Full wwPDB EM Validation Report (i)

May 11, 2025 – 12:58 AM JST

PDB ID	:	9KQB / pdb_00009kqb
EMDB ID	:	EMD-62499
Title	:	PSII-FCPII supercomplex from haptophyte Chrysotila roscoffensis
Authors	:	La Rocca, R.; Kato, K.; Tsai, P.-C.; Nakajima, Y.; Akita, F.; Shen, J.-R.
Deposited on	:	2024-11-25
Resolution	:	2.22 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 (i) 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 (1)) were used in the production of this report:

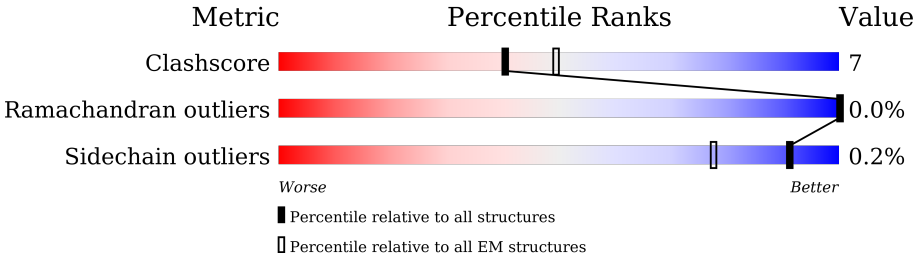
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.22 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	1	166	80% 17% • •
1	5	166	68% 25% • 6%
1	7	166	86% 13% •
1	g	166	78% 16% • 6%
2	6	167	6% 74% 17% • 8%
2	J	167	5% 74% 18% 8%
3	A	360	78% 13% 9%
3	a	360	79% 12% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	B	509	85% 10% 5%
4	b	509	84% 11% 5%
5	E	82	5% 73% 7% 20%
5	e	82	6% 70% 11% 20%
6	F	42	• 67% 10% 24%
6	f	42	5% 74% • 24%
7	H	65	80% 18% •
7	h	65	86% 12% •
8	I	38	92% • 5%
8	i	38	• 87% 8% 5%
9	K	40	5% 80% 12% 8%
9	k	40	5% 78% 12% • 8%
10	L	38	82% 18%
10	l	38	• 84% 16%
11	M	130	38% • 59%
11	m	130	• 36% 5% 59%
12	N	36	• 78% 6% 17%
12	n	36	• 83% 17%
13	T	32	88% 9% •
13	t	32	91% 6% •
14	W	53	• 66% 17% 17%
14	w	53	• 72% 11% 17%
15	X	36	• 89% 6% 6%
15	x	36	• 89% 6% 6%
16	2	225	78% 15% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	8	225	82% 12% 6%
17	D	351	83% 11% 5%
17	d	351	83% 11% 7%
18	C	445	79% 15% 7%
18	c	445	78% 16% 7%
19	3	216	12% 38% 7% 55%
19	9	216	13% 37% 8% 55%
20	4	167	11% 50% 12% 38%
20	G	167	9% 51% 11% 38%

