
10:J:7:TYR:OH	25:J:101:8CT:C06	2.65	0.45
22:1:303:CLA:HBA1	22:1:304:CLA:C1D	2.47	0.45
22:1:303:CLA:C4A	22:1:303:CLA:HBA2	2.46	0.45
14:2:83:GLN:HE21	14:2:148:ARG:HH11	1.65	0.45
16:4:160:ASP:HA	16:4:167:LEU:HD13	1.99	0.45
17:6:200:PHE:CE1	17:6:211:PRO:HB3	2.51	0.45
17:6:232:VAL:HG13	17:6:233:ILE:N	2.31	0.45
18:7:54:GLY:HA2	18:7:59:ASP:HB3	1.98	0.45
30:0:314:XAT:H201	30:0:314:XAT:H15	1.62	0.45
30:0:314:XAT:H202	30:0:314:XAT:H10	1.98	0.45
1:A:327:MET:HB2	1:A:347:TYR:CE1	2.51	0.45
22:A:813:CLA:HAA2	22:A:825:CLA:H52	1.98	0.45
2:B:141:PHE:CZ	22:B:815:CLA:H43	2.51	0.45
22:B:812:CLA:H112	22:B:840:CLA:H12	1.98	0.45
22:B:818:CLA:H3A	22:B:818:CLA:HBA2	1.32	0.45
22:B:830:CLA:H2A	22:B:830:CLA:O1D	2.16	0.45
3:C:25:VAL:O	3:C:27:GLU:HG3	2.17	0.45
4:D:137:CYS:SG	4:D:154:PHE:CG	3.08	0.45
9:I:19:PRO:O	9:I:23:MET:HB2	2.17	0.45
11:K:40:LEU:N	22:K:105:CLA:H43	2.32	0.45
13:1:221:THR:HG23	13:1:222:SER:N	2.32	0.45
14:2:234:PHE:O	14:2:237:ILE:HG22	2.17	0.45
29:2:301:CHL:HED3	15:3:173:ARG:HA	1.98	0.45
29:2:307:CHL:H2A	29:2:307:CHL:HED3	1.97	0.45
22:3:319:CLA:HAA2	22:3:319:CLA:CED	2.46	0.45
22:5:309:CLA:H72	30:5:315:XAT:C9	2.45	0.45
29:7:308:CHL:O1A	22:7:310:CLA:HMD2	2.16	0.45
22:0:304:CLA:H41	22:0:304:CLA:H61	1.56	0.45
1:A:463:HIS:CE1	1:A:467:MET:HG3	2.52	0.45
1:A:467:MET:HB2	1:A:476:MET:HG2	1.98	0.45
22:A:839:CLA:HBB2	22:A:839:CLA:H152	1.97	0.45
2:B:585:ASN:ND2	22:B:803:CLA:HBC2	2.26	0.45
2:B:658:ALA:CB	22:B:806:CLA:HBB2	2.47	0.45
22:B:815:CLA:C4A	22:B:815:CLA:HBA2	2.46	0.45
6:F:126:GLN:HA	6:F:129:PHE:CD2	2.51	0.45
8:H:132:GLY:HA3	8:H:133:PRO:HD3	1.79	0.45
11:K:16:GLY:O	11:K:20:ALA:HB2	2.17	0.45
11:K:68:HIS:ND1	25:K:103:8CT:C15	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:207:HIS:CD2	22:1:311:CLA:HAA2	2.51	0.45
14:2:239:ASP:HB3	14:2:243:ASN:ND2	2.32	0.45
18:7:116:LEU:HB3	18:7:120:VAL:HG23	1.98	0.45
18:7:249:ASP:HB2	18:7:252:GLY:O	2.16	0.45
30:7:319:XAT:H31	30:7:319:XAT:H391	1.58	0.45
16:8:43:ILE:HG22	16:8:44:TRP:H	1.81	0.45
16:8:205:MET:HE2	22:8:302:CLA:HHC	1.99	0.45
22:8:312:CLA:C1B	22:8:313:CLA:HMD3	2.46	0.45
20:0:72:ARG:HH22	22:0:302:CLA:HED3	1.81	0.45
29:0:301:CHL:H92	22:0:312:CLA:H93	1.99	0.45
22:0:311:CLA:C2B	30:0:313:XAT:H363	2.46	0.45
1:A:576:PHE:HE2	1:A:594:TRP:HD1	1.65	0.45
22:A:829:CLA:HMD2	22:A:829:CLA:H8	1.98	0.45
2:B:265:THR:HA	2:B:360:PHE:CE1	2.51	0.45
22:B:811:CLA:CGA	22:B:811:CLA:C1A	2.95	0.45
22:B:825:CLA:H161	22:B:825:CLA:H141	1.63	0.45
4:D:110:GLN:O	4:D:122:MET:HG2	2.17	0.45
14:2:187:PHE:CE1	22:6:304:CLA:H2	2.51	0.45
17:6:180:GLU:OE1	17:6:180:GLU:N	2.41	0.45
29:6:302:CHL:HBB1	29:6:302:CHL:HHC	1.99	0.45
13:5:147:ASP:HB3	13:5:150:LYS:CB	2.47	0.45
16:8:66:PRO:HD2	30:8:317:XAT:H222	1.98	0.45
16:8:196:LYS:HE2	22:8:311:CLA:HAA2	1.99	0.45
20:0:72:ARG:NH2	20:0:164:LEU:HD11	2.28	0.45
1:A:585:ARG:NH1	3:C:49:VAL:HG11	2.32	0.45
1:A:703:GLU:OE2	2:B:545:LYS:HB2	2.16	0.45
2:B:38:THR:OG1	2:B:41:THR:HG22	2.17	0.45
2:B:47:PHE:HA	2:B:50:HIS:HD2	1.82	0.45
2:B:597:LYS:HD2	22:B:836:CLA:HBC1	1.97	0.45
22:B:807:CLA:C4A	22:B:807:CLA:HBA2	2.47	0.45
22:B:813:CLA:C3D	22:B:814:CLA:HMC3	2.47	0.45
14:2:86:LEU:HB3	14:2:90:ARG:NH1	2.32	0.45
15:3:205:PRO:HG3	29:3:306:CHL:HMD2	1.98	0.45
16:4:76:LEU:O	16:4:80:VAL:HG23	2.17	0.45
16:4:196:LYS:HE3	22:4:311:CLA:HAA2	1.99	0.45
29:4:307:CHL:HMB3	25:4:317:8CT:C19	2.47	0.45
17:6:88:ALA:O	17:6:92:VAL:HG12	2.17	0.45
22:6:303:CLA:HBC1	24:6:322:LHG:H261	1.99	0.45
13:5:35:TRP:NE1	13:5:54:GLY:O	2.50	0.45
22:7:316:CLA:H2	22:7:316:CLA:H61	1.58	0.45
16:8:196:LYS:HE3	22:8:311:CLA:HBD	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:8:316:XAT:H191	30:8:316:XAT:H11	1.42	0.45
22:A:801:CLA:H2	22:A:801:CLA:H61	1.79	0.45
22:A:811:CLA:H143	22:A:811:CLA:H161	1.62	0.45
2:B:441:ASP:OD1	2:B:615:TYR:HB2	2.17	0.45
2:B:612:SER:HA	2:B:615:TYR:CE1	2.52	0.45
22:B:823:CLA:H92	22:B:823:CLA:H61	1.73	0.45
4:D:201:LYS:C	4:D:203:THR:H	2.20	0.45
6:F:184:TYR:CZ	6:F:188:THR:HG21	2.51	0.45
7:G:14:LEU:HG	13:1:133:VAL:HG22	1.99	0.45
22:G:102:CLA:H2A	22:G:102:CLA:CED	2.46	0.45
8:H:98:ARG:N	8:H:102:ILE:HD12	2.26	0.45
30:1:315:XAT:H35	30:1:315:XAT:H401	1.65	0.45
22:3:319:CLA:HED2	22:3:319:CLA:HBD	1.47	0.45
22:4:311:CLA:H61	22:4:311:CLA:H41	1.71	0.45
13:5:135:MET:HG2	22:5:308:CLA:OBD	2.17	0.45
16:8:89:PHE:HZ	29:8:305:CHL:HAB	1.81	0.45
16:8:97:MET:HB2	16:8:117:TRP:CB	2.47	0.45
22:8:308:CLA:HHC	22:8:308:CLA:CBB	2.46	0.45
19:9:216:ILE:N	19:9:217:PRO:HD3	2.31	0.45
22:A:826:CLA:C9	25:A:849:8CT:C40	2.95	0.44
22:A:828:CLA:H161	22:A:828:CLA:H202	1.64	0.44
22:A:840:CLA:H172	22:F:301:CLA:HMC3	1.98	0.44
2:B:70:TRP:HE1	9:I:3:ALA:HB3	1.82	0.44
2:B:257:PHE:HE2	2:B:493:TRP:CE3	2.35	0.44
7:G:61:ASN:ND2	22:G:103:CLA:OBD	2.51	0.44
22:G:101:CLA:HAA2	29:1:305:CHL:HBC2	1.99	0.44
13:1:215:ASN:ND2	22:1:312:CLA:O1D	2.50	0.44
16:4:158:ASN:OD1	16:4:162:ILE:HB	2.17	0.44
17:6:55:SER:N	17:6:59:ASP:OD2	2.49	0.44
13:5:34:ASN:ND2	13:5:36:LEU:O	2.50	0.44
13:5:36:LEU:HD12	13:5:38:GLY:H	1.82	0.44
22:7:304:CLA:HBB1	22:7:317:CLA:HMC1	1.99	0.44
22:7:317:CLA:HBA2	22:7:317:CLA:O2D	2.16	0.44
16:8:148:TYR:HB2	22:8:308:CLA:CMA	2.47	0.44
29:8:307:CHL:HMA1	25:8:318:8CT:C39	2.47	0.44
29:0:301:CHL:HBB1	29:0:301:CHL:CHC	2.42	0.44
1:A:379:MET:SD	22:A:818:CLA:HAA2	2.58	0.44
1:A:545:ALA:HB2	22:A:837:CLA:HMA1	1.98	0.44
2:B:96:PHE:O	8:H:126:THR:OG1	2.22	0.44
22:B:837:CLA:H143	22:B:837:CLA:H112	1.80	0.44
28:B:849:DGD:HAV2	28:B:849:DGD:HAF1	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:850:CLA:C3D	6:F:152:GLY:HA3	2.47	0.44
8:H:72:MET:HA	12:L:117:LEU:HD21	1.99	0.44
8:H:81:TYR:HA	22:L:202:CLA:HMD3	1.98	0.44
15:3:277:VAL:O	15:3:277:VAL:HG12	2.17	0.44
16:4:41:ARG:HH12	16:4:50:VAL:HG11	1.82	0.44
22:6:311:CLA:H61	22:6:311:CLA:H121	1.99	0.44
13:5:205:THR:HA	13:5:208:ILE:HG22	1.99	0.44
19:9:82:ARG:HG3	22:9:309:CLA:C4C	2.47	0.44
20:0:84:LEU:HD13	22:0:304:CLA:HBB2	1.98	0.44
22:0:311:CLA:H121	24:0:315:LHG:H172	1.99	0.44
1:A:209:GLY:HA3	22:A:813:CLA:HBB1	2.00	0.44
1:A:652:ARG:HB2	2:B:632:ILE:CG2	2.46	0.44
22:A:807:CLA:H171	22:A:807:CLA:H13	1.50	0.44
22:A:830:CLA:H61	22:A:830:CLA:H92	1.65	0.44
22:A:853:CLA:H142	22:A:853:CLA:H111	1.76	0.44
2:B:438:VAL:HG22	22:B:803:CLA:C2	2.47	0.44
12:L:65:ILE:HD11	22:L:204:CLA:HMA3	1.99	0.44
12:L:85:SER:HA	12:L:88:LEU:HG	1.98	0.44
14:2:86:LEU:CD2	14:2:205:ILE:HD11	2.47	0.44
16:4:150:ASP:CB	16:4:157:VAL:HG22	2.40	0.44
17:6:45:GLY:O	18:7:149:ASN:ND2	2.49	0.44
17:6:52:LEU:HD21	17:6:59:ASP:HB2	1.97	0.44
17:6:182:LEU:HD21	22:6:310:CLA:O1A	2.17	0.44
17:6:214:CYS:HA	17:6:217:ASP:HB2	1.98	0.44
22:7:303:CLA:H41	22:7:303:CLA:H61	1.41	0.44
16:8:132:LEU:HD21	29:8:305:CHL:CHD	2.47	0.44
22:8:304:CLA:C2B	30:8:317:XAT:H183	2.48	0.44
19:9:164:VAL:HG11	22:9:309:CLA:H12	1.99	0.44
22:A:840:CLA:C4A	22:A:840:CLA:HBA2	2.47	0.44
23:A:842:PQN:H261	23:A:842:PQN:H243	1.72	0.44
2:B:581:PHE:O	2:B:585:ASN:ND2	2.51	0.44
2:B:658:ALA:HB3	22:B:806:CLA:HBB2	1.99	0.44
22:B:836:CLA:H62	22:B:836:CLA:H41	1.63	0.44
13:1:80:TRP:HD1	22:1:307:CLA:HMD3	1.81	0.44
22:2:302:CLA:H3A	22:2:302:CLA:CGA	2.48	0.44
22:3:311:CLA:HBB1	22:3:311:CLA:H8	1.99	0.44
16:4:102:LEU:O	16:4:106:ALA:N	2.51	0.44
16:4:239:TRP:HE1	22:4:314:CLA:HMD3	1.81	0.44
22:4:303:CLA:HMD2	22:4:308:CLA:CHD	2.46	0.44
17:6:191:ARG:NH2	22:6:303:CLA:HMD3	2.32	0.44
13:5:123:ASP:O	13:5:127:LEU:N	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:7:51:TYR:CE2	18:7:52:LEU:HG	2.52	0.44
16:8:229:HIS:ND1	16:8:236:ASN:O	2.50	0.44
19:9:69:ARG:NH1	22:9:301:CLA:O2D	2.24	0.44
1:A:20:VAL:HG12	1:A:22:VAL:HG13	2.00	0.44
1:A:193:LEU:HG	1:A:197:GLN:HE21	1.82	0.44
22:A:826:CLA:H91	22:A:826:CLA:H112	1.64	0.44
2:B:61:THR:OG1	2:B:142:LEU:HD13	2.17	0.44
2:B:448:THR:HB	2:B:450:GLU:HG2	2.00	0.44
22:B:803:CLA:H111	22:B:803:CLA:H91	1.55	0.44
22:B:813:CLA:HBA2	22:B:813:CLA:H3A	1.73	0.44
8:H:110:GLY:O	22:H:201:CLA:H142	2.18	0.44
13:1:83:LEU:O	22:1:303:CLA:HMC3	2.17	0.44
22:2:304:CLA:H43	25:2:317:8CT:C34	2.47	0.44
22:3:301:CLA:H3A	22:3:301:CLA:CGA	2.48	0.44
17:6:120:ILE:O	17:6:123:ILE:N	2.50	0.44
22:6:310:CLA:H52	30:6:319:XAT:C30	2.43	0.44
22:6:315:CLA:H2	22:6:315:CLA:H61	1.64	0.44
13:5:123:ASP:OD1	13:5:124:ILE:N	2.47	0.44
13:5:180:ARG:HD3	22:5:302:CLA:CHD	2.48	0.44
29:5:301:CHL:H102	22:5:313:CLA:H71	1.98	0.44
20:0:100:TRP:HB2	30:0:314:XAT:H41	1.99	0.44
1:A:381:PRO:HG3	22:A:819:CLA:HBA1	1.99	0.44
1:A:447:ASN:ND2	2:B:678:LEU:HD21	2.33	0.44
2:B:92:TRP:HB2	22:B:810:CLA:HED1	2.00	0.44
2:B:126:THR:HG21	2:B:358:TYR:HD1	1.82	0.44
2:B:224:PRO:HG2	2:B:233:TYR:CZ	2.52	0.44
6:F:90:PHE:O	6:F:94:GLU:HG2	2.18	0.44
6:F:237:THR:HG22	6:F:238:VAL:N	2.30	0.44
11:K:40:LEU:HB2	22:K:105:CLA:C3	2.48	0.44
13:1:73:CYS:SG	22:1:302:CLA:HBD	2.57	0.44
22:1:301:CLA:HBC2	29:4:301:CHL:HBB2	1.99	0.44
22:3:307:CLA:H3A	22:3:307:CLA:HBA2	1.66	0.44
13:5:216:PHE:HD1	22:5:312:CLA:H12	1.82	0.44
30:7:319:XAT:H15	30:7:319:XAT:H201	1.77	0.44
20:0:173:ALA:HA	22:0:311:CLA:HBB1	1.98	0.44
22:0:302:CLA:H102	22:0:303:CLA:HMB3	1.98	0.44
22:A:808:CLA:H2A	22:A:808:CLA:O2D	2.17	0.44
22:A:818:CLA:HBA2	22:A:818:CLA:H3A	1.41	0.44
22:A:826:CLA:H141	22:A:826:CLA:H161	1.73	0.44
2:B:545:LYS:CE	6:F:236:ILE:HG12	2.47	0.44
2:B:655:LEU:CD2	22:B:840:CLA:HAB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:813:CLA:CGA	22:B:813:CLA:C1A	2.95	0.44
12:L:36:LEU:HD23	22:L:203:CLA:HBD	1.99	0.44
22:2:304:CLA:H8	22:2:304:CLA:H122	1.41	0.44
15:3:104:VAL:HG22	15:3:230:ILE:HD11	2.00	0.44
16:4:54:LEU:HD21	16:4:61:ASP:OD1	2.18	0.44
16:4:176:PRO:HG2	22:4:309:CLA:OBD	2.18	0.44
16:4:238:VAL:O	16:4:240:SER:N	2.50	0.44
17:6:159:LEU:HD12	17:6:160:PRO:HD2	1.99	0.44
17:6:232:VAL:HG13	17:6:233:ILE:H	1.82	0.44
29:6:307:CHL:HHC	29:6:307:CHL:HBB1	2.00	0.44
13:5:61:SER:HB2	13:5:67:MET:HB2	1.99	0.44
22:0:307:CLA:H92	22:0:307:CLA:H61	1.68	0.44
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.52	0.44
1:A:714:VAL:HG11	22:A:839:CLA:HMB3	2.00	0.44
22:A:829:CLA:H72	22:A:829:CLA:H112	1.83	0.44
2:B:71:GLN:NE2	22:B:810:CLA:O1D	2.42	0.44
2:B:203:ARG:NE	2:B:251:GLY:O	2.51	0.44
2:B:345:CYS:HB2	2:B:379:ALA:HB2	1.98	0.44
2:B:609:PHE:O	2:B:613:SER:N	2.49	0.44
6:F:199:ILE:HG22	6:F:200:ILE:HG13	1.98	0.44
8:H:124:ASP:HB3	8:H:127:LEU:CG	2.47	0.44
22:1:312:CLA:H2	22:1:312:CLA:HAA1	2.00	0.44
22:3:301:CLA:H2A	22:3:301:CLA:CED	2.47	0.44
16:4:241:ILE:HD12	16:4:241:ILE:O	2.17	0.44
17:6:159:LEU:HD23	17:6:162:HIS:ND1	2.33	0.44
13:5:192:GLN:HE21	22:5:312:CLA:C4D	2.31	0.44
16:8:43:ILE:HG23	16:8:62:PHE:O	2.18	0.44
20:0:146:PHE:CD1	20:0:151:PRO:HD2	2.53	0.44
1:A:217:GLY:O	22:A:814:CLA:HHC	2.18	0.44
1:A:439:ARG:NH1	1:A:560:LEU:O	2.50	0.44
2:B:8:PHE:HB2	2:B:34:HIS:ND1	2.33	0.44
2:B:32:GLU:HG3	2:B:42:LEU:HD11	2.00	0.44
2:B:60:TRP:HA	22:B:810:CLA:HAB	2.00	0.44
2:B:233:TYR:O	2:B:253:ALA:HB1	2.17	0.44
2:B:320:GLN:O	2:B:406:ASN:ND2	2.51	0.44
22:B:834:CLA:H122	22:B:834:CLA:H161	1.90	0.44
9:I:11:VAL:HA	9:I:14:VAL:HG12	1.99	0.44
11:K:42:ASP:CG	11:K:44:PRO:HD3	2.38	0.44
25:K:103:8CT:C38	22:K:104:CLA:NB	2.80	0.44
13:1:123:ASP:O	13:1:127:LEU:HB2	2.17	0.44
22:1:308:CLA:H112	22:1:308:CLA:H91	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:317:LHG:H341	29:4:301:CHL:HMB1	1.99	0.44
17:6:154:PHE:CZ	29:6:316:CHL:HAA1	2.52	0.44
29:9:302:CHL:HBB1	29:9:302:CHL:HHC	2.00	0.44
29:0:301:CHL:H3A	24:0:315:LHG:H321	1.99	0.44
11:K:38:LEU:HB3	22:K:105:CLA:O2A	2.18	0.43
17:6:87:TRP:CE2	22:6:309:CLA:HBC3	2.53	0.43
29:6:306:CHL:HBB2	29:6:307:CHL:CBB	2.48	0.43
24:5:318:LHG:H321	24:5:318:LHG:H352	1.72	0.43
18:7:67:LEU:CD2	22:7:303:CLA:H43	2.45	0.43
16:8:159:VAL:HG12	16:8:160:ASP:N	2.33	0.43
1:A:198:ASN:HD22	22:A:812:CLA:CED	2.31	0.43
1:A:301:HIS:CD2	22:A:818:CLA:HMB1	2.52	0.43
22:A:803:CLA:H2A	22:A:803:CLA:O1D	2.19	0.43
22:A:806:CLA:H192	22:A:806:CLA:H161	1.75	0.43
2:B:50:HIS:CE1	22:B:808:CLA:NA	2.85	0.43
2:B:684:ARG:HB3	12:L:18:MET:HE3	2.00	0.43
22:B:806:CLA:H72	22:B:840:CLA:HBB2	2.00	0.43
22:1:311:CLA:H122	22:1:311:CLA:H161	1.72	0.43
22:1:311:CLA:H41	22:1:311:CLA:H61	1.46	0.43
30:1:314:XAT:H181	30:1:314:XAT:C8	2.48	0.43
30:2:315:XAT:H15	30:2:315:XAT:H201	1.79	0.43
24:2:318:LHG:H142	22:3:313:CLA:HED1	1.99	0.43
22:5:303:CLA:H141	22:5:303:CLA:H161	1.83	0.43
22:7:312:CLA:H12	22:7:312:CLA:H52	1.85	0.43
16:8:217:VAL:HG11	22:8:312:CLA:HMD1	2.00	0.43
24:9:316:LHG:H192	24:9:316:LHG:H361	2.01	0.43
20:0:82:ALA:HA	30:0:314:XAT:H11	2.00	0.43
20:0:93:ASN:HA	20:0:97:LEU:HD23	2.00	0.43
22:0:312:CLA:H92	22:0:312:CLA:H61	1.77	0.43
1:A:346:LEU:HD21	22:A:824:CLA:HBC3	1.99	0.43
2:B:6:PRO:HG2	2:B:13:ALA:HA	1.99	0.43
2:B:182:LEU:HD12	22:B:814:CLA:CHB	2.47	0.43
2:B:222:LEU:HB3	2:B:226:PHE:CD2	2.52	0.43
2:B:272:ASP:OD1	22:B:818:CLA:HHB	2.18	0.43
2:B:438:VAL:HG22	22:B:803:CLA:H2	1.99	0.43
6:F:147:LEU:HD22	6:F:162:ASP:HB2	2.01	0.43
12:L:60:VAL:O	12:L:63:PRO:HD2	2.17	0.43
13:1:154:PRO:HB3	22:1:306:CLA:HBC2	2.01	0.43
15:3:168:GLN:HE22	22:3:313:CLA:C4D	2.31	0.43
15:3:211:ASN:ND2	15:3:214:ASN:HA	2.33	0.43
15:3:269:ASN:OD1	15:3:270:ILE:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:319:CLA:H41	22:3:319:CLA:H61	1.71	0.43
16:4:146:ARG:HA	29:4:301:CHL:HED1	1.99	0.43
22:6:309:CLA:H3A	22:6:309:CLA:HBA1	1.60	0.43
22:5:312:CLA:H2	22:5:313:CLA:OBD	2.18	0.43
18:7:241:THR:HA	18:7:264:GLN:O	2.18	0.43
29:0:301:CHL:O2A	24:0:315:LHG:H182	2.19	0.43
1:A:97:TYR:HD1	1:A:153:TRP:CZ2	2.36	0.43
1:A:202:MET:HB2	22:A:813:CLA:HBC3	2.00	0.43
1:A:617:TRP:CZ3	1:A:644:ALA:HB2	2.52	0.43
2:B:22:TRP:CZ2	22:B:839:CLA:HMB1	2.53	0.43
2:B:126:THR:HB	2:B:359:ALA:H	1.83	0.43
22:B:823:CLA:HAB	25:B:846:8CT:C08	2.48	0.43
22:B:834:CLA:H142	22:B:834:CLA:H111	1.72	0.43
5:E:9:VAL:O	5:E:22:ALA:HA	2.18	0.43
12:L:38:ALA:HB2	22:L:203:CLA:OBD	2.19	0.43
12:L:127:LEU:HD21	12:L:133:TRP:CE3	2.53	0.43
13:1:127:LEU:HD11	22:1:304:CLA:C2D	2.49	0.43
15:3:180:ASN:HB3	15:3:183:SER:HB3	2.01	0.43
17:6:249:VAL:HG11	29:6:307:CHL:O2D	2.17	0.43
22:6:318:CLA:H2A	22:6:318:CLA:O2D	2.18	0.43
30:6:320:XAT:H15	30:6:320:XAT:H201	1.65	0.43
29:7:308:CHL:HMB1	25:7:321:8CT:C18	2.46	0.43
19:9:85:MET:HA	19:9:175:ALA:HB1	1.99	0.43
22:9:312:CLA:H2	22:9:312:CLA:H72	2.01	0.43
1:A:670:LEU:HB2	1:A:673:TYR:HD2	1.84	0.43
2:B:188:LEU:HB3	22:B:816:CLA:HBB2	1.99	0.43
2:B:493:TRP:HE1	22:B:834:CLA:HED1	1.83	0.43
16:4:192:SER:O	16:4:196:LYS:HG3	2.17	0.43
13:5:139:GLU:O	13:5:143:ALA:N	2.52	0.43
22:5:305:CLA:HMC3	29:5:306:CHL:C2C	2.48	0.43
22:7:310:CLA:CGA	22:7:310:CLA:C4A	2.96	0.43
22:9:306:CLA:H61	22:9:306:CLA:H41	1.81	0.43
22:9:306:CLA:HMC3	29:9:307:CHL:C2C	2.49	0.43
1:A:536:SER:HB3	1:A:641:ALA:HA	2.01	0.43
1:A:586:GLY:O	2:B:668:ARG:HD3	2.19	0.43
22:A:838:CLA:O2D	22:A:838:CLA:H2A	2.18	0.43
22:A:840:CLA:H62	22:A:840:CLA:H41	1.80	0.43
2:B:480:SER:OG	2:B:483:SER:OG	2.31	0.43
22:B:805:CLA:H62	22:B:805:CLA:H2	1.70	0.43
22:B:809:CLA:H61	22:B:809:CLA:H92	1.72	0.43
3:C:23:THR:O	4:D:134:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:2:GLN:NE2	14:2:74:ASP:OD1	2.51	0.43
22:K:102:CLA:H3A	22:K:102:CLA:HBA1	1.65	0.43
13:1:37:PRO:HG3	16:4:162:ILE:HG21	2.00	0.43
22:1:310:CLA:H11	22:1:310:CLA:HMA2	2.00	0.43
14:2:117:ASP:OD1	14:2:120:LYS:HB2	2.19	0.43
14:2:217:GLY:O	14:2:221:GLN:HG2	2.19	0.43
17:6:215:TRP:HE3	30:6:319:XAT:H21	1.82	0.43
29:5:301:CHL:C2C	24:5:318:LHG:HC81	2.48	0.43
18:7:56:LEU:HD11	18:7:74:LEU:HD21	2.01	0.43
18:7:197:ASN:HD22	22:7:310:CLA:CBB	2.31	0.43
22:7:302:CLA:HAC2	24:7:322:LHG:HC32	2.01	0.43
16:8:221:GLY:N	16:8:224:ALA:HB3	2.33	0.43
22:0:307:CLA:H13	22:0:307:CLA:H172	1.79	0.43
1:A:48:PRO:HG3	6:F:199:ILE:HD11	2.00	0.43
22:A:806:CLA:H62	22:A:806:CLA:H102	1.81	0.43
2:B:178:HIS:HE1	22:B:814:CLA:NA	2.17	0.43
2:B:302:LYS:HE2	2:B:323:PHE:CD2	2.53	0.43
3:C:27:GLU:OE2	3:C:44:ARG:NH1	2.47	0.43
13:1:171:LEU:HD13	22:1:308:CLA:O1A	2.18	0.43
22:1:313:CLA:HBA1	22:1:313:CLA:H3A	1.47	0.43
14:2:74:ASP:HB3	14:2:77:MET:HB3	2.01	0.43
15:3:97:SER:HA	15:3:100:ARG:HH21	1.84	0.43
22:3:311:CLA:HBA2	22:3:311:CLA:H3A	1.63	0.43
17:6:114:ILE:HG12	22:6:305:CLA:HAA1	2.01	0.43
17:6:251:PHE:HB3	17:6:256:ILE:HD12	2.00	0.43
29:6:307:CHL:CBA	25:8:301:8CT:C37	2.97	0.43
13:5:92:GLU:HB2	13:5:98:ASN:HA	2.01	0.43
29:5:301:CHL:H111	29:5:301:CHL:H91	1.67	0.43
18:7:81:GLU:OE2	18:7:199:ARG:NH2	2.50	0.43
18:7:226:HIS:NE2	22:7:313:CLA:HBA1	2.34	0.43
22:7:318:CLA:HAA2	22:7:318:CLA:HBD	1.99	0.43
16:8:158:ASN:ND2	29:8:307:CHL:HAC1	2.32	0.43
16:8:168:PRO:HG2	16:8:177:GLY:O	2.18	0.43
22:0:302:CLA:HBC1	24:0:315:LHG:H271	2.00	0.43
1:A:346:LEU:HD13	22:A:824:CLA:HMD3	2.00	0.43
1:A:394:SER:OG	22:A:828:CLA:HHB	2.18	0.43
2:B:393:PHE:HA	2:B:397:ASP:OD1	2.19	0.43
2:B:440:ASN:OD1	2:B:452:GLN:HB3	2.18	0.43
2:B:595:HIS:CD2	2:B:623:TYR:CZ	2.88	0.43
22:B:808:CLA:H62	22:B:808:CLA:H2	1.64	0.43
8:H:89:PHE:CD1	12:L:50:VAL:HG21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:6:THR:HA	11:K:9:LEU:HD12	2.01	0.43
17:6:123:ILE:O	17:6:127:GLN:N	2.46	0.43
22:6:311:CLA:CBB	25:7:321:8CT:C01	2.96	0.43
18:7:92:VAL:HA	18:7:208:PHE:HE2	1.82	0.43
16:8:44:TRP:CE3	16:8:45:LEU:HB2	2.53	0.43
16:8:51:PRO:HB3	16:8:53:TRP:CH2	2.54	0.43
16:8:193:LEU:HD22	22:8:309:CLA:H3A	2.01	0.43
16:8:211:PHE:CE1	16:8:222:PRO:HB3	2.54	0.43
16:8:236:ASN:O	16:8:237:ASN:ND2	2.51	0.43
22:9:312:CLA:H71	24:9:316:LHG:H181	2.01	0.43
1:A:343:HIS:ND1	1:A:431:LEU:HD12	2.34	0.43
1:A:596:HIS:CE1	2:B:670:TYR:HD1	2.37	0.43
1:A:667:GLY:N	2:B:445:ALA:O	2.41	0.43
22:A:808:CLA:H193	22:A:808:CLA:H162	1.76	0.43
22:A:832:CLA:HAA2	25:B:851:8CT:C17	2.49	0.43
2:B:278:LEU:HD21	22:B:817:CLA:HAB	2.00	0.43
2:B:428:PHE:HE2	22:B:832:CLA:C2D	2.32	0.43
2:B:486:PHE:HA	2:B:494:LEU:HD11	2.01	0.43
2:B:553:PHE:HZ	3:C:52:LYS:NZ	2.16	0.43
2:B:599:LEU:HD11	2:B:623:TYR:HE1	1.84	0.43
22:B:818:CLA:H93	22:B:818:CLA:H62	1.69	0.43
22:B:840:CLA:H42	23:B:842:PQN:H271	2.01	0.43
8:H:131:VAL:O	8:H:134:GLN:HG3	2.18	0.43
22:1:301:CLA:H3A	22:1:301:CLA:CGA	2.49	0.43
17:6:100:LEU:CD1	17:6:101:VAL:HG23	2.46	0.43
17:6:153:ILE:HG13	17:6:154:PHE:N	2.34	0.43
29:6:302:CHL:H91	29:6:302:CHL:H111	1.64	0.43
13:5:178:ASN:HD22	22:5:309:CLA:HAB	1.83	0.43
18:7:153:VAL:O	18:7:153:VAL:HG13	2.18	0.43
18:7:208:PHE:CD1	18:7:219:PRO:HB3	2.54	0.43
18:7:260:LEU:HD21	22:7:317:CLA:C4C	2.49	0.43
19:9:189:VAL:HG11	22:9:312:CLA:HED1	2.01	0.43
22:9:310:CLA:HBC3	24:9:316:LHG:HC62	2.00	0.43
20:0:141:CYS:HB3	20:0:144:LEU:HD12	2.00	0.43
20:0:189:VAL:HA	20:0:192:LEU:HD12	1.99	0.43
29:0:301:CHL:C3B	24:0:315:LHG:H301	2.48	0.43
22:0:304:CLA:HMB3	30:0:314:XAT:H22	2.01	0.43
1:A:37:PRO:HB2	1:A:53:TRP:HH2	1.84	0.43
1:A:439:ARG:NH2	1:A:564:SER:O	2.50	0.43
22:A:820:CLA:HMB1	22:A:820:CLA:HBB1	2.01	0.43
2:B:632:ILE:HD11	22:B:805:CLA:HBC1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:809:CLA:H3A	22:B:809:CLA:HBA1	1.42	0.43
7:G:3:SER:HA	7:G:6:LEU:HB2	2.00	0.43
12:L:9:PRO:HA	12:L:19:LEU:HB2	2.00	0.43
12:L:29:VAL:HG13	22:L:201:CLA:H43	2.00	0.43
22:L:201:CLA:H2	22:L:203:CLA:H72	1.99	0.43
22:1:303:CLA:C1B	25:1:316:8CT:C36	2.97	0.43
17:6:46:SER:OG	17:6:47:THR:N	2.52	0.43
22:6:323:CLA:HBB1	31:8:319:LMG:H162	2.00	0.43
16:8:146:ARG:NE	29:8:307:CHL:OMC	2.40	0.43
22:8:310:CLA:C4A	31:8:319:LMG:HC4	2.49	0.43
22:A:825:CLA:H161	22:A:825:CLA:H141	1.64	0.42
22:A:853:CLA:H71	22:A:853:CLA:H112	1.75	0.42
2:B:417:ALA:O	2:B:421:HIS:HD2	2.02	0.42
2:B:438:VAL:HG13	22:B:803:CLA:H62	2.01	0.42
15:3:90:ASP:CG	15:3:91:VAL:H	2.22	0.42
15:3:222:MET:HG3	15:3:226:LYS:HE3	2.00	0.42
16:4:180:PHE:HB3	22:4:309:CLA:HMD1	2.01	0.42
22:4:314:CLA:H61	22:4:314:CLA:H2	1.85	0.42
13:5:170:GLU:OE2	13:5:174:LYS:HD2	2.18	0.42
24:5:318:LHG:H341	24:5:318:LHG:H172	1.99	0.42
18:7:209:ALA:O	18:7:213:GLN:HB2	2.19	0.42
19:9:55:ASP:CG	19:9:57:GLY:H	2.23	0.42
19:9:84:ALA:HB2	30:9:315:XAT:C13	2.48	0.42
1:A:371:ILE:HG12	22:A:826:CLA:HED3	2.00	0.42
22:A:805:CLA:H3A	22:A:805:CLA:HBA1	1.71	0.42
22:A:810:CLA:H111	22:A:810:CLA:H152	1.77	0.42
2:B:177:HIS:O	2:B:181:GLY:N	2.48	0.42
4:D:189:ARG:HB2	4:D:193:GLU:HB2	2.00	0.42
8:H:115:LEU:HD21	9:I:13:LEU:HB2	2.01	0.42
30:2:316:XAT:H15	30:2:316:XAT:H201	1.83	0.42
17:6:102:LYS:HD2	22:6:305:CLA:HMD3	2.01	0.42
17:6:141:ASP:OD2	29:6:308:CHL:HBC1	2.18	0.42
13:5:203:CYS:HA	13:5:206:GLU:HB3	2.00	0.42
18:7:87:TRP:CE2	29:7:308:CHL:HED2	2.54	0.42
22:9:303:CLA:O2D	22:9:303:CLA:H2A	2.18	0.42
20:0:199:PRO:HB2	22:0:312:CLA:HMA1	2.01	0.42
1:A:375:HIS:HE1	22:A:827:CLA:NB	2.17	0.42
22:A:810:CLA:H62	22:A:810:CLA:H2	1.80	0.42
22:A:841:CLA:HMC3	22:B:839:CLA:C4D	2.50	0.42
23:A:842:PQN:H292	23:A:842:PQN:H262	1.84	0.42
2:B:44:GLN:NE2	2:B:162:GLN:HG3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:686:PRO:HG2	22:L:203:CLA:H41	2.00	0.42
22:B:814:CLA:H142	22:B:814:CLA:H112	1.75	0.42
22:B:829:CLA:HHC	22:B:829:CLA:CBB	2.42	0.42
4:D:98:GLU:OE1	4:D:156:ARG:HD3	2.19	0.42
22:H:201:CLA:H2	22:H:201:CLA:H61	1.79	0.42
12:L:91:ILE:O	12:L:94:THR:OG1	2.37	0.42
15:3:109:PHE:CD2	22:3:307:CLA:HMD3	2.55	0.42
15:3:229:GLU:HG3	22:3:308:CLA:C1B	2.49	0.42
22:3:302:CLA:HMD2	22:3:307:CLA:C1D	2.50	0.42
16:4:202:ARG:HD2	22:4:302:CLA:C4C	2.49	0.42
29:4:307:CHL:O1A	22:4:309:CLA:HHD	2.19	0.42
22:6:317:CLA:HMD3	22:6:318:CLA:HBB2	2.01	0.42
22:5:309:CLA:HMC2	30:5:315:XAT:C11	2.49	0.42
22:5:310:CLA:C3D	22:5:311:CLA:HMA3	2.48	0.42
16:8:115:THR:H	16:8:119:ASN:HD21	1.66	0.42
16:8:172:ILE:HB	16:8:175:TYR:O	2.20	0.42
1:A:563:ARG:O	1:A:571:LYS:HB3	2.20	0.42
2:B:91:ILE:HD11	2:B:114:ASN:CG	2.40	0.42
22:B:806:CLA:H161	22:B:806:CLA:H141	1.66	0.42
4:D:104:TRP:HD1	4:D:105:GLU:O	2.01	0.42
8:H:114:LEU:HG	22:H:201:CLA:H152	2.02	0.42
14:2:72:ALA:HB1	14:2:78:LEU:HD13	2.01	0.42
14:2:99:MET:HG2	14:2:115:TRP:CB	2.50	0.42
22:3:301:CLA:H112	22:3:302:CLA:HMB3	2.01	0.42
30:4:316:XAT:H27	30:4:316:XAT:H30	1.70	0.42
17:6:119:ASN:HB3	17:6:120:ILE:H	1.61	0.42
18:7:182:ALA:HB3	22:7:310:CLA:HAA2	2.01	0.42
22:7:306:CLA:HBC2	22:7:307:CLA:HBC3	2.01	0.42
19:9:77:GLU:HB2	22:9:303:CLA:C1B	2.49	0.42
20:0:68:LEU:HD12	20:0:69:ALA:N	2.34	0.42
1:A:40:PHE:CD1	1:A:41:SER:N	2.87	0.42
1:A:79:PHE:HA	1:A:82:HIS:HD2	1.85	0.42
1:A:312:ILE:HG21	22:A:817:CLA:H162	2.02	0.42
1:A:484:LEU:O	1:A:535:THR:HG22	2.18	0.42
2:B:5:PHE:O	2:B:7:LYS:N	2.52	0.42
2:B:209:TRP:NE1	22:B:815:CLA:H11	2.35	0.42
4:D:190:SER:HG	5:E:13:ARG:NH1	2.17	0.42
25:J:104:8CT:C37	25:J:104:8CT:C32	2.98	0.42
12:L:18:MET:HG2	12:L:19:LEU:N	2.34	0.42
12:L:127:LEU:HD21	12:L:133:TRP:HE3	1.84	0.42
13:1:61:SER:OG	13:1:67:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:210:ASP:O	13:1:214:ALA:HB3	2.20	0.42
30:4:315:XAT:H31	30:4:315:XAT:H391	1.79	0.42
22:6:323:CLA:H3A	22:6:323:CLA:HBA1	1.55	0.42
13:5:35:TRP:CG	13:5:36:LEU:N	2.88	0.42
31:5:319:LMG:H331	31:5:319:LMG:H152	2.02	0.42
18:7:109:GLU:HA	22:7:307:CLA:O1D	2.19	0.42
18:7:208:PHE:CE1	30:7:319:XAT:H362	2.54	0.42
22:7:306:CLA:HMC3	22:7:307:CLA:NC	2.35	0.42
16:8:88:ARG:NH1	16:8:175:TYR:CD2	2.88	0.42
22:9:306:CLA:HMC3	29:9:307:CHL:C1C	2.49	0.42
1:A:557:LYS:HG3	1:A:561:TYR:HD2	1.85	0.42
22:A:812:CLA:C3D	22:A:813:CLA:HMC3	2.50	0.42
2:B:509:PHE:CD1	22:B:827:CLA:HBC2	2.53	0.42
2:B:582:TRP:O	2:B:586:THR:HG22	2.19	0.42
22:B:803:CLA:HMB3	22:B:805:CLA:H193	2.02	0.42
22:B:805:CLA:H52	22:B:805:CLA:H8	1.81	0.42
23:B:842:PQN:H241	23:B:842:PQN:H262	1.78	0.42
3:C:28:MET:HB3	3:C:38:GLN:HE21	1.84	0.42
11:K:2:PHE:CE2	11:K:8:ASN:HB2	2.53	0.42
30:1:314:XAT:H31	30:1:314:XAT:H391	1.47	0.42
22:3:312:CLA:O2D	22:3:312:CLA:H2A	2.19	0.42
16:4:91:MET:HE3	22:4:309:CLA:HMC3	2.01	0.42
16:4:97:MET:HG2	16:4:117:TRP:HB2	2.01	0.42
29:4:305:CHL:C4A	25:4:317:8CT:C38	2.95	0.42
22:6:305:CLA:C1B	25:6:321:8CT:C33	2.97	0.42
18:7:226:HIS:ND1	22:7:313:CLA:HAA2	2.35	0.42
16:8:122:ALA:N	29:8:306:CHL:O1D	2.53	0.42
1:A:131:ILE:HD11	1:A:667:GLY:O	2.20	0.42
2:B:29:HIS:CE1	22:B:807:CLA:NB	2.87	0.42
2:B:283:LEU:HD11	22:B:818:CLA:HMC1	2.02	0.42
22:B:827:CLA:H41	22:B:827:CLA:H62	1.76	0.42
22:B:832:CLA:H143	22:B:832:CLA:H112	1.74	0.42
22:B:832:CLA:HAA1	22:B:832:CLA:HBD	2.00	0.42
6:F:78:ILE:HD13	6:F:78:ILE:HA	1.87	0.42
11:K:21:ALA:HB3	11:K:26:LEU:CD2	2.43	0.42
11:K:35:THR:HG22	11:K:36:SER:N	2.34	0.42
12:L:66:LYS:HB3	22:L:204:CLA:HMB3	2.02	0.42
13:1:147:ASP:OD1	13:1:148:MET:N	2.53	0.42
14:2:179:PRO:HB2	14:2:184:PHE:HD2	1.85	0.42
22:2:303:CLA:H91	22:2:303:CLA:H111	1.75	0.42
15:3:121:GLU:HG2	15:3:255:TYR:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:3:196:LEU:HD23	15:3:196:LEU:HA	1.83	0.42
16:4:172:ILE:HD12	16:4:173:PRO:O	2.19	0.42
22:4:314:CLA:H3A	22:4:314:CLA:HBA1	1.57	0.42
17:6:39:ARG:HB2	17:6:40:PRO:HD2	2.02	0.42
17:6:159:LEU:HD22	17:6:168:GLY:CA	2.48	0.42
22:6:311:CLA:C1D	22:6:312:CLA:HMD2	2.50	0.42
22:5:302:CLA:H51	22:5:303:CLA:H3A	2.02	0.42
22:9:303:CLA:H2	30:9:315:XAT:O24	2.20	0.42
20:0:33:ARG:O	20:0:35:MET:HG2	2.20	0.42
20:0:223:TRP:HB3	20:0:224:PRO:HD3	2.01	0.42
1:A:699:GLN:O	1:A:703:GLU:HG3	2.19	0.42
22:A:836:CLA:HBC2	22:A:836:CLA:HHD	2.02	0.42
2:B:95:HIS:HE1	22:H:201:CLA:NA	2.17	0.42
2:B:207:VAL:O	2:B:208:ARG:HD3	2.20	0.42
2:B:273:MET:O	2:B:276:HIS:HB3	2.20	0.42
2:B:559:CYS:HB3	27:B:802:SF4:S3	2.59	0.42
22:B:824:CLA:H112	22:B:824:CLA:H143	1.82	0.42
22:B:827:CLA:H151	22:B:827:CLA:H18	1.77	0.42
22:B:829:CLA:H192	22:B:829:CLA:H162	1.81	0.42
7:G:22:VAL:HG13	7:G:23:PHE:N	2.35	0.42
8:H:124:ASP:CB	8:H:127:LEU:CD1	2.73	0.42
11:K:18:CYS:SG	22:K:105:CLA:HBB2	2.59	0.42
22:L:202:CLA:H203	22:L:202:CLA:H122	2.01	0.42
13:1:127:LEU:HD11	22:1:304:CLA:HMD3	2.01	0.42
16:4:41:ARG:NH1	16:4:50:VAL:HG11	2.35	0.42
22:4:310:CLA:C1D	22:4:311:CLA:HMD2	2.49	0.42
22:4:314:CLA:O2D	22:4:314:CLA:H2A	2.19	0.42
29:6:302:CHL:H101	22:6:314:CLA:C1D	2.50	0.42
22:6:310:CLA:H62	22:6:310:CLA:H41	1.69	0.42
18:7:188:GLU:HA	18:7:191:LYS:HB2	2.02	0.42
30:7:319:XAT:H11	30:7:319:XAT:H191	1.52	0.42
22:9:303:CLA:H102	22:9:304:CLA:HMB3	2.02	0.42
2:B:53:GLN:HE22	22:B:809:CLA:C4D	2.32	0.42
2:B:397:ASP:HA	4:D:198:ILE:CD1	2.49	0.42
22:B:828:CLA:H141	22:B:830:CLA:H162	2.02	0.42
22:B:850:CLA:HBC2	6:F:151:PRO:HG2	2.01	0.42
13:1:31:ARG:HB2	13:1:52:ASN:O	2.20	0.42
22:1:301:CLA:HBB2	30:1:315:XAT:H34	2.02	0.42
15:3:68:LEU:HD12	15:3:84:LEU:HD22	2.02	0.42
16:4:157:VAL:HG11	29:4:307:CHL:HMC	2.02	0.42
17:6:126:PHE:HD1	22:8:313:CLA:HBA1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:233:ILE:HG12	17:6:238:ALA:HB1	2.02	0.42
29:5:301:CHL:C1C	24:5:318:LHG:HC81	2.49	0.42
16:8:166:LYS:HE3	16:8:179:ILE:N	2.32	0.42
19:9:178:ALA:HA	22:9:312:CLA:CBB	2.49	0.42
20:0:36:TRP:CD1	20:0:56:TYR:HB2	2.55	0.42
20:0:52:GLY:H	20:0:161:LEU:HD12	1.85	0.42
22:0:303:CLA:HMC2	30:0:314:XAT:C13	2.50	0.42
1:A:474:GLN:HG3	1:A:475:ASP:OD1	2.20	0.42
1:A:700:GLU:C	2:B:536:LYS:HZ1	2.23	0.42
22:A:806:CLA:H12	22:A:806:CLA:HBA2	1.75	0.42
22:A:809:CLA:CBB	22:B:833:CLA:HMD2	2.50	0.42
22:A:809:CLA:H162	22:A:809:CLA:H141	1.75	0.42
2:B:5:PHE:HB3	2:B:20:ARG:HH12	1.84	0.42
2:B:87:ILE:HG12	2:B:113:VAL:HG21	2.02	0.42
2:B:680:TRP:CE2	2:B:684:ARG:HD2	2.54	0.42
22:B:813:CLA:H93	22:9:301:CLA:O2A	2.20	0.42
5:E:39:VAL:HG12	5:E:40:ARG:H	1.85	0.42
7:G:22:VAL:HG13	7:G:23:PHE:CD2	2.55	0.42
7:G:69:VAL:HA	7:G:72:LEU:HD12	2.01	0.42
10:J:24:SER:HA	25:J:101:8CT:C27	2.49	0.42
22:K:102:CLA:HMC1	25:K:103:8CT:C09	2.50	0.42
13:1:80:TRP:CE2	22:1:306:CLA:HED2	2.55	0.42
13:1:134:LEU:HD13	22:1:304:CLA:H51	2.02	0.42
14:2:46:TRP:CE3	14:2:47:TYR:HB2	2.55	0.42
15:3:249:LEU:CD2	22:3:311:CLA:HMD1	2.49	0.42
16:4:144:GLU:OE2	16:4:147:ARG:NH2	2.44	0.42
17:6:187:LEU:HB3	17:6:191:ARG:HD3	2.01	0.42
20:0:48:GLY:N	20:0:53:ASP:OD2	2.53	0.42
1:A:126:ILE:HG23	1:A:127:VAL:HG23	2.01	0.41
1:A:379:MET:HG3	1:A:379:MET:O	2.19	0.41
22:A:819:CLA:H3A	22:A:819:CLA:HBA2	1.31	0.41
22:A:827:CLA:H61	22:A:827:CLA:H2	1.67	0.41
22:A:828:CLA:H13	22:A:828:CLA:H102	1.27	0.41
22:A:837:CLA:H162	22:A:837:CLA:H121	1.75	0.41
2:B:458:VAL:H	22:B:837:CLA:HMD1	1.84	0.41
2:B:494:LEU:HD23	2:B:494:LEU:HA	1.89	0.41
2:B:608:GLN:O	2:B:612:SER:OG	2.37	0.41
22:B:810:CLA:H92	22:B:810:CLA:H61	1.81	0.41
22:B:828:CLA:HBB1	22:B:828:CLA:HMB1	2.03	0.41
22:B:828:CLA:O1D	22:B:829:CLA:HHB	2.20	0.41
11:K:3:ILE:HA	11:K:8:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:307:CLA:HBA2	22:1:307:CLA:H3A	1.39	0.41
14:2:86:LEU:HB3	14:2:90:ARG:HH12	1.85	0.41
14:2:189:LEU:HD22	22:2:309:CLA:CGA	2.50	0.41
22:3:307:CLA:HMB2	22:3:313:CLA:C2C	2.49	0.41
16:4:199:LYS:HE2	16:4:199:LYS:HB2	1.79	0.41
22:6:305:CLA:C4B	30:6:320:XAT:H163	2.50	0.41
22:6:317:CLA:HBC3	22:6:318:CLA:CHC	2.50	0.41
13:5:183:MET:HB2	22:5:302:CLA:HMC3	2.02	0.41
18:7:142:ARG:HH22	18:7:153:VAL:HG21	1.85	0.41
22:8:310:CLA:H2	22:8:311:CLA:C3D	2.50	0.41
19:9:165:GLU:O	19:9:168:GLU:HB3	2.20	0.41
20:0:131:ARG:NH2	20:0:132:TYR:OH	2.53	0.41
1:A:237:VAL:HG12	1:A:238:ASP:H	1.85	0.41
1:A:267:LYS:HD2	1:A:267:LYS:HA	1.86	0.41
1:A:666:TYR:HE2	2:B:617:MET:HG2	1.84	0.41
1:A:690:PHE:HA	23:A:842:PQN:O1	2.20	0.41
22:A:817:CLA:H2	22:K:101:CLA:HED1	2.02	0.41
22:A:833:CLA:H203	22:A:833:CLA:H141	2.01	0.41
2:B:222:LEU:HD11	22:B:816:CLA:C3D	2.51	0.41
2:B:236:ASN:HD22	2:B:252:ASP:HB3	1.85	0.41
22:B:824:CLA:HBC3	25:B:846:8CT:C26	2.48	0.41
22:B:837:CLA:H3A	22:B:837:CLA:HBA2	1.74	0.41
3:C:9:ASP:OD2	5:E:34:LYS:NZ	2.53	0.41
4:D:195:VAL:O	4:D:208:PRO:HB3	2.21	0.41
22:H:201:CLA:H203	22:H:201:CLA:H161	1.81	0.41
11:K:34:ALA:CA	22:K:105:CLA:H41	2.48	0.41
22:L:202:CLA:H3A	22:L:202:CLA:CGA	2.45	0.41
13:1:85:VAL:HG11	30:1:314:XAT:C11	2.50	0.41
22:1:308:CLA:CGA	22:1:308:CLA:C4A	2.98	0.41
14:2:77:MET:HG2	14:2:81:TRP:NE1	2.35	0.41
14:2:189:LEU:HD23	14:2:190:ALA:H	1.85	0.41
22:2:312:CLA:HMB3	30:2:315:XAT:H372	2.02	0.41
30:2:315:XAT:H27	30:2:315:XAT:H371	1.81	0.41
15:3:230:ILE:O	15:3:233:GLY:N	2.54	0.41
17:6:76:TRP:CE2	22:6:309:CLA:HED1	2.56	0.41
17:6:223:PHE:CD2	18:7:123:LEU:HD22	2.50	0.41
22:5:307:CLA:HED3	22:5:309:CLA:HAC2	2.01	0.41
22:7:317:CLA:H2	22:7:317:CLA:O1D	2.20	0.41
22:8:315:CLA:H152	22:8:315:CLA:C2	2.50	0.41
22:9:309:CLA:C2	30:9:314:XAT:H7	2.50	0.41
22:0:310:CLA:H3A	22:0:310:CLA:HBA1	1.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:PRO:HG2	1:A:277:TYR:CZ	2.56	0.41
1:A:723:LEU:HD22	1:A:727:GLN:HG2	2.01	0.41
22:A:806:CLA:H172	22:A:829:CLA:HBB2	2.02	0.41
22:A:807:CLA:H8	22:A:807:CLA:H51	1.85	0.41
22:A:813:CLA:H142	22:A:813:CLA:C2B	2.51	0.41
22:A:820:CLA:CBB	25:K:103:8CT:C40	2.98	0.41
22:A:822:CLA:H2A	11:K:34:ALA:HB3	2.02	0.41
22:A:834:CLA:NB	25:A:849:8CT:C07	2.83	0.41
22:A:841:CLA:H203	22:A:841:CLA:H162	1.79	0.41
2:B:605:ASN:HB3	2:B:608:GLN:OE1	2.19	0.41
2:B:683:GLU:HG2	4:D:92:ARG:NH1	2.28	0.41
22:B:817:CLA:H93	22:B:817:CLA:H61	1.75	0.41
3:C:3:HIS:HD2	3:C:48:CYS:O	2.04	0.41
6:F:190:GLY:O	6:F:191:GLU:HG3	2.20	0.41
11:K:35:THR:HG22	11:K:36:SER:H	1.85	0.41
22:K:102:CLA:CMC	25:K:103:8CT:C09	2.98	0.41
22:1:311:CLA:H111	22:1:311:CLA:H72	1.63	0.41
16:4:207:ALA:HB1	30:4:315:XAT:H181	2.02	0.41
16:4:239:TRP:HA	16:4:244:ALA:HB3	2.02	0.41
29:6:302:CHL:HAA1	24:6:322:LHG:H122	2.01	0.41
18:7:86:ARG:HB3	22:7:310:CLA:CAC	2.50	0.41
18:7:144:TRP:HB2	22:7:309:CLA:CMA	2.50	0.41
18:7:235:ILE:HG13	22:7:313:CLA:CAD	2.50	0.41
18:7:241:THR:HB	18:7:243:VAL:HG13	2.02	0.41
22:8:302:CLA:HAB	30:8:317:XAT:H32	2.03	0.41
30:9:315:XAT:H15	30:9:315:XAT:H201	1.76	0.41
1:A:237:VAL:HG12	1:A:238:ASP:N	2.36	0.41
1:A:377:TYR:HE1	1:A:619:MET:CE	2.34	0.41
22:A:809:CLA:H91	22:A:809:CLA:H111	1.88	0.41
22:A:837:CLA:H41	22:A:837:CLA:H62	1.67	0.41
2:B:77:TRP:CD2	2:B:121:TYR:HE1	2.38	0.41
2:B:165:LEU:HD21	2:B:169:LYS:NZ	2.35	0.41
2:B:261:PHE:O	2:B:269:TRP:NE1	2.54	0.41
2:B:302:LYS:HE2	2:B:302:LYS:HB3	1.84	0.41
2:B:346:SER:OG	22:B:826:CLA:OBD	2.38	0.41
22:B:833:CLA:HBA1	22:B:833:CLA:H3A	1.87	0.41
24:B:852:LHG:O3	24:B:852:LHG:O1	2.38	0.41
13:1:82:MET:HB3	30:1:314:XAT:C40	2.50	0.41
14:2:43:ARG:HA	14:2:44:PRO:HD3	1.83	0.41
22:2:308:CLA:HHC	22:2:308:CLA:CBB	2.50	0.41
22:3:307:CLA:HBB1	22:3:313:CLA:HBB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:308:CLA:HAB	30:3:314:XAT:C40	2.50	0.41
30:3:315:XAT:H35	30:3:315:XAT:H401	1.91	0.41
16:4:60:GLY:O	22:4:302:CLA:HED3	2.21	0.41
30:6:320:XAT:H23	30:6:320:XAT:H373	1.83	0.41
13:5:218:THR:C	13:5:220:GLY:H	2.23	0.41
22:5:302:CLA:H72	30:5:316:XAT:H30	2.02	0.41
30:5:316:XAT:H15	30:5:316:XAT:H201	1.91	0.41
22:7:313:CLA:O1D	22:7:313:CLA:H2A	2.21	0.41
16:8:94:LEU:HG	16:8:211:PHE:CE2	2.55	0.41
16:8:157:VAL:O	16:8:159:VAL:HG23	2.21	0.41
19:9:129:MET:HG3	22:9:308:CLA:HMC3	2.01	0.41
19:9:200:HIS:ND1	19:9:207:GLN:O	2.51	0.41
20:0:195:HIS:ND1	22:0:311:CLA:HAA2	2.36	0.41
22:0:303:CLA:HMD2	22:0:307:CLA:C1D	2.50	0.41
1:A:172:LEU:HD12	22:A:807:CLA:HMC1	2.03	0.41
22:A:827:CLA:H111	22:A:827:CLA:H151	1.39	0.41
2:B:41:THR:HA	2:B:44:GLN:HG2	2.02	0.41
2:B:284:PHE:CD1	22:B:820:CLA:HMC3	2.54	0.41
22:B:817:CLA:H43	7:G:88:THR:HG22	2.02	0.41
13:1:82:MET:SD	22:1:308:CLA:HMC3	2.59	0.41
22:1:301:CLA:HED2	22:1:301:CLA:H2A	2.03	0.41
22:1:310:CLA:O2D	22:1:310:CLA:HBA2	2.20	0.41
14:2:173:THR:HG22	14:2:178:TYR:O	2.20	0.41
17:6:176:PRO:HG2	22:6:310:CLA:H42	2.02	0.41
22:5:302:CLA:CMB	22:5:303:CLA:HBA2	2.50	0.41
16:8:115:THR:H	16:8:119:ASN:CG	2.23	0.41
16:8:161:PRO:HD2	16:8:166:LYS:H	1.85	0.41
29:8:306:CHL:HBB1	29:8:306:CHL:HHC	2.03	0.41
1:A:104:SER:HA	1:A:120:ALA:HA	2.03	0.41
1:A:291:ASN:HB3	1:A:383:PRO:HA	2.02	0.41
1:A:528:MET:SD	1:A:619:MET:HE1	2.59	0.41
22:A:822:CLA:H2	22:K:105:CLA:HHB	2.03	0.41
22:A:827:CLA:H62	22:A:827:CLA:H102	1.93	0.41
22:A:829:CLA:H18	22:A:829:CLA:H152	1.85	0.41
2:B:130:ARG:NH2	2:B:201:GLU:OE2	2.54	0.41
2:B:187:SER:OG	2:B:277:HIS:O	2.37	0.41
2:B:233:TYR:HB3	2:B:254:ILE:HG13	2.02	0.41
2:B:277:HIS:HE1	22:B:819:CLA:NA	2.19	0.41
22:B:801:CLA:H92	22:B:801:CLA:H62	1.66	0.41
7:G:8:ILE:HD11	7:G:86:LEU:HD12	2.03	0.41
12:L:64:PHE:HB3	12:L:82:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:306:CLA:H141	22:1:306:CLA:H162	1.57	0.41
14:2:139:LEU:HD23	22:4:313:CLA:O2A	2.20	0.41
22:2:309:CLA:H3A	22:2:309:CLA:O1A	2.20	0.41
22:2:312:CLA:H2A	22:2:312:CLA:O1D	2.21	0.41
16:4:222:PRO:O	16:4:226:TRP:N	2.33	0.41
17:6:98:GLN:HE22	22:6:305:CLA:CGD	2.33	0.41
17:6:192:LEU:HD21	30:6:319:XAT:H191	2.02	0.41
18:7:205:TRP:O	18:7:208:PHE:HB2	2.21	0.41
22:7:313:CLA:HBA2	22:7:313:CLA:H3A	1.31	0.41
30:7:319:XAT:H373	30:7:319:XAT:H23	1.63	0.41
19:9:105:GLU:O	19:9:108:GLN:HB3	2.20	0.41
20:0:155:ARG:HH22	20:0:162:LYS:CD	2.30	0.41
1:A:252:ARG:HH21	15:3:277:VAL:HB	1.84	0.41
22:A:809:CLA:HBB2	22:B:833:CLA:HMD2	2.03	0.41
22:A:814:CLA:HBA1	22:A:814:CLA:H3A	1.92	0.41
22:A:817:CLA:O2D	22:A:817:CLA:H2A	2.20	0.41
22:A:839:CLA:H111	22:A:839:CLA:H142	1.79	0.41
2:B:432:HIS:O	2:B:436:LEU:HG	2.20	0.41
2:B:461:GLN:HG3	2:B:512:ILE:HD11	2.02	0.41
11:K:74:ILE:HA	22:K:101:CLA:HBB1	2.02	0.41
22:1:301:CLA:HMB1	22:1:302:CLA:HAA1	2.02	0.41
22:2:302:CLA:H61	22:2:302:CLA:H41	1.60	0.41
22:2:309:CLA:HBB1	22:2:309:CLA:HMB1	2.03	0.41
30:3:314:XAT:H15	30:3:314:XAT:H201	1.52	0.41
16:4:140:MET:O	16:4:143:ALA:N	2.54	0.41
29:4:301:CHL:HAA1	29:4:301:CHL:HBD	2.03	0.41
17:6:267:PRO:HB3	22:6:318:CLA:CBB	2.51	0.41
22:5:304:CLA:HMB2	25:5:317:8CT:C38	2.51	0.41
18:7:260:LEU:HD21	22:7:317:CLA:C3C	2.51	0.41
19:9:41:GLY:O	19:9:42:ALA:C	2.58	0.41
24:9:316:LHG:H111	24:9:316:LHG:HC82	1.66	0.41
20:0:64:ASN:N	20:0:65:PRO:HD3	2.35	0.41
20:0:189:VAL:HG22	20:0:192:LEU:HD12	2.02	0.41
22:M:101:CLA:CED	22:M:101:CLA:H2A	2.50	0.41
1:A:368:LEU:O	1:A:372:VAL:HG23	2.20	0.41
1:A:397:THR:O	1:A:401:TRP:HD1	2.04	0.41
1:A:465:ASP:OD2	1:A:647:ILE:HB	2.21	0.41
1:A:614:HIS:HD2	22:A:836:CLA:HMC2	1.86	0.41
22:A:801:CLA:H202	22:A:801:CLA:H162	1.87	0.41
22:A:802:CLA:H2	2:B:655:LEU:HD13	2.02	0.41
2:B:388:ALA:O	2:B:391:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:662:MET:HB2	22:B:806:CLA:C1C	2.50	0.41
22:B:815:CLA:H102	22:B:815:CLA:H61	1.65	0.41
12:L:40:ARG:HH22	22:L:202:CLA:C3C	2.34	0.41
13:1:31:ARG:HH22	13:1:54:GLY:HA3	1.85	0.41
13:1:102:ALA:O	13:1:106:VAL:HG23	2.20	0.41
14:2:90:ARG:HD2	29:2:307:CHL:OBD	2.20	0.41
14:2:214:SER:O	14:2:217:GLY:N	2.50	0.41
16:4:81:GLN:HE21	16:4:147:ARG:HH11	1.69	0.41
17:6:110:ALA:O	17:6:112:THR:HG23	2.21	0.41
22:6:304:CLA:H92	22:6:304:CLA:H41	2.02	0.41
13:5:106:VAL:HB	13:5:110:GLY:O	2.21	0.41
29:5:301:CHL:HBB1	29:5:301:CHL:CHC	2.45	0.41
22:5:311:CLA:CGA	22:5:311:CLA:H3A	2.51	0.41
25:5:317:8CT:C38	25:5:317:8CT:C28	2.99	0.41
31:5:319:LMG:H242	31:5:319:LMG:H272	1.68	0.41
29:9:302:CHL:C1C	24:9:316:LHG:HC81	2.51	0.41
29:0:301:CHL:HMB2	24:0:315:LHG:H322	2.03	0.41
29:0:306:CHL:HBC3	29:0:306:CHL:HMC	2.02	0.41
1:A:628:SER:OG	1:A:632:VAL:N	2.54	0.41
1:A:662:VAL:HG13	1:A:663:ILE:HG13	2.02	0.41
22:A:803:CLA:H101	10:J:16:PHE:HD1	1.85	0.41
22:A:831:CLA:HAA1	12:L:7:ILE:CD1	2.51	0.41
22:A:841:CLA:H72	22:A:841:CLA:H111	1.64	0.41
24:A:844:LHG:H281	24:A:844:LHG:H252	1.87	0.41
2:B:92:TRP:O	2:B:92:TRP:CG	2.74	0.41
2:B:234:ALA:HA	2:B:256:THR:CG2	2.50	0.41
2:B:243:ILE:HD12	2:B:264:GLN:HE21	1.84	0.41
2:B:658:ALA:O	22:B:806:CLA:HAB	2.21	0.41
22:B:823:CLA:HBA2	22:B:823:CLA:H11	1.78	0.41
22:B:826:CLA:HAA2	22:B:827:CLA:OBD	2.20	0.41
3:C:11:CYS:HB2	3:C:39:ILE:CD1	2.51	0.41
3:C:55:GLU:OE2	3:C:66:ARG:HD3	2.21	0.41
4:D:102:ILE:HG12	4:D:137:CYS:SG	2.61	0.41
6:F:202:ASP:HA	26:J:102:HTG:O2	2.21	0.41
8:H:103:ARG:HG2	8:H:107:PHE:CE2	2.56	0.41
8:H:113:ALA:O	22:H:201:CLA:H91	2.21	0.41
11:K:21:ALA:C	11:K:26:LEU:HG	2.41	0.41
13:1:84:ALA:HA	22:1:303:CLA:HBB1	2.03	0.41
29:2:305:CHL:HBC2	29:2:306:CHL:HHD	2.03	0.41
15:3:105:ILE:HD12	22:3:307:CLA:HED2	2.03	0.41
30:3:315:XAT:H11	30:3:315:XAT:H191	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3:319:CLA:H142	22:3:319:CLA:H112	1.86	0.41
16:4:147:ARG:NH2	22:4:308:CLA:O1D	2.42	0.41
16:4:179:ILE:HA	13:5:58:LEU:HD22	2.03	0.41
16:4:243:LEU:HD12	16:4:244:ALA:N	2.36	0.41
22:4:302:CLA:HMC2	30:4:316:XAT:C31	2.51	0.41
17:6:188:LYS:HD2	22:6:311:CLA:C3D	2.51	0.41
18:7:182:ALA:CB	22:7:310:CLA:HAA2	2.51	0.41
18:7:195:ILE:HD13	18:7:195:ILE:HA	1.88	0.41
18:7:235:ILE:HG13	22:7:313:CLA:C3D	2.50	0.41
22:7:304:CLA:OBD	22:7:309:CLA:HBA2	2.21	0.41
22:7:317:CLA:H12	22:7:317:CLA:O2D	2.20	0.41
16:8:166:LYS:HE2	16:8:168:PRO:CG	2.37	0.41
16:8:238:VAL:HG13	16:8:239:TRP:HD1	1.83	0.41
29:8:314:CHL:HBB1	29:8:314:CHL:CHC	2.46	0.41
30:8:317:XAT:H35	30:8:317:XAT:H401	1.70	0.41
19:9:69:ARG:NH1	22:9:301:CLA:CGD	2.83	0.41
20:0:100:TRP:CE2	20:0:101:TRP:HE3	2.39	0.41
20:0:124:PHE:CZ	22:0:305:CLA:HAC2	2.56	0.41
20:0:162:LYS:NZ	22:0:309:CLA:HBD	2.36	0.41
22:0:311:CLA:H62	22:0:311:CLA:H93	1.80	0.41
1:A:267:LYS:O	1:A:271:THR:N	2.31	0.41
1:A:460:LEU:HD22	1:A:477:PHE:CE2	2.55	0.41
1:A:462:ILE:HG23	22:A:802:CLA:H61	2.03	0.41
22:A:832:CLA:H72	22:A:832:CLA:H111	1.83	0.41
2:B:438:VAL:HG12	22:B:833:CLA:HAC1	2.03	0.41
2:B:577:TYR:OH	2:B:664:LEU:HD22	2.21	0.41
2:B:718:ILE:HD12	28:B:849:DGD:HBV2	2.02	0.41
22:B:814:CLA:H2	22:B:814:CLA:H61	1.81	0.41
22:B:824:CLA:HHB	22:B:841:CLA:O1D	2.21	0.41
22:B:830:CLA:H42	28:B:849:DGD:HB42	2.02	0.41
23:B:842:PQN:H291	28:B:849:DGD:HA81	2.01	0.41
4:D:165:TYR:HE2	4:D:169:LYS:HA	1.86	0.41
13:1:136:GLY:HA2	22:1:307:CLA:HAB	2.02	0.41
15:3:99:LEU:HD22	22:3:301:CLA:H43	2.01	0.41
16:4:146:ARG:HD3	29:4:301:CHL:OBD	2.20	0.41
16:4:203:LEU:HD21	30:4:315:XAT:H191	2.02	0.41
29:4:305:CHL:CGA	25:4:317:8CT:C22	2.99	0.41
30:4:315:XAT:H12	30:4:315:XAT:H15	1.83	0.41
29:6:308:CHL:HBB2	29:6:316:CHL:HHC	2.01	0.41
16:8:132:LEU:HD11	29:8:305:CHL:C3D	2.51	0.41
31:8:319:LMG:O6	31:8:319:LMG:O3	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:M:101:CLA:HBB1	22:M:101:CLA:HHC	2.03	0.41
1:A:231:LYS:HD3	1:A:258:LEU:HD22	2.03	0.40
1:A:461:TYR:HB3	1:A:647:ILE:HG13	2.04	0.40
1:A:484:LEU:O	1:A:535:THR:HA	2.21	0.40
1:A:491:TRP:CH2	1:A:495:ILE:HD11	2.56	0.40
1:A:514:THR:HG22	1:A:528:MET:HE2	2.03	0.40
22:A:825:CLA:H2	22:A:825:CLA:H62	1.80	0.40
22:A:827:CLA:HBB1	22:A:827:CLA:HMB1	2.03	0.40
22:A:841:CLA:HMD3	2:B:678:LEU:HD13	2.03	0.40
2:B:93:ASP:HB2	2:B:96:PHE:CD2	2.55	0.40
2:B:181:GLY:O	2:B:185:VAL:HB	2.21	0.40
2:B:262:HIS:N	2:B:267:SER:O	2.54	0.40
22:B:813:CLA:H43	22:B:813:CLA:C1C	2.51	0.40
22:B:818:CLA:HAA1	22:B:827:CLA:HBB2	2.03	0.40
4:D:70:THR:N	4:D:71:PRO:HD2	2.36	0.40
4:D:105:GLU:OE1	4:D:105:GLU:N	2.54	0.40
6:F:185:LEU:O	6:F:189:ARG:HB2	2.21	0.40
8:H:99:ARG:HB3	12:L:102:GLN:NE2	2.33	0.40
12:L:133:TRP:O	12:L:136:PHE:HB3	2.21	0.40
13:1:85:VAL:HB	13:1:86:PRO:HD3	2.03	0.40
13:1:183:MET:SD	22:1:301:CLA:HMC3	2.61	0.40
29:2:301:CHL:H111	29:2:301:CHL:H91	1.77	0.40
22:2:303:CLA:H2A	22:2:303:CLA:O1D	2.21	0.40
15:3:246:GLN:HG2	15:3:257:ASN:ND2	2.35	0.40
16:8:210:GLY:O	16:8:214:GLN:HG2	2.21	0.40
16:8:217:VAL:HG13	16:8:242:GLU:OE1	2.21	0.40
19:9:134:VAL:HG21	29:0:301:CHL:HED2	2.02	0.40
22:9:309:CLA:HBB1	22:9:309:CLA:H51	2.03	0.40
20:0:168:ARG:HH22	22:0:302:CLA:C2D	2.34	0.40
1:A:447:ASN:HD21	2:B:678:LEU:HD11	1.86	0.40
1:A:582:GLY:N	1:A:588:THR:OG1	2.54	0.40
1:A:589:CYS:O	2:B:669:GLY:N	2.54	0.40
22:A:813:CLA:H161	22:A:813:CLA:H143	1.73	0.40
2:B:67:HIS:O	2:B:71:GLN:N	2.54	0.40
2:B:123:TRP:O	2:B:127:ILE:HG12	2.22	0.40
2:B:462:TRP:NE1	22:B:850:CLA:O2A	2.54	0.40
22:B:809:CLA:H161	22:B:809:CLA:H192	1.66	0.40
7:G:27:GLN:O	7:G:31:VAL:HG23	2.20	0.40
22:G:102:CLA:H2A	22:G:102:CLA:HED3	2.03	0.40
16:4:176:PRO:HB2	16:4:180:PHE:HD2	1.83	0.40
17:6:141:ASP:HB2	17:6:148:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:5:161:ALA:HB1	13:5:163:PHE:CE1	2.56	0.40
30:7:320:XAT:H15	30:7:320:XAT:H201	1.84	0.40
20:0:128:GLU:HG2	20:0:131:ARG:HE	1.86	0.40
1:A:308:VAL:HG21	22:A:817:CLA:HAB	2.02	0.40
1:A:678:LEU:HD11	2:B:617:MET:SD	2.62	0.40
22:A:843:CLA:O1A	22:A:843:CLA:HBD	2.21	0.40
2:B:40:GLU:O	2:B:44:GLN:HG2	2.21	0.40
2:B:199:ILE:O	2:B:202:SER:HB3	2.21	0.40
2:B:373:THR:HG21	2:B:725:LEU:HD13	2.03	0.40
2:B:649:MET:O	2:B:653:GLY:N	2.52	0.40
6:F:129:PHE:N	6:F:129:PHE:CD1	2.88	0.40
12:L:94:THR:HG21	12:L:141:LEU:HD12	2.04	0.40
12:L:111:GLN:HE22	12:L:126:PRO:HA	1.85	0.40
29:1:305:CHL:HBB1	29:1:305:CHL:HHC	2.04	0.40
22:1:309:CLA:HBC3	24:1:317:LHG:C6	2.52	0.40
14:2:215:CYS:HA	14:2:218:TYR:CD2	2.56	0.40
16:4:168:PRO:HG3	16:4:179:ILE:HD11	2.04	0.40
17:6:192:LEU:O	17:6:196:ALA:N	2.53	0.40
22:6:305:CLA:NA	22:6:305:CLA:HBA2	2.34	0.40
18:7:142:ARG:HE	22:7:316:CLA:HMC1	1.86	0.40
16:8:116:GLU:HG2	16:8:116:GLU:O	2.22	0.40
22:9:309:CLA:HBB1	22:9:311:CLA:H3A	2.02	0.40
20:0:107:VAL:HG12	22:0:304:CLA:HED3	2.04	0.40
22:0:312:CLA:HBB1	22:0:312:CLA:HHC	2.03	0.40
1:A:25:ASN:N	1:A:188:LYS:O	2.55	0.40
1:A:288:ASN:OD1	1:A:290:ILE:HG22	2.22	0.40
1:A:319:THR:OG1	1:A:320:ASN:N	2.52	0.40
1:A:612:ILE:HG21	1:A:748:PHE:HE2	1.86	0.40
25:A:849:8CT:C11	25:A:849:8CT:C09	2.97	0.40
6:F:83:PRO:HD2	6:F:86:GLU:OE2	2.21	0.40
6:F:204:PRO:O	6:F:208:LYS:HG2	2.21	0.40
13:1:34:ASN:OD1	13:1:35:TRP:N	2.54	0.40
14:2:92:ALA:O	14:2:95:GLY:N	2.54	0.40
14:2:209:ARG:NH2	22:2:302:CLA:ND	2.69	0.40
15:3:175:LEU:HG	22:3:307:CLA:HMA2	2.03	0.40
29:4:305:CHL:HHC	29:4:306:CHL:CMC	2.52	0.40
22:4:314:CLA:H162	22:4:314:CLA:H192	1.79	0.40
22:7:317:CLA:HBD	22:7:317:CLA:HED2	1.76	0.40
30:8:316:XAT:H391	30:8:316:XAT:H31	1.71	0.40
20:0:188:PRO:O	20:0:192:LEU:HG	2.21	0.40
22:0:302:CLA:HMC2	30:0:314:XAT:C31	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:M:101:CLA:HHC	22:M:101:CLA:CBB	2.52	0.40
1:A:51:THR:HG22	1:A:721:ARG:H	1.85	0.40
22:A:821:CLA:HBC3	22:A:827:CLA:H203	2.03	0.40
22:A:837:CLA:H51	22:A:837:CLA:H11	1.87	0.40
2:B:426:SER:HB2	2:B:529:THR:HG23	2.04	0.40
22:B:812:CLA:H101	22:B:840:CLA:O1A	2.22	0.40
22:B:816:CLA:H13	22:B:816:CLA:H102	1.64	0.40
15:3:164:VAL:HG11	22:3:313:CLA:HMB3	2.03	0.40
22:5:309:CLA:CGA	30:5:315:XAT:H3	2.51	0.40
18:7:125:LEU:HA	18:7:128:ILE:HB	2.04	0.40
16:8:132:LEU:HD21	29:8:305:CHL:C1D	2.52	0.40
22:8:315:CLA:H162	22:8:315:CLA:H121	1.27	0.40
19:9:86:ASN:OD1	30:9:314:XAT:H202	2.22	0.40
22:9:304:CLA:HMC2	30:9:315:XAT:C12	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	738/751 (98%)	680 (92%)	54 (7%)	4 (0%)	25 59
2	B	731/734 (100%)	677 (93%)	53 (7%)	1 (0%)	48 79
3	C	78/81 (96%)	71 (91%)	7 (9%)	0	100 100
4	D	140/198 (71%)	129 (92%)	9 (6%)	2 (1%)	9 40
5	E	59/91 (65%)	55 (93%)	4 (7%)	0	100 100
6	F	161/236 (68%)	153 (95%)	8 (5%)	0	100 100
7	G	90/167 (54%)	85 (94%)	5 (6%)	0	100 100
8	H	86/133 (65%)	74 (86%)	9 (10%)	3 (4%)	3 24
9	I	30/36 (83%)	27 (90%)	3 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
11	K	78/123 (63%)	69 (88%)	7 (9%)	2 (3%)	4	28
12	L	153/204 (75%)	139 (91%)	13 (8%)	1 (1%)	19	53
13	1	191/226 (84%)	175 (92%)	15 (8%)	1 (0%)	25	59
13	5	193/226 (85%)	173 (90%)	19 (10%)	1 (0%)	25	59
14	2	210/256 (82%)	190 (90%)	20 (10%)	0	100	100
15	3	224/281 (80%)	197 (88%)	26 (12%)	1 (0%)	30	64
16	4	205/248 (83%)	176 (86%)	29 (14%)	0	100	100
16	8	203/248 (82%)	173 (85%)	27 (13%)	3 (2%)	8	39
17	6	227/267 (85%)	200 (88%)	26 (12%)	1 (0%)	30	64
18	7	226/264 (86%)	190 (84%)	31 (14%)	5 (2%)	5	31
19	9	181/222 (82%)	156 (86%)	24 (13%)	1 (1%)	22	56
20	0	200/245 (82%)	175 (88%)	25 (12%)	0	100	100
21	M	29/32 (91%)	29 (100%)	0	0	100	100
All	All	4472/5310 (84%)	4029 (90%)	417 (9%)	26 (1%)	24	56

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	8	157	VAL
4	D	168	PRO
11	K	44	PRO
18	7	110	ALA
18	7	158	VAL
15	3	277	VAL
18	7	172	PRO
16	8	159	VAL
1	A	579	PRO
2	B	35	ASP
4	D	167	HIS
8	H	99	ARG
8	H	134	GLN
12	L	116	THR
13	1	160	PRO
18	7	120	VAL
19	9	45	PRO
16	8	176	PRO

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Mol	Chain	Res	Type
8	H	131	VAL
13	5	112	PRO
18	7	105	VAL
1	A	381	PRO
11	K	3	ILE
1	A	21	ILE
1	A	127	VAL
17	6	233	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	603/614 (98%)	602 (100%)	1 (0%)	92 97
2	B	600/601 (100%)	599 (100%)	1 (0%)	92 97
3	C	68/69 (99%)	68 (100%)	0	100 100
4	D	119/162 (74%)	119 (100%)	0	100 100
5	E	53/77 (69%)	53 (100%)	0	100 100
6	F	129/180 (72%)	129 (100%)	0	100 100
7	G	78/145 (54%)	78 (100%)	0	100 100
8	H	67/103 (65%)	66 (98%)	1 (2%)	60 77
9	I	25/28 (89%)	25 (100%)	0	100 100
10	J	38/38 (100%)	38 (100%)	0	100 100
11	K	58/94 (62%)	58 (100%)	0	100 100
12	L	118/157 (75%)	116 (98%)	2 (2%)	56 75
13	1	147/175 (84%)	147 (100%)	0	100 100
13	5	149/175 (85%)	149 (100%)	0	100 100
14	2	164/197 (83%)	164 (100%)	0	100 100
15	3	184/225 (82%)	182 (99%)	2 (1%)	70 83
16	4	161/189 (85%)	161 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	8	159/189 (84%)	159 (100%)	0	100 100
17	6	188/216 (87%)	188 (100%)	0	100 100
18	7	181/209 (87%)	181 (100%)	0	100 100
19	9	144/173 (83%)	144 (100%)	0	100 100
20	0	160/194 (82%)	160 (100%)	0	100 100
21	M	26/27 (96%)	26 (100%)	0	100 100
All	All	3619/4237 (85%)	3612 (100%)	7 (0%)	91 97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
2	B	625	TRP
8	H	124	ASP
12	L	70	LEU
12	L	71	ARG
15	3	193	GLU
15	3	195	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	82	HIS
1	A	85	GLN
1	A	197	GLN
1	A	198	ASN
1	A	205	HIS
1	A	206	HIS
1	A	222	GLN
1	A	230	ASN
1	A	246	HIS
1	A	301	HIS
1	A	303	HIS
1	A	315	HIS
1	A	334	HIS
1	A	375	HIS
1	A	398	HIS
1	A	399	HIS

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Mol	Chain	Res	Type
1	A	445	HIS
1	A	456	HIS
1	A	485	GLN
1	A	541	HIS
1	A	544	HIS
1	A	549	HIS
1	A	596	HIS
1	A	606	ASN
1	A	614	HIS
1	A	620	GLN
1	A	634	HIS
1	A	658	GLN
1	A	709	HIS
1	A	727	GLN
1	A	735	HIS
2	B	44	GLN
2	B	50	HIS
2	B	53	GLN
2	B	95	HIS
2	B	133	GLN
2	B	162	GLN
2	B	177	HIS
2	B	236	ASN
2	B	242	HIS
2	B	264	GLN
2	B	277	HIS
2	B	289	HIS
2	B	294	ASN
2	B	308	HIS
2	B	319	HIS
2	B	321	ASN
2	B	421	HIS
2	B	432	HIS
2	B	528	HIS
2	B	585	ASN
2	B	595	HIS
2	B	598	HIS
2	B	712	HIS
3	C	4	ASN
3	C	38	GLN
4	D	143	GLN
6	F	235	ASN

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Mol	Chain	Res	Type
10	J	2	GLN
11	K	8	ASN
11	K	31	ASN
12	L	5	GLN
12	L	8	GLN
12	L	11	ASN
12	L	128	GLN
13	1	98	ASN
13	1	167	ASN
13	1	192	GLN
13	1	215	ASN
14	2	88	HIS
14	2	114	GLN
14	2	176	ASN
15	3	168	GLN
15	3	257	ASN
15	3	268	ASN
16	4	105	ASN
16	4	119	ASN
16	4	214	GLN
17	6	83	GLN
17	6	119	ASN
17	6	203	GLN
17	6	218	HIS
13	5	192	GLN
18	7	84	HIS
18	7	115	ASN
18	7	211	GLN
18	7	213	GLN
16	8	81	GLN
16	8	158	ASN
16	8	237	ASN
19	9	100	GLN
19	9	102	ASN
19	9	171	ASN
19	9	185	GLN
19	9	207	GLN
20	0	45	HIS
20	0	201	HIS
20	0	202	ASN
20	0	203	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

320 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	6	304	17	65,73,73	1.49	10 (15%)	76,113,113	1.41	8 (10%)
22	CLA	A	818	-	65,73,73	1.46	10 (15%)	76,113,113	1.50	8 (10%)
25	8CT	5	317	22	40,41,41	4.75	23 (57%)	50,56,56	3.48	21 (42%)
22	CLA	9	312	30	59,67,73	1.57	9 (15%)	68,105,113	1.40	8 (11%)
22	CLA	5	308	-	42,50,73	1.85	7 (16%)	48,85,113	1.78	8 (16%)
22	CLA	B	817	-	55,63,73	1.53	9 (16%)	64,101,113	1.49	8 (12%)
22	CLA	A	804	22	55,63,73	1.55	10 (18%)	64,101,113	1.62	9 (14%)
22	CLA	1	310	-	52,60,73	1.61	9 (17%)	60,97,113	1.48	7 (11%)
22	CLA	9	308	-	65,73,73	1.45	10 (15%)	76,113,113	1.42	7 (9%)
27	SF4	B	802	-	0,12,12	-	-	-		
22	CLA	A	828	-	65,73,73	1.42	9 (13%)	76,113,113	1.51	8 (10%)
22	CLA	7	302	18	46,54,73	1.69	10 (21%)	53,90,113	1.57	7 (13%)
22	CLA	4	303	-	46,54,73	1.70	9 (19%)	53,90,113	1.60	7 (13%)
22	CLA	A	825	-	65,73,73	1.46	8 (12%)	76,113,113	1.41	9 (11%)
27	SF4	C	102	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	3	312	-	45,53,73	1.69	7 (15%)	52,89,113	1.68	9 (17%)
22	CLA	7	314	-	45,53,73	1.71	10 (22%)	52,89,113	1.64	7 (13%)
22	CLA	1	301	13	65,73,73	1.49	10 (15%)	76,113,113	1.48	8 (10%)
25	8CT	B	851	22	40,41,41	4.75	25 (62%)	50,56,56	2.52	19 (38%)
22	CLA	5	310	24	41,49,73	1.76	10 (24%)	47,84,113	1.69	7 (14%)
22	CLA	0	302	30	65,73,73	1.49	8 (12%)	76,113,113	1.36	9 (11%)
29	CHL	9	302	19	61,69,74	1.94	14 (22%)	67,108,114	2.61	22 (32%)
22	CLA	7	305	-	45,53,73	1.73	10 (22%)	52,89,113	1.52	7 (13%)
22	CLA	8	303	22,31	46,54,73	1.68	10 (21%)	53,90,113	1.57	7 (13%)
22	CLA	4	309	30	60,68,73	1.46	10 (16%)	70,107,113	1.43	9 (12%)
22	CLA	9	303	19	65,73,73	1.43	10 (15%)	76,113,113	1.49	8 (10%)
22	CLA	B	850	-	55,63,73	1.57	8 (14%)	64,101,113	1.65	13 (20%)
22	CLA	2	314	14	49,57,73	1.67	10 (20%)	55,93,113	1.50	8 (14%)
22	CLA	0	307	22	65,73,73	1.49	7 (10%)	76,113,113	1.45	10 (13%)
24	LHG	3	317	22	19,19,48	0.86	0	21,24,54	1.41	2 (9%)
22	CLA	0	310	30	52,60,73	1.60	9 (17%)	60,97,113	1.55	7 (11%)
22	CLA	7	306	22	42,50,73	1.78	8 (19%)	48,85,113	1.60	7 (14%)
22	CLA	7	307	22	47,55,73	1.69	7 (14%)	54,91,113	1.58	7 (12%)
29	CHL	5	306	-	48,56,74	2.30	16 (33%)	51,92,114	2.72	20 (39%)
22	CLA	A	826	25	65,73,73	1.46	10 (15%)	76,113,113	1.36	5 (6%)
22	CLA	5	302	-	65,73,73	1.44	10 (15%)	76,113,113	1.36	9 (11%)
25	8CT	A	854	-	40,41,41	4.68	24 (60%)	50,56,56	2.70	18 (36%)
22	CLA	5	309	13,30	60,68,73	1.53	9 (15%)	70,107,113	1.42	8 (11%)
29	CHL	8	314	-	43,51,74	2.34	15 (34%)	45,86,114	3.01	22 (48%)
22	CLA	A	821	-	65,73,73	1.42	8 (12%)	76,113,113	1.50	9 (11%)
29	CHL	0	306	30,22	48,56,74	2.33	16 (33%)	51,92,114	2.69	19 (37%)
22	CLA	2	310	24	41,49,73	1.81	10 (24%)	47,84,113	1.66	8 (17%)
22	CLA	A	815	-	47,55,73	1.70	8 (17%)	54,91,113	1.61	8 (14%)
22	CLA	B	811	-	65,73,73	1.46	10 (15%)	76,113,113	1.46	9 (11%)
22	CLA	7	313	-	55,63,73	1.55	10 (18%)	64,101,113	1.62	9 (14%)
22	CLA	B	813	-	55,63,73	1.58	9 (16%)	64,101,113	1.45	6 (9%)
22	CLA	B	836	-	60,68,73	1.49	10 (16%)	70,107,113	1.50	8 (11%)
22	CLA	2	308	-	50,58,73	1.62	10 (20%)	58,95,113	1.48	7 (12%)
30	XAT	6	319	22	39,47,47	0.96	2 (5%)	54,74,74	3.23	24 (44%)
22	CLA	5	313	-	55,63,73	1.60	8 (14%)	64,101,113	1.40	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	8CT	B	844	-	40,41,41	4.69	24 (60%)	50,56,56	2.90	16 (32%)
30	XAT	8	316	29	39,47,47	0.92	1 (2%)	54,74,74	3.74	29 (53%)
22	CLA	7	315	-	46,54,73	1.67	8 (17%)	53,90,113	1.59	7 (13%)
22	CLA	6	323	16	46,54,73	1.68	10 (21%)	53,90,113	1.51	6 (11%)
22	CLA	B	829	-	65,73,73	1.43	10 (15%)	76,113,113	1.52	11 (14%)
22	CLA	A	803	-	65,73,73	1.43	10 (15%)	76,113,113	1.48	10 (13%)
22	CLA	B	821	-	50,58,73	1.66	9 (18%)	58,95,113	1.54	8 (13%)
29	CHL	8	305	-	56,64,74	2.04	14 (25%)	61,102,114	2.70	23 (37%)
24	LHG	2	318	22	31,31,48	0.81	1 (3%)	34,37,54	1.30	3 (8%)
22	CLA	B	805	-	65,73,73	1.44	10 (15%)	76,113,113	1.33	7 (9%)
29	CHL	2	307	-	51,59,74	2.00	13 (25%)	55,96,114	2.87	22 (40%)
22	CLA	A	819	-	65,73,73	1.43	9 (13%)	76,113,113	1.53	8 (10%)
22	CLA	A	810	-	65,73,73	1.47	10 (15%)	76,113,113	1.35	6 (7%)
22	CLA	B	835	-	45,53,73	1.69	8 (17%)	52,89,113	1.62	7 (13%)
25	8CT	8	301	-	40,41,41	4.70	24 (60%)	50,56,56	2.66	18 (36%)
22	CLA	3	319	-	65,73,73	1.50	9 (13%)	76,113,113	1.41	9 (11%)
22	CLA	6	315	-	65,73,73	1.47	9 (13%)	76,113,113	1.32	7 (9%)
22	CLA	A	812	-	54,62,73	1.63	10 (18%)	62,99,113	1.56	8 (12%)
29	CHL	6	306	-	43,51,74	2.17	13 (30%)	45,86,114	2.90	19 (42%)
22	CLA	B	818	-	59,67,73	1.55	11 (18%)	68,105,113	1.68	10 (14%)
31	LMG	8	319	22	44,44,55	0.85	4 (9%)	52,52,63	1.40	5 (9%)
22	CLA	A	806	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	9 (11%)
22	CLA	1	307	-	65,73,73	1.44	9 (13%)	76,113,113	1.40	9 (11%)
22	CLA	B	838	-	47,55,73	1.70	9 (19%)	54,91,113	1.60	6 (11%)
22	CLA	A	824	-	55,63,73	1.55	10 (18%)	64,101,113	1.47	8 (12%)
22	CLA	A	811	22	65,73,73	1.50	10 (15%)	76,113,113	1.38	6 (7%)
29	CHL	4	305	29	56,64,74	2.09	16 (28%)	61,102,114	2.53	21 (34%)
22	CLA	2	302	29	65,73,73	1.41	9 (13%)	76,113,113	1.51	11 (14%)
22	CLA	B	812	2	65,73,73	1.48	10 (15%)	76,113,113	1.41	7 (9%)
22	CLA	M	101	-	46,54,73	1.77	10 (21%)	53,90,113	1.44	7 (13%)
30	XAT	8	317	-	39,47,47	0.97	2 (5%)	54,74,74	2.90	21 (38%)
22	CLA	3	305	15	47,55,73	1.68	10 (21%)	54,91,113	1.49	7 (12%)
25	8CT	J	101	-	40,41,41	4.67	24 (60%)	50,56,56	2.99	18 (36%)
22	CLA	B	819	-	60,68,73	1.49	8 (13%)	70,107,113	1.48	9 (12%)
22	CLA	5	312	30	65,73,73	1.45	7 (10%)	76,113,113	1.46	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	L	201	-	65,73,73	1.43	10 (15%)	76,113,113	1.35	6 (7%)
22	CLA	7	311	24	38,45,73	1.80	8 (21%)	43,78,113	1.61	7 (16%)
22	CLA	A	805	-	65,73,73	1.45	11 (16%)	76,113,113	1.42	9 (11%)
22	CLA	7	309	22	50,58,73	1.65	10 (20%)	58,95,113	1.43	7 (12%)
22	CLA	B	810	-	65,73,73	1.44	10 (15%)	76,113,113	1.45	9 (11%)
22	CLA	4	304	-	50,58,73	1.61	9 (18%)	58,95,113	1.67	9 (15%)
22	CLA	6	314	-	43,51,73	1.72	9 (20%)	49,86,113	1.60	6 (12%)
22	CLA	B	832	-	65,73,73	1.43	10 (15%)	76,113,113	1.49	9 (11%)
22	CLA	A	809	1	65,73,73	1.44	10 (15%)	76,113,113	1.40	10 (13%)
22	CLA	2	303	-	65,73,73	1.46	9 (13%)	76,113,113	1.33	5 (6%)
22	CLA	K	105	-	50,58,73	1.67	9 (18%)	58,95,113	1.64	7 (12%)
22	CLA	A	823	-	51,59,73	1.64	10 (19%)	59,96,113	1.57	8 (13%)
22	CLA	0	304	22	52,60,73	1.66	7 (13%)	60,97,113	1.54	7 (11%)
22	CLA	4	313	-	45,53,73	1.74	10 (22%)	52,89,113	1.68	7 (13%)
29	CHL	4	306	29	51,59,74	2.23	16 (31%)	55,96,114	2.74	21 (38%)
22	CLA	A	834	-	50,58,73	1.70	10 (20%)	58,95,113	1.53	7 (12%)
22	CLA	7	303	18	60,68,73	1.53	10 (16%)	70,107,113	1.51	8 (11%)
22	CLA	3	302	25	50,58,73	1.68	9 (18%)	58,95,113	1.48	6 (10%)
22	CLA	B	827	-	65,73,73	1.42	8 (12%)	76,113,113	1.48	8 (10%)
23	PQN	B	842	-	34,34,34	1.47	2 (5%)	42,45,45	1.10	2 (4%)
22	CLA	A	817	-	65,73,73	1.41	8 (12%)	76,113,113	1.48	8 (10%)
22	CLA	B	830	-	65,73,73	1.42	11 (16%)	76,113,113	1.56	8 (10%)
22	CLA	A	814	-	45,53,73	1.75	10 (22%)	52,89,113	1.54	7 (13%)
22	CLA	B	820	-	65,73,73	1.46	10 (15%)	76,113,113	1.39	7 (9%)
27	SF4	C	101	-	0,12,12	-	-	-		
29	CHL	6	308	-	51,59,74	2.11	14 (27%)	55,96,114	2.73	25 (45%)
30	XAT	3	314	25	39,47,47	0.98	3 (7%)	54,74,74	4.62	28 (51%)
22	CLA	2	311	14	52,60,73	1.62	10 (19%)	60,97,113	1.61	7 (11%)
22	CLA	3	304	-	42,50,73	1.77	10 (23%)	48,85,113	1.56	7 (14%)
22	CLA	5	304	-	52,60,73	1.62	8 (15%)	60,97,113	1.54	7 (11%)
25	8CT	B	847	-	40,41,41	4.69	24 (60%)	50,56,56	2.73	18 (36%)
29	CHL	9	307	-	48,56,74	2.27	15 (31%)	51,92,114	2.77	21 (41%)
30	XAT	1	315	-	39,47,47	0.97	2 (5%)	54,74,74	3.10	21 (38%)
30	XAT	0	314	29,22	39,47,47	0.88	0	54,74,74	3.06	22 (40%)
22	CLA	8	309	-	60,68,73	1.48	10 (16%)	70,107,113	1.54	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	839	25	65,73,73	1.46	8 (12%)	76,113,113	1.37	7 (9%)
31	LMG	5	319	22	44,44,55	0.97	3 (6%)	52,52,63	1.33	6 (11%)
22	CLA	6	309	17	50,58,73	1.64	8 (16%)	58,95,113	1.56	7 (12%)
24	LHG	9	316	22	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
22	CLA	6	311	24	65,73,73	1.42	10 (15%)	76,113,113	1.41	7 (9%)
22	CLA	0	309	24	41,49,73	1.81	7 (17%)	47,84,113	1.59	8 (17%)
25	8CT	2	317	-	40,41,41	4.70	24 (60%)	50,56,56	2.98	19 (38%)
22	CLA	A	841	25	65,73,73	1.46	11 (16%)	76,113,113	1.40	7 (9%)
22	CLA	1	311	-	65,73,73	1.44	10 (15%)	76,113,113	1.44	9 (11%)
22	CLA	6	305	-	60,68,73	1.55	8 (13%)	70,107,113	1.36	6 (8%)
22	CLA	L	202	-	65,73,73	1.43	8 (12%)	76,113,113	1.52	9 (11%)
29	CHL	4	301	13,22	61,69,74	1.90	12 (19%)	67,108,114	2.60	24 (35%)
22	CLA	3	307	15	50,58,73	1.75	10 (20%)	58,95,113	1.55	7 (12%)
22	CLA	6	317	-	45,53,73	1.72	10 (22%)	52,89,113	1.62	8 (15%)
22	CLA	5	311	30	45,53,73	1.73	7 (15%)	52,89,113	1.66	7 (13%)
22	CLA	3	310	-	52,60,73	1.63	9 (17%)	60,97,113	1.50	7 (11%)
22	CLA	6	301	-	52,60,73	1.64	7 (13%)	60,97,113	1.49	8 (13%)
22	CLA	L	204	-	50,58,73	1.65	8 (16%)	58,95,113	1.52	8 (13%)
22	CLA	L	203	-	65,73,73	1.44	6 (9%)	76,113,113	1.37	7 (9%)
25	8CT	6	321	-	40,41,41	4.67	24 (60%)	50,56,56	3.26	18 (36%)
25	8CT	7	321	-	40,41,41	4.66	24 (60%)	50,56,56	3.72	22 (44%)
30	XAT	4	315	22	39,47,47	0.95	1 (2%)	54,74,74	3.14	26 (48%)
31	LMG	4	318	-	44,44,55	0.98	4 (9%)	52,52,63	1.49	9 (17%)
25	8CT	3	318	25,22	40,41,41	4.68	25 (62%)	50,56,56	3.66	22 (44%)
30	XAT	2	316	-	39,47,47	1.01	2 (5%)	54,74,74	3.14	23 (42%)
22	CLA	A	820	-	45,53,73	1.68	8 (17%)	52,89,113	1.71	7 (13%)
25	8CT	B	848	-	40,41,41	4.70	24 (60%)	50,56,56	2.60	16 (32%)
22	CLA	4	302	-	60,68,73	1.50	10 (16%)	70,107,113	1.47	8 (11%)
22	CLA	7	317	-	65,73,73	1.45	8 (12%)	76,113,113	1.36	7 (9%)
24	LHG	B	852	22	22,22,48	0.84	0	25,28,54	1.21	1 (4%)
22	CLA	6	318	17	52,60,73	1.64	10 (19%)	60,97,113	1.62	9 (15%)
22	CLA	B	807	-	45,53,73	1.70	10 (22%)	52,89,113	1.84	9 (17%)
22	CLA	7	312	30	52,60,73	1.67	9 (17%)	60,97,113	1.43	6 (10%)
25	8CT	B	804	-	40,41,41	4.55	23 (57%)	50,56,56	2.90	20 (40%)
29	CHL	1	305	-	48,56,74	2.28	15 (31%)	51,92,114	2.76	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	8CT	I	101	-	40,41,41	4.54	23 (57%)	50,56,56	3.13	19 (38%)
24	LHG	0	315	29,22	48,48,48	0.58	0	51,54,54	1.24	5 (9%)
22	CLA	7	316	18	65,73,73	1.48	9 (13%)	76,113,113	1.39	6 (7%)
29	CHL	3	306	25	47,55,74	2.08	14 (29%)	50,91,114	2.92	22 (44%)
22	CLA	A	840	-	65,73,73	1.44	10 (15%)	76,113,113	1.44	9 (11%)
22	CLA	3	309	24	38,45,73	1.79	8 (21%)	43,78,113	1.78	7 (16%)
22	CLA	8	308	16	50,58,73	1.66	11 (22%)	58,95,113	1.73	11 (18%)
22	CLA	A	813	-	65,73,73	1.42	9 (13%)	76,113,113	1.58	10 (13%)
22	CLA	B	815	-	65,73,73	1.41	10 (15%)	76,113,113	1.53	9 (11%)
22	CLA	1	304	-	52,60,73	1.59	9 (17%)	60,97,113	1.50	8 (13%)
26	HTG	A	851	-	19,19,19	1.11	2 (10%)	23,24,24	0.73	0
22	CLA	A	802	-	65,73,73	1.43	10 (15%)	76,113,113	1.47	7 (9%)
22	CLA	9	305	-	52,60,73	1.64	9 (17%)	60,97,113	1.64	10 (16%)
25	8CT	L	205	22	40,41,41	4.65	24 (60%)	50,56,56	3.13	21 (42%)
22	CLA	A	807	-	65,73,73	1.44	10 (15%)	76,113,113	1.47	9 (11%)
22	CLA	B	831	-	50,58,73	1.67	10 (20%)	58,95,113	1.63	8 (13%)
22	CLA	B	801	-	65,73,73	1.43	11 (16%)	76,113,113	1.49	8 (10%)
24	LHG	5	318	22	48,48,48	0.65	1 (2%)	51,54,54	1.28	6 (11%)
25	8CT	8	318	-	40,41,41	4.69	24 (60%)	50,56,56	2.68	18 (36%)
22	CLA	K	102	-	46,54,73	1.65	8 (17%)	53,90,113	1.68	8 (15%)
22	CLA	A	822	-	49,57,73	1.64	9 (18%)	55,93,113	1.66	10 (18%)
22	CLA	G	101	-	45,53,73	1.79	5 (11%)	52,89,113	1.61	8 (15%)
22	CLA	A	831	-	50,58,73	1.63	10 (20%)	58,95,113	1.64	8 (13%)
22	CLA	7	318	22	65,73,73	1.46	10 (15%)	76,113,113	1.47	9 (11%)
29	CHL	2	305	-	43,51,74	2.14	14 (32%)	45,86,114	2.99	19 (42%)
25	8CT	L	206	-	40,41,41	4.67	24 (60%)	50,56,56	3.02	19 (38%)
22	CLA	8	310	31	55,63,73	1.58	9 (16%)	64,101,113	1.55	6 (9%)
29	CHL	4	307	-	51,59,74	2.04	14 (27%)	55,96,114	2.88	22 (40%)
22	CLA	8	315	-	65,73,73	1.45	7 (10%)	76,113,113	1.34	6 (7%)
22	CLA	1	303	-	52,60,73	1.60	9 (17%)	60,97,113	1.52	9 (15%)
22	CLA	9	310	24	41,49,73	1.79	8 (19%)	47,84,113	1.55	7 (14%)
25	8CT	7	301	29,30	40,41,41	4.63	23 (57%)	50,56,56	2.71	19 (38%)
22	CLA	A	832	-	65,73,73	1.43	10 (15%)	76,113,113	1.42	6 (7%)
22	CLA	B	837	-	65,73,73	1.43	9 (13%)	76,113,113	1.47	9 (11%)
24	LHG	7	322	22	19,19,48	0.93	0	21,24,54	1.36	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	4	308	16	50,58,73	1.60	10 (20%)	58,95,113	1.67	8 (13%)
30	XAT	5	315	22	39,47,47	0.94	1 (2%)	54,74,74	4.68	23 (42%)
22	CLA	B	833	-	58,66,73	1.54	10 (17%)	67,104,113	1.58	9 (13%)
22	CLA	J	103	10	42,50,73	1.78	8 (19%)	48,85,113	1.68	6 (12%)
30	XAT	3	315	-	39,47,47	0.98	2 (5%)	54,74,74	2.75	20 (37%)
29	CHL	8	306	-	51,59,74	2.16	14 (27%)	55,96,114	2.81	23 (41%)
22	CLA	G	102	-	50,58,73	1.65	7 (14%)	58,95,113	1.59	8 (13%)
22	CLA	2	313	-	43,51,73	1.76	10 (23%)	49,86,113	1.59	6 (12%)
22	CLA	H	201	-	65,73,73	1.42	7 (10%)	76,113,113	1.46	9 (11%)
29	CHL	2	306	-	48,56,74	2.23	15 (31%)	51,92,114	2.75	20 (39%)
22	CLA	1	309	24	41,49,73	1.79	10 (24%)	47,84,113	1.72	9 (19%)
22	CLA	0	303	30	65,73,73	1.47	8 (12%)	76,113,113	1.34	7 (9%)
22	CLA	A	836	-	51,59,73	1.62	10 (19%)	59,96,113	1.58	10 (16%)
25	8CT	A	849	22	40,41,41	4.70	24 (60%)	50,56,56	2.63	18 (36%)
22	CLA	B	808	-	65,73,73	1.44	10 (15%)	76,113,113	1.44	9 (11%)
22	CLA	B	841	24	65,73,73	1.43	10 (15%)	76,113,113	1.50	10 (13%)
24	LHG	6	322	22	36,36,48	0.78	1 (2%)	39,42,54	1.26	4 (10%)
29	CHL	7	308	-	47,55,74	2.15	14 (29%)	50,91,114	2.92	19 (38%)
22	CLA	2	319	16	46,54,73	1.70	10 (21%)	53,90,113	1.50	6 (11%)
22	CLA	B	825	-	65,73,73	1.45	10 (15%)	76,113,113	1.45	8 (10%)
22	CLA	8	304	-	50,58,73	1.65	10 (20%)	58,95,113	1.52	6 (10%)
22	CLA	B	816	-	60,68,73	1.51	10 (16%)	70,107,113	1.56	8 (11%)
22	CLA	B	824	-	60,68,73	1.53	9 (15%)	70,107,113	1.45	9 (12%)
30	XAT	9	314	22	39,47,47	0.95	1 (2%)	54,74,74	4.46	27 (50%)
22	CLA	A	843	24	52,60,73	1.62	8 (15%)	60,97,113	1.60	9 (15%)
22	CLA	8	302	-	60,68,73	1.51	10 (16%)	70,107,113	1.41	7 (10%)
22	CLA	8	313	-	45,53,73	1.76	9 (20%)	52,89,113	1.64	8 (15%)
30	XAT	1	314	22	39,47,47	0.91	1 (2%)	54,74,74	4.66	26 (48%)
22	CLA	A	837	-	65,73,73	1.43	8 (12%)	76,113,113	1.45	8 (10%)
22	CLA	A	835	1	45,53,73	1.75	10 (22%)	52,89,113	1.72	7 (13%)
22	CLA	9	313	-	55,63,73	1.56	8 (14%)	64,101,113	1.44	7 (10%)
22	CLA	0	312	29	55,63,73	1.66	7 (12%)	64,101,113	1.53	9 (14%)
22	CLA	B	834	2	65,73,73	1.52	10 (15%)	76,113,113	1.35	8 (10%)
22	CLA	6	303	17	65,73,73	1.44	10 (15%)	76,113,113	1.47	8 (10%)
22	CLA	A	839	-	65,73,73	1.44	10 (15%)	76,113,113	1.47	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CHL	6	302	17,22	61,69,74	1.99	15 (24%)	67,108,114	2.44	24 (35%)
22	CLA	A	830	-	65,73,73	1.49	10 (15%)	76,113,113	1.52	7 (9%)
22	CLA	9	301	-	46,54,73	1.79	9 (19%)	57,90,113	1.64	9 (15%)
22	CLA	3	311	-	55,63,73	1.55	10 (18%)	64,101,113	1.58	8 (12%)
24	LHG	A	844	-	48,48,48	0.73	1 (2%)	51,54,54	1.32	6 (11%)
22	CLA	A	852	-	49,57,73	1.69	9 (18%)	55,93,113	1.56	6 (10%)
22	CLA	4	314	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	8 (10%)
29	CHL	2	301	22	61,69,74	1.89	14 (22%)	67,108,114	2.74	22 (32%)
30	XAT	9	315	-	39,47,47	0.93	2 (5%)	54,74,74	2.88	20 (37%)
30	XAT	4	316	-	39,47,47	1.04	3 (7%)	54,74,74	2.76	21 (38%)
30	XAT	6	320	-	39,47,47	0.96	2 (5%)	54,74,74	4.47	21 (38%)
22	CLA	B	828	-	65,73,73	1.43	8 (12%)	76,113,113	1.55	9 (11%)
25	8CT	A	850	-	40,41,41	4.67	24 (60%)	50,56,56	2.90	18 (36%)
25	8CT	7	323	-	40,41,41	4.70	24 (60%)	50,56,56	2.73	18 (36%)
25	8CT	K	103	-	40,41,41	4.87	24 (60%)	50,56,56	2.64	18 (36%)
22	CLA	5	314	24	46,54,73	1.73	9 (19%)	53,90,113	1.52	6 (11%)
22	CLA	B	803	-	65,73,73	1.43	10 (15%)	76,113,113	1.44	10 (13%)
22	CLA	2	309	-	60,68,73	1.50	11 (18%)	70,107,113	1.45	7 (10%)
22	CLA	B	809	-	65,73,73	1.47	10 (15%)	76,113,113	1.39	8 (10%)
25	8CT	B	843	-	40,41,41	4.73	25 (62%)	50,56,56	2.87	20 (40%)
28	DGD	B	849	-	67,67,67	1.01	5 (7%)	81,81,81	1.51	13 (16%)
22	CLA	A	853	-	65,73,73	1.46	10 (15%)	76,113,113	1.31	9 (11%)
22	CLA	2	304	-	60,68,73	1.49	9 (15%)	70,107,113	1.48	8 (11%)
25	8CT	3	316	-	40,41,41	4.68	24 (60%)	50,56,56	2.87	20 (40%)
25	8CT	B	846	-	40,41,41	4.71	24 (60%)	50,56,56	2.91	17 (34%)
22	CLA	6	312	-	52,60,73	1.61	9 (17%)	60,97,113	1.51	7 (11%)
22	CLA	B	823	-	55,63,73	1.58	10 (18%)	64,101,113	1.53	8 (12%)
22	CLA	B	814	-	65,73,73	1.46	10 (15%)	76,113,113	1.51	9 (11%)
22	CLA	3	301	-	60,68,73	1.49	10 (16%)	70,107,113	1.51	7 (10%)
22	CLA	A	829	-	65,73,73	1.46	10 (15%)	76,113,113	1.45	8 (10%)
24	LHG	A	845	22	26,26,48	0.95	1 (3%)	29,32,54	1.38	3 (10%)
30	XAT	2	315	-	39,47,47	1.14	2 (5%)	54,74,74	5.94	29 (53%)
30	XAT	0	313	22	39,47,47	1.11	2 (5%)	54,74,74	5.03	22 (40%)
22	CLA	0	308	20	60,68,73	1.50	7 (11%)	70,107,113	1.41	6 (8%)
25	8CT	A	848	-	40,41,41	4.64	23 (57%)	50,56,56	2.72	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	HTG	J	102	-	19,19,19	1.12	2 (10%)	23,24,24	0.77	0
30	XAT	7	320	-	39,47,47	1.01	2 (5%)	54,74,74	2.75	20 (37%)
22	CLA	A	801	-	65,73,73	1.46	10 (15%)	76,113,113	1.36	10 (13%)
22	CLA	8	312	16	56,64,73	1.58	10 (17%)	65,102,113	1.55	7 (10%)
22	CLA	8	311	-	52,60,73	1.67	8 (15%)	60,97,113	1.47	7 (11%)
22	CLA	0	305	29,22	52,60,73	1.59	7 (13%)	60,97,113	1.58	9 (15%)
22	CLA	2	312	14	65,73,73	1.40	9 (13%)	76,113,113	1.51	8 (10%)
22	CLA	4	311	22	52,60,73	1.62	9 (17%)	60,97,113	1.54	7 (11%)
22	CLA	A	827	-	65,73,73	1.45	10 (15%)	76,113,113	1.49	9 (11%)
22	CLA	9	311	-	52,60,73	1.62	7 (13%)	60,97,113	1.59	9 (15%)
25	8CT	F	302	-	40,41,41	4.59	23 (57%)	50,56,56	3.19	20 (40%)
22	CLA	A	838	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	9 (11%)
22	CLA	0	311	-	65,73,73	1.46	8 (12%)	76,113,113	1.40	9 (11%)
22	CLA	B	822	-	46,54,73	1.69	10 (21%)	53,90,113	1.63	7 (13%)
22	CLA	K	101	-	45,53,73	1.74	8 (17%)	52,89,113	1.56	8 (15%)
22	CLA	6	310	17,30	60,68,73	1.52	9 (15%)	70,107,113	1.47	10 (14%)
22	CLA	A	808	1	65,73,73	1.45	9 (13%)	76,113,113	1.45	8 (10%)
29	CHL	0	301	22,24	61,69,74	2.08	16 (26%)	67,108,114	2.42	21 (31%)
22	CLA	B	840	-	65,73,73	1.46	9 (13%)	76,113,113	1.45	7 (9%)
22	CLA	9	304	-	48,56,73	1.67	10 (20%)	55,92,113	1.59	7 (12%)
22	CLA	4	312	-	56,64,73	1.56	10 (17%)	65,102,113	1.60	7 (10%)
30	XAT	5	316	-	39,47,47	1.04	2 (5%)	54,74,74	3.14	21 (38%)
22	CLA	B	806	-	65,73,73	1.40	10 (15%)	76,113,113	1.53	9 (11%)
30	XAT	7	319	22	39,47,47	0.98	2 (5%)	54,74,74	3.25	24 (44%)
22	CLA	B	826	-	65,73,73	1.40	8 (12%)	76,113,113	1.46	7 (9%)
22	CLA	5	303	-	65,73,73	1.43	9 (13%)	76,113,113	1.36	7 (9%)
22	CLA	5	305	25	52,60,73	1.66	8 (15%)	60,97,113	1.43	7 (11%)
22	CLA	F	301	-	45,53,73	1.74	10 (22%)	52,89,113	1.59	6 (11%)
25	8CT	4	317	-	40,41,41	4.74	24 (60%)	50,56,56	2.36	15 (30%)
22	CLA	A	833	25	65,73,73	1.44	10 (15%)	76,113,113	1.37	8 (10%)
22	CLA	5	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	9 (11%)
25	8CT	J	104	-	40,41,41	4.70	24 (60%)	50,56,56	2.79	18 (36%)
29	CHL	5	301	13	61,69,74	1.98	14 (22%)	67,108,114	2.53	22 (32%)
22	CLA	3	308	-	50,58,73	1.66	11 (22%)	58,95,113	1.66	9 (15%)
22	CLA	4	310	-	55,63,73	1.60	10 (18%)	64,101,113	1.51	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	LHG	1	317	22	48,48,48	0.68	2 (4%)	51,54,54	1.30	7 (13%)
25	8CT	1	316	13	40,41,41	4.73	24 (60%)	50,56,56	2.61	18 (36%)
29	CHL	8	307	30	51,59,74	2.11	13 (25%)	55,96,114	2.76	25 (45%)
29	CHL	6	307	-	43,51,74	2.33	14 (32%)	45,86,114	2.84	17 (37%)
22	CLA	9	309	-	60,68,73	1.49	9 (15%)	70,107,113	1.52	9 (12%)
22	CLA	1	313	-	46,54,73	1.71	9 (19%)	53,90,113	1.58	7 (13%)
22	CLA	7	310	18	50,58,73	1.60	9 (18%)	58,95,113	1.77	8 (13%)
25	8CT	G	104	-	40,41,41	4.74	24 (60%)	50,56,56	2.59	19 (38%)
22	CLA	1	302	-	65,73,73	1.48	10 (15%)	76,113,113	1.43	9 (11%)
22	CLA	3	313	-	46,54,73	1.68	10 (21%)	53,90,113	1.63	6 (11%)
22	CLA	3	303	-	45,53,73	1.76	9 (20%)	52,89,113	1.59	7 (13%)
22	CLA	9	306	-	52,60,73	1.62	10 (19%)	60,97,113	1.56	7 (11%)
22	CLA	G	103	7	46,54,73	1.67	5 (10%)	53,90,113	1.60	6 (11%)
22	CLA	6	313	29	65,73,73	1.41	10 (15%)	76,113,113	1.46	10 (13%)
29	CHL	6	316	17	43,51,74	2.29	14 (32%)	45,86,114	2.96	19 (42%)
25	8CT	A	846	25	40,41,41	4.64	24 (60%)	50,56,56	2.97	19 (38%)
25	8CT	B	845	-	40,41,41	4.64	24 (60%)	50,56,56	3.16	20 (40%)
22	CLA	1	312	29	55,63,73	1.56	8 (14%)	64,101,113	1.56	6 (9%)
22	CLA	1	306	-	65,73,73	1.49	9 (13%)	76,113,113	1.41	8 (10%)
23	PQN	A	842	-	34,34,34	1.47	2 (5%)	42,45,45	1.31	6 (14%)
22	CLA	K	104	-	46,54,73	1.74	9 (19%)	53,90,113	1.56	6 (11%)
22	CLA	7	304	22	47,55,73	1.69	10 (21%)	54,91,113	1.58	8 (14%)
22	CLA	A	816	-	45,53,73	1.73	9 (20%)	52,89,113	1.57	6 (11%)
22	CLA	1	308	13,30	60,68,73	1.50	8 (13%)	70,107,113	1.48	8 (11%)
25	8CT	A	847	-	40,41,41	4.60	23 (57%)	50,56,56	2.97	20 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	304	17	1/1/15/20	15/37/115/115	-
22	CLA	A	818	-	1/1/15/20	12/37/115/115	-
25	8CT	5	317	22	-	10/29/63/63	0/2/2/2
22	CLA	9	312	30	1/1/13/20	13/30/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	308	-	1/1/10/20	2/10/88/115	-
22	CLA	B	817	-	1/1/13/20	10/25/103/115	-
22	CLA	A	804	22	1/1/13/20	9/25/103/115	-
22	CLA	1	310	-	1/1/12/20	7/22/100/115	-
22	CLA	9	308	-	1/1/15/20	16/37/115/115	-
27	SF4	B	802	-	-	-	0/6/5/5
22	CLA	A	828	-	1/1/15/20	18/37/115/115	-
22	CLA	7	302	18	1/1/11/20	7/15/93/115	-
22	CLA	4	303	-	1/1/11/20	5/15/93/115	-
22	CLA	A	825	-	-	15/37/115/115	-
27	SF4	C	102	3	-	-	0/6/5/5
22	CLA	3	312	-	1/1/11/20	7/13/91/115	-
22	CLA	7	314	-	1/1/11/20	4/13/91/115	-
22	CLA	1	301	13	1/1/15/20	10/37/115/115	-
25	8CT	B	851	22	-	15/29/63/63	0/2/2/2
22	CLA	5	310	24	1/1/10/20	3/8/86/115	-
22	CLA	0	302	30	1/1/15/20	16/37/115/115	-
29	CHL	9	302	19	4/4/19/26	11/33/131/137	-
22	CLA	7	305	-	1/1/11/20	8/13/91/115	-
22	CLA	8	303	22,31	1/1/11/20	3/15/93/115	-
22	CLA	4	309	30	1/1/14/20	14/31/109/115	-
22	CLA	9	303	19	1/1/15/20	12/37/115/115	-
22	CLA	B	850	-	1/1/13/20	11/25/103/115	-
22	CLA	2	314	14	1/1/11/20	7/18/96/115	-
22	CLA	0	307	22	1/1/15/20	26/37/115/115	-
24	LHG	3	317	22	-	12/23/23/53	-
22	CLA	0	310	30	1/1/12/20	2/22/100/115	-
22	CLA	7	306	22	1/1/10/20	4/10/88/115	-
22	CLA	7	307	22	1/1/11/20	3/16/94/115	-
29	CHL	5	306	-	3/3/16/26	7/18/116/137	-
22	CLA	A	826	25	1/1/15/20	13/37/115/115	-
22	CLA	5	302	-	1/1/15/20	9/37/115/115	-
25	8CT	A	854	-	-	12/29/63/63	0/2/2/2
22	CLA	5	309	13,30	1/1/14/20	8/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	8	314	-	3/3/15/26	3/12/110/137	-
22	CLA	A	821	-	1/1/15/20	9/37/115/115	-
29	CHL	0	306	30,22	3/3/16/26	5/18/116/137	-
22	CLA	2	310	24	1/1/10/20	4/8/86/115	-
22	CLA	A	815	-	1/1/11/20	3/16/94/115	-
22	CLA	B	811	-	1/1/15/20	11/37/115/115	-
22	CLA	7	313	-	1/1/13/20	13/25/103/115	-
22	CLA	B	813	-	1/1/13/20	7/25/103/115	-
22	CLA	B	836	-	1/1/14/20	13/31/109/115	-
22	CLA	2	308	-	1/1/12/20	5/19/97/115	-
30	XAT	6	319	22	-	3/31/93/93	0/4/4/4
22	CLA	5	313	-	1/1/13/20	7/25/103/115	-
25	8CT	B	844	-	-	15/29/63/63	0/2/2/2
30	XAT	8	316	29	-	7/31/93/93	0/4/4/4
22	CLA	7	315	-	1/1/11/20	4/15/93/115	-
22	CLA	6	323	16	1/1/11/20	11/15/93/115	-
22	CLA	B	829	-	1/1/15/20	11/37/115/115	-
22	CLA	A	803	-	1/1/15/20	17/37/115/115	-
22	CLA	B	821	-	1/1/12/20	8/19/97/115	-
29	CHL	8	305	-	4/4/18/26	9/27/125/137	-
24	LHG	2	318	22	-	19/36/36/53	-
22	CLA	B	805	-	1/1/15/20	16/37/115/115	-
29	CHL	2	307	-	3/3/17/26	9/21/119/137	-
22	CLA	A	819	-	1/1/15/20	14/37/115/115	-
22	CLA	A	810	-	1/1/15/20	11/37/115/115	-
22	CLA	B	835	-	1/1/11/20	3/13/91/115	-
25	8CT	8	301	-	-	13/29/63/63	0/2/2/2
22	CLA	3	319	-	1/1/15/20	21/37/115/115	-
22	CLA	6	315	-	1/1/15/20	14/37/115/115	-
22	CLA	A	812	-	1/1/12/20	1/24/102/115	-
29	CHL	6	306	-	3/3/15/26	2/12/110/137	-
22	CLA	B	818	-	1/1/13/20	12/30/108/115	-
31	LMG	8	319	22	-	17/39/59/70	0/1/1/1
22	CLA	A	806	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	307	-	1/1/15/20	16/37/115/115	-
22	CLA	B	838	-	1/1/11/20	4/16/94/115	-
22	CLA	A	824	-	1/1/13/20	8/25/103/115	-
22	CLA	A	811	22	1/1/15/20	18/37/115/115	-
29	CHL	4	305	29	4/4/18/26	12/27/125/137	-
22	CLA	2	302	29	1/1/15/20	17/37/115/115	-
22	CLA	B	812	2	1/1/15/20	13/37/115/115	-
22	CLA	M	101	-	-	8/15/93/115	-
30	XAT	8	317	-	-	0/31/93/93	0/4/4/4
22	CLA	3	305	15	1/1/11/20	8/16/94/115	-
25	8CT	J	101	-	-	9/29/63/63	0/2/2/2
22	CLA	B	819	-	1/1/14/20	19/31/109/115	-
22	CLA	5	312	30	1/1/15/20	12/37/115/115	-
22	CLA	L	201	-	1/1/15/20	17/37/115/115	-
22	CLA	7	311	24	1/1/8/20	0/2/76/115	-
22	CLA	A	805	-	1/1/15/20	14/37/115/115	-
22	CLA	7	309	22	1/1/12/20	4/19/97/115	-
22	CLA	B	810	-	1/1/15/20	6/37/115/115	-
22	CLA	4	304	-	1/1/12/20	4/19/97/115	-
22	CLA	6	314	-	1/1/10/20	6/11/89/115	-
22	CLA	B	832	-	1/1/15/20	14/37/115/115	-
22	CLA	A	809	1	1/1/15/20	13/37/115/115	-
22	CLA	2	303	-	1/1/15/20	11/37/115/115	-
22	CLA	K	105	-	1/1/12/20	9/19/97/115	-
22	CLA	A	823	-	1/1/12/20	6/21/99/115	-
22	CLA	0	304	22	1/1/12/20	11/22/100/115	-
22	CLA	4	313	-	1/1/11/20	6/13/91/115	-
29	CHL	4	306	29	3/3/17/26	7/21/119/137	-
22	CLA	A	834	-	1/1/12/20	1/19/97/115	-
22	CLA	7	303	18	1/1/14/20	17/31/109/115	-
22	CLA	3	302	25	1/1/12/20	2/19/97/115	-
22	CLA	B	827	-	1/1/15/20	18/37/115/115	-
23	PQN	B	842	-	-	5/23/43/43	0/2/2/2
22	CLA	A	817	-	1/1/15/20	19/37/115/115	-
22	CLA	B	830	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	814	-	1/1/11/20	10/13/91/115	-
22	CLA	B	820	-	1/1/15/20	9/37/115/115	-
27	SF4	C	101	-	-	-	0/6/5/5
29	CHL	6	308	-	3/3/17/26	6/21/119/137	-
30	XAT	3	314	25	-	4/31/93/93	0/4/4/4
22	CLA	2	311	14	1/1/12/20	7/22/100/115	-
22	CLA	3	304	-	1/1/10/20	3/10/88/115	-
22	CLA	5	304	-	1/1/12/20	8/22/100/115	-
25	8CT	B	847	-	-	10/29/63/63	0/2/2/2
29	CHL	9	307	-	3/3/16/26	10/18/116/137	-
30	XAT	1	315	-	-	1/31/93/93	0/4/4/4
30	XAT	0	314	29,22	-	8/31/93/93	0/4/4/4
22	CLA	8	309	-	1/1/14/20	8/31/109/115	-
22	CLA	B	839	25	1/1/15/20	13/37/115/115	-
31	LMG	5	319	22	-	18/39/59/70	0/1/1/1
22	CLA	6	309	17	1/1/12/20	10/19/97/115	-
24	LHG	9	316	22	-	22/53/53/53	-
22	CLA	6	311	24	1/1/15/20	20/37/115/115	-
22	CLA	0	309	24	1/1/10/20	2/8/86/115	-
25	8CT	2	317	-	-	10/29/63/63	0/2/2/2
22	CLA	A	841	25	1/1/15/20	13/37/115/115	-
22	CLA	1	311	-	1/1/15/20	15/37/115/115	-
22	CLA	6	305	-	1/1/14/20	13/31/109/115	-
22	CLA	L	202	-	1/1/15/20	15/37/115/115	-
29	CHL	4	301	13,22	4/4/19/26	11/33/131/137	-
22	CLA	3	307	15	1/1/12/20	8/19/97/115	-
22	CLA	6	317	-	1/1/11/20	5/13/91/115	-
22	CLA	5	311	30	1/1/11/20	1/13/91/115	-
22	CLA	3	310	-	1/1/12/20	2/22/100/115	-
22	CLA	6	301	-	1/1/12/20	11/22/100/115	-
22	CLA	L	204	-	1/1/12/20	9/19/97/115	-
22	CLA	L	203	-	1/1/15/20	14/37/115/115	-
25	8CT	6	321	-	-	9/29/63/63	0/2/2/2
25	8CT	7	321	-	-	10/29/63/63	0/2/2/2
30	XAT	4	315	22	-	8/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	4	318	-	-	19/39/59/70	0/1/1/1
25	8CT	3	318	25,22	-	6/29/63/63	0/2/2/2
30	XAT	2	316	-	-	3/31/93/93	0/4/4/4
22	CLA	A	820	-	1/1/11/20	4/13/91/115	-
25	8CT	B	848	-	-	10/29/63/63	0/2/2/2
22	CLA	4	302	-	1/1/14/20	8/31/109/115	-
22	CLA	7	317	-	1/1/15/20	19/37/115/115	-
24	LHG	B	852	22	-	10/26/26/53	-
22	CLA	6	318	17	1/1/12/20	6/22/100/115	-
22	CLA	B	807	-	1/1/11/20	5/13/91/115	-
22	CLA	7	312	30	1/1/12/20	3/22/100/115	-
25	8CT	B	804	-	-	15/29/63/63	0/2/2/2
29	CHL	1	305	-	3/3/16/26	7/18/116/137	-
25	8CT	I	101	-	-	10/29/63/63	0/2/2/2
24	LHG	0	315	29,22	-	27/53/53/53	-
22	CLA	7	316	18	1/1/15/20	18/37/115/115	-
29	CHL	3	306	25	3/3/16/26	3/17/115/137	-
22	CLA	A	840	-	1/1/15/20	14/37/115/115	-
22	CLA	3	309	24	1/1/8/20	0/2/76/115	-
22	CLA	8	308	16	1/1/12/20	6/19/97/115	-
22	CLA	A	813	-	1/1/15/20	16/37/115/115	-
22	CLA	B	815	-	1/1/15/20	11/37/115/115	-
22	CLA	1	304	-	1/1/12/20	6/22/100/115	-
26	HTG	A	851	-	-	4/10/30/30	0/1/1/1
22	CLA	A	802	-	1/1/15/20	8/37/115/115	-
22	CLA	9	305	-	1/1/12/20	7/22/100/115	-
25	8CT	L	205	22	-	13/29/63/63	0/2/2/2
22	CLA	A	807	-	1/1/15/20	14/37/115/115	-
22	CLA	B	831	-	1/1/12/20	8/19/97/115	-
22	CLA	B	801	-	1/1/15/20	10/37/115/115	-
24	LHG	5	318	22	-	29/53/53/53	-
25	8CT	8	318	-	-	13/29/63/63	0/2/2/2
22	CLA	K	102	-	1/1/11/20	9/15/93/115	-
22	CLA	A	822	-	1/1/11/20	10/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	G	101	-	1/1/11/20	5/13/91/115	-
22	CLA	A	831	-	1/1/12/20	1/19/97/115	-
22	CLA	7	318	22	1/1/15/20	18/37/115/115	-
29	CHL	2	305	-	3/3/15/26	3/12/110/137	-
29	CHL	4	307	-	3/3/17/26	5/21/119/137	-
22	CLA	8	310	31	1/1/13/20	8/25/103/115	-
25	8CT	L	206	-	-	15/29/63/63	0/2/2/2
22	CLA	8	315	-	1/1/15/20	25/37/115/115	-
22	CLA	1	303	-	1/1/12/20	8/22/100/115	-
22	CLA	9	310	24	1/1/10/20	4/8/86/115	-
25	8CT	7	301	29,30	-	11/29/63/63	0/2/2/2
22	CLA	A	832	-	1/1/15/20	16/37/115/115	-
22	CLA	B	837	-	1/1/15/20	17/37/115/115	-
24	LHG	7	322	22	-	16/23/23/53	-
22	CLA	4	308	16	1/1/12/20	1/19/97/115	-
30	XAT	5	315	22	-	6/31/93/93	0/4/4/4
22	CLA	B	833	-	1/1/13/20	13/29/107/115	-
22	CLA	J	103	10	1/1/10/20	8/10/88/115	-
30	XAT	3	315	-	-	0/31/93/93	0/4/4/4
29	CHL	8	306	-	3/3/17/26	9/21/119/137	-
22	CLA	G	102	-	1/1/12/20	5/19/97/115	-
22	CLA	2	313	-	1/1/10/20	2/11/89/115	-
22	CLA	H	201	-	1/1/15/20	16/37/115/115	-
29	CHL	2	306	-	3/3/16/26	8/18/116/137	-
22	CLA	1	309	24	1/1/10/20	2/8/86/115	-
22	CLA	0	303	30	1/1/15/20	14/37/115/115	-
22	CLA	A	836	-	1/1/12/20	11/21/99/115	-
25	8CT	A	849	22	-	11/29/63/63	0/2/2/2
22	CLA	B	808	-	1/1/15/20	16/37/115/115	-
22	CLA	B	841	24	1/1/15/20	13/37/115/115	-
24	LHG	6	322	22	-	22/41/41/53	-
29	CHL	7	308	-	3/3/16/26	8/17/115/137	-
22	CLA	2	319	16	1/1/11/20	9/15/93/115	-
22	CLA	B	825	-	1/1/15/20	17/37/115/115	-
22	CLA	8	304	-	1/1/12/20	10/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	816	-	1/1/14/20	13/31/109/115	-
22	CLA	B	824	-	1/1/14/20	13/31/109/115	-
30	XAT	9	314	22	-	4/31/93/93	0/4/4/4
22	CLA	A	843	24	1/1/12/20	11/22/100/115	-
22	CLA	8	302	-	1/1/14/20	7/31/109/115	-
22	CLA	8	313	-	1/1/11/20	3/13/91/115	-
30	XAT	1	314	22	-	11/31/93/93	0/4/4/4
22	CLA	A	837	-	1/1/15/20	19/37/115/115	-
22	CLA	A	835	1	1/1/11/20	5/13/91/115	-
22	CLA	9	313	-	1/1/13/20	13/25/103/115	-
22	CLA	0	312	29	1/1/13/20	10/25/103/115	-
22	CLA	B	834	2	1/1/15/20	16/37/115/115	-
22	CLA	6	303	17	1/1/15/20	16/37/115/115	-
22	CLA	A	839	-	1/1/15/20	17/37/115/115	-
29	CHL	6	302	17,22	4/4/19/26	14/33/131/137	-
22	CLA	A	830	-	1/1/15/20	11/37/115/115	-
22	CLA	9	301	-	1/1/11/20	6/16/92/115	-
22	CLA	3	311	-	1/1/13/20	11/25/103/115	-
24	LHG	A	844	-	-	25/53/53/53	-
22	CLA	A	852	-	1/1/11/20	7/18/96/115	-
22	CLA	4	314	-	1/1/15/20	18/37/115/115	-
29	CHL	2	301	22	4/4/19/26	13/33/131/137	-
30	XAT	9	315	-	-	0/31/93/93	0/4/4/4
30	XAT	4	316	-	-	3/31/93/93	0/4/4/4
30	XAT	6	320	-	-	4/31/93/93	0/4/4/4
22	CLA	B	828	-	1/1/15/20	16/37/115/115	-
25	8CT	A	850	-	-	11/29/63/63	0/2/2/2
25	8CT	7	323	-	-	14/29/63/63	0/2/2/2
25	8CT	K	103	-	-	12/29/63/63	0/2/2/2
22	CLA	5	314	24	1/1/11/20	9/15/93/115	-
22	CLA	B	803	-	1/1/15/20	19/37/115/115	-
22	CLA	2	309	-	1/1/14/20	10/31/109/115	-
22	CLA	B	809	-	1/1/15/20	20/37/115/115	-
25	8CT	B	843	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	B	849	-	-	31/55/95/95	0/2/2/2
22	CLA	A	853	-	1/1/15/20	15/37/115/115	-
22	CLA	2	304	-	1/1/14/20	16/31/109/115	-
25	8CT	3	316	-	-	12/29/63/63	0/2/2/2
25	8CT	B	846	-	-	13/29/63/63	0/2/2/2
22	CLA	6	312	-	1/1/12/20	9/22/100/115	-
22	CLA	B	823	-	-	11/25/103/115	-
22	CLA	B	814	-	1/1/15/20	21/37/115/115	-
22	CLA	3	301	-	1/1/14/20	11/31/109/115	-
22	CLA	A	829	-	1/1/15/20	10/37/115/115	-
24	LHG	A	845	22	-	16/31/31/53	-
30	XAT	2	315	-	-	2/31/93/93	0/4/4/4
30	XAT	0	313	22	-	16/31/93/93	0/4/4/4
22	CLA	0	308	20	1/1/14/20	16/31/109/115	-
25	8CT	A	848	-	-	6/29/63/63	0/2/2/2
26	HTG	J	102	-	-	3/10/30/30	0/1/1/1
30	XAT	7	320	-	-	0/31/93/93	0/4/4/4
22	CLA	A	801	-	1/1/15/20	8/37/115/115	-
22	CLA	8	312	16	1/1/13/20	5/27/105/115	-
22	CLA	8	311	-	-	5/22/100/115	-
22	CLA	0	305	29,22	1/1/12/20	8/22/100/115	-
22	CLA	2	312	14	1/1/15/20	15/37/115/115	-
22	CLA	4	311	22	1/1/12/20	8/22/100/115	-
22	CLA	A	827	-	1/1/15/20	15/37/115/115	-
22	CLA	9	311	-	1/1/12/20	4/22/100/115	-
25	8CT	F	302	-	-	9/29/63/63	0/2/2/2
22	CLA	A	838	-	1/1/15/20	16/37/115/115	-
22	CLA	0	311	-	1/1/15/20	14/37/115/115	-
22	CLA	B	822	-	1/1/11/20	6/15/93/115	-
22	CLA	K	101	-	1/1/11/20	7/13/91/115	-
22	CLA	6	310	17,30	1/1/14/20	10/31/109/115	-
22	CLA	A	808	1	1/1/15/20	20/37/115/115	-
29	CHL	0	301	22,24	4/4/19/26	17/33/131/137	-
22	CLA	B	840	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	9	304	-	1/1/11/20	8/17/95/115	-
22	CLA	4	312	-	1/1/13/20	6/27/105/115	-
30	XAT	5	316	-	-	2/31/93/93	0/4/4/4
22	CLA	B	806	-	1/1/15/20	17/37/115/115	-
30	XAT	7	319	22	-	7/31/93/93	0/4/4/4
22	CLA	B	826	-	1/1/15/20	13/37/115/115	-
22	CLA	5	303	-	-	23/37/115/115	-
22	CLA	5	305	25	1/1/12/20	6/22/100/115	-
22	CLA	F	301	-	1/1/11/20	8/13/91/115	-
25	8CT	4	317	-	-	8/29/63/63	0/2/2/2
22	CLA	A	833	25	1/1/15/20	14/37/115/115	-
22	CLA	5	307	-	1/1/15/20	16/37/115/115	-
25	8CT	J	104	-	-	7/29/63/63	0/2/2/2
29	CHL	5	301	13	4/4/19/26	14/33/131/137	-
22	CLA	3	308	-	1/1/12/20	3/19/97/115	-
22	CLA	4	310	-	1/1/13/20	7/25/103/115	-
24	LHG	1	317	22	-	25/53/53/53	-
25	8CT	1	316	13	-	11/29/63/63	0/2/2/2
29	CHL	8	307	30	3/3/17/26	7/21/119/137	-
29	CHL	6	307	-	3/3/15/26	6/12/110/137	-
22	CLA	9	309	-	1/1/14/20	15/31/109/115	-
22	CLA	1	313	-	1/1/11/20	7/15/93/115	-
22	CLA	7	310	18	1/1/12/20	7/19/97/115	-
25	8CT	G	104	-	-	13/29/63/63	0/2/2/2
22	CLA	1	302	-	1/1/15/20	21/37/115/115	-
22	CLA	3	313	-	1/1/11/20	7/15/93/115	-
22	CLA	3	303	-	1/1/11/20	5/13/91/115	-
22	CLA	9	306	-	1/1/12/20	8/22/100/115	-
22	CLA	G	103	7	1/1/11/20	9/15/93/115	-
22	CLA	6	313	29	1/1/15/20	10/37/115/115	-
29	CHL	6	316	17	3/3/15/26	8/12/110/137	-
25	8CT	A	846	25	-	13/29/63/63	0/2/2/2
25	8CT	B	845	-	-	12/29/63/63	0/2/2/2
22	CLA	1	312	29	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	306	-	1/1/15/20	12/37/115/115	-
23	PQN	A	842	-	-	7/23/43/43	0/2/2/2
22	CLA	K	104	-	1/1/11/20	5/15/93/115	-
22	CLA	7	304	22	1/1/11/20	6/16/94/115	-
22	CLA	A	816	-	1/1/11/20	4/13/91/115	-
22	CLA	1	308	13,30	1/1/14/20	11/31/109/115	-
25	8CT	A	847	-	-	9/29/63/63	0/2/2/2

All (3250) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	318	8CT	C02-C03	14.68	1.59	1.34
25	5	317	8CT	C02-C03	14.38	1.59	1.34
25	K	103	8CT	C32-C31	14.37	1.61	1.32
25	7	301	8CT	C02-C03	14.33	1.59	1.34
25	1	316	8CT	C02-C03	14.33	1.59	1.34
25	B	844	8CT	C02-C03	14.33	1.59	1.34
25	J	101	8CT	C02-C03	14.29	1.59	1.34
25	8	301	8CT	C02-C03	14.29	1.59	1.34
25	L	205	8CT	C02-C03	14.29	1.59	1.34
25	A	847	8CT	C02-C03	14.28	1.59	1.34
25	A	848	8CT	C02-C03	14.28	1.59	1.34
25	B	851	8CT	C02-C03	14.28	1.59	1.34
25	A	854	8CT	C02-C03	14.27	1.59	1.34
25	B	847	8CT	C02-C03	14.27	1.59	1.34
25	G	104	8CT	C02-C03	14.26	1.59	1.34
25	L	206	8CT	C02-C03	14.25	1.59	1.34
25	B	848	8CT	C02-C03	14.25	1.59	1.34
25	4	317	8CT	C02-C03	14.22	1.59	1.34
25	8	318	8CT	C02-C03	14.17	1.59	1.34
25	A	849	8CT	C02-C03	14.17	1.59	1.34
25	B	846	8CT	C02-C03	14.16	1.59	1.34
25	2	317	8CT	C02-C03	14.14	1.58	1.34
25	F	302	8CT	C02-C03	14.14	1.58	1.34
25	J	104	8CT	C02-C03	14.14	1.58	1.34
25	7	323	8CT	C02-C03	14.14	1.58	1.34
25	3	316	8CT	C02-C03	14.11	1.58	1.34
25	6	321	8CT	C02-C03	14.08	1.58	1.34
25	K	103	8CT	C02-C03	14.07	1.58	1.34
25	I	101	8CT	C02-C03	14.07	1.58	1.34
25	A	846	8CT	C02-C03	14.04	1.58	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	321	8CT	C02-C03	14.03	1.58	1.34
25	B	845	8CT	C02-C03	14.03	1.58	1.34
25	A	850	8CT	C02-C03	14.02	1.58	1.34
25	B	804	8CT	C02-C03	14.00	1.58	1.34
25	B	843	8CT	C02-C03	14.00	1.58	1.34
25	4	317	8CT	C32-C31	13.97	1.60	1.32
25	L	205	8CT	C32-C31	13.93	1.60	1.32
25	B	843	8CT	C32-C31	13.89	1.60	1.32
25	G	104	8CT	C32-C31	13.86	1.60	1.32
25	7	323	8CT	C32-C31	13.85	1.60	1.32
25	1	316	8CT	C32-C31	13.84	1.59	1.32
25	A	850	8CT	C32-C31	13.82	1.59	1.32
25	A	849	8CT	C32-C31	13.82	1.59	1.32
25	J	104	8CT	C32-C31	13.82	1.59	1.32
25	5	317	8CT	C32-C31	13.82	1.59	1.32
25	3	318	8CT	C32-C31	13.82	1.59	1.32
25	8	318	8CT	C32-C31	13.80	1.59	1.32
25	B	848	8CT	C32-C31	13.79	1.59	1.32
25	6	321	8CT	C32-C31	13.78	1.59	1.32
25	8	301	8CT	C32-C31	13.75	1.59	1.32
25	B	851	8CT	C32-C31	13.73	1.59	1.32
25	2	317	8CT	C32-C31	13.73	1.59	1.32
25	B	847	8CT	C32-C31	13.73	1.59	1.32
25	3	316	8CT	C32-C31	13.73	1.59	1.32
25	7	321	8CT	C32-C31	13.72	1.59	1.32
25	A	854	8CT	C32-C31	13.72	1.59	1.32
25	B	845	8CT	C32-C31	13.69	1.59	1.32
25	B	846	8CT	C32-C31	13.69	1.59	1.32
25	L	206	8CT	C32-C31	13.62	1.59	1.32
25	B	804	8CT	C32-C31	13.58	1.59	1.32
25	J	101	8CT	C32-C31	13.52	1.59	1.32
25	7	301	8CT	C32-C31	13.45	1.59	1.32
25	F	302	8CT	C32-C31	13.44	1.59	1.32
25	A	847	8CT	C32-C31	13.43	1.59	1.32
25	A	846	8CT	C32-C31	13.42	1.59	1.32
25	A	848	8CT	C32-C31	13.38	1.59	1.32
25	B	844	8CT	C32-C31	13.29	1.58	1.32
25	I	101	8CT	C32-C31	13.19	1.58	1.32
25	A	847	8CT	C34-C35	-8.55	1.36	1.54
25	B	843	8CT	C34-C35	-8.25	1.37	1.54
25	B	851	8CT	C34-C35	-8.25	1.37	1.54
25	F	302	8CT	C34-C35	-8.21	1.37	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	318	8CT	C34-C35	-8.20	1.37	1.54
25	L	205	8CT	C34-C35	-8.14	1.37	1.54
25	B	804	8CT	C34-C35	-8.07	1.37	1.54
25	A	849	8CT	C34-C35	-8.06	1.37	1.54
25	A	850	8CT	C34-C35	-8.02	1.37	1.54
25	A	848	8CT	C34-C35	-8.02	1.37	1.54
25	8	301	8CT	C34-C35	-8.01	1.37	1.54
25	B	845	8CT	C34-C35	-8.01	1.37	1.54
25	7	323	8CT	C34-C35	-7.98	1.37	1.54
25	7	321	8CT	C34-C35	-7.98	1.37	1.54
25	8	318	8CT	C34-C35	-7.98	1.37	1.54
25	3	316	8CT	C34-C35	-7.97	1.37	1.54
25	A	854	8CT	C34-C35	-7.97	1.37	1.54
25	I	101	8CT	C34-C35	-7.96	1.37	1.54
25	4	317	8CT	C34-C35	-7.94	1.37	1.54
25	1	316	8CT	C34-C35	-7.94	1.37	1.54
25	B	847	8CT	C34-C35	-7.93	1.37	1.54
25	B	846	8CT	C34-C35	-7.91	1.37	1.54
25	B	848	8CT	C34-C35	-7.91	1.37	1.54
25	7	301	8CT	C34-C35	-7.91	1.37	1.54
25	J	104	8CT	C34-C35	-7.90	1.37	1.54
25	B	844	8CT	C34-C35	-7.88	1.37	1.54
25	2	317	8CT	C34-C35	-7.88	1.37	1.54
25	A	846	8CT	C34-C35	-7.86	1.38	1.54
25	6	321	8CT	C34-C35	-7.86	1.38	1.54
25	G	104	8CT	C34-C35	-7.86	1.38	1.54
22	0	312	CLA	C4B-NB	7.81	1.42	1.35
25	L	206	8CT	C34-C35	-7.70	1.38	1.54
22	G	101	CLA	C4B-NB	7.64	1.42	1.35
25	5	317	8CT	C34-C35	-7.63	1.38	1.54
25	J	101	8CT	C34-C35	-7.62	1.38	1.54
22	0	304	CLA	C4B-NB	7.45	1.41	1.35
25	K	103	8CT	C34-C35	-7.42	1.38	1.54
22	7	312	CLA	C4B-NB	7.38	1.41	1.35
22	9	312	CLA	C4B-NB	7.31	1.41	1.35
23	B	842	PQN	C3-C2	7.19	1.48	1.35
22	B	834	CLA	C4B-NB	7.19	1.41	1.35
22	5	308	CLA	C4B-NB	7.18	1.41	1.35
22	4	314	CLA	C4B-NB	7.17	1.41	1.35
23	A	842	PQN	C3-C2	7.16	1.48	1.35
22	0	303	CLA	C4B-NB	7.16	1.41	1.35
22	7	316	CLA	C4B-NB	7.15	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	306	CLA	C4B-NB	7.15	1.41	1.35
22	K	104	CLA	C4B-NB	7.14	1.41	1.35
22	K	105	CLA	C4B-NB	7.14	1.41	1.35
22	8	311	CLA	C4B-NB	7.13	1.41	1.35
22	9	305	CLA	C4B-NB	7.13	1.41	1.35
22	0	302	CLA	C4B-NB	7.13	1.41	1.35
22	7	306	CLA	C4B-NB	7.12	1.41	1.35
22	M	101	CLA	C4B-NB	7.12	1.41	1.35
22	K	101	CLA	C4B-NB	7.08	1.41	1.35
22	1	301	CLA	C4B-NB	7.08	1.41	1.35
22	0	309	CLA	C4B-NB	7.08	1.41	1.35
22	6	301	CLA	C4B-NB	7.07	1.41	1.35
22	8	313	CLA	C4B-NB	7.06	1.41	1.35
22	L	202	CLA	C4B-NB	7.05	1.41	1.35
22	5	313	CLA	C4B-NB	7.05	1.41	1.35
22	0	307	CLA	C4B-NB	7.03	1.41	1.35
22	5	305	CLA	C4B-NB	7.02	1.41	1.35
22	6	315	CLA	C4B-NB	7.01	1.41	1.35
22	6	305	CLA	C4B-NB	6.99	1.41	1.35
22	5	309	CLA	C4B-NB	6.98	1.41	1.35
22	9	310	CLA	C4B-NB	6.97	1.41	1.35
22	9	301	CLA	C4B-NB	6.96	1.41	1.35
22	0	308	CLA	C4B-NB	6.95	1.41	1.35
22	3	303	CLA	C4B-NB	6.95	1.41	1.35
22	A	811	CLA	C4B-NB	6.94	1.41	1.35
22	B	824	CLA	C4B-NB	6.93	1.41	1.35
22	G	102	CLA	C4B-NB	6.93	1.41	1.35
22	1	302	CLA	C4B-NB	6.92	1.41	1.35
22	A	834	CLA	C4B-NB	6.91	1.41	1.35
22	B	821	CLA	C4B-NB	6.91	1.41	1.35
22	8	315	CLA	C4B-NB	6.90	1.41	1.35
22	8	312	CLA	C4B-NB	6.90	1.41	1.35
22	A	830	CLA	C4B-NB	6.90	1.41	1.35
22	8	310	CLA	C4B-NB	6.89	1.41	1.35
22	7	307	CLA	C4B-NB	6.89	1.41	1.35
22	A	843	CLA	C4B-NB	6.89	1.41	1.35
22	B	839	CLA	C4B-NB	6.88	1.41	1.35
22	5	304	CLA	C4B-NB	6.87	1.41	1.35
22	G	103	CLA	C4B-NB	6.86	1.41	1.35
22	0	311	CLA	C4B-NB	6.86	1.41	1.35
22	5	312	CLA	C4B-NB	6.86	1.41	1.35
25	K	103	8CT	C28-C26	6.85	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	313	CLA	C4B-NB	6.84	1.41	1.35
22	3	307	CLA	C4B-NB	6.84	1.41	1.35
22	5	307	CLA	C4B-NB	6.82	1.41	1.35
22	A	810	CLA	C4B-NB	6.82	1.41	1.35
22	A	835	CLA	C4B-NB	6.82	1.41	1.35
25	B	851	8CT	C15-C16	6.81	1.60	1.45
25	F	302	8CT	C05-C06	-6.80	1.35	1.52
22	B	816	CLA	C4B-NB	6.80	1.41	1.35
22	8	304	CLA	C4B-NB	6.78	1.41	1.35
22	J	103	CLA	C4B-NB	6.78	1.41	1.35
22	3	319	CLA	C4B-NB	6.77	1.41	1.35
22	B	813	CLA	C4B-NB	6.77	1.41	1.35
22	L	203	CLA	C4B-NB	6.77	1.41	1.35
25	3	318	8CT	C05-C06	-6.77	1.35	1.52
22	L	204	CLA	C4B-NB	6.76	1.41	1.35
22	5	314	CLA	C4B-NB	6.75	1.41	1.35
22	5	311	CLA	C4B-NB	6.75	1.41	1.35
22	2	314	CLA	C4B-NB	6.75	1.41	1.35
22	9	311	CLA	C4B-NB	6.75	1.41	1.35
22	6	304	CLA	C4B-NB	6.74	1.41	1.35
22	9	308	CLA	C4B-NB	6.74	1.41	1.35
22	A	852	CLA	C4B-NB	6.74	1.41	1.35
22	7	303	CLA	C4B-NB	6.74	1.41	1.35
22	9	306	CLA	C4B-NB	6.74	1.41	1.35
25	7	301	8CT	C05-C06	-6.73	1.36	1.52
22	3	309	CLA	C4B-NB	6.71	1.41	1.35
25	A	847	8CT	C05-C06	-6.71	1.36	1.52
22	3	312	CLA	C4B-NB	6.71	1.41	1.35
22	6	310	CLA	C4B-NB	6.70	1.41	1.35
25	5	317	8CT	C28-C26	6.70	1.60	1.45
22	3	302	CLA	C4B-NB	6.69	1.41	1.35
22	A	812	CLA	C4B-NB	6.69	1.41	1.35
22	6	309	CLA	C4B-NB	6.68	1.41	1.35
25	B	843	8CT	C05-C06	-6.68	1.36	1.52
22	A	838	CLA	C4B-NB	6.67	1.41	1.35
22	3	310	CLA	C4B-NB	6.67	1.41	1.35
22	A	816	CLA	C4B-NB	6.67	1.41	1.35
22	B	831	CLA	C4B-NB	6.67	1.41	1.35
25	4	317	8CT	C15-C16	6.66	1.60	1.45
25	L	205	8CT	C05-C06	-6.65	1.36	1.52
22	5	310	CLA	C4B-NB	6.64	1.41	1.35
25	I	101	8CT	C05-C06	-6.64	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	318	CLA	C4B-NB	6.64	1.41	1.35
22	2	310	CLA	C4B-NB	6.63	1.41	1.35
22	1	313	CLA	C4B-NB	6.63	1.41	1.35
22	B	850	CLA	C4B-NB	6.63	1.41	1.35
22	9	303	CLA	C4B-NB	6.62	1.41	1.35
22	0	305	CLA	C4B-NB	6.62	1.41	1.35
22	A	825	CLA	C4B-NB	6.61	1.41	1.35
22	B	820	CLA	C4B-NB	6.61	1.41	1.35
22	6	318	CLA	C4B-NB	6.61	1.41	1.35
22	1	308	CLA	C4B-NB	6.61	1.41	1.35
22	1	309	CLA	C4B-NB	6.61	1.41	1.35
22	A	853	CLA	C4B-NB	6.60	1.41	1.35
22	4	310	CLA	C4B-NB	6.60	1.41	1.35
25	A	846	8CT	C05-C06	-6.60	1.36	1.52
22	A	815	CLA	C4B-NB	6.59	1.41	1.35
25	B	844	8CT	C05-C06	-6.59	1.36	1.52
22	A	808	CLA	C4B-NB	6.59	1.41	1.35
22	7	311	CLA	C4B-NB	6.58	1.41	1.35
22	B	809	CLA	C4B-NB	6.58	1.41	1.35
22	B	805	CLA	C4B-NB	6.58	1.41	1.35
22	7	314	CLA	C4B-NB	6.58	1.41	1.35
25	B	845	8CT	C05-C06	-6.57	1.36	1.52
22	B	825	CLA	C4B-NB	6.57	1.41	1.35
25	B	851	8CT	C05-C06	-6.56	1.36	1.52
22	B	812	CLA	C4B-NB	6.56	1.41	1.35
22	1	303	CLA	C4B-NB	6.56	1.41	1.35
25	K	103	8CT	C23-C21	6.56	1.60	1.45
25	B	844	8CT	C15-C16	6.55	1.60	1.45
25	B	846	8CT	C15-C16	6.55	1.60	1.45
22	2	303	CLA	C4B-NB	6.55	1.41	1.35
25	G	104	8CT	C15-C16	6.55	1.60	1.45
22	1	307	CLA	C4B-NB	6.55	1.41	1.35
22	B	837	CLA	C4B-NB	6.54	1.41	1.35
25	K	103	8CT	C15-C16	6.53	1.60	1.45
22	1	310	CLA	C4B-NB	6.53	1.41	1.35
22	6	312	CLA	C4B-NB	6.53	1.41	1.35
25	1	316	8CT	C15-C16	6.53	1.60	1.45
25	L	206	8CT	C05-C06	-6.53	1.36	1.52
22	0	310	CLA	C4B-NB	6.52	1.41	1.35
22	6	314	CLA	C4B-NB	6.52	1.41	1.35
25	J	101	8CT	C05-C06	-6.51	1.36	1.52
22	A	823	CLA	C4B-NB	6.51	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	305	CLA	C4B-NB	6.51	1.41	1.35
22	7	304	CLA	C4B-NB	6.51	1.41	1.35
22	2	313	CLA	C4B-NB	6.51	1.41	1.35
22	B	811	CLA	C4B-NB	6.51	1.41	1.35
22	B	833	CLA	C4B-NB	6.51	1.41	1.35
22	8	308	CLA	C4B-NB	6.50	1.41	1.35
22	A	818	CLA	C4B-NB	6.48	1.41	1.35
22	A	826	CLA	C4B-NB	6.48	1.41	1.35
22	6	303	CLA	C4B-NB	6.48	1.41	1.35
22	2	309	CLA	C4B-NB	6.47	1.41	1.35
25	J	104	8CT	C05-C06	-6.46	1.36	1.52
22	B	810	CLA	C4B-NB	6.46	1.41	1.35
25	8	318	8CT	C05-C06	-6.46	1.36	1.52
25	A	849	8CT	C05-C06	-6.45	1.36	1.52
25	2	317	8CT	C15-C16	6.45	1.59	1.45
22	1	312	CLA	C4B-NB	6.45	1.41	1.35
22	9	309	CLA	C4B-NB	6.45	1.41	1.35
25	6	321	8CT	C05-C06	-6.44	1.36	1.52
22	3	308	CLA	C4B-NB	6.44	1.41	1.35
25	4	317	8CT	C05-C06	-6.44	1.36	1.52
25	8	301	8CT	C15-C16	6.44	1.59	1.45
22	4	304	CLA	C4B-NB	6.43	1.40	1.35
22	7	305	CLA	C4B-NB	6.43	1.40	1.35
22	9	304	CLA	C4B-NB	6.43	1.40	1.35
22	3	304	CLA	C4B-NB	6.43	1.40	1.35
22	B	840	CLA	C4B-NB	6.43	1.40	1.35
22	A	807	CLA	C4B-NB	6.42	1.40	1.35
22	2	311	CLA	C4B-NB	6.42	1.40	1.35
22	4	312	CLA	C4B-NB	6.42	1.40	1.35
25	8	318	8CT	C15-C16	6.42	1.59	1.45
25	B	804	8CT	C05-C06	-6.42	1.36	1.52
22	A	829	CLA	C4B-NB	6.42	1.40	1.35
25	B	847	8CT	C05-C06	-6.42	1.36	1.52
25	B	848	8CT	C05-C06	-6.42	1.36	1.52
22	B	838	CLA	C4B-NB	6.41	1.40	1.35
22	7	315	CLA	C4B-NB	6.41	1.40	1.35
25	3	316	8CT	C15-C16	6.41	1.59	1.45
25	A	854	8CT	C05-C06	-6.41	1.36	1.52
25	1	316	8CT	C05-C06	-6.41	1.36	1.52
25	A	848	8CT	C05-C06	-6.41	1.36	1.52
22	6	323	CLA	C4B-NB	6.40	1.40	1.35
22	7	302	CLA	C4B-NB	6.40	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	101	8CT	C15-C16	6.40	1.59	1.45
22	4	313	CLA	C4B-NB	6.40	1.40	1.35
25	B	848	8CT	C15-C16	6.40	1.59	1.45
25	8	301	8CT	C05-C06	-6.40	1.36	1.52
25	B	843	8CT	C15-C16	6.40	1.59	1.45
25	3	316	8CT	C05-C06	-6.40	1.36	1.52
22	A	836	CLA	C4B-NB	6.40	1.40	1.35
22	5	303	CLA	C4B-NB	6.39	1.40	1.35
25	1	316	8CT	C28-C26	6.39	1.59	1.45
22	A	827	CLA	C4B-NB	6.39	1.40	1.35
22	B	823	CLA	C4B-NB	6.39	1.40	1.35
25	B	846	8CT	C05-C06	-6.39	1.36	1.52
22	A	817	CLA	C4B-NB	6.39	1.40	1.35
22	4	311	CLA	C4B-NB	6.38	1.40	1.35
25	A	850	8CT	C05-C06	-6.38	1.36	1.52
25	F	302	8CT	C04-C03	-6.38	1.45	1.53
25	2	317	8CT	C05-C06	-6.38	1.36	1.52
22	8	303	CLA	C4B-NB	6.38	1.40	1.35
25	5	317	8CT	C05-C06	-6.38	1.36	1.52
25	7	323	8CT	C05-C06	-6.38	1.36	1.52
25	J	104	8CT	C15-C16	6.37	1.59	1.45
25	7	321	8CT	C05-C06	-6.37	1.36	1.52
25	G	104	8CT	C28-C26	6.37	1.59	1.45
22	B	818	CLA	C4B-NB	6.37	1.40	1.35
22	2	304	CLA	C4B-NB	6.37	1.40	1.35
22	A	822	CLA	C4B-NB	6.36	1.40	1.35
22	A	809	CLA	C4B-NB	6.36	1.40	1.35
25	B	847	8CT	C15-C16	6.35	1.59	1.45
25	4	317	8CT	C28-C26	6.35	1.59	1.45
22	A	821	CLA	C4B-NB	6.35	1.40	1.35
22	B	822	CLA	C4B-NB	6.35	1.40	1.35
25	K	103	8CT	C05-C06	-6.35	1.36	1.52
22	K	102	CLA	C4B-NB	6.35	1.40	1.35
22	F	301	CLA	C4B-NB	6.35	1.40	1.35
22	A	837	CLA	C4B-NB	6.35	1.40	1.35
25	A	849	8CT	C15-C16	6.35	1.59	1.45
25	6	321	8CT	C15-C16	6.34	1.59	1.45
22	6	317	CLA	C4B-NB	6.34	1.40	1.35
22	A	840	CLA	C4B-NB	6.34	1.40	1.35
22	2	319	CLA	C4B-NB	6.34	1.40	1.35
22	3	301	CLA	C4B-NB	6.34	1.40	1.35
22	6	311	CLA	C4B-NB	6.34	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	846	8CT	C28-C26	6.33	1.59	1.45
22	5	302	CLA	C4B-NB	6.33	1.40	1.35
25	A	854	8CT	C15-C16	6.33	1.59	1.45
25	5	317	8CT	C15-C16	6.33	1.59	1.45
22	4	303	CLA	C4B-NB	6.32	1.40	1.35
22	A	841	CLA	C4B-NB	6.31	1.40	1.35
22	3	311	CLA	C4B-NB	6.31	1.40	1.35
25	2	317	8CT	C28-C26	6.31	1.59	1.45
22	A	802	CLA	C4B-NB	6.31	1.40	1.35
22	8	309	CLA	C4B-NB	6.31	1.40	1.35
25	L	206	8CT	C28-C26	6.31	1.59	1.45
25	7	323	8CT	C15-C16	6.31	1.59	1.45
25	7	321	8CT	C15-C16	6.30	1.59	1.45
25	7	323	8CT	C28-C26	6.30	1.59	1.45
25	B	845	8CT	C15-C16	6.30	1.59	1.45
25	B	843	8CT	C28-C26	6.29	1.59	1.45
22	L	201	CLA	C4B-NB	6.29	1.40	1.35
22	7	313	CLA	C4B-NB	6.29	1.40	1.35
22	B	832	CLA	C4B-NB	6.29	1.40	1.35
25	G	104	8CT	C05-C06	-6.29	1.37	1.52
25	A	849	8CT	C28-C26	6.28	1.59	1.45
25	B	851	8CT	C23-C21	6.28	1.59	1.45
25	A	850	8CT	C15-C16	6.28	1.59	1.45
22	B	814	CLA	C4B-NB	6.27	1.40	1.35
22	1	304	CLA	C4B-NB	6.27	1.40	1.35
22	B	819	CLA	C4B-NB	6.27	1.40	1.35
25	A	848	8CT	C15-C16	6.27	1.59	1.45
22	B	836	CLA	C4B-NB	6.26	1.40	1.35
22	B	827	CLA	C4B-NB	6.25	1.40	1.35
25	J	104	8CT	C28-C26	6.25	1.59	1.45
22	A	806	CLA	C4B-NB	6.25	1.40	1.35
25	B	847	8CT	C28-C26	6.25	1.59	1.45
25	8	301	8CT	C28-C26	6.25	1.59	1.45
22	A	803	CLA	C4B-NB	6.24	1.40	1.35
22	7	317	CLA	C4B-NB	6.24	1.40	1.35
25	A	846	8CT	C15-C16	6.23	1.59	1.45
22	8	302	CLA	C4B-NB	6.23	1.40	1.35
25	B	851	8CT	C28-C26	6.22	1.59	1.45
22	A	824	CLA	C4B-NB	6.22	1.40	1.35
25	A	850	8CT	C28-C26	6.22	1.59	1.45
25	A	854	8CT	C28-C26	6.22	1.59	1.45
22	1	311	CLA	C4B-NB	6.21	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	814	CLA	C4B-NB	6.21	1.40	1.35
22	B	829	CLA	C4B-NB	6.21	1.40	1.35
22	B	815	CLA	C4B-NB	6.21	1.40	1.35
25	3	316	8CT	C28-C26	6.21	1.59	1.45
25	J	101	8CT	C28-C26	6.21	1.59	1.45
22	A	831	CLA	C4B-NB	6.21	1.40	1.35
22	A	801	CLA	C4B-NB	6.20	1.40	1.35
22	A	833	CLA	C4B-NB	6.20	1.40	1.35
22	B	828	CLA	C4B-NB	6.20	1.40	1.35
22	2	308	CLA	C4B-NB	6.19	1.40	1.35
22	7	309	CLA	C4B-NB	6.19	1.40	1.35
25	8	318	8CT	C28-C26	6.19	1.59	1.45
22	6	313	CLA	C4B-NB	6.18	1.40	1.35
22	H	201	CLA	C4B-NB	6.18	1.40	1.35
22	B	808	CLA	C4B-NB	6.17	1.40	1.35
22	B	835	CLA	C4B-NB	6.17	1.40	1.35
22	B	801	CLA	C4B-NB	6.17	1.40	1.35
22	7	310	CLA	C4B-NB	6.16	1.40	1.35
25	7	321	8CT	C28-C26	6.16	1.59	1.45
25	6	321	8CT	C28-C26	6.16	1.59	1.45
22	A	828	CLA	C4B-NB	6.16	1.40	1.35
22	4	302	CLA	C4B-NB	6.14	1.40	1.35
25	7	301	8CT	C15-C16	6.14	1.59	1.45
22	A	832	CLA	C4B-NB	6.14	1.40	1.35
22	A	839	CLA	C4B-NB	6.14	1.40	1.35
22	B	826	CLA	C4B-NB	6.13	1.40	1.35
25	B	848	8CT	C28-C26	6.13	1.59	1.45
22	2	302	CLA	C4B-NB	6.12	1.40	1.35
22	A	804	CLA	C4B-NB	6.11	1.40	1.35
25	L	206	8CT	C15-C16	6.10	1.59	1.45
22	A	819	CLA	C4B-NB	6.07	1.40	1.35
25	A	847	8CT	C15-C16	6.05	1.58	1.45
22	B	807	CLA	C4B-NB	6.05	1.40	1.35
25	B	843	8CT	C23-C21	6.04	1.58	1.45
25	L	205	8CT	C28-C26	6.04	1.58	1.45
22	3	313	CLA	C4B-NB	6.03	1.40	1.35
25	B	844	8CT	C23-C21	6.02	1.58	1.45
22	A	820	CLA	C4B-NB	6.02	1.40	1.35
25	3	318	8CT	C15-C16	5.98	1.58	1.45
25	B	845	8CT	C28-C26	5.98	1.58	1.45
25	A	847	8CT	C28-C26	5.97	1.58	1.45
25	G	104	8CT	C23-C21	5.96	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	830	CLA	C4B-NB	5.96	1.40	1.35
25	A	848	8CT	C28-C26	5.96	1.58	1.45
22	B	803	CLA	C4B-NB	5.95	1.40	1.35
25	B	848	8CT	C23-C21	5.95	1.58	1.45
25	B	804	8CT	C15-C16	5.94	1.58	1.45
25	B	845	8CT	C23-C21	5.94	1.58	1.45
22	B	841	CLA	C4B-NB	5.94	1.40	1.35
25	2	317	8CT	C23-C21	5.94	1.58	1.45
22	B	817	CLA	C4B-NB	5.94	1.40	1.35
25	F	302	8CT	C28-C26	5.93	1.58	1.45
25	I	101	8CT	C15-C16	5.93	1.58	1.45
25	4	317	8CT	C23-C21	5.92	1.58	1.45
22	2	312	CLA	C4B-NB	5.92	1.40	1.35
25	B	844	8CT	C28-C26	5.92	1.58	1.45
22	A	813	CLA	C4B-NB	5.92	1.40	1.35
25	A	846	8CT	C28-C26	5.91	1.58	1.45
25	1	316	8CT	C23-C21	5.89	1.58	1.45
25	L	205	8CT	C15-C16	5.89	1.58	1.45
25	B	804	8CT	C28-C26	5.88	1.58	1.45
25	J	104	8CT	C23-C21	5.88	1.58	1.45
25	B	847	8CT	C23-C21	5.87	1.58	1.45
22	A	805	CLA	C4B-NB	5.87	1.40	1.35
25	3	316	8CT	C23-C21	5.86	1.58	1.45
25	L	206	8CT	C23-C21	5.86	1.58	1.45
25	8	318	8CT	C23-C21	5.86	1.58	1.45
25	7	323	8CT	C23-C21	5.85	1.58	1.45
25	J	101	8CT	C23-C21	5.84	1.58	1.45
25	8	301	8CT	C23-C21	5.84	1.58	1.45
25	7	301	8CT	C28-C26	5.83	1.58	1.45
25	A	849	8CT	C23-C21	5.83	1.58	1.45
25	3	318	8CT	C28-C26	5.82	1.58	1.45
22	4	309	CLA	C4B-NB	5.80	1.40	1.35
25	B	804	8CT	C04-C03	-5.80	1.45	1.53
25	6	321	8CT	C23-C21	5.80	1.58	1.45
22	4	308	CLA	C4B-NB	5.79	1.40	1.35
25	A	848	8CT	C23-C21	5.79	1.58	1.45
25	A	850	8CT	C23-C21	5.77	1.58	1.45
25	A	854	8CT	C23-C21	5.76	1.58	1.45
25	B	846	8CT	C23-C21	5.76	1.58	1.45
25	5	317	8CT	C23-C21	5.76	1.58	1.45
25	K	103	8CT	C34-C33	5.75	1.66	1.52
25	7	321	8CT	C23-C21	5.75	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	317	8CT	C34-C33	5.72	1.66	1.52
25	I	101	8CT	C04-C03	-5.70	1.45	1.53
25	A	846	8CT	C04-C03	-5.70	1.45	1.53
25	B	843	8CT	C04-C03	-5.69	1.46	1.53
25	7	323	8CT	C04-C03	-5.67	1.46	1.53
25	6	321	8CT	C04-C03	-5.67	1.46	1.53
25	A	849	8CT	C04-C03	-5.67	1.46	1.53
25	F	302	8CT	C15-C16	5.67	1.58	1.45
25	J	101	8CT	C34-C33	5.66	1.65	1.52
25	A	846	8CT	C23-C21	5.65	1.58	1.45
25	A	847	8CT	C04-C03	-5.64	1.46	1.53
25	L	206	8CT	C04-C03	-5.64	1.46	1.53
25	B	845	8CT	C04-C03	-5.63	1.46	1.53
25	I	101	8CT	C28-C26	5.63	1.58	1.45
25	L	206	8CT	C34-C33	5.62	1.65	1.52
25	3	318	8CT	C23-C21	5.62	1.58	1.45
25	7	301	8CT	C23-C21	5.62	1.58	1.45
22	B	806	CLA	C4B-NB	5.61	1.40	1.35
25	L	205	8CT	C23-C21	5.61	1.58	1.45
25	B	844	8CT	C34-C33	5.60	1.65	1.52
25	B	847	8CT	C34-C33	5.60	1.65	1.52
25	7	321	8CT	C04-C03	-5.58	1.46	1.53
25	K	103	8CT	C04-C03	-5.58	1.46	1.53
25	J	104	8CT	C34-C33	5.58	1.65	1.52
25	B	848	8CT	C34-C33	5.57	1.65	1.52
25	I	101	8CT	C34-C33	5.55	1.65	1.52
25	G	104	8CT	C34-C33	5.54	1.65	1.52
25	A	850	8CT	C34-C33	5.54	1.65	1.52
25	F	302	8CT	C23-C21	5.54	1.57	1.45
25	6	321	8CT	C34-C33	5.53	1.65	1.52
25	A	850	8CT	C04-C03	-5.52	1.46	1.53
25	J	104	8CT	C04-C03	-5.52	1.46	1.53
25	G	104	8CT	C04-C03	-5.50	1.46	1.53
25	B	846	8CT	C34-C33	5.50	1.65	1.52
25	B	848	8CT	C04-C03	-5.49	1.46	1.53
25	A	846	8CT	C34-C33	5.49	1.65	1.52
25	7	321	8CT	C34-C33	5.48	1.65	1.52
25	J	101	8CT	C04-C03	-5.48	1.46	1.53
25	8	318	8CT	C04-C03	-5.48	1.46	1.53
25	B	846	8CT	C04-C03	-5.47	1.46	1.53
25	A	854	8CT	C04-C03	-5.47	1.46	1.53
25	2	317	8CT	C04-C03	-5.47	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	316	8CT	C34-C33	5.46	1.65	1.52
25	1	316	8CT	C34-C33	5.46	1.65	1.52
25	2	317	8CT	C34-C33	5.45	1.65	1.52
25	4	317	8CT	C34-C33	5.45	1.65	1.52
25	8	301	8CT	C34-C33	5.45	1.65	1.52
25	8	318	8CT	C34-C33	5.44	1.65	1.52
25	5	317	8CT	C04-C03	-5.44	1.46	1.53
25	4	317	8CT	C04-C03	-5.43	1.46	1.53
25	A	854	8CT	C34-C33	5.43	1.65	1.52
25	I	101	8CT	C23-C21	5.42	1.57	1.45
25	3	316	8CT	C04-C03	-5.42	1.46	1.53
25	3	318	8CT	C04-C03	-5.41	1.46	1.53
25	8	301	8CT	C04-C03	-5.40	1.46	1.53
25	B	844	8CT	C04-C03	-5.40	1.46	1.53
25	7	323	8CT	C34-C33	5.40	1.65	1.52
25	A	848	8CT	C04-C03	-5.39	1.46	1.53
29	1	305	CHL	O2D-CGD	5.38	1.46	1.33
29	3	306	CHL	C3D-C4D	-5.38	1.32	1.44
25	A	849	8CT	C34-C33	5.37	1.65	1.52
29	7	308	CHL	C3D-C4D	-5.35	1.32	1.44
25	1	316	8CT	C04-C03	-5.34	1.46	1.53
25	B	804	8CT	C23-C21	5.34	1.57	1.45
25	B	847	8CT	C04-C03	-5.33	1.46	1.53
25	B	804	8CT	C34-C33	5.33	1.65	1.52
25	7	301	8CT	C34-C33	5.32	1.65	1.52
25	B	845	8CT	C34-C33	5.28	1.65	1.52
25	G	104	8CT	C05-C04	5.25	1.66	1.54
25	A	847	8CT	C23-C21	5.25	1.57	1.45
25	L	205	8CT	C34-C33	5.25	1.64	1.52
25	B	851	8CT	C04-C03	-5.24	1.46	1.53
29	2	306	CHL	C3D-C4D	-5.24	1.32	1.44
25	A	848	8CT	C05-C04	5.22	1.66	1.54
29	8	314	CHL	O2D-CGD	5.21	1.45	1.33
25	A	848	8CT	C34-C33	5.20	1.64	1.52
25	A	850	8CT	C05-C04	5.20	1.66	1.54
25	B	847	8CT	C05-C04	5.20	1.66	1.54
29	2	307	CHL	C3D-C4D	-5.19	1.32	1.44
25	7	321	8CT	C05-C04	5.18	1.66	1.54
29	5	301	CHL	C3D-C4D	-5.17	1.32	1.44
29	6	316	CHL	O2D-CGD	5.16	1.45	1.33
25	5	317	8CT	C05-C04	5.16	1.66	1.54
29	2	305	CHL	C3D-C4D	-5.15	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	316	8CT	C05-C04	5.15	1.66	1.54
29	5	306	CHL	O2D-CGD	5.14	1.45	1.33
25	A	854	8CT	C05-C04	5.14	1.66	1.54
25	8	318	8CT	C05-C04	5.13	1.66	1.54
25	B	843	8CT	C34-C33	5.11	1.64	1.52
25	B	848	8CT	C05-C04	5.11	1.65	1.54
25	B	846	8CT	C05-C04	5.11	1.65	1.54
25	J	101	8CT	C05-C04	5.10	1.65	1.54
25	K	103	8CT	C05-C04	5.10	1.65	1.54
29	4	305	CHL	C3D-C4D	-5.10	1.32	1.44
25	A	849	8CT	C05-C04	5.09	1.65	1.54
25	8	301	8CT	C05-C04	5.09	1.65	1.54
25	F	302	8CT	C34-C33	5.09	1.64	1.52
25	6	321	8CT	C05-C04	5.09	1.65	1.54
29	4	301	CHL	C3D-C4D	-5.09	1.32	1.44
29	0	301	CHL	CHC-C1C	5.08	1.48	1.35
25	2	317	8CT	C05-C04	5.08	1.65	1.54
25	3	316	8CT	C05-C04	5.06	1.65	1.54
29	4	306	CHL	C3D-C4D	-5.05	1.32	1.44
25	B	845	8CT	C05-C04	5.05	1.65	1.54
29	9	307	CHL	O2D-CGD	5.05	1.45	1.33
29	0	306	CHL	C3B-C2B	5.05	1.47	1.40
29	4	307	CHL	C3D-C4D	-5.05	1.32	1.44
29	8	306	CHL	O2D-CGD	5.04	1.45	1.33
29	0	301	CHL	O2D-CGD	5.04	1.45	1.33
29	2	301	CHL	C3D-C4D	-5.03	1.32	1.44
29	6	306	CHL	O2D-CGD	5.03	1.45	1.33
25	3	318	8CT	C34-C33	5.02	1.64	1.52
29	0	306	CHL	O2D-CGD	5.02	1.45	1.33
29	8	307	CHL	C3D-C4D	-5.02	1.32	1.44
25	7	323	8CT	C05-C04	5.02	1.65	1.54
29	6	307	CHL	CHC-C1C	5.01	1.47	1.35
25	A	847	8CT	C34-C33	5.01	1.64	1.52
29	5	306	CHL	C3B-C2B	5.01	1.47	1.40
25	B	851	8CT	C34-C33	5.01	1.64	1.52
25	7	301	8CT	C05-C04	5.01	1.65	1.54
25	J	104	8CT	C05-C04	5.01	1.65	1.54
29	6	307	CHL	C3D-C4D	-5.01	1.32	1.44
29	6	306	CHL	C3D-C4D	-5.00	1.32	1.44
29	6	302	CHL	C3D-C4D	-5.00	1.32	1.44
29	4	306	CHL	CHC-C1C	5.00	1.47	1.35
25	L	206	8CT	C05-C04	4.99	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	317	8CT	C05-C04	4.99	1.65	1.54
29	4	305	CHL	O2D-CGD	4.98	1.45	1.33
29	5	301	CHL	CHC-C1C	4.97	1.47	1.35
29	6	308	CHL	C3D-C4D	-4.97	1.33	1.44
29	8	306	CHL	C3D-C4D	-4.97	1.33	1.44
29	2	306	CHL	CHC-C1C	4.96	1.47	1.35
29	2	306	CHL	O2D-CGD	4.96	1.45	1.33
29	8	314	CHL	C3D-C4D	-4.95	1.33	1.44
29	1	305	CHL	CHC-C1C	4.95	1.47	1.35
29	9	307	CHL	C3D-C4D	-4.95	1.33	1.44
29	8	305	CHL	C3D-C4D	-4.95	1.33	1.44
29	6	316	CHL	C3D-C4D	-4.95	1.33	1.44
29	1	305	CHL	C3D-C4D	-4.94	1.33	1.44
29	9	302	CHL	O2D-CGD	4.94	1.45	1.33
25	B	844	8CT	C05-C04	4.94	1.65	1.54
29	0	306	CHL	C3D-C4D	-4.91	1.33	1.44
25	B	851	8CT	C05-C04	4.91	1.65	1.54
25	L	205	8CT	C05-C04	4.91	1.65	1.54
25	L	205	8CT	C04-C03	-4.91	1.47	1.53
25	B	804	8CT	C05-C04	4.90	1.65	1.54
29	6	307	CHL	O2D-CGD	4.89	1.45	1.33
29	6	302	CHL	CHC-C1C	4.89	1.47	1.35
29	6	302	CHL	O2D-CGD	4.88	1.45	1.33
29	0	301	CHL	C3D-C4D	-4.87	1.33	1.44
29	9	302	CHL	C3D-C4D	-4.86	1.33	1.44
25	A	846	8CT	C05-C04	4.85	1.65	1.54
29	9	307	CHL	CHC-C1C	4.85	1.47	1.35
29	6	308	CHL	CHC-C1C	4.85	1.47	1.35
29	0	301	CHL	C3B-C2B	4.85	1.47	1.40
25	7	301	8CT	C04-C03	-4.84	1.47	1.53
25	B	843	8CT	C05-C04	4.84	1.65	1.54
29	8	314	CHL	CHC-C1C	4.83	1.47	1.35
29	8	307	CHL	O2D-CGD	4.81	1.44	1.33
29	4	306	CHL	O2D-CGD	4.81	1.44	1.33
29	6	316	CHL	CHC-C1C	4.80	1.47	1.35
25	3	318	8CT	C05-C04	4.80	1.65	1.54
29	8	305	CHL	CHC-C1C	4.80	1.47	1.35
29	2	301	CHL	O2D-CGD	4.77	1.44	1.33
29	4	305	CHL	CHC-C1C	4.77	1.47	1.35
29	3	306	CHL	O2D-CGD	4.77	1.44	1.33
29	8	306	CHL	CHC-C1C	4.77	1.47	1.35
29	7	308	CHL	CHC-C1C	4.77	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	7	308	CHL	O2D-CGD	4.77	1.44	1.33
29	5	306	CHL	CHC-C1C	4.75	1.47	1.35
25	I	101	8CT	C05-C04	4.75	1.65	1.54
29	8	305	CHL	O2D-CGD	4.74	1.44	1.33
29	6	316	CHL	C3B-C2B	4.74	1.46	1.40
25	K	103	8CT	C06-C07	4.72	1.67	1.52
25	7	301	8CT	C19-C20	4.72	1.58	1.43
29	5	306	CHL	C3D-C4D	-4.72	1.33	1.44
29	6	307	CHL	C3B-C2B	4.72	1.46	1.40
29	6	308	CHL	O2D-CGD	4.72	1.44	1.33
25	J	104	8CT	C06-C07	4.70	1.67	1.52
29	0	306	CHL	CHC-C1C	4.70	1.47	1.35
25	B	846	8CT	C06-C07	4.69	1.67	1.52
25	B	851	8CT	C19-C20	4.69	1.58	1.43
29	9	302	CHL	CHC-C1C	4.68	1.47	1.35
25	7	323	8CT	C06-C07	4.68	1.67	1.52
25	G	104	8CT	C06-C07	4.68	1.67	1.52
25	B	848	8CT	C06-C07	4.68	1.67	1.52
29	0	306	CHL	C2C-C3C	4.67	1.46	1.36
29	9	307	CHL	C3B-C2B	4.66	1.46	1.40
25	A	850	8CT	C06-C07	4.66	1.67	1.52
25	1	316	8CT	C06-C07	4.66	1.67	1.52
25	A	847	8CT	C05-C04	4.65	1.64	1.54
25	5	317	8CT	C06-C07	4.65	1.67	1.52
25	6	321	8CT	C06-C07	4.64	1.67	1.52
29	5	301	CHL	O2D-CGD	4.64	1.44	1.33
25	4	317	8CT	C19-C20	4.63	1.57	1.43
29	4	301	CHL	CHC-C1C	4.63	1.46	1.35
25	B	844	8CT	C19-C20	4.62	1.57	1.43
25	B	847	8CT	C06-C07	4.62	1.67	1.52
25	7	321	8CT	C06-C07	4.62	1.67	1.52
25	8	318	8CT	C06-C07	4.62	1.67	1.52
25	A	849	8CT	C06-C07	4.61	1.67	1.52
25	3	316	8CT	C06-C07	4.61	1.67	1.52
29	4	306	CHL	CHD-C1D	4.60	1.47	1.38
25	2	317	8CT	C06-C07	4.60	1.67	1.52
29	8	307	CHL	CHC-C1C	4.60	1.46	1.35
25	B	844	8CT	C06-C07	4.60	1.67	1.52
25	B	804	8CT	C06-C07	4.60	1.67	1.52
29	4	307	CHL	CHC-C1C	4.60	1.46	1.35
29	2	305	CHL	CHC-C1C	4.60	1.46	1.35
25	8	301	8CT	C06-C07	4.59	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	854	8CT	C06-C07	4.59	1.66	1.52
25	B	843	8CT	C19-C20	4.59	1.57	1.43
25	A	848	8CT	C06-C07	4.58	1.66	1.52
25	4	317	8CT	C06-C07	4.58	1.66	1.52
25	F	302	8CT	C05-C04	4.58	1.64	1.54
29	1	305	CHL	C3B-C2B	4.58	1.46	1.40
25	1	316	8CT	C19-C20	4.58	1.57	1.43
29	2	307	CHL	CHC-C1C	4.57	1.46	1.35
29	4	307	CHL	O2D-CGD	4.56	1.44	1.33
25	G	104	8CT	C19-C20	4.56	1.57	1.43
25	K	103	8CT	C28-C29	4.56	1.43	1.32
29	5	306	CHL	C2C-C3C	4.55	1.46	1.36
29	6	306	CHL	CHC-C1C	4.53	1.46	1.35
25	8	318	8CT	C19-C20	4.52	1.57	1.43
25	8	301	8CT	C19-C20	4.52	1.57	1.43
25	A	846	8CT	C06-C07	4.52	1.66	1.52
25	I	101	8CT	C06-C07	4.51	1.66	1.52
25	J	101	8CT	C06-C07	4.51	1.66	1.52
25	J	104	8CT	C19-C20	4.51	1.57	1.43
29	4	305	CHL	C3B-C2B	4.51	1.46	1.40
25	K	103	8CT	C24-C25	4.51	1.57	1.43
29	9	307	CHL	C2C-C3C	4.50	1.46	1.36
29	2	307	CHL	O2D-CGD	4.50	1.44	1.33
25	7	323	8CT	C19-C20	4.50	1.57	1.43
29	0	301	CHL	C2C-C3C	4.50	1.46	1.36
25	B	851	8CT	C06-C07	4.49	1.66	1.52
29	0	306	CHL	CHD-C1D	4.49	1.47	1.38
25	B	848	8CT	C19-C20	4.49	1.57	1.43
25	A	854	8CT	C19-C20	4.49	1.57	1.43
29	3	306	CHL	CHC-C1C	4.49	1.46	1.35
29	2	305	CHL	O2D-CGD	4.49	1.44	1.33
25	L	206	8CT	C06-C07	4.48	1.66	1.52
25	3	316	8CT	C19-C20	4.48	1.57	1.43
25	L	206	8CT	C19-C20	4.48	1.57	1.43
25	K	103	8CT	C19-C20	4.47	1.57	1.43
25	B	845	8CT	C06-C07	4.47	1.66	1.52
25	5	317	8CT	C24-C25	4.46	1.57	1.43
25	J	101	8CT	C19-C20	4.46	1.57	1.43
25	B	843	8CT	C06-C07	4.46	1.66	1.52
25	B	847	8CT	C19-C20	4.46	1.57	1.43
25	A	849	8CT	C19-C20	4.45	1.57	1.43
25	B	846	8CT	C19-C20	4.45	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	305	CHL	O2A-CGA	4.44	1.46	1.33
25	A	846	8CT	C19-C20	4.44	1.57	1.43
29	8	314	CHL	C3B-C2B	4.43	1.46	1.40
25	A	847	8CT	C06-C07	4.43	1.66	1.52
25	A	850	8CT	C19-C20	4.43	1.57	1.43
29	4	306	CHL	C2C-C3C	4.42	1.46	1.36
25	5	317	8CT	C19-C20	4.41	1.57	1.43
25	7	321	8CT	C19-C20	4.40	1.57	1.43
29	0	301	CHL	O2A-CGA	4.40	1.46	1.33
25	6	321	8CT	C19-C20	4.40	1.57	1.43
29	8	305	CHL	O2A-CGA	4.40	1.46	1.33
25	L	205	8CT	C06-C07	4.40	1.66	1.52
25	A	848	8CT	C19-C20	4.39	1.57	1.43
29	4	301	CHL	O2A-CGA	4.39	1.46	1.33
29	8	306	CHL	O2A-CGA	4.38	1.46	1.33
25	F	302	8CT	C06-C07	4.38	1.66	1.52
25	7	301	8CT	C06-C07	4.38	1.66	1.52
29	4	306	CHL	C3B-C2B	4.38	1.46	1.40
25	2	317	8CT	C19-C20	4.37	1.57	1.43
29	1	305	CHL	O2A-CGA	4.37	1.46	1.33
29	0	301	CHL	CHD-C1D	4.37	1.46	1.38
25	3	318	8CT	C06-C07	4.37	1.66	1.52
29	5	301	CHL	C2C-C3C	4.36	1.46	1.36
25	B	843	8CT	C24-C25	4.35	1.56	1.43
29	5	306	CHL	CHD-C1D	4.34	1.46	1.38
29	0	306	CHL	O2A-CGA	4.34	1.46	1.33
29	6	302	CHL	C2C-C3C	4.34	1.46	1.36
29	6	307	CHL	C2C-C3C	4.34	1.46	1.36
29	6	316	CHL	C2C-C3C	4.34	1.46	1.36
29	8	314	CHL	C2C-C3C	4.34	1.46	1.36
29	9	307	CHL	O2A-CGA	4.33	1.46	1.33
25	B	804	8CT	C19-C20	4.33	1.56	1.43
29	4	301	CHL	O2D-CGD	4.33	1.43	1.33
29	2	301	CHL	O2A-CGA	4.33	1.46	1.33
29	4	307	CHL	O2A-CGA	4.33	1.46	1.33
25	L	205	8CT	C19-C20	4.32	1.56	1.43
25	A	846	8CT	C24-C25	4.32	1.56	1.43
25	B	845	8CT	C19-C20	4.31	1.56	1.43
29	9	307	CHL	CHD-C1D	4.31	1.46	1.38
29	1	305	CHL	CHD-C1D	4.30	1.46	1.38
29	6	308	CHL	O2A-CGA	4.30	1.45	1.33
29	9	302	CHL	C3B-C2B	4.30	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	L	205	8CT	C24-C25	4.29	1.56	1.43
29	6	307	CHL	CHD-C1D	4.28	1.46	1.38
25	B	851	8CT	C24-C25	4.27	1.56	1.43
29	5	306	CHL	O2A-CGA	4.27	1.45	1.33
29	2	301	CHL	C3B-C2B	4.27	1.46	1.40
25	3	318	8CT	C19-C20	4.27	1.56	1.43
29	5	301	CHL	O2A-CGA	4.26	1.45	1.33
29	6	308	CHL	C2C-C3C	4.25	1.45	1.36
29	8	305	CHL	C2C-C3C	4.25	1.45	1.36
25	B	846	8CT	C24-C25	4.24	1.56	1.43
29	6	316	CHL	CHD-C1D	4.24	1.46	1.38
29	9	302	CHL	O2A-CGA	4.24	1.45	1.33
25	4	317	8CT	C24-C25	4.24	1.56	1.43
25	B	844	8CT	C24-C25	4.23	1.56	1.43
29	2	301	CHL	CHC-C1C	4.23	1.45	1.35
29	6	302	CHL	O2A-CGA	4.22	1.45	1.33
29	8	307	CHL	CHD-C1D	4.22	1.46	1.38
29	2	306	CHL	O2A-CGA	4.22	1.45	1.33
29	8	314	CHL	CHD-C1D	4.21	1.46	1.38
25	I	101	8CT	C19-C20	4.21	1.56	1.43
25	G	104	8CT	C24-C25	4.21	1.56	1.43
29	2	307	CHL	O2A-CGA	4.20	1.45	1.33
25	A	847	8CT	C19-C20	4.20	1.56	1.43
29	4	305	CHL	C2C-C3C	4.20	1.45	1.36
29	8	306	CHL	C3B-C2B	4.19	1.46	1.40
29	4	301	CHL	C2C-C3C	4.19	1.45	1.36
25	1	316	8CT	C24-C25	4.19	1.56	1.43
25	8	318	8CT	C24-C25	4.19	1.56	1.43
25	A	848	8CT	C24-C25	4.18	1.56	1.43
29	8	307	CHL	C2C-C3C	4.18	1.45	1.36
22	B	814	CLA	C4D-ND	-4.18	1.32	1.37
29	8	305	CHL	C3B-C2B	4.18	1.46	1.40
25	2	317	8CT	C24-C25	4.17	1.56	1.43
29	4	306	CHL	O2A-CGA	4.17	1.45	1.33
25	B	848	8CT	C24-C25	4.17	1.56	1.43
25	3	316	8CT	C24-C25	4.16	1.56	1.43
25	B	845	8CT	C24-C25	4.16	1.56	1.43
25	F	302	8CT	C19-C20	4.16	1.56	1.43
25	A	854	8CT	C24-C25	4.16	1.56	1.43
25	B	847	8CT	C24-C25	4.16	1.56	1.43
29	6	302	CHL	C3B-C2B	4.16	1.46	1.40
25	J	104	8CT	C24-C25	4.15	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	305	CHL	CHD-C1D	4.15	1.46	1.38
29	6	306	CHL	C3B-C2B	4.15	1.46	1.40
29	9	302	CHL	C2C-C3C	4.14	1.45	1.36
25	L	206	8CT	C24-C25	4.14	1.56	1.43
29	5	301	CHL	C3B-C2B	4.14	1.46	1.40
25	7	323	8CT	C24-C25	4.14	1.56	1.43
25	8	301	8CT	C24-C25	4.14	1.56	1.43
25	J	101	8CT	C24-C25	4.12	1.56	1.43
22	A	805	CLA	C4D-ND	-4.12	1.32	1.37
29	2	306	CHL	C2C-C3C	4.12	1.45	1.36
29	2	306	CHL	CHD-C1D	4.11	1.46	1.38
23	B	842	PQN	C10-C5	4.10	1.47	1.40
29	6	302	CHL	CHD-C1D	4.10	1.46	1.38
25	A	849	8CT	C24-C25	4.10	1.56	1.43
29	8	306	CHL	C2C-C3C	4.09	1.45	1.36
29	7	308	CHL	C2C-C3C	4.09	1.45	1.36
29	1	305	CHL	C2C-C3C	4.09	1.45	1.36
25	A	850	8CT	C24-C25	4.07	1.56	1.43
22	5	308	CLA	C1D-ND	4.07	1.42	1.37
29	2	305	CHL	C2C-C3C	4.07	1.45	1.36
29	0	306	CHL	CHD-C4C	4.06	1.48	1.39
25	7	321	8CT	C24-C25	4.06	1.56	1.43
25	7	301	8CT	C24-C25	4.06	1.56	1.43
26	J	102	HTG	C1'-S1	-4.06	1.76	1.81
25	B	844	8CT	C14-C13	4.05	1.56	1.43
29	8	306	CHL	CHD-C1D	4.05	1.46	1.38
25	6	321	8CT	C24-C25	4.05	1.56	1.43
29	6	306	CHL	CHD-C1D	4.05	1.46	1.38
29	5	301	CHL	CHD-C1D	4.04	1.46	1.38
22	7	317	CLA	C4D-ND	-4.03	1.32	1.37
29	4	307	CHL	C2C-C3C	4.02	1.45	1.36
29	5	306	CHL	CHD-C4C	4.01	1.48	1.39
29	2	305	CHL	C3B-C2B	4.01	1.45	1.40
29	8	307	CHL	O2A-CGA	4.01	1.45	1.33
29	8	305	CHL	CHD-C1D	4.00	1.46	1.38
25	K	103	8CT	C25-C26	4.00	1.41	1.35
29	6	306	CHL	C2C-C3C	4.00	1.45	1.36
29	4	301	CHL	C3B-C2B	3.99	1.45	1.40
29	2	306	CHL	C3B-C2B	3.99	1.45	1.40
22	B	808	CLA	C4D-ND	-3.98	1.32	1.37
25	B	851	8CT	C14-C13	3.97	1.55	1.43
29	9	307	CHL	CHD-C4C	3.96	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	318	8CT	C24-C25	3.96	1.55	1.43
29	0	301	CHL	CHD-C4C	3.96	1.48	1.39
22	B	826	CLA	C4D-ND	-3.96	1.32	1.37
29	9	302	CHL	CHD-C1D	3.96	1.46	1.38
29	8	307	CHL	C3B-C2B	3.95	1.45	1.40
22	A	837	CLA	C4D-ND	-3.93	1.32	1.37
22	A	813	CLA	C4D-ND	-3.93	1.32	1.37
25	A	848	8CT	C14-C13	3.92	1.55	1.43
29	2	301	CHL	CHD-C1D	3.92	1.46	1.38
23	A	842	PQN	C10-C5	3.92	1.47	1.40
25	5	317	8CT	C28-C29	3.89	1.41	1.32
22	B	838	CLA	C4D-ND	-3.89	1.32	1.37
22	A	814	CLA	C4D-ND	-3.89	1.32	1.37
29	7	308	CHL	O2A-CGA	3.89	1.45	1.33
26	A	851	HTG	C1'-S1	-3.89	1.76	1.81
29	6	308	CHL	CHD-C1D	3.89	1.45	1.38
29	4	306	CHL	CHD-C4C	3.88	1.48	1.39
29	8	314	CHL	CHD-C4C	3.88	1.48	1.39
29	3	306	CHL	C3B-C2B	3.88	1.45	1.40
25	I	101	8CT	C24-C25	3.88	1.55	1.43
25	K	103	8CT	C30-C29	3.88	1.56	1.50
25	G	104	8CT	C14-C13	3.87	1.55	1.43
29	6	316	CHL	CHD-C4C	3.87	1.48	1.39
25	B	843	8CT	C14-C13	3.87	1.55	1.43
25	F	302	8CT	C24-C25	3.86	1.55	1.43
22	1	312	CLA	C1D-ND	3.86	1.42	1.37
25	J	101	8CT	C14-C13	3.86	1.55	1.43
25	2	317	8CT	C14-C13	3.86	1.55	1.43
29	3	306	CHL	O2A-CGA	3.86	1.45	1.33
25	B	804	8CT	C24-C25	3.86	1.55	1.43
22	0	307	CLA	C1D-ND	3.85	1.42	1.37
22	B	806	CLA	C4D-ND	-3.85	1.32	1.37
25	B	846	8CT	C14-C13	3.85	1.55	1.43
22	B	827	CLA	C4D-ND	-3.85	1.32	1.37
25	3	316	8CT	C14-C13	3.85	1.55	1.43
22	9	301	CLA	CAB-C3B	-3.85	1.43	1.51
25	5	317	8CT	C11-C12	3.85	1.54	1.45
25	4	317	8CT	C14-C13	3.85	1.55	1.43
25	B	848	8CT	C14-C13	3.85	1.55	1.43
30	2	315	XAT	O4-C5	-3.84	1.40	1.46
25	G	104	8CT	C11-C12	3.84	1.54	1.45
25	1	316	8CT	C14-C13	3.84	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	303	CLA	C4D-ND	-3.84	1.32	1.37
25	7	301	8CT	C14-C13	3.84	1.55	1.43
22	B	812	CLA	C4D-ND	-3.84	1.32	1.37
25	A	846	8CT	C14-C13	3.84	1.55	1.43
22	0	302	CLA	C4D-ND	-3.84	1.32	1.37
25	A	849	8CT	C14-C13	3.84	1.55	1.43
25	K	103	8CT	C14-C13	3.84	1.55	1.43
25	1	316	8CT	C11-C12	3.84	1.54	1.45
25	8	318	8CT	C14-C13	3.83	1.55	1.43
25	B	847	8CT	C14-C13	3.83	1.55	1.43
29	1	305	CHL	CHD-C4C	3.82	1.48	1.39
22	B	809	CLA	C4D-ND	-3.82	1.32	1.37
22	A	815	CLA	C4D-ND	-3.82	1.32	1.37
29	6	308	CHL	C3B-C2B	3.82	1.45	1.40
25	8	301	8CT	C14-C13	3.82	1.55	1.43
22	B	820	CLA	C4D-ND	-3.81	1.32	1.37
25	8	301	8CT	C11-C12	3.81	1.54	1.45
22	B	828	CLA	C4D-ND	-3.81	1.32	1.37
25	5	317	8CT	C14-C13	3.81	1.55	1.43
22	A	809	CLA	C4D-ND	-3.81	1.32	1.37
29	8	306	CHL	CHD-C4C	3.80	1.47	1.39
22	B	836	CLA	C4D-ND	-3.80	1.32	1.37
22	3	305	CLA	C4D-ND	-3.79	1.32	1.37
25	B	847	8CT	C11-C12	3.79	1.54	1.45
22	2	310	CLA	C4D-ND	-3.79	1.32	1.37
22	A	811	CLA	C4D-ND	-3.79	1.32	1.37
22	L	201	CLA	C4D-ND	-3.79	1.32	1.37
22	7	315	CLA	C4D-ND	-3.79	1.32	1.37
25	J	104	8CT	C11-C12	3.79	1.54	1.45
25	7	323	8CT	C14-C13	3.79	1.55	1.43
22	7	304	CLA	C4D-ND	-3.78	1.32	1.37
22	2	303	CLA	C4D-ND	-3.78	1.32	1.37
25	B	851	8CT	C28-C29	3.78	1.41	1.32
25	4	317	8CT	C28-C29	3.77	1.41	1.32
22	3	307	CLA	C4D-ND	-3.77	1.32	1.37
25	A	854	8CT	C14-C13	3.77	1.55	1.43
22	6	304	CLA	C4D-ND	-3.76	1.32	1.37
25	2	317	8CT	C11-C12	3.76	1.54	1.45
22	5	302	CLA	C4D-ND	-3.76	1.32	1.37
29	8	307	CHL	CHD-C4C	3.76	1.47	1.39
29	8	314	CHL	OBD-CAD	3.76	1.29	1.22
25	4	317	8CT	C11-C12	3.76	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	846	8CT	C11-C12	3.75	1.54	1.45
29	0	306	CHL	OBD-CAD	3.75	1.28	1.22
25	8	318	8CT	C11-C12	3.75	1.54	1.45
30	0	313	XAT	O24-C25	-3.75	1.40	1.46
25	7	321	8CT	C14-C13	3.75	1.55	1.43
25	6	321	8CT	C14-C13	3.74	1.55	1.43
22	A	839	CLA	C4D-ND	-3.74	1.32	1.37
22	2	308	CLA	C4D-ND	-3.74	1.32	1.37
22	B	817	CLA	C4D-ND	-3.74	1.32	1.37
25	L	206	8CT	C14-C13	3.74	1.55	1.43
29	7	308	CHL	C3B-C2B	3.74	1.45	1.40
25	J	101	8CT	C11-C12	3.74	1.54	1.45
29	4	305	CHL	CHD-C4C	3.74	1.47	1.39
29	2	306	CHL	CHD-C4C	3.73	1.47	1.39
25	B	848	8CT	C11-C12	3.73	1.54	1.45
25	J	104	8CT	C14-C13	3.73	1.55	1.43
29	5	301	CHL	CHD-C4C	3.73	1.47	1.39
25	7	323	8CT	C11-C12	3.73	1.54	1.45
22	A	812	CLA	C4D-ND	-3.73	1.32	1.37
22	B	837	CLA	C4D-ND	-3.73	1.32	1.37
22	0	312	CLA	C1D-ND	3.72	1.42	1.37
22	B	821	CLA	C4D-ND	-3.72	1.32	1.37
22	7	305	CLA	C4D-ND	-3.72	1.32	1.37
22	A	808	CLA	C4D-ND	-3.72	1.32	1.37
25	A	854	8CT	C11-C12	3.72	1.53	1.45
22	4	309	CLA	C4D-ND	-3.72	1.32	1.37
29	9	307	CHL	OBD-CAD	3.71	1.28	1.22
22	A	828	CLA	C4D-ND	-3.71	1.32	1.37
29	6	307	CHL	CHD-C4C	3.71	1.47	1.39
29	2	301	CHL	CHD-C4C	3.71	1.47	1.39
29	6	308	CHL	CHD-C4C	3.71	1.47	1.39
22	6	323	CLA	C4D-ND	-3.71	1.32	1.37
25	K	103	8CT	C11-C12	3.70	1.53	1.45
22	3	302	CLA	C4D-ND	-3.70	1.32	1.37
25	A	849	8CT	C11-C12	3.70	1.53	1.45
29	4	301	CHL	CHD-C1D	3.70	1.45	1.38
25	7	301	8CT	C11-C12	3.70	1.53	1.45
22	B	824	CLA	C4D-ND	-3.70	1.32	1.37
25	A	850	8CT	C14-C13	3.70	1.54	1.43
22	B	819	CLA	C4D-ND	-3.70	1.32	1.37
25	B	845	8CT	C14-C13	3.70	1.54	1.43
22	3	301	CLA	C4D-ND	-3.69	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	321	8CT	C11-C12	3.69	1.53	1.45
22	3	319	CLA	C4D-ND	-3.69	1.32	1.37
22	6	310	CLA	C4D-ND	-3.69	1.32	1.37
25	A	847	8CT	C24-C25	3.69	1.54	1.43
22	1	313	CLA	C4D-ND	-3.69	1.32	1.37
22	8	310	CLA	C4D-ND	-3.69	1.32	1.37
22	G	101	CLA	C1D-ND	3.69	1.42	1.37
22	4	311	CLA	C4D-ND	-3.68	1.32	1.37
25	B	851	8CT	C11-C12	3.68	1.53	1.45
25	A	848	8CT	C11-C12	3.68	1.53	1.45
29	1	305	CHL	OBD-CAD	3.68	1.28	1.22
25	B	846	8CT	C28-C29	3.68	1.41	1.32
25	2	317	8CT	C28-C29	3.68	1.41	1.32
22	4	308	CLA	C4D-ND	-3.68	1.32	1.37
22	3	308	CLA	C4D-ND	-3.68	1.32	1.37
22	8	308	CLA	C4D-ND	-3.68	1.32	1.37
22	A	838	CLA	C4D-ND	-3.68	1.32	1.37
25	B	844	8CT	C11-C12	3.68	1.53	1.45
22	A	840	CLA	C4D-ND	-3.68	1.32	1.37
25	F	302	8CT	C14-C13	3.67	1.54	1.43
29	5	306	CHL	OBD-CAD	3.67	1.28	1.22
22	4	310	CLA	C4D-ND	-3.67	1.32	1.37
25	B	843	8CT	C11-C12	3.67	1.53	1.45
22	5	305	CLA	C1D-ND	3.67	1.42	1.37
22	F	301	CLA	C4D-ND	-3.67	1.32	1.37
25	G	104	8CT	C28-C29	3.66	1.41	1.32
22	3	304	CLA	C4D-ND	-3.66	1.32	1.37
22	2	313	CLA	C4D-ND	-3.66	1.32	1.37
22	A	853	CLA	C4D-ND	-3.66	1.32	1.37
25	3	318	8CT	C28-C29	3.65	1.40	1.32
29	6	302	CHL	CHD-C4C	3.65	1.47	1.39
25	A	850	8CT	C11-C12	3.65	1.53	1.45
22	A	826	CLA	C4D-ND	-3.65	1.32	1.37
22	7	310	CLA	C4D-ND	-3.65	1.32	1.37
22	8	303	CLA	C4D-ND	-3.65	1.32	1.37
25	I	101	8CT	C14-C13	3.64	1.54	1.43
25	7	321	8CT	C11-C12	3.64	1.53	1.45
22	2	302	CLA	C4D-ND	-3.64	1.32	1.37
25	L	206	8CT	C28-C29	3.64	1.40	1.32
22	8	311	CLA	C1D-ND	3.64	1.42	1.37
22	A	831	CLA	C4D-ND	-3.64	1.32	1.37
22	L	204	CLA	C1D-ND	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	316	8CT	C11-C12	3.64	1.53	1.45
22	A	830	CLA	C4D-ND	-3.64	1.32	1.37
25	A	846	8CT	C11-C12	3.64	1.53	1.45
22	B	835	CLA	C4D-ND	-3.63	1.32	1.37
22	B	840	CLA	C4D-ND	-3.63	1.32	1.37
22	A	852	CLA	C4D-ND	-3.63	1.32	1.37
22	B	841	CLA	C4D-ND	-3.63	1.32	1.37
22	2	312	CLA	C4D-ND	-3.63	1.32	1.37
29	2	301	CHL	C2C-C3C	3.63	1.44	1.36
22	A	827	CLA	C4D-ND	-3.62	1.32	1.37
25	L	205	8CT	C14-C13	3.62	1.54	1.43
22	H	201	CLA	C4D-ND	-3.62	1.32	1.37
22	A	834	CLA	C4D-ND	-3.62	1.32	1.37
22	A	836	CLA	C4D-ND	-3.62	1.32	1.37
22	3	310	CLA	C4D-ND	-3.62	1.32	1.37
22	7	309	CLA	C4D-ND	-3.62	1.32	1.37
22	6	305	CLA	C4D-ND	-3.62	1.32	1.37
25	3	318	8CT	C14-C13	3.62	1.54	1.43
25	7	323	8CT	C28-C29	3.62	1.40	1.32
25	J	104	8CT	C28-C29	3.61	1.40	1.32
25	3	316	8CT	C28-C29	3.61	1.40	1.32
22	A	803	CLA	C4D-ND	-3.61	1.32	1.37
29	4	307	CHL	C3B-C2B	3.61	1.45	1.40
29	7	308	CHL	CHD-C1D	3.61	1.45	1.38
22	8	311	CLA	C4D-ND	-3.61	1.32	1.37
22	A	833	CLA	C4D-ND	-3.61	1.32	1.37
25	1	316	8CT	C28-C29	3.61	1.40	1.32
22	2	309	CLA	C4D-ND	-3.61	1.32	1.37
29	2	307	CHL	CHD-C1D	3.60	1.45	1.38
29	3	306	CHL	C2C-C3C	3.60	1.44	1.36
25	A	847	8CT	C14-C13	3.60	1.54	1.43
22	A	819	CLA	C4D-ND	-3.60	1.32	1.37
29	9	302	CHL	CHD-C4C	3.59	1.47	1.39
25	A	846	8CT	C28-C29	3.59	1.40	1.32
25	B	848	8CT	C28-C29	3.59	1.40	1.32
25	L	205	8CT	C28-C29	3.59	1.40	1.32
29	9	302	CHL	OBD-CAD	3.59	1.28	1.22
22	B	831	CLA	C4D-ND	-3.59	1.32	1.37
25	B	804	8CT	C14-C13	3.59	1.54	1.43
29	2	305	CHL	CHD-C1D	3.59	1.45	1.38
25	8	301	8CT	C28-C29	3.59	1.40	1.32
22	A	802	CLA	C4D-ND	-3.59	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	305	CHL	CHD-C4C	3.58	1.47	1.39
22	1	303	CLA	C4D-ND	-3.58	1.32	1.37
25	L	206	8CT	C11-C12	3.58	1.53	1.45
25	A	854	8CT	C28-C29	3.58	1.40	1.32
22	4	304	CLA	C4D-ND	-3.57	1.32	1.37
22	A	824	CLA	C4D-ND	-3.57	1.32	1.37
29	2	307	CHL	CHD-C4C	3.57	1.47	1.39
22	A	829	CLA	C4D-ND	-3.57	1.32	1.37
22	A	843	CLA	C4D-ND	-3.57	1.32	1.37
25	B	844	8CT	C28-C29	3.57	1.40	1.32
22	M	101	CLA	C4D-ND	-3.56	1.32	1.37
22	0	309	CLA	C1D-ND	3.56	1.42	1.37
22	A	820	CLA	C4D-ND	-3.56	1.32	1.37
25	A	850	8CT	C28-C29	3.56	1.40	1.32
25	A	849	8CT	C28-C29	3.56	1.40	1.32
25	B	843	8CT	C28-C29	3.56	1.40	1.32
22	1	309	CLA	C4D-ND	-3.55	1.32	1.37
25	7	321	8CT	C28-C29	3.55	1.40	1.32
29	6	306	CHL	CHD-C4C	3.55	1.47	1.39
29	8	307	CHL	OBD-CAD	3.54	1.28	1.22
22	3	313	CLA	C4D-ND	-3.54	1.32	1.37
29	4	305	CHL	OBD-CAD	3.54	1.28	1.22
25	B	847	8CT	C28-C29	3.53	1.40	1.32
22	6	318	CLA	C1D-ND	3.53	1.42	1.37
22	0	304	CLA	C1D-ND	3.53	1.42	1.37
22	B	811	CLA	C1D-ND	3.53	1.42	1.37
25	6	321	8CT	C28-C29	3.53	1.40	1.32
22	9	304	CLA	C4D-ND	-3.53	1.32	1.37
22	A	823	CLA	C4D-ND	-3.53	1.32	1.37
22	B	829	CLA	C4D-ND	-3.53	1.32	1.37
22	L	203	CLA	C4D-ND	-3.53	1.32	1.37
29	5	301	CHL	OBD-CAD	3.53	1.28	1.22
22	B	822	CLA	C4D-ND	-3.52	1.32	1.37
29	4	307	CHL	CHD-C1D	3.52	1.45	1.38
29	2	307	CHL	C3B-C2B	3.52	1.45	1.40
25	J	101	8CT	C28-C29	3.52	1.40	1.32
22	6	313	CLA	C4D-ND	-3.52	1.32	1.37
29	7	308	CHL	CHD-C4C	3.52	1.47	1.39
25	5	317	8CT	C30-C29	3.52	1.55	1.50
29	8	306	CHL	OBD-CAD	3.52	1.28	1.22
22	B	823	CLA	C4D-ND	-3.51	1.32	1.37
22	8	312	CLA	C4D-ND	-3.51	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	306	CLA	C1D-ND	3.51	1.42	1.37
22	9	310	CLA	C1D-ND	3.51	1.42	1.37
22	A	818	CLA	C4D-ND	-3.51	1.32	1.37
22	A	821	CLA	C4D-ND	-3.51	1.32	1.37
22	6	315	CLA	C4D-ND	-3.51	1.32	1.37
22	7	302	CLA	C4D-ND	-3.51	1.32	1.37
22	8	302	CLA	C4D-ND	-3.51	1.32	1.37
22	B	834	CLA	C4D-ND	-3.50	1.32	1.37
22	6	309	CLA	C4D-ND	-3.50	1.32	1.37
29	4	307	CHL	CHD-C4C	3.50	1.47	1.39
22	1	301	CLA	C4D-ND	-3.50	1.32	1.37
22	7	310	CLA	C1D-ND	3.50	1.42	1.37
22	8	309	CLA	C4D-ND	-3.50	1.32	1.37
22	2	311	CLA	C4D-ND	-3.50	1.32	1.37
22	B	818	CLA	C4D-ND	-3.50	1.32	1.37
22	B	801	CLA	C4D-ND	-3.49	1.32	1.37
22	7	303	CLA	C4D-ND	-3.49	1.32	1.37
22	6	301	CLA	C1D-ND	3.49	1.42	1.37
22	A	816	CLA	C4D-ND	-3.49	1.32	1.37
29	6	316	CHL	OBD-CAD	3.49	1.28	1.22
22	A	806	CLA	C4D-ND	-3.49	1.32	1.37
29	4	301	CHL	CHD-C4C	3.48	1.47	1.39
25	7	301	8CT	C28-C29	3.48	1.40	1.32
22	B	805	CLA	C4D-ND	-3.48	1.32	1.37
22	K	104	CLA	C4D-ND	-3.48	1.32	1.37
22	5	311	CLA	C1D-ND	3.48	1.42	1.37
22	1	307	CLA	C4D-ND	-3.47	1.32	1.37
22	9	312	CLA	C1D-ND	3.47	1.42	1.37
22	0	310	CLA	C1D-ND	3.47	1.42	1.37
29	4	301	CHL	OBD-CAD	3.46	1.28	1.22
22	6	318	CLA	C4D-ND	-3.46	1.32	1.37
22	5	313	CLA	C4D-ND	-3.46	1.32	1.37
25	B	843	8CT	C30-C29	3.46	1.55	1.50
22	6	312	CLA	C4D-ND	-3.46	1.32	1.37
22	B	830	CLA	C4D-ND	-3.46	1.32	1.37
22	1	311	CLA	C4D-ND	-3.46	1.32	1.37
22	9	311	CLA	C4D-ND	-3.46	1.32	1.37
25	A	848	8CT	C28-C29	3.46	1.40	1.32
22	B	813	CLA	C4D-ND	-3.45	1.32	1.37
22	B	803	CLA	C4D-ND	-3.45	1.32	1.37
29	3	306	CHL	CHD-C1D	3.45	1.45	1.38
22	6	317	CLA	C4D-ND	-3.45	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	I	101	8CT	C01-C02	3.45	1.56	1.50
22	A	830	CLA	CMB-C2B	-3.45	1.44	1.51
25	A	846	8CT	C30-C29	3.45	1.55	1.50
29	4	306	CHL	OBD-CAD	3.45	1.28	1.22
22	4	314	CLA	C1D-ND	3.45	1.42	1.37
22	7	307	CLA	C4D-ND	-3.45	1.33	1.37
22	B	825	CLA	C4D-ND	-3.45	1.33	1.37
22	3	319	CLA	C1D-ND	3.44	1.42	1.37
22	0	311	CLA	C1D-ND	3.44	1.42	1.37
29	2	307	CHL	C2C-C3C	3.44	1.44	1.36
22	1	310	CLA	C4D-ND	-3.44	1.33	1.37
22	4	313	CLA	C4D-ND	-3.44	1.33	1.37
22	B	832	CLA	C4D-ND	-3.43	1.33	1.37
22	2	319	CLA	C4D-ND	-3.43	1.33	1.37
22	2	304	CLA	C4D-ND	-3.43	1.33	1.37
22	9	301	CLA	C4D-ND	-3.43	1.33	1.37
22	7	318	CLA	C4D-ND	-3.43	1.33	1.37
29	0	301	CHL	OBD-CAD	3.43	1.28	1.22
22	5	314	CLA	C1D-ND	3.43	1.42	1.37
22	5	314	CLA	C4D-ND	-3.42	1.33	1.37
22	7	313	CLA	C4D-ND	-3.42	1.33	1.37
25	A	847	8CT	C28-C29	3.42	1.40	1.32
22	B	833	CLA	C4D-ND	-3.42	1.33	1.37
22	5	304	CLA	C4D-ND	-3.42	1.33	1.37
29	6	302	CHL	OBD-CAD	3.42	1.28	1.22
22	9	309	CLA	C1D-ND	3.42	1.42	1.37
22	7	318	CLA	C1D-ND	3.42	1.42	1.37
25	8	318	8CT	C28-C29	3.42	1.40	1.32
25	B	846	8CT	C01-C02	3.42	1.56	1.50
22	3	311	CLA	C4D-ND	-3.42	1.33	1.37
22	8	304	CLA	C4D-ND	-3.41	1.33	1.37
22	0	303	CLA	C1D-ND	3.41	1.42	1.37
22	0	311	CLA	C4D-ND	-3.41	1.33	1.37
29	6	308	CHL	OBD-CAD	3.41	1.28	1.22
25	3	318	8CT	C01-C02	3.41	1.56	1.50
22	A	801	CLA	C4D-ND	-3.41	1.33	1.37
22	3	303	CLA	C4D-ND	-3.41	1.33	1.37
22	0	308	CLA	C1D-ND	3.40	1.42	1.37
22	B	807	CLA	C4D-ND	-3.40	1.33	1.37
22	A	807	CLA	C4D-ND	-3.40	1.33	1.37
22	2	314	CLA	C4D-ND	-3.40	1.33	1.37
25	7	323	8CT	C01-C02	3.40	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	305	CHL	OBD-CAD	3.40	1.28	1.22
22	1	308	CLA	C1D-ND	3.40	1.42	1.37
22	9	308	CLA	C1D-ND	3.40	1.42	1.37
22	K	101	CLA	C4D-ND	-3.40	1.33	1.37
25	F	302	8CT	C28-C29	3.40	1.40	1.32
25	7	321	8CT	C01-C02	3.39	1.56	1.50
22	4	314	CLA	C4D-ND	-3.39	1.33	1.37
25	B	843	8CT	C35-C30	3.39	1.65	1.56
25	F	302	8CT	C01-C02	3.39	1.56	1.50
22	3	307	CLA	CMB-C2B	-3.39	1.44	1.51
22	6	314	CLA	C4D-ND	-3.39	1.33	1.37
22	A	804	CLA	C4D-ND	-3.39	1.33	1.37
22	B	815	CLA	C4D-ND	-3.39	1.33	1.37
22	7	311	CLA	C4D-ND	-3.39	1.33	1.37
22	9	312	CLA	C4D-ND	-3.39	1.33	1.37
25	B	845	8CT	C28-C29	3.39	1.40	1.32
22	1	307	CLA	C1D-ND	3.39	1.41	1.37
22	4	313	CLA	C1D-ND	3.39	1.41	1.37
22	8	315	CLA	C4D-ND	-3.38	1.33	1.37
25	A	847	8CT	C11-C12	3.38	1.53	1.45
29	2	305	CHL	OBD-CAD	3.38	1.28	1.22
22	A	801	CLA	C1D-ND	3.38	1.41	1.37
22	A	823	CLA	C1D-ND	3.38	1.41	1.37
22	M	101	CLA	C1D-ND	3.38	1.41	1.37
22	A	832	CLA	C4D-ND	-3.38	1.33	1.37
25	B	845	8CT	C11-C12	3.38	1.53	1.45
22	K	102	CLA	C4D-ND	-3.38	1.33	1.37
22	A	822	CLA	C1D-ND	3.38	1.41	1.37
29	6	307	CHL	OBD-CAD	3.38	1.28	1.22
22	B	839	CLA	C4D-ND	-3.38	1.33	1.37
22	3	307	CLA	C1D-ND	3.38	1.41	1.37
22	A	833	CLA	C1D-ND	3.37	1.41	1.37
22	9	311	CLA	C1D-ND	3.37	1.41	1.37
22	2	304	CLA	C1D-ND	3.37	1.41	1.37
22	7	316	CLA	C4D-ND	-3.37	1.33	1.37
29	2	301	CHL	OBD-CAD	3.37	1.28	1.22
22	B	816	CLA	C4D-ND	-3.37	1.33	1.37
25	1	316	8CT	C01-C02	3.36	1.56	1.50
29	3	306	CHL	CHD-C4C	3.36	1.46	1.39
25	B	848	8CT	C01-C02	3.36	1.56	1.50
22	G	102	CLA	C1D-ND	3.36	1.41	1.37
25	3	316	8CT	C01-C02	3.36	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	313	CLA	C1D-ND	3.36	1.41	1.37
22	5	312	CLA	C4D-ND	-3.36	1.33	1.37
22	1	304	CLA	C4D-ND	-3.35	1.33	1.37
22	A	835	CLA	C4D-ND	-3.35	1.33	1.37
22	5	307	CLA	C1D-ND	3.35	1.41	1.37
22	K	105	CLA	C4D-ND	-3.35	1.33	1.37
22	7	312	CLA	C4D-ND	-3.34	1.33	1.37
22	5	309	CLA	C1D-ND	3.34	1.41	1.37
22	6	310	CLA	C1D-ND	3.34	1.41	1.37
25	3	318	8CT	C11-C12	3.34	1.53	1.45
22	6	305	CLA	C1D-ND	3.34	1.41	1.37
22	9	305	CLA	C4D-ND	-3.34	1.33	1.37
22	0	305	CLA	C1D-ND	3.33	1.41	1.37
22	3	309	CLA	C4D-ND	-3.33	1.33	1.37
25	6	321	8CT	C01-C02	3.33	1.56	1.50
22	7	306	CLA	C4D-ND	-3.33	1.33	1.37
22	B	841	CLA	C1D-ND	3.33	1.41	1.37
22	8	313	CLA	C4D-ND	-3.33	1.33	1.37
25	5	317	8CT	C01-C02	3.33	1.56	1.50
25	B	851	8CT	C18-C17	3.33	1.53	1.43
22	A	825	CLA	C4D-ND	-3.33	1.33	1.37
25	8	301	8CT	C01-C02	3.33	1.56	1.50
25	J	101	8CT	C01-C02	3.32	1.56	1.50
22	5	307	CLA	C4D-ND	-3.32	1.33	1.37
25	G	104	8CT	C01-C02	3.32	1.56	1.50
25	K	103	8CT	C01-C02	3.32	1.56	1.50
22	H	201	CLA	C1D-ND	3.32	1.41	1.37
25	K	103	8CT	C35-C30	3.32	1.65	1.56
29	6	306	CHL	OBD-CAD	3.32	1.28	1.22
22	9	303	CLA	C1D-ND	3.31	1.41	1.37
22	1	308	CLA	C4D-ND	-3.31	1.33	1.37
25	J	104	8CT	C01-C02	3.31	1.56	1.50
25	L	206	8CT	C35-C30	3.31	1.65	1.56
25	A	849	8CT	C01-C02	3.31	1.56	1.50
22	9	313	CLA	C4D-ND	-3.31	1.33	1.37
25	I	101	8CT	C11-C12	3.31	1.53	1.45
22	6	314	CLA	C1D-ND	3.30	1.41	1.37
25	A	854	8CT	C01-C02	3.30	1.56	1.50
22	1	311	CLA	C1D-ND	3.30	1.41	1.37
22	7	314	CLA	C1D-ND	3.30	1.41	1.37
22	A	810	CLA	C1D-ND	3.30	1.41	1.37
22	0	312	CLA	C4D-ND	-3.30	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	317	8CT	C18-C17	3.30	1.53	1.43
22	B	818	CLA	C1D-ND	3.30	1.41	1.37
22	L	204	CLA	C4D-ND	-3.29	1.33	1.37
22	1	310	CLA	C1D-ND	3.29	1.41	1.37
22	A	810	CLA	C4D-ND	-3.29	1.33	1.37
25	4	317	8CT	C01-C02	3.29	1.56	1.50
22	9	306	CLA	C4D-ND	-3.29	1.33	1.37
22	5	310	CLA	C4D-ND	-3.29	1.33	1.37
22	5	309	CLA	C4D-ND	-3.29	1.33	1.37
22	A	841	CLA	C4D-ND	-3.29	1.33	1.37
22	B	822	CLA	C1D-ND	3.28	1.41	1.37
25	8	318	8CT	C01-C02	3.28	1.56	1.50
29	2	305	CHL	CHD-C4C	3.28	1.46	1.39
22	2	311	CLA	C1D-ND	3.28	1.41	1.37
22	B	811	CLA	C4D-ND	-3.28	1.33	1.37
22	A	820	CLA	C1D-ND	3.28	1.41	1.37
22	A	843	CLA	C1D-ND	3.28	1.41	1.37
22	B	810	CLA	C4D-ND	-3.27	1.33	1.37
22	A	822	CLA	C4D-ND	-3.27	1.33	1.37
22	B	818	CLA	CMB-C2B	-3.27	1.44	1.51
25	L	205	8CT	C11-C12	3.27	1.53	1.45
22	1	309	CLA	C1D-ND	3.27	1.41	1.37
22	0	309	CLA	C4D-ND	-3.27	1.33	1.37
22	1	302	CLA	C4D-ND	-3.26	1.33	1.37
25	L	206	8CT	C01-C02	3.26	1.56	1.50
22	7	305	CLA	C1D-ND	3.26	1.41	1.37
25	A	850	8CT	C01-C02	3.26	1.56	1.50
25	B	804	8CT	C11-C12	3.26	1.52	1.45
22	6	311	CLA	C1D-ND	3.26	1.41	1.37
22	8	315	CLA	C1D-ND	3.26	1.41	1.37
22	4	302	CLA	C4D-ND	-3.26	1.33	1.37
22	L	202	CLA	C4D-ND	-3.25	1.33	1.37
25	B	844	8CT	C01-C02	3.25	1.56	1.50
25	B	851	8CT	C01-C02	3.25	1.56	1.50
22	A	819	CLA	C1D-ND	3.25	1.41	1.37
22	8	312	CLA	C1D-ND	3.25	1.41	1.37
25	B	804	8CT	C28-C29	3.25	1.40	1.32
25	A	848	8CT	C01-C02	3.25	1.56	1.50
22	G	103	CLA	C1D-ND	3.25	1.41	1.37
22	5	312	CLA	C1D-ND	3.25	1.41	1.37
22	1	306	CLA	C4D-ND	-3.25	1.33	1.37
22	5	311	CLA	C4D-ND	-3.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	312	CLA	C4D-ND	-3.25	1.33	1.37
22	J	103	CLA	C1D-ND	3.25	1.41	1.37
22	1	302	CLA	C1D-ND	3.25	1.41	1.37
22	9	309	CLA	C4D-ND	-3.25	1.33	1.37
22	7	307	CLA	C1D-ND	3.24	1.41	1.37
25	B	847	8CT	C01-C02	3.24	1.56	1.50
22	5	308	CLA	C4D-ND	-3.24	1.33	1.37
22	B	839	CLA	C1D-ND	3.24	1.41	1.37
22	7	314	CLA	C4D-ND	-3.24	1.33	1.37
22	5	305	CLA	C4D-ND	-3.24	1.33	1.37
22	1	313	CLA	C1D-ND	3.23	1.41	1.37
22	6	312	CLA	C1D-ND	3.23	1.41	1.37
25	2	317	8CT	C01-C02	3.23	1.56	1.50
22	2	314	CLA	C1D-ND	3.23	1.41	1.37
22	G	102	CLA	CHC-C1C	3.23	1.43	1.35
25	A	847	8CT	C01-C02	3.23	1.56	1.50
22	8	310	CLA	C1D-ND	3.23	1.41	1.37
25	F	302	8CT	C11-C12	3.22	1.52	1.45
24	A	844	LHG	O7-C5	-3.22	1.38	1.46
25	7	301	8CT	C35-C30	3.22	1.65	1.56
29	7	308	CHL	OBD-CAD	3.22	1.28	1.22
25	B	851	8CT	C35-C30	3.22	1.65	1.56
22	4	312	CLA	C4D-ND	-3.22	1.33	1.37
25	A	846	8CT	C35-C30	3.22	1.65	1.56
22	9	308	CLA	C4D-ND	-3.22	1.33	1.37
22	7	312	CLA	CHC-C1C	3.21	1.43	1.35
22	0	302	CLA	C1D-ND	3.21	1.41	1.37
22	5	303	CLA	C4D-ND	-3.21	1.33	1.37
22	B	815	CLA	C1D-ND	3.21	1.41	1.37
22	B	816	CLA	C1D-ND	3.21	1.41	1.37
22	3	302	CLA	C1D-ND	3.21	1.41	1.37
22	A	814	CLA	C1D-ND	3.21	1.41	1.37
22	7	306	CLA	C1D-ND	3.21	1.41	1.37
22	A	817	CLA	C4D-ND	-3.20	1.33	1.37
22	B	850	CLA	C4D-ND	-3.20	1.33	1.37
22	B	834	CLA	CMB-C2B	-3.20	1.45	1.51
22	B	835	CLA	C1D-ND	3.20	1.41	1.37
22	5	310	CLA	C1D-ND	3.20	1.41	1.37
22	9	301	CLA	C1D-ND	3.20	1.41	1.37
25	A	846	8CT	C01-C02	3.20	1.56	1.50
22	B	833	CLA	C1D-ND	3.20	1.41	1.37
22	3	312	CLA	C1D-ND	3.20	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	306	CLA	C1D-ND	3.20	1.41	1.37
25	G	104	8CT	C18-C17	3.20	1.53	1.43
22	L	203	CLA	C1D-ND	3.19	1.41	1.37
22	7	316	CLA	C1D-ND	3.19	1.41	1.37
22	3	311	CLA	C1D-ND	3.19	1.41	1.37
22	6	304	CLA	C1D-ND	3.19	1.41	1.37
22	J	103	CLA	C4D-ND	-3.19	1.33	1.37
22	A	853	CLA	C1D-ND	3.19	1.41	1.37
22	A	817	CLA	C1D-ND	3.19	1.41	1.37
22	B	830	CLA	CMB-C2B	-3.19	1.45	1.51
22	K	104	CLA	C1D-ND	3.19	1.41	1.37
22	3	309	CLA	C1D-ND	3.19	1.41	1.37
22	K	105	CLA	C1D-ND	3.19	1.41	1.37
25	B	845	8CT	C01-C02	3.19	1.56	1.50
22	A	835	CLA	C1D-ND	3.19	1.41	1.37
22	2	319	CLA	C1D-ND	3.18	1.41	1.37
22	6	317	CLA	C1D-ND	3.18	1.41	1.37
22	5	313	CLA	C1D-ND	3.18	1.41	1.37
22	B	828	CLA	CHC-C1C	3.18	1.43	1.35
22	A	834	CLA	C1D-ND	3.18	1.41	1.37
22	5	304	CLA	C1D-ND	3.18	1.41	1.37
22	G	103	CLA	C4D-ND	-3.18	1.33	1.37
22	0	308	CLA	C4D-ND	-3.17	1.33	1.37
22	A	832	CLA	C1D-ND	3.17	1.41	1.37
22	8	313	CLA	C1D-ND	3.17	1.41	1.37
25	B	846	8CT	C30-C29	3.17	1.55	1.50
25	B	848	8CT	C18-C17	3.17	1.53	1.43
22	4	303	CLA	C1D-ND	3.17	1.41	1.37
25	A	846	8CT	C18-C17	3.17	1.53	1.43
25	2	317	8CT	C18-C17	3.17	1.53	1.43
22	2	310	CLA	C1D-ND	3.17	1.41	1.37
25	L	205	8CT	C01-C02	3.17	1.56	1.50
22	1	312	CLA	C4D-ND	-3.16	1.33	1.37
22	9	303	CLA	C4D-ND	-3.16	1.33	1.37
29	2	307	CHL	OBD-CAD	3.16	1.27	1.22
25	1	316	8CT	C18-C17	3.16	1.53	1.43
25	L	206	8CT	C18-C17	3.16	1.53	1.43
25	L	205	8CT	C35-C30	3.16	1.65	1.56
22	8	302	CLA	C1D-ND	3.16	1.41	1.37
25	B	851	8CT	C30-C29	3.16	1.54	1.50
22	B	832	CLA	C1D-ND	3.16	1.41	1.37
22	4	312	CLA	C1D-ND	3.16	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	834	CLA	CMB-C2B	-3.16	1.45	1.51
25	5	317	8CT	C35-C30	3.16	1.65	1.56
25	I	101	8CT	C35-C30	3.16	1.65	1.56
22	7	313	CLA	C1D-ND	3.15	1.41	1.37
22	A	827	CLA	C1D-ND	3.15	1.41	1.37
22	0	307	CLA	CHC-C1C	3.15	1.43	1.35
22	B	819	CLA	C1D-ND	3.15	1.41	1.37
22	2	302	CLA	C1D-ND	3.15	1.41	1.37
22	4	311	CLA	C1D-ND	3.15	1.41	1.37
25	A	847	8CT	C30-C29	3.15	1.54	1.50
22	A	835	CLA	CHC-C1C	3.15	1.43	1.35
22	6	311	CLA	C4D-ND	-3.15	1.33	1.37
22	A	841	CLA	CMB-C2B	-3.15	1.45	1.51
25	I	101	8CT	C28-C29	3.15	1.39	1.32
25	B	846	8CT	C35-C30	3.15	1.65	1.56
25	A	849	8CT	C18-C17	3.15	1.53	1.43
22	8	304	CLA	C1D-ND	3.14	1.41	1.37
22	7	306	CLA	CHC-C1C	3.14	1.43	1.35
25	7	301	8CT	C01-C02	3.14	1.56	1.50
22	A	825	CLA	C1D-ND	3.14	1.41	1.37
22	A	815	CLA	C1D-ND	3.14	1.41	1.37
22	B	823	CLA	C1D-ND	3.14	1.41	1.37
25	B	847	8CT	C18-C17	3.14	1.53	1.43
25	3	316	8CT	C18-C17	3.14	1.53	1.43
25	B	846	8CT	C18-C17	3.14	1.53	1.43
25	8	301	8CT	C18-C17	3.14	1.53	1.43
22	1	301	CLA	C1D-ND	3.14	1.41	1.37
25	J	101	8CT	C18-C17	3.14	1.53	1.43
22	0	309	CLA	CHC-C1C	3.14	1.43	1.35
22	G	101	CLA	CHC-C1C	3.13	1.43	1.35
22	B	850	CLA	CHC-C1C	3.13	1.43	1.35
25	A	854	8CT	C18-C17	3.13	1.53	1.43
22	B	812	CLA	CMB-C2B	-3.13	1.45	1.51
29	8	314	CHL	MG-NA	-3.13	1.98	2.06
25	8	318	8CT	C18-C17	3.13	1.53	1.43
22	K	101	CLA	C1D-ND	3.13	1.41	1.37
25	A	848	8CT	C18-C17	3.13	1.53	1.43
22	6	303	CLA	C4D-ND	-3.13	1.33	1.37
25	K	103	8CT	C18-C17	3.12	1.53	1.43
22	5	308	CLA	CHC-C1C	3.12	1.43	1.35
25	G	104	8CT	C35-C30	3.12	1.65	1.56
22	A	841	CLA	C1D-ND	3.12	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	315	XAT	O24-C25	-3.12	1.41	1.46
25	J	104	8CT	C18-C17	3.12	1.53	1.43
25	7	323	8CT	C18-C17	3.12	1.53	1.43
22	9	305	CLA	C1D-ND	3.12	1.41	1.37
22	A	852	CLA	C1D-ND	3.11	1.41	1.37
25	7	321	8CT	C18-C17	3.11	1.53	1.43
22	5	307	CLA	CHC-C1C	3.11	1.42	1.35
25	A	847	8CT	C35-C30	3.11	1.65	1.56
22	1	303	CLA	CHC-C1C	3.11	1.42	1.35
22	L	202	CLA	C1D-ND	3.11	1.41	1.37
25	2	317	8CT	C35-C30	3.11	1.65	1.56
22	2	312	CLA	C1D-ND	3.11	1.41	1.37
22	3	310	CLA	C1D-ND	3.10	1.41	1.37
22	A	807	CLA	C1D-ND	3.10	1.41	1.37
22	B	831	CLA	CMB-C2B	-3.09	1.45	1.51
22	6	301	CLA	C4D-ND	-3.09	1.33	1.37
22	0	303	CLA	C4D-ND	-3.09	1.33	1.37
22	A	811	CLA	C1D-ND	3.09	1.41	1.37
25	7	301	8CT	C07-C02	-3.09	1.44	1.51
22	A	829	CLA	CHC-C1C	3.09	1.42	1.35
29	4	307	CHL	OBD-CAD	3.09	1.27	1.22
29	2	306	CHL	OBD-CAD	3.09	1.27	1.22
22	G	102	CLA	C4D-ND	-3.09	1.33	1.37
22	B	838	CLA	C1D-ND	3.09	1.41	1.37
22	3	308	CLA	C1D-ND	3.09	1.41	1.37
22	0	305	CLA	C4D-ND	-3.08	1.33	1.37
22	A	821	CLA	C1D-ND	3.08	1.41	1.37
22	3	313	CLA	C1D-ND	3.08	1.41	1.37
22	B	836	CLA	CHC-C1C	3.08	1.42	1.35
22	3	303	CLA	C1D-ND	3.08	1.41	1.37
22	A	819	CLA	CHC-C1C	3.08	1.42	1.35
25	B	843	8CT	C01-C02	3.08	1.56	1.50
29	0	301	CHL	MG-NA	-3.08	1.99	2.06
22	K	102	CLA	C1D-ND	3.08	1.41	1.37
25	A	854	8CT	C35-C30	3.08	1.64	1.56
22	6	301	CLA	CHC-C1C	3.07	1.42	1.35
22	1	301	CLA	CHC-C1C	3.07	1.42	1.35
22	B	850	CLA	C1D-ND	3.07	1.41	1.37
22	1	304	CLA	C1D-ND	3.07	1.41	1.37
22	B	840	CLA	CMB-C2B	-3.07	1.45	1.51
25	A	849	8CT	C35-C30	3.07	1.64	1.56
25	3	316	8CT	C35-C30	3.07	1.64	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	301	8CT	C10-C03	3.07	1.56	1.45
25	B	804	8CT	C01-C02	3.07	1.56	1.50
22	B	813	CLA	C1D-ND	3.07	1.41	1.37
22	B	829	CLA	CMB-C2B	-3.07	1.45	1.51
29	0	301	CHL	C3D-C2D	3.07	1.47	1.39
22	9	309	CLA	CHC-C1C	3.07	1.42	1.35
25	B	845	8CT	C18-C17	3.07	1.52	1.43
22	A	816	CLA	C1D-ND	3.07	1.41	1.37
25	5	317	8CT	C18-C17	3.06	1.52	1.43
22	4	304	CLA	C1D-ND	3.06	1.41	1.37
22	5	309	CLA	CHC-C1C	3.06	1.42	1.35
25	3	318	8CT	C35-C30	3.06	1.64	1.56
25	A	848	8CT	C35-C30	3.06	1.64	1.56
22	A	805	CLA	CMB-C2B	-3.06	1.45	1.51
22	A	839	CLA	C1D-ND	3.05	1.41	1.37
22	6	323	CLA	C1D-ND	3.05	1.41	1.37
22	0	304	CLA	C4D-ND	-3.05	1.33	1.37
25	1	316	8CT	C35-C30	3.05	1.64	1.56
25	B	844	8CT	C18-C17	3.05	1.52	1.43
22	5	302	CLA	CMB-C2B	-3.05	1.45	1.51
25	A	850	8CT	C18-C17	3.05	1.52	1.43
25	G	104	8CT	C30-C29	3.05	1.54	1.50
22	L	204	CLA	CHC-C1C	3.05	1.42	1.35
22	6	309	CLA	C1D-ND	3.05	1.41	1.37
22	B	808	CLA	C1D-ND	3.05	1.41	1.37
22	B	831	CLA	C1D-ND	3.05	1.41	1.37
22	8	311	CLA	CHC-C1C	3.05	1.42	1.35
29	0	306	CHL	C3D-C2D	3.05	1.47	1.39
29	4	306	CHL	C3D-C2D	3.05	1.47	1.39
25	4	317	8CT	C35-C30	3.04	1.64	1.56
22	A	827	CLA	CHC-C1C	3.04	1.42	1.35
22	9	310	CLA	C4D-ND	-3.04	1.33	1.37
22	9	304	CLA	C1D-ND	3.04	1.41	1.37
22	0	303	CLA	CHC-C1C	3.04	1.42	1.35
25	8	318	8CT	C35-C30	3.04	1.64	1.56
22	8	302	CLA	CHC-C1C	3.04	1.42	1.35
22	7	311	CLA	C1D-ND	3.04	1.41	1.37
25	6	321	8CT	C35-C30	3.03	1.64	1.56
22	1	308	CLA	CHC-C1C	3.03	1.42	1.35
22	F	301	CLA	CMB-C2B	-3.03	1.45	1.51
25	8	301	8CT	C10-C03	3.03	1.55	1.45
25	1	316	8CT	C10-C03	3.03	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	312	CLA	CHC-C1C	3.03	1.42	1.35
22	4	302	CLA	C1D-ND	3.03	1.41	1.37
22	3	303	CLA	CMB-C2B	-3.03	1.45	1.51
25	A	848	8CT	C10-C03	3.03	1.55	1.45
25	7	323	8CT	C35-C30	3.03	1.64	1.56
22	G	101	CLA	C4D-ND	-3.02	1.33	1.37
22	6	315	CLA	C1D-ND	3.02	1.41	1.37
25	B	844	8CT	C10-C03	3.02	1.55	1.45
25	6	321	8CT	C18-C17	3.02	1.52	1.43
22	5	303	CLA	C1D-ND	3.02	1.41	1.37
29	6	307	CHL	C3D-C2D	3.02	1.47	1.39
29	5	306	CHL	C3D-C2D	3.02	1.47	1.39
29	6	307	CHL	MG-NA	-3.02	1.99	2.06
22	8	309	CLA	C1D-ND	3.02	1.41	1.37
22	5	313	CLA	CHC-C1C	3.02	1.42	1.35
22	4	313	CLA	CHC-C1C	3.02	1.42	1.35
22	0	311	CLA	CHC-C1C	3.02	1.42	1.35
22	A	825	CLA	CMB-C2B	-3.01	1.45	1.51
25	B	848	8CT	C35-C30	3.01	1.64	1.56
22	2	313	CLA	CHC-C1C	3.01	1.42	1.35
25	B	847	8CT	C10-C03	3.01	1.55	1.45
25	L	205	8CT	C18-C17	3.01	1.52	1.43
25	5	317	8CT	C10-C03	3.01	1.55	1.45
22	A	802	CLA	C1D-ND	3.01	1.41	1.37
22	6	310	CLA	CMB-C2B	-3.01	1.45	1.51
22	0	308	CLA	CHC-C1C	3.01	1.42	1.35
22	2	309	CLA	CHC-C1C	3.01	1.42	1.35
22	B	810	CLA	C1D-ND	3.01	1.41	1.37
25	B	843	8CT	C18-C17	3.00	1.52	1.43
22	J	103	CLA	CHC-C1C	3.00	1.42	1.35
22	2	310	CLA	CMB-C2B	-3.00	1.45	1.51
22	4	310	CLA	C1D-ND	3.00	1.41	1.37
22	3	319	CLA	CHC-C1C	3.00	1.42	1.35
22	1	306	CLA	CHC-C1C	3.00	1.42	1.35
25	2	317	8CT	C10-C03	3.00	1.55	1.45
25	B	848	8CT	C10-C03	3.00	1.55	1.45
25	4	317	8CT	C10-C03	3.00	1.55	1.45
25	8	301	8CT	C35-C30	3.00	1.64	1.56
22	4	310	CLA	CHC-C1C	3.00	1.42	1.35
22	A	813	CLA	CHC-C1C	3.00	1.42	1.35
25	A	846	8CT	C10-C03	3.00	1.55	1.45
22	K	101	CLA	CHC-C1C	3.00	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	0	310	CLA	C4D-ND	-3.00	1.33	1.37
22	B	834	CLA	C1D-ND	2.99	1.41	1.37
25	J	101	8CT	C35-C30	2.99	1.64	1.56
25	G	104	8CT	C10-C03	2.99	1.55	1.45
22	7	315	CLA	CHC-C1C	2.99	1.42	1.35
22	1	301	CLA	CMB-C2B	-2.99	1.45	1.51
22	9	305	CLA	CHC-C1C	2.99	1.42	1.35
25	4	317	8CT	C30-C29	2.99	1.54	1.50
22	A	809	CLA	C1D-ND	2.99	1.41	1.37
25	3	318	8CT	C07-C02	-2.99	1.45	1.51
22	H	201	CLA	CHC-C1C	2.99	1.42	1.35
22	2	319	CLA	CHC-C1C	2.99	1.42	1.35
22	L	203	CLA	CHC-C1C	2.99	1.42	1.35
22	3	307	CLA	C3B-C2B	-2.99	1.36	1.40
29	9	307	CHL	C3D-C2D	2.98	1.47	1.39
22	7	302	CLA	C1D-ND	2.98	1.41	1.37
22	A	815	CLA	CHC-C1C	2.98	1.42	1.35
22	8	313	CLA	CHC-C1C	2.98	1.42	1.35
22	3	303	CLA	CHC-C1C	2.98	1.42	1.35
22	0	307	CLA	C4D-ND	-2.98	1.33	1.37
25	7	321	8CT	C35-C30	2.98	1.64	1.56
22	B	834	CLA	CHC-C1C	2.98	1.42	1.35
29	6	302	CHL	MG-NA	-2.98	1.99	2.06
22	A	806	CLA	CHC-C1C	2.97	1.42	1.35
29	6	302	CHL	C3D-C2D	2.97	1.47	1.39
22	8	308	CLA	C1D-ND	2.97	1.41	1.37
25	K	103	8CT	C10-C03	2.97	1.55	1.45
22	2	310	CLA	CHC-C1C	2.97	1.42	1.35
25	J	104	8CT	C35-C30	2.97	1.64	1.56
22	0	302	CLA	CHC-C1C	2.97	1.42	1.35
25	3	318	8CT	C18-C17	2.97	1.52	1.43
29	1	305	CHL	C3D-C2D	2.97	1.47	1.39
22	8	303	CLA	C1D-ND	2.97	1.41	1.37
25	B	845	8CT	C07-C02	-2.97	1.45	1.51
25	8	318	8CT	C10-C03	2.97	1.55	1.45
22	0	312	CLA	CHC-C1C	2.96	1.42	1.35
25	7	301	8CT	C18-C17	2.96	1.52	1.43
22	0	304	CLA	CHC-C1C	2.96	1.42	1.35
22	A	806	CLA	C1D-ND	2.96	1.41	1.37
22	9	310	CLA	CHC-C1C	2.96	1.42	1.35
22	2	302	CLA	CHC-C1C	2.96	1.42	1.35
22	6	304	CLA	CHC-C1C	2.96	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	839	CLA	CMB-C2B	-2.96	1.45	1.51
25	J	104	8CT	C10-C03	2.96	1.55	1.45
22	B	814	CLA	CHC-C1C	2.96	1.42	1.35
29	6	307	CHL	C1D-ND	-2.96	1.34	1.37
22	B	824	CLA	CHC-C1C	2.96	1.42	1.35
25	F	302	8CT	C18-C17	2.96	1.52	1.43
25	B	846	8CT	C10-C03	2.96	1.55	1.45
22	A	824	CLA	CHC-C1C	2.96	1.42	1.35
22	A	824	CLA	C1D-ND	2.95	1.41	1.37
22	3	302	CLA	CMB-C2B	-2.95	1.45	1.51
22	F	301	CLA	C1D-ND	2.95	1.41	1.37
25	B	851	8CT	C10-C03	2.95	1.55	1.45
25	3	318	8CT	C10-C03	2.95	1.55	1.45
25	A	850	8CT	C35-C30	2.95	1.64	1.56
22	7	303	CLA	C1D-ND	2.95	1.41	1.37
22	4	302	CLA	CHC-C1C	2.95	1.42	1.35
22	A	818	CLA	CHC-C1C	2.95	1.42	1.35
22	2	309	CLA	C1D-ND	2.95	1.41	1.37
22	A	804	CLA	CHC-C1C	2.95	1.42	1.35
22	3	312	CLA	CHC-C1C	2.95	1.42	1.35
22	6	304	CLA	CMB-C2B	-2.95	1.45	1.51
22	1	303	CLA	C1D-ND	2.95	1.41	1.37
22	B	801	CLA	CHC-C1C	2.95	1.42	1.35
22	B	807	CLA	CHC-C1C	2.95	1.42	1.35
22	9	311	CLA	CHC-C1C	2.95	1.42	1.35
22	B	820	CLA	CHC-C1C	2.95	1.42	1.35
22	B	834	CLA	C3B-C2B	-2.95	1.36	1.40
22	2	303	CLA	C1D-ND	2.95	1.41	1.37
22	B	812	CLA	CHC-C1C	2.95	1.42	1.35
22	B	803	CLA	C1D-ND	2.94	1.41	1.37
22	3	308	CLA	CHC-C1C	2.94	1.42	1.35
22	A	801	CLA	CHC-C1C	2.94	1.42	1.35
22	A	808	CLA	C1D-ND	2.94	1.41	1.37
22	A	831	CLA	C1D-ND	2.94	1.41	1.37
22	2	303	CLA	CMB-C2B	-2.94	1.45	1.51
22	B	819	CLA	CHC-C1C	2.94	1.42	1.35
22	7	312	CLA	C1D-ND	2.94	1.41	1.37
22	A	853	CLA	CHC-C1C	2.94	1.42	1.35
22	A	852	CLA	CHC-C1C	2.94	1.42	1.35
25	B	845	8CT	C30-C29	2.94	1.54	1.50
22	L	202	CLA	CHC-C1C	2.94	1.42	1.35
22	A	812	CLA	CMB-C2B	-2.94	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	311	CLA	CHC-C1C	2.94	1.42	1.35
22	3	304	CLA	C1D-ND	2.94	1.41	1.37
22	7	309	CLA	CHC-C1C	2.94	1.42	1.35
22	A	837	CLA	C1D-ND	2.94	1.41	1.37
22	B	817	CLA	C1D-ND	2.94	1.41	1.37
22	A	828	CLA	CHC-C1C	2.94	1.42	1.35
22	2	313	CLA	C1D-ND	2.94	1.41	1.37
22	7	317	CLA	CHC-C1C	2.94	1.42	1.35
22	8	309	CLA	CHC-C1C	2.94	1.42	1.35
22	A	821	CLA	CHC-C1C	2.93	1.42	1.35
25	B	843	8CT	C10-C03	2.93	1.55	1.45
29	0	306	CHL	MG-NA	-2.93	1.99	2.06
22	A	812	CLA	C1D-ND	2.93	1.41	1.37
22	B	832	CLA	CHC-C1C	2.93	1.42	1.35
22	4	314	CLA	CHC-C1C	2.93	1.42	1.35
22	6	303	CLA	CHC-C1C	2.93	1.42	1.35
25	A	854	8CT	C10-C03	2.93	1.55	1.45
22	1	312	CLA	CHC-C1C	2.93	1.42	1.35
29	8	314	CHL	C3D-C2D	2.93	1.47	1.39
25	3	316	8CT	C10-C03	2.93	1.55	1.45
22	B	812	CLA	C1D-ND	2.92	1.41	1.37
22	5	305	CLA	CHC-C1C	2.92	1.42	1.35
22	A	836	CLA	CHC-C1C	2.92	1.42	1.35
22	B	816	CLA	CHC-C1C	2.92	1.42	1.35
22	8	312	CLA	CHC-C1C	2.92	1.42	1.35
29	8	306	CHL	C3D-C2D	2.92	1.47	1.39
25	L	205	8CT	C07-C02	-2.92	1.45	1.51
22	4	310	CLA	CMB-C2B	-2.92	1.45	1.51
22	B	839	CLA	CHC-C1C	2.92	1.42	1.35
22	B	825	CLA	C1D-ND	2.92	1.41	1.37
25	5	317	8CT	C25-C26	2.92	1.39	1.35
22	7	316	CLA	CHC-C1C	2.92	1.42	1.35
25	L	205	8CT	C10-C03	2.92	1.55	1.45
22	B	831	CLA	CHC-C1C	2.92	1.42	1.35
22	1	311	CLA	CHC-C1C	2.92	1.42	1.35
29	6	316	CHL	C3D-C2D	2.92	1.47	1.39
22	6	315	CLA	CHC-C1C	2.91	1.42	1.35
22	B	827	CLA	C1D-ND	2.91	1.41	1.37
22	7	309	CLA	CMB-C2B	-2.91	1.45	1.51
25	A	850	8CT	C30-C29	2.91	1.54	1.50
25	J	101	8CT	C10-C03	2.91	1.55	1.45
22	F	301	CLA	CHC-C1C	2.91	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	829	CLA	C1D-ND	2.91	1.41	1.37
22	B	822	CLA	CHC-C1C	2.91	1.42	1.35
22	B	830	CLA	C1D-ND	2.91	1.41	1.37
25	A	847	8CT	C18-C17	2.91	1.52	1.43
22	3	302	CLA	CHC-C1C	2.91	1.42	1.35
22	A	804	CLA	C1D-ND	2.91	1.41	1.37
22	B	820	CLA	C1D-ND	2.91	1.41	1.37
22	A	803	CLA	CMB-C2B	-2.91	1.45	1.51
22	0	310	CLA	CHC-C1C	2.91	1.42	1.35
22	4	312	CLA	CMB-C2B	-2.91	1.45	1.51
22	A	834	CLA	CHC-C1C	2.90	1.42	1.35
22	G	103	CLA	CHC-C1C	2.90	1.42	1.35
25	A	849	8CT	C10-C03	2.90	1.55	1.45
22	B	806	CLA	CHC-C1C	2.90	1.42	1.35
22	A	812	CLA	CHC-C1C	2.90	1.42	1.35
22	9	313	CLA	CHC-C1C	2.90	1.42	1.35
22	A	826	CLA	C1D-ND	2.90	1.41	1.37
28	B	849	DGD	O2G-C2G	-2.90	1.39	1.46
25	7	323	8CT	C10-C03	2.90	1.55	1.45
22	9	301	CLA	CHC-C1C	2.90	1.42	1.35
25	A	850	8CT	C10-C03	2.90	1.55	1.45
22	B	837	CLA	CHC-C1C	2.90	1.42	1.35
25	B	804	8CT	C18-C17	2.90	1.52	1.43
22	B	825	CLA	CHC-C1C	2.90	1.42	1.35
25	7	321	8CT	C10-C03	2.90	1.55	1.45
25	2	317	8CT	C30-C29	2.90	1.54	1.50
22	A	831	CLA	CMB-C2B	-2.90	1.45	1.51
25	B	847	8CT	C35-C30	2.90	1.64	1.56
22	A	832	CLA	CMB-C2B	-2.90	1.45	1.51
22	6	305	CLA	CMB-C2B	-2.90	1.45	1.51
22	A	822	CLA	CHC-C1C	2.90	1.42	1.35
22	B	803	CLA	CHC-C1C	2.90	1.42	1.35
25	A	847	8CT	C10-C03	2.90	1.55	1.45
22	9	304	CLA	CHC-C1C	2.89	1.42	1.35
22	B	809	CLA	CHC-C1C	2.89	1.42	1.35
22	2	314	CLA	CHC-C1C	2.89	1.42	1.35
22	4	308	CLA	CMD-C2D	-2.89	1.44	1.50
22	1	304	CLA	CMB-C2B	-2.89	1.45	1.51
22	A	818	CLA	CMB-C2B	-2.89	1.45	1.51
22	7	309	CLA	C3B-C2B	-2.89	1.36	1.40
22	7	317	CLA	C1D-ND	2.89	1.41	1.37
22	B	807	CLA	C1D-ND	2.89	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	313	CLA	CHC-C1C	2.89	1.42	1.35
22	3	310	CLA	CHC-C1C	2.89	1.42	1.35
22	6	317	CLA	CHC-C1C	2.89	1.42	1.35
22	5	310	CLA	CHC-C1C	2.89	1.42	1.35
22	7	303	CLA	CHC-C1C	2.88	1.42	1.35
22	4	304	CLA	CHC-C1C	2.88	1.42	1.35
22	K	104	CLA	CHC-C1C	2.88	1.42	1.35
22	9	301	CLA	CMB-C2B	-2.88	1.45	1.51
25	A	848	8CT	C07-C02	-2.88	1.45	1.51
25	I	101	8CT	C18-C17	2.88	1.52	1.43
22	A	813	CLA	C1D-ND	2.88	1.41	1.37
22	7	310	CLA	CHC-C1C	2.87	1.42	1.35
22	B	823	CLA	CHC-C1C	2.87	1.42	1.35
22	5	302	CLA	CHC-C1C	2.87	1.42	1.35
25	1	316	8CT	C30-C29	2.87	1.54	1.50
22	2	311	CLA	CHC-C1C	2.87	1.42	1.35
22	A	818	CLA	C1D-ND	2.87	1.41	1.37
22	A	811	CLA	CHC-C1C	2.87	1.42	1.35
22	B	823	CLA	CMB-C2B	-2.87	1.45	1.51
22	7	303	CLA	CMB-C2B	-2.87	1.45	1.51
22	A	833	CLA	CMB-C2B	-2.87	1.45	1.51
22	6	318	CLA	CHC-C1C	2.87	1.42	1.35
25	L	206	8CT	C30-C29	2.87	1.54	1.50
31	4	318	LMG	O6-C5	-2.87	1.37	1.44
29	4	306	CHL	MG-NA	-2.86	1.99	2.06
25	B	845	8CT	C35-C30	2.86	1.64	1.56
22	B	807	CLA	CMB-C2B	-2.86	1.45	1.51
22	6	305	CLA	CHC-C1C	2.86	1.42	1.35
22	5	303	CLA	CMB-C2B	-2.86	1.45	1.51
22	8	303	CLA	CHC-C1C	2.86	1.42	1.35
22	2	304	CLA	CHC-C1C	2.86	1.42	1.35
22	2	308	CLA	CMB-C2B	-2.86	1.45	1.51
25	6	321	8CT	C10-C03	2.86	1.55	1.45
28	B	849	DGD	O1G-C1G	-2.86	1.38	1.45
22	B	809	CLA	CMB-C2B	-2.86	1.45	1.51
25	7	323	8CT	C30-C29	2.86	1.54	1.50
22	B	815	CLA	CHC-C1C	2.86	1.42	1.35
22	3	305	CLA	C1D-ND	2.86	1.41	1.37
22	6	323	CLA	CHC-C1C	2.86	1.42	1.35
22	A	806	CLA	CMB-C2B	-2.85	1.45	1.51
22	B	826	CLA	CHC-C1C	2.85	1.42	1.35
25	F	302	8CT	C30-C29	2.85	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	314	CLA	CHC-C1C	2.85	1.42	1.35
22	8	304	CLA	CMB-C2B	-2.85	1.45	1.51
22	B	820	CLA	CMB-C2B	-2.85	1.45	1.51
22	7	311	CLA	CHC-C1C	2.85	1.42	1.35
25	A	847	8CT	C07-C02	-2.85	1.45	1.51
25	A	854	8CT	C30-C29	2.85	1.54	1.50
22	3	309	CLA	CHC-C1C	2.85	1.42	1.35
22	B	808	CLA	CHC-C1C	2.85	1.42	1.35
22	1	309	CLA	CHC-C1C	2.85	1.42	1.35
22	5	308	CLA	CMB-C2B	-2.85	1.45	1.51
22	2	304	CLA	CMB-C2B	-2.85	1.45	1.51
22	A	839	CLA	CHC-C1C	2.85	1.42	1.35
22	B	833	CLA	CHC-C1C	2.85	1.42	1.35
22	K	105	CLA	CHC-C1C	2.85	1.42	1.35
22	B	829	CLA	C1D-ND	2.84	1.41	1.37
22	5	314	CLA	CHC-C1C	2.84	1.42	1.35
25	F	302	8CT	C35-C30	2.84	1.64	1.56
22	B	821	CLA	CHC-C1C	2.84	1.42	1.35
22	6	303	CLA	C1D-ND	2.84	1.41	1.37
25	8	318	8CT	C30-C29	2.84	1.54	1.50
22	4	311	CLA	CHC-C1C	2.84	1.42	1.35
22	5	304	CLA	CHC-C1C	2.84	1.42	1.35
22	A	838	CLA	CHC-C1C	2.84	1.42	1.35
22	6	318	CLA	CMB-C2B	-2.84	1.45	1.51
22	B	840	CLA	C1D-ND	2.84	1.41	1.37
22	3	305	CLA	CHC-C1C	2.84	1.42	1.35
22	7	304	CLA	C1D-ND	2.84	1.41	1.37
22	6	312	CLA	CHC-C1C	2.84	1.42	1.35
22	B	824	CLA	C1D-ND	2.84	1.41	1.37
29	2	306	CHL	C3D-C2D	2.84	1.46	1.39
22	A	821	CLA	CMB-C2B	-2.84	1.45	1.51
22	B	816	CLA	CMB-C2B	-2.84	1.45	1.51
22	A	814	CLA	CHC-C1C	2.84	1.42	1.35
22	9	308	CLA	CHC-C1C	2.84	1.42	1.35
22	7	304	CLA	CMB-C2B	-2.84	1.45	1.51
22	A	831	CLA	CHC-C1C	2.83	1.42	1.35
22	B	838	CLA	CHC-C1C	2.83	1.42	1.35
22	B	805	CLA	CHC-C1C	2.83	1.42	1.35
22	6	314	CLA	CHC-C1C	2.83	1.42	1.35
22	7	307	CLA	CHC-C1C	2.83	1.42	1.35
22	3	301	CLA	C1D-ND	2.83	1.41	1.37
25	B	847	8CT	C07-C02	-2.83	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	813	CLA	CMB-C2B	-2.83	1.45	1.51
22	A	841	CLA	CMD-C2D	-2.83	1.44	1.50
22	A	838	CLA	C1D-ND	2.83	1.41	1.37
25	L	205	8CT	C30-C29	2.83	1.54	1.50
22	3	304	CLA	CHC-C1C	2.83	1.42	1.35
22	B	827	CLA	CHC-C1C	2.82	1.42	1.35
25	J	101	8CT	C30-C29	2.82	1.54	1.50
29	9	307	CHL	C1D-C2D	2.82	1.50	1.45
22	4	311	CLA	CMB-C2B	-2.82	1.45	1.51
29	6	316	CHL	C1D-C2D	2.82	1.50	1.45
29	8	305	CHL	C3D-C2D	2.82	1.46	1.39
22	3	308	CLA	CMB-C2B	-2.82	1.45	1.51
25	B	844	8CT	C30-C29	2.82	1.54	1.50
22	4	309	CLA	CHC-C1C	2.82	1.42	1.35
22	5	312	CLA	CHC-C1C	2.82	1.42	1.35
25	8	301	8CT	C30-C29	2.82	1.54	1.50
22	1	306	CLA	CMB-C2B	-2.82	1.45	1.51
25	3	316	8CT	C30-C29	2.82	1.54	1.50
22	A	810	CLA	CMB-C2B	-2.82	1.45	1.51
22	7	302	CLA	CHC-C1C	2.82	1.42	1.35
25	A	848	8CT	C30-C29	2.82	1.54	1.50
22	8	304	CLA	CHC-C1C	2.82	1.42	1.35
22	M	101	CLA	CHC-C1C	2.82	1.42	1.35
22	L	201	CLA	CHC-C1C	2.82	1.42	1.35
22	7	305	CLA	CHC-C1C	2.81	1.42	1.35
22	B	803	CLA	C3B-C2B	-2.81	1.36	1.40
22	A	802	CLA	CHC-C1C	2.81	1.42	1.35
29	5	306	CHL	MG-NA	-2.81	1.99	2.06
22	A	819	CLA	CMB-C2B	-2.81	1.45	1.51
22	A	814	CLA	C3B-C2B	-2.81	1.36	1.40
22	A	816	CLA	CHC-C1C	2.81	1.42	1.35
22	3	301	CLA	CHC-C1C	2.81	1.42	1.35
22	A	816	CLA	CMB-C2B	-2.81	1.45	1.51
25	A	850	8CT	C07-C02	-2.81	1.45	1.51
22	A	829	CLA	CMB-C2B	-2.80	1.45	1.51
22	1	310	CLA	CMB-C2B	-2.80	1.45	1.51
22	8	308	CLA	CMB-C2B	-2.80	1.45	1.51
22	3	301	CLA	CMB-C2B	-2.80	1.45	1.51
22	3	319	CLA	CMB-C2B	-2.80	1.45	1.51
29	8	306	CHL	MG-NA	-2.80	1.99	2.06
22	7	315	CLA	C1D-ND	2.80	1.41	1.37
22	7	309	CLA	C1D-ND	2.80	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	313	CLA	CHC-C1C	2.80	1.42	1.35
25	7	321	8CT	C07-C02	-2.80	1.45	1.51
25	I	101	8CT	C07-C02	-2.80	1.45	1.51
22	B	825	CLA	CMB-C2B	-2.80	1.45	1.51
22	4	309	CLA	C1D-ND	2.80	1.41	1.37
22	B	809	CLA	C1D-ND	2.79	1.41	1.37
22	A	826	CLA	CMB-C2B	-2.79	1.45	1.51
22	B	813	CLA	CHC-C1C	2.79	1.42	1.35
22	2	308	CLA	CHC-C1C	2.79	1.42	1.35
22	A	801	CLA	CMB-C2B	-2.79	1.45	1.51
25	B	843	8CT	C07-C02	-2.79	1.45	1.51
22	B	810	CLA	CHC-C1C	2.79	1.42	1.35
25	B	804	8CT	C35-C30	2.79	1.64	1.56
25	L	206	8CT	C10-C03	2.79	1.55	1.45
29	2	306	CHL	C1D-ND	-2.79	1.34	1.37
22	6	311	CLA	CHC-C1C	2.79	1.42	1.35
22	7	302	CLA	CMB-C2B	-2.79	1.45	1.51
22	1	302	CLA	CHC-C1C	2.79	1.42	1.35
22	A	837	CLA	CMB-C2B	-2.79	1.45	1.51
22	B	814	CLA	CMB-C2B	-2.78	1.45	1.51
22	4	308	CLA	C1D-ND	2.78	1.41	1.37
29	5	301	CHL	MG-NA	-2.78	1.99	2.06
22	A	814	CLA	CMB-C2B	-2.78	1.45	1.51
22	B	819	CLA	CMB-C2B	-2.78	1.45	1.51
22	4	303	CLA	CMB-C2B	-2.78	1.45	1.51
22	3	313	CLA	CMB-C2B	-2.78	1.45	1.51
22	4	312	CLA	CHC-C1C	2.78	1.42	1.35
22	A	827	CLA	CMB-C2B	-2.78	1.45	1.51
22	4	302	CLA	CMB-C2B	-2.78	1.45	1.51
22	A	803	CLA	CHC-C1C	2.78	1.42	1.35
22	A	807	CLA	CMB-C2B	-2.78	1.45	1.51
22	A	825	CLA	CHC-C1C	2.78	1.42	1.35
25	2	317	8CT	C07-C02	-2.77	1.45	1.51
29	8	314	CHL	C1D-C2D	2.77	1.50	1.45
22	3	307	CLA	CHC-C1C	2.77	1.42	1.35
25	7	301	8CT	C30-C29	2.77	1.54	1.50
22	A	805	CLA	C1D-ND	2.77	1.41	1.37
22	A	852	CLA	CMB-C2B	-2.77	1.45	1.51
22	2	314	CLA	CMB-C2B	-2.77	1.45	1.51
22	A	808	CLA	CHC-C1C	2.77	1.42	1.35
22	A	826	CLA	C3B-C2B	-2.77	1.36	1.40
25	A	849	8CT	C30-C29	2.77	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	F	302	8CT	C07-C02	-2.77	1.45	1.51
22	A	820	CLA	CHC-C1C	2.77	1.42	1.35
22	A	811	CLA	CMB-C2B	-2.77	1.45	1.51
22	7	316	CLA	CMB-C2B	-2.77	1.45	1.51
29	9	302	CHL	C3D-C2D	2.77	1.46	1.39
22	B	835	CLA	CHC-C1C	2.76	1.42	1.35
22	3	311	CLA	CHC-C1C	2.76	1.42	1.35
22	9	306	CLA	CHC-C1C	2.76	1.42	1.35
22	A	837	CLA	CHC-C1C	2.76	1.42	1.35
22	B	801	CLA	CMB-C2B	-2.76	1.45	1.51
22	A	804	CLA	CMB-C2B	-2.76	1.45	1.51
22	A	832	CLA	CHC-C1C	2.76	1.42	1.35
29	8	307	CHL	C3D-C2D	2.76	1.46	1.39
22	A	840	CLA	CHC-C1C	2.76	1.42	1.35
29	0	306	CHL	C4C-C3C	2.76	1.49	1.45
22	1	310	CLA	CHC-C1C	2.76	1.42	1.35
22	B	810	CLA	CMB-C2B	-2.76	1.45	1.51
25	B	844	8CT	C35-C30	2.76	1.64	1.56
22	6	303	CLA	CMB-C2B	-2.76	1.45	1.51
25	A	846	8CT	C07-C02	-2.76	1.45	1.51
22	A	807	CLA	CHC-C1C	2.76	1.42	1.35
22	2	312	CLA	CMB-C2B	-2.76	1.45	1.51
22	7	304	CLA	CHC-C1C	2.75	1.42	1.35
22	2	303	CLA	CHC-C1C	2.75	1.42	1.35
22	6	305	CLA	C3B-C2B	-2.75	1.36	1.40
25	B	851	8CT	C07-C02	-2.75	1.45	1.51
25	J	104	8CT	C30-C29	2.75	1.54	1.50
22	8	312	CLA	CMB-C2B	-2.75	1.45	1.51
22	L	204	CLA	CMB-C2B	-2.75	1.45	1.51
29	4	305	CHL	C3D-C2D	2.75	1.46	1.39
22	A	808	CLA	CMB-C2B	-2.75	1.45	1.51
22	B	808	CLA	CMB-C2B	-2.75	1.45	1.51
22	B	841	CLA	CMB-C2B	-2.75	1.45	1.51
22	B	805	CLA	CMB-C2B	-2.75	1.45	1.51
22	7	318	CLA	CHC-C1C	2.75	1.42	1.35
22	A	840	CLA	C1D-ND	2.75	1.41	1.37
22	L	201	CLA	C1D-ND	2.75	1.41	1.37
22	A	812	CLA	C3B-C2B	-2.75	1.36	1.40
22	K	104	CLA	CMB-C2B	-2.75	1.45	1.51
22	9	309	CLA	CMB-C2B	-2.75	1.45	1.51
22	A	839	CLA	CMB-C2B	-2.75	1.45	1.51
29	8	314	CHL	C1D-ND	-2.75	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	836	CLA	CMB-C2B	-2.75	1.45	1.51
29	0	306	CHL	C1D-C2D	2.74	1.50	1.45
29	6	308	CHL	MG-NA	-2.74	1.99	2.06
25	B	845	8CT	C10-C03	2.74	1.54	1.45
22	2	309	CLA	CMB-C2B	-2.74	1.45	1.51
22	B	817	CLA	CHC-C1C	2.74	1.42	1.35
25	B	848	8CT	C30-C29	2.74	1.54	1.50
22	A	807	CLA	C3B-C2B	-2.74	1.36	1.40
22	B	821	CLA	C1D-ND	2.74	1.41	1.37
29	3	306	CHL	C1D-ND	-2.74	1.34	1.37
22	B	803	CLA	CMB-C2B	-2.74	1.45	1.51
22	B	811	CLA	CMB-C2B	-2.74	1.45	1.51
25	F	302	8CT	C10-C03	2.74	1.54	1.45
22	A	843	CLA	CHC-C1C	2.74	1.42	1.35
29	6	306	CHL	C3D-C2D	2.74	1.46	1.39
29	0	301	CHL	C1D-ND	-2.74	1.34	1.37
29	1	305	CHL	MG-NA	-2.74	1.99	2.06
22	B	841	CLA	CHC-C1C	2.74	1.42	1.35
22	4	313	CLA	CMB-C2B	-2.73	1.46	1.51
22	A	805	CLA	CHC-C1C	2.73	1.42	1.35
22	B	811	CLA	CHC-C1C	2.73	1.42	1.35
22	A	835	CLA	CMB-C2B	-2.73	1.46	1.51
25	I	101	8CT	C10-C03	2.73	1.54	1.45
22	B	836	CLA	CMB-C2B	-2.73	1.46	1.51
29	8	305	CHL	C1D-C2D	2.73	1.50	1.45
22	B	818	CLA	CHC-C1C	2.73	1.42	1.35
22	B	832	CLA	CMB-C2B	-2.73	1.46	1.51
25	3	316	8CT	C07-C02	-2.73	1.45	1.51
22	6	315	CLA	CMB-C2B	-2.72	1.46	1.51
22	4	308	CLA	CMB-C2B	-2.72	1.46	1.51
22	A	802	CLA	CMB-C2B	-2.72	1.46	1.51
22	8	302	CLA	CMB-C2B	-2.72	1.46	1.51
22	A	826	CLA	CHC-C1C	2.72	1.41	1.35
22	A	830	CLA	CHC-C1C	2.72	1.41	1.35
22	B	837	CLA	CMB-C2B	-2.72	1.46	1.51
22	3	302	CLA	C3B-C2B	-2.72	1.36	1.40
22	5	303	CLA	C3B-C2B	-2.72	1.36	1.40
22	5	302	CLA	C1D-ND	2.72	1.41	1.37
22	A	809	CLA	CMB-C2B	-2.72	1.46	1.51
22	6	313	CLA	CHC-C1C	2.72	1.41	1.35
22	9	304	CLA	CMB-C2B	-2.71	1.46	1.51
29	9	302	CHL	C1D-C2D	2.71	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	828	CLA	CMB-C2B	-2.71	1.46	1.51
22	B	827	CLA	CMB-C2B	-2.71	1.46	1.51
22	A	824	CLA	CMB-C2B	-2.71	1.46	1.51
22	A	810	CLA	CHC-C1C	2.71	1.41	1.35
22	5	303	CLA	CHC-C1C	2.71	1.41	1.35
25	A	854	8CT	C07-C02	-2.71	1.45	1.51
22	A	822	CLA	C3B-C2B	-2.71	1.36	1.40
25	B	847	8CT	C30-C29	2.71	1.54	1.50
25	8	301	8CT	C07-C02	-2.71	1.45	1.51
22	2	312	CLA	CHC-C1C	2.71	1.41	1.35
22	3	313	CLA	CHC-C1C	2.71	1.41	1.35
22	0	305	CLA	CHC-C1C	2.71	1.41	1.35
29	8	306	CHL	C1D-C2D	2.71	1.50	1.45
22	5	314	CLA	CMB-C2B	-2.70	1.46	1.51
22	9	306	CLA	CMB-C2B	-2.70	1.46	1.51
22	A	822	CLA	CMB-C2B	-2.70	1.46	1.51
29	5	301	CHL	C3D-C2D	2.70	1.46	1.39
22	4	309	CLA	CMB-C2B	-2.70	1.46	1.51
22	1	304	CLA	CHC-C1C	2.70	1.41	1.35
22	A	836	CLA	C1D-ND	2.70	1.41	1.37
25	4	317	8CT	C07-C02	-2.70	1.45	1.51
22	A	840	CLA	CMB-C2B	-2.70	1.46	1.51
22	3	310	CLA	CMB-C2B	-2.70	1.46	1.51
22	B	837	CLA	C1D-ND	2.70	1.41	1.37
22	6	310	CLA	CHC-C1C	2.70	1.41	1.35
29	4	306	CHL	C1D-ND	-2.70	1.34	1.37
22	B	810	CLA	C3B-C2B	-2.69	1.36	1.40
22	B	818	CLA	C3B-C2B	-2.69	1.36	1.40
22	6	314	CLA	CMB-C2B	-2.69	1.46	1.51
24	1	317	LHG	O7-C5	-2.69	1.39	1.46
22	A	823	CLA	CMB-C2B	-2.69	1.46	1.51
22	B	823	CLA	C3B-C2B	-2.69	1.36	1.40
22	A	817	CLA	CHC-C1C	2.69	1.41	1.35
22	4	302	CLA	C3B-C2B	-2.69	1.36	1.40
22	B	821	CLA	CMB-C2B	-2.69	1.46	1.51
22	K	102	CLA	CMB-C2B	-2.69	1.46	1.51
25	6	321	8CT	C30-C29	2.69	1.54	1.50
22	6	301	CLA	CMB-C2B	-2.69	1.46	1.51
25	8	318	8CT	C07-C02	-2.69	1.45	1.51
22	3	311	CLA	CMB-C2B	-2.69	1.46	1.51
22	B	806	CLA	CMC-C2C	-2.69	1.45	1.50
22	B	822	CLA	CMB-C2B	-2.69	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	305	CLA	CMB-C2B	-2.69	1.46	1.51
22	B	805	CLA	C1D-ND	2.68	1.41	1.37
22	B	840	CLA	C3B-C2B	-2.68	1.36	1.40
22	9	312	CLA	CMB-C2B	-2.68	1.46	1.51
29	4	306	CHL	C1D-C2D	2.68	1.50	1.45
22	6	309	CLA	CHC-C1C	2.68	1.41	1.35
22	2	313	CLA	CMB-C2B	-2.68	1.46	1.51
25	K	103	8CT	C07-C02	-2.68	1.45	1.51
22	8	315	CLA	CHC-C1C	2.68	1.41	1.35
22	6	313	CLA	C1D-ND	2.68	1.41	1.37
22	1	302	CLA	CMB-C2B	-2.68	1.46	1.51
25	J	101	8CT	C07-C02	-2.68	1.45	1.51
22	A	823	CLA	CHC-C1C	2.67	1.41	1.35
22	B	824	CLA	CMB-C2B	-2.67	1.46	1.51
22	1	308	CLA	CMB-C2B	-2.67	1.46	1.51
22	3	304	CLA	CMB-C2B	-2.67	1.46	1.51
25	A	849	8CT	C07-C02	-2.67	1.45	1.51
22	A	834	CLA	C3B-C2B	-2.67	1.36	1.40
22	B	830	CLA	CHC-C1C	2.67	1.41	1.35
22	A	817	CLA	CMB-C2B	-2.67	1.46	1.51
22	B	835	CLA	CMB-C2B	-2.67	1.46	1.51
29	6	308	CHL	C3D-C2D	2.67	1.46	1.39
22	5	305	CLA	CMB-C2B	-2.67	1.46	1.51
22	A	833	CLA	CHC-C1C	2.67	1.41	1.35
25	7	321	8CT	C30-C29	2.66	1.54	1.50
22	B	811	CLA	C3B-C2B	-2.66	1.36	1.40
22	6	312	CLA	CMB-C2B	-2.66	1.46	1.51
22	M	101	CLA	C3B-C2B	-2.66	1.36	1.40
22	A	828	CLA	C1D-ND	2.66	1.41	1.37
22	B	801	CLA	C1D-ND	2.66	1.41	1.37
25	5	317	8CT	C07-C02	-2.66	1.45	1.51
22	4	309	CLA	C3B-C2B	-2.66	1.36	1.40
29	4	301	CHL	C1D-ND	-2.66	1.34	1.37
22	8	313	CLA	CMB-C2B	-2.66	1.46	1.51
22	4	314	CLA	CMB-C2B	-2.66	1.46	1.51
29	9	307	CHL	MG-NA	-2.66	2.00	2.06
29	7	308	CHL	C1D-ND	-2.66	1.34	1.37
22	8	310	CLA	CHC-C1C	2.66	1.41	1.35
22	B	814	CLA	CMC-C2C	-2.65	1.45	1.50
22	A	830	CLA	C3B-C2B	-2.65	1.36	1.40
22	A	841	CLA	CHC-C1C	2.65	1.41	1.35
22	2	302	CLA	CMB-C2B	-2.65	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	318	CLA	C3B-C2B	-2.65	1.36	1.40
22	5	312	CLA	CMB-C2B	-2.65	1.46	1.51
22	2	311	CLA	CMB-C2B	-2.65	1.46	1.51
22	K	102	CLA	CHC-C1C	2.65	1.41	1.35
22	1	312	CLA	CMB-C2B	-2.65	1.46	1.51
22	2	303	CLA	C3B-C2B	-2.65	1.36	1.40
22	9	303	CLA	CHC-C1C	2.65	1.41	1.35
22	A	838	CLA	CMB-C2B	-2.65	1.46	1.51
25	B	846	8CT	C07-C02	-2.65	1.45	1.51
29	1	305	CHL	C1D-C2D	2.65	1.50	1.45
22	9	303	CLA	CMB-C2B	-2.65	1.46	1.51
31	4	318	LMG	O1-C7	-2.65	1.38	1.43
22	7	307	CLA	CMB-C2B	-2.65	1.46	1.51
22	9	308	CLA	CMB-C2B	-2.64	1.46	1.51
22	2	319	CLA	CMB-C2B	-2.64	1.46	1.51
22	7	317	CLA	CMB-C2B	-2.64	1.46	1.51
29	2	305	CHL	C1D-ND	-2.64	1.34	1.37
25	1	316	8CT	C07-C02	-2.64	1.45	1.51
22	A	813	CLA	CMB-C2B	-2.64	1.46	1.51
25	B	844	8CT	C07-C02	-2.64	1.45	1.51
22	M	101	CLA	CMB-C2B	-2.64	1.46	1.51
22	H	201	CLA	CMB-C2B	-2.63	1.46	1.51
26	A	851	HTG	C1-S1	-2.63	1.76	1.80
29	6	316	CHL	C1D-ND	-2.63	1.34	1.37
22	A	832	CLA	C3B-C2B	-2.63	1.36	1.40
22	B	838	CLA	CMB-C2B	-2.63	1.46	1.51
22	B	850	CLA	CMB-C2B	-2.63	1.46	1.51
22	5	309	CLA	CMB-C2B	-2.63	1.46	1.51
22	7	306	CLA	CMB-C2B	-2.63	1.46	1.51
22	9	311	CLA	CMB-C2B	-2.63	1.46	1.51
22	A	803	CLA	C1D-ND	2.63	1.41	1.37
22	8	311	CLA	CMB-C2B	-2.63	1.46	1.51
22	A	852	CLA	C3B-C2B	-2.63	1.36	1.40
25	G	104	8CT	C07-C02	-2.63	1.45	1.51
22	3	305	CLA	CMB-C2B	-2.63	1.46	1.51
22	4	310	CLA	C3B-C2B	-2.63	1.36	1.40
22	A	804	CLA	CMD-C2D	-2.63	1.45	1.50
25	B	804	8CT	C07-C02	-2.62	1.45	1.51
22	B	826	CLA	CMB-C2B	-2.62	1.46	1.51
22	4	308	CLA	CHC-C1C	2.62	1.41	1.35
22	A	828	CLA	CMB-C2B	-2.62	1.46	1.51
22	A	810	CLA	C3B-C2B	-2.62	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	3	306	CHL	OBD-CAD	2.62	1.27	1.22
24	5	318	LHG	O7-C5	-2.62	1.40	1.46
22	A	809	CLA	CHC-C1C	2.62	1.41	1.35
22	8	315	CLA	CMB-C2B	-2.62	1.46	1.51
22	B	840	CLA	CHC-C1C	2.61	1.41	1.35
22	1	307	CLA	CHC-C1C	2.61	1.41	1.35
22	8	308	CLA	CHC-C1C	2.61	1.41	1.35
22	4	303	CLA	CHC-C1C	2.61	1.41	1.35
22	1	311	CLA	CMB-C2B	-2.61	1.46	1.51
22	8	309	CLA	CMB-C2B	-2.61	1.46	1.51
25	L	206	8CT	C07-C02	-2.61	1.45	1.51
25	B	848	8CT	C07-C02	-2.61	1.45	1.51
25	6	321	8CT	C07-C02	-2.61	1.45	1.51
25	7	323	8CT	C07-C02	-2.61	1.45	1.51
22	5	310	CLA	CMB-C2B	-2.61	1.46	1.51
22	1	309	CLA	CMB-C2B	-2.61	1.46	1.51
22	8	303	CLA	CMB-C2B	-2.61	1.46	1.51
22	7	312	CLA	CMB-C2B	-2.61	1.46	1.51
22	6	309	CLA	CMB-C2B	-2.61	1.46	1.51
22	L	203	CLA	CMB-C2B	-2.61	1.46	1.51
22	0	303	CLA	CMB-C2B	-2.61	1.46	1.51
25	J	104	8CT	C07-C02	-2.61	1.45	1.51
29	4	305	CHL	C1D-ND	-2.60	1.34	1.37
22	6	323	CLA	CMB-C2B	-2.60	1.46	1.51
22	B	801	CLA	C3B-C2B	-2.60	1.36	1.40
22	A	801	CLA	CMD-C2D	-2.60	1.45	1.50
22	5	307	CLA	CMB-C2B	-2.60	1.46	1.51
29	6	302	CHL	C1D-ND	-2.60	1.34	1.37
29	2	306	CHL	MG-NA	-2.60	2.00	2.06
22	2	309	CLA	CMC-C2C	-2.60	1.45	1.50
22	A	803	CLA	C3B-C2B	-2.60	1.36	1.40
22	L	201	CLA	CMB-C2B	-2.60	1.46	1.51
22	9	313	CLA	CMB-C2B	-2.60	1.46	1.51
25	B	804	8CT	C10-C03	2.60	1.54	1.45
22	A	843	CLA	CMB-C2B	-2.60	1.46	1.51
22	6	313	CLA	CMB-C2B	-2.60	1.46	1.51
22	2	308	CLA	C1D-ND	2.59	1.41	1.37
22	B	825	CLA	CMD-C2D	-2.59	1.45	1.50
22	A	829	CLA	C3B-C2B	-2.59	1.36	1.40
22	6	304	CLA	C3B-C2B	-2.59	1.36	1.40
29	2	307	CHL	C1D-ND	-2.59	1.34	1.37
22	6	311	CLA	CMB-C2B	-2.59	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	314	CLA	CMB-C2B	-2.59	1.46	1.51
22	B	836	CLA	C1D-ND	2.59	1.41	1.37
29	5	301	CHL	C1D-ND	-2.59	1.34	1.37
25	3	318	8CT	C30-C29	2.59	1.54	1.50
22	6	317	CLA	CMB-C2B	-2.59	1.46	1.51
22	1	307	CLA	CMB-C2B	-2.59	1.46	1.51
22	7	315	CLA	CMB-C2B	-2.58	1.46	1.51
22	0	312	CLA	CMB-C2B	-2.58	1.46	1.51
22	7	318	CLA	CMB-C2B	-2.58	1.46	1.51
22	A	833	CLA	C3B-C2B	-2.58	1.36	1.40
29	8	307	CHL	C1D-ND	-2.58	1.34	1.37
22	4	304	CLA	CMB-C2B	-2.58	1.46	1.51
22	3	308	CLA	CMD-C2D	-2.58	1.45	1.50
22	3	312	CLA	CMB-C2B	-2.58	1.46	1.51
22	A	830	CLA	C1D-ND	2.58	1.41	1.37
22	A	825	CLA	CMD-C2D	-2.58	1.45	1.50
22	7	311	CLA	CMB-C2B	-2.58	1.46	1.51
22	0	304	CLA	CMB-C2B	-2.57	1.46	1.51
22	0	309	CLA	CMB-C2B	-2.57	1.46	1.51
29	2	307	CHL	MG-NA	-2.57	2.00	2.06
29	6	308	CHL	C1D-C2D	2.57	1.50	1.45
22	B	828	CLA	C1D-ND	2.57	1.40	1.37
22	1	313	CLA	CMB-C2B	-2.57	1.46	1.51
29	4	307	CHL	MG-NA	-2.57	2.00	2.06
29	6	306	CHL	C1D-C2D	2.56	1.50	1.45
22	7	313	CLA	CMB-C2B	-2.56	1.46	1.51
22	B	831	CLA	CMD-C2D	-2.56	1.45	1.50
22	0	305	CLA	CMB-C2B	-2.56	1.46	1.51
22	7	302	CLA	C3B-C2B	-2.56	1.36	1.40
22	B	819	CLA	CMD-C2D	-2.56	1.45	1.50
25	B	804	8CT	C30-C29	2.56	1.54	1.50
29	1	305	CHL	C1D-ND	-2.56	1.34	1.37
29	5	306	CHL	C1D-C2D	2.56	1.50	1.45
22	2	308	CLA	C3B-C2B	-2.56	1.36	1.40
29	4	305	CHL	MG-NA	-2.56	2.00	2.06
22	B	806	CLA	CMB-C2B	-2.56	1.46	1.51
29	0	301	CHL	C1D-C2D	2.55	1.50	1.45
22	7	310	CLA	CMB-C2B	-2.55	1.46	1.51
24	2	318	LHG	O7-C5	-2.55	1.40	1.46
22	7	305	CLA	CMB-C2B	-2.55	1.46	1.51
25	F	302	8CT	C33-C32	-2.55	1.43	1.50
22	3	313	CLA	C3B-C2B	-2.55	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	2	306	CHL	C1D-C2D	2.55	1.50	1.45
22	A	827	CLA	CMC-C2C	-2.55	1.45	1.50
22	8	308	CLA	C3B-C2B	-2.55	1.36	1.40
25	B	844	8CT	C25-C26	2.55	1.39	1.35
22	A	815	CLA	CMB-C2B	-2.54	1.46	1.51
22	0	310	CLA	CMB-C2B	-2.54	1.46	1.51
29	9	302	CHL	MG-NA	-2.54	2.00	2.06
22	B	820	CLA	C3B-C2B	-2.54	1.36	1.40
22	A	853	CLA	CMB-C2B	-2.54	1.46	1.51
29	2	301	CHL	MG-NA	-2.54	2.00	2.06
22	3	311	CLA	CMD-C2D	-2.54	1.45	1.50
29	6	316	CHL	MG-NA	-2.54	2.00	2.06
29	8	307	CHL	MG-NA	-2.54	2.00	2.06
29	5	301	CHL	C1D-C2D	2.53	1.50	1.45
22	K	105	CLA	CMB-C2B	-2.53	1.46	1.51
29	8	307	CHL	C1D-C2D	2.53	1.50	1.45
22	1	303	CLA	CMB-C2B	-2.53	1.46	1.51
22	B	812	CLA	CMD-C2D	-2.53	1.45	1.50
22	A	841	CLA	C3B-C2B	-2.53	1.36	1.40
29	4	307	CHL	C1D-ND	-2.53	1.34	1.37
22	0	307	CLA	CMB-C2B	-2.53	1.46	1.51
22	B	820	CLA	CMC-C2C	-2.53	1.45	1.50
22	5	311	CLA	CMB-C2B	-2.52	1.46	1.51
22	6	303	CLA	C3B-CAB	-2.52	1.42	1.47
22	B	829	CLA	C3B-C2B	-2.52	1.36	1.40
22	5	311	CLA	CMD-C2D	-2.52	1.45	1.50
25	A	847	8CT	C33-C32	-2.52	1.43	1.50
22	B	806	CLA	CMD-C2D	-2.52	1.45	1.50
22	A	820	CLA	CMB-C2B	-2.52	1.46	1.51
22	B	806	CLA	MG-ND	-2.52	2.00	2.05
22	2	314	CLA	C3B-C2B	-2.52	1.36	1.40
22	5	304	CLA	CMB-C2B	-2.51	1.46	1.51
22	A	805	CLA	C3B-C2B	-2.51	1.36	1.40
22	B	833	CLA	CMD-C2D	-2.51	1.45	1.50
29	6	306	CHL	C1D-ND	-2.51	1.34	1.37
22	5	313	CLA	CMB-C2B	-2.51	1.46	1.51
29	6	302	CHL	C1D-C2D	2.51	1.50	1.45
22	7	317	CLA	C3B-C2B	-2.51	1.36	1.40
25	B	851	8CT	C25-C26	2.51	1.39	1.35
29	5	306	CHL	C1D-ND	-2.51	1.34	1.37
25	B	846	8CT	C25-C26	2.51	1.39	1.35
29	5	301	CHL	C4B-CHC	2.51	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	303	CLA	C3B-C2B	-2.50	1.36	1.40
22	0	308	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	833	CLA	CMC-C2C	-2.50	1.45	1.50
22	4	303	CLA	CMD-C2D	-2.50	1.45	1.50
22	B	829	CLA	CHC-C1C	2.50	1.41	1.35
22	B	836	CLA	CMD-C2D	-2.50	1.45	1.50
29	8	306	CHL	C1D-ND	-2.50	1.34	1.37
22	5	314	CLA	CMD-C2D	-2.50	1.45	1.50
22	3	304	CLA	C3B-C2B	-2.50	1.36	1.40
22	8	310	CLA	CMB-C2B	-2.50	1.46	1.51
22	7	304	CLA	CMD-C2D	-2.50	1.45	1.50
22	A	809	CLA	C3B-C2B	-2.50	1.36	1.40
22	B	814	CLA	C1D-ND	2.50	1.40	1.37
22	K	105	CLA	CMC-C2C	-2.50	1.45	1.50
22	A	840	CLA	C3B-C2B	-2.50	1.36	1.40
22	8	308	CLA	CAC-C3C	-2.49	1.44	1.51
22	7	309	CLA	C3B-CAB	-2.49	1.42	1.47
22	6	315	CLA	C3B-C2B	-2.49	1.36	1.40
22	A	825	CLA	C3B-C2B	-2.49	1.36	1.40
22	F	301	CLA	C3B-C2B	-2.49	1.36	1.40
22	K	101	CLA	CMB-C2B	-2.49	1.46	1.51
22	A	839	CLA	C3B-C2B	-2.49	1.36	1.40
22	B	815	CLA	CMB-C2B	-2.49	1.46	1.51
22	A	806	CLA	C3B-C2B	-2.48	1.36	1.40
22	B	808	CLA	CMC-C2C	-2.48	1.45	1.50
22	A	831	CLA	CMD-C2D	-2.48	1.45	1.50
31	4	318	LMG	O7-C8	-2.48	1.40	1.46
22	J	103	CLA	CMB-C2B	-2.48	1.46	1.51
30	2	315	XAT	O24-C25	-2.48	1.42	1.46
22	B	806	CLA	C1D-ND	2.48	1.40	1.37
22	B	817	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	833	CLA	CMB-C2B	-2.48	1.46	1.51
29	7	308	CHL	MG-NA	-2.48	2.00	2.06
22	A	802	CLA	CMC-C2C	-2.47	1.45	1.50
22	2	310	CLA	C3B-C2B	-2.47	1.36	1.40
29	6	308	CHL	C1D-ND	-2.47	1.34	1.37
22	6	311	CLA	C3B-C2B	-2.47	1.36	1.40
22	B	821	CLA	CMD-C2D	-2.47	1.45	1.50
24	6	322	LHG	O7-C5	-2.47	1.40	1.46
22	4	312	CLA	C3B-C2B	-2.47	1.36	1.40
22	2	319	CLA	CMD-C2D	-2.47	1.45	1.50
22	A	820	CLA	CMD-C2D	-2.47	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	313	CLA	CMD-C2D	-2.46	1.45	1.50
25	4	317	8CT	C25-C26	2.46	1.39	1.35
22	G	103	CLA	CMB-C2B	-2.46	1.46	1.51
26	J	102	HTG	C1-S1	-2.46	1.76	1.80
22	B	810	CLA	C3B-CAB	-2.46	1.42	1.47
29	2	301	CHL	C1D-ND	-2.46	1.34	1.37
22	3	303	CLA	C3B-C2B	-2.46	1.37	1.40
22	B	827	CLA	CMD-C2D	-2.46	1.45	1.50
22	7	309	CLA	CMD-C2D	-2.46	1.45	1.50
22	8	302	CLA	C3B-C2B	-2.46	1.37	1.40
22	9	304	CLA	CMD-C2D	-2.46	1.45	1.50
22	A	829	CLA	CMD-C2D	-2.46	1.45	1.50
25	3	318	8CT	C22-C21	2.45	1.56	1.50
22	4	314	CLA	CMD-C2D	-2.45	1.45	1.50
22	A	803	CLA	CMD-C2D	-2.45	1.45	1.50
22	A	840	CLA	C3B-CAB	-2.45	1.42	1.47
25	I	101	8CT	C33-C32	-2.45	1.43	1.50
22	6	304	CLA	CMD-C2D	-2.45	1.45	1.50
22	4	313	CLA	CMD-C2D	-2.45	1.45	1.50
22	B	826	CLA	CMD-C2D	-2.45	1.45	1.50
22	G	102	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	817	CLA	C3B-C2B	-2.45	1.37	1.40
22	4	302	CLA	C3B-CAB	-2.44	1.43	1.47
22	B	801	CLA	CMD-C2D	-2.44	1.45	1.50
22	B	828	CLA	CMC-C2C	-2.44	1.45	1.50
22	A	811	CLA	C3B-C2B	-2.44	1.37	1.40
28	B	849	DGD	O3G-C3G	-2.44	1.39	1.43
22	0	302	CLA	CMB-C2B	-2.44	1.46	1.51
22	B	801	CLA	CMC-C2C	-2.44	1.45	1.50
25	K	103	8CT	C24-C23	2.44	1.40	1.34
22	B	841	CLA	CMD-C2D	-2.43	1.45	1.50
22	A	831	CLA	C3B-C2B	-2.43	1.37	1.40
22	2	319	CLA	C3B-C2B	-2.43	1.37	1.40
22	3	310	CLA	C3B-C2B	-2.43	1.37	1.40
22	2	311	CLA	CMC-C2C	-2.43	1.45	1.50
22	3	301	CLA	CMD-C2D	-2.43	1.45	1.50
22	1	304	CLA	MG-ND	-2.43	2.01	2.05
22	2	314	CLA	CMD-C2D	-2.43	1.45	1.50
22	B	834	CLA	CMD-C2D	-2.43	1.45	1.50
22	B	833	CLA	C3B-C2B	-2.43	1.37	1.40
22	3	304	CLA	CMD-C2D	-2.43	1.45	1.50
22	8	313	CLA	CMD-C2D	-2.43	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	4	305	CHL	C1D-C2D	2.43	1.50	1.45
22	B	805	CLA	CMD-C2D	-2.42	1.45	1.50
29	4	306	CHL	C4B-CHC	2.42	1.47	1.41
22	3	307	CLA	C3B-CAB	-2.42	1.43	1.47
22	A	840	CLA	CMD-C2D	-2.42	1.45	1.50
22	A	827	CLA	CMD-C2D	-2.42	1.45	1.50
22	2	313	CLA	CMD-C2D	-2.42	1.45	1.50
30	3	315	XAT	O4-C5	-2.42	1.42	1.46
29	0	301	CHL	C4B-CHC	2.42	1.47	1.41
22	B	807	CLA	CMD-C2D	-2.42	1.45	1.50
22	4	311	CLA	CMD-C2D	-2.42	1.45	1.50
22	4	309	CLA	CMD-C2D	-2.42	1.45	1.50
29	9	302	CHL	C1D-ND	-2.42	1.34	1.37
22	L	201	CLA	C3B-C2B	-2.41	1.37	1.40
29	2	301	CHL	C1D-C2D	2.41	1.50	1.45
22	1	310	CLA	CMD-C2D	-2.41	1.45	1.50
22	9	310	CLA	CMB-C2B	-2.41	1.46	1.51
22	A	819	CLA	CMD-C2D	-2.41	1.45	1.50
22	B	830	CLA	CMC-C2C	-2.41	1.45	1.50
25	1	316	8CT	C25-C26	2.41	1.39	1.35
22	A	805	CLA	CMC-C2C	-2.41	1.45	1.50
22	0	311	CLA	CMB-C2B	-2.41	1.46	1.51
22	1	304	CLA	C3B-C2B	-2.41	1.37	1.40
22	3	308	CLA	CMC-C2C	-2.41	1.45	1.50
22	7	307	CLA	CMC-C2C	-2.41	1.45	1.50
22	2	313	CLA	C3B-CAB	-2.41	1.43	1.47
22	B	827	CLA	MG-ND	-2.41	2.01	2.05
22	A	803	CLA	MG-ND	-2.41	2.01	2.05
22	3	313	CLA	CMC-C2C	-2.40	1.45	1.50
22	A	837	CLA	CMD-C2D	-2.40	1.45	1.50
22	8	308	CLA	CMD-C2D	-2.40	1.45	1.50
22	A	838	CLA	C3B-C2B	-2.40	1.37	1.40
22	3	319	CLA	C3B-C2B	-2.40	1.37	1.40
22	7	313	CLA	CMD-C2D	-2.40	1.45	1.50
22	B	825	CLA	C3B-C2B	-2.40	1.37	1.40
22	6	312	CLA	C3B-C2B	-2.40	1.37	1.40
25	L	206	8CT	C25-C26	2.40	1.39	1.35
29	0	301	CHL	C1B-CHB	2.40	1.47	1.41
22	2	319	CLA	C3B-CAB	-2.40	1.43	1.47
22	9	312	CLA	C3B-C2B	-2.40	1.37	1.40
22	7	316	CLA	CMC-C2C	-2.40	1.45	1.50
22	2	303	CLA	CMD-C2D	-2.40	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	302	CLA	CMD-C2D	-2.40	1.45	1.50
22	A	823	CLA	CMD-C2D	-2.40	1.45	1.50
22	2	308	CLA	CMD-C2D	-2.40	1.45	1.50
22	A	812	CLA	C3B-CAB	-2.40	1.43	1.47
22	8	311	CLA	CMD-C2D	-2.40	1.45	1.50
22	A	813	CLA	CMC-C2C	-2.39	1.45	1.50
29	2	307	CHL	C3D-C2D	2.39	1.45	1.39
22	A	809	CLA	MG-ND	-2.39	2.01	2.05
22	B	811	CLA	CMC-C2C	-2.39	1.45	1.50
22	1	306	CLA	CMD-C2D	-2.39	1.45	1.50
22	3	309	CLA	CMB-C2B	-2.39	1.46	1.51
22	B	839	CLA	CMD-C2D	-2.39	1.45	1.50
22	7	303	CLA	CMC-C2C	-2.39	1.45	1.50
22	A	832	CLA	CMD-C2D	-2.39	1.45	1.50
25	3	318	8CT	C33-C32	-2.39	1.43	1.50
30	3	315	XAT	O24-C25	-2.39	1.42	1.46
22	B	803	CLA	MG-ND	-2.39	2.01	2.05
22	B	807	CLA	C3B-C2B	-2.39	1.37	1.40
22	B	810	CLA	CMD-C2D	-2.39	1.45	1.50
22	7	309	CLA	CMC-C2C	-2.39	1.45	1.50
22	A	816	CLA	C3B-C2B	-2.39	1.37	1.40
22	B	809	CLA	C3B-C2B	-2.39	1.37	1.40
22	3	301	CLA	C3B-C2B	-2.39	1.37	1.40
22	A	812	CLA	CMD-C2D	-2.39	1.45	1.50
22	3	305	CLA	C3B-C2B	-2.39	1.37	1.40
22	A	811	CLA	C3B-CAB	-2.39	1.43	1.47
22	B	813	CLA	CMD-C2D	-2.39	1.45	1.50
22	4	312	CLA	CMD-C2D	-2.39	1.45	1.50
22	B	826	CLA	MG-ND	-2.38	2.01	2.05
22	7	303	CLA	CMD-C2D	-2.38	1.45	1.50
22	A	853	CLA	C3B-C2B	-2.38	1.37	1.40
22	7	317	CLA	MG-ND	-2.38	2.01	2.05
22	A	824	CLA	CMD-C2D	-2.38	1.45	1.50
22	2	311	CLA	C3B-C2B	-2.38	1.37	1.40
22	F	301	CLA	MG-ND	-2.38	2.01	2.05
22	A	852	CLA	CMD-C2D	-2.38	1.45	1.50
25	J	104	8CT	C25-C26	2.38	1.38	1.35
22	A	828	CLA	CMD-C2D	-2.38	1.45	1.50
22	B	832	CLA	C3B-C2B	-2.38	1.37	1.40
22	A	840	CLA	MG-ND	-2.38	2.01	2.05
22	8	302	CLA	C3B-CAB	-2.38	1.43	1.47
22	0	302	CLA	CMC-C2C	-2.38	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	311	CLA	CMD-C2D	-2.38	1.45	1.50
22	4	302	CLA	CMD-C2D	-2.37	1.45	1.50
22	A	836	CLA	C3B-CAB	-2.37	1.43	1.47
22	3	304	CLA	C3B-CAB	-2.37	1.43	1.47
29	2	305	CHL	C3D-C2D	2.37	1.45	1.39
22	3	302	CLA	CMD-C2D	-2.37	1.45	1.50
22	A	824	CLA	C3B-C2B	-2.37	1.37	1.40
22	B	823	CLA	CMD-C2D	-2.37	1.45	1.50
29	6	302	CHL	C4B-CHC	2.37	1.47	1.41
22	9	306	CLA	C3B-C2B	-2.37	1.37	1.40
22	A	830	CLA	CMC-C2C	-2.37	1.45	1.50
22	3	313	CLA	CMD-C2D	-2.37	1.45	1.50
22	8	309	CLA	C3B-C2B	-2.37	1.37	1.40
22	3	307	CLA	CMD-C2D	-2.37	1.45	1.50
25	B	844	8CT	C33-C32	-2.37	1.43	1.50
22	1	309	CLA	C3B-C2B	-2.37	1.37	1.40
29	8	305	CHL	MG-NA	-2.37	2.00	2.06
29	6	307	CHL	C4B-CHC	2.37	1.47	1.41
22	A	814	CLA	C3B-CAB	-2.37	1.43	1.47
22	2	302	CLA	CMC-C2C	-2.37	1.45	1.50
22	1	310	CLA	C3B-C2B	-2.36	1.37	1.40
31	8	319	LMG	O8-C9	-2.36	1.39	1.45
22	1	309	CLA	CMD-C2D	-2.36	1.45	1.50
22	3	308	CLA	C3B-CAB	-2.36	1.43	1.47
22	B	838	CLA	CMD-C2D	-2.36	1.45	1.50
22	8	303	CLA	CMC-C2C	-2.36	1.45	1.50
22	B	813	CLA	C3B-C2B	-2.36	1.37	1.40
22	1	302	CLA	C3B-C2B	-2.36	1.37	1.40
22	A	804	CLA	MG-ND	-2.36	2.01	2.05
29	8	314	CHL	C1B-CHB	2.36	1.47	1.41
22	B	840	CLA	MG-ND	-2.36	2.01	2.05
22	B	822	CLA	C3B-C2B	-2.36	1.37	1.40
22	A	801	CLA	C3B-C2B	-2.35	1.37	1.40
22	B	830	CLA	CMD-C2D	-2.35	1.45	1.50
22	B	824	CLA	C3B-C2B	-2.35	1.37	1.40
31	8	319	LMG	O1-C7	-2.35	1.39	1.43
22	4	310	CLA	C3B-CAB	-2.35	1.43	1.47
22	A	828	CLA	CMC-C2C	-2.35	1.45	1.50
22	K	102	CLA	CMD-C2D	-2.35	1.45	1.50
22	L	202	CLA	CMB-C2B	-2.35	1.46	1.51
25	A	848	8CT	C33-C32	-2.35	1.44	1.50
29	2	306	CHL	C4B-CHC	2.35	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	8	305	CHL	C1D-ND	-2.35	1.34	1.37
29	4	301	CHL	C3D-C2D	2.35	1.45	1.39
22	A	809	CLA	CMD-C2D	-2.35	1.45	1.50
22	9	308	CLA	CMD-C2D	-2.35	1.45	1.50
22	A	801	CLA	CMC-C2C	-2.35	1.45	1.50
22	8	303	CLA	MG-ND	-2.35	2.01	2.05
22	6	317	CLA	CMD-C2D	-2.35	1.45	1.50
22	9	309	CLA	C3B-C2B	-2.35	1.37	1.40
22	1	301	CLA	CMD-C2D	-2.34	1.45	1.50
30	7	320	XAT	O4-C5	-2.34	1.42	1.46
22	A	805	CLA	CMD-C2D	-2.34	1.45	1.50
29	0	306	CHL	C1D-ND	-2.34	1.34	1.37
22	A	811	CLA	CMC-C2C	-2.34	1.45	1.50
22	1	311	CLA	CMD-C2D	-2.34	1.45	1.50
22	A	818	CLA	CMC-C2C	-2.34	1.45	1.50
22	5	302	CLA	C3B-C2B	-2.34	1.37	1.40
22	A	828	CLA	MG-ND	-2.34	2.01	2.05
22	B	803	CLA	C3B-CAB	-2.34	1.43	1.47
25	G	104	8CT	C25-C26	2.34	1.38	1.35
22	1	303	CLA	CMC-C2C	-2.34	1.45	1.50
22	A	823	CLA	C3B-C2B	-2.34	1.37	1.40
22	A	836	CLA	C3B-C2B	-2.34	1.37	1.40
22	A	831	CLA	MG-ND	-2.34	2.01	2.05
29	2	301	CHL	C3D-C2D	2.34	1.45	1.39
22	A	811	CLA	CMD-C2D	-2.34	1.45	1.50
22	B	831	CLA	MG-ND	-2.34	2.01	2.05
22	B	823	CLA	C3B-CAB	-2.34	1.43	1.47
22	B	829	CLA	CMC-C2C	-2.34	1.45	1.50
29	6	307	CHL	C1D-C2D	2.34	1.49	1.45
22	A	841	CLA	MG-ND	-2.34	2.01	2.05
22	B	829	CLA	CMD-C2D	-2.34	1.45	1.50
22	A	815	CLA	CMD-C2D	-2.34	1.45	1.50
22	7	310	CLA	CMD-C2D	-2.34	1.45	1.50
30	6	320	XAT	O4-C5	-2.34	1.42	1.46
22	B	814	CLA	CMD-C2D	-2.34	1.45	1.50
22	4	310	CLA	CMD-C2D	-2.34	1.45	1.50
22	B	841	CLA	C3B-C2B	-2.34	1.37	1.40
22	7	302	CLA	CMD-C2D	-2.34	1.45	1.50
22	4	308	CLA	MG-ND	-2.34	2.01	2.05
29	2	305	CHL	MG-NA	-2.34	2.00	2.06
22	8	315	CLA	CMD-C2D	-2.33	1.45	1.50
29	4	307	CHL	C1D-C2D	2.33	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	312	CLA	CMC-C2C	-2.33	1.45	1.50
22	1	301	CLA	C3B-C2B	-2.33	1.37	1.40
22	1	311	CLA	C3B-C2B	-2.33	1.37	1.40
22	5	303	CLA	CMD-C2D	-2.33	1.45	1.50
22	0	311	CLA	CMD-C2D	-2.33	1.45	1.50
22	3	305	CLA	C3B-CAB	-2.33	1.43	1.47
22	A	807	CLA	C3B-CAB	-2.33	1.43	1.47
22	7	318	CLA	CMD-C2D	-2.33	1.45	1.50
22	6	309	CLA	CMD-C2D	-2.33	1.45	1.50
22	B	814	CLA	C3B-C2B	-2.33	1.37	1.40
22	4	308	CLA	C3B-C2B	-2.33	1.37	1.40
22	8	304	CLA	C3B-C2B	-2.33	1.37	1.40
22	2	309	CLA	CMD-C2D	-2.33	1.45	1.50
24	A	845	LHG	O7-C5	-2.33	1.40	1.46
31	5	319	LMG	O1-C1	2.33	1.44	1.40
22	A	853	CLA	CMD-C2D	-2.33	1.45	1.50
22	B	818	CLA	CMC-C2C	-2.33	1.45	1.50
22	6	312	CLA	CMD-C2D	-2.33	1.45	1.50
22	B	824	CLA	CMD-C2D	-2.33	1.45	1.50
22	8	302	CLA	CMD-C2D	-2.32	1.45	1.50
29	4	307	CHL	C3D-C2D	2.32	1.45	1.39
22	6	304	CLA	CMC-C2C	-2.32	1.45	1.50
22	A	836	CLA	MG-ND	-2.32	2.01	2.05
22	A	822	CLA	CMD-C2D	-2.32	1.45	1.50
22	7	304	CLA	CMC-C2C	-2.32	1.45	1.50
22	A	802	CLA	MG-ND	-2.32	2.01	2.05
22	8	313	CLA	C3B-C2B	-2.32	1.37	1.40
22	9	304	CLA	MG-ND	-2.32	2.01	2.05
31	8	319	LMG	O6-C5	-2.32	1.38	1.44
22	2	304	CLA	CMD-C2D	-2.32	1.45	1.50
25	2	317	8CT	C25-C26	2.32	1.38	1.35
30	2	316	XAT	O24-C25	-2.32	1.42	1.46
25	B	845	8CT	C33-C32	-2.32	1.44	1.50
22	A	806	CLA	MG-ND	-2.32	2.01	2.05
29	8	305	CHL	C4B-CHC	2.32	1.47	1.41
22	1	302	CLA	CMD-C2D	-2.31	1.45	1.50
22	A	852	CLA	CMC-C2C	-2.31	1.45	1.50
25	7	301	8CT	C33-C32	-2.31	1.44	1.50
22	7	313	CLA	C3B-C2B	-2.31	1.37	1.40
22	A	808	CLA	CMC-C2C	-2.31	1.45	1.50
22	8	312	CLA	CMD-C2D	-2.31	1.45	1.50
22	6	313	CLA	MG-ND	-2.31	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	806	CLA	CMC-C2C	-2.31	1.45	1.50
22	L	202	CLA	CMD-C2D	-2.31	1.45	1.50
22	6	323	CLA	CMD-C2D	-2.31	1.45	1.50
22	B	803	CLA	CMD-C2D	-2.31	1.45	1.50
22	B	820	CLA	CMD-C2D	-2.31	1.45	1.50
22	B	826	CLA	C1D-ND	2.31	1.40	1.37
22	B	820	CLA	MG-ND	-2.31	2.01	2.05
22	A	811	CLA	MG-ND	-2.31	2.01	2.05
22	A	833	CLA	CMD-C2D	-2.31	1.45	1.50
22	A	840	CLA	CMC-C2C	-2.31	1.45	1.50
22	3	301	CLA	CMC-C2C	-2.31	1.45	1.50
22	7	315	CLA	CMD-C2D	-2.31	1.45	1.50
22	B	817	CLA	CMD-C2D	-2.30	1.45	1.50
22	A	818	CLA	C3B-C2B	-2.30	1.37	1.40
22	B	825	CLA	MG-ND	-2.30	2.01	2.05
22	4	308	CLA	C3B-CAB	-2.30	1.43	1.47
22	B	817	CLA	CMC-C2C	-2.30	1.45	1.50
22	4	311	CLA	CMC-C2C	-2.30	1.45	1.50
25	B	804	8CT	C33-C32	-2.30	1.44	1.50
29	8	314	CHL	C4B-CHC	2.30	1.47	1.41
22	4	313	CLA	C3B-C2B	-2.30	1.37	1.40
22	L	201	CLA	C3B-CAB	-2.30	1.43	1.47
22	B	809	CLA	CMC-C2C	-2.30	1.45	1.50
22	A	814	CLA	CMC-C2C	-2.30	1.45	1.50
22	1	307	CLA	CMD-C2D	-2.30	1.45	1.50
22	6	311	CLA	CMD-C2D	-2.30	1.45	1.50
22	4	304	CLA	CMD-C2D	-2.30	1.45	1.50
30	5	316	XAT	O4-C5	-2.30	1.42	1.46
22	7	312	CLA	CMD-C2D	-2.30	1.45	1.50
22	B	803	CLA	CMC-C2C	-2.30	1.45	1.50
22	1	301	CLA	CMC-C2C	-2.30	1.45	1.50
22	7	307	CLA	CMD-C2D	-2.30	1.45	1.50
22	B	840	CLA	CMC-C2C	-2.30	1.45	1.50
29	7	308	CHL	C4B-CHC	2.29	1.47	1.41
22	A	812	CLA	MG-ND	-2.29	2.01	2.05
22	A	825	CLA	CMC-C2C	-2.29	1.45	1.50
22	A	839	CLA	CMD-C2D	-2.29	1.45	1.50
22	9	306	CLA	CMD-C2D	-2.29	1.45	1.50
25	B	843	8CT	C25-C26	2.29	1.38	1.35
22	9	303	CLA	CMD-C2D	-2.29	1.45	1.50
30	4	316	XAT	O24-C25	-2.29	1.42	1.46
22	A	814	CLA	MG-ND	-2.29	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	311	CLA	CMD-C2D	-2.29	1.45	1.50
22	6	303	CLA	C3B-C2B	-2.29	1.37	1.40
22	A	853	CLA	C3B-CAB	-2.29	1.43	1.47
22	A	806	CLA	C3B-CAB	-2.29	1.43	1.47
29	3	306	CHL	MG-NA	-2.29	2.00	2.06
22	7	306	CLA	CMC-C2C	-2.29	1.45	1.50
25	3	316	8CT	C25-C26	2.29	1.38	1.35
22	0	310	CLA	C3B-C2B	-2.29	1.37	1.40
22	A	816	CLA	CMC-C2C	-2.29	1.46	1.50
22	A	836	CLA	CMD-C2D	-2.29	1.46	1.50
22	B	840	CLA	CMD-C2D	-2.29	1.46	1.50
22	B	806	CLA	C3B-CAB	-2.29	1.43	1.47
22	A	814	CLA	CMD-C2D	-2.29	1.46	1.50
22	6	318	CLA	CMD-C2D	-2.29	1.46	1.50
22	H	201	CLA	CMD-C2D	-2.29	1.46	1.50
30	7	319	XAT	O24-C25	-2.29	1.42	1.46
22	2	312	CLA	CMC-C2C	-2.29	1.46	1.50
22	2	308	CLA	MG-ND	-2.29	2.01	2.05
22	7	318	CLA	MG-ND	-2.29	2.01	2.05
22	5	304	CLA	C3B-C2B	-2.28	1.37	1.40
22	A	806	CLA	CMD-C2D	-2.28	1.46	1.50
22	A	826	CLA	C3B-CAB	-2.28	1.43	1.47
22	B	807	CLA	C3B-CAB	-2.28	1.43	1.47
22	A	808	CLA	C3B-C2B	-2.28	1.37	1.40
29	4	301	CHL	MG-NA	-2.28	2.00	2.06
22	A	818	CLA	C3B-CAB	-2.28	1.43	1.47
22	B	821	CLA	MG-ND	-2.28	2.01	2.05
22	2	304	CLA	C3B-C2B	-2.28	1.37	1.40
22	1	312	CLA	CMD-C2D	-2.28	1.46	1.50
22	A	815	CLA	CMC-C2C	-2.28	1.46	1.50
22	B	805	CLA	CMC-C2C	-2.28	1.46	1.50
30	6	320	XAT	O24-C25	-2.28	1.43	1.46
22	A	829	CLA	C3B-CAB	-2.28	1.43	1.47
29	5	306	CHL	C4B-CHC	2.28	1.47	1.41
22	0	302	CLA	CMD-C2D	-2.28	1.46	1.50
22	B	831	CLA	C3B-C2B	-2.28	1.37	1.40
25	8	301	8CT	C25-C26	2.28	1.38	1.35
22	9	310	CLA	CMD-C2D	-2.28	1.46	1.50
22	B	830	CLA	MG-ND	-2.28	2.01	2.05
22	8	309	CLA	CMD-C2D	-2.28	1.46	1.50
22	A	818	CLA	MG-ND	-2.28	2.01	2.05
22	B	836	CLA	MG-ND	-2.28	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	816	CLA	CMC-C2C	-2.28	1.46	1.50
22	B	828	CLA	CMD-C2D	-2.28	1.46	1.50
22	7	312	CLA	C3B-C2B	-2.28	1.37	1.40
30	1	314	XAT	O4-C5	-2.27	1.43	1.46
22	B	838	CLA	MG-ND	-2.27	2.01	2.05
22	6	317	CLA	MG-ND	-2.27	2.01	2.05
22	B	830	CLA	C3B-C2B	-2.27	1.37	1.40
22	3	313	CLA	MG-ND	-2.27	2.01	2.05
22	1	308	CLA	CMC-C2C	-2.27	1.46	1.50
22	6	315	CLA	CMD-C2D	-2.27	1.46	1.50
22	7	316	CLA	C3B-C2B	-2.27	1.37	1.40
22	B	809	CLA	CMD-C2D	-2.27	1.46	1.50
22	3	319	CLA	CMD-C2D	-2.27	1.46	1.50
22	A	834	CLA	CMD-C2D	-2.27	1.46	1.50
22	4	311	CLA	C3B-C2B	-2.27	1.37	1.40
22	B	837	CLA	CMD-C2D	-2.27	1.46	1.50
25	B	843	8CT	C33-C32	-2.27	1.44	1.50
22	B	812	CLA	C3B-C2B	-2.27	1.37	1.40
22	L	201	CLA	MG-ND	-2.27	2.01	2.05
29	4	305	CHL	C4B-CHC	2.27	1.47	1.41
22	F	301	CLA	C3B-CAB	-2.27	1.43	1.47
22	4	302	CLA	MG-ND	-2.27	2.01	2.05
29	7	308	CHL	C3D-C2D	2.27	1.45	1.39
22	A	835	CLA	CMD-C2D	-2.26	1.46	1.50
22	7	314	CLA	CMD-C2D	-2.26	1.46	1.50
22	B	838	CLA	CMC-C2C	-2.26	1.46	1.50
22	3	311	CLA	C3B-C2B	-2.26	1.37	1.40
22	6	317	CLA	C3B-C2B	-2.26	1.37	1.40
29	2	305	CHL	C1D-C2D	2.26	1.49	1.45
22	A	836	CLA	CMC-C2C	-2.26	1.46	1.50
22	A	816	CLA	CMD-C2D	-2.26	1.46	1.50
22	7	317	CLA	CMD-C2D	-2.26	1.46	1.50
22	A	838	CLA	CMD-C2D	-2.26	1.46	1.50
22	8	310	CLA	C3B-C2B	-2.26	1.37	1.40
22	B	808	CLA	C3B-C2B	-2.26	1.37	1.40
22	J	103	CLA	C3B-C2B	-2.26	1.37	1.40
22	4	310	CLA	MG-ND	-2.26	2.01	2.05
22	1	313	CLA	CMD-C2D	-2.26	1.46	1.50
22	2	303	CLA	MG-ND	-2.26	2.01	2.05
22	6	313	CLA	CMC-C2C	-2.26	1.46	1.50
22	B	822	CLA	CMD-C2D	-2.25	1.46	1.50
22	A	826	CLA	MG-ND	-2.25	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	818	CLA	CMD-C2D	-2.25	1.46	1.50
22	B	812	CLA	CMC-C2C	-2.25	1.46	1.50
22	6	310	CLA	MG-ND	-2.25	2.01	2.05
22	3	308	CLA	C3B-C2B	-2.25	1.37	1.40
22	A	826	CLA	CMD-C2D	-2.25	1.46	1.50
22	8	303	CLA	CMD-C2D	-2.25	1.46	1.50
29	7	308	CHL	C1D-C2D	2.25	1.49	1.45
25	8	318	8CT	C25-C26	2.25	1.38	1.35
22	A	809	CLA	CMC-C2C	-2.25	1.46	1.50
22	A	823	CLA	C3B-CAB	-2.25	1.43	1.47
22	3	311	CLA	CMC-C2C	-2.25	1.46	1.50
22	7	306	CLA	MG-ND	-2.25	2.01	2.05
22	6	318	CLA	C3B-CAB	-2.25	1.43	1.47
22	1	303	CLA	MG-ND	-2.25	2.01	2.05
22	B	839	CLA	C3B-C2B	-2.25	1.37	1.40
30	3	314	XAT	O24-C25	-2.25	1.43	1.46
22	B	833	CLA	C3B-CAB	-2.25	1.43	1.47
22	B	835	CLA	C3B-C2B	-2.25	1.37	1.40
22	G	101	CLA	CMB-C2B	-2.25	1.47	1.51
22	A	821	CLA	CMD-C2D	-2.24	1.46	1.50
22	2	310	CLA	C3B-CAB	-2.24	1.43	1.47
29	8	306	CHL	C4B-CHC	2.24	1.47	1.41
22	5	309	CLA	CMC-C2C	-2.24	1.46	1.50
25	B	851	8CT	C33-C32	-2.24	1.44	1.50
22	6	311	CLA	C3B-CAB	-2.24	1.43	1.47
22	B	835	CLA	CMC-C2C	-2.24	1.46	1.50
29	0	306	CHL	C1B-CHB	2.24	1.47	1.41
22	B	801	CLA	C3B-CAB	-2.24	1.43	1.47
30	4	315	XAT	O4-C5	-2.24	1.43	1.46
22	B	824	CLA	CMC-C2C	-2.24	1.46	1.50
29	6	316	CHL	C4B-CHC	2.24	1.47	1.41
22	K	105	CLA	C3B-C2B	-2.24	1.37	1.40
22	7	304	CLA	MG-ND	-2.24	2.01	2.05
22	A	827	CLA	C3B-CAB	-2.24	1.43	1.47
22	A	832	CLA	C3B-CAB	-2.24	1.43	1.47
22	7	306	CLA	CMD-C2D	-2.24	1.46	1.50
22	0	308	CLA	CMD-C2D	-2.24	1.46	1.50
22	7	305	CLA	C3B-C2B	-2.24	1.37	1.40
22	A	810	CLA	CMC-C2C	-2.24	1.46	1.50
22	5	314	CLA	C3B-C2B	-2.23	1.37	1.40
22	1	313	CLA	MG-ND	-2.23	2.01	2.05
22	4	304	CLA	CMC-C2C	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	302	CLA	CMC-C2C	-2.23	1.46	1.50
29	9	307	CHL	C1D-ND	-2.23	1.35	1.37
22	5	309	CLA	C3B-C2B	-2.23	1.37	1.40
22	A	830	CLA	MG-ND	-2.23	2.01	2.05
22	4	303	CLA	CMC-C2C	-2.23	1.46	1.50
22	5	303	CLA	CMC-C2C	-2.23	1.46	1.50
22	3	305	CLA	MG-ND	-2.23	2.01	2.05
29	3	306	CHL	C3D-C2D	2.23	1.45	1.39
22	A	820	CLA	MG-ND	-2.23	2.01	2.05
22	K	101	CLA	CMC-C2C	-2.23	1.46	1.50
22	3	303	CLA	CMD-C2D	-2.23	1.46	1.50
22	0	310	CLA	C3B-CAB	-2.23	1.43	1.47
22	2	312	CLA	CMD-C2D	-2.23	1.46	1.50
22	3	309	CLA	CMD-C2D	-2.23	1.46	1.50
22	4	313	CLA	CMC-C2C	-2.23	1.46	1.50
22	B	834	CLA	C3B-CAB	-2.23	1.43	1.47
22	0	308	CLA	CMC-C2C	-2.23	1.46	1.50
22	9	301	CLA	CMD-C2D	-2.23	1.46	1.50
30	8	317	XAT	O4-C5	-2.23	1.43	1.46
22	A	808	CLA	MG-ND	-2.23	2.01	2.05
22	6	303	CLA	MG-ND	-2.23	2.01	2.05
22	A	835	CLA	CMC-C2C	-2.23	1.46	1.50
30	4	316	XAT	C22-C21	-2.23	1.51	1.54
25	3	316	8CT	C33-C32	-2.23	1.44	1.50
22	B	812	CLA	MG-ND	-2.23	2.01	2.05
25	B	848	8CT	C25-C26	2.22	1.38	1.35
22	5	312	CLA	CMD-C2D	-2.22	1.46	1.50
22	B	817	CLA	MG-ND	-2.22	2.01	2.05
22	A	807	CLA	CMC-C2C	-2.22	1.46	1.50
25	7	323	8CT	C25-C26	2.22	1.38	1.35
22	9	305	CLA	C3B-C2B	-2.22	1.37	1.40
22	B	818	CLA	C3B-CAB	-2.22	1.43	1.47
22	1	303	CLA	C3B-C2B	-2.22	1.37	1.40
22	B	841	CLA	CMC-C2C	-2.22	1.46	1.50
22	1	302	CLA	CMC-C2C	-2.22	1.46	1.50
22	9	306	CLA	MG-ND	-2.22	2.01	2.05
22	B	850	CLA	C3B-C2B	-2.22	1.37	1.40
22	F	301	CLA	CMC-C2C	-2.22	1.46	1.50
25	B	845	8CT	C25-C26	2.22	1.38	1.35
22	5	302	CLA	CMC-C2C	-2.22	1.46	1.50
29	2	307	CHL	C1D-C2D	2.22	1.49	1.45
22	B	837	CLA	C3B-CAB	-2.22	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	2	301	CHL	C1C-NC	-2.22	1.34	1.37
22	6	312	CLA	MG-ND	-2.22	2.01	2.05
22	A	808	CLA	CMD-C2D	-2.22	1.46	1.50
22	1	311	CLA	CMC-C2C	-2.22	1.46	1.50
22	8	309	CLA	C3B-CAB	-2.22	1.43	1.47
22	3	305	CLA	CMD-C2D	-2.22	1.46	1.50
22	7	304	CLA	C3B-C2B	-2.22	1.37	1.40
22	9	304	CLA	C3B-C2B	-2.22	1.37	1.40
22	K	102	CLA	CMC-C2C	-2.22	1.46	1.50
22	7	305	CLA	MG-ND	-2.21	2.01	2.05
22	B	811	CLA	CMD-C2D	-2.21	1.46	1.50
22	A	819	CLA	CMC-C2C	-2.21	1.46	1.50
22	5	305	CLA	CMD-C2D	-2.21	1.46	1.50
22	3	304	CLA	MG-ND	-2.21	2.01	2.05
22	3	310	CLA	CMD-C2D	-2.21	1.46	1.50
22	L	201	CLA	CMD-C2D	-2.21	1.46	1.50
22	A	804	CLA	C3B-CAB	-2.21	1.43	1.47
22	B	831	CLA	CMC-C2C	-2.21	1.46	1.50
22	2	313	CLA	C3B-C2B	-2.21	1.37	1.40
22	B	821	CLA	CMC-C2C	-2.21	1.46	1.50
22	3	309	CLA	CMC-C2C	-2.21	1.46	1.50
25	B	847	8CT	C25-C26	2.21	1.38	1.35
22	5	310	CLA	CMD-C2D	-2.21	1.46	1.50
22	K	102	CLA	MG-ND	-2.21	2.01	2.05
22	A	827	CLA	C3B-C2B	-2.21	1.37	1.40
22	4	303	CLA	MG-ND	-2.21	2.01	2.05
22	2	312	CLA	MG-ND	-2.21	2.01	2.05
22	2	314	CLA	MG-ND	-2.21	2.01	2.05
22	B	806	CLA	C3B-C2B	-2.21	1.37	1.40
22	A	824	CLA	CMC-C2C	-2.21	1.46	1.50
29	6	306	CHL	MG-NA	-2.21	2.01	2.06
22	A	812	CLA	CMC-C2C	-2.21	1.46	1.50
22	5	308	CLA	C3B-C2B	-2.21	1.37	1.40
22	B	825	CLA	C3B-CAB	-2.21	1.43	1.47
25	A	846	8CT	C33-C32	-2.21	1.44	1.50
22	A	803	CLA	CMC-C2C	-2.21	1.46	1.50
22	5	304	CLA	CMC-C2C	-2.21	1.46	1.50
22	A	824	CLA	MG-ND	-2.21	2.01	2.05
22	7	309	CLA	MG-ND	-2.21	2.01	2.05
22	B	832	CLA	CMC-C2C	-2.20	1.46	1.50
22	B	834	CLA	CMC-C2C	-2.20	1.46	1.50
22	A	841	CLA	CMC-C2C	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	843	CLA	CMD-C2D	-2.20	1.46	1.50
22	4	312	CLA	CMC-C2C	-2.20	1.46	1.50
22	9	301	CLA	CMC-C2C	-2.20	1.46	1.50
22	A	807	CLA	CMD-C2D	-2.20	1.46	1.50
22	7	304	CLA	C3B-CAB	-2.20	1.43	1.47
22	0	303	CLA	CMD-C2D	-2.20	1.46	1.50
22	A	826	CLA	CMC-C2C	-2.20	1.46	1.50
22	B	816	CLA	C3B-C2B	-2.20	1.37	1.40
22	4	311	CLA	MG-ND	-2.20	2.01	2.05
22	B	815	CLA	C3B-C2B	-2.20	1.37	1.40
22	B	815	CLA	CMD-C2D	-2.20	1.46	1.50
22	6	303	CLA	CMC-C2C	-2.20	1.46	1.50
29	1	305	CHL	C4B-CHC	2.20	1.47	1.41
22	7	311	CLA	MG-ND	-2.20	2.01	2.05
22	A	802	CLA	CMD-C2D	-2.20	1.46	1.50
22	B	815	CLA	CMC-C2C	-2.20	1.46	1.50
22	B	850	CLA	CMD-C2D	-2.20	1.46	1.50
22	6	314	CLA	CMD-C2D	-2.20	1.46	1.50
22	1	307	CLA	CMC-C2C	-2.20	1.46	1.50
22	3	312	CLA	CMD-C2D	-2.20	1.46	1.50
22	B	816	CLA	C3B-CAB	-2.20	1.43	1.47
22	1	310	CLA	MG-ND	-2.20	2.01	2.05
22	2	319	CLA	CMC-C2C	-2.20	1.46	1.50
22	7	305	CLA	CMD-C2D	-2.20	1.46	1.50
24	9	316	LHG	O7-C5	-2.20	1.41	1.46
22	B	824	CLA	C3B-CAB	-2.20	1.43	1.47
22	2	312	CLA	C3B-C2B	-2.20	1.37	1.40
22	3	313	CLA	C3B-CAB	-2.19	1.43	1.47
22	A	829	CLA	MG-ND	-2.19	2.01	2.05
22	B	828	CLA	MG-ND	-2.19	2.01	2.05
22	5	302	CLA	MG-ND	-2.19	2.01	2.05
22	3	307	CLA	CMC-C2C	-2.19	1.46	1.50
22	K	104	CLA	C3B-C2B	-2.19	1.37	1.40
30	9	314	XAT	O4-C5	-2.19	1.43	1.46
22	6	310	CLA	C3B-C2B	-2.19	1.37	1.40
22	B	805	CLA	C3B-CAB	-2.19	1.43	1.47
22	B	809	CLA	C3B-CAB	-2.19	1.43	1.47
22	7	316	CLA	CMD-C2D	-2.19	1.46	1.50
25	A	849	8CT	C25-C26	2.19	1.38	1.35
22	6	314	CLA	C3B-C2B	-2.19	1.37	1.40
22	B	816	CLA	CMD-C2D	-2.19	1.46	1.50
22	B	826	CLA	CMC-C2C	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	J	103	CLA	CMD-C2D	-2.19	1.46	1.50
22	7	310	CLA	CMC-C2C	-2.19	1.46	1.50
22	A	813	CLA	C3B-CAB	-2.19	1.43	1.47
25	L	205	8CT	C33-C32	-2.19	1.44	1.50
22	A	831	CLA	C3B-CAB	-2.19	1.43	1.47
29	6	316	CHL	C4C-C3C	2.19	1.48	1.45
22	6	310	CLA	CMC-C2C	-2.19	1.46	1.50
22	A	804	CLA	CMC-C2C	-2.18	1.46	1.50
29	4	305	CHL	C4C-C3C	2.18	1.48	1.45
22	7	313	CLA	CMC-C2C	-2.18	1.46	1.50
22	8	311	CLA	CMC-C2C	-2.18	1.46	1.50
22	B	837	CLA	CMC-C2C	-2.18	1.46	1.50
22	5	302	CLA	C3B-CAB	-2.18	1.43	1.47
25	J	101	8CT	C25-C26	2.18	1.38	1.35
22	A	804	CLA	C3B-C2B	-2.18	1.37	1.40
29	5	306	CHL	C4C-C3C	2.18	1.48	1.45
22	6	310	CLA	CMD-C2D	-2.18	1.46	1.50
22	1	309	CLA	MG-ND	-2.18	2.01	2.05
22	2	308	CLA	CMC-C2C	-2.18	1.46	1.50
22	9	304	CLA	CMC-C2C	-2.18	1.46	1.50
22	1	306	CLA	C3B-C2B	-2.18	1.37	1.40
22	0	304	CLA	CMD-C2D	-2.18	1.46	1.50
22	6	323	CLA	CMC-C2C	-2.18	1.46	1.50
22	8	310	CLA	CMD-C2D	-2.18	1.46	1.50
22	A	805	CLA	C3B-CAB	-2.18	1.43	1.47
25	7	321	8CT	C25-C26	2.18	1.38	1.35
22	4	312	CLA	MG-ND	-2.18	2.01	2.05
22	A	813	CLA	CMD-C2D	-2.18	1.46	1.50
30	4	316	XAT	O4-C5	-2.18	1.43	1.46
22	A	841	CLA	C3B-CAB	-2.18	1.43	1.47
30	7	320	XAT	O24-C25	-2.17	1.43	1.46
22	8	304	CLA	MG-ND	-2.17	2.01	2.05
22	B	836	CLA	CMC-C2C	-2.17	1.46	1.50
22	5	313	CLA	CMD-C2D	-2.17	1.46	1.50
25	2	317	8CT	C33-C32	-2.17	1.44	1.50
22	3	305	CLA	CMC-C2C	-2.17	1.46	1.50
29	3	306	CHL	C1D-C2D	2.17	1.49	1.45
22	7	310	CLA	C3B-CAB	-2.17	1.43	1.47
22	B	815	CLA	C3B-CAB	-2.17	1.43	1.47
22	2	310	CLA	CMD-C2D	-2.17	1.46	1.50
22	M	101	CLA	CMC-C2C	-2.17	1.46	1.50
22	6	315	CLA	CMC-C2C	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	318	CLA	CMC-C2C	-2.17	1.46	1.50
22	A	813	CLA	MG-ND	-2.17	2.01	2.05
22	2	313	CLA	MG-ND	-2.17	2.01	2.05
22	1	304	CLA	C3B-CAB	-2.17	1.43	1.47
22	2	309	CLA	C3B-CAB	-2.17	1.43	1.47
30	8	317	XAT	O24-C25	-2.17	1.43	1.46
22	7	318	CLA	C3B-CAB	-2.17	1.43	1.47
22	B	809	CLA	MG-ND	-2.17	2.01	2.05
25	L	205	8CT	C25-C26	2.17	1.38	1.35
22	6	313	CLA	C3B-CAB	-2.17	1.43	1.47
31	8	319	LMG	O7-C8	-2.17	1.41	1.46
22	A	829	CLA	CMC-C2C	-2.17	1.46	1.50
22	5	314	CLA	CMC-C2C	-2.17	1.46	1.50
22	3	307	CLA	MG-ND	-2.16	2.01	2.05
22	3	308	CLA	MG-ND	-2.16	2.01	2.05
22	8	315	CLA	MG-ND	-2.16	2.01	2.05
22	9	312	CLA	MG-ND	-2.16	2.01	2.05
22	B	808	CLA	CMD-C2D	-2.16	1.46	1.50
22	1	311	CLA	C3B-CAB	-2.16	1.43	1.47
22	7	313	CLA	C3B-CAB	-2.16	1.43	1.47
22	8	308	CLA	CMC-C2C	-2.16	1.46	1.50
22	2	310	CLA	MG-ND	-2.16	2.01	2.05
22	B	825	CLA	CMC-C2C	-2.16	1.46	1.50
22	L	202	CLA	CMC-C2C	-2.16	1.46	1.50
22	B	813	CLA	CMC-C2C	-2.16	1.46	1.50
22	6	309	CLA	MG-ND	-2.16	2.01	2.05
22	6	304	CLA	C3B-CAB	-2.16	1.43	1.47
22	L	204	CLA	CMD-C2D	-2.16	1.46	1.50
22	7	315	CLA	MG-ND	-2.16	2.01	2.05
22	8	310	CLA	MG-ND	-2.16	2.01	2.05
22	M	101	CLA	C3B-CAB	-2.16	1.43	1.47
25	A	850	8CT	C25-C26	2.16	1.38	1.35
30	5	316	XAT	O24-C25	-2.16	1.43	1.46
22	A	824	CLA	C3B-CAB	-2.16	1.43	1.47
22	4	309	CLA	CMC-C2C	-2.15	1.46	1.50
29	2	305	CHL	C4B-CHC	2.15	1.47	1.41
22	6	301	CLA	CMD-C2D	-2.15	1.46	1.50
22	1	308	CLA	C3B-C2B	-2.15	1.37	1.40
22	5	307	CLA	C3B-C2B	-2.15	1.37	1.40
22	5	304	CLA	CMD-C2D	-2.15	1.46	1.50
22	4	314	CLA	MG-ND	-2.15	2.01	2.05
22	A	817	CLA	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	853	CLA	CMC-C2C	-2.15	1.46	1.50
22	7	315	CLA	CMC-C2C	-2.15	1.46	1.50
22	4	312	CLA	C3B-CAB	-2.15	1.43	1.47
22	7	314	CLA	CMC-C2C	-2.15	1.46	1.50
29	9	307	CHL	C4B-CHC	2.15	1.47	1.41
22	B	819	CLA	CMC-C2C	-2.15	1.46	1.50
30	0	313	XAT	O4-C5	-2.15	1.43	1.46
22	6	309	CLA	CMC-C2C	-2.15	1.46	1.50
22	7	311	CLA	CMC-C2C	-2.15	1.46	1.50
22	K	105	CLA	CMD-C2D	-2.15	1.46	1.50
22	B	808	CLA	MG-ND	-2.15	2.01	2.05
22	A	852	CLA	C3B-CAB	-2.15	1.43	1.47
22	B	819	CLA	MG-ND	-2.15	2.01	2.05
22	L	203	CLA	CMD-C2D	-2.15	1.46	1.50
22	7	302	CLA	MG-ND	-2.15	2.01	2.05
22	B	827	CLA	CMC-C2C	-2.15	1.46	1.50
22	6	311	CLA	CMC-C2C	-2.15	1.46	1.50
22	7	305	CLA	CMC-C2C	-2.15	1.46	1.50
22	4	313	CLA	C3B-CAB	-2.15	1.43	1.47
22	9	308	CLA	C3B-CAB	-2.15	1.43	1.47
22	A	822	CLA	CMC-C2C	-2.15	1.46	1.50
22	F	301	CLA	CMD-C2D	-2.15	1.46	1.50
22	2	309	CLA	C3B-C2B	-2.15	1.37	1.40
22	0	311	CLA	C3B-C2B	-2.15	1.37	1.40
25	B	846	8CT	C33-C32	-2.15	1.44	1.50
22	7	302	CLA	C3B-CAB	-2.15	1.43	1.47
29	2	306	CHL	C1B-CHB	2.14	1.47	1.41
22	8	303	CLA	C3B-C2B	-2.14	1.37	1.40
22	A	810	CLA	C3B-CAB	-2.14	1.43	1.47
22	J	103	CLA	C3B-CAB	-2.14	1.43	1.47
22	B	818	CLA	CMD-C2D	-2.14	1.46	1.50
22	7	310	CLA	MG-ND	-2.14	2.01	2.05
30	7	319	XAT	O4-C5	-2.14	1.43	1.46
22	A	801	CLA	C3B-CAB	-2.14	1.43	1.47
22	A	839	CLA	C3B-CAB	-2.14	1.43	1.47
22	2	314	CLA	CMC-C2C	-2.14	1.46	1.50
22	9	312	CLA	CMD-C2D	-2.14	1.46	1.50
22	A	805	CLA	MG-ND	-2.14	2.01	2.05
22	0	312	CLA	CMD-C2D	-2.14	1.46	1.50
22	B	810	CLA	CMC-C2C	-2.14	1.46	1.50
22	B	823	CLA	CMC-C2C	-2.14	1.46	1.50
25	8	318	8CT	C33-C32	-2.14	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	318	8CT	C25-C26	2.14	1.38	1.35
22	5	313	CLA	C3B-C2B	-2.14	1.37	1.40
22	A	838	CLA	MG-ND	-2.14	2.01	2.05
22	1	312	CLA	CMC-C2C	-2.13	1.46	1.50
30	1	315	XAT	O24-C25	-2.13	1.43	1.46
22	5	310	CLA	MG-ND	-2.13	2.01	2.05
22	5	305	CLA	C3B-CAB	-2.13	1.43	1.47
25	8	301	8CT	C33-C32	-2.13	1.44	1.50
22	A	821	CLA	MG-ND	-2.13	2.01	2.05
22	2	311	CLA	MG-ND	-2.13	2.01	2.05
22	0	312	CLA	C3B-C2B	-2.13	1.37	1.40
22	1	307	CLA	MG-ND	-2.13	2.01	2.05
22	7	305	CLA	C3B-CAB	-2.13	1.43	1.47
30	9	315	XAT	O24-C25	-2.13	1.43	1.46
22	B	832	CLA	CMD-C2D	-2.13	1.46	1.50
22	9	311	CLA	CMD-C2D	-2.13	1.46	1.50
22	3	309	CLA	MG-ND	-2.13	2.01	2.05
22	A	822	CLA	C3B-CAB	-2.13	1.43	1.47
22	6	312	CLA	CMC-C2C	-2.13	1.46	1.50
25	1	316	8CT	C33-C32	-2.13	1.44	1.50
22	B	801	CLA	CAC-C3C	-2.13	1.45	1.51
22	A	827	CLA	MG-ND	-2.13	2.01	2.05
22	B	811	CLA	C3B-CAB	-2.13	1.43	1.47
22	1	302	CLA	C3B-CAB	-2.13	1.43	1.47
22	4	304	CLA	MG-ND	-2.13	2.01	2.05
22	A	834	CLA	CMC-C2C	-2.13	1.46	1.50
22	9	310	CLA	C3B-C2B	-2.13	1.37	1.40
22	A	820	CLA	CMC-C2C	-2.12	1.46	1.50
22	B	831	CLA	C3B-CAB	-2.12	1.43	1.47
22	3	302	CLA	MG-ND	-2.12	2.01	2.05
29	6	307	CHL	C1B-CHB	2.12	1.46	1.41
22	B	812	CLA	C3B-CAB	-2.12	1.43	1.47
22	B	822	CLA	MG-ND	-2.12	2.01	2.05
22	A	823	CLA	MG-ND	-2.12	2.01	2.05
22	5	309	CLA	CMD-C2D	-2.12	1.46	1.50
22	1	308	CLA	CMD-C2D	-2.12	1.46	1.50
22	4	302	CLA	CMC-C2C	-2.12	1.46	1.50
22	A	839	CLA	MG-ND	-2.12	2.01	2.05
22	A	843	CLA	MG-ND	-2.12	2.01	2.05
22	3	303	CLA	CMC-C2C	-2.12	1.46	1.50
22	5	305	CLA	C3B-C2B	-2.12	1.37	1.40
22	3	311	CLA	MG-ND	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	309	CLA	C3B-CAB	-2.12	1.43	1.47
22	6	323	CLA	MG-ND	-2.12	2.01	2.05
22	9	309	CLA	CMD-C2D	-2.12	1.46	1.50
22	6	313	CLA	C3B-C2B	-2.12	1.37	1.40
22	B	815	CLA	MG-ND	-2.12	2.01	2.05
22	A	843	CLA	CMC-C2C	-2.12	1.46	1.50
22	1	310	CLA	CMC-C2C	-2.12	1.46	1.50
22	2	304	CLA	CMC-C2C	-2.12	1.46	1.50
22	B	832	CLA	C3B-CAB	-2.12	1.43	1.47
22	5	309	CLA	C3B-CAB	-2.12	1.43	1.47
22	A	807	CLA	MG-ND	-2.12	2.01	2.05
22	K	101	CLA	CMD-C2D	-2.12	1.46	1.50
22	5	310	CLA	CMC-C2C	-2.12	1.46	1.50
25	A	849	8CT	C33-C32	-2.12	1.44	1.50
22	A	835	CLA	MG-ND	-2.12	2.01	2.05
22	2	319	CLA	MG-ND	-2.12	2.01	2.05
22	7	303	CLA	MG-ND	-2.12	2.01	2.05
22	1	309	CLA	C3B-CAB	-2.12	1.43	1.47
22	2	309	CLA	MG-ND	-2.12	2.01	2.05
22	2	310	CLA	CMC-C2C	-2.11	1.46	1.50
22	B	836	CLA	C3B-CAB	-2.11	1.43	1.47
22	K	104	CLA	MG-ND	-2.11	2.01	2.05
31	4	318	LMG	O8-C9	-2.11	1.40	1.45
22	B	807	CLA	CMC-C2C	-2.11	1.46	1.50
22	A	834	CLA	MG-ND	-2.11	2.01	2.05
22	B	801	CLA	MG-ND	-2.11	2.01	2.05
22	8	302	CLA	MG-ND	-2.11	2.01	2.05
22	5	310	CLA	C3B-C2B	-2.11	1.37	1.40
30	6	319	XAT	O24-C25	-2.11	1.43	1.46
30	6	319	XAT	O4-C5	-2.11	1.43	1.46
22	8	304	CLA	CMC-C2C	-2.11	1.46	1.50
25	6	321	8CT	C25-C26	2.11	1.38	1.35
22	B	841	CLA	C3B-CAB	-2.11	1.43	1.47
22	0	305	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	830	CLA	C3B-CAB	-2.11	1.43	1.47
22	B	805	CLA	MG-ND	-2.11	2.01	2.05
22	B	814	CLA	MG-ND	-2.11	2.01	2.05
25	L	206	8CT	C33-C32	-2.11	1.44	1.50
22	4	309	CLA	C3B-CAB	-2.11	1.43	1.47
22	8	312	CLA	C3B-C2B	-2.11	1.37	1.40
22	0	309	CLA	C3B-C2B	-2.11	1.37	1.40
22	A	837	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	I	101	8CT	C30-C29	2.11	1.53	1.50
29	6	302	CHL	C1B-CHB	2.10	1.46	1.41
22	A	832	CLA	CMC-C2C	-2.10	1.46	1.50
22	A	819	CLA	MG-ND	-2.10	2.01	2.05
22	B	837	CLA	MG-ND	-2.10	2.01	2.05
22	A	830	CLA	C3B-CAB	-2.10	1.43	1.47
22	3	301	CLA	MG-ND	-2.10	2.01	2.05
25	B	851	8CT	C24-C23	2.10	1.40	1.34
22	A	831	CLA	CMC-C2C	-2.10	1.46	1.50
22	B	814	CLA	C3B-CAB	-2.10	1.43	1.47
22	3	304	CLA	CMC-C2C	-2.10	1.46	1.50
22	B	839	CLA	MG-ND	-2.10	2.01	2.05
25	A	854	8CT	C25-C26	2.10	1.38	1.35
29	4	306	CHL	C1B-CHB	2.10	1.46	1.41
29	5	306	CHL	C1B-CHB	2.10	1.46	1.41
22	5	314	CLA	MG-ND	-2.10	2.01	2.05
22	3	301	CLA	C3B-CAB	-2.10	1.43	1.47
22	9	311	CLA	C3B-C2B	-2.10	1.37	1.40
22	6	318	CLA	MG-ND	-2.10	2.01	2.05
22	A	817	CLA	CMC-C2C	-2.10	1.46	1.50
25	A	854	8CT	C33-C32	-2.10	1.44	1.50
22	A	810	CLA	MG-ND	-2.10	2.01	2.05
22	8	304	CLA	CMD-C2D	-2.10	1.46	1.50
29	8	314	CHL	C1C-NC	-2.10	1.34	1.37
22	0	310	CLA	CMC-C2C	-2.10	1.46	1.50
22	B	835	CLA	CMD-C2D	-2.10	1.46	1.50
22	8	309	CLA	MG-ND	-2.10	2.01	2.05
25	7	321	8CT	C33-C32	-2.10	1.44	1.50
22	6	317	CLA	CMC-C2C	-2.10	1.46	1.50
22	9	312	CLA	CMC-C2C	-2.10	1.46	1.50
22	B	829	CLA	MG-ND	-2.10	2.01	2.05
22	8	312	CLA	C3B-CAB	-2.10	1.43	1.47
22	7	318	CLA	C3B-C2B	-2.10	1.37	1.40
22	A	830	CLA	CMD-C2D	-2.10	1.46	1.50
22	B	822	CLA	CMC-C2C	-2.10	1.46	1.50
22	4	309	CLA	MG-ND	-2.10	2.01	2.05
22	A	815	CLA	C3B-CAB	-2.10	1.43	1.47
22	A	828	CLA	C3B-CAB	-2.10	1.43	1.47
22	B	841	CLA	MG-ND	-2.09	2.01	2.05
22	2	314	CLA	C3B-CAB	-2.09	1.43	1.47
22	L	202	CLA	MG-ND	-2.09	2.01	2.05
22	8	303	CLA	C3B-CAB	-2.09	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	313	CLA	CMC-C2C	-2.09	1.46	1.50
22	9	313	CLA	CMD-C2D	-2.09	1.46	1.50
22	9	303	CLA	C3B-C2B	-2.09	1.37	1.40
25	7	323	8CT	C33-C32	-2.09	1.44	1.50
22	3	310	CLA	C3B-CAB	-2.09	1.43	1.47
22	3	319	CLA	CMC-C2C	-2.09	1.46	1.50
22	0	307	CLA	CMD-C2D	-2.09	1.46	1.50
22	7	312	CLA	MG-ND	-2.09	2.01	2.05
22	9	308	CLA	MG-ND	-2.09	2.01	2.05
30	1	315	XAT	O4-C5	-2.09	1.43	1.46
22	7	303	CLA	C3B-CAB	-2.09	1.43	1.47
22	9	303	CLA	C3B-CAB	-2.09	1.43	1.47
22	A	810	CLA	CMD-C2D	-2.09	1.46	1.50
22	K	104	CLA	CMD-C2D	-2.09	1.46	1.50
22	7	318	CLA	CMC-C2C	-2.09	1.46	1.50
22	2	313	CLA	CMC-C2C	-2.09	1.46	1.50
22	9	303	CLA	CMC-C2C	-2.09	1.46	1.50
22	H	201	CLA	CMC-C2C	-2.09	1.46	1.50
22	1	307	CLA	C3B-CAB	-2.09	1.43	1.47
22	2	302	CLA	C3B-C2B	-2.09	1.37	1.40
22	M	101	CLA	CMD-C2D	-2.09	1.46	1.50
22	1	302	CLA	MG-ND	-2.08	2.01	2.05
22	B	807	CLA	MG-ND	-2.08	2.01	2.05
22	B	810	CLA	MG-ND	-2.08	2.01	2.05
22	5	311	CLA	MG-ND	-2.08	2.01	2.05
22	9	313	CLA	MG-ND	-2.08	2.01	2.05
22	1	306	CLA	CMC-C2C	-2.08	1.46	1.50
22	6	304	CLA	MG-ND	-2.08	2.01	2.05
22	2	311	CLA	C3B-CAB	-2.08	1.43	1.47
22	2	303	CLA	CMC-C2C	-2.08	1.46	1.50
22	0	310	CLA	CMD-C2D	-2.08	1.46	1.50
22	6	317	CLA	C3B-CAB	-2.08	1.43	1.47
22	G	102	CLA	CMD-C2D	-2.08	1.46	1.50
31	5	319	LMG	C1-C2	2.08	1.58	1.52
22	4	310	CLA	CMC-C2C	-2.08	1.46	1.50
22	A	835	CLA	C3B-C2B	-2.08	1.37	1.40
22	9	306	CLA	C3B-CAB	-2.08	1.43	1.47
22	A	823	CLA	CMC-C2C	-2.08	1.46	1.50
22	B	820	CLA	C3B-CAB	-2.08	1.43	1.47
22	5	312	CLA	CMC-C2C	-2.08	1.46	1.50
22	5	303	CLA	MG-ND	-2.08	2.01	2.05
28	B	849	DGD	O6E-C5E	-2.08	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	313	CLA	CMC-C2C	-2.08	1.46	1.50
22	B	850	CLA	CMC-C2C	-2.07	1.46	1.50
22	B	821	CLA	C3B-CAB	-2.07	1.43	1.47
22	3	319	CLA	MG-ND	-2.07	2.01	2.05
22	1	304	CLA	CMD-C2D	-2.07	1.46	1.50
22	6	305	CLA	CMC-C2C	-2.07	1.46	1.50
22	6	315	CLA	MG-ND	-2.07	2.01	2.05
22	6	323	CLA	C3B-C2B	-2.07	1.37	1.40
22	B	833	CLA	MG-ND	-2.07	2.01	2.05
29	6	306	CHL	C4B-CHC	2.07	1.46	1.41
22	A	832	CLA	MG-ND	-2.07	2.01	2.05
25	J	104	8CT	C33-C32	-2.07	1.44	1.50
22	6	311	CLA	MG-ND	-2.07	2.01	2.05
22	A	802	CLA	C3B-C2B	-2.07	1.37	1.40
28	B	849	DGD	O4D-C4D	-2.07	1.38	1.43
22	7	303	CLA	C3B-C2B	-2.07	1.37	1.40
22	8	308	CLA	MG-ND	-2.07	2.01	2.05
30	3	314	XAT	O4-C5	-2.07	1.43	1.46
22	3	308	CLA	CAC-C3C	-2.07	1.45	1.51
29	9	307	CHL	C1B-CHB	2.06	1.46	1.41
22	9	303	CLA	MG-ND	-2.06	2.01	2.05
22	9	305	CLA	C3B-CAB	-2.06	1.43	1.47
22	L	201	CLA	CMC-C2C	-2.06	1.46	1.50
22	K	104	CLA	CMC-C2C	-2.06	1.46	1.50
22	8	310	CLA	C3B-CAB	-2.06	1.43	1.47
22	B	834	CLA	MG-ND	-2.06	2.01	2.05
29	4	306	CHL	C4C-C3C	2.06	1.48	1.45
22	1	303	CLA	CMD-C2D	-2.06	1.46	1.50
22	3	310	CLA	CMC-C2C	-2.06	1.46	1.50
24	1	317	LHG	O8-C6	-2.06	1.40	1.45
22	5	308	CLA	CMD-C2D	-2.06	1.46	1.50
29	6	308	CHL	C4B-CHC	2.06	1.46	1.41
22	A	833	CLA	MG-ND	-2.06	2.01	2.05
22	6	314	CLA	CMC-C2C	-2.06	1.46	1.50
22	0	311	CLA	CMC-C2C	-2.06	1.46	1.50
25	G	104	8CT	C33-C32	-2.06	1.44	1.50
22	5	307	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	822	CLA	C3B-CAB	-2.06	1.43	1.47
22	3	311	CLA	C3B-CAB	-2.06	1.43	1.47
29	4	307	CHL	C4B-CHC	2.06	1.46	1.41
22	B	836	CLA	C3B-C2B	-2.06	1.37	1.40
22	0	309	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	853	CLA	MG-ND	-2.06	2.01	2.05
22	7	314	CLA	MG-ND	-2.06	2.01	2.05
22	6	303	CLA	CMD-C2D	-2.06	1.46	1.50
25	J	101	8CT	C33-C32	-2.06	1.44	1.50
22	1	306	CLA	MG-ND	-2.06	2.01	2.05
29	9	302	CHL	C4B-CHC	2.05	1.46	1.41
22	A	803	CLA	C3B-CAB	-2.05	1.43	1.47
22	B	813	CLA	MG-ND	-2.05	2.01	2.05
22	B	823	CLA	MG-ND	-2.05	2.01	2.05
22	K	105	CLA	MG-ND	-2.05	2.01	2.05
22	B	829	CLA	C4B-CHC	-2.05	1.35	1.41
22	1	309	CLA	CMC-C2C	-2.05	1.46	1.50
22	B	818	CLA	C4B-CHC	-2.05	1.35	1.41
22	A	819	CLA	C3B-CAB	-2.05	1.43	1.47
22	A	821	CLA	CMC-C2C	-2.05	1.46	1.50
25	A	846	8CT	C25-C26	2.05	1.38	1.35
22	9	304	CLA	C3B-CAB	-2.05	1.43	1.47
22	9	306	CLA	CMC-C2C	-2.05	1.46	1.50
22	B	818	CLA	MG-ND	-2.05	2.01	2.05
22	A	838	CLA	C3B-CAB	-2.05	1.43	1.47
22	0	303	CLA	CMC-C2C	-2.05	1.46	1.50
22	2	302	CLA	C3B-CAB	-2.05	1.43	1.47
22	K	101	CLA	MG-ND	-2.05	2.01	2.05
22	B	808	CLA	C3B-CAB	-2.05	1.43	1.47
22	B	838	CLA	C3B-CAB	-2.05	1.43	1.47
22	B	805	CLA	C3B-C2B	-2.04	1.37	1.40
22	4	314	CLA	C3B-C2B	-2.04	1.37	1.40
22	0	302	CLA	MG-ND	-2.04	2.01	2.05
22	4	308	CLA	CMC-C2C	-2.04	1.46	1.50
22	1	311	CLA	MG-ND	-2.04	2.01	2.05
22	6	301	CLA	CMC-C2C	-2.04	1.46	1.50
22	B	830	CLA	C4B-CHC	-2.04	1.35	1.41
22	A	833	CLA	C3B-CAB	-2.04	1.43	1.47
22	9	305	CLA	CMD-C2D	-2.04	1.46	1.50
29	1	305	CHL	C1B-CHB	2.04	1.46	1.41
22	A	817	CLA	C3B-CAB	-2.04	1.43	1.47
30	9	315	XAT	O4-C5	-2.04	1.43	1.46
22	9	305	CLA	CMC-C2C	-2.04	1.46	1.50
22	3	312	CLA	CMC-C2C	-2.04	1.46	1.50
25	4	317	8CT	C33-C32	-2.04	1.44	1.50
22	3	302	CLA	CMC-C2C	-2.04	1.46	1.50
22	4	314	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	805	CLA	CAC-C3C	-2.04	1.45	1.51
22	9	301	CLA	MG-ND	-2.04	2.01	2.05
22	A	837	CLA	MG-ND	-2.04	2.01	2.05
22	9	310	CLA	C3B-CAB	-2.04	1.43	1.47
22	A	816	CLA	MG-ND	-2.04	2.01	2.05
22	A	834	CLA	C3B-CAB	-2.04	1.43	1.47
29	0	306	CHL	C4B-CHC	2.03	1.46	1.41
22	A	802	CLA	C3B-CAB	-2.03	1.43	1.47
22	1	313	CLA	C3B-C2B	-2.03	1.37	1.40
22	2	308	CLA	C3B-CAB	-2.03	1.43	1.47
22	8	313	CLA	C3B-CAB	-2.03	1.43	1.47
22	7	314	CLA	C3B-CAB	-2.03	1.43	1.47
30	2	316	XAT	O4-C5	-2.03	1.43	1.46
22	L	204	CLA	C3B-C2B	-2.03	1.37	1.40
22	8	309	CLA	CMC-C2C	-2.03	1.46	1.50
22	A	841	CLA	C4B-CHC	-2.03	1.35	1.41
22	9	308	CLA	CMC-C2C	-2.03	1.46	1.50
22	5	310	CLA	C3B-CAB	-2.03	1.43	1.47
22	4	313	CLA	MG-ND	-2.03	2.01	2.05
25	B	848	8CT	C33-C32	-2.03	1.44	1.50
22	7	313	CLA	MG-ND	-2.02	2.01	2.05
22	6	314	CLA	C3B-CAB	-2.02	1.43	1.47
22	8	304	CLA	C3B-CAB	-2.02	1.43	1.47
22	0	305	CLA	MG-ND	-2.02	2.01	2.05
25	A	850	8CT	C33-C32	-2.02	1.44	1.50
22	2	304	CLA	MG-ND	-2.02	2.01	2.05
22	1	301	CLA	MG-ND	-2.02	2.01	2.05
29	2	305	CHL	C1C-NC	-2.02	1.34	1.37
22	G	102	CLA	C3B-CAB	-2.02	1.43	1.47
22	2	309	CLA	CAC-C3C	-2.02	1.45	1.51
22	M	101	CLA	MG-ND	-2.02	2.01	2.05
30	8	316	XAT	O4-C5	-2.02	1.43	1.46
22	8	313	CLA	CMC-C2C	-2.02	1.46	1.50
22	1	312	CLA	MG-ND	-2.02	2.01	2.05
22	6	305	CLA	MG-ND	-2.02	2.01	2.05
22	7	312	CLA	CMC-C2C	-2.02	1.46	1.50
22	1	301	CLA	C3B-CAB	-2.02	1.43	1.47
22	7	314	CLA	C3B-C2B	-2.02	1.37	1.40
22	B	816	CLA	MG-ND	-2.01	2.01	2.05
22	8	311	CLA	C3B-C2B	-2.01	1.37	1.40
25	B	843	8CT	C24-C23	2.01	1.39	1.34
31	5	319	LMG	O6-C5	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	302	CLA	CMD-C2D	-2.01	1.46	1.50
29	3	306	CHL	C1B-CHB	2.01	1.46	1.41
22	A	835	CLA	C3B-CAB	-2.01	1.43	1.47
22	A	839	CLA	CMC-C2C	-2.01	1.46	1.50
22	A	809	CLA	C3B-CAB	-2.01	1.43	1.47
22	0	303	CLA	MG-ND	-2.01	2.01	2.05
25	6	321	8CT	C33-C32	-2.01	1.44	1.50
22	6	323	CLA	C3B-CAB	-2.01	1.43	1.47
22	B	832	CLA	MG-ND	-2.01	2.01	2.05
22	9	309	CLA	CMC-C2C	-2.01	1.46	1.50
22	3	303	CLA	C3B-CAB	-2.01	1.43	1.47
22	4	304	CLA	C3B-CAB	-2.00	1.43	1.47
22	0	307	CLA	CMC-C2C	-2.00	1.46	1.50
22	8	312	CLA	MG-ND	-2.00	2.01	2.05
30	3	314	XAT	C22-C21	-2.00	1.51	1.54
29	0	301	CHL	C4C-C3C	2.00	1.48	1.45
22	L	204	CLA	CMC-C2C	-2.00	1.46	1.50
25	B	847	8CT	C33-C32	-2.00	1.44	1.50
22	7	302	CLA	CMC-C2C	-2.00	1.46	1.50
22	B	811	CLA	CAC-C3C	-2.00	1.46	1.51
29	4	305	CHL	C1B-CHB	2.00	1.46	1.41
22	A	801	CLA	MG-ND	-2.00	2.01	2.05
22	A	833	CLA	CMC-C2C	-2.00	1.46	1.50
22	9	313	CLA	CMC-C2C	-2.00	1.46	1.50
22	0	304	CLA	C3B-C2B	-2.00	1.37	1.40
22	8	308	CLA	C3B-CAB	-2.00	1.43	1.47
22	9	308	CLA	C3B-C2B	-2.00	1.37	1.40
22	7	316	CLA	MG-ND	-2.00	2.01	2.05