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
21	CLA	1	301	X	-	-	-
21	CLA	1	302	X	-	-	-
21	CLA	1	303	X	-	-	-
21	CLA	1	304	X	-	-	-
21	CLA	1	306	X	-	-	-
21	CLA	1	307	X	-	-	-
21	CLA	1	309	X	-	-	-
21	CLA	2	301	X	-	-	-
21	CLA	2	302	X	-	-	-
21	CLA	2	303	X	-	-	-
21	CLA	2	305	X	-	-	-
21	CLA	3	301	X	-	-	-
21	CLA	3	302	X	-	-	-
21	CLA	4	300	X	-	-	-
21	CLA	4	301	X	-	-	-
21	CLA	4	303	X	-	-	-
21	CLA	4	304	X	-	-	-
21	CLA	5	302	X	-	-	-
21	CLA	5	303	X	-	-	-
21	CLA	5	305	X	-	-	-
21	CLA	5	306	X	-	-	-
21	CLA	5	309	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	6	300	X	-	-	-
21	CLA	6	301	X	-	-	-
21	CLA	6	302	X	-	-	-
21	CLA	6	303	X	-	-	-
21	CLA	6	304	X	-	-	-
21	CLA	6	305	X	-	-	-
21	CLA	6	306	X	-	-	-
21	CLA	6	307	X	-	-	-
21	CLA	6	308	X	-	-	-
21	CLA	7	300	X	-	-	-
21	CLA	7	301	X	-	-	-
21	CLA	7	302	X	-	-	-
21	CLA	7	303	X	-	-	-
21	CLA	7	304	X	-	-	-
21	CLA	7	305	X	-	-	-
21	CLA	7	306	X	-	-	-
21	CLA	7	307	X	-	-	-
21	CLA	7	308	X	-	-	-
21	CLA	8	302	X	-	-	-
21	CLA	8	303	X	-	-	-
21	CLA	8	306	X	-	-	-
21	CLA	8	307	X	-	-	-
21	CLA	9	300	X	-	-	-
21	CLA	9	302	X	-	-	-
21	CLA	9	303	X	-	-	-
21	CLA	9	304	X	-	-	-
21	CLA	B	602	X	-	-	-
21	CLA	B	603	X	-	-	-
21	CLA	B	604	X	-	-	-
21	CLA	B	610	X	-	-	-
21	CLA	B	612	X	-	-	-
21	CLA	B	613	X	-	-	-
21	CLA	B	614	X	-	-	-
21	CLA	B	615	X	-	-	-
21	CLA	B	616	X	-	-	-
21	CLA	C	503	X	-	-	-
21	CLA	C	508	X	-	-	-
21	CLA	C	509	X	-	-	-
21	CLA	C	511	X	-	-	-
21	CLA	C	512	X	-	-	-
21	CLA	C	514	X	-	-	-
21	CLA	D	404	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	D	406	X	-	-	-
21	CLA	G	300	X	-	-	-
21	CLA	G	301	X	-	-	-
21	CLA	G	303	X	-	-	-
21	CLA	G	304	X	-	-	-
21	CLA	J	300	X	-	-	-
21	CLA	J	301	X	-	-	-
21	CLA	J	302	X	-	-	-
21	CLA	J	304	X	-	-	-
21	CLA	J	305	X	-	-	-
21	CLA	J	306	X	-	-	-
21	CLA	J	307	X	-	-	-
21	CLA	J	308	X	-	-	-
21	CLA	b	603	X	-	-	-
21	CLA	b	604	X	-	-	-
21	CLA	b	605	X	-	-	-
21	CLA	b	611	X	-	-	-
21	CLA	b	613	X	-	-	-
21	CLA	b	614	X	-	-	-
21	CLA	b	615	X	-	-	-
21	CLA	b	616	X	-	-	-
21	CLA	b	617	X	-	-	-
21	CLA	b	623	X	-	-	-
21	CLA	c	502	X	-	-	-
21	CLA	c	507	X	-	-	-
21	CLA	c	508	X	-	-	-
21	CLA	c	510	X	-	-	-
21	CLA	c	511	X	-	-	-
21	CLA	c	512	X	-	-	-
21	CLA	c	513	X	-	-	-
21	CLA	d	404	X	-	-	-
21	CLA	d	405	X	-	-	-
21	CLA	g	302	X	-	-	-
21	CLA	g	303	X	-	-	-
21	CLA	g	305	X	-	-	-
21	CLA	g	306	X	-	-	-
21	CLA	g	309	X	-	-	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 61348 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 Fucoxanthin chlorophyll a/c binding protein II (FCPII-1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	164	1281	834	206	238	3	0	0
1	7	164	1278	833	206	236	3	0	0
1	5	156	1217	789	198	227	3	0	0
1	g	156	1217	789	198	227	3	0	0

- Molecule 2 is a protein called Fucoxanthin chlorophyll a/c binding protein II (FCPII-5).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	6	154	1191	778	197	213	3	0	0
2	J	154	1191	778	197	213	3	0	0

- Molecule 3 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	328	2565	1678	418	454	15	0	0
3	a	329	2575	1684	421	455	15	0	0