All (3454) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	315	XAT	O4-C5-C4	-26.68	93.34	113.38
30	0	313	XAT	O24-C25-C24	-23.72	95.57	113.38
30	5	315	XAT	O24-C25-C38	-20.89	90.03	115.06
30	5	315	XAT	O24-C25-C24	-18.04	99.83	113.38
30	2	315	XAT	O4-C5-C18	-18.03	93.46	115.06
30	0	313	XAT	O24-C25-C38	-17.92	93.58	115.06
30	6	320	XAT	C17-C1-C16	-17.70	81.27	107.37
30	2	315	XAT	C37-C21-C36	-16.56	82.94	107.37
30	1	314	XAT	C17-C1-C16	-16.28	83.35	107.37
30	9	314	XAT	C37-C21-C36	-16.15	83.54	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	314	XAT	C17-C1-C16	-16.01	83.75	107.37
30	1	314	XAT	C17-C1-C2	-15.50	82.05	108.98
30	6	320	XAT	C17-C1-C2	-14.32	84.10	108.98
30	9	314	XAT	C37-C21-C22	-13.49	85.55	108.98
30	3	314	XAT	C17-C1-C2	-13.33	85.82	108.98
30	2	315	XAT	C37-C21-C22	-12.85	86.65	108.98
25	3	318	8CT	C24-C25-C26	-11.71	110.60	127.31
25	I	101	8CT	C33-C32-C31	-11.51	113.81	124.85
25	J	101	8CT	C33-C32-C31	-11.40	113.92	124.85
30	9	314	XAT	O4-C5-C4	11.36	121.92	113.38
25	B	844	8CT	C33-C32-C31	-11.24	114.07	124.85
25	3	318	8CT	C18-C17-C16	-11.07	111.50	127.31
25	7	321	8CT	C18-C17-C16	-10.93	111.71	127.31
25	A	846	8CT	C33-C32-C31	-10.92	114.38	124.85
30	7	319	XAT	O24-C25-C24	10.83	121.52	113.38
25	L	205	8CT	C18-C17-C16	-10.82	111.87	127.31
30	1	315	XAT	O24-C25-C24	10.69	121.41	113.38
25	5	317	8CT	C33-C32-C31	-10.53	114.76	124.85
25	A	848	8CT	C33-C32-C31	-10.51	114.77	124.85
30	9	315	XAT	O24-C25-C24	10.19	121.04	113.38
25	7	321	8CT	C19-C20-C21	-10.06	112.95	127.31
25	B	845	8CT	C33-C32-C31	-9.96	115.30	124.85
30	2	316	XAT	C18-C5-C6	-9.93	105.62	122.26
25	B	846	8CT	C33-C32-C31	-9.91	115.34	124.85
25	2	317	8CT	C33-C32-C31	-9.88	115.38	124.85
25	A	847	8CT	C33-C32-C31	-9.86	115.40	124.85
25	8	318	8CT	C33-C32-C31	-9.84	115.42	124.85
25	3	316	8CT	C33-C32-C31	-9.77	115.48	124.85
30	2	316	XAT	O24-C25-C24	9.71	120.68	113.38
30	5	316	XAT	O24-C25-C24	9.67	120.64	113.38
30	8	317	XAT	O24-C25-C24	9.67	120.64	113.38
30	3	314	XAT	O24-C25-C24	9.62	120.61	113.38
30	8	316	XAT	C15-C14-C13	-9.55	113.67	127.31
30	6	320	XAT	O24-C25-C24	9.50	120.52	113.38
25	5	317	8CT	C19-C20-C21	-9.49	113.77	127.31
25	L	206	8CT	C33-C32-C31	-9.41	115.83	124.85
30	7	320	XAT	O24-C25-C24	9.41	120.45	113.38
25	3	318	8CT	C19-C20-C21	-9.40	113.89	127.31
25	F	302	8CT	C33-C32-C31	-9.38	115.86	124.85
30	2	316	XAT	O4-C5-C18	9.33	126.23	115.06
25	A	854	8CT	C33-C32-C31	-9.28	115.95	124.85
30	0	313	XAT	O4-C5-C4	9.23	120.31	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	847	8CT	C33-C32-C31	-9.17	116.06	124.85
25	F	302	8CT	C14-C13-C12	-9.14	114.26	127.31
25	B	804	8CT	C33-C32-C31	-9.11	116.11	124.85
25	7	321	8CT	C33-C32-C31	-9.09	116.14	124.85
29	2	301	CHL	CMD-C2D-C1D	9.00	140.58	124.71
29	7	308	CHL	CMD-C2D-C1D	8.99	140.56	124.71
30	1	314	XAT	C7-C8-C9	-8.86	111.78	125.53
29	3	306	CHL	CMD-C2D-C1D	8.80	140.22	124.71
25	6	321	8CT	C18-C17-C16	-8.80	114.76	127.31
30	3	314	XAT	C15-C14-C13	-8.70	114.89	127.31
30	0	314	XAT	O4-C5-C4	8.70	119.92	113.38
25	7	301	8CT	C33-C32-C31	-8.69	116.52	124.85
30	3	314	XAT	C35-C34-C33	-8.60	115.03	127.31
29	4	307	CHL	CMD-C2D-C1D	8.57	139.81	124.71
25	8	301	8CT	C33-C32-C31	-8.57	116.64	124.85
29	2	305	CHL	CMD-C2D-C1D	8.54	139.77	124.71
30	8	316	XAT	C11-C10-C9	-8.40	115.32	127.31
25	G	104	8CT	C33-C32-C31	-8.35	116.85	124.85
29	2	307	CHL	CMD-C2D-C1D	8.34	139.41	124.71
25	B	848	8CT	C33-C32-C31	-8.33	116.87	124.85
29	2	305	CHL	C2C-C3C-C4C	-8.32	100.56	106.49
25	L	206	8CT	C24-C25-C26	-8.32	115.43	127.31
25	A	849	8CT	C33-C32-C31	-8.31	116.88	124.85
29	8	305	CHL	CMD-C2D-C1D	8.29	139.33	124.71
25	B	845	8CT	C24-C25-C26	-8.26	115.52	127.31
22	7	310	CLA	C4A-NA-C1A	8.26	110.42	106.71
29	5	301	CHL	C2C-C3C-C4C	-8.24	100.61	106.49
29	6	316	CHL	CMD-C2D-C1D	8.24	139.23	124.71
29	4	301	CHL	C2C-C3C-C4C	-8.24	100.62	106.49
25	J	104	8CT	C33-C32-C31	-8.23	116.95	124.85
30	6	320	XAT	C18-C5-C6	-8.23	108.47	122.26
29	9	302	CHL	C2C-C3C-C4C	-8.21	100.64	106.49
29	9	307	CHL	CMD-C2D-C1D	8.20	139.16	124.71
29	6	308	CHL	CMD-C2D-C1D	8.19	139.15	124.71
29	2	301	CHL	C2C-C3C-C4C	-8.17	100.66	106.49
25	5	317	8CT	C24-C25-C26	-8.16	115.67	127.31
29	1	305	CHL	CMD-C2D-C1D	8.15	139.07	124.71
25	A	850	8CT	C33-C32-C31	-8.13	117.05	124.85
25	7	321	8CT	C24-C25-C26	-8.13	115.71	127.31
25	1	316	8CT	C33-C32-C31	-8.12	117.07	124.85
25	6	321	8CT	C33-C32-C31	-8.09	117.10	124.85
25	6	321	8CT	C14-C13-C12	-8.06	115.80	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	4	301	CHL	CMD-C2D-C1D	8.06	138.92	124.71
29	9	302	CHL	CMD-C2D-C1D	8.06	138.91	124.71
30	6	319	XAT	C15-C14-C13	-8.05	115.83	127.31
25	B	846	8CT	C24-C25-C26	-8.04	115.84	127.31
29	4	305	CHL	CMD-C2D-C1D	8.03	138.86	124.71
29	5	301	CHL	CMD-C2D-C1D	8.01	138.84	124.71
29	8	314	CHL	CMD-C2D-C1D	8.01	138.83	124.71
29	0	306	CHL	CMD-C2D-C1D	8.00	138.81	124.71
29	8	306	CHL	CMD-C2D-C1D	7.98	138.78	124.71
29	6	306	CHL	CMD-C2D-C1D	7.98	138.77	124.71
29	2	306	CHL	CMD-C2D-C1D	7.96	138.75	124.71
25	6	321	8CT	C24-C25-C26	-7.96	115.95	127.31
29	8	307	CHL	CMD-C2D-C1D	7.95	138.72	124.71
25	3	318	8CT	C33-C32-C31	-7.93	117.25	124.85
25	B	804	8CT	C14-C13-C12	-7.89	116.05	127.31
29	8	305	CHL	C2C-C3C-C4C	-7.87	100.88	106.49
25	7	301	8CT	C24-C25-C26	-7.86	116.09	127.31
30	8	316	XAT	C38-C25-C26	-7.86	109.09	122.26
30	1	314	XAT	C31-C30-C29	-7.85	116.11	127.31
25	5	317	8CT	C30-C31-C32	-7.83	111.83	121.47
29	4	306	CHL	CMD-C2D-C1D	7.81	138.48	124.71
25	L	205	8CT	C33-C32-C31	-7.80	117.37	124.85
25	B	843	8CT	C33-C32-C31	-7.77	117.40	124.85
29	5	306	CHL	CMD-C2D-C1D	7.77	138.41	124.71
29	0	301	CHL	CMD-C2D-C1D	7.75	138.38	124.71
22	7	317	CLA	C4A-NA-C1A	7.75	110.19	106.71
25	7	323	8CT	C33-C32-C31	-7.74	117.42	124.85
30	0	314	XAT	C38-C25-C26	-7.74	109.30	122.26
29	2	306	CHL	C2C-C3C-C4C	-7.72	100.98	106.49
22	B	806	CLA	C4A-NA-C1A	7.72	110.18	106.71
30	4	316	XAT	O24-C25-C24	7.71	119.17	113.38
30	4	315	XAT	C35-C34-C33	-7.70	116.32	127.31
30	1	314	XAT	C17-C1-C6	-7.70	89.27	110.05
29	6	302	CHL	C2C-C3C-C4C	-7.68	101.01	106.49
25	B	851	8CT	C33-C32-C31	-7.66	117.51	124.85
29	4	306	CHL	C2C-C3C-C4C	-7.65	101.03	106.49
22	K	105	CLA	C4A-NA-C1A	7.65	110.15	106.71
22	9	305	CLA	C4A-NA-C1A	7.64	110.14	106.71
22	B	818	CLA	C4A-NA-C1A	7.60	110.12	106.71
29	6	307	CHL	C2C-C3C-C4C	-7.60	101.07	106.49
22	B	833	CLA	C4A-NA-C1A	7.60	110.12	106.71
30	2	315	XAT	C26-C27-C28	-7.58	109.97	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	313	XAT	C18-C5-C6	-7.58	109.56	122.26
25	4	317	8CT	C33-C32-C31	-7.57	117.59	124.85
25	A	850	8CT	C19-C20-C21	-7.57	116.51	127.31
29	8	314	CHL	C2C-C3C-C4C	-7.54	101.11	106.49
25	I	101	8CT	C18-C17-C16	-7.53	116.56	127.31
22	A	804	CLA	C4A-NA-C1A	7.52	110.09	106.71
29	4	306	CHL	CHD-C1D-ND	-7.51	117.56	124.45
22	9	303	CLA	C4A-NA-C1A	7.51	110.08	106.71
30	6	320	XAT	C17-C1-C6	-7.48	89.84	110.05
30	2	315	XAT	C37-C21-C26	-7.48	89.86	110.05
30	5	315	XAT	C31-C30-C29	-7.47	116.65	127.31
29	4	305	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
29	7	308	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
25	F	302	8CT	C19-C20-C21	-7.46	116.66	127.31
30	3	314	XAT	C17-C1-C6	-7.45	89.93	110.05
25	K	103	8CT	C33-C32-C31	-7.45	117.71	124.85
29	6	302	CHL	CMD-C2D-C1D	7.45	137.84	124.71
29	6	307	CHL	CMD-C2D-C1D	7.45	137.84	124.71
22	5	308	CLA	C4A-NA-C1A	7.44	110.05	106.71
22	B	815	CLA	C4A-NA-C1A	7.44	110.05	106.71
22	7	318	CLA	C4A-NA-C1A	7.42	110.04	106.71
30	4	315	XAT	O24-C25-C24	7.40	118.94	113.38
22	8	310	CLA	C4A-NA-C1A	7.38	110.02	106.71
30	7	319	XAT	C11-C10-C9	-7.37	116.80	127.31
29	3	306	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
25	J	104	8CT	C24-C25-C26	-7.34	116.83	127.31
22	L	202	CLA	C4A-NA-C1A	7.32	110.00	106.71
29	4	307	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
30	5	316	XAT	C35-C34-C33	-7.31	116.87	127.31
25	B	843	8CT	C19-C20-C21	-7.31	116.88	127.31
29	8	307	CHL	C2C-C3C-C4C	-7.31	101.28	106.49
29	2	307	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
22	B	807	CLA	C4A-NA-C1A	7.28	109.98	106.71
22	B	840	CLA	C4A-NA-C1A	7.28	109.98	106.71
22	A	822	CLA	C4A-NA-C1A	7.27	109.97	106.71
30	3	314	XAT	C6-C7-C8	-7.24	110.69	125.99
22	A	832	CLA	C4A-NA-C1A	7.23	109.95	106.71
22	7	313	CLA	C4A-NA-C1A	7.22	109.95	106.71
22	3	311	CLA	C4A-NA-C1A	7.22	109.95	106.71
25	A	846	8CT	C30-C31-C32	-7.22	112.59	121.47
22	B	829	CLA	C4A-NA-C1A	7.22	109.95	106.71
22	5	312	CLA	C4A-NA-C1A	7.21	109.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	9	307	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
22	A	820	CLA	C4A-NA-C1A	7.20	109.94	106.71
30	1	315	XAT	C26-C27-C28	-7.19	110.79	125.99
29	5	306	CHL	C2C-C3C-C4C	-7.18	101.37	106.49
30	0	314	XAT	O24-C25-C24	7.17	118.77	113.38
30	9	314	XAT	C37-C21-C26	-7.17	90.69	110.05
22	3	308	CLA	C4A-NA-C1A	7.16	109.92	106.71
22	3	319	CLA	C4A-NA-C1A	7.15	109.92	106.71
25	8	301	8CT	C24-C25-C26	-7.14	117.12	127.31
22	6	318	CLA	C4A-NA-C1A	7.12	109.91	106.71
30	5	316	XAT	C18-C5-C6	-7.12	110.33	122.26
25	B	843	8CT	C18-C17-C16	-7.12	117.15	127.31
22	B	824	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	A	808	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	B	808	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	A	805	CLA	C4A-NA-C1A	7.09	109.89	106.71
30	8	316	XAT	O4-C5-C4	7.09	118.71	113.38
29	1	305	CHL	C2C-C3C-C4C	-7.09	101.44	106.49
25	F	302	8CT	C24-C25-C26	-7.08	117.20	127.31
25	F	302	8CT	C18-C17-C16	-7.07	117.21	127.31
30	8	316	XAT	C18-C5-C6	-7.07	110.41	122.26
30	2	315	XAT	C36-C21-C22	7.06	121.25	108.98
30	8	317	XAT	C18-C5-C6	-7.06	110.43	122.26
22	7	307	CLA	C4A-NA-C1A	7.06	109.88	106.71
30	6	320	XAT	O4-C5-C4	7.06	118.68	113.38
22	4	308	CLA	C4A-NA-C1A	7.04	109.87	106.71
30	5	316	XAT	C26-C27-C28	-7.03	111.12	125.99
22	B	820	CLA	C4A-NA-C1A	7.03	109.87	106.71
22	9	309	CLA	C4A-NA-C1A	7.03	109.87	106.71
30	4	316	XAT	C27-C28-C29	-7.02	114.63	125.53
22	A	817	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	9	311	CLA	C4A-NA-C1A	7.02	109.86	106.71
29	6	316	CHL	C2C-C3C-C4C	-7.00	101.50	106.49
30	4	316	XAT	C18-C5-C6	-7.00	110.53	122.26
22	4	311	CLA	C4A-NA-C1A	7.00	109.85	106.71
22	6	313	CLA	C4A-NA-C1A	7.00	109.85	106.71
29	0	301	CHL	C2C-C3C-C4C	-6.99	101.50	106.49
30	1	314	XAT	O4-C5-C18	6.98	123.42	115.06
22	B	801	CLA	C4A-NA-C1A	6.98	109.84	106.71
22	A	826	CLA	C4A-NA-C1A	6.97	109.84	106.71
25	I	101	8CT	C10-C11-C12	-6.97	115.70	126.23
29	6	306	CHL	C2C-C3C-C4C	-6.96	101.53	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	305	CHL	CHD-C1D-ND	-6.96	118.06	124.45
22	4	312	CLA	C4A-NA-C1A	6.95	109.83	106.71
30	9	314	XAT	C36-C21-C22	6.95	121.06	108.98
25	A	847	8CT	C30-C31-C32	-6.95	112.92	121.47
22	J	103	CLA	C4A-NA-C1A	6.94	109.82	106.71
30	1	314	XAT	C38-C25-C26	-6.93	110.64	122.26
29	0	306	CHL	C2C-C3C-C4C	-6.93	101.55	106.49
30	3	315	XAT	C38-C25-C26	-6.93	110.65	122.26
29	2	306	CHL	CHD-C1D-ND	-6.92	118.10	124.45
29	8	305	CHL	CHD-C1D-ND	-6.92	118.10	124.45
25	J	104	8CT	C10-C11-C12	-6.91	115.79	126.23
30	5	316	XAT	O4-C5-C4	6.90	118.57	113.38
22	A	812	CLA	C4A-NA-C1A	6.90	109.81	106.71
25	7	321	8CT	C10-C11-C12	-6.90	115.81	126.23
22	1	310	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	B	835	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	A	837	CLA	C4A-NA-C1A	6.88	109.80	106.71
30	5	315	XAT	O4-C5-C4	6.87	118.54	113.38
22	L	203	CLA	C4A-NA-C1A	6.86	109.79	106.71
30	4	315	XAT	C38-C25-C26	-6.86	110.76	122.26
22	4	310	CLA	C4A-NA-C1A	6.86	109.79	106.71
29	6	308	CHL	C2C-C3C-C4C	-6.85	101.60	106.49
22	6	309	CLA	C4A-NA-C1A	6.85	109.79	106.71
22	A	807	CLA	C4A-NA-C1A	6.85	109.78	106.71
22	3	307	CLA	C4A-NA-C1A	6.85	109.78	106.71
29	9	307	CHL	CHD-C1D-ND	-6.84	118.17	124.45
25	B	804	8CT	C10-C11-C12	-6.84	115.90	126.23
22	A	816	CLA	C4A-NA-C1A	6.84	109.78	106.71
29	8	314	CHL	CHD-C1D-ND	-6.83	118.18	124.45
22	A	810	CLA	C4A-NA-C1A	6.82	109.77	106.71
30	6	319	XAT	C18-C5-C6	-6.82	110.83	122.26
22	L	201	CLA	C4A-NA-C1A	6.82	109.77	106.71
25	J	101	8CT	C30-C31-C32	-6.82	113.08	121.47
30	9	314	XAT	C38-C25-C26	-6.82	110.84	122.26
29	8	306	CHL	C2C-C3C-C4C	-6.81	101.63	106.49
22	4	303	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	A	824	CLA	C4A-NA-C1A	6.79	109.76	106.71
22	8	312	CLA	C4A-NA-C1A	6.79	109.76	106.71
22	6	314	CLA	C4A-NA-C1A	6.79	109.76	106.71
30	9	315	XAT	C18-C5-C6	-6.78	110.89	122.26
25	L	205	8CT	C19-C20-C21	-6.78	117.63	127.31
22	6	311	CLA	C4A-NA-C1A	6.78	109.75	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	844	8CT	C35-C30-C29	-6.78	104.14	112.70
22	1	311	CLA	C4A-NA-C1A	6.78	109.75	106.71
22	6	304	CLA	C4A-NA-C1A	6.77	109.75	106.71
22	B	816	CLA	C4A-NA-C1A	6.76	109.75	106.71
29	0	301	CHL	CHD-C1D-ND	-6.76	118.24	124.45
30	6	320	XAT	C38-C25-C26	-6.76	110.93	122.26
22	A	823	CLA	C4A-NA-C1A	6.75	109.74	106.71
30	0	313	XAT	C15-C14-C13	-6.75	117.68	127.31
22	5	311	CLA	C4A-NA-C1A	6.75	109.74	106.71
29	6	316	CHL	CHD-C1D-ND	-6.75	118.25	124.45
30	6	320	XAT	C16-C1-C2	6.75	120.70	108.98
22	G	103	CLA	C4A-NA-C1A	6.74	109.73	106.71
22	2	308	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	B	811	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	5	309	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	1	301	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	1	307	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	0	308	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	2	303	CLA	C4A-NA-C1A	6.72	109.73	106.71
30	3	314	XAT	C16-C1-C2	6.72	120.66	108.98
30	7	320	XAT	C18-C5-C6	-6.72	111.00	122.26
22	A	843	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	A	830	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	5	303	CLA	C4A-NA-C1A	6.72	109.72	106.71
22	1	303	CLA	C4A-NA-C1A	6.71	109.72	106.71
30	5	316	XAT	C38-C25-C26	-6.71	111.01	122.26
22	3	312	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	B	810	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	B	836	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	7	316	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	K	102	CLA	C4A-NA-C1A	6.70	109.72	106.71
25	3	318	8CT	C14-C13-C12	-6.70	117.75	127.31
22	2	313	CLA	C4A-NA-C1A	6.69	109.71	106.71
25	B	845	8CT	C19-C20-C21	-6.69	117.76	127.31
22	2	311	CLA	C4A-NA-C1A	6.69	109.71	106.71
22	6	312	CLA	C4A-NA-C1A	6.68	109.71	106.71
22	8	304	CLA	C4A-NA-C1A	6.68	109.71	106.71
22	3	313	CLA	C4A-NA-C1A	6.67	109.71	106.71
22	6	310	CLA	C4A-NA-C1A	6.67	109.70	106.71
30	9	315	XAT	C38-C25-C26	-6.67	111.08	122.26
22	0	305	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	0	304	CLA	C4A-NA-C1A	6.64	109.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	317	XAT	C38-C25-C26	-6.64	111.14	122.26
22	2	304	CLA	C4A-NA-C1A	6.64	109.69	106.71
30	2	315	XAT	C38-C25-C26	-6.63	111.14	122.26
30	7	319	XAT	C38-C25-C26	-6.63	111.14	122.26
22	1	308	CLA	C4A-NA-C1A	6.63	109.69	106.71
25	A	848	8CT	C04-C03-C02	-6.62	113.28	122.61
22	K	104	CLA	C4A-NA-C1A	6.62	109.68	106.71
30	6	319	XAT	C38-C25-C26	-6.61	111.17	122.26
22	6	303	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	8	313	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	B	825	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	2	312	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	5	304	CLA	C4A-NA-C1A	6.60	109.67	106.71
29	6	307	CHL	CHD-C1D-ND	-6.60	118.39	124.45
25	A	848	8CT	C30-C31-C32	-6.60	113.35	121.47
22	6	317	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	B	837	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	1	313	CLA	C4A-NA-C1A	6.58	109.66	106.71
25	L	206	8CT	C10-C11-C12	-6.57	116.30	126.23
22	8	315	CLA	C4A-NA-C1A	6.57	109.66	106.71
22	9	306	CLA	C4A-NA-C1A	6.55	109.65	106.71
25	A	846	8CT	C18-C17-C16	-6.54	117.98	127.31
25	J	101	8CT	C14-C13-C12	-6.53	117.99	127.31
22	B	813	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	A	831	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	3	301	CLA	C4A-NA-C1A	6.51	109.64	106.71
22	G	102	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	0	310	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	0	312	CLA	C4A-NA-C1A	6.50	109.63	106.71
30	3	315	XAT	C18-C5-C6	-6.50	111.36	122.26
30	3	314	XAT	C18-C5-C6	-6.50	111.37	122.26
29	6	308	CHL	CHD-C1D-ND	-6.49	118.49	124.45
25	7	323	8CT	C14-C13-C12	-6.49	118.05	127.31
22	A	815	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	3	305	CLA	C4A-NA-C1A	6.49	109.62	106.71
29	8	306	CHL	CHD-C1D-ND	-6.48	118.50	124.45
22	A	838	CLA	C4A-NA-C1A	6.47	109.61	106.71
22	1	302	CLA	C4A-NA-C1A	6.47	109.61	106.71
29	5	301	CHL	CHD-C1D-ND	-6.46	118.52	124.45
22	4	314	CLA	C4A-NA-C1A	6.46	109.61	106.71
30	4	316	XAT	O4-C5-C4	6.45	118.23	113.38
22	A	825	CLA	C4A-NA-C1A	6.45	109.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	834	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	G	101	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	B	817	CLA	C4A-NA-C1A	6.43	109.60	106.71
22	7	304	CLA	C4A-NA-C1A	6.43	109.60	106.71
30	5	315	XAT	C18-C5-C6	-6.43	111.49	122.26
22	8	303	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	B	821	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	9	308	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	A	852	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	7	302	CLA	C4A-NA-C1A	6.41	109.59	106.71
30	3	314	XAT	C38-C25-C26	-6.41	111.52	122.26
30	3	314	XAT	O4-C5-C4	6.41	118.19	113.38
22	B	822	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	A	811	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	3	310	CLA	C4A-NA-C1A	6.40	109.58	106.71
30	0	314	XAT	C18-C5-C6	-6.39	111.55	122.26
22	A	840	CLA	C4A-NA-C1A	6.39	109.58	106.71
30	4	315	XAT	C18-C5-C6	-6.39	111.56	122.26
30	7	319	XAT	C31-C30-C29	-6.38	118.21	127.31
22	0	307	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	A	828	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	B	814	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	B	832	CLA	C4A-NA-C1A	6.37	109.57	106.71
30	1	315	XAT	C35-C34-C33	-6.37	118.22	127.31
22	A	833	CLA	C4A-NA-C1A	6.36	109.57	106.71
22	5	302	CLA	C4A-NA-C1A	6.36	109.56	106.71
29	2	301	CHL	CHD-C1D-ND	-6.35	118.62	124.45
30	8	316	XAT	O24-C25-C38	6.35	122.66	115.06
25	B	847	8CT	C30-C31-C32	-6.35	113.66	121.47
22	1	306	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	1	309	CLA	C4A-NA-C1A	6.35	109.56	106.71
29	9	302	CHL	CHD-C1D-ND	-6.34	118.63	124.45
22	4	302	CLA	C4A-NA-C1A	6.33	109.55	106.71
25	6	321	8CT	C10-C11-C12	-6.32	116.68	126.23
22	L	204	CLA	C4A-NA-C1A	6.32	109.55	106.71
29	4	307	CHL	CHD-C1D-ND	-6.31	118.65	124.45
22	A	802	CLA	C4A-NA-C1A	6.31	109.54	106.71
30	5	315	XAT	C27-C28-C29	-6.31	115.74	125.53
22	A	841	CLA	C4A-NA-C1A	6.30	109.54	106.71
30	7	319	XAT	C18-C5-C6	-6.30	111.70	122.26
22	A	821	CLA	C4A-NA-C1A	6.29	109.53	106.71
22	B	823	CLA	C4A-NA-C1A	6.29	109.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	829	CLA	C4A-NA-C1A	6.29	109.53	106.71
30	9	314	XAT	C31-C30-C29	-6.28	118.35	127.31
22	3	303	CLA	C4A-NA-C1A	6.28	109.53	106.71
29	2	307	CHL	CHD-C1D-ND	-6.28	118.68	124.45
25	L	206	8CT	C18-C17-C16	-6.27	118.36	127.31
22	5	310	CLA	C4A-NA-C1A	6.27	109.53	106.71
22	2	310	CLA	C4A-NA-C1A	6.27	109.52	106.71
30	1	314	XAT	O24-C25-C24	6.25	118.08	113.38
29	0	306	CHL	CHD-C1D-ND	-6.25	118.71	124.45
30	0	313	XAT	C35-C34-C33	-6.25	118.39	127.31
22	8	309	CLA	C4A-NA-C1A	6.25	109.51	106.71
29	5	306	CHL	CHD-C1D-ND	-6.24	118.72	124.45
22	6	301	CLA	C4A-NA-C1A	6.24	109.51	106.71
22	8	308	CLA	C4A-NA-C1A	6.23	109.51	106.71
25	B	851	8CT	C18-C17-C16	-6.22	118.43	127.31
29	4	301	CHL	O2D-CGD-CBD	6.22	122.33	111.27
22	A	836	CLA	C4A-NA-C1A	6.22	109.50	106.71
22	B	819	CLA	C4A-NA-C1A	6.22	109.50	106.71
22	3	309	CLA	C4A-NA-C1A	6.21	109.50	106.71
25	L	205	8CT	C10-C11-C12	-6.21	116.85	126.23
30	1	315	XAT	C18-C5-C6	-6.20	111.87	122.26
22	7	309	CLA	C4A-NA-C1A	6.18	109.48	106.71
22	A	803	CLA	C4A-NA-C1A	6.17	109.48	106.71
30	4	315	XAT	O4-C5-C4	6.17	118.02	113.38
22	2	302	CLA	C4A-NA-C1A	6.16	109.48	106.71
30	6	319	XAT	O24-C25-C24	6.16	118.01	113.38
25	3	316	8CT	C10-C11-C12	-6.15	116.94	126.23
25	A	847	8CT	C14-C13-C12	-6.14	118.54	127.31
22	5	314	CLA	C4A-NA-C1A	6.14	109.47	106.71
22	1	312	CLA	C4A-NA-C1A	6.13	109.46	106.71
22	7	314	CLA	C4A-NA-C1A	6.13	109.46	106.71
22	B	827	CLA	C4A-NA-C1A	6.12	109.46	106.71
25	7	323	8CT	C19-C20-C21	-6.12	118.57	127.31
22	A	814	CLA	C4A-NA-C1A	6.12	109.46	106.71
22	4	304	CLA	C4A-NA-C1A	6.11	109.45	106.71
22	B	809	CLA	C4A-NA-C1A	6.11	109.45	106.71
22	7	315	CLA	C4A-NA-C1A	6.11	109.45	106.71
25	3	316	8CT	C24-C25-C26	-6.11	118.60	127.31
30	1	315	XAT	C6-C7-C8	-6.10	113.09	125.99
22	B	828	CLA	C4A-NA-C1A	6.10	109.45	106.71
22	B	830	CLA	C4A-NA-C1A	6.10	109.45	106.71
25	K	103	8CT	C18-C17-C16	-6.10	118.61	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	839	CLA	C4A-NA-C1A	6.09	109.44	106.71
22	2	314	CLA	C4A-NA-C1A	6.09	109.44	106.71
25	5	317	8CT	C14-C13-C12	-6.09	118.62	127.31
22	A	813	CLA	C4A-NA-C1A	6.08	109.44	106.71
25	3	316	8CT	C18-C17-C16	-6.08	118.64	127.31
29	4	305	CHL	CHD-C1D-ND	-6.07	118.87	124.45
25	J	101	8CT	C10-C11-C12	-6.07	117.06	126.23
29	4	306	CHL	O2D-CGD-CBD	6.07	122.05	111.27
22	9	313	CLA	C4A-NA-C1A	6.07	109.43	106.71
30	1	314	XAT	C18-C5-C6	-6.07	112.09	122.26
25	A	847	8CT	C19-C20-C21	-6.06	118.66	127.31
30	3	315	XAT	C6-C7-C8	-6.06	113.18	125.99
30	6	320	XAT	C15-C14-C13	-6.06	118.66	127.31
22	A	809	CLA	C4A-NA-C1A	6.06	109.43	106.71
29	8	307	CHL	CHD-C1D-ND	-6.05	118.89	124.45
22	9	310	CLA	C4A-NA-C1A	6.05	109.43	106.71
25	K	103	8CT	C19-C20-C21	-6.05	118.68	127.31
22	7	305	CLA	C4A-NA-C1A	6.04	109.42	106.71
22	9	301	CLA	C4A-NA-C1A	6.04	109.42	106.71
29	5	306	CHL	C1B-CHB-C4A	-6.04	118.16	130.12
22	4	309	CLA	C4A-NA-C1A	6.04	109.42	106.71
25	1	316	8CT	C14-C13-C12	-6.03	118.70	127.31
22	0	309	CLA	C4A-NA-C1A	6.03	109.42	106.71
29	9	302	CHL	O2D-CGD-CBD	6.03	121.98	111.27
29	7	308	CHL	CHD-C1D-ND	-6.02	118.92	124.45
25	B	846	8CT	C10-C11-C12	-6.02	117.14	126.23
30	1	315	XAT	C38-C25-C26	-6.02	112.17	122.26
30	9	314	XAT	C18-C5-C6	-6.02	112.18	122.26
22	6	305	CLA	C4A-NA-C1A	5.99	109.40	106.71
25	2	317	8CT	C18-C17-C16	-5.99	118.77	127.31
29	6	302	CHL	CHD-C1D-ND	-5.99	118.95	124.45
22	A	827	CLA	C4A-NA-C1A	5.99	109.40	106.71
29	3	306	CHL	CHD-C1D-ND	-5.98	118.96	124.45
22	2	309	CLA	C4A-NA-C1A	5.98	109.39	106.71
22	4	313	CLA	C4A-NA-C1A	5.97	109.39	106.71
22	B	841	CLA	C4A-NA-C1A	5.95	109.38	106.71
22	7	311	CLA	C4A-NA-C1A	5.95	109.38	106.71
30	7	320	XAT	C38-C25-C26	-5.95	112.29	122.26
30	9	314	XAT	O24-C25-C38	5.95	122.18	115.06
25	B	848	8CT	C10-C11-C12	-5.95	117.25	126.23
22	A	834	CLA	C4A-NA-C1A	5.95	109.38	106.71
25	2	317	8CT	C24-C25-C26	-5.94	118.83	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	323	8CT	C04-C03-C02	-5.93	114.25	122.61
30	0	313	XAT	C31-C30-C29	-5.93	118.84	127.31
22	B	839	CLA	C4A-NA-C1A	5.93	109.37	106.71
22	A	819	CLA	C4A-NA-C1A	5.92	109.37	106.71
22	F	301	CLA	C4A-NA-C1A	5.92	109.37	106.71
22	0	303	CLA	C4A-NA-C1A	5.91	109.36	106.71
30	1	314	XAT	C10-C11-C12	5.89	141.61	123.22
22	B	838	CLA	C4A-NA-C1A	5.88	109.35	106.71
22	B	812	CLA	C4A-NA-C1A	5.87	109.34	106.71
22	0	302	CLA	C4A-NA-C1A	5.87	109.34	106.71
22	5	307	CLA	C4A-NA-C1A	5.86	109.34	106.71
22	9	312	CLA	C4A-NA-C1A	5.86	109.34	106.71
22	0	311	CLA	C4A-NA-C1A	5.85	109.34	106.71
25	L	205	8CT	C14-C13-C12	-5.85	118.96	127.31
22	A	818	CLA	C4A-NA-C1A	5.85	109.34	106.71
22	3	304	CLA	C4A-NA-C1A	5.85	109.34	106.71
30	2	316	XAT	C38-C25-C26	-5.85	112.46	122.26
22	7	303	CLA	C4A-NA-C1A	5.83	109.33	106.71
25	I	101	8CT	C24-C25-C26	-5.82	119.00	127.31
30	0	313	XAT	C7-C8-C9	-5.82	116.50	125.53
25	B	847	8CT	C18-C17-C16	-5.81	119.02	127.31
25	B	845	8CT	C14-C13-C12	-5.80	119.03	127.31
22	2	319	CLA	C4A-NA-C1A	5.80	109.31	106.71
25	B	844	8CT	C30-C31-C32	-5.80	114.33	121.47
22	B	803	CLA	C4A-NA-C1A	5.80	109.31	106.71
22	B	850	CLA	C4A-NA-C1A	5.80	109.31	106.71
29	6	306	CHL	CHD-C1D-ND	-5.79	119.13	124.45
22	A	835	CLA	C4A-NA-C1A	5.76	109.30	106.71
22	5	313	CLA	C4A-NA-C1A	5.76	109.30	106.71
30	8	316	XAT	C31-C30-C29	-5.75	119.10	127.31
22	K	101	CLA	C4A-NA-C1A	5.75	109.29	106.71
22	6	323	CLA	C4A-NA-C1A	5.74	109.29	106.71
29	2	305	CHL	C3C-C4C-NC	5.73	117.00	110.57
29	2	305	CHL	CHD-C1D-ND	-5.73	119.19	124.45
22	B	826	CLA	C4A-NA-C1A	5.73	109.28	106.71
22	3	302	CLA	C4A-NA-C1A	5.72	109.28	106.71
25	B	843	8CT	C14-C13-C12	-5.72	119.15	127.31
25	J	104	8CT	C18-C17-C16	-5.69	119.19	127.31
29	8	306	CHL	O2D-CGD-CBD	5.69	121.38	111.27
29	6	316	CHL	O2D-CGD-CBD	5.69	121.37	111.27
22	9	304	CLA	C4A-NA-C1A	5.68	109.26	106.71
25	3	316	8CT	C19-C20-C21	-5.68	119.20	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	849	8CT	C24-C25-C26	-5.68	119.21	127.31
25	2	317	8CT	C14-C13-C12	-5.67	119.21	127.31
25	B	844	8CT	C01-C02-C03	-5.67	118.16	124.53
25	A	854	8CT	C18-C17-C16	-5.67	119.22	127.31
25	I	101	8CT	C35-C30-C29	-5.66	105.55	112.70
22	5	305	CLA	C4A-NA-C1A	5.65	109.24	106.71
30	9	314	XAT	C7-C8-C9	5.64	134.28	125.53
29	4	301	CHL	C3C-C4C-NC	5.64	116.90	110.57
25	A	850	8CT	C10-C11-C12	-5.63	117.73	126.23
29	9	307	CHL	O2D-CGD-CBD	5.59	121.20	111.27
25	K	103	8CT	C04-C03-C02	-5.59	114.74	122.61
29	8	314	CHL	O2D-CGD-CBD	5.58	121.18	111.27
22	H	201	CLA	C4A-NA-C1A	5.57	109.21	106.71
25	I	101	8CT	C01-C02-C03	-5.56	118.28	124.53
30	8	317	XAT	C6-C7-C8	-5.56	114.24	125.99
22	A	801	CLA	C4A-NA-C1A	5.54	109.19	106.71
22	8	311	CLA	C4A-NA-C1A	5.53	109.19	106.71
25	7	321	8CT	C04-C03-C02	-5.51	114.85	122.61
22	1	304	CLA	C4A-NA-C1A	5.51	109.18	106.71
25	A	850	8CT	C07-C02-C03	-5.50	114.75	122.73
25	4	317	8CT	C14-C13-C12	-5.48	119.49	127.31
22	8	302	CLA	C4A-NA-C1A	5.47	109.17	106.71
30	2	316	XAT	C26-C27-C28	-5.47	114.44	125.99
25	B	848	8CT	C04-C03-C02	-5.46	114.93	122.61
29	7	308	CHL	C3C-C4C-NC	5.46	116.69	110.57
25	7	301	8CT	C30-C31-C32	-5.45	114.76	121.47
22	6	315	CLA	C4A-NA-C1A	5.45	109.16	106.71
30	6	320	XAT	C26-C27-C28	-5.45	114.47	125.99
22	A	853	CLA	C4A-NA-C1A	5.45	109.16	106.71
30	9	315	XAT	O4-C5-C4	5.44	117.47	113.38
29	7	308	CHL	CHD-C4C-C3C	-5.44	116.85	124.84
25	A	847	8CT	C24-C25-C26	-5.43	119.57	127.31
30	3	315	XAT	O4-C5-C18	5.42	121.55	115.06
30	7	320	XAT	O4-C5-C4	5.41	117.44	113.38
29	8	314	CHL	C1B-CHB-C4A	-5.40	119.42	130.12
30	8	317	XAT	O4-C5-C4	5.39	117.43	113.38
29	3	306	CHL	C3D-C2D-C1D	-5.39	98.47	105.83
25	B	846	8CT	C30-C31-C32	-5.39	114.84	121.47
22	B	805	CLA	C4A-NA-C1A	5.39	109.13	106.71
25	A	854	8CT	C14-C13-C12	-5.38	119.62	127.31
25	B	804	8CT	C24-C25-C26	-5.38	119.63	127.31
22	B	831	CLA	C4A-NA-C1A	5.37	109.12	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	850	8CT	C30-C31-C32	-5.36	114.88	121.47
30	7	319	XAT	C27-C28-C29	-5.36	117.22	125.53
29	8	305	CHL	C3C-C4C-NC	5.34	116.56	110.57
30	6	319	XAT	O4-C5-C4	5.34	117.39	113.38
25	B	804	8CT	C01-C02-C03	-5.34	118.54	124.53
25	A	846	8CT	C19-C18-C17	-5.33	112.55	123.47
29	8	307	CHL	O2D-CGD-CBD	5.33	120.73	111.27
30	8	316	XAT	C7-C8-C9	-5.32	117.27	125.53
22	B	831	CLA	CMB-C2B-C1B	-5.32	120.28	128.46
25	G	104	8CT	C18-C17-C16	-5.32	119.71	127.31
25	B	846	8CT	C04-C03-C02	-5.32	115.13	122.61
30	1	314	XAT	O24-C25-C38	5.31	121.42	115.06
30	0	314	XAT	C27-C28-C29	-5.30	117.30	125.53
29	0	306	CHL	O2D-CGD-CBD	5.29	120.66	111.27
25	2	317	8CT	C30-C31-C32	-5.29	114.97	121.47
30	6	319	XAT	C11-C10-C9	-5.28	119.78	127.31
30	3	315	XAT	O24-C25-C24	5.28	117.34	113.38
29	9	302	CHL	C3C-C4C-NC	5.26	116.47	110.57
30	7	319	XAT	O4-C5-C4	5.26	117.33	113.38
30	1	314	XAT	C11-C10-C9	-5.25	119.81	127.31
25	7	301	8CT	C10-C11-C12	-5.25	118.30	126.23
30	6	320	XAT	O4-C5-C18	5.25	121.34	115.06
25	J	101	8CT	C19-C20-C21	-5.25	119.82	127.31
22	M	101	CLA	C4A-NA-C1A	5.25	109.06	106.71
22	A	806	CLA	C4A-NA-C1A	5.24	109.06	106.71
25	A	849	8CT	C10-C11-C12	-5.24	118.32	126.23
25	1	316	8CT	C19-C20-C21	-5.23	119.84	127.31
22	A	835	CLA	CMB-C2B-C1B	-5.23	120.43	128.46
30	8	316	XAT	C32-C33-C34	5.22	126.95	118.94
25	F	302	8CT	C04-C03-C02	-5.21	115.27	122.61
30	8	317	XAT	C26-C27-C28	-5.19	115.03	125.99
30	7	320	XAT	C6-C7-C8	-5.18	115.03	125.99
30	2	315	XAT	O24-C25-C24	5.18	117.27	113.38
29	6	306	CHL	C3C-C4C-NC	5.18	116.38	110.57
30	7	319	XAT	C35-C34-C33	-5.18	119.92	127.31
25	B	847	8CT	C14-C13-C12	-5.17	119.93	127.31
30	6	319	XAT	C31-C32-C33	-5.17	111.90	126.42
25	1	316	8CT	C10-C11-C12	-5.17	118.43	126.23
25	7	321	8CT	C30-C31-C32	-5.16	115.12	121.47
30	8	316	XAT	O4-C5-C18	5.15	121.23	115.06
30	9	315	XAT	C6-C7-C8	-5.15	115.10	125.99
29	3	306	CHL	C3C-C4C-NC	5.15	116.35	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	318	8CT	C19-C20-C21	-5.14	119.98	127.31
30	4	315	XAT	C7-C8-C9	-5.14	117.56	125.53
22	A	830	CLA	CMB-C2B-C1B	-5.14	120.57	128.46
22	7	306	CLA	C4A-NA-C1A	5.13	109.01	106.71
30	9	315	XAT	O4-C5-C18	5.12	121.19	115.06
25	A	850	8CT	C24-C25-C26	-5.12	120.00	127.31
22	A	819	CLA	CMB-C2B-C1B	-5.12	120.60	128.46
25	B	845	8CT	C30-C31-C32	-5.11	115.18	121.47
30	8	316	XAT	C15-C35-C34	-5.11	113.01	123.47
25	2	317	8CT	C04-C03-C02	-5.10	115.43	122.61
25	7	321	8CT	C14-C15-C16	-5.10	112.08	126.42
22	7	312	CLA	C4A-NA-C1A	5.10	109.00	106.71
29	4	307	CHL	C3D-C2D-C1D	-5.09	98.89	105.83
25	A	847	8CT	C10-C11-C12	-5.09	118.55	126.23
25	2	317	8CT	C10-C11-C12	-5.09	118.55	126.23
25	A	849	8CT	C18-C17-C16	-5.06	120.09	127.31
25	B	844	8CT	C10-C11-C12	-5.06	118.60	126.23
25	7	321	8CT	C07-C02-C03	-5.05	115.40	122.73
29	6	306	CHL	O2D-CGD-CBD	5.05	120.24	111.27
30	9	314	XAT	O24-C25-C24	5.05	117.17	113.38
25	A	846	8CT	C04-C03-C02	-5.05	115.50	122.61
29	2	305	CHL	CHD-C4C-C3C	-5.05	117.42	124.84
30	8	317	XAT	C35-C34-C33	-5.04	120.11	127.31
25	5	317	8CT	C10-C11-C12	-5.04	118.62	126.23
30	2	315	XAT	O24-C25-C38	5.04	121.09	115.06
29	4	307	CHL	C3C-C4C-NC	5.04	116.22	110.57
29	4	301	CHL	CHD-C1D-ND	-5.04	119.83	124.45
25	8	318	8CT	C14-C13-C12	-5.04	120.12	127.31
29	3	306	CHL	CHD-C4C-C3C	-5.04	117.44	124.84
22	B	830	CLA	CMB-C2B-C1B	-5.03	120.73	128.46
25	J	104	8CT	C01-C02-C03	-5.03	118.88	124.53
25	J	104	8CT	C30-C31-C32	-5.02	115.29	121.47
29	4	307	CHL	CHD-C4C-C3C	-5.02	117.47	124.84
30	8	316	XAT	C40-C33-C34	-5.00	115.92	122.92
25	A	846	8CT	C24-C25-C26	-5.00	120.18	127.31
22	7	306	CLA	CMB-C2B-C1B	-4.99	120.79	128.46
29	8	305	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
29	8	305	CHL	O2D-CGD-CBD	4.97	120.09	111.27
29	6	307	CHL	O2D-CGD-CBD	4.96	120.08	111.27
25	8	318	8CT	C18-C17-C16	-4.96	120.23	127.31
30	6	319	XAT	C15-C35-C34	-4.96	113.31	123.47
22	B	828	CLA	CMB-C2B-C1B	-4.96	120.84	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	6	307	CHL	C1B-CHB-C4A	-4.95	120.31	130.12
30	0	314	XAT	C15-C14-C13	-4.95	120.25	127.31
29	2	301	CHL	OMC-CMC-C2C	-4.95	114.50	125.69
30	1	314	XAT	C16-C1-C2	4.94	117.57	108.98
25	A	849	8CT	C19-C20-C21	-4.94	120.26	127.31
25	6	321	8CT	C04-C03-C02	-4.94	115.66	122.61
30	9	315	XAT	C26-C27-C28	-4.93	115.56	125.99
29	8	307	CHL	C3C-C4C-NC	4.93	116.10	110.57
25	B	804	8CT	C18-C17-C16	-4.89	120.34	127.31
30	7	319	XAT	O4-C5-C18	4.88	120.91	115.06
29	2	306	CHL	C3C-C4C-NC	4.88	116.05	110.57
25	7	301	8CT	C01-C02-C03	-4.88	119.05	124.53
30	4	316	XAT	O4-C5-C18	4.88	120.90	115.06
29	5	301	CHL	C3C-C4C-NC	4.87	116.04	110.57
25	B	843	8CT	C24-C25-C26	-4.87	120.35	127.31
29	6	302	CHL	C3C-C4C-NC	4.87	116.04	110.57
25	A	847	8CT	C01-C02-C03	-4.87	119.06	124.53
25	B	845	8CT	C10-C11-C12	-4.87	118.88	126.23
30	6	319	XAT	C32-C33-C34	4.86	126.40	118.94
30	4	315	XAT	C20-C13-C14	-4.86	116.12	122.92
25	A	848	8CT	C18-C17-C16	-4.86	120.38	127.31
25	J	101	8CT	C18-C17-C16	-4.86	120.38	127.31
25	3	318	8CT	C10-C11-C12	-4.86	118.90	126.23
25	L	206	8CT	C19-C20-C21	-4.85	120.38	127.31
29	0	306	CHL	C1B-CHB-C4A	-4.85	120.50	130.12
29	4	307	CHL	C2D-C1D-ND	4.85	113.68	110.10
25	7	323	8CT	C07-C02-C03	-4.85	115.69	122.73
25	2	317	8CT	C35-C30-C29	-4.85	106.57	112.70
29	6	302	CHL	O2D-CGD-CBD	4.85	119.89	111.27
29	2	307	CHL	C3C-C4C-NC	4.85	116.01	110.57
29	2	301	CHL	C3C-C4C-NC	4.84	116.00	110.57
25	J	104	8CT	C04-C03-C02	-4.83	115.80	122.61
25	K	103	8CT	C07-C02-C03	-4.83	115.71	122.73
25	B	848	8CT	C30-C31-C32	-4.82	115.53	121.47
25	L	206	8CT	C30-C31-C32	-4.82	115.53	121.47
29	9	302	CHL	C3D-C2D-C1D	-4.82	99.25	105.83
25	A	854	8CT	C19-C20-C21	-4.82	120.43	127.31
22	4	304	CLA	CMB-C2B-C1B	-4.82	121.06	128.46
25	6	321	8CT	C01-C02-C03	-4.82	119.12	124.53
25	B	847	8CT	C19-C20-C21	-4.81	120.45	127.31
22	B	814	CLA	CMB-C2B-C1B	-4.80	121.08	128.46
25	1	316	8CT	C04-C03-C02	-4.80	115.86	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	4	305	CHL	C3C-C4C-NC	4.79	115.94	110.57
22	B	826	CLA	CMB-C2B-C1B	-4.78	121.11	128.46
29	2	306	CHL	O2D-CGD-CBD	4.78	119.76	111.27
29	2	301	CHL	O2D-CGD-CBD	4.78	119.76	111.27
25	2	317	8CT	C07-C02-C03	-4.78	115.80	122.73
22	A	813	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
30	4	315	XAT	O4-C5-C18	4.77	120.77	115.06
30	5	315	XAT	O4-C5-C18	4.77	120.77	115.06
25	G	104	8CT	C19-C20-C21	-4.77	120.51	127.31
25	L	205	8CT	C01-C02-C03	-4.76	119.18	124.53
29	6	302	CHL	C3D-C2D-C1D	-4.76	99.33	105.83
30	0	314	XAT	C11-C10-C9	-4.76	120.52	127.31
25	1	316	8CT	C18-C17-C16	-4.75	120.53	127.31
30	5	316	XAT	C35-C15-C14	-4.75	113.75	123.47
30	3	315	XAT	O24-C25-C38	4.75	120.74	115.06
29	0	301	CHL	C1B-CHB-C4A	-4.74	120.72	130.12
25	L	205	8CT	C14-C15-C16	-4.74	113.10	126.42
29	1	305	CHL	O2D-CGD-CBD	4.73	119.67	111.27
25	B	848	8CT	C18-C19-C20	-4.73	113.79	123.47
29	6	308	CHL	C3C-C4C-NC	4.71	115.86	110.57
29	8	306	CHL	C3C-C4C-NC	4.71	115.86	110.57
25	G	104	8CT	C07-C02-C03	-4.71	115.89	122.73
25	A	850	8CT	C14-C13-C12	-4.71	120.59	127.31
30	8	316	XAT	C11-C12-C13	-4.71	113.19	126.42
29	2	307	CHL	CHD-C4C-C3C	-4.71	117.92	124.84
30	6	319	XAT	C31-C30-C29	-4.71	120.59	127.31
30	2	315	XAT	C15-C14-C13	-4.70	120.60	127.31
29	2	301	CHL	C3B-C4B-NB	4.70	115.28	109.21
30	3	314	XAT	C40-C33-C34	-4.70	116.34	122.92
29	3	306	CHL	C2D-C1D-ND	4.69	113.56	110.10
29	5	301	CHL	O2D-CGD-CBD	4.69	119.60	111.27
29	2	301	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
25	A	848	8CT	C07-C02-C03	-4.69	115.93	122.73
29	5	301	CHL	C3D-C2D-C1D	-4.69	99.44	105.83
29	2	307	CHL	C3D-C2D-C1D	-4.68	99.44	105.83
25	B	847	8CT	C07-C02-C03	-4.68	115.93	122.73
30	4	315	XAT	C15-C14-C13	-4.68	120.63	127.31
25	K	103	8CT	C10-C11-C12	-4.67	119.17	126.23
29	7	308	CHL	O2D-CGD-CBD	4.67	119.57	111.27
25	B	844	8CT	C39-C16-C17	-4.66	116.39	122.92
25	A	850	8CT	C04-C03-C02	-4.66	116.05	122.61
29	6	307	CHL	C3C-C4C-NC	4.66	115.80	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	846	8CT	C07-C02-C03	-4.66	115.97	122.73
29	6	316	CHL	C3D-C2D-C1D	-4.65	99.49	105.83
30	0	313	XAT	O4-C5-C18	4.65	120.62	115.06
29	6	316	CHL	C3C-C4C-NC	4.65	115.78	110.57
25	L	206	8CT	C01-C02-C03	-4.65	119.31	124.53
25	A	849	8CT	C04-C03-C02	-4.64	116.07	122.61
25	A	848	8CT	C19-C20-C21	-4.64	120.69	127.31
25	B	845	8CT	C18-C17-C16	-4.64	120.69	127.31
25	3	316	8CT	C04-C03-C02	-4.64	116.08	122.61
30	4	316	XAT	C35-C34-C33	-4.63	120.70	127.31
25	A	847	8CT	C18-C17-C16	-4.63	120.70	127.31
25	B	848	8CT	C07-C02-C03	-4.63	116.02	122.73
25	5	317	8CT	C04-C03-C02	-4.62	116.10	122.61
29	4	306	CHL	C3C-C4C-NC	4.62	115.75	110.57
30	1	315	XAT	O4-C5-C4	4.62	116.85	113.38
29	8	306	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
29	6	308	CHL	CHD-C4C-C3C	-4.62	118.06	124.84
22	1	312	CLA	CMB-C2B-C1B	-4.61	121.37	128.46
30	1	315	XAT	O4-C5-C18	4.60	120.57	115.06
25	7	323	8CT	C01-C02-C03	-4.60	119.36	124.53
22	B	827	CLA	CMB-C2B-C1B	-4.60	121.39	128.46
29	4	301	CHL	CHD-C4C-C3C	-4.60	118.08	124.84
29	8	314	CHL	C3C-C4C-NC	4.60	115.73	110.57
29	8	314	CHL	C3D-C2D-C1D	-4.59	99.56	105.83
29	2	306	CHL	C3D-C2D-C1D	-4.59	99.56	105.83
22	B	838	CLA	CMB-C2B-C1B	-4.59	121.40	128.46
25	B	843	8CT	C01-C02-C03	-4.58	119.38	124.53
22	A	818	CLA	CMB-C2B-C1B	-4.58	121.42	128.46
29	4	301	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
29	0	301	CHL	O2D-CGD-CBD	4.58	119.41	111.27
25	8	301	8CT	C14-C13-C12	-4.58	120.78	127.31
29	7	308	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
29	6	308	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
25	1	316	8CT	C24-C25-C26	-4.56	120.81	127.31
30	5	315	XAT	C20-C13-C14	-4.56	116.54	122.92
22	B	819	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
22	A	827	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
29	5	306	CHL	O2D-CGD-CBD	4.54	119.34	111.27
30	9	315	XAT	C15-C14-C13	-4.54	120.83	127.31
22	B	812	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
29	2	307	CHL	C1-C2-C3	-4.53	119.42	126.75
29	4	305	CHL	C3D-C2D-C1D	-4.53	99.65	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	301	8CT	C30-C31-C32	-4.53	115.90	121.47
25	A	854	8CT	C24-C25-C26	-4.53	120.85	127.31
25	8	301	8CT	C10-C11-C12	-4.52	119.41	126.23
29	8	305	CHL	CHD-C4C-C3C	-4.52	118.20	124.84
22	3	309	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
30	5	316	XAT	C6-C7-C8	-4.51	116.45	125.99
30	1	314	XAT	C28-C29-C30	4.51	125.86	118.94
25	B	804	8CT	C30-C31-C32	-4.50	115.93	121.47
29	2	305	CHL	C3D-C2D-C1D	-4.50	99.70	105.83
25	B	843	8CT	C10-C11-C12	-4.49	119.44	126.23
29	4	306	CHL	C3D-C2D-C1D	-4.49	99.70	105.83
30	4	315	XAT	O24-C25-C38	4.49	120.44	115.06
30	6	319	XAT	O4-C5-C18	4.49	120.44	115.06
30	8	317	XAT	C18-C5-C4	4.49	119.33	114.28
29	4	305	CHL	O2D-CGD-CBD	4.49	119.24	111.27
30	6	319	XAT	C26-C27-C28	-4.48	116.52	125.99
25	6	321	8CT	C07-C02-C03	-4.48	116.23	122.73
29	0	301	CHL	C3D-C2D-C1D	-4.48	99.72	105.83
25	7	321	8CT	C24-C23-C21	-4.48	113.84	126.42
25	K	103	8CT	C01-C02-C03	-4.47	119.51	124.53
25	6	321	8CT	C30-C31-C32	-4.47	115.97	121.47
29	5	306	CHL	C3C-C4C-NC	4.47	115.58	110.57
22	3	308	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
25	5	317	8CT	C24-C23-C21	-4.45	113.91	126.42
25	8	318	8CT	C30-C31-C32	-4.45	115.99	121.47
22	7	303	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
30	6	319	XAT	C20-C13-C14	-4.44	116.70	122.92
22	A	837	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
25	G	104	8CT	C24-C25-C26	-4.43	120.98	127.31
25	A	850	8CT	C01-C02-C03	-4.43	119.55	124.53
29	4	307	CHL	C1D-ND-C4D	-4.43	103.19	106.33
29	6	306	CHL	C3D-C2D-C1D	-4.43	99.78	105.83
30	3	314	XAT	C31-C30-C29	-4.43	120.99	127.31
29	1	305	CHL	C3D-C2D-C1D	-4.42	99.80	105.83
24	1	317	LHG	O4-P-O5	4.42	134.09	112.24
30	9	315	XAT	C35-C34-C33	-4.42	121.00	127.31
22	2	309	CLA	CMB-C2B-C1B	-4.42	121.68	128.46
25	G	104	8CT	C14-C13-C12	-4.41	121.01	127.31
25	2	317	8CT	C01-C02-C03	-4.41	119.57	124.53
25	B	846	8CT	C19-C20-C21	-4.41	121.01	127.31
25	K	103	8CT	C14-C13-C12	-4.41	121.01	127.31
30	5	315	XAT	C12-C13-C14	4.41	125.70	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	305	CHL	C3C-C4C-NC	4.41	115.51	110.57
30	3	315	XAT	C26-C27-C28	-4.41	116.68	125.99
22	L	202	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
22	H	201	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
30	3	314	XAT	O4-C5-C18	4.40	120.33	115.06
25	G	104	8CT	C01-C02-C03	-4.40	119.59	124.53
30	8	316	XAT	C12-C13-C14	4.40	125.69	118.94
29	3	306	CHL	O2D-CGD-CBD	4.40	119.08	111.27
25	3	316	8CT	C07-C02-C03	-4.39	116.35	122.73
25	B	851	8CT	C19-C20-C21	-4.39	121.04	127.31
22	7	310	CLA	CMB-C2B-C1B	-4.39	121.71	128.46
29	2	307	CHL	O2D-CGD-CBD	4.39	119.06	111.27
29	8	307	CHL	C3D-C2D-C1D	-4.38	99.85	105.83
22	B	837	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
30	0	314	XAT	O24-C25-C38	4.38	120.30	115.06
29	8	306	CHL	CHD-C4C-C3C	-4.38	118.41	124.84
30	4	316	XAT	C6-C7-C8	-4.37	116.74	125.99
24	2	318	LHG	O4-P-O5	4.37	133.85	112.24
25	B	846	8CT	C01-C02-C03	-4.37	119.62	124.53
30	7	319	XAT	C6-C7-C8	-4.37	116.76	125.99
30	7	320	XAT	O4-C5-C18	4.37	120.29	115.06
24	5	318	LHG	O4-P-O5	4.36	133.80	112.24
29	9	307	CHL	C3D-C2D-C1D	-4.36	99.88	105.83
29	9	302	CHL	CHD-C4C-C3C	-4.36	118.44	124.84
24	B	852	LHG	O4-P-O5	4.35	133.76	112.24
22	A	817	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
22	A	802	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
30	3	315	XAT	C18-C5-C4	4.35	119.17	114.28
30	6	319	XAT	C40-C33-C34	-4.34	116.84	122.92
24	3	317	LHG	O4-P-O5	4.34	133.71	112.24
22	1	301	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
25	A	849	8CT	C07-C02-C03	-4.34	116.43	122.73
22	A	821	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
30	9	314	XAT	C27-C28-C29	-4.33	118.81	125.53
22	5	311	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
22	A	819	CLA	CMB-C2B-C3B	4.33	132.78	124.68
29	2	307	CHL	C1D-ND-C4D	-4.33	103.26	106.33
22	3	301	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
30	6	319	XAT	O24-C25-C38	4.32	120.24	115.06
29	9	307	CHL	C3C-C4C-NC	4.32	115.42	110.57
25	A	854	8CT	C30-C31-C32	-4.32	116.15	121.47
29	2	307	CHL	C2D-C1D-ND	4.32	113.29	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	847	8CT	C10-C11-C12	-4.32	119.71	126.23
22	1	306	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
25	G	104	8CT	C04-C03-C02	-4.31	116.54	122.61
22	B	807	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
30	1	314	XAT	C32-C33-C34	4.31	125.56	118.94
29	0	306	CHL	C3D-C2D-C1D	-4.31	99.95	105.83
22	B	829	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
22	B	832	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
25	B	845	8CT	C39-C16-C15	4.30	124.85	118.08
25	A	854	8CT	C10-C11-C12	-4.30	119.74	126.23
29	5	306	CHL	C3D-C2D-C1D	-4.29	99.97	105.83
25	B	848	8CT	C01-C02-C03	-4.29	119.71	124.53
25	7	321	8CT	C35-C30-C29	-4.29	107.28	112.70
25	8	301	8CT	C07-C02-C03	-4.28	116.51	122.73
30	0	314	XAT	C31-C30-C29	-4.27	121.21	127.31
29	1	305	CHL	C1B-CHB-C4A	-4.27	121.66	130.12
22	B	836	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
22	K	102	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
25	3	318	8CT	C24-C23-C21	-4.26	114.45	126.42
25	2	317	8CT	C19-C20-C21	-4.26	121.23	127.31
24	A	844	LHG	O4-P-O5	4.26	133.30	112.24
25	B	848	8CT	C35-C30-C29	-4.26	107.32	112.70
25	J	101	8CT	C01-C02-C03	-4.25	119.75	124.53
25	B	851	8CT	C30-C31-C32	-4.25	116.24	121.47
25	8	318	8CT	C07-C02-C03	-4.25	116.56	122.73
25	I	101	8CT	C19-C20-C21	-4.25	121.25	127.31
24	9	316	LHG	O4-P-O5	4.24	133.22	112.24
25	7	323	8CT	C35-C30-C29	-4.24	107.34	112.70
22	A	813	CLA	CMB-C2B-C3B	4.24	132.61	124.68
25	I	101	8CT	C30-C31-C32	-4.24	116.25	121.47
22	3	312	CLA	CMB-C2B-C1B	-4.23	121.95	128.46
22	A	831	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
22	2	302	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
29	9	302	CHL	C2D-C1D-ND	4.23	113.22	110.10
25	8	318	8CT	C10-C11-C12	-4.21	119.87	126.23
22	2	304	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
25	A	854	8CT	C07-C02-C03	-4.21	116.62	122.73
24	A	845	LHG	O4-P-O5	4.21	133.05	112.24
25	5	317	8CT	C01-C02-C03	-4.21	119.81	124.53
29	5	301	CHL	CHD-C4C-C3C	-4.20	118.66	124.84
30	8	316	XAT	C31-C32-C33	-4.20	114.61	126.42
25	3	318	8CT	C14-C15-C16	-4.20	114.61	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	828	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
22	A	835	CLA	CMB-C2B-C3B	4.20	132.53	124.68
22	8	312	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
25	B	851	8CT	C10-C11-C12	-4.19	119.90	126.23
22	4	312	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
29	6	306	CHL	CHD-C4C-C3C	-4.19	118.68	124.84
25	B	847	8CT	C01-C02-C03	-4.19	119.82	124.53
25	L	206	8CT	C04-C03-C02	-4.19	116.71	122.61
22	G	103	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
22	9	304	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
25	G	104	8CT	C30-C31-C32	-4.19	116.31	121.47
25	6	321	8CT	C35-C30-C29	-4.18	107.41	112.70
25	A	854	8CT	C01-C02-C03	-4.18	119.83	124.53
22	2	312	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
25	B	845	8CT	C01-C02-C03	-4.17	119.84	124.53
24	0	315	LHG	O4-P-O5	4.17	132.87	112.24
22	4	304	CLA	CMB-C2B-C3B	4.17	132.48	124.68
29	2	301	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
25	7	323	8CT	C30-C31-C32	-4.17	116.34	121.47
30	9	314	XAT	C19-C9-C8	4.16	124.64	118.08
24	6	322	LHG	O4-P-O5	4.16	132.79	112.24
22	8	308	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
29	8	305	CHL	C2D-C1D-ND	4.15	113.16	110.10
29	6	307	CHL	C3D-C2D-C1D	-4.15	100.17	105.83
22	F	301	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
30	7	319	XAT	C15-C14-C13	-4.14	121.40	127.31
25	B	843	8CT	C04-C03-C02	-4.14	116.78	122.61
22	7	315	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
29	4	307	CHL	O2D-CGD-CBD	4.14	118.62	111.27
22	4	308	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
29	6	306	CHL	CAC-C3C-C4C	4.14	130.18	124.81
22	A	843	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
22	6	303	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
29	2	301	CHL	C2D-C1D-ND	4.13	113.15	110.10
22	B	816	CLA	O2D-CGD-O1D	-4.13	115.76	123.84
22	B	818	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
25	5	317	8CT	C19-C18-C17	-4.13	115.02	123.47
30	0	313	XAT	C20-C13-C14	-4.13	117.14	122.92
29	0	301	CHL	C3C-C4C-NC	4.12	115.20	110.57
30	8	316	XAT	O24-C25-C24	4.12	116.48	113.38
25	B	844	8CT	C14-C13-C12	-4.12	121.43	127.31
25	4	317	8CT	C35-C30-C29	-4.11	107.51	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	8	316	XAT	C20-C13-C14	-4.11	117.17	122.92
30	5	315	XAT	C11-C10-C9	-4.10	121.46	127.31
25	4	317	8CT	C18-C19-C20	-4.10	115.08	123.47
28	B	849	DGD	O3G-C3G-C2G	-4.09	101.02	110.90
29	6	308	CHL	O2D-CGD-CBD	4.09	118.54	111.27
29	0	306	CHL	CAC-C3C-C4C	4.09	130.12	124.81
30	2	316	XAT	C35-C34-C33	-4.09	121.47	127.31
29	2	301	CHL	CAC-C3C-C4C	4.08	130.11	124.81
22	B	839	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
22	B	841	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
25	8	318	8CT	C01-C02-C03	-4.07	119.96	124.53
22	B	838	CLA	CMB-C2B-C3B	4.07	132.29	124.68
22	8	302	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
25	G	104	8CT	C10-C11-C12	-4.05	120.12	126.23
25	7	323	8CT	C18-C17-C16	-4.04	121.54	127.31
25	B	851	8CT	C39-C16-C17	-4.04	117.26	122.92
22	9	301	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
25	7	301	8CT	C07-C02-C03	-4.04	116.86	122.73
30	3	315	XAT	C15-C14-C13	-4.04	121.55	127.31
30	8	317	XAT	O4-C5-C18	4.04	119.89	115.06
22	B	823	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
25	3	318	8CT	C28-C26-C25	4.04	125.13	118.94
30	7	320	XAT	C26-C27-C28	-4.03	117.47	125.99
25	L	205	8CT	C24-C23-C21	-4.03	115.10	126.42
25	A	849	8CT	C01-C02-C03	-4.03	120.00	124.53
22	3	308	CLA	CMB-C2B-C3B	4.03	132.21	124.68
24	7	322	LHG	O4-P-O5	4.02	132.13	112.24
29	2	301	CHL	C1D-ND-C4D	-4.02	103.48	106.33
25	8	318	8CT	C04-C03-C02	-4.02	116.95	122.61
25	8	301	8CT	C01-C02-C03	-4.02	120.02	124.53
25	4	317	8CT	C04-C03-C02	-4.02	116.96	122.61
22	1	308	CLA	CMB-C2B-C1B	-4.01	122.29	128.46
30	9	314	XAT	C26-C27-C28	-4.01	117.51	125.99
25	A	854	8CT	C04-C03-C02	-4.01	116.97	122.61
22	B	828	CLA	CMB-C2B-C3B	3.99	132.15	124.68
22	A	829	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
22	7	306	CLA	CMB-C2B-C3B	3.99	132.15	124.68
22	B	821	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
29	4	301	CHL	C2D-C1D-ND	3.98	113.04	110.10
22	0	308	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
22	B	831	CLA	CMB-C2B-C3B	3.98	132.12	124.68
25	B	844	8CT	C24-C25-C26	-3.97	121.64	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	843	8CT	C22-C21-C20	-3.97	117.36	122.92
30	6	319	XAT	C6-C7-C8	-3.97	117.59	125.99
30	0	314	XAT	C20-C13-C14	-3.97	117.36	122.92
25	J	104	8CT	C07-C02-C03	-3.97	116.97	122.73
30	7	320	XAT	C24-C23-C22	-3.97	103.11	110.77
22	A	808	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
22	6	304	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
22	A	806	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
30	8	316	XAT	C24-C23-C22	-3.97	103.11	110.77
29	8	307	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
30	7	319	XAT	C8-C9-C10	3.96	125.02	118.94
25	7	321	8CT	C15-C16-C17	3.96	125.02	118.94
22	B	830	CLA	CMB-C2B-C3B	3.96	132.08	124.68
25	F	302	8CT	C10-C11-C12	-3.96	120.25	126.23
29	6	308	CHL	C2D-C1D-ND	3.96	113.02	110.10
25	L	206	8CT	C14-C13-C12	-3.95	121.67	127.31
25	B	843	8CT	C35-C30-C29	-3.95	107.71	112.70
22	2	311	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
25	4	317	8CT	C10-C11-C12	-3.95	120.27	126.23
29	6	302	CHL	CHD-C4C-C3C	-3.94	119.04	124.84
30	5	316	XAT	O4-C5-C18	3.94	119.78	115.06
30	0	313	XAT	C27-C28-C29	-3.94	119.42	125.53
25	B	804	8CT	C19-C20-C21	-3.93	121.70	127.31
30	0	313	XAT	C20-C13-C12	3.93	124.27	118.08
30	3	315	XAT	C5-C4-C3	-3.93	104.97	112.75
29	7	308	CHL	C1D-ND-C4D	-3.93	103.54	106.33
22	4	313	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
22	B	814	CLA	CMB-C2B-C3B	3.93	132.03	124.68
25	A	846	8CT	C01-C02-C03	-3.92	120.12	124.53
22	K	101	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
25	J	101	8CT	C24-C25-C26	-3.92	121.72	127.31
22	B	803	CLA	O2D-CGD-O1D	-3.92	116.18	123.84
22	7	303	CLA	C1-C2-C3	-3.92	119.27	126.04
22	B	850	CLA	CAA-CBA-CGA	-3.91	101.81	113.25
22	B	816	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
25	5	317	8CT	C07-C02-C03	-3.91	117.05	122.73
29	6	308	CHL	C1D-ND-C4D	-3.91	103.56	106.33
25	8	301	8CT	C35-C30-C29	-3.90	107.77	112.70
22	A	803	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
22	A	834	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
22	A	820	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
25	B	848	8CT	C14-C15-C16	-3.89	115.50	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	4	307	CHL	C1-C2-C3	-3.88	120.47	126.75
25	L	205	8CT	C19-C18-C17	3.88	131.43	123.47
22	B	822	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
22	4	309	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
22	B	828	CLA	C1-C2-C3	-3.88	119.33	126.04
25	J	101	8CT	C04-C03-C02	-3.88	117.15	122.61
25	6	321	8CT	C18-C19-C20	-3.88	115.54	123.47
22	A	828	CLA	C1-C2-C3	-3.88	119.34	126.04
25	1	316	8CT	C07-C02-C03	-3.87	117.11	122.73
30	7	320	XAT	C18-C5-C4	3.87	118.64	114.28
30	4	316	XAT	C24-C23-C22	-3.87	103.30	110.77
30	5	315	XAT	C40-C33-C34	-3.87	117.50	122.92
29	0	306	CHL	C3B-C4B-NB	3.87	114.21	109.21
22	B	826	CLA	CMB-C2B-C3B	3.87	131.92	124.68
22	G	101	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
29	6	316	CHL	CAC-C3C-C4C	3.85	129.81	124.81
30	2	316	XAT	C7-C8-C9	-3.85	119.55	125.53
29	2	305	CHL	C2D-C1D-ND	3.85	112.94	110.10
30	4	315	XAT	C24-C23-C22	-3.85	103.34	110.77
22	3	303	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
29	4	305	CHL	CAC-C3C-C4C	3.85	129.80	124.81
29	8	307	CHL	C1-C2-C3	-3.85	120.53	126.75
25	6	321	8CT	C14-C15-C16	-3.84	115.62	126.42
25	B	851	8CT	C04-C03-C02	-3.84	117.20	122.61
30	2	316	XAT	C18-C5-C4	3.84	118.60	114.28
22	7	310	CLA	CMB-C2B-C3B	3.84	131.87	124.68
29	8	306	CHL	C2D-C1D-ND	3.83	112.93	110.10
30	1	315	XAT	C5-C4-C3	-3.83	105.17	112.75
22	B	819	CLA	CMB-C2B-C3B	3.82	131.83	124.68
22	B	827	CLA	CMB-C2B-C3B	3.82	131.83	124.68
29	2	306	CHL	CHD-C4C-C3C	-3.82	119.22	124.84
25	A	850	8CT	C14-C15-C16	-3.82	115.68	126.42
30	0	314	XAT	O4-C5-C18	3.82	119.63	115.06
29	2	305	CHL	C1D-ND-C4D	-3.81	103.62	106.33
22	8	313	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
25	3	316	8CT	C30-C31-C32	-3.81	116.78	121.47
25	B	845	8CT	C19-C18-C17	-3.81	115.67	123.47
29	9	302	CHL	C1D-ND-C4D	-3.81	103.63	106.33
22	9	308	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
22	B	850	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
30	9	314	XAT	C6-C7-C8	3.80	134.03	125.99
22	L	202	CLA	CMB-C2B-C3B	3.80	131.79	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	316	8CT	C01-C02-C03	-3.80	120.26	124.53
29	4	301	CHL	C4-C3-C5	3.80	121.66	115.27
22	A	818	CLA	CMB-C2B-C3B	3.79	131.77	124.68
30	5	315	XAT	C31-C32-C33	-3.79	115.77	126.42
30	3	315	XAT	C24-C23-C22	-3.79	103.46	110.77
29	2	307	CHL	C3B-C4B-NB	3.79	114.11	109.21
30	1	315	XAT	C18-C5-C4	3.79	118.54	114.28
29	4	306	CHL	C1-C2-C3	-3.78	120.63	126.75
30	4	316	XAT	C31-C30-C29	-3.78	121.91	127.31
22	3	302	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
22	1	312	CLA	CMB-C2B-C3B	3.78	131.75	124.68
22	9	306	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
22	5	312	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
22	A	807	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
22	B	850	CLA	CAA-C2A-C1A	-3.78	99.60	111.97
22	4	312	CLA	O2D-CGD-O1D	-3.78	116.46	123.84
22	9	313	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
25	A	846	8CT	C07-C02-C03	-3.77	117.25	122.73
22	9	312	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
29	3	306	CHL	C1D-ND-C4D	-3.77	103.66	106.33
30	4	315	XAT	C32-C33-C34	3.77	124.72	118.94
30	1	314	XAT	C31-C32-C33	-3.76	115.84	126.42
29	9	302	CHL	CAC-C3C-C4C	3.76	129.69	124.81
22	8	311	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
22	3	309	CLA	CMB-C2B-C3B	3.76	131.71	124.68
22	B	801	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
25	B	851	8CT	C01-C02-C03	-3.75	120.31	124.53
30	3	315	XAT	C38-C25-C24	3.75	118.50	114.28
30	8	316	XAT	C38-C25-C24	3.75	118.50	114.28
30	4	315	XAT	C31-C30-C29	-3.75	121.96	127.31
22	5	302	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
25	I	101	8CT	C14-C13-C12	-3.74	121.97	127.31
29	7	308	CHL	C2D-C1D-ND	3.74	112.86	110.10
22	1	311	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
25	4	317	8CT	C01-C02-C07	3.74	120.81	113.62
25	L	206	8CT	C35-C30-C29	-3.74	107.97	112.70
25	3	318	8CT	C01-C02-C03	-3.74	120.33	124.53
25	7	321	8CT	C39-C16-C17	-3.74	117.69	122.92
22	0	311	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
29	4	306	CHL	CAC-C3C-C4C	3.73	129.65	124.81
30	5	316	XAT	C28-C29-C30	-3.73	113.22	118.94
22	8	309	CLA	C1-C2-C3	-3.73	119.59	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	308	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
22	H	201	CLA	CMB-C2B-C3B	3.73	131.65	124.68
25	A	849	8CT	C35-C30-C29	-3.73	107.99	112.70
25	8	318	8CT	C24-C25-C26	-3.73	121.99	127.31
22	A	817	CLA	CMB-C2B-C3B	3.72	131.64	124.68
25	7	301	8CT	C05-C04-C03	3.72	116.20	110.48
22	A	804	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
29	9	302	CHL	C3B-C4B-NB	3.71	114.00	109.21
22	B	837	CLA	CMB-C2B-C3B	3.71	131.62	124.68
22	7	304	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
29	2	307	CHL	CAC-C3C-C4C	3.70	129.61	124.81
29	5	301	CHL	C1B-CHB-C4A	-3.70	122.79	130.12
29	6	308	CHL	C3D-C4D-ND	3.70	116.22	110.24
22	6	310	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
25	A	849	8CT	C30-C31-C32	-3.70	116.92	121.47
25	5	317	8CT	C14-C15-C16	-3.69	116.05	126.42
30	9	314	XAT	C40-C33-C32	3.69	123.89	118.08
29	6	307	CHL	CAC-C3C-C4C	3.69	129.59	124.81
25	7	321	8CT	C01-C02-C07	3.69	120.70	113.62
22	A	815	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
22	2	302	CLA	CMB-C2B-C3B	3.68	131.57	124.68
22	A	827	CLA	CMB-C2B-C3B	3.68	131.57	124.68
25	B	851	8CT	C07-C02-C03	-3.68	117.39	122.73
29	6	302	CHL	C2D-C1D-ND	3.68	112.82	110.10
25	L	205	8CT	C18-C19-C20	3.68	131.01	123.47
25	3	318	8CT	C35-C30-C29	-3.68	108.05	112.70
22	7	312	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
25	5	317	8CT	C27-C26-C25	-3.68	117.77	122.92
22	B	836	CLA	CMB-C2B-C3B	3.68	131.56	124.68
25	B	851	8CT	C27-C26-C25	-3.67	117.78	122.92
25	5	317	8CT	C28-C26-C25	3.67	124.58	118.94
22	8	303	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
22	A	823	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
25	8	301	8CT	C18-C17-C16	-3.66	122.08	127.31
22	B	809	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
29	8	307	CHL	C3B-C4B-NB	3.66	113.94	109.21
22	A	828	CLA	CMB-C2B-C3B	3.66	131.53	124.68
29	0	301	CHL	C4A-NA-C1A	3.66	108.35	106.71
22	4	311	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
30	0	314	XAT	C20-C13-C12	3.66	123.84	118.08
22	G	102	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
22	4	314	CLA	CMB-C2B-C1B	-3.66	122.85	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	0	306	CHL	C3C-C4C-NC	3.65	114.67	110.57
22	6	309	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
22	8	309	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
29	4	301	CHL	C3B-C4B-NB	3.65	113.93	109.21
22	A	839	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
22	A	802	CLA	CMB-C2B-C3B	3.65	131.50	124.68
25	B	845	8CT	C05-C04-C03	3.64	116.09	110.48
22	A	836	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
29	9	307	CHL	CHD-C4C-C3C	-3.64	119.49	124.84
29	2	306	CHL	CAC-C3C-C4C	3.64	129.53	124.81
22	0	305	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
22	7	318	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
22	2	302	CLA	O2D-CGD-O1D	-3.64	116.73	123.84
23	A	842	PQN	C11-C12-C13	-3.63	120.75	126.79
22	B	807	CLA	CHB-C4A-NA	3.63	129.53	124.51
22	2	303	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
29	5	301	CHL	C2D-C1D-ND	3.63	112.78	110.10
22	A	821	CLA	CMB-C2B-C3B	3.63	131.46	124.68
22	7	305	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
30	5	315	XAT	C11-C12-C13	-3.62	116.24	126.42
22	5	311	CLA	CMB-C2B-C3B	3.62	131.45	124.68
22	7	314	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
30	1	315	XAT	C28-C29-C30	-3.62	113.39	118.94
22	A	830	CLA	CMB-C2B-C3B	3.62	131.45	124.68
22	B	832	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
30	5	315	XAT	C39-C29-C30	-3.62	117.86	122.92
22	L	203	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
22	B	807	CLA	CMB-C2B-C3B	3.61	131.44	124.68
25	4	317	8CT	C30-C31-C32	-3.61	117.03	121.47
29	6	316	CHL	CHD-C4C-C3C	-3.61	119.53	124.84
22	A	837	CLA	CMB-C2B-C3B	3.61	131.43	124.68
22	7	303	CLA	CMB-C2B-C3B	3.61	131.43	124.68
25	F	302	8CT	C01-C02-C03	-3.61	120.48	124.53
25	L	206	8CT	C14-C15-C16	-3.60	116.29	126.42
22	6	311	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
29	6	306	CHL	C2D-C1D-ND	3.60	112.76	110.10
22	0	302	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
29	4	305	CHL	C1B-CHB-C4A	-3.59	123.00	130.12
22	A	821	CLA	C1-C2-C3	-3.59	119.83	126.04
30	2	316	XAT	C5-C4-C3	-3.59	105.65	112.75
25	I	101	8CT	C07-C02-C03	-3.59	117.52	122.73
29	6	316	CHL	C2D-C1D-ND	3.59	112.75	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	307	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
22	4	308	CLA	CMB-C2B-C3B	3.59	131.39	124.68
29	2	307	CHL	C3D-C4D-ND	3.58	116.04	110.24
25	A	847	8CT	C07-C02-C03	-3.58	117.53	122.73
29	9	307	CHL	C1B-CHB-C4A	-3.58	123.03	130.12
29	9	302	CHL	C3D-C4D-ND	3.58	116.03	110.24
30	5	315	XAT	O24-C25-C26	-3.58	56.00	58.96
22	7	314	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
29	6	306	CHL	C3B-C4B-NB	3.57	113.83	109.21
25	3	318	8CT	C15-C16-C17	3.57	124.42	118.94
30	8	317	XAT	C10-C11-C12	-3.57	112.07	123.22
29	6	316	CHL	C1B-CHB-C4A	-3.57	123.05	130.12
30	4	316	XAT	C35-C15-C14	-3.57	116.16	123.47
30	0	313	XAT	O24-C25-C26	-3.57	56.01	58.96
22	2	309	CLA	CMB-C2B-C3B	3.57	131.35	124.68
22	4	310	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
25	B	851	8CT	C28-C26-C25	3.57	124.41	118.94
22	B	806	CLA	CMB-C2B-C1B	-3.56	122.98	128.46
25	B	845	8CT	C07-C02-C03	-3.56	117.56	122.73
22	J	103	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
30	5	315	XAT	C32-C33-C34	3.56	124.41	118.94
29	9	307	CHL	C3D-C4D-ND	3.56	116.00	110.24
29	1	305	CHL	CAC-C3C-C4C	3.56	129.43	124.81
25	B	844	8CT	C22-C21-C20	-3.56	117.93	122.92
25	7	321	8CT	C01-C02-C03	-3.56	120.53	124.53
22	A	803	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
22	6	318	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
22	6	301	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
22	5	307	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
30	2	316	XAT	C4-C3-C2	-3.55	103.91	110.77
25	1	316	8CT	C01-C02-C07	3.55	120.44	113.62
22	3	309	CLA	CAA-C2A-C3A	-3.55	107.81	116.10
22	B	817	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
22	2	313	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
22	6	313	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
22	1	313	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
22	3	301	CLA	CMB-C2B-C3B	3.55	131.32	124.68
22	5	308	CLA	CHB-C4A-NA	3.55	129.42	124.51
22	A	824	CLA	CMB-C2B-C1B	-3.55	123.02	128.46
29	8	306	CHL	C3D-C4D-ND	3.54	115.97	110.24
24	A	845	LHG	O8-C23-C24	3.54	120.67	111.38
22	L	204	CLA	CMB-C2B-C1B	-3.54	123.02	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	301	CLA	CAB-C3B-C4B	-3.54	123.02	128.46
29	7	308	CHL	C3D-C4D-ND	3.54	115.96	110.24
30	1	314	XAT	C11-C12-C13	3.54	136.36	126.42
25	B	845	8CT	C22-C21-C20	-3.54	117.97	122.92
29	0	301	CHL	CAC-C3C-C4C	3.54	129.40	124.81
22	8	315	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
30	4	315	XAT	C20-C13-C12	3.53	123.64	118.08
29	5	301	CHL	C1-C2-C3	-3.53	119.94	126.04
30	4	315	XAT	C4-C3-C2	-3.53	103.96	110.77
22	2	310	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
22	0	307	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
25	6	321	8CT	C19-C20-C21	-3.53	122.28	127.31
22	6	315	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
22	B	815	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
22	8	304	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
25	4	317	8CT	C01-C02-C03	-3.52	120.58	124.53
22	2	308	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
29	4	307	CHL	C3B-C4B-NB	3.52	113.76	109.21
29	4	301	CHL	C1D-ND-C4D	-3.51	103.84	106.33
22	2	312	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
29	5	301	CHL	CAC-C3C-C4C	3.51	129.36	124.81
29	2	301	CHL	CHB-C4A-NA	3.51	129.37	124.51
25	B	844	8CT	C07-C02-C03	-3.51	117.64	122.73
22	A	807	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
30	4	316	XAT	C38-C25-C26	-3.51	116.39	122.26
22	2	304	CLA	CMB-C2B-C3B	3.50	131.23	124.68
22	7	315	CLA	CMB-C2B-C3B	3.50	131.23	124.68
25	B	845	8CT	C39-C16-C17	-3.50	118.02	122.92
22	A	805	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	B	805	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	5	310	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
25	8	301	8CT	C04-C03-C02	-3.50	117.69	122.61
29	6	308	CHL	C3B-C4B-NB	3.50	113.73	109.21
29	8	306	CHL	C3B-C4B-NB	3.50	113.73	109.21
22	B	825	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
25	3	316	8CT	C01-C02-C07	3.49	120.33	113.62
25	B	845	8CT	C22-C21-C23	3.49	123.58	118.08
29	8	314	CHL	CAC-C3C-C4C	3.49	129.34	124.81
22	7	311	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
30	1	314	XAT	C8-C9-C10	3.49	124.30	118.94
22	8	302	CLA	CMB-C2B-C3B	3.49	131.20	124.68
22	3	313	CLA	CMB-C2B-C1B	-3.48	123.11	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	303	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
25	7	301	8CT	C14-C15-C16	-3.48	116.64	126.42
25	J	101	8CT	C01-C02-C07	3.48	120.30	113.62
22	B	850	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
25	3	316	8CT	C35-C30-C29	-3.48	108.30	112.70
22	L	202	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
30	9	314	XAT	O4-C5-C18	3.48	119.22	115.06
22	A	819	CLA	O2D-CGD-O1D	-3.47	117.04	123.84
30	1	315	XAT	C38-C25-C24	3.47	118.19	114.28
22	B	811	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
22	A	814	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	0	304	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
29	5	301	CHL	C4-C3-C5	3.47	121.11	115.27
22	9	311	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	B	825	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
22	A	811	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
22	7	313	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
22	B	832	CLA	CMB-C2B-C3B	3.46	131.16	124.68
22	3	312	CLA	CMB-C2B-C3B	3.46	131.16	124.68
25	A	848	8CT	C11-C10-C03	-3.46	117.48	127.20
25	A	850	8CT	C19-C18-C17	-3.46	116.38	123.47
25	I	101	8CT	C18-C19-C20	-3.46	116.39	123.47
31	8	319	LMG	O6-C1-O1	-3.46	101.78	109.97
30	2	316	XAT	C30-C31-C32	-3.46	112.42	123.22
22	B	808	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
29	5	306	CHL	CAC-C3C-C4C	3.46	129.30	124.81
29	8	305	CHL	C1D-ND-C4D	-3.46	103.88	106.33
29	5	301	CHL	C3D-C4D-ND	3.46	115.83	110.24
22	A	840	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
22	6	303	CLA	CMB-C2B-C3B	3.45	131.14	124.68
25	L	205	8CT	C01-C02-C07	3.45	120.25	113.62
22	B	813	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
30	6	319	XAT	C4-C3-C2	-3.45	104.12	110.77
22	5	305	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
22	9	303	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
29	8	307	CHL	CAC-C3C-C4C	3.44	129.28	124.81
29	8	306	CHL	C1D-ND-C4D	-3.44	103.89	106.33
22	0	303	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
22	4	312	CLA	CMB-C2B-C3B	3.44	131.11	124.68
22	A	822	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
22	0	312	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
25	A	854	8CT	C01-C02-C07	3.43	120.21	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	0	301	CHL	C1-C2-C3	-3.43	120.11	126.04
29	2	301	CHL	C1-C2-C3	-3.43	120.11	126.04
22	9	309	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
29	8	307	CHL	C2D-C1D-ND	3.43	112.63	110.10
22	9	304	CLA	CMB-C2B-C3B	3.43	131.10	124.68
29	4	305	CHL	CHD-C4C-C3C	-3.43	119.80	124.84
22	A	812	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
22	5	314	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
29	2	305	CHL	C3D-C4D-ND	3.43	115.78	110.24
29	1	305	CHL	CHD-C4C-C3C	-3.43	119.80	124.84
29	8	307	CHL	C3D-C4D-ND	3.42	115.78	110.24
22	1	304	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
22	B	812	CLA	CMB-C2B-C3B	3.42	131.08	124.68
22	2	312	CLA	CMB-C2B-C3B	3.42	131.08	124.68
22	3	301	CLA	O2D-CGD-O1D	-3.42	117.14	123.84
30	2	315	XAT	C36-C21-C26	3.42	119.28	110.05
22	6	318	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	4	313	CLA	CMB-C2B-C3B	3.42	131.08	124.68
22	8	308	CLA	CBC-CAC-C3C	-3.42	103.00	112.43
25	5	317	8CT	C22-C21-C20	-3.42	118.13	122.92
22	7	310	CLA	C1-C2-C3	-3.42	121.22	126.75
22	B	850	CLA	CMB-C2B-C3B	3.42	131.07	124.68
25	B	846	8CT	C39-C16-C17	-3.42	118.14	122.92
25	8	301	8CT	C19-C20-C21	-3.42	122.43	127.31
22	4	302	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	9	305	CLA	O2D-CGD-CBD	3.42	117.34	111.27
22	4	303	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
30	5	316	XAT	C30-C31-C32	-3.41	112.56	123.22
25	A	847	8CT	C04-C03-C02	-3.41	117.80	122.61
22	1	312	CLA	O2D-CGD-O1D	-3.41	117.16	123.84
30	7	320	XAT	C15-C14-C13	-3.41	122.44	127.31
30	8	316	XAT	C8-C9-C10	3.41	124.18	118.94
22	1	306	CLA	CMB-C2B-C3B	3.41	131.06	124.68
22	6	305	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
30	2	315	XAT	O4-C5-C6	-3.41	56.14	58.96
22	9	312	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
30	3	314	XAT	C16-C1-C6	3.41	119.25	110.05
29	4	307	CHL	C3D-C4D-ND	3.40	115.75	110.24
22	7	316	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
29	2	301	CHL	C3D-C4D-ND	3.40	115.74	110.24
22	1	301	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
25	8	318	8CT	C01-C02-C07	3.40	120.15	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	314	XAT	C26-C27-C28	-3.40	118.80	125.99
22	9	305	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
24	3	317	LHG	O8-C23-C24	3.40	120.29	111.38
22	K	102	CLA	CMB-C2B-C3B	3.40	131.03	124.68
25	7	323	8CT	C10-C11-C12	-3.40	121.10	126.23
25	G	104	8CT	C35-C30-C29	-3.40	108.41	112.70
22	6	314	CLA	CMB-C2B-C1B	-3.40	123.25	128.46
25	4	317	8CT	C27-C26-C25	-3.39	118.17	122.92
30	1	315	XAT	C10-C11-C12	-3.39	112.62	123.22
29	4	305	CHL	OMC-CMC-C2C	-3.39	118.01	125.69
25	A	846	8CT	C01-C02-C07	3.39	120.13	113.62
22	4	313	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
22	1	307	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
22	3	311	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
29	7	308	CHL	CMD-C2D-C3D	-3.39	119.83	127.61
22	G	103	CLA	CMB-C2B-C3B	3.38	131.01	124.68
22	0	310	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
22	B	822	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
29	8	314	CHL	CHD-C4C-C3C	-3.38	119.88	124.84
29	6	306	CHL	C3D-C4D-ND	3.37	115.70	110.24
22	9	305	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
22	K	104	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
22	A	829	CLA	CMB-C2B-C3B	3.37	130.98	124.68
25	A	849	8CT	C01-C02-C07	3.37	120.09	113.62
30	1	314	XAT	C40-C33-C34	-3.37	118.20	122.92
22	B	815	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
25	F	302	8CT	C11-C10-C03	-3.37	117.75	127.20
25	B	845	8CT	C01-C02-C07	3.36	120.08	113.62
22	A	831	CLA	CMB-C2B-C3B	3.36	130.97	124.68
30	2	316	XAT	C11-C10-C9	-3.36	122.51	127.31
25	5	317	8CT	C39-C16-C17	-3.36	118.21	122.92
29	8	306	CHL	C1-C2-C3	-3.36	121.31	126.75
25	1	316	8CT	C01-C02-C03	-3.36	120.75	124.53
22	A	820	CLA	CMB-C2B-C3B	3.36	130.97	124.68
22	A	838	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
22	5	304	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
22	4	302	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
22	A	830	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
22	0	302	CLA	CMB-C2B-C3B	3.36	130.96	124.68
25	7	321	8CT	C22-C21-C20	-3.36	118.22	122.92
25	A	850	8CT	C01-C02-C07	3.36	120.06	113.62
29	8	305	CHL	C3D-C4D-ND	3.35	115.66	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	841	CLA	CMB-C2B-C3B	3.35	130.95	124.68
22	B	840	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
29	9	307	CHL	C3B-C4B-NB	3.35	113.54	109.21
22	3	311	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
29	9	307	CHL	CAC-C3C-C4C	3.35	129.15	124.81
22	B	830	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
30	8	316	XAT	C19-C9-C10	-3.34	118.24	122.92
25	1	316	8CT	C30-C31-C32	-3.34	117.36	121.47
29	6	306	CHL	C1D-ND-C4D	-3.34	103.96	106.33
22	6	323	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
22	0	309	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
29	6	302	CHL	C1B-CHB-C4A	-3.33	123.51	130.12
22	1	310	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
25	4	317	8CT	C07-C02-C03	-3.33	117.89	122.73
22	B	803	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
30	0	314	XAT	C38-C25-C24	3.33	118.03	114.28
30	0	313	XAT	C38-C25-C24	-3.33	110.53	114.28
25	A	848	8CT	C01-C02-C07	3.33	120.01	113.62
22	A	853	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
22	1	302	CLA	CMB-C2B-C1B	-3.32	123.35	128.46
22	6	303	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
25	7	323	8CT	C24-C25-C26	-3.32	122.57	127.31
30	3	314	XAT	C27-C28-C29	-3.32	120.37	125.53
22	B	810	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	A	834	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
25	B	847	8CT	C04-C03-C02	-3.32	117.94	122.61
22	1	309	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
22	1	308	CLA	CMB-C2B-C3B	3.32	130.88	124.68
25	B	843	8CT	C07-C02-C03	-3.32	117.92	122.73
29	2	301	CHL	CMD-C2D-C3D	-3.32	119.99	127.61
22	1	301	CLA	CMB-C2B-C3B	3.31	130.88	124.68
22	1	313	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
30	3	314	XAT	O24-C25-C38	3.31	119.02	115.06
30	7	320	XAT	C4-C3-C2	-3.31	104.39	110.77
22	B	826	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
25	5	317	8CT	C01-C02-C07	3.30	119.96	113.62
22	A	841	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
22	7	313	CLA	C1-C2-C3	-3.29	120.35	126.04
30	6	319	XAT	C20-C13-C12	3.29	123.26	118.08
25	8	301	8CT	C01-C02-C07	3.29	119.94	113.62
22	A	806	CLA	CMB-C2B-C3B	3.29	130.83	124.68
25	B	804	8CT	C18-C19-C20	-3.29	116.74	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	843	8CT	C01-C02-C07	3.29	119.93	113.62
22	A	808	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
29	6	316	CHL	C3B-C4B-NB	3.29	113.46	109.21
29	3	306	CHL	CAC-C3C-C4C	3.28	129.07	124.81
22	8	308	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
29	5	301	CHL	C1D-ND-C4D	-3.28	104.00	106.33
30	1	314	XAT	C39-C29-C30	-3.28	118.33	122.92
30	6	319	XAT	C18-C5-C4	3.28	117.97	114.28
29	8	314	CHL	C2D-C1D-ND	3.27	112.52	110.10
22	A	836	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
22	7	302	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
22	K	102	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
25	K	103	8CT	C30-C31-C32	-3.27	117.45	121.47
29	2	307	CHL	OMC-CMC-C2C	-3.27	118.30	125.69
22	3	313	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
29	4	307	CHL	CAA-CBA-CGA	-3.26	103.72	113.25
24	7	322	LHG	O8-C23-C24	3.26	119.94	111.38
30	9	314	XAT	C10-C11-C12	-3.26	113.03	123.22
31	5	319	LMG	O6-C1-O1	-3.26	102.25	109.97
22	3	312	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
22	0	308	CLA	CMB-C2B-C3B	3.26	130.78	124.68
22	B	826	CLA	CAA-CBA-CGA	-3.26	103.73	113.25
30	0	313	XAT	C11-C10-C9	-3.26	122.66	127.31
25	B	847	8CT	C01-C02-C07	3.26	119.88	113.62
25	6	321	8CT	C39-C16-C17	-3.26	118.36	122.92
22	G	101	CLA	CMB-C2B-C3B	3.25	130.76	124.68
25	7	301	8CT	C14-C13-C12	-3.25	122.67	127.31
29	3	306	CHL	C3B-C4B-NB	3.25	113.41	109.21
22	B	827	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
29	6	316	CHL	C3D-C4D-ND	3.25	115.49	110.24
22	L	201	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
22	B	806	CLA	CMB-C2B-C3B	3.25	130.75	124.68
22	3	319	CLA	CMB-C2B-C1B	-3.25	123.48	128.46
30	0	313	XAT	C40-C33-C32	3.25	123.19	118.08
22	B	823	CLA	CMB-C2B-C3B	3.24	130.75	124.68
22	G	101	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
22	K	105	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
22	M	101	CLA	C1B-CHB-C4A	-3.24	123.71	130.12
30	8	317	XAT	C4-C3-C2	-3.24	104.53	110.77
25	B	804	8CT	C07-C02-C03	-3.23	118.04	122.73
22	F	301	CLA	CMB-C2B-C3B	3.23	130.73	124.68
29	2	305	CHL	O2D-CGD-CBD	3.23	117.01	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	310	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
22	7	316	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
22	B	839	CLA	CMB-C2B-C3B	3.23	130.72	124.68
29	1	305	CHL	C3B-C4B-NB	3.23	113.39	109.21
22	A	828	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
29	6	302	CHL	O2A-CGA-CBA	3.23	122.03	111.91
25	B	847	8CT	C24-C23-C21	-3.22	117.36	126.42
22	A	808	CLA	CMB-C2B-C3B	3.22	130.71	124.68
25	B	848	8CT	C14-C13-C12	-3.22	122.71	127.31
22	8	312	CLA	CMB-C2B-C3B	3.22	130.71	124.68
22	6	317	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
30	0	313	XAT	C40-C33-C34	-3.22	118.41	122.92
29	6	302	CHL	C3D-C4D-ND	3.22	115.45	110.24
25	A	846	8CT	C10-C11-C12	-3.22	121.37	126.23
29	2	306	CHL	C3D-C4D-ND	3.22	115.44	110.24
30	5	315	XAT	C28-C29-C30	3.22	123.88	118.94
25	B	846	8CT	C27-C26-C25	-3.22	118.42	122.92
22	2	314	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
22	B	807	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
22	A	831	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
29	4	306	CHL	C1B-CHB-C4A	-3.21	123.75	130.12
29	6	302	CHL	CAC-C3C-C4C	3.21	128.97	124.81
30	2	315	XAT	C10-C11-C12	-3.21	113.20	123.22
22	2	319	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
30	6	319	XAT	C38-C25-C24	3.21	117.89	114.28
22	2	311	CLA	CMB-C2B-C3B	3.20	130.67	124.68
30	9	314	XAT	C8-C9-C10	-3.20	114.03	118.94
25	B	848	8CT	C01-C02-C07	3.20	119.77	113.62
25	L	206	8CT	C24-C23-C21	-3.20	117.43	126.42
30	9	315	XAT	C4-C3-C2	-3.20	104.59	110.77
30	6	320	XAT	C35-C34-C33	-3.20	122.74	127.31
25	L	206	8CT	C07-C02-C03	-3.20	118.08	122.73
29	8	314	CHL	C3B-C4B-NB	3.20	113.35	109.21
30	8	316	XAT	C37-C21-C36	3.20	112.08	107.37
22	A	804	CLA	CMB-C2B-C3B	3.19	130.65	124.68
30	5	316	XAT	C38-C25-C24	3.19	117.87	114.28
30	1	315	XAT	C35-C15-C14	-3.19	116.93	123.47
22	5	308	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
30	7	319	XAT	O24-C25-C38	3.19	118.88	115.06
29	4	306	CHL	O2D-CGD-O1D	-3.19	117.60	123.84
22	7	318	CLA	CMB-C2B-C3B	3.19	130.65	124.68
22	3	307	CLA	CMB-C2B-C1B	-3.19	123.56	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	801	CLA	CMB-C2B-C3B	3.19	130.64	124.68
22	A	815	CLA	CMB-C2B-C3B	3.19	130.64	124.68
30	9	314	XAT	C36-C21-C26	3.19	118.65	110.05
25	8	318	8CT	C35-C30-C29	-3.19	108.67	112.70
25	7	323	8CT	C11-C10-C03	-3.18	118.26	127.20
22	A	831	CLA	C1-C2-C3	-3.18	121.60	126.75
22	J	103	CLA	CMB-C2B-C3B	3.18	130.63	124.68
22	9	306	CLA	CMB-C2B-C3B	3.18	130.63	124.68
30	1	315	XAT	C4-C3-C2	-3.18	104.63	110.77
22	B	824	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
29	4	301	CHL	C3D-C4D-ND	3.18	115.38	110.24
29	8	314	CHL	C3D-C4D-ND	3.17	115.37	110.24
29	2	305	CHL	C3B-C4B-NB	3.17	113.31	109.21
22	5	309	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
30	0	314	XAT	C6-C7-C8	-3.17	119.29	125.99
22	K	101	CLA	CMB-C2B-C3B	3.17	130.61	124.68
22	9	313	CLA	CMB-C2B-C3B	3.17	130.60	124.68
22	G	102	CLA	CMB-C2B-C3B	3.16	130.60	124.68
25	3	318	8CT	C27-C26-C25	-3.16	118.49	122.92
29	8	307	CHL	C1D-ND-C4D	-3.16	104.09	106.33
22	6	317	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
22	B	835	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
22	B	801	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
22	0	304	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
30	2	315	XAT	C6-C7-C8	-3.16	119.31	125.99
22	6	312	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
29	4	307	CHL	O2A-CGA-CBA	3.16	121.81	111.91
30	5	316	XAT	C18-C5-C4	3.16	117.83	114.28
25	A	848	8CT	C14-C13-C12	-3.16	122.81	127.31
22	9	304	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
22	B	808	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
22	A	801	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
25	B	851	8CT	C01-C02-C07	3.15	119.67	113.62
30	5	316	XAT	C4-C3-C2	-3.15	104.69	110.77
25	K	103	8CT	C01-C02-C07	3.15	119.67	113.62
22	M	101	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
28	B	849	DGD	O3G-C1D-C2D	-3.15	103.39	108.30
22	A	804	CLA	CHB-C4A-NA	3.15	128.87	124.51
22	4	309	CLA	CMB-C2B-C3B	3.15	130.57	124.68
22	5	313	CLA	CMB-C2B-C1B	-3.15	123.63	128.46
22	8	303	CLA	CMB-C2B-C3B	3.15	130.56	124.68
22	6	305	CLA	C1B-CHB-C4A	-3.15	123.89	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	308	CLA	CMB-C2B-C3B	3.14	130.56	124.68
22	B	818	CLA	CMB-C2B-C3B	3.14	130.56	124.68
22	8	309	CLA	CMB-C2B-C3B	3.14	130.56	124.68
30	6	319	XAT	C7-C8-C9	-3.14	120.66	125.53
22	A	852	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
22	A	836	CLA	CMB-C2B-C3B	3.14	130.55	124.68
29	4	305	CHL	C3B-C4B-NB	3.14	113.27	109.21
30	5	315	XAT	C35-C15-C14	-3.14	117.05	123.47
29	8	314	CHL	C4A-NA-C1A	3.13	108.11	106.71
22	B	833	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
25	J	104	8CT	C40-C12-C13	-3.13	118.53	122.92
22	5	309	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
22	2	319	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
29	8	306	CHL	C2A-C3A-C4A	-3.13	96.81	101.87
30	6	319	XAT	C24-C23-C22	-3.13	104.72	110.77
25	L	205	8CT	C15-C16-C17	3.13	123.74	118.94
22	A	840	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
29	2	306	CHL	C2D-C1D-ND	3.13	112.41	110.10
25	7	323	8CT	C18-C19-C20	-3.13	117.07	123.47
22	A	825	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
22	A	804	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
25	A	850	8CT	C35-C30-C29	-3.12	108.75	112.70
22	8	308	CLA	CMB-C2B-C3B	3.12	130.52	124.68
29	6	316	CHL	CMB-C2B-C3B	3.12	130.52	124.68
30	2	315	XAT	C15-C35-C34	-3.12	117.08	123.47
22	A	833	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
25	G	104	8CT	C01-C02-C07	3.12	119.61	113.62
22	5	307	CLA	CMB-C2B-C3B	3.12	130.51	124.68
22	A	843	CLA	CMB-C2B-C3B	3.12	130.51	124.68
29	4	301	CHL	CAC-C3C-C4C	3.12	128.86	124.81
22	A	816	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
30	4	315	XAT	C8-C9-C10	3.12	123.72	118.94
22	A	832	CLA	CMB-C2B-C1B	-3.12	123.68	128.46
22	5	302	CLA	CMB-C2B-C3B	3.11	130.50	124.68
22	5	307	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
22	6	313	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
22	3	305	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
22	0	311	CLA	CMB-C2B-C3B	3.11	130.50	124.68
22	B	816	CLA	CMB-C2B-C3B	3.11	130.49	124.68
22	B	821	CLA	CMB-C2B-C3B	3.11	130.49	124.68
29	5	306	CHL	C3B-C4B-NB	3.10	113.22	109.21
31	4	318	LMG	C1-O6-C5	-3.10	107.60	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	827	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
30	1	314	XAT	C18-C5-C4	3.10	117.77	114.28
29	4	301	CHL	O2D-CGD-O1D	-3.10	117.78	123.84
29	6	308	CHL	O2A-CGA-CBA	3.10	121.63	111.91
22	L	203	CLA	CMB-C2B-C3B	3.10	130.47	124.68
22	3	310	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
22	6	311	CLA	CMB-C2B-C3B	3.10	130.47	124.68
22	K	105	CLA	CHB-C4A-NA	3.09	128.79	124.51
22	A	841	CLA	C2D-C1D-ND	-3.09	107.83	110.10
22	8	310	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
29	9	307	CHL	C2D-C1D-ND	3.09	112.38	110.10
25	B	846	8CT	C01-C02-C07	3.09	119.55	113.62
22	6	323	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
29	0	306	CHL	C3D-C4D-ND	3.09	115.23	110.24
22	2	309	CLA	O2A-CGA-O1A	-3.09	115.80	123.59
30	3	315	XAT	C4-C3-C2	-3.09	104.81	110.77
29	5	306	CHL	CHD-C4C-C3C	-3.09	120.30	124.84
30	0	313	XAT	C35-C15-C14	3.09	129.80	123.47
22	7	314	CLA	CMB-C2B-C3B	3.09	130.45	124.68
22	3	304	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
22	B	841	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
29	7	308	CHL	C2A-C1A-CHA	-3.08	118.47	123.86
29	2	305	CHL	CAC-C3C-C4C	3.08	128.81	124.81
30	7	319	XAT	C39-C29-C30	-3.08	118.61	122.92
29	2	305	CHL	CMD-C2D-C3D	-3.08	120.53	127.61
22	B	824	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
22	5	307	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
30	8	316	XAT	C4-C3-C2	-3.07	104.84	110.77
30	3	315	XAT	O4-C5-C4	3.07	115.69	113.38
22	1	311	CLA	CMB-C2B-C3B	3.07	130.42	124.68
30	4	315	XAT	C26-C27-C28	-3.07	119.50	125.99
22	B	815	CLA	CMB-C2B-C3B	3.07	130.42	124.68
29	6	307	CHL	CHD-C4C-C3C	-3.07	120.33	124.84
22	5	304	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
22	B	818	CLA	CHB-C4A-NA	3.06	128.75	124.51
29	8	306	CHL	C1B-CHB-C4A	-3.06	124.05	130.12
30	3	314	XAT	C40-C33-C32	3.06	122.90	118.08
30	0	313	XAT	C19-C9-C10	-3.06	118.64	122.92
22	4	304	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
25	B	851	8CT	C22-C21-C20	-3.06	118.64	122.92
30	4	316	XAT	O24-C25-C38	3.06	118.72	115.06
25	7	321	8CT	C23-C21-C20	3.06	123.63	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	303	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
25	B	851	8CT	C05-C04-C03	3.05	115.18	110.48
22	5	312	CLA	CMB-C2B-C3B	3.05	130.39	124.68
25	A	849	8CT	C14-C13-C12	-3.05	122.96	127.31
25	5	317	8CT	C23-C21-C20	3.05	123.62	118.94
25	3	316	8CT	C40-C12-C13	-3.05	118.65	122.92
29	6	307	CHL	C3D-C4D-ND	3.05	115.17	110.24
25	J	104	8CT	C01-C02-C07	3.05	119.47	113.62
25	F	302	8CT	C14-C15-C16	-3.04	117.86	126.42
22	0	305	CLA	CMB-C2B-C3B	3.04	130.38	124.68
22	A	835	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	6	305	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	7	313	CLA	CMB-C2B-C3B	3.04	130.37	124.68
25	A	850	8CT	C24-C23-C21	-3.04	117.87	126.42
22	7	312	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	4	314	CLA	CMB-C2B-C3B	3.04	130.36	124.68
22	6	304	CLA	CMB-C2B-C3B	3.04	130.36	124.68
22	0	311	CLA	C1-C2-C3	-3.04	120.79	126.04
25	F	302	8CT	C40-C12-C13	-3.04	118.67	122.92
22	0	310	CLA	CMB-C2B-C3B	3.04	130.36	124.68
29	8	305	CHL	CAC-C3C-C4C	3.04	128.75	124.81
22	6	311	CLA	CHB-C4A-NA	3.04	128.71	124.51
22	L	204	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
22	B	815	CLA	C1-C2-C3	-3.03	120.80	126.04
22	A	839	CLA	CMB-C2B-C3B	3.03	130.35	124.68
25	B	848	8CT	C27-C26-C25	-3.03	118.67	122.92
22	8	313	CLA	CMB-C2B-C3B	3.03	130.35	124.68
29	1	305	CHL	C3D-C4D-ND	3.03	115.14	110.24
22	B	820	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
22	9	308	CLA	CMB-C2B-C3B	3.03	130.35	124.68
22	A	825	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
22	B	806	CLA	CHB-C4A-NA	3.03	128.70	124.51
22	7	311	CLA	CMB-C2B-C3B	3.03	130.34	124.68
22	4	313	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
22	6	309	CLA	CMB-C2B-C3B	3.02	130.34	124.68
22	B	813	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	K	103	8CT	C24-C25-C26	-3.02	123.00	127.31
29	8	305	CHL	OMC-CMC-C2C	-3.02	118.85	125.69
22	0	310	CLA	CHB-C4A-NA	3.02	128.69	124.51
22	A	826	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	J	104	8CT	C35-C30-C29	-3.02	108.88	112.70
25	4	317	8CT	C28-C26-C25	3.02	123.57	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	321	8CT	C01-C02-C07	3.02	119.41	113.62
22	A	838	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
23	A	842	PQN	C14-C13-C15	3.02	120.34	115.27
22	7	318	CLA	CHB-C4A-NA	3.01	128.68	124.51
30	7	319	XAT	C19-C9-C10	-3.01	118.70	122.92
22	A	809	CLA	CAA-CBA-CGA	-3.01	104.46	113.25
22	A	821	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
22	6	310	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
22	L	201	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
25	1	316	8CT	C35-C30-C29	-3.01	108.90	112.70
29	7	308	CHL	CMB-C2B-C3B	3.01	130.30	124.68
22	7	318	CLA	C2A-C1A-CHA	3.00	129.11	123.86
25	B	845	8CT	C11-C10-C03	-3.00	118.76	127.20
30	1	315	XAT	C30-C31-C32	-3.00	113.84	123.22
25	B	847	8CT	C35-C30-C29	-3.00	108.91	112.70
22	8	311	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
30	5	316	XAT	C39-C29-C28	3.00	122.81	118.08
22	B	834	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
31	4	318	LMG	O1-C7-C8	-3.00	103.66	110.90
25	2	317	8CT	C01-C02-C07	3.00	119.38	113.62
22	B	828	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
29	7	308	CHL	CHB-C4A-NA	3.00	128.66	124.51
22	B	825	CLA	CMB-C2B-C3B	3.00	130.28	124.68
28	B	849	DGD	O6D-C1D-O3G	-2.99	102.89	109.97
22	5	313	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
30	7	319	XAT	C18-C5-C4	2.99	117.65	114.28
22	6	315	CLA	CMB-C2B-C3B	2.99	130.27	124.68
22	B	818	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
29	8	307	CHL	CMB-C2B-C3B	2.98	130.26	124.68
29	4	305	CHL	C2D-C1D-ND	2.98	112.30	110.10
22	0	312	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	A	849	8CT	C14-C15-C16	-2.98	118.04	126.42
22	3	305	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
30	2	316	XAT	C15-C14-C13	-2.98	123.06	127.31
25	B	804	8CT	C14-C15-C16	-2.98	118.05	126.42
22	L	202	CLA	CHB-C4A-NA	2.98	128.63	124.51
22	0	307	CLA	CMB-C2B-C3B	2.98	130.25	124.68
29	4	305	CHL	C4-C3-C5	2.97	120.27	115.27
30	6	320	XAT	C30-C31-C32	-2.97	113.94	123.22
29	4	307	CHL	OMC-CMC-C2C	-2.97	118.97	125.69
22	B	834	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
30	0	314	XAT	C31-C32-C33	-2.97	118.07	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	0	303	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	B	829	CLA	CMB-C2B-C3B	2.97	130.23	124.68
22	G	101	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
22	A	832	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	L	204	CLA	CMB-C2B-C3B	2.96	130.22	124.68
22	B	823	CLA	C1-C2-C3	-2.96	120.92	126.04
22	K	101	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	A	817	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	G	102	CLA	CHB-C4A-NA	2.96	128.60	124.51
22	B	801	CLA	C1-C2-C3	-2.96	120.92	126.04
22	A	840	CLA	CMB-C2B-C3B	2.96	130.21	124.68
29	4	305	CHL	C3D-C4D-ND	2.96	115.02	110.24
29	6	302	CHL	C3B-C4B-NB	2.96	113.03	109.21
30	9	315	XAT	C10-C11-C12	-2.96	113.99	123.22
30	4	315	XAT	C31-C32-C33	-2.95	118.12	126.42
25	7	301	8CT	C24-C23-C21	-2.95	118.13	126.42
25	A	846	8CT	C18-C19-C20	2.95	129.52	123.47
25	L	206	8CT	C27-C26-C25	-2.95	118.79	122.92
22	B	817	CLA	CMB-C2B-C3B	2.95	130.20	124.68
29	9	307	CHL	C1D-ND-C4D	-2.95	104.24	106.33
22	7	307	CLA	CMB-C2B-C3B	2.95	130.19	124.68
22	J	103	CLA	CHB-C4A-NA	2.95	128.59	124.51
30	7	320	XAT	C10-C11-C12	-2.95	114.02	123.22
22	4	311	CLA	CMB-C2B-C3B	2.95	130.19	124.68
22	8	302	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
30	2	315	XAT	C30-C31-C32	-2.95	114.03	123.22
22	5	303	CLA	CMB-C2B-C1B	-2.95	123.94	128.46
22	A	813	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
25	2	317	8CT	C14-C15-C16	-2.94	118.14	126.42
22	B	805	CLA	CMB-C2B-C3B	2.94	130.19	124.68
25	7	301	8CT	C35-C30-C29	-2.94	108.98	112.70
29	4	306	CHL	C3D-C4D-ND	2.94	115.00	110.24
22	B	810	CLA	CMB-C2B-C3B	2.94	130.18	124.68
22	2	313	CLA	CMB-C2B-C3B	2.94	130.18	124.68
25	7	301	8CT	C27-C26-C25	-2.94	118.80	122.92
22	8	311	CLA	CMB-C2B-C3B	2.94	130.18	124.68
22	7	304	CLA	CMB-C2B-C3B	2.94	130.18	124.68
22	B	803	CLA	CMB-C2B-C3B	2.94	130.18	124.68
22	6	318	CLA	CHB-C4A-NA	2.94	128.57	124.51
25	7	323	8CT	C01-C02-C07	2.94	119.26	113.62
22	7	305	CLA	CMB-C2B-C3B	2.94	130.17	124.68
25	F	302	8CT	C24-C23-C21	-2.93	118.18	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	845	8CT	C35-C30-C29	-2.93	109.00	112.70
25	3	318	8CT	C19-C18-C17	2.93	129.47	123.47
22	2	310	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
30	8	316	XAT	C26-C27-C28	-2.92	119.81	125.99
25	A	850	8CT	C18-C17-C16	-2.92	123.14	127.31
29	3	306	CHL	C3D-C4D-ND	2.92	114.96	110.24
29	2	307	CHL	C2A-C1A-CHA	-2.92	118.75	123.86
22	1	313	CLA	CMB-C2B-C3B	2.92	130.14	124.68
25	B	804	8CT	C04-C03-C02	-2.92	118.51	122.61
22	9	310	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
25	B	843	8CT	C22-C21-C23	2.91	122.67	118.08
22	7	316	CLA	CMB-C2B-C3B	2.91	130.13	124.68
22	B	850	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	B	805	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	9	310	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	9	301	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
29	9	302	CHL	O2D-CGD-O1D	-2.91	118.15	123.84
25	B	846	8CT	C40-C12-C13	-2.91	118.85	122.92
25	7	301	8CT	C04-C03-C02	-2.91	118.52	122.61
29	1	305	CHL	C2D-C1D-ND	2.91	112.25	110.10
22	9	311	CLA	CMB-C2B-C3B	2.91	130.12	124.68
30	7	320	XAT	C30-C31-C32	-2.91	114.15	123.22
29	0	301	CHL	O2A-CGA-CBA	2.90	121.02	111.91
22	0	309	CLA	CMB-C2B-C3B	2.90	130.11	124.68
25	7	323	8CT	C14-C15-C16	-2.90	118.26	126.42
22	B	837	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	J	104	8CT	C19-C20-C21	-2.90	123.17	127.31
22	4	314	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	7	318	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
22	B	823	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	8	312	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	A	829	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
30	4	316	XAT	C4-C3-C2	-2.90	105.18	110.77
22	6	313	CLA	CMB-C2B-C3B	2.90	130.10	124.68
29	5	301	CHL	CMB-C2B-C3B	2.90	130.10	124.68
22	A	820	CLA	CHB-C4A-NA	2.90	128.52	124.51
29	6	306	CHL	C1C-C2C-C3C	-2.90	104.81	107.11
22	4	309	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
22	9	306	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
29	0	301	CHL	C2D-C1D-ND	2.89	112.24	110.10
25	5	317	8CT	C15-C16-C17	2.89	123.38	118.94
22	9	301	CLA	CMB-C2B-C3B	2.89	130.35	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	815	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	5	312	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
29	6	316	CHL	C1D-ND-C4D	-2.89	104.28	106.33
30	8	317	XAT	C15-C14-C13	-2.89	123.18	127.31
22	B	827	CLA	C1-C2-C3	-2.89	121.04	126.04
29	9	307	CHL	CMD-C2D-C3D	-2.89	120.96	127.61
22	7	313	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	3	313	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	5	313	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
22	6	301	CLA	CMB-C2B-C3B	2.89	130.08	124.68
30	7	319	XAT	C4-C3-C2	-2.89	105.19	110.77
22	0	304	CLA	CMB-C2B-C3B	2.89	130.08	124.68
28	B	849	DGD	C3G-C2G-C1G	-2.89	104.96	111.79
22	7	313	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
22	9	303	CLA	CMB-C2B-C3B	2.88	130.07	124.68
22	0	309	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
25	6	321	8CT	C40-C12-C13	-2.88	118.89	122.92
29	4	306	CHL	CHD-C4C-C3C	-2.88	120.60	124.84
22	3	313	CLA	CMB-C2B-C3B	2.88	130.07	124.68
22	B	821	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	B	806	CLA	CAC-C3C-C4C	2.88	128.54	124.81
22	2	311	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	6	314	CLA	CMB-C2B-C3B	2.88	130.06	124.68
22	M	101	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	7	302	CLA	CAA-CBA-CGA	-2.87	104.85	113.25
22	3	310	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
29	0	306	CHL	C4A-NA-C1A	2.87	108.00	106.71
22	4	310	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
22	K	104	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
30	6	320	XAT	O24-C25-C38	2.87	118.49	115.06
22	5	310	CLA	CMB-C2B-C3B	2.87	130.04	124.68
29	2	307	CHL	CHB-C4A-NA	2.87	128.48	124.51
25	3	318	8CT	C07-C02-C03	-2.87	118.57	122.73
22	1	310	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	0	303	CLA	CMB-C2B-C3B	2.87	130.04	124.68
22	0	310	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
29	4	306	CHL	C3B-C4B-NB	2.86	112.91	109.21
25	B	846	8CT	C28-C26-C25	2.86	123.34	118.94
29	4	305	CHL	CMB-C2B-C3B	2.86	130.03	124.68
22	A	822	CLA	CHB-C4A-NA	2.86	128.47	124.51
22	6	314	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	8	309	CLA	O2D-CGD-O1D	-2.86	118.24	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	803	CLA	CMB-C2B-C3B	2.86	130.03	124.68
22	A	824	CLA	CMB-C2B-C3B	2.86	130.03	124.68
22	2	310	CLA	CAA-C2A-C3A	-2.86	109.43	116.10
30	2	316	XAT	C35-C15-C14	-2.86	117.62	123.47
22	4	302	CLA	CMB-C2B-C3B	2.86	130.02	124.68
30	8	317	XAT	C24-C23-C22	-2.86	105.25	110.77
25	J	101	8CT	C07-C02-C03	-2.86	118.58	122.73
30	2	316	XAT	C6-C7-C8	-2.85	119.96	125.99
25	A	846	8CT	C39-C16-C17	-2.85	118.92	122.92
22	A	810	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	4	310	CLA	CMB-C2B-C3B	2.85	130.01	124.68
29	0	301	CHL	C3D-C4D-ND	2.85	114.85	110.24
22	A	818	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	G	103	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	4	303	CLA	CMB-C2B-C3B	2.85	130.01	124.68
22	B	831	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	6	306	CHL	C2A-C1A-CHA	-2.85	118.88	123.86
22	B	829	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
22	7	309	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
30	0	314	XAT	C24-C23-C22	-2.84	105.28	110.77
25	A	846	8CT	C28-C26-C25	2.84	123.30	118.94
29	2	306	CHL	C3B-C4B-NB	2.84	112.89	109.21
22	7	312	CLA	CMB-C2B-C3B	2.84	130.00	124.68
22	9	309	CLA	CMB-C2B-C3B	2.84	130.00	124.68
22	5	310	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	B	810	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	A	814	CLA	CMB-C2B-C3B	2.84	129.99	124.68
22	B	818	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	1	311	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
29	5	306	CHL	C3D-C4D-ND	2.84	114.83	110.24
30	7	320	XAT	O24-C25-C38	2.84	118.45	115.06
30	6	320	XAT	C16-C1-C6	2.84	117.70	110.05
22	B	815	CLA	O2D-CGD-CBD	2.84	116.31	111.27
22	9	306	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
30	5	315	XAT	C6-C7-C8	-2.83	120.00	125.99
30	2	315	XAT	C18-C5-C4	-2.83	111.09	114.28
22	5	312	CLA	CHB-C4A-NA	2.83	128.43	124.51
29	6	307	CHL	C4A-NA-C1A	2.83	107.98	106.71
29	3	306	CHL	OMC-CMC-C2C	-2.83	119.28	125.69
30	6	320	XAT	C20-C13-C14	-2.83	118.96	122.92
22	B	811	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	B	807	CLA	C1B-CHB-C4A	-2.83	124.51	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	808	CLA	CMB-C2B-C3B	2.83	129.97	124.68
22	3	311	CLA	CMB-C2B-C3B	2.83	129.97	124.68
29	2	307	CHL	O2A-CGA-CBA	2.83	120.79	111.91
22	A	829	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	6	323	CLA	CMB-C2B-C3B	2.83	129.97	124.68
22	A	812	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	0	305	CLA	CBC-CAC-C3C	2.82	120.22	112.43
25	F	302	8CT	C07-C02-C03	-2.82	118.63	122.73
22	B	830	CLA	C2D-C1D-ND	-2.82	108.03	110.10
25	3	318	8CT	C18-C19-C20	2.82	129.25	123.47
22	B	809	CLA	CMB-C2B-C3B	2.82	129.95	124.68
29	1	305	CHL	CMD-C2D-C3D	-2.82	121.13	127.61
25	A	846	8CT	C11-C10-C03	-2.82	119.28	127.20
22	7	315	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	B	809	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	1	304	CLA	CMB-C2B-C3B	2.82	129.95	124.68
29	8	305	CHL	CMB-C2B-C3B	2.82	129.95	124.68
22	5	314	CLA	CMB-C2B-C3B	2.82	129.95	124.68
22	A	809	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	A	814	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
29	2	307	CHL	CMD-C2D-C3D	-2.81	121.15	127.61
22	A	824	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	A	838	CLA	CMB-C2B-C3B	2.81	129.93	124.68
29	6	307	CHL	OMC-CMC-C2C	-2.81	119.34	125.69
30	4	315	XAT	C19-C9-C10	-2.81	118.99	122.92
22	2	303	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
22	9	309	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
22	2	304	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	7	321	8CT	C27-C26-C25	-2.80	119.00	122.92
24	A	844	LHG	O8-C23-C24	2.80	120.70	111.91
29	5	306	CHL	C2D-C1D-ND	2.80	112.17	110.10
22	2	308	CLA	CMB-C2B-C3B	2.80	129.91	124.68
25	L	205	8CT	C35-C30-C31	2.80	116.43	111.42
22	1	302	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
29	8	307	CHL	CHB-C4A-NA	2.80	128.38	124.51
22	5	305	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	A	810	CLA	CMB-C2B-C1B	-2.80	124.17	128.46
22	3	304	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
25	F	302	8CT	C30-C31-C32	-2.80	118.03	121.47
22	1	306	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
22	A	823	CLA	CMB-C2B-C3B	2.79	129.91	124.68
22	J	103	CLA	O2D-CGD-O1D	-2.79	118.38	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	820	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
30	1	314	XAT	C24-C23-C22	-2.79	105.38	110.77
22	3	303	CLA	CMB-C2B-C3B	2.79	129.90	124.68
25	8	301	8CT	C19-C18-C17	-2.79	117.76	123.47
29	8	306	CHL	CMB-C2B-C3B	2.79	129.90	124.68
22	K	105	CLA	CMB-C2B-C3B	2.79	129.90	124.68
22	A	840	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
25	7	301	8CT	C18-C17-C16	-2.79	123.33	127.31
22	B	825	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
25	L	206	8CT	C28-C26-C25	2.79	123.22	118.94
29	8	306	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
25	8	301	8CT	C14-C15-C16	-2.79	118.59	126.42
22	4	310	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
25	A	850	8CT	C22-C21-C20	-2.79	119.02	122.92
29	4	301	CHL	CMB-C2B-C3B	2.79	129.89	124.68
29	8	305	CHL	C3B-C4B-NB	2.78	112.81	109.21
22	6	309	CLA	CHB-C4A-NA	2.78	128.36	124.51
22	1	307	CLA	CMB-C2B-C3B	2.78	129.88	124.68
22	3	304	CLA	CMB-C2B-C3B	2.78	129.88	124.68
22	6	312	CLA	CHB-C4A-NA	2.78	128.36	124.51
22	9	311	CLA	C1-C2-C3	-2.78	121.23	126.04
22	B	838	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
25	B	846	8CT	C18-C17-C16	-2.78	123.34	127.31
22	5	313	CLA	CMB-C2B-C3B	2.78	129.88	124.68
22	8	315	CLA	CMB-C2B-C3B	2.78	129.88	124.68
25	8	318	8CT	C11-C10-C03	-2.78	119.39	127.20
30	1	315	XAT	C15-C14-C13	-2.78	123.34	127.31
22	B	841	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
22	2	314	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	K	103	8CT	C39-C16-C17	-2.78	119.03	122.92
22	5	314	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
22	A	827	CLA	C1-C2-C3	-2.78	121.24	126.04
22	A	807	CLA	CMB-C2B-C3B	2.77	129.87	124.68
22	A	853	CLA	CMB-C2B-C3B	2.77	129.87	124.68
29	6	308	CHL	CAC-C3C-C4C	2.77	128.41	124.81
30	3	314	XAT	C8-C9-C10	-2.77	114.69	118.94
22	B	816	CLA	O2D-CGD-CBD	2.77	116.19	111.27
22	5	304	CLA	CMB-C2B-C3B	2.77	129.86	124.68
25	6	321	8CT	C27-C26-C25	-2.77	119.04	122.92
29	6	308	CHL	C1-C2-C3	-2.77	122.27	126.75
22	1	303	CLA	CMB-C2B-C3B	2.77	129.86	124.68
22	8	304	CLA	CMB-C2B-C3B	2.77	129.86	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	6	308	CHL	CMD-C2D-C3D	-2.77	121.24	127.61
22	1	302	CLA	CMB-C2B-C3B	2.77	129.86	124.68
29	0	306	CHL	CMD-C2D-C3D	-2.77	121.25	127.61
22	9	301	CLA	CAB-C3B-C2B	2.77	130.11	124.69
22	A	819	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
29	7	308	CHL	C3B-C4B-NB	2.77	112.79	109.21
22	7	304	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	6	318	CLA	CMB-C2B-C3B	2.77	129.85	124.68
25	A	854	8CT	C11-C10-C03	-2.77	119.44	127.20
25	I	101	8CT	C35-C30-C31	2.76	116.37	111.42
22	A	843	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
22	A	812	CLA	CHB-C4A-NA	2.76	128.33	124.51
30	7	320	XAT	C27-C28-C29	-2.76	121.24	125.53
22	A	806	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	3	318	8CT	C39-C16-C17	-2.76	119.06	122.92
22	7	302	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	3	313	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
22	B	822	CLA	O2D-CGD-CBD	2.76	116.17	111.27
25	4	317	8CT	C11-C10-C03	-2.76	119.46	127.20
22	1	304	CLA	O2A-CGA-O1A	-2.76	116.64	123.59
29	6	307	CHL	C3B-C4B-NB	2.76	112.77	109.21
22	1	304	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	A	832	CLA	CHB-C4A-NA	2.76	128.32	124.51
25	A	854	8CT	C35-C30-C29	-2.75	109.22	112.70
24	A	844	LHG	C11-C10-C9	-2.75	100.45	114.42
22	9	303	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	0	302	CLA	C1-C2-C3	-2.75	121.28	126.04
22	B	830	CLA	C1-C2-C3	-2.75	121.28	126.04
25	L	206	8CT	C01-C02-C07	2.75	118.90	113.62
22	1	303	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
29	6	316	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
29	8	305	CHL	C1-C2-C3	-2.75	121.28	126.04
22	1	309	CLA	CMB-C2B-C3B	2.75	129.82	124.68
25	B	844	8CT	C39-C16-C15	2.75	122.41	118.08
25	K	103	8CT	C27-C26-C25	-2.75	119.07	122.92
22	L	201	CLA	CMB-C2B-C3B	2.75	129.82	124.68
22	7	317	CLA	CHB-C4A-NA	2.75	128.31	124.51
25	B	843	8CT	C39-C16-C15	2.75	122.41	118.08
22	A	812	CLA	CMB-C2B-C3B	2.75	129.82	124.68
30	0	314	XAT	C40-C33-C34	-2.75	119.07	122.92
22	B	815	CLA	CHB-C4A-NA	2.75	128.31	124.51
22	B	822	CLA	CMB-C2B-C3B	2.75	129.82	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	315	LHG	O8-C23-C24	2.75	120.53	111.91
30	7	319	XAT	C11-C12-C13	-2.75	118.70	126.42
25	A	848	8CT	C01-C02-C03	-2.75	121.44	124.53
29	8	307	CHL	CAA-CBA-CGA	-2.75	105.22	113.25
22	A	828	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
22	2	309	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
22	1	309	CLA	CAA-C2A-C3A	-2.74	109.69	116.10
29	3	306	CHL	CMD-C2D-C3D	-2.74	121.30	127.61
25	2	317	8CT	C22-C21-C20	-2.74	119.08	122.92
22	A	813	CLA	C1-C2-C3	-2.74	121.30	126.04
29	4	307	CHL	CMD-C2D-C3D	-2.74	121.30	127.61
29	8	306	CHL	CAC-C3C-C4C	2.74	128.37	124.81
23	B	842	PQN	C14-C13-C15	2.74	119.88	115.27
29	1	305	CHL	CMB-C2B-C3B	2.74	129.81	124.68
25	B	843	8CT	C27-C26-C25	-2.74	119.08	122.92
25	F	302	8CT	C27-C26-C25	-2.74	119.09	122.92
29	8	305	CHL	O2A-CGA-CBA	2.74	120.50	111.91
30	5	316	XAT	C15-C14-C13	-2.74	123.40	127.31
30	4	315	XAT	C15-C35-C34	2.74	129.08	123.47
22	2	319	CLA	CMB-C2B-C3B	2.74	129.80	124.68
30	0	313	XAT	C39-C29-C30	-2.74	119.09	122.92
29	2	301	CHL	O2A-CGA-CBA	2.74	120.50	111.91
29	5	301	CHL	O2A-CGA-CBA	2.74	120.49	111.91
25	B	804	8CT	C27-C26-C28	2.73	122.39	118.08
25	7	301	8CT	C01-C02-C07	2.73	118.87	113.62
22	B	811	CLA	C1-C2-C3	-2.73	121.31	126.04
22	9	311	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
22	B	822	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
22	2	311	CLA	CHB-C4A-NA	2.73	128.29	124.51
22	6	315	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
22	3	311	CLA	CHB-C4A-NA	2.73	128.29	124.51
29	9	307	CHL	CMB-C2B-C3B	2.73	129.79	124.68
25	A	847	8CT	C24-C23-C21	-2.73	118.74	126.42
25	J	104	8CT	C11-C12-C13	2.73	123.13	118.94
22	9	309	CLA	C1-C2-C3	-2.73	121.32	126.04
25	B	851	8CT	C11-C10-C03	-2.73	119.54	127.20
22	G	102	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	1	309	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
22	8	309	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
22	B	811	CLA	CMB-C2B-C3B	2.73	129.78	124.68
22	4	311	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	B	825	CLA	CHB-C4A-NA	2.73	128.28	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	315	XAT	C4-C3-C2	-2.73	105.51	110.77
29	6	302	CHL	C1D-ND-C4D	-2.73	104.40	106.33
22	H	201	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
29	4	305	CHL	O2A-CGA-CBA	2.73	120.46	111.91
22	2	304	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
25	B	804	8CT	C25-C24-C23	-2.73	114.71	123.22
22	9	305	CLA	CMB-C2B-C3B	2.73	129.78	124.68
22	7	307	CLA	CHB-C4A-NA	2.72	128.28	124.51
22	F	301	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	A	834	CLA	CMB-C2B-C3B	2.72	129.78	124.68
29	5	301	CHL	C3B-C4B-NB	2.72	112.73	109.21
22	0	310	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
29	3	306	CHL	CMB-C2B-C3B	2.72	129.77	124.68
22	A	806	CLA	C1-C2-C3	-2.72	121.33	126.04
25	B	851	8CT	C14-C13-C12	-2.72	123.42	127.31
22	A	802	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
22	3	303	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
22	B	850	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	B	835	CLA	CMB-C2B-C3B	2.72	129.76	124.68
25	8	301	8CT	C27-C26-C25	-2.72	119.12	122.92
29	8	306	CHL	O2A-CGA-CBA	2.72	120.43	111.91
22	9	309	CLA	CHB-C4A-NA	2.71	128.26	124.51
30	6	320	XAT	C6-C7-C8	-2.71	120.26	125.99
22	K	105	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
22	B	803	CLA	O2D-CGD-CBD	2.71	116.09	111.27
22	B	840	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	A	810	CLA	CHB-C4A-NA	2.71	128.26	124.51
22	5	303	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	1	309	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	5	310	CLA	CAA-C2A-C3A	-2.71	109.78	116.10
22	3	302	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
22	A	852	CLA	CHB-C4A-NA	2.71	128.26	124.51
29	4	307	CHL	CHB-C4A-NA	2.71	128.25	124.51
22	A	823	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
22	B	806	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
30	8	317	XAT	O24-C25-C38	2.71	118.30	115.06
29	1	305	CHL	O2A-CGA-CBA	2.71	120.40	111.91
30	3	315	XAT	C30-C31-C32	-2.71	114.77	123.22
22	1	306	CLA	C1-C2-C3	-2.71	121.36	126.04
22	A	843	CLA	CHB-C4A-NA	2.71	128.25	124.51
22	7	304	CLA	O2A-CGA-O1A	-2.71	116.77	123.59
22	9	309	CLA	O2D-CGD-O1D	-2.70	118.55	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	311	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
22	B	817	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
22	A	839	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
22	3	310	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	B	842	PQN	C11-C12-C13	-2.70	122.30	126.79
31	8	319	LMG	O1-C1-C2	-2.70	104.09	108.30
25	F	302	8CT	C01-C02-C07	2.70	118.80	113.62
22	3	319	CLA	O1D-CGD-CBD	2.69	130.00	124.48
30	3	314	XAT	C11-C12-C13	-2.69	118.85	126.42
25	L	205	8CT	C35-C30-C29	-2.69	109.30	112.70
30	9	315	XAT	C18-C5-C4	2.69	117.31	114.28
22	A	811	CLA	CMB-C2B-C3B	2.69	129.71	124.68
22	7	306	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
22	A	853	CLA	C1-C2-C3	-2.69	121.39	126.04
29	0	306	CHL	O2A-CGA-CBA	2.69	120.35	111.91
29	9	302	CHL	O2A-CGA-CBA	2.69	120.35	111.91
22	A	841	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
29	8	307	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
22	A	822	CLA	O2D-CGD-CBD	2.69	116.05	111.27
25	I	101	8CT	C01-C02-C07	2.69	118.78	113.62
22	4	303	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
22	6	314	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	B	835	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	0	314	XAT	C35-C34-C33	-2.69	123.48	127.31
22	1	302	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
22	7	317	CLA	CMB-C2B-C1B	-2.69	124.34	128.46
22	A	839	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
22	B	830	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
29	8	307	CHL	O2A-CGA-CBA	2.68	120.33	111.91
22	1	307	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
29	4	306	CHL	C2D-C1D-ND	2.68	112.08	110.10
22	1	313	CLA	O2D-CGD-CBD	2.68	116.03	111.27
22	B	833	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
29	6	306	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
22	6	305	CLA	CMB-C2B-C3B	2.68	129.69	124.68
28	B	849	DGD	CDB-CCB-CBB	-2.68	100.83	114.42
22	A	833	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
22	K	105	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
25	3	318	8CT	C11-C10-C03	-2.68	119.69	127.20
22	A	823	CLA	CHB-C4A-NA	2.68	128.21	124.51
22	B	819	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
25	B	804	8CT	C01-C02-C07	2.67	118.75	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	833	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	3	302	CLA	CMB-C2B-C3B	2.67	129.68	124.68
25	3	318	8CT	C05-C04-C03	2.67	114.60	110.48
22	0	312	CLA	CMB-C2B-C3B	2.67	129.68	124.68
25	B	848	8CT	C28-C26-C25	2.67	123.04	118.94
22	A	809	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
22	0	304	CLA	C1-C2-C3	-2.67	121.42	126.04
30	3	315	XAT	C19-C9-C8	2.67	122.28	118.08
25	L	205	8CT	C10-C03-C02	-2.67	115.00	121.46
25	B	844	8CT	C04-C03-C02	-2.67	118.85	122.61
22	6	318	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
30	8	317	XAT	C38-C25-C24	2.67	117.28	114.28
30	8	316	XAT	C27-C28-C29	-2.66	121.39	125.53
30	3	314	XAT	C39-C29-C30	-2.66	119.19	122.92
22	B	840	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
29	0	301	CHL	CHD-C4C-C3C	-2.66	120.92	124.84
22	B	833	CLA	CAA-CBA-CGA	-2.66	105.47	113.25
22	9	305	CLA	CHB-C4A-NA	2.66	128.20	124.51
22	8	310	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
22	B	811	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	A	805	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
22	1	308	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
29	2	305	CHL	C2A-C1A-CHA	-2.66	119.20	123.86
30	5	315	XAT	C7-C8-C9	-2.66	121.40	125.53
22	2	309	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
29	4	305	CHL	CMD-C2D-C3D	-2.66	121.49	127.61
29	4	301	CHL	CMD-C2D-C3D	-2.66	121.49	127.61
22	8	308	CLA	C3C-C4C-NC	-2.66	107.59	110.57
22	6	303	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	A	838	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
22	7	316	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
31	8	319	LMG	O3-C3-C2	-2.65	104.21	110.35
22	0	311	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
30	6	320	XAT	C28-C29-C30	-2.65	114.87	118.94
22	A	837	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
29	5	306	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
22	B	814	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	A	847	8CT	C35-C30-C29	-2.65	109.35	112.70
22	A	805	CLA	CMB-C2B-C3B	2.65	129.64	124.68
22	H	201	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
22	2	313	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
29	6	316	CHL	C1C-C2C-C3C	-2.65	105.01	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	2	306	CHL	O2A-CGA-CBA	2.65	120.22	111.91
25	3	316	8CT	C11-C12-C13	2.65	123.01	118.94
22	B	818	CLA	CHD-C1D-ND	-2.65	122.02	124.45
22	B	836	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	4	310	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	7	310	CLA	CHB-C4A-NA	2.65	128.18	124.51
29	2	306	CHL	OMC-CMC-C2C	-2.65	119.70	125.69
22	9	312	CLA	CMB-C2B-C3B	2.65	129.63	124.68
22	4	302	CLA	CHB-C4A-NA	2.65	128.17	124.51
30	4	316	XAT	C15-C14-C13	-2.65	123.53	127.31
22	7	314	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
22	9	304	CLA	C2D-C1D-ND	-2.64	108.16	110.10
22	2	303	CLA	CMB-C2B-C3B	2.64	129.62	124.68
22	B	836	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	A	807	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	4	311	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	3	303	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	7	302	CLA	CMB-C2B-C3B	2.64	129.62	124.68
24	6	322	LHG	O8-C23-C24	2.64	120.19	111.91
22	8	312	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	B	813	CLA	CMB-C2B-C3B	2.64	129.61	124.68
22	0	304	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
22	6	310	CLA	CMB-C2B-C3B	2.64	129.61	124.68
22	B	828	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
22	0	309	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
29	8	314	CHL	O2D-CGD-O1D	-2.64	118.69	123.84
22	4	309	CLA	C1-C2-C3	-2.63	121.49	126.04
25	J	101	8CT	C40-C12-C13	-2.63	119.23	122.92
22	A	811	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
29	8	305	CHL	C1B-CHB-C4A	-2.63	124.90	130.12
22	3	307	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
22	1	306	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
22	9	313	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
31	5	319	LMG	C7-O1-C1	2.63	118.87	113.74
29	9	302	CHL	C2A-C1A-CHA	-2.63	119.27	123.86
22	B	801	CLA	CHB-C4A-NA	2.63	128.14	124.51
22	8	309	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
22	2	310	CLA	CMB-C2B-C3B	2.63	129.59	124.68
22	5	304	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
25	B	843	8CT	C35-C30-C31	2.62	116.12	111.42
22	A	841	CLA	CHB-C4A-NA	2.62	128.14	124.51
22	9	311	CLA	CHB-C4A-NA	2.62	128.14	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	314	XAT	C15-C14-C13	-2.62	123.57	127.31
22	4	309	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	L	203	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
22	A	820	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	A	833	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	A	822	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
22	1	313	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
25	B	843	8CT	C11-C10-C03	-2.62	119.84	127.20
22	H	201	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
22	F	301	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
22	A	816	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	B	848	8CT	C25-C24-C23	-2.62	115.05	123.22
25	A	846	8CT	C19-C20-C21	-2.62	123.58	127.31
31	4	318	LMG	O2-C2-C1	-2.62	103.69	110.05
22	3	308	CLA	CHB-C4A-NA	2.61	128.13	124.51
22	0	312	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
22	J	103	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
22	M	101	CLA	CMB-C2B-C3B	2.61	129.57	124.68
25	F	302	8CT	C11-C12-C13	2.61	122.95	118.94
22	A	809	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
22	6	318	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
29	8	314	CHL	CMD-C2D-C3D	-2.61	121.60	127.61
22	0	307	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	A	830	CLA	O2D-CGD-CBD	2.61	115.91	111.27
22	A	829	CLA	C1-C2-C3	-2.61	121.53	126.04
22	A	853	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	7	305	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
22	B	816	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	7	302	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	B	846	8CT	C14-C13-C12	-2.61	123.59	127.31
22	F	301	CLA	CHB-C4A-NA	2.61	128.12	124.51
29	5	306	CHL	CMD-C2D-C3D	-2.61	121.62	127.61
22	A	802	CLA	O2A-CGA-O1A	-2.61	117.02	123.59
30	7	319	XAT	C28-C29-C30	2.61	122.94	118.94
22	A	843	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
22	B	810	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	8	313	CLA	CHD-C1D-ND	-2.60	122.06	124.45
24	5	318	LHG	O8-C23-C24	2.60	120.07	111.91
22	4	308	CLA	C1-C2-C3	-2.60	122.54	126.75
22	A	834	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
22	1	302	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	A	818	CLA	CHB-C4A-NA	2.60	128.11	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	803	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
29	6	307	CHL	C2D-C1D-ND	2.60	112.02	110.10
22	K	102	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	B	834	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
22	7	310	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
22	A	807	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
29	4	301	CHL	CHB-C4A-NA	2.60	128.10	124.51
22	A	852	CLA	CMB-C2B-C3B	2.60	129.54	124.68
29	8	305	CHL	CMD-C2D-C3D	-2.60	121.64	127.61
22	A	815	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	0	308	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	B	806	CLA	C1B-CHB-C4A	-2.60	124.98	130.12
22	4	308	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	A	840	CLA	C1B-CHB-C4A	-2.60	124.98	130.12
22	A	832	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
25	2	317	8CT	C27-C26-C25	-2.59	119.29	122.92
22	7	311	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	3	304	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
30	2	316	XAT	O24-C25-C38	2.59	118.16	115.06
30	0	314	XAT	C39-C29-C30	-2.59	119.29	122.92
25	A	847	8CT	C18-C19-C20	-2.59	118.17	123.47
22	6	301	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	B	812	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
22	A	817	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	0	307	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	A	804	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
29	5	306	CHL	C4A-NA-C1A	2.59	107.87	106.71
22	A	836	CLA	CHB-C4A-NA	2.59	128.09	124.51
29	4	301	CHL	O2A-CGA-CBA	2.59	120.03	111.91
29	6	308	CHL	CMB-C2B-C3B	2.59	129.52	124.68
29	9	302	CHL	CMB-C2B-C3B	2.59	129.52	124.68
23	A	842	PQN	C21-C20-C18	-2.59	107.56	115.92
24	2	318	LHG	C11-C10-C9	-2.59	101.30	114.42
30	9	315	XAT	C24-C23-C22	-2.59	105.78	110.77
22	4	303	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	5	305	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
29	4	301	CHL	C1-C2-C3	-2.59	121.57	126.04
30	2	315	XAT	C38-C25-C24	2.58	117.19	114.28
28	B	849	DGD	O5D-C6D-C5D	-2.58	104.26	109.05
22	B	840	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	8	302	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	5	312	CLA	C1B-CHB-C4A	-2.58	125.00	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	321	8CT	C15-C16-C17	2.58	122.90	118.94
22	2	314	CLA	CMB-C2B-C3B	2.58	129.50	124.68
29	8	306	CHL	CMD-C2D-C3D	-2.58	121.68	127.61
22	B	814	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
30	3	315	XAT	C31-C30-C29	-2.58	123.63	127.31
29	0	301	CHL	CMB-C2B-C3B	2.58	129.50	124.68
22	A	824	CLA	CHB-C4A-NA	2.58	128.07	124.51
25	J	104	8CT	C18-C19-C20	-2.58	118.20	123.47
29	2	306	CHL	CMD-C2D-C3D	-2.57	121.69	127.61
22	4	312	CLA	CHB-C4A-NA	2.57	128.07	124.51
25	B	804	8CT	C40-C12-C13	-2.57	119.32	122.92
25	A	846	8CT	C35-C30-C29	2.57	115.95	112.70
30	2	316	XAT	C20-C13-C12	2.57	122.13	118.08
22	B	832	CLA	O2D-CGD-CBD	2.57	115.84	111.27
30	9	315	XAT	C30-C31-C32	-2.57	115.19	123.22
29	0	301	CHL	C3B-C4B-NB	2.57	112.53	109.21
22	8	311	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
30	9	315	XAT	C38-C25-C24	2.57	117.17	114.28
22	A	818	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
25	A	846	8CT	C15-C16-C17	2.57	122.88	118.94
22	5	304	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	3	316	8CT	C24-C23-C21	-2.57	119.20	126.42
22	B	832	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	9	313	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	B	847	8CT	C14-C15-C16	-2.57	119.20	126.42
29	6	302	CHL	C4-C3-C5	2.57	119.59	115.27
25	G	104	8CT	C11-C10-C03	-2.57	119.99	127.20
22	A	829	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	1	307	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	8	308	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	4	313	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	B	827	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
22	6	315	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
24	9	316	LHG	C11-C10-C9	-2.56	101.41	114.42
25	A	854	8CT	C14-C15-C16	-2.56	119.21	126.42
22	3	312	CLA	CHB-C4A-NA	2.56	128.06	124.51
22	7	303	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	6	317	CLA	CMB-C2B-C3B	2.56	129.47	124.68
29	5	301	CHL	CMD-C2D-C3D	-2.56	121.73	127.61
22	B	822	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	3	311	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
22	7	315	CLA	C1B-CHB-C4A	-2.56	125.05	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	308	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	A	808	CLA	O2D-CGD-CBD	2.56	115.81	111.27
22	B	841	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	3	319	CLA	CHB-C4A-NA	2.56	128.05	124.51
29	9	307	CHL	O2A-CGA-CBA	2.56	119.93	111.91
29	8	307	CHL	C1C-C2C-C3C	-2.56	105.09	107.11
22	B	824	CLA	CMB-C2B-C3B	2.55	129.46	124.68
29	8	305	CHL	C4-C3-C5	2.55	119.57	115.27
22	1	308	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
22	2	314	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	2	316	XAT	C39-C29-C28	2.55	122.10	118.08
30	3	314	XAT	C18-C5-C4	2.55	117.15	114.28
29	8	306	CHL	O2D-CGD-O1D	-2.55	118.84	123.84
30	2	315	XAT	C39-C29-C28	2.55	122.10	118.08
22	8	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	6	312	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
22	1	307	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
29	8	307	CHL	C2A-C1A-CHA	-2.55	119.40	123.86
25	J	104	8CT	C27-C26-C25	-2.55	119.35	122.92
24	2	318	LHG	O8-C23-C24	2.55	119.91	111.91
22	A	840	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	B	809	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	5	316	XAT	C24-C23-C22	-2.55	105.85	110.77
22	B	839	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
22	8	310	CLA	CHB-C4A-NA	2.55	128.03	124.51
29	0	306	CHL	C2D-C1D-ND	2.55	111.98	110.10
22	2	302	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
22	1	309	CLA	CHB-C4A-NA	2.55	128.03	124.51
25	3	316	8CT	C13-C14-C15	-2.55	115.27	123.22
29	2	305	CHL	OMC-CMC-C2C	-2.55	119.93	125.69
22	A	839	CLA	CAC-C3C-C2C	2.54	131.88	127.53
22	A	801	CLA	CMB-C2B-C3B	2.54	129.44	124.68
30	2	315	XAT	C24-C23-C22	-2.54	105.86	110.77
22	B	839	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
22	6	301	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	4	309	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
22	9	313	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
22	B	805	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
22	4	308	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
22	A	822	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
22	5	314	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
22	B	823	CLA	C1B-CHB-C4A	-2.54	125.09	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	814	CLA	C1-C2-C3	-2.54	121.65	126.04
22	6	318	CLA	O2D-CGD-CBD	2.54	115.78	111.27
22	A	825	CLA	C1-C2-C3	-2.54	121.65	126.04
22	8	308	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
22	A	821	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
25	A	847	8CT	C11-C10-C03	-2.54	120.08	127.20
22	5	311	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	A	810	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
22	6	310	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
22	1	312	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
22	A	816	CLA	CHB-C4A-NA	2.53	128.02	124.51
25	B	846	8CT	C19-C18-C17	-2.53	118.28	123.47
30	4	316	XAT	C10-C11-C12	-2.53	115.31	123.22
22	7	313	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
22	2	312	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
29	5	306	CHL	O2A-CGA-CBA	2.53	119.85	111.91
22	A	853	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
22	B	831	CLA	C2D-C1D-ND	-2.53	108.24	110.10
25	A	847	8CT	C40-C12-C13	-2.53	119.38	122.92
29	0	306	CHL	C1C-C2C-C3C	-2.53	105.11	107.11
22	A	835	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
22	3	310	CLA	CMB-C2B-C3B	2.53	129.41	124.68
22	A	820	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
22	9	313	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
24	A	845	LHG	C11-C10-C9	-2.53	101.61	114.42
22	A	852	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
22	9	311	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
22	G	102	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
29	1	305	CHL	OMC-CMC-C2C	-2.52	119.98	125.69
30	0	314	XAT	C19-C9-C10	-2.52	119.39	122.92
25	2	317	8CT	C24-C23-C21	-2.52	119.33	126.42
29	4	306	CHL	CMD-C2D-C3D	-2.52	121.81	127.61
22	1	301	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
22	A	805	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
22	A	804	CLA	CAA-CBA-CGA	-2.52	105.89	113.25
22	1	303	CLA	CHB-C4A-NA	2.52	128.00	124.51
30	2	315	XAT	C35-C34-C33	-2.52	123.71	127.31
22	9	308	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
25	1	316	8CT	C40-C12-C13	-2.52	119.39	122.92
22	6	312	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
22	4	312	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
22	A	812	CLA	C1B-CHB-C4A	-2.52	125.13	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	304	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	B	820	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	B	812	CLA	C1-C2-C3	-2.52	121.69	126.04
22	8	309	CLA	CHB-C4A-NA	2.52	127.99	124.51
30	3	314	XAT	C15-C35-C34	2.52	128.63	123.47
29	6	306	CHL	CMB-C2B-C3B	2.51	129.38	124.68
22	9	308	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
22	0	312	CLA	CAA-C2A-C3A	-2.51	105.89	112.78
22	5	311	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
22	K	104	CLA	CMB-C2B-C3B	2.51	129.38	124.68
22	6	304	CLA	CHB-C4A-NA	2.51	127.99	124.51
29	9	302	CHL	CMD-C2D-C3D	-2.51	121.83	127.61
22	2	308	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
22	6	303	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
30	5	316	XAT	C10-C11-C12	-2.51	115.38	123.22
22	4	304	CLA	C1-C2-C3	-2.51	122.69	126.75
22	A	830	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
22	B	809	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
22	B	813	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	9	306	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	B	801	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
22	B	831	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
22	3	308	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
22	B	810	CLA	C1-C2-C3	-2.51	121.70	126.04
22	L	203	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
22	B	820	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
22	5	303	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	A	823	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
25	F	302	8CT	C22-C21-C20	-2.51	119.41	122.92
30	5	316	XAT	C19-C9-C8	2.50	122.02	118.08
22	8	312	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
22	A	807	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
22	A	815	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
30	3	314	XAT	C19-C9-C8	2.50	122.02	118.08
22	9	310	CLA	CMB-C2B-C3B	2.50	129.36	124.68
22	7	307	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
30	4	315	XAT	C40-C33-C34	-2.50	119.42	122.92
22	5	309	CLA	CMB-C2B-C3B	2.50	129.35	124.68
22	0	307	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
22	3	303	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	4	303	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	B	847	8CT	C11-C10-C03	-2.50	120.19	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	303	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
22	B	817	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	B	810	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
22	0	308	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
22	7	309	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
22	B	829	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	1	304	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
22	3	301	CLA	O2D-CGD-CBD	2.49	115.70	111.27
22	4	304	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	A	832	CLA	CMB-C2B-C3B	2.49	129.34	124.68
30	9	314	XAT	C20-C13-C12	2.49	122.00	118.08
22	A	841	CLA	CMB-C2B-C3B	2.49	129.34	124.68
22	B	807	CLA	O2D-CGD-CBD	2.49	115.70	111.27
25	7	301	8CT	C39-C16-C15	2.49	122.00	118.08
22	3	319	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
22	A	802	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
22	3	305	CLA	CMB-C2B-C3B	2.49	129.34	124.68
22	8	310	CLA	CMB-C2B-C3B	2.49	129.34	124.68
22	A	827	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
22	4	311	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
22	6	311	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
22	3	319	CLA	CMB-C2B-C3B	2.49	129.33	124.68
29	2	305	CHL	CHB-C4A-NA	2.49	127.95	124.51
22	A	831	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
29	2	301	CHL	CMB-C2B-C3B	2.49	129.33	124.68
22	A	803	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	3	307	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
30	9	315	XAT	C39-C29-C28	2.49	121.99	118.08
22	A	838	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	L	204	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	A	833	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	7	304	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	0	307	CLA	CBC-CAC-C3C	2.48	119.28	112.43
22	A	803	CLA	C1-C2-C3	-2.48	121.75	126.04
22	5	305	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
29	0	301	CHL	CMD-C2D-C3D	-2.48	121.90	127.61
22	2	313	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	8	308	CLA	CHD-C1D-ND	-2.48	122.17	124.45
22	2	303	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
22	H	201	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	0	302	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
22	B	816	CLA	C1B-CHB-C4A	-2.48	125.21	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	314	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
30	3	315	XAT	C35-C34-C33	-2.48	123.77	127.31
29	6	316	CHL	O2D-CGD-O1D	-2.48	118.99	123.84
22	B	834	CLA	C2D-C1D-ND	-2.48	108.28	110.10
22	B	836	CLA	C1-C2-C3	-2.48	121.76	126.04
22	0	311	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
29	6	306	CHL	CHB-C4A-NA	2.47	127.93	124.51
22	B	837	CLA	CHB-C4A-NA	2.47	127.93	124.51
29	2	306	CHL	C1D-ND-C4D	-2.47	104.58	106.33
22	3	312	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
22	6	312	CLA	CMB-C2B-C3B	2.47	129.30	124.68
29	4	307	CHL	C2A-C1A-CHA	-2.47	119.54	123.86
29	8	306	CHL	OMC-CMC-C2C	-2.47	120.10	125.69
22	B	811	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
24	6	322	LHG	C11-C10-C9	-2.47	101.89	114.42
22	B	835	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
30	2	316	XAT	C24-C23-C22	-2.47	106.00	110.77
24	0	315	LHG	C11-C10-C9	-2.47	101.89	114.42
22	4	314	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	A	852	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
25	3	316	8CT	C39-C16-C17	-2.47	119.47	122.92
22	A	801	CLA	C1-C2-C3	-2.47	121.78	126.04
29	6	308	CHL	C1C-C2C-C3C	-2.47	105.16	107.11
29	6	316	CHL	OMC-CMC-C2C	-2.47	120.11	125.69
29	5	306	CHL	CMB-C2B-C3B	2.47	129.29	124.68
22	H	201	CLA	C1-C2-C3	-2.47	121.78	126.04
25	L	206	8CT	C39-C16-C17	-2.47	119.47	122.92
25	A	849	8CT	C19-C18-C17	-2.47	118.42	123.47
22	5	310	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
22	B	827	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	B	841	CLA	C1-C2-C3	-2.46	121.78	126.04
24	1	317	LHG	O8-C23-C24	2.46	119.63	111.91
25	3	316	8CT	C19-C18-C17	-2.46	118.43	123.47
22	B	819	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	3	311	CLA	C1-C2-C3	-2.46	121.79	126.04
22	5	307	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	A	821	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	9	310	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
22	0	304	CLA	CHB-C4A-NA	2.46	127.91	124.51
29	9	302	CHL	CHB-C4A-NA	2.46	127.91	124.51
29	8	307	CHL	C5-C3-C4	2.46	120.03	114.60
22	B	829	CLA	C1B-CHB-C4A	-2.46	125.25	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	306	CLA	CHB-C4A-NA	2.46	127.91	124.51
24	5	318	LHG	C11-C10-C9	-2.46	101.96	114.42
22	B	812	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
22	B	805	CLA	O2A-CGA-O1A	-2.46	117.40	123.59
22	0	303	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
22	A	833	CLA	CMB-C2B-C3B	2.45	129.26	124.68
22	5	309	CLA	C1-C2-C3	-2.45	121.80	126.04
25	7	323	8CT	C40-C12-C13	-2.45	119.49	122.92
24	1	317	LHG	C11-C10-C9	-2.45	101.98	114.42
22	0	312	CLA	O2D-CGD-CBD	2.45	115.62	111.27
22	2	311	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
29	6	307	CHL	CMD-C2D-C3D	-2.45	121.98	127.61
22	9	304	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
22	A	813	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
22	L	203	CLA	CHD-C1D-ND	-2.45	122.20	124.45
29	6	308	CHL	C2A-C1A-CHA	-2.45	119.58	123.86
22	1	307	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
30	7	320	XAT	C35-C15-C14	-2.45	118.46	123.47
22	K	104	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
22	5	310	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	5	308	CLA	C2A-C1A-CHA	2.45	128.13	123.86
22	7	310	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
22	B	819	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
22	B	838	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
25	7	323	8CT	C22-C21-C20	-2.44	119.50	122.92
22	6	310	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
22	8	315	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	4	314	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
30	0	313	XAT	C5-C4-C3	2.44	117.58	112.75
22	L	201	CLA	CHB-C4A-NA	2.44	127.89	124.51
29	2	306	CHL	C1B-CHB-C4A	-2.44	125.28	130.12
29	8	314	CHL	C1D-ND-C4D	-2.44	104.60	106.33
22	7	314	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	7	305	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
30	4	315	XAT	C18-C5-C4	2.44	117.02	114.28
22	A	811	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
22	1	310	CLA	CHB-C4A-NA	2.44	127.88	124.51
29	2	307	CHL	CMB-C2B-C3B	2.44	129.24	124.68
22	G	103	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
30	9	315	XAT	O24-C25-C38	2.44	117.98	115.06
22	0	305	CLA	CBA-CAA-C2A	-2.44	106.67	113.86
22	A	804	CLA	C1-C2-C3	-2.44	121.83	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	316	LHG	O8-C23-C24	2.43	119.55	111.91
22	A	839	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	8	315	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
22	2	302	CLA	O2D-CGD-CBD	2.43	115.59	111.27
22	B	808	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
29	9	307	CHL	O1D-CGD-CBD	-2.43	119.50	124.48
25	5	317	8CT	C40-C12-C13	-2.43	119.51	122.92
22	B	837	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
25	4	317	8CT	C40-C12-C13	-2.43	119.52	122.92
25	A	849	8CT	C11-C10-C03	-2.43	120.37	127.20
25	B	846	8CT	C11-C12-C13	2.43	122.67	118.94
22	6	310	CLA	C1-C2-C3	-2.43	121.84	126.04
29	3	306	CHL	C1B-CHB-C4A	-2.43	125.30	130.12
22	2	304	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	1	308	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
22	G	101	CLA	CHD-C1D-ND	-2.43	122.22	124.45
25	A	848	8CT	C24-C25-C26	-2.43	123.84	127.31
22	6	312	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	B	835	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	5	303	CLA	CHD-C1D-ND	-2.43	122.22	124.45
22	A	824	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	G	103	CLA	CHB-C4A-NA	2.43	127.87	124.51
30	8	317	XAT	C30-C31-C32	-2.43	115.65	123.22
22	8	313	CLA	O2D-CGD-O1D	-2.43	119.10	123.84
22	6	305	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
22	4	302	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
29	1	305	CHL	CED-O2D-CGD	2.42	121.42	115.94
22	5	314	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	2	310	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	A	808	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	J	101	8CT	C05-C04-C03	2.42	114.21	110.48
29	1	305	CHL	C4A-NA-C1A	2.42	107.80	106.71
22	B	821	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	1	312	CLA	CHB-C4A-NA	2.42	127.86	124.51
29	5	301	CHL	O2D-CGD-O1D	-2.42	119.11	123.84
22	9	303	CLA	O2D-CGD-CBD	2.42	115.57	111.27
24	9	316	LHG	C5-O7-C7	-2.42	111.84	117.79
31	4	318	LMG	O1-C1-C2	-2.42	104.53	108.30
22	2	302	CLA	CAC-C3C-C4C	2.42	127.95	124.81
25	J	104	8CT	C14-C13-C12	-2.42	123.86	127.31
22	8	302	CLA	C2D-C1D-ND	-2.42	108.32	110.10
22	2	309	CLA	CHB-C4A-NA	2.42	127.85	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	314	XAT	C4-C3-C2	-2.42	106.11	110.77
22	B	806	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
22	8	304	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	B	833	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
22	A	825	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
22	6	310	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	K	103	8CT	C11-C10-C03	-2.41	120.44	127.20
25	B	844	8CT	C28-C26-C25	2.41	122.64	118.94
22	5	304	CLA	CHD-C1D-ND	-2.41	122.24	124.45
22	7	303	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
30	1	314	XAT	C19-C9-C10	-2.41	119.55	122.92
25	2	317	8CT	C39-C16-C17	-2.41	119.55	122.92
22	4	308	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
25	I	101	8CT	C24-C23-C21	-2.41	119.66	126.42
22	2	312	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	A	803	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
25	K	103	8CT	C22-C21-C20	-2.41	119.55	122.92
25	L	205	8CT	C27-C26-C25	-2.41	119.55	122.92
22	6	304	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
22	A	835	CLA	CHB-C4A-NA	2.40	127.84	124.51
22	3	301	CLA	CHB-C4A-NA	2.40	127.84	124.51
22	A	816	CLA	CMB-C2B-C3B	2.40	129.17	124.68
22	2	310	CLA	CMA-C3A-C2A	-2.40	110.49	116.10
29	2	306	CHL	O1D-CGD-CBD	-2.40	119.57	124.48
30	1	315	XAT	C39-C29-C28	2.40	121.86	118.08
22	6	317	CLA	CHB-C4A-NA	2.40	127.83	124.51
29	5	306	CHL	OMC-CMC-C2C	-2.40	120.26	125.69
22	1	310	CLA	CMB-C2B-C3B	2.40	129.17	124.68
22	A	836	CLA	C1-C2-C3	-2.40	121.89	126.04
22	B	829	CLA	C2D-C1D-ND	-2.40	108.34	110.10
29	4	306	CHL	CMB-C2B-C3B	2.40	129.17	124.68
22	0	303	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	K	102	CLA	O2D-CGD-CBD	2.40	115.53	111.27
22	B	809	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
22	8	302	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
22	B	830	CLA	CHB-C4A-NA	2.39	127.82	124.51
22	1	311	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	1	317	LHG	C20-C19-C18	-2.39	102.28	114.42
22	5	307	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
28	B	849	DGD	O3E-C3E-C2E	-2.39	104.82	110.35
22	6	313	CLA	CHB-C4A-NA	2.39	127.82	124.51
30	2	316	XAT	C28-C29-C30	-2.39	115.27	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	309	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
22	L	203	CLA	CHB-C4A-NA	2.39	127.81	124.51
22	2	308	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	8	304	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	A	814	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	A	819	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	9	310	CLA	CHB-C4A-NA	2.38	127.81	124.51
29	6	307	CHL	O1D-CGD-CBD	-2.38	119.61	124.48
22	B	837	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
24	A	844	LHG	C18-C17-C16	-2.38	102.33	114.42
22	B	836	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
22	5	308	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
25	B	804	8CT	C11-C10-C03	-2.38	120.52	127.20
22	4	304	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
22	4	310	CLA	CAA-CBA-CGA	-2.38	106.30	113.25
31	4	318	LMG	C6-C5-C4	-2.38	107.44	113.00
22	A	801	CLA	C1D-ND-C4D	-2.38	104.65	106.33
30	1	314	XAT	C16-C1-C6	2.38	116.46	110.05
29	7	308	CHL	O2A-CGA-CBA	2.38	121.63	112.23
22	8	315	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
29	2	305	CHL	CMB-C2B-C3B	2.38	129.12	124.68
24	A	844	LHG	C20-C19-C18	-2.38	102.37	114.42
22	A	817	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
22	1	311	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
25	G	104	8CT	C14-C15-C16	-2.37	119.75	126.42
22	A	836	CLA	CHD-C1D-ND	-2.37	122.27	124.45
22	B	811	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
22	3	309	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	5	302	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
22	B	839	CLA	CHB-C4A-NA	2.37	127.79	124.51
29	6	316	CHL	O1D-CGD-CBD	-2.37	119.63	124.48
22	B	850	CLA	O2D-CGD-CBD	2.37	115.48	111.27
29	4	306	CHL	O2A-CGA-CBA	2.37	119.34	111.91
30	8	317	XAT	C39-C29-C28	2.37	121.81	118.08
29	8	305	CHL	C2A-C1A-CHA	-2.37	119.72	123.86
22	A	803	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
25	1	316	8CT	C24-C23-C21	-2.37	119.77	126.42
30	7	320	XAT	C35-C34-C33	-2.37	123.93	127.31
22	6	311	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
29	7	308	CHL	C1C-C2C-C3C	-2.37	105.24	107.11
22	5	309	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
22	A	813	CLA	O1D-CGD-CBD	2.36	129.32	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	0	311	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	L	205	8CT	C05-C04-C03	2.36	114.12	110.48
29	6	307	CHL	CMB-C2B-C3B	2.36	129.10	124.68
22	K	104	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	1	304	CLA	C2D-C1D-ND	-2.36	108.36	110.10
30	3	314	XAT	O4-C5-C6	-2.36	57.00	58.96
22	B	808	CLA	CHB-C4A-NA	2.36	127.78	124.51
30	7	320	XAT	C5-C4-C3	-2.36	108.08	112.75
22	A	837	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
29	4	306	CHL	OMC-CMC-C2C	-2.36	120.35	125.69
22	5	311	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
22	0	307	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
25	A	854	8CT	C39-C16-C17	-2.36	119.62	122.92
30	4	316	XAT	C18-C5-C4	2.36	116.93	114.28
25	A	849	8CT	C24-C23-C21	-2.36	119.80	126.42
29	6	308	CHL	CHB-C4A-NA	2.36	127.77	124.51
22	B	833	CLA	CMB-C2B-C3B	2.35	129.08	124.68
22	3	305	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
22	9	312	CLA	O2D-CGD-CBD	2.35	115.45	111.27
22	7	309	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	B	833	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
22	3	302	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	A	806	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
22	A	813	CLA	CHD-C1D-ND	-2.35	122.29	124.45
30	7	320	XAT	C19-C9-C8	2.35	121.78	118.08
22	0	305	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
22	2	319	CLA	O2D-CGD-CBD	2.35	115.44	111.27
25	3	316	8CT	C22-C21-C20	-2.35	119.63	122.92
22	A	805	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	A	806	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	6	304	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
29	2	301	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
22	A	834	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	2	310	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	9	312	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
22	4	304	CLA	CAA-CBA-CGA	-2.35	106.40	113.25
22	B	820	CLA	CMB-C2B-C3B	2.34	129.06	124.68
22	3	310	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
30	4	316	XAT	C30-C31-C32	-2.34	115.91	123.22
22	B	839	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
29	2	307	CHL	CAA-CBA-CGA	-2.34	106.41	113.25
22	9	305	CLA	C1B-CHB-C4A	-2.34	125.48	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	0	309	CLA	CHB-C4A-NA	2.34	127.75	124.51
29	9	302	CHL	C4-C3-C5	2.34	119.21	115.27
22	A	807	CLA	CHD-C1D-ND	-2.34	122.31	124.45
22	8	310	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
25	B	847	8CT	C24-C25-C26	-2.34	123.97	127.31
22	7	307	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
25	B	843	8CT	C30-C31-C32	-2.34	118.59	121.47
22	0	308	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
22	K	102	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
31	4	318	LMG	O3-C3-C2	-2.33	104.95	110.35
22	A	831	CLA	CHB-C4A-NA	2.33	127.74	124.51
22	8	313	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
25	4	317	8CT	C25-C24-C23	-2.33	115.94	123.22
25	K	103	8CT	C40-C12-C13	-2.33	119.66	122.92
30	9	314	XAT	C5-C4-C3	2.33	117.36	112.75
22	9	301	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	6	309	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	A	826	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	2	302	CLA	CHD-C1D-ND	-2.33	122.31	124.45
30	3	314	XAT	C24-C23-C22	-2.33	106.28	110.77
22	3	304	CLA	C2D-C1D-ND	-2.33	108.39	110.10
22	7	314	CLA	O2D-CGD-CBD	2.33	115.40	111.27
22	3	305	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	7	317	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
22	1	308	CLA	CHB-C4A-NA	2.33	127.73	124.51
29	9	307	CHL	O2D-CGD-O1D	-2.32	119.29	123.84
22	7	316	CLA	CHB-C4A-NA	2.32	127.73	124.51
22	7	309	CLA	CMB-C2B-C3B	2.32	129.03	124.68
22	3	308	CLA	C1-C2-C3	-2.32	122.99	126.75
23	A	842	PQN	C2M-C2-C3	-2.32	120.61	124.40
22	5	305	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
22	A	827	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	6	301	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
22	A	825	CLA	CHB-C4A-NA	2.32	127.72	124.51
25	B	843	8CT	C40-C12-C13	-2.32	119.67	122.92
22	B	807	CLA	CMA-C3A-C4A	-2.32	105.53	111.77
25	I	101	8CT	C14-C15-C16	-2.32	119.90	126.42
22	6	313	CLA	CMD-C2D-C1D	-2.32	120.62	124.71
22	8	311	CLA	CHB-C4A-NA	2.32	127.72	124.51
29	2	306	CHL	CMB-C2B-C3B	2.32	129.02	124.68
29	8	305	CHL	O1D-CGD-CBD	-2.32	119.74	124.48
22	3	302	CLA	CHB-C4A-NA	2.32	127.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	307	CLA	CHD-C1D-ND	-2.32	122.32	124.45
22	8	309	CLA	CHD-C1D-ND	-2.32	122.32	124.45
29	0	301	CHL	C1C-C2C-C3C	-2.32	105.28	107.11
22	B	833	CLA	C1-C2-C3	-2.32	122.03	126.04
30	7	319	XAT	C5-C4-C3	-2.32	108.17	112.75
22	B	814	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
22	B	831	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	1	313	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	B	829	CLA	CMC-C2C-C1C	-2.32	121.51	125.04
25	I	101	8CT	C11-C10-C03	-2.31	120.70	127.20
29	8	306	CHL	C5-C3-C4	2.31	119.71	114.60
30	2	315	XAT	C28-C29-C30	-2.31	115.39	118.94
29	3	306	CHL	O2A-CGA-CBA	2.31	121.37	112.23
22	A	836	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
22	A	826	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
22	B	831	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
22	1	301	CLA	C1-C2-C3	-2.31	122.05	126.04
30	8	317	XAT	C40-C33-C34	-2.31	119.69	122.92
30	9	314	XAT	C31-C32-C33	2.31	132.91	126.42
29	4	306	CHL	CHD-C1D-C2D	2.31	130.32	125.48
24	1	317	LHG	C27-C26-C25	-2.31	102.70	114.42
29	0	306	CHL	OMC-CMC-C2C	-2.31	120.47	125.69
22	M	101	CLA	CAA-C2A-C1A	-2.31	104.41	111.97
22	B	818	CLA	C1-C2-C3	-2.31	122.05	126.04
22	3	309	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	A	809	CLA	C2D-C1D-ND	-2.31	108.40	110.10
30	8	316	XAT	C35-C15-C14	2.31	128.20	123.47
23	A	842	PQN	C21-C22-C23	-2.31	108.46	115.92
22	A	807	CLA	O2D-CGD-CBD	2.31	115.37	111.27
25	F	302	8CT	C10-C03-C02	-2.31	115.87	121.46
25	7	321	8CT	C19-C18-C17	2.31	128.20	123.47
22	3	301	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
22	5	309	CLA	CHB-C4A-NA	2.30	127.70	124.51
29	6	302	CHL	OMC-CMC-C2C	-2.30	120.48	125.69
25	G	104	8CT	C39-C16-C17	-2.30	119.69	122.92
29	3	306	CHL	C2A-C1A-CHA	-2.30	119.83	123.86
29	3	306	CHL	OBD-CAD-C3D	-2.30	122.98	128.52
22	3	304	CLA	CHB-C4A-NA	2.30	127.70	124.51
22	A	825	CLA	O2D-CGD-CBD	2.30	115.36	111.27
29	8	306	CHL	O1D-CGD-CBD	-2.30	119.77	124.48
22	9	304	CLA	CHB-C4A-NA	2.30	127.69	124.51
30	0	313	XAT	C8-C9-C10	2.30	122.47	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	841	CLA	C16-C15-C13	-2.30	108.48	115.92
25	7	321	8CT	C40-C12-C11	2.30	121.70	118.08
22	7	304	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	B	821	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	8	301	8CT	C11-C10-C03	-2.30	120.75	127.20
22	L	202	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
22	1	301	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	B	840	CLA	CMB-C2B-C3B	2.30	128.98	124.68
22	A	853	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
22	K	101	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	9	312	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	5	318	LHG	C20-C19-C18	-2.30	102.77	114.42
22	B	817	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
29	4	305	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
22	7	309	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	8	303	CLA	CHB-C4A-NA	2.30	127.69	124.51
30	1	315	XAT	C24-C23-C22	-2.30	106.34	110.77
22	5	305	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	B	823	CLA	C2D-C1D-ND	-2.29	108.41	110.10
25	A	847	8CT	C38-C31-C32	-2.29	114.17	122.33
31	4	318	LMG	O6-C1-O1	-2.29	104.54	109.97
22	2	308	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
22	8	303	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
29	4	307	CHL	CMB-C2B-C3B	2.29	128.97	124.68
22	B	814	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
30	3	315	XAT	C25-C24-C23	-2.29	108.22	112.75
22	7	305	CLA	CHB-C4A-NA	2.29	127.68	124.51
25	2	317	8CT	C40-C12-C13	-2.29	119.71	122.92
30	4	315	XAT	C38-C25-C24	2.29	116.86	114.28
22	A	837	CLA	CHB-C4A-NA	2.29	127.68	124.51
29	3	306	CHL	CHB-C4A-NA	2.29	127.68	124.51
25	B	851	8CT	C40-C12-C13	-2.29	119.72	122.92
25	I	101	8CT	C04-C03-C02	-2.29	119.39	122.61
22	2	314	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
22	6	303	CLA	O1D-CGD-CBD	2.29	129.17	124.48
29	9	302	CHL	OMC-CMC-C2C	-2.29	120.51	125.69
22	B	850	CLA	C1-C2-C3	-2.29	122.09	126.04
30	3	314	XAT	C35-C15-C14	2.29	128.16	123.47
22	6	323	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
29	8	307	CHL	O2D-CGD-O1D	-2.29	119.37	123.84
22	B	817	CLA	C1-C2-C3	-2.29	122.09	126.04
22	L	204	CLA	C1B-CHB-C4A	-2.29	125.59	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	809	CLA	C1-C2-C3	-2.28	122.09	126.04
22	3	319	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
22	4	309	CLA	C2D-C1D-ND	-2.28	108.42	110.10
22	A	822	CLA	CMB-C2B-C3B	2.28	128.95	124.68
22	8	308	CLA	O2D-CGD-CBD	2.28	115.32	111.27
22	A	801	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
22	0	310	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
22	A	801	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	5	308	CLA	C3A-C2A-C1A	2.28	104.75	101.34
22	6	313	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	A	825	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
31	4	318	LMG	C1-C2-C3	-2.27	105.26	110.00
22	6	309	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
22	0	312	CLA	CHD-C1D-ND	-2.27	122.37	124.45
24	0	315	LHG	C20-C19-C18	-2.27	102.90	114.42
30	8	316	XAT	C25-C24-C23	-2.27	108.26	112.75
22	0	311	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
22	3	307	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	1	311	CLA	CHD-C1D-ND	-2.27	122.37	124.45
22	B	840	CLA	C1-C2-C3	-2.27	122.12	126.04
22	B	811	CLA	CHD-C1D-ND	-2.27	122.37	124.45
22	7	317	CLA	CMB-C2B-C3B	2.27	128.92	124.68
22	5	313	CLA	CHD-C1D-ND	-2.27	122.37	124.45
25	8	318	8CT	C19-C18-C17	-2.26	118.84	123.47
22	4	314	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
28	B	849	DGD	O2E-C2E-C1E	-2.26	104.55	110.05
22	B	814	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	A	818	CLA	C2D-C1D-ND	-2.26	108.44	110.10
29	4	301	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
29	8	314	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
25	B	804	8CT	C05-C04-C03	2.26	113.96	110.48
22	A	809	CLA	CMB-C2B-C3B	2.26	128.91	124.68
30	8	317	XAT	C19-C9-C8	2.26	121.64	118.08
29	6	308	CHL	C5-C3-C4	2.26	119.60	114.60
22	B	810	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
22	A	840	CLA	C11-C12-C13	-2.26	108.61	115.92
25	L	205	8CT	C04-C03-C02	-2.26	119.43	122.61
29	0	306	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
30	0	314	XAT	C32-C33-C34	2.26	122.41	118.94
29	6	302	CHL	O2A-CGA-O1A	-2.26	117.89	123.59
29	9	302	CHL	O1D-CGD-CBD	-2.26	119.87	124.48
22	B	810	CLA	CHD-C1D-ND	-2.26	122.38	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	316	LHG	C20-C19-C18	-2.26	102.97	114.42
22	5	302	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
25	A	850	8CT	C11-C10-C03	-2.26	120.87	127.20
25	B	847	8CT	C40-C12-C13	-2.26	119.76	122.92
22	A	838	CLA	CAA-CBA-CGA	-2.26	106.66	113.25
30	4	316	XAT	C20-C13-C12	2.26	121.63	118.08
24	5	318	LHG	C27-C26-C25	-2.25	102.98	114.42
22	B	818	CLA	CHC-C1C-NC	2.25	127.62	124.20
22	A	813	CLA	CHB-C4A-NA	2.25	127.63	124.51
22	0	302	CLA	O1D-CGD-CBD	2.25	129.10	124.48
29	2	306	CHL	CAA-C2A-C3A	-2.25	106.61	112.78
22	0	305	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
25	B	844	8CT	C19-C20-C21	-2.25	124.09	127.31
22	G	101	CLA	O2A-CGA-O1A	-2.25	117.69	123.30
22	8	304	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
22	4	314	CLA	O2D-CGD-CBD	2.25	115.27	111.27
22	B	823	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	A	818	CLA	CHD-C1D-ND	-2.25	122.39	124.45
22	A	836	CLA	CAC-C3C-C4C	2.25	127.73	124.81
22	1	302	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
22	B	808	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
29	8	307	CHL	O1D-CGD-CBD	-2.25	119.89	124.48
22	A	822	CLA	CHD-C1D-ND	-2.25	122.39	124.45
29	2	305	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
22	A	816	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
29	6	308	CHL	OMC-CMC-C2C	-2.25	120.61	125.69
22	B	825	CLA	C2D-C1D-ND	-2.25	108.45	110.10
22	7	312	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
22	7	306	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
22	B	835	CLA	CHD-C1D-ND	-2.24	122.39	124.45
22	A	811	CLA	CHB-C4A-NA	2.24	127.62	124.51
29	8	314	CHL	OMC-CMC-C2C	-2.24	120.61	125.69
29	4	307	CHL	C1C-C2C-C3C	-2.24	105.33	107.11
30	9	314	XAT	C30-C31-C32	2.24	130.22	123.22
22	A	841	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
29	2	305	CHL	CGD-CBD-CAD	-2.24	103.47	110.73
22	6	311	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
25	7	301	8CT	C06-C07-C02	-2.24	110.08	114.08
22	6	317	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
22	6	323	CLA	CHB-C4A-NA	2.24	127.61	124.51
29	5	301	CHL	OMC-CMC-C2C	-2.24	120.63	125.69
22	5	312	CLA	C1-C2-C3	-2.24	122.17	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	9	315	XAT	C20-C13-C12	2.24	121.60	118.08
22	3	308	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
22	A	803	CLA	O2D-CGD-CBD	2.24	115.24	111.27
22	0	305	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	8	303	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
22	A	804	CLA	O2D-CGD-CBD	2.24	115.24	111.27
22	A	815	CLA	CAA-CBA-CGA	-2.24	106.72	113.25
22	B	826	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
30	9	314	XAT	C35-C34-C33	-2.24	124.12	127.31
25	A	849	8CT	C27-C26-C25	-2.24	119.79	122.92
30	9	315	XAT	C19-C9-C8	2.23	121.60	118.08
29	0	306	CHL	O2D-CGD-O1D	-2.23	119.47	123.84
30	4	315	XAT	C11-C12-C13	2.23	132.69	126.42
22	0	302	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
22	A	822	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
25	L	205	8CT	C39-C16-C17	-2.23	119.80	122.92
22	7	315	CLA	CHD-C1D-ND	-2.23	122.40	124.45
25	F	302	8CT	C35-C30-C29	-2.23	109.88	112.70
22	B	815	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
30	5	316	XAT	C11-C10-C9	-2.23	124.13	127.31
22	A	829	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
22	A	822	CLA	C3A-C2A-C1A	2.23	104.68	101.34
22	B	803	CLA	CHB-C4A-NA	2.23	127.59	124.51
24	1	317	LHG	C18-C17-C16	-2.23	103.12	114.42
22	2	313	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
30	6	319	XAT	C27-C28-C29	-2.22	122.08	125.53
22	B	836	CLA	CBA-CAA-C2A	-2.22	107.30	113.86
22	6	315	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
29	6	308	CHL	CBC-CAC-C3C	-2.22	106.31	112.43
22	7	318	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
22	A	839	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
29	4	307	CHL	C5-C3-C4	2.22	119.51	114.60
30	4	316	XAT	C19-C9-C8	2.22	121.58	118.08
22	0	302	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
22	3	319	CLA	C1-C2-C3	2.22	129.88	126.04
22	1	310	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	A	823	CLA	C2D-C1D-ND	-2.22	108.47	110.10
22	0	307	CLA	CMC-C2C-C1C	-2.22	121.66	125.04
22	6	301	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
29	6	302	CHL	CAA-CBA-CGA	-2.22	106.78	113.25
28	B	849	DGD	CBB-CAB-C9B	-2.21	103.18	114.42
22	B	827	CLA	O2A-CGA-O1A	-2.21	118.00	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	311	CLA	CAA-C2A-C3A	-2.21	110.93	116.10
22	B	826	CLA	O2D-CGD-CBD	2.21	115.20	111.27
25	A	848	8CT	C14-C15-C16	-2.21	120.20	126.42
22	A	828	CLA	CAA-CBA-CGA	-2.21	106.79	113.25
22	B	837	CLA	CHD-C1D-ND	-2.21	122.42	124.45
29	4	301	CHL	CGD-CBD-CAD	-2.21	103.57	110.73
29	6	308	CHL	CAA-CBA-CGA	-2.21	106.79	113.25
22	B	803	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
22	9	305	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
22	A	839	CLA	CAC-C3C-C4C	-2.21	121.94	124.81
22	K	101	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
22	A	823	CLA	C1-C2-C3	-2.21	122.22	126.04
22	A	813	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
29	6	306	CHL	O1D-CGD-CBD	-2.21	119.97	124.48
22	2	319	CLA	CHB-C4A-NA	2.21	127.56	124.51
25	A	854	8CT	C24-C23-C21	-2.21	120.22	126.42
22	5	302	CLA	CHB-C4A-NA	2.20	127.56	124.51
29	8	307	CHL	C1B-CHB-C4A	-2.20	125.75	130.12
22	B	837	CLA	C1-C2-C3	-2.20	122.23	126.04
29	0	306	CHL	CHD-C4C-C3C	-2.20	121.60	124.84
22	B	801	CLA	O2D-CGD-CBD	2.20	115.18	111.27
30	5	316	XAT	O24-C25-C38	2.20	117.69	115.06
22	B	828	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
22	7	302	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
29	7	308	CHL	CAC-C3C-C4C	2.20	127.67	124.81
22	9	305	CLA	CHD-C1D-ND	-2.20	122.43	124.45
22	A	819	CLA	CAA-CBA-CGA	-2.20	106.83	113.25
25	B	848	8CT	C22-C21-C23	2.20	121.54	118.08
22	9	311	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
22	7	317	CLA	C2A-C1A-CHA	2.20	127.70	123.86
29	8	307	CHL	OMC-CMC-C2C	-2.20	120.72	125.69
25	7	301	8CT	C40-C12-C13	-2.20	119.84	122.92
22	9	309	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
30	6	320	XAT	C38-C25-C24	2.20	116.75	114.28
22	A	812	CLA	C1-C2-C3	-2.20	122.24	126.04
22	7	313	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
22	A	814	CLA	O2A-CGA-O1A	-2.20	117.83	123.30
29	4	301	CHL	C2A-C1A-CHA	-2.20	120.02	123.86
22	7	303	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
30	4	316	XAT	O24-C25-C26	-2.19	57.14	58.96
30	2	315	XAT	C19-C9-C8	2.19	121.53	118.08
22	4	308	CLA	C2D-C1D-ND	-2.19	108.49	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	847	8CT	C27-C26-C28	2.19	121.53	118.08
22	A	826	CLA	C1-C2-C3	-2.19	122.25	126.04
30	7	320	XAT	C38-C25-C24	2.19	116.74	114.28
22	A	802	CLA	CHB-C4A-NA	2.19	127.54	124.51
22	6	315	CLA	CHB-C4A-NA	2.19	127.54	124.51
22	A	839	CLA	CBC-CAC-C3C	2.19	118.46	112.43
25	3	318	8CT	C01-C02-C07	2.19	117.82	113.62
22	6	313	CLA	CMD-C2D-C3D	2.19	132.64	127.61
25	B	847	8CT	C39-C16-C17	-2.19	119.86	122.92
22	1	303	CLA	C1-C2-C3	-2.19	122.26	126.04
22	A	843	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
22	B	834	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
30	2	315	XAT	O24-C25-C26	-2.18	57.15	58.96
25	L	205	8CT	C24-C25-C26	-2.18	124.20	127.31
30	3	314	XAT	C20-C13-C14	-2.18	119.87	122.92
22	A	821	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
22	A	801	CLA	O1D-CGD-CBD	2.18	128.94	124.48
22	A	801	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
22	L	202	CLA	C1-C2-C3	-2.18	122.28	126.04
30	6	320	XAT	C12-C13-C14	2.18	122.28	118.94
29	6	302	CHL	CMB-C2B-C3B	2.18	128.75	124.68
31	8	319	LMG	C3-C4-C5	-2.18	106.35	110.24
30	4	316	XAT	O4-C5-C6	-2.18	57.16	58.96
30	6	319	XAT	O4-C5-C6	-2.18	57.16	58.96
25	7	321	8CT	C14-C13-C12	-2.18	124.20	127.31
22	A	814	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
22	B	832	CLA	CHD-C1D-ND	-2.18	122.45	124.45
25	A	847	8CT	C35-C30-C31	2.18	115.32	111.42
22	B	828	CLA	CHB-C4A-NA	2.18	127.52	124.51
22	9	301	CLA	CHB-C4A-NA	2.18	127.52	124.51
22	9	305	CLA	CGD-CBD-CAD	-2.18	103.69	110.73
22	A	817	CLA	O2D-CGD-CBD	2.18	115.13	111.27
22	9	301	CLA	CHD-C1D-ND	-2.18	122.45	124.45
25	G	104	8CT	C22-C21-C20	-2.17	119.88	122.92
22	G	102	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	A	830	CLA	CHB-C4A-NA	2.17	127.52	124.51
24	9	316	LHG	C27-C26-C25	-2.17	103.39	114.42
22	7	318	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
22	7	312	CLA	CHB-C4A-NA	2.17	127.52	124.51
22	3	308	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	B	805	CLA	C16-C15-C13	-2.17	108.90	115.92
22	6	304	CLA	O2A-CGA-O1A	-2.17	118.11	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	0	301	CHL	C4D-CHA-C1A	-2.17	118.61	121.25
25	A	854	8CT	C40-C12-C13	-2.17	119.88	122.92
22	B	841	CLA	O1D-CGD-CBD	2.17	128.92	124.48
22	A	833	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
22	A	806	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
22	B	828	CLA	O2D-CGD-CBD	2.17	115.12	111.27
22	B	816	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	4	311	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
29	4	305	CHL	C1D-ND-C4D	-2.17	104.80	106.33
22	0	309	CLA	CAA-C2A-C3A	-2.16	111.05	116.10
25	1	316	8CT	C19-C18-C17	-2.16	119.04	123.47
22	7	313	CLA	CHD-C1D-ND	-2.16	122.47	124.45
22	6	318	CLA	C1-C2-C3	-2.16	122.30	126.04
22	3	308	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
22	A	838	CLA	C1-C2-C3	-2.16	122.30	126.04
29	2	301	CHL	C6-C5-C3	-2.16	107.78	113.45
22	B	834	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	B	841	CLA	C2D-C1D-ND	-2.16	108.51	110.10
22	B	812	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	1	303	CLA	C6-C5-C3	-2.16	111.08	114.62
30	7	319	XAT	C35-C15-C14	-2.16	119.05	123.47
22	A	805	CLA	CHD-C1D-ND	-2.16	122.47	124.45
29	6	302	CHL	C4-C3-C2	-2.16	118.14	123.68
22	2	312	CLA	C1-C2-C3	-2.16	122.31	126.04
29	2	301	CHL	C2A-C1A-CHA	-2.16	120.08	123.86
22	A	828	CLA	C16-C15-C13	-2.16	108.94	115.92
29	4	306	CHL	C5-C3-C4	2.16	119.37	114.60
22	5	302	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	7	306	CLA	CHB-C4A-NA	2.16	127.50	124.51
28	B	849	DGD	CFB-CEB-CDB	-2.16	103.47	114.42
29	2	307	CHL	O2D-CGD-O1D	-2.16	119.62	123.84
29	8	314	CHL	C4D-CHA-C1A	-2.16	118.62	121.25
22	A	825	CLA	CMB-C2B-C3B	2.16	128.72	124.68
22	5	303	CLA	CMB-C2B-C3B	2.16	128.71	124.68
29	2	307	CHL	C5-C3-C4	2.16	119.37	114.60
22	2	304	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
25	5	317	8CT	C11-C10-C03	-2.16	121.14	127.20
24	A	844	LHG	C27-C26-C25	-2.16	103.48	114.42
22	2	302	CLA	CHB-C4A-NA	2.16	127.49	124.51
25	K	103	8CT	C34-C33-C32	-2.16	108.42	112.00
30	8	317	XAT	C5-C4-C3	-2.16	108.48	112.75
22	A	837	CLA	O1D-CGD-CBD	2.16	128.90	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	105	CLA	CMA-C3A-C4A	-2.16	105.98	111.77
22	4	303	CLA	C2D-C1D-ND	-2.15	108.52	110.10
25	B	845	8CT	C08-C04-C03	-2.15	106.80	110.30
22	4	312	CLA	O1D-CGD-CBD	2.15	128.89	124.48
22	L	202	CLA	O2D-CGD-CBD	2.15	115.09	111.27
22	8	313	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
25	B	848	8CT	C39-C16-C15	2.15	121.47	118.08
22	B	808	CLA	C11-C10-C8	-2.15	108.97	115.92
25	B	843	8CT	C39-C16-C17	-2.15	119.91	122.92
25	3	318	8CT	C35-C30-C31	2.15	115.27	111.42
22	A	806	CLA	C2D-C1D-ND	-2.15	108.52	110.10
24	5	318	LHG	C18-C17-C16	-2.15	103.51	114.42
22	B	824	CLA	CHB-C4A-NA	2.15	127.48	124.51
22	A	843	CLA	C2D-C1D-ND	-2.15	108.52	110.10
25	3	318	8CT	C40-C12-C13	-2.15	119.92	122.92
30	3	315	XAT	C10-C11-C12	-2.15	116.52	123.22
22	9	310	CLA	CAA-C2A-C3A	-2.15	111.09	116.10
22	L	204	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
30	8	316	XAT	C36-C21-C26	-2.15	104.25	110.05
28	B	849	DGD	CAB-C9B-C8B	-2.15	103.53	114.42
29	5	301	CHL	CAA-CBA-CGA	-2.15	106.98	113.25
22	B	815	CLA	C1B-CHB-C4A	-2.15	125.87	130.12
22	B	819	CLA	CHD-C1D-ND	-2.14	122.48	124.45
22	B	838	CLA	CHD-C1D-ND	-2.14	122.48	124.45
30	8	316	XAT	O24-C25-C26	-2.14	57.18	58.96
29	2	301	CHL	C4A-NA-C1A	2.14	107.67	106.71
30	8	317	XAT	C28-C29-C30	-2.14	115.66	118.94
22	B	832	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
29	4	305	CHL	C1-C2-C3	-2.14	122.34	126.04
25	A	849	8CT	C22-C21-C20	-2.14	119.92	122.92
22	2	314	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
22	7	311	CLA	C2D-C1D-ND	-2.14	108.53	110.10
22	A	836	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
25	B	804	8CT	C27-C26-C25	-2.14	119.93	122.92
22	B	824	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
22	A	805	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
25	8	301	8CT	C40-C12-C13	-2.13	119.94	122.92
22	1	309	CLA	CMA-C3A-C2A	-2.13	111.12	116.10
29	2	306	CHL	CED-O2D-CGD	2.13	120.76	115.94
22	K	101	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	1	316	8CT	C22-C21-C20	-2.13	119.94	122.92
29	8	305	CHL	CHB-C4A-NA	2.13	127.46	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	8	314	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
25	3	316	8CT	C27-C26-C25	-2.13	119.94	122.92
29	9	307	CHL	C2A-C1A-CHA	-2.13	120.14	123.86
22	L	201	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
30	4	315	XAT	C37-C21-C36	2.13	110.51	107.37
24	0	315	LHG	C27-C26-C25	-2.13	103.63	114.42
22	1	310	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
30	2	315	XAT	C7-C8-C9	-2.13	122.23	125.53
22	B	850	CLA	C4-C3-C5	2.13	118.85	115.27
29	9	307	CHL	OMC-CMC-C2C	-2.13	120.88	125.69
22	B	818	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
22	B	850	CLA	CAC-C3C-C4C	2.12	127.57	124.81
22	6	310	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
22	3	307	CLA	C1-C2-C3	-2.12	123.32	126.75
25	B	804	8CT	C11-C12-C13	2.12	122.20	118.94
22	0	312	CLA	CHB-C4A-NA	2.12	127.45	124.51
22	B	819	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
29	1	305	CHL	C1C-C2C-C3C	-2.12	105.43	107.11
22	1	301	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
29	4	301	CHL	C1C-C2C-C3C	-2.12	105.43	107.11
22	0	307	CLA	C2D-C1D-ND	-2.12	108.54	110.10
25	8	318	8CT	C39-C16-C17	-2.12	119.95	122.92
29	5	301	CHL	C2A-C1A-CHA	-2.12	120.15	123.86
22	3	307	CLA	CMB-C2B-C3B	2.12	128.64	124.68
22	3	310	CLA	C1-C2-C3	-2.12	122.38	126.04
22	1	309	CLA	O2D-CGD-CBD	2.12	115.03	111.27
25	3	316	8CT	C11-C10-C03	-2.12	121.25	127.20
29	0	301	CHL	O2D-CGD-O1D	-2.12	119.70	123.84
22	6	313	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	B	813	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
29	9	307	CHL	C1C-C2C-C3C	-2.12	105.44	107.11
25	A	846	8CT	C14-C13-C12	-2.12	124.29	127.31
29	9	302	CHL	C1B-CHB-C4A	-2.12	125.93	130.12
22	B	850	CLA	CHD-C1D-ND	-2.11	122.51	124.45
25	B	844	8CT	C19-C18-C17	-2.11	119.15	123.47
22	8	303	CLA	O1D-CGD-CBD	2.11	128.81	124.48
29	5	306	CHL	O1D-CGD-CBD	-2.11	120.16	124.48
30	5	315	XAT	C18-C5-C4	2.11	116.65	114.28
22	B	821	CLA	C1-C2-C3	-2.11	123.34	126.75
22	B	821	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
22	G	101	CLA	CHB-C4A-NA	2.11	127.42	124.51
22	A	819	CLA	CHD-C1D-ND	-2.11	122.52	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	0	311	CLA	CHD-C1D-ND	-2.11	122.52	124.45
22	2	302	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
22	1	302	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
22	9	308	CLA	C2D-C1D-ND	-2.10	108.55	110.10
22	4	309	CLA	CHB-C4A-NA	2.10	127.42	124.51
22	7	317	CLA	C1-C2-C3	-2.10	122.41	126.04
22	B	824	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
25	J	104	8CT	C39-C16-C17	-2.10	119.98	122.92
22	7	315	CLA	CHB-C4A-NA	2.10	127.42	124.51
25	J	101	8CT	C22-C21-C20	-2.10	119.98	122.92
25	8	318	8CT	C14-C15-C16	-2.10	120.52	126.42
22	9	303	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
22	1	307	CLA	O2D-CGD-CBD	2.10	114.99	111.27
22	A	812	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
29	3	306	CHL	C1C-C2C-C3C	-2.10	105.45	107.11
30	2	315	XAT	C11-C10-C9	-2.10	124.32	127.31
22	1	302	CLA	C2D-C1D-ND	-2.10	108.56	110.10
22	A	808	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	B	824	CLA	C1-C2-C3	-2.09	122.42	126.04
22	B	819	CLA	C2D-C1D-ND	-2.09	108.56	110.10
22	3	312	CLA	O2D-CGD-CBD	2.09	114.99	111.27
25	A	848	8CT	C25-C24-C23	-2.09	116.69	123.22
22	B	803	CLA	C2D-C1D-ND	-2.09	108.56	110.10
22	2	302	CLA	C11-C10-C8	-2.09	109.16	115.92
25	8	318	8CT	C22-C21-C20	-2.09	119.99	122.92
22	A	834	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	2	311	CLA	C1-C2-C3	-2.09	122.43	126.04
22	5	307	CLA	O1D-CGD-CBD	2.09	128.76	124.48
22	2	304	CLA	CHD-C1D-ND	-2.09	122.53	124.45
31	5	319	LMG	O2-C2-C1	-2.09	104.97	110.05
22	7	303	CLA	CHB-C4A-NA	2.09	127.40	124.51
22	1	311	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
22	A	820	CLA	C2D-C1D-ND	-2.09	108.57	110.10
29	6	302	CHL	O1D-CGD-CBD	-2.08	120.22	124.48
22	A	853	CLA	O2D-CGD-CBD	2.08	114.97	111.27
22	8	308	CLA	C2D-C1D-ND	-2.08	108.57	110.10
22	3	311	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	A	837	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	4	302	CLA	O2D-CGD-CBD	2.08	114.97	111.27
29	6	302	CHL	CMD-C2D-C3D	-2.08	122.83	127.61
25	B	851	8CT	C39-C16-C15	2.08	121.36	118.08
30	2	315	XAT	C31-C30-C29	-2.08	124.34	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	7	319	XAT	C20-C13-C14	-2.08	120.01	122.92
25	A	848	8CT	C10-C11-C12	-2.08	123.09	126.23
29	8	305	CHL	C1C-C2C-C3C	-2.08	105.46	107.11
30	9	314	XAT	O24-C25-C26	-2.08	57.24	58.96
22	A	840	CLA	C11-C10-C8	-2.08	109.20	115.92
22	A	835	CLA	CHD-C1D-ND	-2.08	122.54	124.45
25	7	301	8CT	C28-C26-C25	2.08	122.13	118.94
22	2	314	CLA	O2D-CGD-CBD	2.08	114.96	111.27
22	L	204	CLA	C1-C2-C3	-2.08	123.39	126.75
29	5	306	CHL	C2A-C3A-C4A	-2.08	98.51	101.87
31	4	318	LMG	C4-C3-C2	-2.08	107.20	110.82
29	6	306	CHL	O2D-CGD-O1D	-2.08	119.78	123.84
25	G	104	8CT	C18-C19-C20	-2.08	119.22	123.47
25	2	317	8CT	C11-C10-C03	-2.08	121.37	127.20
22	A	833	CLA	C2D-C1D-ND	-2.07	108.58	110.10
25	L	205	8CT	C07-C02-C03	-2.07	119.72	122.73
22	3	312	CLA	CHD-C1D-ND	-2.07	122.55	124.45
22	A	809	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
22	0	303	CLA	C2D-C1D-ND	-2.07	108.58	110.10
30	7	319	XAT	C40-C33-C34	-2.07	120.02	122.92
22	6	309	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
25	K	103	8CT	C28-C26-C25	2.07	122.12	118.94
22	1	303	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	8	314	CHL	CMB-C2B-C1B	2.07	131.65	128.46
22	B	825	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
22	B	829	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
29	1	305	CHL	C1D-ND-C4D	-2.07	104.87	106.33
29	6	308	CHL	C1B-CHB-C4A	-2.07	126.02	130.12
25	G	104	8CT	C24-C23-C21	-2.07	120.61	126.42
22	6	301	CLA	C1-C2-C3	-2.07	122.47	126.04
25	J	104	8CT	C22-C21-C23	2.07	121.33	118.08
22	9	303	CLA	C1-C2-C3	-2.07	122.47	126.04
22	7	304	CLA	CHD-C1D-ND	-2.07	122.56	124.45
30	9	314	XAT	C40-C33-C34	-2.07	120.03	122.92
22	A	808	CLA	C1B-CHB-C4A	-2.07	126.03	130.12
22	0	302	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	3	319	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
29	4	301	CHL	OMC-CMC-C2C	-2.06	121.02	125.69
30	6	320	XAT	C24-C23-C22	-2.06	106.79	110.77
25	1	316	8CT	C11-C10-C03	-2.06	121.41	127.20
30	7	319	XAT	C31-C32-C33	-2.06	120.63	126.42
22	7	318	CLA	CHA-C1A-NA	-2.06	121.68	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	850	8CT	C39-C16-C15	2.06	121.32	118.08
25	J	101	8CT	C18-C19-C20	-2.06	119.26	123.47
25	7	321	8CT	C18-C19-C20	2.06	127.69	123.47
22	5	311	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
22	A	827	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	5	309	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	6	317	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
22	4	313	CLA	CHD-C1D-ND	-2.06	122.56	124.45
30	2	315	XAT	C40-C33-C32	2.06	121.32	118.08
22	5	303	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
25	J	101	8CT	C35-C30-C29	-2.06	110.10	112.70
22	K	102	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	7	307	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	K	101	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
23	A	842	PQN	C16-C17-C18	-2.05	109.28	115.92
22	H	201	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	9	311	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	B	847	8CT	C18-C19-C20	-2.05	119.27	123.47
29	4	307	CHL	CBC-CAC-C3C	-2.05	106.77	112.43
30	4	315	XAT	O4-C5-C6	-2.05	57.26	58.96
22	B	820	CLA	O2D-CGD-CBD	2.05	114.91	111.27
25	I	101	8CT	C39-C16-C17	-2.05	120.05	122.92
22	A	824	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
22	9	312	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	A	847	8CT	C01-C02-C07	2.05	117.55	113.62
22	A	831	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	3	303	CLA	O1A-CGA-CBA	2.05	129.66	123.08
22	A	817	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	A	853	CLA	CHB-C4A-NA	2.05	127.34	124.51
29	6	302	CHL	C1C-C2C-C3C	-2.05	105.49	107.11
22	B	829	CLA	CHC-C1C-NC	2.05	127.31	124.20
22	1	307	CLA	C2D-C1D-ND	-2.05	108.59	110.10
22	B	829	CLA	CMC-C2C-C3C	2.05	131.67	126.12
22	5	302	CLA	C1-C2-C3	-2.05	122.50	126.04
22	3	312	CLA	O2A-CGA-O1A	-2.04	118.20	123.30
22	6	303	CLA	C7-C6-C5	-2.04	107.81	113.36
22	6	310	CLA	O1D-CGD-CBD	2.04	128.67	124.48
25	A	847	8CT	C14-C15-C16	-2.04	120.68	126.42
25	7	323	8CT	C25-C24-C23	-2.04	116.84	123.22
22	7	306	CLA	CHD-C1D-ND	-2.04	122.58	124.45
28	B	849	DGD	C3D-C4D-C5D	-2.04	106.60	110.24
25	B	851	8CT	C22-C21-C23	2.04	121.29	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	827	CLA	CHD-C1D-ND	-2.04	122.58	124.45
30	2	316	XAT	C10-C11-C12	-2.04	116.85	123.22
25	8	301	8CT	C04-C03-C10	2.04	121.55	115.78
22	4	302	CLA	C6-C5-C3	-2.04	108.11	113.45
31	8	319	LMG	O1-C7-C8	-2.04	105.98	110.90
28	B	849	DGD	O2D-C2D-C1D	-2.04	105.09	110.05
22	G	102	CLA	C1-C2-C3	-2.04	123.45	126.75
29	1	305	CHL	O1D-CGD-CBD	-2.04	120.32	124.48
22	A	805	CLA	CAA-CBA-CGA	-2.04	107.31	113.25
22	0	305	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
22	2	312	CLA	CHD-C1D-ND	-2.03	122.58	124.45
22	A	809	CLA	CHB-C4A-NA	2.03	127.32	124.51
29	6	308	CHL	O2A-CGA-O1A	-2.03	118.46	123.59
22	A	824	CLA	CHD-C1D-ND	-2.03	122.59	124.45
31	5	319	LMG	O3-C3-C2	-2.03	105.65	110.35
22	9	306	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	2	308	CLA	C1-C2-C3	-2.03	123.47	126.75
22	A	821	CLA	C2D-C1D-ND	-2.03	108.61	110.10
25	A	854	8CT	C22-C21-C20	-2.03	120.08	122.92
25	G	104	8CT	C27-C26-C25	-2.03	120.08	122.92
31	5	319	LMG	O7-C10-O9	-2.03	118.79	123.70
31	5	319	LMG	O1-C1-C2	2.03	111.47	108.30
29	4	306	CHL	O1D-CGD-CBD	-2.03	120.33	124.48
29	8	314	CHL	CMA-C3A-C2A	-2.03	105.64	113.83
25	B	845	8CT	C25-C24-C23	2.03	129.55	123.22
22	5	302	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
22	B	834	CLA	CMB-C2B-C3B	2.03	128.47	124.68
22	5	312	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	L	202	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
29	6	302	CHL	O2D-CGD-O1D	-2.03	119.88	123.84
25	A	848	8CT	C18-C19-C20	-2.03	119.33	123.47
30	1	315	XAT	C19-C9-C8	2.03	121.27	118.08
25	8	318	8CT	C40-C12-C13	-2.02	120.09	122.92
22	1	308	CLA	C1-C2-C3	-2.02	122.54	126.04
25	I	101	8CT	C40-C12-C11	2.02	121.27	118.08
22	B	817	CLA	C2D-C1D-ND	-2.02	108.61	110.10
30	9	315	XAT	O4-C5-C6	-2.02	57.28	58.96
25	B	844	8CT	C11-C10-C03	-2.02	121.52	127.20
22	B	808	CLA	C16-C15-C13	-2.02	109.38	115.92
22	8	311	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
22	6	317	CLA	O2D-CGD-CBD	2.02	114.86	111.27
22	3	305	CLA	O2A-CGA-O1A	-2.02	118.49	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	0	301	CHL	OMC-CMC-C2C	-2.02	121.12	125.69
22	B	832	CLA	C3C-C4C-NC	-2.02	108.31	110.57
22	6	313	CLA	C1-C2-C3	-2.02	122.55	126.04
25	A	846	8CT	C04-C03-C10	2.02	121.49	115.78
25	L	206	8CT	C22-C21-C20	-2.02	120.09	122.92
22	3	309	CLA	CMA-C3A-C2A	-2.02	111.39	116.10
22	B	803	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
22	8	312	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	4	304	CLA	C2D-C1D-ND	-2.02	108.62	110.10
29	3	306	CHL	CAA-CBA-CGA	-2.01	107.37	113.25
30	5	315	XAT	C35-C34-C33	-2.01	124.44	127.31
22	B	806	CLA	O1D-CGD-CBD	2.01	128.60	124.48
22	9	309	CLA	CHD-C1D-ND	-2.01	122.60	124.45
22	B	807	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
22	6	304	CLA	CHD-C1D-ND	-2.01	122.61	124.45
25	1	316	8CT	C39-C16-C17	-2.01	120.11	122.92
22	1	311	CLA	C3C-C4C-NC	-2.01	108.32	110.57
25	L	206	8CT	C11-C10-C03	-2.01	121.56	127.20
29	4	305	CHL	O2D-CGD-O1D	-2.01	119.91	123.84
24	1	317	LHG	O8-C23-O10	-2.01	118.52	123.59
25	J	101	8CT	C24-C23-C21	-2.01	120.77	126.42
30	2	316	XAT	C20-C13-C14	-2.01	120.11	122.92
22	B	824	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
30	1	315	XAT	O24-C25-C26	-2.01	57.30	58.96
22	0	309	CLA	CHD-C1D-ND	-2.01	122.61	124.45
29	7	308	CHL	O2D-CGD-O1D	-2.01	119.92	123.84
22	M	101	CLA	O2D-CGD-CBD	2.01	114.83	111.27
22	A	843	CLA	CAC-C3C-C4C	2.01	127.41	124.81
22	A	810	CLA	CMB-C2B-C3B	2.01	128.43	124.68
22	A	803	CLA	CAA-CBA-CGA	-2.00	107.39	113.25
24	6	322	LHG	C27-C26-C25	-2.00	104.25	114.42
30	2	316	XAT	C38-C25-C24	2.00	116.53	114.28
25	J	101	8CT	C39-C16-C17	-2.00	120.12	122.92
22	1	306	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	A	809	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	A	838	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	A	839	CLA	CMC-C2C-C1C	-2.00	121.99	125.04
29	1	305	CHL	CHD-C1D-C2D	2.00	129.68	125.48
22	5	313	CLA	O2D-CGD-CBD	2.00	114.83	111.27
22	7	305	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
22	A	801	CLA	CAC-C3C-C4C	2.00	127.41	124.81
22	A	815	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (299) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	801	CLA	ND
22	A	802	CLA	ND
22	A	803	CLA	ND
22	A	804	CLA	ND
22	A	805	CLA	ND
22	A	806	CLA	ND
22	A	807	CLA	ND
22	A	808	CLA	ND
22	A	809	CLA	ND
22	A	810	CLA	ND
22	A	811	CLA	ND
22	A	812	CLA	ND
22	A	813	CLA	ND
22	A	814	CLA	ND
22	A	815	CLA	ND
22	A	816	CLA	ND
22	A	817	CLA	ND
22	A	818	CLA	ND
22	A	819	CLA	ND
22	A	820	CLA	ND
22	A	821	CLA	ND
22	A	822	CLA	ND
22	A	823	CLA	ND
22	A	824	CLA	ND
22	A	826	CLA	ND
22	A	827	CLA	ND
22	A	828	CLA	ND
22	A	829	CLA	ND
22	A	830	CLA	ND
22	A	831	CLA	ND
22	A	832	CLA	ND
22	A	833	CLA	ND
22	A	834	CLA	ND
22	A	835	CLA	ND
22	A	836	CLA	ND
22	A	837	CLA	ND
22	A	838	CLA	ND
22	A	839	CLA	ND
22	A	840	CLA	ND
22	A	841	CLA	ND
22	A	843	CLA	ND
22	A	852	CLA	ND

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Mol	Chain	Res	Type	Atom
22	A	853	CLA	ND
22	B	801	CLA	ND
22	B	803	CLA	ND
22	B	805	CLA	ND
22	B	806	CLA	ND
22	B	807	CLA	ND
22	B	808	CLA	ND
22	B	809	CLA	ND
22	B	810	CLA	ND
22	B	811	CLA	ND
22	B	812	CLA	ND
22	B	813	CLA	ND
22	B	814	CLA	ND
22	B	815	CLA	ND
22	B	816	CLA	ND
22	B	817	CLA	ND
22	B	818	CLA	ND
22	B	819	CLA	ND
22	B	820	CLA	ND
22	B	821	CLA	ND
22	B	822	CLA	ND
22	B	824	CLA	ND
22	B	825	CLA	ND
22	B	826	CLA	ND
22	B	827	CLA	ND
22	B	828	CLA	ND
22	B	829	CLA	ND
22	B	830	CLA	ND
22	B	831	CLA	ND
22	B	832	CLA	ND
22	B	833	CLA	ND
22	B	834	CLA	ND
22	B	835	CLA	ND
22	B	836	CLA	ND
22	B	837	CLA	ND
22	B	838	CLA	ND
22	B	839	CLA	ND
22	B	840	CLA	ND
22	B	841	CLA	ND
22	B	850	CLA	ND
22	F	301	CLA	ND
22	G	101	CLA	ND

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Mol	Chain	Res	Type	Atom
22	G	102	CLA	ND
22	G	103	CLA	ND
22	H	201	CLA	ND
22	J	103	CLA	ND
22	K	101	CLA	ND
22	K	102	CLA	ND
22	K	104	CLA	ND
22	K	105	CLA	ND
22	L	201	CLA	ND
22	L	202	CLA	ND
22	L	203	CLA	ND
22	L	204	CLA	ND
22	1	301	CLA	ND
22	1	302	CLA	ND
22	1	303	CLA	ND
22	1	304	CLA	ND
22	1	306	CLA	ND
22	1	307	CLA	ND
22	1	308	CLA	ND
22	1	309	CLA	ND
22	1	310	CLA	ND
22	1	311	CLA	ND
22	1	312	CLA	ND
22	1	313	CLA	ND
22	2	302	CLA	ND
22	2	303	CLA	ND
22	2	304	CLA	ND
22	2	308	CLA	ND
22	2	309	CLA	ND
22	2	310	CLA	ND
22	2	311	CLA	ND
22	2	312	CLA	ND
22	2	313	CLA	ND
22	2	314	CLA	ND
22	2	319	CLA	ND
22	3	301	CLA	ND
22	3	302	CLA	ND
22	3	303	CLA	ND
22	3	304	CLA	ND
22	3	305	CLA	ND
22	3	307	CLA	ND
22	3	308	CLA	ND

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Mol	Chain	Res	Type	Atom
22	3	309	CLA	ND
22	3	310	CLA	ND
22	3	311	CLA	ND
22	3	312	CLA	ND
22	3	313	CLA	ND
22	3	319	CLA	ND
22	4	302	CLA	ND
22	4	303	CLA	ND
22	4	304	CLA	ND
22	4	308	CLA	ND
22	4	309	CLA	ND
22	4	310	CLA	ND
22	4	311	CLA	ND
22	4	312	CLA	ND
22	4	313	CLA	ND
22	4	314	CLA	ND
22	6	301	CLA	ND
22	6	303	CLA	ND
22	6	304	CLA	ND
22	6	305	CLA	ND
22	6	309	CLA	ND
22	6	310	CLA	ND
22	6	311	CLA	ND
22	6	312	CLA	ND
22	6	313	CLA	ND
22	6	314	CLA	ND
22	6	315	CLA	ND
22	6	317	CLA	ND
22	6	318	CLA	ND
22	6	323	CLA	ND
22	5	302	CLA	ND
22	5	304	CLA	ND
22	5	305	CLA	ND
22	5	307	CLA	ND
22	5	308	CLA	ND
22	5	309	CLA	ND
22	5	310	CLA	ND
22	5	311	CLA	ND
22	5	312	CLA	ND
22	5	313	CLA	ND
22	5	314	CLA	ND
22	7	302	CLA	ND

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Mol	Chain	Res	Type	Atom
22	7	303	CLA	ND
22	7	304	CLA	ND
22	7	305	CLA	ND
22	7	306	CLA	ND
22	7	307	CLA	ND
22	7	309	CLA	ND
22	7	310	CLA	ND
22	7	311	CLA	ND
22	7	312	CLA	ND
22	7	313	CLA	ND
22	7	314	CLA	ND
22	7	315	CLA	ND
22	7	316	CLA	ND
22	7	317	CLA	ND
22	7	318	CLA	ND
22	8	302	CLA	ND
22	8	303	CLA	ND
22	8	304	CLA	ND
22	8	308	CLA	ND
22	8	309	CLA	ND
22	8	310	CLA	ND
22	8	312	CLA	ND
22	8	313	CLA	ND
22	8	315	CLA	ND
22	9	301	CLA	ND
22	9	303	CLA	ND
22	9	304	CLA	ND
22	9	305	CLA	ND
22	9	306	CLA	ND
22	9	308	CLA	ND
22	9	309	CLA	ND
22	9	310	CLA	ND
22	9	311	CLA	ND
22	9	312	CLA	ND
22	9	313	CLA	ND
22	0	302	CLA	ND
22	0	303	CLA	ND
22	0	304	CLA	ND
22	0	305	CLA	ND
22	0	307	CLA	ND
22	0	308	CLA	ND
22	0	309	CLA	ND

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Mol	Chain	Res	Type	Atom
22	0	310	CLA	ND
22	0	311	CLA	ND
22	0	312	CLA	ND
29	1	305	CHL	ND
29	1	305	CHL	NC
29	1	305	CHL	NA
29	2	301	CHL	C8
29	2	301	CHL	ND
29	2	301	CHL	NC
29	2	301	CHL	NA
29	2	305	CHL	ND
29	2	305	CHL	NC
29	2	305	CHL	NA
29	2	306	CHL	ND
29	2	306	CHL	NC
29	2	306	CHL	NA
29	2	307	CHL	ND
29	2	307	CHL	NC
29	2	307	CHL	NA
29	3	306	CHL	ND
29	3	306	CHL	NC
29	3	306	CHL	NA
29	4	301	CHL	C8
29	4	301	CHL	ND
29	4	301	CHL	NC
29	4	301	CHL	NA
29	4	305	CHL	C8
29	4	305	CHL	ND
29	4	305	CHL	NC
29	4	305	CHL	NA
29	4	306	CHL	ND
29	4	306	CHL	NC
29	4	306	CHL	NA
29	4	307	CHL	ND
29	4	307	CHL	NC
29	4	307	CHL	NA
29	6	302	CHL	C8
29	6	302	CHL	ND
29	6	302	CHL	NC
29	6	302	CHL	NA
29	6	306	CHL	ND
29	6	306	CHL	NC

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Mol	Chain	Res	Type	Atom
29	6	306	CHL	NA
29	6	307	CHL	ND
29	6	307	CHL	NC
29	6	307	CHL	NA
29	6	308	CHL	ND
29	6	308	CHL	NC
29	6	308	CHL	NA
29	6	316	CHL	ND
29	6	316	CHL	NC
29	6	316	CHL	NA
29	5	301	CHL	C8
29	5	301	CHL	ND
29	5	301	CHL	NC
29	5	301	CHL	NA
29	5	306	CHL	ND
29	5	306	CHL	NC
29	5	306	CHL	NA
29	7	308	CHL	ND
29	7	308	CHL	NC
29	7	308	CHL	NA
29	8	305	CHL	C8
29	8	305	CHL	ND
29	8	305	CHL	NC
29	8	305	CHL	NA
29	8	306	CHL	ND
29	8	306	CHL	NC
29	8	306	CHL	NA
29	8	307	CHL	ND
29	8	307	CHL	NC
29	8	307	CHL	NA
29	8	314	CHL	ND
29	8	314	CHL	NC
29	8	314	CHL	NA
29	9	302	CHL	C8
29	9	302	CHL	ND
29	9	302	CHL	NC
29	9	302	CHL	NA
29	9	307	CHL	ND
29	9	307	CHL	NC
29	9	307	CHL	NA
29	0	301	CHL	C8
29	0	301	CHL	ND

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Mol	Chain	Res	Type	Atom
29	0	301	CHL	NC
29	0	301	CHL	NA
29	0	306	CHL	ND
29	0	306	CHL	NC
29	0	306	CHL	NA

All (3256) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	803	CLA	CAD-CBD-CGD-O1D
22	A	803	CLA	CAD-CBD-CGD-O2D
22	A	804	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	805	CLA	C14-C13-C15-C16
22	A	806	CLA	O1A-CGA-O2A-C1
22	A	808	CLA	C1A-C2A-CAA-CBA
22	A	808	CLA	C3A-C2A-CAA-CBA
22	A	809	CLA	C1A-C2A-CAA-CBA
22	A	809	CLA	C3A-C2A-CAA-CBA
22	A	811	CLA	CBD-CGD-O2D-CED
22	A	811	CLA	O1D-CGD-O2D-CED
22	A	811	CLA	C14-C13-C15-C16
22	A	813	CLA	CHA-CBD-CGD-O1D
22	A	813	CLA	CHA-CBD-CGD-O2D
22	A	813	CLA	CAD-CBD-CGD-O1D
22	A	814	CLA	CHA-CBD-CGD-O1D
22	A	814	CLA	CHA-CBD-CGD-O2D
22	A	814	CLA	CAD-CBD-CGD-O1D
22	A	814	CLA	CAD-CBD-CGD-O2D
22	A	815	CLA	CBD-CGD-O2D-CED
22	A	816	CLA	CAD-CBD-CGD-O1D
22	A	816	CLA	CAD-CBD-CGD-O2D
22	A	818	CLA	C3A-C2A-CAA-CBA
22	A	819	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C3A-C2A-CAA-CBA
22	A	823	CLA	C1A-C2A-CAA-CBA
22	A	823	CLA	C3A-C2A-CAA-CBA
22	A	824	CLA	CHA-CBD-CGD-O1D
22	A	824	CLA	CHA-CBD-CGD-O2D
22	A	826	CLA	C3A-C2A-CAA-CBA
22	A	828	CLA	C1A-C2A-CAA-CBA
22	A	832	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	833	CLA	C3A-C2A-CAA-CBA
22	A	836	CLA	C1A-C2A-CAA-CBA
22	A	836	CLA	C3A-C2A-CAA-CBA
22	A	836	CLA	CHA-CBD-CGD-O1D
22	A	839	CLA	C11-C12-C13-C14
22	A	840	CLA	C4-C3-C5-C6
22	A	843	CLA	CHA-CBD-CGD-O1D
22	A	843	CLA	CHA-CBD-CGD-O2D
22	A	853	CLA	CBD-CGD-O2D-CED
22	B	801	CLA	C2-C3-C5-C6
22	B	801	CLA	C4-C3-C5-C6
22	B	803	CLA	CAD-CBD-CGD-O1D
22	B	803	CLA	CAD-CBD-CGD-O2D
22	B	803	CLA	O2A-C1-C2-C3
22	B	806	CLA	CBD-CGD-O2D-CED
22	B	807	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	C1A-C2A-CAA-CBA
22	B	808	CLA	C3A-C2A-CAA-CBA
22	B	812	CLA	CBD-CGD-O2D-CED
22	B	814	CLA	CHA-CBD-CGD-O1D
22	B	814	CLA	CHA-CBD-CGD-O2D
22	B	814	CLA	C11-C12-C13-C14
22	B	815	CLA	CBD-CGD-O2D-CED
22	B	816	CLA	CAD-CBD-CGD-O1D
22	B	816	CLA	CAD-CBD-CGD-O2D
22	B	817	CLA	CBD-CGD-O2D-CED
22	B	817	CLA	O1D-CGD-O2D-CED
22	B	818	CLA	C3A-C2A-CAA-CBA
22	B	819	CLA	C1A-C2A-CAA-CBA
22	B	819	CLA	C3A-C2A-CAA-CBA
22	B	820	CLA	CBD-CGD-O2D-CED
22	B	821	CLA	CHA-CBD-CGD-O1D
22	B	821	CLA	CHA-CBD-CGD-O2D
22	B	821	CLA	CAD-CBD-CGD-O1D
22	B	821	CLA	CAD-CBD-CGD-O2D
22	B	822	CLA	CBA-CGA-O2A-C1
22	B	823	CLA	CBD-CGD-O2D-CED
22	B	825	CLA	CHA-CBD-CGD-O1D
22	B	825	CLA	CHA-CBD-CGD-O2D
22	B	825	CLA	CAD-CBD-CGD-O1D
22	B	825	CLA	CAD-CBD-CGD-O2D
22	B	826	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	826	CLA	C3A-C2A-CAA-CBA
22	B	827	CLA	C1A-C2A-CAA-CBA
22	B	827	CLA	C3A-C2A-CAA-CBA
22	B	827	CLA	CAD-CBD-CGD-O1D
22	B	827	CLA	CAD-CBD-CGD-O2D
22	B	828	CLA	C1A-C2A-CAA-CBA
22	B	828	CLA	C3A-C2A-CAA-CBA
22	B	828	CLA	CBD-CGD-O2D-CED
22	B	829	CLA	C1A-C2A-CAA-CBA
22	B	829	CLA	CHA-CBD-CGD-O1D
22	B	829	CLA	CHA-CBD-CGD-O2D
22	B	829	CLA	CBD-CGD-O2D-CED
22	B	831	CLA	C1A-C2A-CAA-CBA
22	B	831	CLA	C3A-C2A-CAA-CBA
22	B	832	CLA	C1A-C2A-CAA-CBA
22	B	833	CLA	C1A-C2A-CAA-CBA
22	B	833	CLA	C3A-C2A-CAA-CBA
22	B	835	CLA	CBD-CGD-O2D-CED
22	B	836	CLA	C2-C3-C5-C6
22	B	836	CLA	C4-C3-C5-C6
22	B	837	CLA	C11-C12-C13-C14
22	B	841	CLA	C1A-C2A-CAA-CBA
22	B	850	CLA	CHA-CBD-CGD-O1D
22	B	850	CLA	CHA-CBD-CGD-O2D
22	G	102	CLA	CHA-CBD-CGD-O1D
22	G	102	CLA	CHA-CBD-CGD-O2D
22	G	103	CLA	C1A-C2A-CAA-CBA
22	G	103	CLA	C3A-C2A-CAA-CBA
22	H	201	CLA	C1A-C2A-CAA-CBA
22	J	103	CLA	C1A-C2A-CAA-CBA
22	J	103	CLA	CHA-CBD-CGD-O1D
22	J	103	CLA	CHA-CBD-CGD-O2D
22	J	103	CLA	CAD-CBD-CGD-O1D
22	J	103	CLA	CAD-CBD-CGD-O2D
22	J	103	CLA	CBD-CGD-O2D-CED
22	K	102	CLA	C1A-C2A-CAA-CBA
22	K	102	CLA	C3A-C2A-CAA-CBA
22	K	102	CLA	CHA-CBD-CGD-O2D
22	K	104	CLA	CHA-CBD-CGD-O1D
22	K	104	CLA	CHA-CBD-CGD-O2D
22	K	105	CLA	CBD-CGD-O2D-CED
22	L	201	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	L	201	CLA	C6-C7-C8-C9
22	L	202	CLA	C3A-C2A-CAA-CBA
22	L	204	CLA	C3A-C2A-CAA-CBA
22	L	204	CLA	O1A-CGA-O2A-C1
22	L	204	CLA	CBD-CGD-O2D-CED
22	1	302	CLA	CBD-CGD-O2D-CED
22	1	302	CLA	C2-C3-C5-C6
22	1	302	CLA	C4-C3-C5-C6
22	1	303	CLA	CBD-CGD-O2D-CED
22	1	307	CLA	C1A-C2A-CAA-CBA
22	1	307	CLA	C3A-C2A-CAA-CBA
22	1	308	CLA	CHA-CBD-CGD-O1D
22	1	308	CLA	CHA-CBD-CGD-O2D
22	1	310	CLA	C1A-C2A-CAA-CBA
22	1	312	CLA	C1A-C2A-CAA-CBA
22	1	312	CLA	C3A-C2A-CAA-CBA
22	2	302	CLA	C4-C3-C5-C6
22	2	304	CLA	CBD-CGD-O2D-CED
22	2	304	CLA	C2-C3-C5-C6
22	2	304	CLA	C4-C3-C5-C6
22	2	308	CLA	CBD-CGD-O2D-CED
22	2	310	CLA	CBD-CGD-O2D-CED
22	2	314	CLA	CHA-CBD-CGD-O1D
22	2	314	CLA	CHA-CBD-CGD-O2D
22	2	319	CLA	C3A-C2A-CAA-CBA
22	2	319	CLA	CHA-CBD-CGD-O1D
22	3	301	CLA	CHA-CBD-CGD-O1D
22	3	301	CLA	CHA-CBD-CGD-O2D
22	3	305	CLA	C1A-C2A-CAA-CBA
22	3	305	CLA	C3A-C2A-CAA-CBA
22	3	311	CLA	C1A-C2A-CAA-CBA
22	3	313	CLA	C1A-C2A-CAA-CBA
22	3	313	CLA	C3A-C2A-CAA-CBA
22	3	313	CLA	CBA-CGA-O2A-C1
22	3	319	CLA	CHA-CBD-CGD-O1D
22	3	319	CLA	CHA-CBD-CGD-O2D
22	3	319	CLA	CBD-CGD-O2D-CED
22	3	319	CLA	O2A-C1-C2-C3
22	4	302	CLA	CHA-CBD-CGD-O1D
22	4	302	CLA	CHA-CBD-CGD-O2D
22	4	302	CLA	CBD-CGD-O2D-CED
22	4	309	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	4	311	CLA	CBD-CGD-O2D-CED
22	4	313	CLA	CAD-CBD-CGD-O1D
22	4	313	CLA	CAD-CBD-CGD-O2D
22	6	301	CLA	C1A-C2A-CAA-CBA
22	6	301	CLA	C3A-C2A-CAA-CBA
22	6	301	CLA	CBD-CGD-O2D-CED
22	6	304	CLA	C2-C3-C5-C6
22	6	304	CLA	C4-C3-C5-C6
22	6	304	CLA	C6-C7-C8-C9
22	6	309	CLA	CBD-CGD-O2D-CED
22	6	310	CLA	CBD-CGD-O2D-CED
22	6	312	CLA	CBD-CGD-O2D-CED
22	6	312	CLA	C2-C3-C5-C6
22	6	312	CLA	C4-C3-C5-C6
22	6	314	CLA	CHA-CBD-CGD-O1D
22	6	314	CLA	CHA-CBD-CGD-O2D
22	6	314	CLA	CAD-CBD-CGD-O1D
22	6	314	CLA	CAD-CBD-CGD-O2D
22	6	314	CLA	CBD-CGD-O2D-CED
22	6	315	CLA	CBD-CGD-O2D-CED
22	6	318	CLA	C1A-C2A-CAA-CBA
22	6	318	CLA	C3A-C2A-CAA-CBA
22	6	323	CLA	C1A-C2A-CAA-CBA
22	5	302	CLA	CBD-CGD-O2D-CED
22	5	303	CLA	CBD-CGD-O2D-CED
22	5	304	CLA	CBD-CGD-O2D-CED
22	5	307	CLA	CAD-CBD-CGD-O1D
22	5	308	CLA	CBD-CGD-O2D-CED
22	5	312	CLA	CBD-CGD-O2D-CED
22	5	312	CLA	C6-C7-C8-C9
22	5	314	CLA	CHA-CBD-CGD-O1D
22	5	314	CLA	CHA-CBD-CGD-O2D
22	5	314	CLA	CBD-CGD-O2D-CED
22	7	303	CLA	CHA-CBD-CGD-O1D
22	7	303	CLA	CHA-CBD-CGD-O2D
22	7	303	CLA	CAD-CBD-CGD-O1D
22	7	303	CLA	C4-C3-C5-C6
22	7	304	CLA	CBD-CGD-O2D-CED
22	7	306	CLA	C1A-C2A-CAA-CBA
22	7	306	CLA	C3A-C2A-CAA-CBA
22	7	310	CLA	CHA-CBD-CGD-O1D
22	7	310	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	7	313	CLA	C1A-C2A-CAA-CBA
22	7	313	CLA	C3A-C2A-CAA-CBA
22	7	315	CLA	CBA-CGA-O2A-C1
22	7	317	CLA	C1A-C2A-CAA-CBA
22	7	317	CLA	C3A-C2A-CAA-CBA
22	7	317	CLA	CBD-CGD-O2D-CED
22	7	318	CLA	C1A-C2A-CAA-CBA
22	8	302	CLA	CBD-CGD-O2D-CED
22	8	304	CLA	CBD-CGD-O2D-CED
22	8	308	CLA	C3A-C2A-CAA-CBA
22	8	310	CLA	CBD-CGD-O2D-CED
22	8	311	CLA	C3-C5-C6-C7
22	8	315	CLA	CHA-CBD-CGD-O1D
22	8	315	CLA	CHA-CBD-CGD-O2D
22	8	315	CLA	CBD-CGD-O2D-CED
22	8	315	CLA	C11-C12-C13-C14
22	9	306	CLA	CBD-CGD-O2D-CED
22	9	309	CLA	CHA-CBD-CGD-O1D
22	9	309	CLA	CHA-CBD-CGD-O2D
22	9	311	CLA	CBD-CGD-O2D-CED
22	9	312	CLA	CHA-CBD-CGD-O1D
22	9	312	CLA	CHA-CBD-CGD-O2D
22	9	312	CLA	CAD-CBD-CGD-O1D
22	9	312	CLA	CAD-CBD-CGD-O2D
22	9	313	CLA	C3A-C2A-CAA-CBA
22	9	313	CLA	CBD-CGD-O2D-CED
22	9	313	CLA	C2-C3-C5-C6
22	9	313	CLA	C4-C3-C5-C6
22	0	303	CLA	C2-C3-C5-C6
22	0	303	CLA	C4-C3-C5-C6
22	0	304	CLA	C1A-C2A-CAA-CBA
22	0	304	CLA	C3A-C2A-CAA-CBA
22	0	304	CLA	C2-C3-C5-C6
22	0	304	CLA	C4-C3-C5-C6
22	0	305	CLA	C1A-C2A-CAA-CBA
22	0	307	CLA	CBD-CGD-O2D-CED
22	0	308	CLA	CBD-CGD-O2D-CED
22	0	309	CLA	CBD-CGD-O2D-CED
22	0	310	CLA	C1A-C2A-CAA-CBA
22	0	310	CLA	C3A-C2A-CAA-CBA
22	0	311	CLA	CBD-CGD-O2D-CED
22	M	101	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	M	101	CLA	CHA-CBD-CGD-O2D
24	A	844	LHG	C1-C2-C3-O3
24	A	844	LHG	C3-O3-P-O6
24	A	845	LHG	O2-C2-C3-O3
24	A	845	LHG	C3-O3-P-O4
24	A	845	LHG	C3-O3-P-O5
24	A	845	LHG	C4-O6-P-O4
24	A	845	LHG	C4-O6-P-O5
24	A	845	LHG	O6-C4-C5-O7
24	A	845	LHG	C8-C7-O7-C5
24	B	852	LHG	C3-O3-P-O5
24	B	852	LHG	C6-C5-O7-C7
24	B	852	LHG	O9-C7-O7-C5
24	B	852	LHG	C8-C7-O7-C5
24	1	317	LHG	O2-C2-C3-O3
24	1	317	LHG	C4-O6-P-O5
24	2	318	LHG	C1-C2-C3-O3
24	2	318	LHG	C3-O3-P-O4
24	2	318	LHG	C4-O6-P-O4
24	3	317	LHG	O1-C1-C2-C3
24	3	317	LHG	C3-O3-P-O5
24	3	317	LHG	C4-C5-O7-C7
24	6	322	LHG	O1-C1-C2-C3
24	6	322	LHG	C1-C2-C3-O3
24	6	322	LHG	C3-O3-P-O4
24	5	318	LHG	C1-C2-C3-O3
24	5	318	LHG	O2-C2-C3-O3
24	5	318	LHG	C4-O6-P-O5
24	7	322	LHG	O1-C1-C2-C3
24	7	322	LHG	C4-O6-P-O5
24	7	322	LHG	C6-C5-O7-C7
24	9	316	LHG	C3-O3-P-O4
24	9	316	LHG	C3-O3-P-O6
24	9	316	LHG	O7-C5-C6-O8
24	0	315	LHG	C1-C2-C3-O3
24	0	315	LHG	C3-O3-P-O4
24	0	315	LHG	C4-O6-P-O3
24	0	315	LHG	C4-O6-P-O4
25	A	846	8CT	C02-C03-C10-C11
25	A	846	8CT	C04-C03-C10-C11
25	A	846	8CT	C18-C19-C20-C21
25	A	846	8CT	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	A	846	8CT	C28-C29-C30-C35
25	A	847	8CT	C10-C11-C12-C13
25	A	847	8CT	C10-C11-C12-C40
25	A	848	8CT	C12-C13-C14-C15
25	A	849	8CT	C04-C03-C10-C11
25	A	849	8CT	C10-C11-C12-C13
25	A	849	8CT	C10-C11-C12-C40
25	A	849	8CT	C14-C15-C16-C17
25	A	849	8CT	C14-C15-C16-C39
25	A	850	8CT	C02-C03-C10-C11
25	A	850	8CT	C10-C11-C12-C13
25	A	850	8CT	C10-C11-C12-C40
25	A	850	8CT	C12-C13-C14-C15
25	A	850	8CT	C28-C29-C30-C35
25	A	854	8CT	C04-C03-C10-C11
25	A	854	8CT	C12-C13-C14-C15
25	A	854	8CT	C14-C15-C16-C17
25	A	854	8CT	C14-C15-C16-C39
25	A	854	8CT	C20-C21-C23-C24
25	A	854	8CT	C22-C21-C23-C24
25	A	854	8CT	C28-C29-C30-C31
25	A	854	8CT	C28-C29-C30-C35
25	B	804	8CT	C25-C26-C28-C29
25	B	804	8CT	C27-C26-C28-C29
25	B	804	8CT	C28-C29-C30-C35
25	B	843	8CT	C10-C11-C12-C13
25	B	843	8CT	C10-C11-C12-C40
25	B	843	8CT	C14-C15-C16-C17
25	B	843	8CT	C14-C15-C16-C39
25	B	843	8CT	C20-C21-C23-C24
25	B	843	8CT	C22-C21-C23-C24
25	B	843	8CT	C28-C29-C30-C35
25	B	844	8CT	C10-C11-C12-C13
25	B	844	8CT	C10-C11-C12-C40
25	B	844	8CT	C18-C19-C20-C21
25	B	844	8CT	C20-C21-C23-C24
25	B	844	8CT	C22-C21-C23-C24
25	B	845	8CT	C25-C26-C28-C29
25	B	845	8CT	C27-C26-C28-C29
25	B	846	8CT	C14-C15-C16-C17
25	B	846	8CT	C14-C15-C16-C39
25	B	846	8CT	C27-C26-C28-C29

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Mol	Chain	Res	Type	Atoms
25	B	846	8CT	C28-C29-C30-C35
25	B	847	8CT	C10-C11-C12-C13
25	B	847	8CT	C10-C11-C12-C40
25	B	847	8CT	C20-C21-C23-C24
25	B	847	8CT	C22-C21-C23-C24
25	B	847	8CT	C23-C24-C25-C26
25	B	851	8CT	C10-C11-C12-C13
25	B	851	8CT	C10-C11-C12-C40
25	B	851	8CT	C12-C13-C14-C15
25	B	851	8CT	C14-C15-C16-C17
25	B	851	8CT	C14-C15-C16-C39
25	B	851	8CT	C20-C21-C23-C24
25	B	851	8CT	C22-C21-C23-C24
25	F	302	8CT	C28-C29-C30-C31
25	F	302	8CT	C28-C29-C30-C35
25	G	104	8CT	C02-C03-C10-C11
25	G	104	8CT	C10-C11-C12-C13
25	G	104	8CT	C10-C11-C12-C40
25	G	104	8CT	C18-C19-C20-C21
25	G	104	8CT	C25-C26-C28-C29
25	G	104	8CT	C27-C26-C28-C29
25	G	104	8CT	C28-C29-C30-C35
25	I	101	8CT	C10-C11-C12-C13
25	I	101	8CT	C10-C11-C12-C40
25	I	101	8CT	C25-C26-C28-C29
25	I	101	8CT	C27-C26-C28-C29
25	I	101	8CT	C28-C29-C30-C31
25	I	101	8CT	C28-C29-C30-C35
25	J	101	8CT	C28-C29-C30-C35
25	J	104	8CT	C04-C03-C10-C11
25	J	104	8CT	C28-C29-C30-C31
25	J	104	8CT	C28-C29-C30-C35
25	K	103	8CT	C14-C15-C16-C17
25	K	103	8CT	C14-C15-C16-C39
25	L	205	8CT	C02-C03-C10-C11
25	L	205	8CT	C10-C11-C12-C13
25	L	205	8CT	C10-C11-C12-C40
25	L	205	8CT	C20-C21-C23-C24
25	L	205	8CT	C22-C21-C23-C24
25	L	206	8CT	C20-C21-C23-C24
25	L	206	8CT	C22-C21-C23-C24
25	L	206	8CT	C28-C29-C30-C35

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Mol	Chain	Res	Type	Atoms
25	1	316	8CT	C02-C03-C10-C11
25	1	316	8CT	C04-C03-C10-C11
25	1	316	8CT	C20-C21-C23-C24
25	1	316	8CT	C22-C21-C23-C24
25	1	316	8CT	C25-C26-C28-C29
25	1	316	8CT	C27-C26-C28-C29
25	1	316	8CT	C28-C29-C30-C35
25	2	317	8CT	C10-C11-C12-C13
25	2	317	8CT	C10-C11-C12-C40
25	2	317	8CT	C28-C29-C30-C35
25	3	316	8CT	C23-C24-C25-C26
25	3	316	8CT	C25-C26-C28-C29
25	3	316	8CT	C27-C26-C28-C29
25	3	318	8CT	C10-C11-C12-C13
25	3	318	8CT	C10-C11-C12-C40
25	3	318	8CT	C20-C21-C23-C24
25	3	318	8CT	C22-C21-C23-C24
25	3	318	8CT	C23-C24-C25-C26
25	6	321	8CT	C10-C11-C12-C13
25	6	321	8CT	C10-C11-C12-C40
25	5	317	8CT	C04-C03-C10-C11
25	5	317	8CT	C28-C29-C30-C31
25	5	317	8CT	C28-C29-C30-C35
25	7	301	8CT	C12-C13-C14-C15
25	7	321	8CT	C22-C21-C23-C24
25	7	321	8CT	C25-C26-C28-C29
25	7	321	8CT	C27-C26-C28-C29
25	7	321	8CT	C28-C29-C30-C31
25	7	321	8CT	C28-C29-C30-C35
25	7	323	8CT	C04-C03-C10-C11
25	7	323	8CT	C23-C24-C25-C26
25	7	323	8CT	C25-C26-C28-C29
25	7	323	8CT	C27-C26-C28-C29
25	8	301	8CT	C18-C19-C20-C21
25	8	301	8CT	C20-C21-C23-C24
25	8	301	8CT	C22-C21-C23-C24
25	8	301	8CT	C23-C24-C25-C26
25	8	301	8CT	C28-C29-C30-C35
25	8	318	8CT	C04-C03-C10-C11
25	8	318	8CT	C27-C26-C28-C29
25	8	318	8CT	C28-C29-C30-C35
26	A	851	HTG	O5-C1-S1-C1'

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Mol	Chain	Res	Type	Atoms
29	2	301	CHL	C1C-C2C-CMC-OMC
29	2	301	CHL	CHA-CBD-CGD-O1D
29	2	301	CHL	CHA-CBD-CGD-O2D
29	2	301	CHL	CAD-CBD-CGD-O1D
29	2	305	CHL	C3C-C2C-CMC-OMC
29	2	307	CHL	C3C-C2C-CMC-OMC
29	2	307	CHL	CBD-CGD-O2D-CED
29	4	305	CHL	C1C-C2C-CMC-OMC
29	4	305	CHL	C3C-C2C-CMC-OMC
29	4	305	CHL	C2-C3-C5-C6
29	4	305	CHL	C4-C3-C5-C6
29	4	306	CHL	C1A-C2A-CAA-CBA
29	4	306	CHL	C3A-C2A-CAA-CBA
29	4	307	CHL	C1C-C2C-CMC-OMC
29	4	307	CHL	C3C-C2C-CMC-OMC
29	6	306	CHL	C1A-C2A-CAA-CBA
29	6	307	CHL	C1A-C2A-CAA-CBA
29	6	307	CHL	C3A-C2A-CAA-CBA
29	6	307	CHL	C1C-C2C-CMC-OMC
29	6	307	CHL	C3C-C2C-CMC-OMC
29	6	308	CHL	C1A-C2A-CAA-CBA
29	6	308	CHL	C3A-C2A-CAA-CBA
29	6	308	CHL	CBD-CGD-O2D-CED
29	6	316	CHL	C3C-C2C-CMC-OMC
29	5	306	CHL	C3C-C2C-CMC-OMC
29	8	305	CHL	C1C-C2C-CMC-OMC
29	8	306	CHL	C1A-C2A-CAA-CBA
29	8	306	CHL	CHA-CBD-CGD-O1D
29	8	306	CHL	CHA-CBD-CGD-O2D
29	0	301	CHL	C1A-C2A-CAA-CBA
29	0	301	CHL	C3A-C2A-CAA-CBA
29	0	301	CHL	C11-C10-C8-C9
30	1	314	XAT	C1-C6-C7-C8
30	1	314	XAT	C7-C8-C9-C10
30	1	314	XAT	C7-C8-C9-C19
30	1	314	XAT	C11-C12-C13-C14
30	1	314	XAT	C11-C12-C13-C20
30	2	315	XAT	C1-C6-C7-C8
30	2	316	XAT	O4-C6-C7-C8
30	3	314	XAT	C31-C32-C33-C40
30	4	315	XAT	O24-C26-C27-C28
30	6	320	XAT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
30	6	320	XAT	C7-C8-C9-C19
30	6	320	XAT	C9-C10-C11-C12
30	5	315	XAT	O4-C6-C7-C8
30	5	315	XAT	C25-C26-C27-C28
30	7	319	XAT	C7-C8-C9-C10
30	7	319	XAT	C7-C8-C9-C19
30	7	319	XAT	C11-C12-C13-C14
30	7	319	XAT	C11-C12-C13-C20
30	7	319	XAT	O24-C26-C27-C28
30	8	316	XAT	C25-C26-C27-C28
30	8	316	XAT	O24-C26-C27-C28
30	0	313	XAT	O4-C6-C7-C8
30	0	313	XAT	C7-C8-C9-C19
30	0	313	XAT	C13-C14-C15-C35
30	0	313	XAT	C21-C26-C27-C28
30	0	313	XAT	C25-C26-C27-C28
30	0	313	XAT	O24-C26-C27-C28
30	0	313	XAT	C31-C32-C33-C34
30	0	313	XAT	C31-C32-C33-C40
30	0	314	XAT	O4-C6-C7-C8
30	0	314	XAT	O24-C26-C27-C28
31	4	318	LMG	O6-C1-O1-C7
31	5	319	LMG	C2-C1-O1-C7
31	5	319	LMG	O6-C1-O1-C7
31	8	319	LMG	C2-C1-O1-C7
31	8	319	LMG	O6-C1-O1-C7
22	A	816	CLA	O1D-CGD-O2D-CED
22	A	853	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	O1D-CGD-O2D-CED
22	K	105	CLA	O1D-CGD-O2D-CED
22	2	310	CLA	O1D-CGD-O2D-CED
22	3	303	CLA	O1D-CGD-O2D-CED
22	4	313	CLA	O1D-CGD-O2D-CED
22	5	303	CLA	O1D-CGD-O2D-CED
22	5	307	CLA	O1D-CGD-O2D-CED
22	7	302	CLA	O1D-CGD-O2D-CED
22	7	303	CLA	O1D-CGD-O2D-CED
22	7	306	CLA	O1D-CGD-O2D-CED
22	8	315	CLA	O1D-CGD-O2D-CED
22	9	306	CLA	O1D-CGD-O2D-CED
22	9	311	CLA	O1D-CGD-O2D-CED
22	A	839	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	A	839	CLA	C4C-C3C-CAC-CBC
22	A	815	CLA	O1D-CGD-O2D-CED
22	B	812	CLA	O1D-CGD-O2D-CED
22	B	823	CLA	O1D-CGD-O2D-CED
22	G	103	CLA	O1D-CGD-O2D-CED
22	L	204	CLA	O1D-CGD-O2D-CED
22	2	304	CLA	O1D-CGD-O2D-CED
22	3	302	CLA	O1D-CGD-O2D-CED
22	3	319	CLA	O1D-CGD-O2D-CED
22	6	304	CLA	O1D-CGD-O2D-CED
22	6	315	CLA	O1D-CGD-O2D-CED
22	5	308	CLA	O1D-CGD-O2D-CED
22	7	304	CLA	O1D-CGD-O2D-CED
22	7	317	CLA	O1D-CGD-O2D-CED
22	9	313	CLA	O1D-CGD-O2D-CED
22	0	308	CLA	O1D-CGD-O2D-CED
29	7	308	CHL	O1D-CGD-O2D-CED
22	A	814	CLA	CBD-CGD-O2D-CED
22	A	816	CLA	CBD-CGD-O2D-CED
22	A	829	CLA	CBD-CGD-O2D-CED
22	A	832	CLA	CBD-CGD-O2D-CED
22	A	837	CLA	CBD-CGD-O2D-CED
22	A	839	CLA	CBD-CGD-O2D-CED
22	A	841	CLA	CBD-CGD-O2D-CED
22	B	805	CLA	CBD-CGD-O2D-CED
22	B	814	CLA	CBD-CGD-O2D-CED
22	B	825	CLA	CBD-CGD-O2D-CED
22	F	301	CLA	CBD-CGD-O2D-CED
22	G	101	CLA	CBD-CGD-O2D-CED
22	G	103	CLA	CBD-CGD-O2D-CED
22	H	201	CLA	CBD-CGD-O2D-CED
22	K	101	CLA	CBD-CGD-O2D-CED
22	1	308	CLA	CBD-CGD-O2D-CED
22	2	302	CLA	CBD-CGD-O2D-CED
22	3	302	CLA	CBD-CGD-O2D-CED
22	3	303	CLA	CBD-CGD-O2D-CED
22	3	305	CLA	CBD-CGD-O2D-CED
22	4	310	CLA	CBD-CGD-O2D-CED
22	4	313	CLA	CBD-CGD-O2D-CED
22	4	314	CLA	CBD-CGD-O2D-CED
22	6	303	CLA	CBD-CGD-O2D-CED
22	6	304	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	6	305	CLA	CBD-CGD-O2D-CED
22	6	311	CLA	CBD-CGD-O2D-CED
22	5	307	CLA	CBD-CGD-O2D-CED
22	5	310	CLA	CBD-CGD-O2D-CED
22	7	302	CLA	CBD-CGD-O2D-CED
22	7	303	CLA	CBD-CGD-O2D-CED
22	7	306	CLA	CBD-CGD-O2D-CED
22	7	310	CLA	CBD-CGD-O2D-CED
22	7	316	CLA	CBD-CGD-O2D-CED
22	9	303	CLA	CBD-CGD-O2D-CED
22	9	310	CLA	CBD-CGD-O2D-CED
22	0	302	CLA	CBD-CGD-O2D-CED
22	M	101	CLA	CBD-CGD-O2D-CED
29	4	305	CHL	CBD-CGD-O2D-CED
29	6	307	CHL	CBD-CGD-O2D-CED
29	7	308	CHL	CBD-CGD-O2D-CED
29	8	314	CHL	CBD-CGD-O2D-CED
22	A	808	CLA	O1A-CGA-O2A-C1
22	A	819	CLA	O1A-CGA-O2A-C1
22	A	852	CLA	O1A-CGA-O2A-C1
22	7	317	CLA	O1A-CGA-O2A-C1
22	0	305	CLA	O1A-CGA-O2A-C1
24	7	322	LHG	O10-C23-O8-C6
22	A	832	CLA	O1D-CGD-O2D-CED
22	B	829	CLA	O1D-CGD-O2D-CED
22	G	101	CLA	O1D-CGD-O2D-CED
22	1	302	CLA	O1D-CGD-O2D-CED
22	4	310	CLA	O1D-CGD-O2D-CED
22	6	301	CLA	O1D-CGD-O2D-CED
22	0	302	CLA	O1D-CGD-O2D-CED
22	K	104	CLA	CBA-CGA-O2A-C1
22	4	303	CLA	CBA-CGA-O2A-C1
22	0	307	CLA	C4C-C3C-CAC-CBC
22	A	837	CLA	O1D-CGD-O2D-CED
22	B	814	CLA	O1D-CGD-O2D-CED
22	B	815	CLA	O1D-CGD-O2D-CED
22	B	828	CLA	O1D-CGD-O2D-CED
22	J	103	CLA	O1D-CGD-O2D-CED
22	1	303	CLA	O1D-CGD-O2D-CED
22	2	308	CLA	O1D-CGD-O2D-CED
22	6	309	CLA	O1D-CGD-O2D-CED
22	6	311	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	6	312	CLA	O1D-CGD-O2D-CED
22	5	302	CLA	O1D-CGD-O2D-CED
22	5	312	CLA	O1D-CGD-O2D-CED
22	8	310	CLA	O1D-CGD-O2D-CED
22	0	307	CLA	O1D-CGD-O2D-CED
22	0	311	CLA	O1D-CGD-O2D-CED
22	A	805	CLA	CBA-CGA-O2A-C1
22	A	808	CLA	CBA-CGA-O2A-C1
22	7	317	CLA	CBA-CGA-O2A-C1
22	9	301	CLA	CBA-CGA-O2A-C1
24	1	317	LHG	C24-C23-O8-C6
22	A	804	CLA	CBD-CGD-O2D-CED
22	A	817	CLA	CBD-CGD-O2D-CED
22	A	819	CLA	CBD-CGD-O2D-CED
22	A	833	CLA	CBD-CGD-O2D-CED
22	B	810	CLA	CBD-CGD-O2D-CED
22	G	102	CLA	CBD-CGD-O2D-CED
22	L	203	CLA	CBD-CGD-O2D-CED
22	1	301	CLA	CBD-CGD-O2D-CED
22	2	303	CLA	CBD-CGD-O2D-CED
22	3	301	CLA	CBD-CGD-O2D-CED
22	3	308	CLA	CBD-CGD-O2D-CED
22	4	304	CLA	CBD-CGD-O2D-CED
22	6	323	CLA	CBD-CGD-O2D-CED
22	7	314	CLA	CBD-CGD-O2D-CED
22	7	315	CLA	CBD-CGD-O2D-CED
22	0	304	CLA	CBD-CGD-O2D-CED
29	1	305	CHL	CBD-CGD-O2D-CED
29	2	306	CHL	CBD-CGD-O2D-CED
29	4	307	CHL	CBD-CGD-O2D-CED
29	8	305	CHL	CBD-CGD-O2D-CED
29	0	301	CHL	CBD-CGD-O2D-CED
22	A	805	CLA	O1A-CGA-O2A-C1
22	A	810	CLA	O1A-CGA-O2A-C1
22	A	811	CLA	O1A-CGA-O2A-C1
22	B	823	CLA	O1A-CGA-O2A-C1
22	B	850	CLA	O1A-CGA-O2A-C1
22	L	202	CLA	O1A-CGA-O2A-C1
22	1	302	CLA	O1A-CGA-O2A-C1
22	4	314	CLA	O1A-CGA-O2A-C1
22	7	316	CLA	O1A-CGA-O2A-C1
22	9	301	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	9	304	CLA	O1A-CGA-O2A-C1
24	1	317	LHG	O10-C23-O8-C6
24	3	317	LHG	O10-C23-O8-C6
24	5	318	LHG	O10-C23-O8-C6
29	2	307	CHL	O1A-CGA-O2A-C1
29	8	307	CHL	O1A-CGA-O2A-C1
22	B	822	CLA	O1A-CGA-O2A-C1
22	K	104	CLA	O1A-CGA-O2A-C1
22	3	313	CLA	O1A-CGA-O2A-C1
22	7	315	CLA	O1A-CGA-O2A-C1
22	B	807	CLA	O1D-CGD-O2D-CED
22	B	835	CLA	O1D-CGD-O2D-CED
22	5	304	CLA	O1D-CGD-O2D-CED
29	2	307	CHL	O1D-CGD-O2D-CED
29	6	308	CHL	O1D-CGD-O2D-CED
22	2	304	CLA	C8-C10-C11-C12
22	4	302	CLA	O1D-CGD-O2D-CED
22	4	311	CLA	O1D-CGD-O2D-CED
22	6	310	CLA	O1D-CGD-O2D-CED
22	5	314	CLA	O1D-CGD-O2D-CED
22	8	302	CLA	O1D-CGD-O2D-CED
22	8	304	CLA	O1D-CGD-O2D-CED
22	0	309	CLA	O1D-CGD-O2D-CED
22	6	317	CLA	C4C-C3C-CAC-CBC
22	A	810	CLA	CBD-CGD-O2D-CED
22	A	820	CLA	CBD-CGD-O2D-CED
22	B	819	CLA	CBD-CGD-O2D-CED
22	B	837	CLA	CBD-CGD-O2D-CED
22	5	309	CLA	CBD-CGD-O2D-CED
22	7	313	CLA	CBD-CGD-O2D-CED
22	B	820	CLA	O1D-CGD-O2D-CED
22	H	201	CLA	O1D-CGD-O2D-CED
22	6	314	CLA	O1D-CGD-O2D-CED
24	A	844	LHG	O9-C7-O7-C5
31	5	319	LMG	O9-C10-O7-C8
22	2	319	CLA	CBA-CGA-O2A-C1
22	5	314	CLA	O1A-CGA-O2A-C1
22	A	817	CLA	C3-C5-C6-C7
22	A	828	CLA	C3-C5-C6-C7
22	A	832	CLA	C3-C5-C6-C7
22	A	833	CLA	C3-C5-C6-C7
22	A	838	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	A	841	CLA	C3-C5-C6-C7
22	B	816	CLA	C3-C5-C6-C7
22	B	817	CLA	C3-C5-C6-C7
22	B	833	CLA	C3-C5-C6-C7
22	B	834	CLA	C3-C5-C6-C7
22	2	309	CLA	C3-C5-C6-C7
22	7	303	CLA	C3-C5-C6-C7
22	9	313	CLA	C3-C5-C6-C7
22	0	308	CLA	C3-C5-C6-C7
29	4	301	CHL	C3-C5-C6-C7
29	0	301	CHL	C3-C5-C6-C7
22	A	806	CLA	CBA-CGA-O2A-C1
22	A	819	CLA	CBA-CGA-O2A-C1
22	A	822	CLA	CBA-CGA-O2A-C1
22	A	852	CLA	CBA-CGA-O2A-C1
22	B	823	CLA	CBA-CGA-O2A-C1
22	B	850	CLA	CBA-CGA-O2A-C1
22	L	204	CLA	CBA-CGA-O2A-C1
22	5	313	CLA	CBA-CGA-O2A-C1
22	7	304	CLA	CBA-CGA-O2A-C1
22	7	316	CLA	CBA-CGA-O2A-C1
22	9	304	CLA	CBA-CGA-O2A-C1
22	9	308	CLA	CBA-CGA-O2A-C1
22	0	305	CLA	CBA-CGA-O2A-C1
24	7	322	LHG	C24-C23-O8-C6
29	8	307	CHL	CBA-CGA-O2A-C1
31	5	319	LMG	C11-C10-O7-C8
22	A	841	CLA	O1D-CGD-O2D-CED
22	B	805	CLA	O1D-CGD-O2D-CED
22	7	316	CLA	O1D-CGD-O2D-CED
22	B	841	CLA	CBD-CGD-O2D-CED
22	9	304	CLA	CBD-CGD-O2D-CED
22	6	317	CLA	C2C-C3C-CAC-CBC
22	0	307	CLA	C2C-C3C-CAC-CBC
22	2	319	CLA	O1A-CGA-O2A-C1
22	4	303	CLA	O1A-CGA-O2A-C1
22	6	323	CLA	CBA-CGA-O2A-C1
22	5	314	CLA	CBA-CGA-O2A-C1
22	3	310	CLA	C3-C5-C6-C7
22	B	840	CLA	C4-C3-C5-C6
22	5	303	CLA	C4-C3-C5-C6
22	9	309	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	B	849	DGD	C4E-C5E-C6E-O5E
31	5	319	LMG	C4-C5-C6-O5
22	A	840	CLA	C2-C3-C5-C6
22	L	201	CLA	C2-C3-C5-C6
22	2	302	CLA	C2-C3-C5-C6
22	4	309	CLA	C2-C3-C5-C6
22	7	303	CLA	C2-C3-C5-C6
22	9	309	CLA	C2-C3-C5-C6
22	1	312	CLA	CBD-CGD-O2D-CED
29	6	316	CHL	CBD-CGD-O2D-CED
22	A	819	CLA	C2A-CAA-CBA-CGA
22	B	823	CLA	C2A-CAA-CBA-CGA
22	B	829	CLA	C2A-CAA-CBA-CGA
22	K	105	CLA	C2A-CAA-CBA-CGA
22	L	201	CLA	C2A-CAA-CBA-CGA
22	3	307	CLA	C2A-CAA-CBA-CGA
22	4	303	CLA	C2A-CAA-CBA-CGA
22	6	301	CLA	C2A-CAA-CBA-CGA
22	6	303	CLA	C2A-CAA-CBA-CGA
22	6	305	CLA	C2A-CAA-CBA-CGA
22	5	303	CLA	C2A-CAA-CBA-CGA
22	5	304	CLA	C2A-CAA-CBA-CGA
22	5	305	CLA	C2A-CAA-CBA-CGA
22	5	313	CLA	C2A-CAA-CBA-CGA
22	5	314	CLA	C2A-CAA-CBA-CGA
22	7	318	CLA	C2A-CAA-CBA-CGA
22	8	308	CLA	C2A-CAA-CBA-CGA
22	8	310	CLA	C2A-CAA-CBA-CGA
22	8	311	CLA	C2A-CAA-CBA-CGA
22	8	315	CLA	C2A-CAA-CBA-CGA
22	9	301	CLA	C2A-CAA-CBA-CGA
29	2	307	CHL	C2A-CAA-CBA-CGA
22	F	301	CLA	O1D-CGD-O2D-CED
22	K	101	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	C3-C5-C6-C7
22	2	302	CLA	C3-C5-C6-C7
22	5	303	CLA	C3-C5-C6-C7
22	7	316	CLA	C3-C5-C6-C7
23	A	842	PQN	C13-C15-C16-C17
22	A	810	CLA	CBA-CGA-O2A-C1
22	A	811	CLA	CBA-CGA-O2A-C1
22	A	817	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	A	821	CLA	CBA-CGA-O2A-C1
22	A	837	CLA	CBA-CGA-O2A-C1
22	A	843	CLA	CBA-CGA-O2A-C1
22	B	817	CLA	CBA-CGA-O2A-C1
22	B	819	CLA	CBA-CGA-O2A-C1
22	L	202	CLA	CBA-CGA-O2A-C1
22	1	302	CLA	CBA-CGA-O2A-C1
22	2	304	CLA	CBA-CGA-O2A-C1
22	4	314	CLA	CBA-CGA-O2A-C1
22	6	303	CLA	CBA-CGA-O2A-C1
22	0	308	CLA	CBA-CGA-O2A-C1
29	2	301	CHL	CBA-CGA-O2A-C1
29	2	307	CHL	CBA-CGA-O2A-C1
29	4	306	CHL	CBA-CGA-O2A-C1
31	8	319	LMG	C29-C28-O8-C9
22	A	814	CLA	O1D-CGD-O2D-CED
22	4	314	CLA	O1D-CGD-O2D-CED
22	9	303	CLA	O1D-CGD-O2D-CED
29	6	307	CHL	O1D-CGD-O2D-CED
22	0	312	CLA	CBD-CGD-O2D-CED
29	8	307	CHL	CBD-CGD-O2D-CED
26	A	851	HTG	S1-C1'-C2'-C3'
22	A	829	CLA	O1D-CGD-O2D-CED
22	6	303	CLA	O1D-CGD-O2D-CED
22	6	305	CLA	O1D-CGD-O2D-CED
22	9	310	CLA	O1D-CGD-O2D-CED
22	M	101	CLA	O1D-CGD-O2D-CED
24	A	845	LHG	O9-C7-O7-C5
28	B	849	DGD	O1B-C1B-O2G-C2G
22	A	843	CLA	O1A-CGA-O2A-C1
22	B	817	CLA	O1A-CGA-O2A-C1
22	B	819	CLA	O1A-CGA-O2A-C1
22	B	824	CLA	O1A-CGA-O2A-C1
22	B	833	CLA	O1A-CGA-O2A-C1
22	B	834	CLA	O1A-CGA-O2A-C1
22	K	105	CLA	O1A-CGA-O2A-C1
22	2	304	CLA	O1A-CGA-O2A-C1
22	6	301	CLA	O1A-CGA-O2A-C1
22	6	303	CLA	O1A-CGA-O2A-C1
22	9	308	CLA	O1A-CGA-O2A-C1
31	8	319	LMG	O10-C28-O8-C9
22	7	310	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	847	8CT	C18-C19-C20-C21
25	J	101	8CT	C12-C13-C14-C15
25	J	101	8CT	C18-C19-C20-C21
25	L	205	8CT	C18-C19-C20-C21
25	L	206	8CT	C23-C24-C25-C26
25	3	316	8CT	C16-C17-C18-C19
25	4	317	8CT	C16-C17-C18-C19
25	6	321	8CT	C12-C13-C14-C15
25	7	301	8CT	C16-C17-C18-C19
25	7	301	8CT	C18-C19-C20-C21
25	7	321	8CT	C12-C13-C14-C15
25	7	323	8CT	C18-C19-C20-C21
25	8	301	8CT	C16-C17-C18-C19
22	B	805	CLA	C5-C6-C7-C8
22	A	809	CLA	CBD-CGD-O2D-CED
22	B	850	CLA	CBD-CGD-O2D-CED
22	2	313	CLA	CBD-CGD-O2D-CED
22	8	309	CLA	CBD-CGD-O2D-CED
22	9	301	CLA	CBD-CGD-O2D-CED
29	8	306	CHL	CBD-CGD-O2D-CED
22	2	302	CLA	O1D-CGD-O2D-CED
24	A	844	LHG	O2-C2-C3-O3
24	2	318	LHG	O2-C2-C3-O3
24	6	322	LHG	O2-C2-C3-O3
24	9	316	LHG	O2-C2-C3-O3
24	0	315	LHG	O2-C2-C3-O3
22	A	813	CLA	C3-C5-C6-C7
22	6	315	CLA	C3-C5-C6-C7
22	B	831	CLA	CBA-CGA-O2A-C1
22	B	833	CLA	CBA-CGA-O2A-C1
22	B	834	CLA	CBA-CGA-O2A-C1
22	K	105	CLA	CBA-CGA-O2A-C1
22	6	301	CLA	CBA-CGA-O2A-C1
22	5	307	CLA	CBA-CGA-O2A-C1
22	9	313	CLA	CBA-CGA-O2A-C1
24	3	317	LHG	C24-C23-O8-C6
24	5	318	LHG	C24-C23-O8-C6
29	4	301	CHL	CBA-CGA-O2A-C1
22	A	817	CLA	O1A-CGA-O2A-C1
22	A	822	CLA	O1A-CGA-O2A-C1
22	3	305	CLA	O1A-CGA-O2A-C1
22	5	313	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	7	304	CLA	O1A-CGA-O2A-C1
22	9	313	CLA	O1A-CGA-O2A-C1
29	2	301	CHL	O1A-CGA-O2A-C1
29	4	306	CHL	O1A-CGA-O2A-C1
28	B	849	DGD	C2B-C1B-O2G-C2G
31	8	319	LMG	C11-C10-O7-C8
22	7	302	CLA	CBA-CGA-O2A-C1
22	A	835	CLA	CBD-CGD-O2D-CED
22	B	818	CLA	CBD-CGD-O2D-CED
22	2	311	CLA	CBD-CGD-O2D-CED
22	4	309	CLA	CBD-CGD-O2D-CED
29	3	306	CHL	CBD-CGD-O2D-CED
22	1	309	CLA	C2C-C3C-CAC-CBC
22	A	837	CLA	O1A-CGA-O2A-C1
22	A	813	CLA	CBD-CGD-O2D-CED
22	B	824	CLA	CBD-CGD-O2D-CED
22	A	811	CLA	C3-C5-C6-C7
22	4	312	CLA	C3-C5-C6-C7
22	B	816	CLA	CBA-CGA-O2A-C1
22	B	824	CLA	CBA-CGA-O2A-C1
22	3	305	CLA	CBA-CGA-O2A-C1
29	5	301	CHL	CBA-CGA-O2A-C1
22	3	305	CLA	O1D-CGD-O2D-CED
29	4	305	CHL	O1D-CGD-O2D-CED
31	8	319	LMG	O6-C5-C6-O5
22	A	821	CLA	O1A-CGA-O2A-C1
22	6	312	CLA	C3-C5-C6-C7
31	5	319	LMG	O6-C5-C6-O5
22	B	830	CLA	C4-C3-C5-C6
22	B	837	CLA	C4-C3-C5-C6
22	1	311	CLA	C4-C3-C5-C6
29	4	301	CHL	C4-C3-C5-C6
22	B	830	CLA	C2-C3-C5-C6
22	B	837	CLA	C2-C3-C5-C6
22	1	311	CLA	C2-C3-C5-C6
29	4	301	CHL	C2-C3-C5-C6
22	A	836	CLA	CBD-CGD-O2D-CED
22	A	839	CLA	C2A-CAA-CBA-CGA
22	A	841	CLA	C2A-CAA-CBA-CGA
22	B	817	CLA	C2A-CAA-CBA-CGA
22	B	832	CLA	C2A-CAA-CBA-CGA
22	K	104	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	8	313	CLA	C2A-CAA-CBA-CGA
22	B	806	CLA	C2C-C3C-CAC-CBC
22	B	816	CLA	O1A-CGA-O2A-C1
22	B	831	CLA	O1A-CGA-O2A-C1
22	0	308	CLA	O1A-CGA-O2A-C1
22	B	825	CLA	O1D-CGD-O2D-CED
22	1	309	CLA	C4C-C3C-CAC-CBC
22	6	323	CLA	O1A-CGA-O2A-C1
22	A	840	CLA	CBA-CGA-O2A-C1
22	1	312	CLA	CBA-CGA-O2A-C1
22	4	310	CLA	CBA-CGA-O2A-C1
22	9	303	CLA	CBA-CGA-O2A-C1
29	0	301	CHL	O1D-CGD-O2D-CED
28	B	849	DGD	O6E-C5E-C6E-O5E
22	A	839	CLA	O1D-CGD-O2D-CED
22	1	308	CLA	O1D-CGD-O2D-CED
22	5	310	CLA	O1D-CGD-O2D-CED
29	8	314	CHL	O1D-CGD-O2D-CED
22	5	307	CLA	O1A-CGA-O2A-C1
29	4	301	CHL	O1A-CGA-O2A-C1
29	5	301	CHL	O1A-CGA-O2A-C1
22	3	301	CLA	O1D-CGD-O2D-CED
22	1	312	CLA	O1A-CGA-O2A-C1
22	4	310	CLA	O1A-CGA-O2A-C1
22	0	305	CLA	C2C-C3C-CAC-CBC
22	B	832	CLA	C3-C5-C6-C7
22	B	810	CLA	O1D-CGD-O2D-CED
29	4	307	CHL	O1D-CGD-O2D-CED
22	A	823	CLA	CBA-CGA-O2A-C1
22	A	841	CLA	CBA-CGA-O2A-C1
22	1	304	CLA	CBA-CGA-O2A-C1
22	1	311	CLA	CBA-CGA-O2A-C1
22	5	303	CLA	CBA-CGA-O2A-C1
22	7	312	CLA	CBA-CGA-O2A-C1
22	8	310	CLA	CBA-CGA-O2A-C1
22	0	304	CLA	CBA-CGA-O2A-C1
29	0	301	CHL	CBA-CGA-O2A-C1
29	4	301	CHL	C5-C6-C7-C8
22	B	821	CLA	CBD-CGD-O2D-CED
22	9	305	CLA	CBD-CGD-O2D-CED
25	A	847	8CT	C23-C24-C25-C26
25	A	849	8CT	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	B	804	8CT	C12-C13-C14-C15
25	B	804	8CT	C23-C24-C25-C26
25	B	848	8CT	C16-C17-C18-C19
25	1	316	8CT	C12-C13-C14-C15
25	7	323	8CT	C12-C13-C14-C15
30	1	314	XAT	C9-C10-C11-C12
24	1	317	LHG	C23-C24-C25-C26
22	H	201	CLA	C5-C6-C7-C8
22	5	312	CLA	C10-C11-C12-C13
22	9	303	CLA	O1A-CGA-O2A-C1
31	8	319	LMG	C4-C5-C6-O5
22	A	809	CLA	C8-C10-C11-C12
22	B	819	CLA	C10-C11-C12-C13
22	B	834	CLA	C8-C10-C11-C12
22	B	840	CLA	C5-C6-C7-C8
22	G	103	CLA	CBA-CGA-O2A-C1
31	5	319	LMG	C28-C29-C30-C31
22	1	303	CLA	C3-C5-C6-C7
22	6	301	CLA	C3-C5-C6-C7
22	0	304	CLA	C3-C5-C6-C7
22	3	308	CLA	O1D-CGD-O2D-CED
22	7	314	CLA	O1D-CGD-O2D-CED
24	A	844	LHG	O7-C5-C6-O8
22	8	310	CLA	O1A-CGA-O2A-C1
22	6	310	CLA	C4-C3-C5-C6
23	A	842	PQN	C14-C13-C15-C16
22	B	840	CLA	C2-C3-C5-C6
22	A	825	CLA	C6-C7-C8-C9
22	A	826	CLA	C14-C13-C15-C16
22	A	838	CLA	C11-C10-C8-C9
22	A	839	CLA	C6-C7-C8-C9
22	A	853	CLA	C6-C7-C8-C9
22	B	801	CLA	C6-C7-C8-C9
22	B	806	CLA	C6-C7-C8-C9
22	B	806	CLA	C14-C13-C15-C16
22	B	808	CLA	C11-C12-C13-C14
22	B	811	CLA	C6-C7-C8-C9
22	B	811	CLA	C14-C13-C15-C16
22	B	819	CLA	C6-C7-C8-C9
22	B	839	CLA	C11-C12-C13-C14
22	L	203	CLA	C11-C10-C8-C9
22	1	301	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	1	306	CLA	C6-C7-C8-C9
22	1	306	CLA	C14-C13-C15-C16
22	1	307	CLA	C6-C7-C8-C9
22	1	307	CLA	C11-C12-C13-C14
22	1	307	CLA	C14-C13-C15-C16
22	2	309	CLA	C11-C10-C8-C9
22	3	301	CLA	C11-C10-C8-C9
22	3	319	CLA	C11-C12-C13-C14
22	5	303	CLA	C11-C12-C13-C14
22	5	309	CLA	C6-C7-C8-C9
22	7	317	CLA	C11-C10-C8-C9
22	9	309	CLA	C6-C7-C8-C9
22	9	312	CLA	C11-C10-C8-C9
22	0	307	CLA	C6-C7-C8-C9
29	9	302	CHL	C6-C7-C8-C9
22	A	817	CLA	O1D-CGD-O2D-CED
22	A	833	CLA	O1D-CGD-O2D-CED
22	4	304	CLA	O1D-CGD-O2D-CED
22	6	323	CLA	O1D-CGD-O2D-CED
29	1	305	CHL	O1D-CGD-O2D-CED
22	1	311	CLA	CBD-CGD-O2D-CED
22	1	302	CLA	C15-C16-C17-C18
22	5	311	CLA	C2A-CAA-CBA-CGA
29	8	307	CHL	C2A-CAA-CBA-CGA
25	A	846	8CT	C10-C11-C12-C40
25	A	846	8CT	C14-C15-C16-C39
25	A	846	8CT	C22-C21-C23-C24
25	A	847	8CT	C27-C26-C28-C29
25	A	848	8CT	C10-C11-C12-C40
25	A	850	8CT	C14-C15-C16-C39
25	A	850	8CT	C27-C26-C28-C29
25	B	804	8CT	C10-C11-C12-C40
25	B	804	8CT	C22-C21-C23-C24
25	B	845	8CT	C10-C11-C12-C40
25	B	847	8CT	C27-C26-C28-C29
25	B	848	8CT	C14-C15-C16-C39
25	G	104	8CT	C14-C15-C16-C39
25	L	206	8CT	C14-C15-C16-C39
25	2	317	8CT	C27-C26-C28-C29
25	3	316	8CT	C14-C15-C16-C39
25	4	317	8CT	C14-C15-C16-C39
25	5	317	8CT	C10-C11-C12-C40

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Mol	Chain	Res	Type	Atoms
25	7	301	8CT	C14-C15-C16-C39
25	7	323	8CT	C10-C11-C12-C40
25	7	323	8CT	C14-C15-C16-C39
25	8	301	8CT	C10-C11-C12-C40
25	8	301	8CT	C14-C15-C16-C39
25	8	318	8CT	C10-C11-C12-C40
25	8	318	8CT	C22-C21-C23-C24
30	1	314	XAT	C27-C28-C29-C39
30	2	316	XAT	C7-C8-C9-C19
30	4	315	XAT	C27-C28-C29-C39
30	7	319	XAT	C31-C32-C33-C40
30	8	316	XAT	C27-C28-C29-C39
25	A	846	8CT	C10-C11-C12-C13
25	A	846	8CT	C14-C15-C16-C17
25	A	847	8CT	C25-C26-C28-C29
25	A	848	8CT	C10-C11-C12-C13
25	A	849	8CT	C25-C26-C28-C29
25	A	850	8CT	C14-C15-C16-C17
25	A	850	8CT	C25-C26-C28-C29
25	B	804	8CT	C10-C11-C12-C13
25	B	804	8CT	C20-C21-C23-C24
25	B	845	8CT	C10-C11-C12-C13
25	B	847	8CT	C25-C26-C28-C29
25	B	848	8CT	C14-C15-C16-C17
25	G	104	8CT	C14-C15-C16-C17
25	L	206	8CT	C14-C15-C16-C17
25	2	317	8CT	C25-C26-C28-C29
25	5	317	8CT	C10-C11-C12-C13
25	7	301	8CT	C14-C15-C16-C17
25	7	321	8CT	C10-C11-C12-C13
25	7	323	8CT	C10-C11-C12-C13
25	7	323	8CT	C14-C15-C16-C17
25	8	301	8CT	C10-C11-C12-C13
25	8	301	8CT	C14-C15-C16-C17
25	8	318	8CT	C10-C11-C12-C13
30	1	314	XAT	C27-C28-C29-C30
30	2	316	XAT	C7-C8-C9-C10
30	4	315	XAT	C27-C28-C29-C30
30	4	316	XAT	C27-C28-C29-C30
30	7	319	XAT	C31-C32-C33-C34
30	8	316	XAT	C27-C28-C29-C30
22	A	841	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	5	303	CLA	O1A-CGA-O2A-C1
29	0	301	CHL	O1A-CGA-O2A-C1
22	A	811	CLA	C13-C15-C16-C17
22	A	818	CLA	C15-C16-C17-C18
22	A	829	CLA	C13-C15-C16-C17
22	6	313	CLA	C13-C15-C16-C17
29	2	301	CHL	C10-C11-C12-C13
29	4	305	CHL	C5-C6-C7-C8
22	G	102	CLA	O1D-CGD-O2D-CED
22	L	203	CLA	O1D-CGD-O2D-CED
26	A	851	HTG	O5-C5-C6-O6
22	2	303	CLA	O1D-CGD-O2D-CED
22	B	813	CLA	C3-C5-C6-C7
22	A	807	CLA	CBA-CGA-O2A-C1
22	8	315	CLA	CBA-CGA-O2A-C1
22	A	825	CLA	C13-C15-C16-C17
22	A	827	CLA	C8-C10-C11-C12
22	B	801	CLA	C5-C6-C7-C8
22	B	812	CLA	C8-C10-C11-C12
22	B	820	CLA	C8-C10-C11-C12
22	B	832	CLA	C8-C10-C11-C12
22	B	836	CLA	C5-C6-C7-C8
22	1	306	CLA	C10-C11-C12-C13
22	0	311	CLA	C15-C16-C17-C18
29	5	301	CHL	C5-C6-C7-C8
24	6	322	LHG	C23-C24-C25-C26
29	2	306	CHL	O1D-CGD-O2D-CED
22	1	307	CLA	CBD-CGD-O2D-CED
22	8	312	CLA	CBD-CGD-O2D-CED
29	0	306	CHL	C2C-C3C-CAC-CBC
22	A	828	CLA	C10-C11-C12-C13
22	A	828	CLA	C15-C16-C17-C18
22	A	840	CLA	C13-C15-C16-C17
22	B	808	CLA	C15-C16-C17-C18
22	B	809	CLA	C5-C6-C7-C8
22	B	809	CLA	C15-C16-C17-C18
22	B	810	CLA	C13-C15-C16-C17
22	B	811	CLA	C8-C10-C11-C12
22	B	817	CLA	C5-C6-C7-C8
22	B	830	CLA	C5-C6-C7-C8
22	B	832	CLA	C15-C16-C17-C18
22	2	303	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	6	303	CLA	C10-C11-C12-C13
22	6	304	CLA	C5-C6-C7-C8
22	6	304	CLA	C15-C16-C17-C18
22	6	310	CLA	C8-C10-C11-C12
22	6	311	CLA	C15-C16-C17-C18
22	8	309	CLA	C10-C11-C12-C13
22	9	308	CLA	C5-C6-C7-C8
23	A	842	PQN	C15-C16-C17-C18
29	6	302	CHL	C10-C11-C12-C13
29	0	301	CHL	C8-C10-C11-C12
22	7	302	CLA	O1A-CGA-O2A-C1
24	3	317	LHG	O1-C1-C2-O2
24	A	844	LHG	C23-C24-C25-C26
24	6	322	LHG	C7-C8-C9-C10
22	1	313	CLA	CBD-CGD-O2D-CED
22	A	838	CLA	C5-C6-C7-C8
22	B	834	CLA	C5-C6-C7-C8
22	2	309	CLA	C8-C10-C11-C12
22	7	318	CLA	C10-C11-C12-C13
22	A	805	CLA	C2-C1-O2A-CGA
22	A	841	CLA	C2-C1-O2A-CGA
22	B	834	CLA	C2-C1-O2A-CGA
22	5	303	CLA	C2-C1-O2A-CGA
22	8	315	CLA	C2-C1-O2A-CGA
24	5	318	LHG	C32-C33-C34-C35
22	B	816	CLA	C5-C6-C7-C8
22	6	311	CLA	C5-C6-C7-C8
22	5	307	CLA	C10-C11-C12-C13
22	0	302	CLA	C5-C6-C7-C8
24	9	316	LHG	C23-C24-C25-C26
22	7	318	CLA	CBD-CGD-O2D-CED
22	3	319	CLA	C5-C6-C7-C8
22	6	313	CLA	C15-C16-C17-C18
22	1	301	CLA	O1D-CGD-O2D-CED
22	0	304	CLA	O1D-CGD-O2D-CED
22	A	809	CLA	C6-C7-C8-C10
22	A	827	CLA	C6-C7-C8-C10
22	A	828	CLA	C11-C10-C8-C7
22	A	838	CLA	C11-C12-C13-C15
22	A	840	CLA	C6-C7-C8-C10
22	B	803	CLA	C6-C7-C8-C10
22	B	809	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	B	833	CLA	C6-C7-C8-C10
22	B	837	CLA	C6-C7-C8-C10
22	H	201	CLA	C11-C12-C13-C15
22	3	301	CLA	C11-C10-C8-C7
22	5	307	CLA	C12-C13-C15-C16
22	7	316	CLA	C12-C13-C15-C16
22	8	315	CLA	C12-C13-C15-C16
22	9	308	CLA	C12-C13-C15-C16
22	A	821	CLA	C3-C5-C6-C7
22	B	819	CLA	C3-C5-C6-C7
22	6	304	CLA	C3-C5-C6-C7
23	B	842	PQN	C13-C15-C16-C17
22	1	311	CLA	O1A-CGA-O2A-C1
22	7	312	CLA	O1A-CGA-O2A-C1
25	A	846	8CT	C12-C13-C14-C15
25	A	854	8CT	C23-C24-C25-C26
25	B	847	8CT	C12-C13-C14-C15
25	B	851	8CT	C18-C19-C20-C21
25	G	104	8CT	C16-C17-C18-C19
25	I	101	8CT	C18-C19-C20-C21
25	J	101	8CT	C23-C24-C25-C26
25	3	316	8CT	C18-C19-C20-C21
25	6	321	8CT	C18-C19-C20-C21
25	8	301	8CT	C12-C13-C14-C15
25	8	318	8CT	C16-C17-C18-C19
30	0	313	XAT	C33-C34-C35-C15
22	9	312	CLA	CBA-CGA-O2A-C1
22	A	808	CLA	C2A-CAA-CBA-CGA
22	A	840	CLA	C2A-CAA-CBA-CGA
22	B	803	CLA	C2A-CAA-CBA-CGA
22	B	822	CLA	C2A-CAA-CBA-CGA
22	K	102	CLA	C2A-CAA-CBA-CGA
22	4	310	CLA	C2A-CAA-CBA-CGA
22	6	317	CLA	C2A-CAA-CBA-CGA
22	7	305	CLA	C2A-CAA-CBA-CGA
22	8	304	CLA	C2A-CAA-CBA-CGA
29	5	306	CHL	C2A-CAA-CBA-CGA
22	A	804	CLA	O1D-CGD-O2D-CED
22	A	819	CLA	O1D-CGD-O2D-CED
22	A	820	CLA	O1D-CGD-O2D-CED
22	B	819	CLA	O1D-CGD-O2D-CED
22	B	837	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	7	313	CLA	O1D-CGD-O2D-CED
22	7	315	CLA	O1D-CGD-O2D-CED
29	8	305	CHL	O1D-CGD-O2D-CED
22	A	826	CLA	C13-C15-C16-C17
22	A	832	CLA	C10-C11-C12-C13
22	B	809	CLA	C10-C11-C12-C13
22	B	818	CLA	C5-C6-C7-C8
22	2	302	CLA	C5-C6-C7-C8
22	2	302	CLA	C13-C15-C16-C17
22	2	309	CLA	C10-C11-C12-C13
22	4	309	CLA	C10-C11-C12-C13
22	9	309	CLA	C5-C6-C7-C8
23	B	842	PQN	C18-C20-C21-C22
22	0	304	CLA	O1A-CGA-O2A-C1
22	B	809	CLA	CBD-CGD-O2D-CED
29	2	301	CHL	CBD-CGD-O2D-CED
22	A	836	CLA	C2C-C3C-CAC-CBC
24	7	322	LHG	O2-C2-C3-O3
31	8	319	LMG	O9-C10-O7-C8
22	A	827	CLA	C3-C5-C6-C7
29	6	302	CHL	C3-C5-C6-C7
22	B	803	CLA	C13-C15-C16-C17
22	B	810	CLA	C10-C11-C12-C13
22	B	811	CLA	C13-C15-C16-C17
22	B	828	CLA	C8-C10-C11-C12
22	B	836	CLA	C8-C10-C11-C12
22	1	306	CLA	C8-C10-C11-C12
22	5	307	CLA	C5-C6-C7-C8
22	8	309	CLA	C5-C6-C7-C8
22	0	307	CLA	C10-C11-C12-C13
22	A	823	CLA	O1A-CGA-O2A-C1
22	A	840	CLA	O1A-CGA-O2A-C1
22	1	304	CLA	O1A-CGA-O2A-C1
22	1	313	CLA	CBA-CGA-O2A-C1
22	A	810	CLA	O1D-CGD-O2D-CED
22	A	821	CLA	C15-C16-C17-C18
22	A	826	CLA	C15-C16-C17-C18
22	B	808	CLA	C8-C10-C11-C12
22	B	820	CLA	C10-C11-C12-C13
22	B	824	CLA	C5-C6-C7-C8
22	B	825	CLA	C13-C15-C16-C17
22	B	841	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	L	202	CLA	C13-C15-C16-C17
22	1	302	CLA	C5-C6-C7-C8
22	1	311	CLA	C13-C15-C16-C17
22	4	314	CLA	C8-C10-C11-C12
22	7	318	CLA	C5-C6-C7-C8
22	0	303	CLA	C5-C6-C7-C8
29	4	301	CHL	C10-C11-C12-C13
22	B	841	CLA	O1D-CGD-O2D-CED
22	5	309	CLA	O1D-CGD-O2D-CED
22	A	807	CLA	O1A-CGA-O2A-C1
22	8	315	CLA	O1A-CGA-O2A-C1
22	0	305	CLA	C4C-C3C-CAC-CBC
22	A	828	CLA	C13-C15-C16-C17
22	A	839	CLA	C8-C10-C11-C12
22	A	841	CLA	C15-C16-C17-C18
22	B	806	CLA	C8-C10-C11-C12
22	B	814	CLA	C10-C11-C12-C13
22	2	304	CLA	C10-C11-C12-C13
22	3	319	CLA	C10-C11-C12-C13
22	6	305	CLA	C10-C11-C12-C13
22	8	315	CLA	C13-C15-C16-C17
22	0	308	CLA	C10-C11-C12-C13
23	B	842	PQN	C20-C21-C22-C23
24	A	845	LHG	C3-O3-P-O6
24	A	845	LHG	C4-O6-P-O3
24	2	318	LHG	C3-O3-P-O6
24	2	318	LHG	C4-O6-P-O3
24	5	318	LHG	C4-O6-P-O3
24	7	322	LHG	C3-O3-P-O6
24	7	322	LHG	C4-O6-P-O3
24	0	315	LHG	C3-O3-P-O6
24	5	318	LHG	C7-C8-C9-C10
22	9	308	CLA	C3-C5-C6-C7
22	3	307	CLA	CBA-CGA-O2A-C1
22	4	304	CLA	CBA-CGA-O2A-C1
22	6	313	CLA	CBA-CGA-O2A-C1
29	5	306	CHL	CBA-CGA-O2A-C1
29	9	302	CHL	CBA-CGA-O2A-C1
22	A	806	CLA	C8-C10-C11-C12
22	B	832	CLA	C10-C11-C12-C13
22	9	304	CLA	O1D-CGD-O2D-CED
24	A	845	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
24	1	317	LHG	C1-C2-C3-O3
24	7	322	LHG	C1-C2-C3-O3
22	A	828	CLA	C4-C3-C5-C6
22	A	832	CLA	C4-C3-C5-C6
22	9	308	CLA	C4-C3-C5-C6
22	5	303	CLA	C2-C3-C5-C6
22	A	825	CLA	C10-C11-C12-C13
22	1	302	CLA	C10-C11-C12-C13
22	7	303	CLA	C5-C6-C7-C8
22	B	815	CLA	C2A-CAA-CBA-CGA
22	7	313	CLA	C2A-CAA-CBA-CGA
22	9	306	CLA	C2A-CAA-CBA-CGA
22	0	308	CLA	C2A-CAA-CBA-CGA
22	M	101	CLA	C2A-CAA-CBA-CGA
22	B	803	CLA	C16-C17-C18-C19
22	L	203	CLA	C16-C17-C18-C19
22	2	304	CLA	C11-C12-C13-C15
22	3	319	CLA	C16-C17-C18-C19
22	7	303	CLA	C11-C12-C13-C15
22	A	808	CLA	C3-C5-C6-C7
22	A	809	CLA	C3-C5-C6-C7
22	1	302	CLA	C3-C5-C6-C7
22	A	824	CLA	CBA-CGA-O2A-C1
22	2	314	CLA	CBA-CGA-O2A-C1
22	0	311	CLA	CBA-CGA-O2A-C1
29	6	316	CHL	O1D-CGD-O2D-CED
25	A	846	8CT	C16-C17-C18-C19
25	F	302	8CT	C12-C13-C14-C15
25	I	101	8CT	C16-C17-C18-C19
25	L	206	8CT	C12-C13-C14-C15
25	L	206	8CT	C16-C17-C18-C19
25	L	206	8CT	C18-C19-C20-C21
25	1	316	8CT	C23-C24-C25-C26
24	5	318	LHG	C11-C10-C9-C8
31	5	319	LMG	C17-C18-C19-C20
22	6	318	CLA	CBD-CGD-O2D-CED
24	A	844	LHG	C8-C7-O7-C5
24	0	315	LHG	C8-C7-O7-C5
22	A	830	CLA	C13-C15-C16-C17
22	B	830	CLA	C10-C11-C12-C13
22	5	312	CLA	C13-C15-C16-C17
22	0	312	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	B	809	CLA	C3-C5-C6-C7
22	B	812	CLA	C3-C5-C6-C7
22	B	841	CLA	C3-C5-C6-C7
22	0	307	CLA	C3-C5-C6-C7
24	A	844	LHG	C27-C28-C29-C30
24	A	845	LHG	C9-C10-C11-C12
24	1	317	LHG	C13-C14-C15-C16
24	1	317	LHG	C14-C15-C16-C17
22	A	827	CLA	C16-C17-C18-C19
22	B	813	CLA	C6-C7-C8-C10
22	L	201	CLA	C16-C17-C18-C19
22	6	305	CLA	C11-C12-C13-C14
22	6	311	CLA	C16-C17-C18-C19
22	8	302	CLA	C11-C12-C13-C15
22	9	309	CLA	C11-C12-C13-C14
29	4	305	CHL	C6-C7-C8-C9
22	A	801	CLA	CBA-CGA-O2A-C1
22	B	826	CLA	CBA-CGA-O2A-C1
22	9	306	CLA	CBA-CGA-O2A-C1
24	6	322	LHG	C26-C27-C28-C29
24	5	318	LHG	C13-C14-C15-C16
22	A	807	CLA	C13-C15-C16-C17
22	2	302	CLA	C15-C16-C17-C18
31	8	319	LMG	C10-C11-C12-C13
22	A	828	CLA	CBD-CGD-O2D-CED
31	4	318	LMG	C21-C22-C23-C24
22	A	809	CLA	O1D-CGD-O2D-CED
22	1	312	CLA	O1D-CGD-O2D-CED
22	5	305	CLA	C3-C5-C6-C7
28	B	849	DGD	C2E-C1E-O5D-C6D
22	2	312	CLA	CBA-CGA-O2A-C1
29	8	305	CHL	CBA-CGA-O2A-C1
24	0	315	LHG	C34-C35-C36-C37
22	1	301	CLA	C16-C17-C18-C19
22	7	317	CLA	C16-C17-C18-C19
22	0	307	CLA	C16-C17-C18-C19
29	6	302	CHL	C11-C12-C13-C15
22	A	801	CLA	C4-C3-C5-C6
22	A	808	CLA	C4-C3-C5-C6
22	B	805	CLA	C4-C3-C5-C6
22	2	312	CLA	C4-C3-C5-C6
22	5	305	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	0	307	CLA	C4-C3-C5-C6
24	A	844	LHG	C10-C11-C12-C13
24	1	317	LHG	C9-C10-C11-C12
24	6	322	LHG	C24-C25-C26-C27
24	0	315	LHG	C9-C10-C11-C12
24	0	315	LHG	C12-C13-C14-C15
22	A	808	CLA	C2-C3-C5-C6
22	9	308	CLA	C2-C3-C5-C6
22	A	805	CLA	C11-C12-C13-C14
22	A	808	CLA	C11-C12-C13-C14
22	A	826	CLA	C11-C12-C13-C14
22	A	827	CLA	C6-C7-C8-C9
22	A	837	CLA	C6-C7-C8-C9
22	A	838	CLA	C6-C7-C8-C9
22	B	806	CLA	C11-C10-C8-C9
22	B	827	CLA	C11-C10-C8-C9
22	3	319	CLA	C11-C10-C8-C9
22	0	308	CLA	C6-C7-C8-C9
22	9	301	CLA	O1D-CGD-O2D-CED
29	8	307	CHL	O1D-CGD-O2D-CED
31	4	318	LMG	C28-C29-C30-C31
24	1	317	LHG	C15-C16-C17-C18
24	1	317	LHG	C32-C33-C34-C35
22	A	826	CLA	C8-C10-C11-C12
22	3	311	CLA	C5-C6-C7-C8
29	5	301	CHL	C8-C10-C11-C12
22	A	829	CLA	C2A-CAA-CBA-CGA
22	A	843	CLA	C2A-CAA-CBA-CGA
22	3	312	CLA	C2A-CAA-CBA-CGA
22	6	313	CLA	C2A-CAA-CBA-CGA
22	7	303	CLA	C2A-CAA-CBA-CGA
22	9	312	CLA	O1A-CGA-O2A-C1
25	A	849	8CT	C27-C26-C28-C29
25	B	804	8CT	C14-C15-C16-C39
25	F	302	8CT	C10-C11-C12-C40
25	L	206	8CT	C10-C11-C12-C40
25	2	317	8CT	C22-C21-C23-C24
25	6	321	8CT	C22-C21-C23-C24
25	7	301	8CT	C22-C21-C23-C24
25	7	321	8CT	C10-C11-C12-C40
25	7	323	8CT	C22-C21-C23-C24
30	4	316	XAT	C27-C28-C29-C39

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Mol	Chain	Res	Type	Atoms
24	B	852	LHG	O1-C1-C2-C3
24	1	317	LHG	O1-C1-C2-C3
24	2	318	LHG	O1-C1-C2-C3
24	5	318	LHG	O1-C1-C2-C3
24	9	316	LHG	O1-C1-C2-C3
25	B	804	8CT	C14-C15-C16-C17
25	B	846	8CT	C25-C26-C28-C29
25	B	848	8CT	C10-C11-C12-C13
25	F	302	8CT	C10-C11-C12-C13
25	L	206	8CT	C10-C11-C12-C13
25	2	317	8CT	C20-C21-C23-C24
25	3	316	8CT	C14-C15-C16-C17
25	6	321	8CT	C20-C21-C23-C24
25	7	301	8CT	C20-C21-C23-C24
25	7	321	8CT	C20-C21-C23-C24
25	7	323	8CT	C20-C21-C23-C24
30	0	313	XAT	C7-C8-C9-C10
22	B	834	CLA	C10-C11-C12-C13
22	6	310	CLA	C5-C6-C7-C8
24	5	318	LHG	C27-C28-C29-C30
28	B	849	DGD	C8A-C9A-CAA-CBA
28	B	849	DGD	CAA-CBA-CCA-CDA
22	3	312	CLA	CBD-CGD-O2D-CED
24	2	318	LHG	C23-C24-C25-C26
24	9	316	LHG	C16-C17-C18-C19
22	A	824	CLA	C6-C7-C8-C10
22	B	803	CLA	C16-C17-C18-C20
22	B	815	CLA	C16-C17-C18-C19
22	B	825	CLA	C16-C17-C18-C19
22	B	825	CLA	C16-C17-C18-C20
22	L	201	CLA	C16-C17-C18-C20
22	L	203	CLA	C16-C17-C18-C20
22	2	304	CLA	C11-C12-C13-C14
22	2	312	CLA	C16-C17-C18-C20
22	7	303	CLA	C11-C12-C13-C14
22	8	302	CLA	C11-C12-C13-C14
29	4	305	CHL	C6-C7-C8-C10
28	B	849	DGD	O6E-C1E-O5D-C6D
22	A	853	CLA	C15-C16-C17-C18
22	1	308	CLA	C8-C10-C11-C12
22	0	302	CLA	C15-C16-C17-C18
28	B	849	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
22	3	304	CLA	CBD-CGD-O2D-CED
22	2	313	CLA	O1D-CGD-O2D-CED
31	4	318	LMG	C17-C18-C19-C20
24	A	844	LHG	C7-C8-C9-C10
24	5	318	LHG	C23-C24-C25-C26
22	0	307	CLA	C8-C10-C11-C12
29	9	302	CHL	C5-C6-C7-C8
22	2	314	CLA	O1A-CGA-O2A-C1
22	4	304	CLA	O1A-CGA-O2A-C1
29	5	306	CHL	O1A-CGA-O2A-C1
24	1	317	LHG	C27-C28-C29-C30
22	A	818	CLA	C3-C5-C6-C7
22	0	302	CLA	C3-C5-C6-C7
22	2	308	CLA	CBA-CGA-O2A-C1
22	2	311	CLA	CBA-CGA-O2A-C1
24	A	844	LHG	C9-C10-C11-C12
31	4	318	LMG	C18-C19-C20-C21
22	0	312	CLA	O1D-CGD-O2D-CED
29	8	306	CHL	O1D-CGD-O2D-CED
22	A	803	CLA	C3A-C2A-CAA-CBA
22	A	806	CLA	C3A-C2A-CAA-CBA
22	A	813	CLA	C3A-C2A-CAA-CBA
22	A	853	CLA	C3A-C2A-CAA-CBA
22	B	829	CLA	C3A-C2A-CAA-CBA
22	B	832	CLA	C3A-C2A-CAA-CBA
22	B	850	CLA	C3A-C2A-CAA-CBA
22	H	201	CLA	C3A-C2A-CAA-CBA
22	1	302	CLA	C3A-C2A-CAA-CBA
22	1	304	CLA	C3A-C2A-CAA-CBA
22	1	310	CLA	C3A-C2A-CAA-CBA
22	3	311	CLA	C3A-C2A-CAA-CBA
22	7	318	CLA	C3A-C2A-CAA-CBA
22	9	311	CLA	C3A-C2A-CAA-CBA
22	0	312	CLA	C3A-C2A-CAA-CBA
22	5	303	CLA	C15-C16-C17-C18
22	A	835	CLA	O1D-CGD-O2D-CED
22	8	309	CLA	O1D-CGD-O2D-CED
22	3	307	CLA	O1A-CGA-O2A-C1
22	6	313	CLA	O1A-CGA-O2A-C1
22	B	815	CLA	C16-C17-C18-C20
22	B	836	CLA	C11-C12-C13-C14
22	1	301	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	2	312	CLA	C16-C17-C18-C19
22	3	301	CLA	C11-C12-C13-C14
22	9	309	CLA	C11-C12-C13-C15
29	6	302	CHL	C11-C12-C13-C14
29	0	301	CHL	C11-C12-C13-C15
24	A	844	LHG	C12-C13-C14-C15
29	5	301	CHL	CBD-CGD-O2D-CED
22	L	202	CLA	C3-C5-C6-C7
22	7	316	CLA	C10-C11-C12-C13
22	9	308	CLA	C15-C16-C17-C18
22	0	307	CLA	C15-C16-C17-C18
22	A	817	CLA	C4-C3-C5-C6
22	A	825	CLA	C4-C3-C5-C6
22	B	808	CLA	C4-C3-C5-C6
22	1	306	CLA	C4-C3-C5-C6
22	1	307	CLA	C4-C3-C5-C6
22	3	311	CLA	C4-C3-C5-C6
22	A	801	CLA	C2-C3-C5-C6
22	A	825	CLA	C2-C3-C5-C6
22	B	808	CLA	C2-C3-C5-C6
22	1	306	CLA	C2-C3-C5-C6
22	3	311	CLA	C2-C3-C5-C6
22	5	305	CLA	C2-C3-C5-C6
24	6	322	LHG	C8-C7-O7-C5
24	1	317	LHG	O1-C1-C2-O2
24	6	322	LHG	O1-C1-C2-O2
24	7	322	LHG	O1-C1-C2-O2
24	6	322	LHG	C25-C26-C27-C28
31	5	319	LMG	C18-C19-C20-C21
31	8	319	LMG	C16-C17-C18-C19
24	B	852	LHG	C7-C8-C9-C10
22	A	824	CLA	O1A-CGA-O2A-C1
29	9	302	CHL	O1A-CGA-O2A-C1
22	B	813	CLA	C6-C7-C8-C9
22	B	819	CLA	C11-C12-C13-C14
22	1	302	CLA	C16-C17-C18-C19
22	6	311	CLA	C16-C17-C18-C20
22	B	806	CLA	C4C-C3C-CAC-CBC
22	G	103	CLA	O1A-CGA-O2A-C1
22	0	311	CLA	O1A-CGA-O2A-C1
22	A	825	CLA	C15-C16-C17-C18
22	B	814	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	6	303	CLA	C13-C15-C16-C17
24	A	844	LHG	C11-C10-C9-C8
24	1	317	LHG	C11-C10-C9-C8
28	B	849	DGD	C7B-C8B-C9B-CAB
22	A	843	CLA	C2-C1-O2A-CGA
22	4	314	CLA	C2-C1-O2A-CGA
22	B	801	CLA	C10-C11-C12-C13
22	B	803	CLA	C8-C10-C11-C12
22	L	201	CLA	C15-C16-C17-C18
22	L	203	CLA	C5-C6-C7-C8
22	B	826	CLA	O1A-CGA-O2A-C1
22	2	312	CLA	O1A-CGA-O2A-C1
22	9	306	CLA	O1A-CGA-O2A-C1
29	8	305	CHL	O1A-CGA-O2A-C1
22	6	305	CLA	C11-C12-C13-C15
22	0	307	CLA	C16-C17-C18-C20
22	B	811	CLA	C3-C5-C6-C7
25	A	848	8CT	C04-C03-C10-C11
25	B	804	8CT	C02-C03-C10-C11
25	B	843	8CT	C02-C03-C10-C11
25	B	843	8CT	C04-C03-C10-C11
25	B	851	8CT	C02-C03-C10-C11
25	F	302	8CT	C04-C03-C10-C11
25	G	104	8CT	C04-C03-C10-C11
25	I	101	8CT	C02-C03-C10-C11
25	I	101	8CT	C04-C03-C10-C11
25	J	101	8CT	C02-C03-C10-C11
25	J	101	8CT	C04-C03-C10-C11
25	K	103	8CT	C02-C03-C10-C11
25	L	205	8CT	C04-C03-C10-C11
25	L	206	8CT	C02-C03-C10-C11
25	3	316	8CT	C02-C03-C10-C11
25	6	321	8CT	C02-C03-C10-C11
25	5	317	8CT	C02-C03-C10-C11
25	7	321	8CT	C02-C03-C10-C11
25	8	318	8CT	C02-C03-C10-C11
24	0	315	LHG	C33-C34-C35-C36
22	A	807	CLA	C8-C10-C11-C12
22	A	807	CLA	C15-C16-C17-C18
22	A	833	CLA	C8-C10-C11-C12
22	B	806	CLA	C10-C11-C12-C13
22	B	814	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	0	303	CLA	C15-C16-C17-C18
22	0	311	CLA	C5-C6-C7-C8
22	4	309	CLA	O1D-CGD-O2D-CED
22	A	801	CLA	O1A-CGA-O2A-C1
31	4	318	LMG	C10-C11-C12-C13
24	5	318	LHG	C30-C31-C32-C33
31	8	319	LMG	C19-C20-C21-C22
22	A	838	CLA	C4-C3-C5-C6
22	B	850	CLA	O1D-CGD-O2D-CED
22	2	311	CLA	O1D-CGD-O2D-CED
22	A	803	CLA	C12-C13-C15-C16
22	A	805	CLA	C11-C12-C13-C15
22	A	806	CLA	C11-C12-C13-C15
22	A	807	CLA	C11-C12-C13-C15
22	A	811	CLA	C12-C13-C15-C16
22	A	818	CLA	C11-C12-C13-C15
22	A	825	CLA	C11-C10-C8-C7
22	A	826	CLA	C11-C12-C13-C15
22	A	837	CLA	C6-C7-C8-C10
22	A	837	CLA	C12-C13-C15-C16
22	A	838	CLA	C2-C3-C5-C6
22	A	838	CLA	C6-C7-C8-C10
22	A	838	CLA	C11-C10-C8-C7
22	A	838	CLA	C12-C13-C15-C16
22	A	839	CLA	C6-C7-C8-C10
22	B	805	CLA	C2-C3-C5-C6
22	B	806	CLA	C11-C10-C8-C7
22	B	811	CLA	C6-C7-C8-C10
22	B	827	CLA	C11-C10-C8-C7
22	B	832	CLA	C2-C3-C5-C6
22	1	306	CLA	C6-C7-C8-C10
22	1	307	CLA	C2-C3-C5-C6
22	2	304	CLA	C11-C10-C8-C7
22	2	312	CLA	C2-C3-C5-C6
22	3	319	CLA	C11-C10-C8-C7
22	5	303	CLA	C6-C7-C8-C10
22	7	316	CLA	C11-C12-C13-C15
22	7	317	CLA	C11-C10-C8-C7
22	7	318	CLA	C11-C12-C13-C15
22	0	303	CLA	C11-C12-C13-C15
22	0	307	CLA	C11-C12-C13-C15
22	0	308	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	2	308	CLA	O1A-CGA-O2A-C1
22	2	311	CLA	O1A-CGA-O2A-C1
24	2	318	LHG	O10-C23-O8-C6
22	2	309	CLA	C5-C6-C7-C8
22	2	312	CLA	C13-C15-C16-C17
25	B	845	8CT	C12-C13-C14-C15
22	6	303	CLA	C16-C17-C18-C19
22	7	317	CLA	C16-C17-C18-C20
24	0	315	LHG	O9-C7-O7-C5
22	A	804	CLA	CBA-CGA-O2A-C1
22	A	830	CLA	CBA-CGA-O2A-C1
22	B	813	CLA	CBA-CGA-O2A-C1
22	B	829	CLA	CBA-CGA-O2A-C1
22	B	839	CLA	CBA-CGA-O2A-C1
22	8	304	CLA	CBA-CGA-O2A-C1
22	9	305	CLA	CBA-CGA-O2A-C1
22	9	309	CLA	CBA-CGA-O2A-C1
26	A	851	HTG	C4-C5-C6-O6
22	A	817	CLA	C2A-CAA-CBA-CGA
22	B	807	CLA	C2A-CAA-CBA-CGA
22	G	101	CLA	C2A-CAA-CBA-CGA
22	1	307	CLA	C2A-CAA-CBA-CGA
29	8	306	CHL	C2A-CAA-CBA-CGA
22	1	306	CLA	C13-C15-C16-C17
22	5	307	CLA	C13-C15-C16-C17
22	0	307	CLA	C5-C6-C7-C8
31	4	318	LMG	O6-C5-C6-O5
24	2	318	LHG	C7-C8-C9-C10
22	A	811	CLA	C8-C10-C11-C12
22	B	806	CLA	C5-C6-C7-C8
22	A	853	CLA	C3-C5-C6-C7
29	6	316	CHL	C2C-C3C-CAC-CBC
31	5	319	LMG	C16-C17-C18-C19
22	7	318	CLA	O1D-CGD-O2D-CED
29	3	306	CHL	O1D-CGD-O2D-CED
24	9	316	LHG	C8-C7-O7-C5
22	A	803	CLA	C5-C6-C7-C8
22	A	808	CLA	C15-C16-C17-C18
22	0	311	CLA	C10-C11-C12-C13
24	0	315	LHG	C27-C28-C29-C30
22	A	819	CLA	C3-C5-C6-C7
28	B	849	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
24	5	318	LHG	O7-C5-C6-O8
26	J	102	HTG	O5-C5-C6-O6
28	B	849	DGD	C4B-C5B-C6B-C7B
22	A	827	CLA	C16-C17-C18-C20
22	3	319	CLA	C16-C17-C18-C20
22	5	303	CLA	C16-C17-C18-C19
24	A	844	LHG	C29-C30-C31-C32
22	6	315	CLA	C5-C6-C7-C8
22	B	818	CLA	O1D-CGD-O2D-CED
22	A	829	CLA	C4-C3-C5-C6
22	B	832	CLA	C4-C3-C5-C6
22	0	302	CLA	C4-C3-C5-C6
22	A	828	CLA	C2-C3-C5-C6
22	A	832	CLA	C2-C3-C5-C6
22	6	310	CLA	C2-C3-C5-C6
22	0	307	CLA	C2-C3-C5-C6
23	A	842	PQN	C12-C13-C15-C16
26	J	102	HTG	C3'-C4'-C5'-C6'
22	A	803	CLA	C14-C13-C15-C16
22	A	806	CLA	C11-C12-C13-C14
22	A	807	CLA	C6-C7-C8-C9
22	A	817	CLA	C11-C10-C8-C9
22	A	817	CLA	C11-C12-C13-C14
22	A	818	CLA	C11-C12-C13-C14
22	A	826	CLA	C11-C10-C8-C9
22	A	828	CLA	C11-C10-C8-C9
22	A	838	CLA	C11-C12-C13-C14
22	B	809	CLA	C14-C13-C15-C16
22	B	832	CLA	C6-C7-C8-C9
22	B	833	CLA	C6-C7-C8-C9
22	B	836	CLA	C6-C7-C8-C9
22	B	837	CLA	C6-C7-C8-C9
22	B	839	CLA	C14-C13-C15-C16
22	H	201	CLA	C11-C12-C13-C14
22	2	304	CLA	C11-C10-C8-C9
22	4	314	CLA	C14-C13-C15-C16
22	6	315	CLA	C14-C13-C15-C16
22	7	303	CLA	C6-C7-C8-C9
22	7	316	CLA	C11-C12-C13-C14
22	7	318	CLA	C11-C12-C13-C14
22	9	308	CLA	C14-C13-C15-C16
22	0	303	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	2	301	CHL	C6-C7-C8-C9
22	A	838	CLA	CBD-CGD-O2D-CED
22	B	831	CLA	CBD-CGD-O2D-CED
22	2	309	CLA	CBD-CGD-O2D-CED
29	5	301	CHL	C3-C5-C6-C7
22	A	806	CLA	C2A-CAA-CBA-CGA
22	A	828	CLA	C2A-CAA-CBA-CGA
22	A	852	CLA	C2A-CAA-CBA-CGA
22	B	828	CLA	C2A-CAA-CBA-CGA
22	1	303	CLA	C2A-CAA-CBA-CGA
22	3	311	CLA	C2A-CAA-CBA-CGA
22	9	303	CLA	C2A-CAA-CBA-CGA
24	1	317	LHG	C12-C13-C14-C15
25	B	848	8CT	C10-C11-C12-C40
25	4	317	8CT	C10-C11-C12-C40
22	1	311	CLA	O1D-CGD-O2D-CED
22	B	837	CLA	C15-C16-C17-C18
24	A	844	LHG	C24-C25-C26-C27
24	1	317	LHG	C30-C31-C32-C33
24	9	316	LHG	C24-C25-C26-C27
22	A	830	CLA	O1A-CGA-O2A-C1
22	B	813	CLA	O1A-CGA-O2A-C1
22	B	829	CLA	O1A-CGA-O2A-C1
22	B	839	CLA	O1A-CGA-O2A-C1
22	A	803	CLA	C1A-C2A-CAA-CBA
22	A	806	CLA	C1A-C2A-CAA-CBA
22	A	813	CLA	C1A-C2A-CAA-CBA
22	A	818	CLA	C1A-C2A-CAA-CBA
22	A	826	CLA	C1A-C2A-CAA-CBA
22	A	829	CLA	C1A-C2A-CAA-CBA
22	A	833	CLA	C1A-C2A-CAA-CBA
22	A	841	CLA	C1A-C2A-CAA-CBA
22	A	843	CLA	C1A-C2A-CAA-CBA
22	A	853	CLA	C1A-C2A-CAA-CBA
22	B	816	CLA	C1A-C2A-CAA-CBA
22	B	818	CLA	C1A-C2A-CAA-CBA
22	B	823	CLA	C1A-C2A-CAA-CBA
22	B	839	CLA	C1A-C2A-CAA-CBA
22	K	101	CLA	C1A-C2A-CAA-CBA
22	K	105	CLA	C1A-C2A-CAA-CBA
22	L	202	CLA	C1A-C2A-CAA-CBA
22	L	204	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	1	304	CLA	C1A-C2A-CAA-CBA
22	1	306	CLA	C1A-C2A-CAA-CBA
22	1	308	CLA	C1A-C2A-CAA-CBA
22	1	313	CLA	C1A-C2A-CAA-CBA
22	2	319	CLA	C1A-C2A-CAA-CBA
22	4	309	CLA	C1A-C2A-CAA-CBA
22	6	305	CLA	C1A-C2A-CAA-CBA
22	5	309	CLA	C1A-C2A-CAA-CBA
22	5	313	CLA	C1A-C2A-CAA-CBA
22	7	305	CLA	C1A-C2A-CAA-CBA
22	8	308	CLA	C1A-C2A-CAA-CBA
22	8	309	CLA	C1A-C2A-CAA-CBA
22	9	309	CLA	C1A-C2A-CAA-CBA
22	9	311	CLA	C1A-C2A-CAA-CBA
22	9	313	CLA	C1A-C2A-CAA-CBA
22	0	312	CLA	C1A-C2A-CAA-CBA
29	4	307	CHL	C1A-C2A-CAA-CBA
29	8	307	CHL	C1A-C2A-CAA-CBA
22	B	836	CLA	C11-C12-C13-C15
22	1	302	CLA	C16-C17-C18-C20
22	6	303	CLA	C16-C17-C18-C20
24	1	317	LHG	O9-C7-O7-C5
25	1	316	8CT	C16-C17-C18-C19
25	8	318	8CT	C23-C24-C25-C26
22	L	201	CLA	C13-C15-C16-C17
22	L	203	CLA	C13-C15-C16-C17
24	6	322	LHG	C4-O6-P-O3
22	9	312	CLA	C11-C12-C13-C14
22	A	839	CLA	C3-C5-C6-C7
22	B	823	CLA	C3-C5-C6-C7
22	B	805	CLA	C8-C10-C11-C12
24	0	315	LHG	C28-C29-C30-C31
22	A	853	CLA	C10-C11-C12-C13
22	B	812	CLA	C15-C16-C17-C18
22	A	824	CLA	C6-C7-C8-C9
22	1	308	CLA	C11-C12-C13-C15
22	7	313	CLA	C3-C5-C6-C7
22	A	807	CLA	C10-C11-C12-C13
28	B	849	DGD	C2A-C1A-O1G-C1G
29	6	306	CHL	C3A-C2A-CAA-CBA
22	A	804	CLA	O1A-CGA-O2A-C1
22	9	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	B	849	DGD	C8B-C9B-CAB-CBB
22	A	840	CLA	C5-C6-C7-C8
22	B	827	CLA	C10-C11-C12-C13
22	1	304	CLA	C2A-CAA-CBA-CGA
29	4	305	CHL	C2A-CAA-CBA-CGA
22	A	810	CLA	C16-C17-C18-C19
22	A	825	CLA	C16-C17-C18-C19
22	3	301	CLA	C11-C12-C13-C15
22	B	824	CLA	O1D-CGD-O2D-CED
22	L	203	CLA	C3-C5-C6-C7
31	4	318	LMG	C7-C8-C9-O8
31	8	319	LMG	O1-C7-C8-C9
26	J	102	HTG	C1'-C2'-C3'-C4'
22	L	203	CLA	CBA-CGA-O2A-C1
22	8	304	CLA	O1A-CGA-O2A-C1
22	9	309	CLA	O1A-CGA-O2A-C1
28	B	849	DGD	C5D-C6D-O5D-C1E
22	A	813	CLA	O1D-CGD-O2D-CED
22	2	302	CLA	C10-C11-C12-C13
22	B	805	CLA	CAA-CBA-CGA-O2A
22	M	101	CLA	CBA-CGA-O2A-C1
24	2	318	LHG	O1-C1-C2-O2
24	5	318	LHG	O1-C1-C2-O2
22	A	801	CLA	C5-C6-C7-C8
22	A	841	CLA	C13-C15-C16-C17
22	A	853	CLA	C8-C10-C11-C12
22	B	837	CLA	C8-C10-C11-C12
22	2	303	CLA	C10-C11-C12-C13
22	6	311	CLA	C8-C10-C11-C12
22	1	313	CLA	O1A-CGA-O2A-C1
22	B	828	CLA	C4-C3-C5-C6
22	B	833	CLA	C4-C3-C5-C6
22	7	318	CLA	C16-C17-C18-C20
29	4	301	CHL	C11-C12-C13-C15
29	0	301	CHL	C11-C12-C13-C14
22	6	315	CLA	CBA-CGA-O2A-C1
22	B	806	CLA	C13-C15-C16-C17
22	7	317	CLA	C8-C10-C11-C12
29	8	305	CHL	C5-C6-C7-C8
24	9	316	LHG	C28-C29-C30-C31
22	B	821	CLA	O1D-CGD-O2D-CED
22	A	813	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	A	808	CLA	C5-C6-C7-C8
22	B	837	CLA	C3-C5-C6-C7
22	B	839	CLA	C3-C5-C6-C7
29	0	306	CHL	C4C-C3C-CAC-CBC
22	A	836	CLA	O1D-CGD-O2D-CED
22	B	832	CLA	C5-C6-C7-C8
24	0	315	LHG	C15-C16-C17-C18
31	4	318	LMG	C31-C32-C33-C34
22	1	307	CLA	CBA-CGA-O2A-C1
31	4	318	LMG	C29-C28-O8-C9
22	3	307	CLA	CAA-CBA-CGA-O2A
22	A	830	CLA	C5-C6-C7-C8
22	B	809	CLA	O1D-CGD-O2D-CED
22	1	313	CLA	O1D-CGD-O2D-CED
22	6	318	CLA	O1D-CGD-O2D-CED
22	B	812	CLA	C13-C15-C16-C17
22	B	834	CLA	C13-C15-C16-C17
29	2	306	CHL	CAA-CBA-CGA-O2A
31	4	318	LMG	O7-C8-C9-O8
24	6	322	LHG	C27-C28-C29-C30
22	A	821	CLA	C13-C15-C16-C17
22	A	818	CLA	C16-C17-C18-C19
22	9	303	CLA	C16-C17-C18-C20
24	0	315	LHG	C11-C10-C9-C8
22	B	823	CLA	C4-C3-C5-C6
22	L	203	CLA	C4-C3-C5-C6
22	4	311	CLA	C4-C3-C5-C6
22	B	806	CLA	C15-C16-C17-C18
22	A	803	CLA	C6-C7-C8-C10
22	A	806	CLA	C12-C13-C15-C16
22	A	807	CLA	C6-C7-C8-C10
22	A	808	CLA	C11-C10-C8-C7
22	A	810	CLA	C12-C13-C15-C16
22	A	817	CLA	C11-C10-C8-C7
22	A	817	CLA	C12-C13-C15-C16
22	A	827	CLA	C11-C12-C13-C15
22	A	829	CLA	C2-C3-C5-C6
22	A	830	CLA	C11-C10-C8-C7
22	A	830	CLA	C12-C13-C15-C16
22	B	803	CLA	C12-C13-C15-C16
22	B	809	CLA	C12-C13-C15-C16
22	B	814	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	825	CLA	C6-C7-C8-C10
22	B	825	CLA	C11-C10-C8-C7
22	B	825	CLA	C11-C12-C13-C15
22	B	827	CLA	C6-C7-C8-C10
22	B	827	CLA	C12-C13-C15-C16
22	B	828	CLA	C2-C3-C5-C6
22	B	829	CLA	C12-C13-C15-C16
22	B	832	CLA	C6-C7-C8-C10
22	B	836	CLA	C6-C7-C8-C10
22	B	839	CLA	C12-C13-C15-C16
22	B	840	CLA	C12-C13-C15-C16
22	L	201	CLA	C6-C7-C8-C10
22	L	201	CLA	C11-C12-C13-C15
22	1	311	CLA	C11-C12-C13-C15
22	2	302	CLA	C11-C12-C13-C15
22	2	303	CLA	C11-C12-C13-C15
22	2	309	CLA	C11-C10-C8-C7
22	4	314	CLA	C12-C13-C15-C16
22	6	315	CLA	C12-C13-C15-C16
22	5	302	CLA	C11-C10-C8-C7
22	5	309	CLA	C6-C7-C8-C10
22	5	312	CLA	C6-C7-C8-C10
22	8	315	CLA	C6-C7-C8-C10
22	9	303	CLA	C12-C13-C15-C16
22	9	309	CLA	C11-C10-C8-C7
22	0	307	CLA	C12-C13-C15-C16
29	9	302	CHL	C6-C7-C8-C10
29	9	302	CHL	C11-C10-C8-C7
22	A	803	CLA	C6-C7-C8-C9
22	A	803	CLA	C11-C12-C13-C14
22	A	806	CLA	C14-C13-C15-C16
22	A	809	CLA	C6-C7-C8-C9
22	A	817	CLA	C14-C13-C15-C16
22	A	818	CLA	C14-C13-C15-C16
22	A	825	CLA	C11-C10-C8-C9
22	A	827	CLA	C14-C13-C15-C16
22	A	830	CLA	C11-C10-C8-C9
22	A	830	CLA	C14-C13-C15-C16
22	A	838	CLA	C14-C13-C15-C16
22	B	803	CLA	C6-C7-C8-C9
22	B	805	CLA	C6-C7-C8-C9
22	B	809	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	814	CLA	C14-C13-C15-C16
22	B	819	CLA	C11-C10-C8-C9
22	B	825	CLA	C11-C12-C13-C14
22	B	827	CLA	C11-C12-C13-C14
22	B	827	CLA	C14-C13-C15-C16
22	B	839	CLA	C6-C7-C8-C9
22	H	201	CLA	C11-C10-C8-C9
22	L	201	CLA	C11-C12-C13-C14
22	2	303	CLA	C11-C12-C13-C14
22	4	314	CLA	C6-C7-C8-C9
22	6	303	CLA	C11-C10-C8-C9
22	6	305	CLA	C6-C7-C8-C9
22	6	315	CLA	C11-C10-C8-C9
22	5	302	CLA	C11-C10-C8-C9
22	5	307	CLA	C11-C12-C13-C14
22	8	315	CLA	C6-C7-C8-C9
22	8	315	CLA	C14-C13-C15-C16
22	9	303	CLA	C14-C13-C15-C16
22	9	309	CLA	C11-C10-C8-C9
22	0	302	CLA	C14-C13-C15-C16
22	0	308	CLA	C11-C10-C8-C9
23	A	842	PQN	C16-C17-C18-C19
29	5	301	CHL	C11-C10-C8-C9
25	A	849	8CT	C12-C13-C14-C15
31	4	318	LMG	C30-C31-C32-C33
22	0	312	CLA	CBA-CGA-O2A-C1
22	5	303	CLA	C2C-C3C-CAC-CBC
25	J	101	8CT	C27-C26-C28-C29
25	3	316	8CT	C22-C21-C23-C24
25	7	301	8CT	C10-C11-C12-C40
22	L	202	CLA	C15-C16-C17-C18
22	A	810	CLA	C16-C17-C18-C20
22	B	824	CLA	C11-C12-C13-C15
22	4	310	CLA	C6-C7-C8-C10
29	8	305	CHL	C6-C7-C8-C9
29	7	308	CHL	C2C-C3C-CAC-CBC
22	9	305	CLA	O1D-CGD-O2D-CED
25	J	101	8CT	C25-C26-C28-C29
25	4	317	8CT	C10-C11-C12-C13
25	7	301	8CT	C10-C11-C12-C13
25	8	318	8CT	C25-C26-C28-C29
22	1	311	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	2	301	CHL	O1D-CGD-O2D-CED
22	A	810	CLA	C13-C15-C16-C17
22	6	309	CLA	CBA-CGA-O2A-C1
22	6	311	CLA	CBA-CGA-O2A-C1
22	B	815	CLA	C13-C15-C16-C17
22	B	819	CLA	C5-C6-C7-C8
24	9	316	LHG	C32-C33-C34-C35
28	B	849	DGD	CFB-CGB-CHB-CIB
22	1	308	CLA	C11-C12-C13-C14
24	A	845	LHG	O6-C4-C5-C6
24	0	315	LHG	O6-C4-C5-C6
22	B	814	CLA	CBA-CGA-O2A-C1
22	5	313	CLA	CBD-CGD-O2D-CED
22	1	307	CLA	O1D-CGD-O2D-CED
22	3	319	CLA	C4-C3-C5-C6
22	A	817	CLA	C2-C3-C5-C6
22	B	823	CLA	C2-C3-C5-C6
22	L	203	CLA	C2-C3-C5-C6
22	L	203	CLA	C8-C10-C11-C12
22	4	302	CLA	C5-C6-C7-C8
22	L	203	CLA	O1A-CGA-O2A-C1
22	8	312	CLA	O1D-CGD-O2D-CED
22	5	302	CLA	C16-C17-C18-C20
22	B	809	CLA	CBA-CGA-O2A-C1
22	0	303	CLA	CBA-CGA-O2A-C1
24	7	322	LHG	C2-C3-O3-P
22	A	828	CLA	C3A-C2A-CAA-CBA
22	A	832	CLA	C3A-C2A-CAA-CBA
22	A	841	CLA	C3A-C2A-CAA-CBA
22	B	841	CLA	C3A-C2A-CAA-CBA
22	K	105	CLA	C3A-C2A-CAA-CBA
22	L	201	CLA	C3A-C2A-CAA-CBA
22	1	303	CLA	C3A-C2A-CAA-CBA
22	1	313	CLA	C3A-C2A-CAA-CBA
22	4	314	CLA	C3A-C2A-CAA-CBA
22	6	309	CLA	C3A-C2A-CAA-CBA
22	6	311	CLA	C3A-C2A-CAA-CBA
22	6	323	CLA	C3A-C2A-CAA-CBA
22	7	305	CLA	C3A-C2A-CAA-CBA
22	8	304	CLA	C3A-C2A-CAA-CBA
22	8	315	CLA	C3A-C2A-CAA-CBA
22	0	305	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	A	849	8CT	C18-C19-C20-C21
30	0	314	XAT	C33-C34-C35-C15
22	4	309	CLA	C3-C5-C6-C7
22	A	803	CLA	C13-C15-C16-C17
22	4	310	CLA	C6-C7-C8-C9
22	0	307	CLA	CBA-CGA-O2A-C1
29	9	302	CHL	C8-C10-C11-C12
24	B	852	LHG	C4-C5-C6-O8
24	2	318	LHG	C4-C5-C6-O8
24	5	318	LHG	C4-C5-C6-O8
28	B	849	DGD	O1G-C1G-C2G-C3G
28	B	849	DGD	C1G-C2G-C3G-O3G
22	2	304	CLA	C3-C5-C6-C7
22	B	819	CLA	C4-C3-C5-C6
22	A	825	CLA	C16-C17-C18-C20
22	5	302	CLA	C16-C17-C18-C19
22	5	307	CLA	C16-C17-C18-C19
29	4	301	CHL	C11-C12-C13-C14
22	3	304	CLA	O1D-CGD-O2D-CED
29	2	301	CHL	C3C-C2C-CMC-OMC
29	6	302	CHL	C3C-C2C-CMC-OMC
29	8	305	CHL	C3C-C2C-CMC-OMC
29	9	307	CHL	C3C-C2C-CMC-OMC
22	1	307	CLA	O1A-CGA-O2A-C1
31	4	318	LMG	C4-C5-C6-O5
22	B	816	CLA	C2A-CAA-CBA-CGA
24	B	852	LHG	O1-C1-C2-O2
24	3	317	LHG	O6-C4-C5-O7
24	0	315	LHG	O6-C4-C5-O7
22	B	812	CLA	CBA-CGA-O2A-C1
22	1	310	CLA	CBA-CGA-O2A-C1
22	5	312	CLA	CBA-CGA-O2A-C1
22	6	315	CLA	O1A-CGA-O2A-C1
22	B	809	CLA	C16-C17-C18-C19
22	B	824	CLA	C11-C12-C13-C14
29	8	305	CHL	C6-C7-C8-C10
22	B	818	CLA	C8-C10-C11-C12
31	8	319	LMG	C31-C32-C33-C34
29	7	308	CHL	CBA-CGA-O2A-C1
22	8	310	CLA	C2C-C3C-CAC-CBC
28	B	849	DGD	CFA-CGA-CHA-CIA
22	0	312	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	B	849	DGD	O2G-C2G-C3G-O3G
22	A	827	CLA	CBA-CGA-O2A-C1
22	3	312	CLA	O1D-CGD-O2D-CED
25	B	845	8CT	C18-C19-C20-C21
25	B	848	8CT	C12-C13-C14-C15
25	7	323	8CT	C16-C17-C18-C19
22	A	818	CLA	C16-C17-C18-C20
22	B	805	CLA	C16-C17-C18-C20
24	9	316	LHG	C1-C2-C3-O3
22	A	817	CLA	C2-C1-O2A-CGA
22	A	824	CLA	C2-C1-O2A-CGA
22	B	808	CLA	C2-C1-O2A-CGA
22	2	314	CLA	C2-C1-O2A-CGA
22	6	303	CLA	C2-C1-O2A-CGA
22	9	303	CLA	C2-C1-O2A-CGA
29	8	307	CHL	C2-C1-O2A-CGA
24	9	316	LHG	C29-C30-C31-C32
24	0	315	LHG	C32-C33-C34-C35
31	5	319	LMG	C23-C24-C25-C26
22	A	802	CLA	C14-C13-C15-C16
22	A	808	CLA	C11-C10-C8-C9
22	A	809	CLA	C11-C12-C13-C14
22	A	810	CLA	C14-C13-C15-C16
22	A	833	CLA	C6-C7-C8-C9
22	A	837	CLA	C11-C10-C8-C9
22	B	803	CLA	C14-C13-C15-C16
22	B	818	CLA	C6-C7-C8-C9
22	B	820	CLA	C11-C10-C8-C9
22	B	826	CLA	C11-C12-C13-C14
22	B	828	CLA	C11-C12-C13-C14
22	B	837	CLA	C14-C13-C15-C16
22	B	841	CLA	C6-C7-C8-C9
22	1	301	CLA	C14-C13-C15-C16
22	1	311	CLA	C11-C12-C13-C14
22	2	302	CLA	C6-C7-C8-C9
22	3	301	CLA	C6-C7-C8-C9
22	3	319	CLA	C14-C13-C15-C16
22	6	303	CLA	C14-C13-C15-C16
22	5	307	CLA	C14-C13-C15-C16
22	7	317	CLA	C11-C12-C13-C14
22	7	310	CLA	CBA-CGA-O2A-C1
24	9	316	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
22	B	825	CLA	C8-C10-C11-C12
22	B	839	CLA	C13-C15-C16-C17
22	1	301	CLA	C8-C10-C11-C12
24	2	318	LHG	C2-C3-O3-P
24	5	318	LHG	C2-C3-O3-P
24	5	318	LHG	C25-C26-C27-C28
22	G	103	CLA	C2A-CAA-CBA-CGA
22	6	313	CLA	C16-C17-C18-C20
22	5	303	CLA	C16-C17-C18-C20
25	A	849	8CT	C02-C03-C10-C11
25	B	844	8CT	C02-C03-C10-C11
25	B	844	8CT	C04-C03-C10-C11
25	B	848	8CT	C02-C03-C10-C11
25	7	301	8CT	C02-C03-C10-C11
22	A	827	CLA	C10-C11-C12-C13
22	5	303	CLA	C5-C6-C7-C8
25	L	205	8CT	C14-C15-C16-C39
25	A	846	8CT	C20-C21-C23-C24
25	4	317	8CT	C14-C15-C16-C17
25	8	318	8CT	C20-C21-C23-C24
30	3	314	XAT	C31-C32-C33-C34
22	2	312	CLA	C5-C6-C7-C8
22	6	304	CLA	C10-C11-C12-C13
24	5	318	LHG	C11-C12-C13-C14
24	9	316	LHG	C27-C28-C29-C30
22	9	304	CLA	O2A-C1-C2-C3
22	A	804	CLA	C6-C7-C8-C10
22	B	819	CLA	C11-C12-C13-C15
22	9	303	CLA	C16-C17-C18-C19
22	A	801	CLA	C3-C5-C6-C7
29	9	307	CHL	CBD-CGD-O2D-CED
22	6	309	CLA	O1A-CGA-O2A-C1
22	A	828	CLA	O1D-CGD-O2D-CED
24	2	318	LHG	O6-C4-C5-C6
24	3	317	LHG	O6-C4-C5-C6
24	6	322	LHG	O6-C4-C5-C6
22	A	838	CLA	O1D-CGD-O2D-CED
24	0	315	LHG	C14-C15-C16-C17
22	A	802	CLA	C12-C13-C15-C16
22	A	803	CLA	C11-C12-C13-C15
22	A	805	CLA	C12-C13-C15-C16
22	A	811	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	A	826	CLA	C12-C13-C15-C16
22	A	837	CLA	C11-C10-C8-C7
22	B	803	CLA	C11-C12-C13-C15
22	B	805	CLA	C6-C7-C8-C10
22	B	805	CLA	C11-C10-C8-C7
22	B	811	CLA	C12-C13-C15-C16
22	B	814	CLA	C12-C13-C15-C16
22	B	819	CLA	C11-C10-C8-C7
22	B	827	CLA	C11-C12-C13-C15
22	B	828	CLA	C11-C12-C13-C15
22	B	837	CLA	C11-C12-C13-C15
22	B	837	CLA	C12-C13-C15-C16
22	B	839	CLA	C6-C7-C8-C10
22	H	201	CLA	C11-C10-C8-C7
22	L	203	CLA	C11-C10-C8-C7
22	1	301	CLA	C12-C13-C15-C16
22	1	306	CLA	C11-C12-C13-C15
22	1	308	CLA	C6-C7-C8-C10
22	2	312	CLA	C11-C12-C13-C15
22	3	301	CLA	C6-C7-C8-C10
22	3	319	CLA	C12-C13-C15-C16
22	4	314	CLA	C6-C7-C8-C10
22	6	303	CLA	C11-C10-C8-C7
22	6	303	CLA	C12-C13-C15-C16
22	6	305	CLA	C6-C7-C8-C10
22	6	311	CLA	C11-C10-C8-C7
22	6	315	CLA	C11-C10-C8-C7
22	5	307	CLA	C11-C12-C13-C15
22	7	316	CLA	C6-C7-C8-C10
22	7	317	CLA	C12-C13-C15-C16
22	8	315	CLA	C11-C12-C13-C15
22	9	309	CLA	C6-C7-C8-C10
22	9	312	CLA	C11-C10-C8-C7
22	0	302	CLA	C11-C10-C8-C7
22	0	302	CLA	C12-C13-C15-C16
22	0	308	CLA	C11-C10-C8-C7
23	A	842	PQN	C16-C17-C18-C20
29	0	301	CHL	C6-C7-C8-C10
31	8	319	LMG	C11-C12-C13-C14
22	A	829	CLA	C5-C6-C7-C8
25	A	847	8CT	C18-C19-C20-C21
25	A	854	8CT	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	B	804	8CT	C16-C17-C18-C19
25	B	848	8CT	C18-C19-C20-C21
25	G	104	8CT	C12-C13-C14-C15
25	5	317	8CT	C18-C19-C20-C21
25	7	301	8CT	C23-C24-C25-C26
25	8	318	8CT	C18-C19-C20-C21
22	A	808	CLA	C16-C17-C18-C19
22	A	808	CLA	C16-C17-C18-C20
22	H	201	CLA	C16-C17-C18-C20
28	B	849	DGD	C2A-C3A-C4A-C5A
22	A	824	CLA	C2A-CAA-CBA-CGA
22	1	306	CLA	C2A-CAA-CBA-CGA
29	1	305	CHL	C2A-CAA-CBA-CGA
29	2	306	CHL	C2A-CAA-CBA-CGA
22	9	308	CLA	C13-C15-C16-C17
22	B	805	CLA	C16-C17-C18-C19
22	5	307	CLA	C16-C17-C18-C20
22	B	809	CLA	C8-C10-C11-C12
22	B	815	CLA	CBA-CGA-O2A-C1
22	4	311	CLA	CBA-CGA-O2A-C1
22	8	311	CLA	CBA-CGA-O2A-C1
22	4	311	CLA	C3-C5-C6-C7
24	1	317	LHG	C28-C29-C30-C31
22	B	826	CLA	C13-C15-C16-C17
31	4	318	LMG	C16-C17-C18-C19
22	A	806	CLA	CAD-CBD-CGD-O2D
22	A	807	CLA	CAD-CBD-CGD-O2D
22	A	811	CLA	CAD-CBD-CGD-O2D
22	A	820	CLA	CAD-CBD-CGD-O2D
22	A	835	CLA	CAD-CBD-CGD-O2D
22	A	852	CLA	CAD-CBD-CGD-O2D
22	B	805	CLA	CAD-CBD-CGD-O2D
22	B	811	CLA	CAD-CBD-CGD-O2D
22	B	819	CLA	CAD-CBD-CGD-O2D
22	B	826	CLA	CAD-CBD-CGD-O2D
22	B	835	CLA	CAD-CBD-CGD-O2D
22	B	838	CLA	CAD-CBD-CGD-O2D
22	2	308	CLA	CAD-CBD-CGD-O2D
22	3	311	CLA	CAD-CBD-CGD-O2D
22	4	308	CLA	CAD-CBD-CGD-O2D
22	4	309	CLA	CAD-CBD-CGD-O2D
22	6	301	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	6	311	CLA	CAD-CBD-CGD-O2D
22	6	312	CLA	CAD-CBD-CGD-O2D
22	5	309	CLA	CAD-CBD-CGD-O2D
22	7	303	CLA	CAD-CBD-CGD-O2D
22	8	308	CLA	CAD-CBD-CGD-O2D
22	8	309	CLA	CAD-CBD-CGD-O2D
22	9	303	CLA	CAD-CBD-CGD-O2D
22	9	304	CLA	CAD-CBD-CGD-O2D
29	1	305	CHL	CAD-CBD-CGD-O2D
29	2	301	CHL	CAD-CBD-CGD-O2D
29	4	306	CHL	CAD-CBD-CGD-O2D
22	2	309	CLA	O1D-CGD-O2D-CED
24	A	844	LHG	C32-C33-C34-C35
24	A	844	LHG	C34-C35-C36-C37
22	7	309	CLA	CBA-CGA-O2A-C1
29	9	307	CHL	CBA-CGA-O2A-C1
22	A	803	CLA	C4-C3-C5-C6
22	A	837	CLA	C4-C3-C5-C6
22	7	318	CLA	C16-C17-C18-C19
22	0	312	CLA	C6-C7-C8-C9
24	5	318	LHG	C16-C17-C18-C19
24	A	844	LHG	C4-C5-C6-O8
31	4	318	LMG	O1-C7-C8-C9
31	5	319	LMG	O1-C7-C8-C9
22	A	827	CLA	O1A-CGA-O2A-C1
22	6	311	CLA	O1A-CGA-O2A-C1
22	8	311	CLA	O1A-CGA-O2A-C1
24	6	322	LHG	O6-C4-C5-O7
22	A	832	CLA	C5-C6-C7-C8
22	B	823	CLA	C5-C6-C7-C8
22	B	808	CLA	CAA-CBA-CGA-O2A
28	B	849	DGD	C2B-C3B-C4B-C5B
22	B	812	CLA	O1A-CGA-O2A-C1
22	5	312	CLA	O1A-CGA-O2A-C1
22	B	801	CLA	C16-C17-C18-C19
22	A	808	CLA	CHA-CBD-CGD-O1D
22	A	808	CLA	CHA-CBD-CGD-O2D
22	A	817	CLA	CHA-CBD-CGD-O1D
22	A	817	CLA	CHA-CBD-CGD-O2D
22	A	833	CLA	CHA-CBD-CGD-O1D
22	A	836	CLA	CHA-CBD-CGD-O2D
22	A	838	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	838	CLA	CHA-CBD-CGD-O2D
22	B	801	CLA	CHA-CBD-CGD-O1D
22	B	801	CLA	CHA-CBD-CGD-O2D
22	B	808	CLA	CHA-CBD-CGD-O1D
22	B	833	CLA	CHA-CBD-CGD-O1D
22	F	301	CLA	CHA-CBD-CGD-O1D
22	F	301	CLA	CHA-CBD-CGD-O2D
22	K	102	CLA	CHA-CBD-CGD-O1D
22	1	301	CLA	CHA-CBD-CGD-O1D
22	1	301	CLA	CHA-CBD-CGD-O2D
22	1	303	CLA	CHA-CBD-CGD-O1D
22	2	319	CLA	CHA-CBD-CGD-O2D
22	3	303	CLA	CHA-CBD-CGD-O1D
22	3	303	CLA	CHA-CBD-CGD-O2D
22	3	312	CLA	CHA-CBD-CGD-O1D
22	4	314	CLA	CHA-CBD-CGD-O1D
22	6	323	CLA	CHA-CBD-CGD-O1D
22	6	323	CLA	CHA-CBD-CGD-O2D
22	7	302	CLA	CHA-CBD-CGD-O1D
22	7	302	CLA	CHA-CBD-CGD-O2D
22	7	305	CLA	CHA-CBD-CGD-O1D
22	7	305	CLA	CHA-CBD-CGD-O2D
22	8	304	CLA	CHA-CBD-CGD-O1D
22	9	305	CLA	CHA-CBD-CGD-O1D
22	9	305	CLA	CHA-CBD-CGD-O2D
22	0	302	CLA	CHA-CBD-CGD-O1D
22	0	303	CLA	CHA-CBD-CGD-O1D
22	0	303	CLA	CHA-CBD-CGD-O2D
29	6	302	CHL	CHA-CBD-CGD-O1D
29	6	302	CHL	CHA-CBD-CGD-O2D
29	6	316	CHL	CHA-CBD-CGD-O1D
29	6	316	CHL	CHA-CBD-CGD-O2D
22	A	837	CLA	C3-C5-C6-C7
22	B	809	CLA	O1A-CGA-O2A-C1
22	B	814	CLA	O1A-CGA-O2A-C1
22	0	303	CLA	O1A-CGA-O2A-C1
22	0	307	CLA	O1A-CGA-O2A-C1
28	B	849	DGD	CBA-CCA-CDA-CEA
24	B	852	LHG	O7-C5-C6-O8
24	2	318	LHG	O7-C5-C6-O8
28	B	849	DGD	O1G-C1G-C2G-O2G
31	4	318	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
22	A	822	CLA	CBD-CGD-O2D-CED
22	2	312	CLA	C8-C10-C11-C12
22	1	310	CLA	O1A-CGA-O2A-C1
22	7	310	CLA	O1A-CGA-O2A-C1
22	B	826	CLA	C16-C17-C18-C19
22	B	834	CLA	C16-C17-C18-C19
22	K	101	CLA	C2C-C3C-CAC-CBC
22	B	814	CLA	C4-C3-C5-C6
22	A	812	CLA	C5-C6-C7-C8
22	B	850	CLA	C2C-C3C-CAC-CBC
24	A	845	LHG	C10-C11-C12-C13
24	6	322	LHG	O9-C7-O7-C5
22	B	812	CLA	C5-C6-C7-C8
22	A	811	CLA	C11-C12-C13-C14
22	A	840	CLA	C14-C13-C15-C16
22	A	853	CLA	C11-C12-C13-C14
22	B	826	CLA	C6-C7-C8-C9
22	B	828	CLA	C6-C7-C8-C9
22	2	312	CLA	C11-C12-C13-C14
22	0	302	CLA	C11-C10-C8-C9
23	B	842	PQN	C21-C22-C23-C24
24	0	315	LHG	C30-C31-C32-C33
22	A	806	CLA	C15-C16-C17-C18
22	B	837	CLA	C13-C15-C16-C17
22	8	310	CLA	C4C-C3C-CAC-CBC
22	B	814	CLA	C2A-CAA-CBA-CGA
22	5	312	CLA	C2A-CAA-CBA-CGA
25	A	854	8CT	C10-C11-C12-C40
24	A	844	LHG	C28-C29-C30-C31
25	A	854	8CT	C10-C11-C12-C13
25	3	316	8CT	C20-C21-C23-C24
22	A	811	CLA	C1A-C2A-CAA-CBA
22	1	302	CLA	C1A-C2A-CAA-CBA
22	4	314	CLA	C1A-C2A-CAA-CBA
22	6	310	CLA	C1A-C2A-CAA-CBA
22	6	311	CLA	C1A-C2A-CAA-CBA
22	7	310	CLA	C1A-C2A-CAA-CBA
22	8	315	CLA	C1A-C2A-CAA-CBA
29	2	307	CHL	C1A-C2A-CAA-CBA
29	3	306	CHL	C1A-C2A-CAA-CBA
22	A	806	CLA	C16-C17-C18-C19
22	A	809	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	B	817	CLA	C6-C7-C8-C9
22	1	312	CLA	C6-C7-C8-C9
22	8	315	CLA	C16-C17-C18-C20
22	A	808	CLA	C13-C15-C16-C17
24	0	315	LHG	C24-C25-C26-C27
24	B	852	LHG	C3-O3-P-O6
24	5	318	LHG	C3-O3-P-O6
24	5	318	LHG	C28-C29-C30-C31
22	6	305	CLA	C3-C5-C6-C7
22	0	302	CLA	C2-C3-C5-C6
22	7	309	CLA	O1A-CGA-O2A-C1
29	9	307	CHL	O1A-CGA-O2A-C1
24	A	844	LHG	C3-O3-P-O4
24	2	318	LHG	C4-O6-P-O5
24	6	322	LHG	C4-O6-P-O4
24	5	318	LHG	C3-O3-P-O4
24	5	318	LHG	C4-O6-P-O4
24	7	322	LHG	C3-O3-P-O5
24	7	322	LHG	C4-O6-P-O4
22	A	821	CLA	C16-C17-C18-C20
22	B	809	CLA	C16-C17-C18-C20
22	4	309	CLA	C11-C12-C13-C15
22	6	304	CLA	C16-C17-C18-C20
22	3	311	CLA	CBA-CGA-O2A-C1
24	2	318	LHG	C24-C23-O8-C6
22	A	801	CLA	CAA-CBA-CGA-O2A
22	G	102	CLA	C2A-CAA-CBA-CGA
22	1	311	CLA	C2A-CAA-CBA-CGA
22	9	312	CLA	C3-C5-C6-C7
22	4	311	CLA	O1A-CGA-O2A-C1
22	A	823	CLA	C2-C3-C5-C6
22	A	832	CLA	CAD-CBD-CGD-O1D
22	A	836	CLA	CAD-CBD-CGD-O1D
22	B	808	CLA	CAD-CBD-CGD-O1D
22	B	814	CLA	CAD-CBD-CGD-O1D
22	2	319	CLA	CAD-CBD-CGD-O1D
22	3	303	CLA	CAD-CBD-CGD-O1D
22	6	303	CLA	CAD-CBD-CGD-O1D
22	6	323	CLA	CAD-CBD-CGD-O1D
22	5	304	CLA	CAD-CBD-CGD-O1D
22	5	312	CLA	CAD-CBD-CGD-O1D
22	7	305	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	7	314	CLA	CAD-CBD-CGD-O1D
22	8	304	CLA	CAD-CBD-CGD-O1D
22	8	311	CLA	CAD-CBD-CGD-O1D
22	0	302	CLA	CAD-CBD-CGD-O1D
22	0	303	CLA	CAD-CBD-CGD-O1D
29	2	305	CHL	CAD-CBD-CGD-O1D
29	6	302	CHL	CAD-CBD-CGD-O1D
22	B	837	CLA	C10-C11-C12-C13
22	B	815	CLA	O1A-CGA-O2A-C1
22	2	303	CLA	C15-C16-C17-C18
24	9	316	LHG	C9-C10-C11-C12
22	B	836	CLA	CBA-CGA-O2A-C1
29	4	305	CHL	CBA-CGA-O2A-C1
22	4	309	CLA	O1A-CGA-O2A-C1
22	L	202	CLA	CBD-CGD-O2D-CED
22	A	833	CLA	C4-C3-C5-C6
22	A	819	CLA	C11-C12-C13-C15
22	A	819	CLA	C12-C13-C15-C16
22	A	828	CLA	C11-C12-C13-C15
22	A	833	CLA	C6-C7-C8-C10
22	A	840	CLA	C12-C13-C15-C16
22	A	841	CLA	C6-C7-C8-C10
22	B	806	CLA	C6-C7-C8-C10
22	B	808	CLA	C11-C10-C8-C7
22	B	808	CLA	C11-C12-C13-C15
22	B	809	CLA	C11-C12-C13-C15
22	B	826	CLA	C6-C7-C8-C10
22	B	828	CLA	C6-C7-C8-C10
22	B	830	CLA	C11-C12-C13-C15
22	B	834	CLA	C11-C10-C8-C7
22	J	103	CLA	C3A-C2A-CAA-CBA
22	2	302	CLA	C12-C13-C15-C16
22	2	303	CLA	C6-C7-C8-C10
22	3	319	CLA	C6-C7-C8-C10
22	0	307	CLA	C6-C7-C8-C10
25	B	843	8CT	C28-C29-C30-C31
25	B	846	8CT	C28-C29-C30-C31
25	L	206	8CT	C28-C29-C30-C31
25	1	316	8CT	C28-C29-C30-C31
25	2	317	8CT	C28-C29-C30-C31
25	8	301	8CT	C28-C29-C30-C31
25	8	318	8CT	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	0	301	CHL	C11-C10-C8-C7
25	4	317	8CT	C12-C13-C14-C15
22	7	307	CLA	CBD-CGD-O2D-CED
22	9	312	CLA	C8-C10-C11-C12
22	B	803	CLA	C2C-C3C-CAC-CBC
29	6	316	CHL	C4C-C3C-CAC-CBC
22	A	832	CLA	C2A-CAA-CBA-CGA
22	A	836	CLA	C2A-CAA-CBA-CGA
22	9	305	CLA	C2A-CAA-CBA-CGA
22	B	814	CLA	C16-C17-C18-C19
22	B	828	CLA	C16-C17-C18-C19
24	7	322	LHG	C4-C5-C6-O8
24	9	316	LHG	C4-C5-C6-O8
29	2	305	CHL	C1C-C2C-CMC-OMC
29	2	307	CHL	C1C-C2C-CMC-OMC
29	6	302	CHL	C1C-C2C-CMC-OMC
29	6	316	CHL	C1C-C2C-CMC-OMC
29	5	306	CHL	C1C-C2C-CMC-OMC
29	9	307	CHL	C1C-C2C-CMC-OMC
31	5	319	LMG	O1-C7-C8-O7
31	8	319	LMG	O1-C7-C8-O7
31	5	319	LMG	C29-C30-C31-C32
22	1	312	CLA	C6-C7-C8-C10
22	B	827	CLA	C13-C15-C16-C17
22	6	310	CLA	C10-C11-C12-C13
22	0	311	CLA	C13-C15-C16-C17
22	A	826	CLA	C2C-C3C-CAC-CBC
22	K	102	CLA	C2C-C3C-CAC-CBC
22	B	836	CLA	O1A-CGA-O2A-C1
22	3	311	CLA	O1A-CGA-O2A-C1
22	4	314	CLA	C5-C6-C7-C8
22	8	315	CLA	C4-C3-C5-C6
22	5	304	CLA	CBA-CGA-O2A-C1
22	A	803	CLA	C2-C3-C5-C6
22	B	828	CLA	CAA-CBA-CGA-O2A
22	1	312	CLA	CAA-CBA-CGA-O2A
22	B	813	CLA	C5-C6-C7-C8
22	L	201	CLA	C8-C10-C11-C12
22	A	811	CLA	C6-C7-C8-C9
22	A	840	CLA	C6-C7-C8-C9
22	A	841	CLA	C6-C7-C8-C9
22	B	803	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	B	805	CLA	C11-C10-C8-C9
22	B	809	CLA	C11-C12-C13-C14
22	B	825	CLA	C6-C7-C8-C9
22	B	827	CLA	C6-C7-C8-C9
22	B	829	CLA	C14-C13-C15-C16
22	B	840	CLA	C14-C13-C15-C16
22	1	306	CLA	C11-C12-C13-C14
22	1	308	CLA	C6-C7-C8-C9
22	2	303	CLA	C11-C10-C8-C9
22	4	312	CLA	C6-C7-C8-C9
22	6	311	CLA	C11-C10-C8-C9
22	7	316	CLA	C6-C7-C8-C9
22	7	317	CLA	C14-C13-C15-C16
22	8	302	CLA	C11-C10-C8-C9
22	0	311	CLA	C6-C7-C8-C9
29	9	302	CHL	C11-C10-C8-C9
29	0	301	CHL	C6-C7-C8-C9
22	B	834	CLA	C16-C17-C18-C20
22	4	309	CLA	C11-C12-C13-C14
29	4	305	CHL	O1A-CGA-O2A-C1
22	7	316	CLA	C2A-CAA-CBA-CGA
22	3	319	CLA	C15-C16-C17-C18
25	B	843	8CT	C13-C14-C15-C16
25	B	843	8CT	C21-C23-C24-C25
25	B	844	8CT	C13-C14-C15-C16
25	B	844	8CT	C21-C23-C24-C25
25	B	845	8CT	C13-C14-C15-C16
25	B	845	8CT	C21-C23-C24-C25
25	B	846	8CT	C13-C14-C15-C16
25	B	846	8CT	C21-C23-C24-C25
25	B	851	8CT	C13-C14-C15-C16
25	B	851	8CT	C21-C23-C24-C25
25	J	104	8CT	C21-C23-C24-C25
25	K	103	8CT	C13-C14-C15-C16
25	K	103	8CT	C21-C23-C24-C25
25	L	205	8CT	C21-C23-C24-C25
25	6	321	8CT	C21-C23-C24-C25
30	1	314	XAT	C10-C11-C12-C13
30	3	314	XAT	C30-C31-C32-C33
30	4	315	XAT	C10-C11-C12-C13
30	6	319	XAT	C10-C11-C12-C13
30	9	314	XAT	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
30	0	313	XAT	C10-C11-C12-C13
30	0	313	XAT	C30-C31-C32-C33
30	0	314	XAT	C10-C11-C12-C13
25	A	847	8CT	C16-C17-C18-C19
22	A	821	CLA	C16-C17-C18-C19
22	8	315	CLA	C16-C17-C18-C19
22	8	315	CLA	C4C-C3C-CAC-CBC
25	L	205	8CT	C14-C15-C16-C17
22	1	308	CLA	C5-C6-C7-C8
22	5	304	CLA	O1A-CGA-O2A-C1
22	B	814	CLA	C2-C3-C5-C6
22	B	833	CLA	C2-C3-C5-C6
22	4	311	CLA	C2-C3-C5-C6
22	B	831	CLA	O1D-CGD-O2D-CED
22	A	806	CLA	C10-C11-C12-C13
22	B	840	CLA	C16-C17-C18-C19
22	B	850	CLA	C6-C7-C8-C9
22	9	313	CLA	C6-C7-C8-C10
22	A	822	CLA	C1-C2-C3-C4
22	A	852	CLA	C1-C2-C3-C4
22	2	314	CLA	C1-C2-C3-C4
22	A	813	CLA	C13-C15-C16-C17
22	L	202	CLA	C2A-CAA-CBA-CGA
22	2	314	CLA	C2A-CAA-CBA-CGA
22	5	302	CLA	C2A-CAA-CBA-CGA
22	0	311	CLA	C2A-CAA-CBA-CGA
22	B	810	CLA	C5-C6-C7-C8
22	B	814	CLA	C2-C1-O2A-CGA
22	B	819	CLA	C2-C1-O2A-CGA
22	B	820	CLA	C2-C1-O2A-CGA
22	B	821	CLA	C2-C1-O2A-CGA
22	H	201	CLA	C2-C1-O2A-CGA
22	2	309	CLA	C2-C1-O2A-CGA
22	6	305	CLA	C2-C1-O2A-CGA
29	4	301	CHL	C2-C1-O2A-CGA
29	9	302	CHL	C2-C1-O2A-CGA
29	7	308	CHL	C4C-C3C-CAC-CBC
29	9	307	CHL	O1D-CGD-O2D-CED
22	L	201	CLA	C3-C5-C6-C7
24	1	317	LHG	C24-C25-C26-C27
22	M	101	CLA	O1A-CGA-O2A-C1
24	1	317	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
25	J	101	8CT	C16-C17-C18-C19
24	2	318	LHG	O6-C4-C5-O7
22	6	311	CLA	C4-C3-C5-C6
25	A	847	8CT	C04-C03-C10-C11
22	4	309	CLA	CBA-CGA-O2A-C1
22	A	833	CLA	C13-C15-C16-C17
22	B	821	CLA	C2C-C3C-CAC-CBC
22	5	303	CLA	C4C-C3C-CAC-CBC
22	5	309	CLA	C11-C12-C13-C14
22	3	319	CLA	C2A-CAA-CBA-CGA
22	5	313	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	O1A-CGA-O2A-C1
24	1	317	LHG	C3-O3-P-O6
24	1	317	LHG	C4-O6-P-O3
24	3	317	LHG	C3-O3-P-O6
22	A	811	CLA	C16-C17-C18-C20
22	B	817	CLA	C6-C7-C8-C10
22	B	824	CLA	C10-C11-C12-C13
22	B	815	CLA	C4C-C3C-CAC-CBC
22	A	805	CLA	C4-C3-C5-C6
22	B	827	CLA	C4-C3-C5-C6
22	A	808	CLA	C11-C12-C13-C15
22	A	811	CLA	C6-C7-C8-C10
22	A	818	CLA	C12-C13-C15-C16
22	A	827	CLA	C12-C13-C15-C16
22	A	853	CLA	C6-C7-C8-C10
22	B	816	CLA	C11-C10-C8-C7
22	6	315	CLA	C6-C7-C8-C10
23	B	842	PQN	C21-C22-C23-C25
29	2	301	CHL	C6-C7-C8-C10
22	6	309	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	C11-C12-C13-C14
22	A	819	CLA	C11-C12-C13-C14
22	A	819	CLA	C14-C13-C15-C16
22	A	828	CLA	C11-C12-C13-C14
22	A	837	CLA	C14-C13-C15-C16
22	B	808	CLA	C11-C10-C8-C9
22	B	830	CLA	C11-C12-C13-C14
22	2	302	CLA	C11-C12-C13-C14
22	2	302	CLA	C14-C13-C15-C16
22	2	303	CLA	C6-C7-C8-C9
22	7	316	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	0	307	CLA	C14-C13-C15-C16
22	H	201	CLA	C13-C15-C16-C17
22	7	307	CLA	O1D-CGD-O2D-CED
25	A	848	8CT	C16-C17-C18-C19
25	B	846	8CT	C12-C13-C14-C15
25	J	104	8CT	C16-C17-C18-C19
25	K	103	8CT	C12-C13-C14-C15
25	3	318	8CT	C18-C19-C20-C21
22	9	308	CLA	C16-C17-C18-C19
22	B	830	CLA	C15-C16-C17-C18
24	5	318	LHG	C9-C10-C11-C12
22	B	805	CLA	CAA-CBA-CGA-O1A
22	B	825	CLA	C2A-CAA-CBA-CGA
22	B	834	CLA	C2A-CAA-CBA-CGA
22	6	311	CLA	C3-C5-C6-C7
22	6	313	CLA	C16-C17-C18-C19
31	8	319	LMG	C30-C31-C32-C33
22	L	201	CLA	C5-C6-C7-C8
29	9	307	CHL	C2C-C3C-CAC-CBC
22	B	819	CLA	C2-C3-C5-C6
22	8	315	CLA	C2-C3-C5-C6
22	A	807	CLA	C16-C17-C18-C20
22	6	304	CLA	C16-C17-C18-C19
22	B	806	CLA	CBA-CGA-O2A-C1
22	4	309	CLA	C8-C10-C11-C12
28	B	849	DGD	O1A-C1A-O1G-C1G
22	A	828	CLA	CAA-CBA-CGA-O2A
22	B	826	CLA	C2C-C3C-CAC-CBC
24	0	315	LHG	C16-C17-C18-C19
22	K	102	CLA	CBA-CGA-O2A-C1
25	B	843	8CT	C18-C19-C20-C21
25	L	205	8CT	C12-C13-C14-C15
22	A	840	CLA	C3-C5-C6-C7
22	9	310	CLA	C2C-C3C-CAC-CBC
28	B	849	DGD	O6D-C5D-C6D-O5D
22	7	303	CLA	C10-C11-C12-C13
22	7	305	CLA	CAA-CBA-CGA-O1A
22	H	201	CLA	C16-C17-C18-C19
22	0	308	CLA	C11-C12-C13-C15
22	L	202	CLA	O1D-CGD-O2D-CED
22	A	802	CLA	C4-C3-C5-C6
22	B	839	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	F	301	CLA	CAA-CBA-CGA-O1A
22	7	317	CLA	C10-C11-C12-C13
22	B	839	CLA	C2-C3-C5-C6
22	A	803	CLA	O1A-CGA-O2A-C1
22	A	839	CLA	C10-C11-C12-C13
23	A	842	PQN	C23-C25-C26-C27
28	B	849	DGD	CAB-CBB-CCB-CDB
31	4	318	LMG	C22-C23-C24-C25
22	A	832	CLA	C2-C1-O2A-CGA
22	B	841	CLA	C2-C1-O2A-CGA
22	1	302	CLA	C2-C1-O2A-CGA
22	6	313	CLA	C2-C1-O2A-CGA
29	0	301	CHL	C2-C1-O2A-CGA
22	8	315	CLA	C2C-C3C-CAC-CBC
22	3	319	CLA	C8-C10-C11-C12
22	A	818	CLA	C2A-CAA-CBA-CGA
22	A	837	CLA	C2A-CAA-CBA-CGA
22	A	853	CLA	C2A-CAA-CBA-CGA
22	B	809	CLA	C2A-CAA-CBA-CGA
22	B	810	CLA	C2A-CAA-CBA-CGA
22	4	302	CLA	C2A-CAA-CBA-CGA
22	4	312	CLA	C2A-CAA-CBA-CGA
22	7	304	CLA	C2A-CAA-CBA-CGA
22	9	304	CLA	C2A-CAA-CBA-CGA
24	9	316	LHG	C31-C32-C33-C34
22	B	809	CLA	C3A-C2A-CAA-CBA
22	3	307	CLA	C3A-C2A-CAA-CBA
29	2	306	CHL	C3A-C2A-CAA-CBA
29	8	306	CHL	C3A-C2A-CAA-CBA
22	B	815	CLA	C2C-C3C-CAC-CBC
22	A	822	CLA	O2A-C1-C2-C3
24	A	844	LHG	C13-C14-C15-C16
30	3	314	XAT	C33-C34-C35-C15
22	A	813	CLA	C11-C10-C8-C9
22	A	837	CLA	C11-C12-C13-C14
22	B	841	CLA	C11-C10-C8-C9
22	2	312	CLA	C11-C10-C8-C9
22	5	302	CLA	C11-C12-C13-C14
22	5	312	CLA	C14-C13-C15-C16
29	6	302	CHL	C11-C10-C8-C9
22	A	817	CLA	C16-C17-C18-C20
24	A	845	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
25	B	843	8CT	C39-C16-C17-C18
25	B	844	8CT	C39-C16-C17-C18
25	B	844	8CT	C19-C20-C21-C22
25	B	844	8CT	C24-C25-C26-C27
25	B	845	8CT	C39-C16-C17-C18
25	B	845	8CT	C24-C25-C26-C27
25	B	846	8CT	C40-C12-C13-C14
25	B	846	8CT	C39-C16-C17-C18
25	B	848	8CT	C24-C25-C26-C27
25	B	851	8CT	C40-C12-C13-C14
25	B	851	8CT	C24-C25-C26-C27
25	J	104	8CT	C40-C12-C13-C14
25	K	103	8CT	C40-C12-C13-C14
25	K	103	8CT	C19-C20-C21-C22
25	K	103	8CT	C24-C25-C26-C27
25	L	205	8CT	C24-C25-C26-C27
25	2	317	8CT	C19-C20-C21-C22
25	3	316	8CT	C40-C12-C13-C14
25	4	317	8CT	C24-C25-C26-C27
25	5	317	8CT	C39-C16-C17-C18
30	1	314	XAT	C40-C33-C34-C35
30	4	315	XAT	C11-C10-C9-C19
30	4	315	XAT	C20-C13-C14-C15
30	6	319	XAT	C40-C33-C34-C35
30	5	315	XAT	C20-C13-C14-C15
30	5	315	XAT	C40-C33-C34-C35
30	8	316	XAT	C40-C33-C34-C35
30	9	314	XAT	C39-C29-C30-C31
30	0	313	XAT	C11-C10-C9-C19
30	0	313	XAT	C40-C33-C34-C35
30	0	314	XAT	C39-C29-C30-C31
30	0	314	XAT	C40-C33-C34-C35
22	5	309	CLA	C11-C12-C13-C15
22	9	308	CLA	C16-C17-C18-C20
22	A	803	CLA	CBA-CGA-O2A-C1
22	2	310	CLA	C4C-C3C-CAC-CBC
22	F	301	CLA	CAA-CBA-CGA-O2A
25	L	206	8CT	C27-C26-C28-C29
29	5	301	CHL	O1D-CGD-O2D-CED
22	A	843	CLA	C2C-C3C-CAC-CBC
22	0	308	CLA	C8-C10-C11-C12
22	A	853	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	802	CLA	C1A-C2A-CAA-CBA
22	A	831	CLA	C1A-C2A-CAA-CBA
22	B	809	CLA	C1A-C2A-CAA-CBA
22	B	830	CLA	C1A-C2A-CAA-CBA
22	B	838	CLA	C1A-C2A-CAA-CBA
22	B	840	CLA	C1A-C2A-CAA-CBA
22	B	850	CLA	C1A-C2A-CAA-CBA
22	L	201	CLA	C1A-C2A-CAA-CBA
22	2	309	CLA	C1A-C2A-CAA-CBA
22	3	307	CLA	C1A-C2A-CAA-CBA
22	6	309	CLA	C1A-C2A-CAA-CBA
22	8	304	CLA	C1A-C2A-CAA-CBA
29	5	301	CHL	C1A-C2A-CAA-CBA
22	A	817	CLA	C11-C12-C13-C15
22	A	825	CLA	C6-C7-C8-C10
22	A	853	CLA	C2-C3-C5-C6
22	B	812	CLA	C11-C12-C13-C15
22	B	824	CLA	C6-C7-C8-C10
22	B	840	CLA	C11-C12-C13-C15
22	1	302	CLA	C6-C7-C8-C10
22	3	319	CLA	C2-C3-C5-C6
22	5	303	CLA	C11-C10-C8-C7
22	8	302	CLA	C11-C10-C8-C7
25	6	321	8CT	C16-C17-C18-C19
22	A	835	CLA	CAA-CBA-CGA-O1A
22	A	835	CLA	CAA-CBA-CGA-O2A
22	A	804	CLA	C6-C7-C8-C9
22	B	823	CLA	C6-C7-C8-C9
24	0	315	LHG	C13-C14-C15-C16
22	B	824	CLA	C2A-CAA-CBA-CGA
22	2	304	CLA	C2A-CAA-CBA-CGA
22	2	312	CLA	C2A-CAA-CBA-CGA
22	3	305	CLA	C2A-CAA-CBA-CGA
22	6	318	CLA	C2A-CAA-CBA-CGA
22	A	826	CLA	C5-C6-C7-C8
22	1	307	CLA	C10-C11-C12-C13
22	5	302	CLA	C13-C15-C16-C17
22	5	303	CLA	C13-C15-C16-C17
22	9	309	CLA	C8-C10-C11-C12
24	6	322	LHG	C12-C13-C14-C15
22	B	807	CLA	CAA-CBA-CGA-O2A
22	B	811	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	4	312	CLA	C4-C3-C5-C6
22	9	306	CLA	C4-C3-C5-C6
22	8	315	CLA	C10-C11-C12-C13
29	6	302	CHL	C5-C6-C7-C8
22	A	802	CLA	C2-C3-C5-C6
31	4	318	LMG	C19-C20-C21-C22
22	7	305	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	C16-C17-C18-C19
25	B	843	8CT	C15-C16-C17-C18
25	B	844	8CT	C15-C16-C17-C18
25	B	844	8CT	C19-C20-C21-C23
25	B	844	8CT	C24-C25-C26-C28
25	B	845	8CT	C15-C16-C17-C18
25	B	845	8CT	C24-C25-C26-C28
25	B	846	8CT	C11-C12-C13-C14
25	B	846	8CT	C15-C16-C17-C18
25	B	848	8CT	C24-C25-C26-C28
25	B	851	8CT	C11-C12-C13-C14
25	B	851	8CT	C24-C25-C26-C28
25	J	104	8CT	C11-C12-C13-C14
25	K	103	8CT	C11-C12-C13-C14
25	K	103	8CT	C19-C20-C21-C23
25	K	103	8CT	C24-C25-C26-C28
25	L	205	8CT	C24-C25-C26-C28
25	2	317	8CT	C19-C20-C21-C23
25	3	316	8CT	C11-C12-C13-C14
25	4	317	8CT	C24-C25-C26-C28
25	5	317	8CT	C15-C16-C17-C18
30	1	314	XAT	C32-C33-C34-C35
30	4	315	XAT	C11-C10-C9-C8
30	4	315	XAT	C12-C13-C14-C15
30	6	319	XAT	C32-C33-C34-C35
30	5	315	XAT	C12-C13-C14-C15
30	5	315	XAT	C32-C33-C34-C35
30	8	316	XAT	C32-C33-C34-C35
30	9	314	XAT	C28-C29-C30-C31
30	0	313	XAT	C11-C10-C9-C8
30	0	313	XAT	C32-C33-C34-C35
30	0	314	XAT	C28-C29-C30-C31
30	0	314	XAT	C32-C33-C34-C35
24	0	315	LHG	O7-C5-C6-O8
22	3	307	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	3	313	CLA	C2A-CAA-CBA-CGA
25	B	804	8CT	C18-C19-C20-C21
25	F	302	8CT	C16-C17-C18-C19
25	F	302	8CT	C18-C19-C20-C21
30	1	315	XAT	C29-C30-C31-C32
30	5	316	XAT	C29-C30-C31-C32
22	4	313	CLA	CAA-CBA-CGA-O2A
22	B	816	CLA	C10-C11-C12-C13
22	B	820	CLA	C16-C17-C18-C19
22	8	309	CLA	C11-C12-C13-C14
22	7	318	CLA	C15-C16-C17-C18
24	3	317	LHG	C1-C2-C3-O3
22	B	807	CLA	CAA-CBA-CGA-O1A
22	8	313	CLA	CAA-CBA-CGA-O2A
22	B	836	CLA	C4C-C3C-CAC-CBC
29	0	306	CHL	C2-C1-O2A-CGA
22	A	843	CLA	C4-C3-C5-C6
22	0	305	CLA	C4-C3-C5-C6
22	A	819	CLA	C2-C1-O2A-CGA
22	A	837	CLA	C2-C1-O2A-CGA
22	2	302	CLA	C2-C1-O2A-CGA
29	7	308	CHL	O1A-CGA-O2A-C1
22	A	805	CLA	C2-C3-C5-C6
22	B	840	CLA	C16-C17-C18-C20
22	A	807	CLA	C14-C13-C15-C16
22	B	812	CLA	C6-C7-C8-C9
22	9	303	CLA	C6-C7-C8-C9
22	9	308	CLA	C11-C10-C8-C9
22	B	808	CLA	C3-C5-C6-C7
22	7	316	CLA	C5-C6-C7-C8
29	6	302	CHL	C2A-CAA-CBA-CGA
22	A	832	CLA	O1A-CGA-O2A-C1
25	8	301	8CT	C02-C03-C10-C11
22	A	837	CLA	C10-C11-C12-C13
22	A	836	CLA	C4C-C3C-CAC-CBC
22	1	311	CLA	C10-C11-C12-C13
28	B	849	DGD	C3A-C4A-C5A-C6A
25	A	848	8CT	C18-C19-C20-C21
31	5	319	LMG	C30-C31-C32-C33
22	7	318	CLA	C4-C3-C5-C6
22	A	811	CLA	C15-C16-C17-C18
24	5	318	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
22	A	833	CLA	C2-C3-C5-C6
22	6	311	CLA	C2-C3-C5-C6
22	B	850	CLA	C3-C5-C6-C7
22	8	313	CLA	CAA-CBA-CGA-O1A
29	2	306	CHL	CAA-CBA-CGA-O1A
29	1	305	CHL	C2-C1-O2A-CGA
29	4	301	CHL	C8-C10-C11-C12
22	A	811	CLA	C16-C17-C18-C19
22	8	310	CLA	C6-C7-C8-C10
29	5	301	CHL	C11-C12-C13-C15
22	4	313	CLA	CAA-CBA-CGA-O1A
22	A	810	CLA	C15-C16-C17-C18
29	9	302	CHL	C4-C3-C5-C6
22	A	801	CLA	C12-C13-C15-C16
22	A	806	CLA	C6-C7-C8-C10
22	A	843	CLA	C2-C3-C5-C6
22	B	819	CLA	C6-C7-C8-C10
22	B	839	CLA	C11-C12-C13-C15
22	1	311	CLA	C12-C13-C15-C16
22	6	304	CLA	C6-C7-C8-C10
22	7	318	CLA	C2-C3-C5-C6
22	9	308	CLA	C11-C10-C8-C7
22	0	311	CLA	C11-C12-C13-C15
22	6	309	CLA	C4C-C3C-CAC-CBC
24	3	317	LHG	O8-C23-C24-C25
24	7	322	LHG	O8-C23-C24-C25
22	5	314	CLA	CAA-CBA-CGA-O2A
22	A	839	CLA	C16-C17-C18-C20
22	A	825	CLA	O1A-CGA-O2A-C1
22	A	832	CLA	CBA-CGA-O2A-C1
24	1	317	LHG	C29-C30-C31-C32
22	A	852	CLA	O2A-C1-C2-C3
22	B	820	CLA	C15-C16-C17-C18
22	6	311	CLA	C10-C11-C12-C13
22	A	853	CLA	C16-C17-C18-C19
22	B	801	CLA	C16-C17-C18-C20
22	0	308	CLA	C11-C12-C13-C14
22	A	825	CLA	CBA-CGA-O2A-C1
24	0	315	LHG	C24-C23-O8-C6
22	B	832	CLA	CAA-CBA-CGA-O2A
22	1	307	CLA	CAA-CBA-CGA-O2A
22	0	312	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	A	830	CLA	C4-C3-C5-C6
22	L	202	CLA	C4-C3-C5-C6
22	9	312	CLA	C4-C3-C5-C6
22	A	837	CLA	C2-C3-C5-C6
22	B	834	CLA	CAA-CBA-CGA-O2A
22	7	318	CLA	CAA-CBA-CGA-O2A
22	A	802	CLA	C6-C7-C8-C9
22	A	818	CLA	C11-C10-C8-C9
22	A	826	CLA	C6-C7-C8-C9
22	B	803	CLA	C11-C10-C8-C9
22	B	816	CLA	C11-C10-C8-C9
22	B	824	CLA	C6-C7-C8-C9
22	B	824	CLA	C11-C10-C8-C9
22	B	825	CLA	C14-C13-C15-C16
22	B	834	CLA	C11-C10-C8-C9
22	B	840	CLA	C11-C12-C13-C14
22	1	302	CLA	C6-C7-C8-C9
22	5	303	CLA	C6-C7-C8-C9
22	5	303	CLA	C11-C10-C8-C9
22	7	317	CLA	C6-C7-C8-C9
22	0	307	CLA	C11-C12-C13-C14
22	6	317	CLA	CAA-CBA-CGA-O1A
22	A	814	CLA	C3A-C2A-CAA-CBA
22	B	822	CLA	C3A-C2A-CAA-CBA
22	B	837	CLA	C3A-C2A-CAA-CBA
22	F	301	CLA	C3A-C2A-CAA-CBA
22	5	304	CLA	C3A-C2A-CAA-CBA
22	7	316	CLA	C3A-C2A-CAA-CBA
22	9	306	CLA	C3A-C2A-CAA-CBA
29	5	306	CHL	C3A-C2A-CAA-CBA
24	A	844	LHG	C33-C34-C35-C36
22	B	838	CLA	CAA-CBA-CGA-O2A
22	H	201	CLA	CAA-CBA-CGA-O2A
22	A	813	CLA	CAD-CBD-CGD-O2D
22	A	823	CLA	CAD-CBD-CGD-O2D
22	A	827	CLA	CAD-CBD-CGD-O2D
22	A	828	CLA	CAD-CBD-CGD-O2D
22	A	833	CLA	CAD-CBD-CGD-O2D
22	A	840	CLA	CAD-CBD-CGD-O2D
22	B	818	CLA	CAD-CBD-CGD-O2D
22	B	820	CLA	CAD-CBD-CGD-O2D
22	B	822	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	830	CLA	CAD-CBD-CGD-O2D
22	B	831	CLA	CAD-CBD-CGD-O2D
22	1	313	CLA	CAD-CBD-CGD-O2D
22	2	311	CLA	CAD-CBD-CGD-O2D
22	3	304	CLA	CAD-CBD-CGD-O2D
22	3	305	CLA	CAD-CBD-CGD-O2D
22	3	307	CLA	CAD-CBD-CGD-O2D
22	3	308	CLA	CAD-CBD-CGD-O2D
22	4	312	CLA	CAD-CBD-CGD-O2D
22	4	314	CLA	CAD-CBD-CGD-O2D
22	6	310	CLA	CAD-CBD-CGD-O2D
22	6	318	CLA	CAD-CBD-CGD-O2D
22	5	310	CLA	CAD-CBD-CGD-O2D
22	5	313	CLA	CAD-CBD-CGD-O2D
22	7	304	CLA	CAD-CBD-CGD-O2D
22	7	307	CLA	CAD-CBD-CGD-O2D
22	7	312	CLA	CAD-CBD-CGD-O2D
22	7	313	CLA	CAD-CBD-CGD-O2D
22	7	316	CLA	CAD-CBD-CGD-O2D
22	8	303	CLA	CAD-CBD-CGD-O2D
22	0	304	CLA	CAD-CBD-CGD-O2D
22	0	305	CLA	CAD-CBD-CGD-O2D
22	0	307	CLA	CAD-CBD-CGD-O2D
22	0	311	CLA	CAD-CBD-CGD-O2D
29	5	301	CHL	CAD-CBD-CGD-O2D
24	5	318	LHG	C19-C20-C21-C22
22	B	811	CLA	C10-C11-C12-C13
22	4	314	CLA	C10-C11-C12-C13
22	A	809	CLA	C10-C11-C12-C13
22	6	309	CLA	C2-C1-O2A-CGA
22	G	101	CLA	CAA-CBA-CGA-O2A
22	A	822	CLA	CAA-CBA-CGA-O2A
22	2	319	CLA	CAA-CBA-CGA-O2A
31	5	319	LMG	O7-C10-C11-C12
22	2	310	CLA	C2C-C3C-CAC-CBC
22	B	818	CLA	C4-C3-C5-C6
22	7	313	CLA	C4-C3-C5-C6
22	7	313	CLA	C6-C7-C8-C10
22	A	815	CLA	C2-C1-O2A-CGA
22	B	818	CLA	C11-C12-C13-C14
22	B	811	CLA	C2-C3-C5-C6
22	L	202	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	4	312	CLA	C2-C3-C5-C6
22	A	806	CLA	CAA-CBA-CGA-O2A
22	1	302	CLA	CAA-CBA-CGA-O2A
22	3	311	CLA	CAA-CBA-CGA-O2A
22	6	301	CLA	CAA-CBA-CGA-O2A
29	0	301	CHL	CAA-CBA-CGA-O2A
24	9	316	LHG	C18-C19-C20-C21
25	B	843	8CT	C25-C26-C28-C29
25	L	206	8CT	C25-C26-C28-C29
22	1	310	CLA	C3-C5-C6-C7
30	2	315	XAT	O4-C6-C7-C8
30	4	316	XAT	O24-C26-C27-C28
30	6	320	XAT	O4-C6-C7-C8
30	5	316	XAT	O24-C26-C27-C28
30	8	316	XAT	O4-C6-C7-C8
22	A	822	CLA	O1D-CGD-O2D-CED
22	6	304	CLA	CAA-CBA-CGA-O2A
29	5	301	CHL	CAA-CBA-CGA-O2A
24	6	322	LHG	C10-C11-C12-C13
22	K	101	CLA	CAA-CBA-CGA-O2A
22	A	805	CLA	O2A-C1-C2-C3
22	A	808	CLA	O2A-C1-C2-C3
22	A	810	CLA	O2A-C1-C2-C3
22	A	840	CLA	O2A-C1-C2-C3
22	B	834	CLA	O2A-C1-C2-C3
22	L	204	CLA	O2A-C1-C2-C3
22	8	315	CLA	O2A-C1-C2-C3
22	9	313	CLA	O2A-C1-C2-C3
29	6	308	CHL	O2A-C1-C2-C3
29	9	302	CHL	O2A-C1-C2-C3
22	B	836	CLA	C2C-C3C-CAC-CBC
28	B	849	DGD	C6A-C7A-C8A-C9A
29	5	301	CHL	C2A-CAA-CBA-CGA
22	A	829	CLA	CAA-CBA-CGA-O2A
22	1	310	CLA	CAA-CBA-CGA-O2A
22	3	312	CLA	CAA-CBA-CGA-O2A
22	H	201	CLA	C15-C16-C17-C18
22	9	313	CLA	C6-C7-C8-C9
22	6	309	CLA	C2C-C3C-CAC-CBC
22	A	809	CLA	CHA-CBD-CGD-O1D
22	A	809	CLA	CHA-CBD-CGD-O2D
22	A	822	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	822	CLA	CHA-CBD-CGD-O2D
22	A	830	CLA	CHA-CBD-CGD-O1D
22	A	830	CLA	CHA-CBD-CGD-O2D
22	A	833	CLA	CHA-CBD-CGD-O2D
22	A	837	CLA	CHA-CBD-CGD-O1D
22	A	837	CLA	CHA-CBD-CGD-O2D
22	B	803	CLA	CHA-CBD-CGD-O1D
22	B	803	CLA	CHA-CBD-CGD-O2D
22	B	816	CLA	CHA-CBD-CGD-O1D
22	B	816	CLA	CHA-CBD-CGD-O2D
22	B	824	CLA	CHA-CBD-CGD-O2D
22	B	827	CLA	CHA-CBD-CGD-O1D
22	B	827	CLA	CHA-CBD-CGD-O2D
22	B	833	CLA	CHA-CBD-CGD-O2D
22	G	103	CLA	CHA-CBD-CGD-O1D
22	1	302	CLA	CHA-CBD-CGD-O1D
22	1	302	CLA	CHA-CBD-CGD-O2D
22	1	303	CLA	CHA-CBD-CGD-O2D
22	2	302	CLA	CHA-CBD-CGD-O1D
22	3	312	CLA	CHA-CBD-CGD-O2D
22	4	314	CLA	CHA-CBD-CGD-O2D
22	6	303	CLA	CHA-CBD-CGD-O1D
22	6	305	CLA	CHA-CBD-CGD-O2D
22	6	315	CLA	CHA-CBD-CGD-O1D
22	6	315	CLA	CHA-CBD-CGD-O2D
22	5	303	CLA	CHA-CBD-CGD-O1D
22	5	303	CLA	CHA-CBD-CGD-O2D
22	5	305	CLA	CHA-CBD-CGD-O1D
22	5	305	CLA	CHA-CBD-CGD-O2D
22	7	318	CLA	CHA-CBD-CGD-O1D
22	8	304	CLA	CHA-CBD-CGD-O2D
22	8	312	CLA	CHA-CBD-CGD-O1D
22	8	312	CLA	CHA-CBD-CGD-O2D
22	9	304	CLA	CHA-CBD-CGD-O2D
22	0	302	CLA	CHA-CBD-CGD-O2D
29	2	306	CHL	CHA-CBD-CGD-O1D
29	2	306	CHL	CHA-CBD-CGD-O2D
22	G	101	CLA	CAA-CBA-CGA-O1A
22	K	101	CLA	CAA-CBA-CGA-O1A
22	3	312	CLA	CAA-CBA-CGA-O1A
22	B	812	CLA	C4-C3-C5-C6
29	6	302	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	A	819	CLA	C16-C17-C18-C20
22	B	833	CLA	CAA-CBA-CGA-O2A
22	7	313	CLA	CAA-CBA-CGA-O2A
29	7	308	CHL	CAA-CBA-CGA-O2A
24	7	322	LHG	O7-C5-C6-O8
22	8	308	CLA	O1A-CGA-O2A-C1
22	B	818	CLA	C3-C5-C6-C7
22	A	839	CLA	CAA-CBA-CGA-O2A
22	3	313	CLA	CAA-CBA-CGA-O2A
22	6	312	CLA	CAA-CBA-CGA-O2A
22	0	308	CLA	CAA-CBA-CGA-O2A
29	4	306	CHL	CAA-CBA-CGA-O2A
22	B	831	CLA	C2A-CAA-CBA-CGA
22	6	317	CLA	CAA-CBA-CGA-O2A
24	2	318	LHG	C24-C25-C26-C27
22	A	813	CLA	C11-C12-C13-C15
22	A	839	CLA	C11-C10-C8-C7
22	A	839	CLA	C11-C12-C13-C15
22	B	805	CLA	C12-C13-C15-C16
22	B	826	CLA	C11-C12-C13-C15
22	7	313	CLA	C2-C3-C5-C6
22	7	317	CLA	C11-C12-C13-C15
22	0	303	CLA	C6-C7-C8-C10
22	0	307	CLA	C11-C10-C8-C7
22	A	806	CLA	C16-C17-C18-C20
22	8	308	CLA	CBA-CGA-O2A-C1
22	A	805	CLA	CAA-CBA-CGA-O2A
22	A	821	CLA	CAA-CBA-CGA-O2A
22	K	105	CLA	CAA-CBA-CGA-O2A
22	A	806	CLA	C11-C10-C8-C9
22	B	841	CLA	C11-C12-C13-C14
22	2	304	CLA	C6-C7-C8-C9
22	6	315	CLA	C6-C7-C8-C9
22	8	309	CLA	C6-C7-C8-C9
25	5	317	8CT	C16-C17-C18-C19
24	3	317	LHG	O2-C2-C3-O3
22	7	317	CLA	CAA-CBA-CGA-O2A
22	B	834	CLA	CAA-CBA-CGA-O1A
22	0	311	CLA	C3-C5-C6-C7
22	B	815	CLA	C15-C16-C17-C18
22	A	802	CLA	C2A-CAA-CBA-CGA
22	8	302	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	8	312	CLA	C2A-CAA-CBA-CGA
24	A	844	LHG	O10-C23-C24-C25
29	0	301	CHL	CAA-CBA-CGA-O1A
29	9	307	CHL	C4C-C3C-CAC-CBC
22	B	838	CLA	CAA-CBA-CGA-O1A
22	A	813	CLA	C15-C16-C17-C18
22	6	305	CLA	C5-C6-C7-C8
22	9	310	CLA	C4C-C3C-CAC-CBC
24	0	315	LHG	O1-C1-C2-C3
22	A	843	CLA	C3-C5-C6-C7
22	A	806	CLA	CAA-CBA-CGA-O1A
22	0	312	CLA	CAA-CBA-CGA-O1A
22	0	302	CLA	C13-C15-C16-C17
22	A	814	CLA	C1A-C2A-CAA-CBA
22	A	852	CLA	C1A-C2A-CAA-CBA
22	B	822	CLA	C1A-C2A-CAA-CBA
22	F	301	CLA	C1A-C2A-CAA-CBA
22	1	303	CLA	C1A-C2A-CAA-CBA
22	2	303	CLA	C1A-C2A-CAA-CBA
22	6	312	CLA	C1A-C2A-CAA-CBA
22	7	316	CLA	C1A-C2A-CAA-CBA
22	9	301	CLA	C1A-C2A-CAA-CBA
22	9	306	CLA	C1A-C2A-CAA-CBA
22	0	307	CLA	C1A-C2A-CAA-CBA
29	5	306	CHL	C1A-C2A-CAA-CBA
22	B	832	CLA	CAA-CBA-CGA-O1A
22	1	310	CLA	CAA-CBA-CGA-O1A
22	2	319	CLA	CAA-CBA-CGA-O1A
22	6	323	CLA	CAA-CBA-CGA-O2A
22	A	805	CLA	C8-C10-C11-C12
24	6	322	LHG	C11-C12-C13-C14
22	A	825	CLA	O1D-CGD-O2D-CED
22	1	304	CLA	C2-C1-O2A-CGA
28	B	849	DGD	C6B-C7B-C8B-C9B
22	A	804	CLA	C5-C6-C7-C8
22	9	308	CLA	C8-C10-C11-C12
22	1	302	CLA	CAA-CBA-CGA-O1A
22	1	307	CLA	CAA-CBA-CGA-O1A
24	5	318	LHG	O10-C23-C24-C25
22	0	307	CLA	C13-C15-C16-C17
22	9	312	CLA	C2A-CAA-CBA-CGA
22	0	304	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	K	102	CLA	CBD-CGD-O2D-CED
22	A	813	CLA	C16-C17-C18-C20
22	5	314	CLA	CAA-CBA-CGA-O1A
22	7	318	CLA	CAA-CBA-CGA-O1A
31	5	319	LMG	O10-C28-C29-C30
31	4	318	LMG	C11-C12-C13-C14
29	8	306	CHL	O1A-CGA-O2A-C1
22	7	303	CLA	CAA-CBA-CGA-O2A
22	8	303	CLA	CAA-CBA-CGA-O2A
24	A	844	LHG	O8-C23-C24-C25
24	6	322	LHG	C5-C4-O6-P
22	H	201	CLA	CAA-CBA-CGA-O1A
22	K	105	CLA	CAA-CBA-CGA-O1A
22	3	311	CLA	CAA-CBA-CGA-O1A
22	B	827	CLA	C2-C3-C5-C6
29	9	307	CHL	C2-C1-O2A-CGA
24	1	317	LHG	C3-O3-P-O5
24	6	322	LHG	C4-O6-P-O5
24	9	316	LHG	C4-O6-P-O5
24	A	845	LHG	O7-C5-C6-O8
22	A	821	CLA	CAA-CBA-CGA-O1A
22	7	317	CLA	CAA-CBA-CGA-O1A
29	7	308	CHL	CAA-CBA-CGA-O1A
22	L	204	CLA	CAA-CBA-CGA-O2A
22	5	307	CLA	CAA-CBA-CGA-O2A
22	7	302	CLA	CAA-CBA-CGA-O2A
22	A	827	CLA	C15-C16-C17-C18
22	B	803	CLA	C4C-C3C-CAC-CBC
22	A	814	CLA	CAA-CBA-CGA-O2A
25	A	850	8CT	C04-C03-C10-C11
25	F	302	8CT	C02-C03-C10-C11
25	7	323	8CT	C02-C03-C10-C11
22	6	304	CLA	C13-C15-C16-C17
30	9	314	XAT	C6-C7-C8-C9
22	A	805	CLA	CAA-CBA-CGA-O1A
22	A	829	CLA	CAA-CBA-CGA-O1A
22	6	301	CLA	CAA-CBA-CGA-O1A
22	0	308	CLA	CAA-CBA-CGA-O1A
22	6	311	CLA	CAA-CBA-CGA-O2A
22	L	202	CLA	C16-C17-C18-C20
22	7	313	CLA	C6-C7-C8-C9
22	0	303	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	7	316	CLA	CAA-CBA-CGA-O2A
22	9	313	CLA	CAA-CBA-CGA-O2A
22	A	822	CLA	CAA-CBA-CGA-O1A
22	6	304	CLA	CAA-CBA-CGA-O1A
22	A	828	CLA	C16-C17-C18-C20
22	A	805	CLA	CAD-CBD-CGD-O1D
22	A	817	CLA	CAD-CBD-CGD-O1D
22	A	827	CLA	CAD-CBD-CGD-O1D
22	A	836	CLA	C2-C3-C5-C6
22	B	836	CLA	CAD-CBD-CGD-O1D
22	B	840	CLA	CAD-CBD-CGD-O1D
22	B	841	CLA	CAD-CBD-CGD-O1D
22	G	103	CLA	CAD-CBD-CGD-O1D
22	K	101	CLA	CAD-CBD-CGD-O1D
22	2	302	CLA	CAD-CBD-CGD-O1D
22	3	310	CLA	CAD-CBD-CGD-O1D
22	4	303	CLA	CAD-CBD-CGD-O1D
22	4	311	CLA	CAD-CBD-CGD-O1D
22	7	318	CLA	CAD-CBD-CGD-O1D
29	8	314	CHL	CAD-CBD-CGD-O1D
22	B	833	CLA	CAA-CBA-CGA-O1A
22	7	303	CLA	CAA-CBA-CGA-O1A
29	5	301	CHL	CAA-CBA-CGA-O1A
22	B	840	CLA	CAA-CBA-CGA-O2A
22	A	802	CLA	C11-C12-C13-C14
22	A	813	CLA	C11-C12-C13-C14
22	A	839	CLA	C11-C10-C8-C9
22	B	828	CLA	C14-C13-C15-C16
22	L	202	CLA	C6-C7-C8-C9
22	1	311	CLA	C6-C7-C8-C9
22	6	313	CLA	C11-C10-C8-C9
22	9	308	CLA	C6-C7-C8-C9
22	0	303	CLA	C6-C7-C8-C9
22	0	307	CLA	C11-C10-C8-C9
22	0	311	CLA	C11-C12-C13-C14
22	2	312	CLA	C15-C16-C17-C18
29	4	306	CHL	CAA-CBA-CGA-O1A
29	8	306	CHL	CBA-CGA-O2A-C1
22	1	312	CLA	C3-C5-C6-C7
22	B	814	CLA	CAA-CBA-CGA-O2A
22	B	841	CLA	CAA-CBA-CGA-O2A
22	4	302	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	5	319	LMG	O8-C28-C29-C30
22	6	310	CLA	O1A-CGA-O2A-C1
22	3	313	CLA	CAA-CBA-CGA-O1A
22	6	312	CLA	CAA-CBA-CGA-O1A
22	4	309	CLA	C5-C6-C7-C8
22	B	837	CLA	C2A-CAA-CBA-CGA
22	3	301	CLA	C2A-CAA-CBA-CGA
22	0	302	CLA	C2A-CAA-CBA-CGA
22	B	801	CLA	CAA-CBA-CGA-O2A
22	2	311	CLA	CAA-CBA-CGA-O2A
22	4	303	CLA	CAA-CBA-CGA-O2A
22	M	101	CLA	CAA-CBA-CGA-O2A
29	1	305	CHL	CAA-CBA-CGA-O2A
29	2	307	CHL	CAA-CBA-CGA-O2A
29	9	307	CHL	CAA-CBA-CGA-O2A
31	8	319	LMG	O7-C10-C11-C12
22	A	839	CLA	CAA-CBA-CGA-O1A
22	A	806	CLA	C11-C10-C8-C7
22	B	812	CLA	C11-C10-C8-C7
22	B	814	CLA	C11-C10-C8-C7
22	B	818	CLA	C6-C7-C8-C10
22	B	826	CLA	C12-C13-C15-C16
22	B	828	CLA	C12-C13-C15-C16
22	B	841	CLA	C11-C12-C13-C15
22	L	201	CLA	C11-C10-C8-C7
22	L	202	CLA	C6-C7-C8-C10
22	1	307	CLA	C6-C7-C8-C10
22	1	311	CLA	C6-C7-C8-C10
22	2	304	CLA	C6-C7-C8-C10
22	2	312	CLA	C6-C7-C8-C10
22	3	319	CLA	C11-C12-C13-C15
22	5	312	CLA	C12-C13-C15-C16
25	A	847	8CT	C28-C29-C30-C31
25	B	804	8CT	C28-C29-C30-C31
25	B	847	8CT	C28-C29-C30-C31
25	G	104	8CT	C28-C29-C30-C31
22	L	204	CLA	CAA-CBA-CGA-O1A
22	A	820	CLA	CAA-CBA-CGA-O2A
28	B	849	DGD	C5B-C6B-C7B-C8B
22	A	832	CLA	CAA-CBA-CGA-O2A
22	B	813	CLA	CAA-CBA-CGA-O2A
22	6	313	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	7	309	CLA	CAA-CBA-CGA-O2A
24	9	316	LHG	O7-C7-C8-C9
29	6	302	CHL	CAA-CBA-CGA-O2A
29	0	306	CHL	CAA-CBA-CGA-O2A
22	A	803	CLA	C3-C5-C6-C7
25	A	850	8CT	C20-C21-C23-C24
22	A	832	CLA	CAA-CBA-CGA-O1A
22	6	311	CLA	CAA-CBA-CGA-O1A
22	7	314	CLA	CAA-CBA-CGA-O1A
24	A	844	LHG	C15-C16-C17-C18
22	5	304	CLA	CAA-CBA-CGA-O2A
22	B	840	CLA	C15-C16-C17-C18
22	4	314	CLA	C15-C16-C17-C18
22	A	834	CLA	O1A-CGA-O2A-C1
22	B	840	CLA	CAA-CBA-CGA-O1A
22	2	311	CLA	CAA-CBA-CGA-O1A
22	4	302	CLA	CAA-CBA-CGA-O1A
22	5	307	CLA	CAA-CBA-CGA-O1A
22	7	313	CLA	CAA-CBA-CGA-O1A
29	1	305	CHL	CAA-CBA-CGA-O1A
29	0	306	CHL	CAA-CBA-CGA-O1A
22	B	808	CLA	CAA-CBA-CGA-O1A
22	6	323	CLA	CAA-CBA-CGA-O1A
22	7	309	CLA	CAA-CBA-CGA-O1A
22	8	303	CLA	CAA-CBA-CGA-O1A
29	6	308	CHL	C2A-CAA-CBA-CGA
24	9	316	LHG	C17-C18-C19-C20
22	B	817	CLA	C4-C3-C5-C6
22	K	102	CLA	O1A-CGA-O2A-C1
22	A	825	CLA	CAA-CBA-CGA-O2A
22	A	814	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

302 monomers are involved in 1491 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	304	CLA	5	0
22	A	818	CLA	4	0
25	5	317	8CT	6	0
22	9	312	CLA	9	0
22	5	308	CLA	6	0
22	B	817	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	804	CLA	4	0
22	1	310	CLA	6	0
22	9	308	CLA	5	0
27	B	802	SF4	1	0
22	A	828	CLA	11	0
22	7	302	CLA	1	0
22	4	303	CLA	2	0
22	A	825	CLA	9	0
22	3	312	CLA	2	0
22	7	314	CLA	2	0
22	1	301	CLA	8	0
25	B	851	8CT	1	0
22	5	310	CLA	2	0
22	0	302	CLA	15	0
29	9	302	CHL	2	0
22	7	305	CLA	3	0
22	8	303	CLA	1	0
22	4	309	CLA	8	0
22	9	303	CLA	7	0
22	B	850	CLA	17	0
22	2	314	CLA	1	0
22	0	307	CLA	7	0
24	3	317	LHG	4	0
22	0	310	CLA	2	0
22	7	306	CLA	6	0
22	7	307	CLA	13	0
29	5	306	CHL	5	0
22	A	826	CLA	12	0
22	5	302	CLA	8	0
25	A	854	8CT	3	0
22	5	309	CLA	10	0
29	8	314	CHL	11	0
22	A	821	CLA	4	0
29	0	306	CHL	2	0
22	A	815	CLA	3	0
22	B	811	CLA	4	0
22	7	313	CLA	7	0
22	B	813	CLA	10	0
22	B	836	CLA	2	0
22	2	308	CLA	7	0
30	6	319	XAT	7	0
22	5	313	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	8	316	XAT	12	0
22	7	315	CLA	2	0
22	6	323	CLA	5	0
22	B	829	CLA	8	0
22	A	803	CLA	5	0
29	8	305	CHL	6	0
24	2	318	LHG	3	0
22	B	805	CLA	7	0
29	2	307	CHL	4	0
22	A	819	CLA	6	0
22	A	810	CLA	4	0
22	B	835	CLA	1	0
25	8	301	8CT	11	0
22	3	319	CLA	8	0
22	6	315	CLA	5	0
22	A	812	CLA	4	0
29	6	306	CHL	2	0
22	B	818	CLA	6	0
31	8	319	LMG	6	0
22	A	806	CLA	4	0
22	1	307	CLA	6	0
22	B	838	CLA	1	0
22	A	824	CLA	3	0
22	A	811	CLA	5	0
29	4	305	CHL	9	0
22	2	302	CLA	8	0
22	B	812	CLA	4	0
22	M	101	CLA	5	0
30	8	317	XAT	9	0
25	J	101	8CT	10	0
22	B	819	CLA	4	0
22	5	312	CLA	6	0
22	L	201	CLA	5	0
22	A	805	CLA	8	0
22	7	309	CLA	5	0
22	B	810	CLA	8	0
22	4	304	CLA	1	0
22	6	314	CLA	4	0
22	B	832	CLA	8	0
22	A	809	CLA	14	0
22	2	303	CLA	3	0
22	K	105	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	823	CLA	1	0
22	0	304	CLA	4	0
22	4	313	CLA	5	0
29	4	306	CHL	2	0
22	A	834	CLA	1	0
22	7	303	CLA	10	0
22	3	302	CLA	3	0
22	B	827	CLA	8	0
23	B	842	PQN	3	0
22	A	817	CLA	7	0
22	B	830	CLA	8	0
22	A	814	CLA	4	0
22	B	820	CLA	5	0
27	C	101	SF4	1	0
29	6	308	CHL	4	0
30	3	314	XAT	8	0
22	2	311	CLA	1	0
22	3	304	CLA	1	0
22	5	304	CLA	8	0
25	B	847	8CT	13	0
29	9	307	CHL	4	0
30	1	315	XAT	5	0
30	0	314	XAT	11	0
22	8	309	CLA	11	0
22	B	839	CLA	4	0
31	5	319	LMG	5	0
22	6	309	CLA	5	0
24	9	316	LHG	8	0
22	6	311	CLA	5	0
22	0	309	CLA	2	0
25	2	317	8CT	13	0
22	A	841	CLA	6	0
22	1	311	CLA	12	0
22	6	305	CLA	11	0
22	L	202	CLA	12	0
29	4	301	CHL	9	0
22	3	307	CLA	9	0
22	6	317	CLA	6	0
22	5	311	CLA	6	0
22	3	310	CLA	1	0
22	6	301	CLA	4	0
22	L	204	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	L	203	CLA	5	0
25	6	321	8CT	14	0
25	7	321	8CT	14	0
30	4	315	XAT	9	0
31	4	318	LMG	1	0
30	2	316	XAT	7	0
22	A	820	CLA	4	0
25	B	848	8CT	12	0
22	4	302	CLA	4	0
22	7	317	CLA	12	0
24	B	852	LHG	1	0
22	6	318	CLA	8	0
22	B	807	CLA	5	0
22	7	312	CLA	3	0
29	1	305	CHL	3	0
24	0	315	LHG	12	0
22	7	316	CLA	7	0
29	3	306	CHL	4	0
22	A	840	CLA	7	0
22	3	309	CLA	1	0
22	8	308	CLA	9	0
22	A	813	CLA	14	0
22	B	815	CLA	6	0
22	1	304	CLA	15	0
22	A	802	CLA	4	0
22	A	807	CLA	4	0
22	B	831	CLA	2	0
22	B	801	CLA	4	0
24	5	318	LHG	8	0
25	8	318	8CT	2	0
22	K	102	CLA	6	0
22	A	822	CLA	4	0
22	G	101	CLA	1	0
22	A	831	CLA	3	0
22	7	318	CLA	4	0
29	2	305	CHL	8	0
22	8	310	CLA	9	0
29	4	307	CHL	11	0
22	8	315	CLA	3	0
22	1	303	CLA	11	0
22	9	310	CLA	2	0
22	A	832	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	837	CLA	6	0
24	7	322	LHG	2	0
22	4	308	CLA	4	0
30	5	315	XAT	8	0
22	B	833	CLA	10	0
22	J	103	CLA	1	0
30	3	315	XAT	9	0
29	8	306	CHL	4	0
22	G	102	CLA	8	0
22	2	313	CLA	1	0
22	H	201	CLA	18	0
29	2	306	CHL	2	0
22	1	309	CLA	3	0
22	0	303	CLA	4	0
22	A	836	CLA	4	0
25	A	849	8CT	8	0
22	B	808	CLA	10	0
22	B	841	CLA	7	0
24	6	322	LHG	4	0
29	7	308	CHL	11	0
22	2	319	CLA	1	0
22	B	825	CLA	4	0
22	8	304	CLA	2	0
22	B	816	CLA	5	0
22	B	824	CLA	8	0
30	9	314	XAT	5	0
22	A	843	CLA	2	0
22	8	302	CLA	4	0
22	8	313	CLA	4	0
30	1	314	XAT	10	0
22	A	837	CLA	6	0
22	A	835	CLA	2	0
22	9	313	CLA	3	0
22	0	312	CLA	6	0
22	B	834	CLA	5	0
22	6	303	CLA	6	0
22	A	839	CLA	9	0
29	6	302	CHL	7	0
22	A	830	CLA	3	0
22	9	301	CLA	5	0
22	3	311	CLA	10	0
24	A	844	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	852	CLA	1	0
22	4	314	CLA	5	0
29	2	301	CHL	3	0
30	9	315	XAT	8	0
30	4	316	XAT	7	0
30	6	320	XAT	7	0
22	B	828	CLA	7	0
25	A	850	8CT	20	0
25	7	323	8CT	22	0
25	K	103	8CT	14	0
22	5	314	CLA	1	0
22	B	803	CLA	18	0
22	2	309	CLA	6	0
22	B	809	CLA	8	0
25	B	843	8CT	3	0
28	B	849	DGD	11	0
22	A	853	CLA	5	0
22	2	304	CLA	5	0
25	3	316	8CT	10	0
25	B	846	8CT	11	0
22	6	312	CLA	2	0
22	B	823	CLA	3	0
22	B	814	CLA	9	0
22	3	301	CLA	5	0
22	A	829	CLA	6	0
24	A	845	LHG	2	0
30	2	315	XAT	7	0
30	0	313	XAT	8	0
22	0	308	CLA	4	0
26	J	102	HTG	1	0
30	7	320	XAT	8	0
22	A	801	CLA	7	0
22	8	312	CLA	5	0
22	8	311	CLA	8	0
22	0	305	CLA	4	0
22	2	312	CLA	5	0
22	4	311	CLA	5	0
22	A	827	CLA	9	0
22	9	311	CLA	3	0
22	A	838	CLA	3	0
22	0	311	CLA	7	0
22	K	101	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	310	CLA	9	0
22	A	808	CLA	10	0
29	0	301	CHL	16	0
22	B	840	CLA	14	0
22	9	304	CLA	6	0
22	4	312	CLA	6	0
30	5	316	XAT	5	0
22	B	806	CLA	10	0
30	7	319	XAT	7	0
22	B	826	CLA	9	0
22	5	303	CLA	11	0
22	5	305	CLA	3	0
22	F	301	CLA	5	0
25	4	317	8CT	12	0
22	A	833	CLA	6	0
22	5	307	CLA	3	0
25	J	104	8CT	16	0
29	5	301	CHL	12	0
22	3	308	CLA	6	0
22	4	310	CLA	1	0
24	1	317	LHG	3	0
25	1	316	8CT	13	0
29	8	307	CHL	6	0
29	6	307	CHL	8	0
22	9	309	CLA	8	0
22	1	313	CLA	1	0
22	7	310	CLA	9	0
25	G	104	8CT	20	0
22	1	302	CLA	6	0
22	3	313	CLA	5	0
22	3	303	CLA	2	0
22	9	306	CLA	5	0
22	G	103	CLA	7	0
22	6	313	CLA	5	0
29	6	316	CHL	3	0
25	A	846	8CT	1	0
22	1	312	CLA	8	0
22	1	306	CLA	5	0
23	A	842	PQN	3	0
22	K	104	CLA	6	0
22	7	304	CLA	4	0
22	A	816	CLA	3	0

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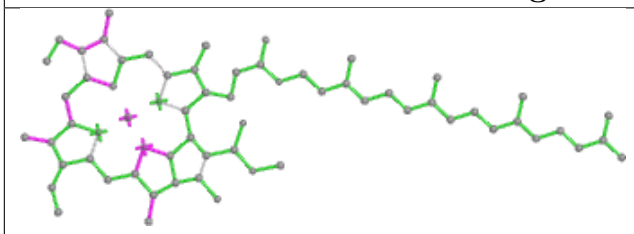
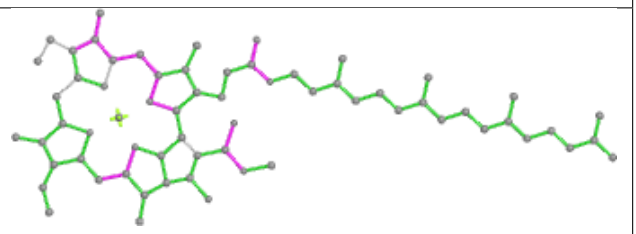
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	308	CLA	6	0
25	A	847	8CT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

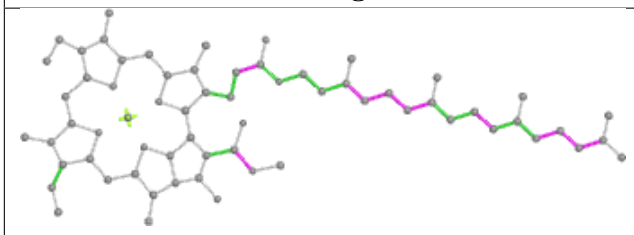
Ligand CLA 6 304



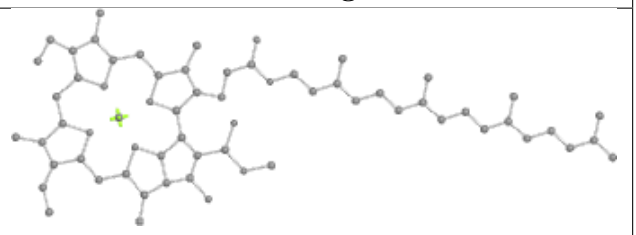
Bond lengths



Bond angles

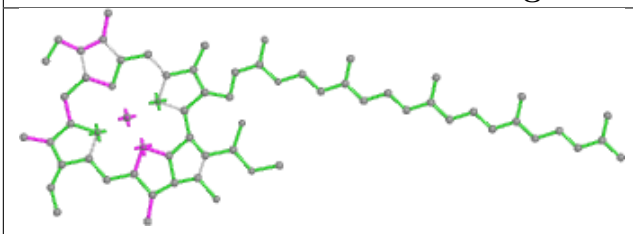


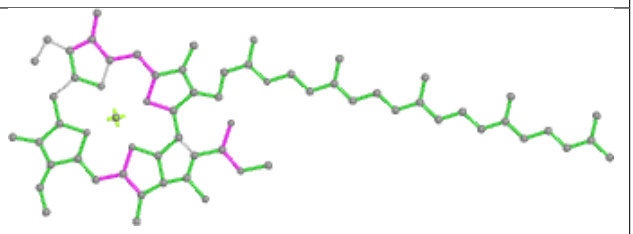
Torsions

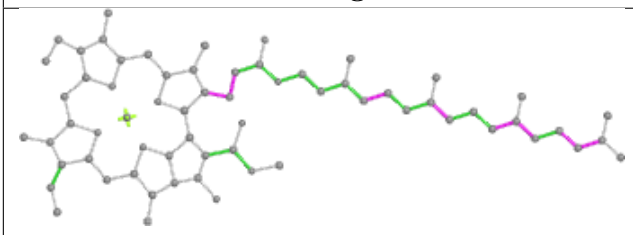


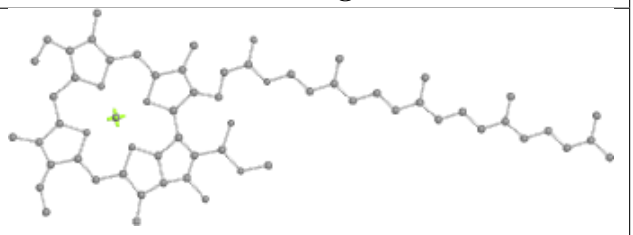
Rings

Ligand CLA A 818

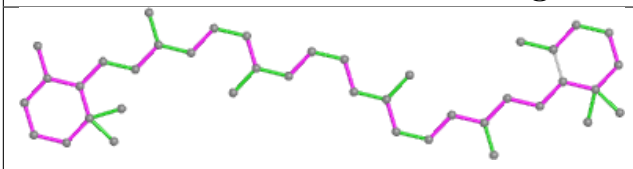

Bond lengths


Bond angles


Torsions


Rings

Ligand 8CT 5 317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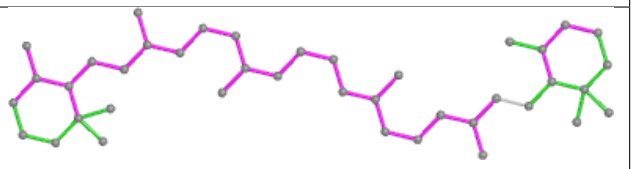
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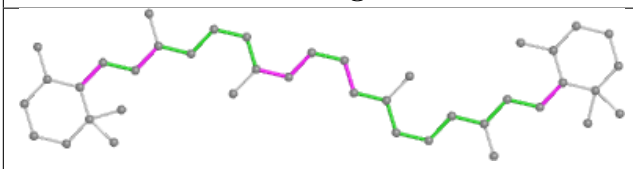
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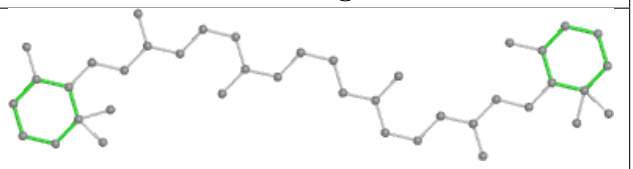
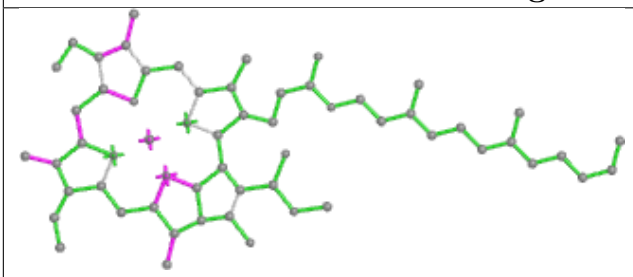

Rings

Ligand CLA 9 312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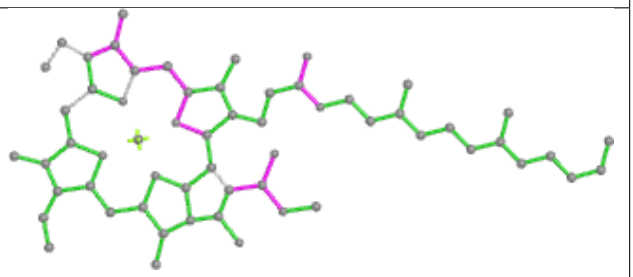
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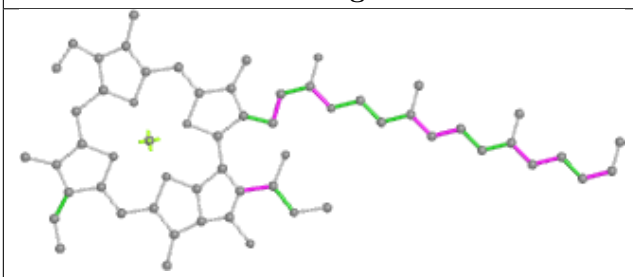
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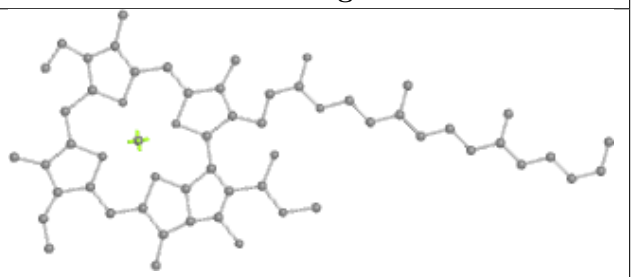
Rings

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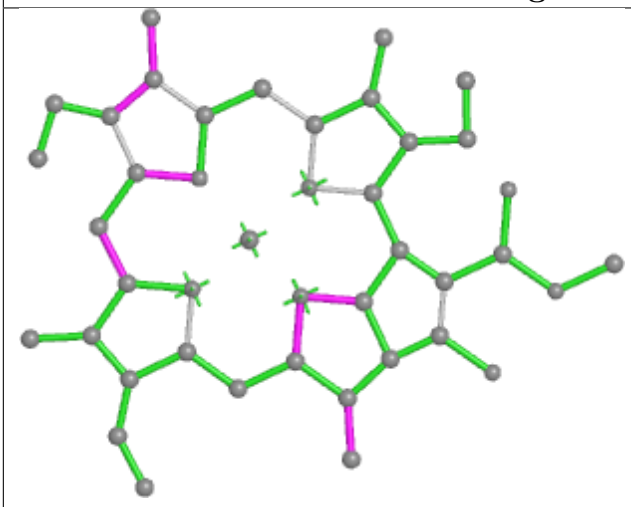

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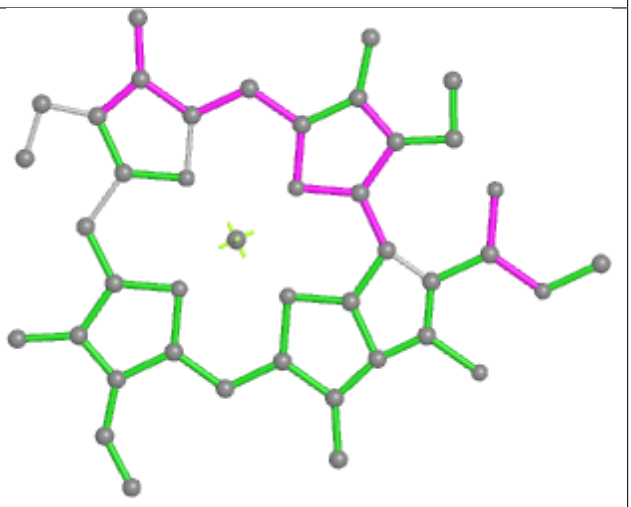

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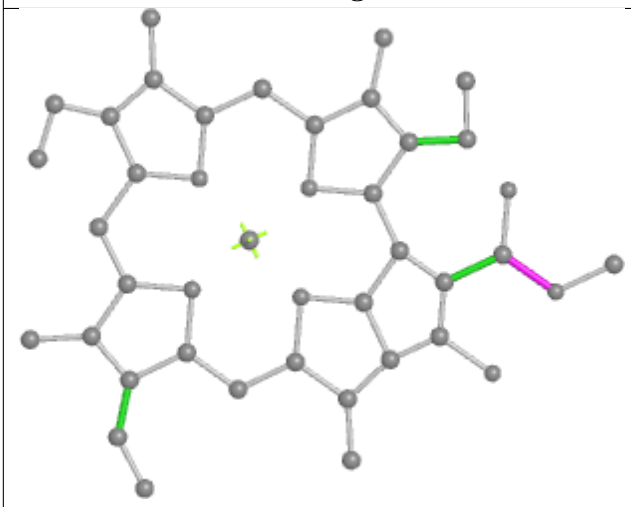

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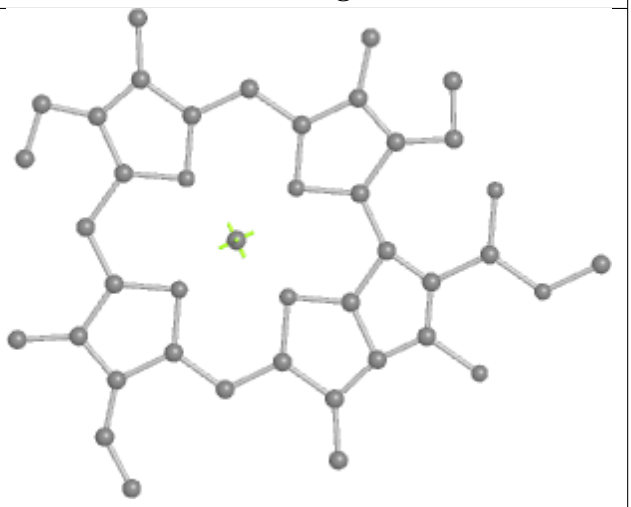

Rings

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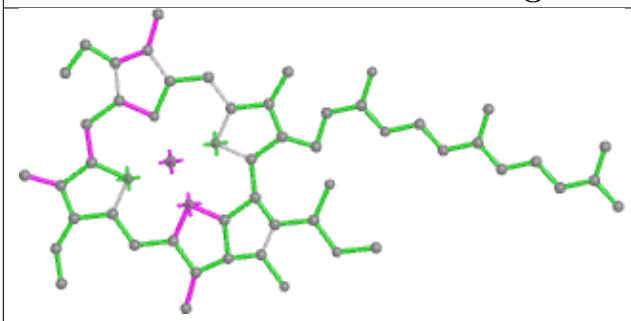

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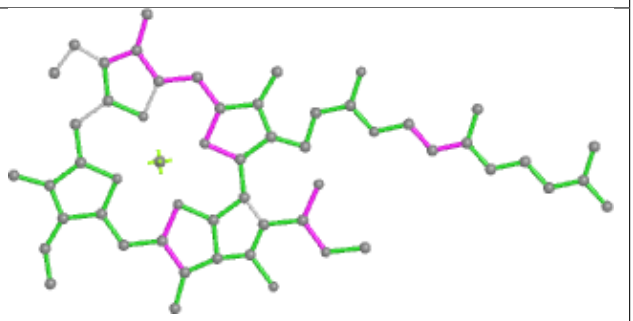

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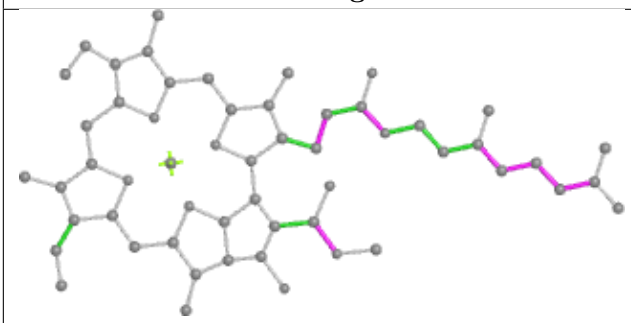

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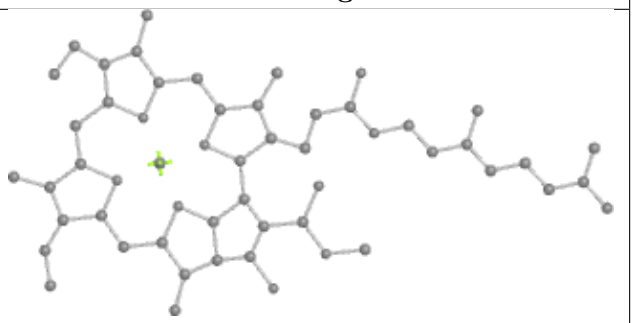

Rings

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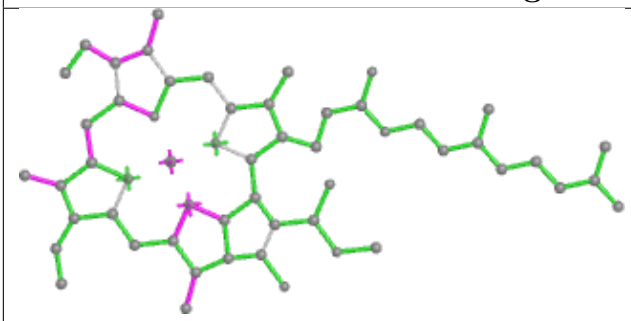

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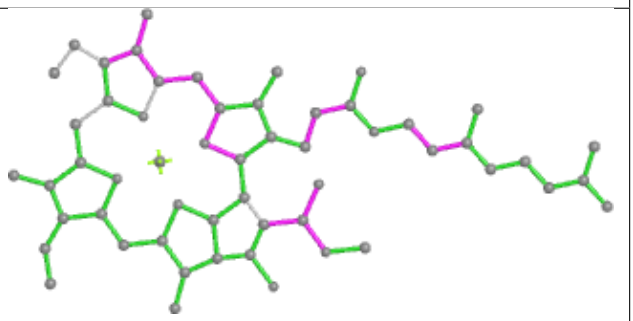

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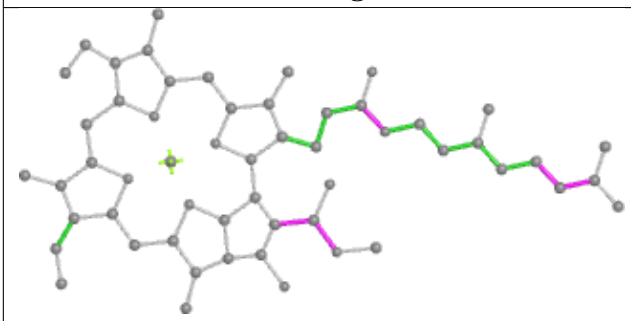

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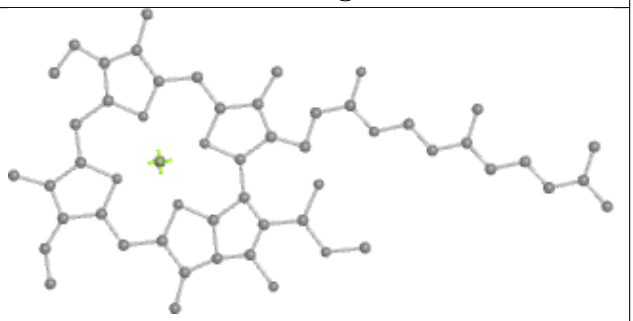

Rings

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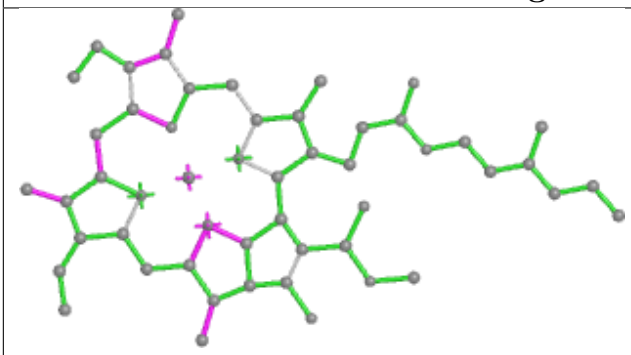
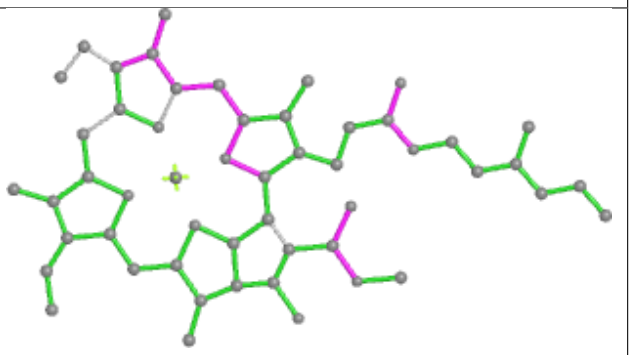
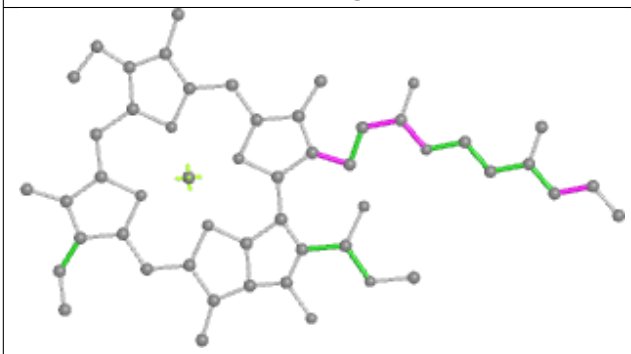
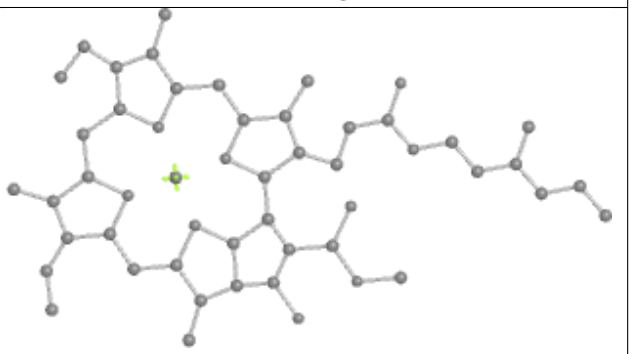
	
Bond lengths	Bond angles
	
Torsions	Rings

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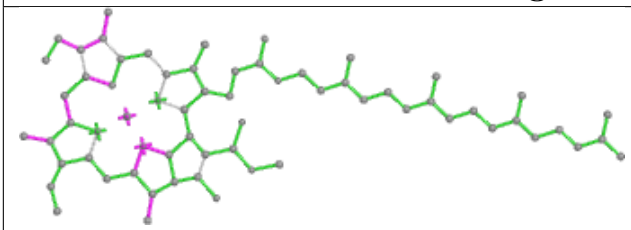
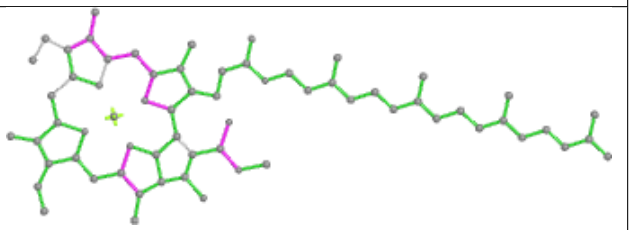
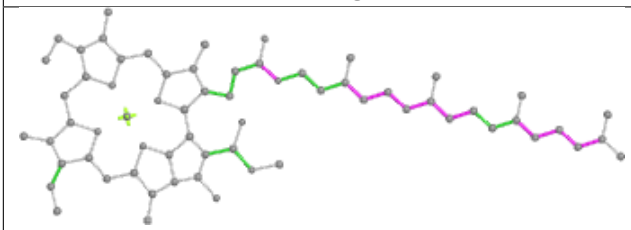
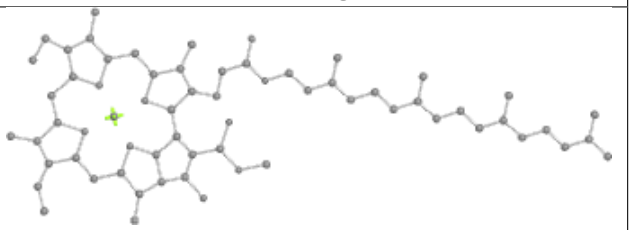
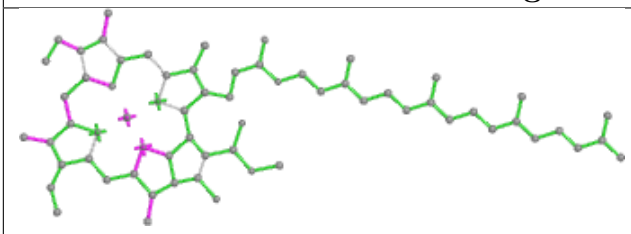
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 828



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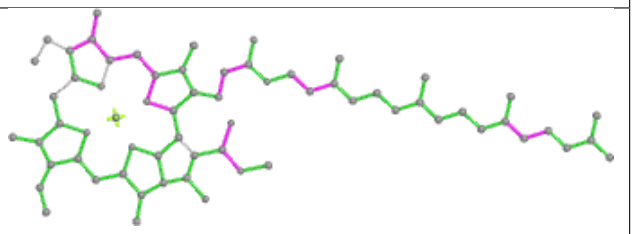

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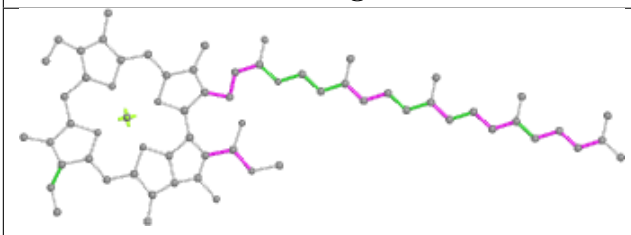

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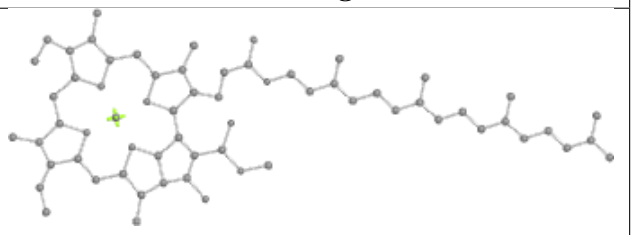
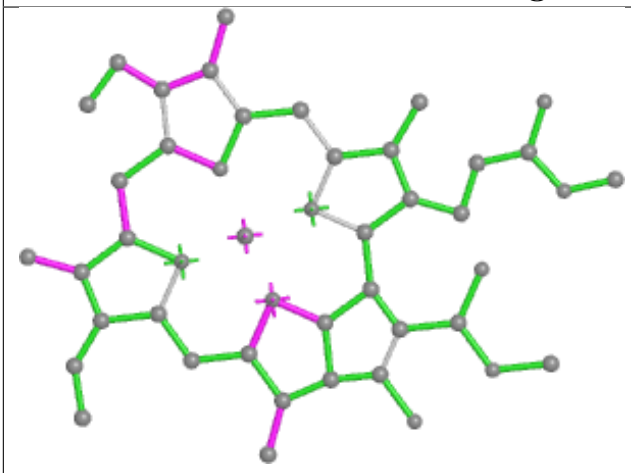


Rings

Ligand CLA 7 302



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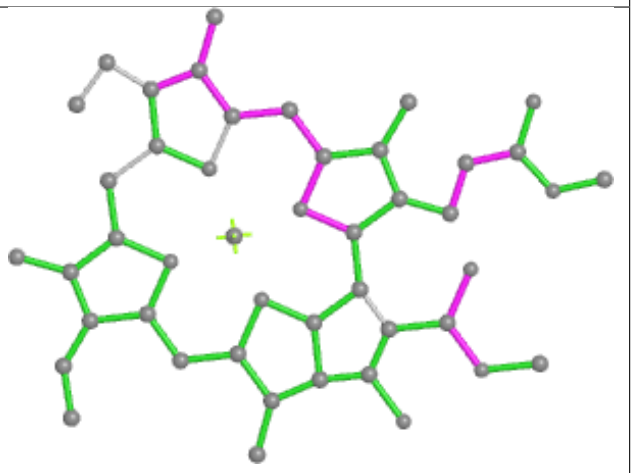
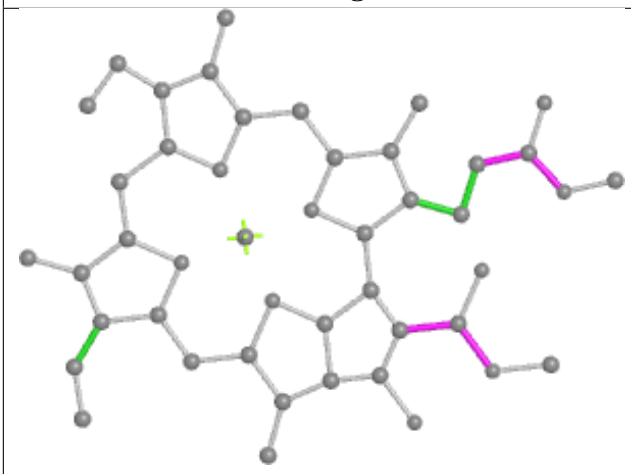


Bond angles



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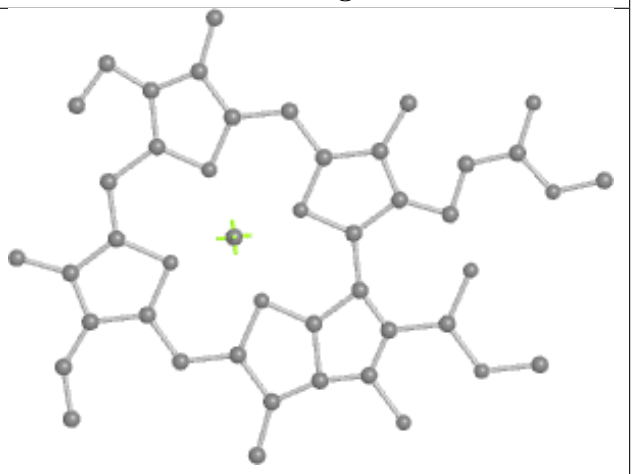
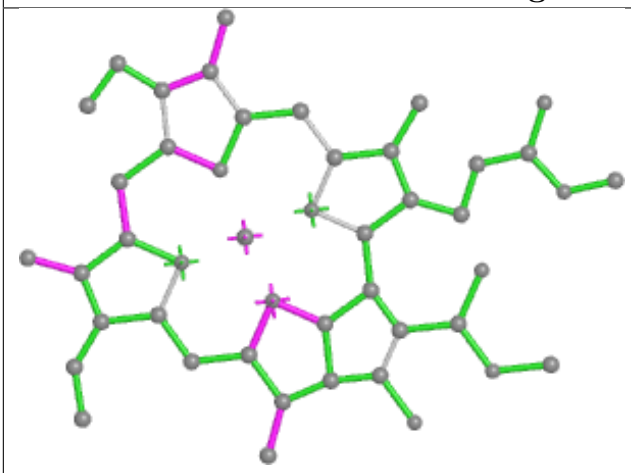


Rings

Ligand CLA 4 303



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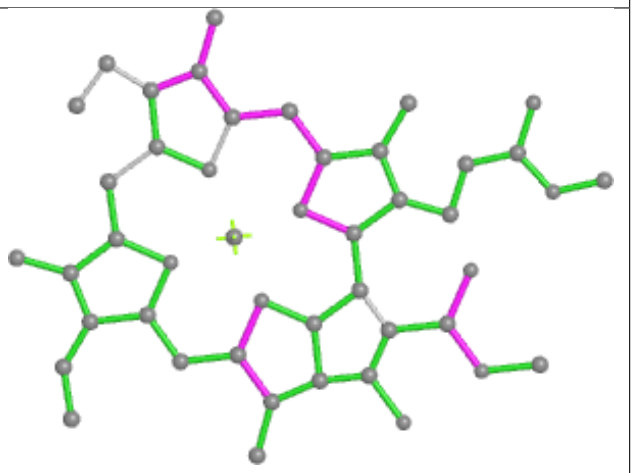
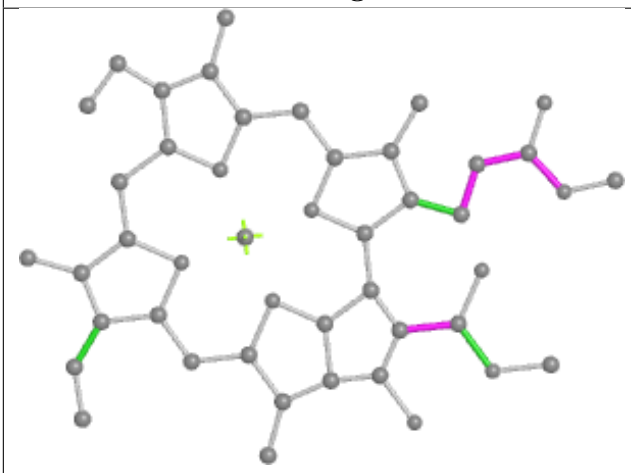


Bond angles



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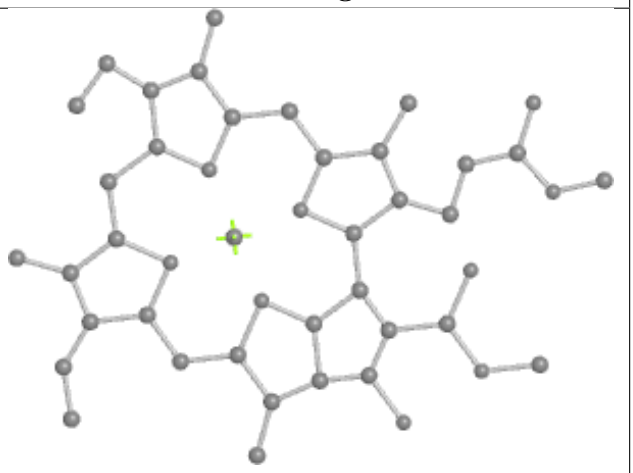
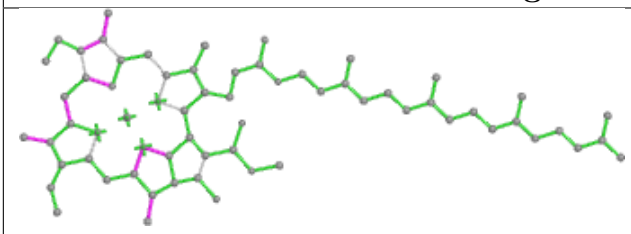


Rings

Ligand CLA A 825



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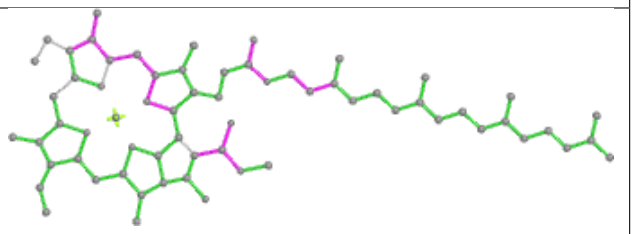
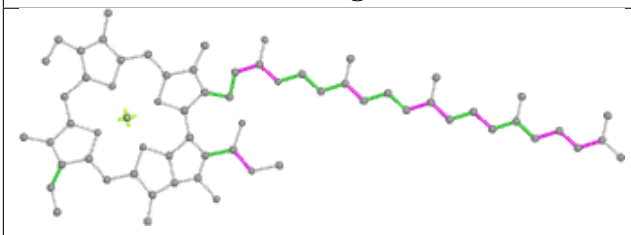


Bond angles



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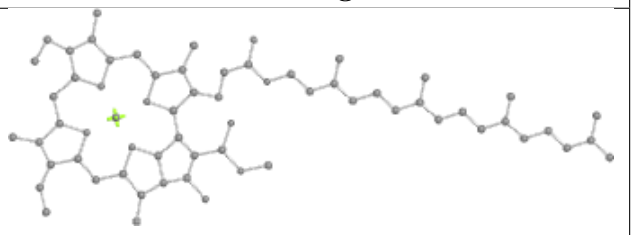
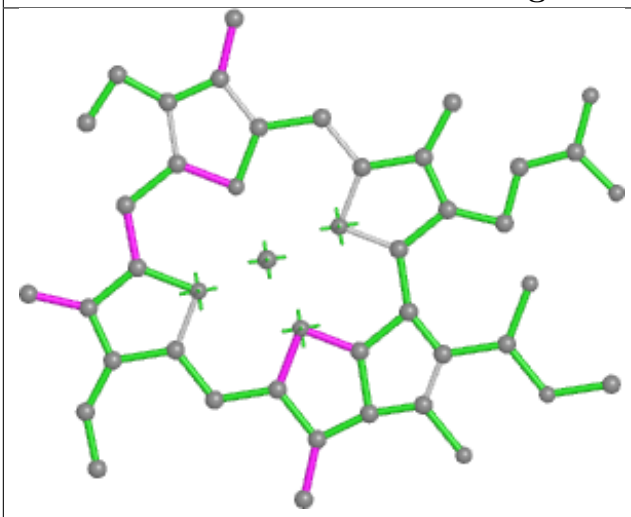


Rings

Ligand CLA 3 312



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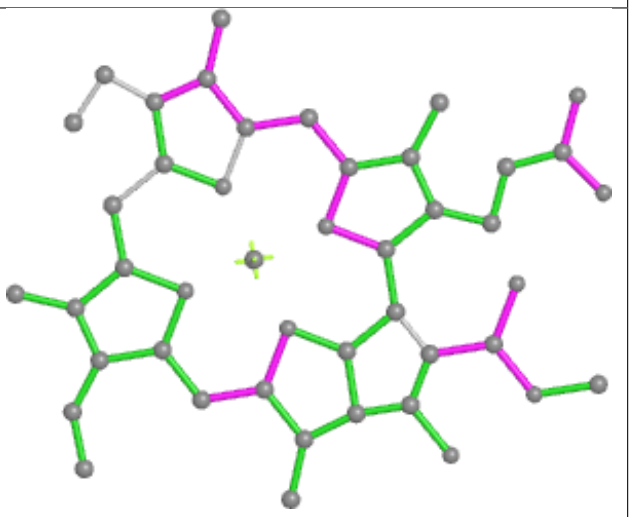
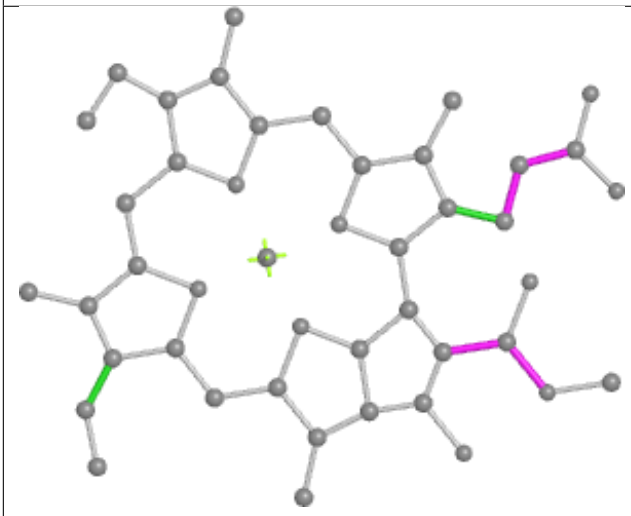


Bond angles



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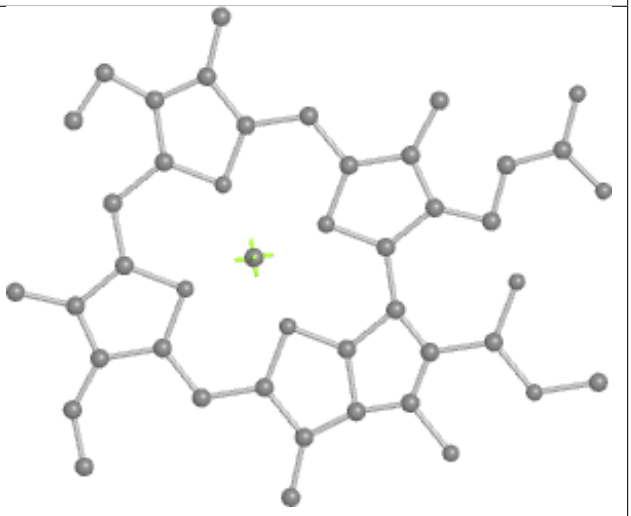
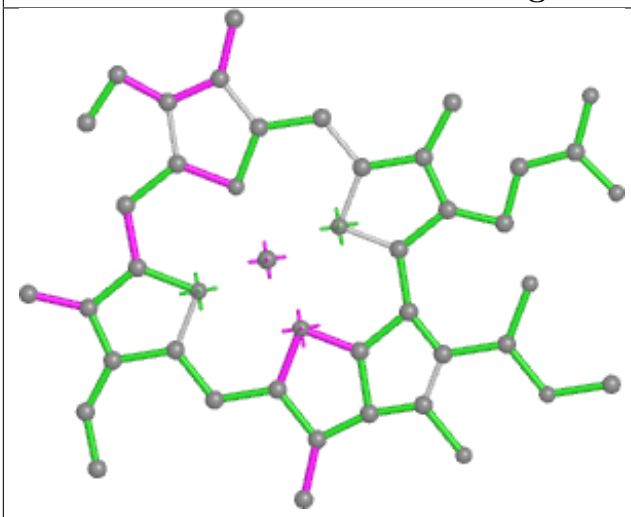


Rings

Ligand CLA 7 314



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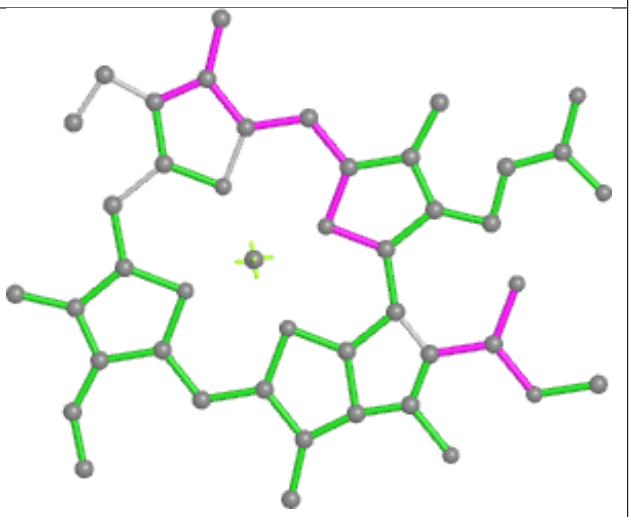
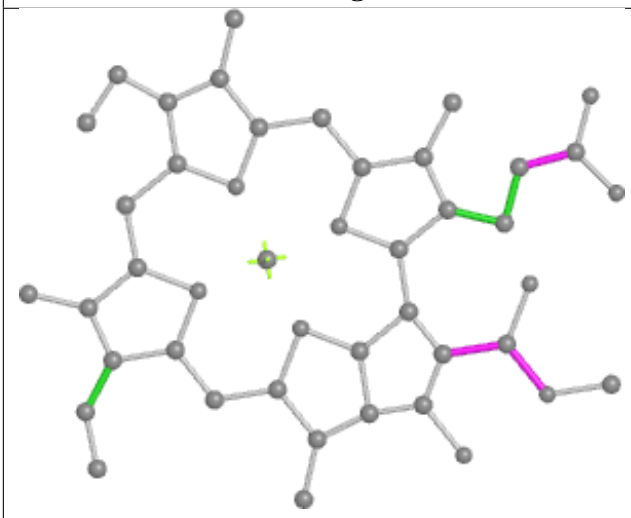


Bond angles



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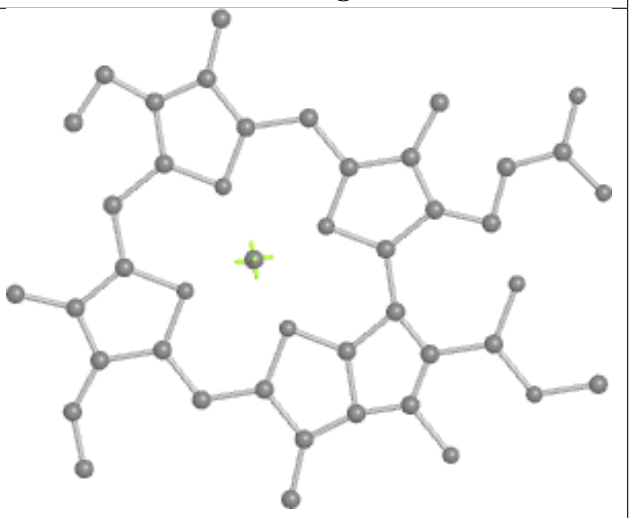
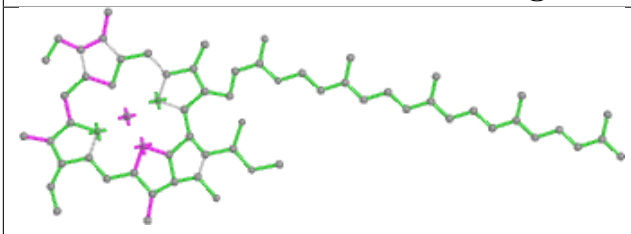
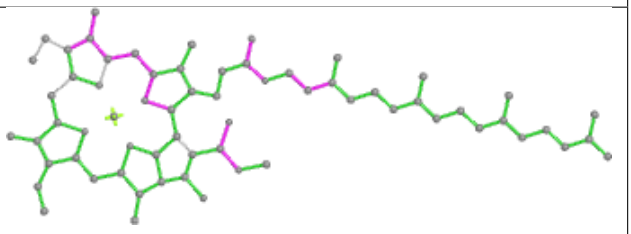


Rings

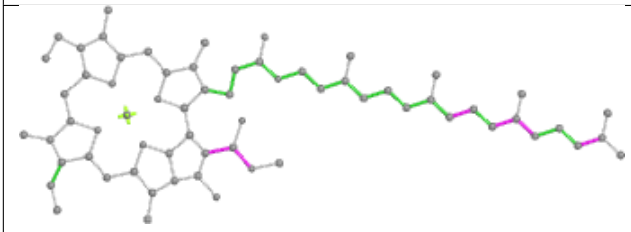
Ligand CLA 1 301



Bond lengths



Bond angles



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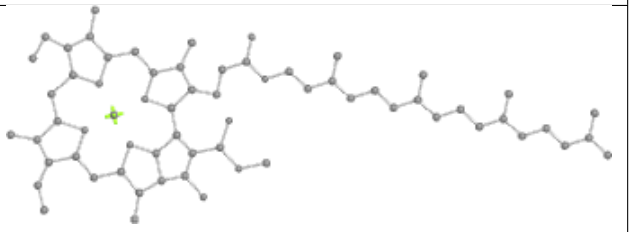
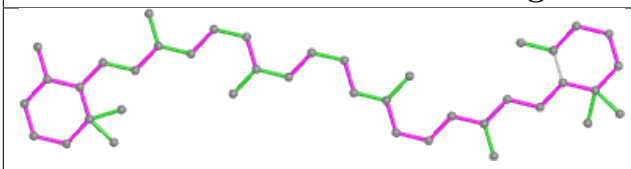


Rings

Ligand 8CT B 851



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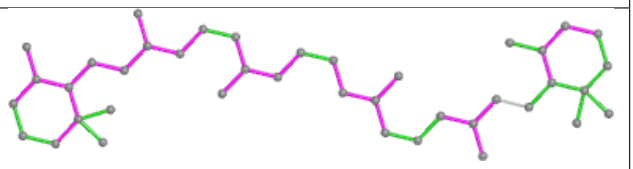

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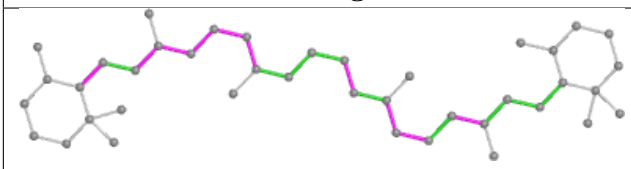

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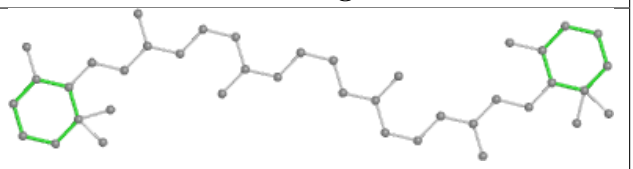
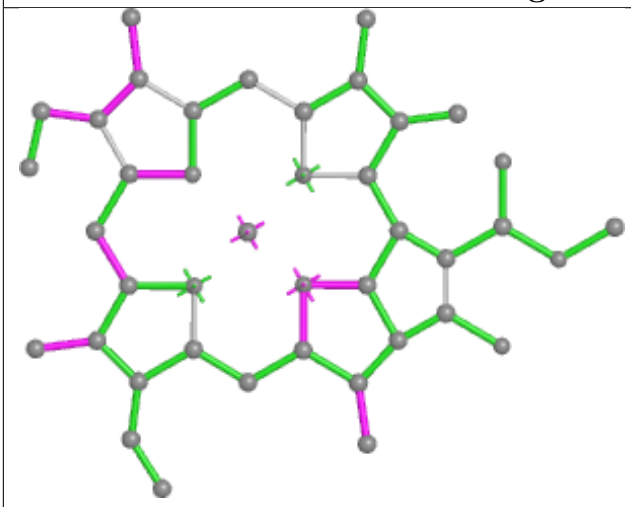


Rings

Ligand CLA 5 310



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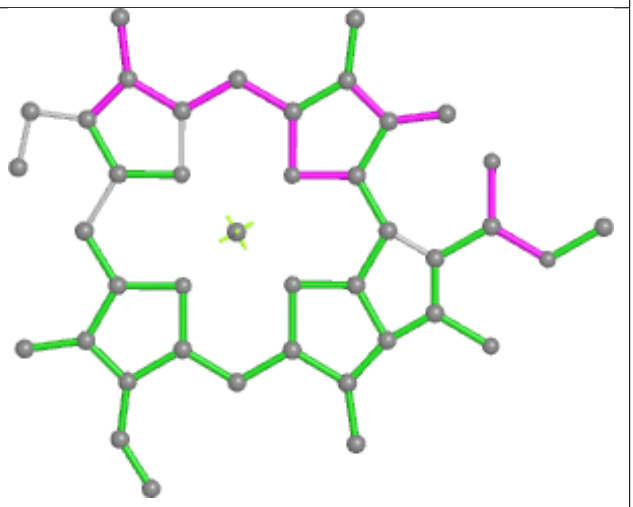

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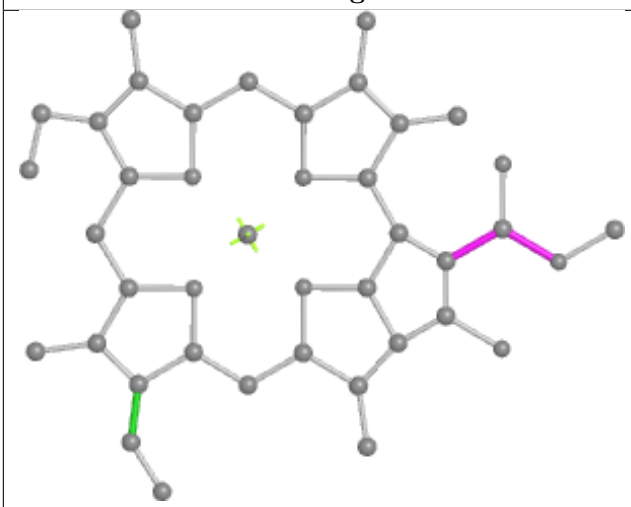

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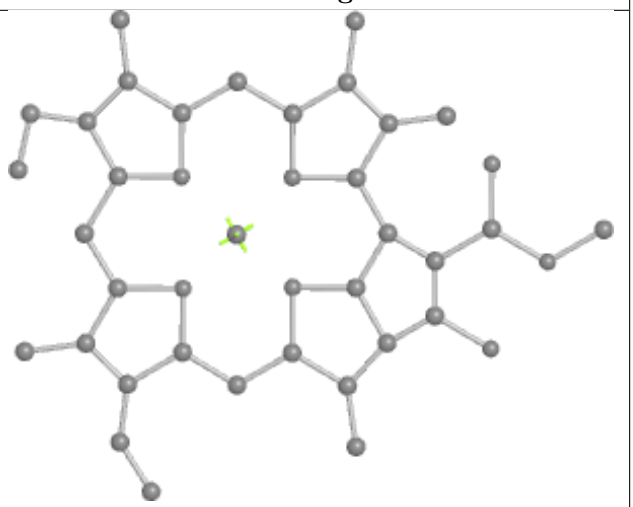
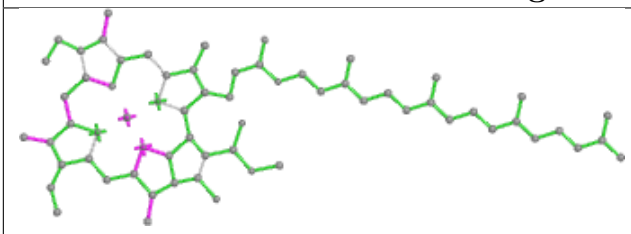


Rings

Ligand CLA 0 302



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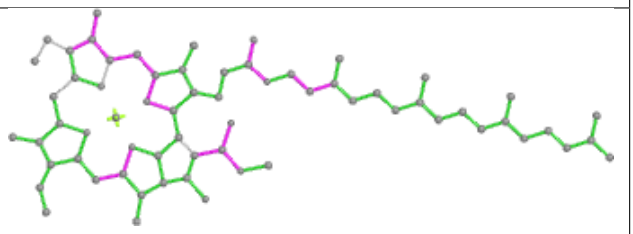
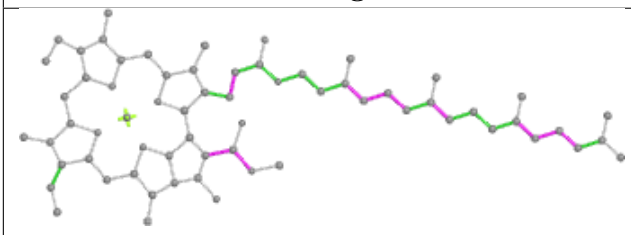


Bond angles



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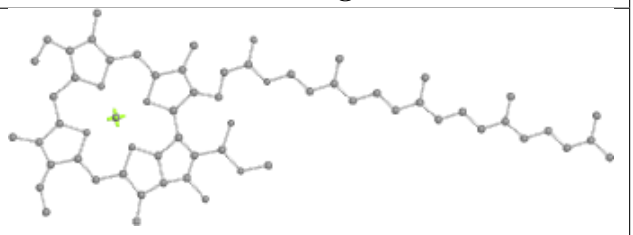
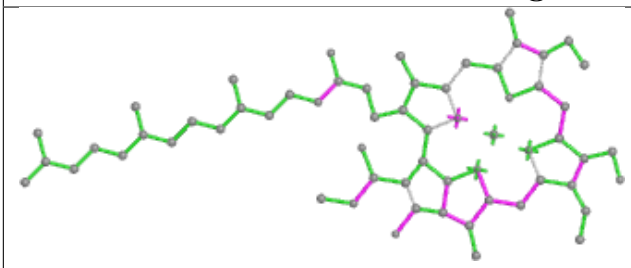


Rings

Ligand CHL 9 302



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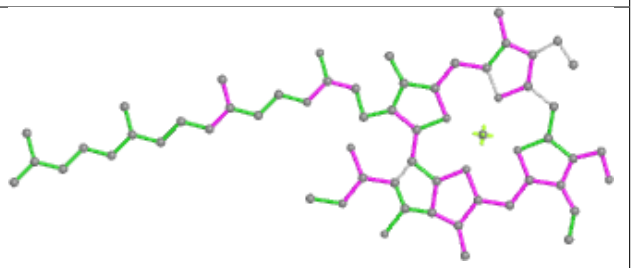

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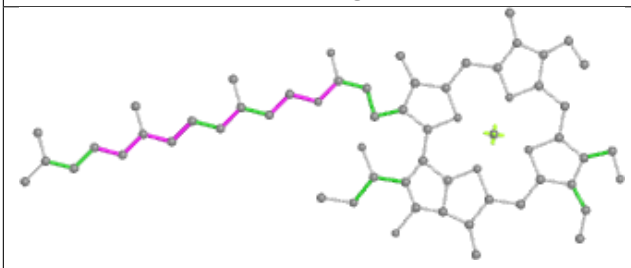

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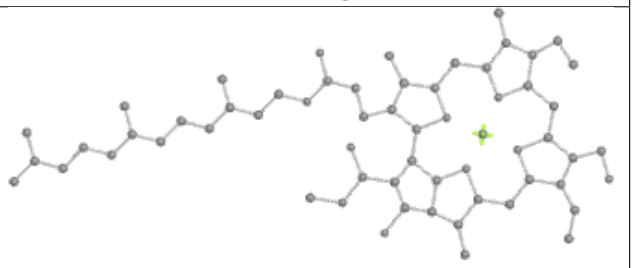

Rings

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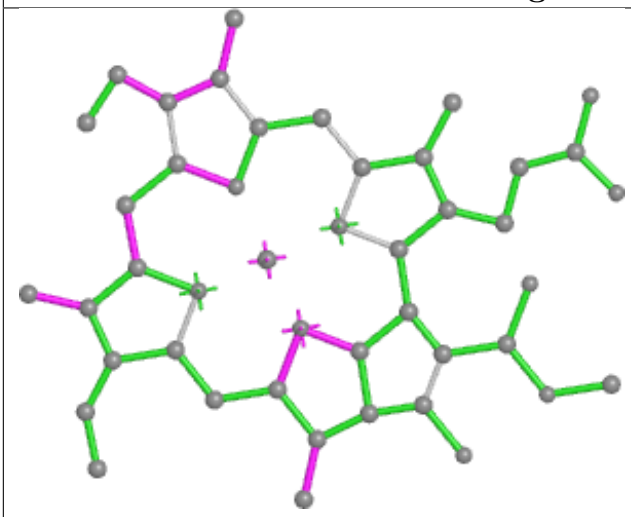

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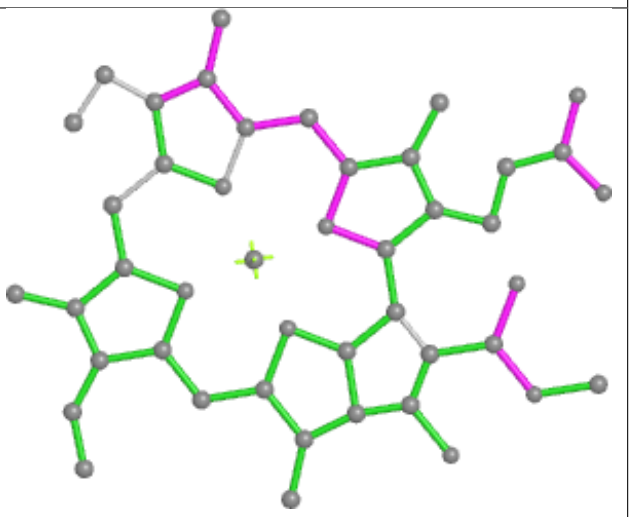

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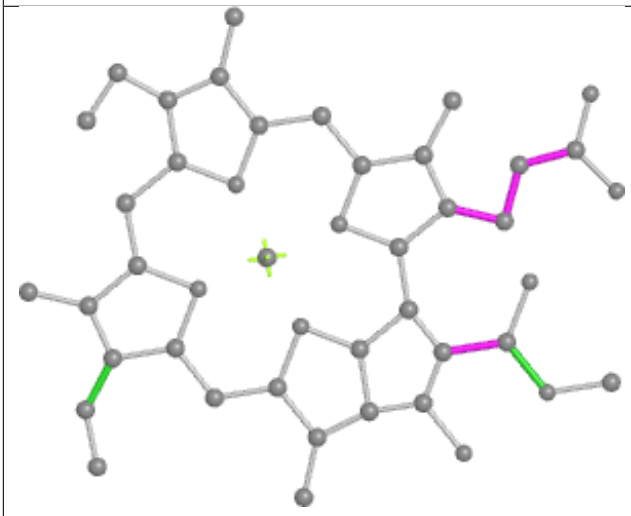

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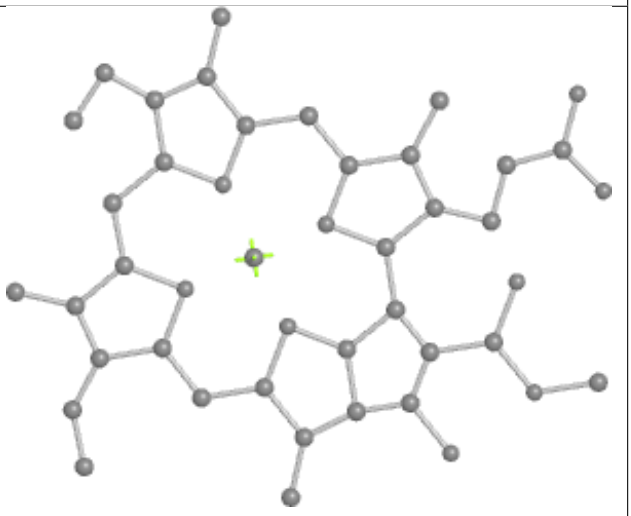

Rings

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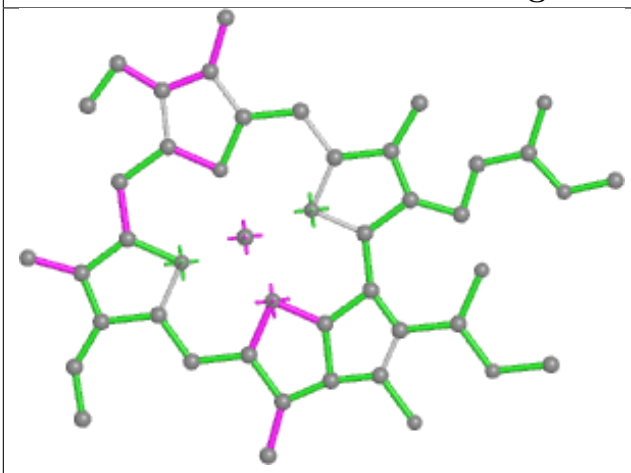

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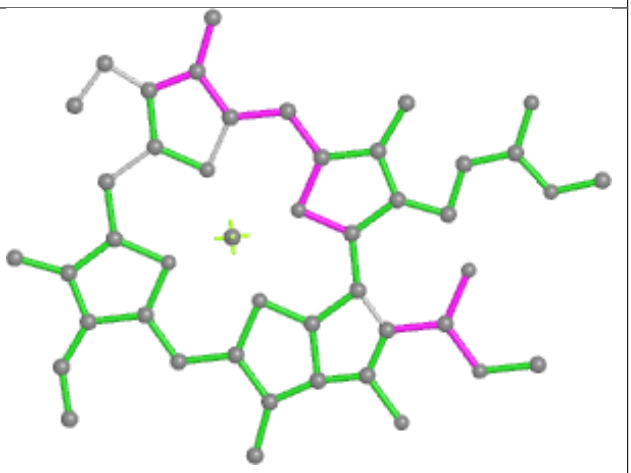

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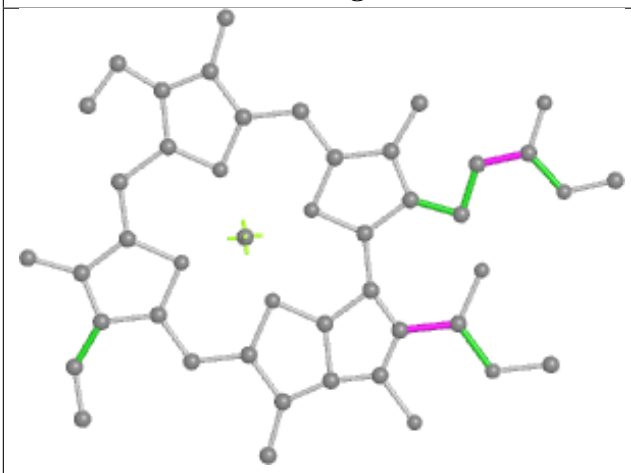

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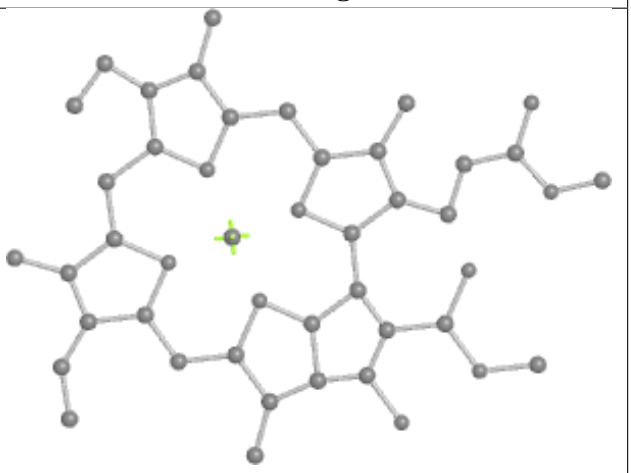
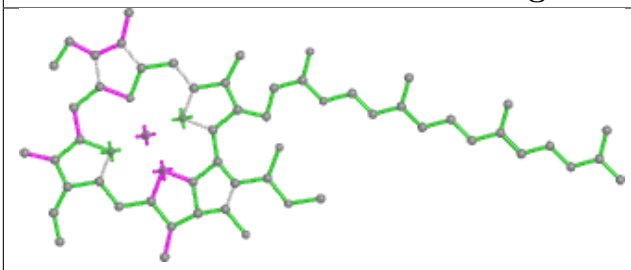


Rings

Ligand CLA 4 309



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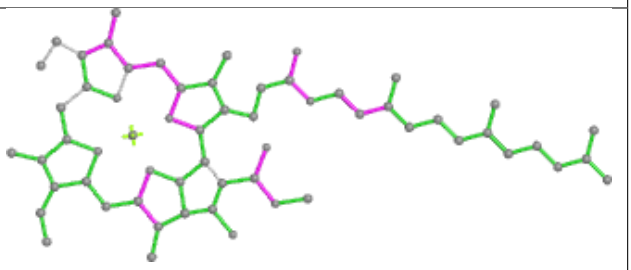
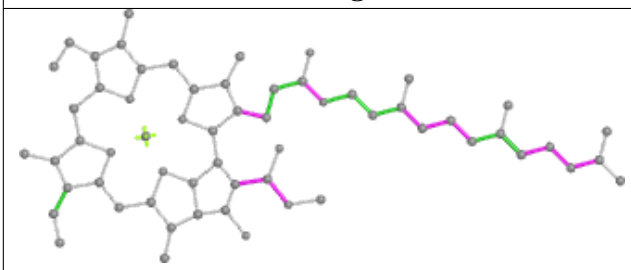


Bond angles



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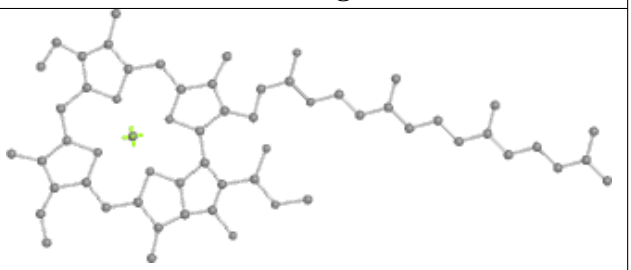
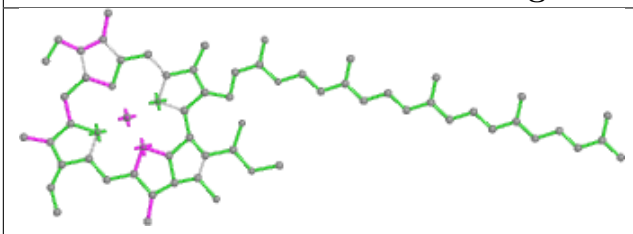


Rings

Ligand CLA 9 303



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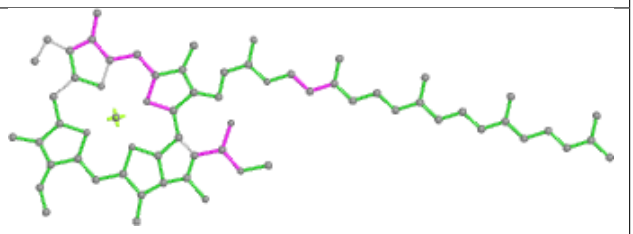

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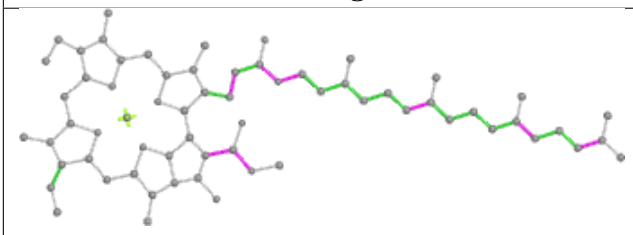

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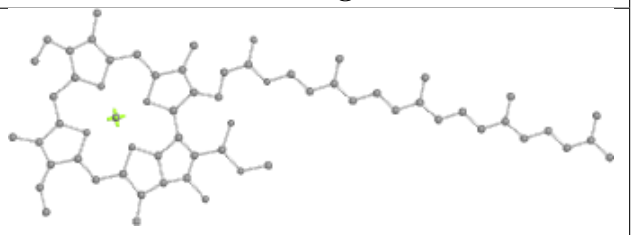
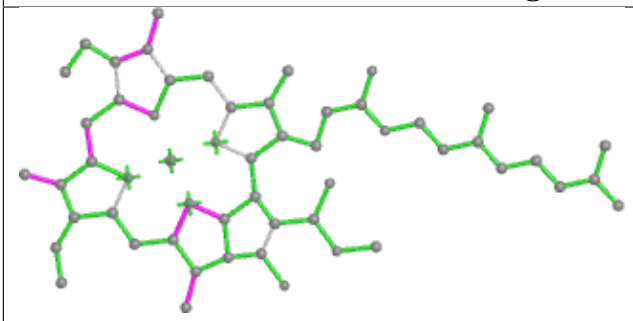


Rings

Ligand CLA B 850



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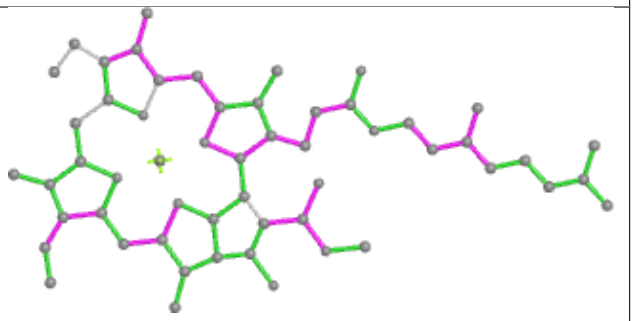
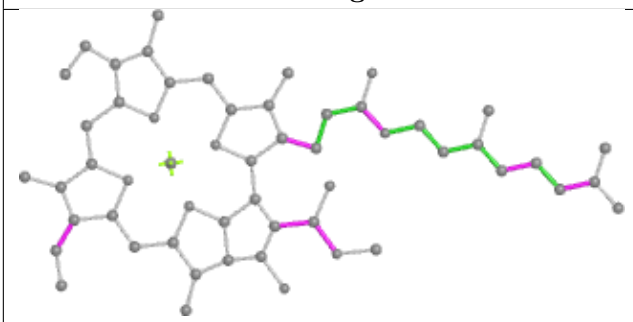


Bond angles



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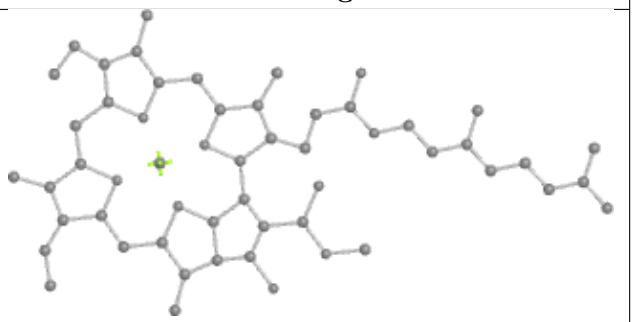
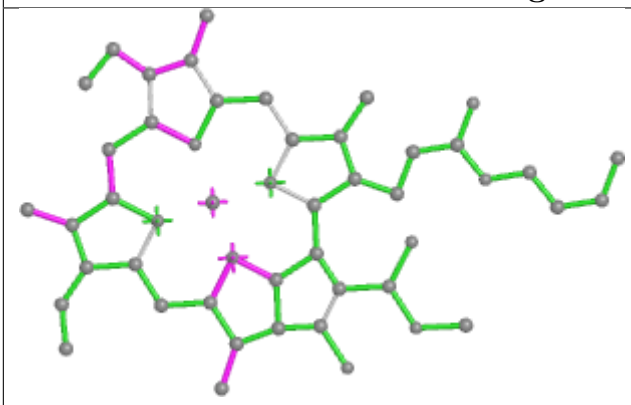


Rings

Ligand CLA 2 314



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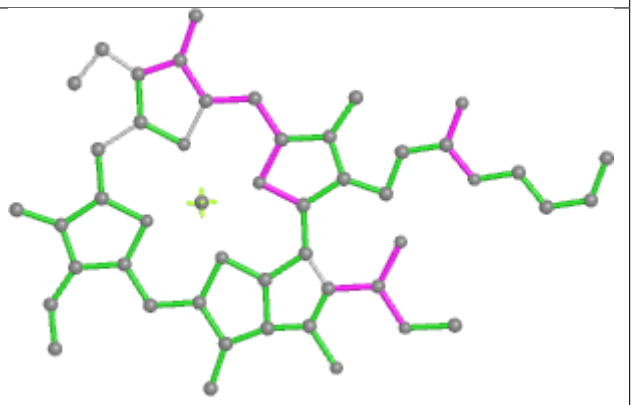
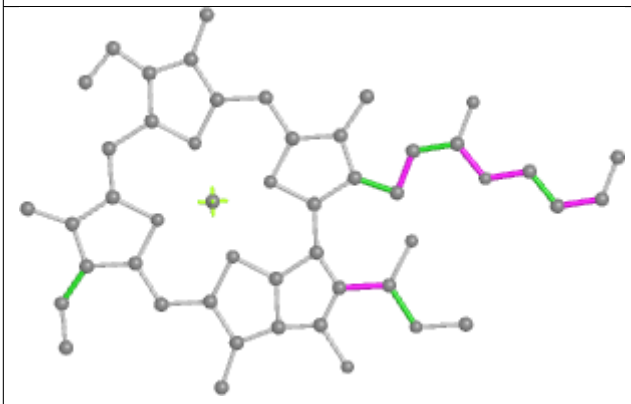


Bond angles



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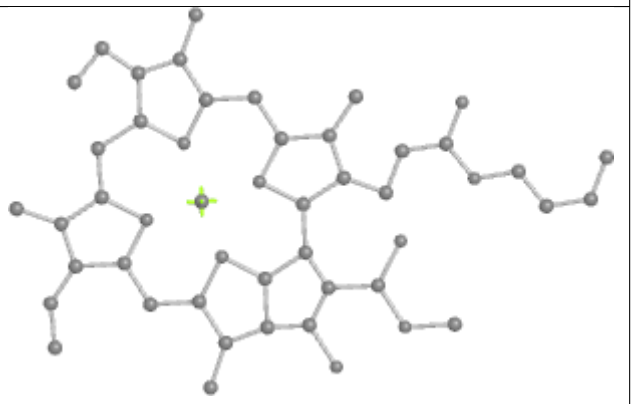
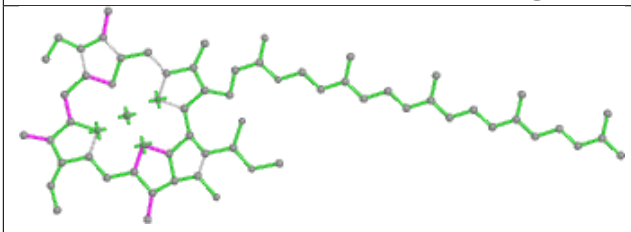


Rings

Ligand CLA 0 307



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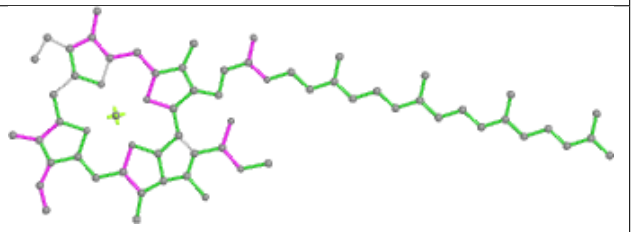
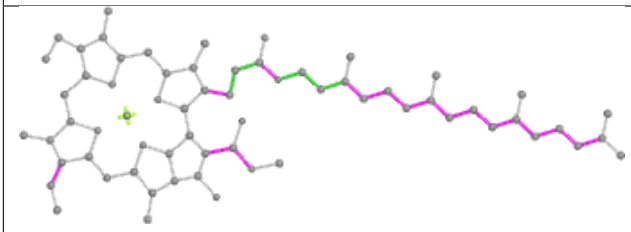


Bond angles



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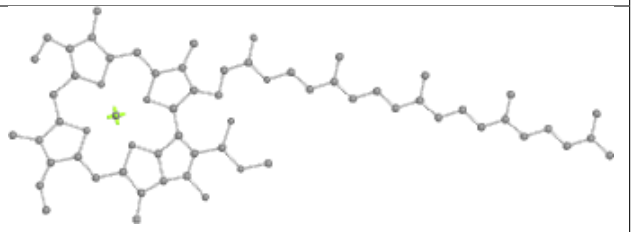
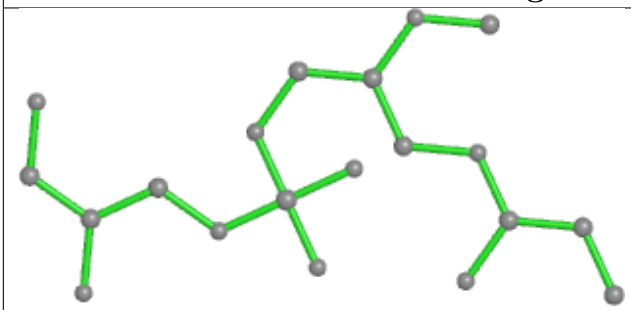


Rings

Ligand LHG 3 317



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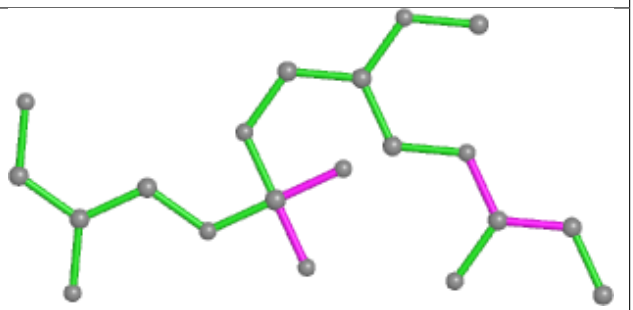
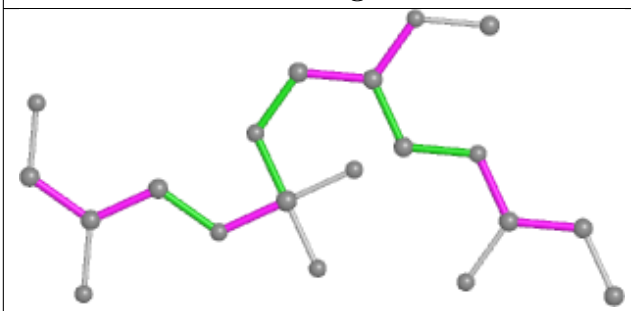
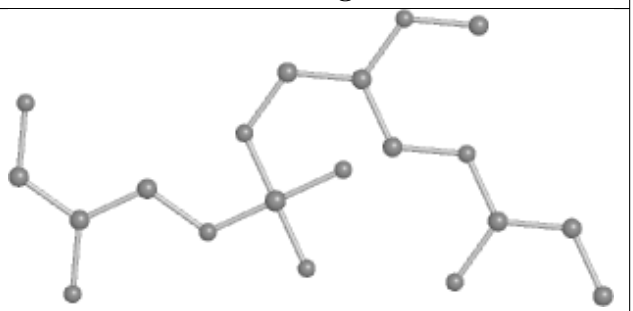


Bond angles

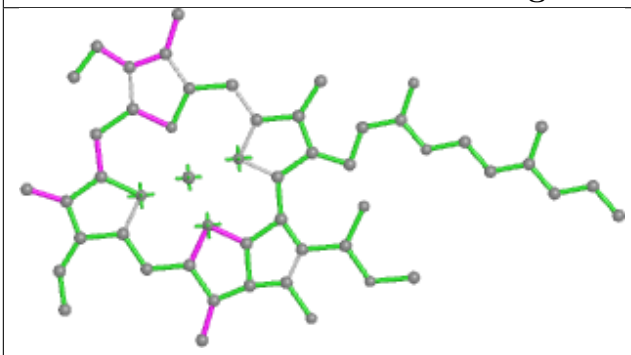


Torsions

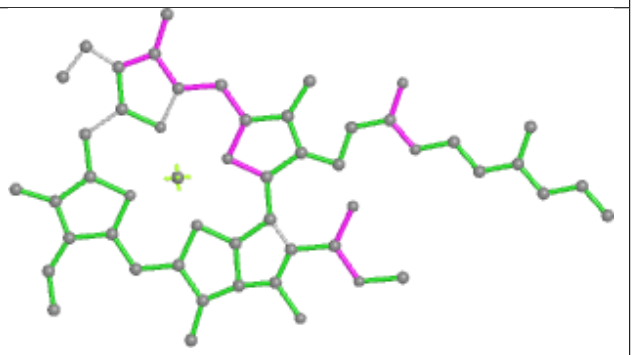


Rings

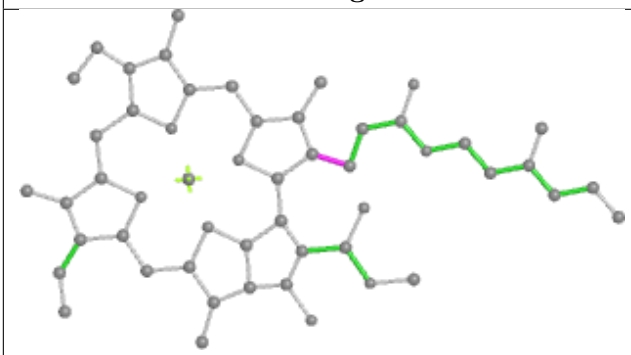
Ligand CLA 0 310



Bond lengths



Bond angles



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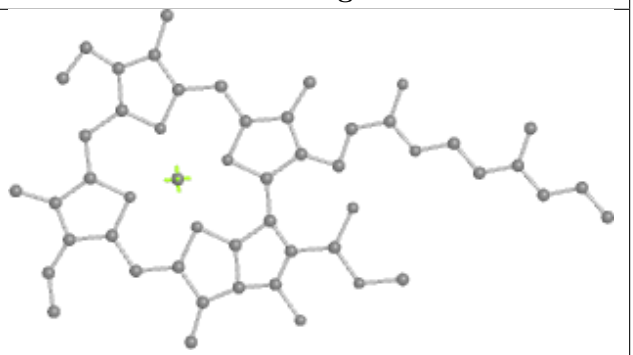
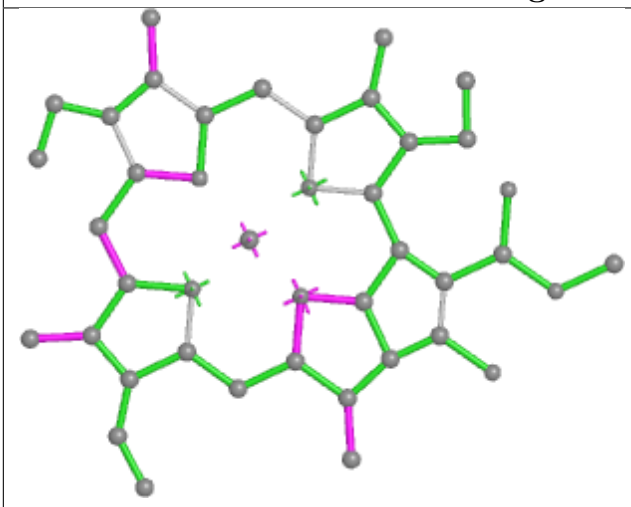


Rings

Ligand CLA 7 306



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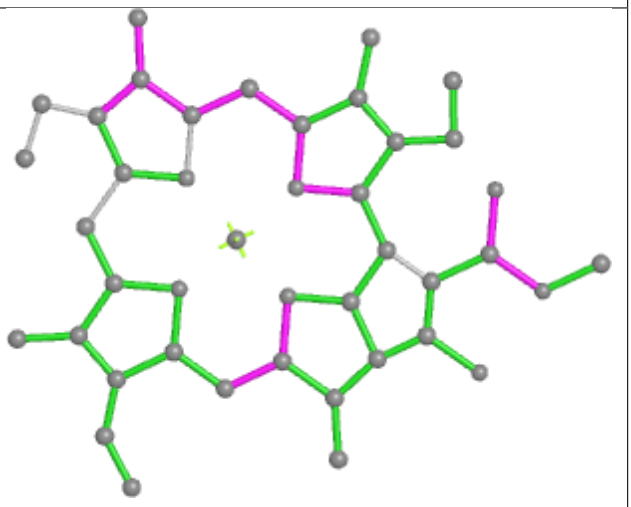

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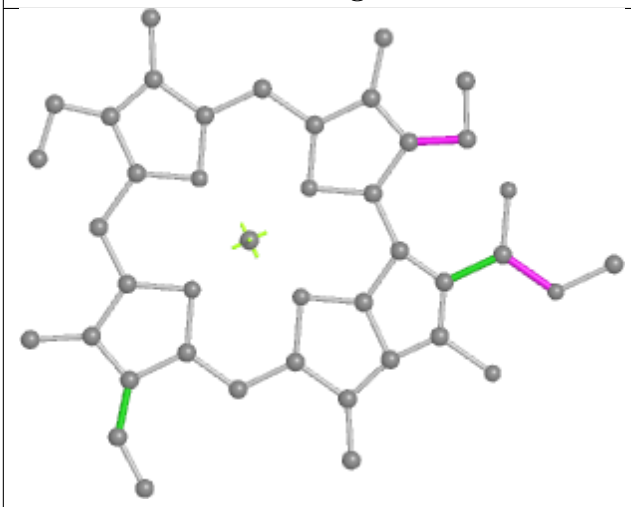

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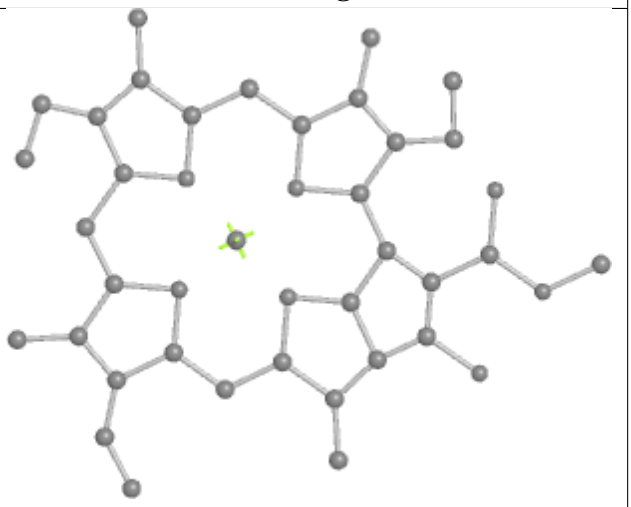
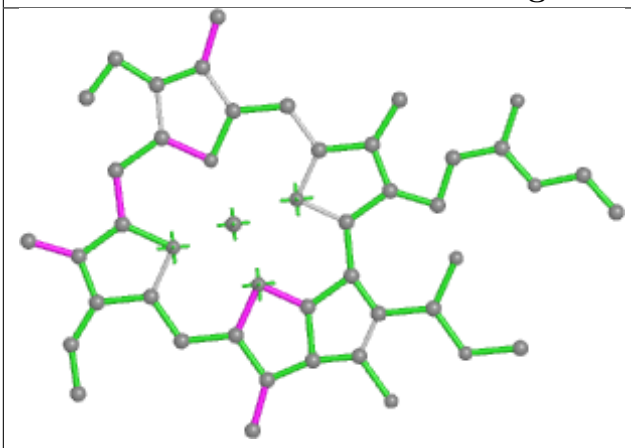


Rings

Ligand CLA 7 307



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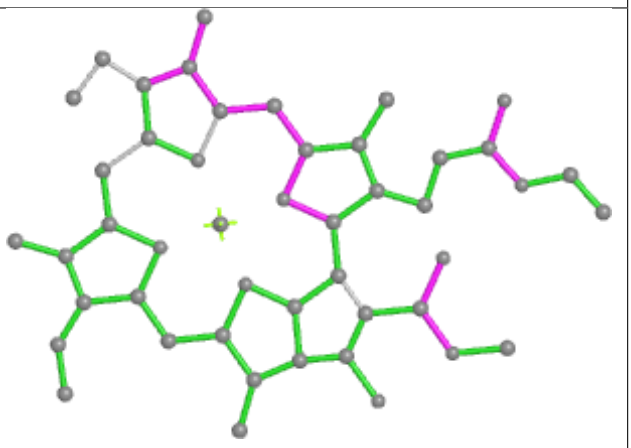

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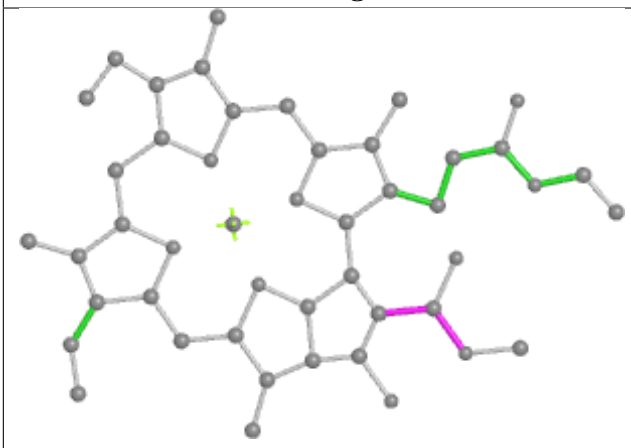

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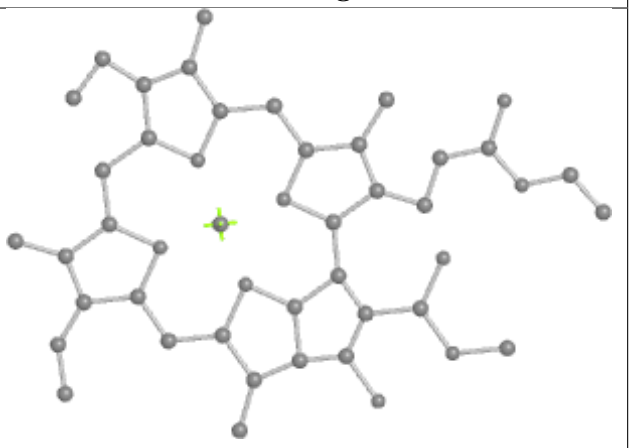
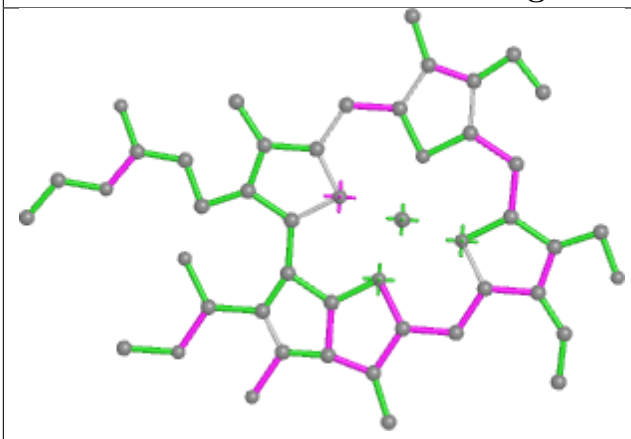


Rings

Ligand CHL 5 306



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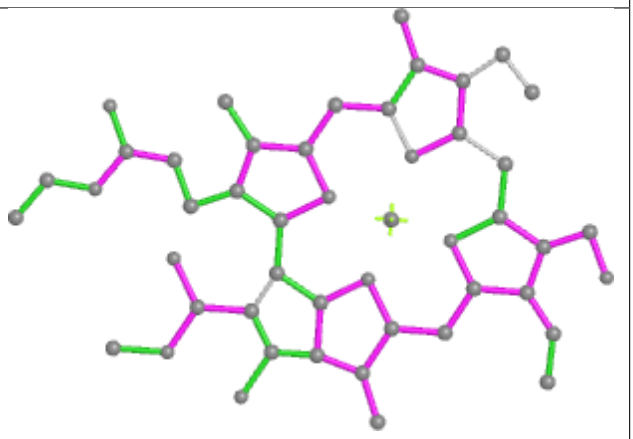

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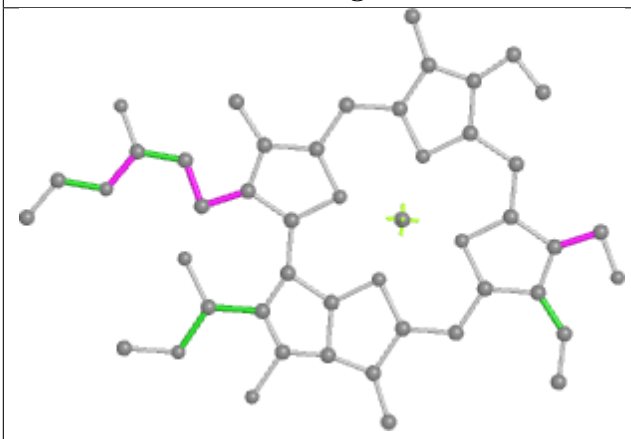

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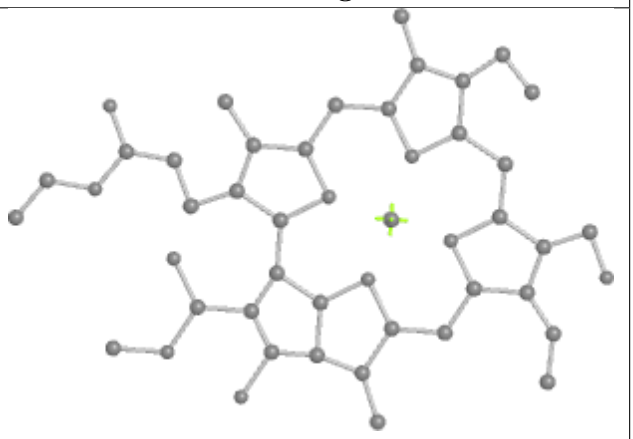
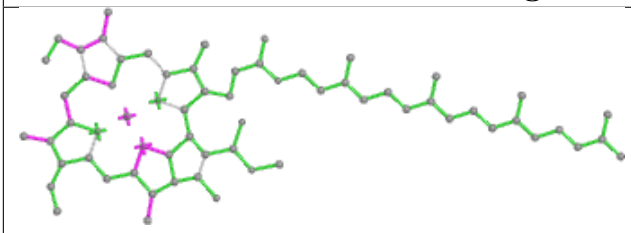


Rings

Ligand CLA A 826



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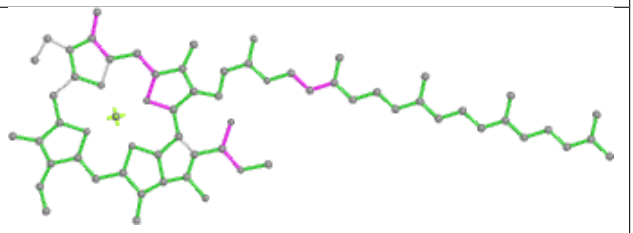
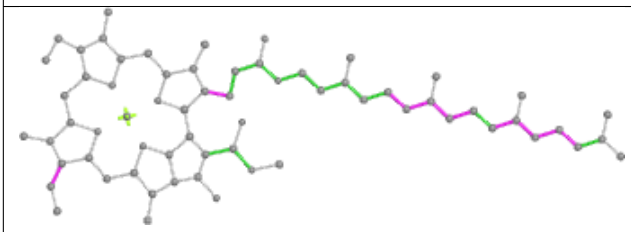


Bond angles



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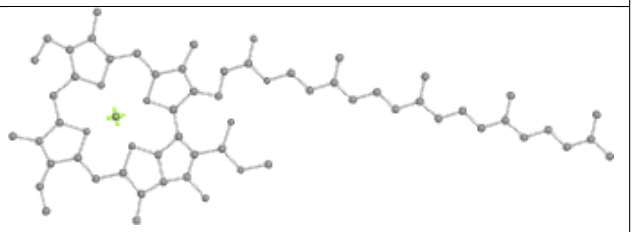
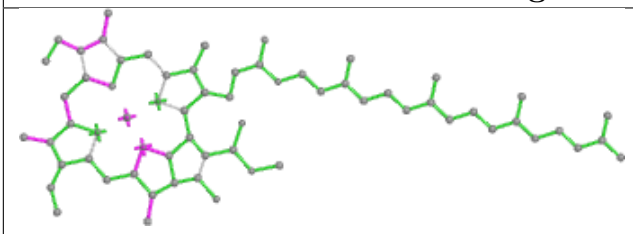


Rings

Ligand CLA 5 302



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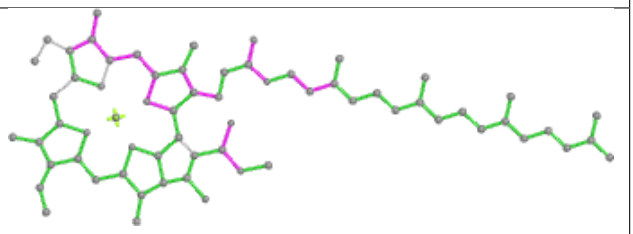
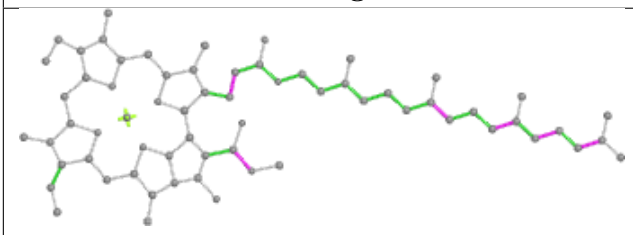


Bond angles



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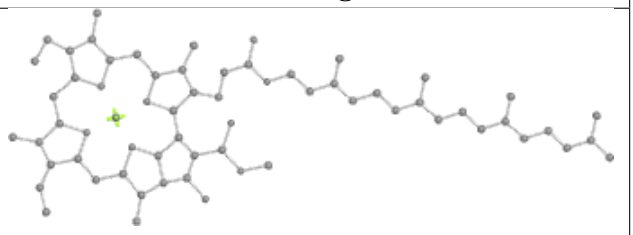
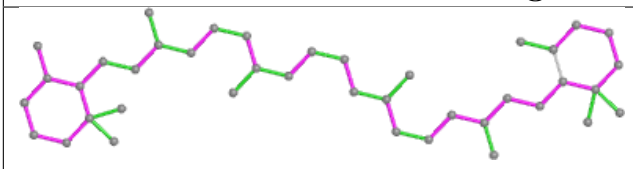


Rings

Ligand 8CT A 854



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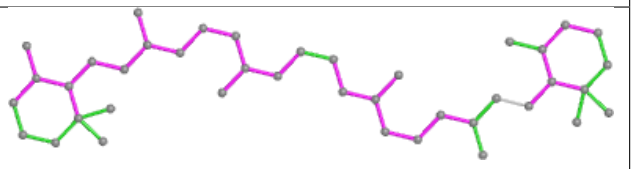

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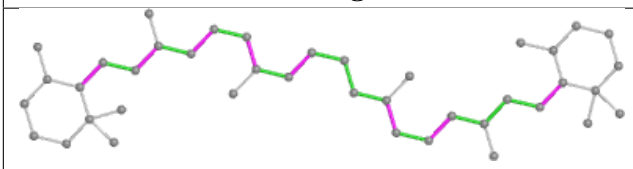

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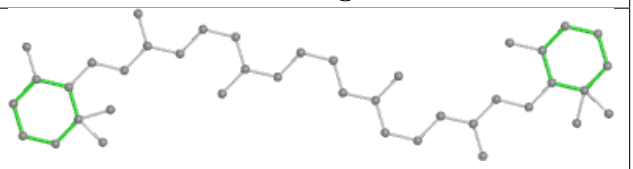
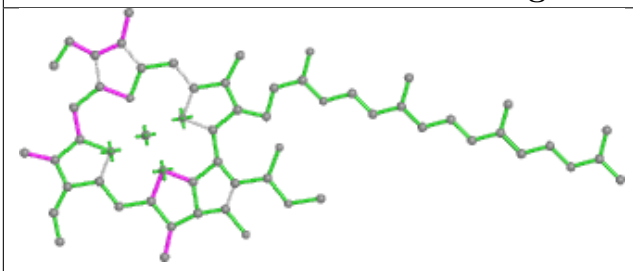


Rings

Ligand CLA 5 309



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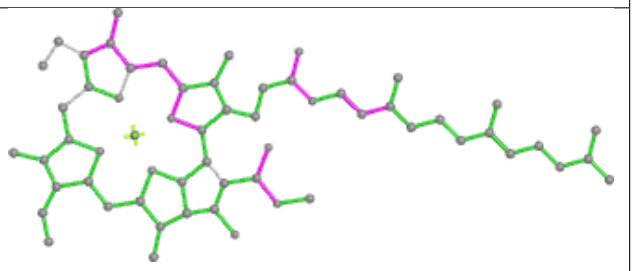
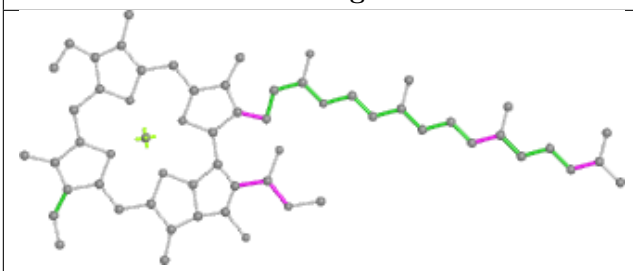


Bond angles



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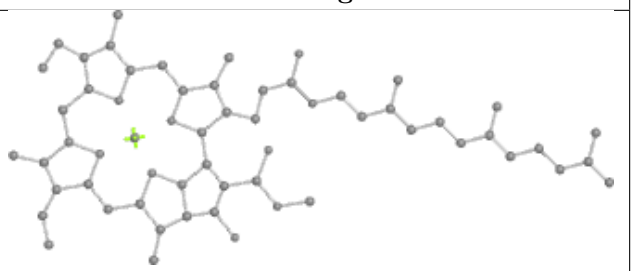
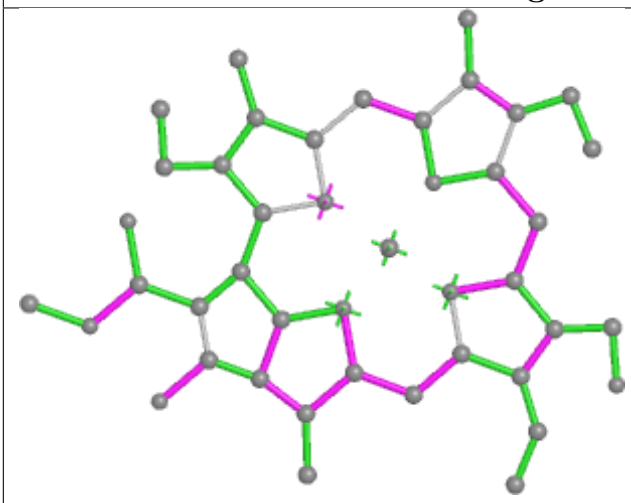


Rings

Ligand CHL 8 314



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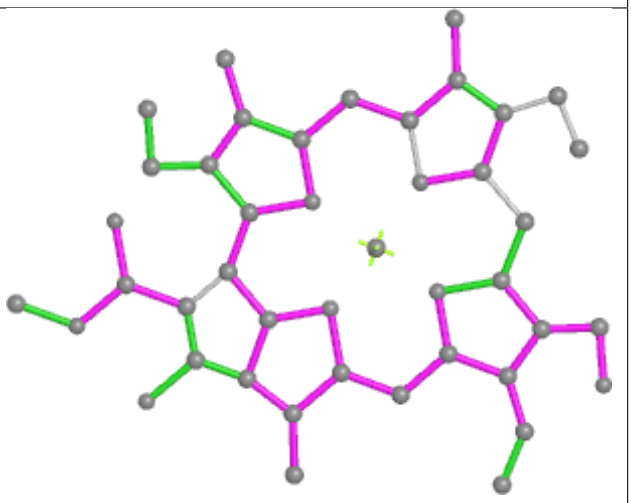

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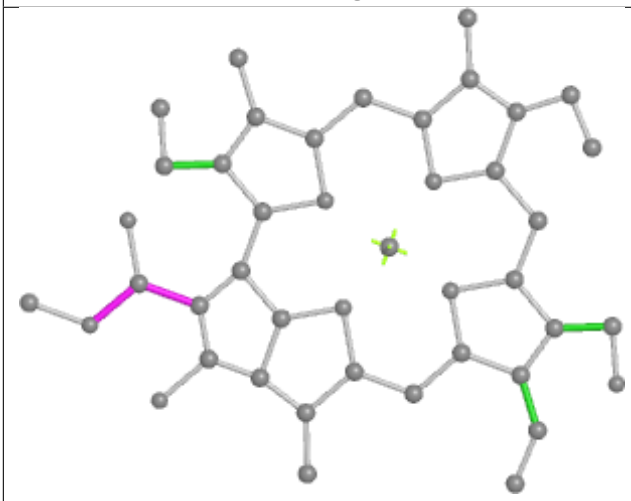

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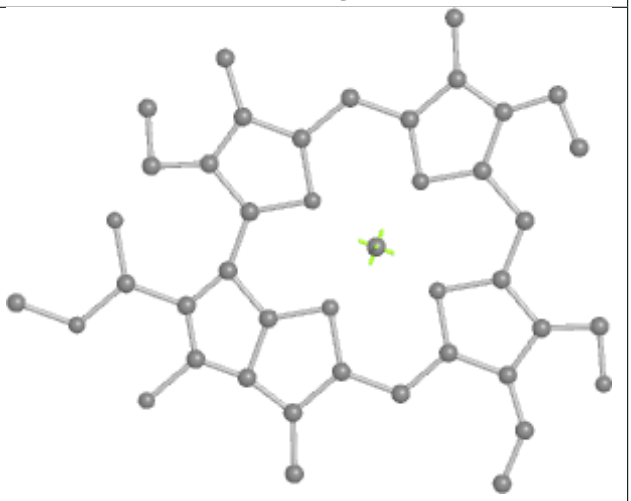
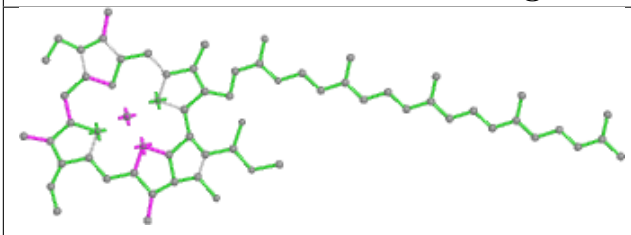


Rings

Ligand CLA A 821



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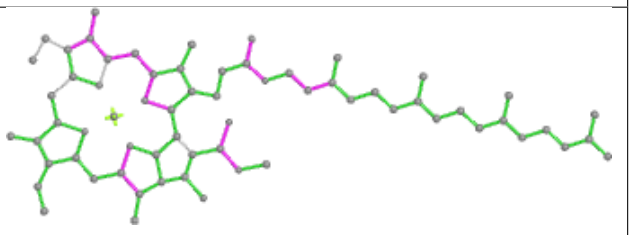
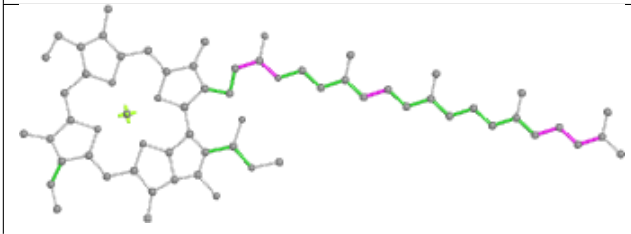


Bond angles



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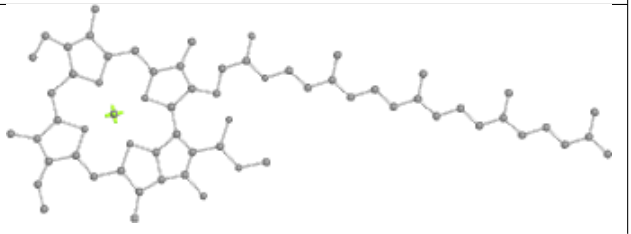
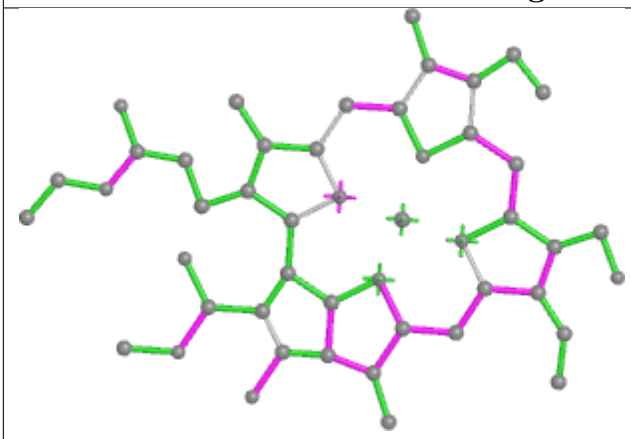


Rings

Ligand CHL 0 306



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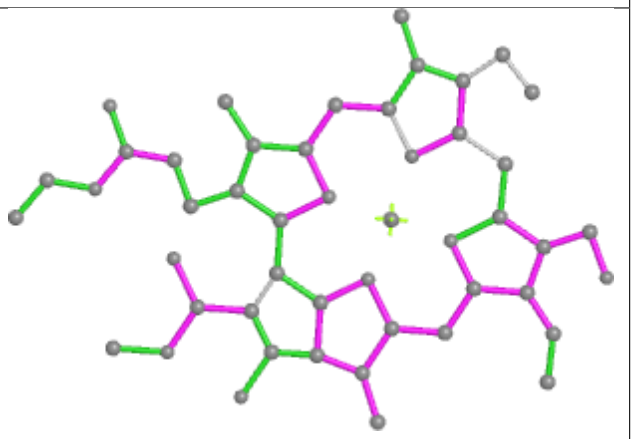
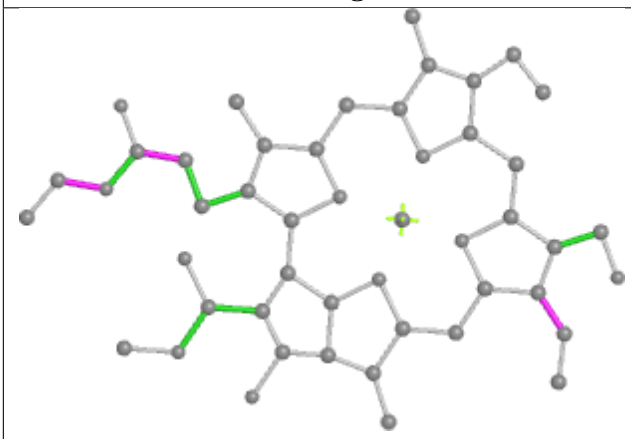


Bond angles



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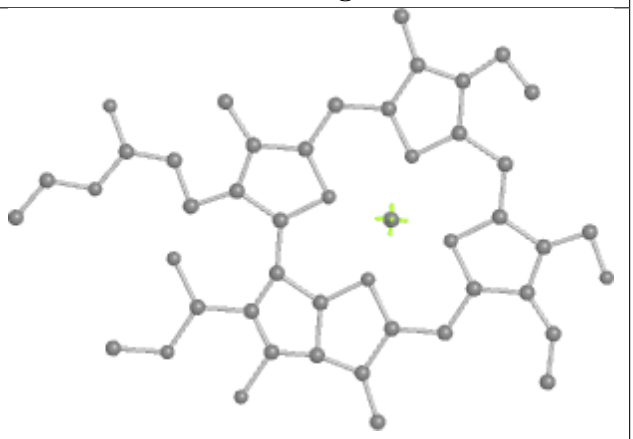
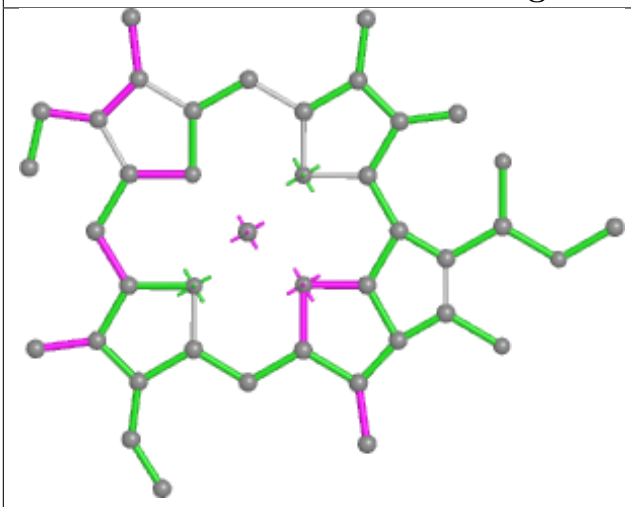


Rings

Ligand CLA 2 310



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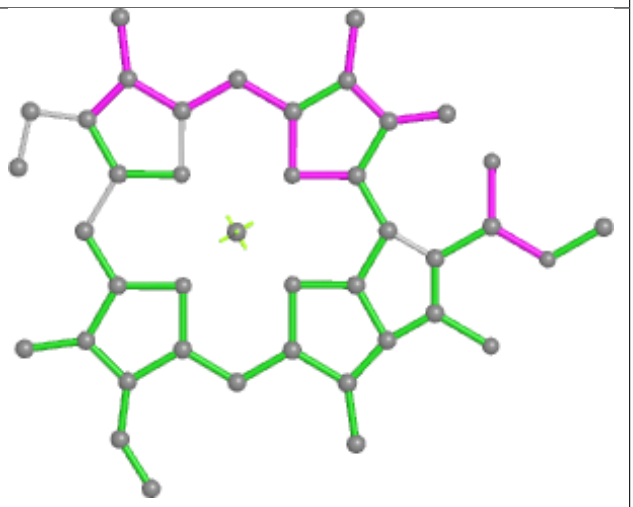
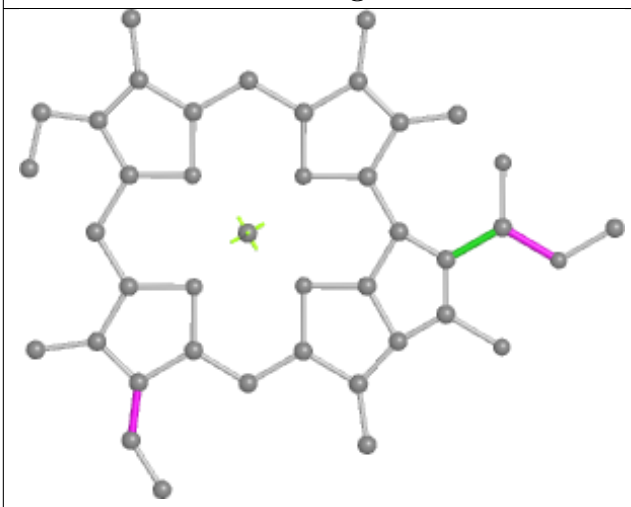


Bond angles



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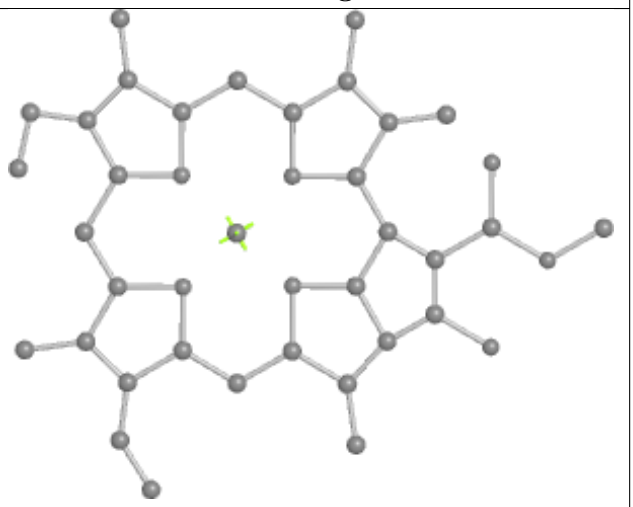
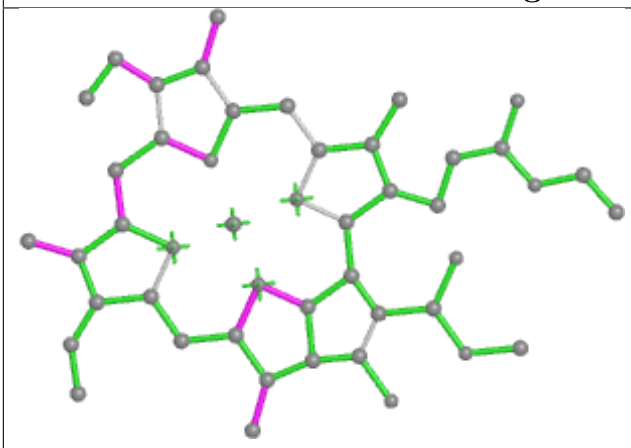


Rings

Ligand CLA A 815



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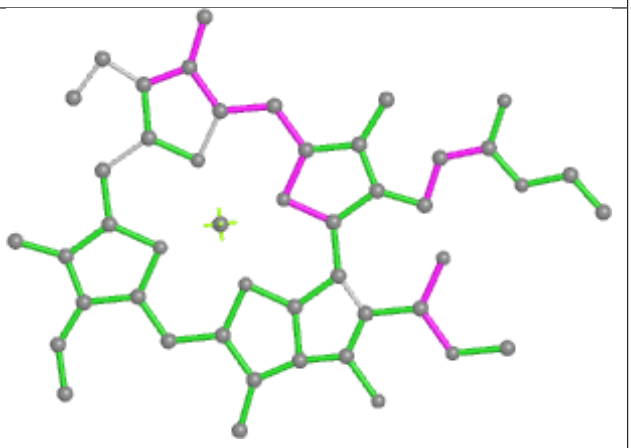
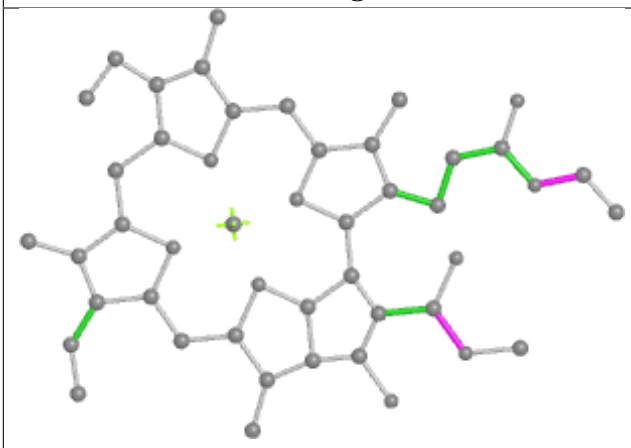
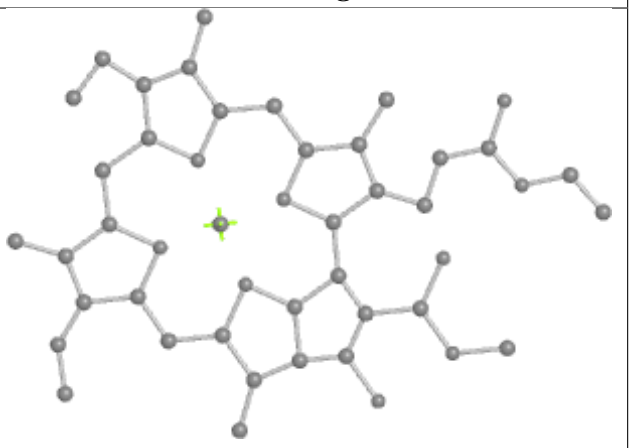


Bond angles

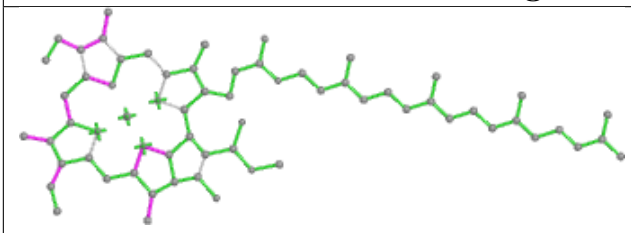


Torsions



Rings

Ligand CLA B 811



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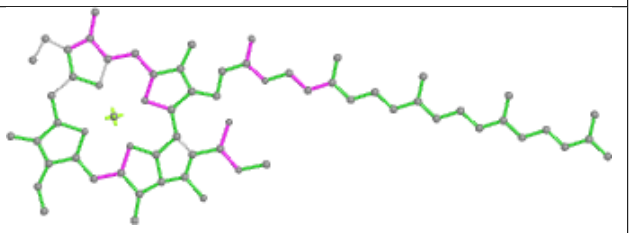

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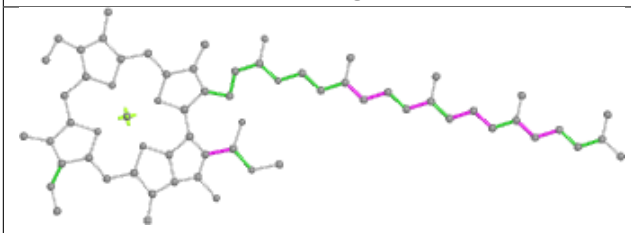

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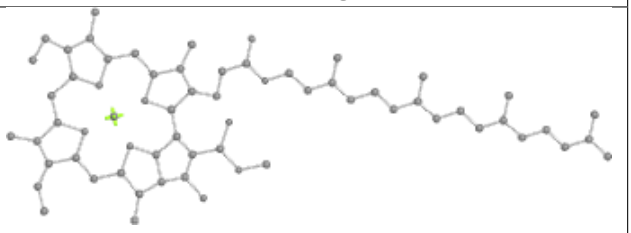
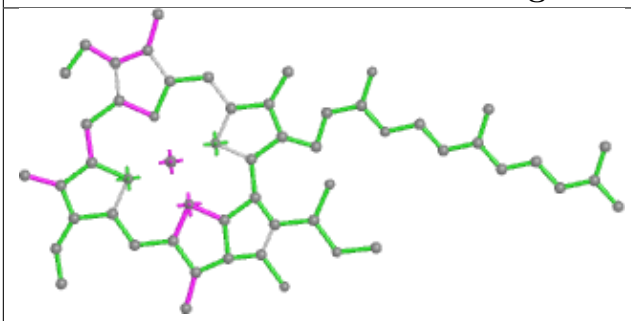


Rings

Ligand CLA 7 313



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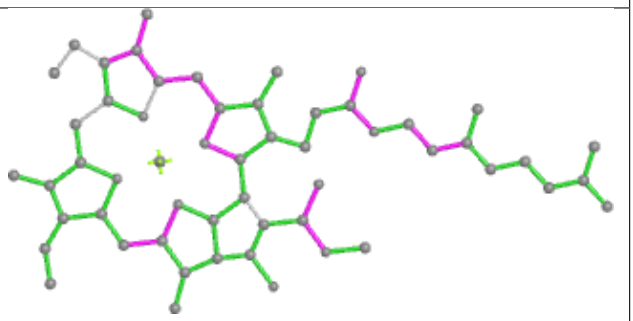
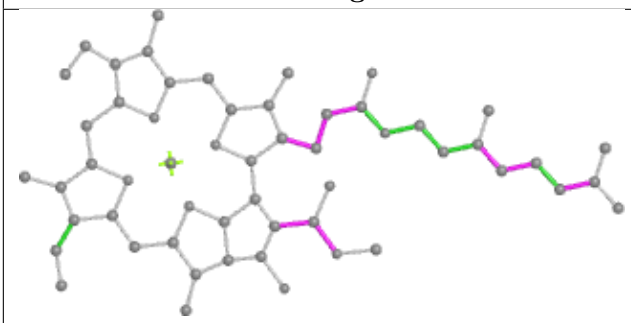


Bond angles



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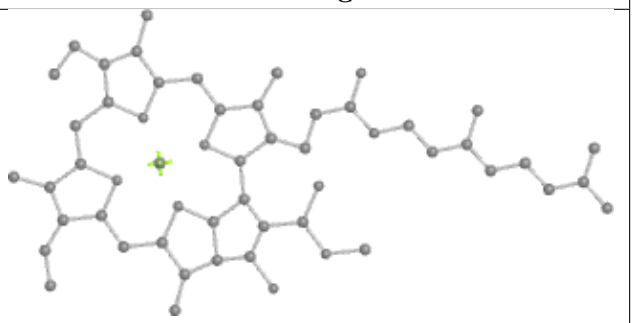
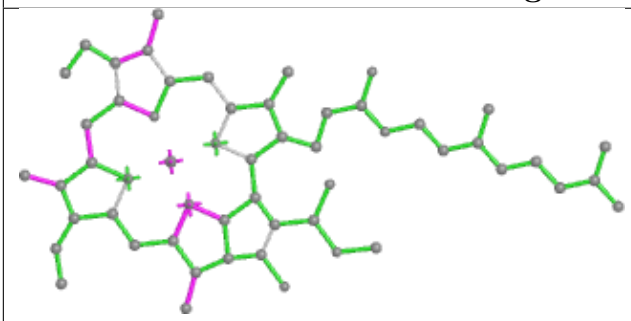


Rings

Ligand CLA B 813



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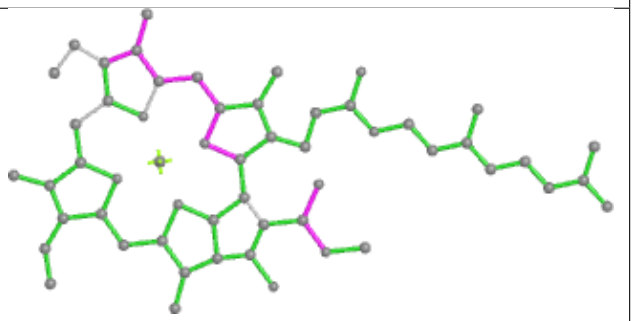

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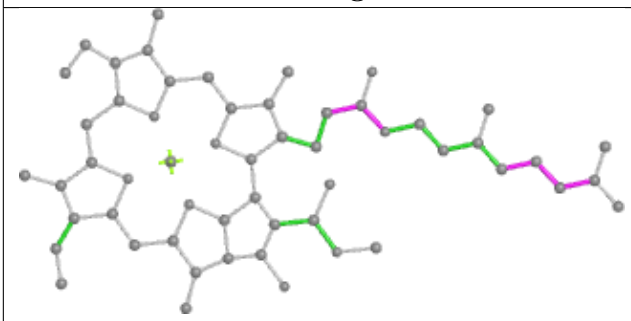

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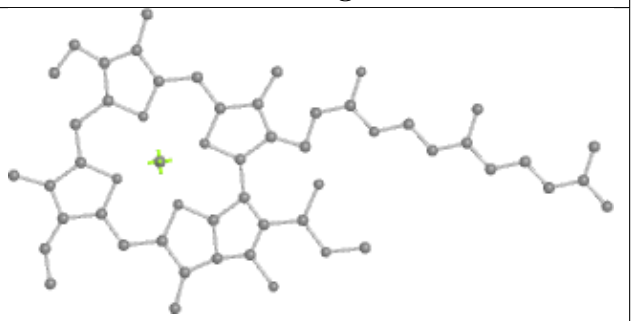
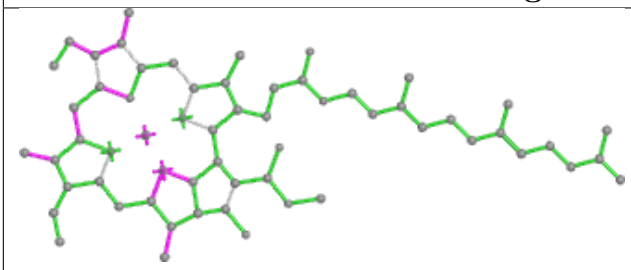


Rings

Ligand CLA B 836



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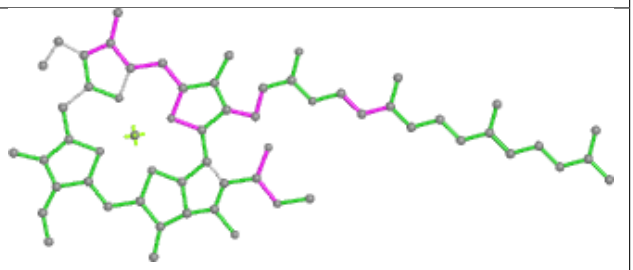

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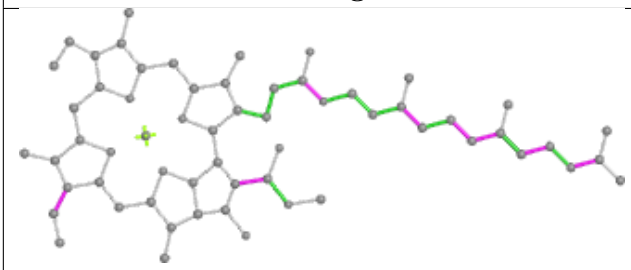

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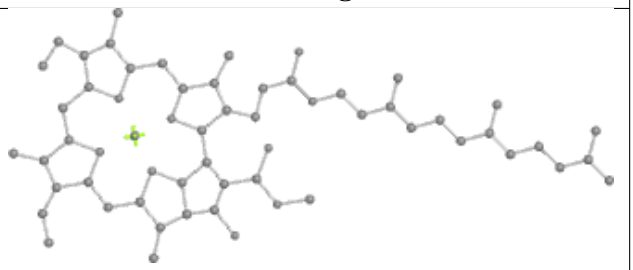
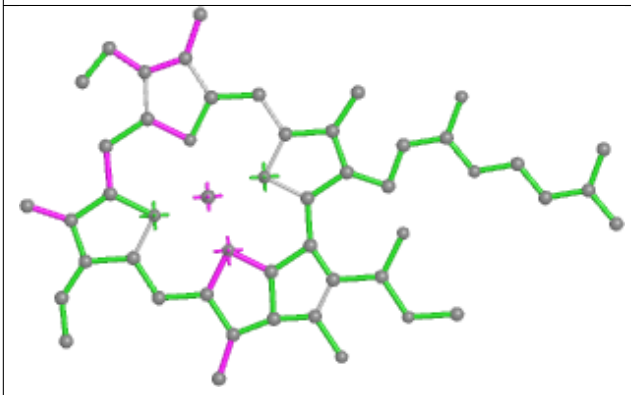


Rings

Ligand CLA 2 308



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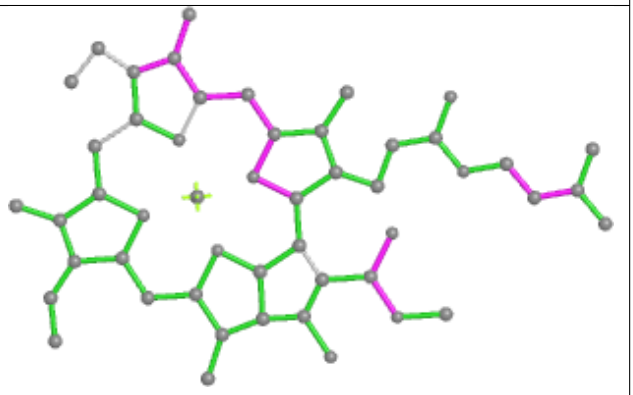

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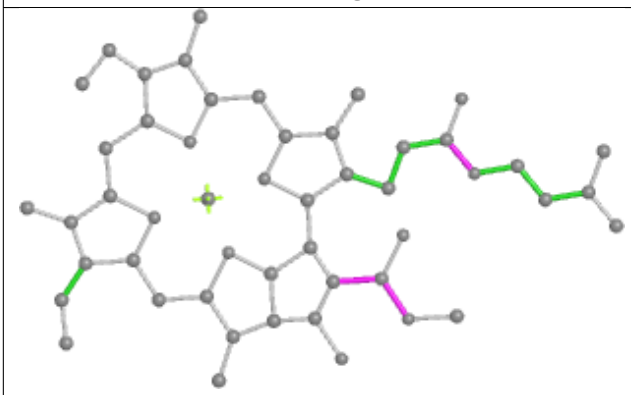

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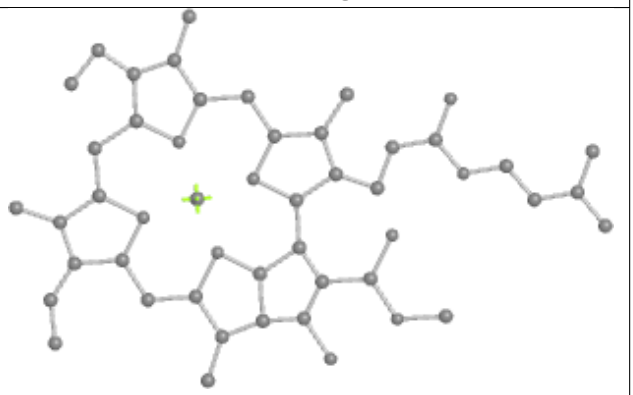
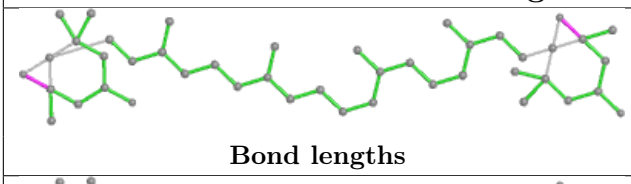


Rings

Ligand XAT 6 319



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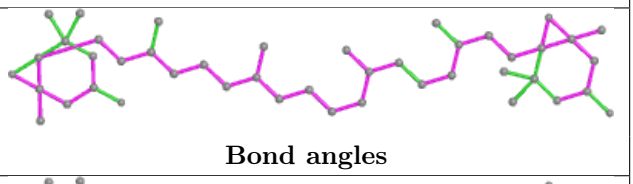

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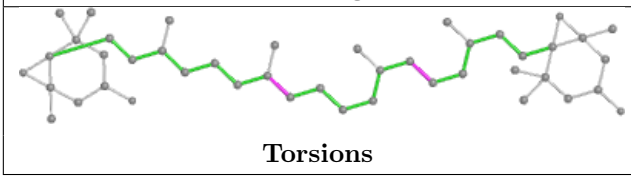

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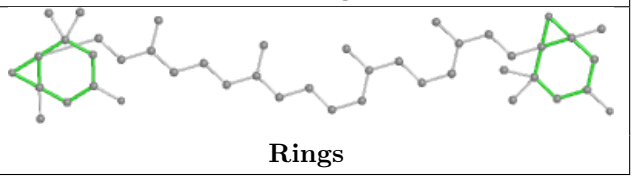
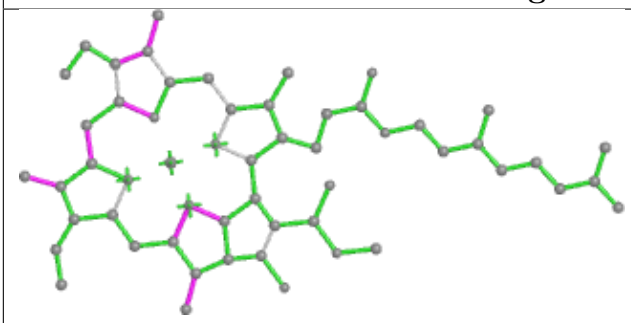


Rings

Ligand CLA 5 313



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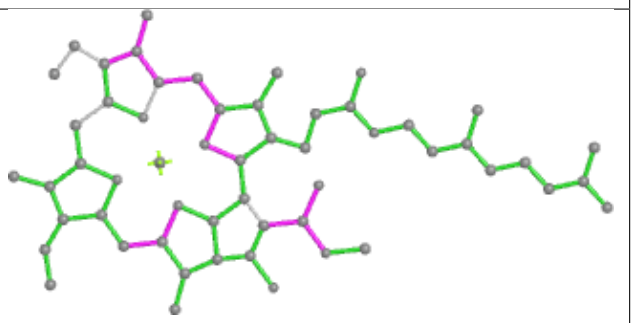

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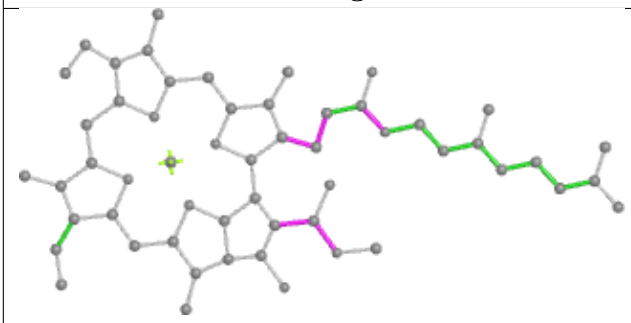

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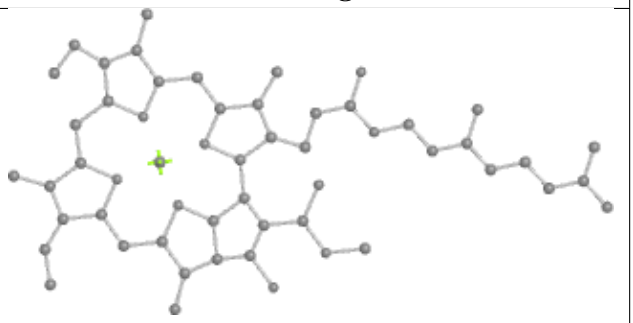
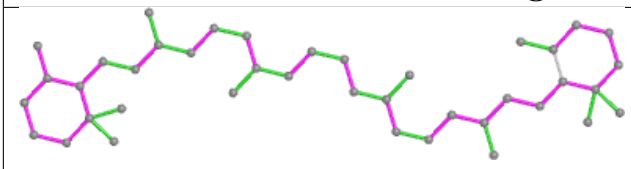


Rings

Ligand 8CT B 844



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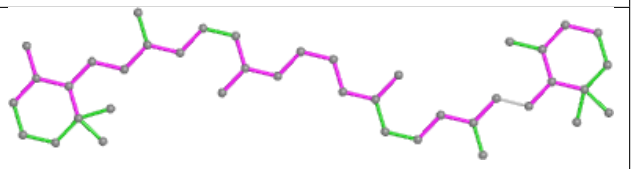
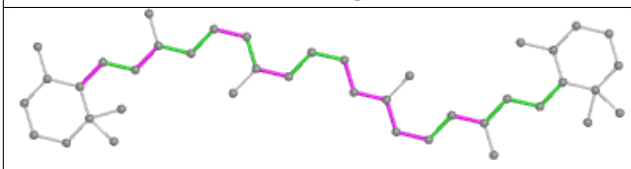


Bond angles



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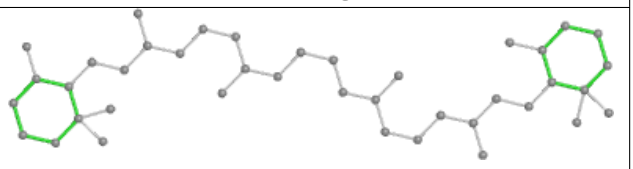
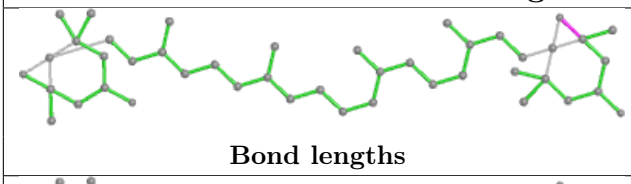


Rings

Ligand XAT 8 316



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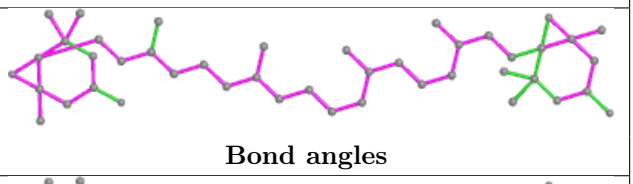
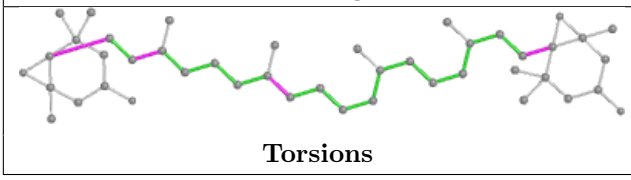


Bond angles



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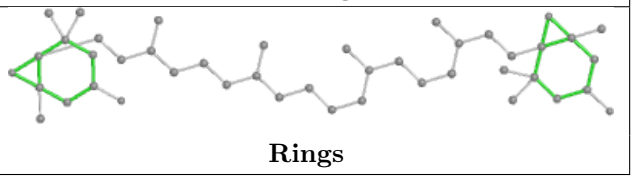
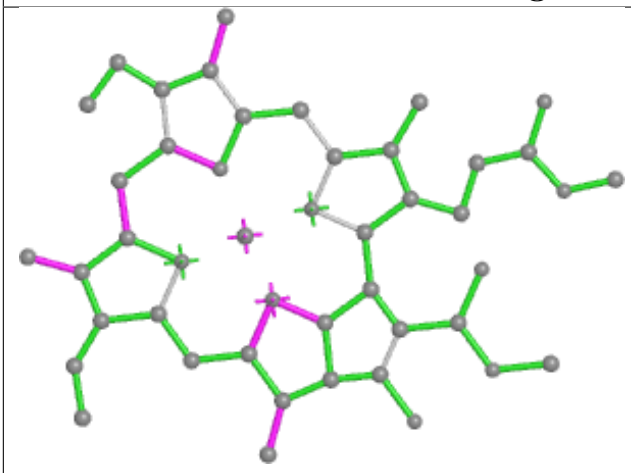


Rings

Ligand CLA 7 315



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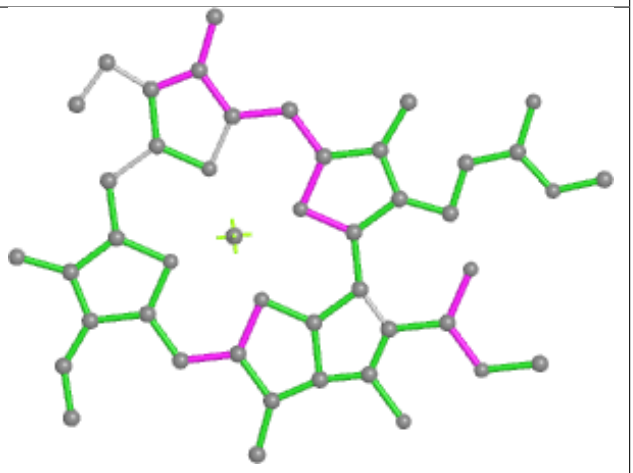
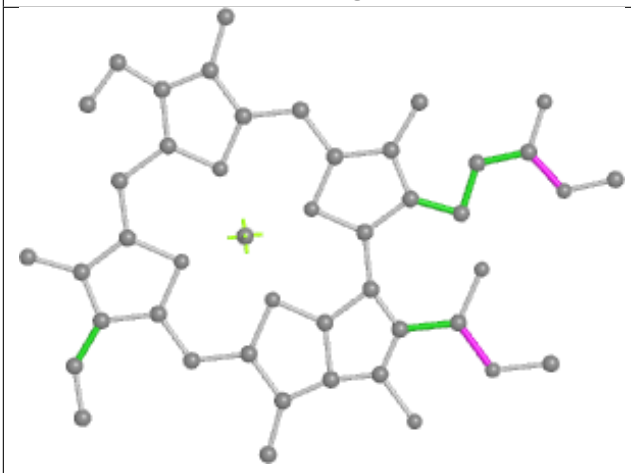


Bond angles



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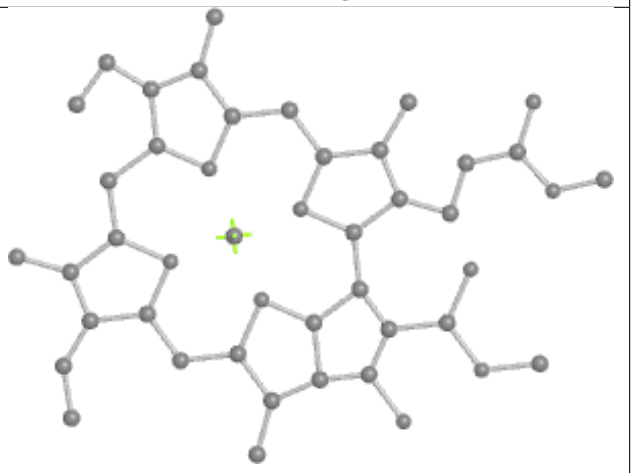
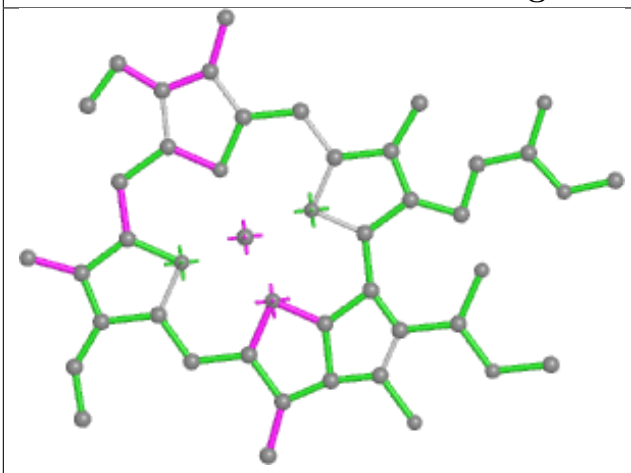


Rings

Ligand CLA 6 323



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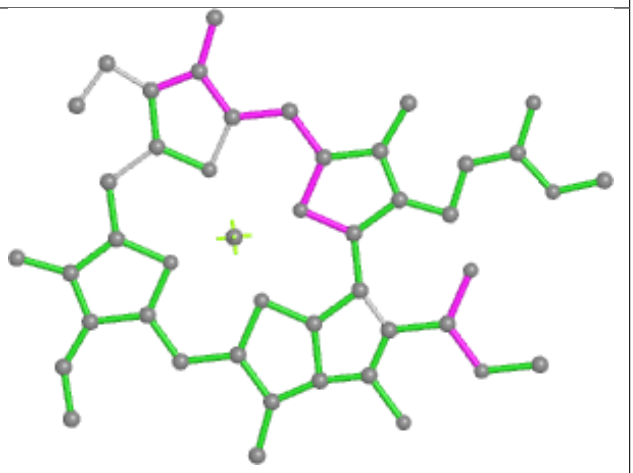
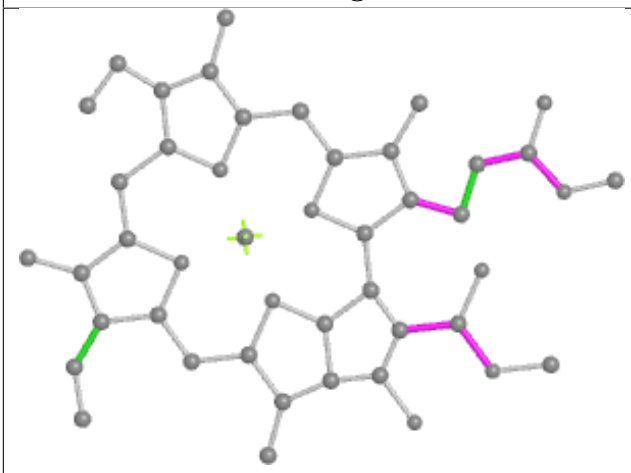
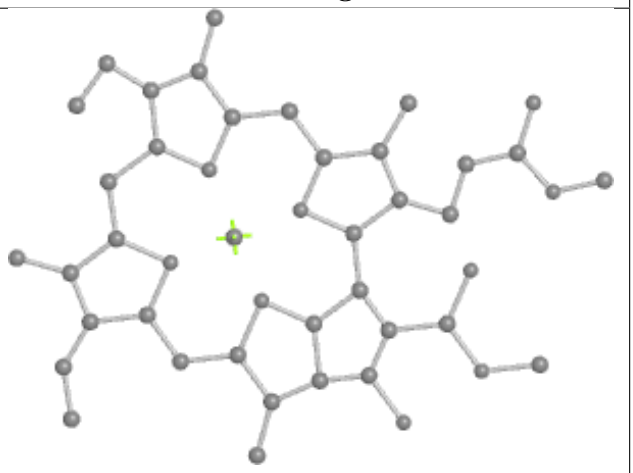


Bond angles

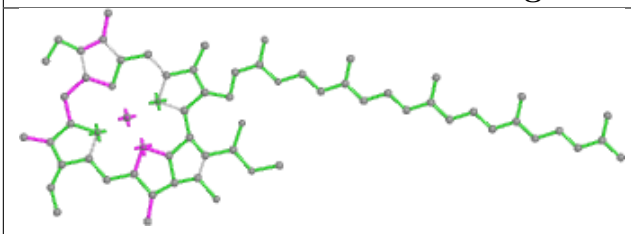


Torsions



Rings

Ligand CLA B 829



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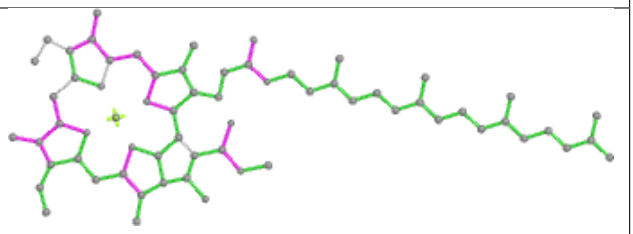
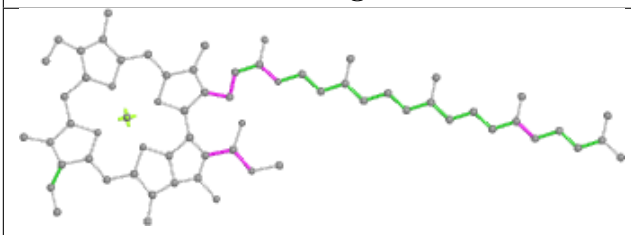
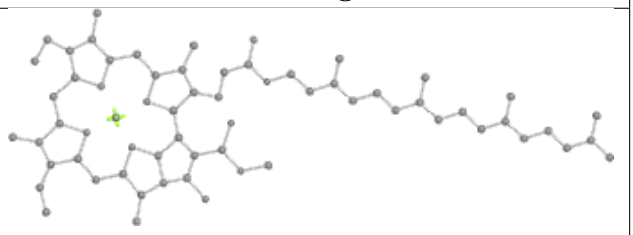


Bond angles

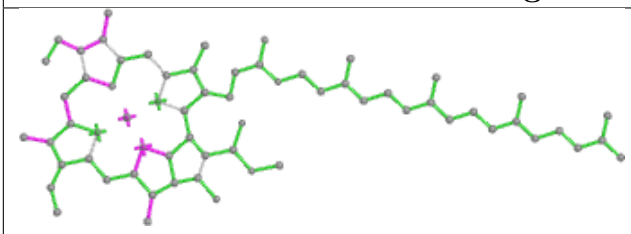


Torsions

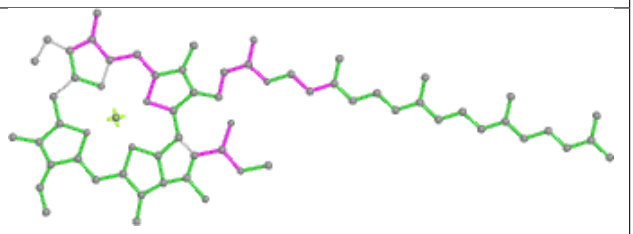


Rings

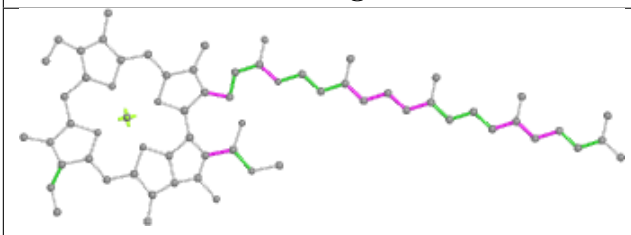
Ligand CLA A 803



Bond lengths



Bond angles



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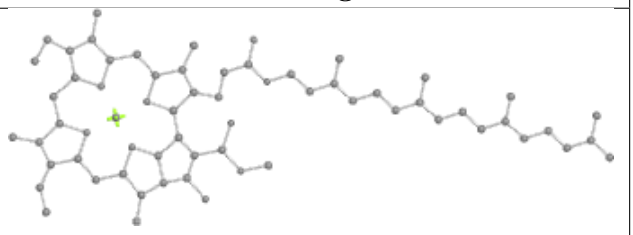
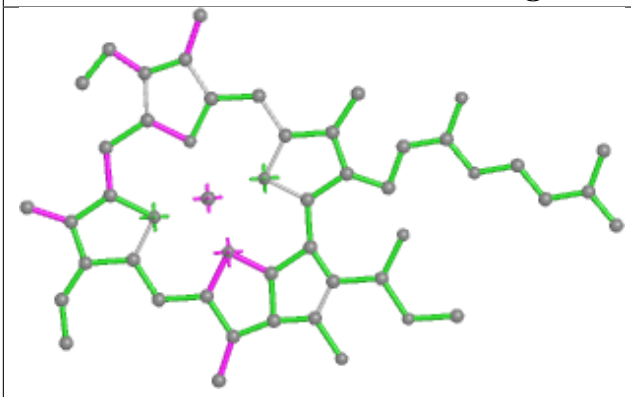


Rings

Ligand CLA B 821



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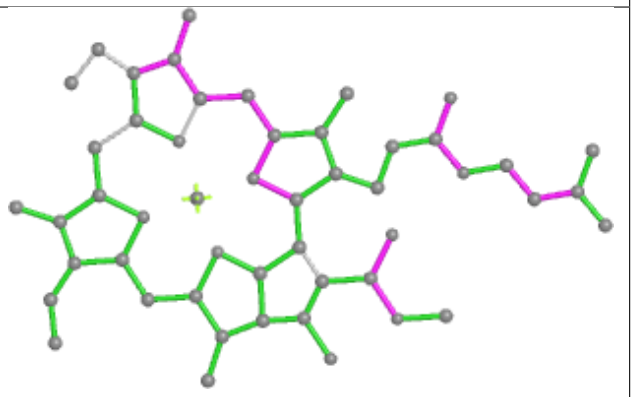

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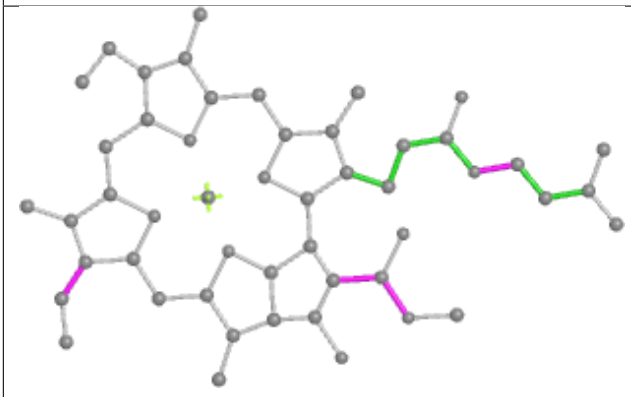

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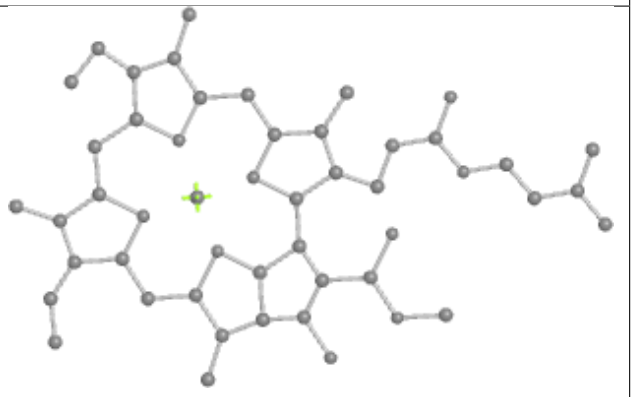
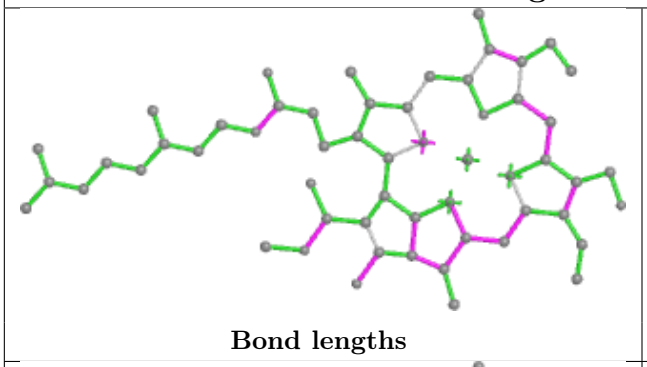


Rings

Ligand CHL 8 305



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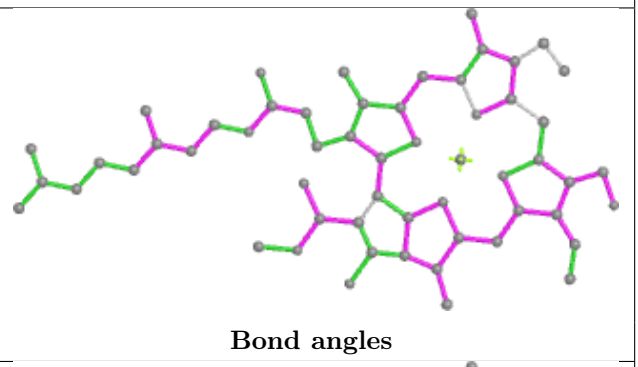

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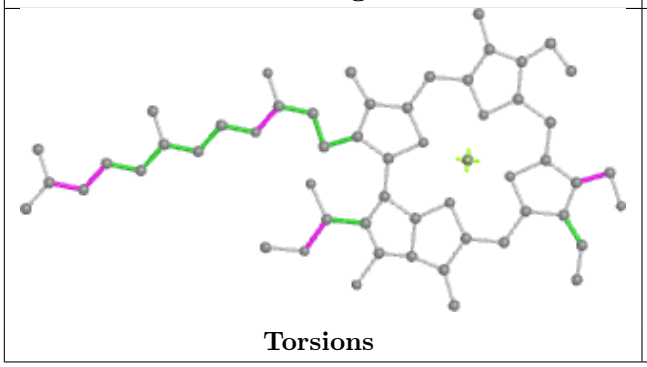

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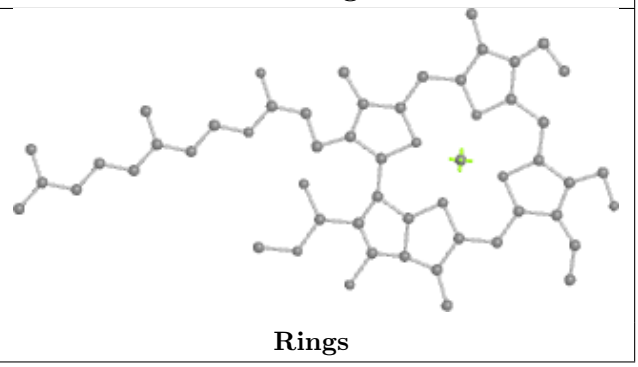
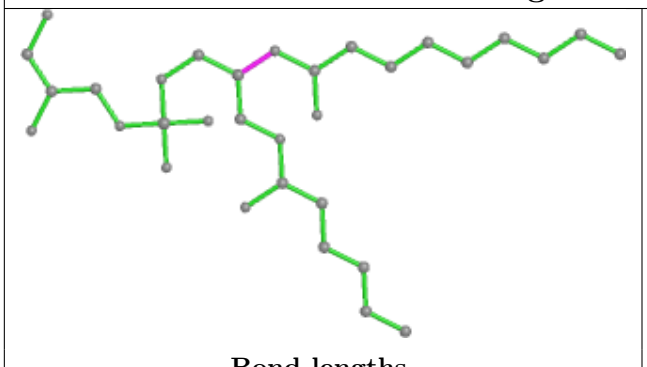


Rings

Ligand LHG 2 318



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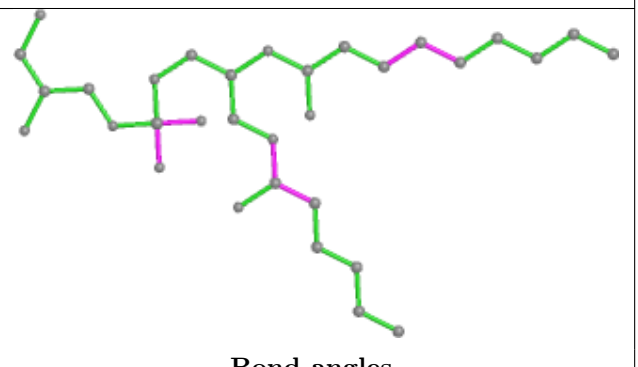
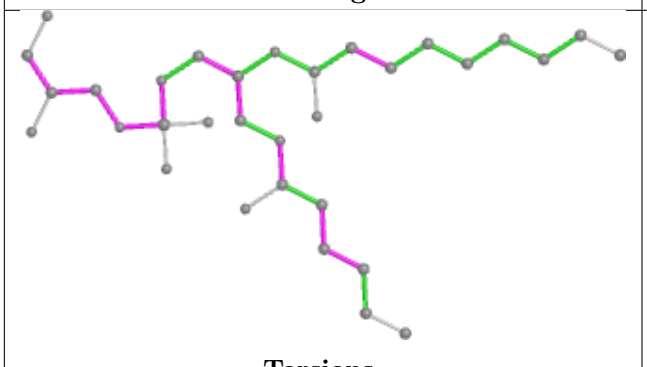


Bond angles



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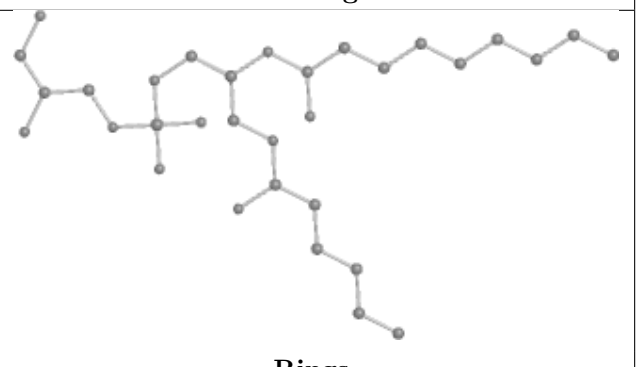
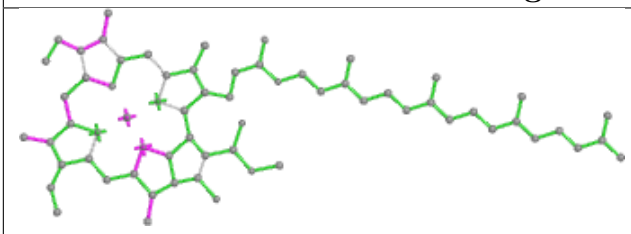


Rings

Ligand CLA B 805



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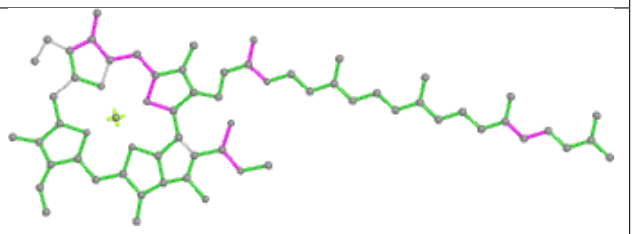
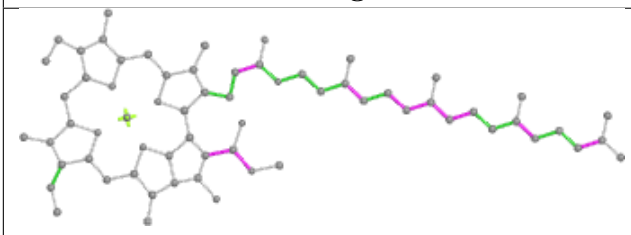


Bond angles



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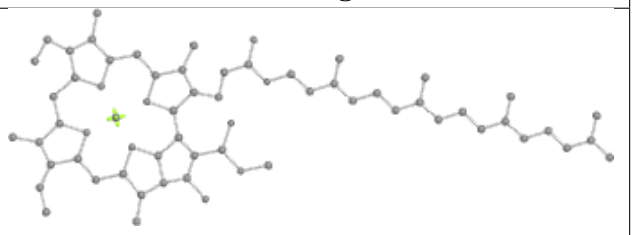
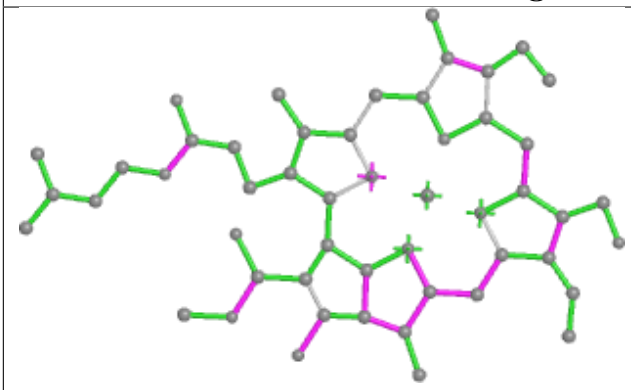


Rings

Ligand CHL 2 307



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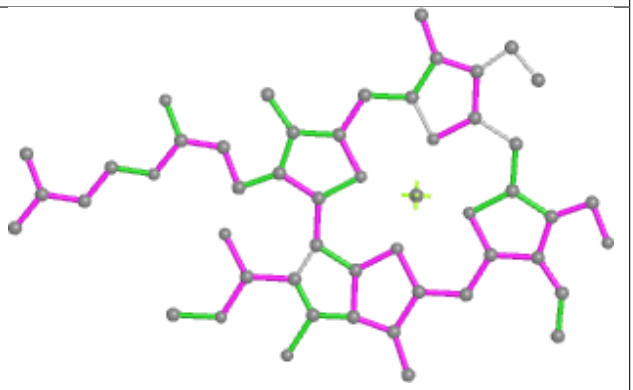
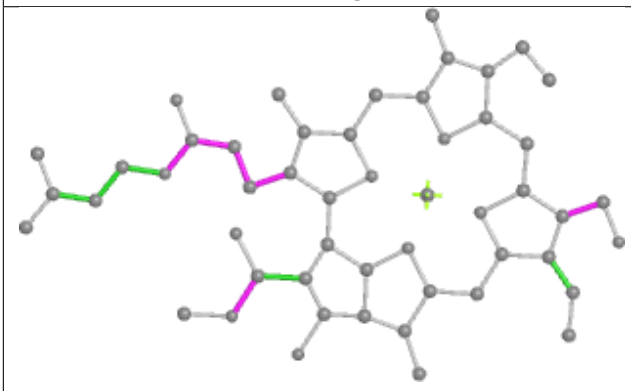


Bond angles



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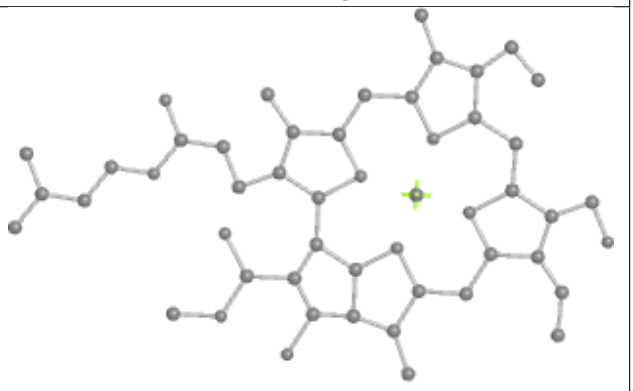
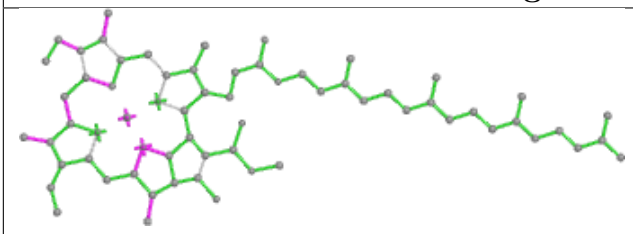


Rings

Ligand CLA A 819



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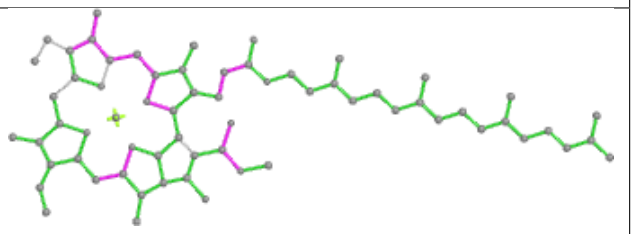

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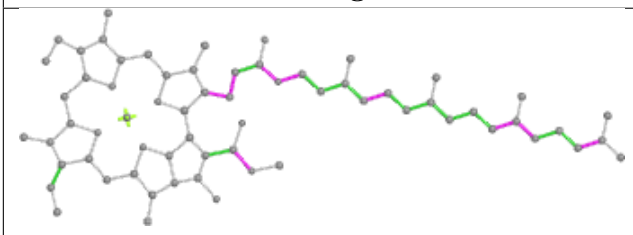

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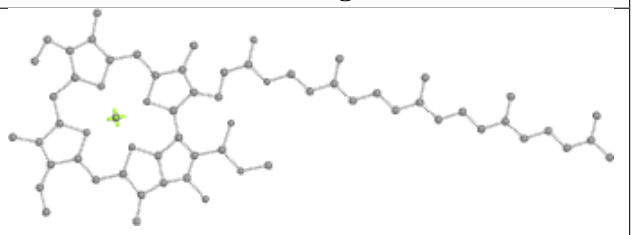
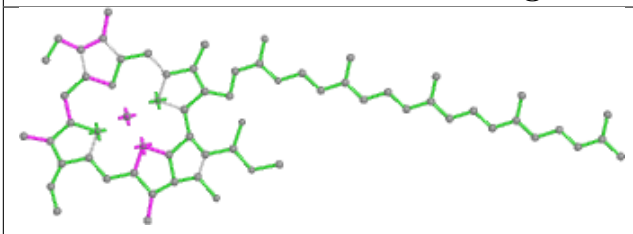


Rings

Ligand CLA A 810



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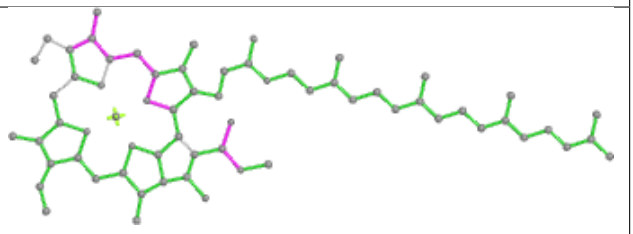
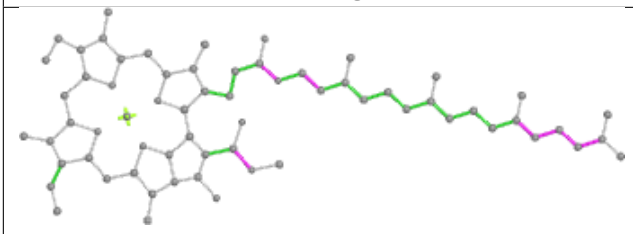


Bond angles



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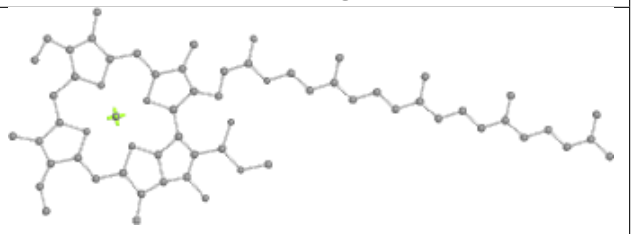
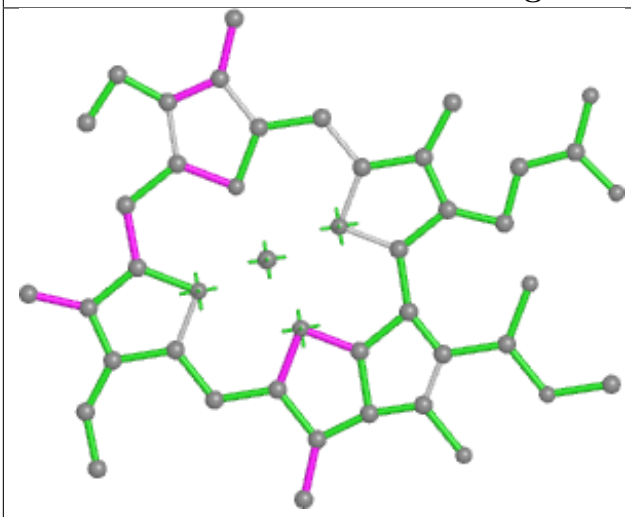


Rings

Ligand CLA B 835



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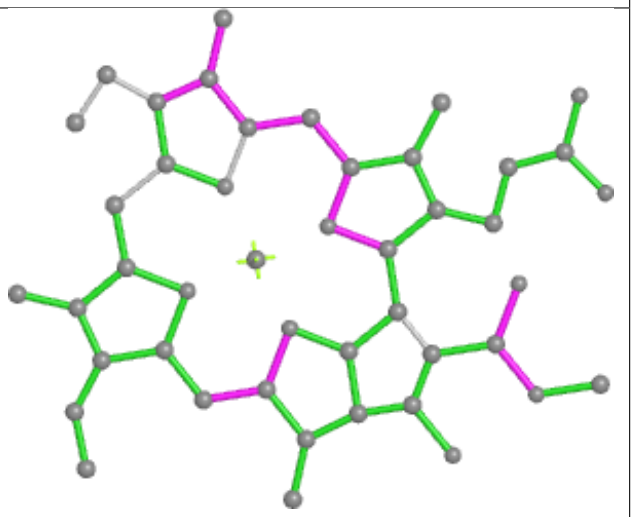

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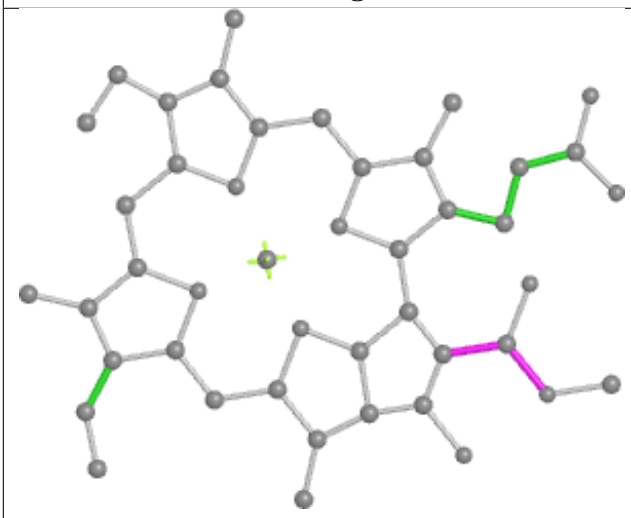

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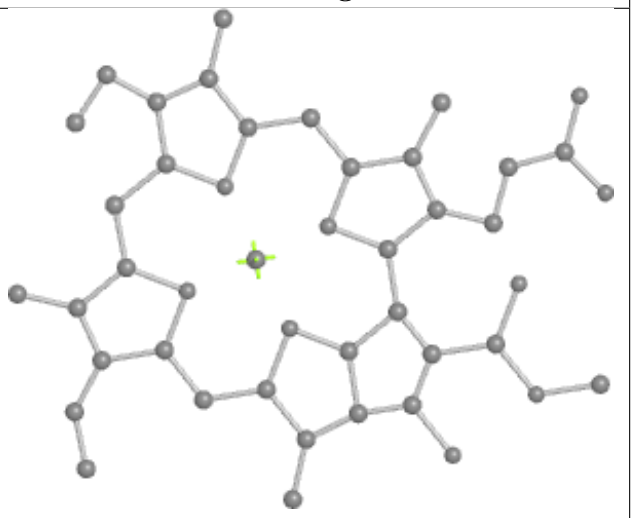
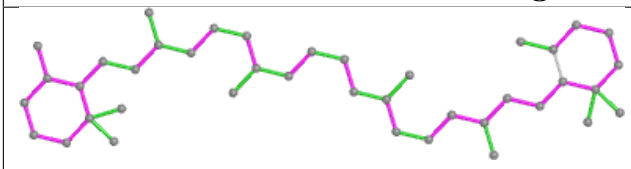


Rings

Ligand 8CT 8 301



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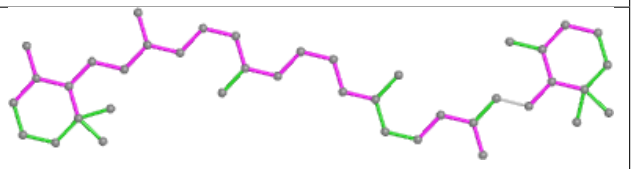

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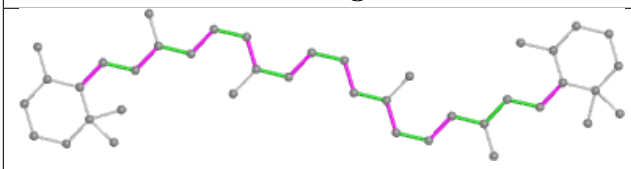

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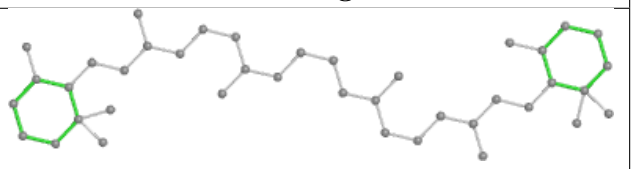
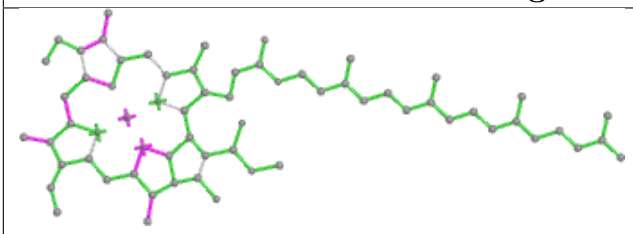


Rings

Ligand CLA 3 319



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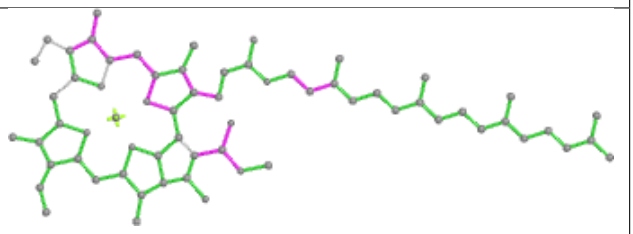
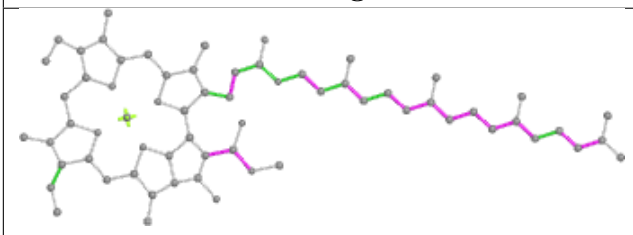


Bond angles



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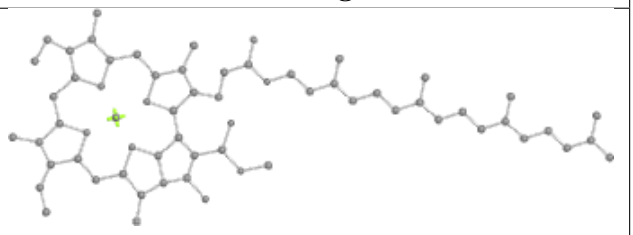
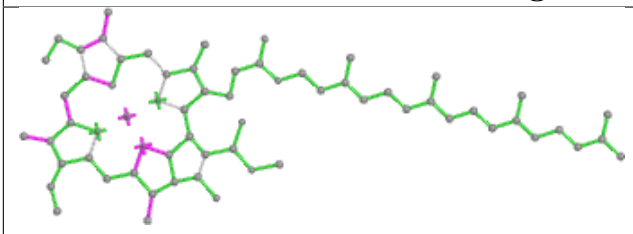


Rings

Ligand CLA 6 315



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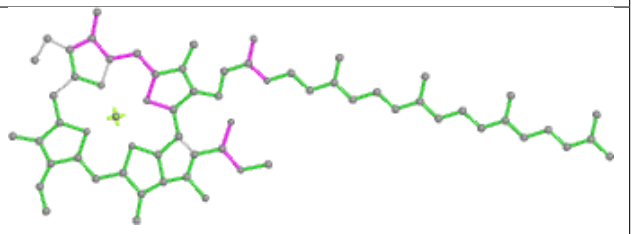
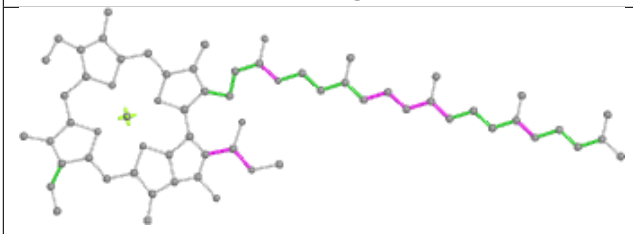


Bond angles



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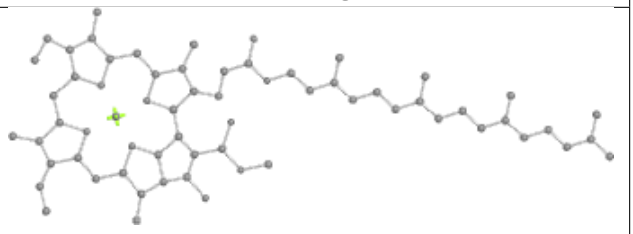
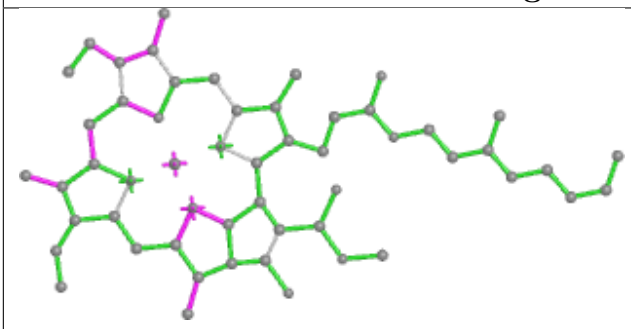
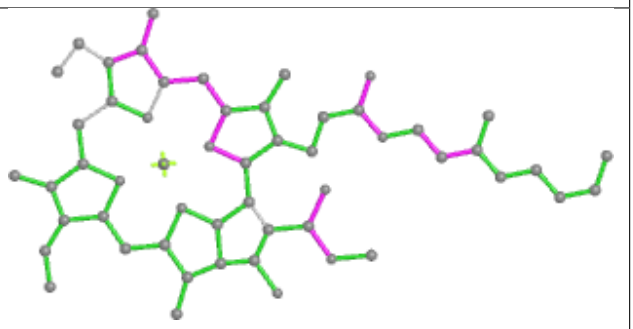


Rings

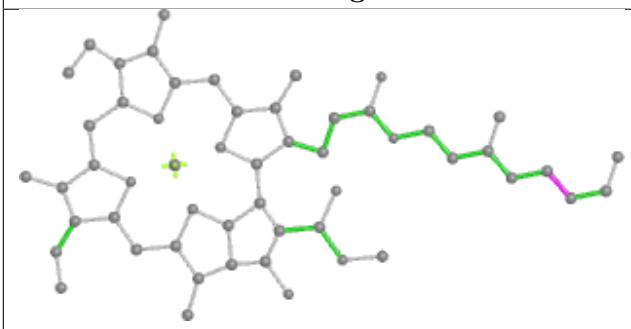
Ligand CLA A 812



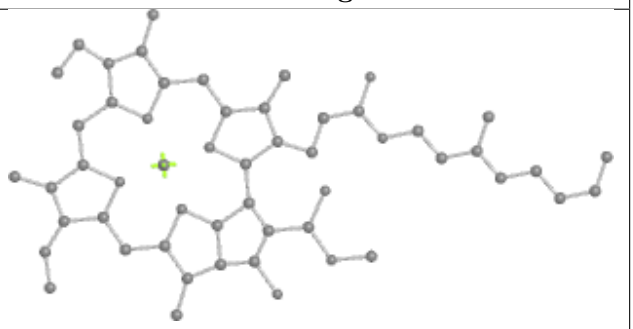
Bond lengths



Bond angles

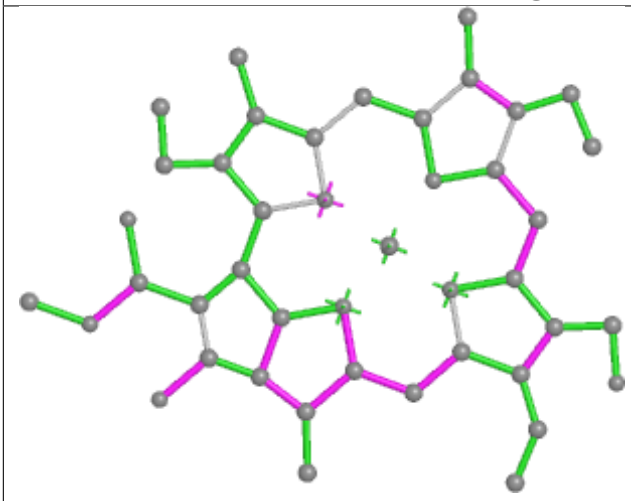


Torsions



Rings

Ligand CHL 6 306



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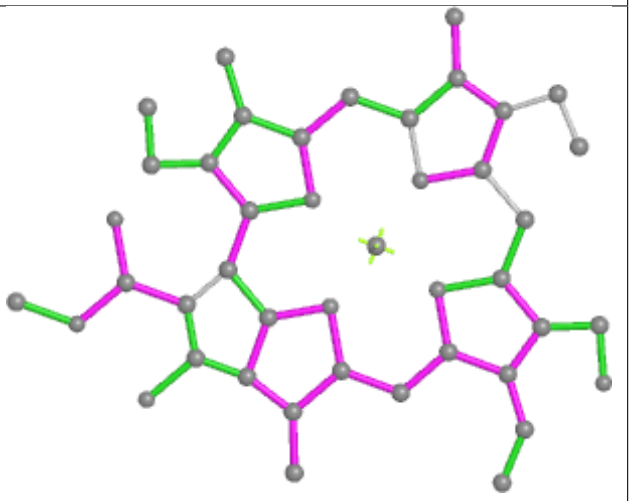

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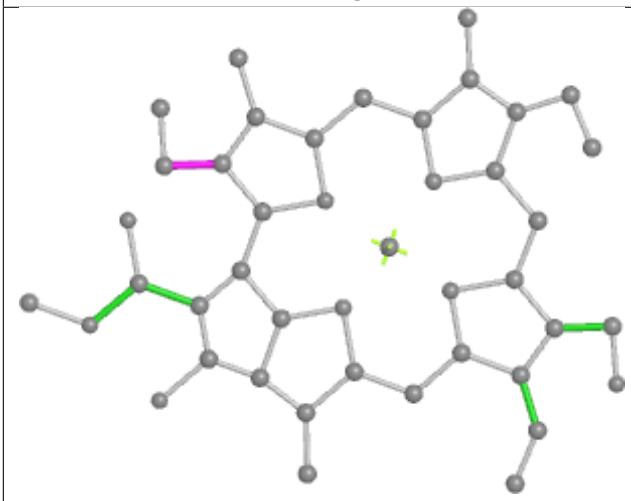

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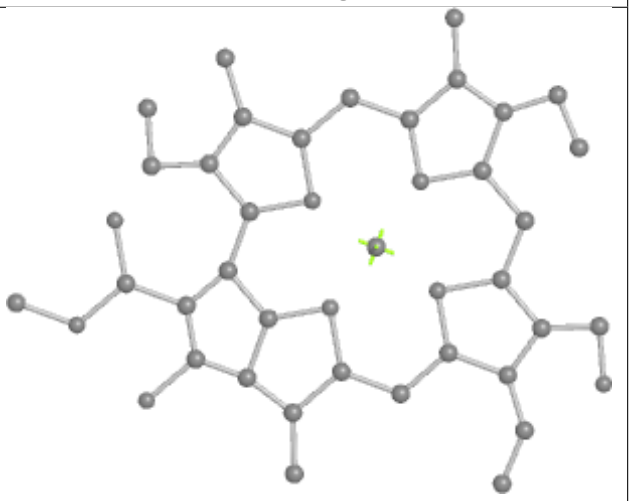
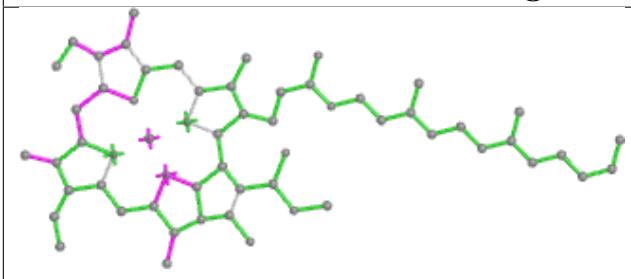


Rings

Ligand CLA B 818



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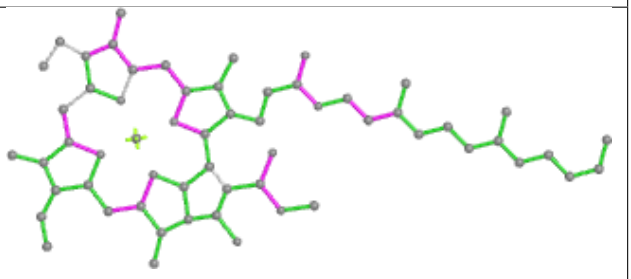

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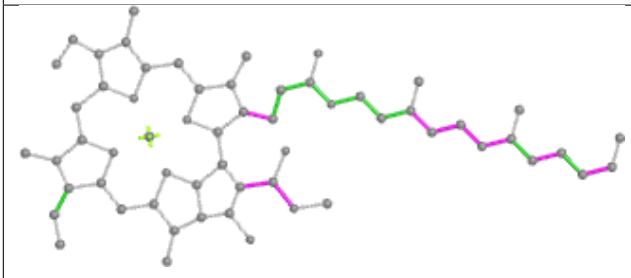

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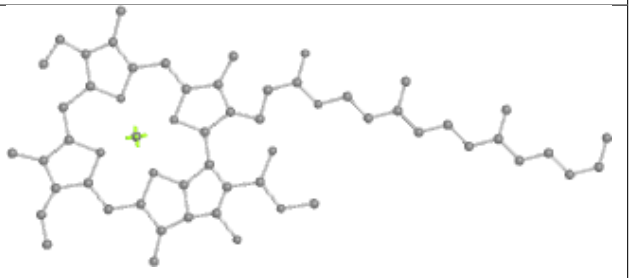
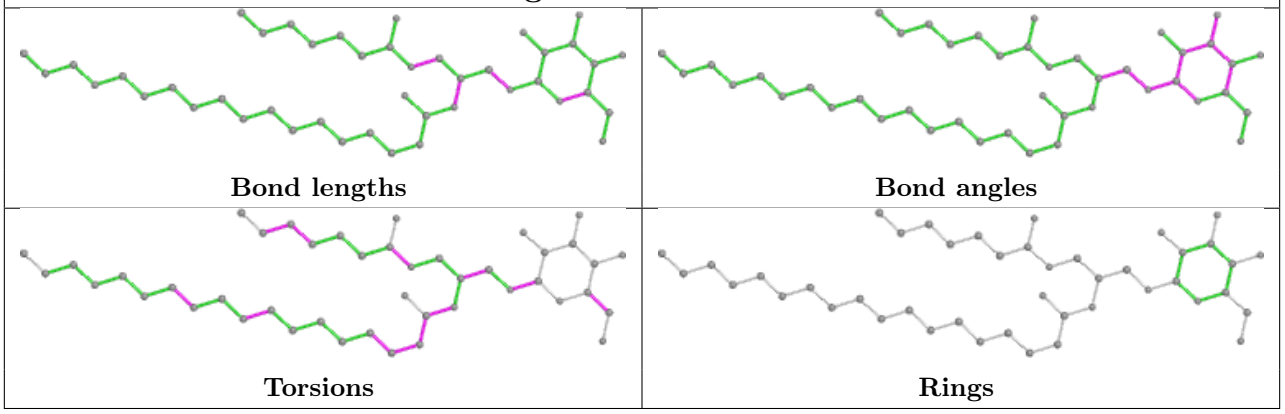
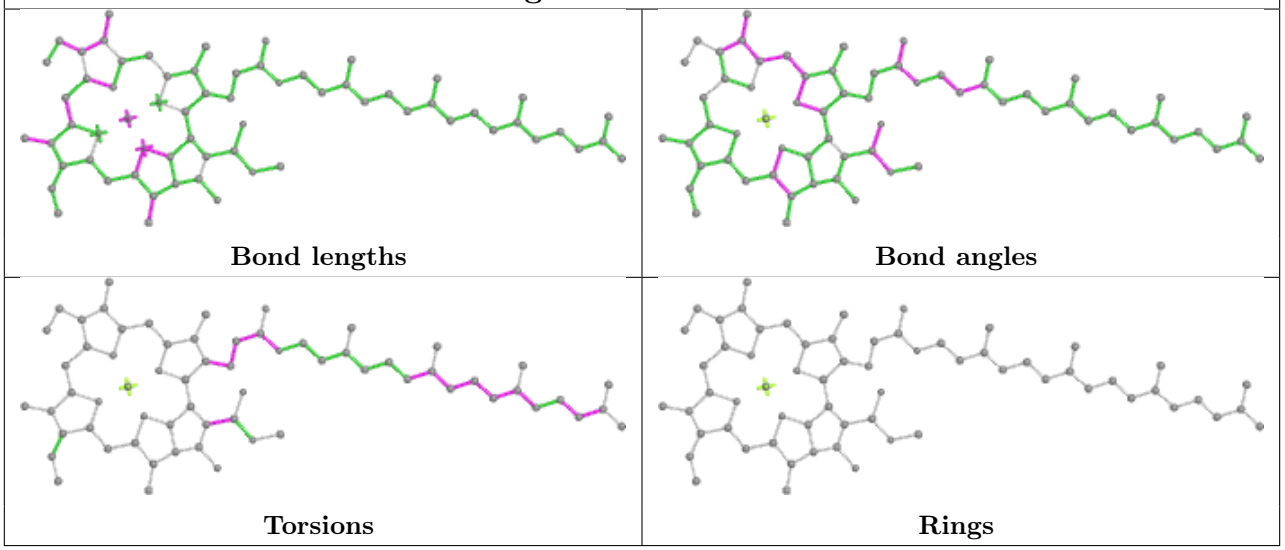


Rings

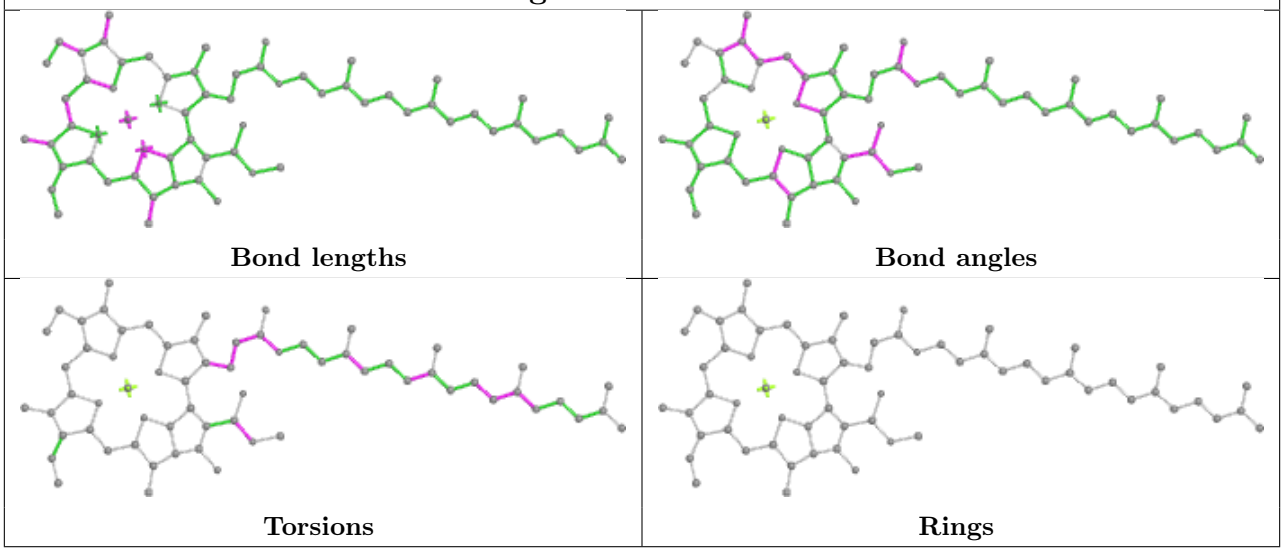
Ligand LMG 8 319



Ligand CLA A 806



Ligand CLA 1 307



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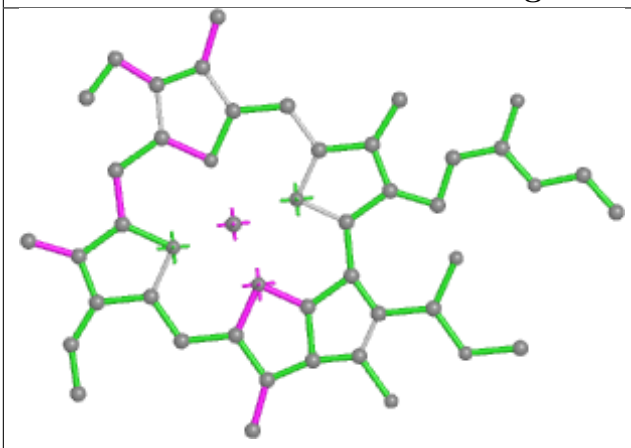
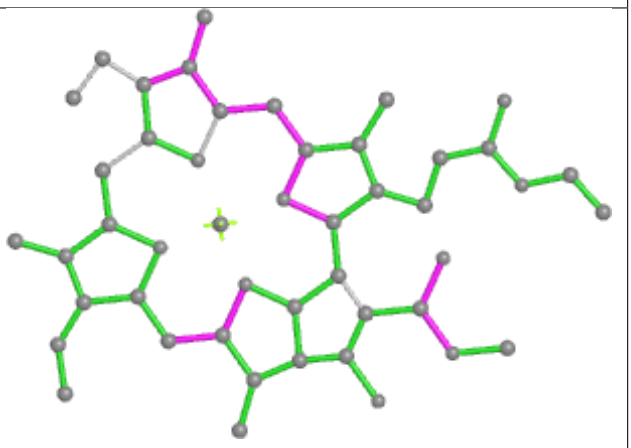
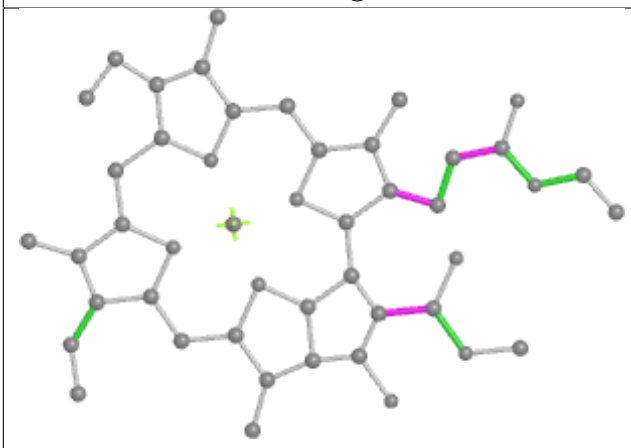


Bond lengths



Bond angles



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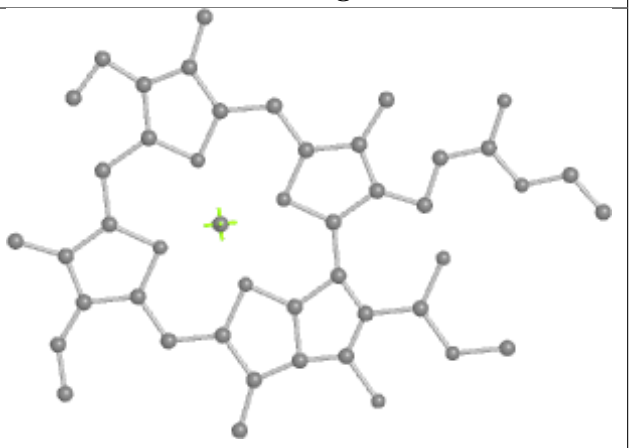
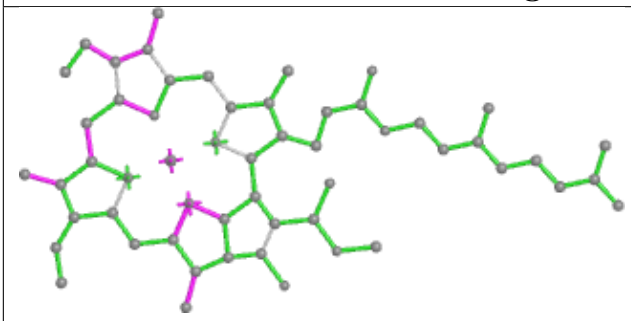


Rings

Ligand CLA A 824



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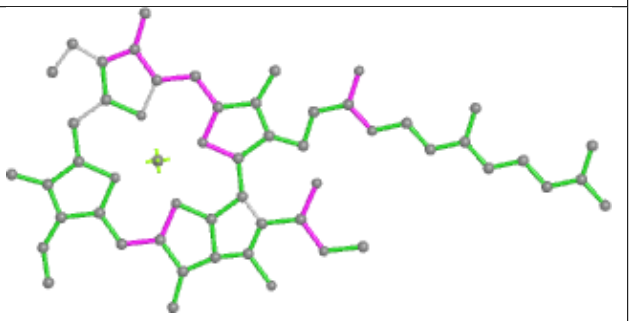
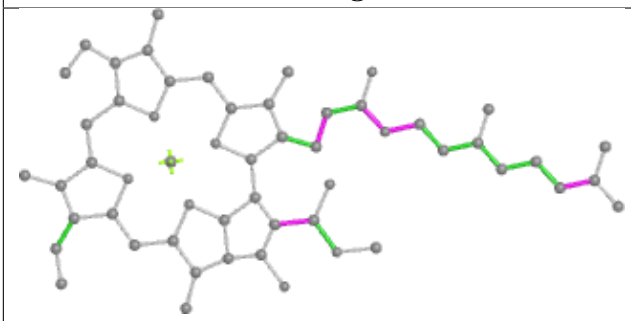


Bond angles



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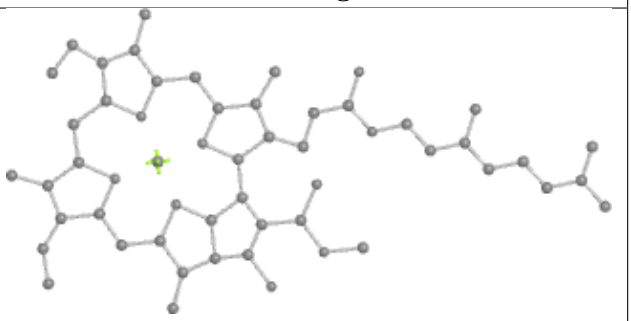
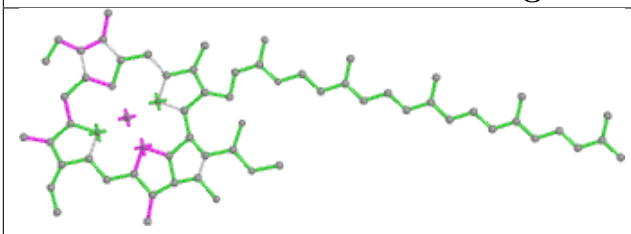


Rings

Ligand CLA A 811



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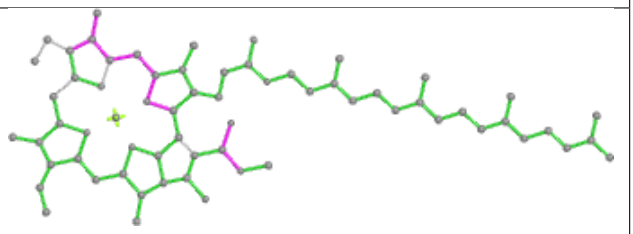
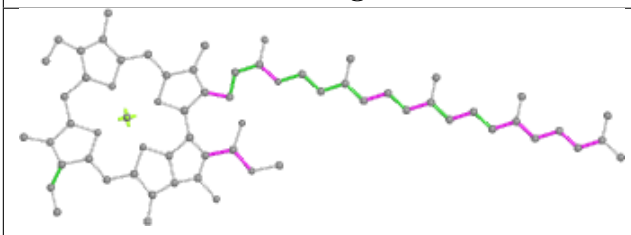


Bond angles



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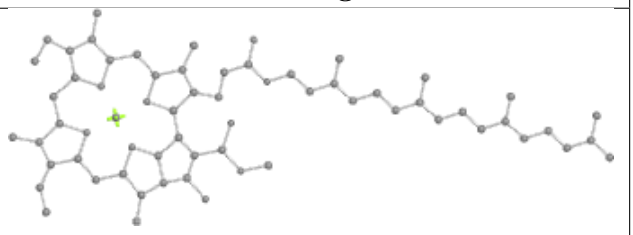
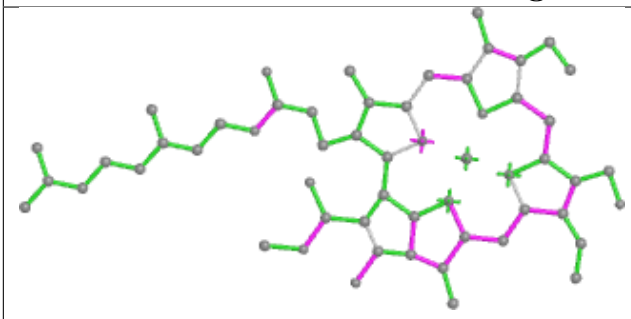


Rings

Ligand CHL 4 305



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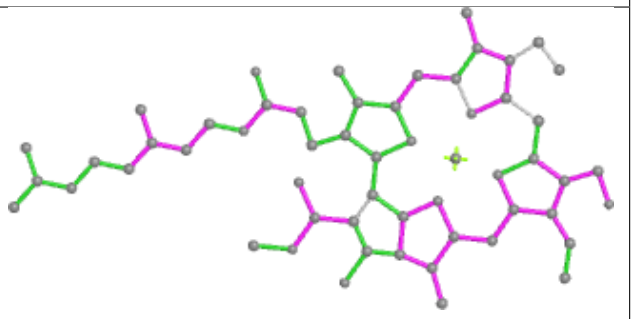

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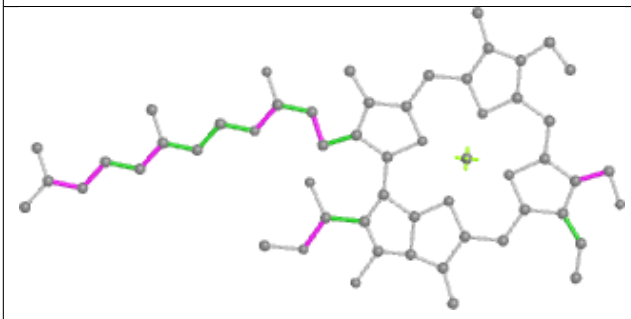

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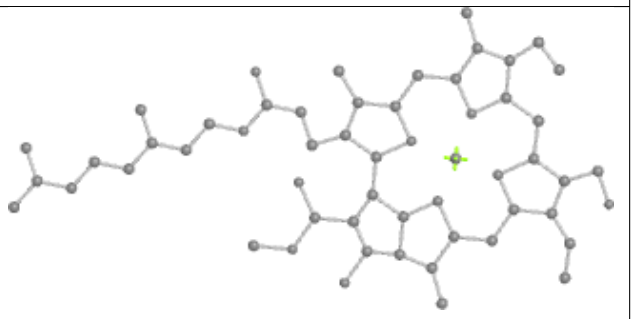
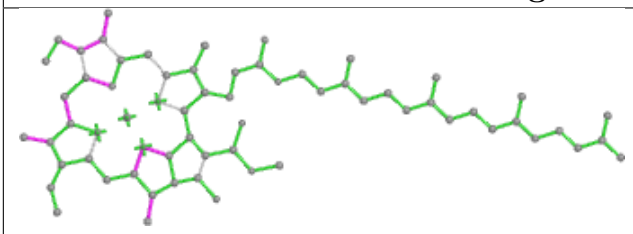
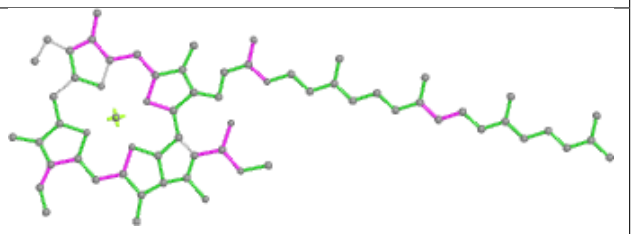


Rings

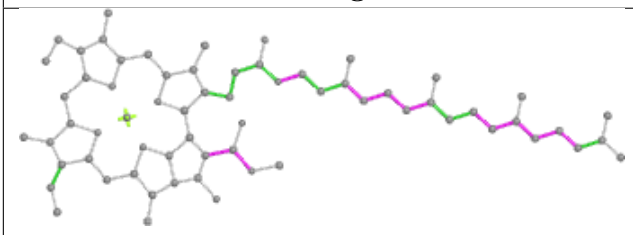
Ligand CLA 2 302



Bond lengths



Bond angles



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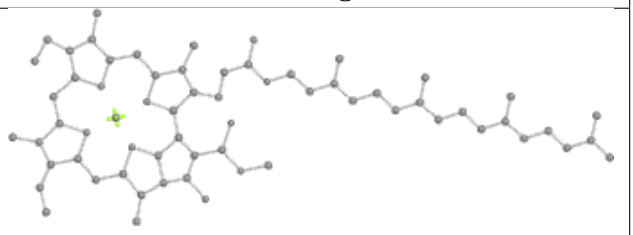
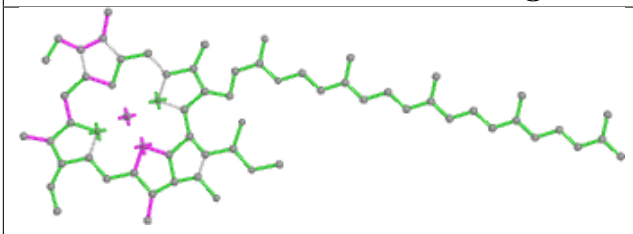


Rings

Ligand CLA B 812



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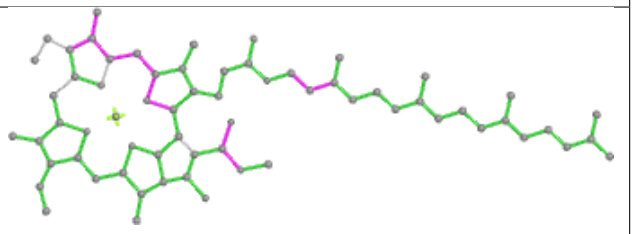
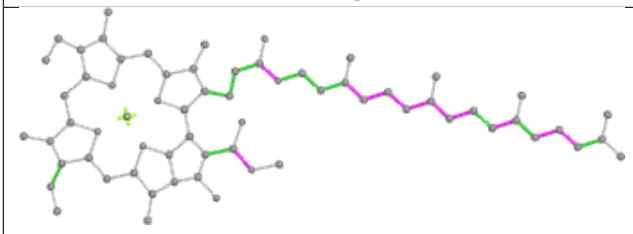


Bond angles



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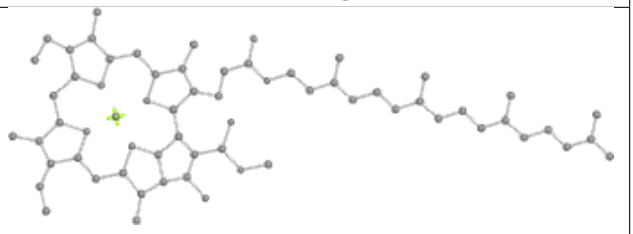
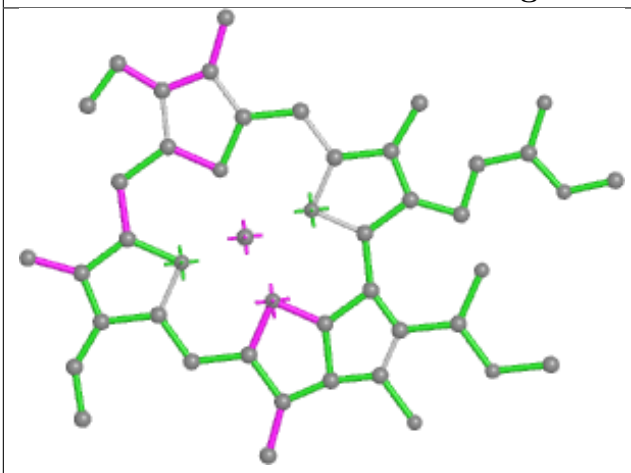


Rings

Ligand CLA M 101



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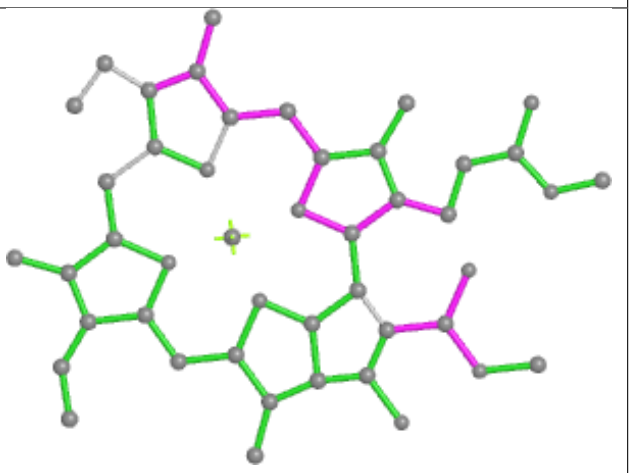

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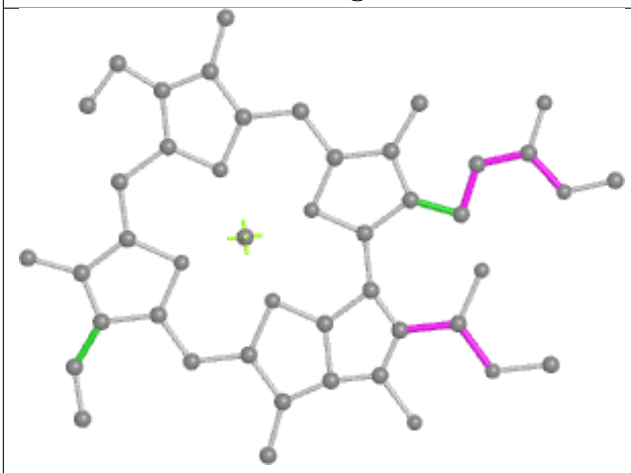

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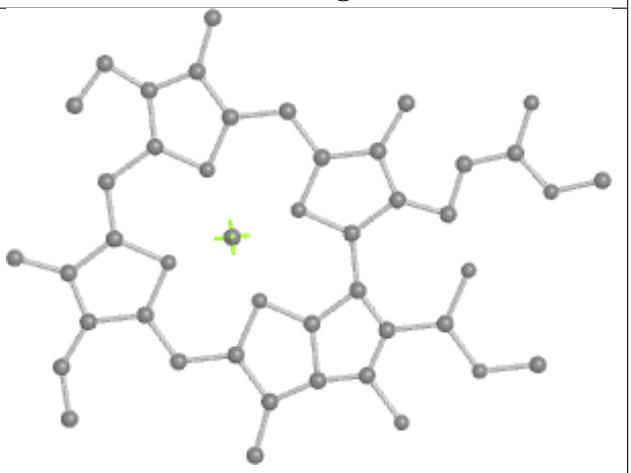
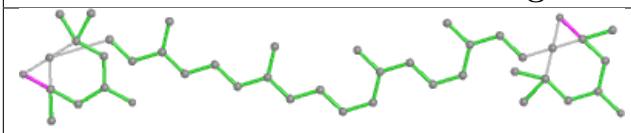


Rings

Ligand XAT 8 317



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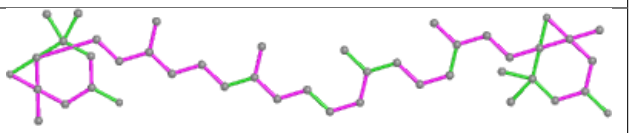
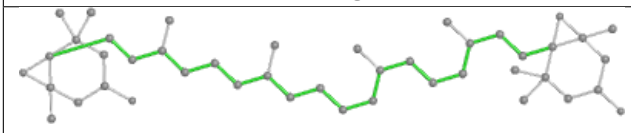


Bond angles



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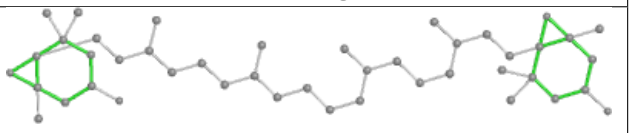
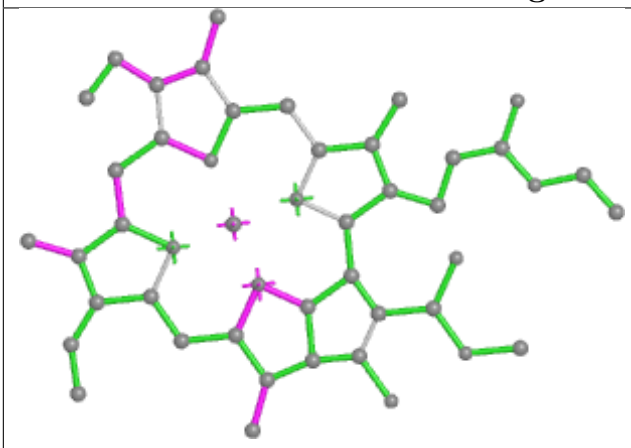


Rings

Ligand CLA 3 305



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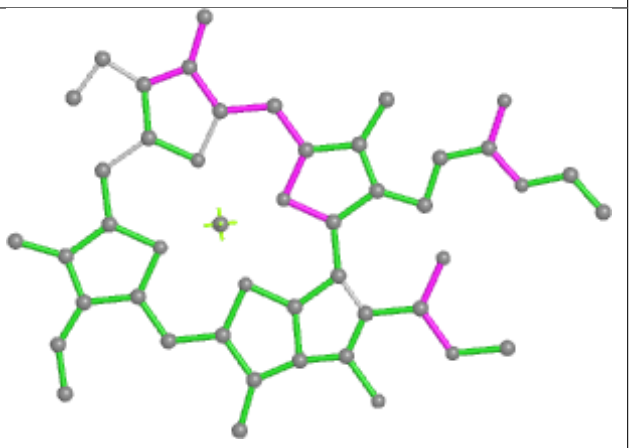
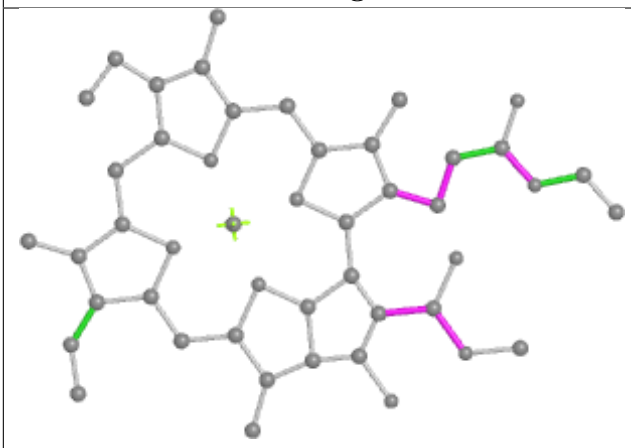


Bond angles



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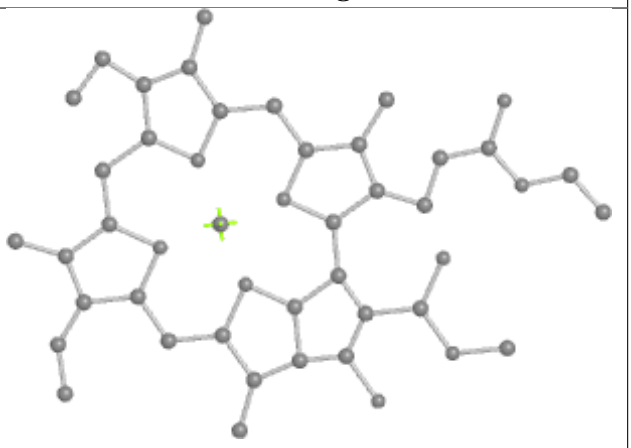
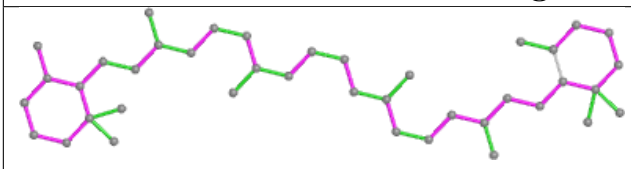
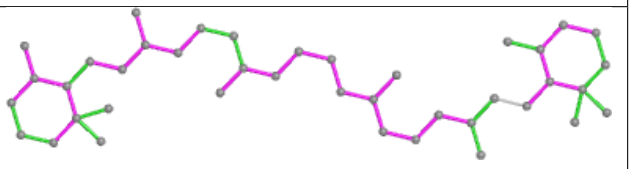


Rings

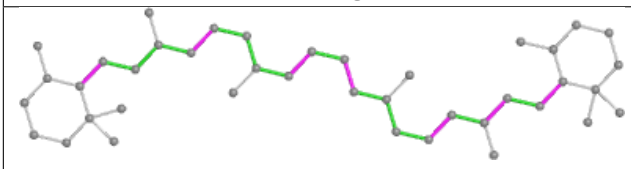
Ligand 8CT J 101



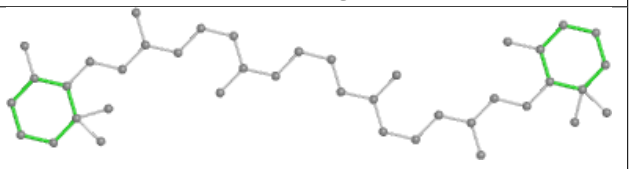
Bond lengths



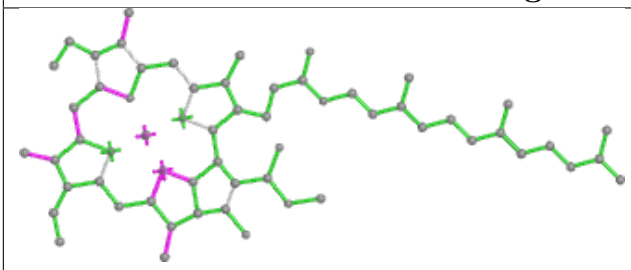
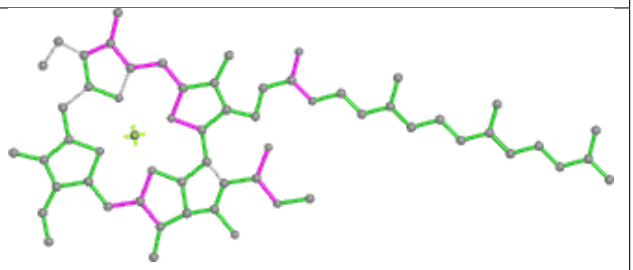
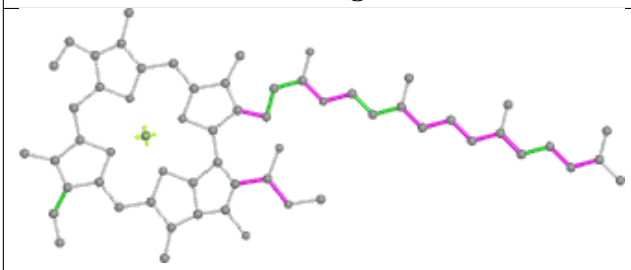
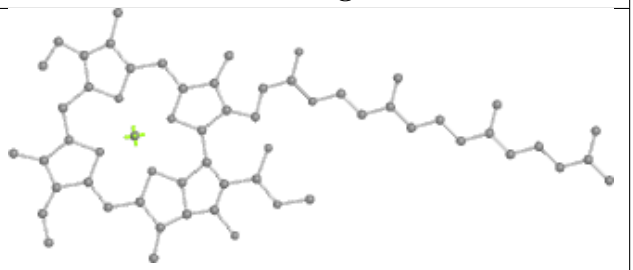
Bond angles



Torsions



Rings

Ligand CLA B 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

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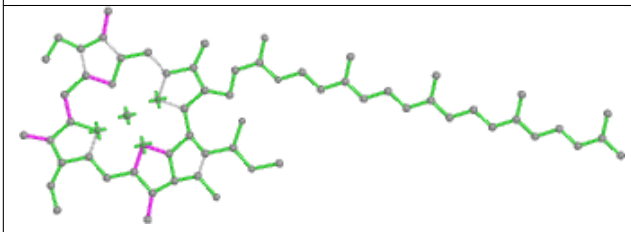
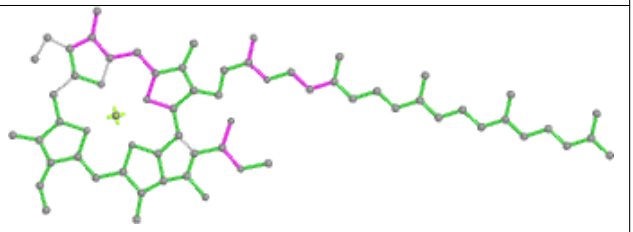
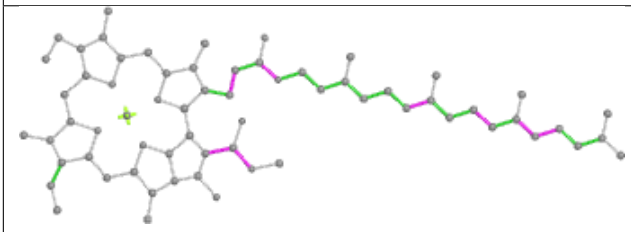
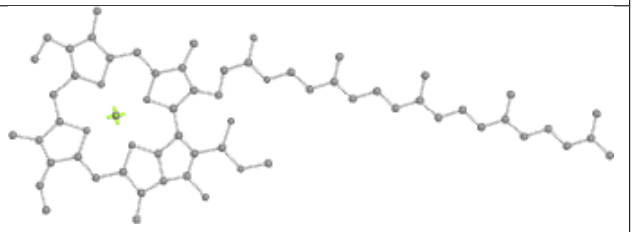
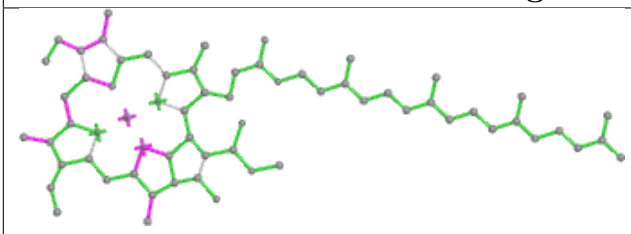
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L 201



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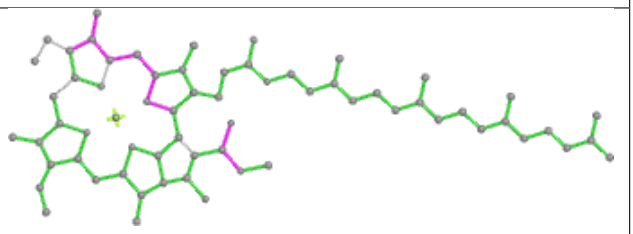
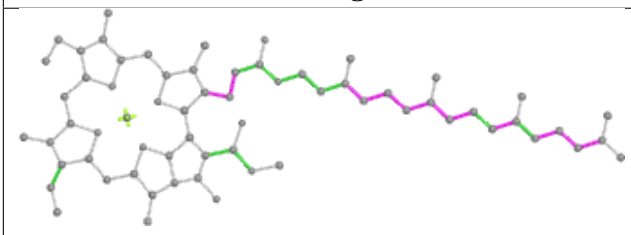


Bond angles



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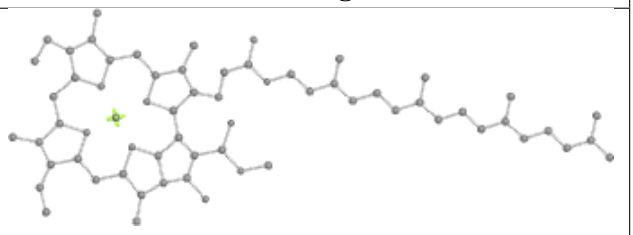
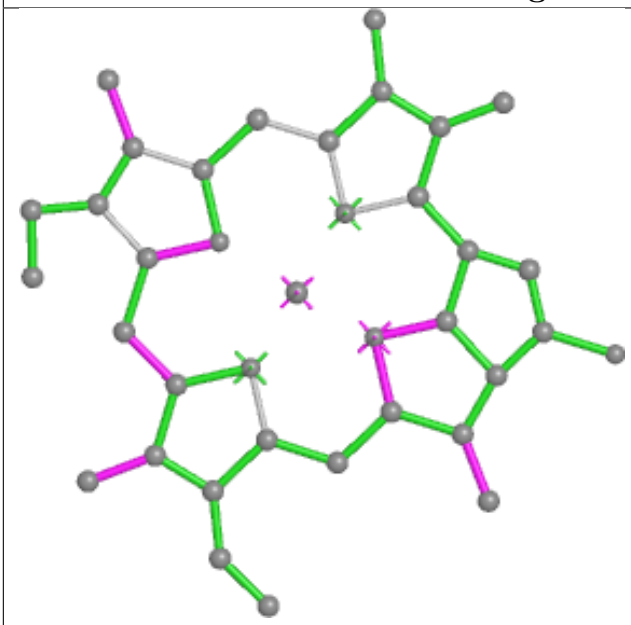


Rings

Ligand CLA 7 311



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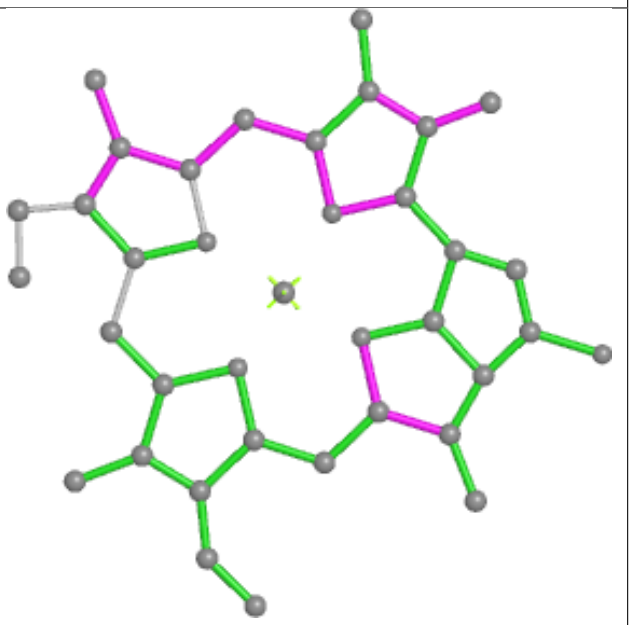

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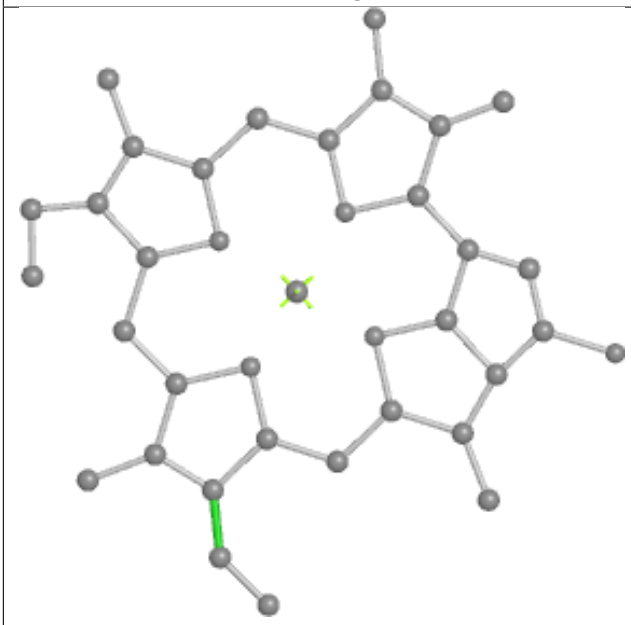

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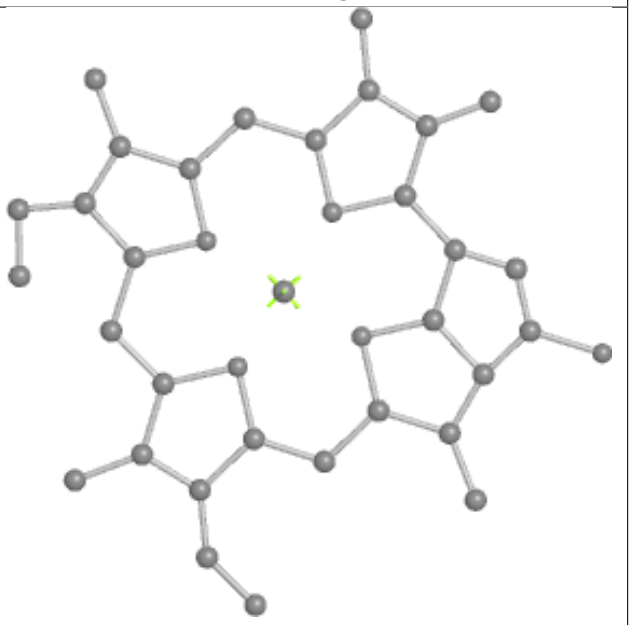
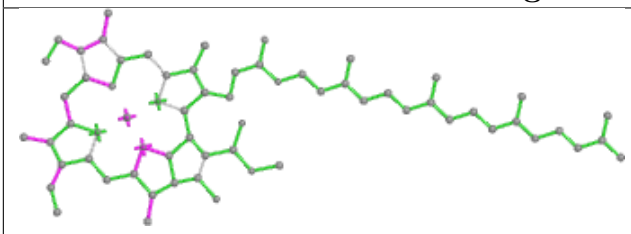


Rings

Ligand CLA A 805



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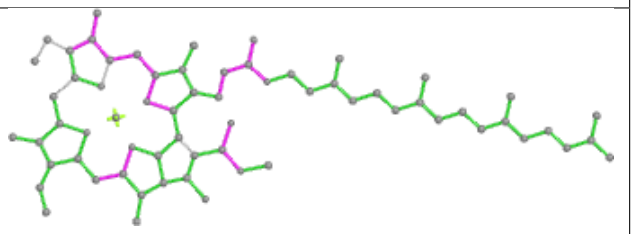
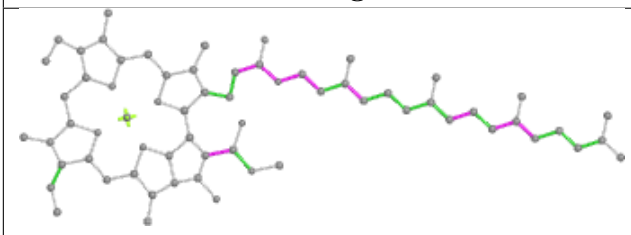


Bond angles



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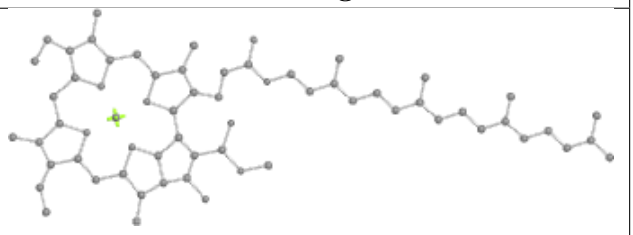
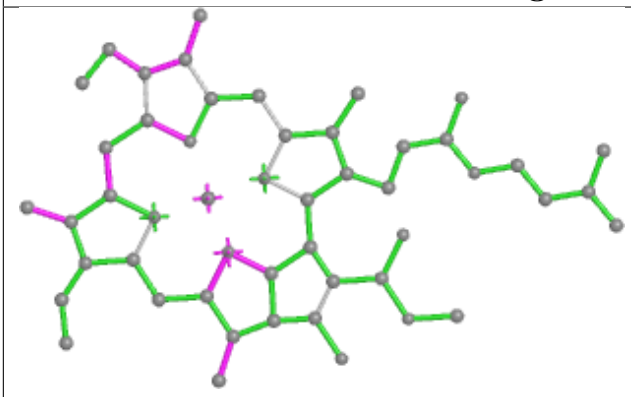


Rings

Ligand CLA 7 309



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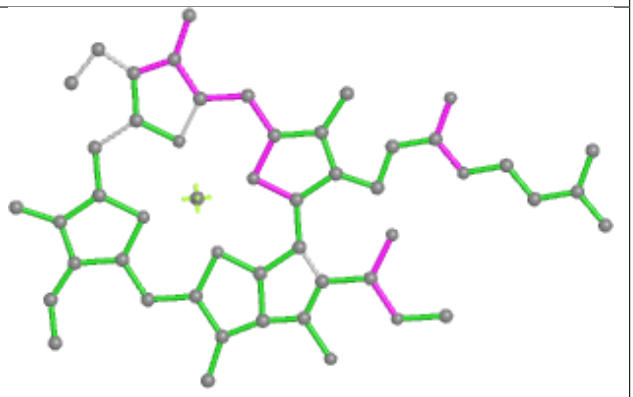
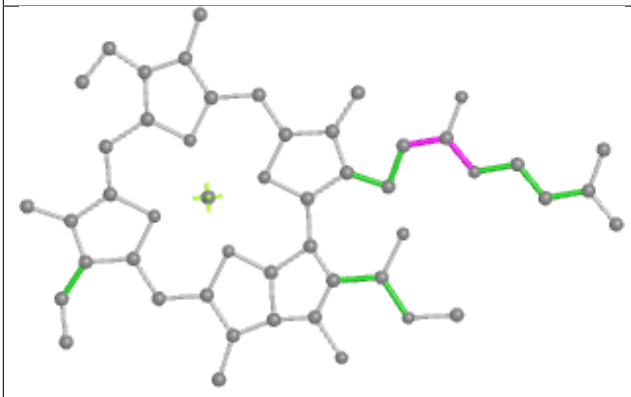


Bond angles



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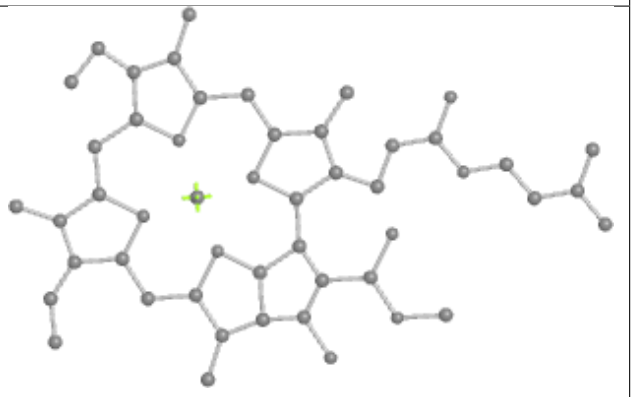
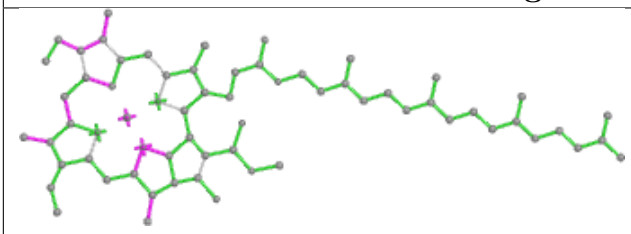


Rings

Ligand CLA B 810



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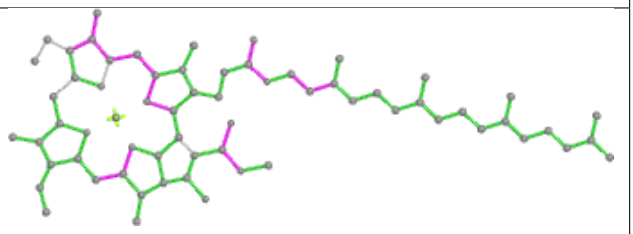
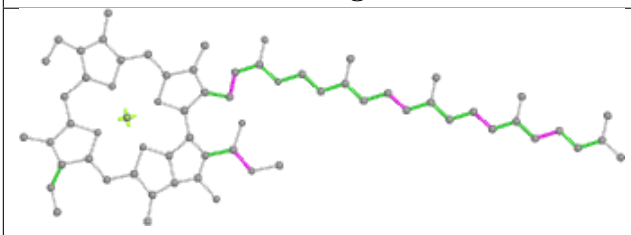


Bond angles



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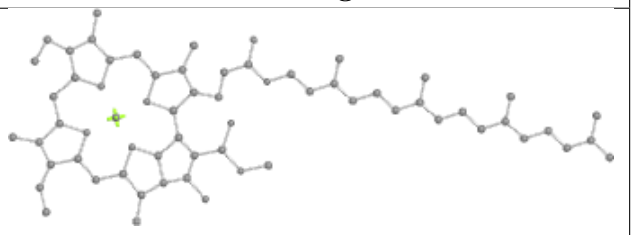
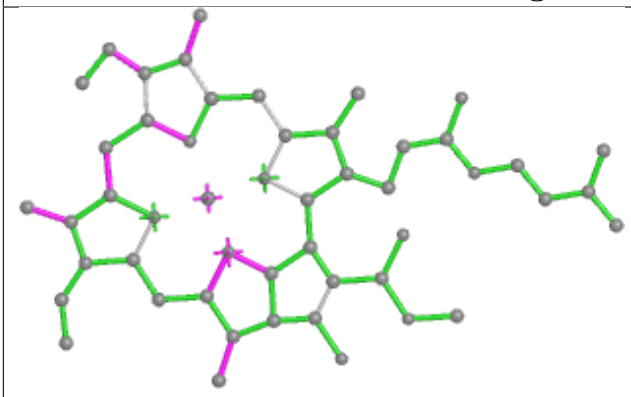


Rings

Ligand CLA 4 304



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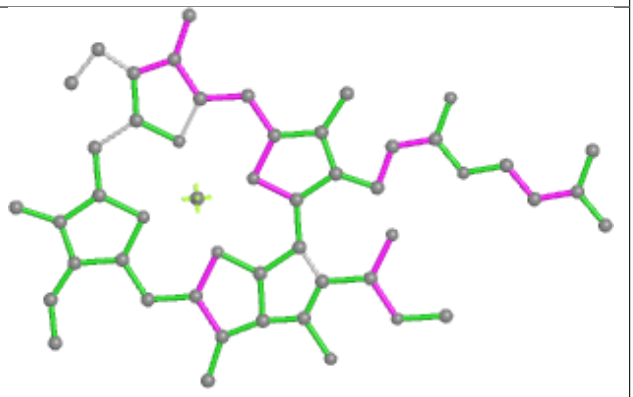
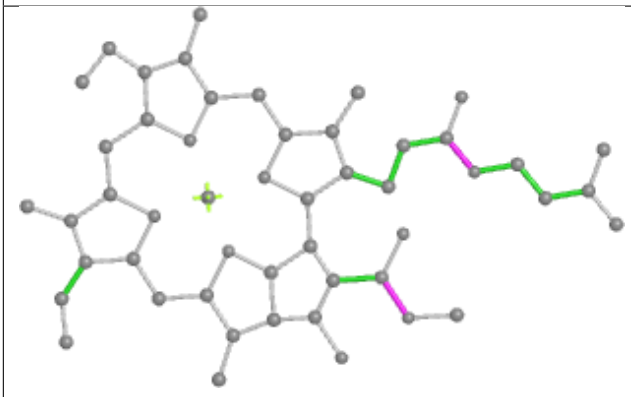


Bond angles



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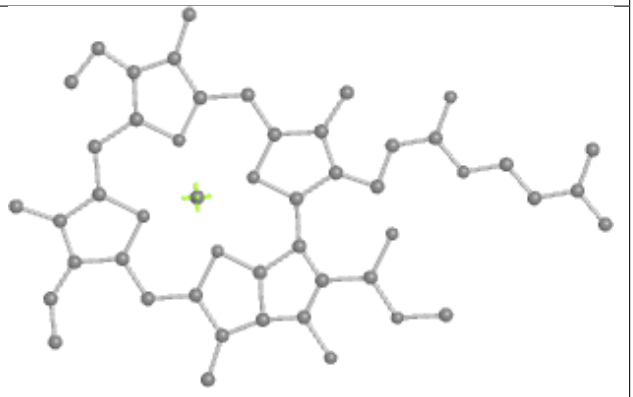
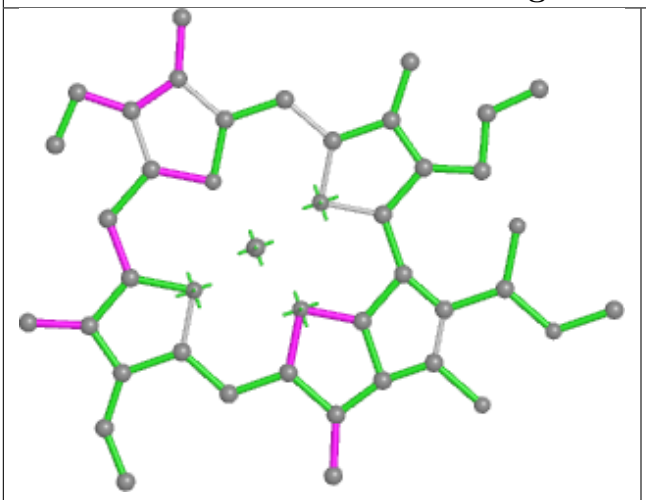


Rings

Ligand CLA 6 314



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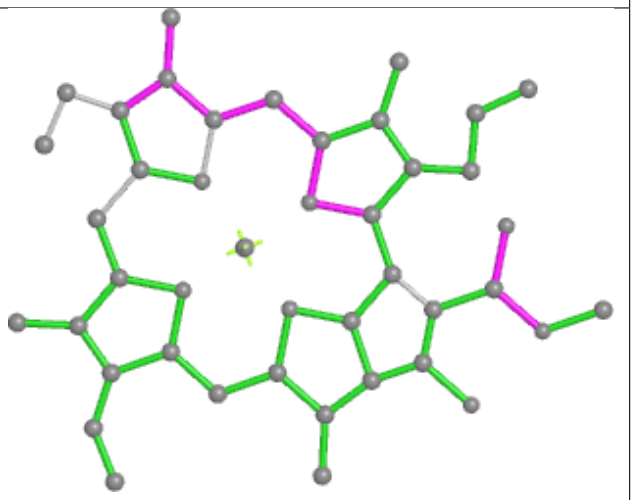

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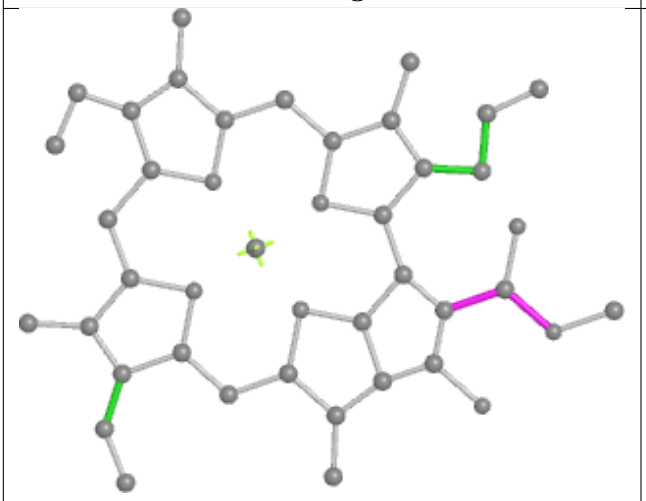

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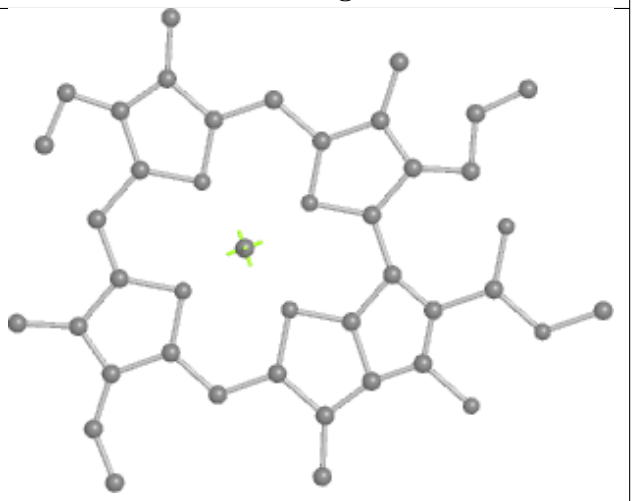
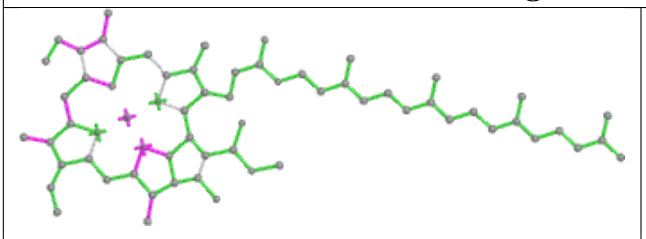


Rings

Ligand CLA B 832



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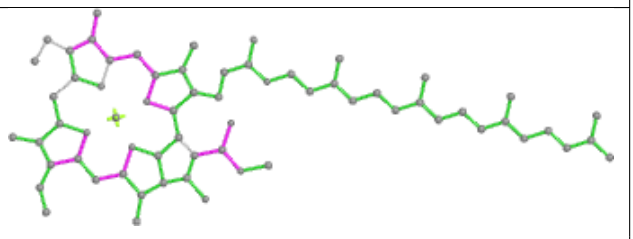
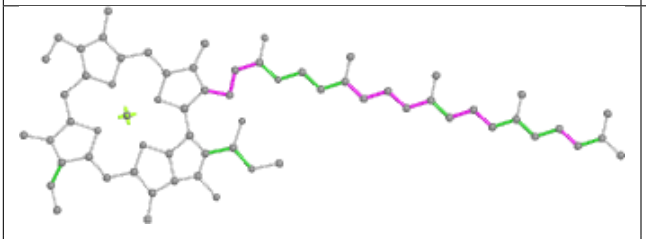


Bond angles



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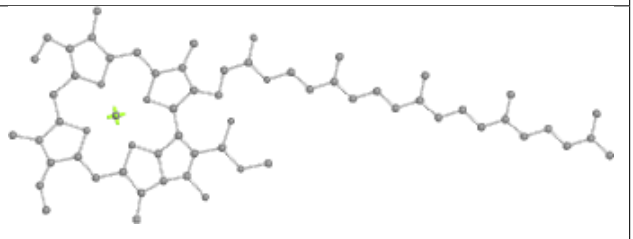
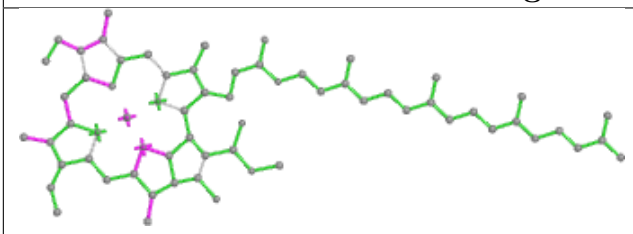


Rings

Ligand CLA A 809



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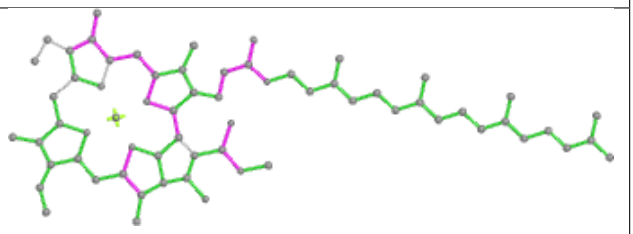
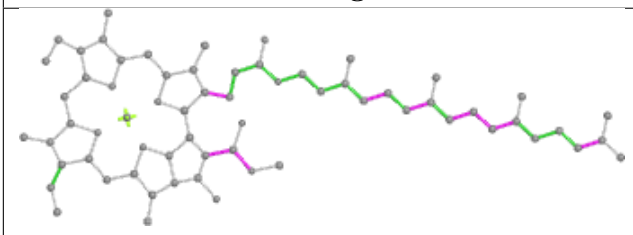


Bond angles



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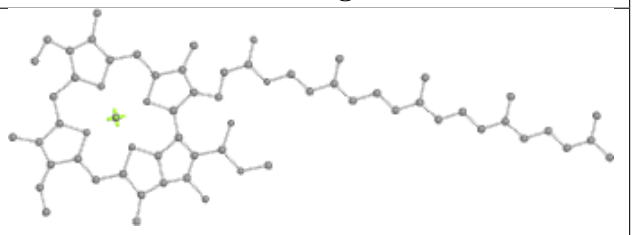
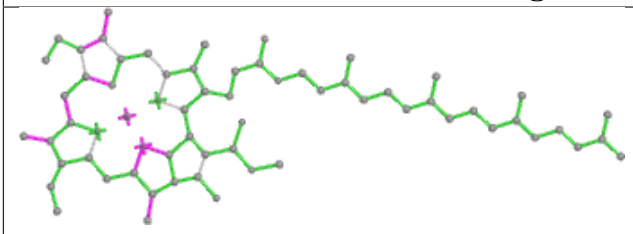


Rings

Ligand CLA 2 303



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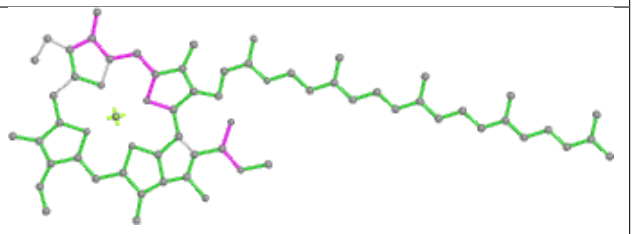
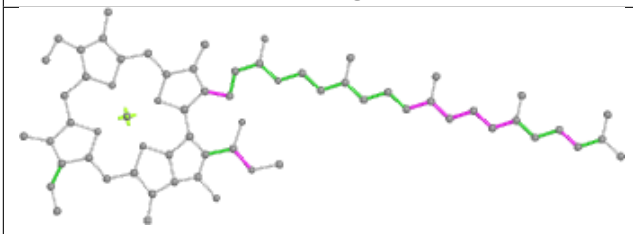
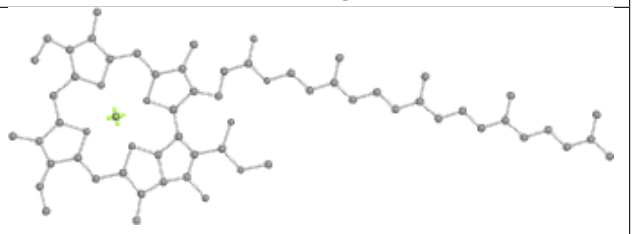


Bond angles

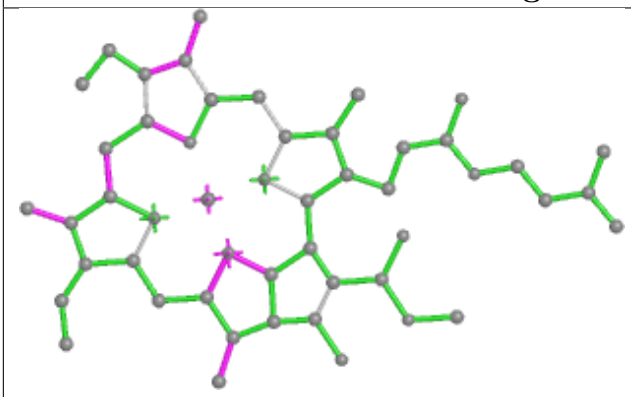


Torsions



Rings

Ligand CLA K 105



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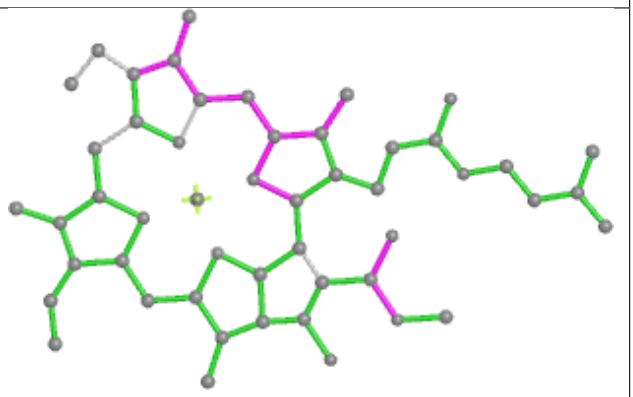
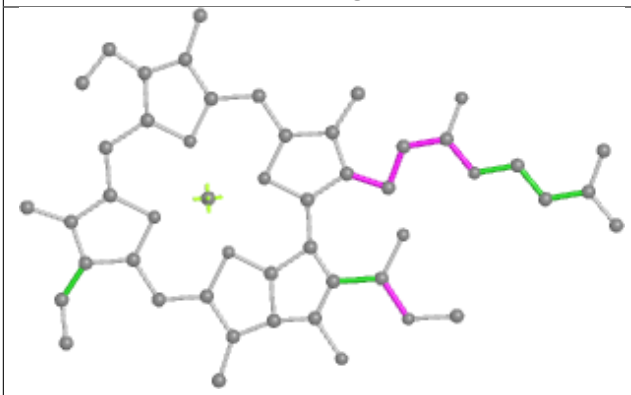


Bond angles



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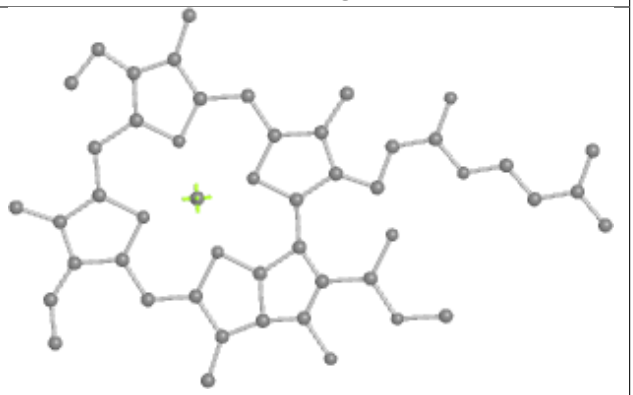
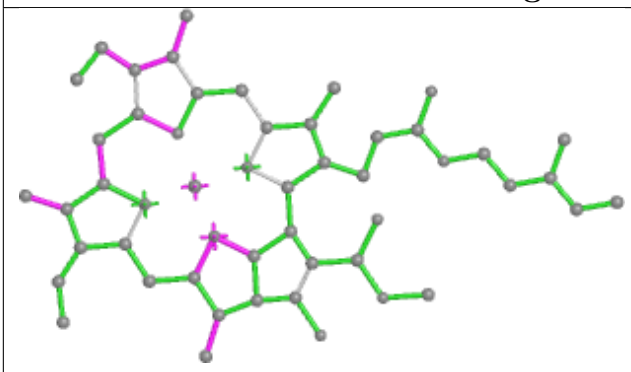


Rings

Ligand CLA A 823



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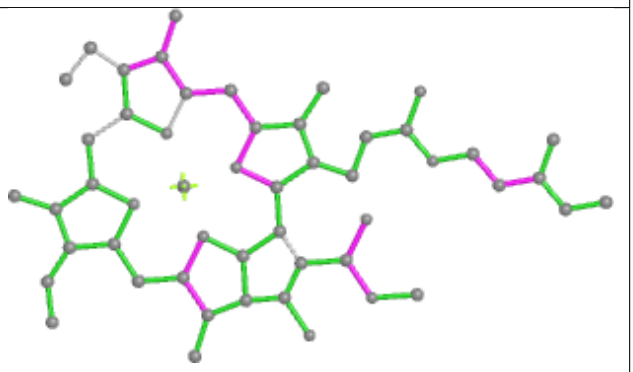

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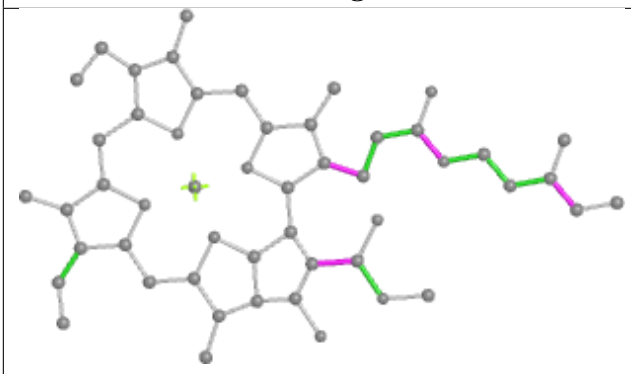

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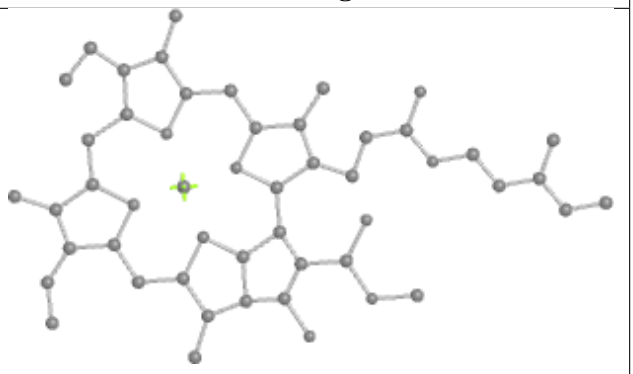
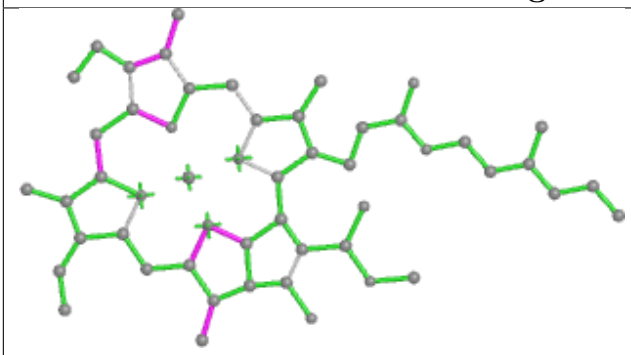


Rings

Ligand CLA 0 304



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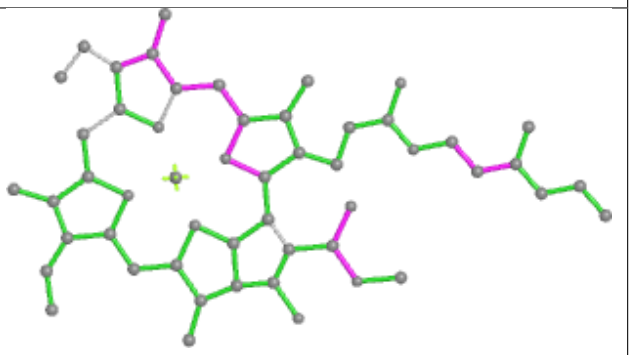

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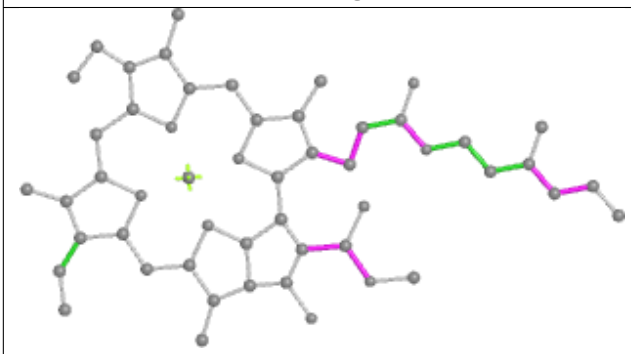

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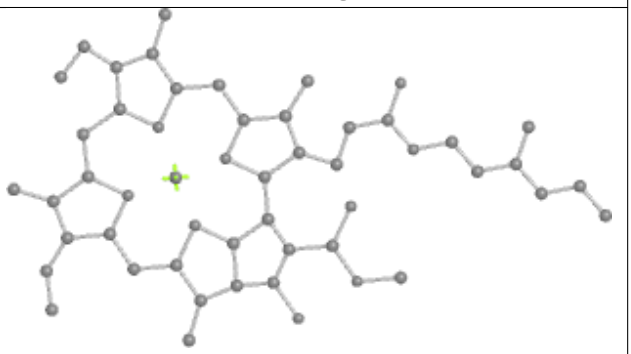
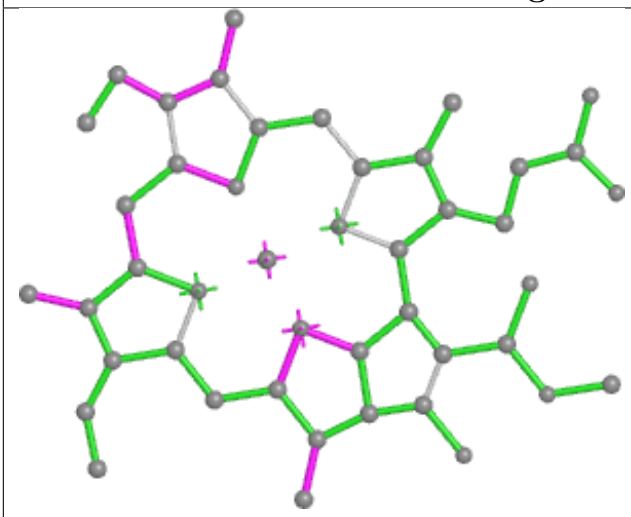


Rings

Ligand CLA 4 313



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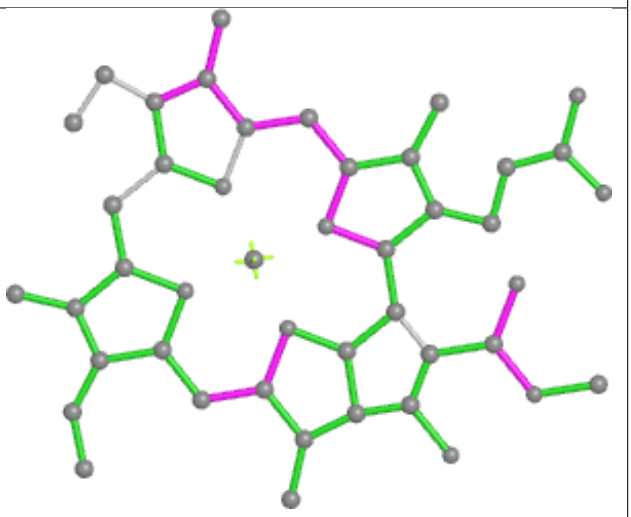
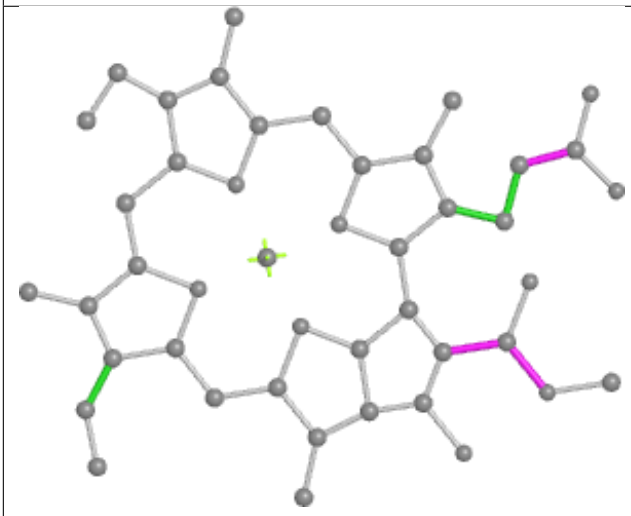


Bond angles



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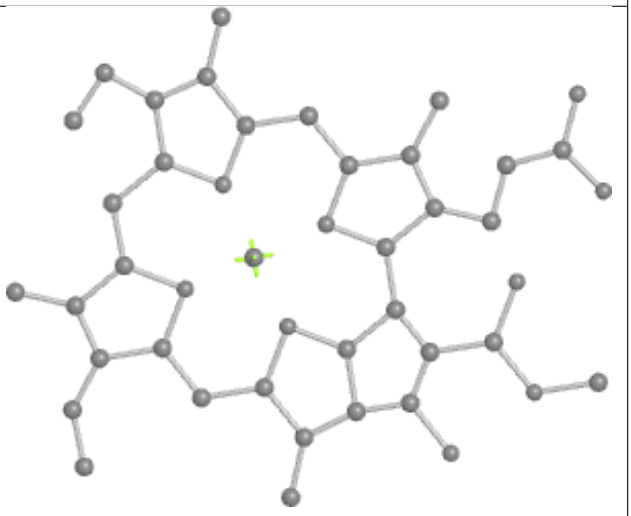
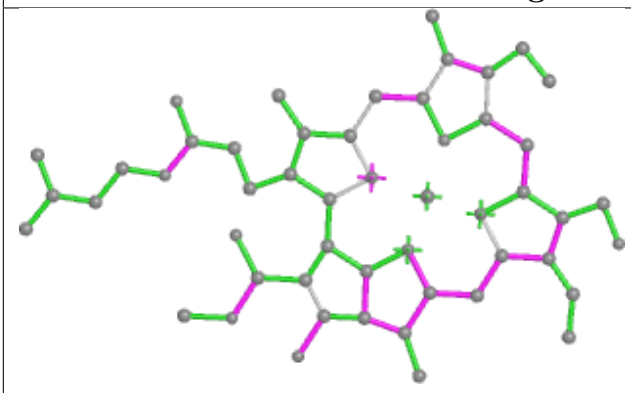


Rings

Ligand CHL 4 306



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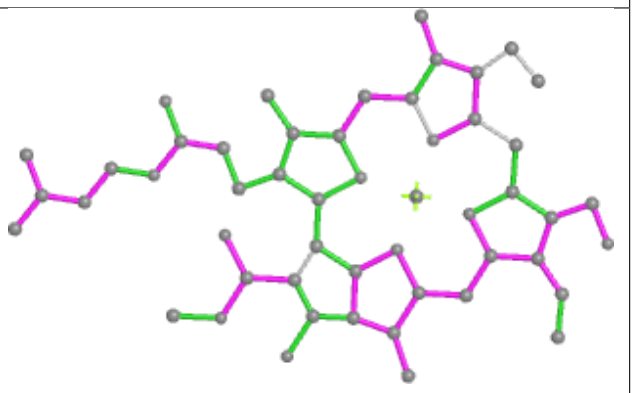

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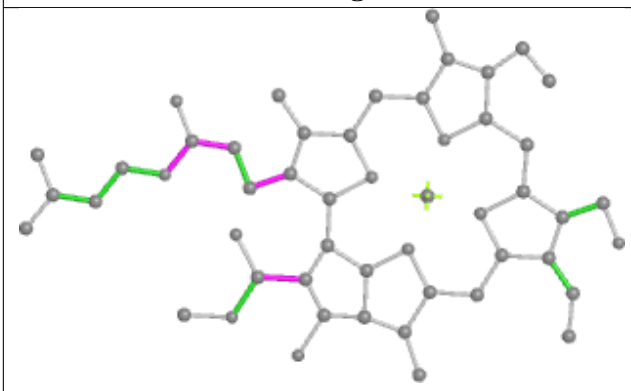

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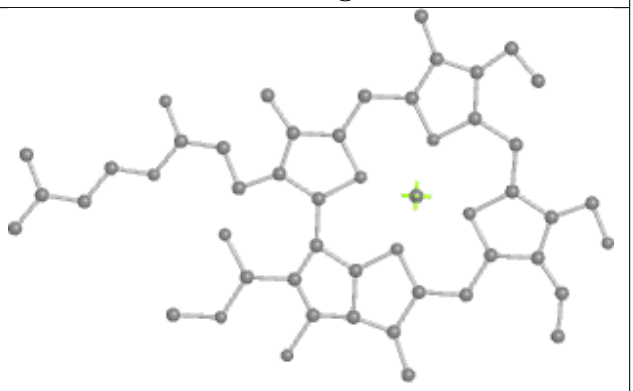
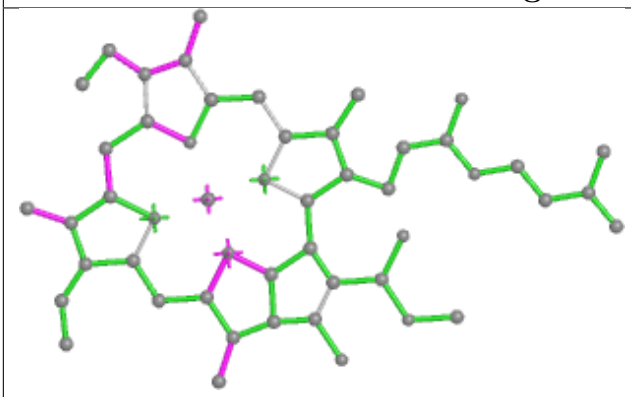


Rings

Ligand CLA A 834



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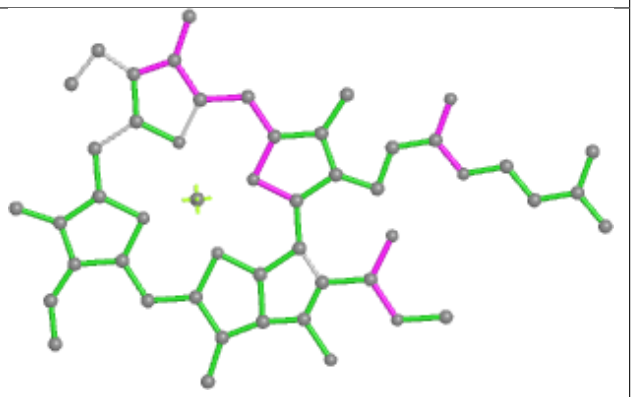

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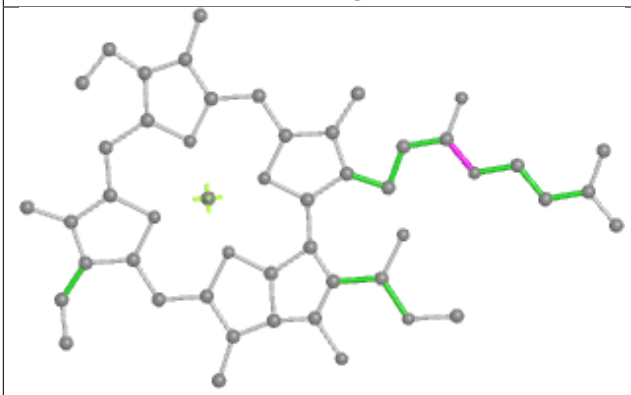

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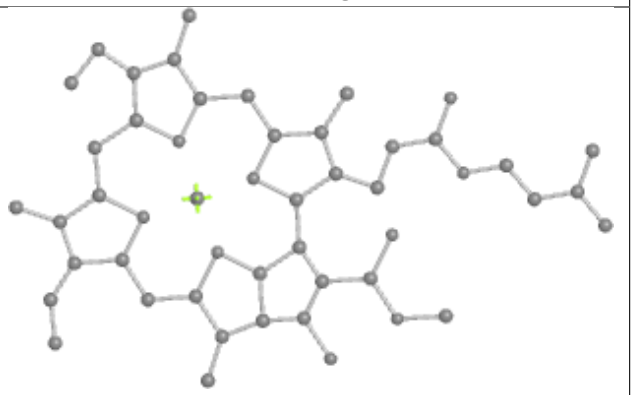
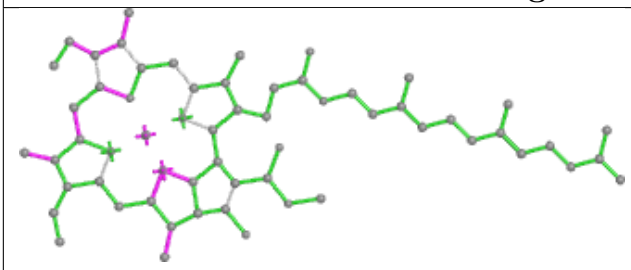


Rings

Ligand CLA 7 303



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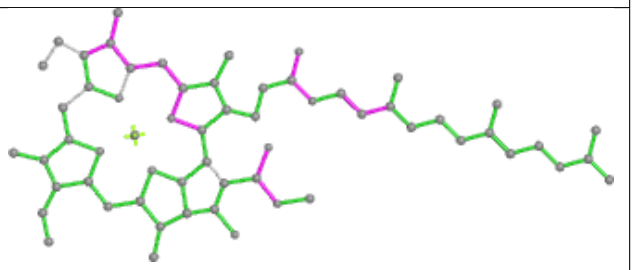
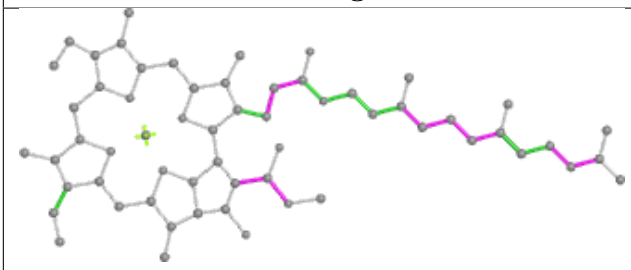


Bond angles



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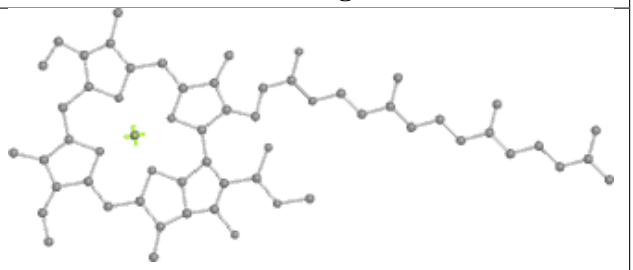
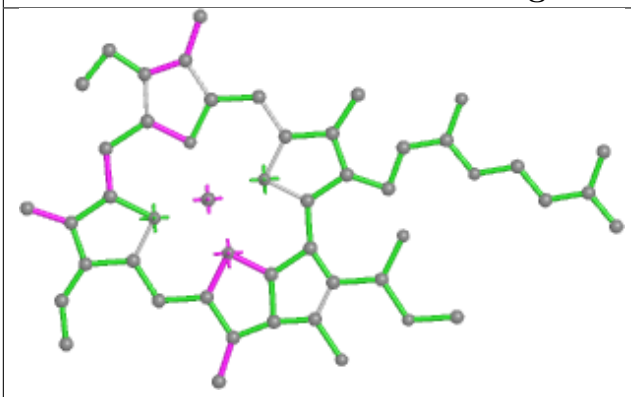
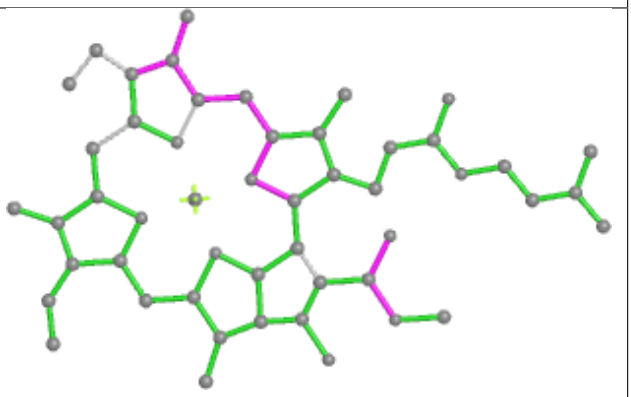
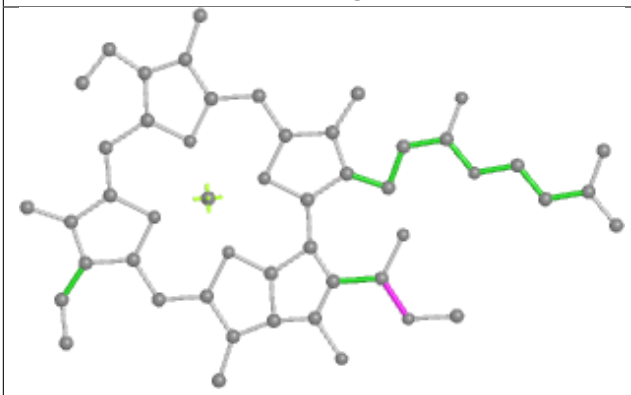
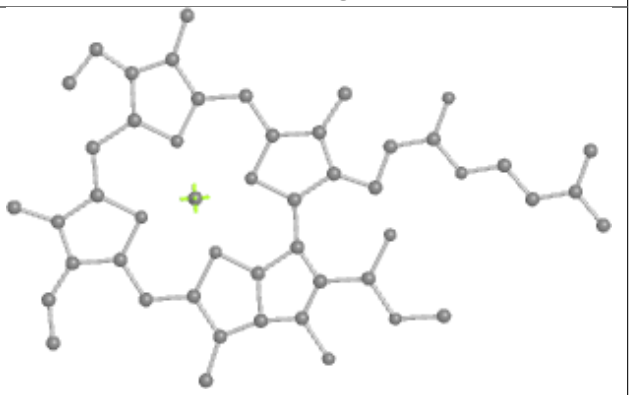


Rings

Ligand CLA 3 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

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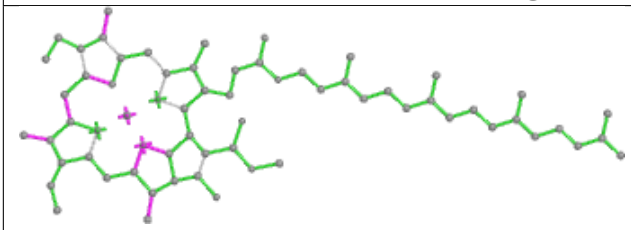
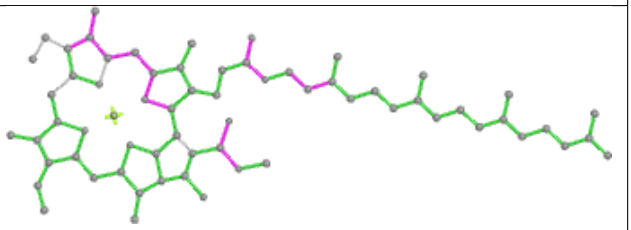
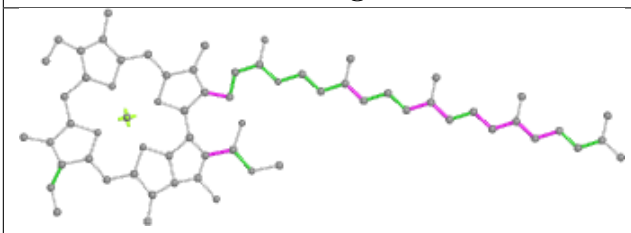
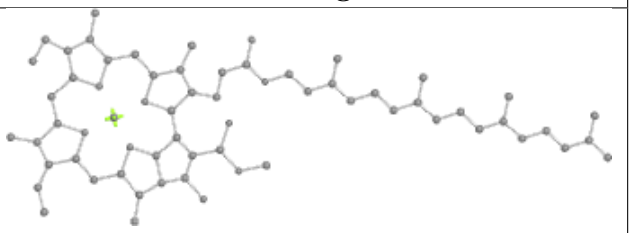
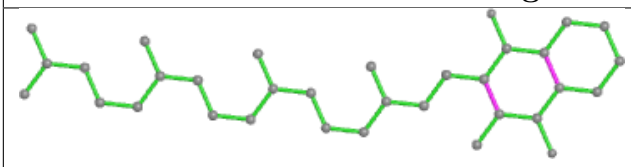
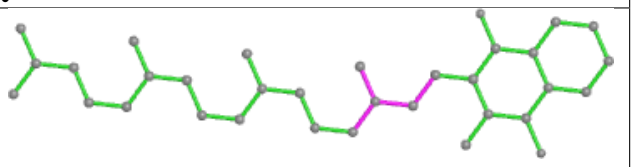
	
Bond lengths	Bond angles
	
Torsions	Rings

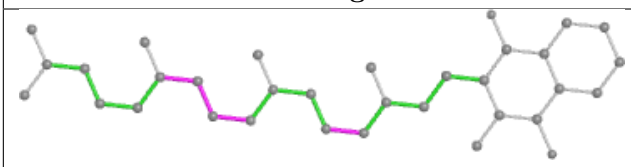
Ligand PQN B 842



Bond lengths



Bond angles



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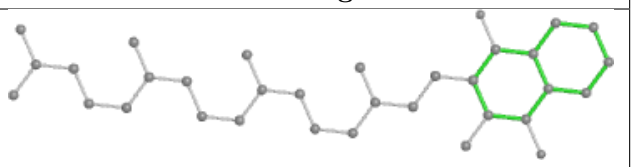
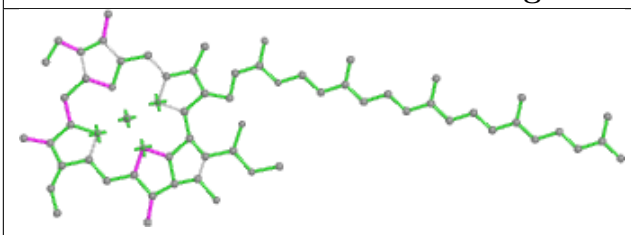


Rings

Ligand CLA A 817



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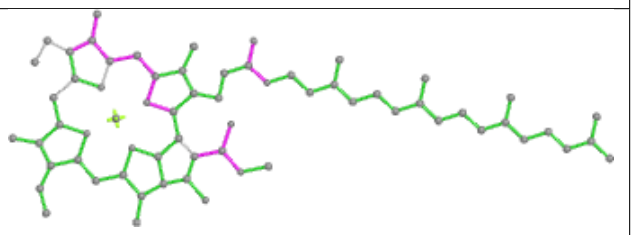
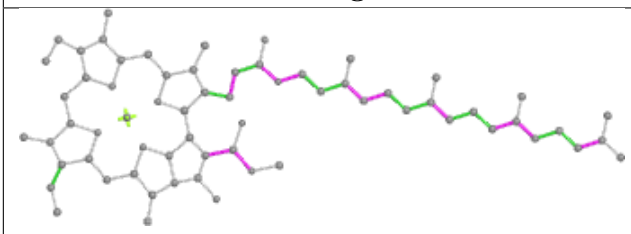


Bond angles



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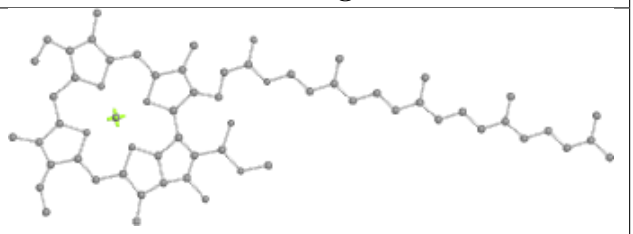
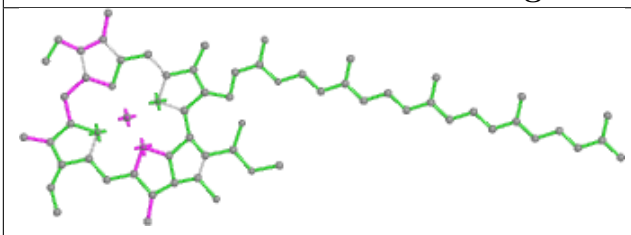
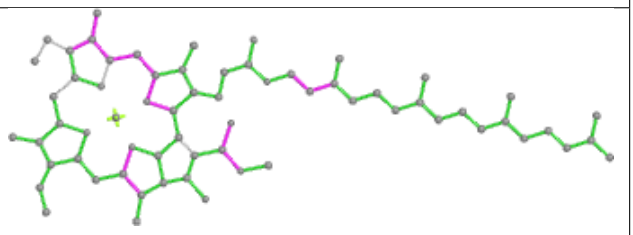


Rings

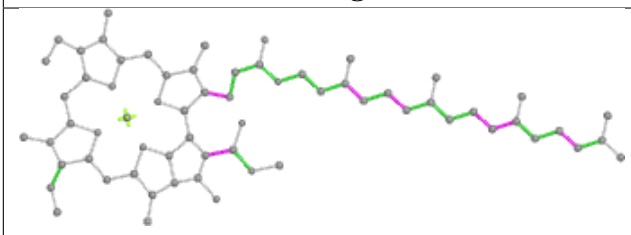
Ligand CLA B 830



Bond lengths



Bond angles



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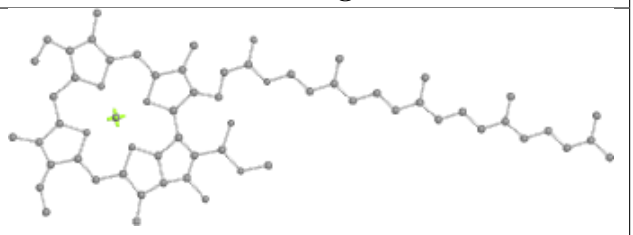
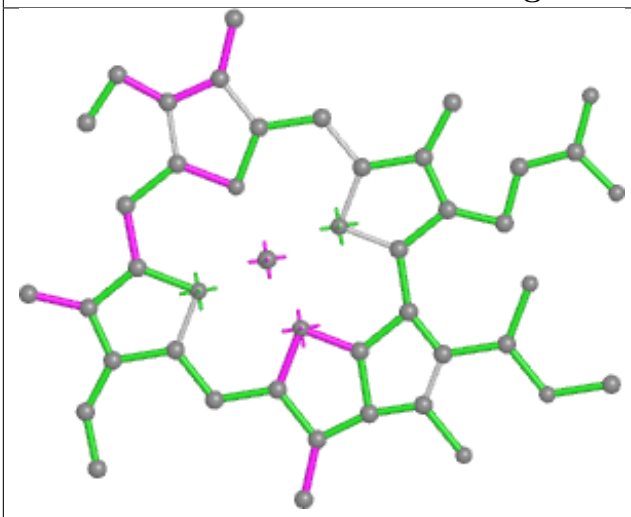
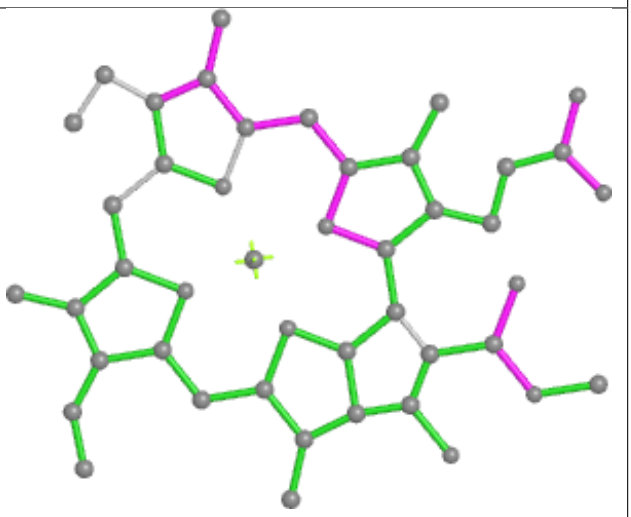


Rings

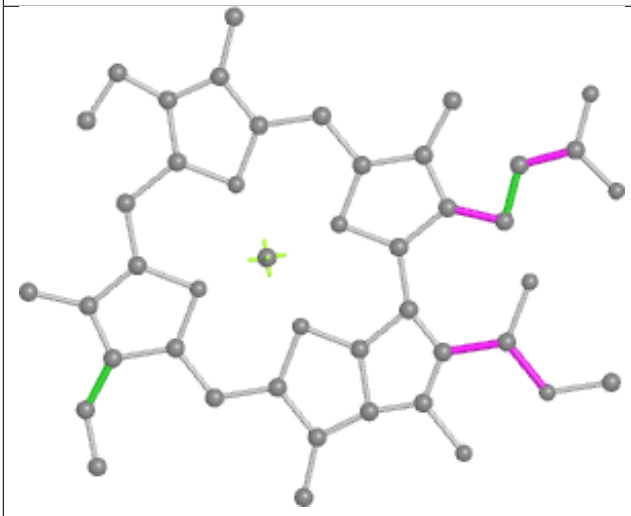
Ligand CLA A 814



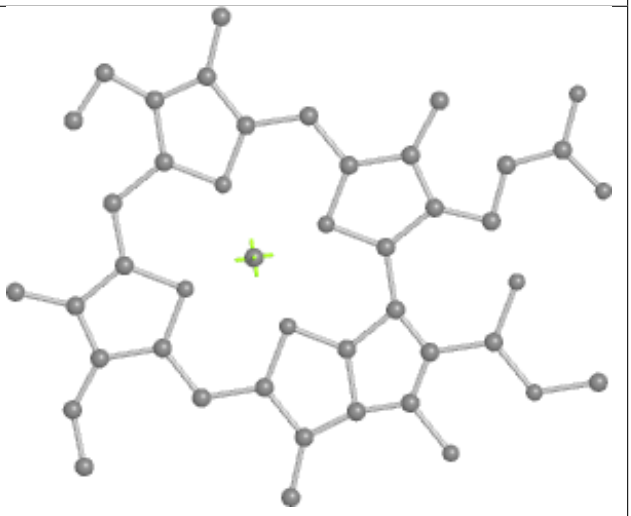
Bond lengths



Bond angles

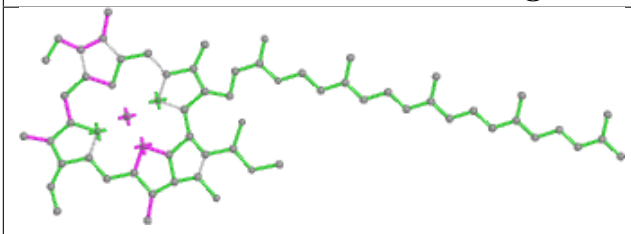


Torsions



Rings

Ligand CLA B 820



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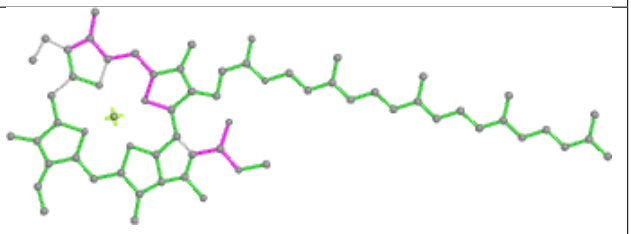
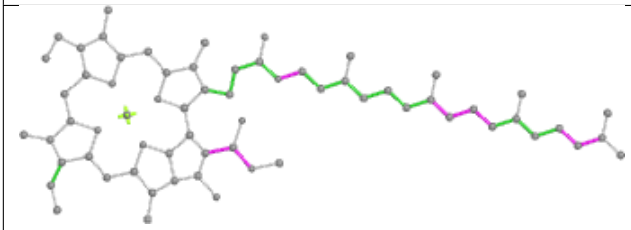


Bond angles



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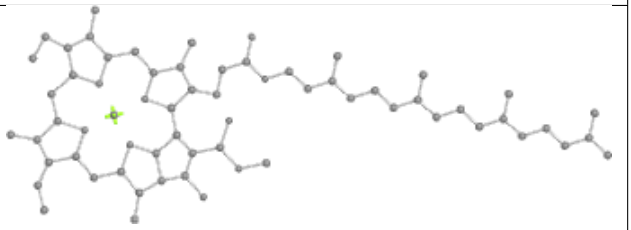
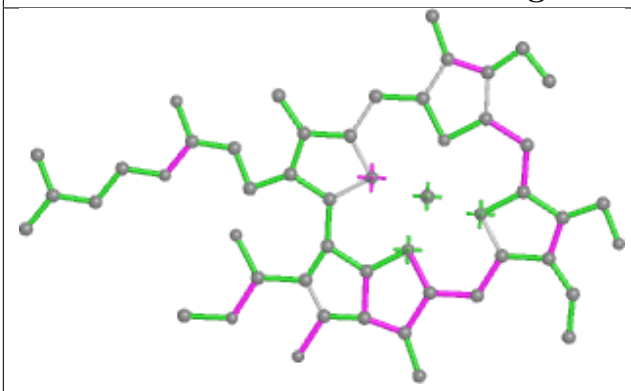


Rings

Ligand CHL 6 308



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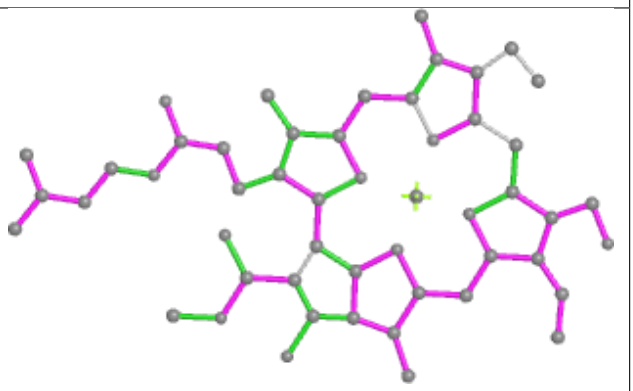
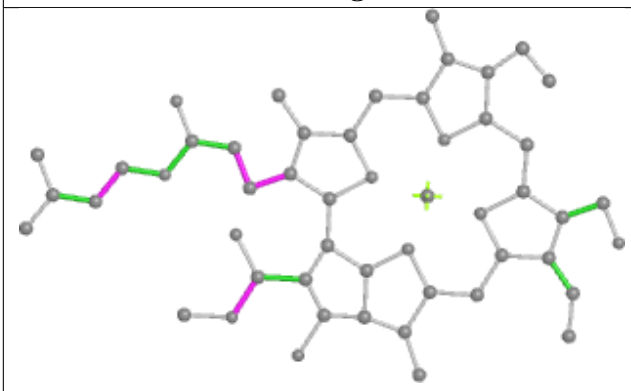


Bond angles



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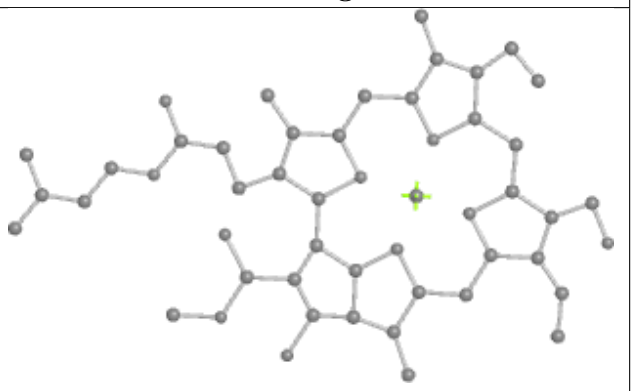
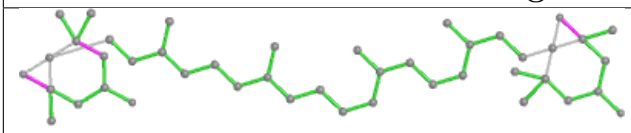


Rings

Ligand XAT 3 314



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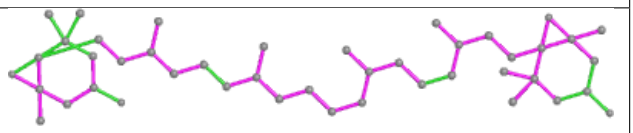

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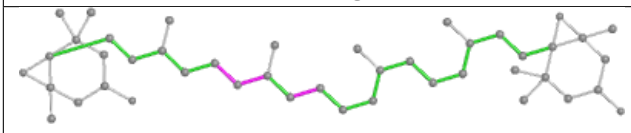

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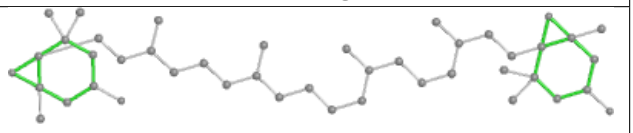
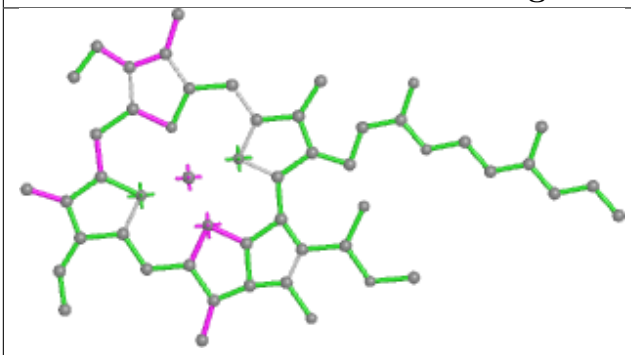


Rings

Ligand CLA 2 311



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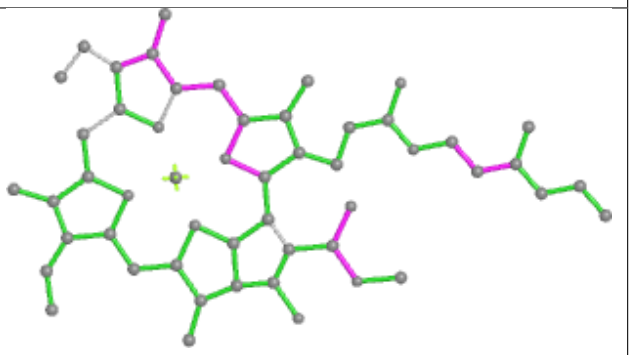
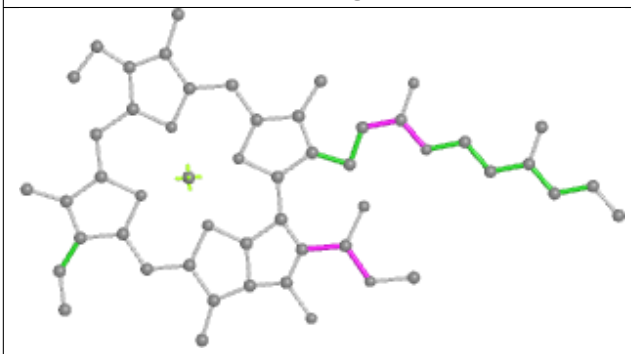


Bond angles



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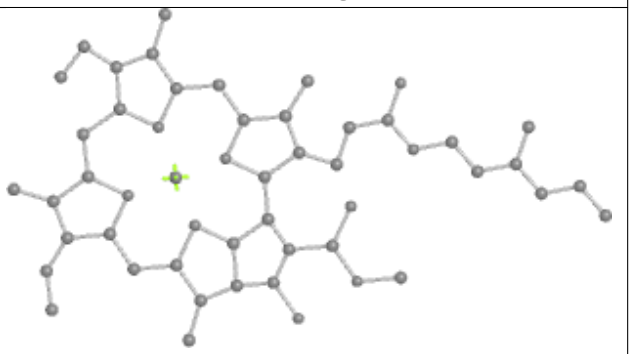

Rings

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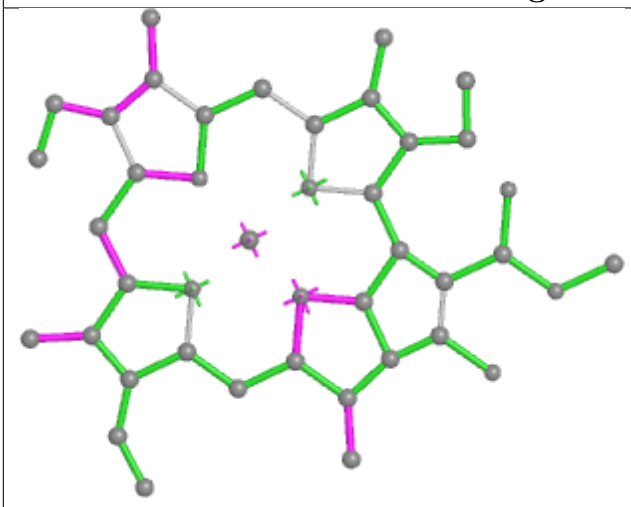

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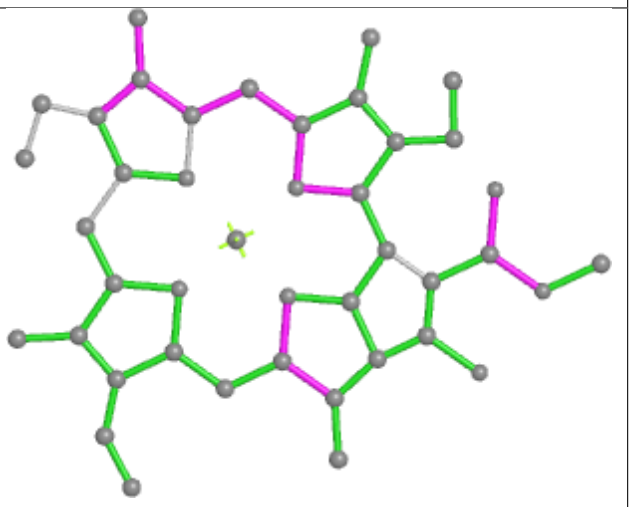
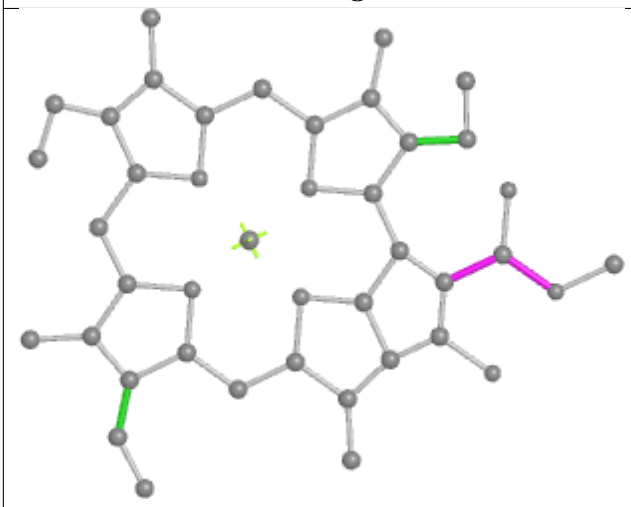


Bond angles



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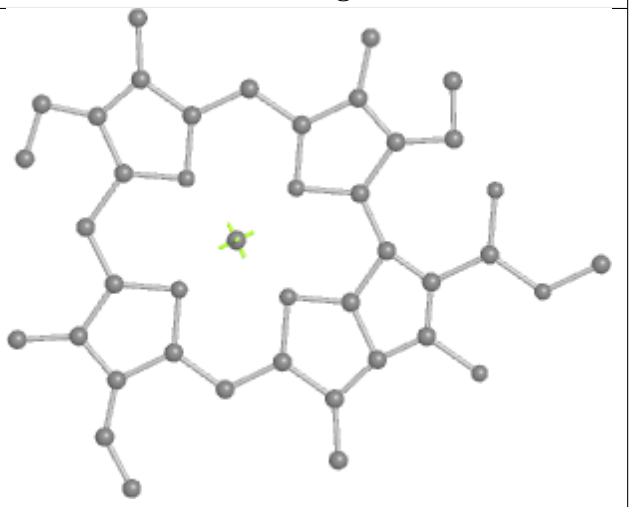
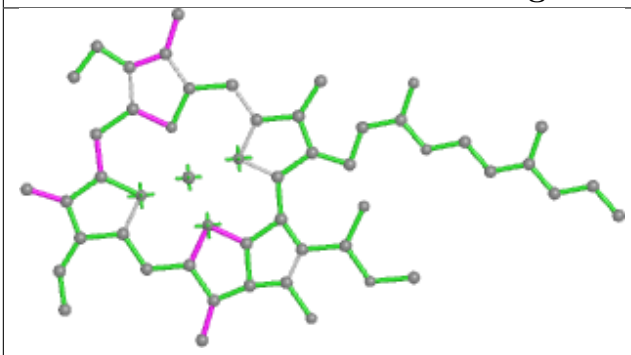
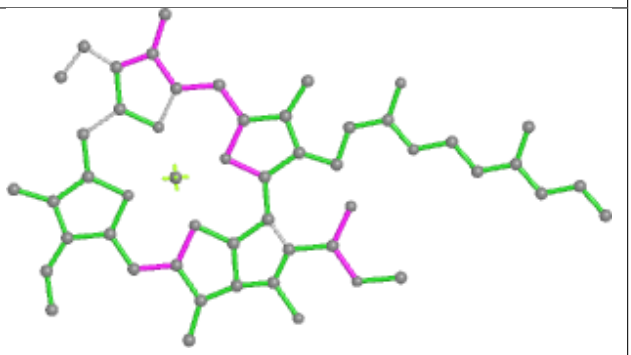
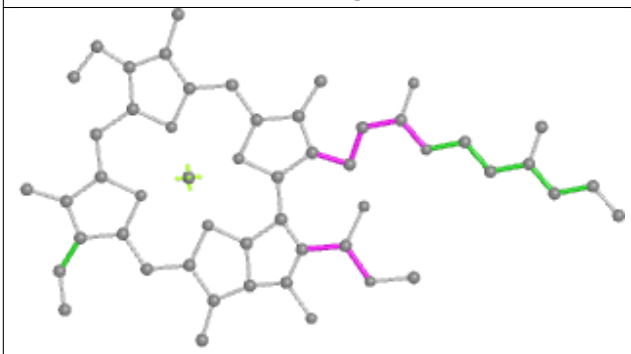
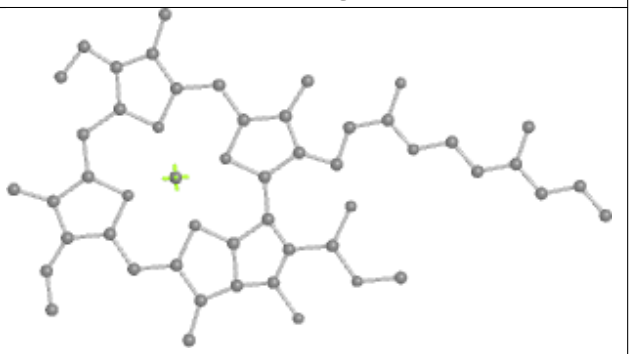
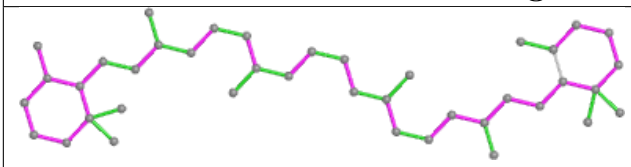
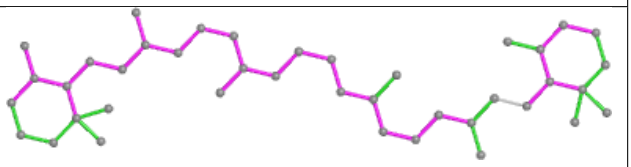
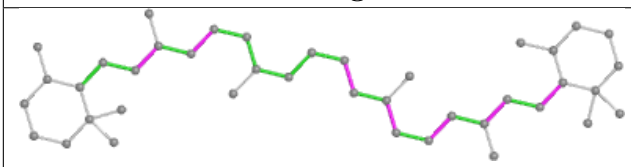
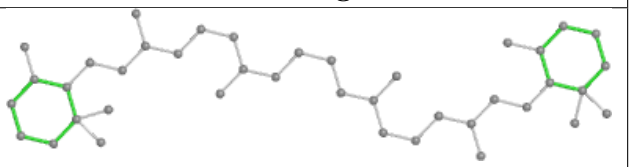
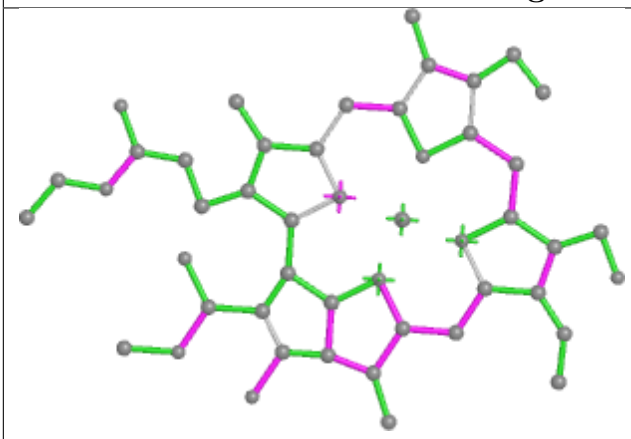


Rings

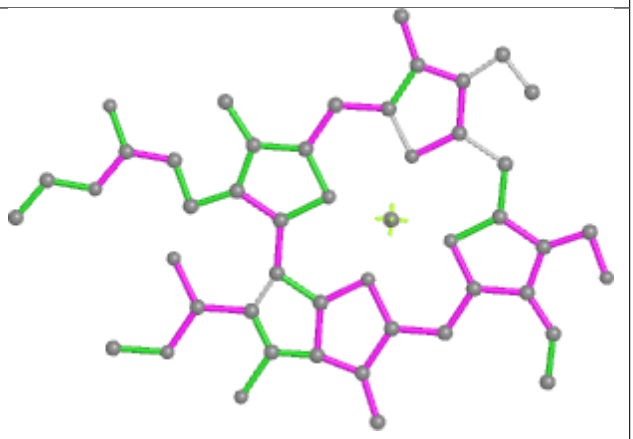
Ligand CLA 5 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT B 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

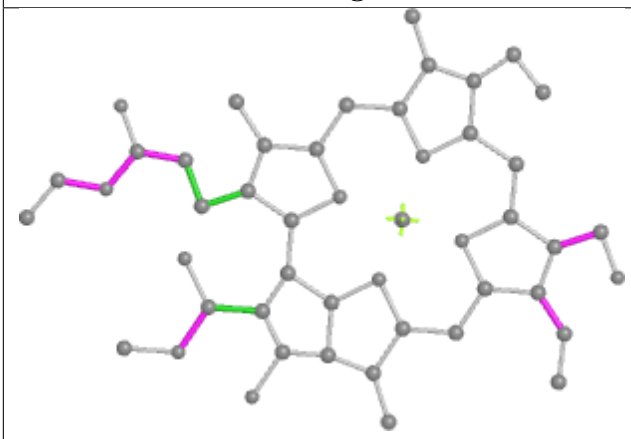
Ligand CHL 9 307



Bond lengths



Bond angles



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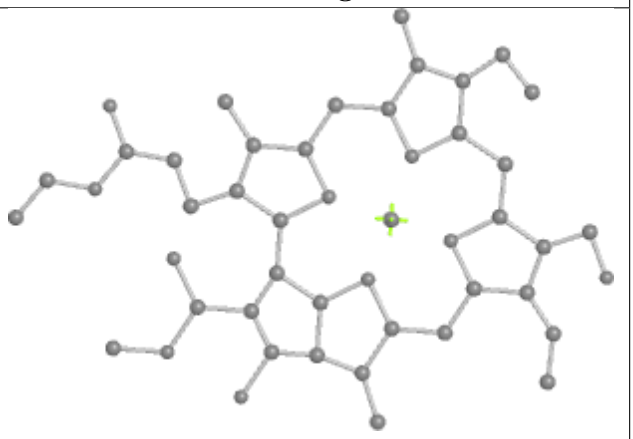
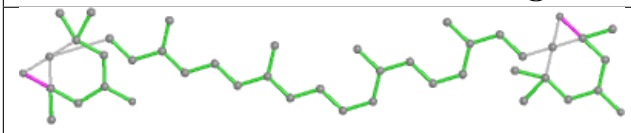


Rings

Ligand XAT 1 315



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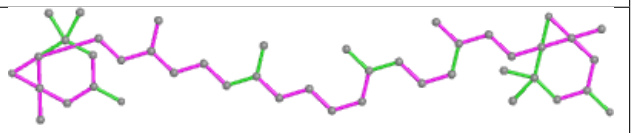

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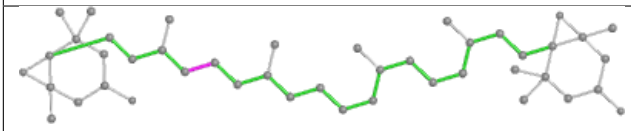

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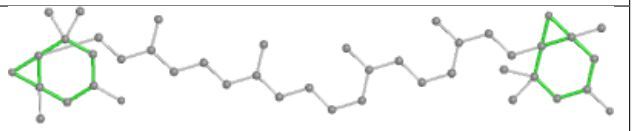
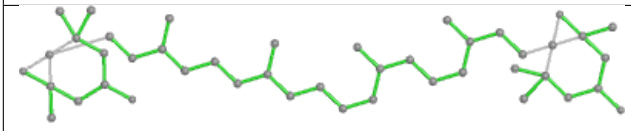


Rings

Ligand XAT 0 314



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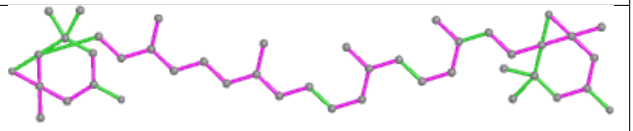
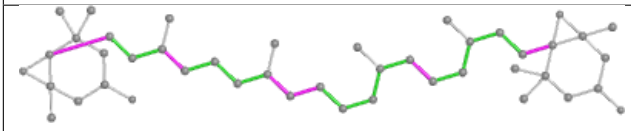


Bond angles



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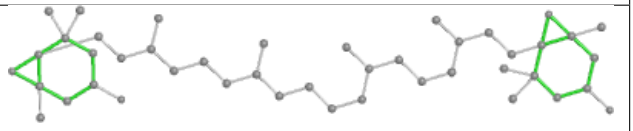
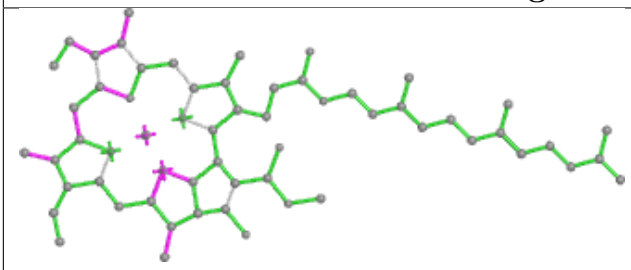
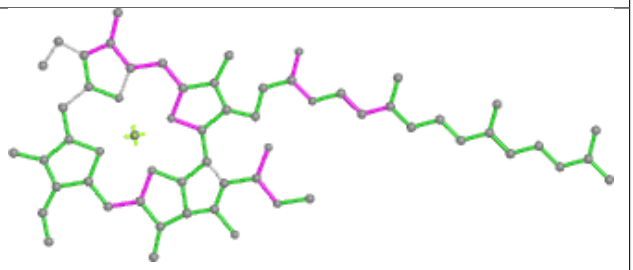


Rings

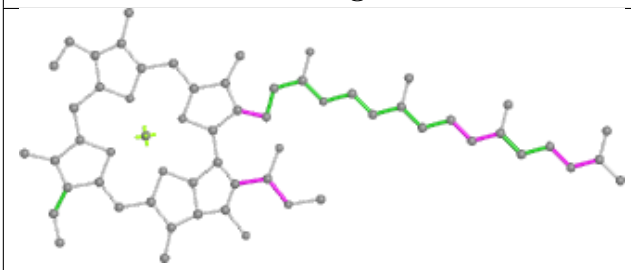
Ligand CLA 8 309



Bond lengths



Bond angles



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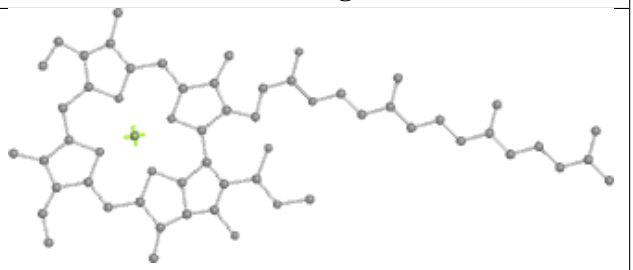
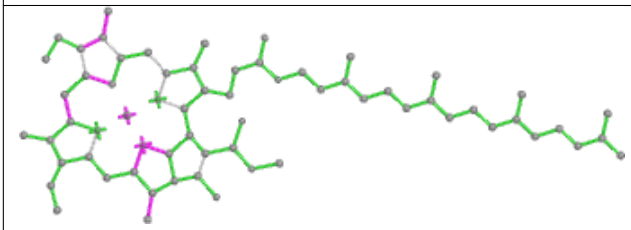
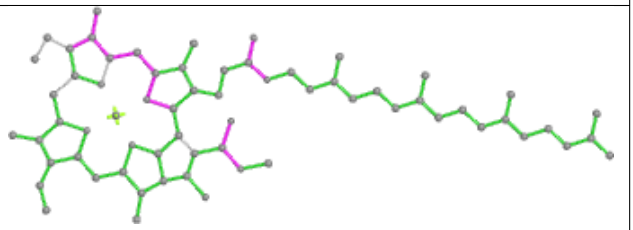


Rings

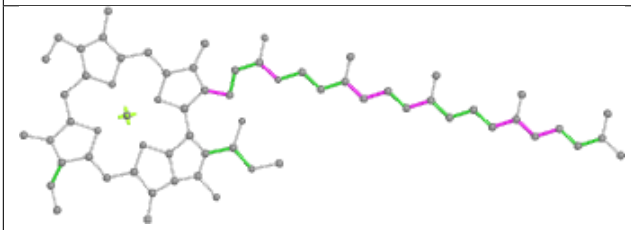
Ligand CLA B 839



Bond lengths



Bond angles



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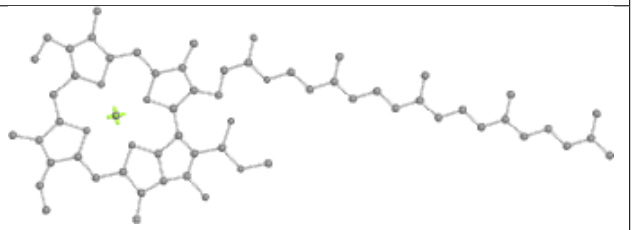
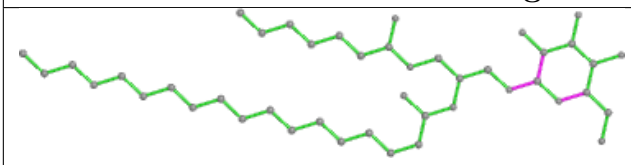
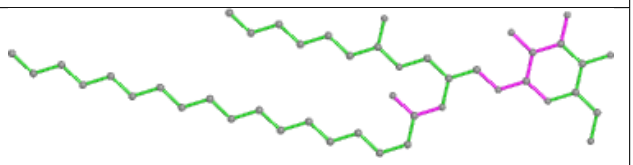


Rings

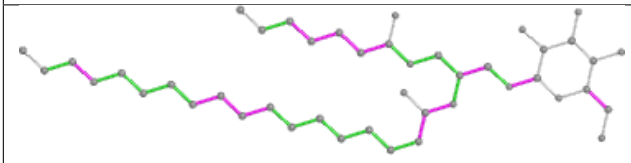
Ligand LMG 5 319



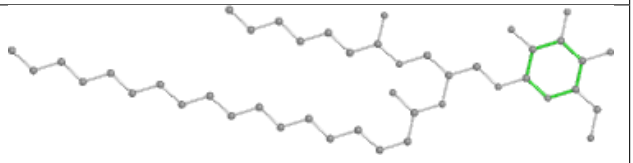
Bond lengths



Bond angles

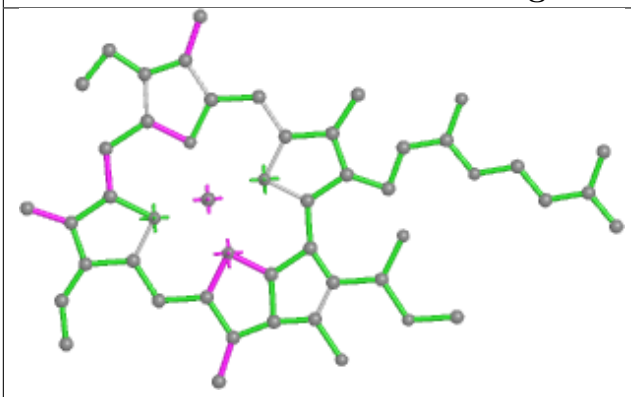


Torsions

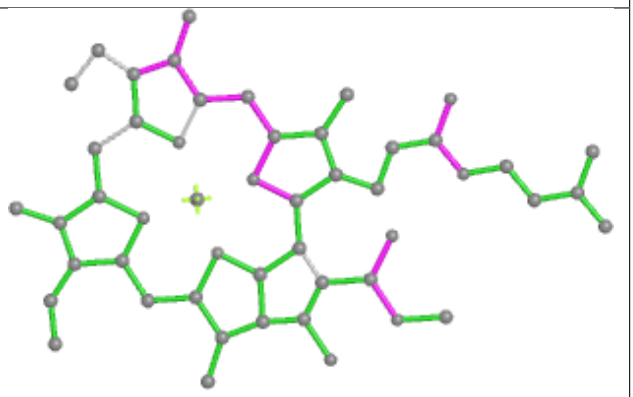


Rings

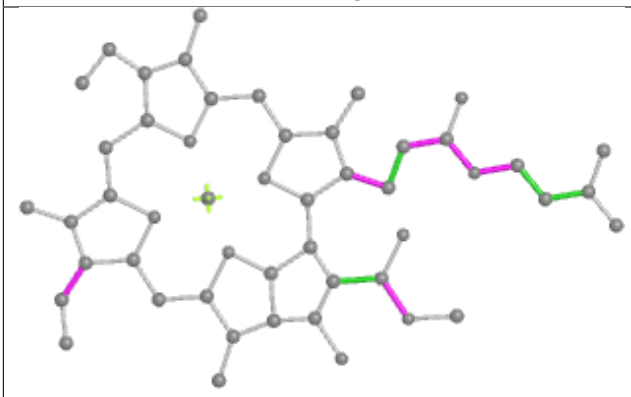
Ligand CLA 6 309



Bond lengths



Bond angles



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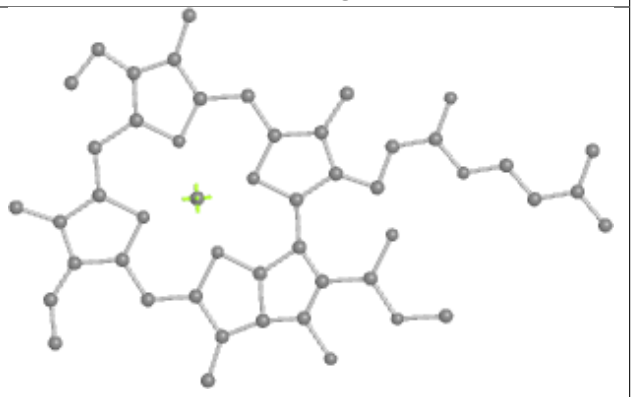
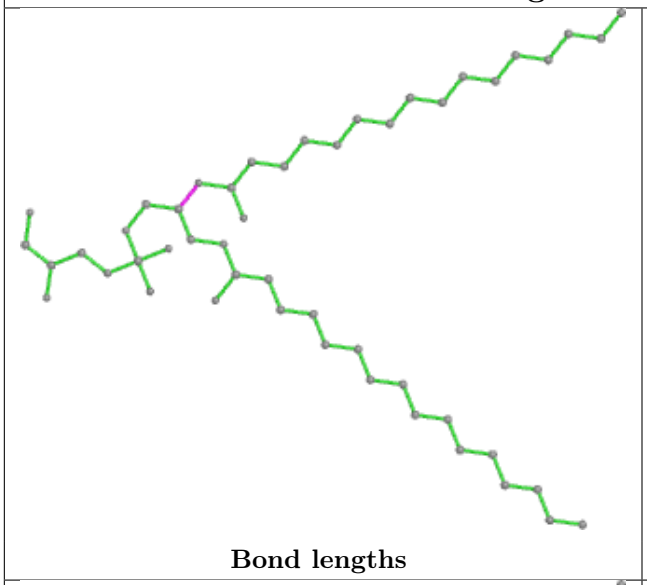


Rings

Ligand LHG 9 316



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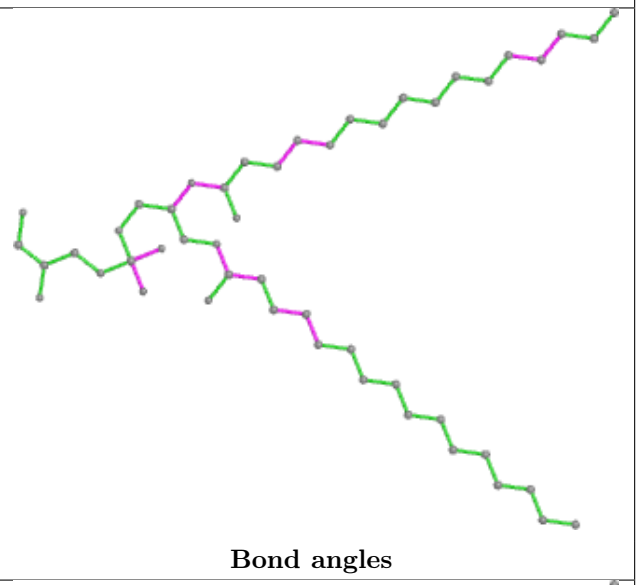
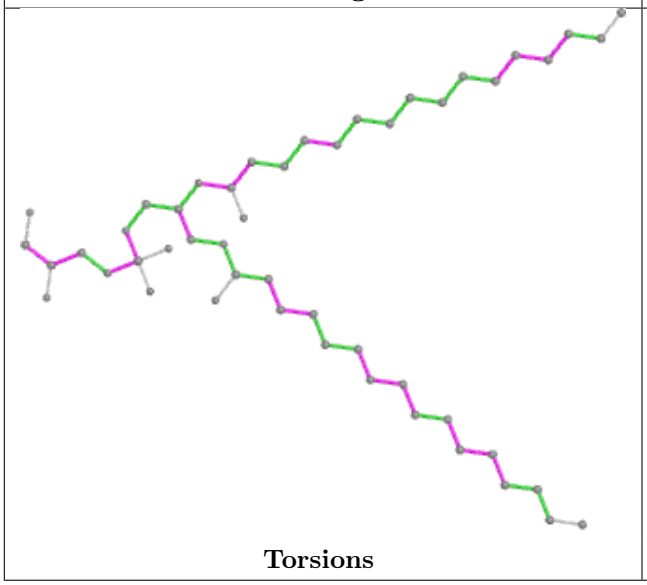


Bond angles



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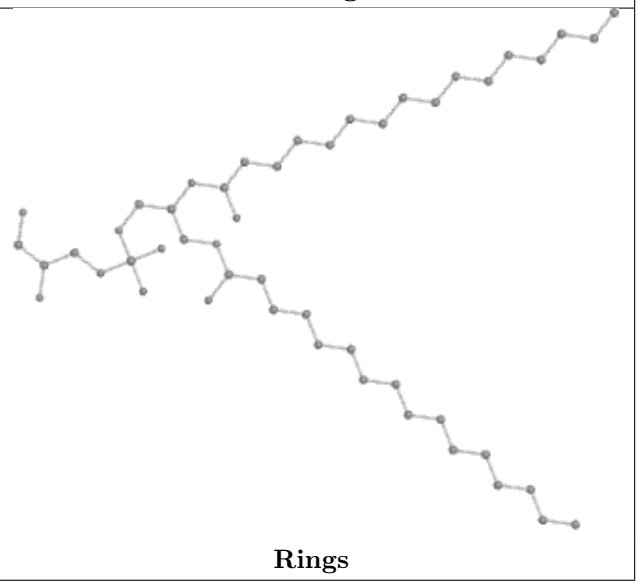
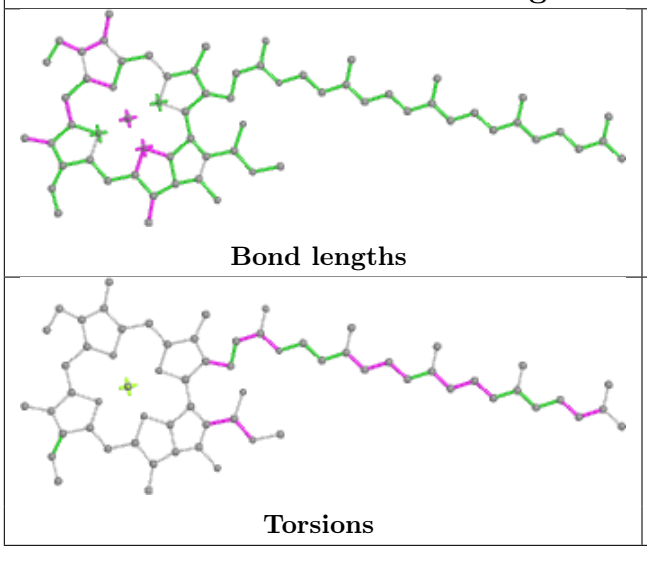


Rings

Ligand CLA 6 311



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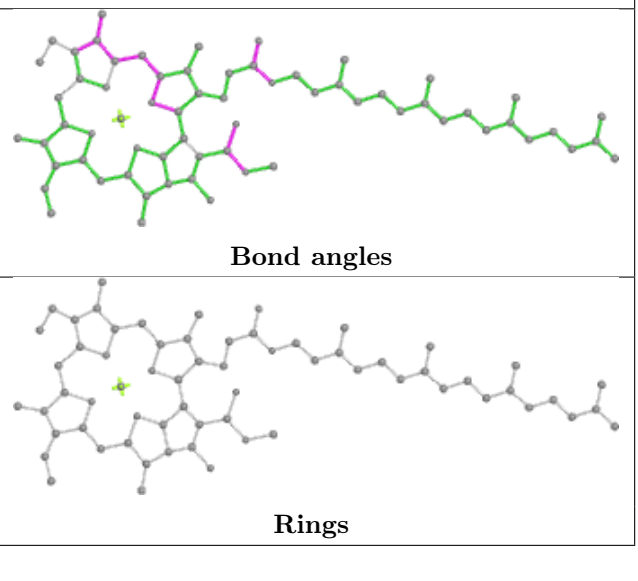
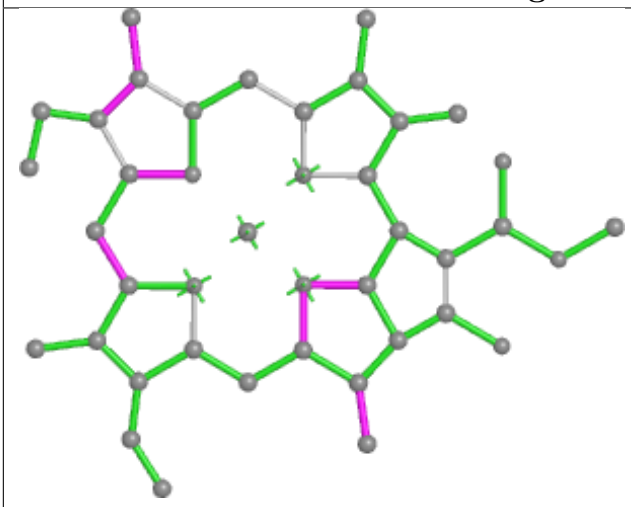


Bond angles

Torsions

Rings

Ligand CLA 0 309



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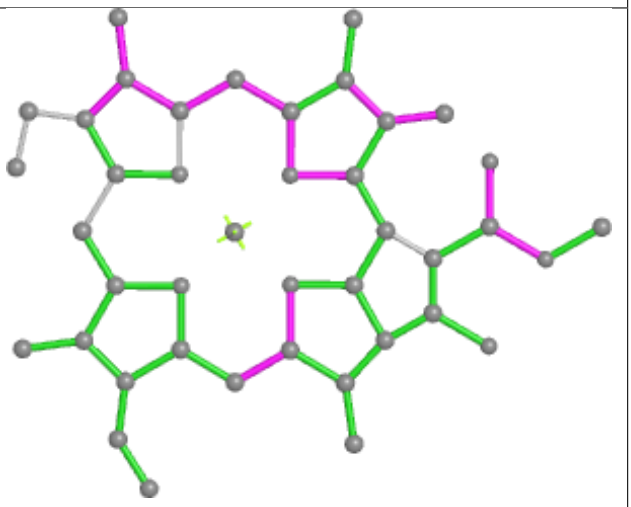
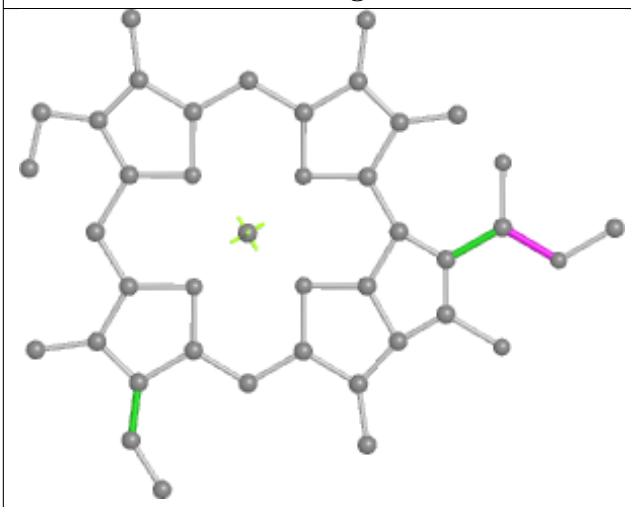


Bond angles



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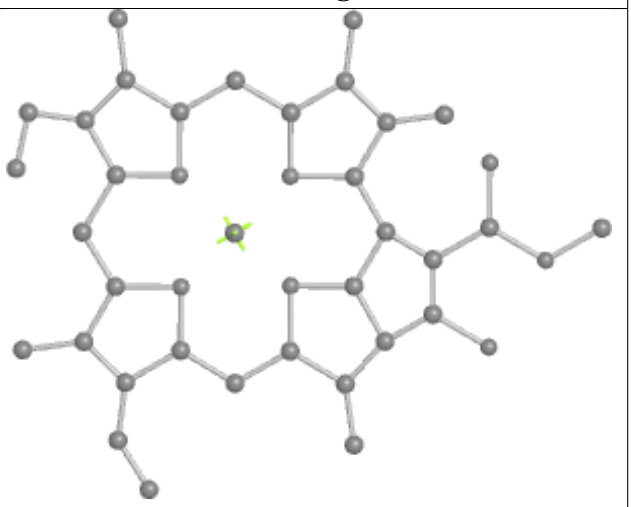
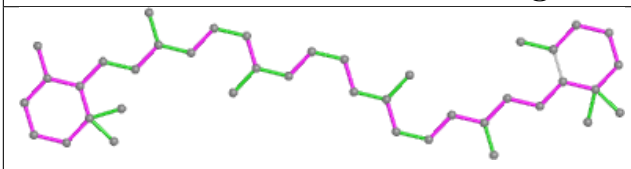


Rings

Ligand 8CT 2 317



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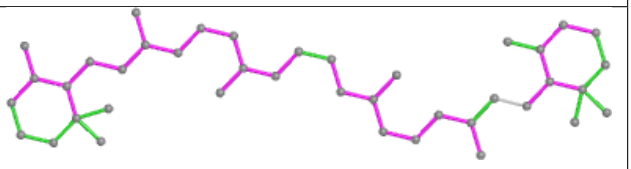
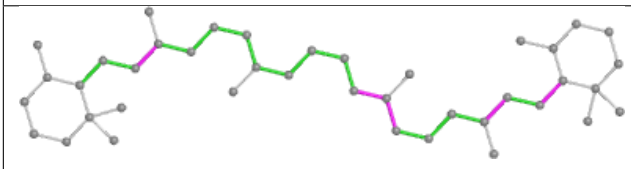


Bond angles



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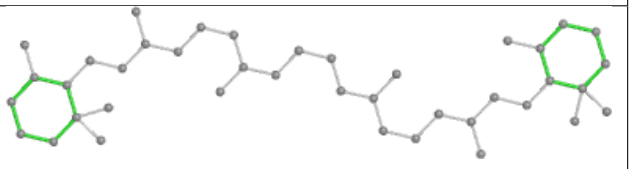
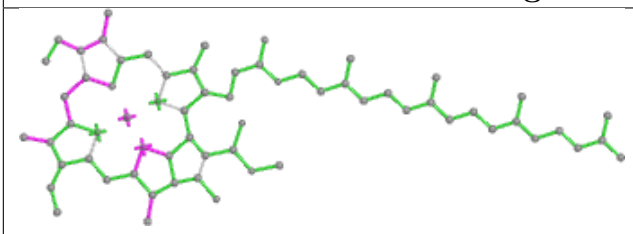


Rings

Ligand CLA A 841



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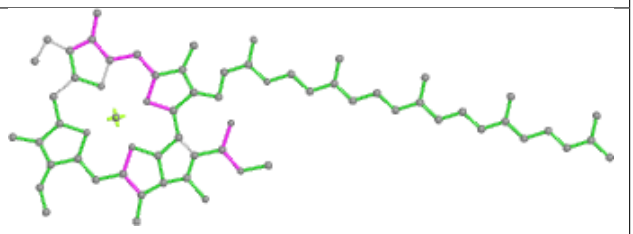
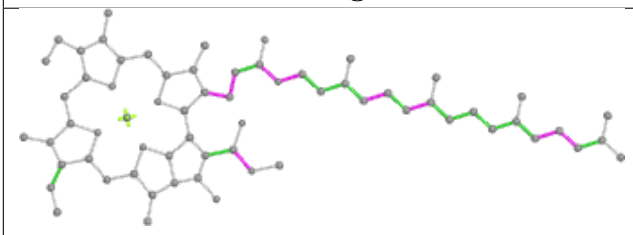


Bond angles



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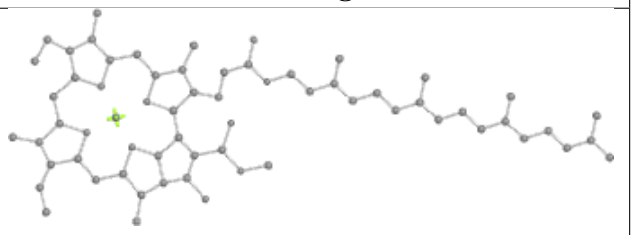
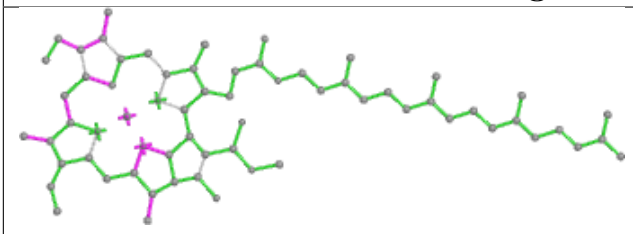


Rings

Ligand CLA 1 311



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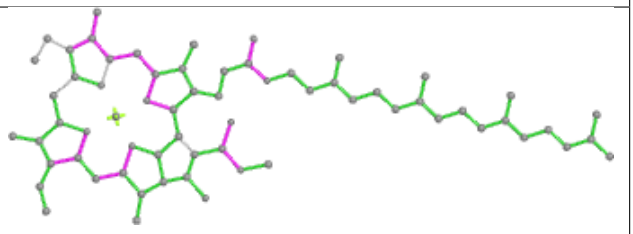
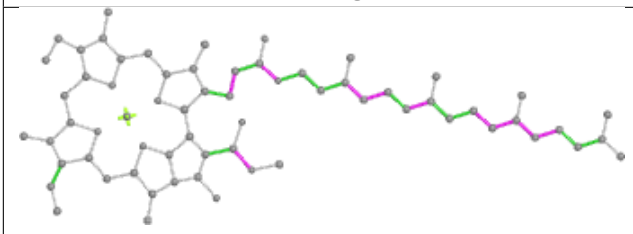


Bond angles



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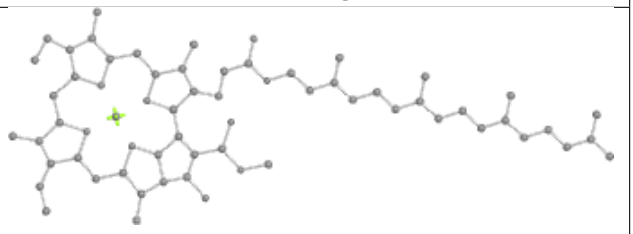
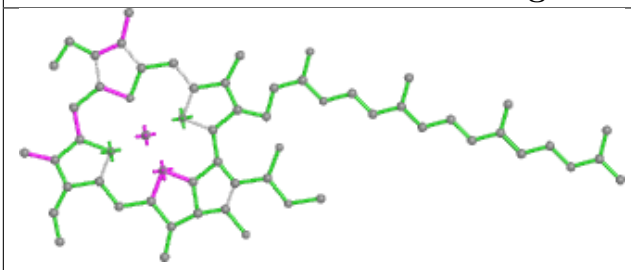


Rings

Ligand CLA 6 305



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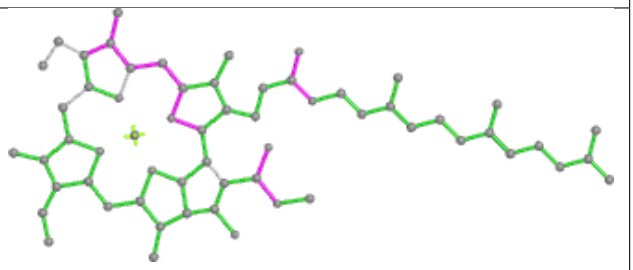
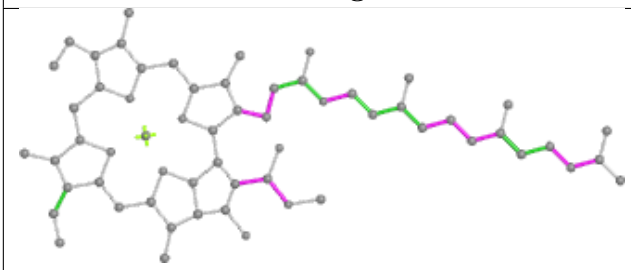


Bond angles



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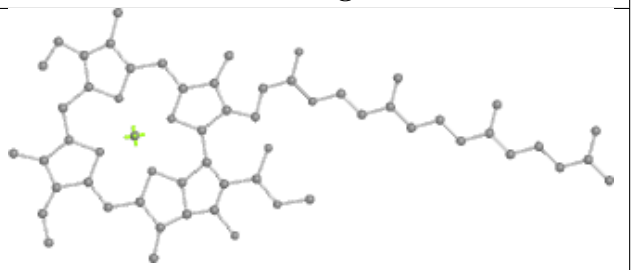
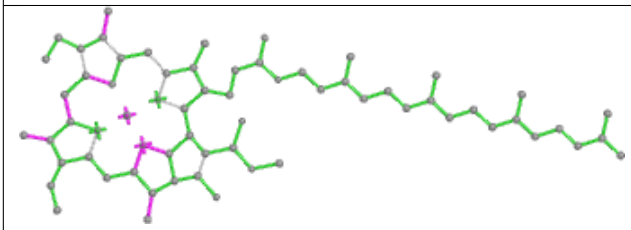


Rings

Ligand CLA L 202



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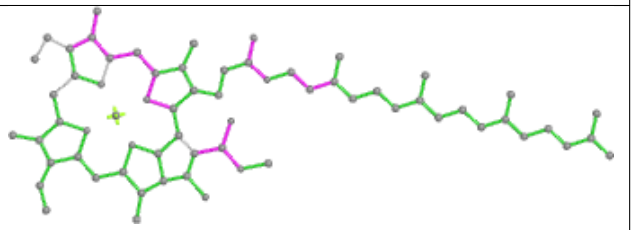
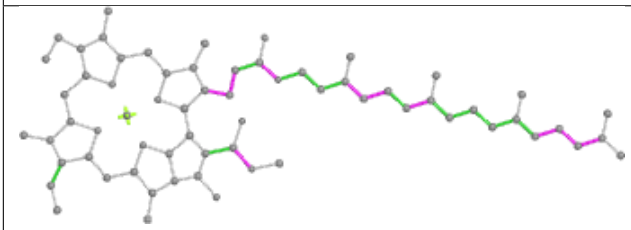


Bond angles



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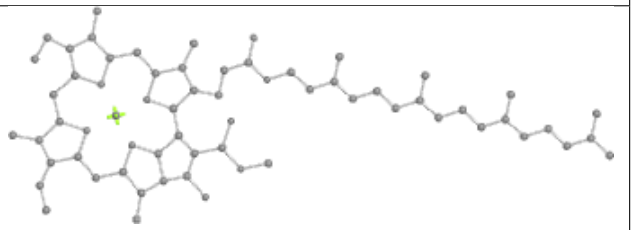
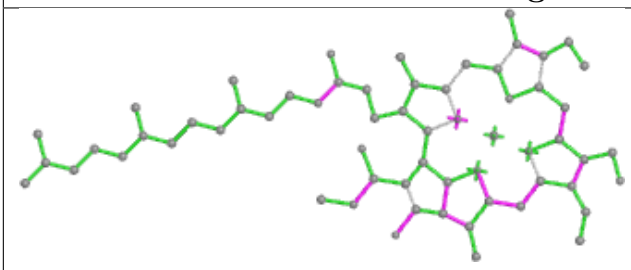


Rings

Ligand CHL 4 301



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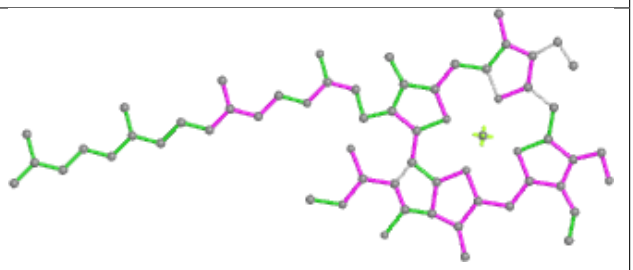
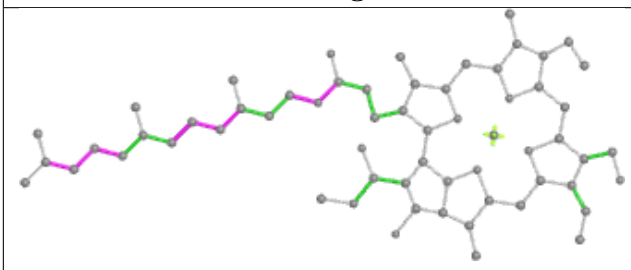


Bond angles



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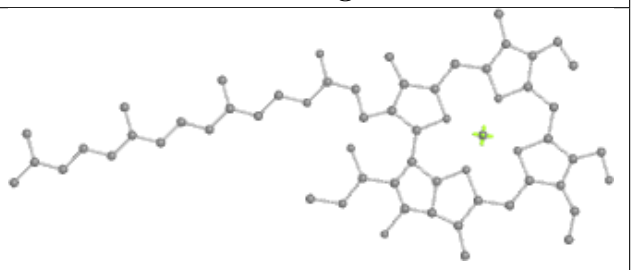
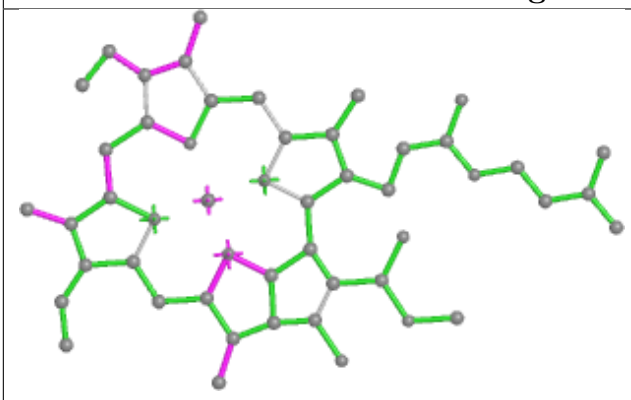


Rings

Ligand CLA 3 307



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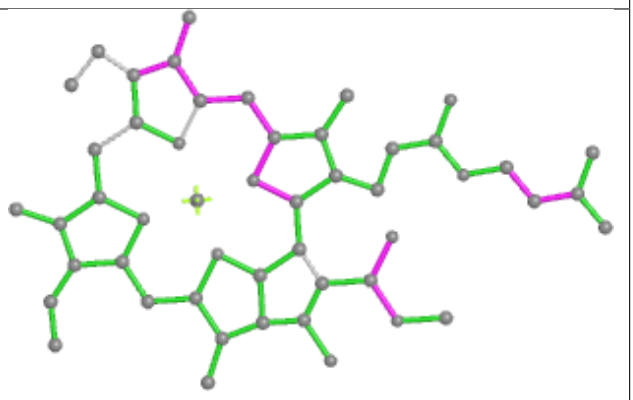
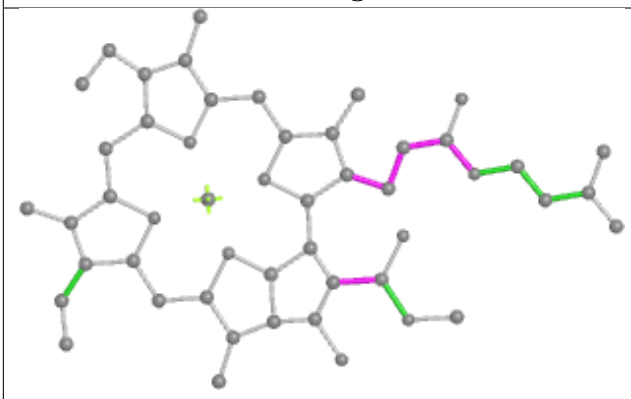


Bond angles



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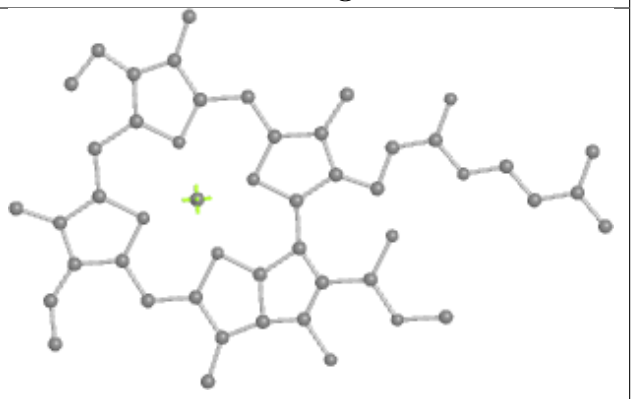
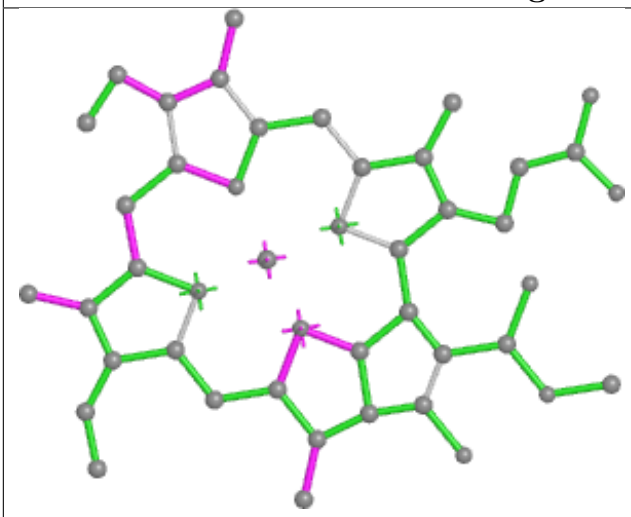
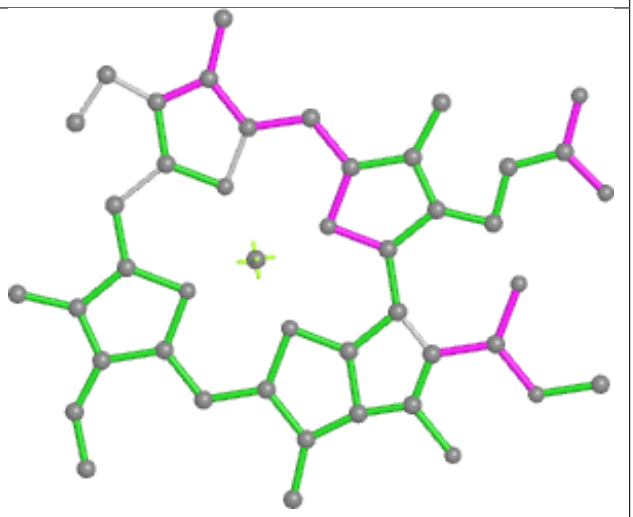


Rings

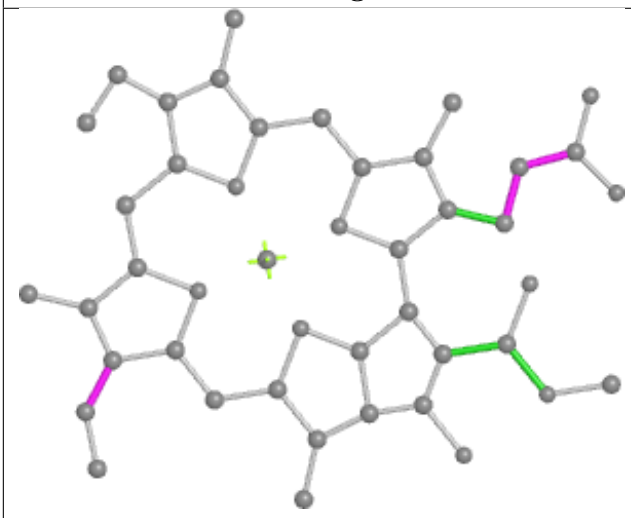
Ligand CLA 6 317



Bond lengths



Bond angles



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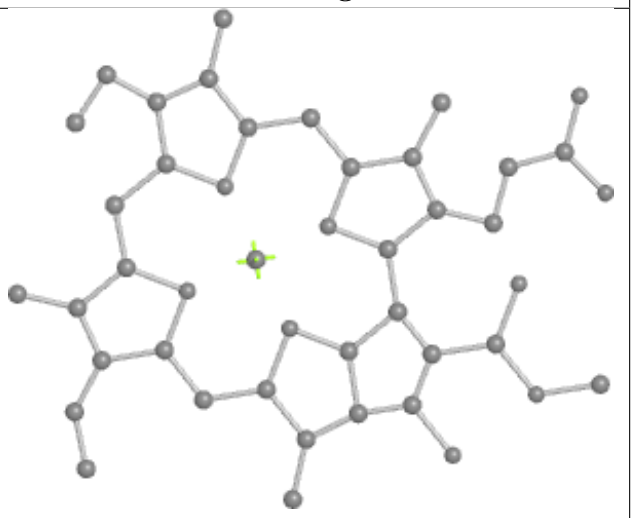
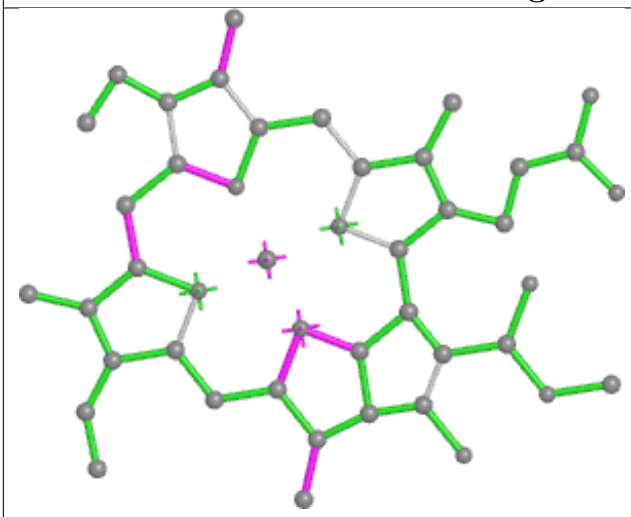


Rings

Ligand CLA 5 311



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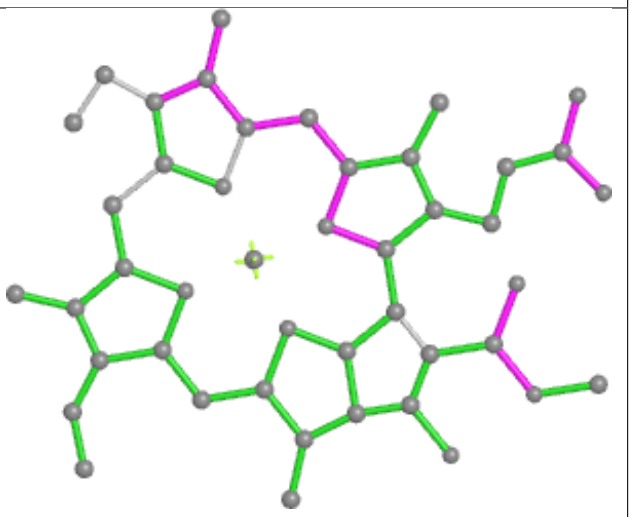
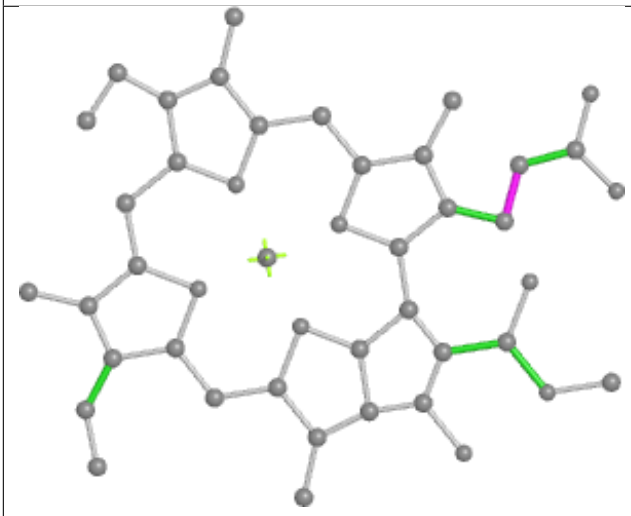
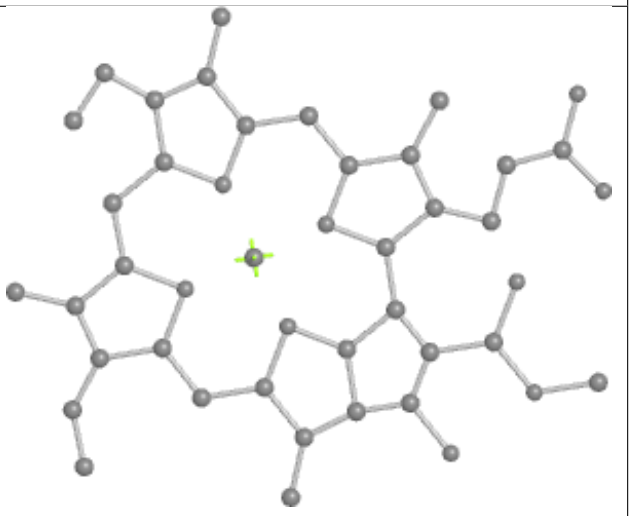


Bond angles

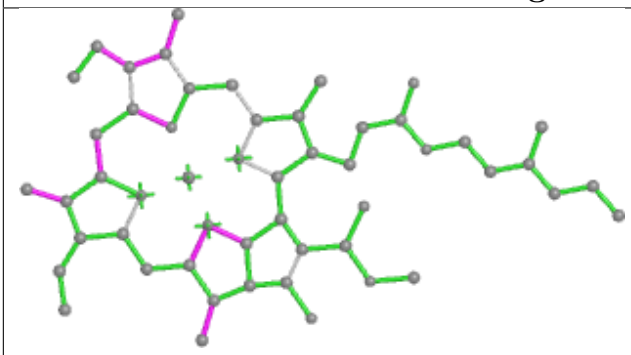


Torsions



Rings

Ligand CLA 3 310



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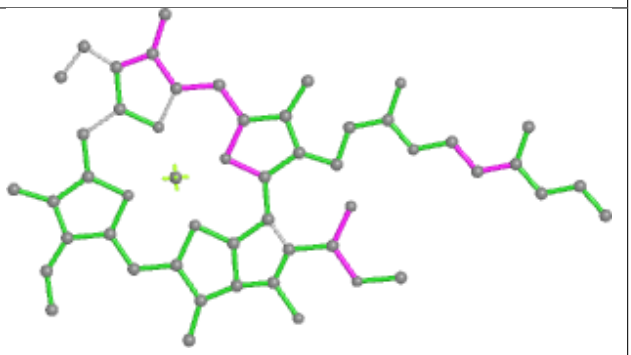

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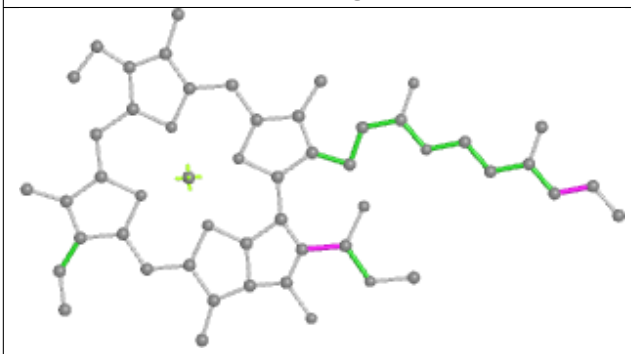

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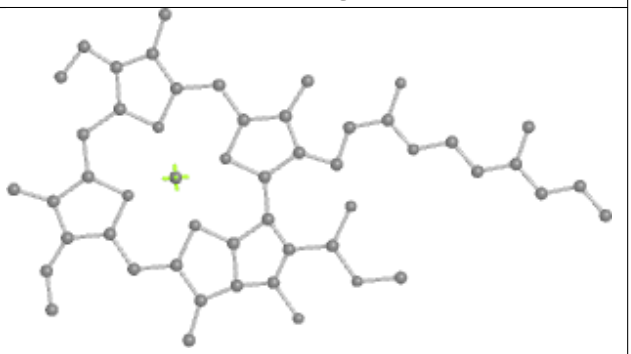
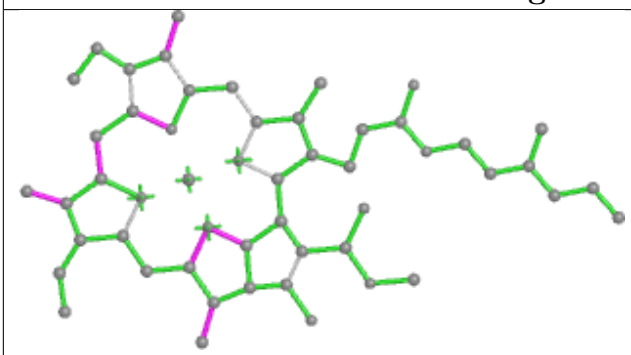
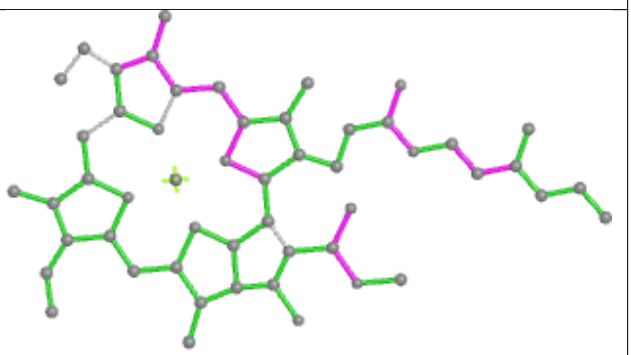


Rings

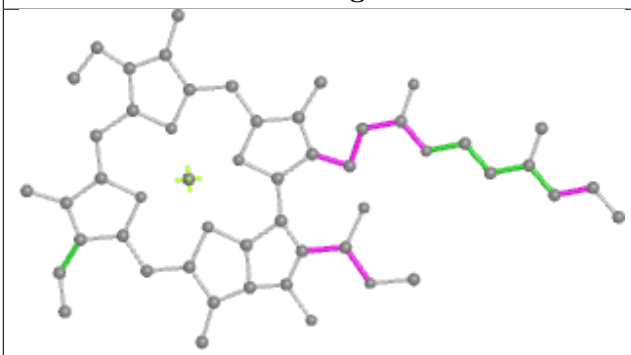
Ligand CLA 6 301



Bond lengths



Bond angles



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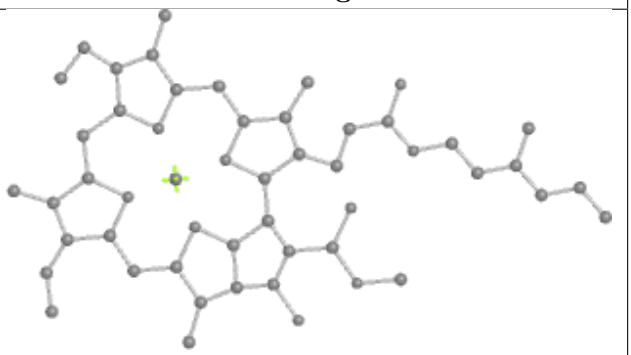
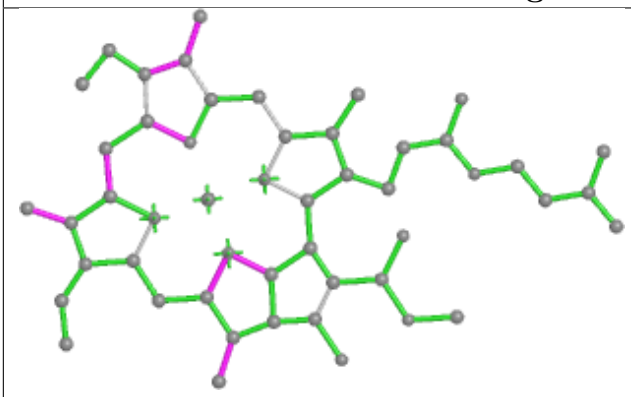
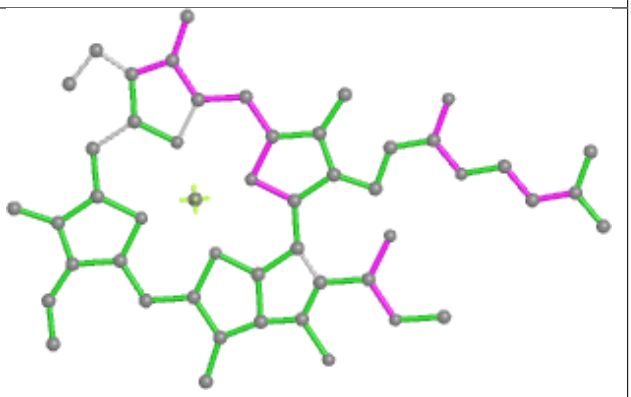
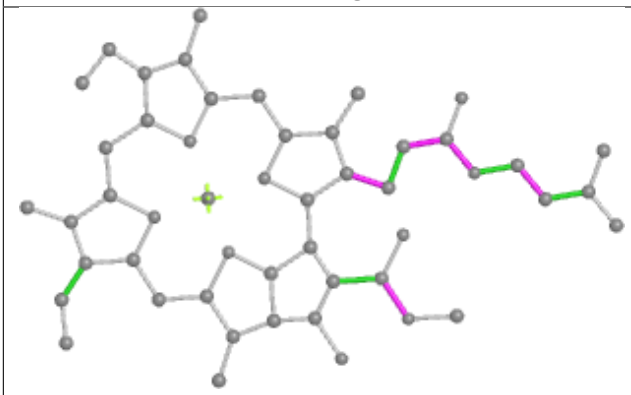
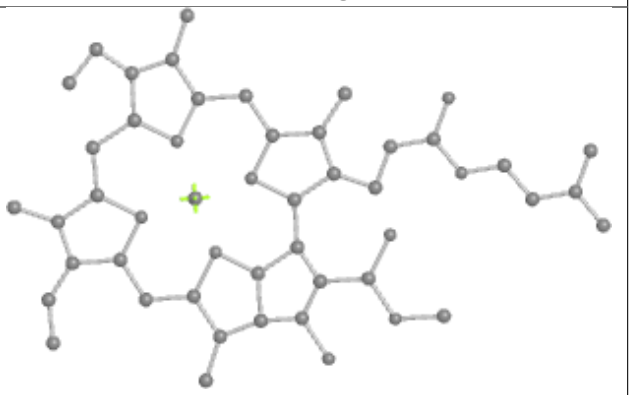
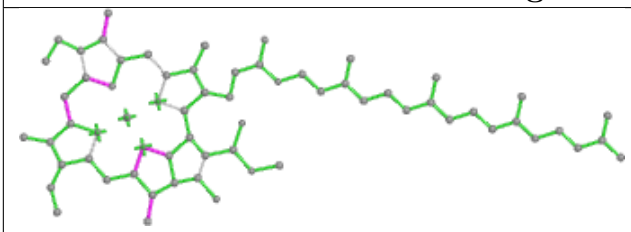
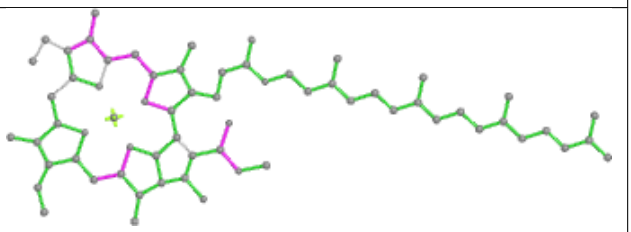
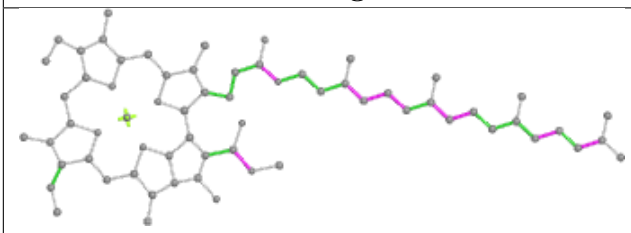
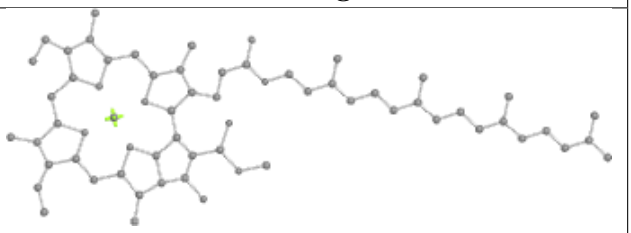
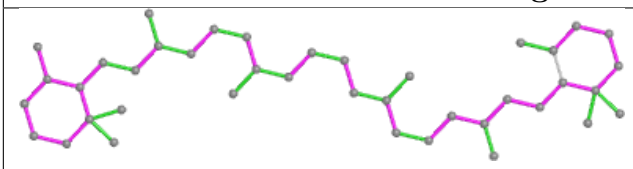


Rings

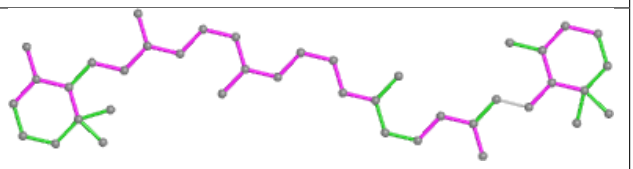
Ligand CLA L 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

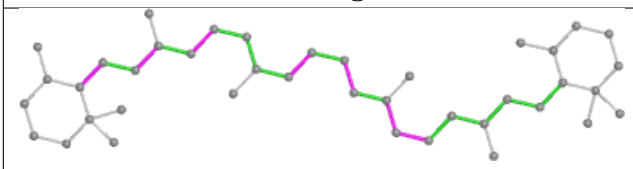
Ligand 8CT 6 321



Bond lengths



Bond angles



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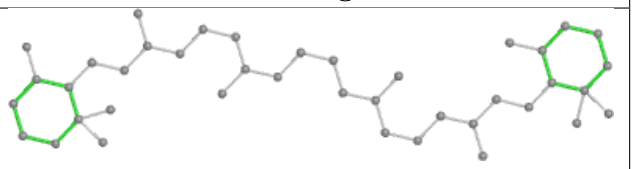
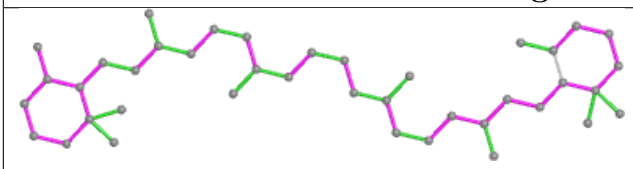


Rings

Ligand 8CT 7 321



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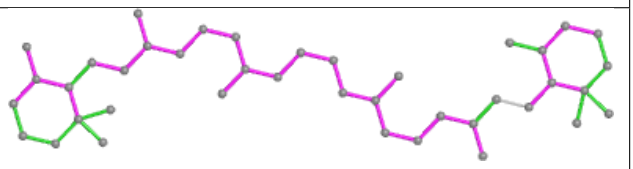
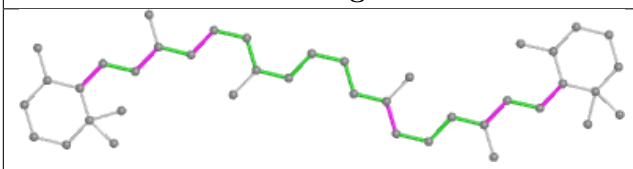


Bond angles



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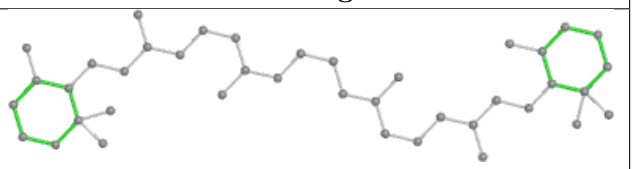
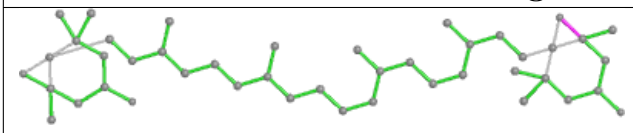


Rings

Ligand XAT 4 315



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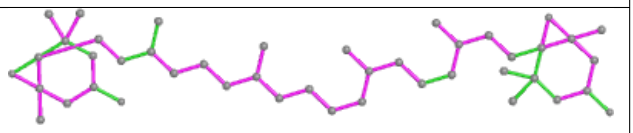

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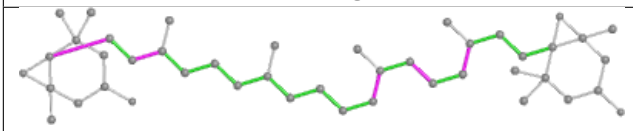

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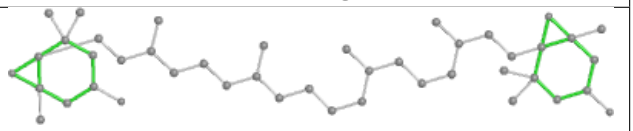
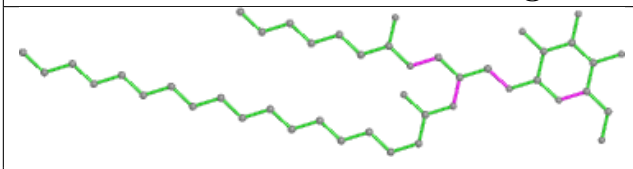
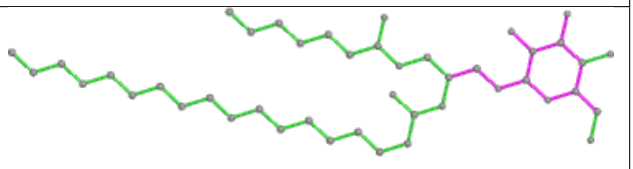


Rings

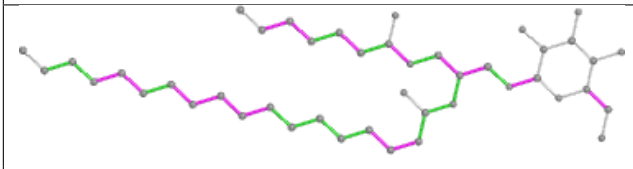
Ligand LMG 4 318



Bond lengths



Bond angles



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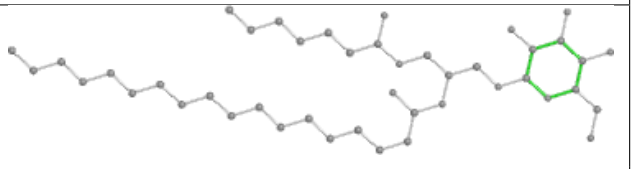
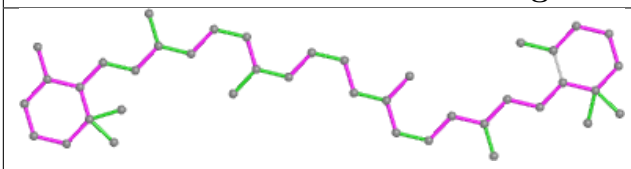
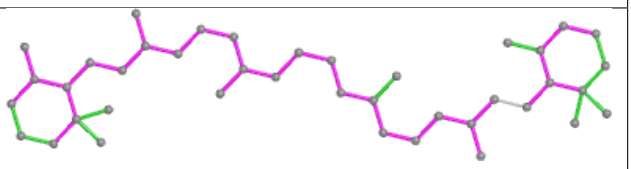
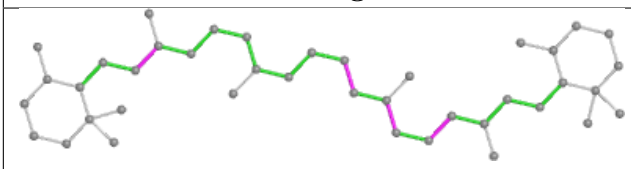
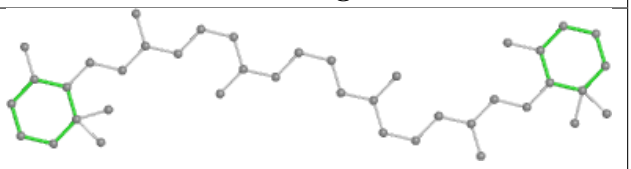
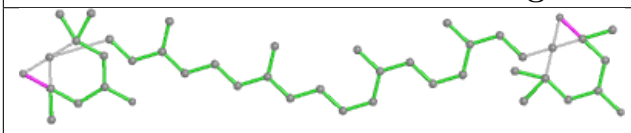
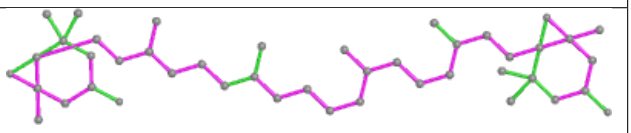
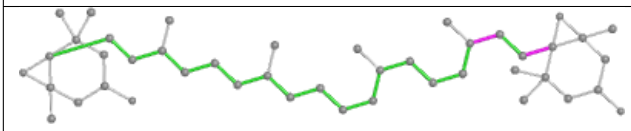
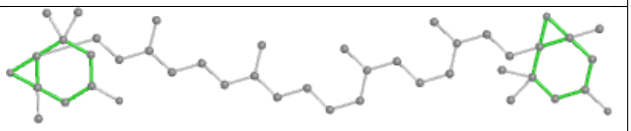
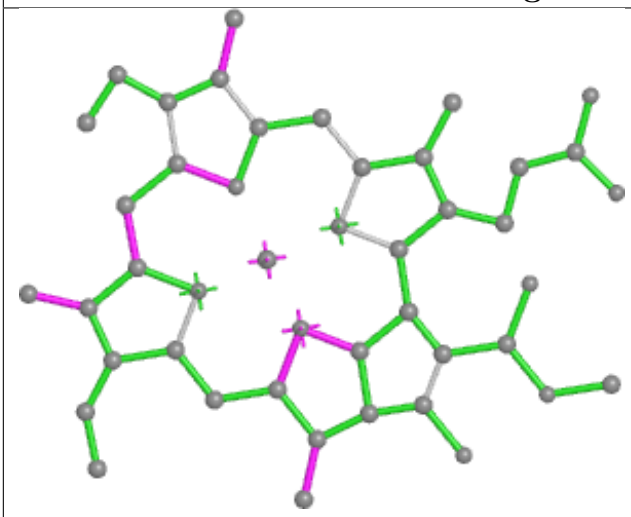


Rings

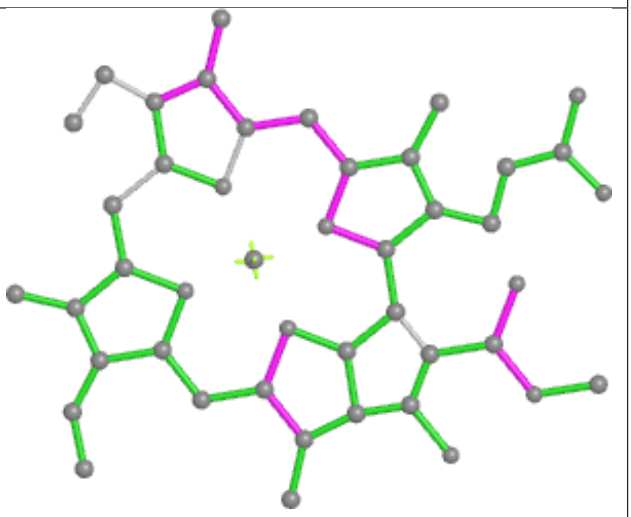
Ligand 8CT 3 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT 2 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

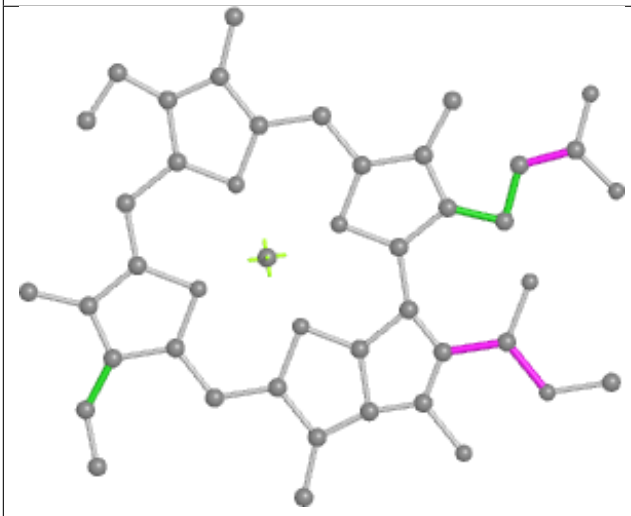
Ligand CLA A 820



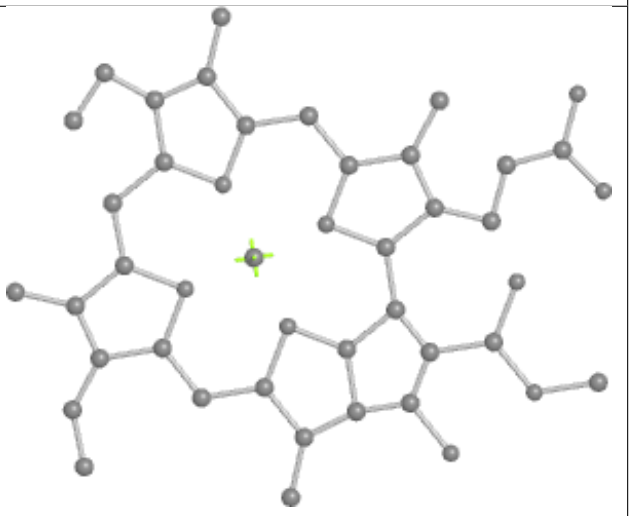
Bond lengths



Bond angles

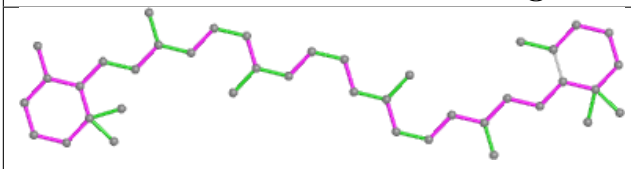


Torsions



Rings

Ligand 8CT B 848



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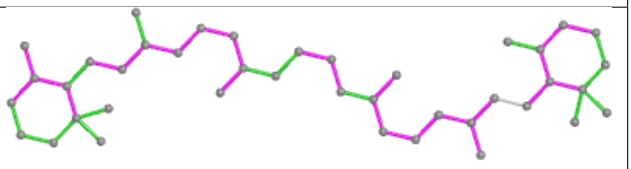
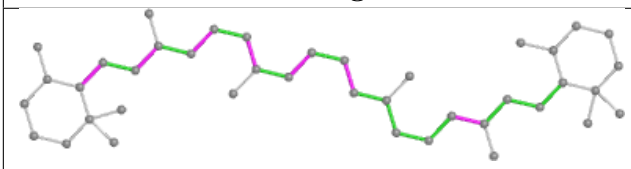


Bond angles



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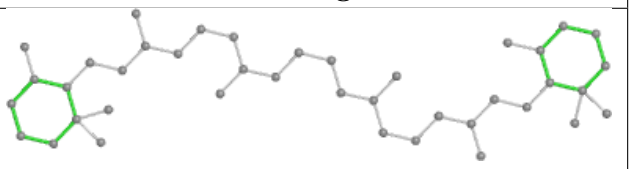
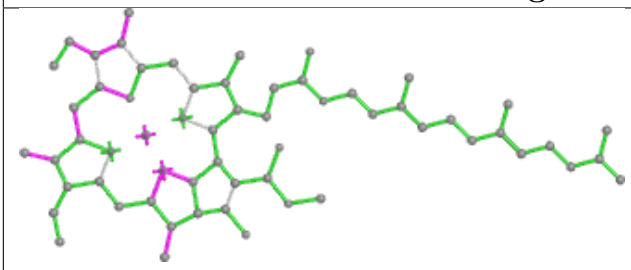
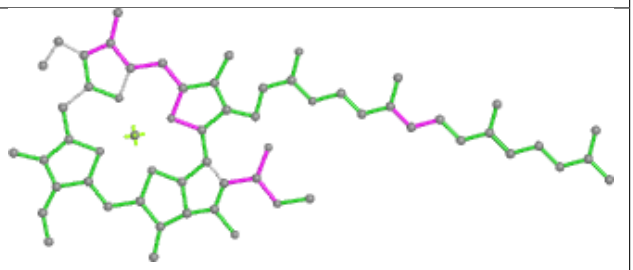
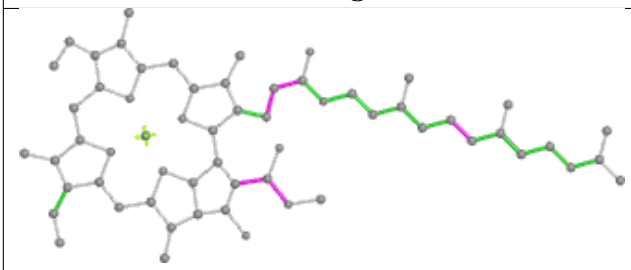
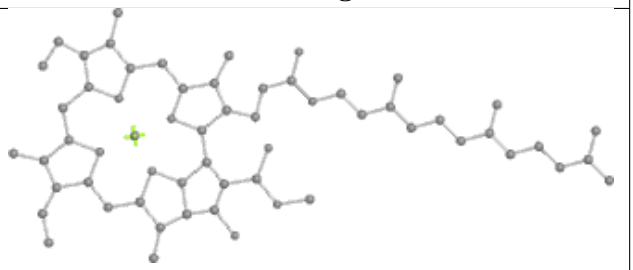
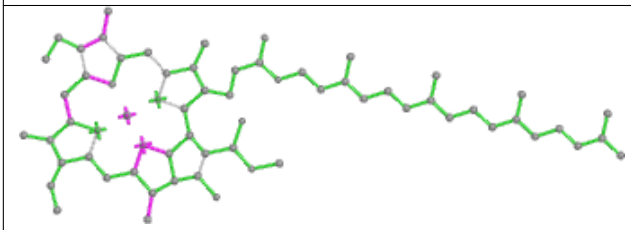
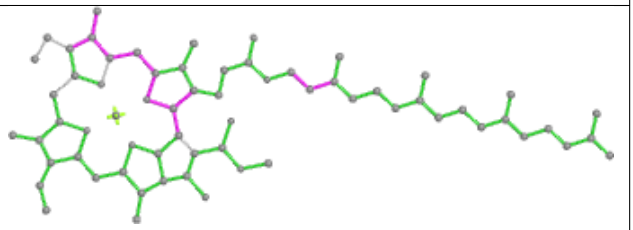
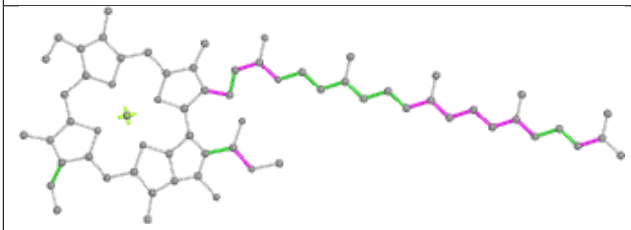
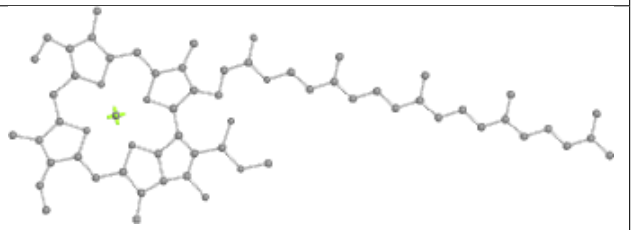
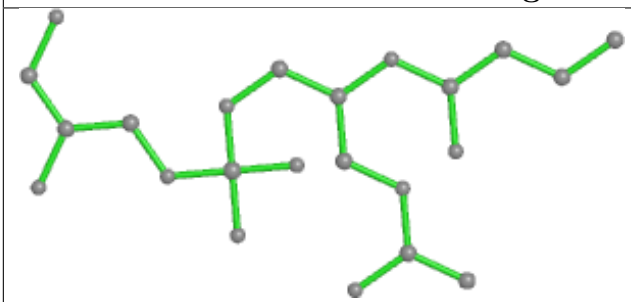


Rings

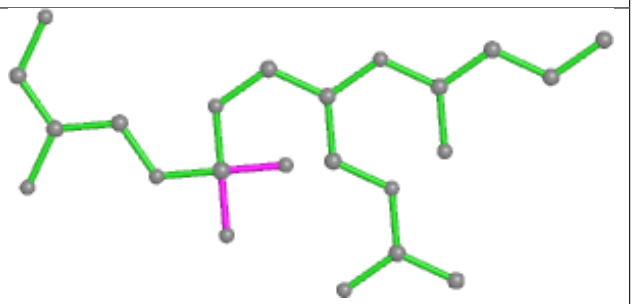
Ligand CLA 4 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG B 852



Bond lengths



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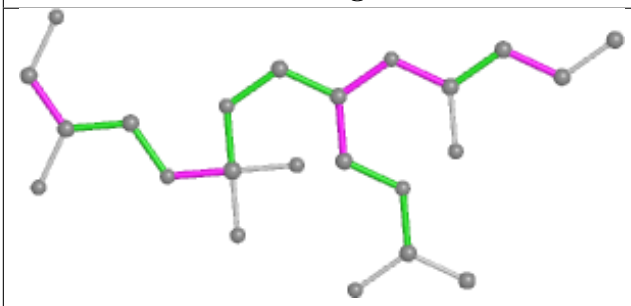

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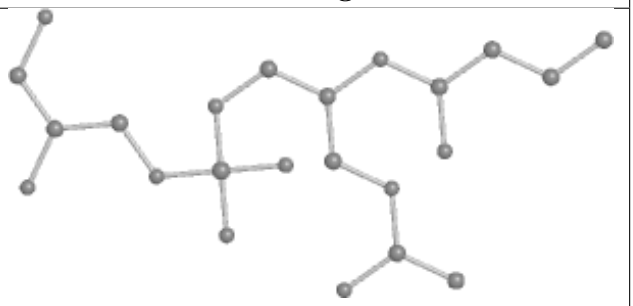
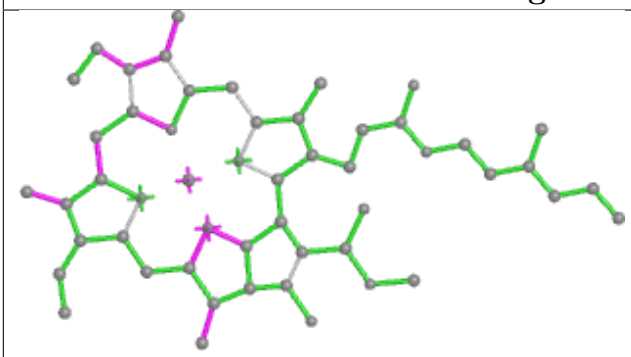


Rings

Ligand CLA 6 318



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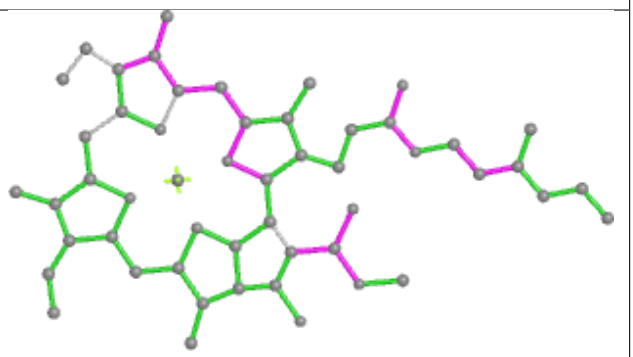

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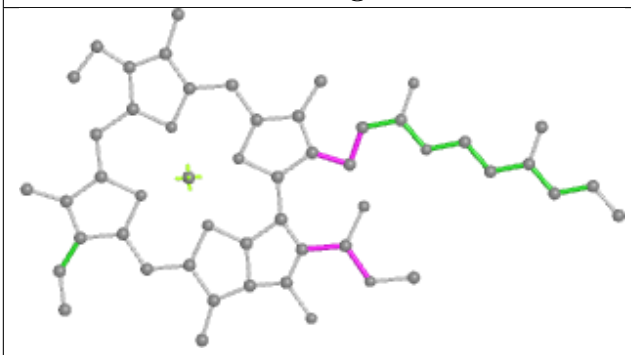

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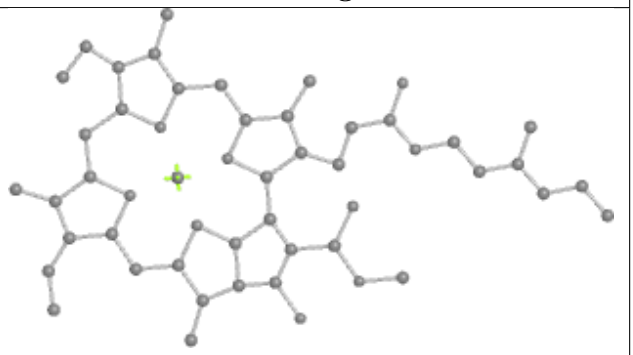

Rings

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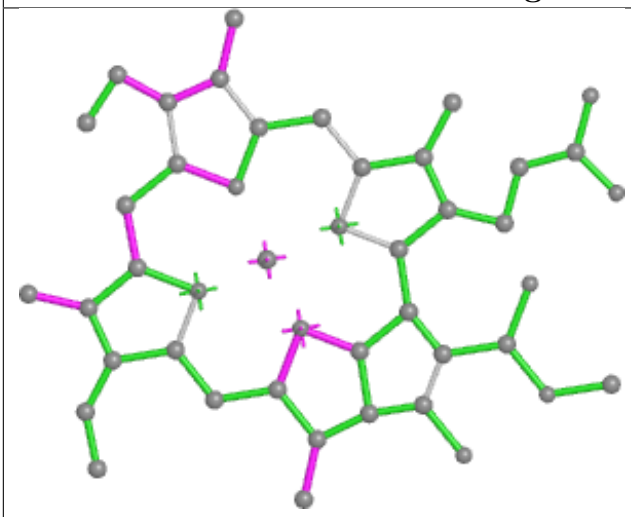

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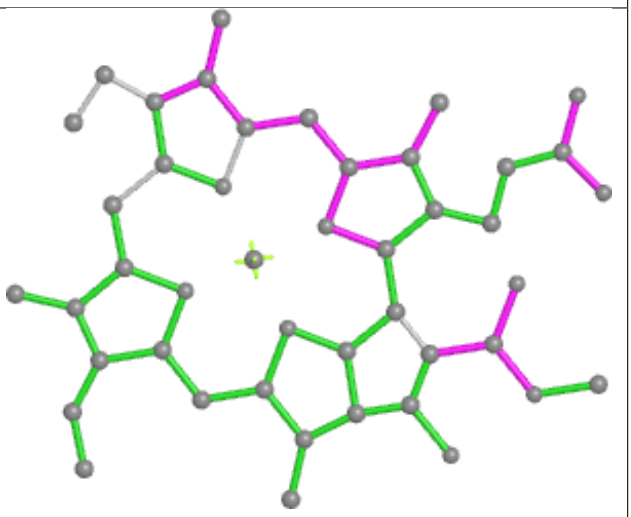

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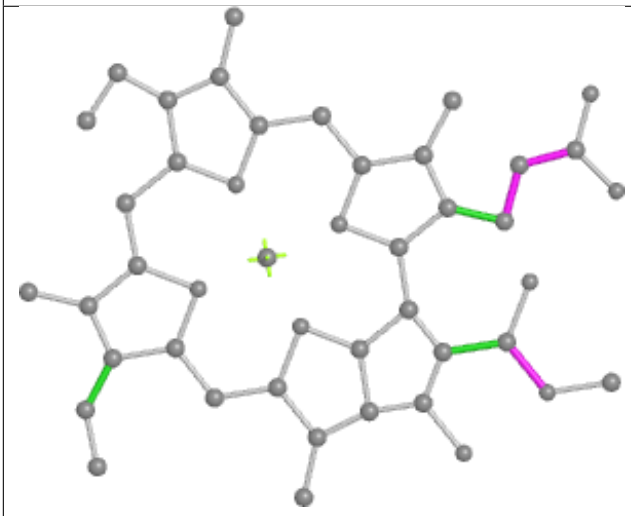

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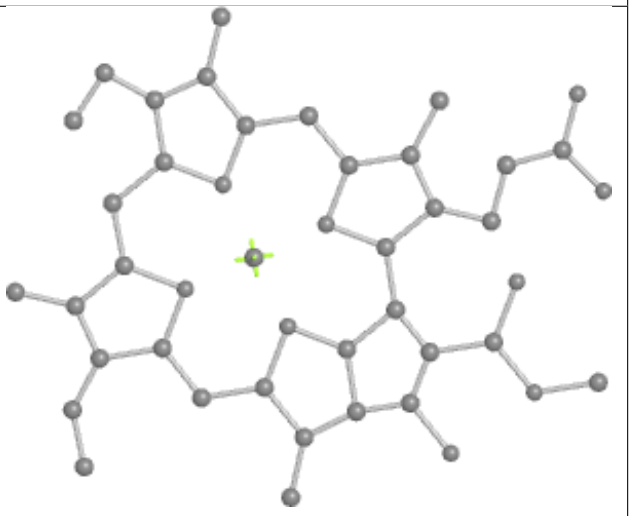

Rings

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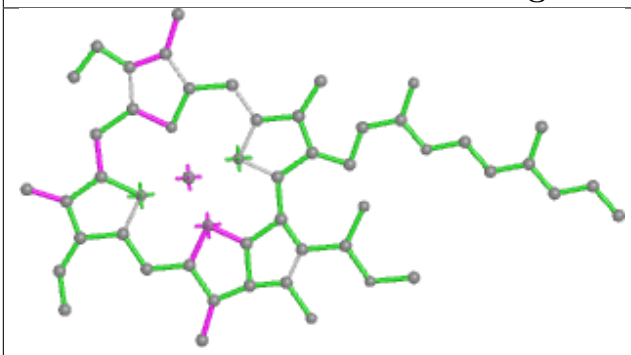
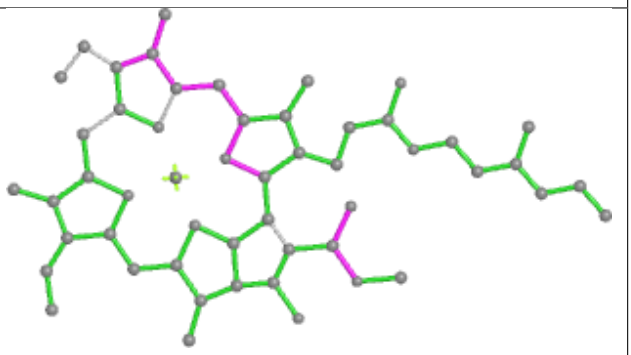
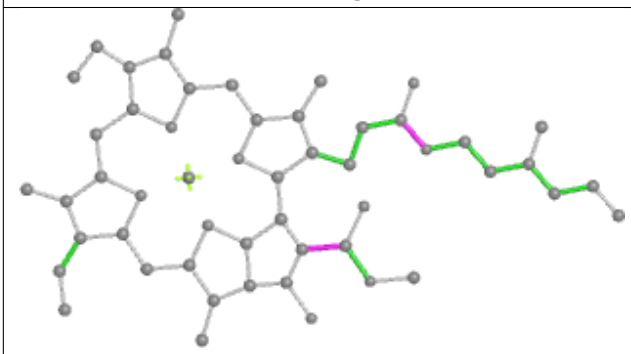
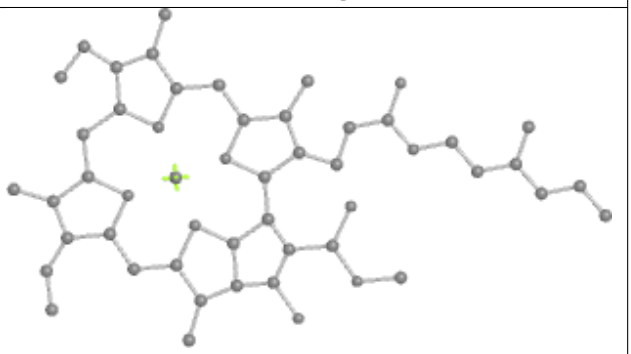
 Bond lengths	 Bond angles
 Torsions	 Rings

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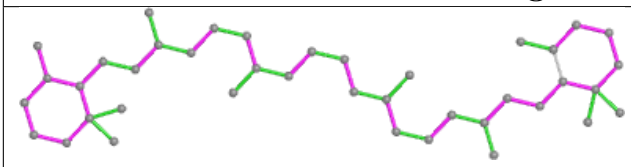
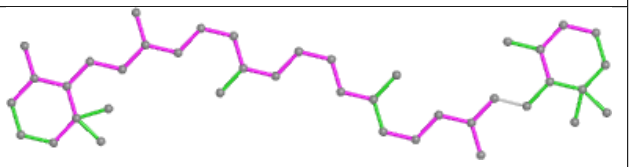
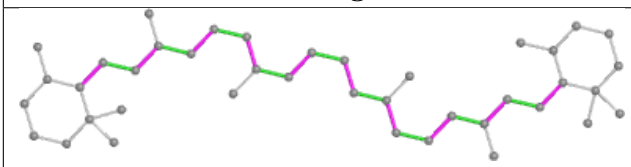
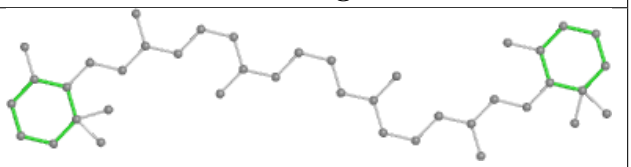
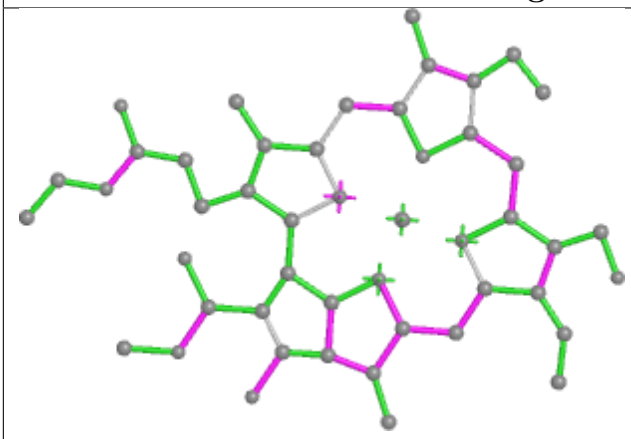
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 1 305



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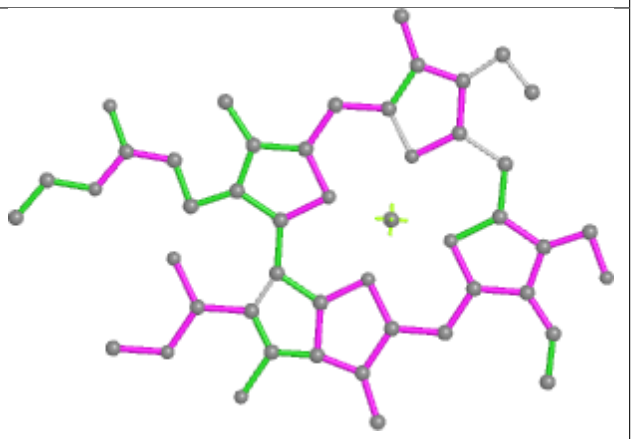
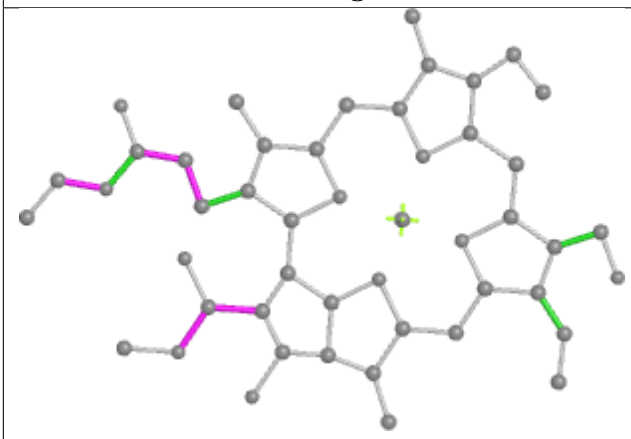


Bond angles



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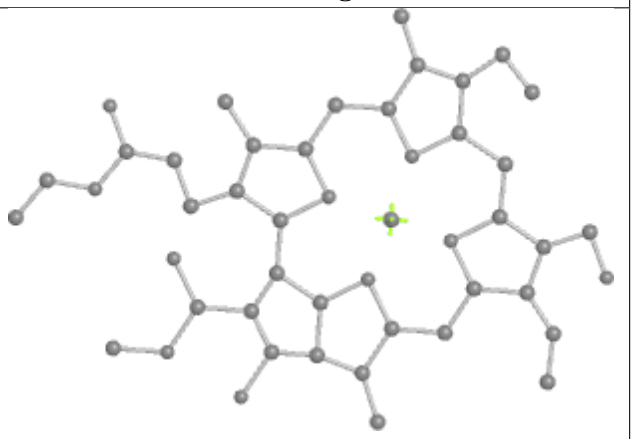
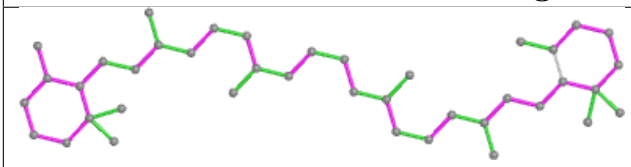


Rings

Ligand 8CT I 101



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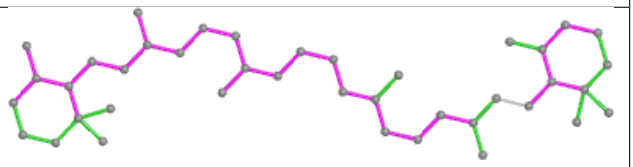

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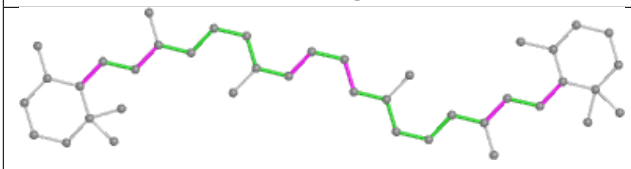

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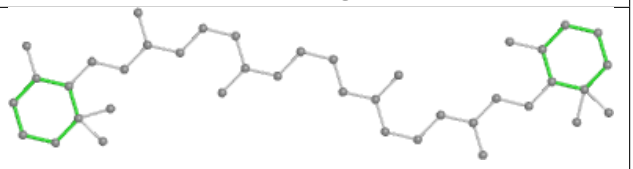
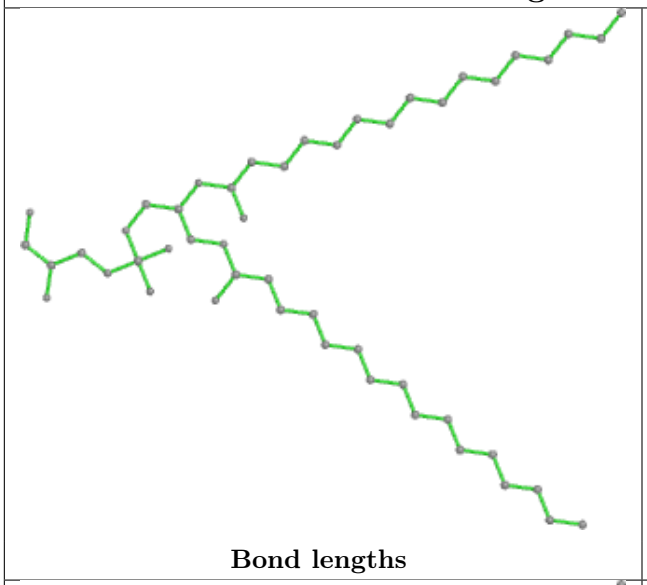


Rings

Ligand LHG 0 315



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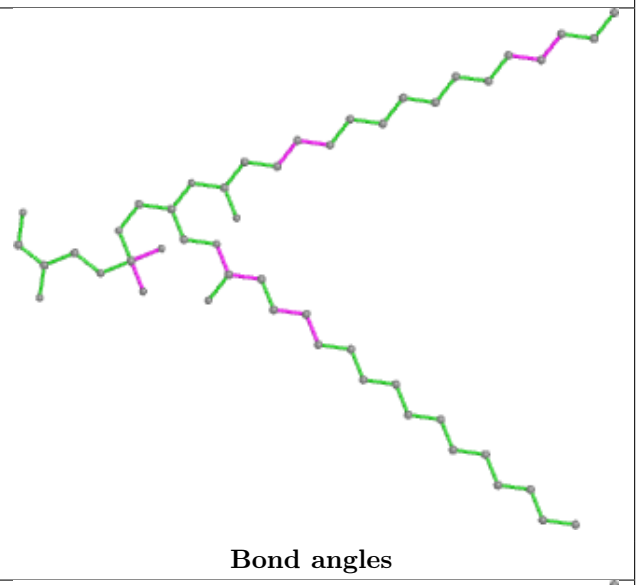

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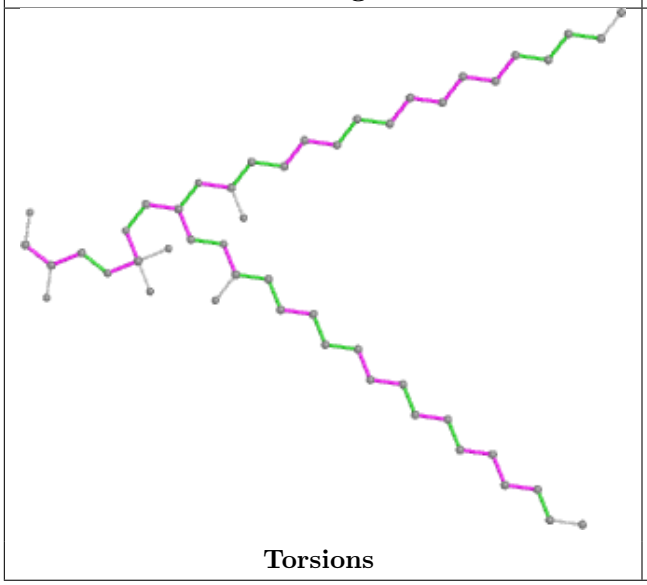

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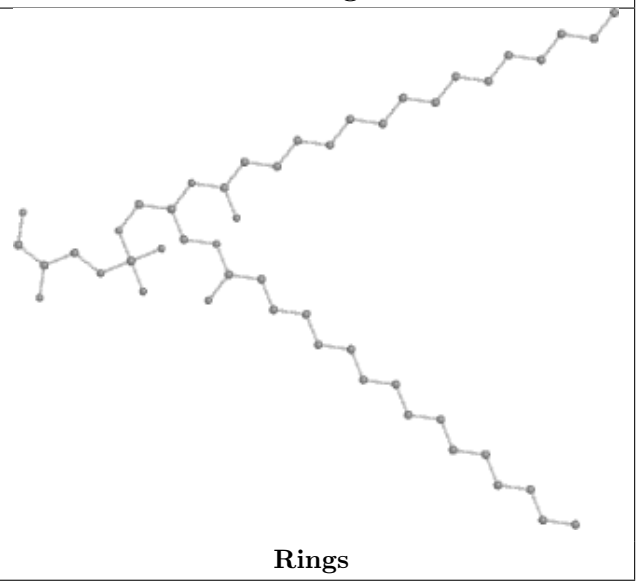
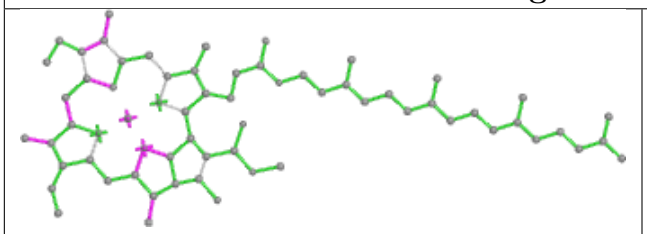


Rings

Ligand CLA 7 316



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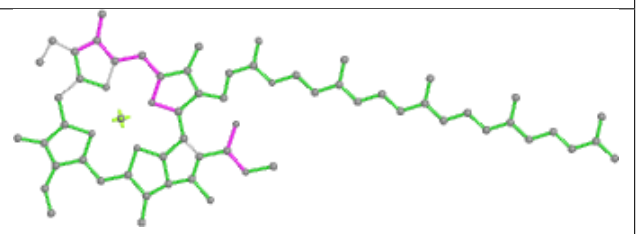

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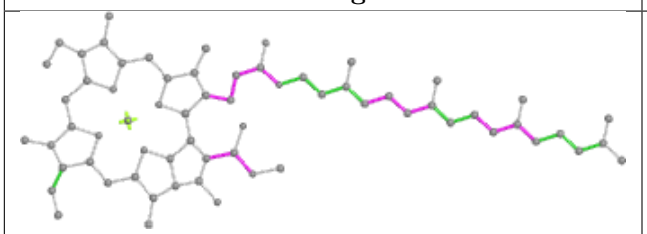

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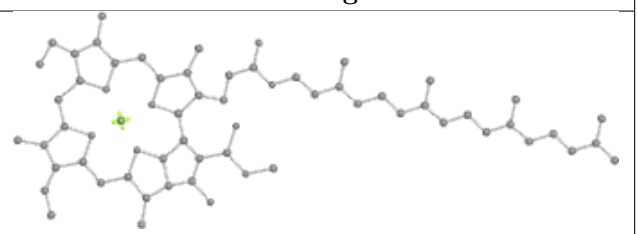
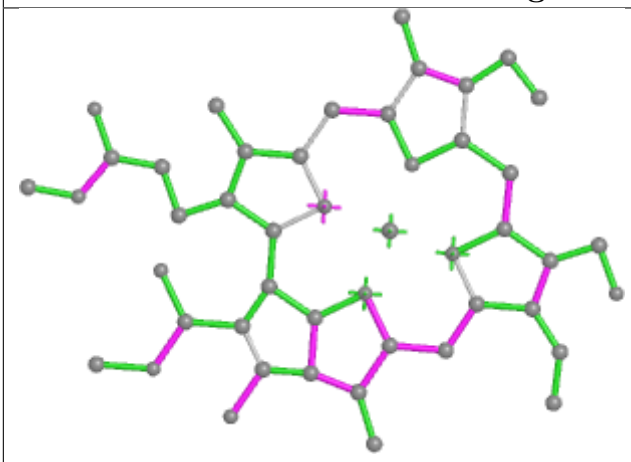


Rings

Ligand CHL 3 306



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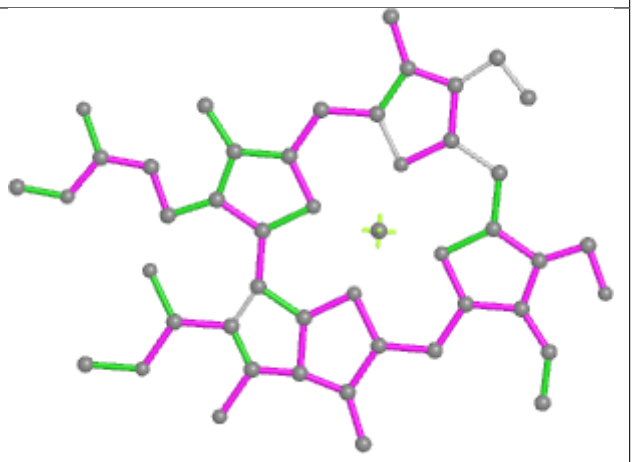
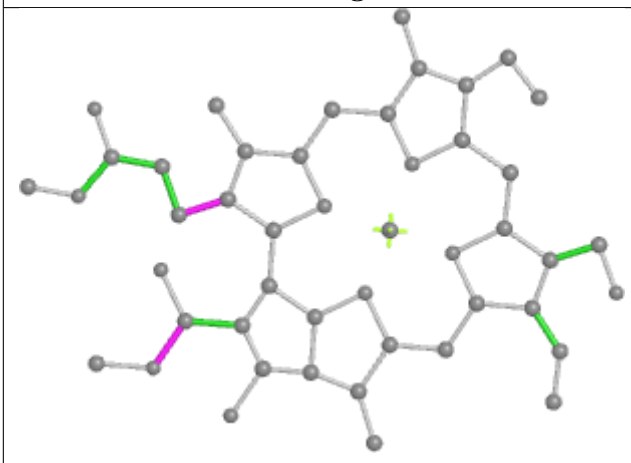


Bond angles



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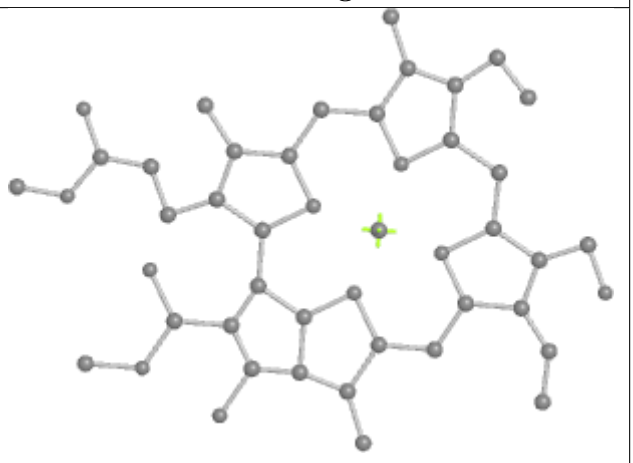
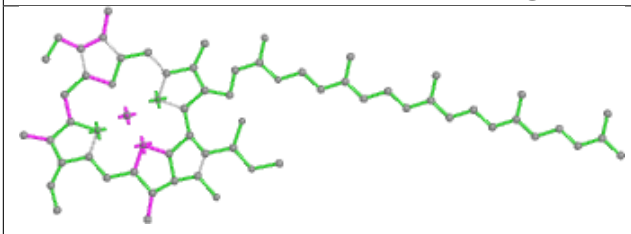


Rings

Ligand CLA A 840



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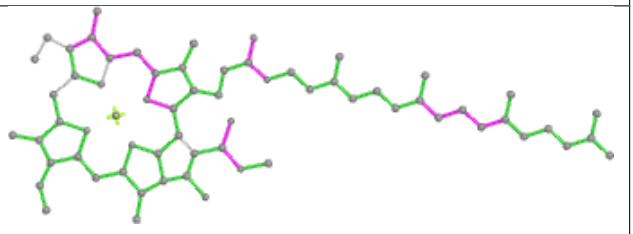
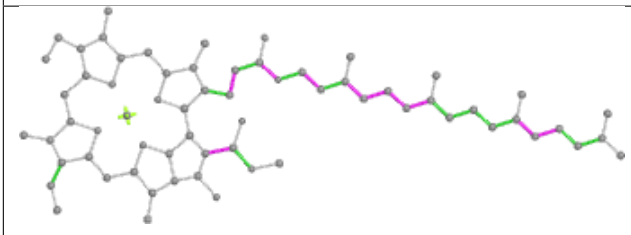


Bond angles



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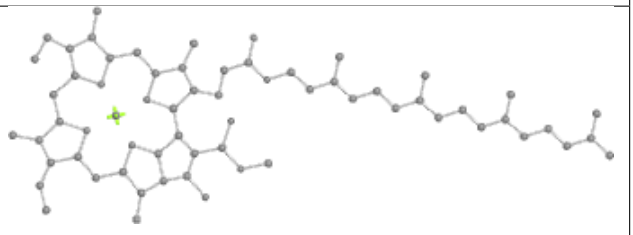
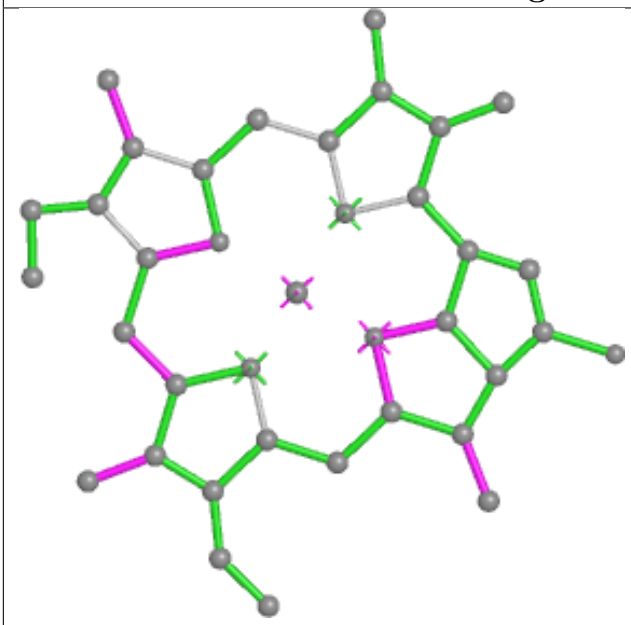
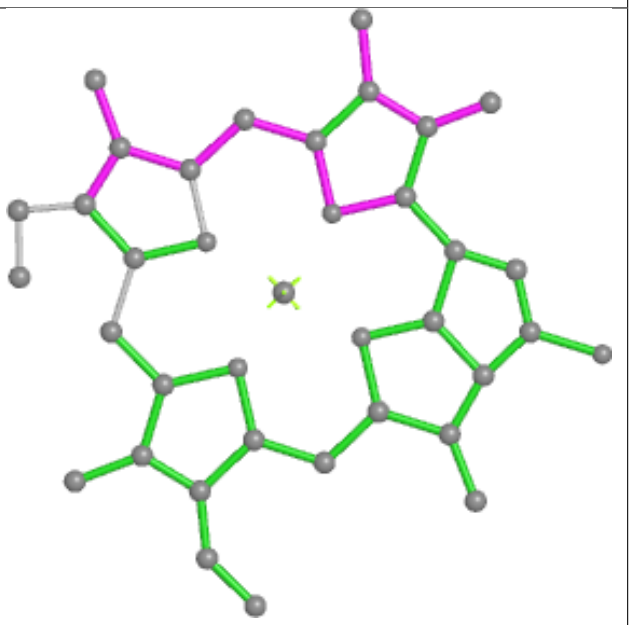


Rings

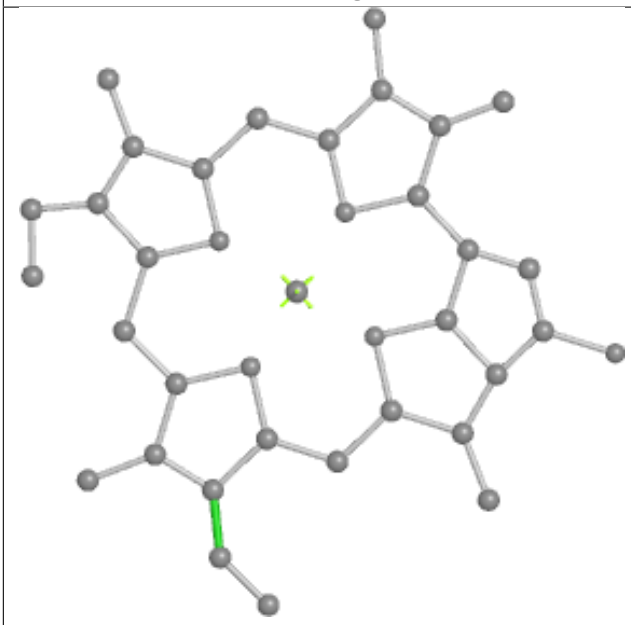
Ligand CLA 3 309



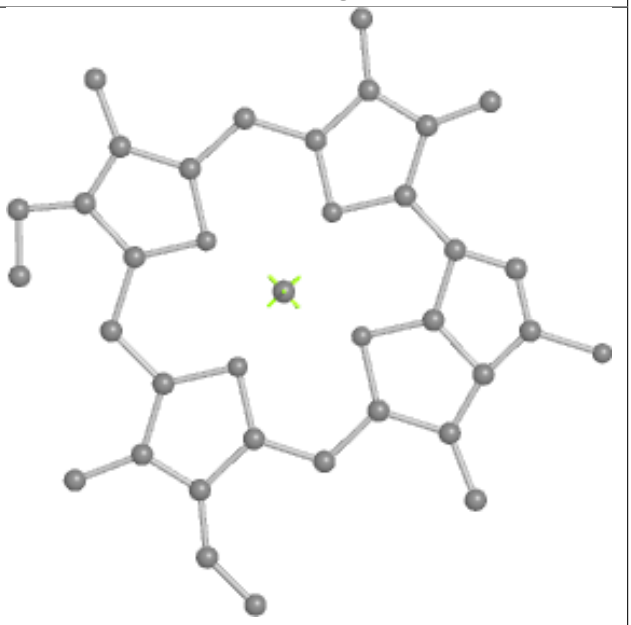
Bond lengths



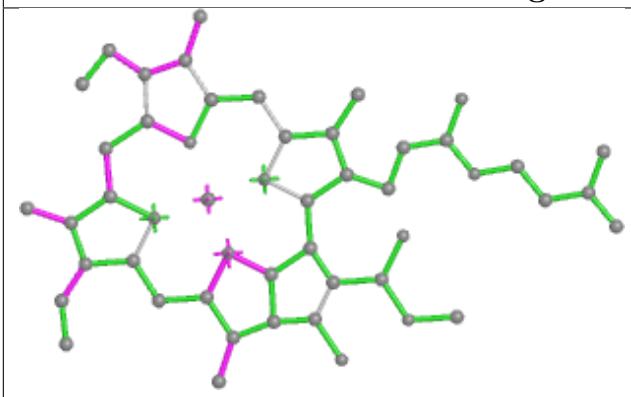
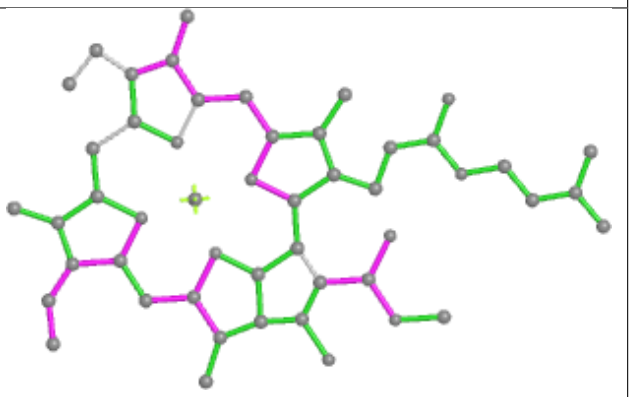
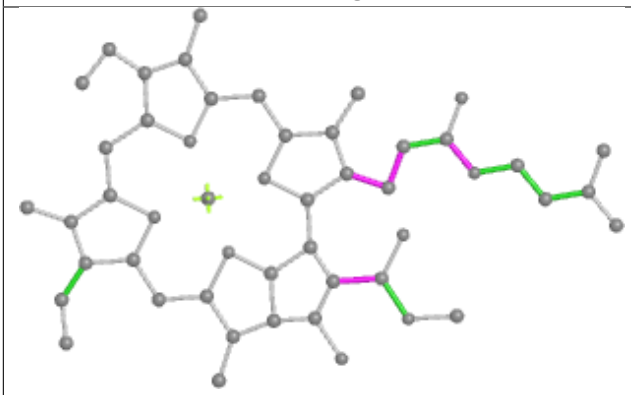
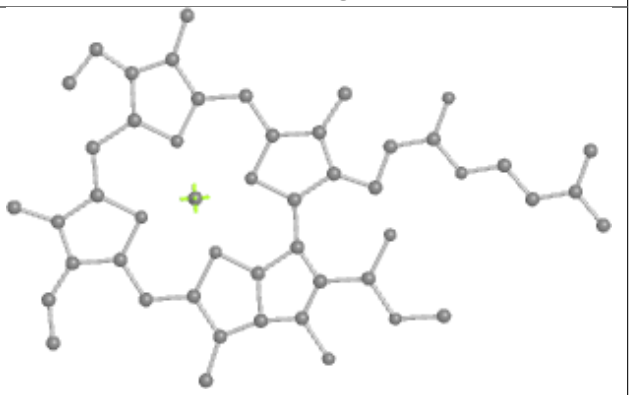
Bond angles

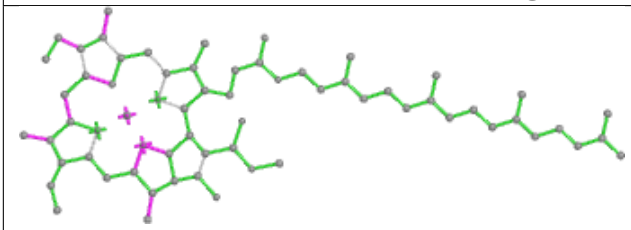
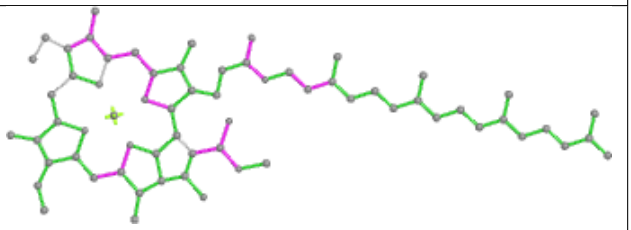
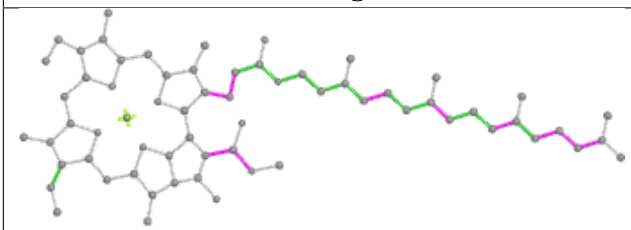
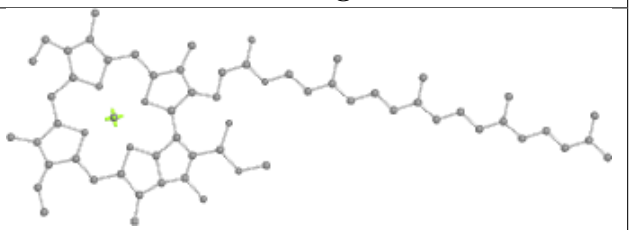


Torsions

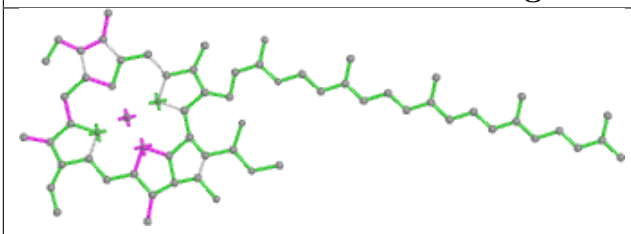


Rings

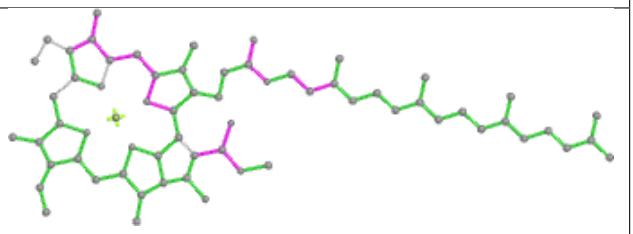
Ligand CLA 8 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

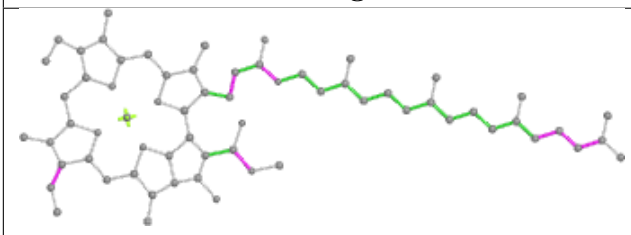
Ligand CLA B 815



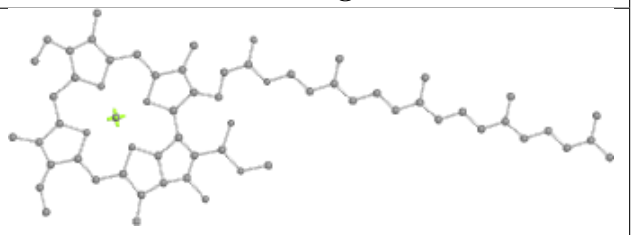
Bond lengths



Bond angles

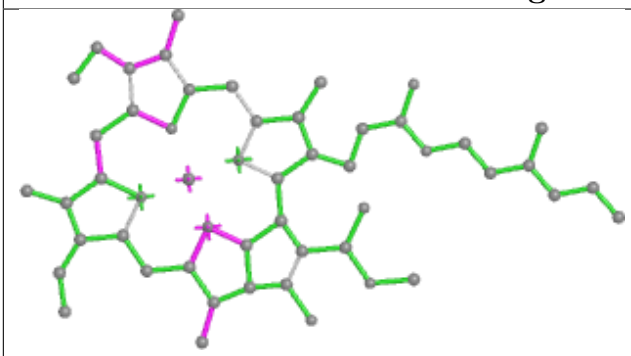


Torsions

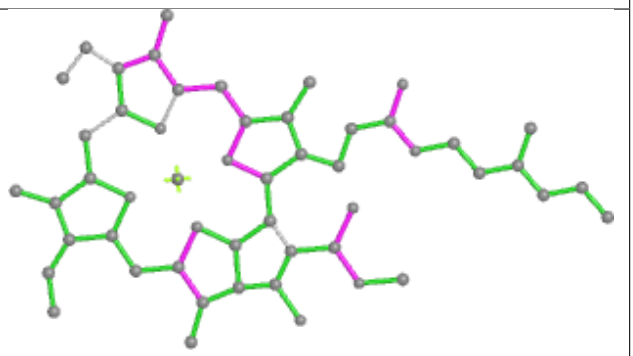


Rings

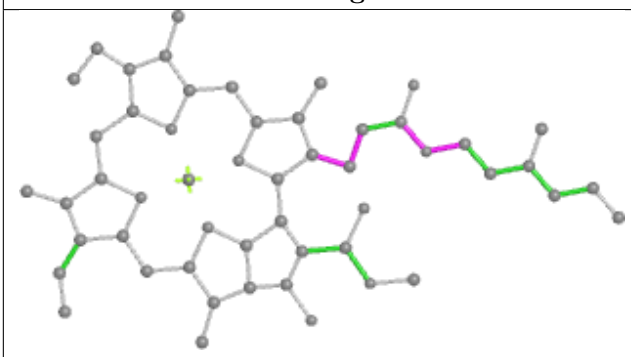
Ligand CLA 1 304



Bond lengths



Bond angles



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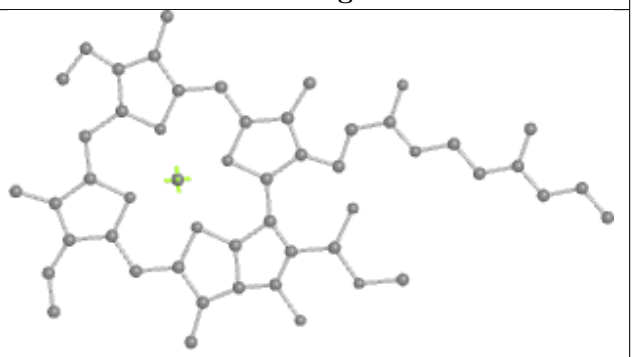
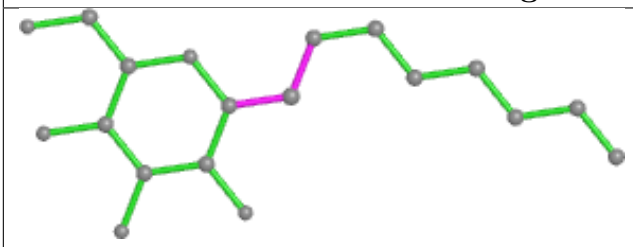


Rings

Ligand HTG A 851



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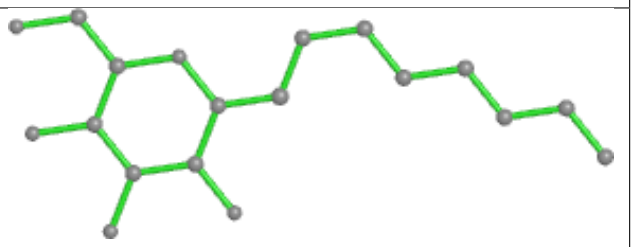
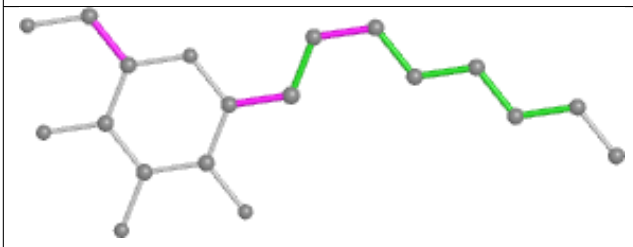


Bond angles



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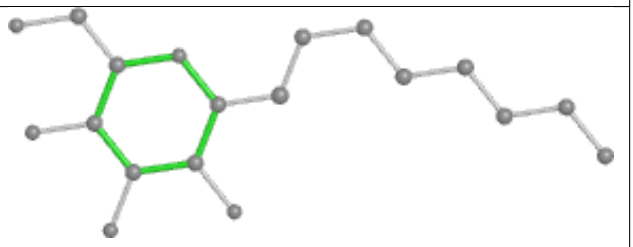
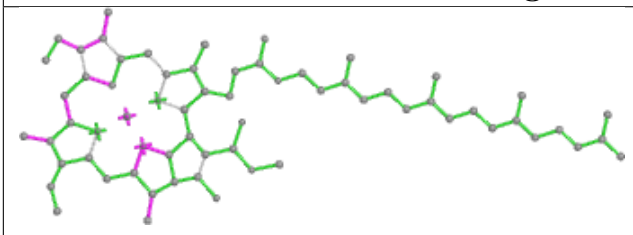


Rings

Ligand CLA A 802



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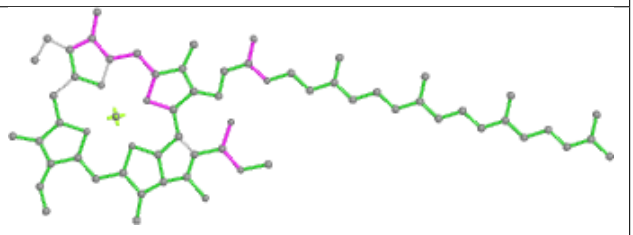
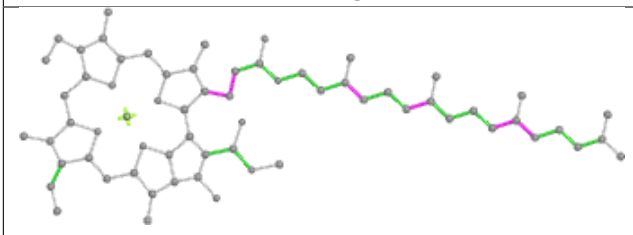


Bond angles



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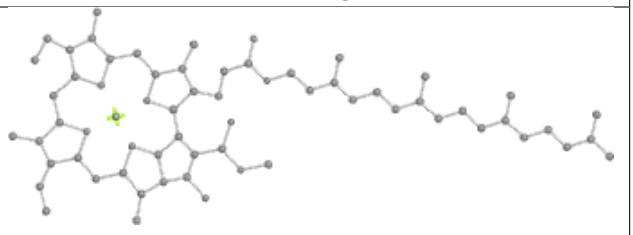
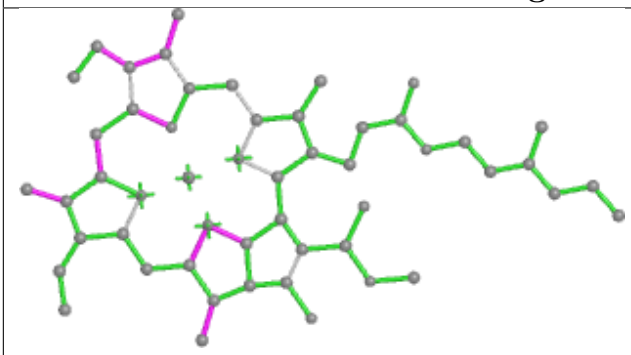
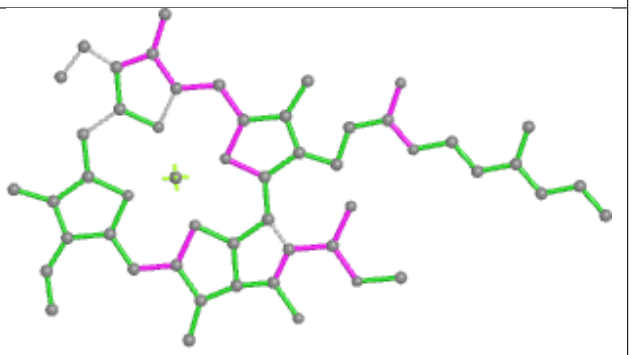


Rings

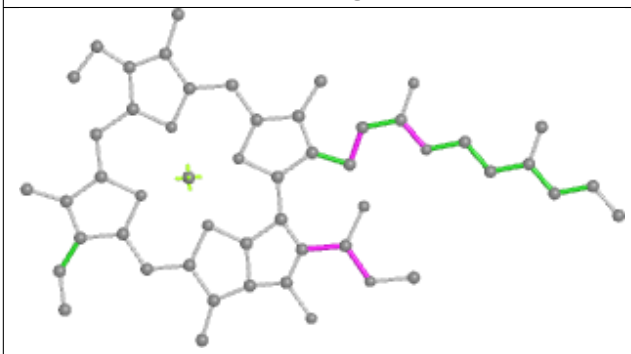
Ligand CLA 9 305



Bond lengths



Bond angles



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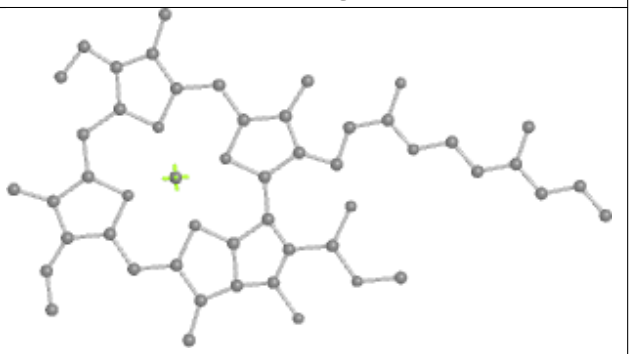
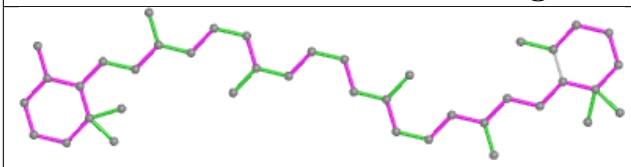
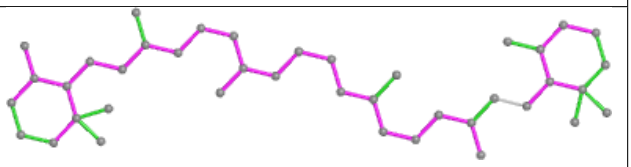


Rings

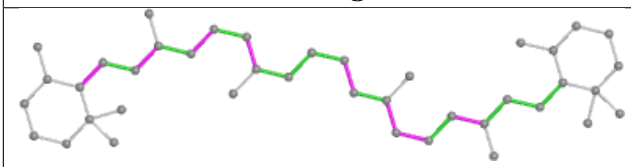
Ligand 8CT L 205



Bond lengths



Bond angles



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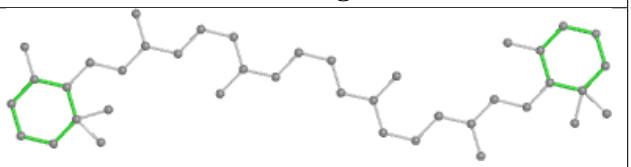
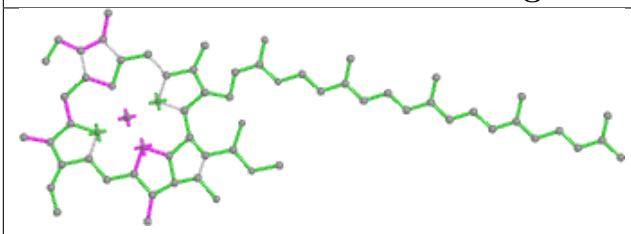


Rings

Ligand CLA A 807



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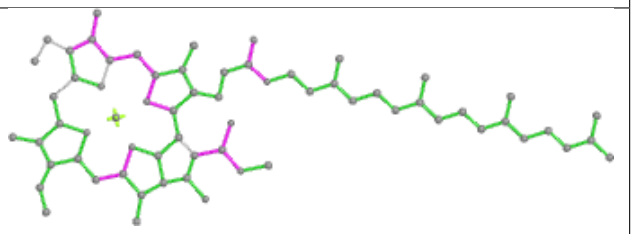
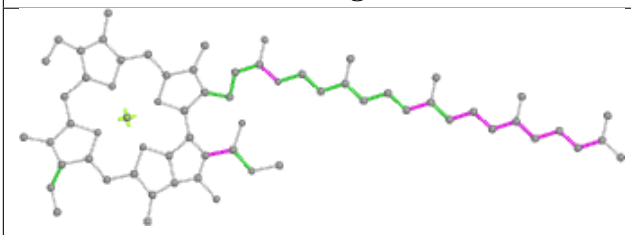


Bond angles



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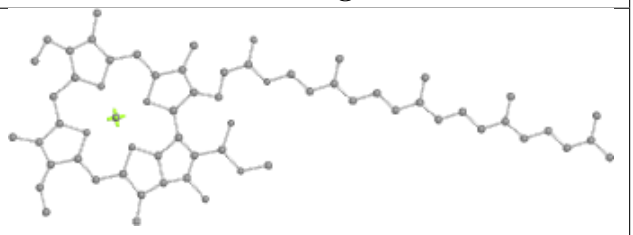
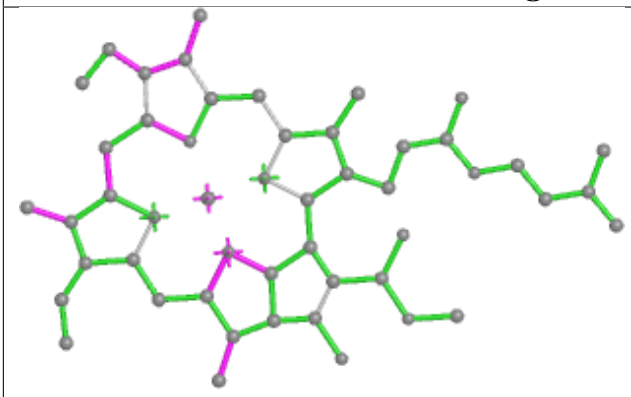


Rings

Ligand CLA B 831



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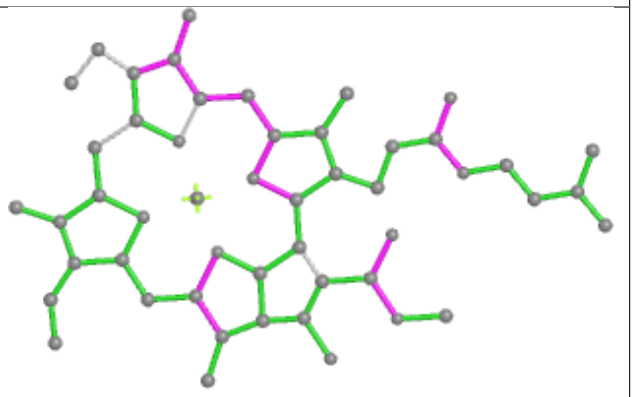
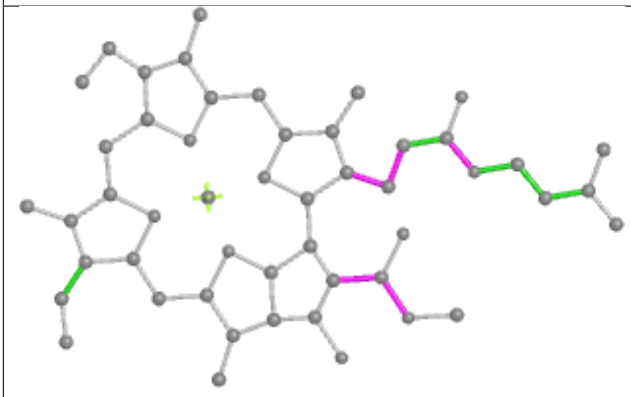


Bond angles



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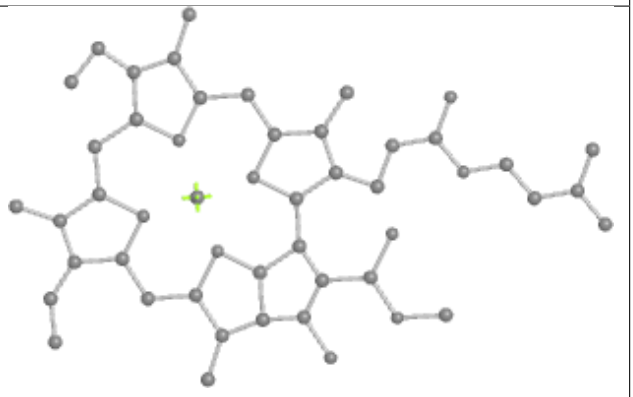
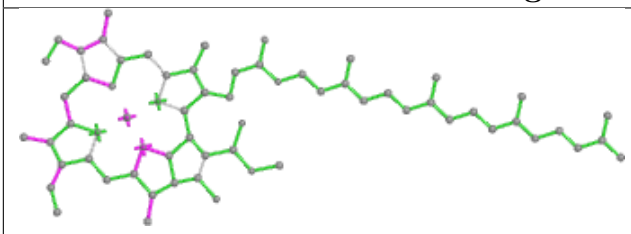
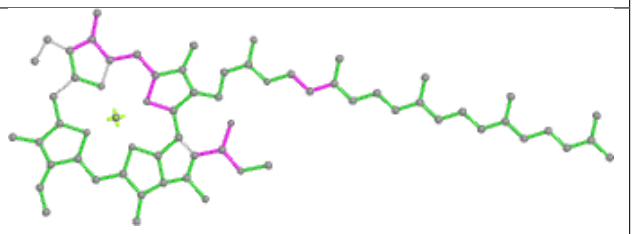


Rings

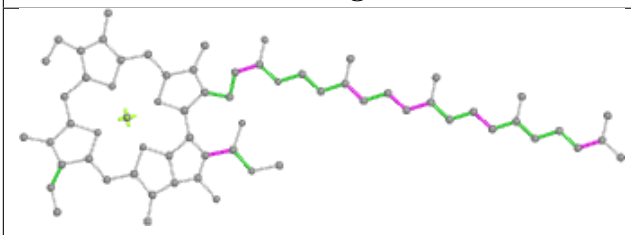
Ligand CLA B 801



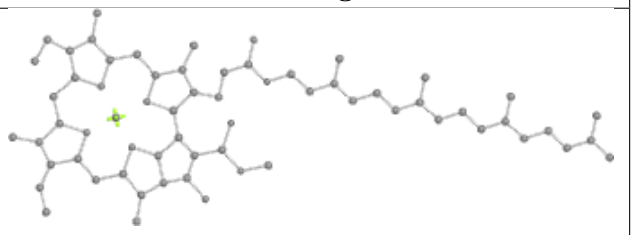
Bond lengths



Bond angles

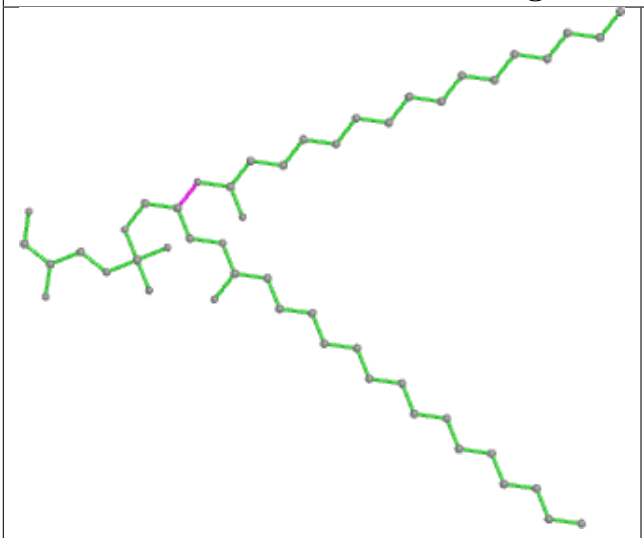


Torsions



Rings

Ligand LHG 5 318



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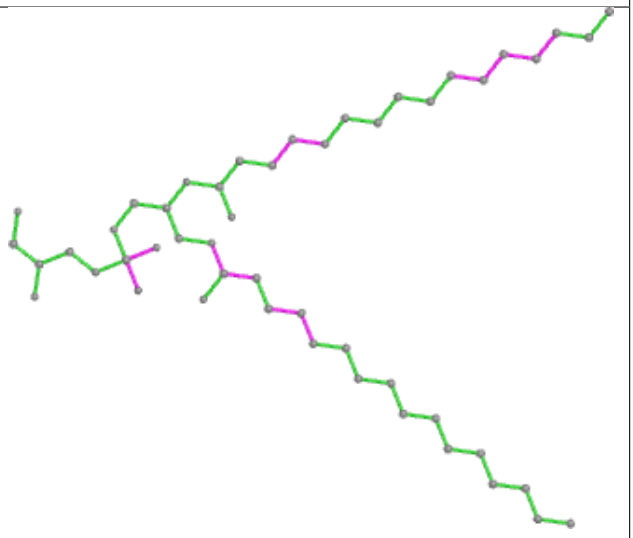
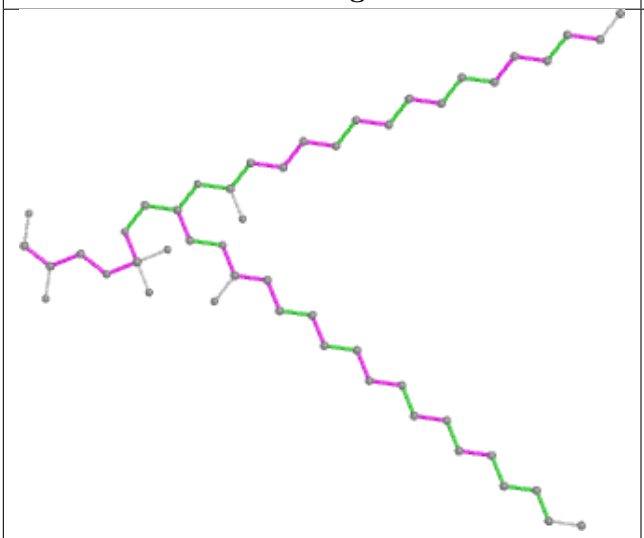
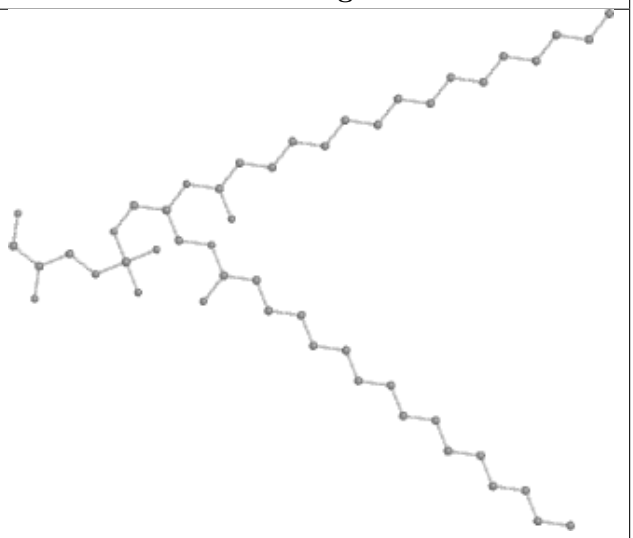


Bond angles

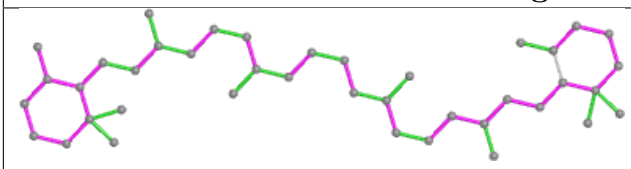


Torsions

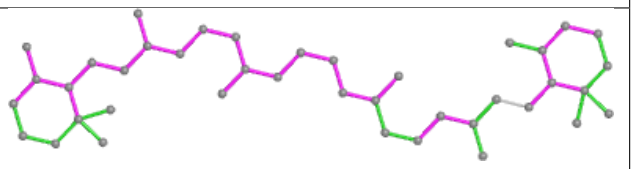


Rings

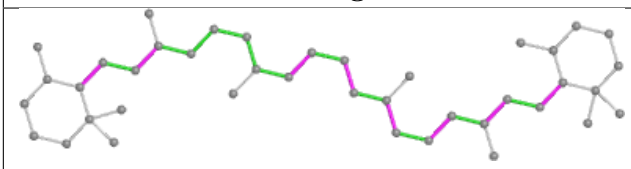
Ligand 8CT 8 318



Bond lengths



Bond angles



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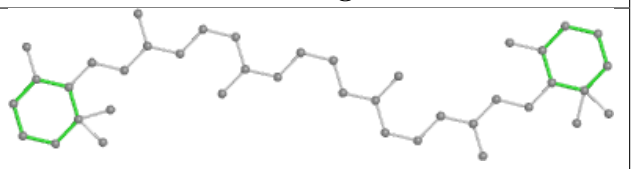
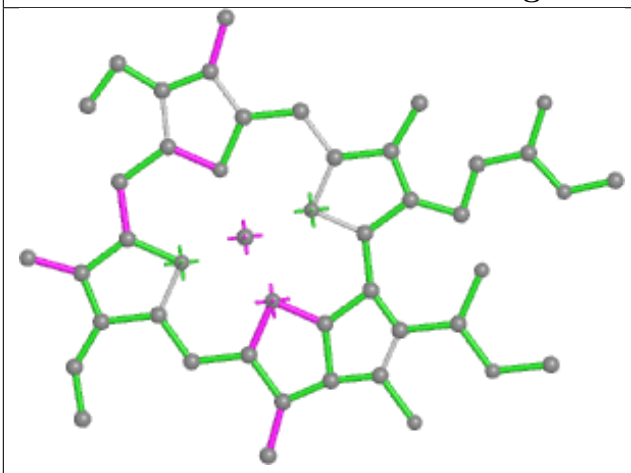


Rings

Ligand CLA K 102



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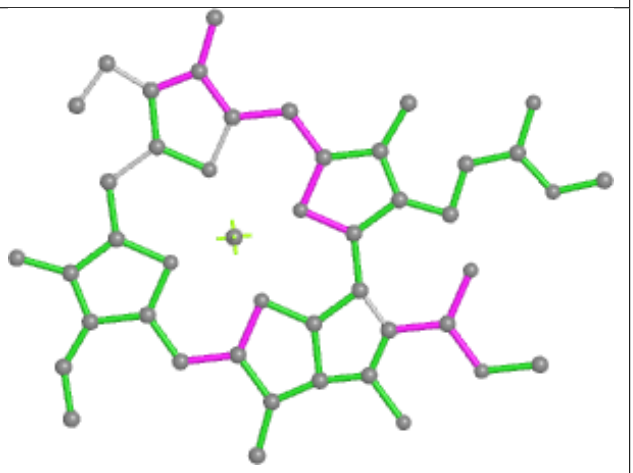

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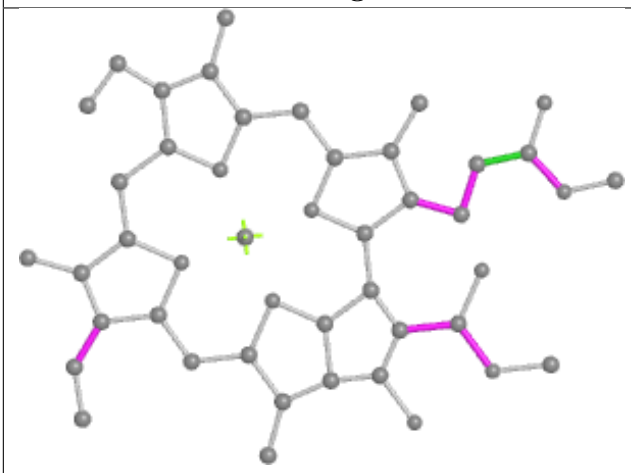

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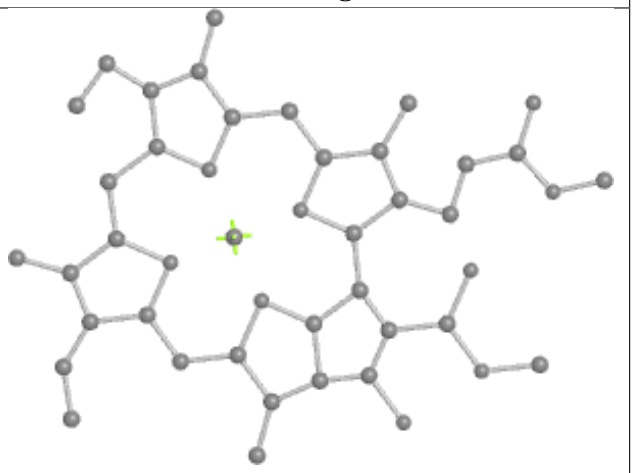
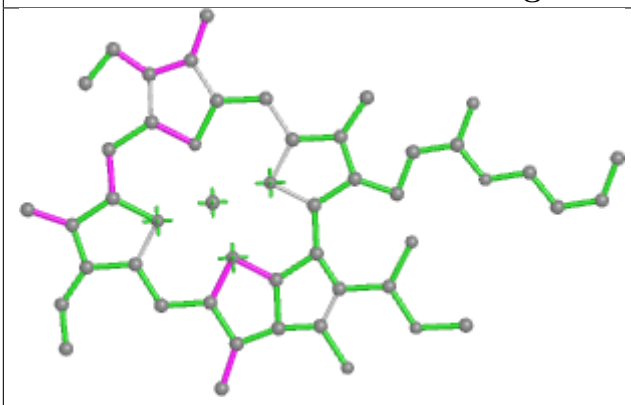


Rings

Ligand CLA A 822



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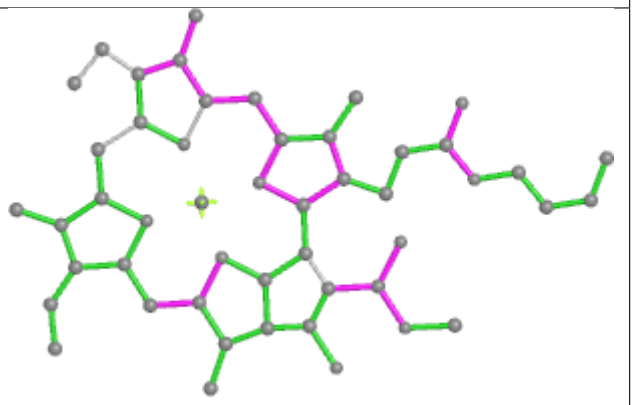
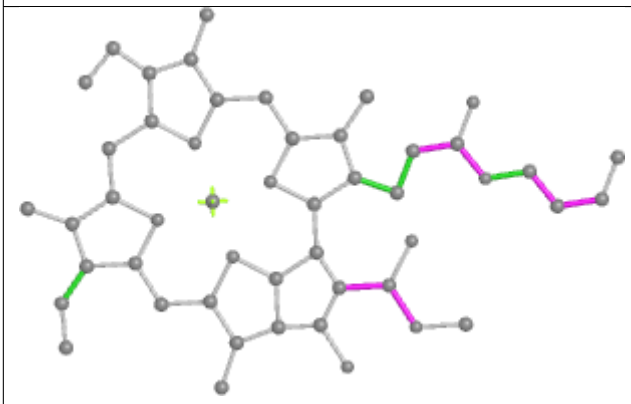


Bond angles



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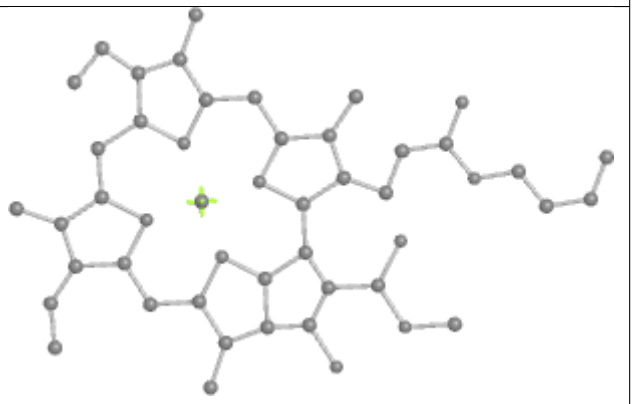
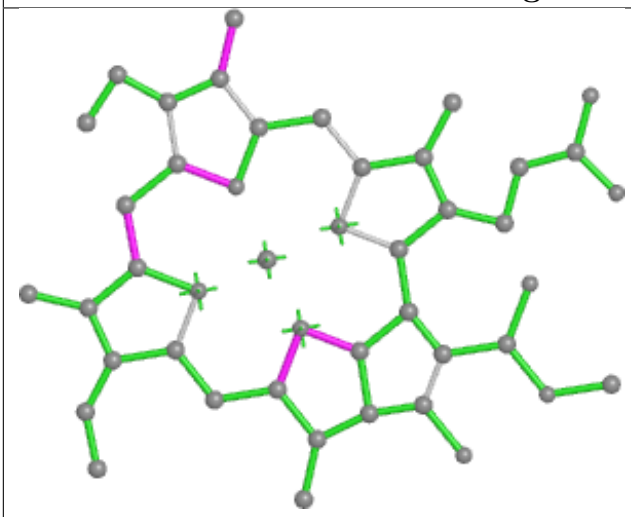


Rings

Ligand CLA G 101



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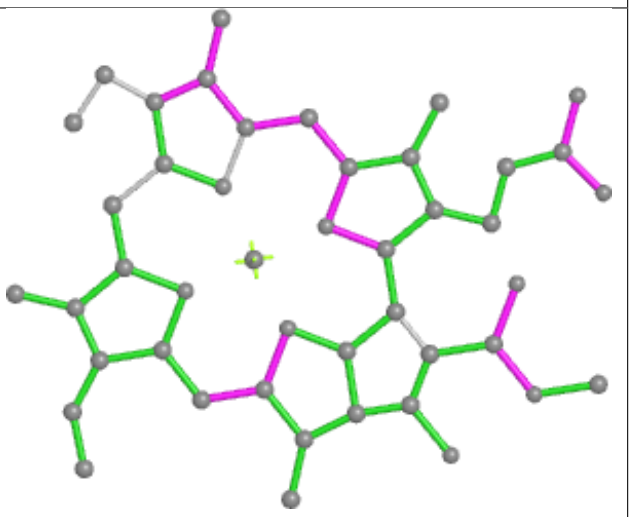
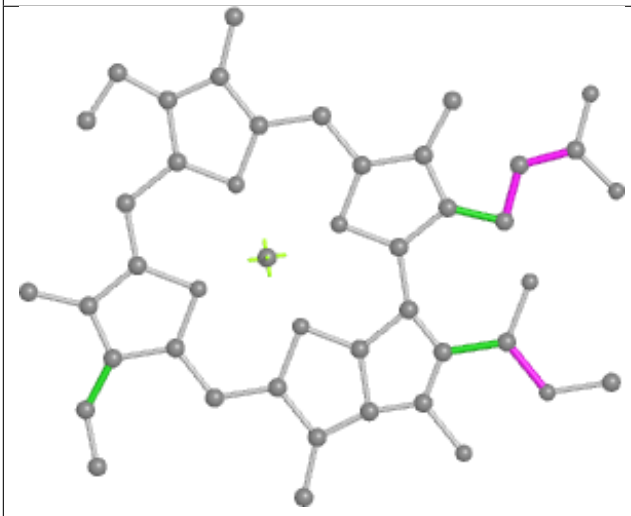


Bond angles



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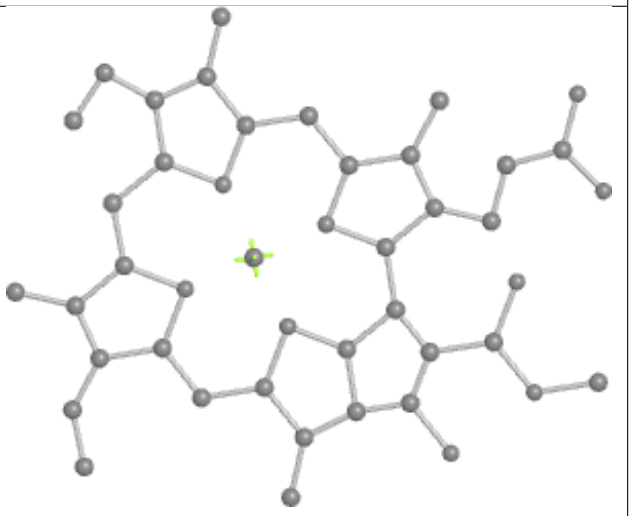

Rings

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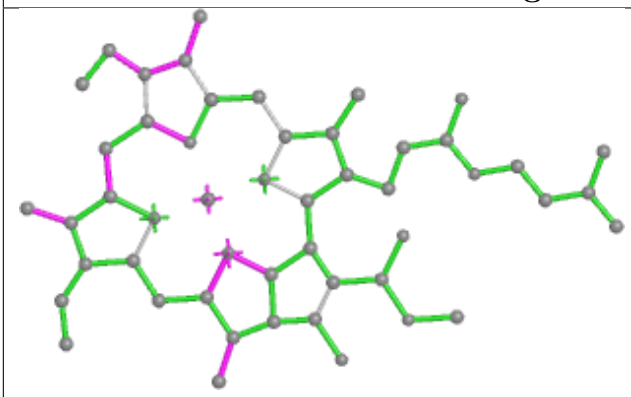
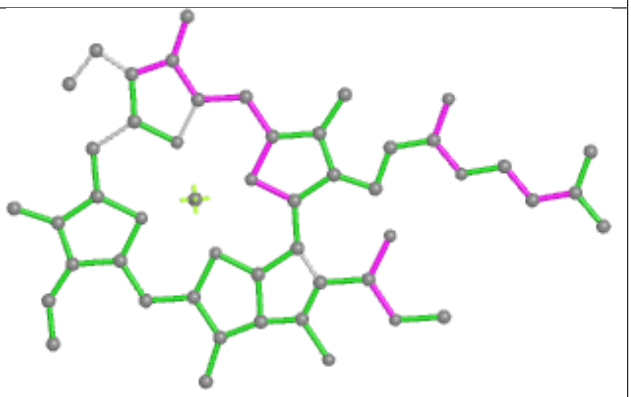
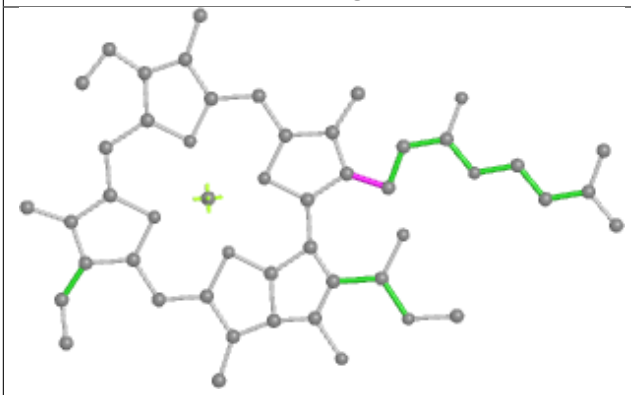
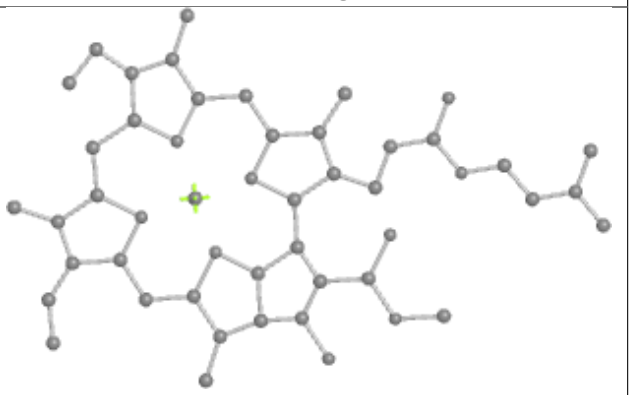
 Bond lengths	 Bond angles
 Torsions	 Rings

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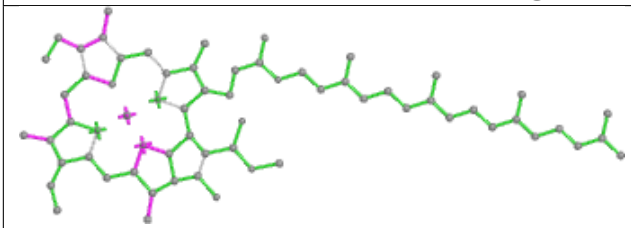
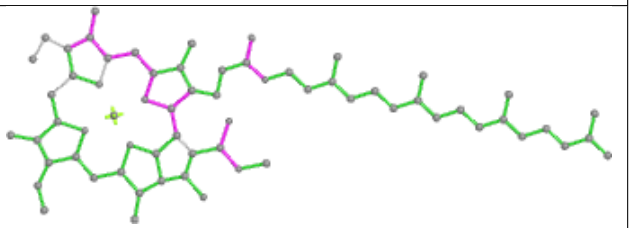
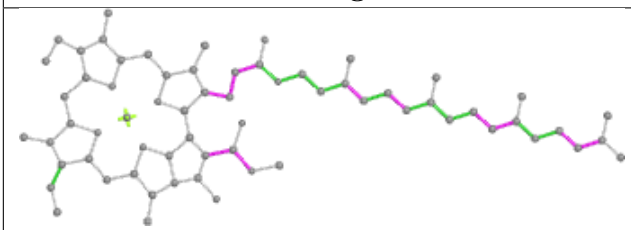
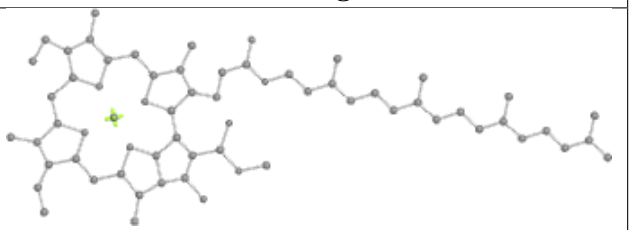
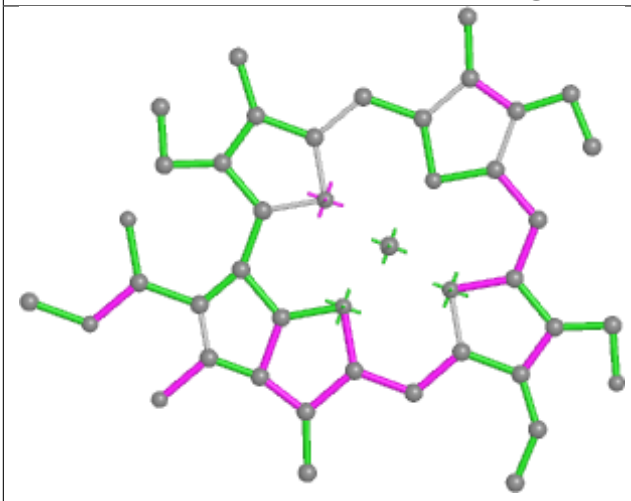
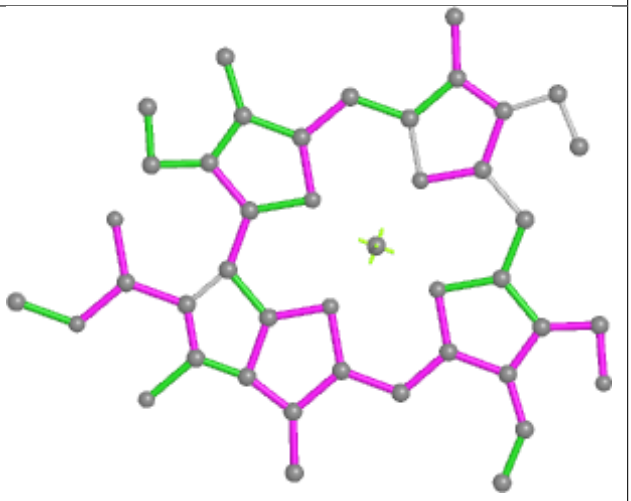
 Bond lengths	 Bond angles
 Torsions	 Rings

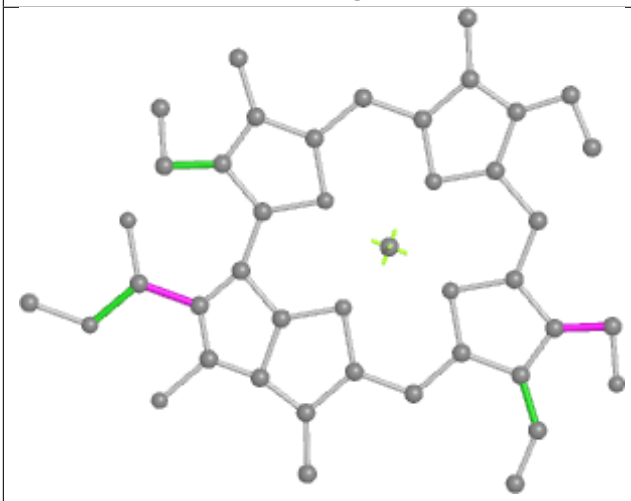
Ligand CHL 2 305



Bond lengths



Bond angles



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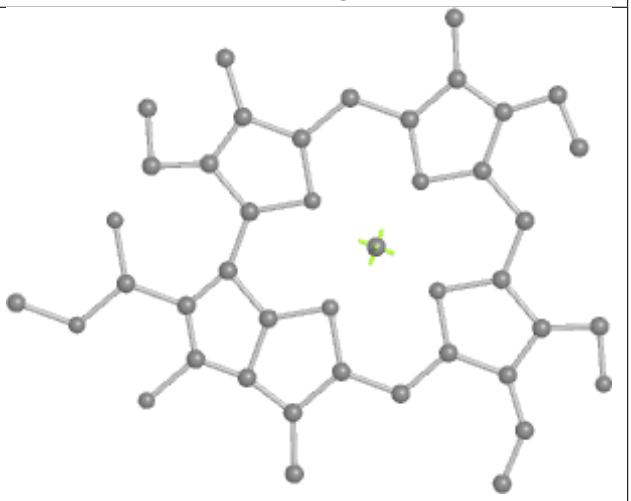
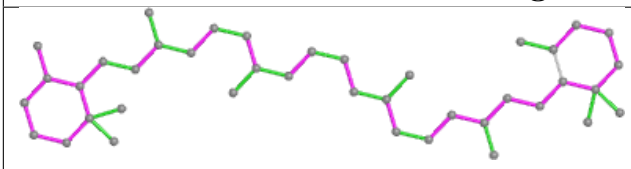
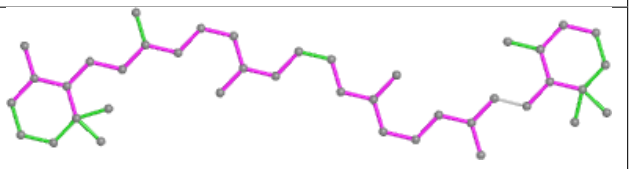


Rings

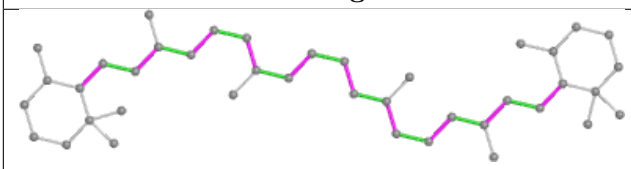
Ligand 8CT L 206



Bond lengths



Bond angles



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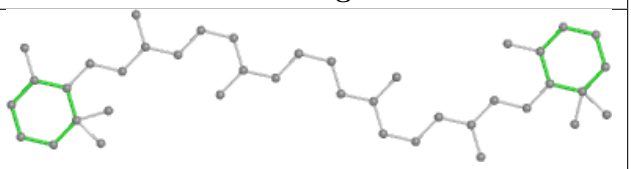
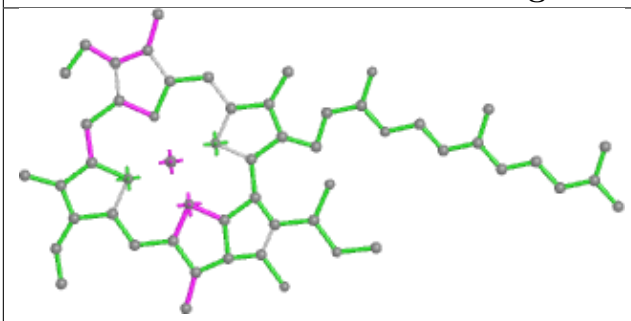


Rings

Ligand CLA 8 310



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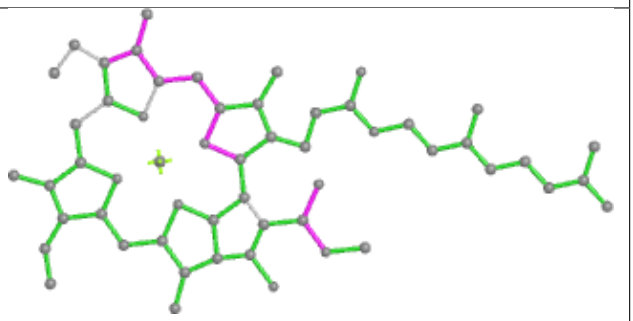
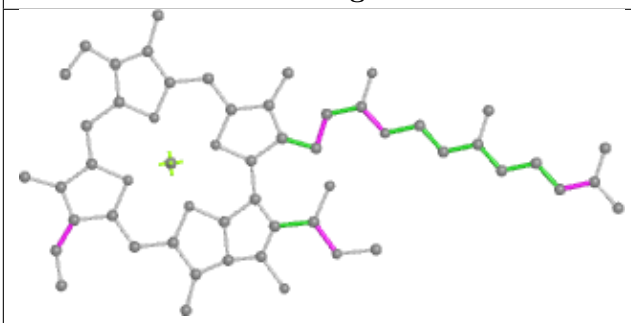


Bond angles



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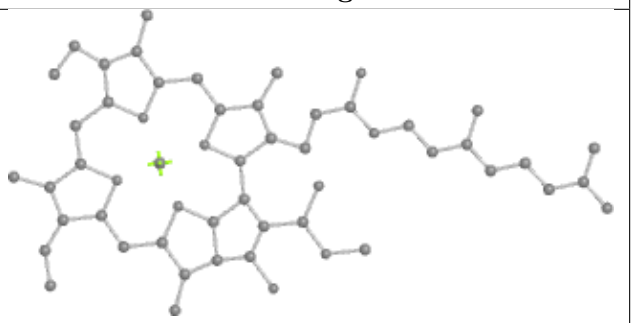
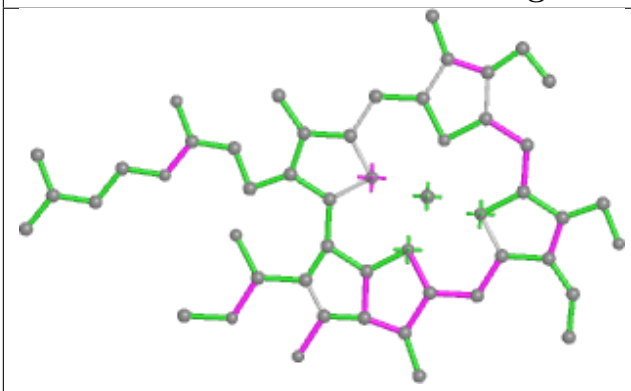


Rings

Ligand CHL 4 307



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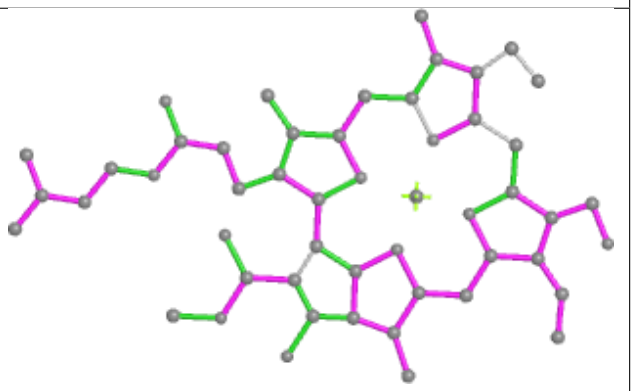
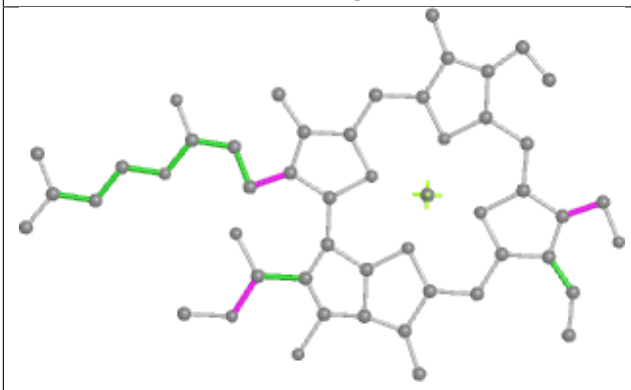


Bond angles



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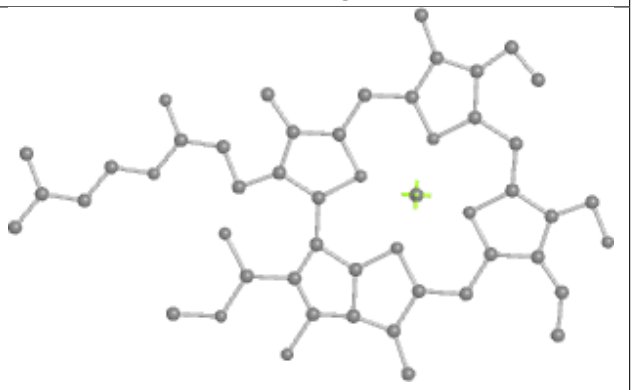
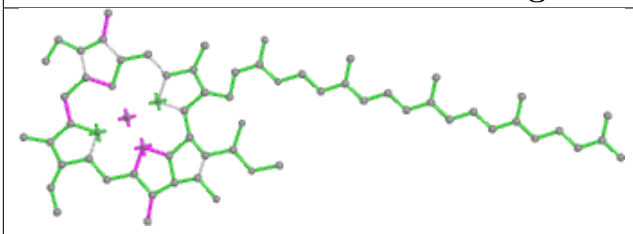


Rings

Ligand CLA 8 315



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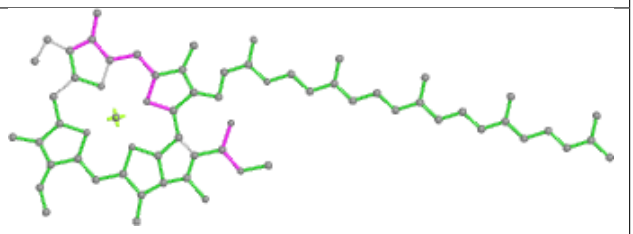
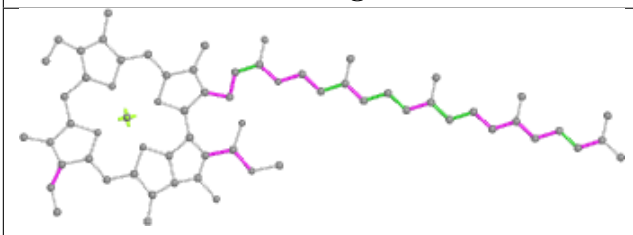


Bond angles



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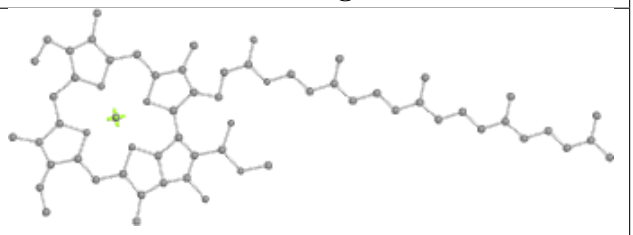
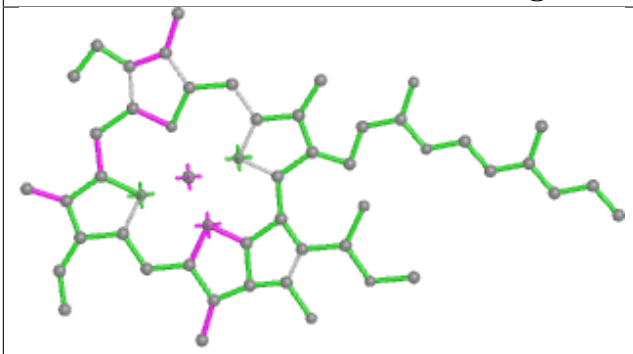


Rings

Ligand CLA 1 303



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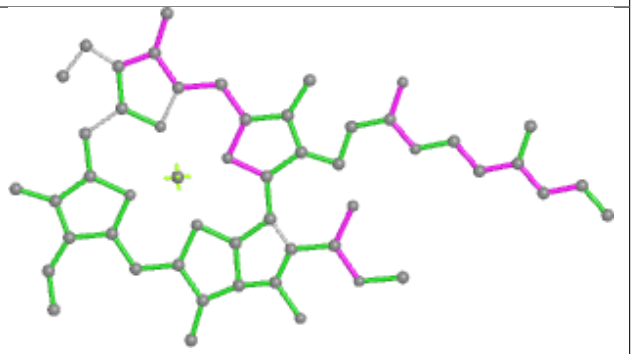
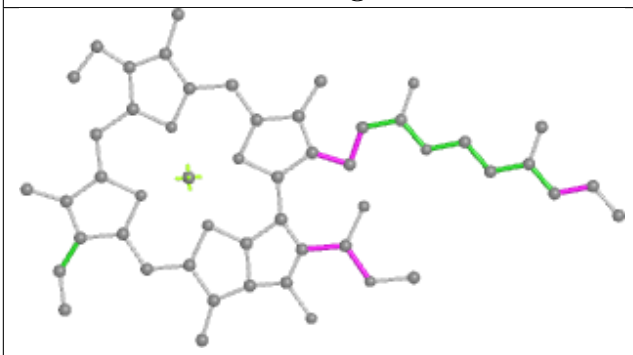


Bond angles



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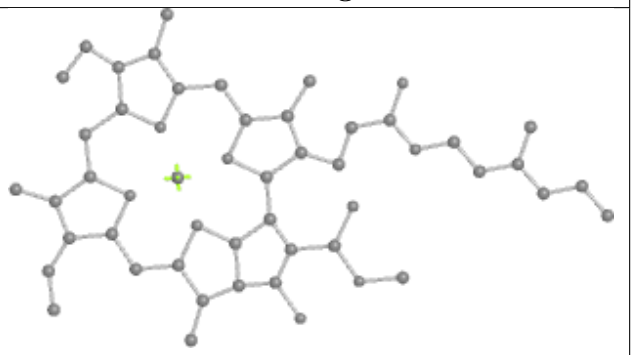
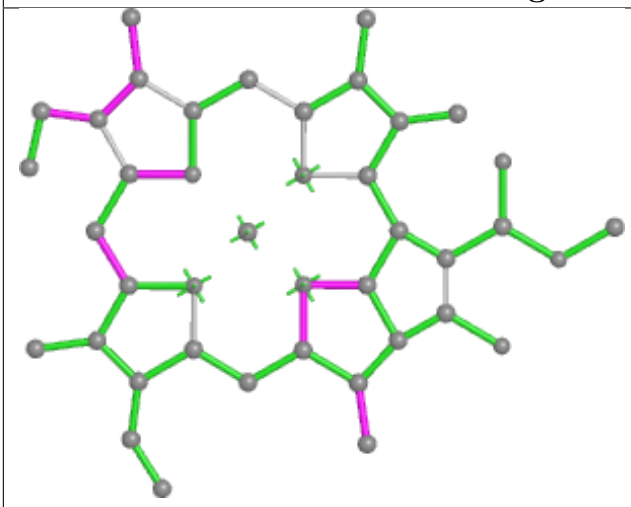


Rings

Ligand CLA 9 310



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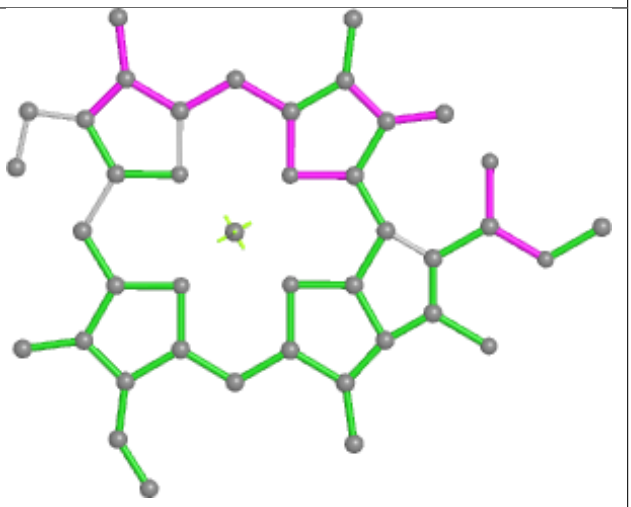
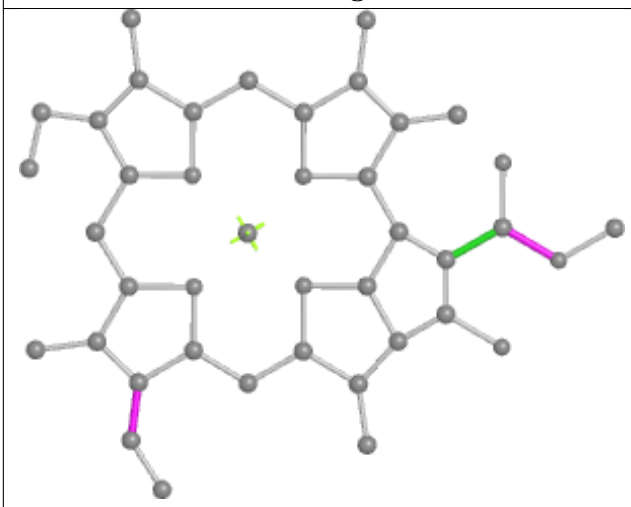
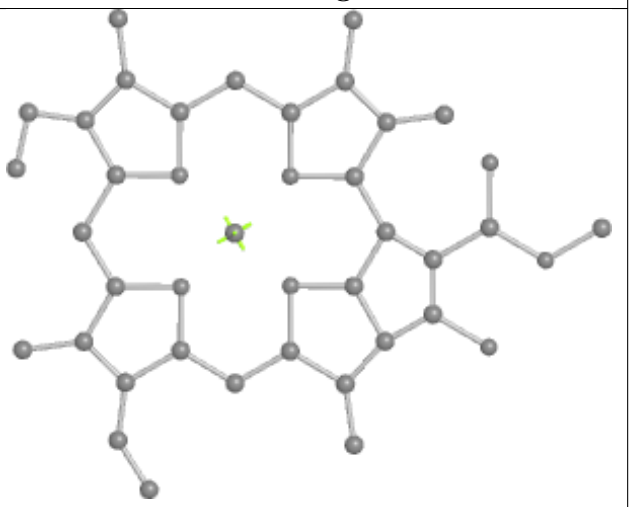


Bond angles

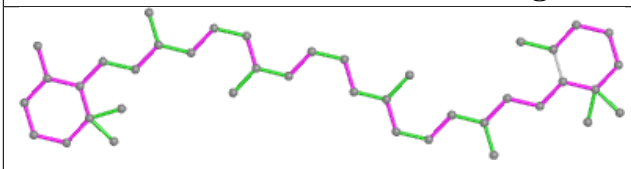


Torsions



Rings

Ligand 8CT 7 301



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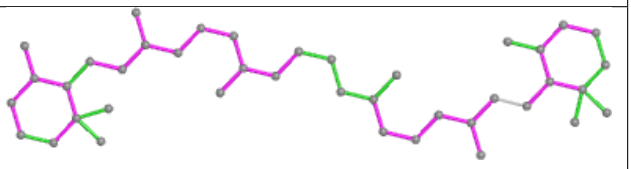
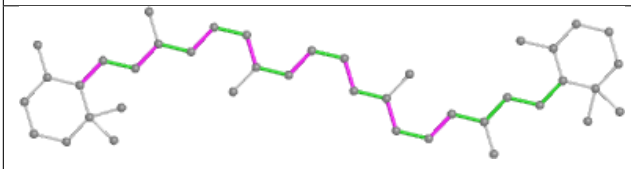


Bond angles



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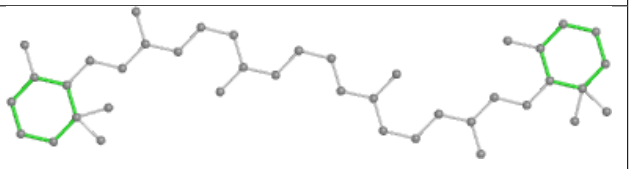
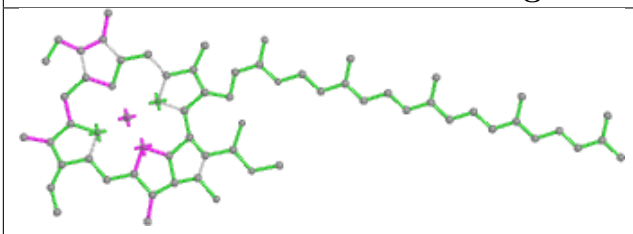


Rings

Ligand CLA A 832



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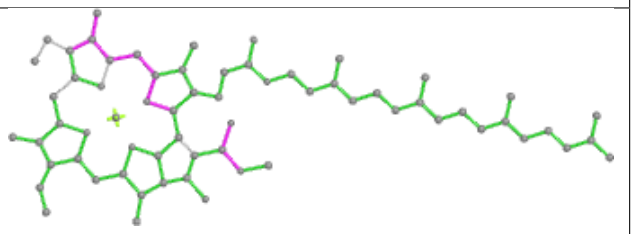
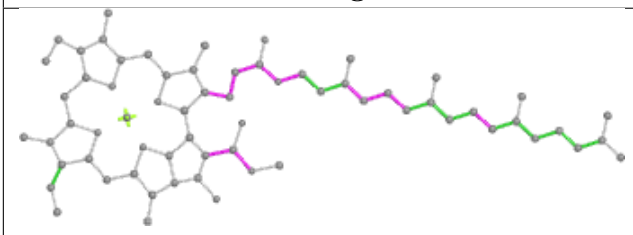


Bond angles



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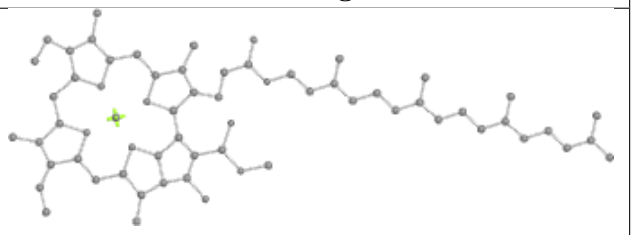

Rings

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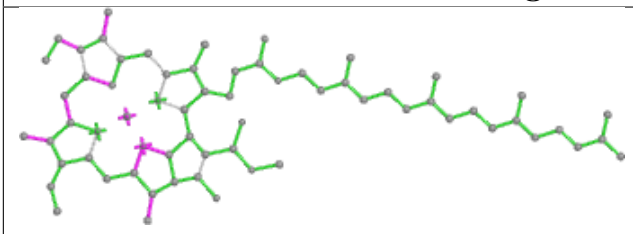

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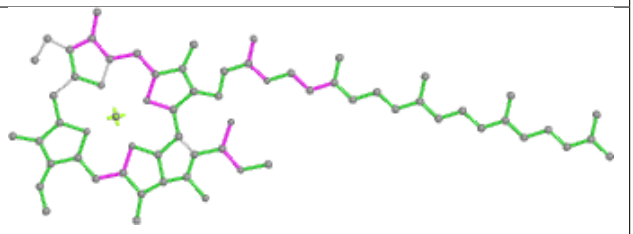
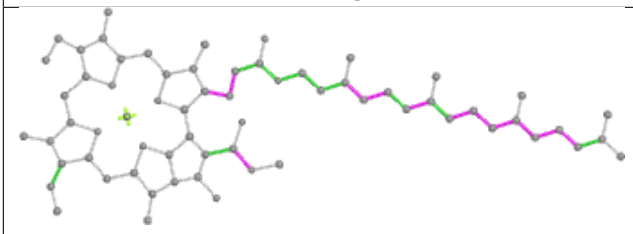


Bond angles



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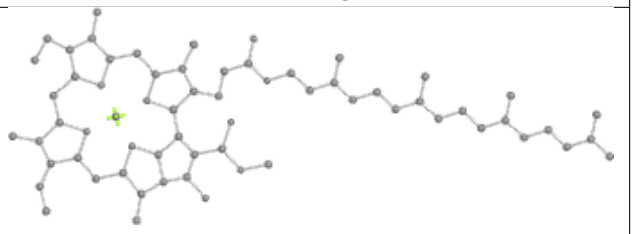
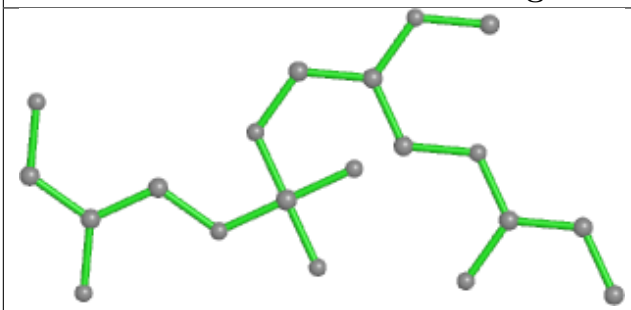


Rings

Ligand LHG 7 322



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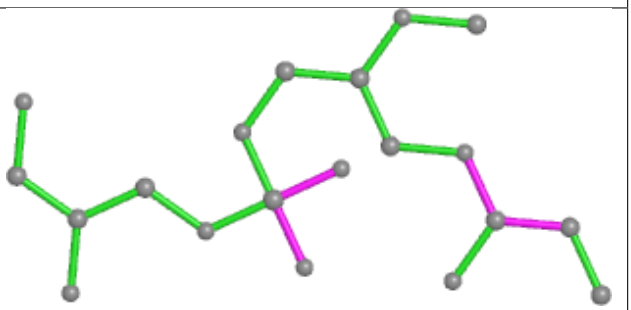
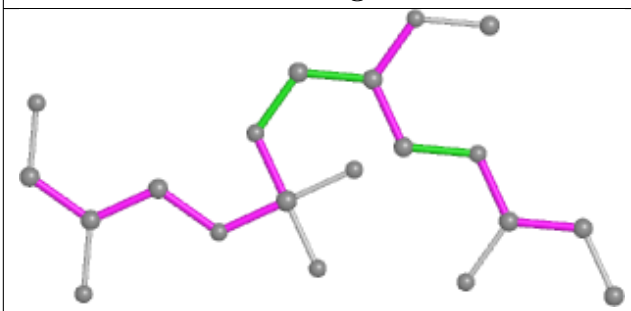


Bond angles



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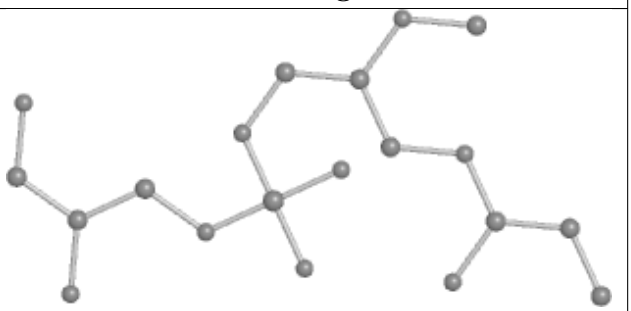
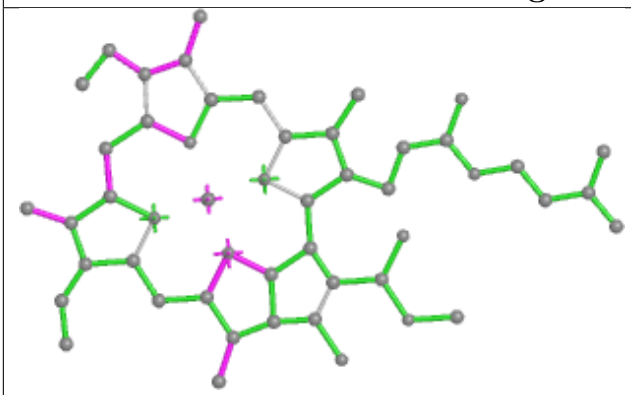


Rings

Ligand CLA 4 308



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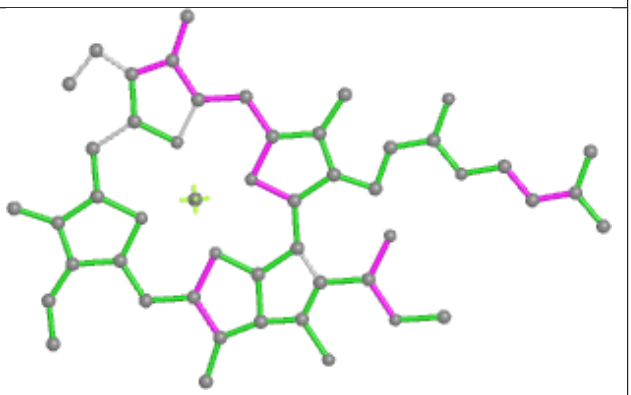
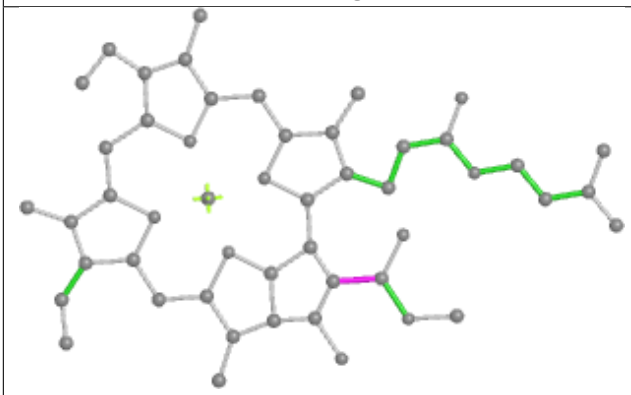


Bond angles



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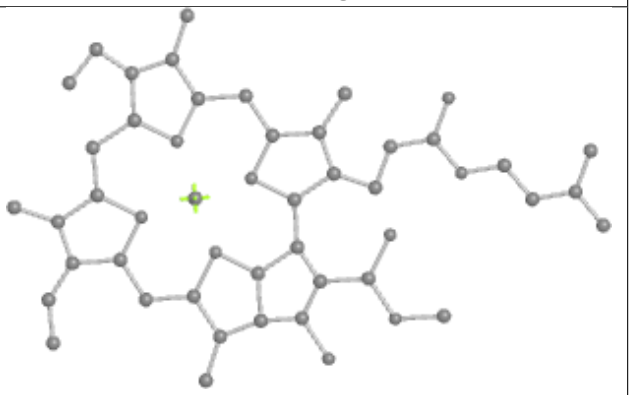
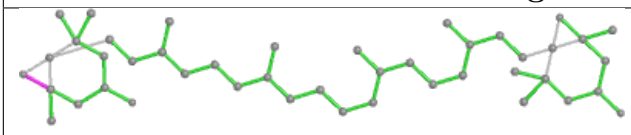
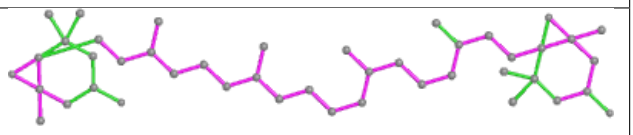
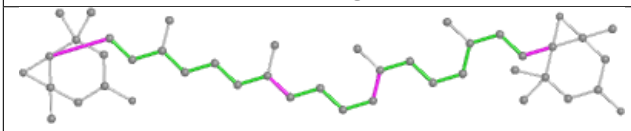
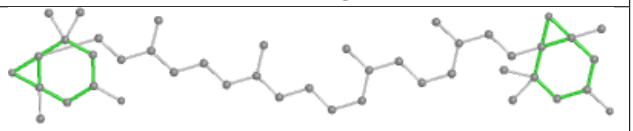


Rings

Ligand XAT 5 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

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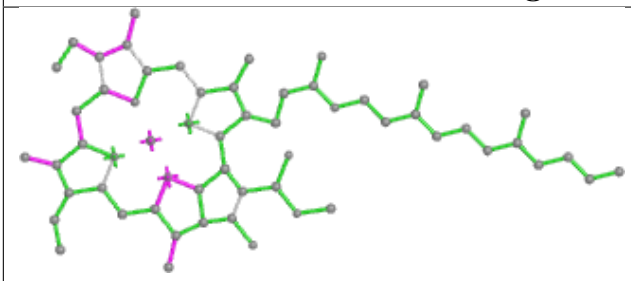
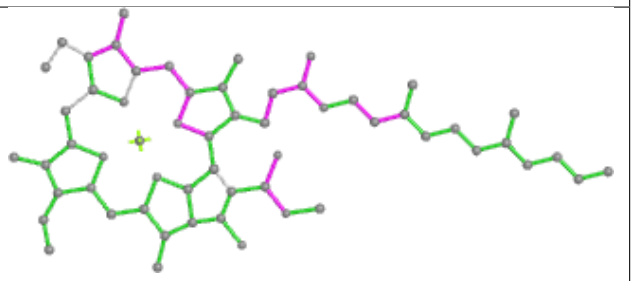
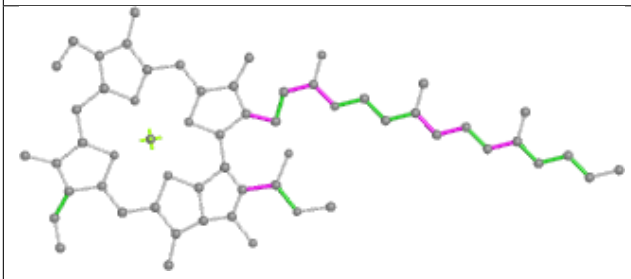
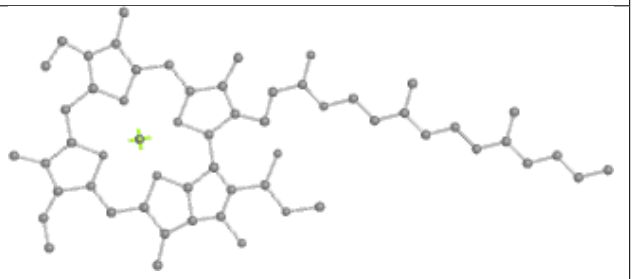
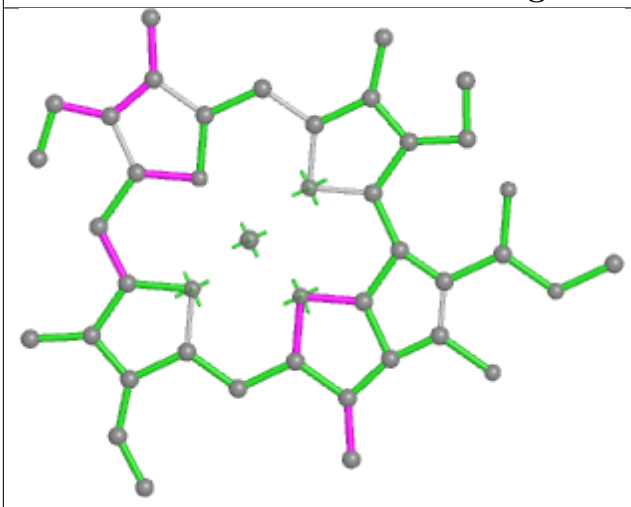
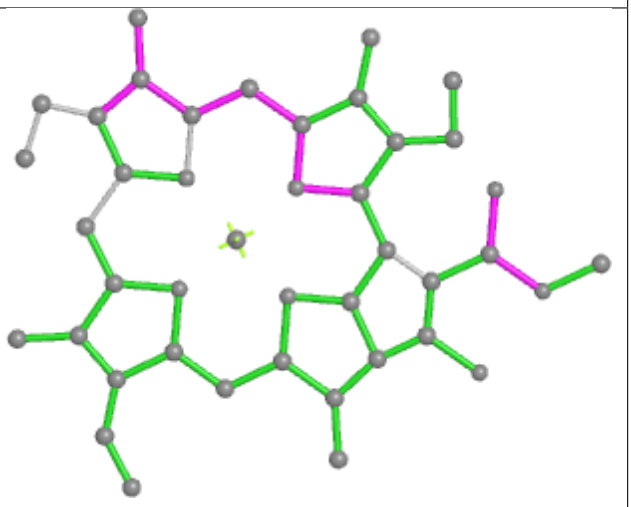
 Bond lengths	 Bond angles
 Torsions	 Rings

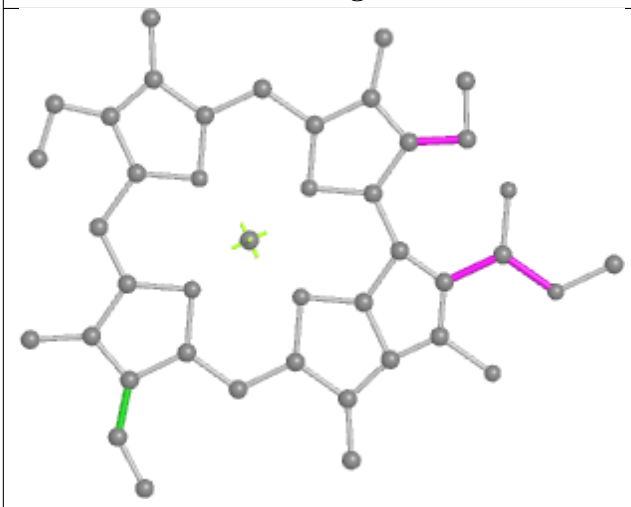
Ligand CLA J 103



Bond lengths



Bond angles



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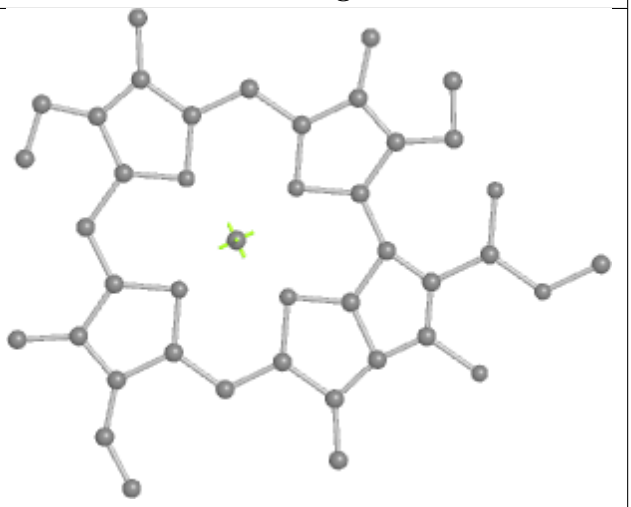
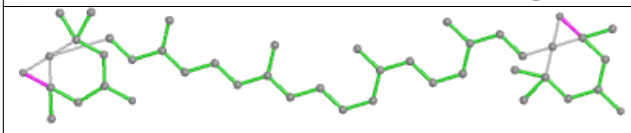


Rings

Ligand XAT 3 315



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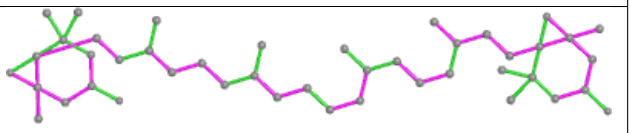
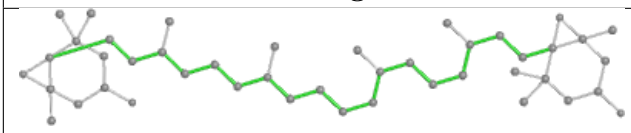


Bond angles



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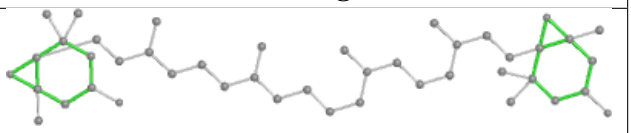
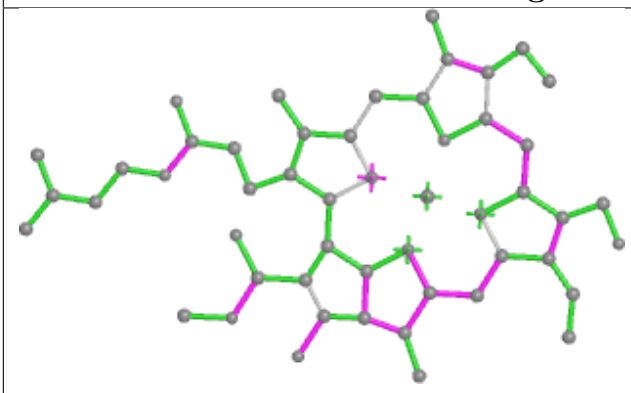


Rings

Ligand CHL 8 306



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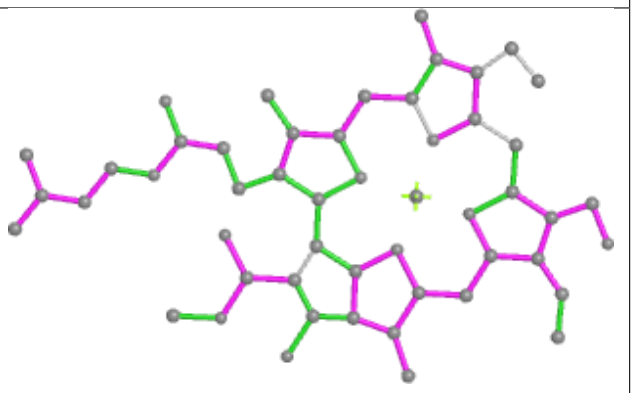
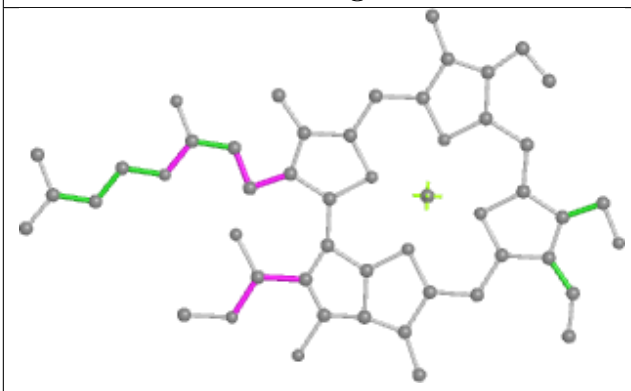


Bond angles



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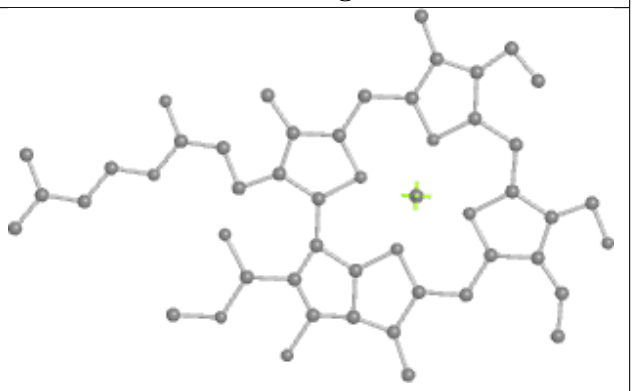
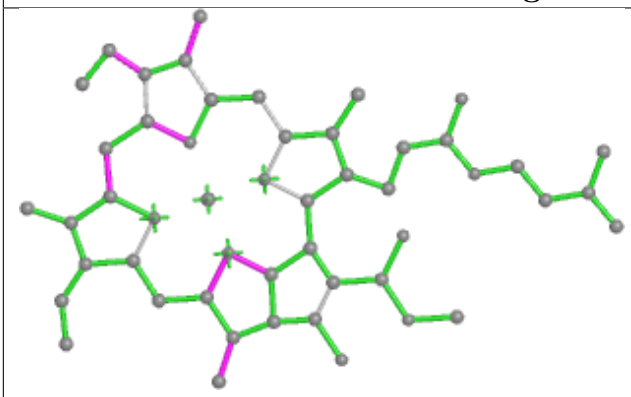
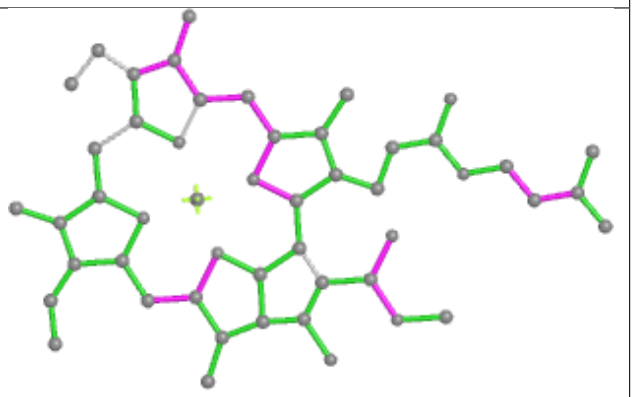


Rings

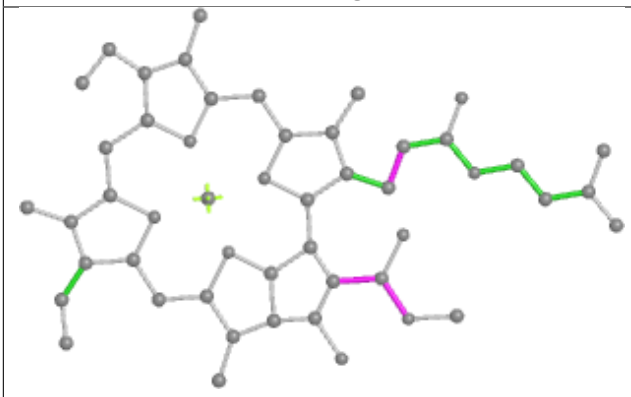
Ligand CLA G 102



Bond lengths



Bond angles



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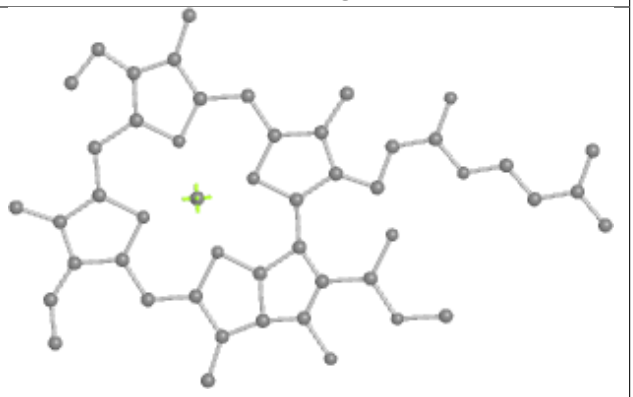
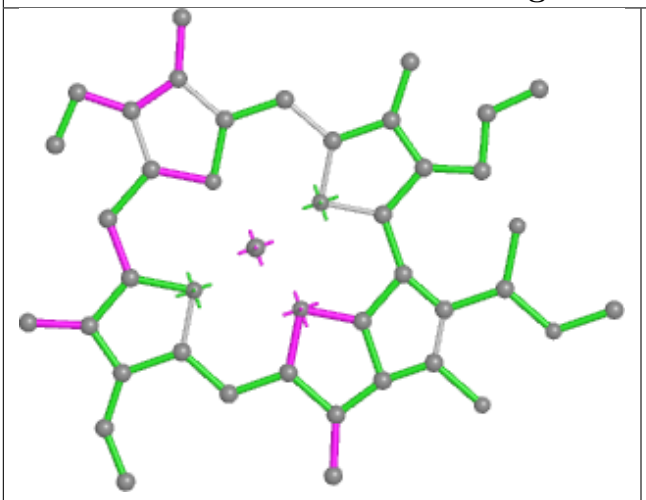


Rings

Ligand CLA 2 313



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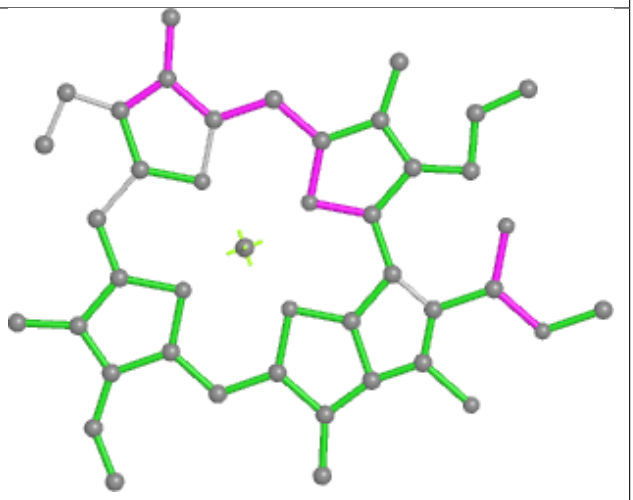
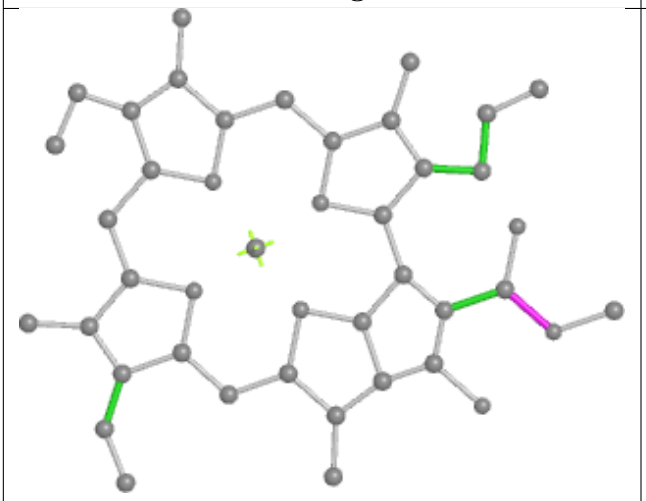


Bond angles



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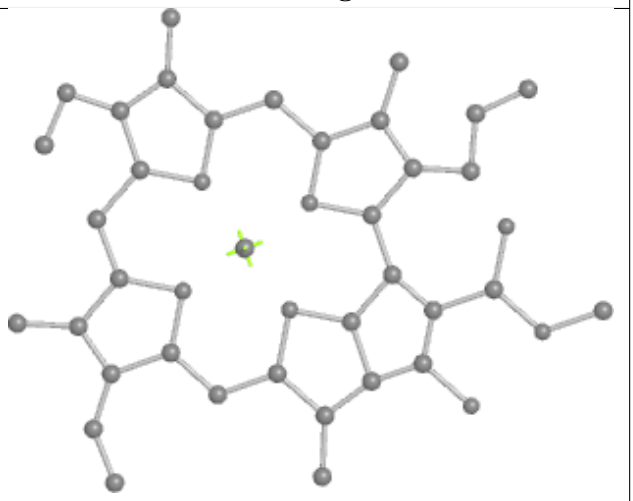
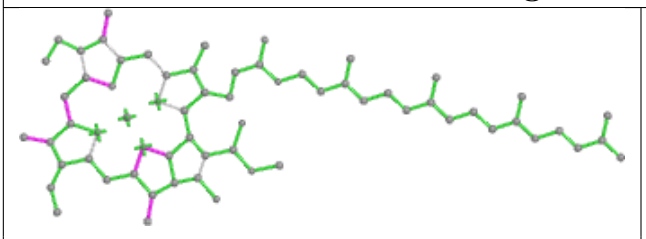
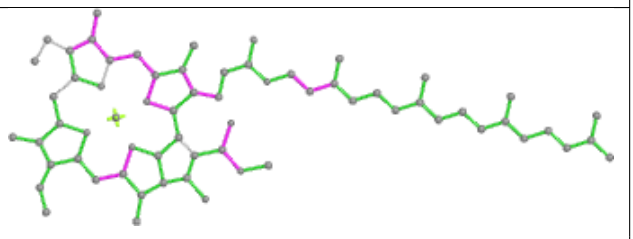


Rings

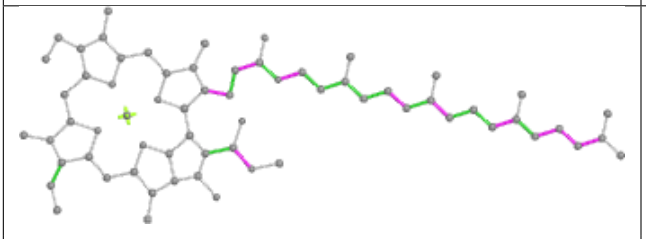
Ligand CLA H 201



Bond lengths



Bond angles



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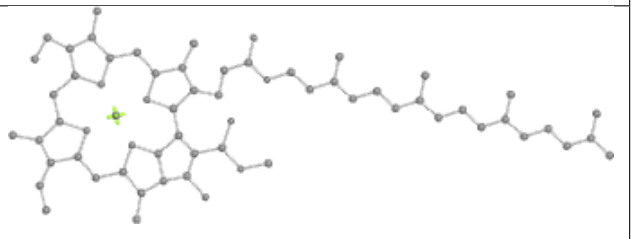
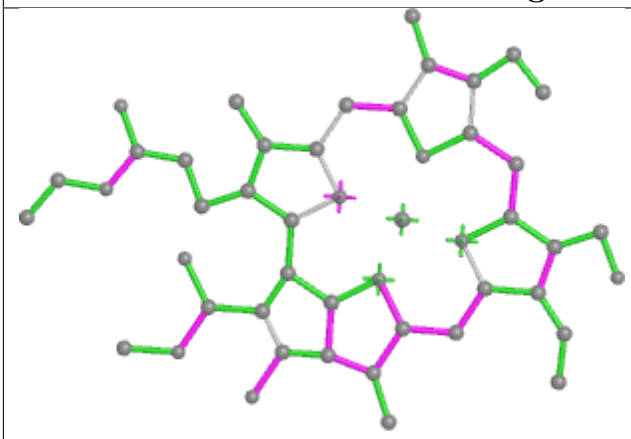


Rings

Ligand CHL 2 306



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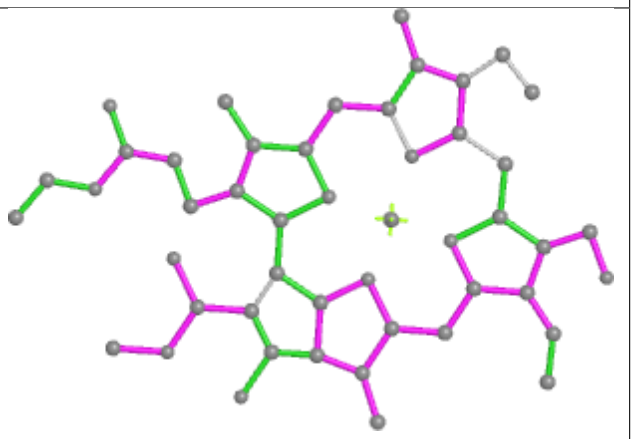

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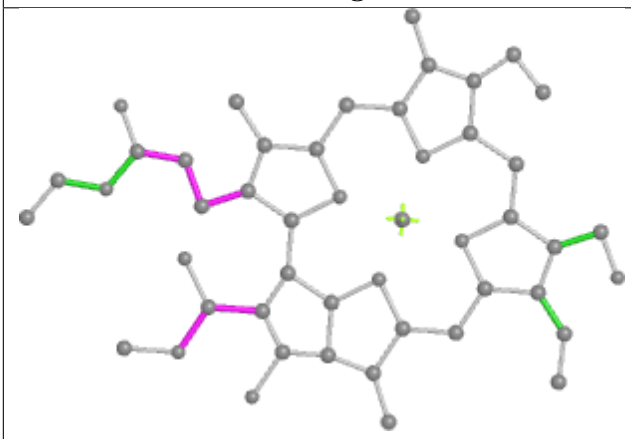

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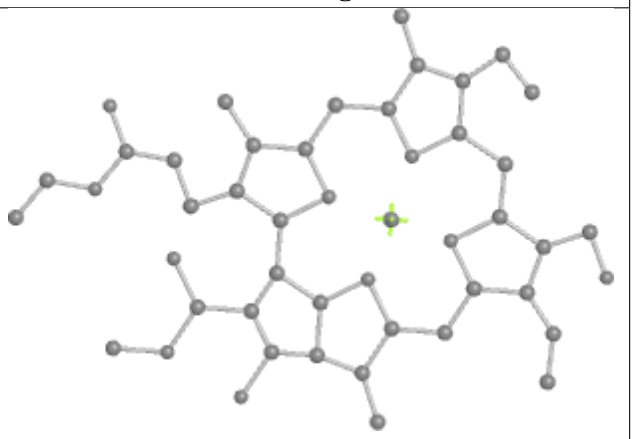
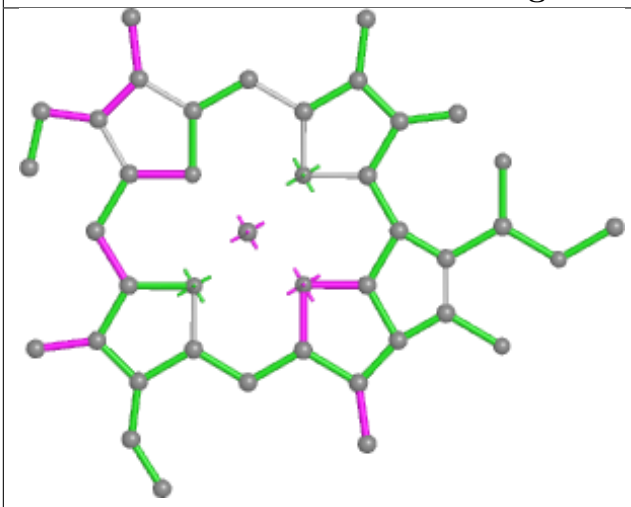


Rings

Ligand CLA 1 309



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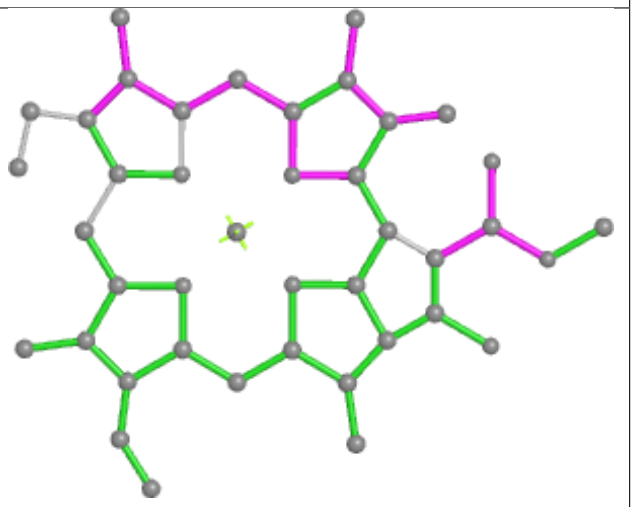

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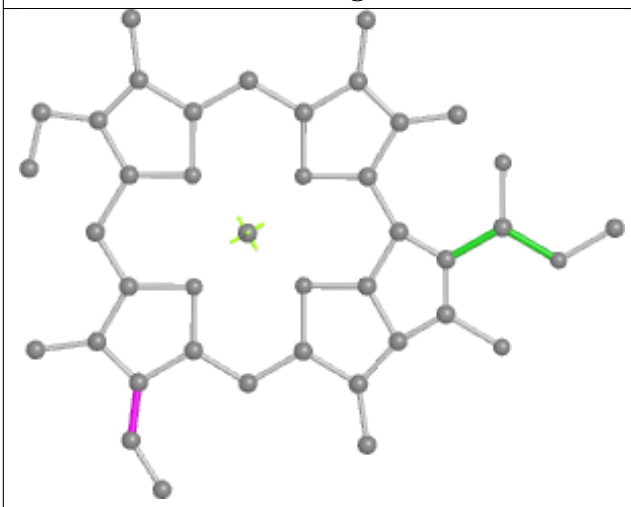

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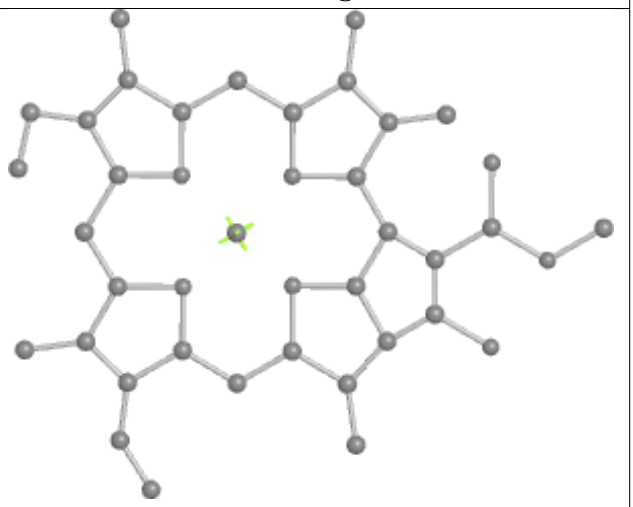
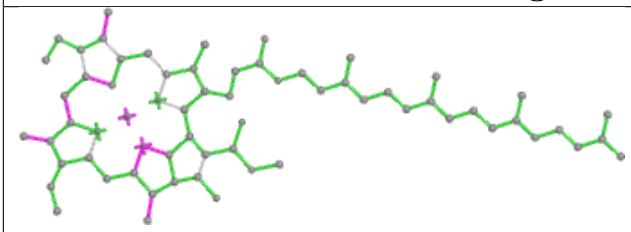


Rings

Ligand CLA 0 303



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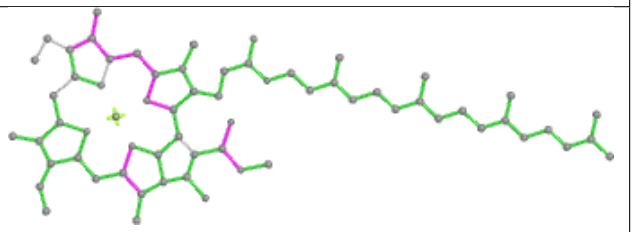

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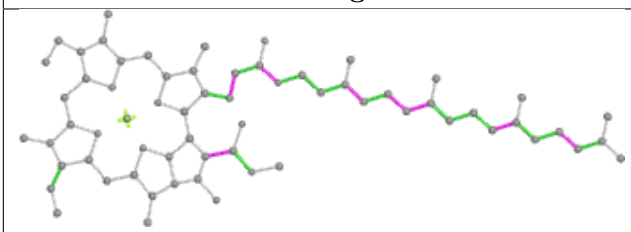

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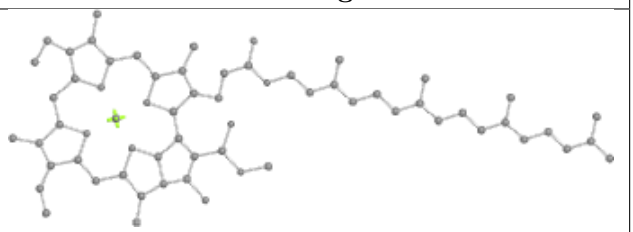
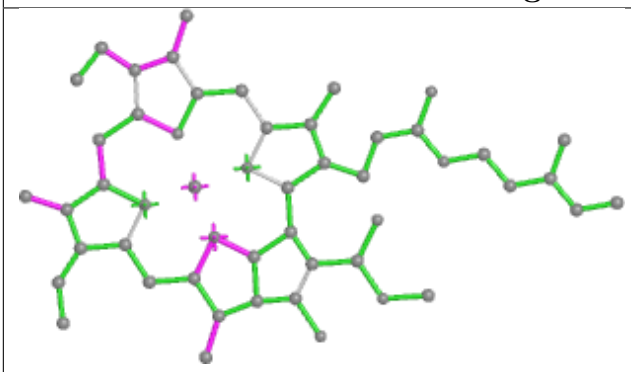


Rings

Ligand CLA A 836



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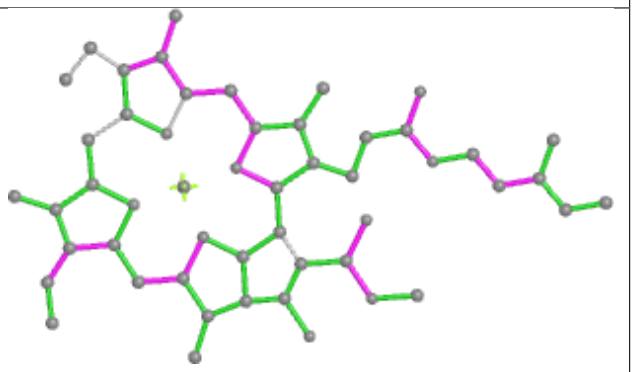

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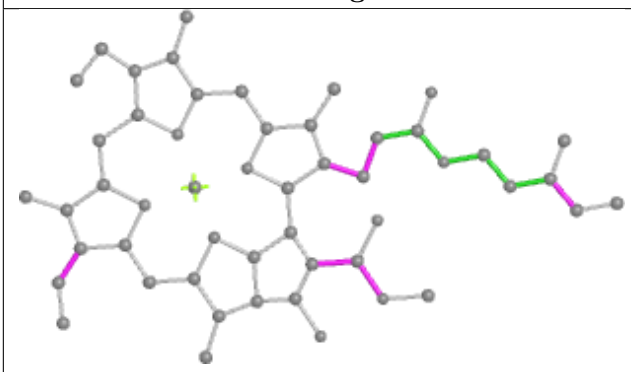

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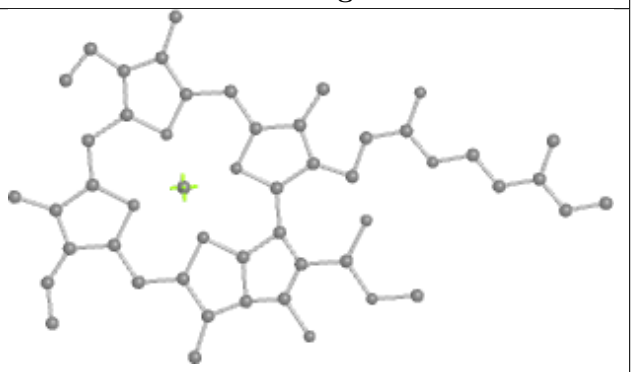
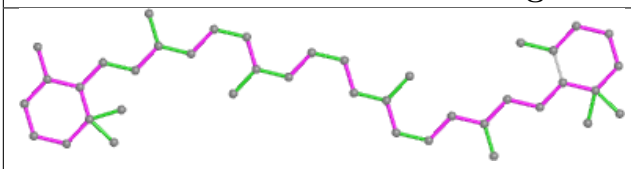


Rings

Ligand 8CT A 849



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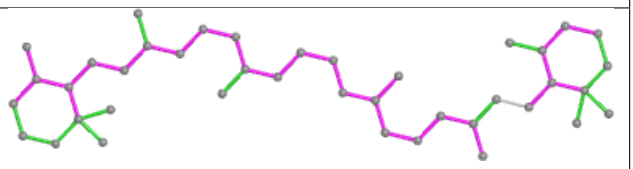

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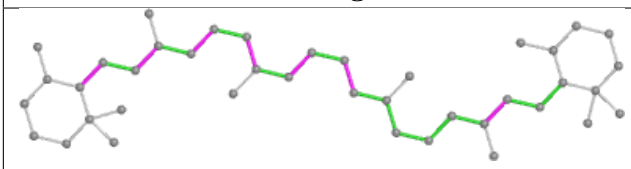

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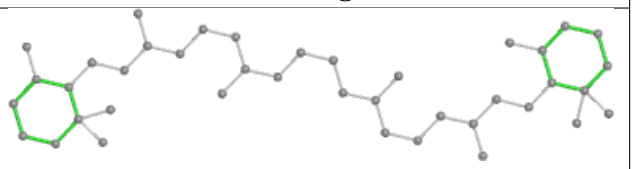
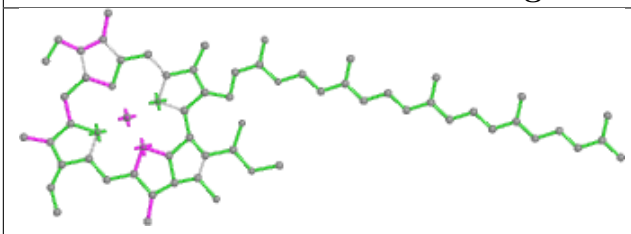


Rings

Ligand CLA B 808



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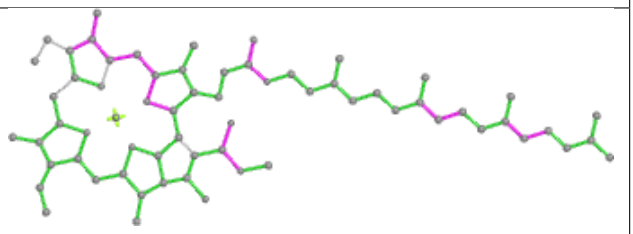
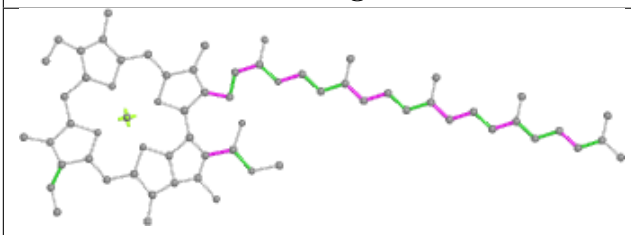


Bond angles



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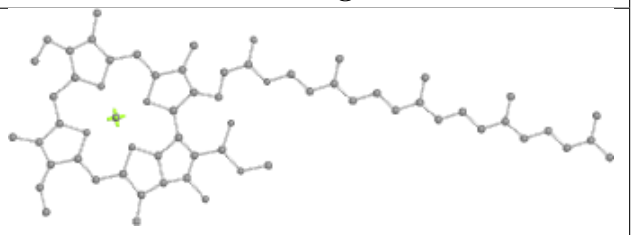
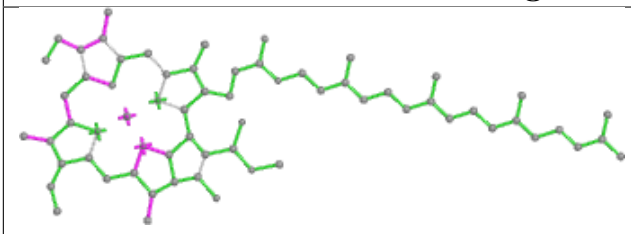


Rings

Ligand CLA B 841



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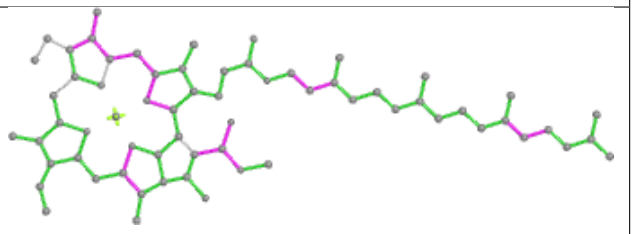
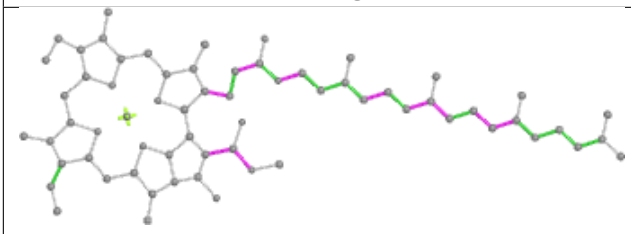


Bond angles



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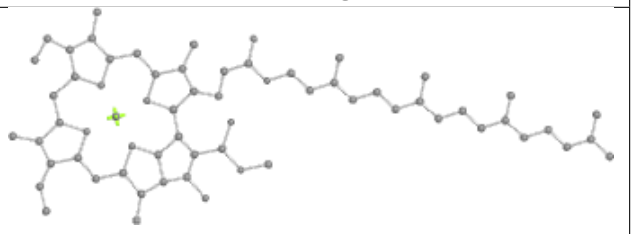
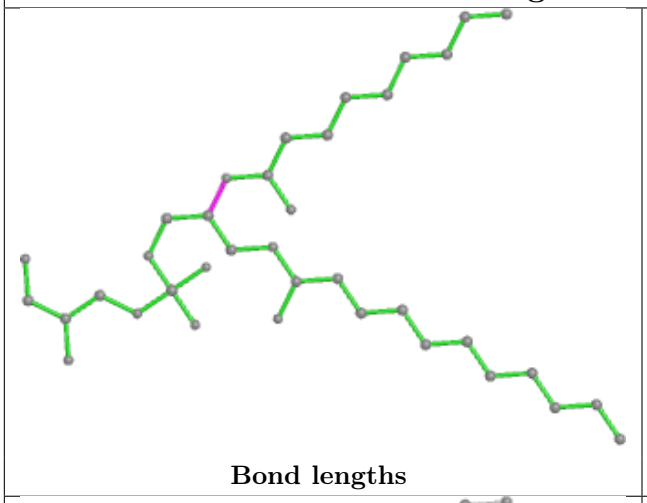


Rings

Ligand LHG 6 322



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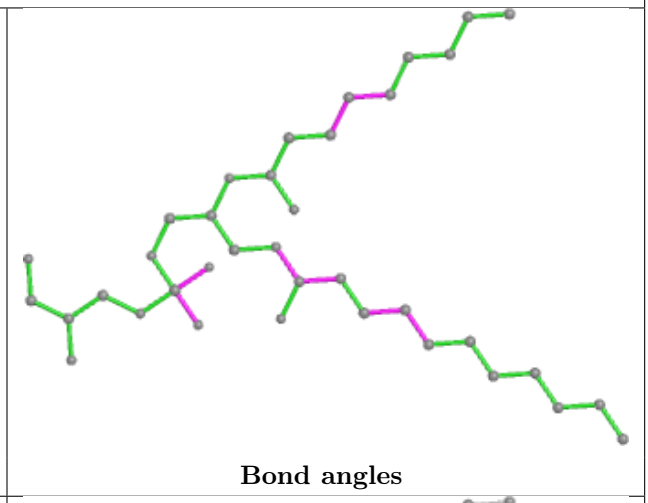
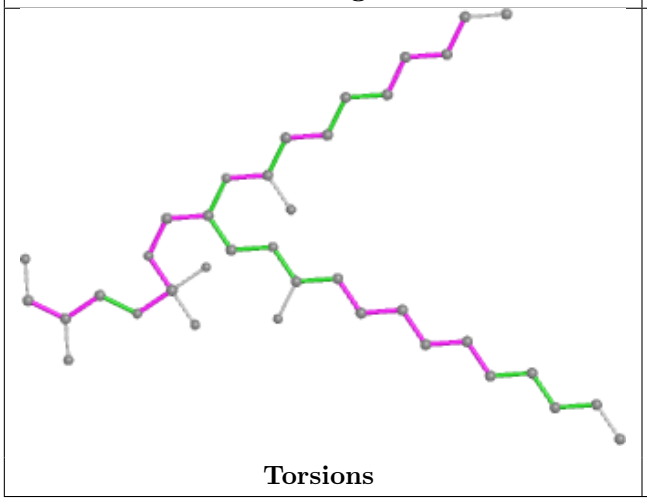


Bond angles



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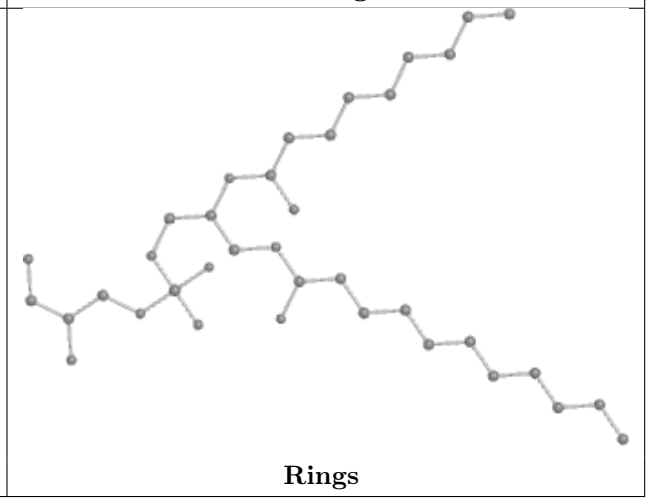
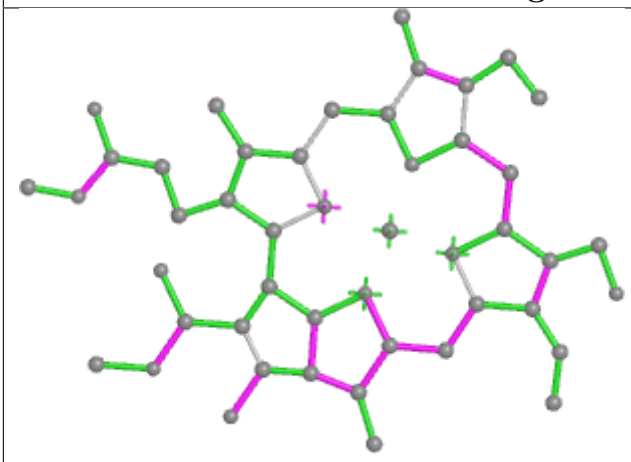


Rings

Ligand CHL 7 308



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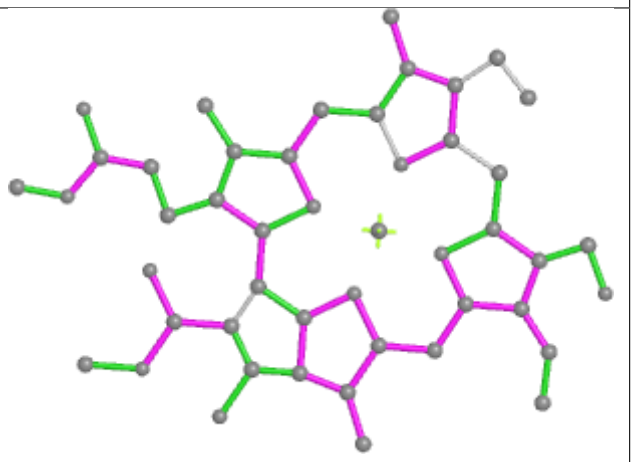

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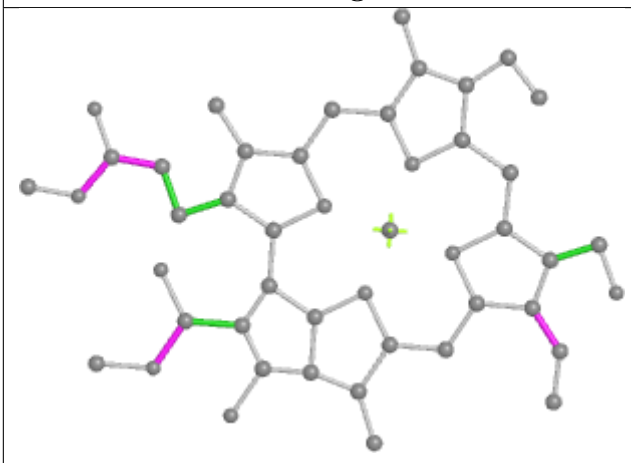

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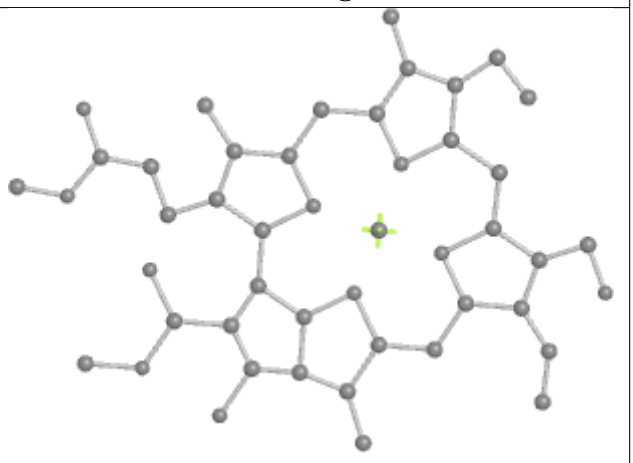
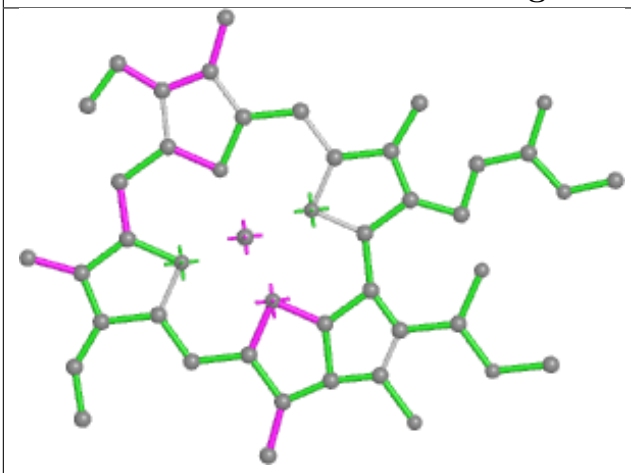


Rings

Ligand CLA 2 319



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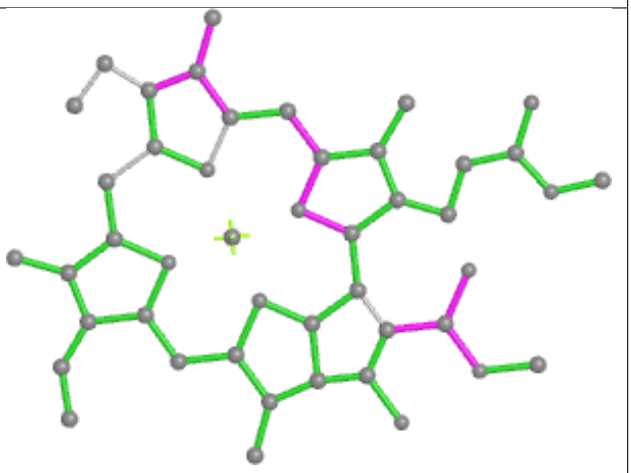
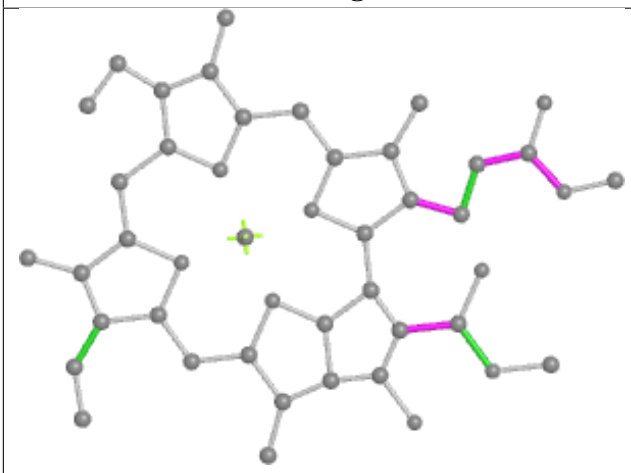


Bond angles



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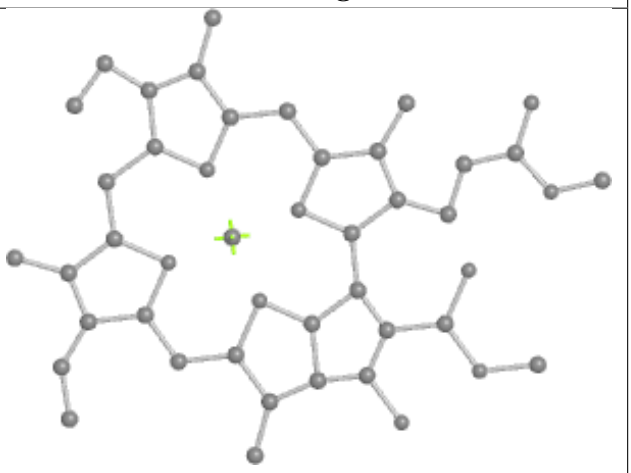
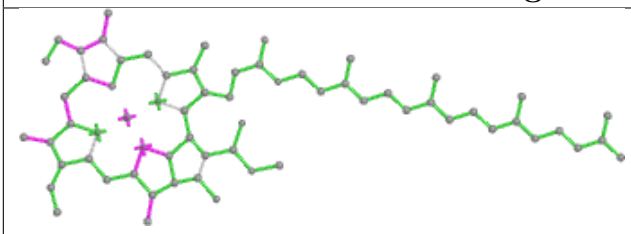


Rings

Ligand CLA B 825



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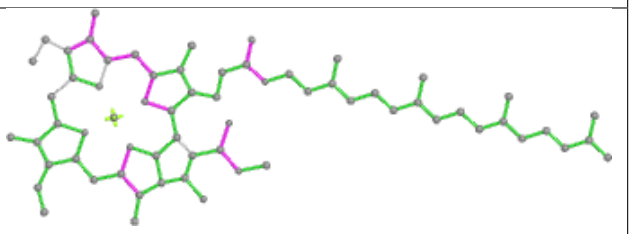
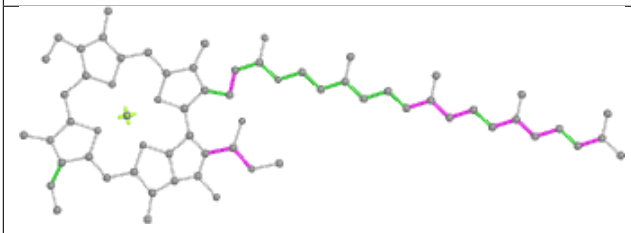


Bond angles



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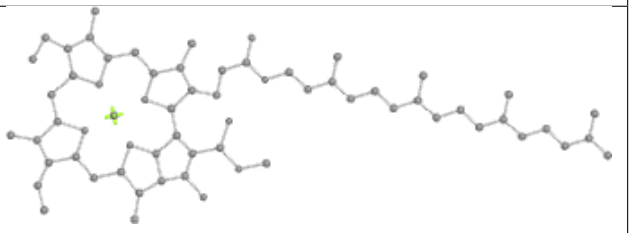
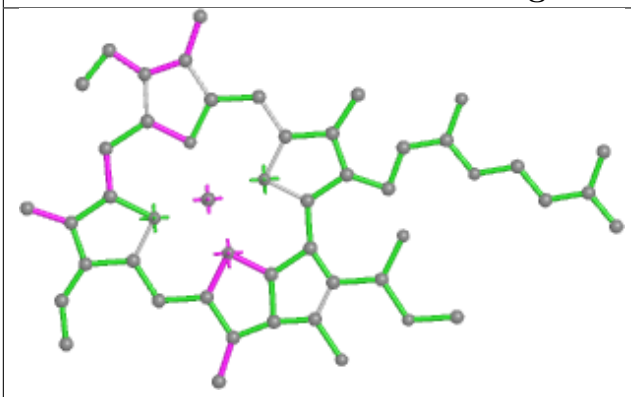


Rings

Ligand CLA 8 304



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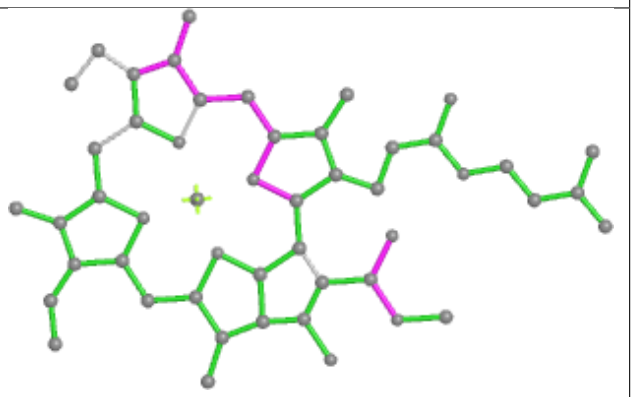
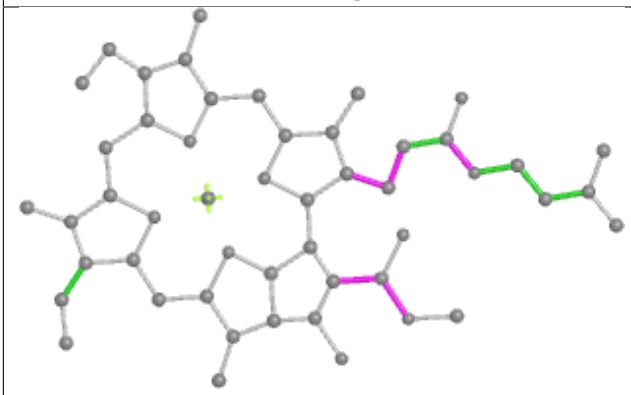
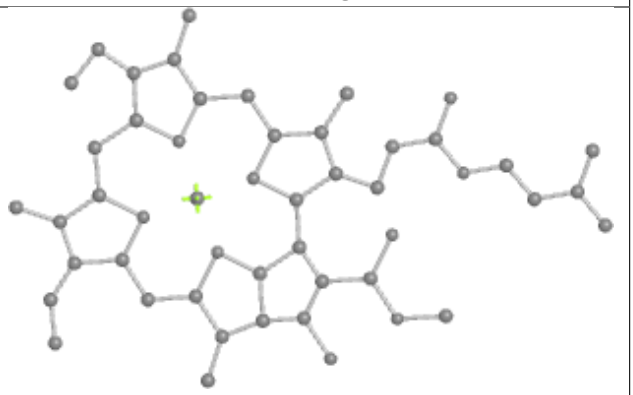


Bond angles

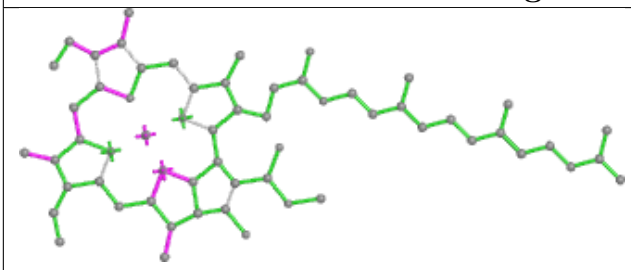


Torsions

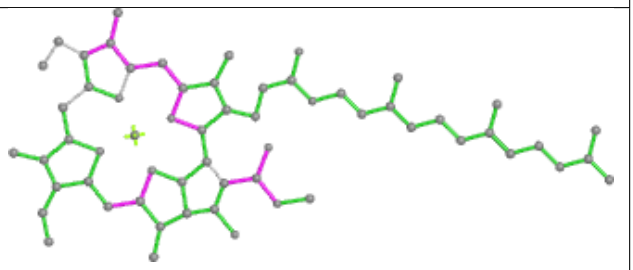


Rings

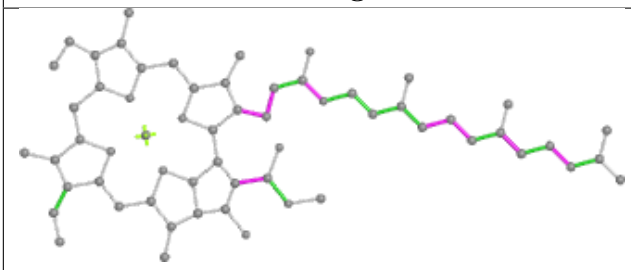
Ligand CLA B 816



Bond lengths



Bond angles



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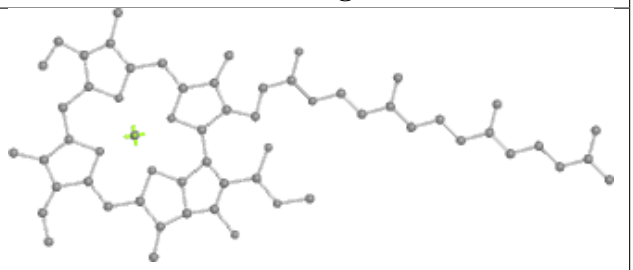
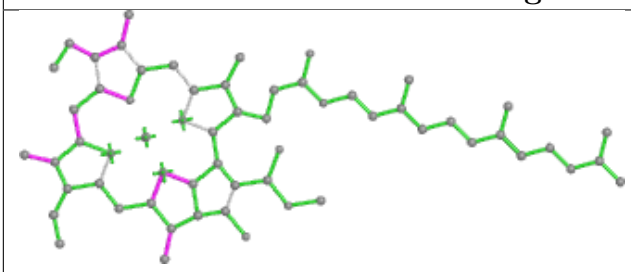


Rings

Ligand CLA B 824



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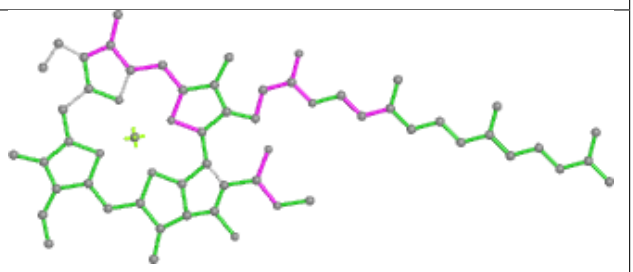

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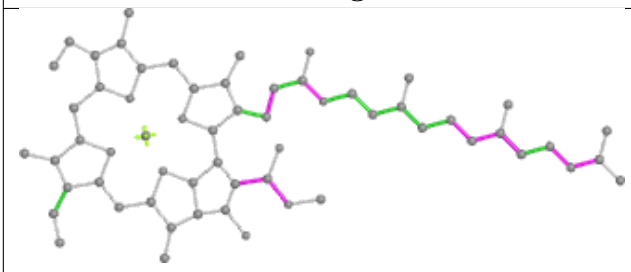

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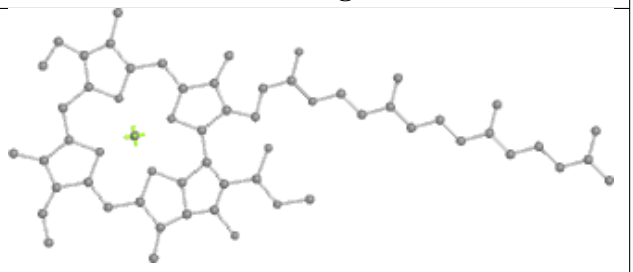
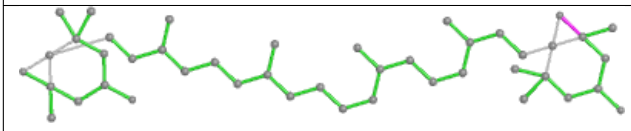


Rings

Ligand XAT 9 314



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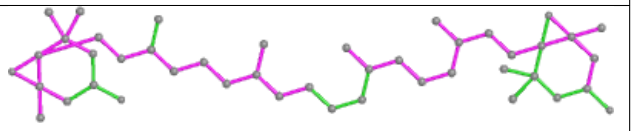

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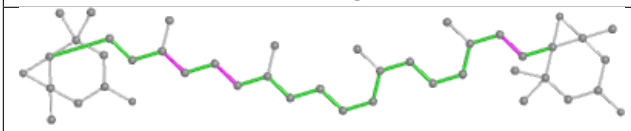

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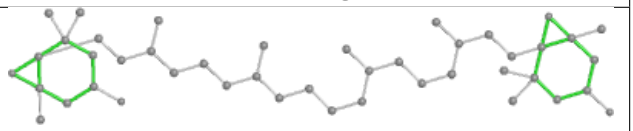
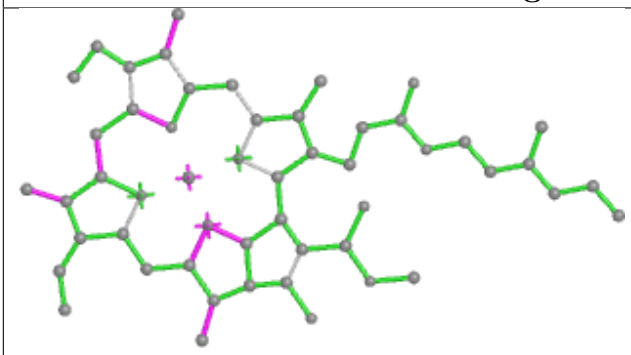


Rings

Ligand CLA A 843



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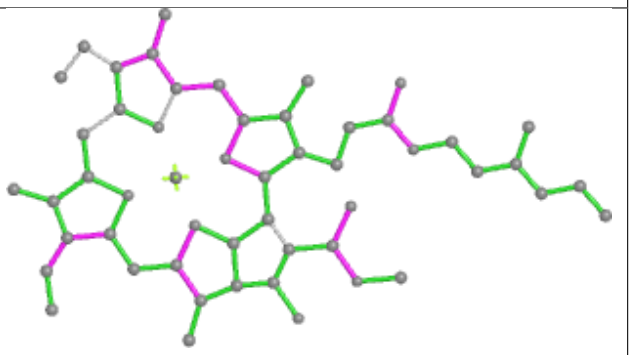

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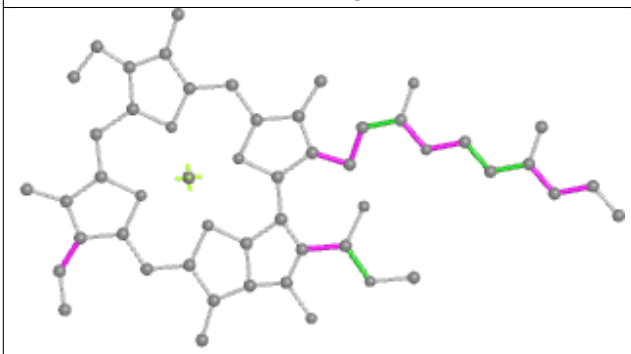

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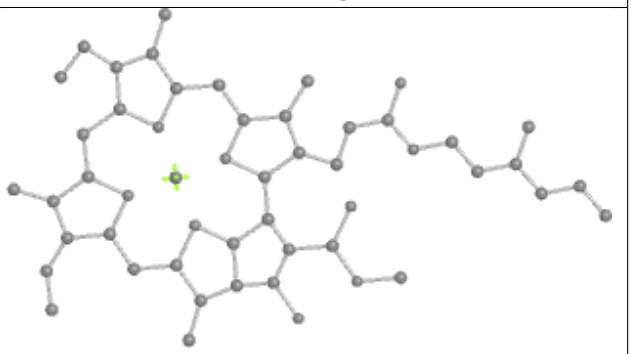
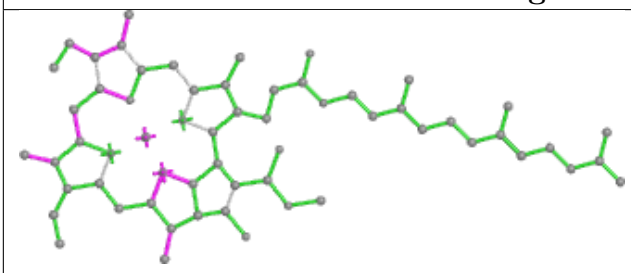


Rings

Ligand CLA 8 302



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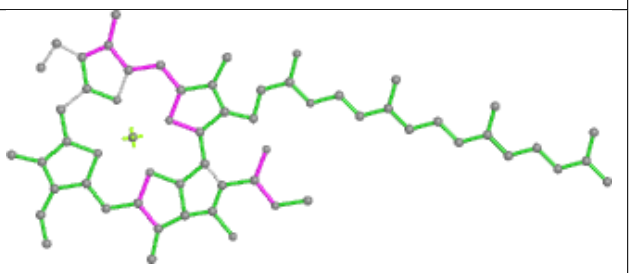

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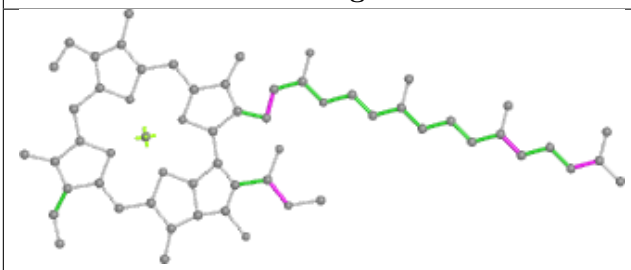

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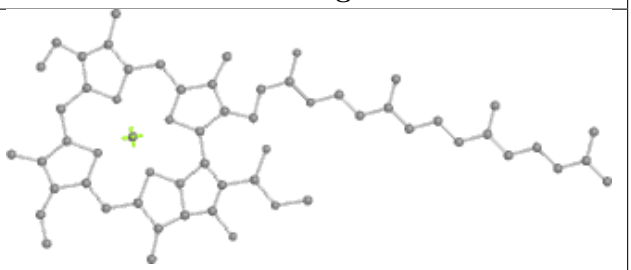
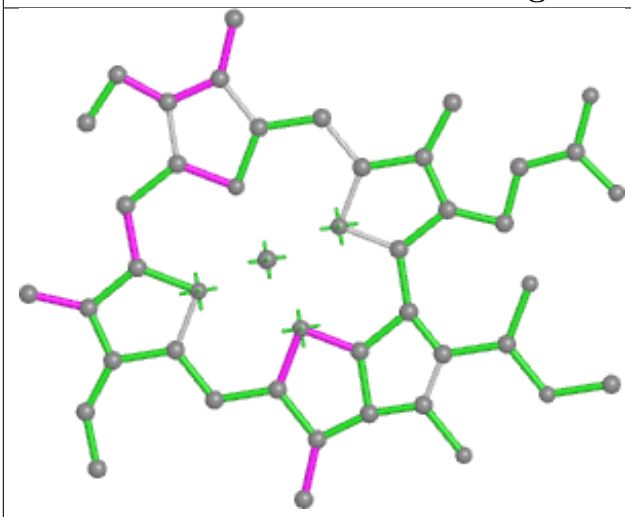


Rings

Ligand CLA 8 313



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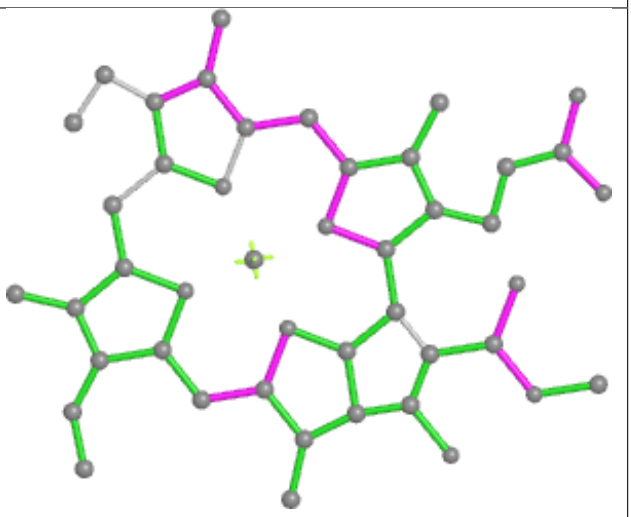

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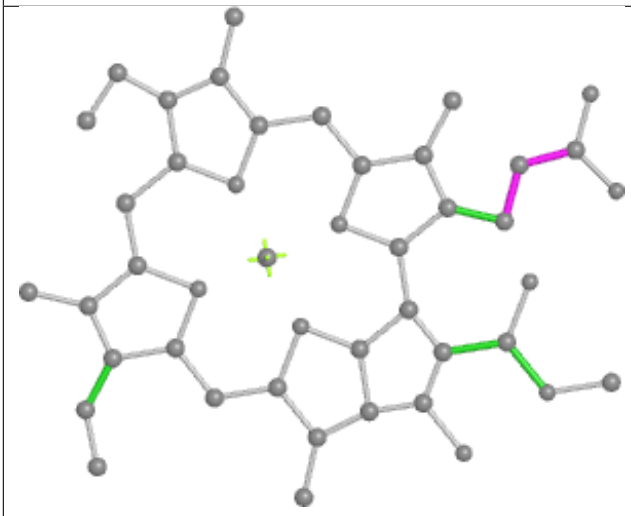

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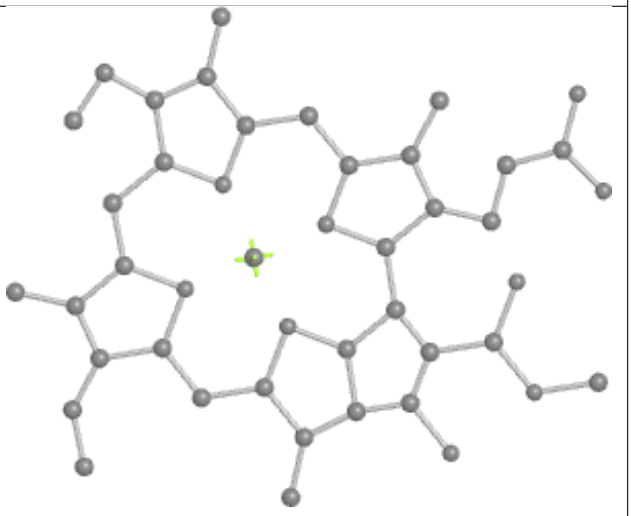
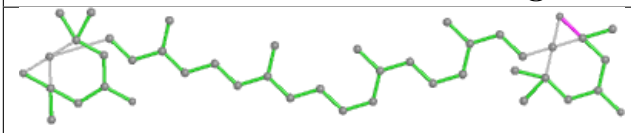


Rings

Ligand XAT 1 314



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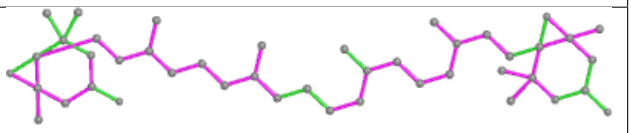

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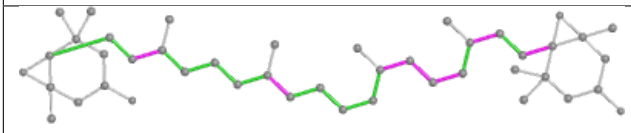

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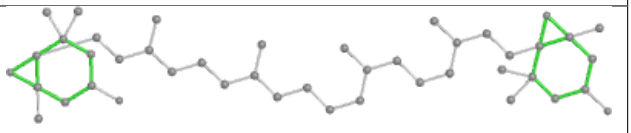
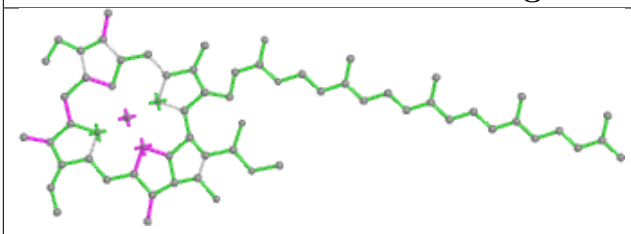


Rings

Ligand CLA A 837



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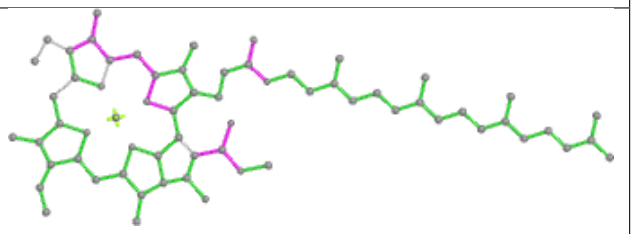

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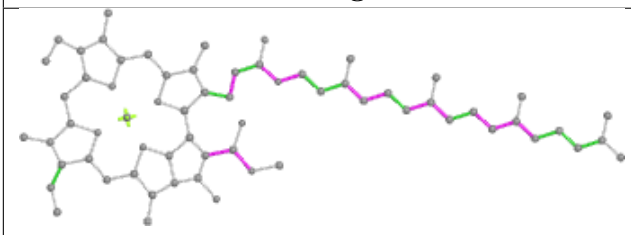

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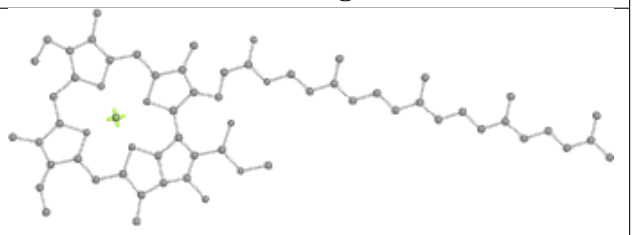
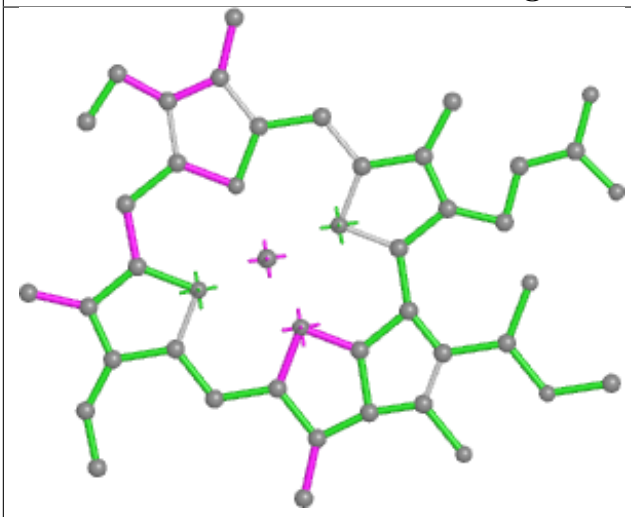


Rings

Ligand CLA A 835



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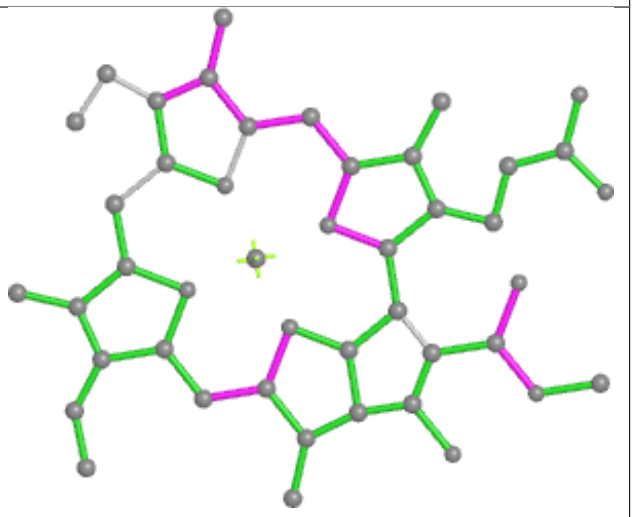
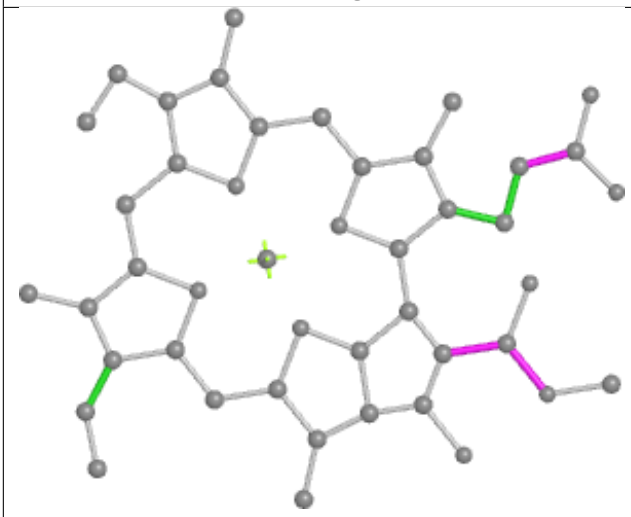


Bond angles



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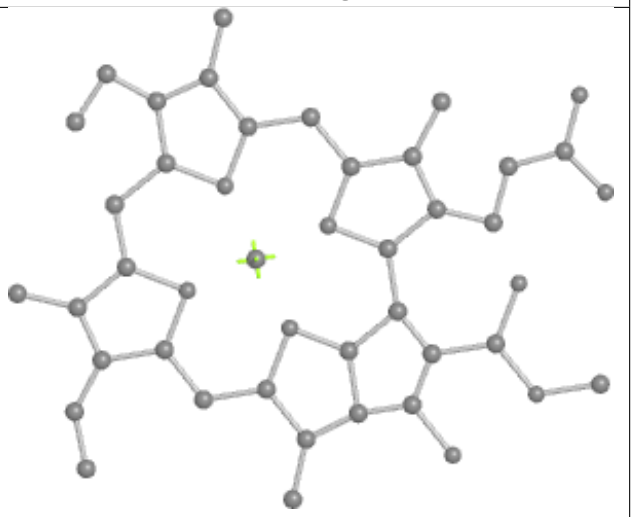
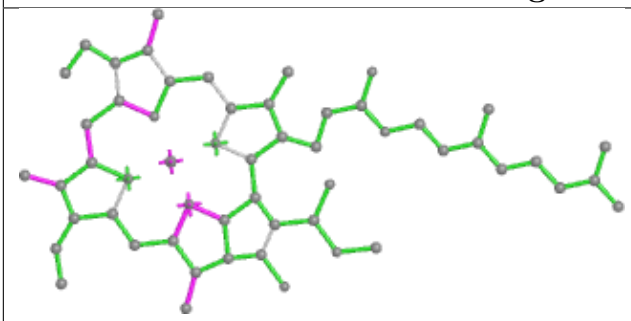


Rings

Ligand CLA 9 313



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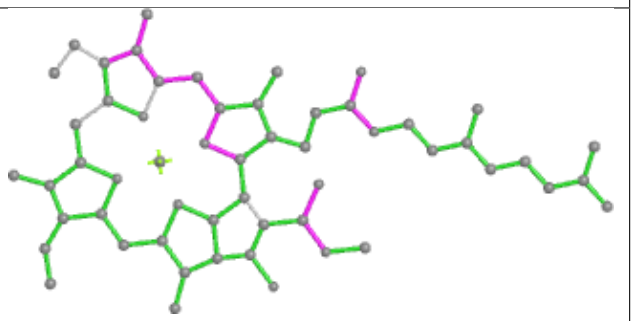
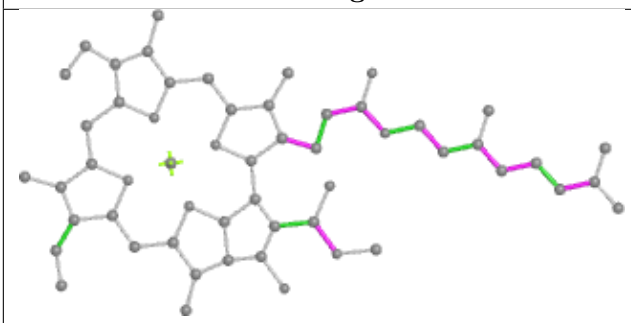


Bond angles



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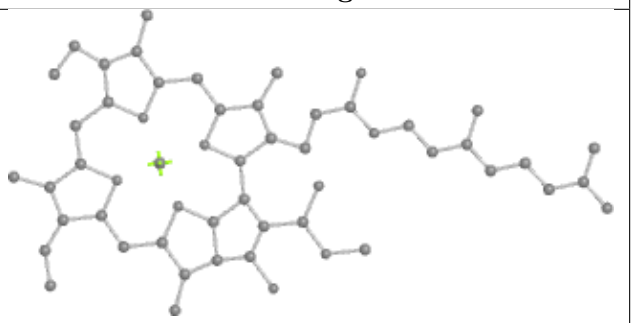
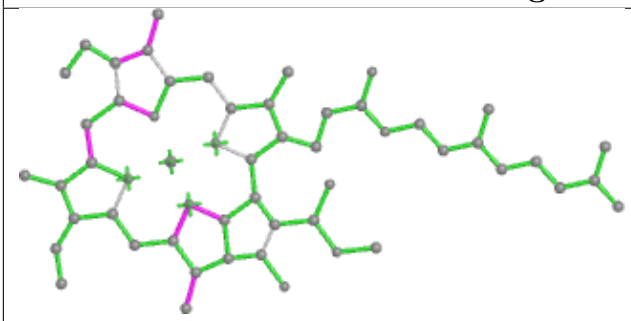


Rings

Ligand CLA 0 312



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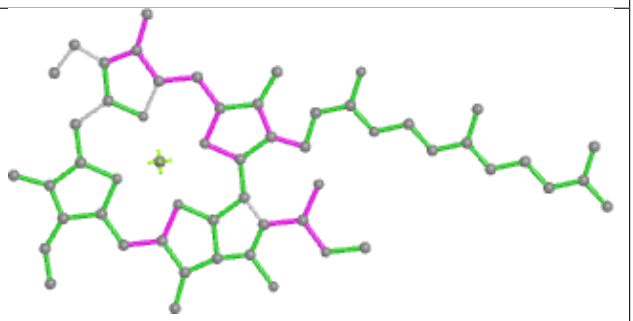
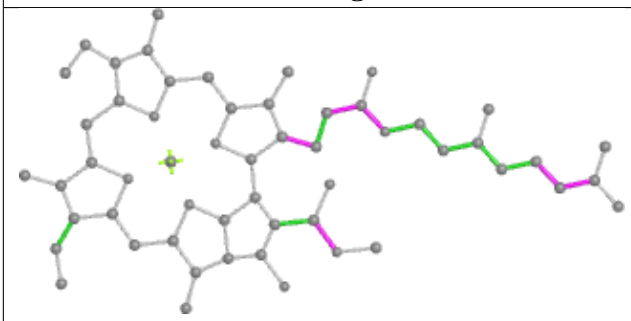


Bond angles



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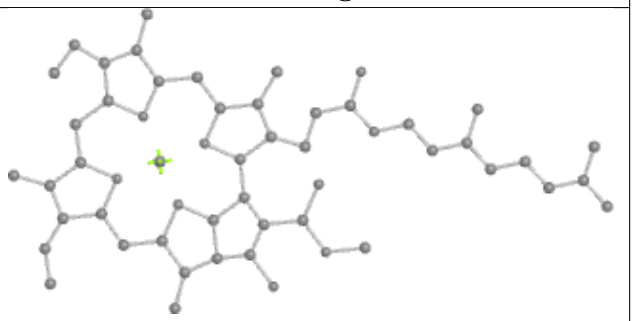
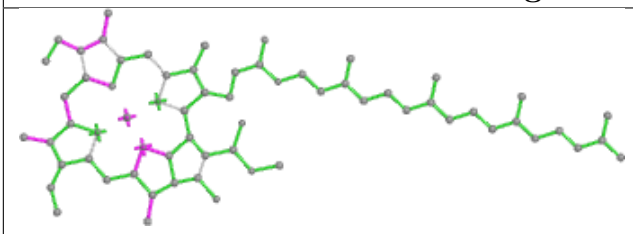


Rings

Ligand CLA B 834



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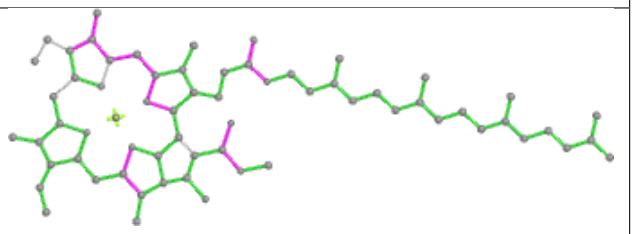
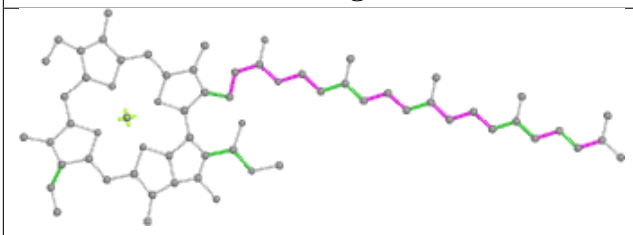


Bond angles



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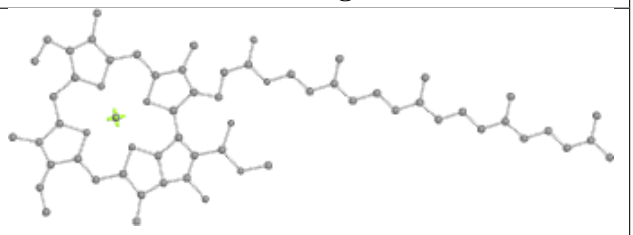

Rings

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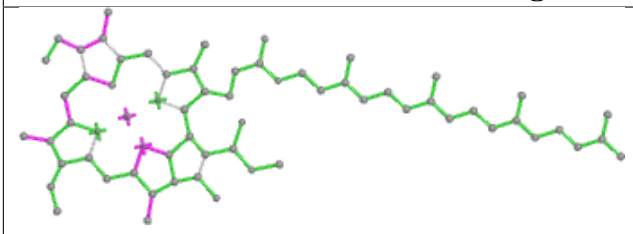
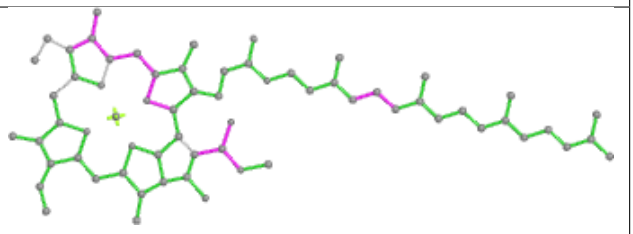
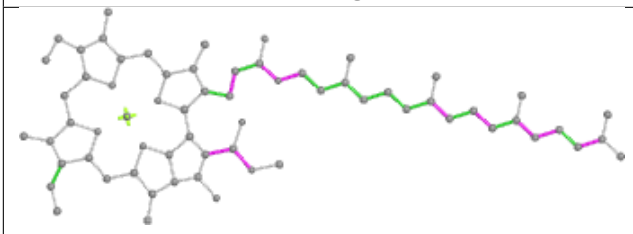


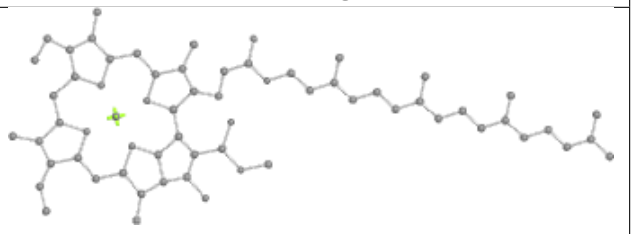
Bond lengths



Bond angles

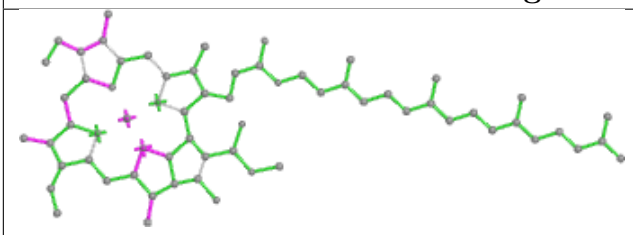


Torsions



Rings

Ligand CLA A 839



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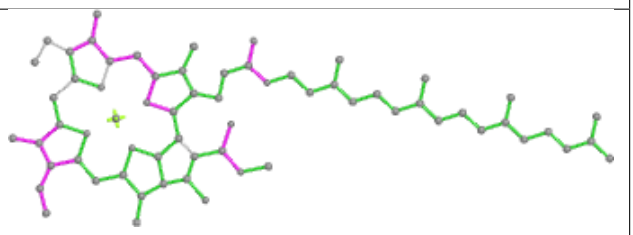
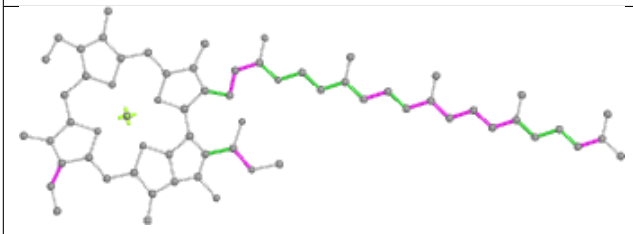


Bond angles



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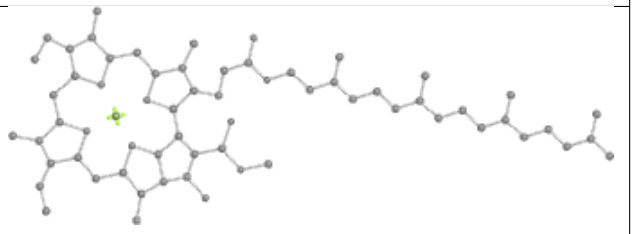
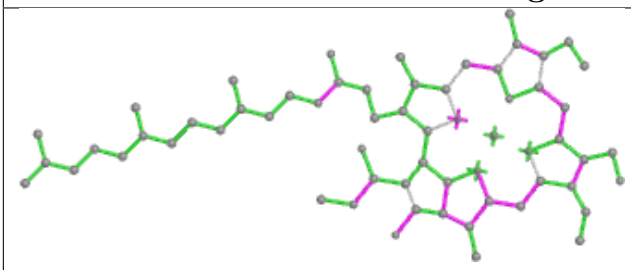


Rings

Ligand CHL 6 302



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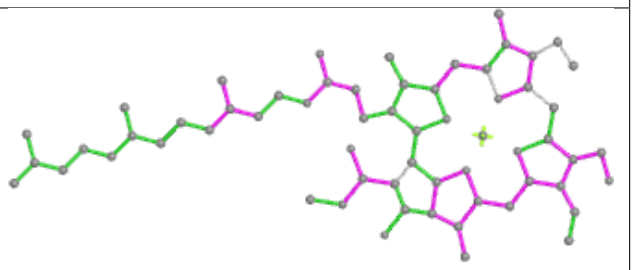
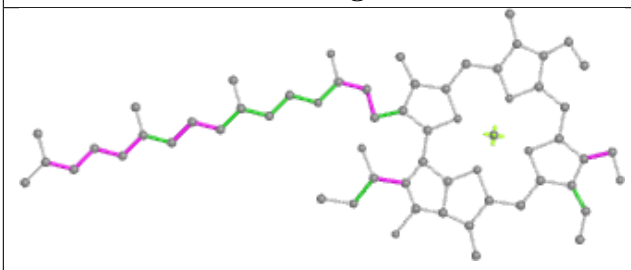


Bond angles



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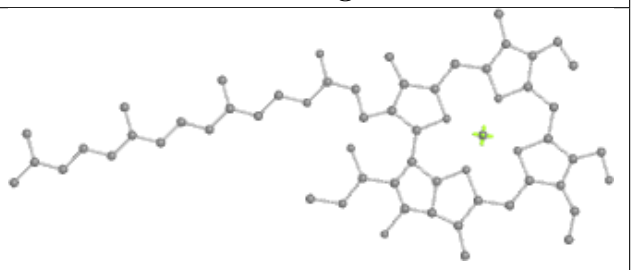
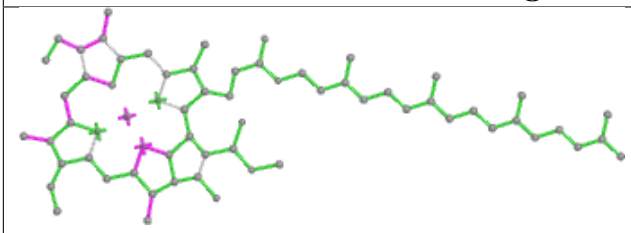


Rings

Ligand CLA A 830



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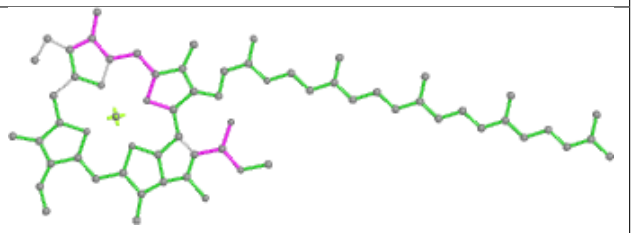
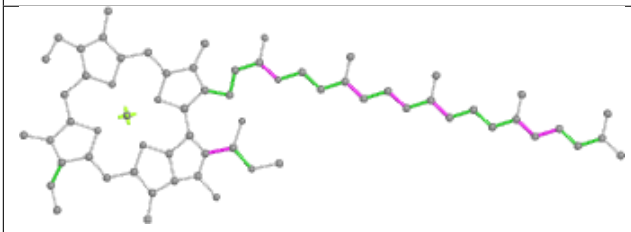


Bond angles



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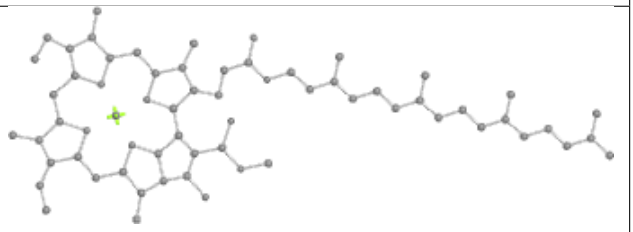
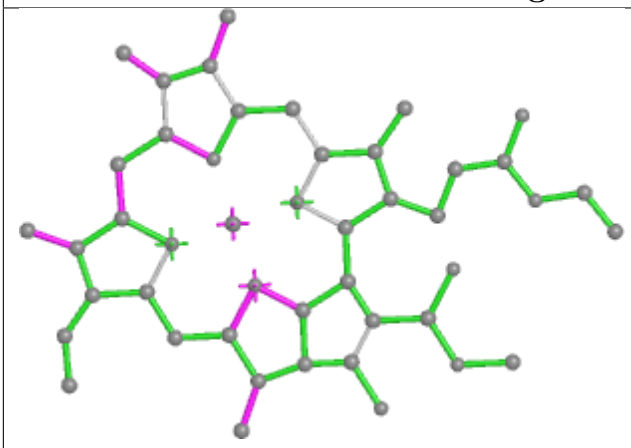


Rings

Ligand CLA 9 301



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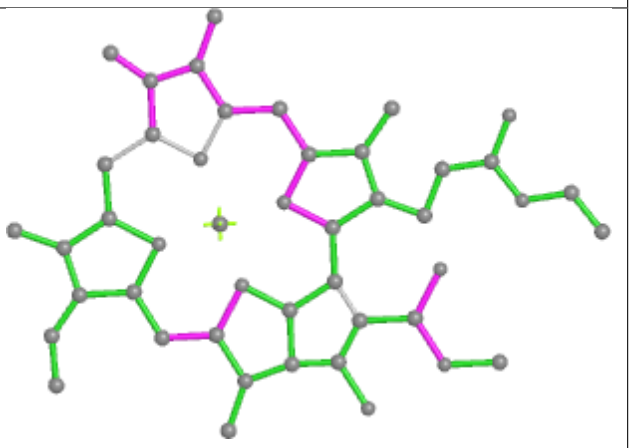

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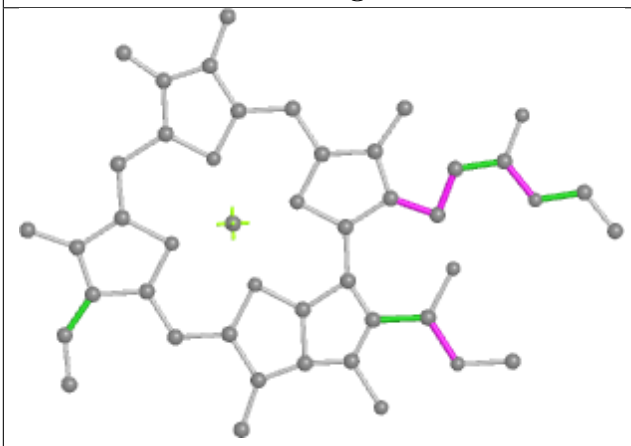

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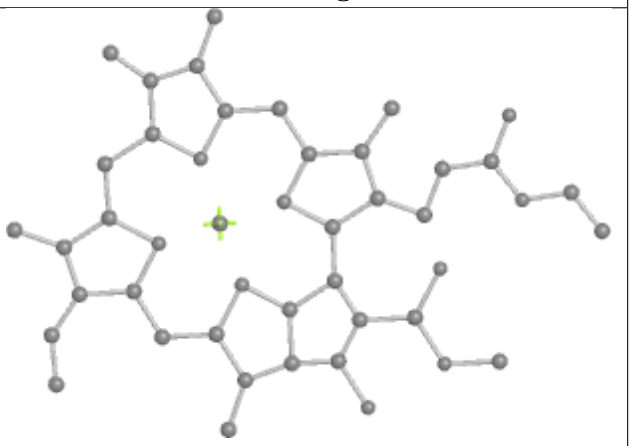
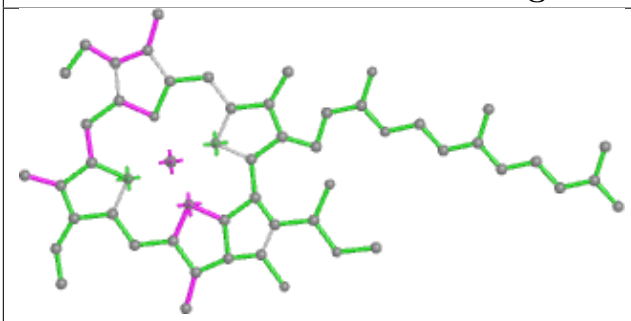


Rings

Ligand CLA 3 311



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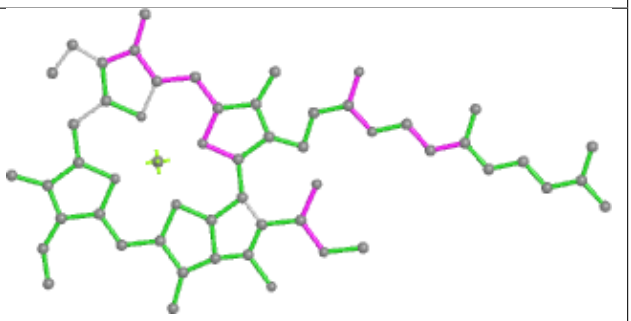
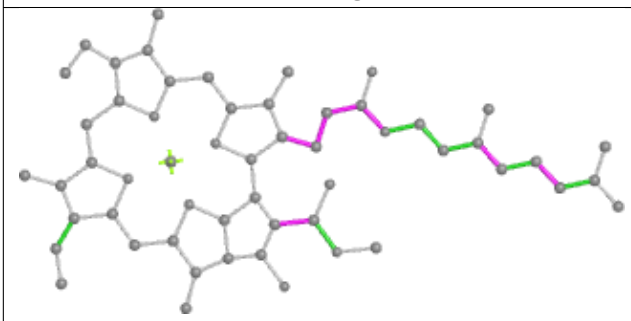


Bond angles



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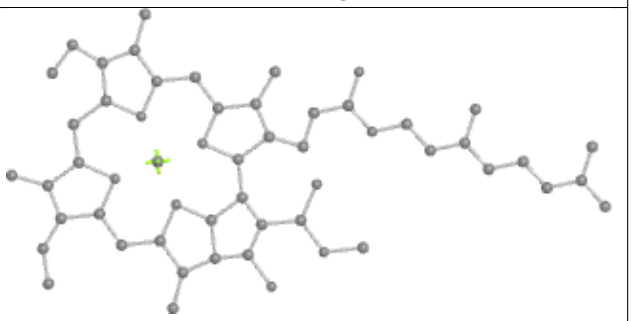
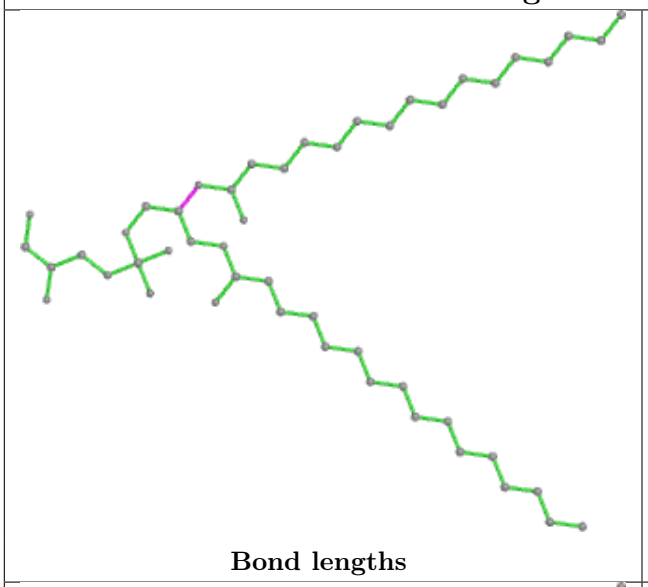
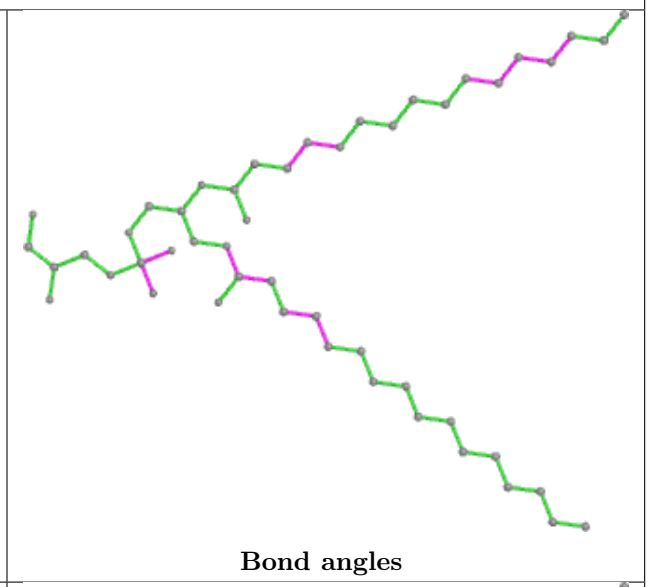


Rings

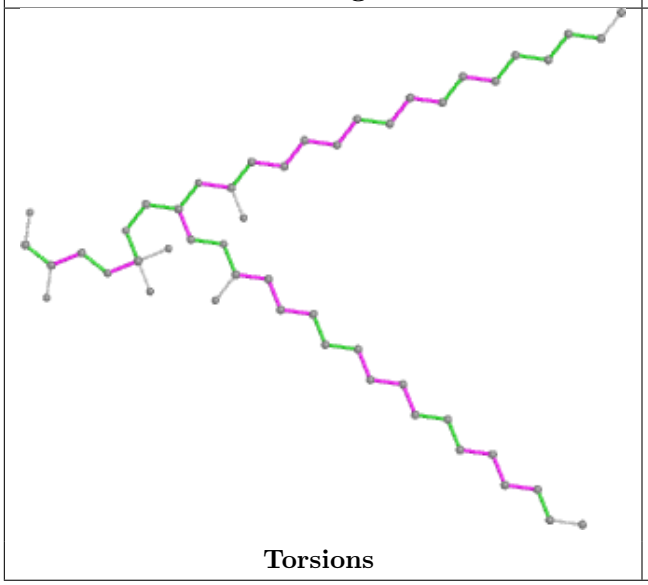
Ligand LHG A 844



Bond lengths



Bond angles



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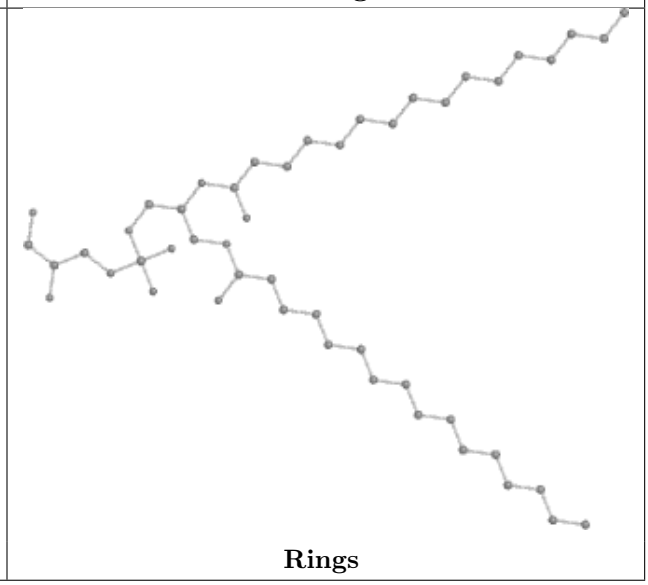
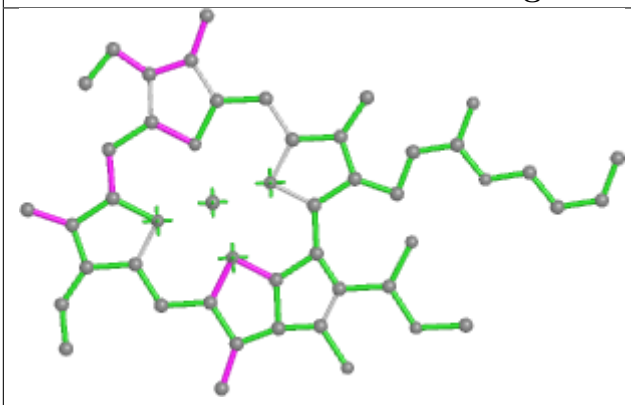


Rings

Ligand CLA A 852



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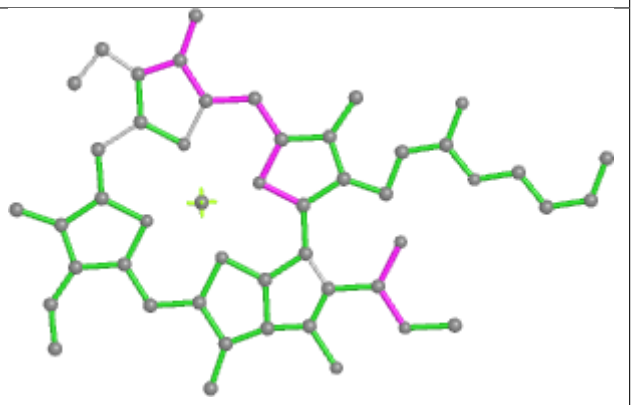
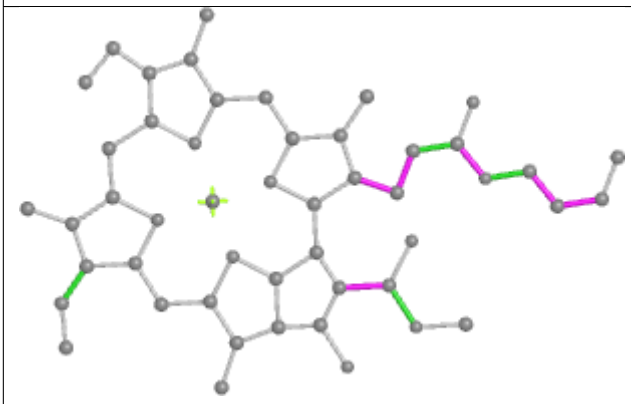


Bond angles



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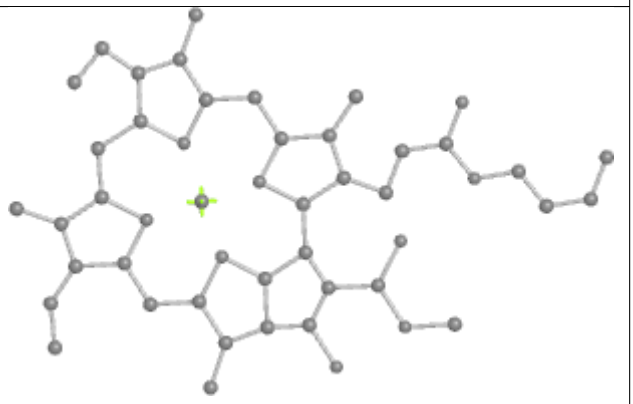
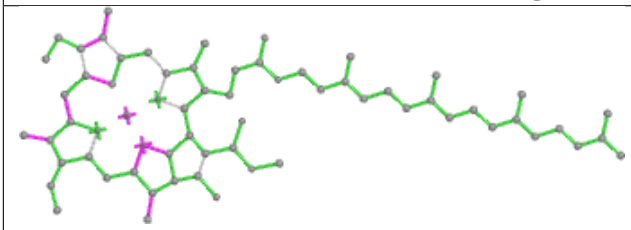


Rings

Ligand CLA 4 314



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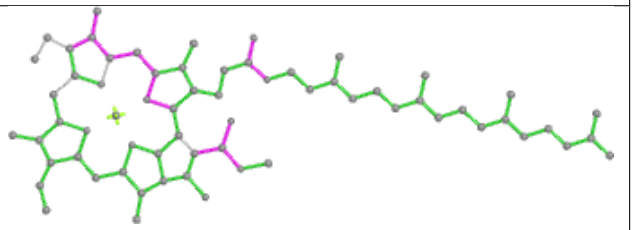
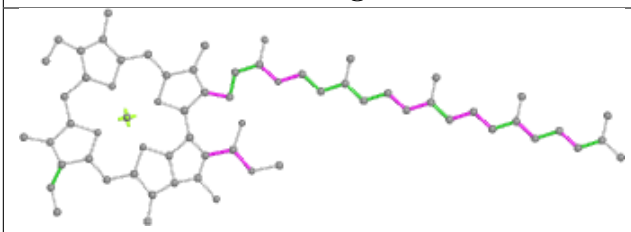


Bond angles



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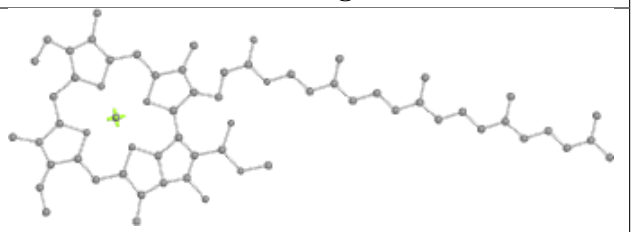
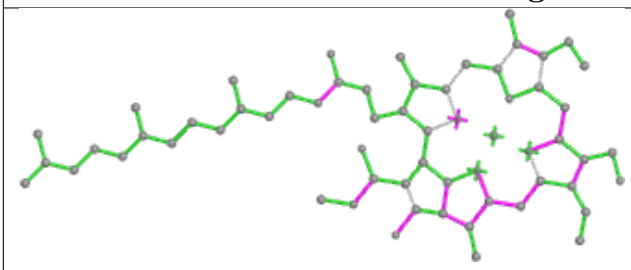


Rings

Ligand CHL 2 301



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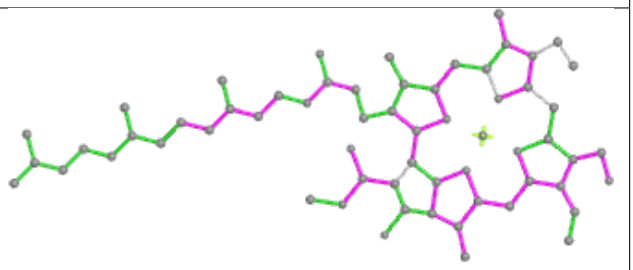
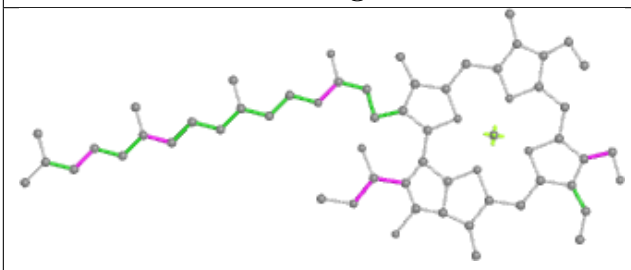


Bond angles



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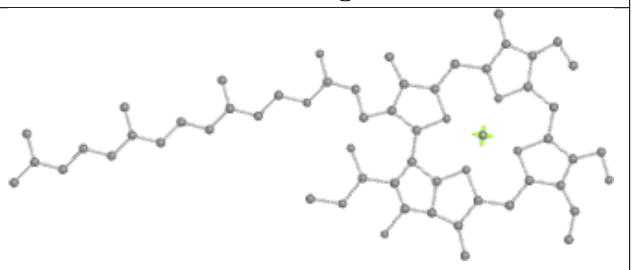
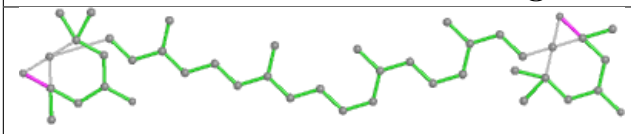


Rings

Ligand XAT 9 315



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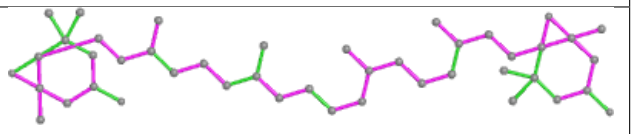
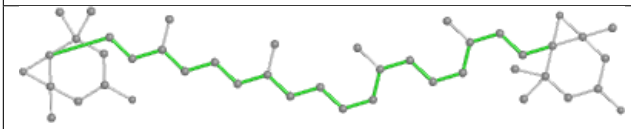


Bond angles



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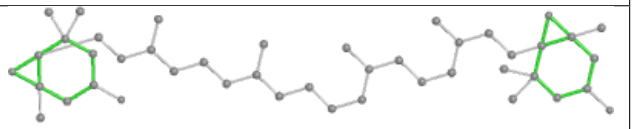
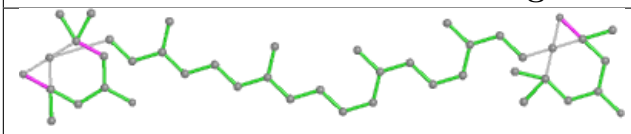


Rings

Ligand XAT 4 316



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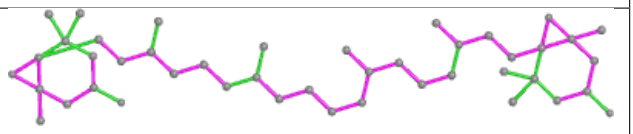
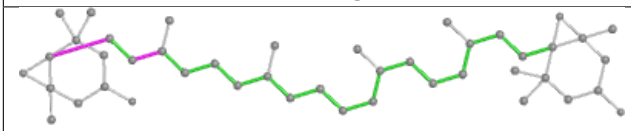


Bond angles



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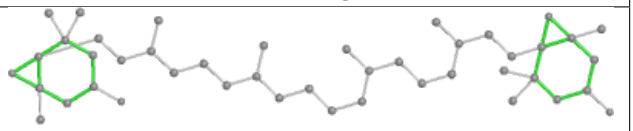
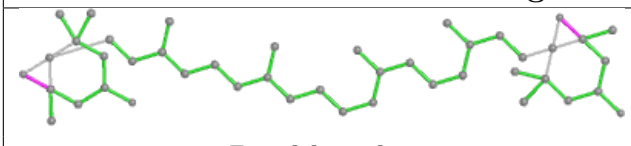


Rings

Ligand XAT 6 320



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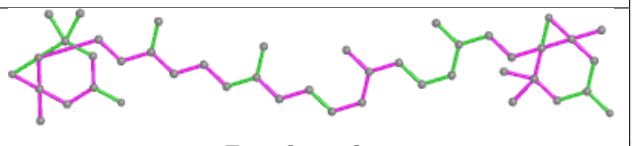
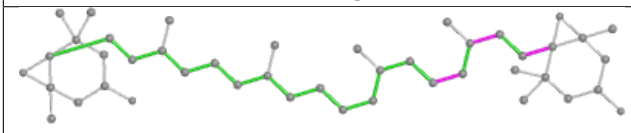
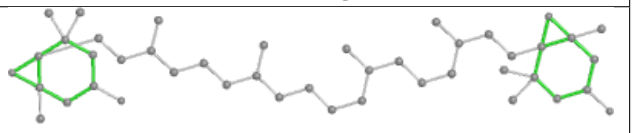


Bond angles

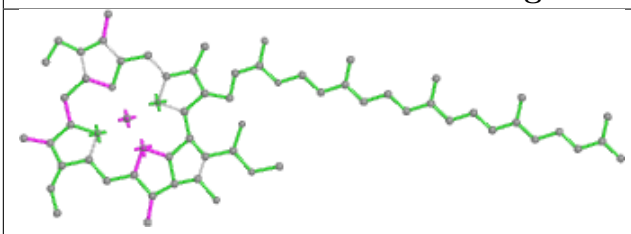


Torsions

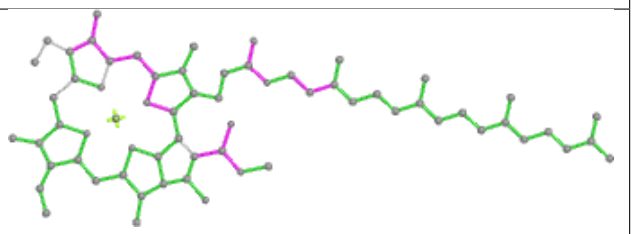


Rings

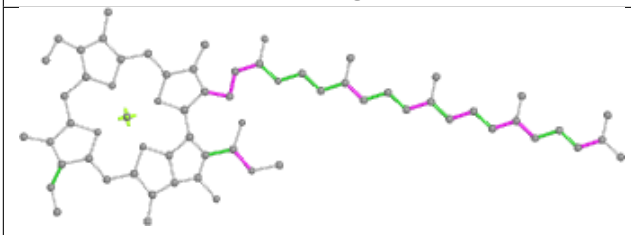
Ligand CLA B 828



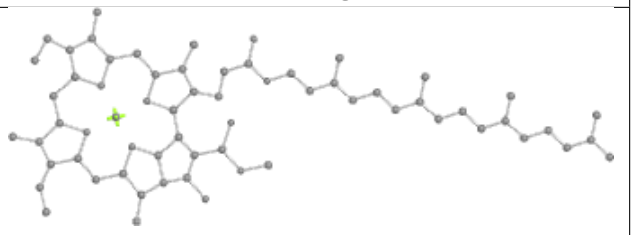
Bond lengths



Bond angles

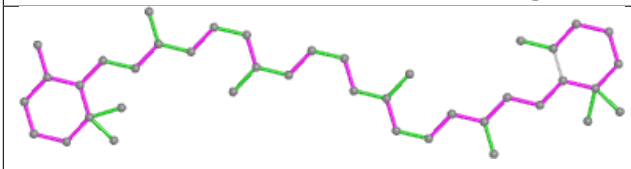


Torsions

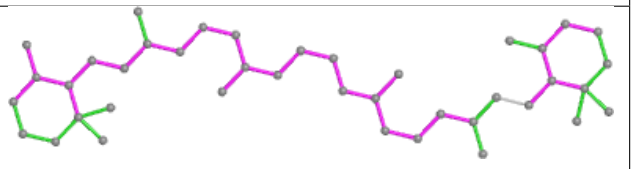


Rings

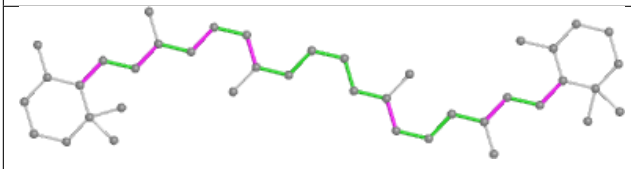
Ligand 8CT A 850



Bond lengths



Bond angles



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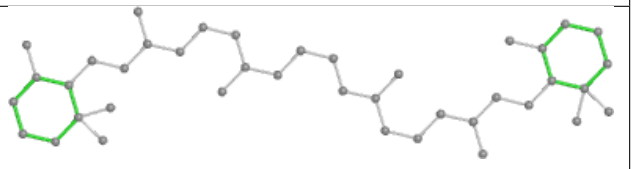
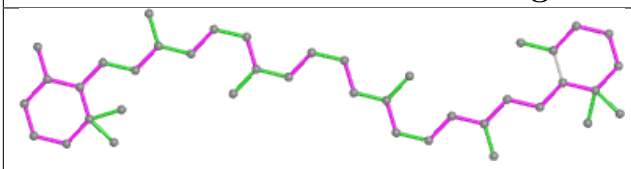
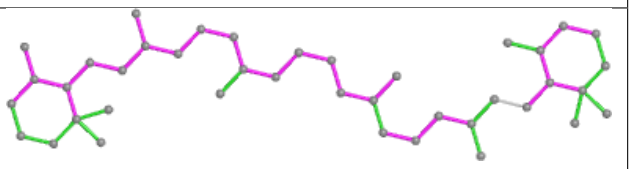
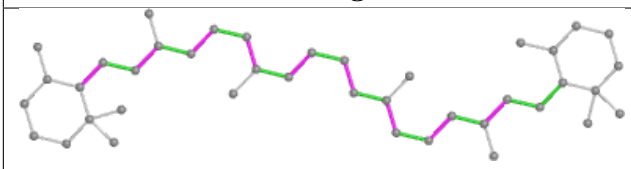
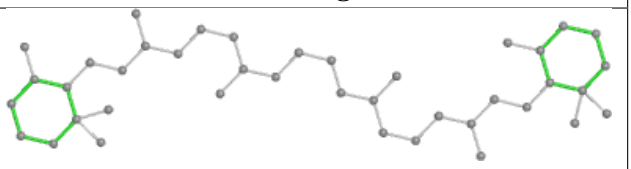
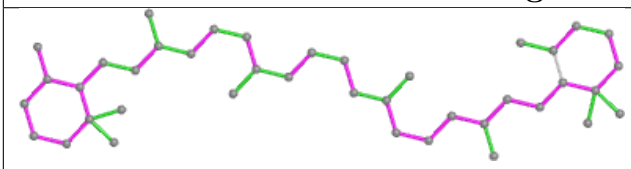
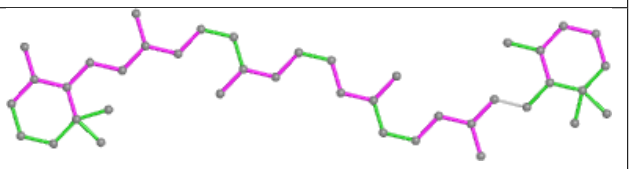
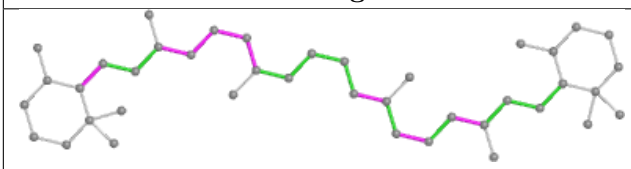
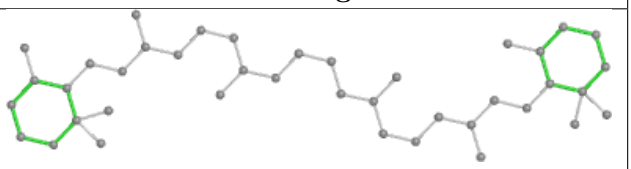
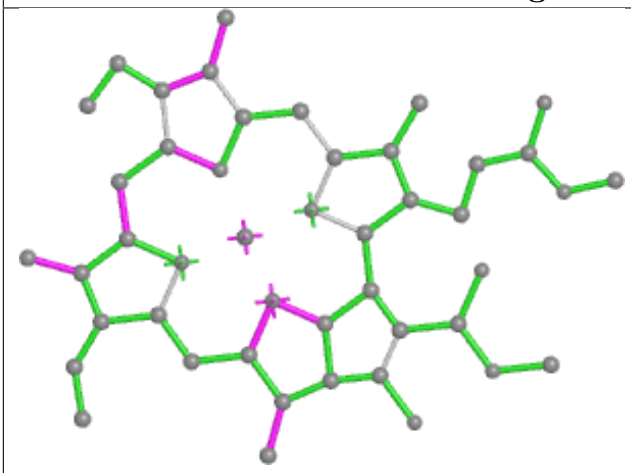


Rings

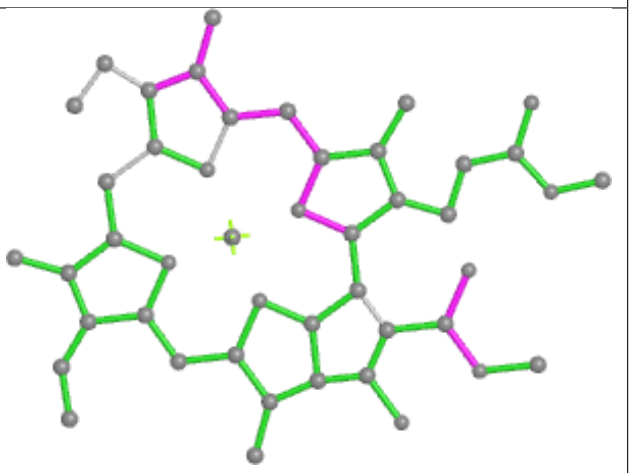
Ligand 8CT 7 323	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT K 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

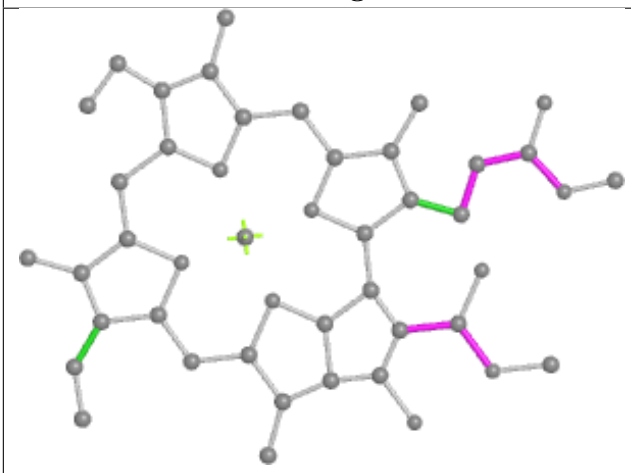
Ligand CLA 5 314



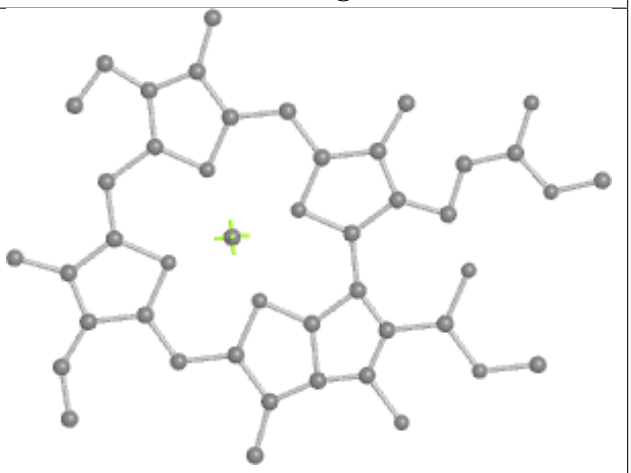
Bond lengths



Bond angles

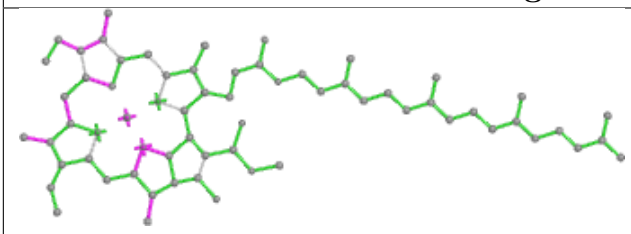


Torsions

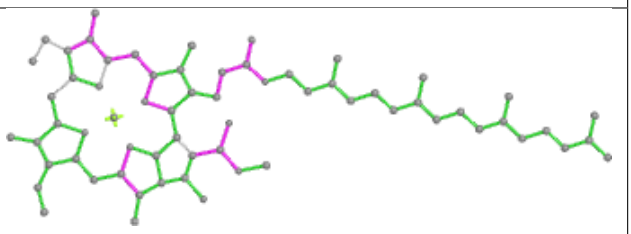


Rings

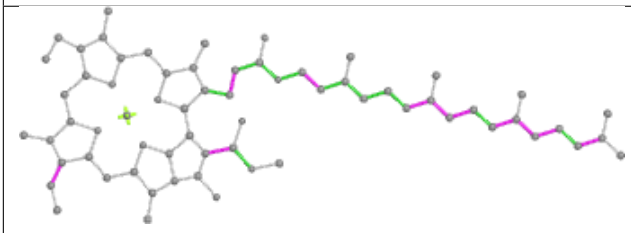
Ligand CLA B 803



Bond lengths



Bond angles



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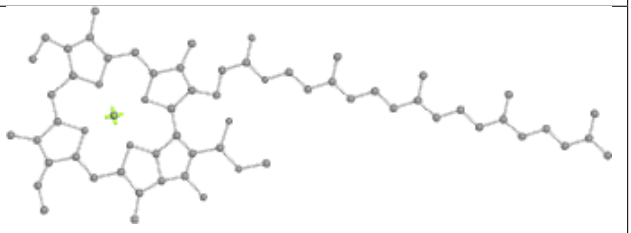
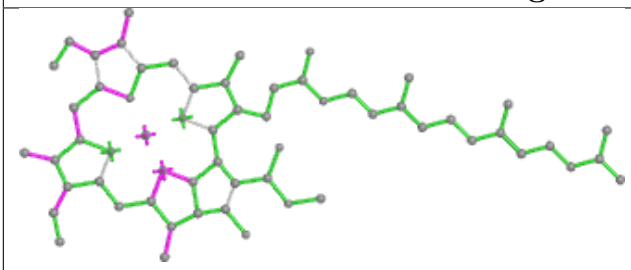
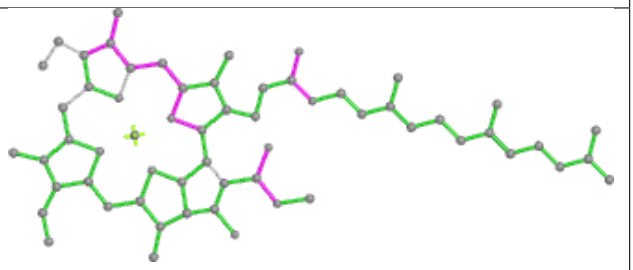


Rings

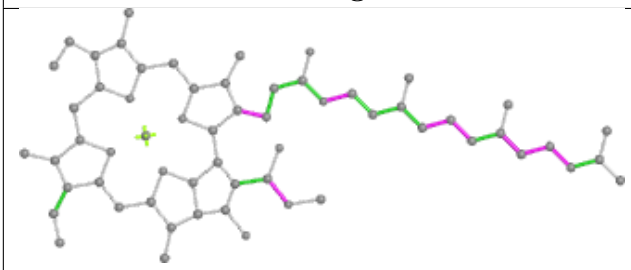
Ligand CLA 2 309



Bond lengths



Bond angles



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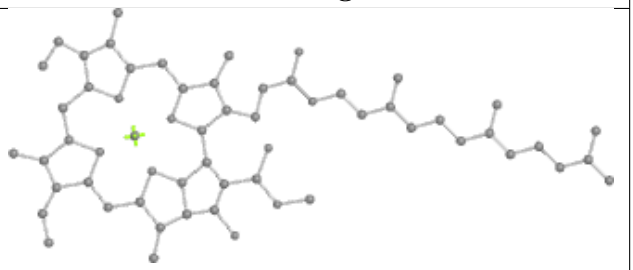
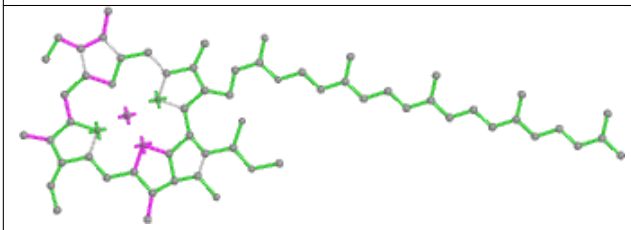
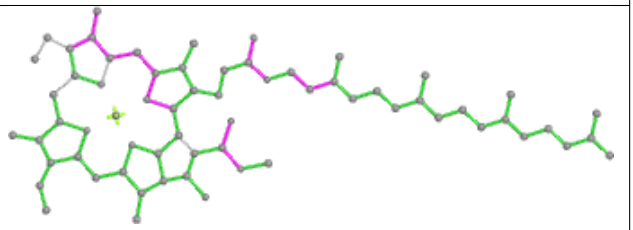


Rings

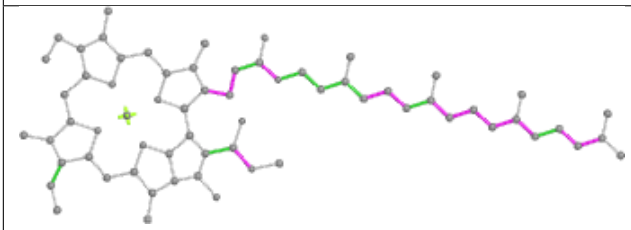
Ligand CLA B 809



Bond lengths



Bond angles



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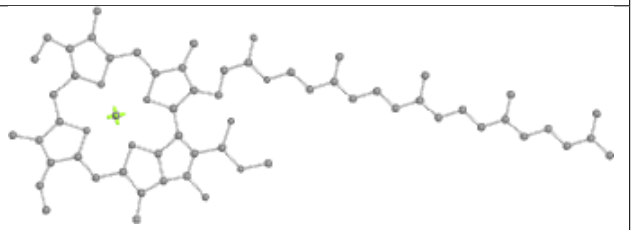
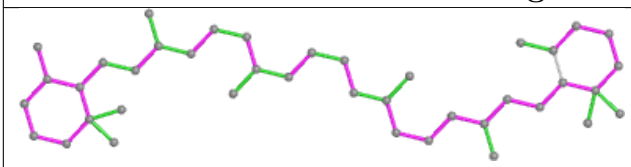
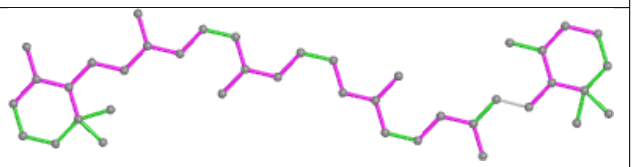


Rings

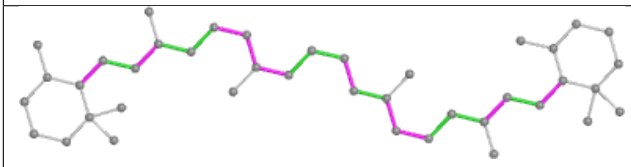
Ligand 8CT B 843



Bond lengths



Bond angles



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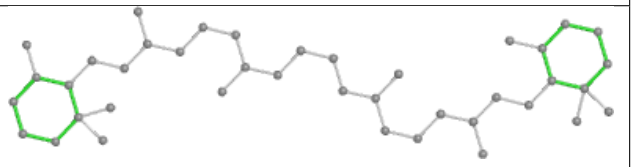
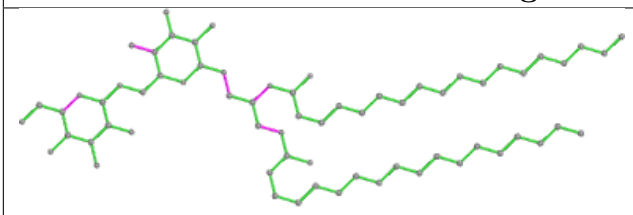
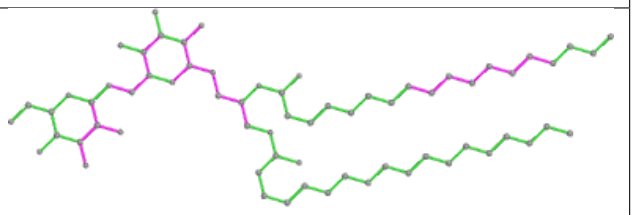


Rings

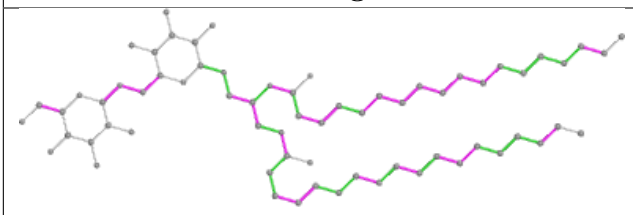
Ligand DGD B 849



Bond lengths



Bond angles



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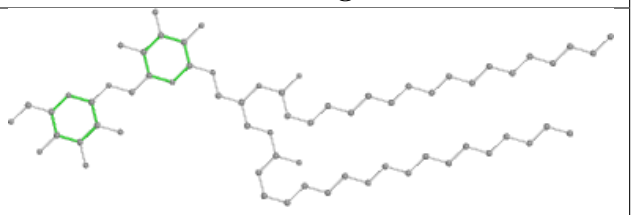
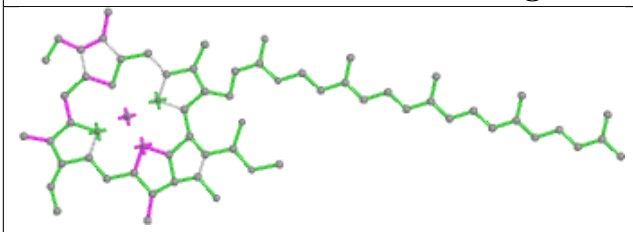


Rings

Ligand CLA A 853



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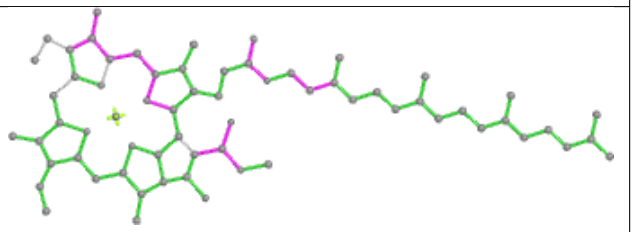
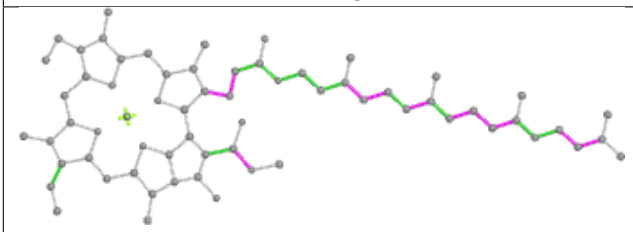


Bond angles



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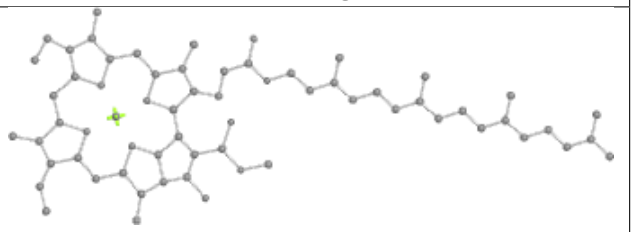
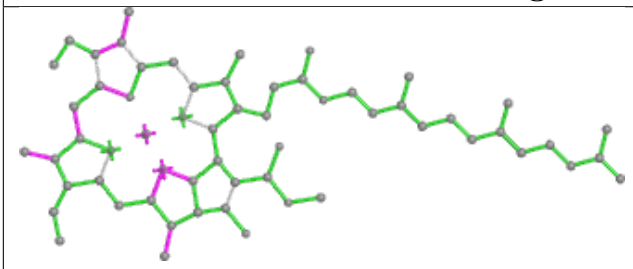
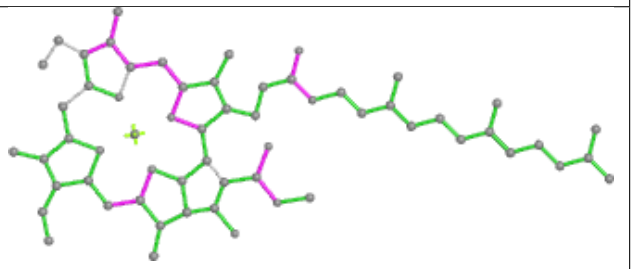


Rings

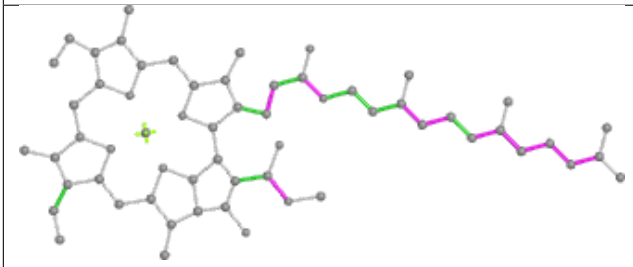
Ligand CLA 2 304



Bond lengths



Bond angles



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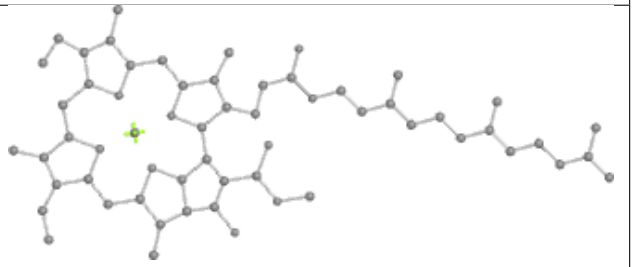
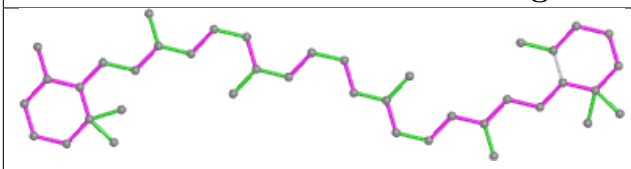
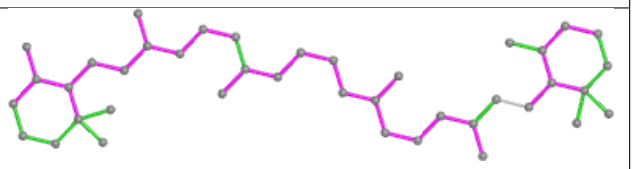


Rings

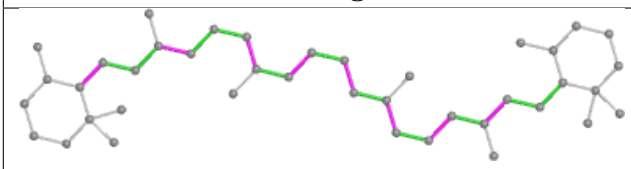
Ligand 8CT 3 316



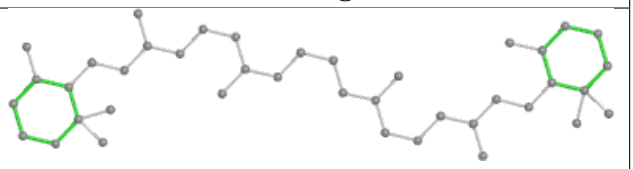
Bond lengths



Bond angles

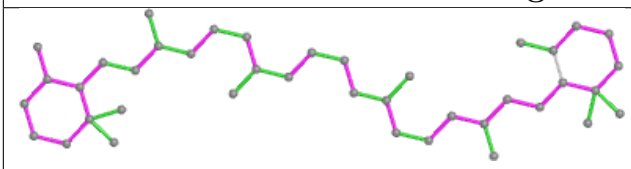


Torsions

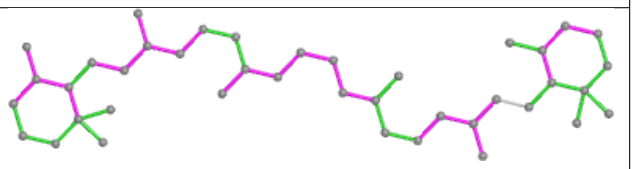


Rings

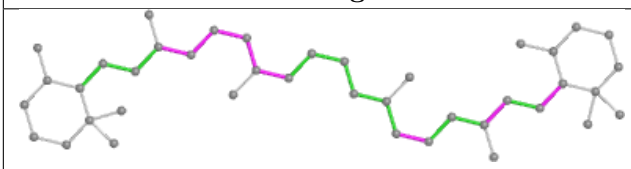
Ligand 8CT B 846



Bond lengths



Bond angles



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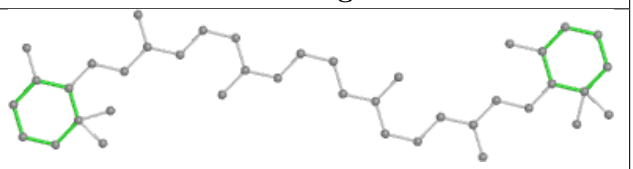
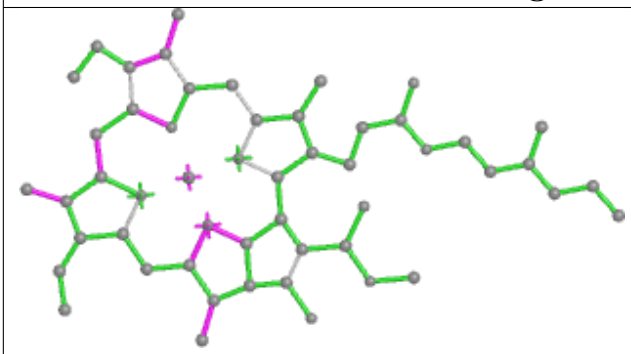
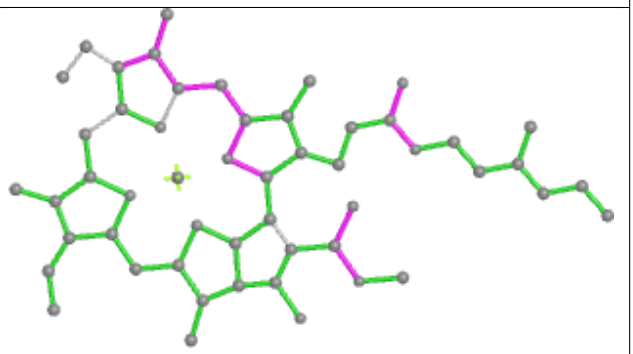


Rings

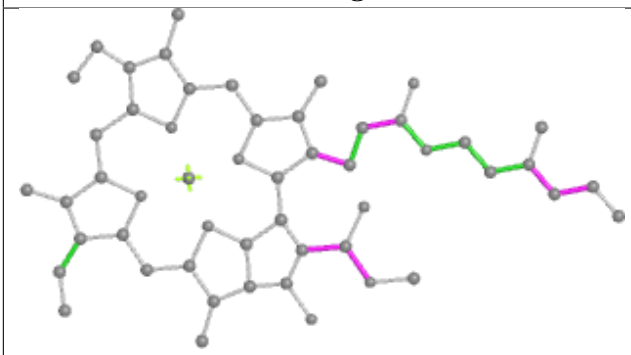
Ligand CLA 6 312



Bond lengths



Bond angles



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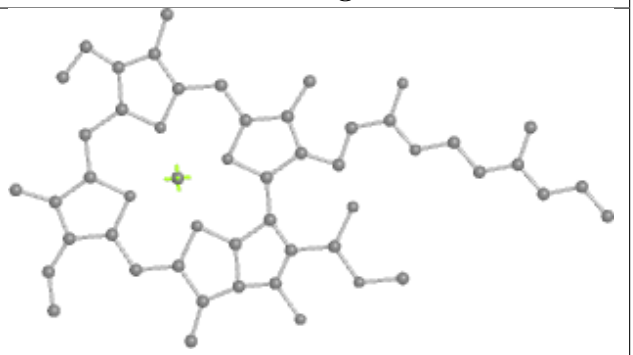
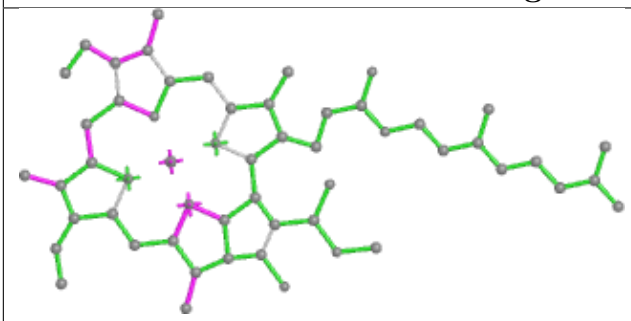
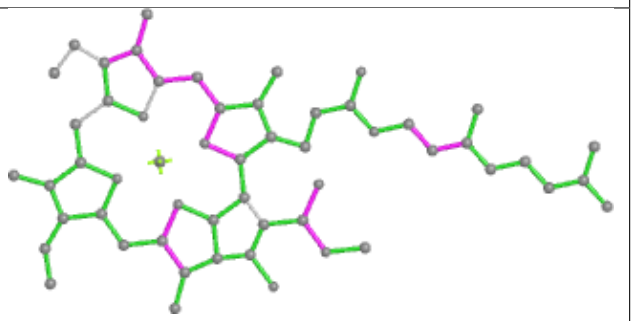


Rings

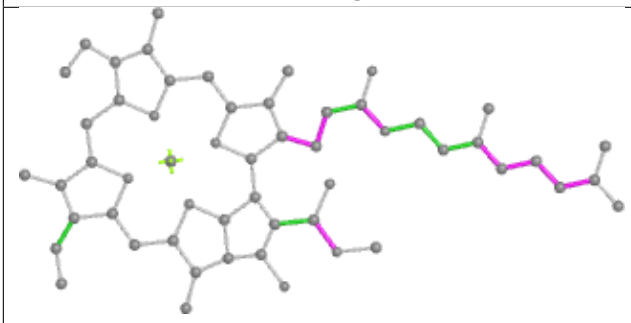
Ligand CLA B 823



Bond lengths



Bond angles



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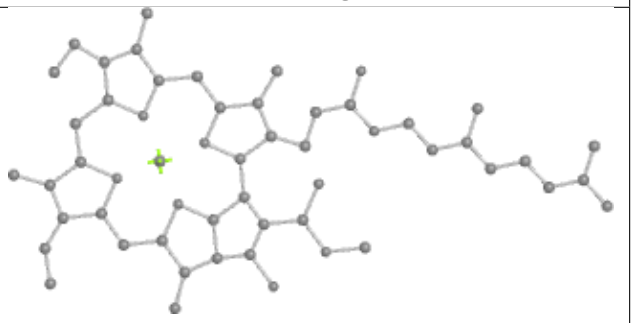
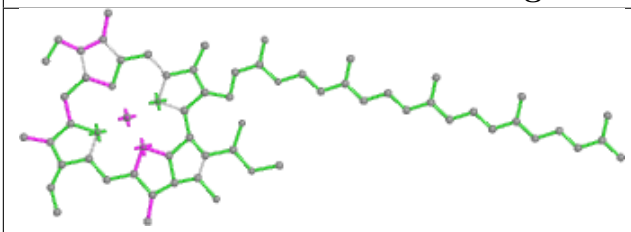
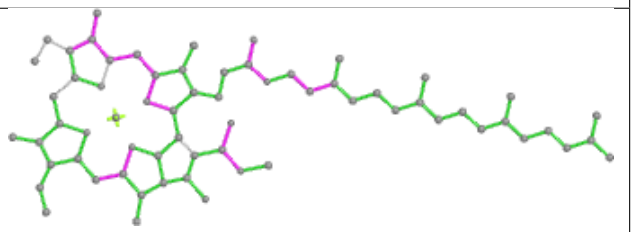


Rings

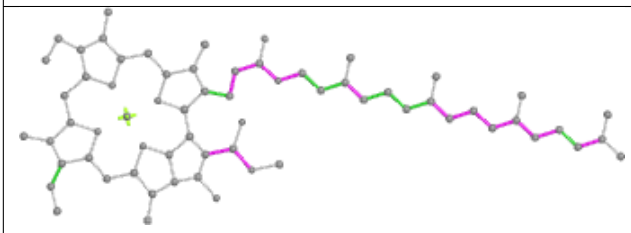
Ligand CLA B 814



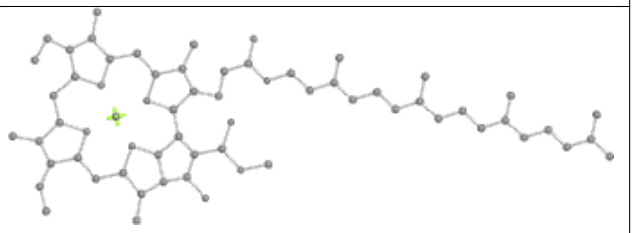
Bond lengths



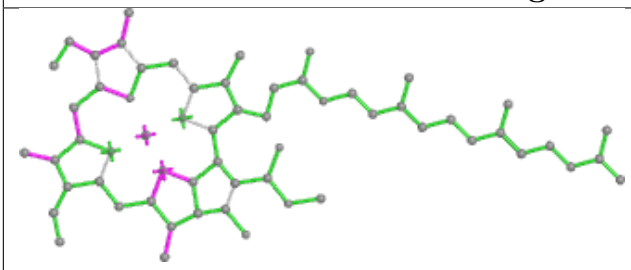
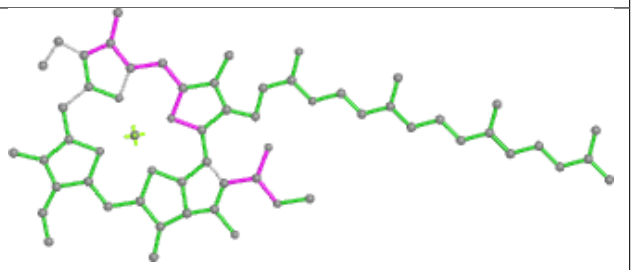
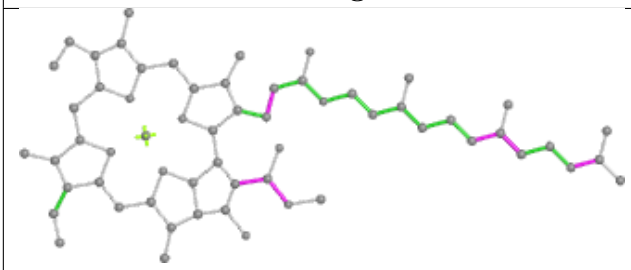
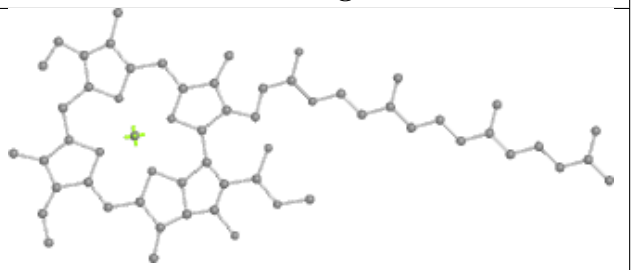
Bond angles



Torsions



Rings

Ligand CLA 3 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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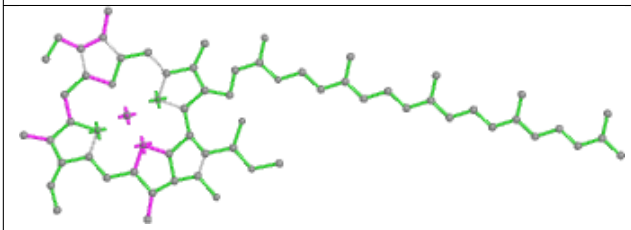
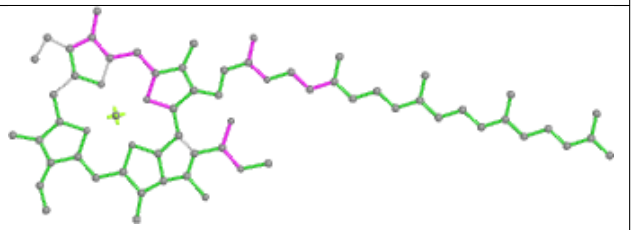
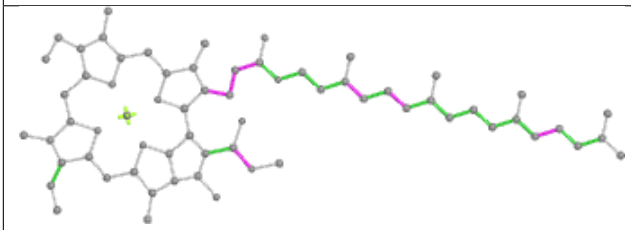
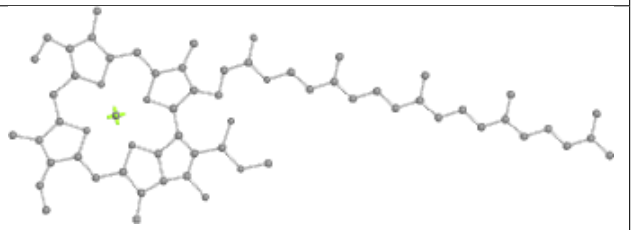
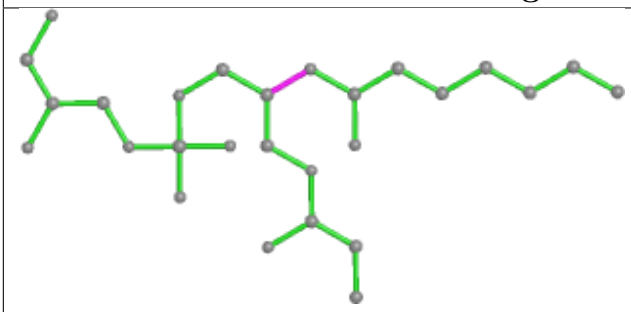
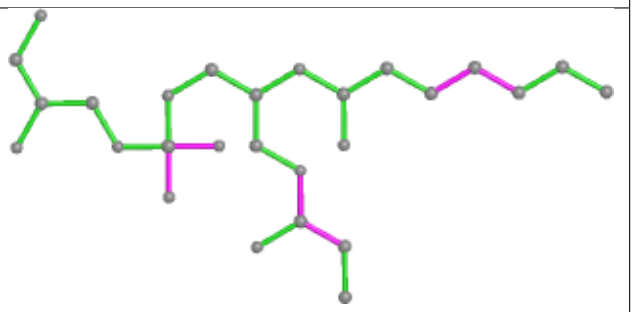
 Bond lengths	 Bond angles
 Torsions	 Rings

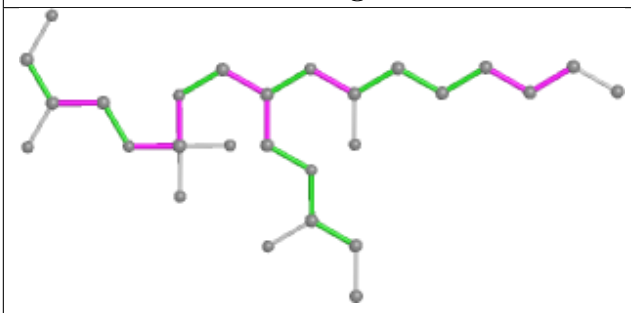
Ligand LHG A 845



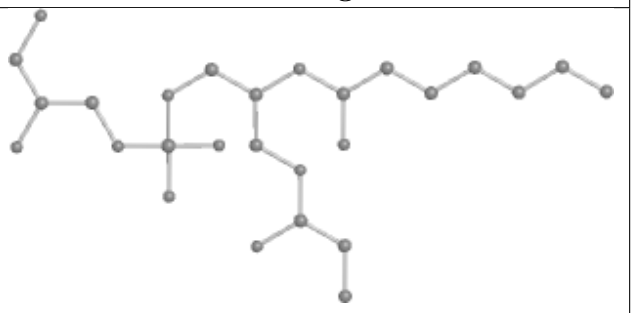
Bond lengths



Bond angles

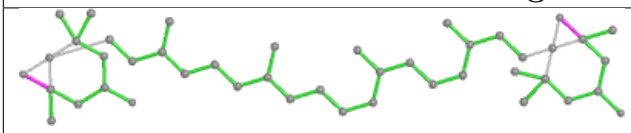


Torsions

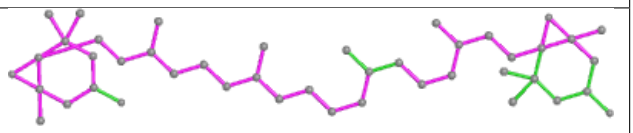


Rings

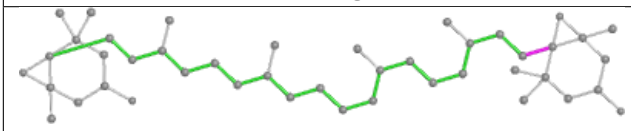
Ligand XAT 2 315



Bond lengths



Bond angles



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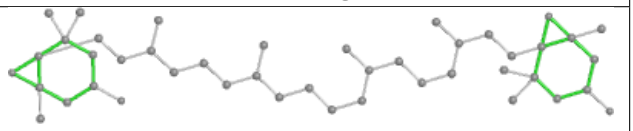
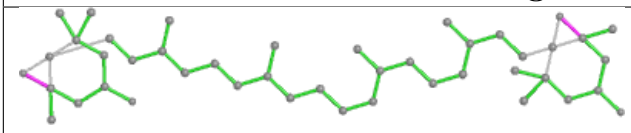
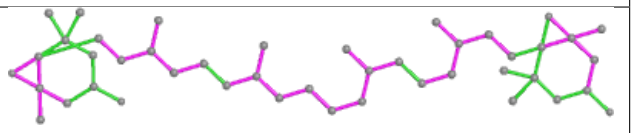


Rings

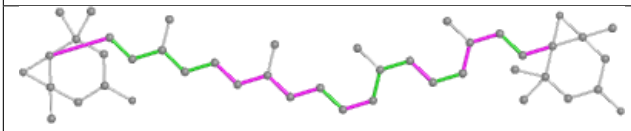
Ligand XAT 0 313



Bond lengths



Bond angles



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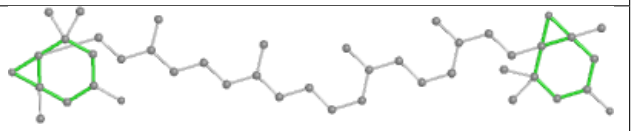
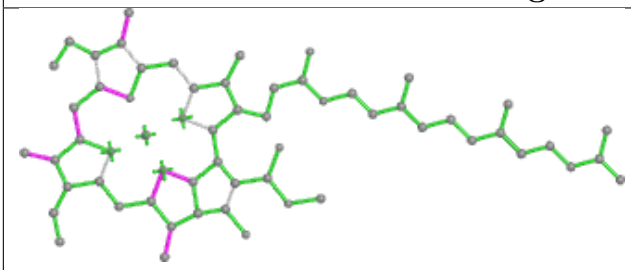
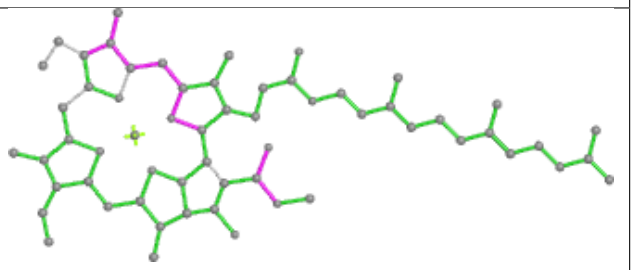


Rings

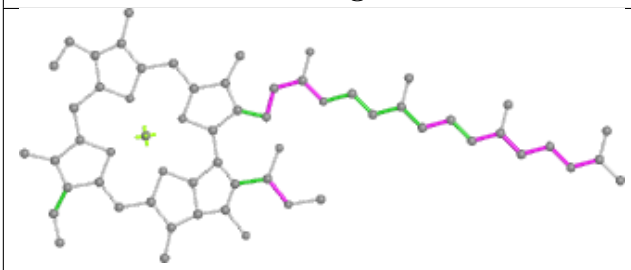
Ligand CLA 0 308



Bond lengths



Bond angles



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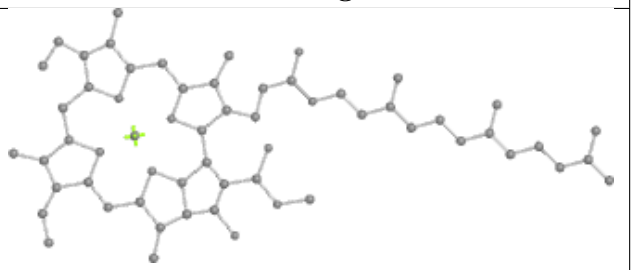
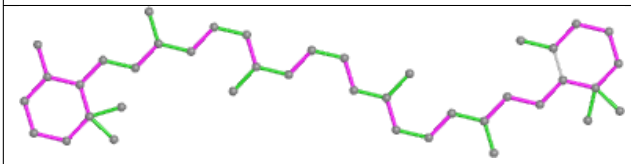


Rings

Ligand 8CT A 848



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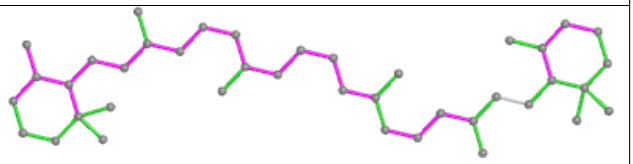
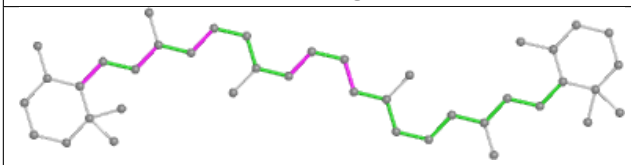


Bond angles



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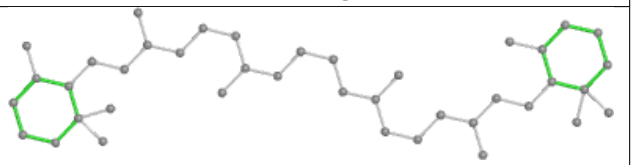
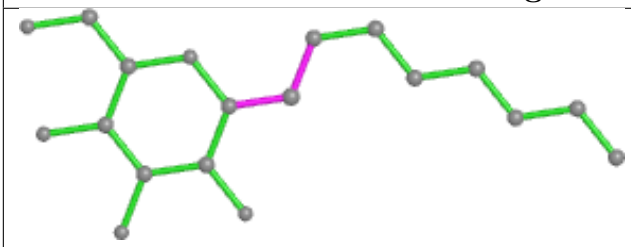
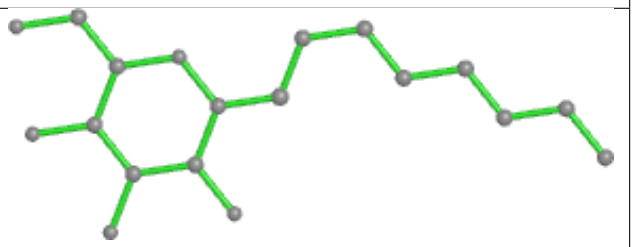


Rings

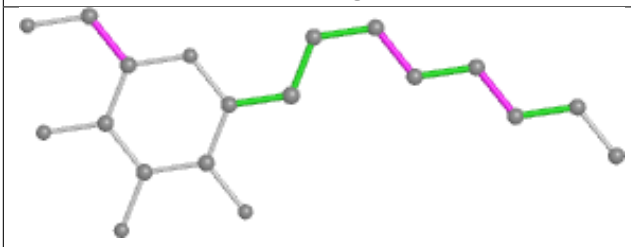
Ligand HTG J 102



Bond lengths



Bond angles



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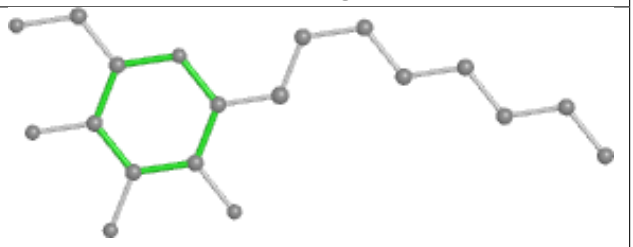
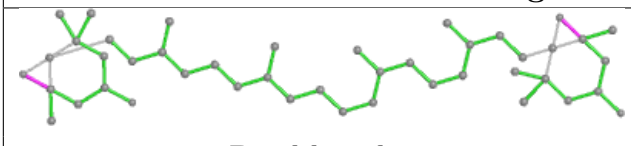
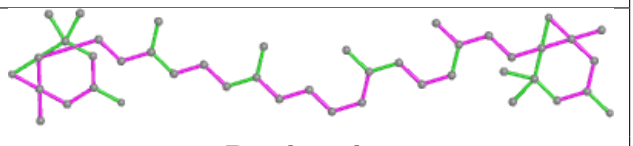


Rings

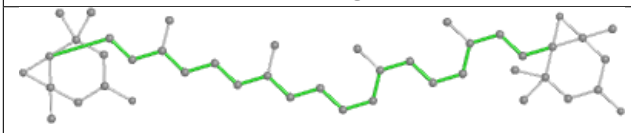
Ligand XAT 7 320



Bond lengths



Bond angles



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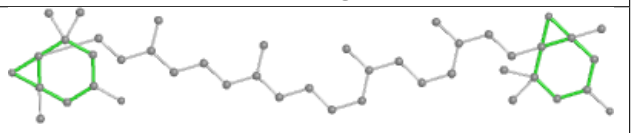
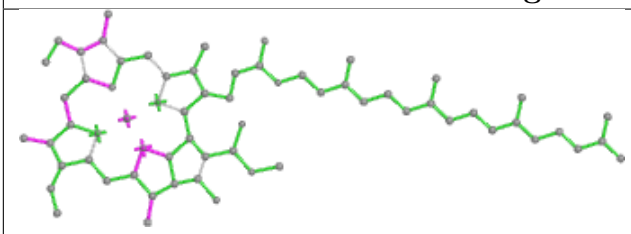


Rings

Ligand CLA A 801



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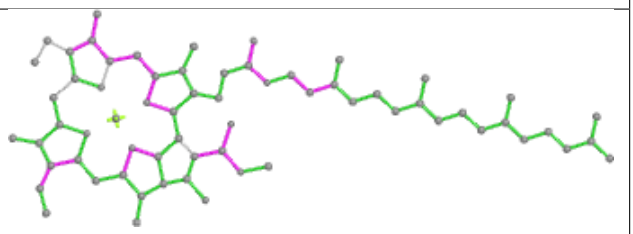

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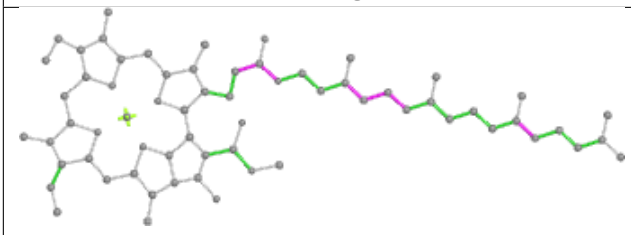

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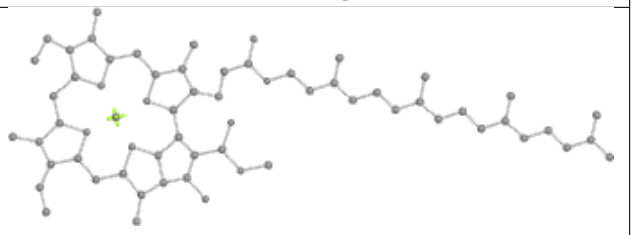
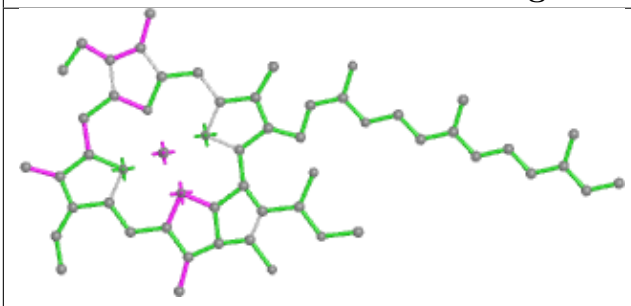


Rings

Ligand CLA 8 312



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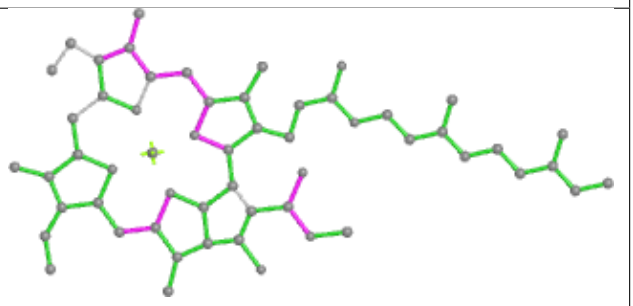

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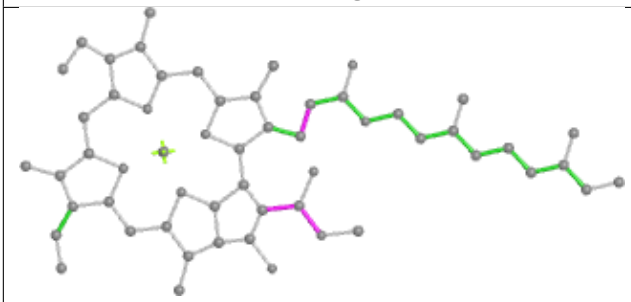

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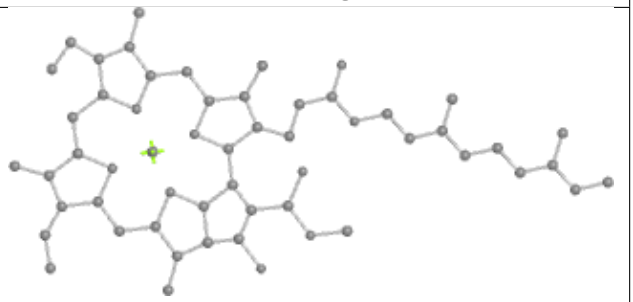

Rings

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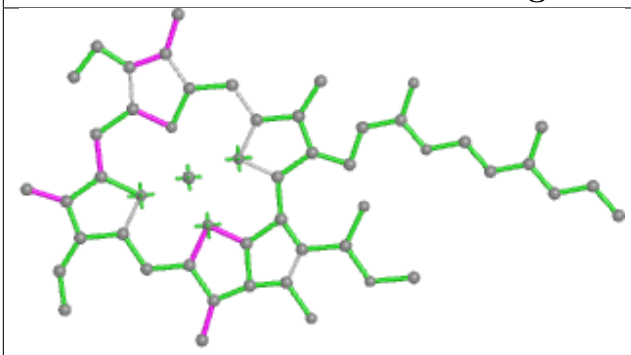
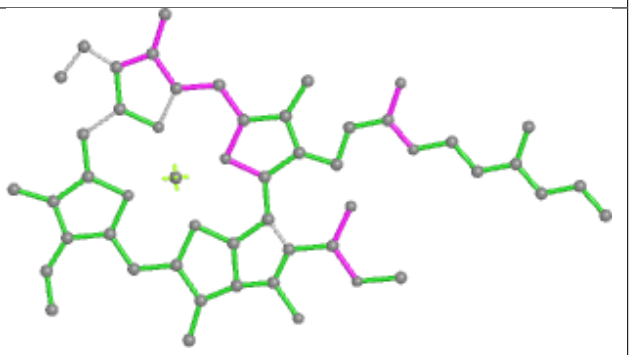
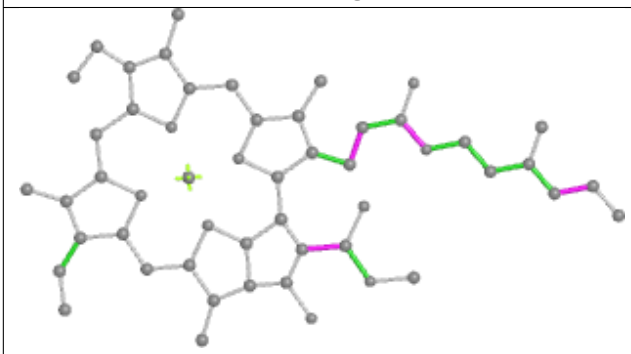
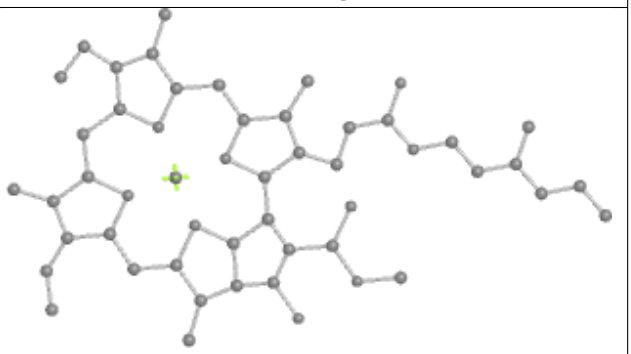
 Bond lengths	 Bond angles
 Torsions	 Rings

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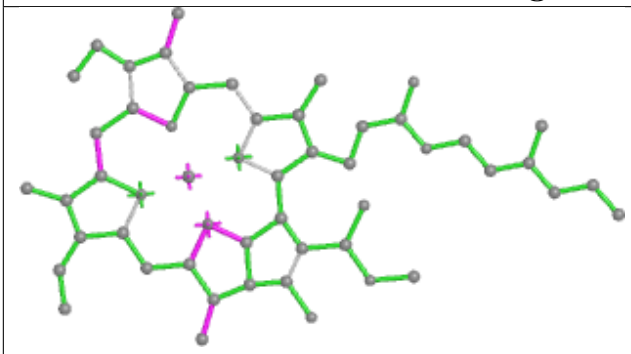
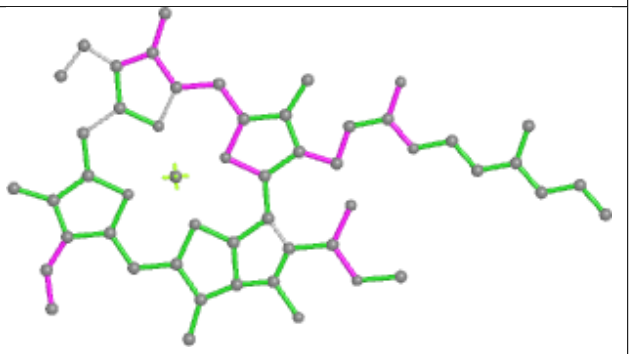
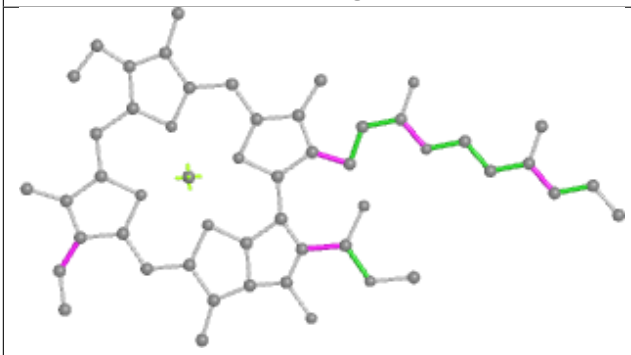
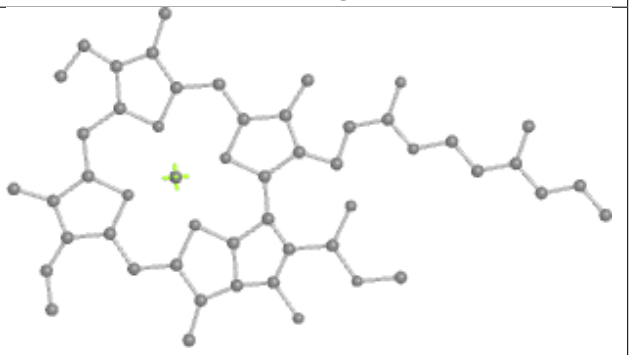
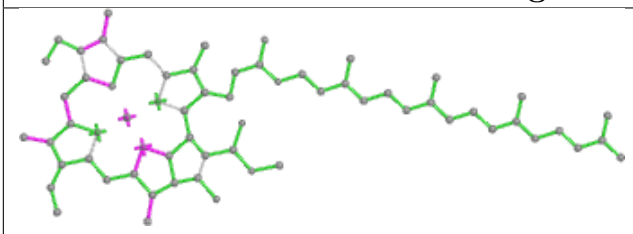
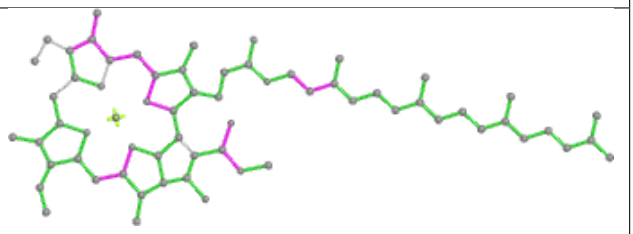
 Bond lengths	 Bond angles
 Torsions	 Rings

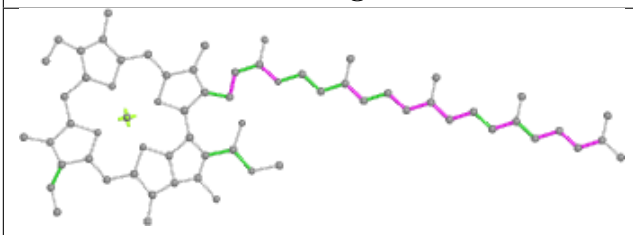
Ligand CLA 2 312



Bond lengths



Bond angles



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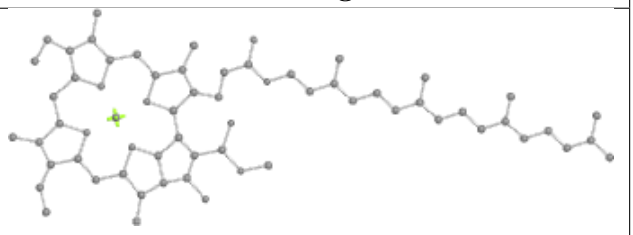
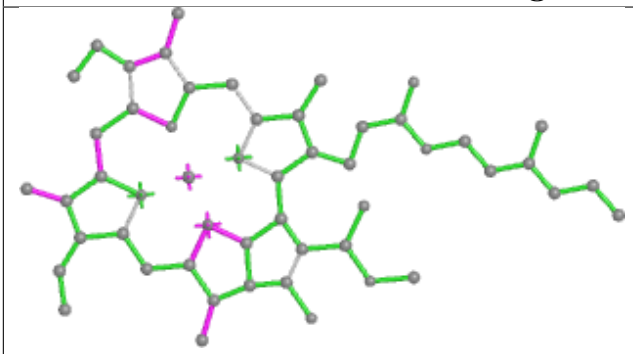


Rings

Ligand CLA 4 311



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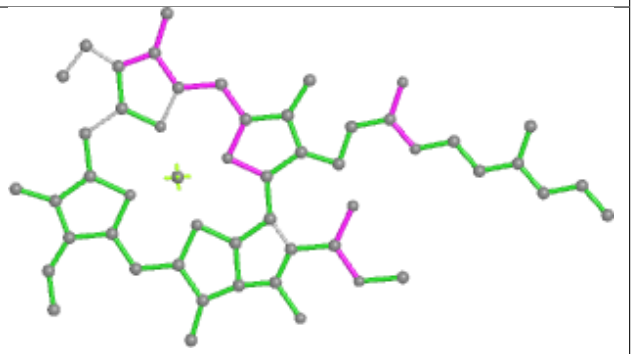
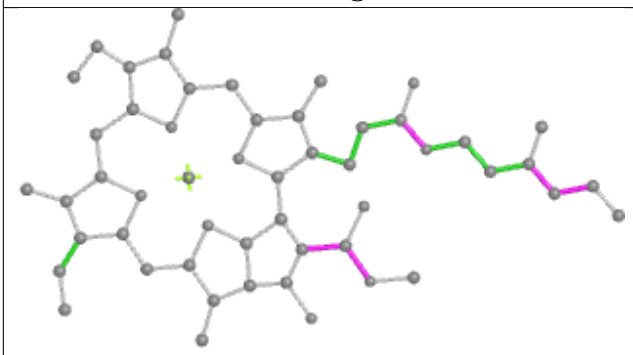


Bond angles



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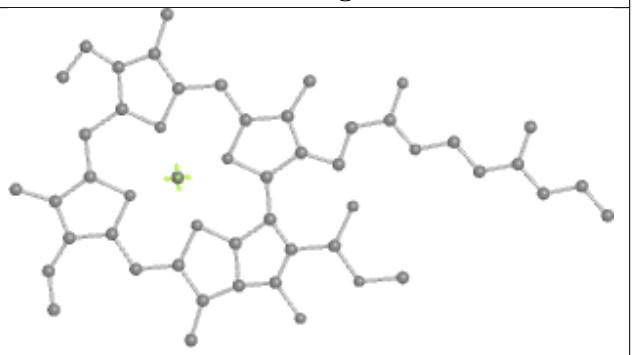
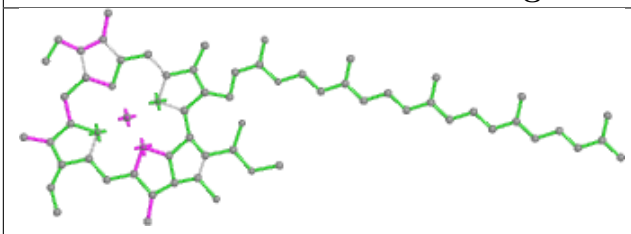


Rings

Ligand CLA A 827



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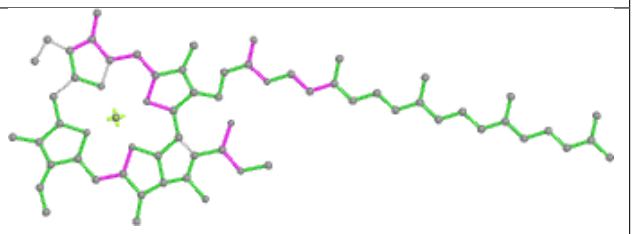

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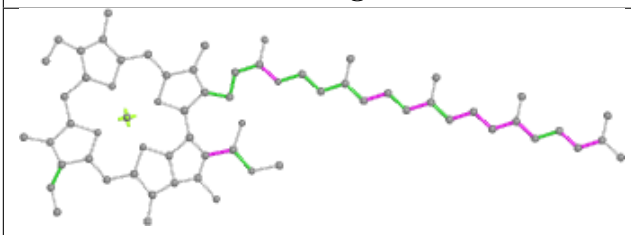

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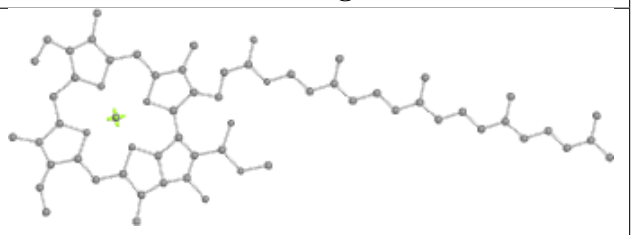
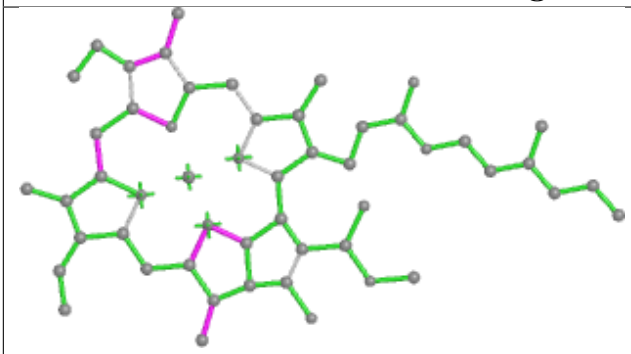


Rings

Ligand CLA 9 311



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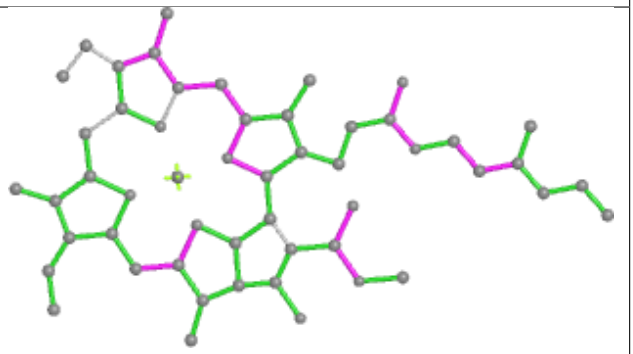
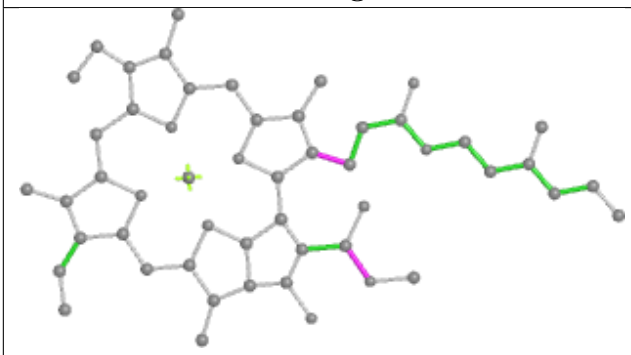


Bond angles



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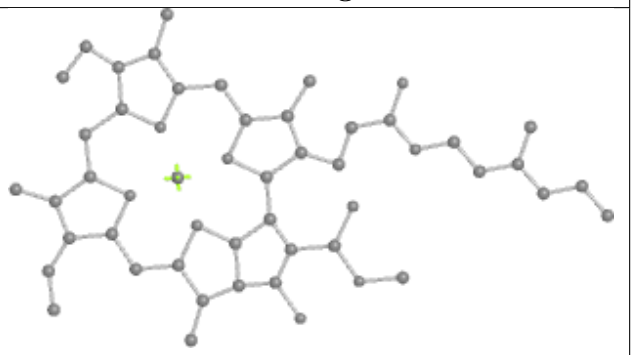
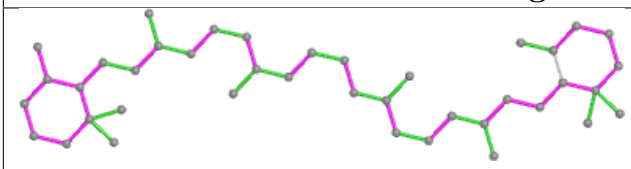


Rings

Ligand 8CT F 302



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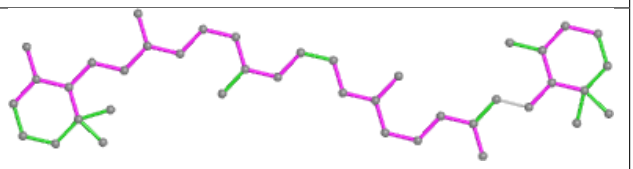

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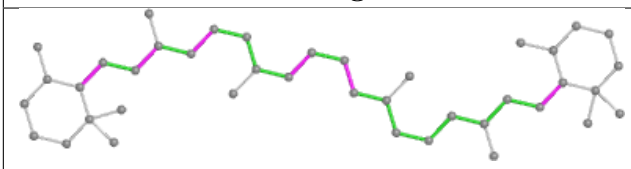

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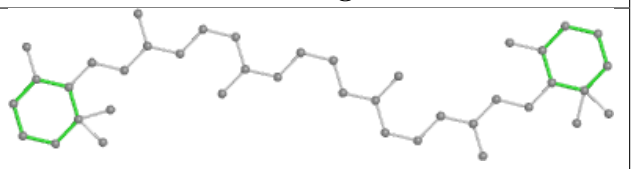
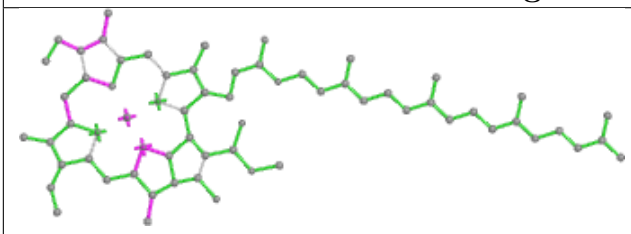


Rings

Ligand CLA A 838



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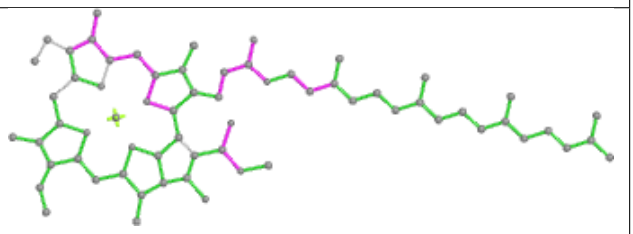

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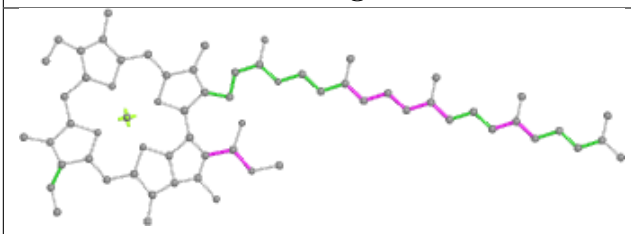

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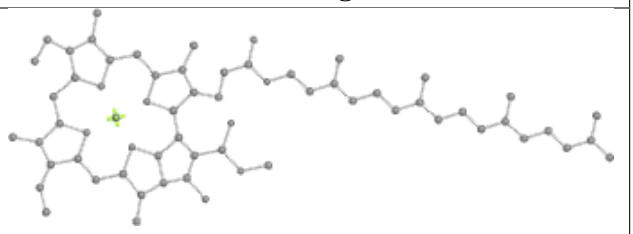
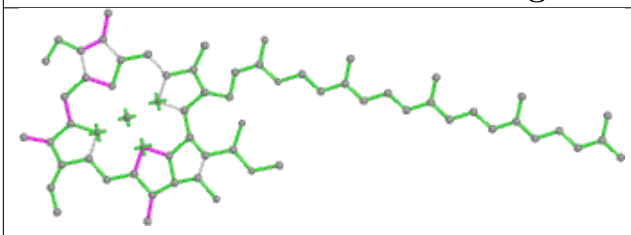


Rings

Ligand CLA 0 311



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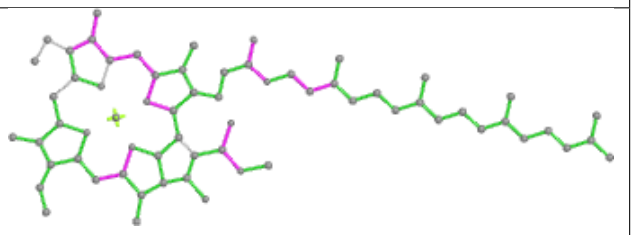

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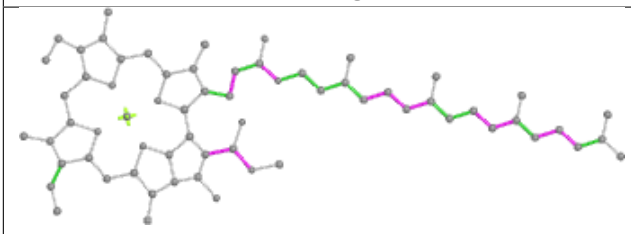

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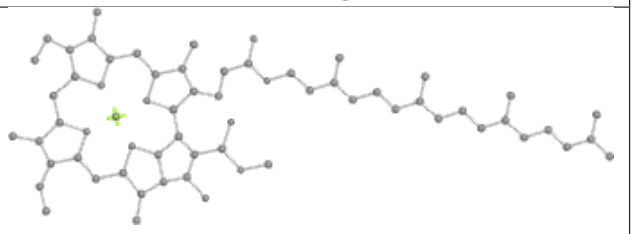
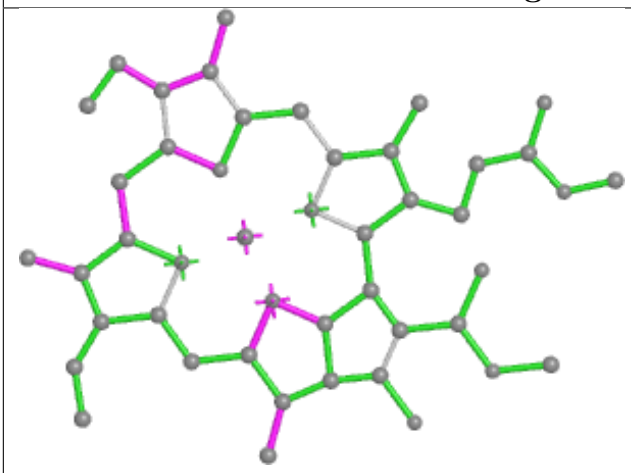


Rings

Ligand CLA B 822



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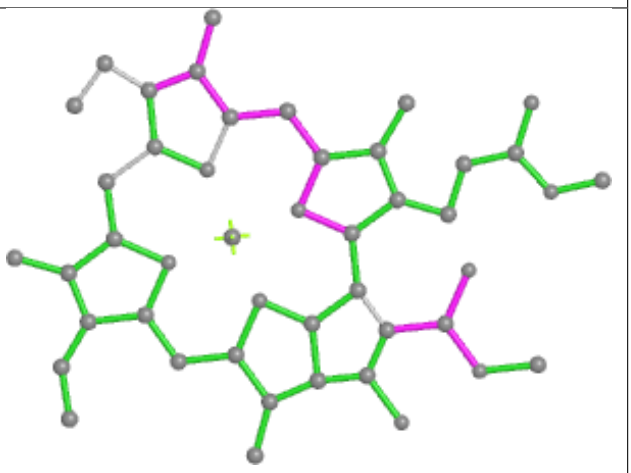

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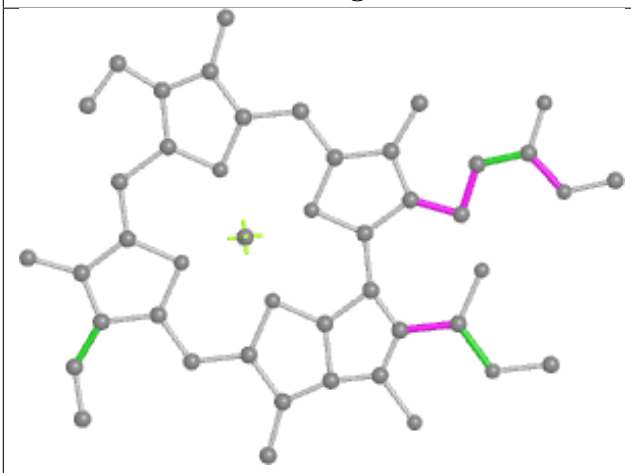

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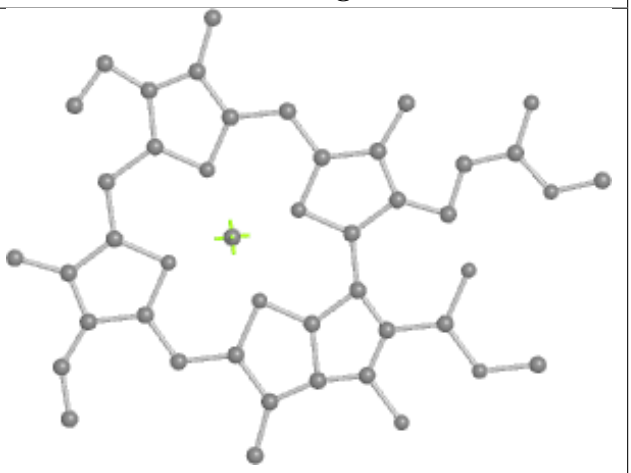
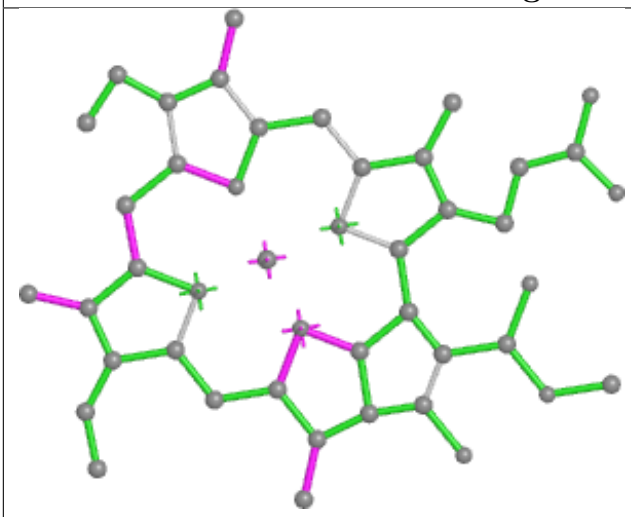


Rings

Ligand CLA K 101



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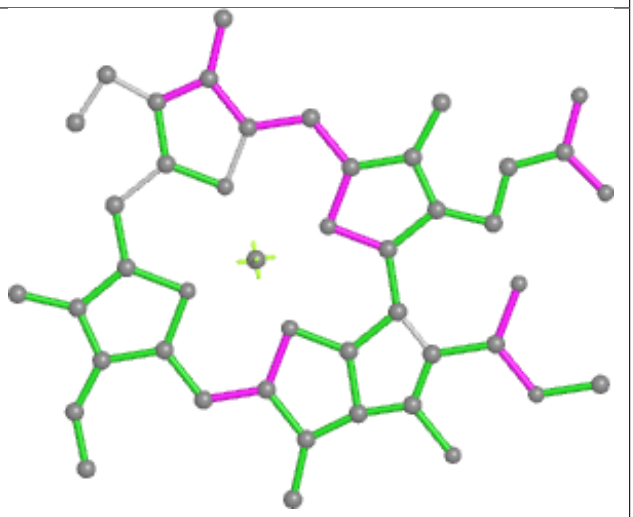
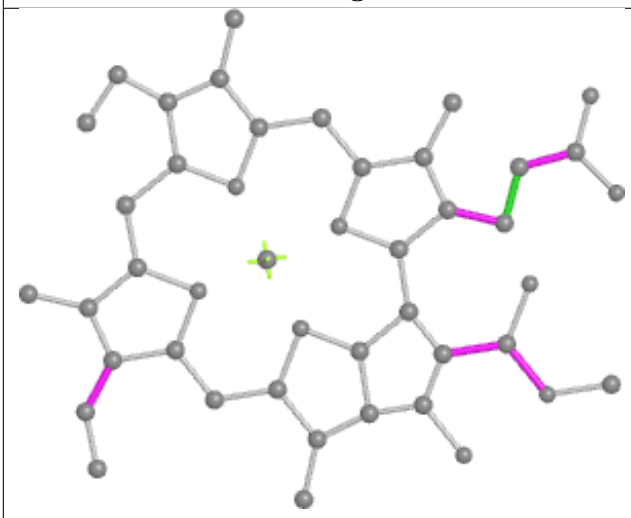
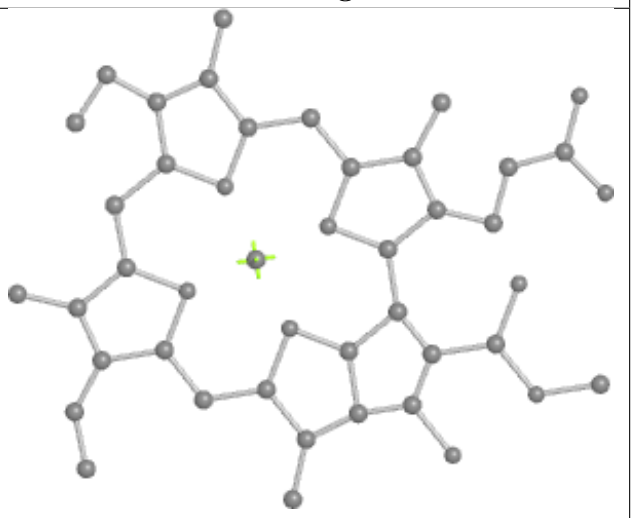


Bond angles

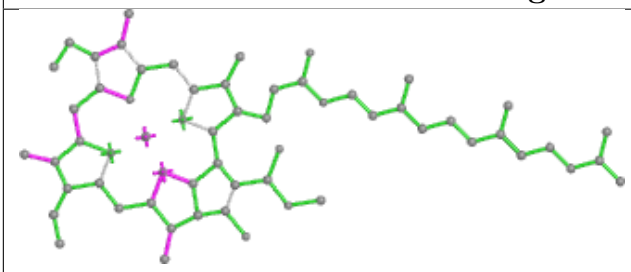


Torsions



Rings

Ligand CLA 6 310



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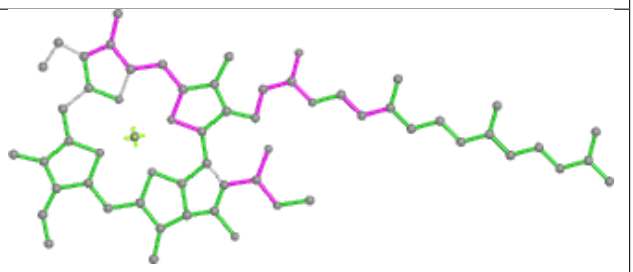

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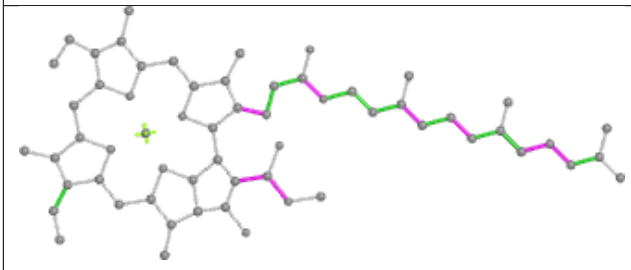

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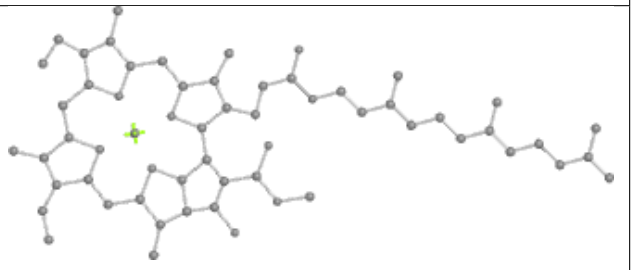
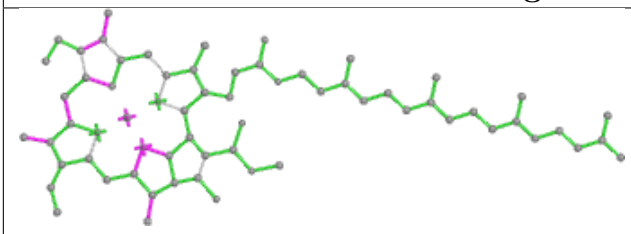


Rings

Ligand CLA A 808



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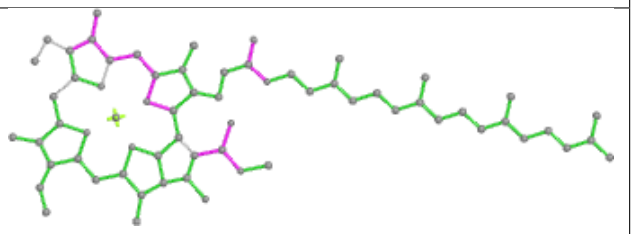

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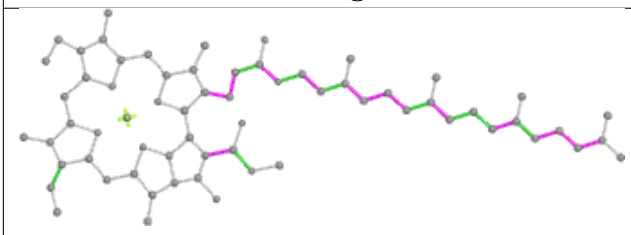

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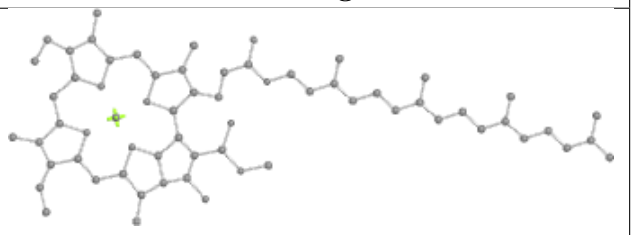
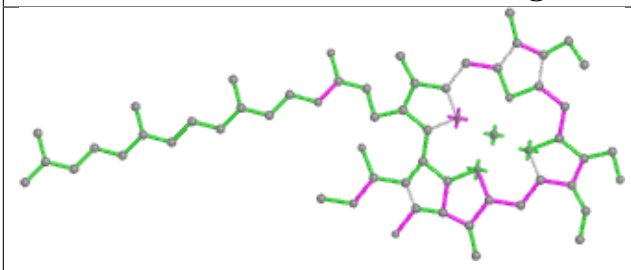


Rings

Ligand CHL 0 301



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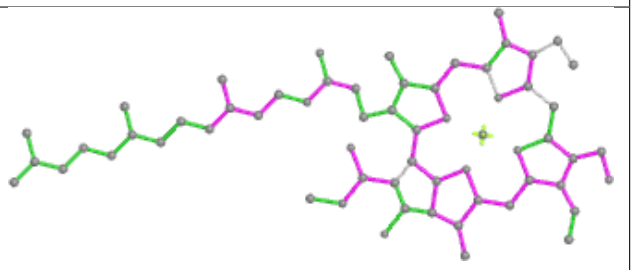

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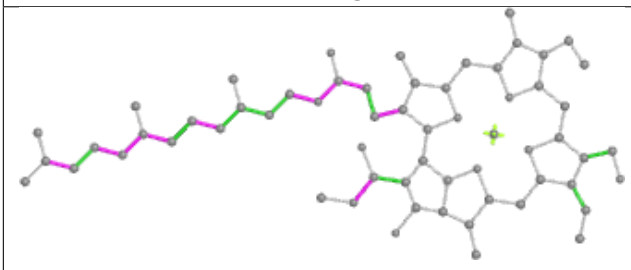

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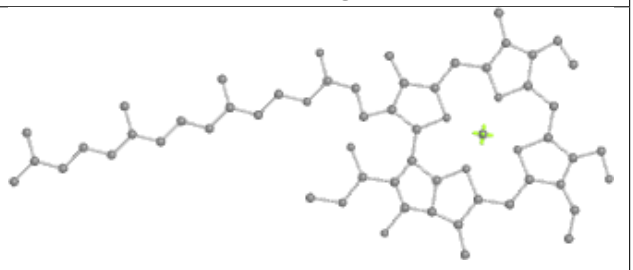
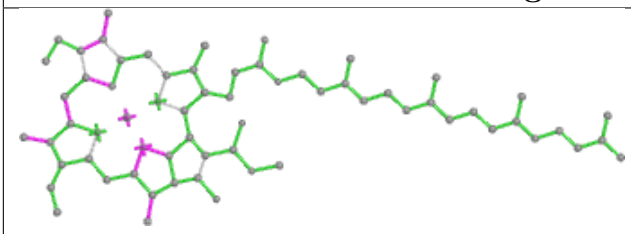


Rings

Ligand CLA B 840



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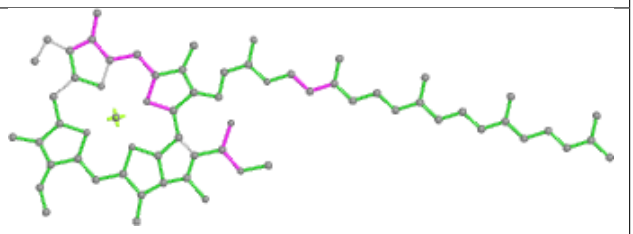

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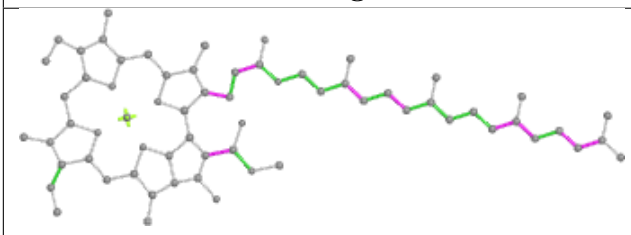

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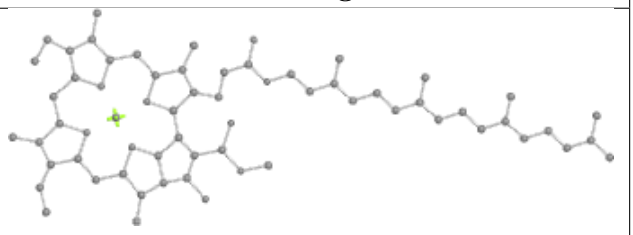
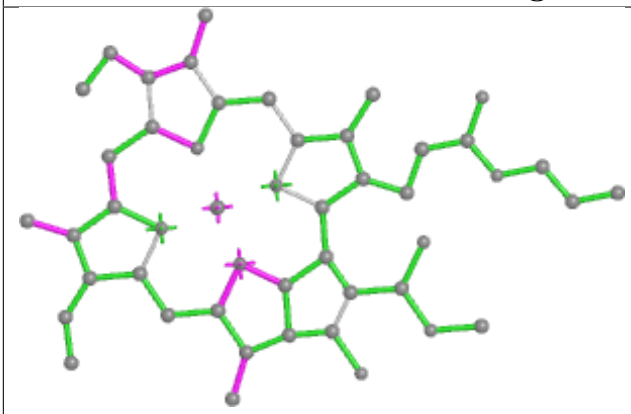


Rings

Ligand CLA 9 304



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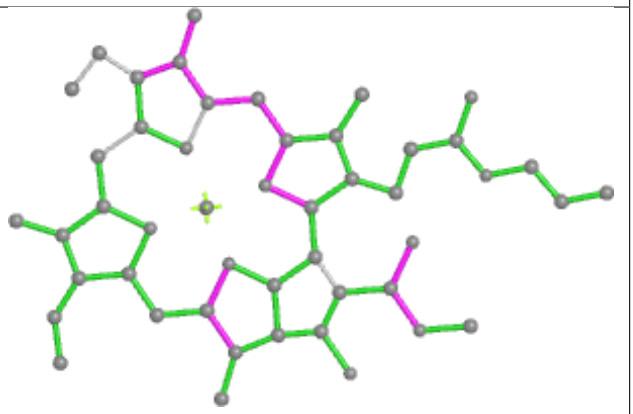

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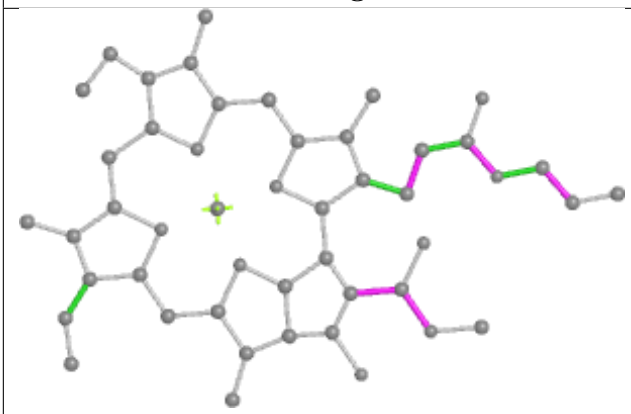

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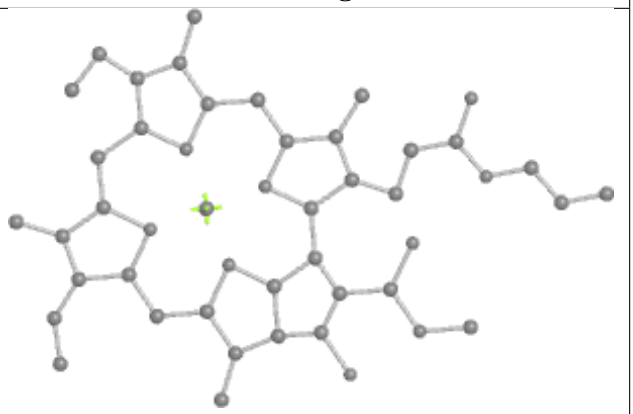
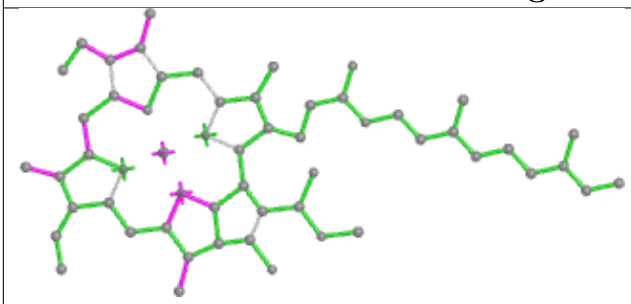


Rings

Ligand CLA 4 312



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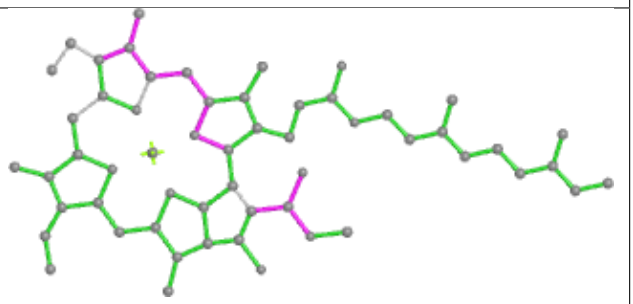

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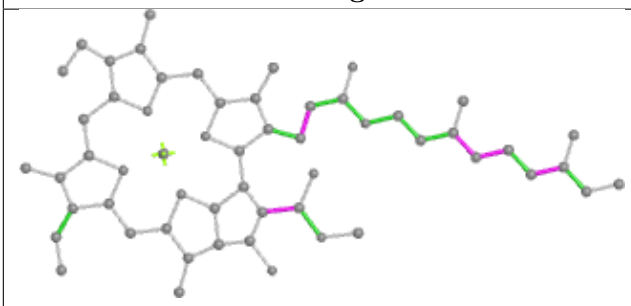

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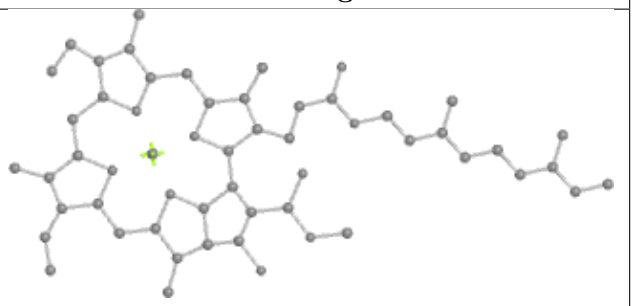
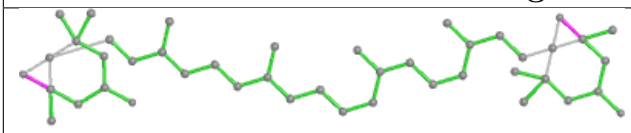


Rings

Ligand XAT 5 316



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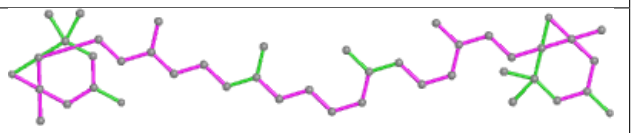

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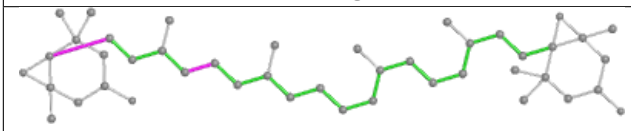

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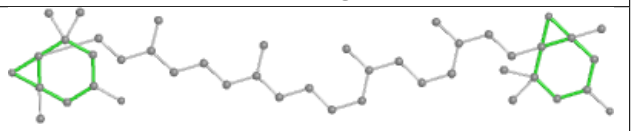
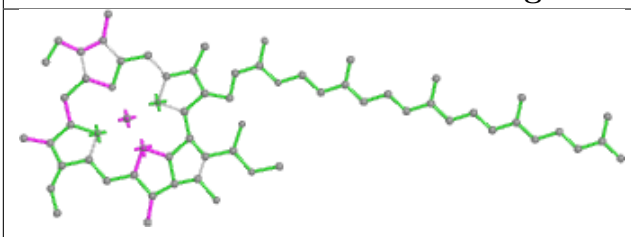


Rings

Ligand CLA B 806



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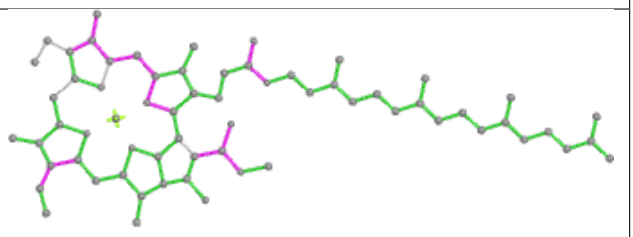

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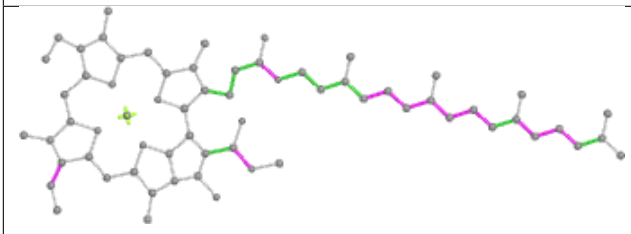

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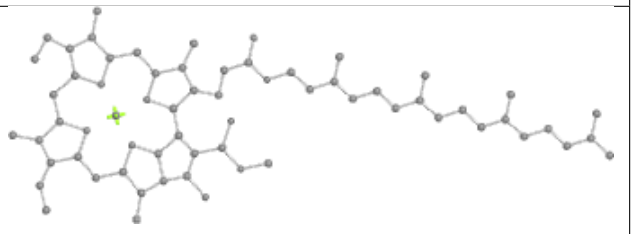
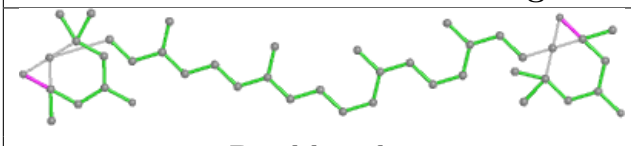


Rings

Ligand XAT 7 319



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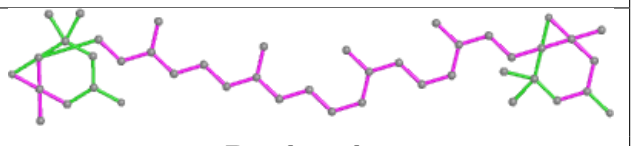
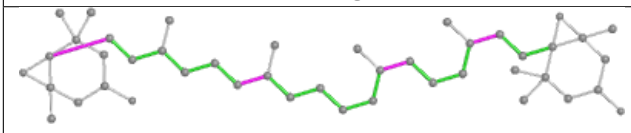


Bond angles



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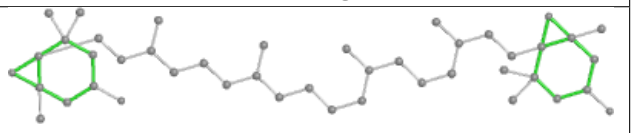

Rings

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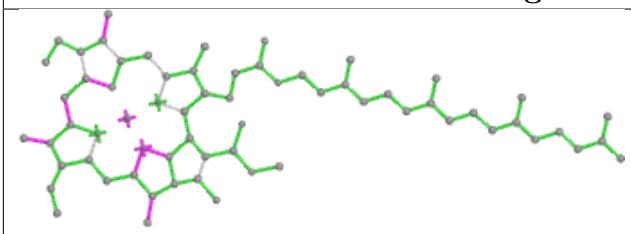

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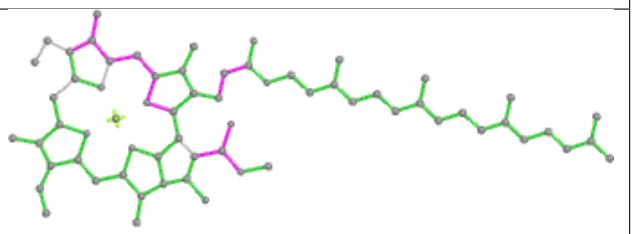
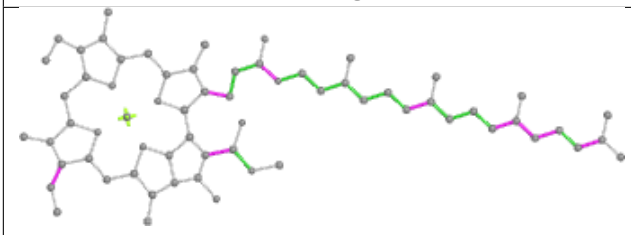


Bond angles



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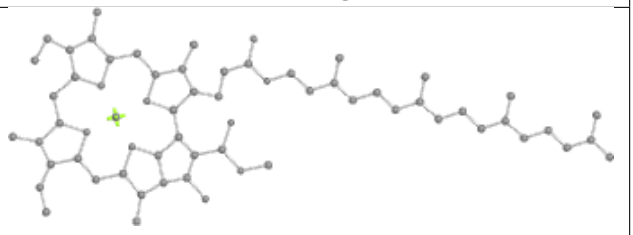
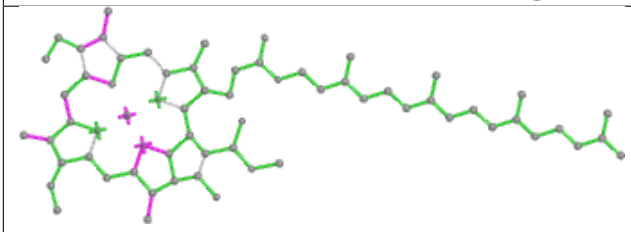


Rings

Ligand CLA 5 303



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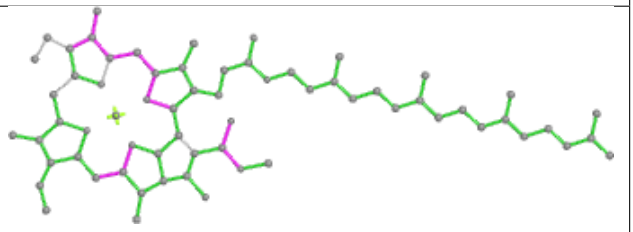
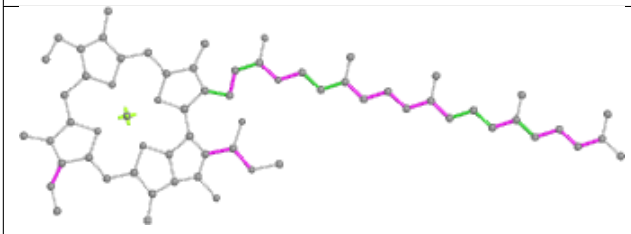


Bond angles



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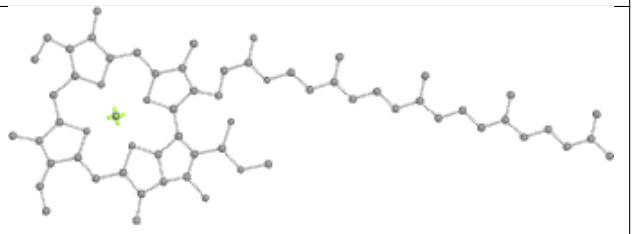
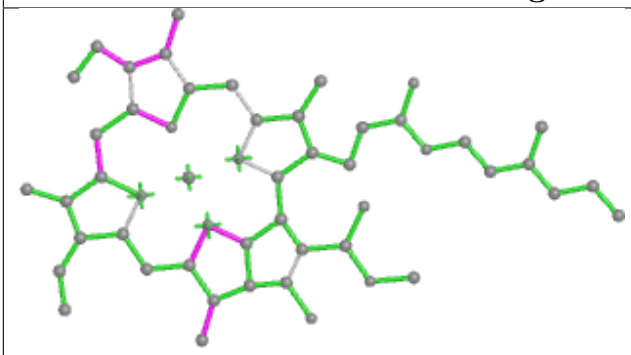


Rings

Ligand CLA 5 305



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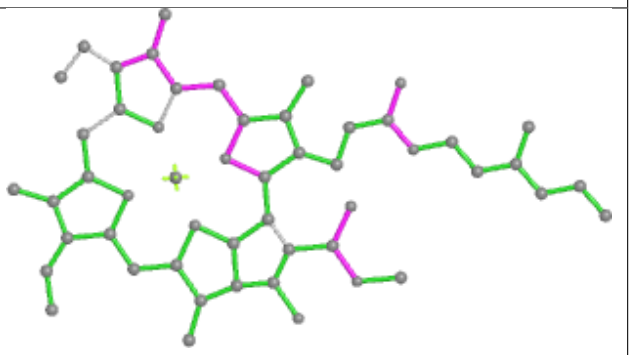
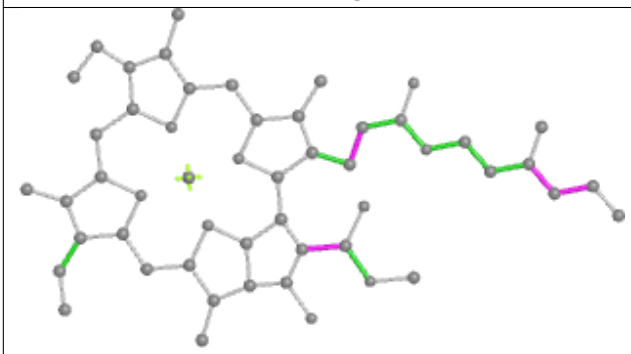
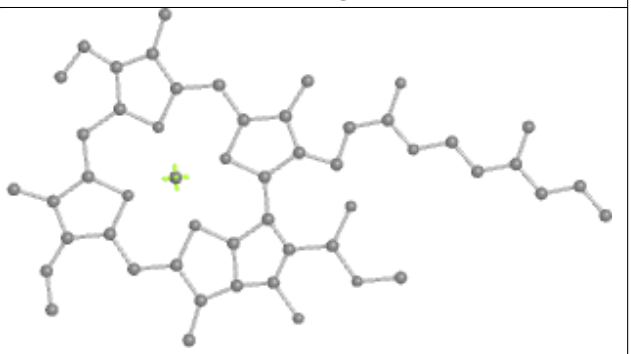


Bond angles

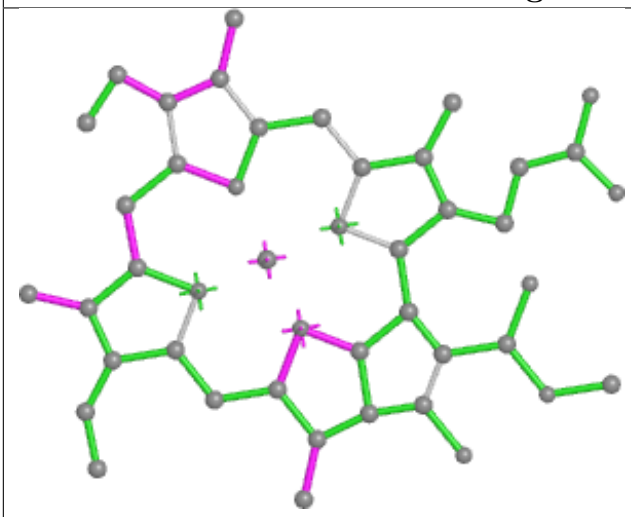


Torsions



Rings

Ligand CLA F 301



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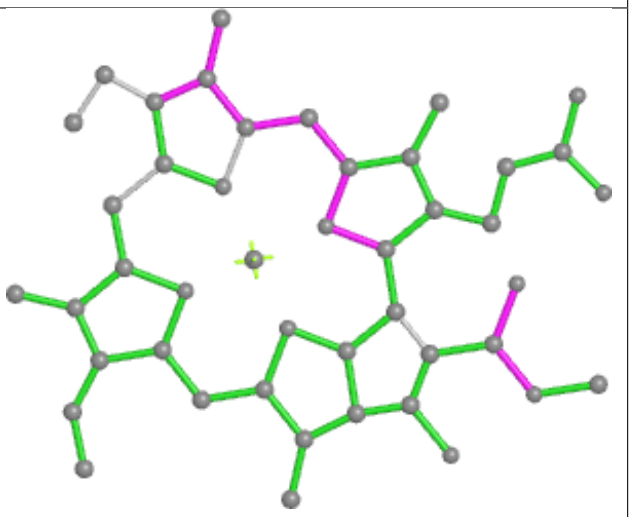
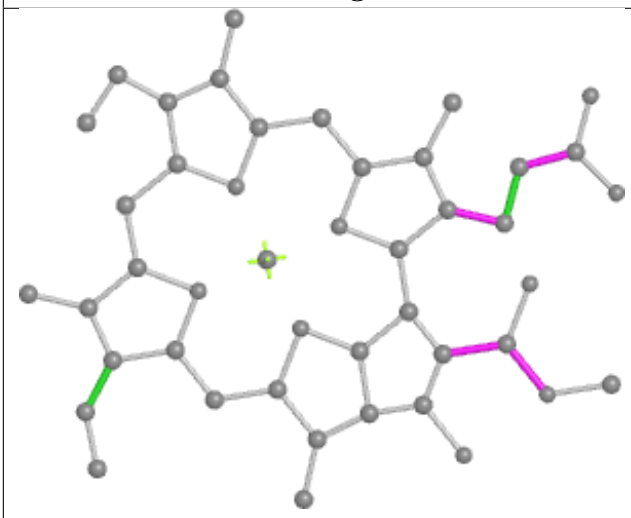


Bond angles



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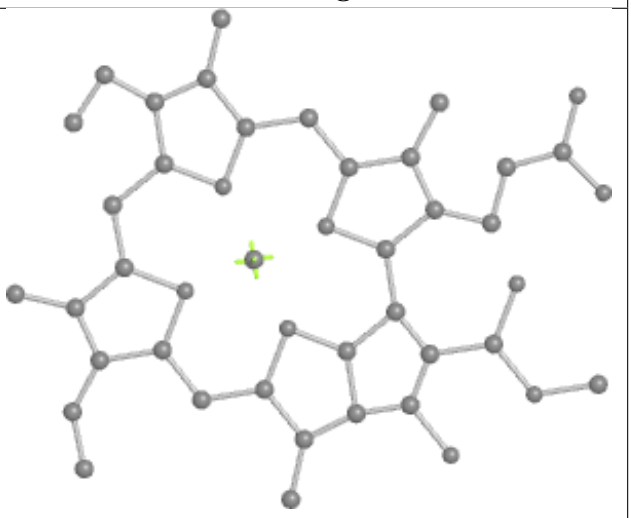
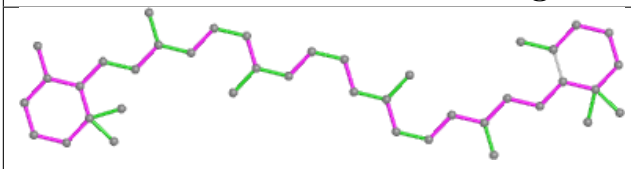


Rings

Ligand 8CT 4 317



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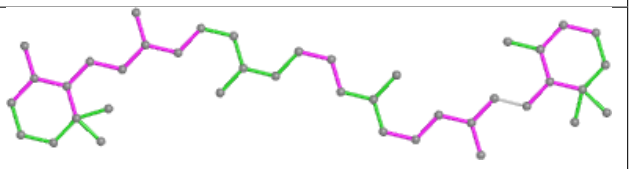

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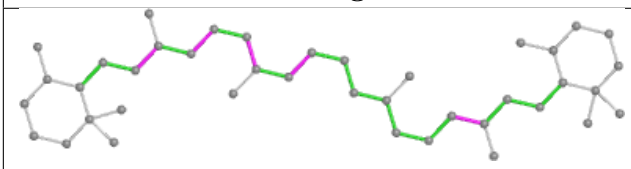

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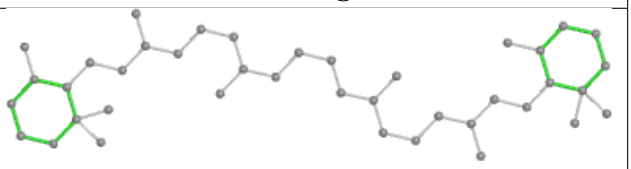
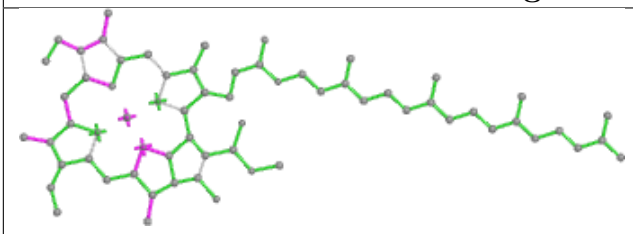


Rings

Ligand CLA A 833



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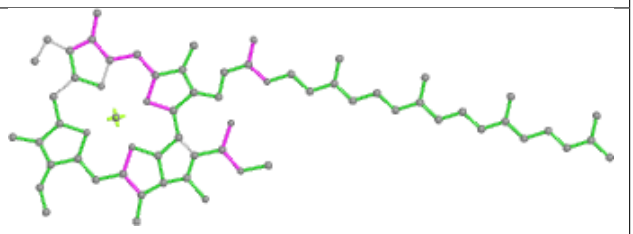

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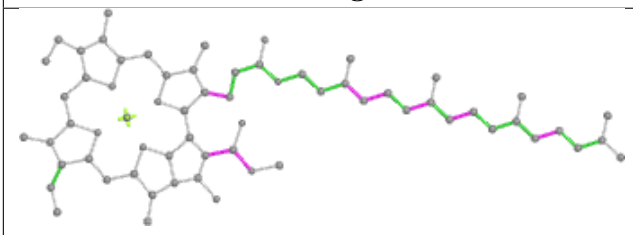

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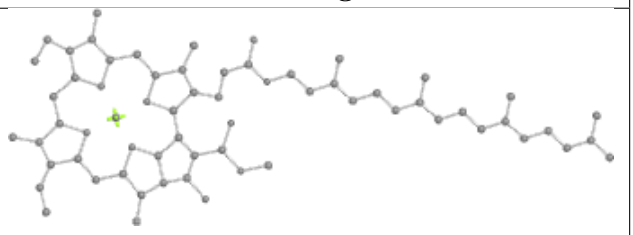
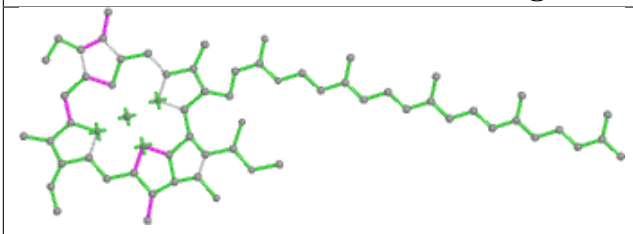


Rings

Ligand CLA 5 307



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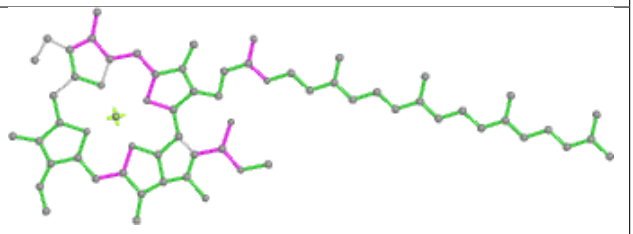

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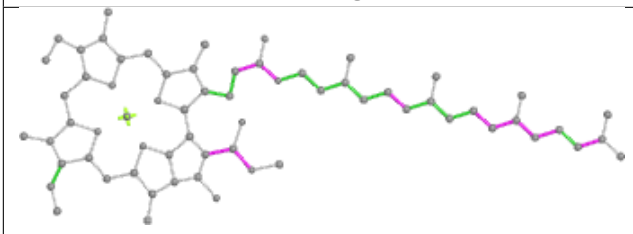

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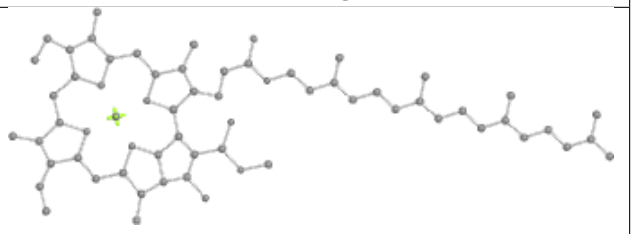
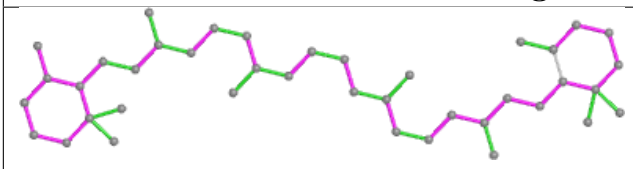


Rings

Ligand 8CT J 104



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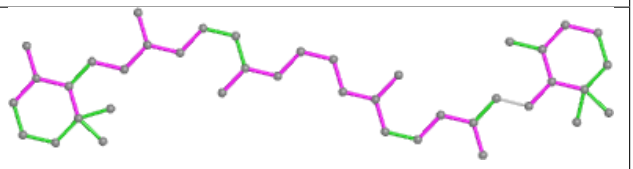

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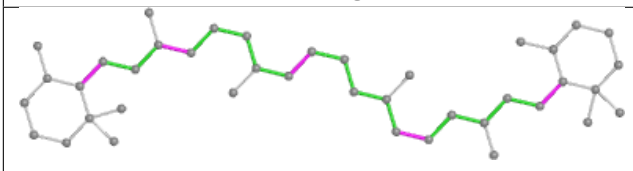

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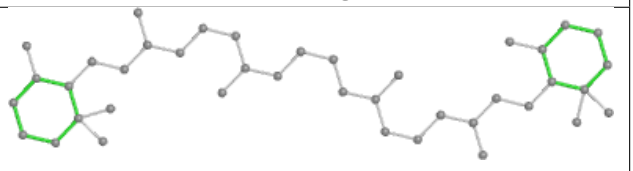
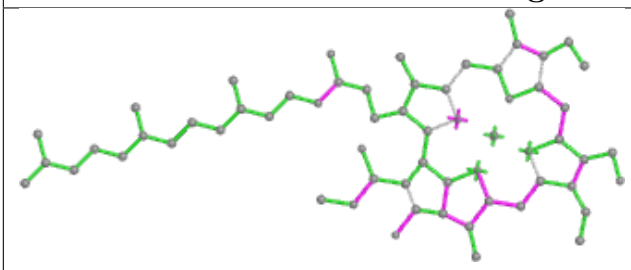


Rings

Ligand CHL 5 301



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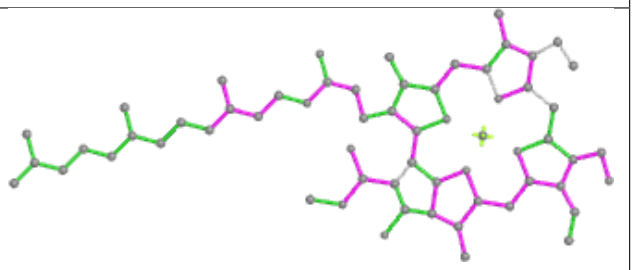

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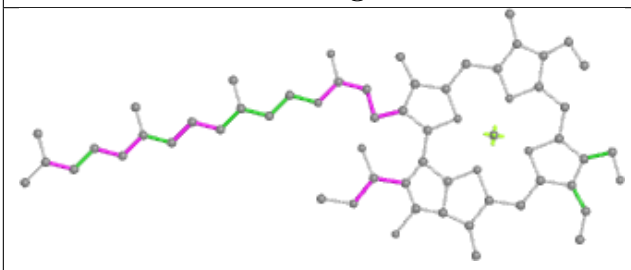

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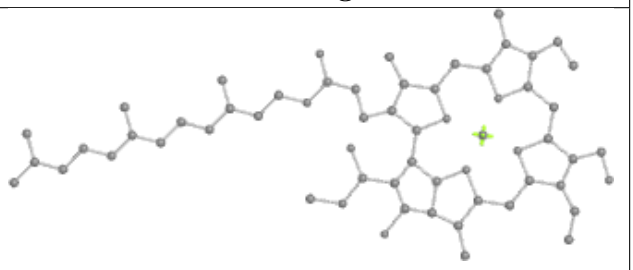
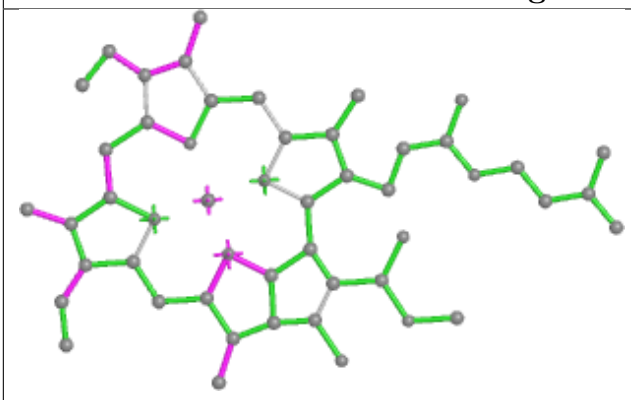


Rings

Ligand CLA 3 308



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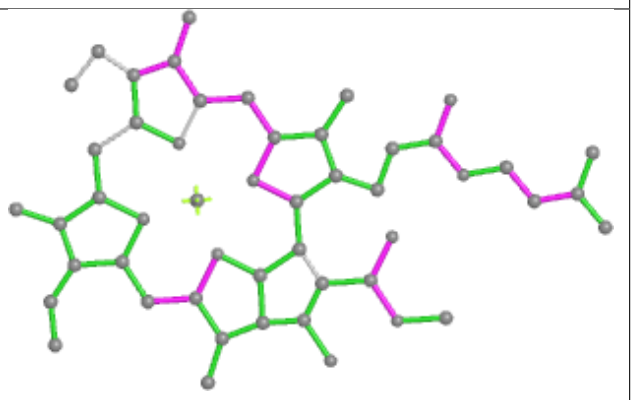

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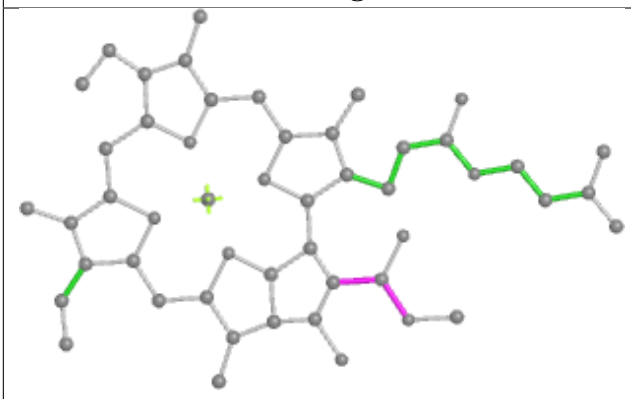

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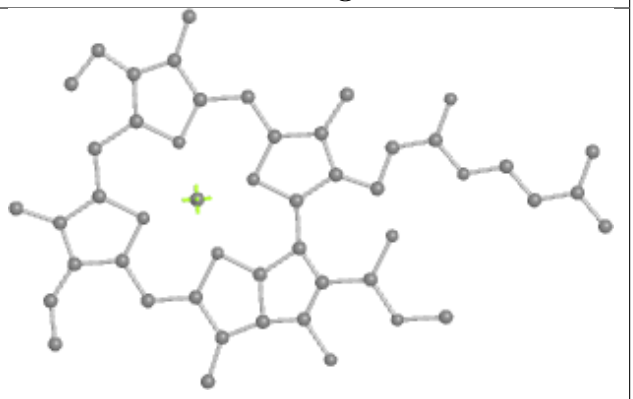

Rings

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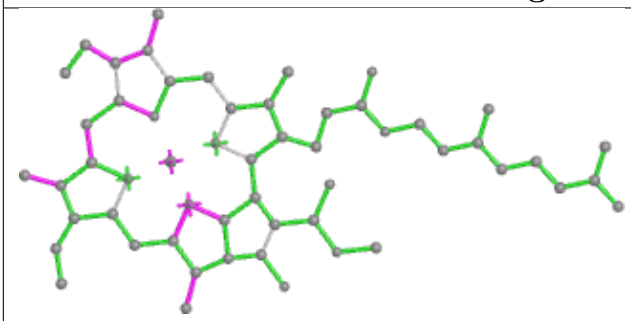

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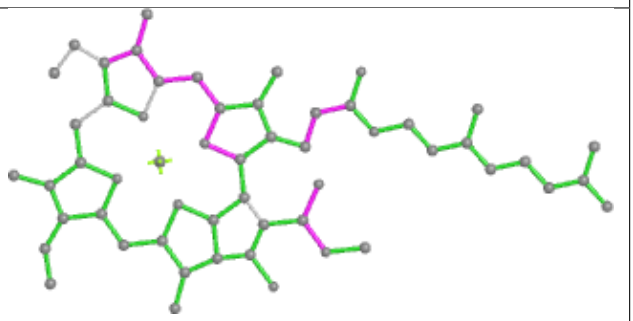

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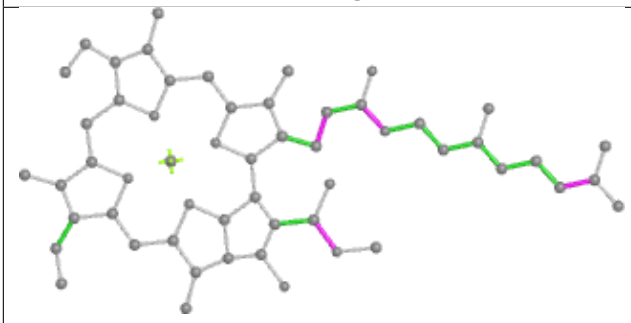

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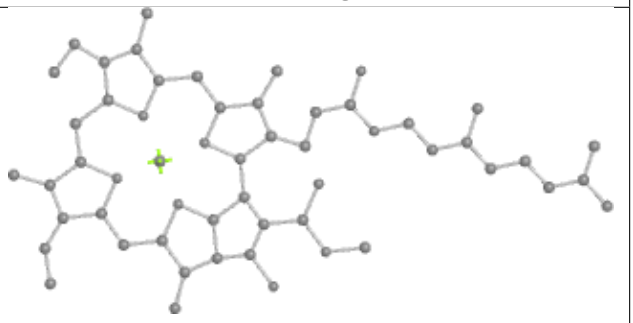
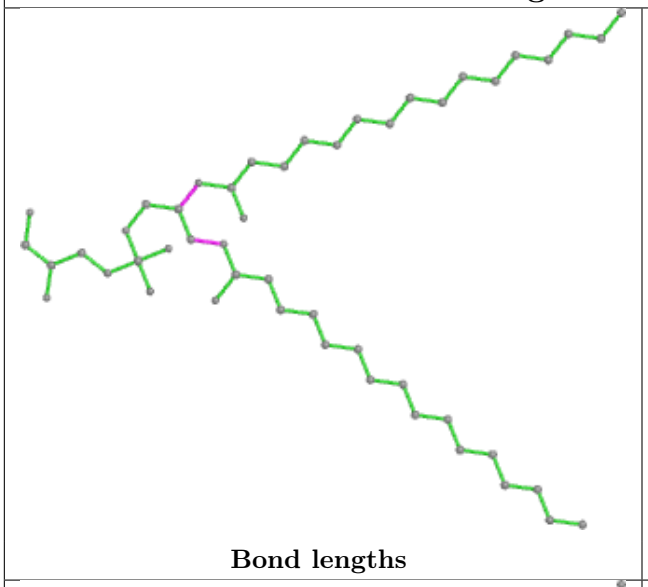


Rings

Ligand LHG 1 317



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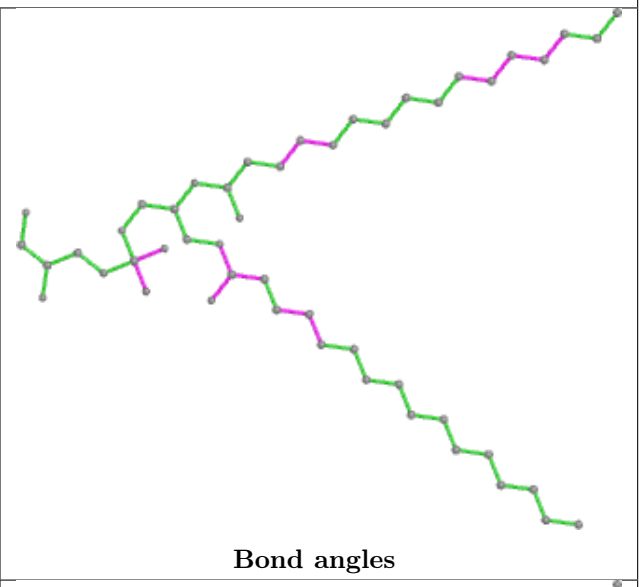

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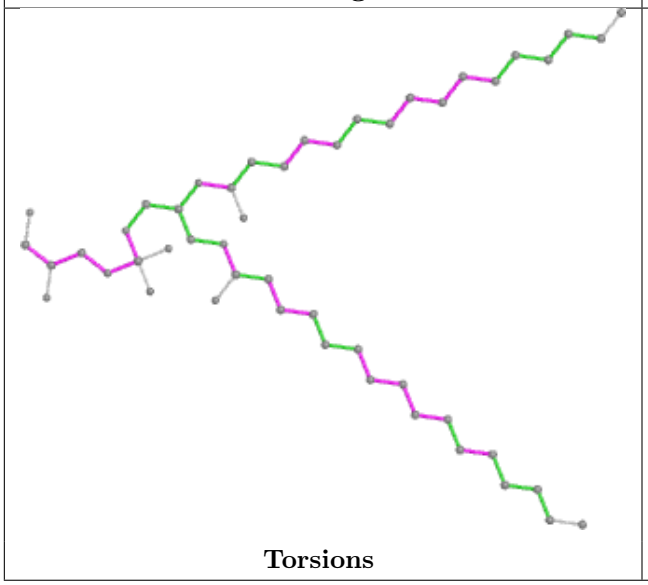

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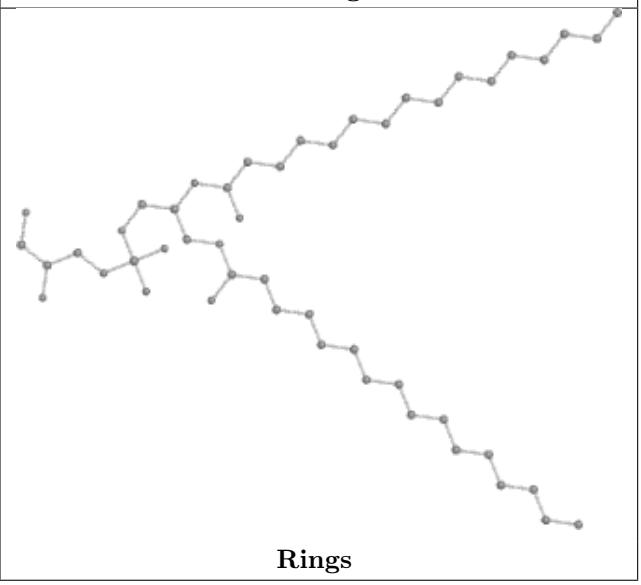

Rings

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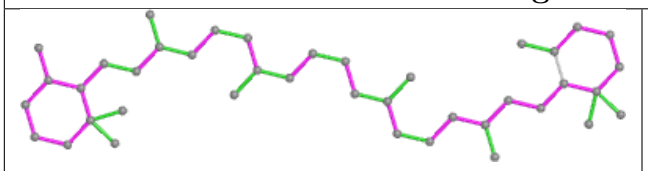

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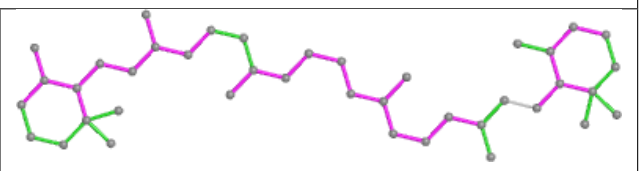

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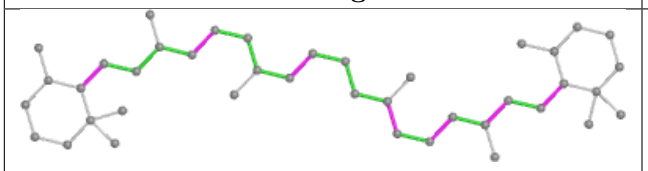

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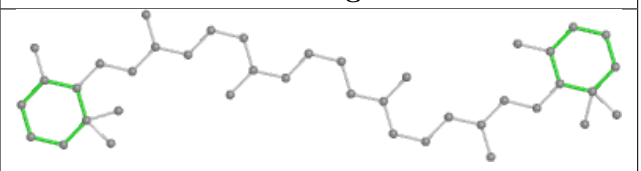
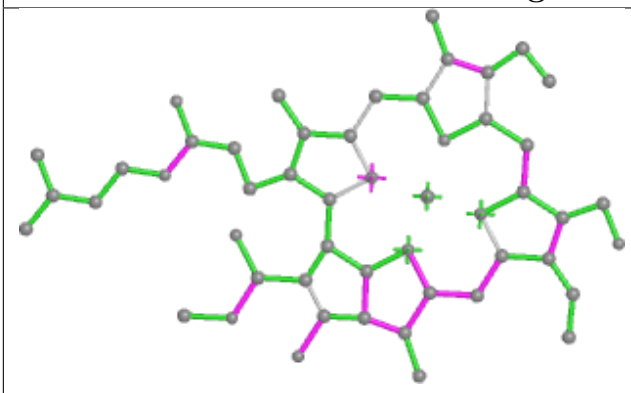


Rings

Ligand CHL 8 307



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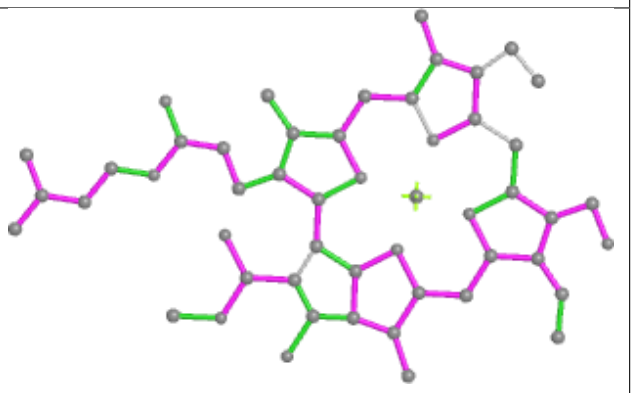

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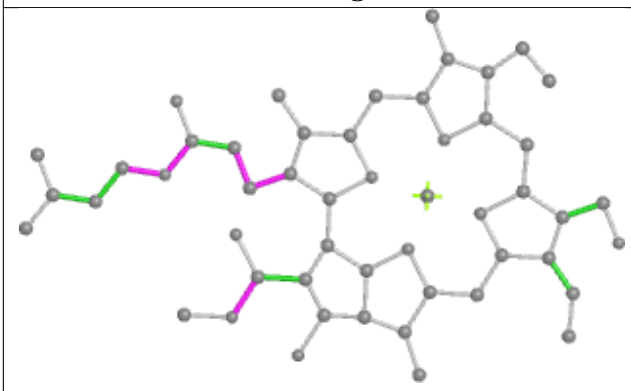

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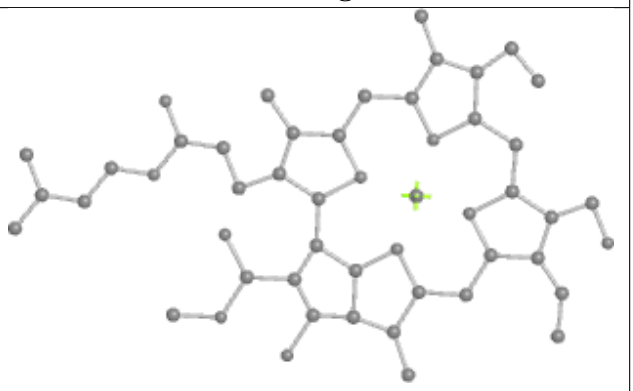

Rings

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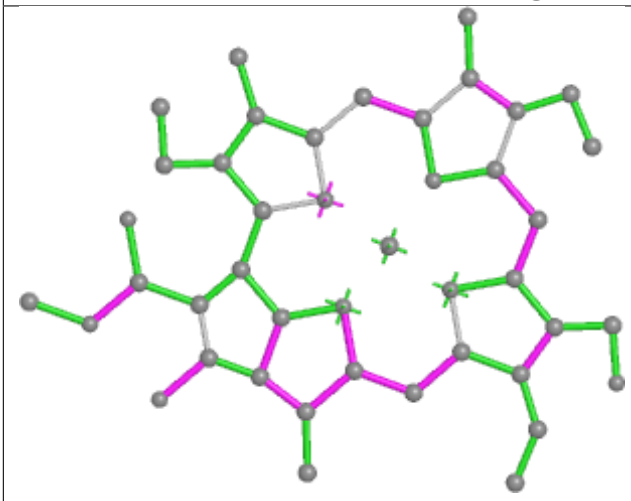

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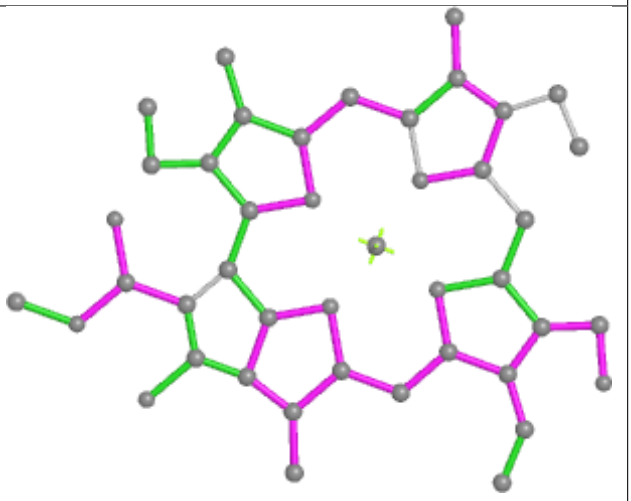
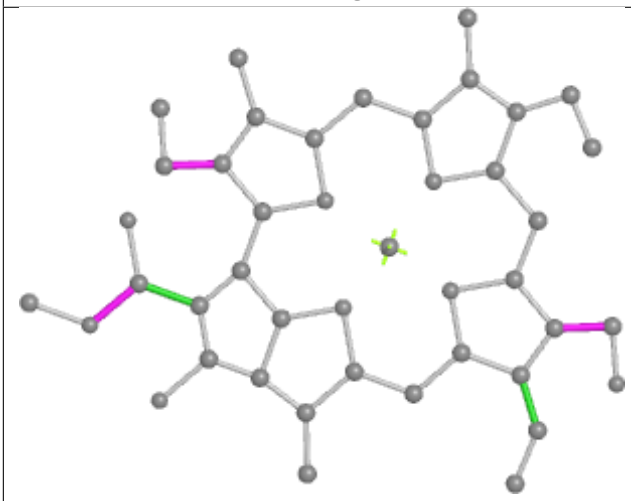


Bond angles



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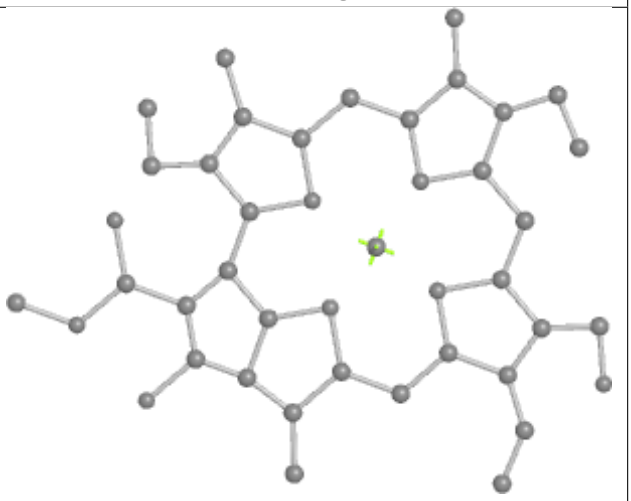
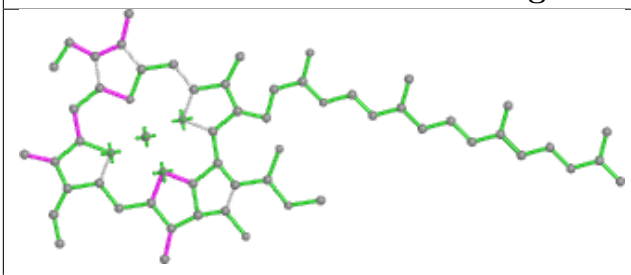


Rings

Ligand CLA 9 309



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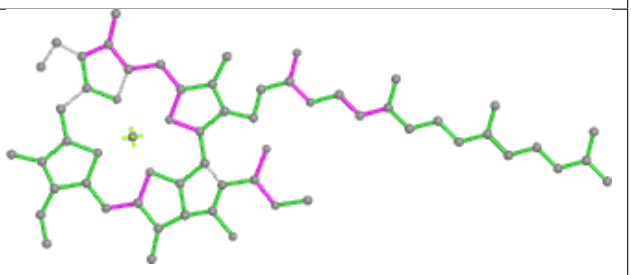
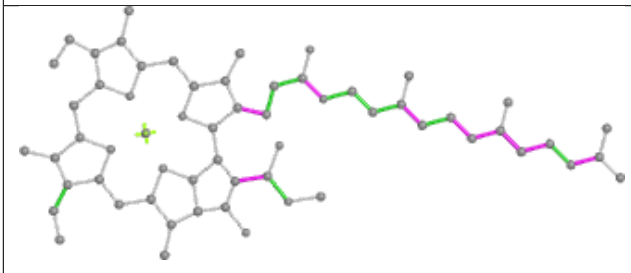
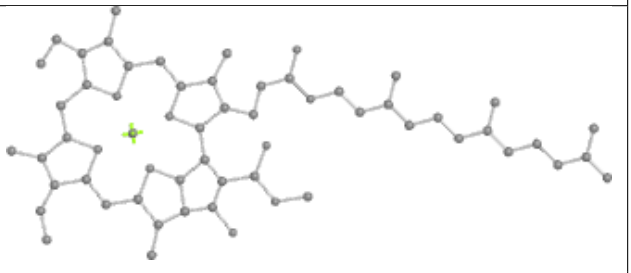


Bond angles

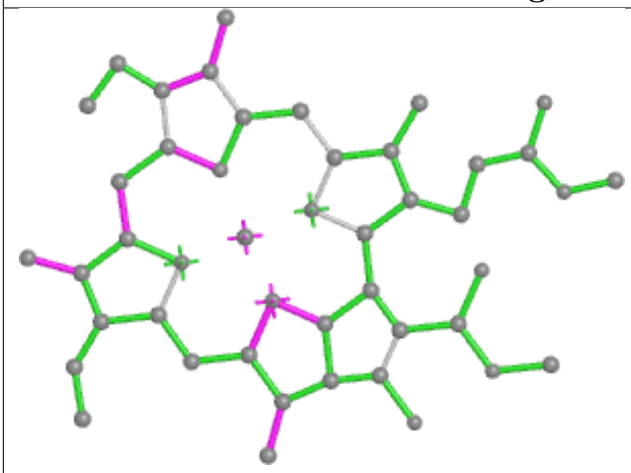


Torsions



Rings

Ligand CLA 1 313



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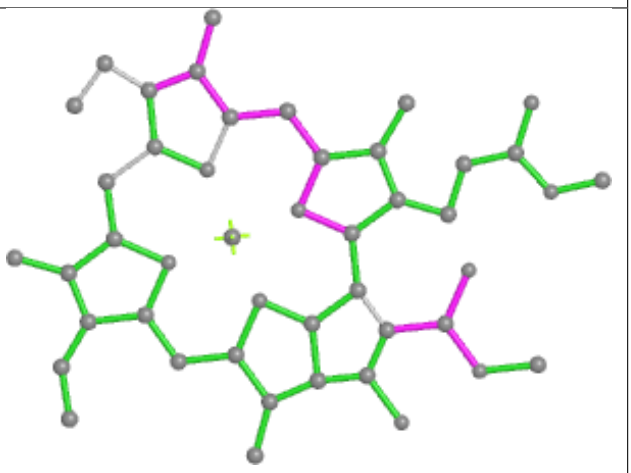

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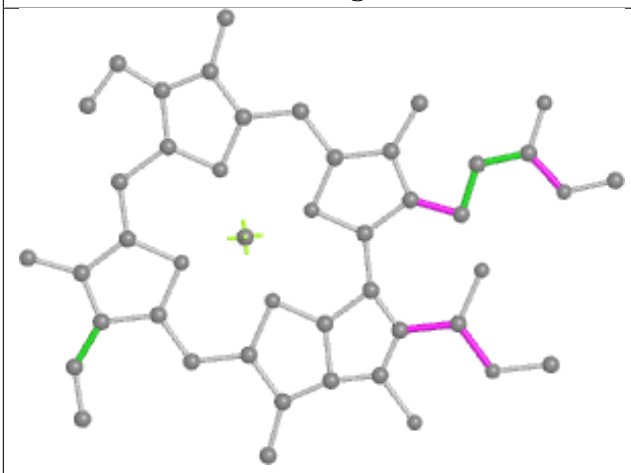

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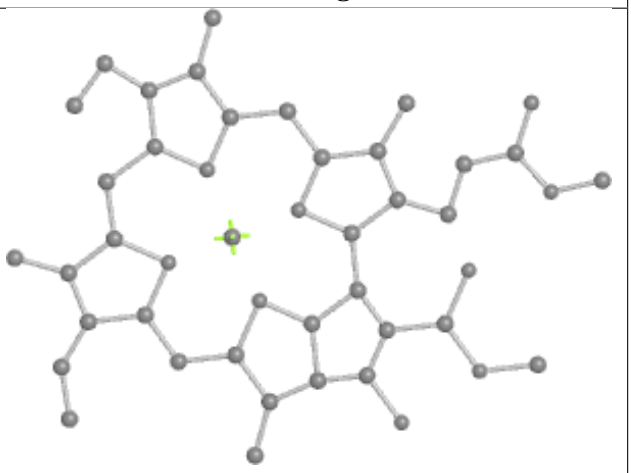
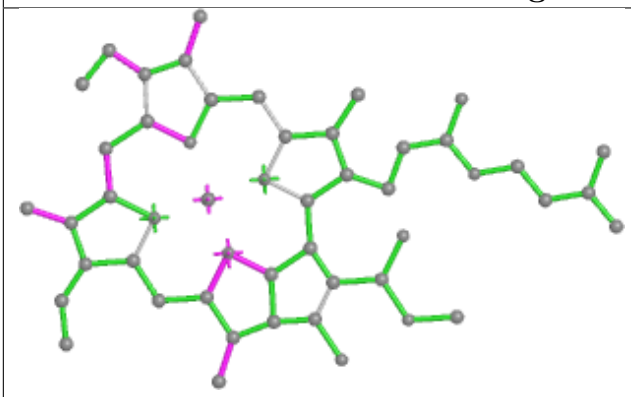


Rings

Ligand CLA 7 310



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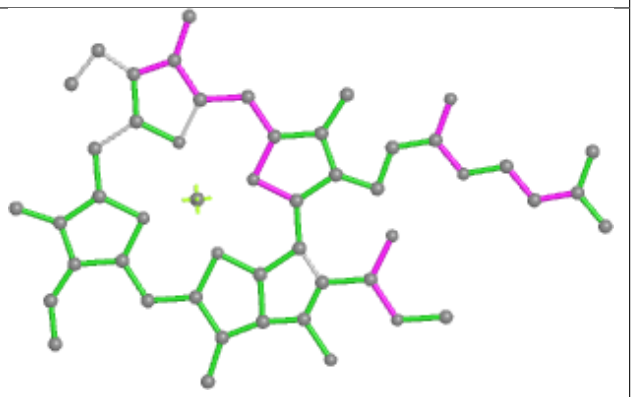

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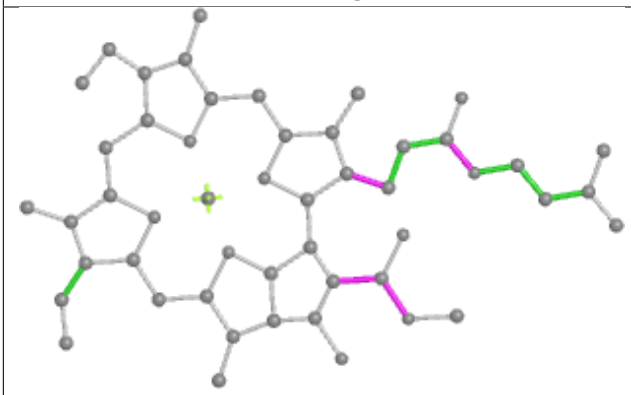

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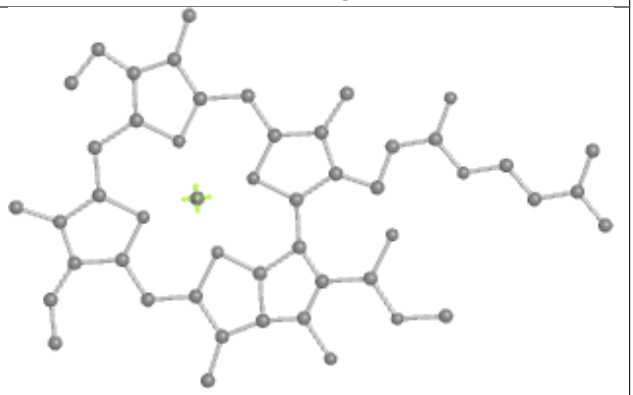
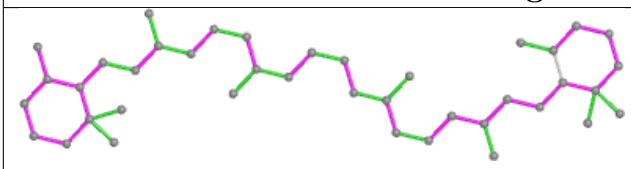


Rings

Ligand 8CT G 104



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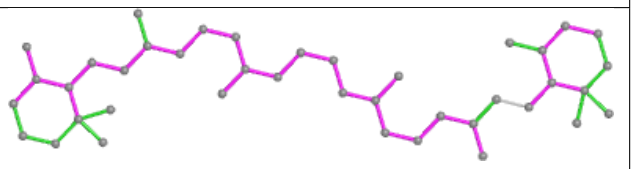
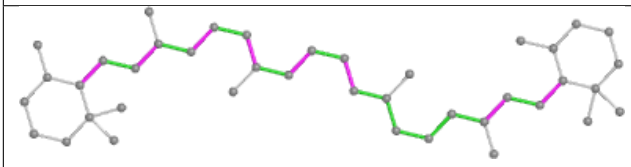


Bond angles



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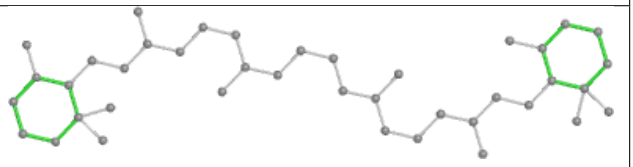
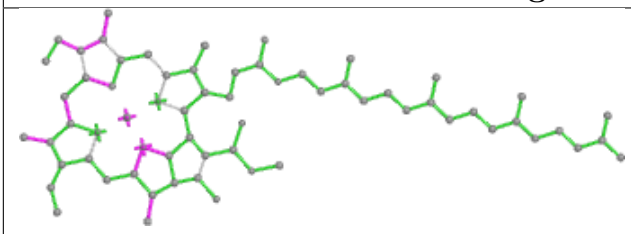


Rings

Ligand CLA 1 302



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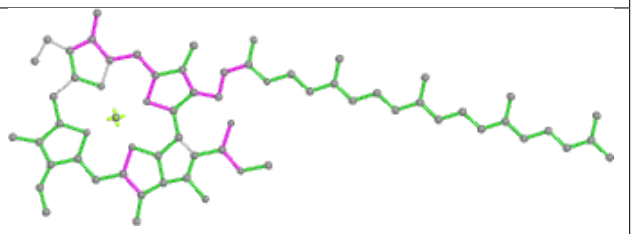

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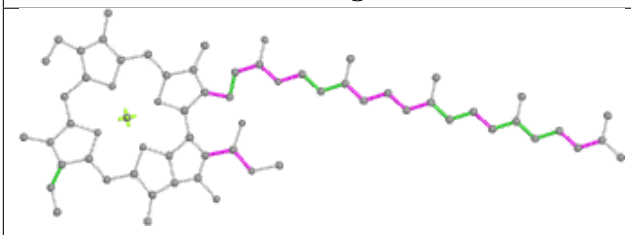

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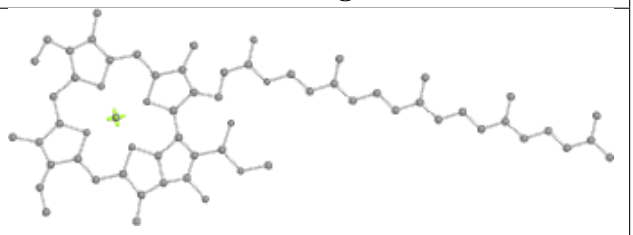
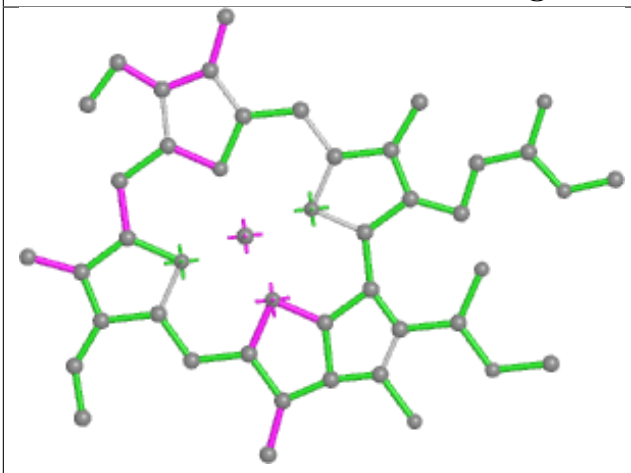


Rings

Ligand CLA 3 313



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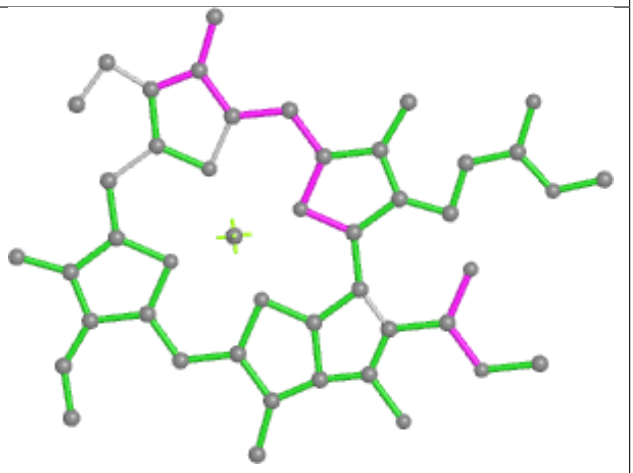
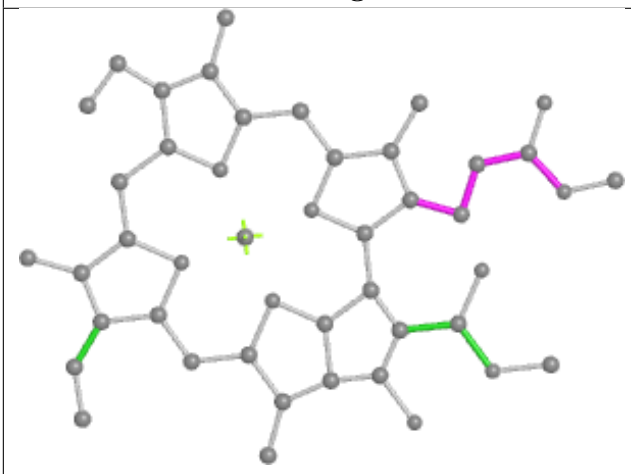


Bond angles



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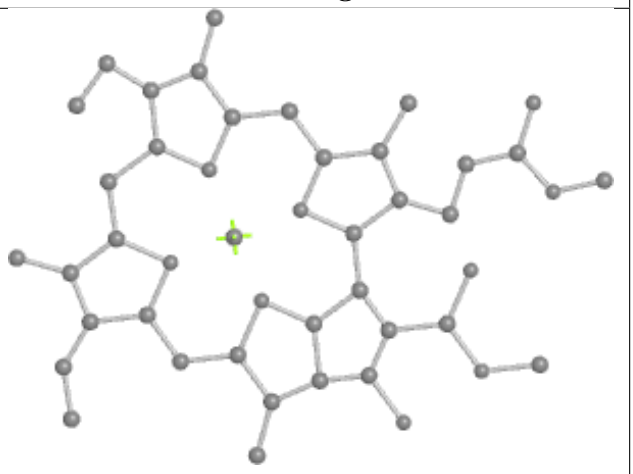
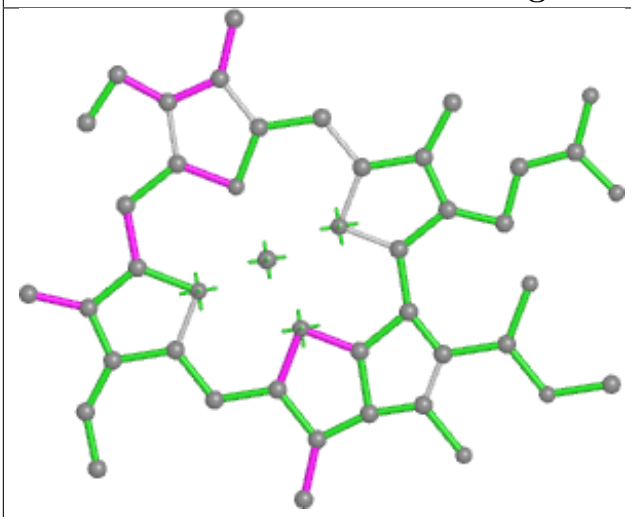


Rings

Ligand CLA 3 303



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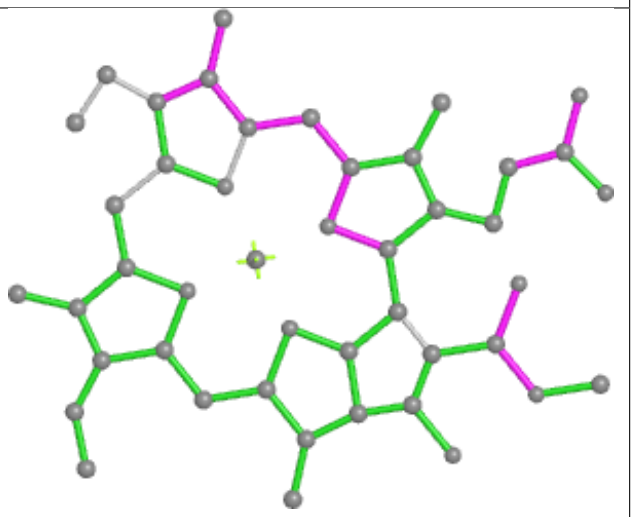

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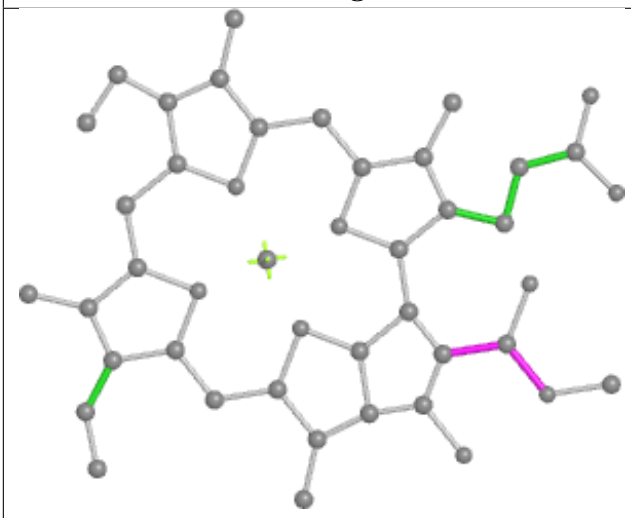

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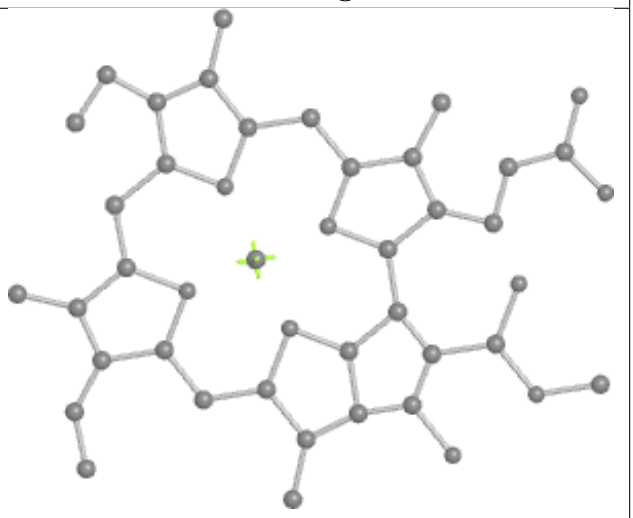
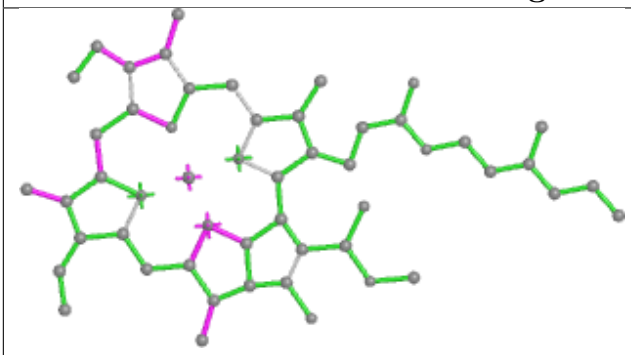


Rings

Ligand CLA 9 306



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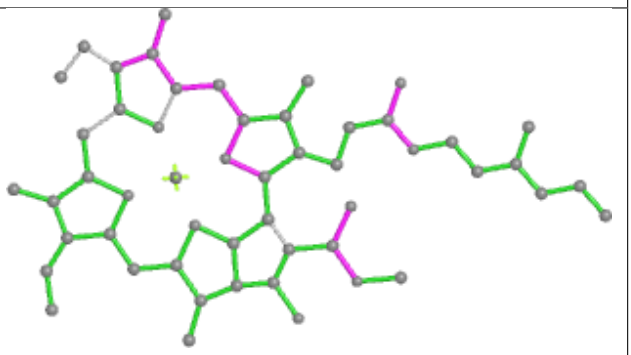

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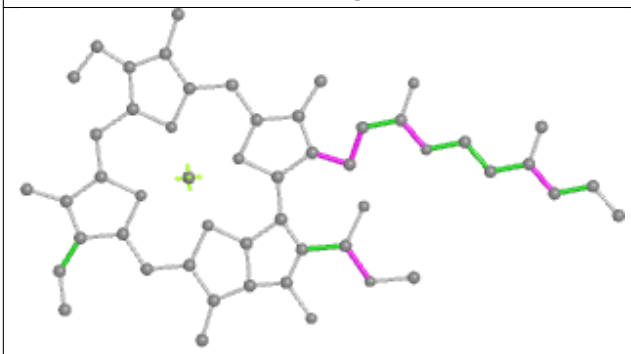

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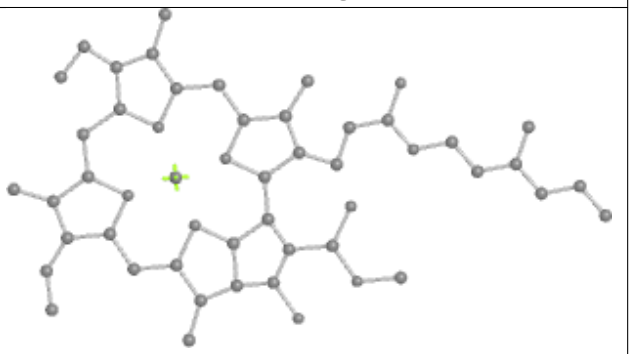
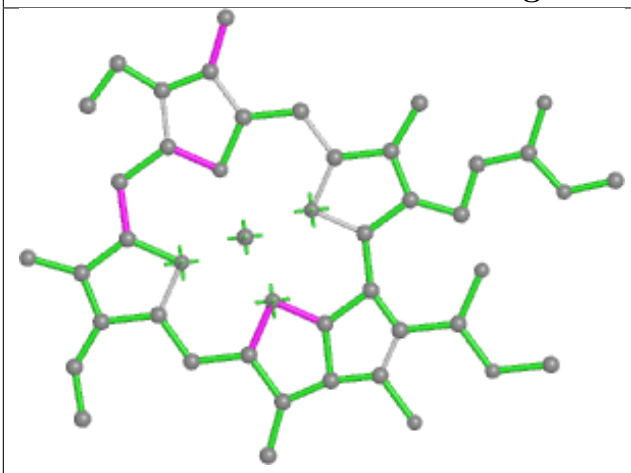


Rings

Ligand CLA G 103



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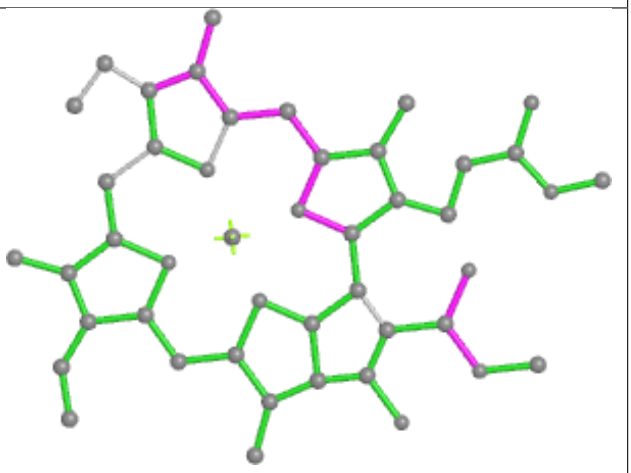
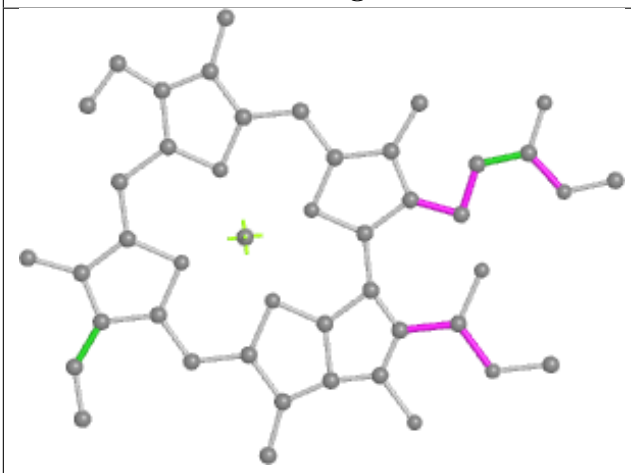


Bond angles



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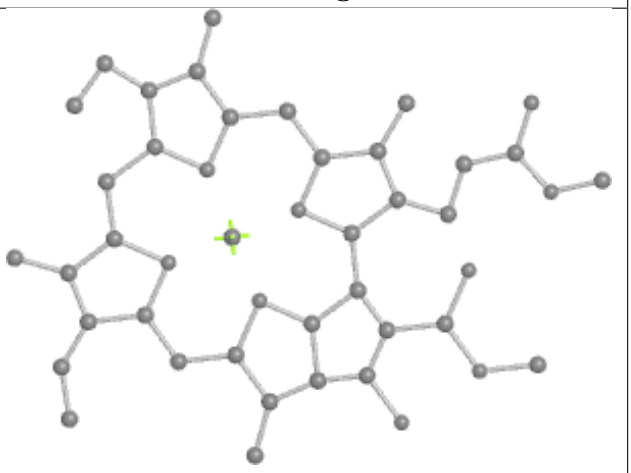
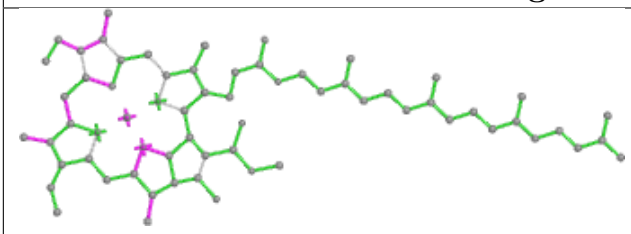


Rings

Ligand CLA 6 313



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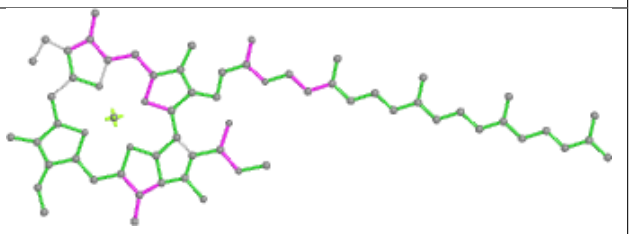

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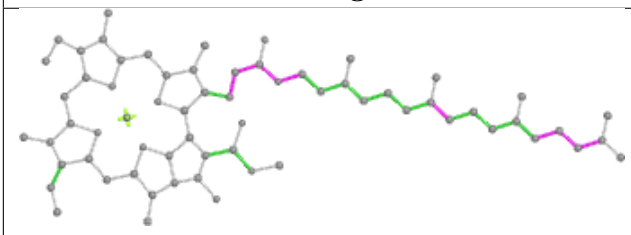

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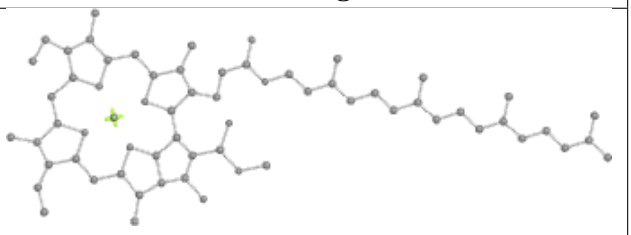
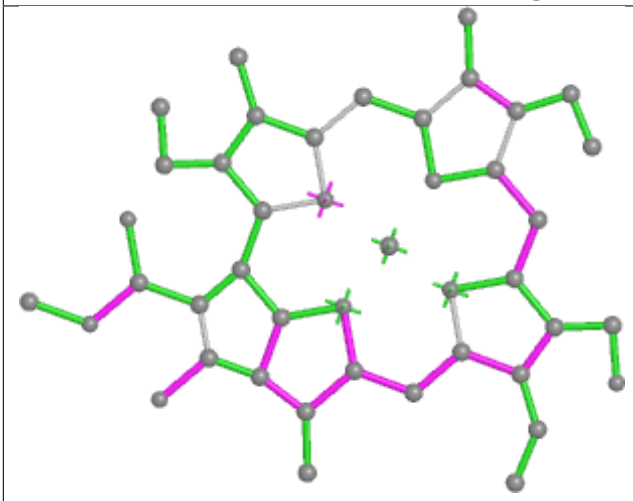


Rings

Ligand CHL 6 316



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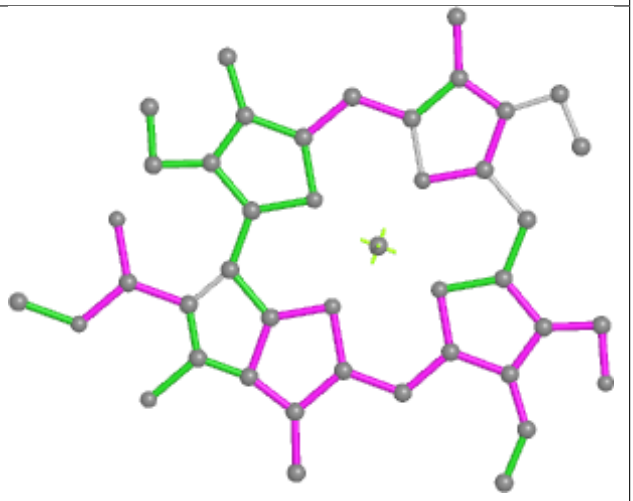

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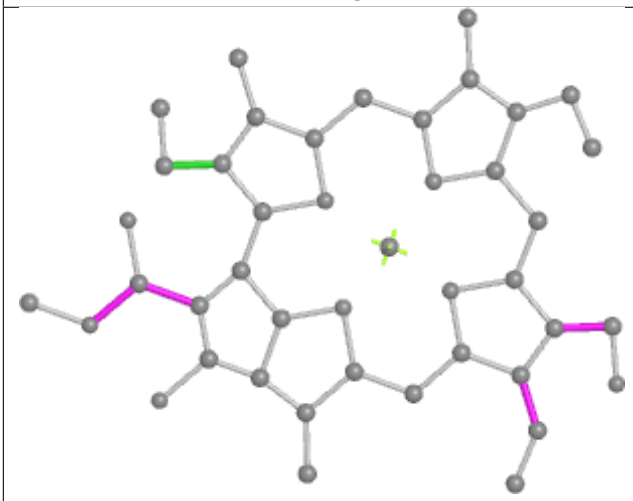

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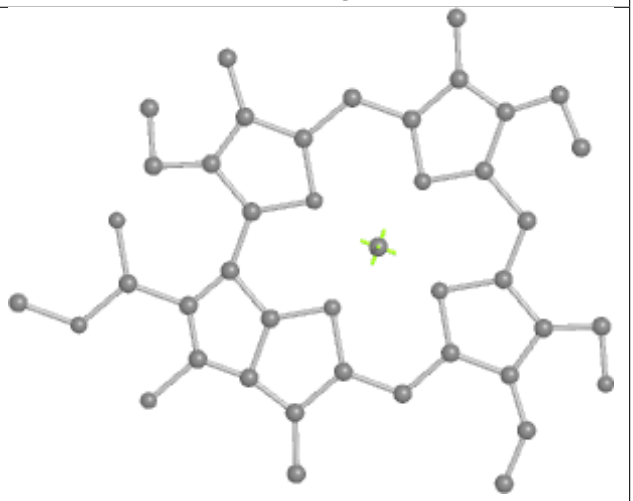
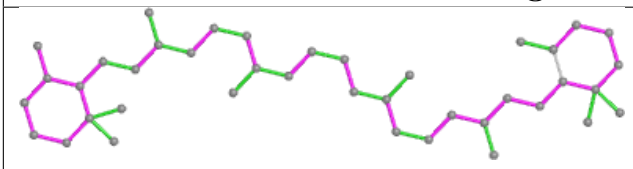


Rings

Ligand 8CT A 846



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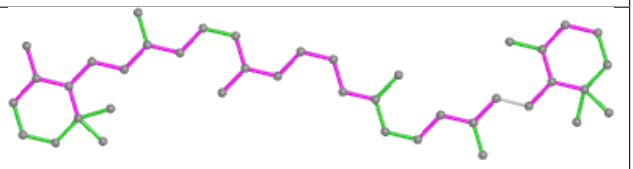
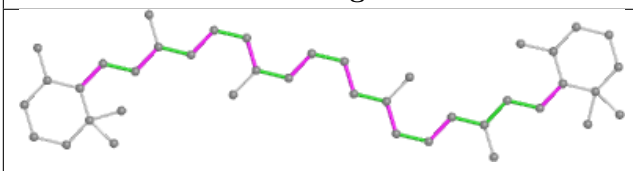


Bond angles



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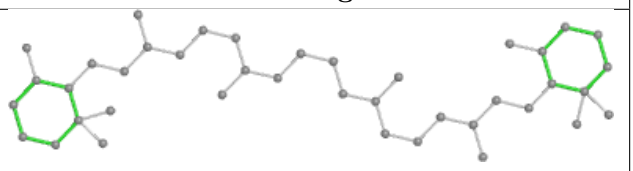
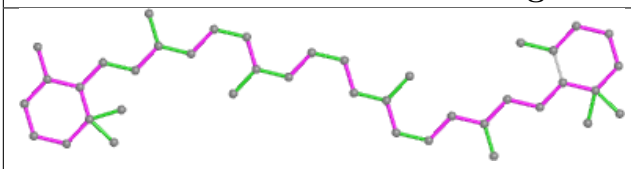
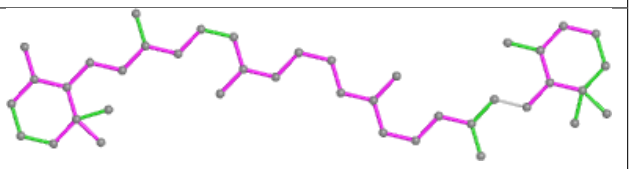
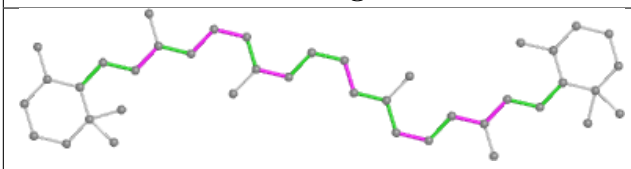
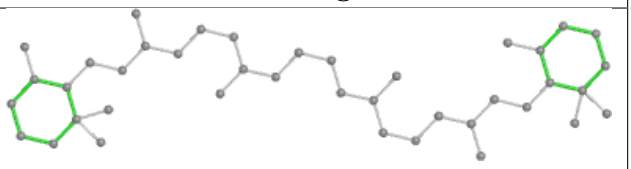
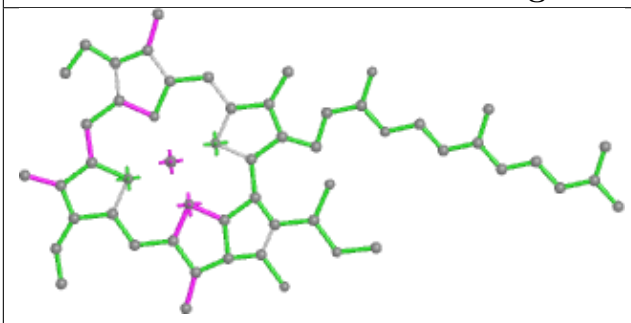
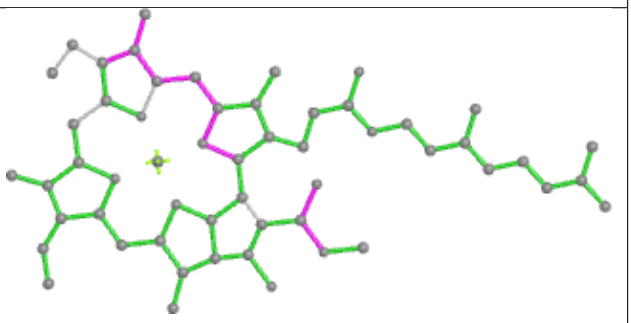
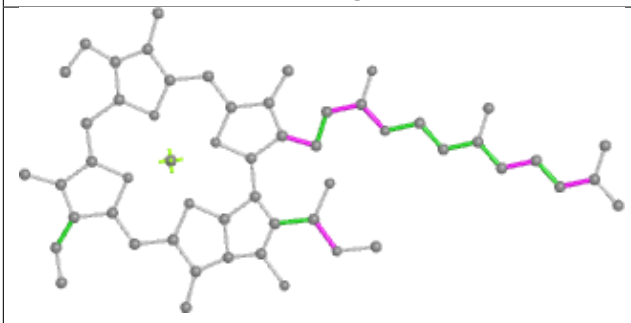
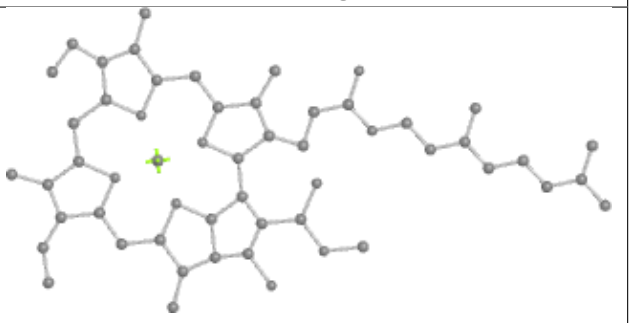
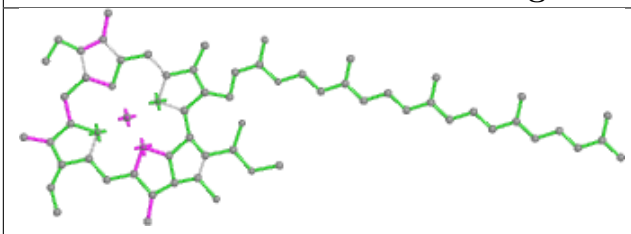


Rings

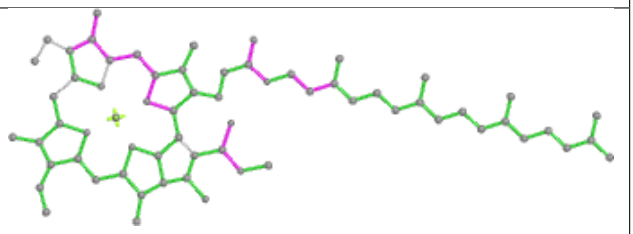
Ligand 8CT B 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

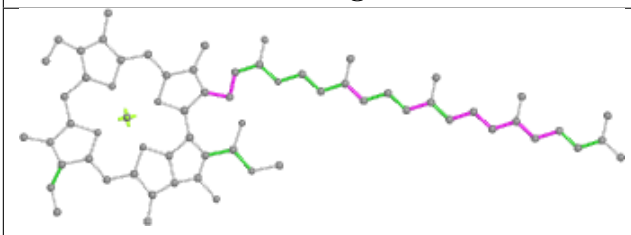
Ligand CLA 1 306



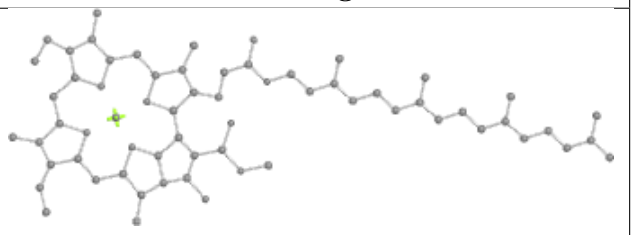
Bond lengths



Bond angles

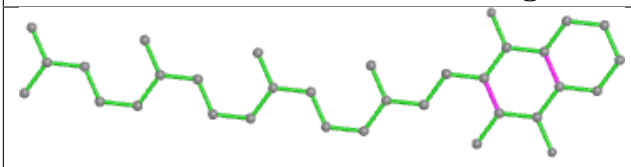


Torsions

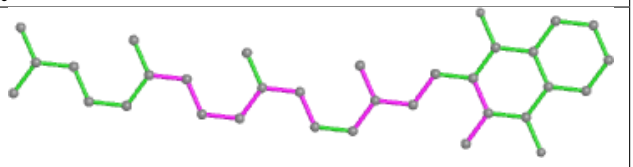


Rings

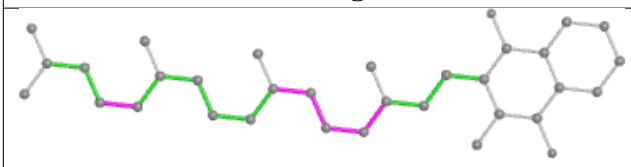
Ligand PQN A 842



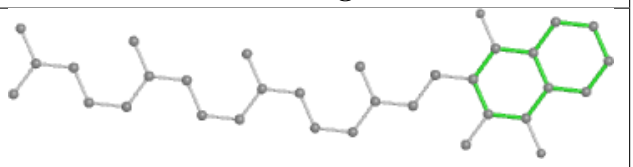
Bond lengths



Bond angles

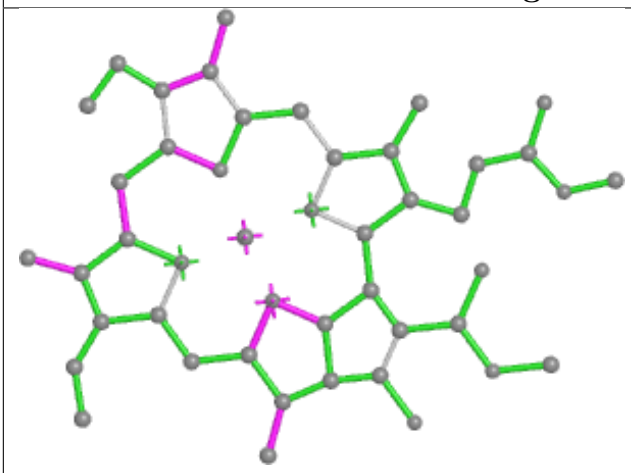


Torsions

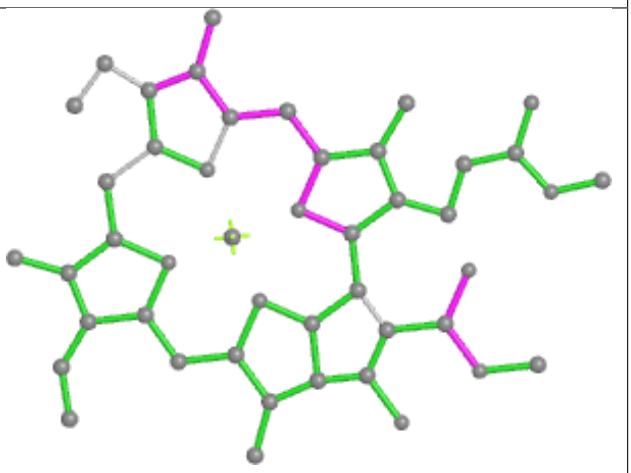


Rings

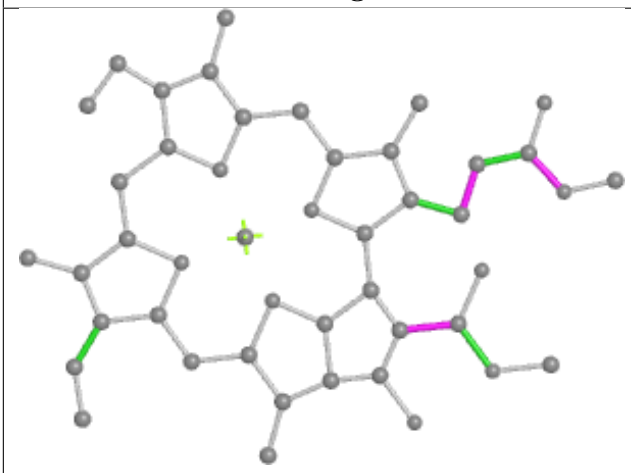
Ligand CLA K 104



Bond lengths



Bond angles



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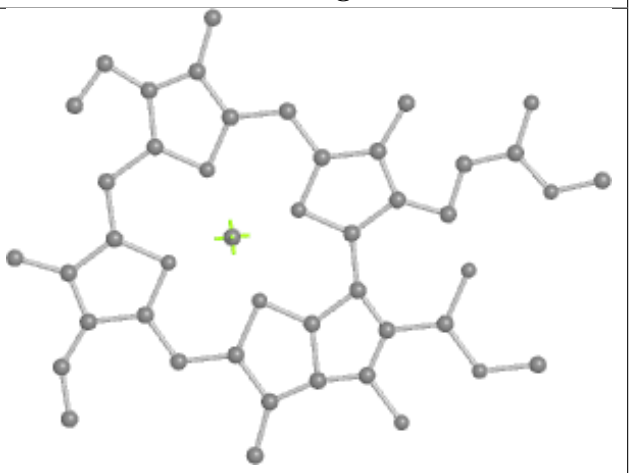
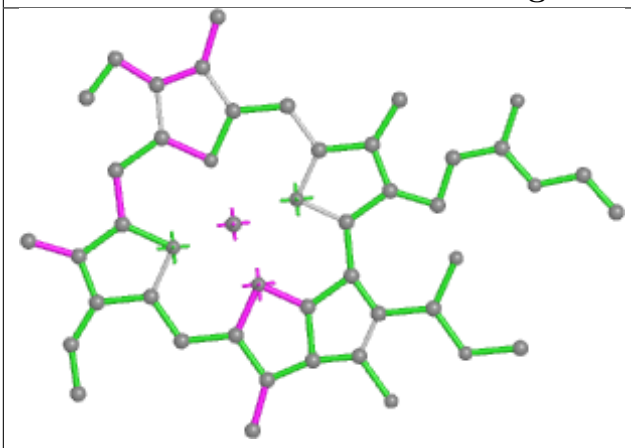
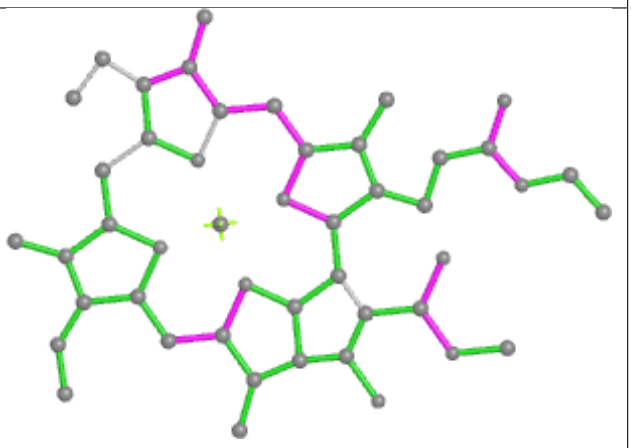


Rings

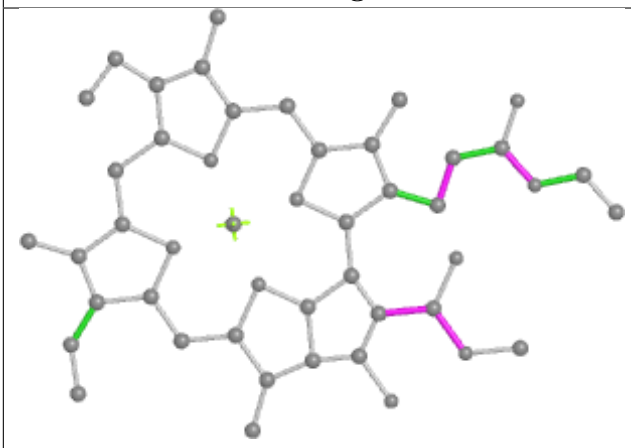
Ligand CLA 7 304



Bond lengths



Bond angles



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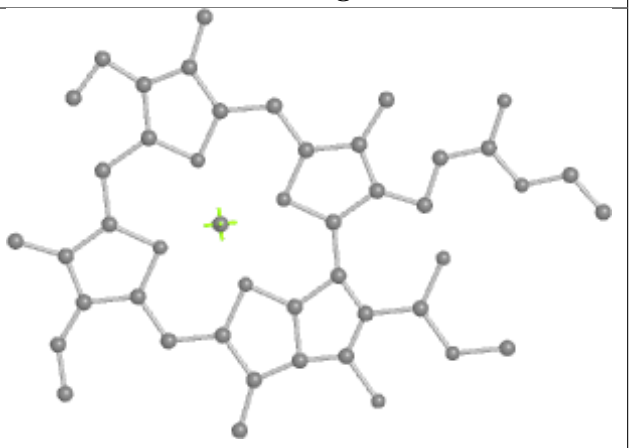
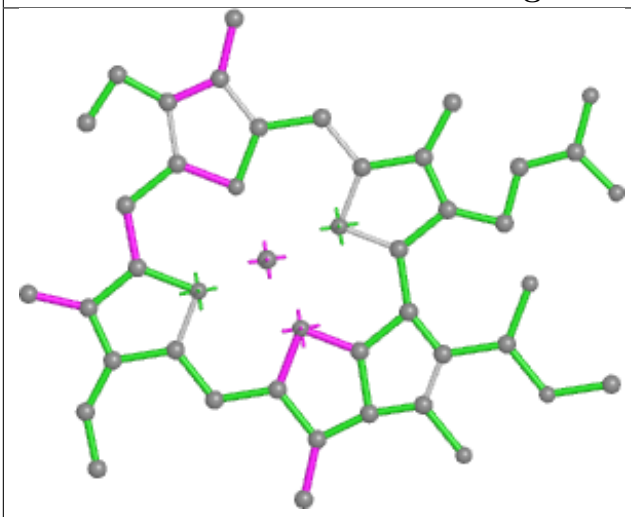
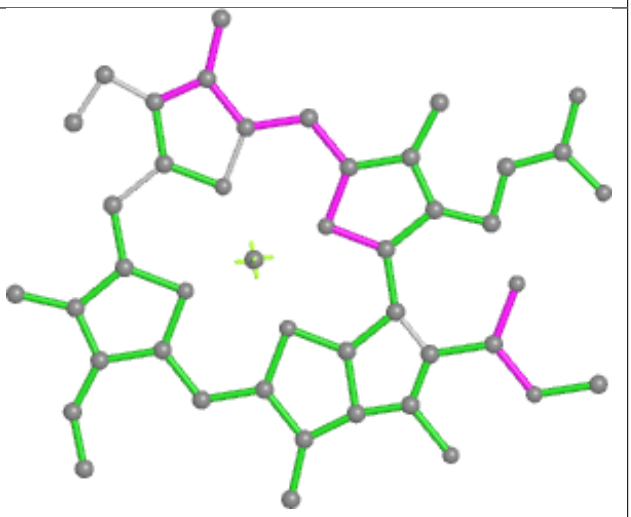


Rings

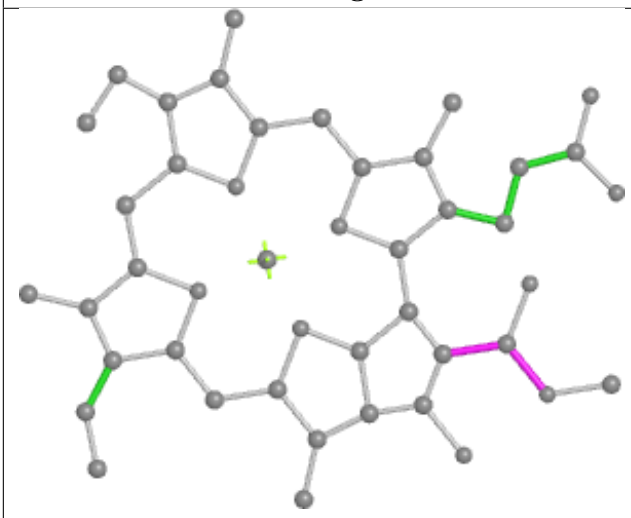
Ligand CLA A 816



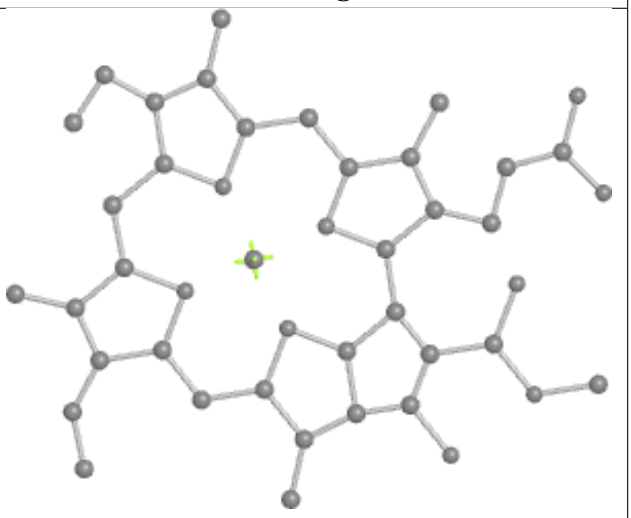
Bond lengths



Bond angles

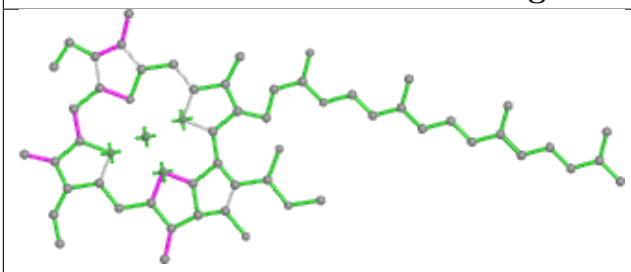


Torsions

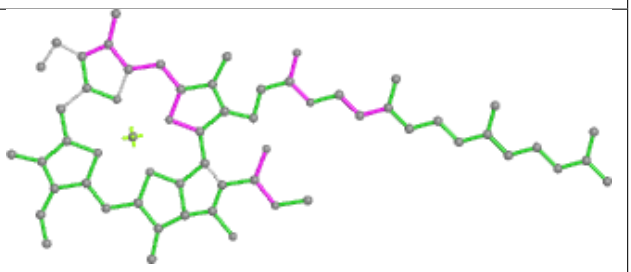


Rings

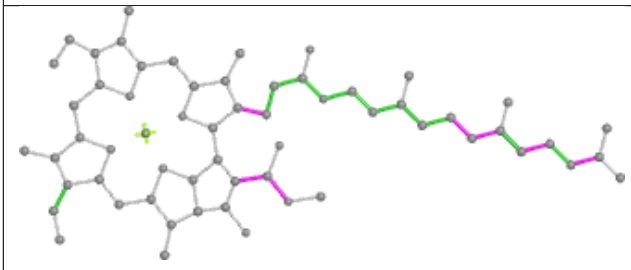
Ligand CLA 1 308



Bond lengths



Bond angles



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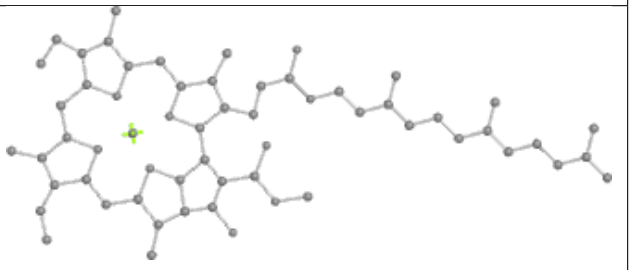
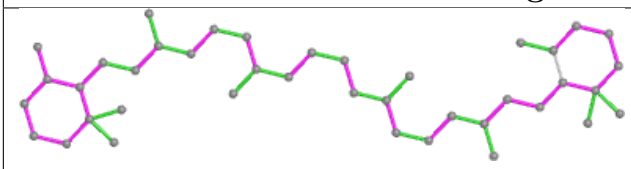
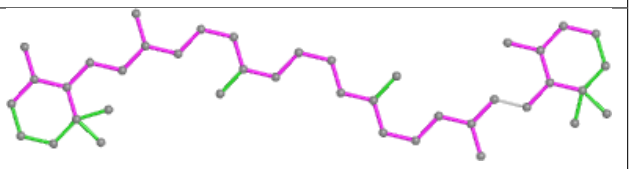
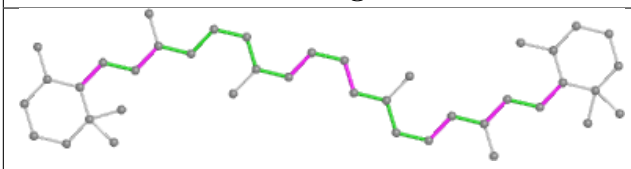
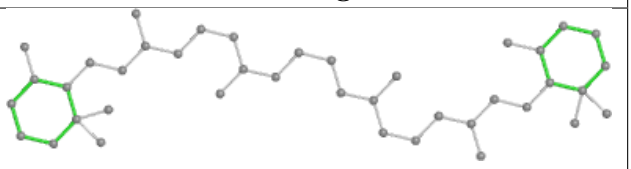


Rings

Ligand 8CT A 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

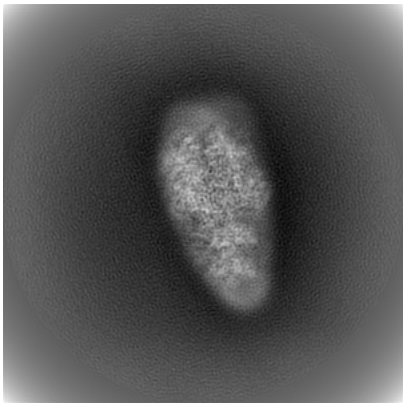
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9670. These allow visual inspection of the internal detail of the map and identification of artifacts.

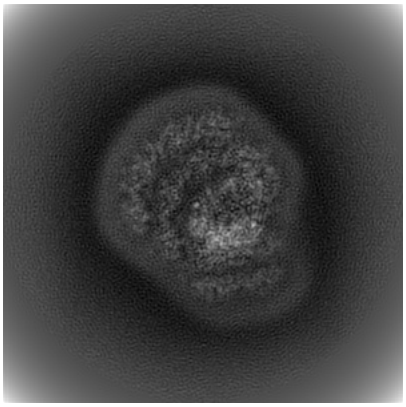
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

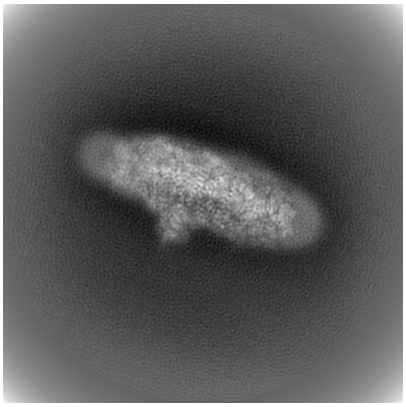
6.1.1 Primary map



X



Y

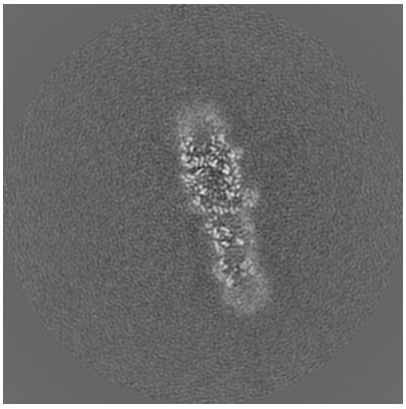


Z

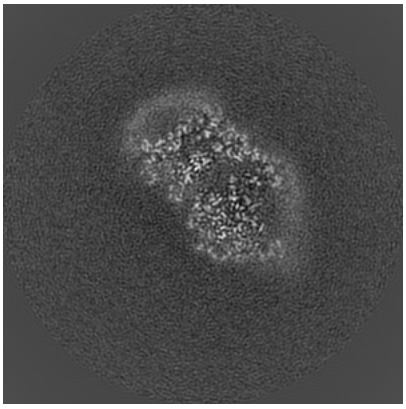
The images above show the map projected in three orthogonal directions.

6.2 Central slices

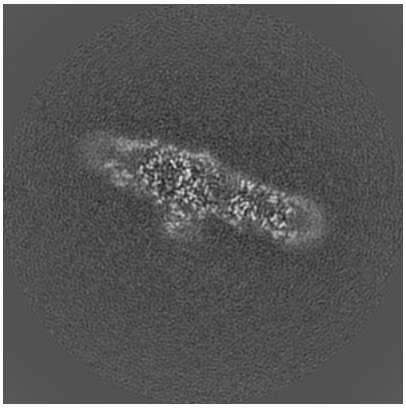
6.2.1 Primary map



X Index: 230



Y Index: 230

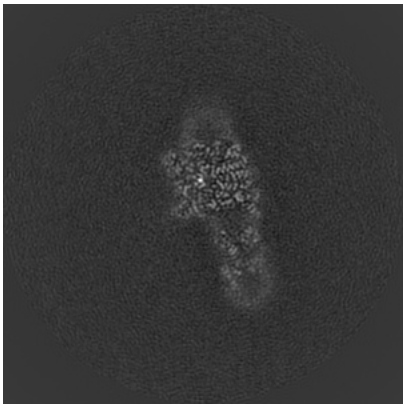


Z Index: 230

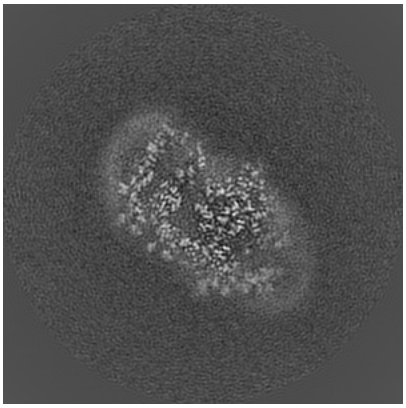
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

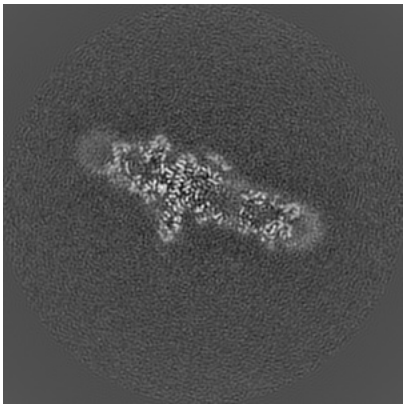
6.3.1 Primary map



X Index: 202



Y Index: 254

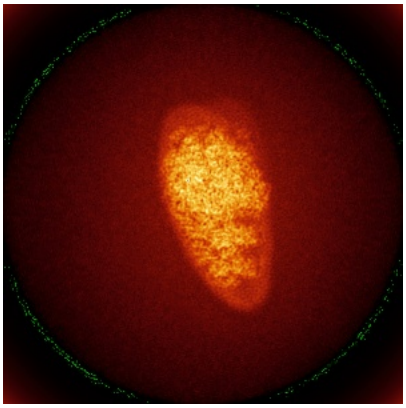


Z Index: 250

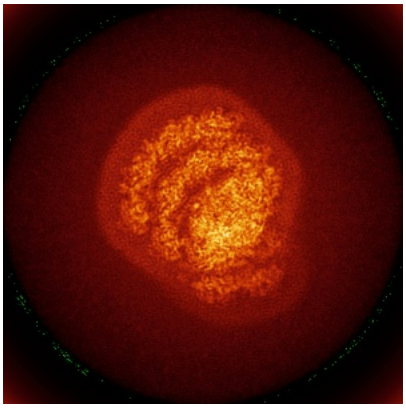
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

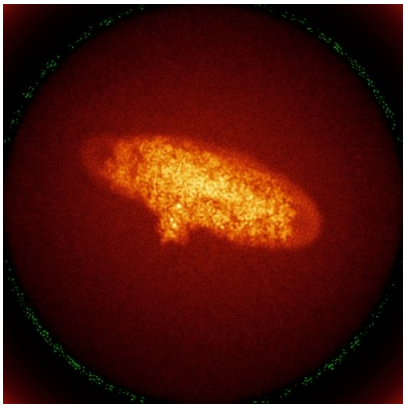
6.4.1 Primary map



X



Y

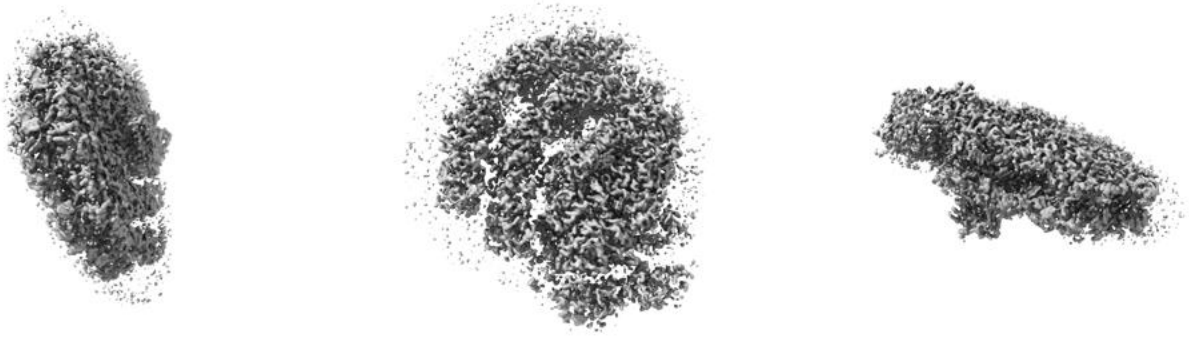


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

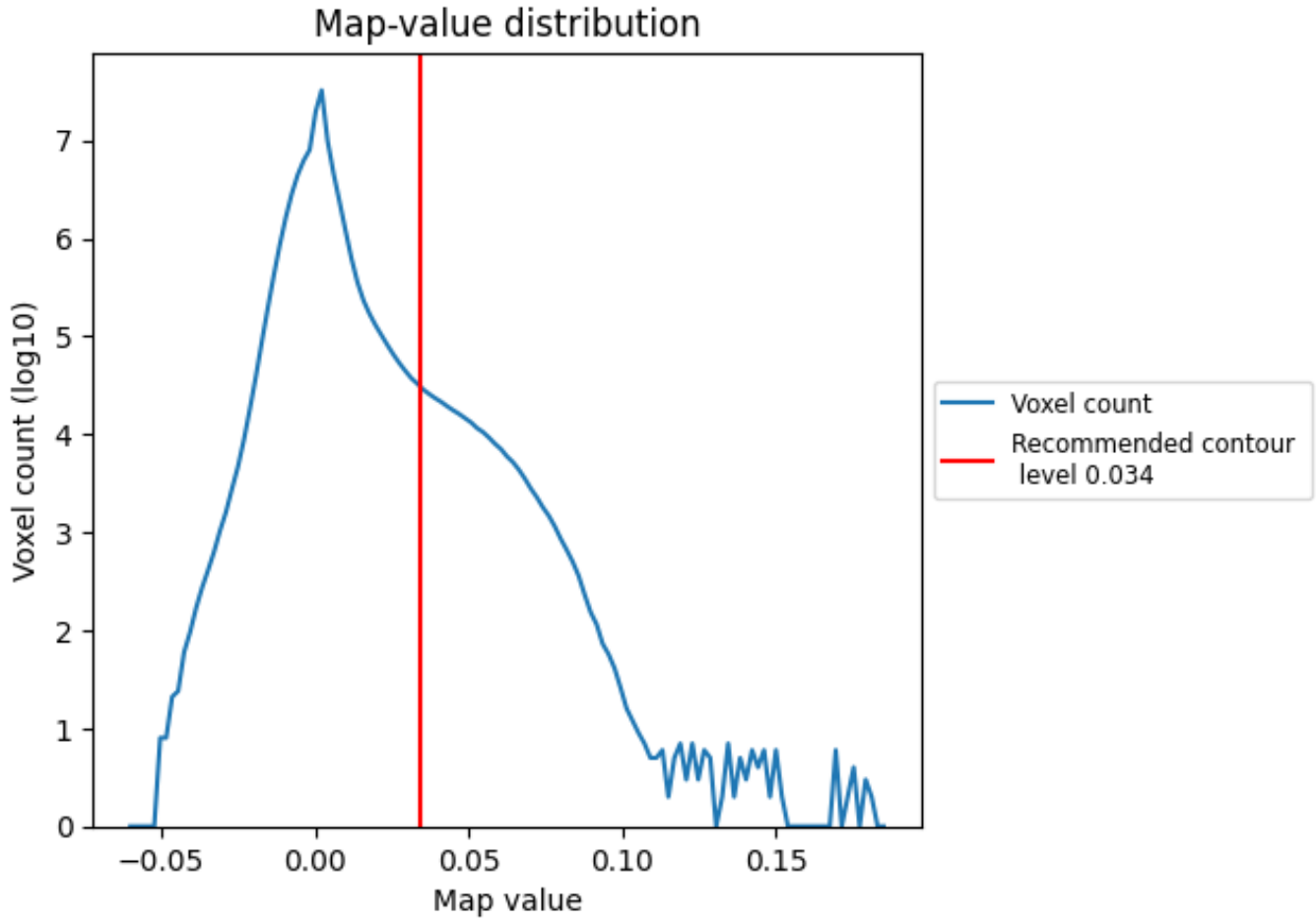
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

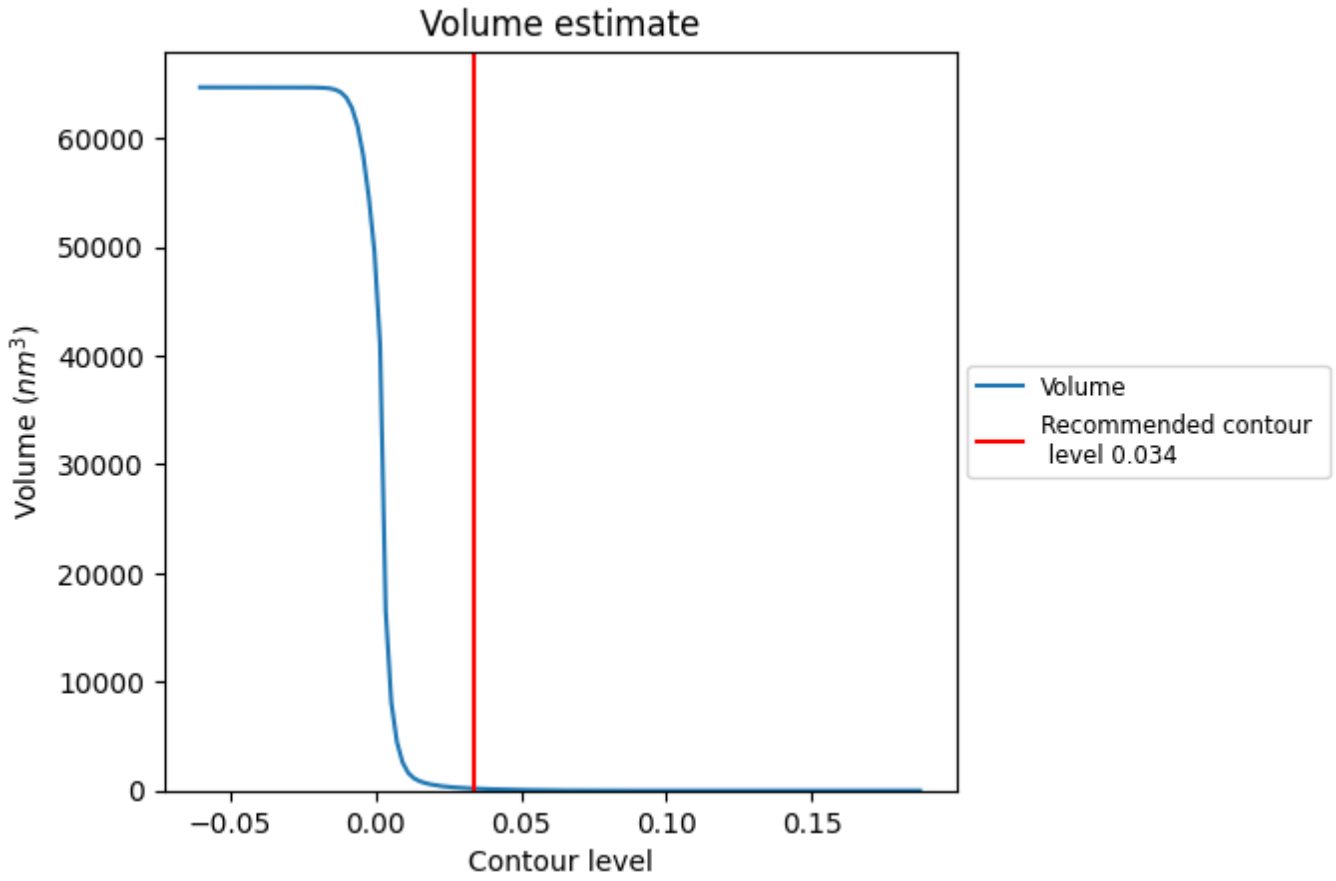
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

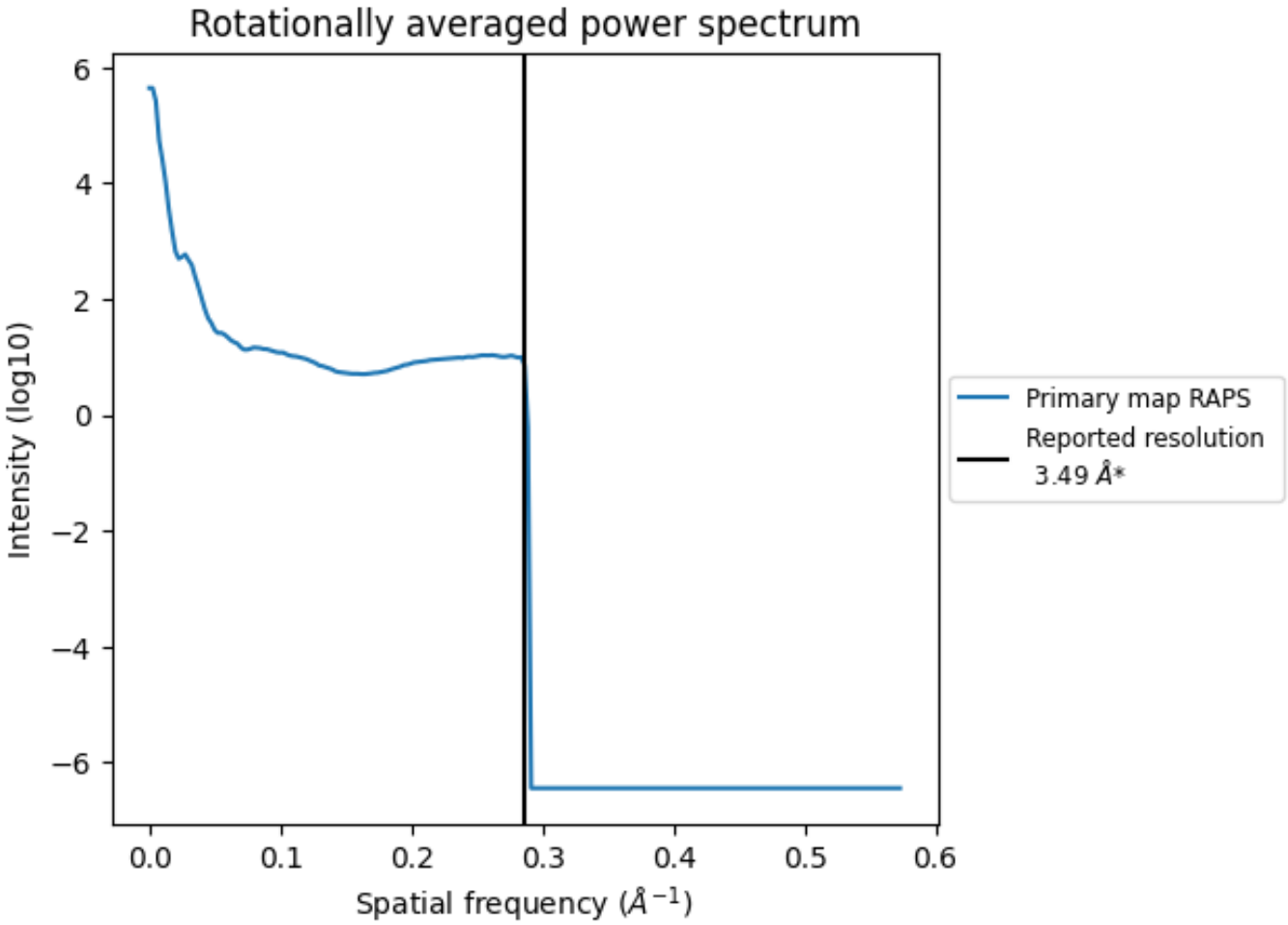
7.2 Volume estimate



The volume at the recommended contour level is 186 nm^3; this corresponds to an approximate mass of 168 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

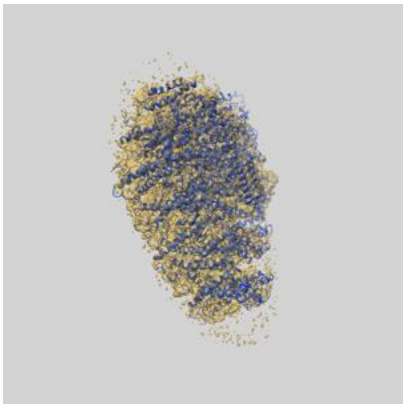
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

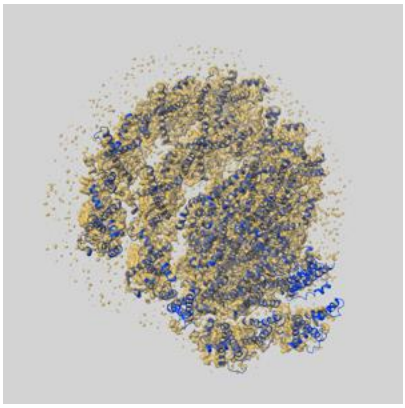
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9670 and PDB model 6IGZ. Per-residue inclusion information can be found in section 3 on page 34.

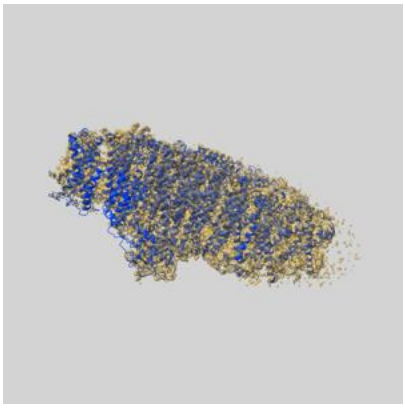
9.1 Map-model overlay



X



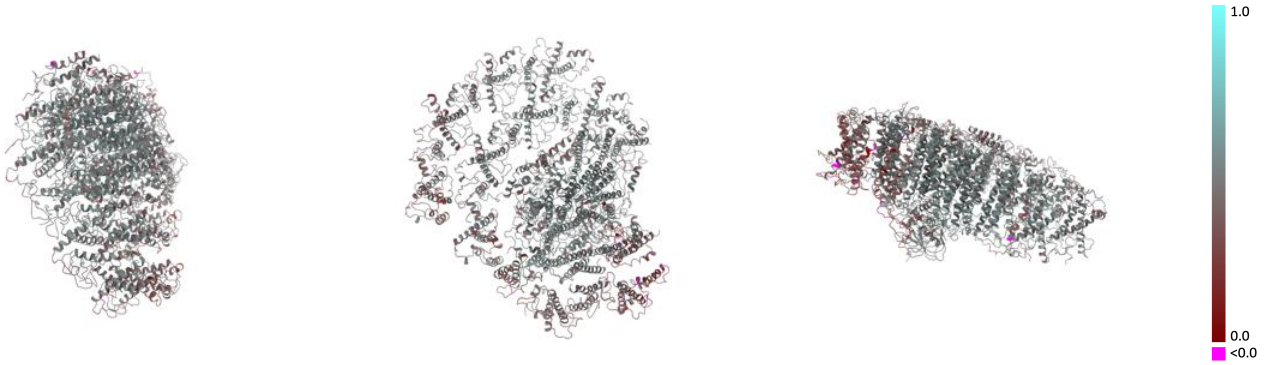
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

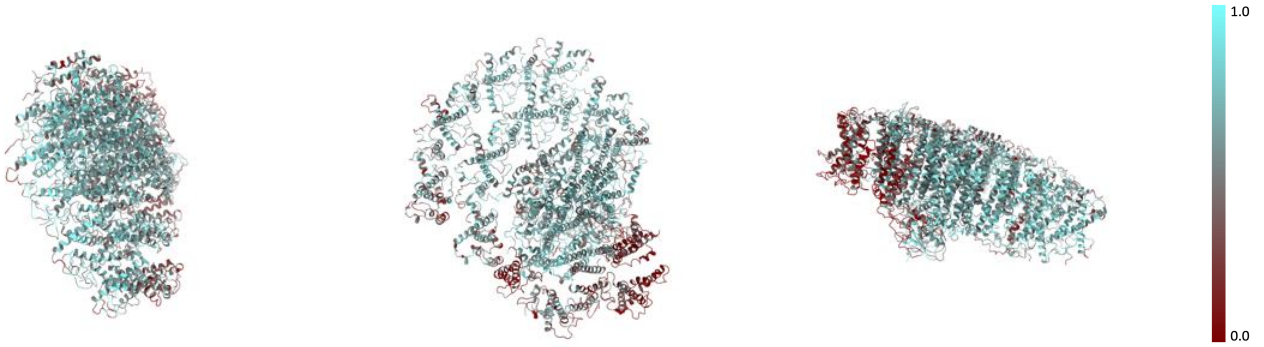
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

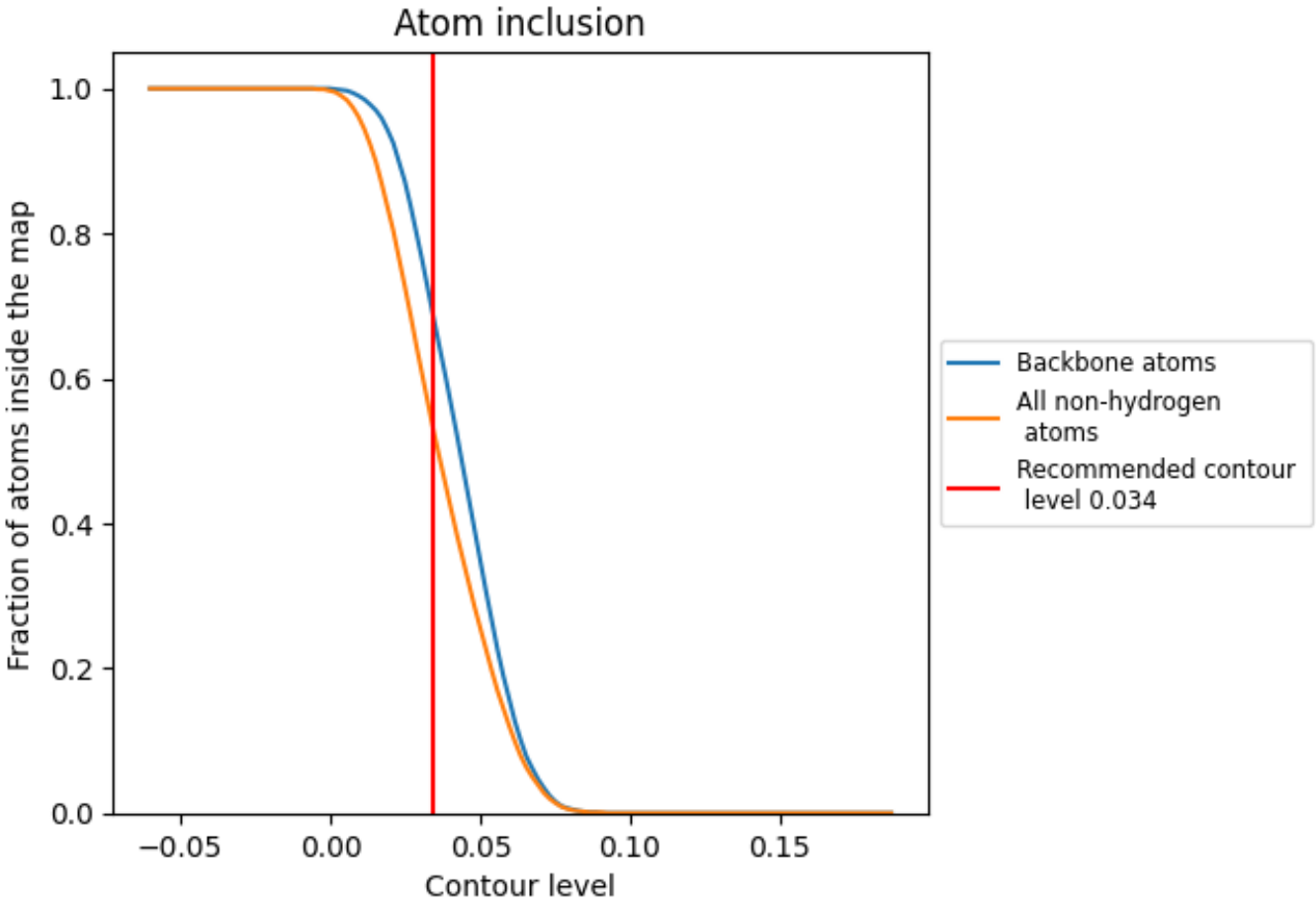
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.034).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5360	0.4750
0	0.2070	0.3440
1	0.5270	0.4620
2	0.6430	0.5160
3	0.6390	0.5010
4	0.5880	0.4810
5	0.4560	0.4250
6	0.5840	0.4770
7	0.5990	0.4760
8	0.5460	0.4490
9	0.4150	0.4280
A	0.6220	0.5250
B	0.6010	0.5160
C	0.7150	0.4740
D	0.5960	0.4680
E	0.5750	0.4740
F	0.5360	0.4700
G	0.1210	0.3640
H	0.0650	0.2890
I	0.4310	0.4880
J	0.4920	0.4980
K	0.4900	0.4400
L	0.2280	0.4030
M	0.5130	0.4760