- Molecule 4 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	484	3796	2479	647	657	13	0	0
4	b	484	3796	2479	647	657	13	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	106	LEU	MET	conflict	UNP Q4G3C5
B	146	ALA	SER	conflict	UNP Q4G3C5
B	161	ALA	THR	conflict	UNP Q4G3C5
B	174	VAL	ILE	conflict	UNP Q4G3C5
B	187	PRO	ALA	conflict	UNP Q4G3C5
B	210	ILE	LEU	conflict	UNP Q4G3C5
B	290	ALA	SER	conflict	UNP Q4G3C5
B	292	ILE	LEU	conflict	UNP Q4G3C5
b	106	LEU	MET	conflict	UNP Q4G3C5
b	146	ALA	SER	conflict	UNP Q4G3C5
b	161	ALA	THR	conflict	UNP Q4G3C5
b	174	VAL	ILE	conflict	UNP Q4G3C5
b	187	PRO	ALA	conflict	UNP Q4G3C5
b	210	ILE	LEU	conflict	UNP Q4G3C5
b	290	ALA	SER	conflict	UNP Q4G3C5
b	292	ILE	LEU	conflict	UNP Q4G3C5

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	66	539	352	89	98	0	0
5	e	66	539	352	89	98	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	32	265	181	43	40	1	0	0
6	f	32	265	181	43	40	1	0	0

- Molecule 7 is a protein called Photosystem II reaction center protein H (psbH).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	64	502	333	80	87	2	0	0
7	h	64	502	333	80	87	2	0	0

- Molecule 8 is a protein called Photosystem II reaction center protein I (psbI).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	36	298	201	46	50	1	0	0
8	i	36	298	201	46	50	1	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein K (psbK).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	37	295	203	45	46	1	0	0
9	k	37	295	203	45	46	1	0	0

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	38	312	210	48	53	1	0	0
10	l	38	312	210	48	53	1	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein M (psbM).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	M	53	397	261	63	73	0	0
11	m	53	397	261	63	73	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein Psb36.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	N	30	202	133	31	38	0	0
12	n	30	202	133	31	38	0	0

- Molecule 13 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	T	31	258	181	38	38	1	0	0
13	t	31	258	181	38	38	1	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein W (psbW).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	W	44	342	217	55	70	0	0
14	w	44	342	217	55	70	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein X (psbX).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	X	34	240	161	34	44	1	0	0
15	x	34	240	161	34	44	1	0	0

- Molecule 16 is a protein called Fucoxanthin chlorophyll a/c binding protein II (FCPII-2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	2	211	1657	1074	280	296	7	0	0
16	8	212	1664	1079	281	297	7	0	0

- Molecule 17 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	D	333	2644	1750	431	452	11	0	0
17	d	327	2597	1720	424	442	11	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	282	SER	ALA	conflict	UNP Q4G395
D	283	LEU	ILE	conflict	UNP Q4G395

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	294	SER	ALA	conflict	UNP Q4G395
d	282	SER	ALA	conflict	UNP Q4G395
d	283	LEU	ILE	conflict	UNP Q4G395
d	294	SER	ALA	conflict	UNP Q4G395

- Molecule 18 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	C	416	3268	2148	547	560	13	0	0
18	c	416	3268	2148	547	560	13	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	79	ASP	ASN	conflict	UNP A0A075DWU3
C	144	SER	CYS	conflict	UNP A0A075DWU3
C	170	ILE	VAL	conflict	UNP A0A075DWU3
C	172	THR	SER	conflict	UNP A0A075DWU3
C	253	VAL	GLY	conflict	UNP A0A075DWU3
C	259	SER	ALA	conflict	UNP A0A075DWU3
C	399	THR	CYS	conflict	UNP A0A075DWU3
C	400	THR	CYS	conflict	UNP A0A075DWU3
c	79	ASP	ASN	conflict	UNP A0A075DWU3
c	144	SER	CYS	conflict	UNP A0A075DWU3
c	170	ILE	VAL	conflict	UNP A0A075DWU3
c	172	THR	SER	conflict	UNP A0A075DWU3
c	253	VAL	GLY	conflict	UNP A0A075DWU3
c	259	SER	ALA	conflict	UNP A0A075DWU3
c	399	THR	CYS	conflict	UNP A0A075DWU3
c	400	THR	CYS	conflict	UNP A0A075DWU3

- Molecule 19 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	9	98	770	495	136	133	6	0	0
19	3	98	770	495	136	133	6	0	0

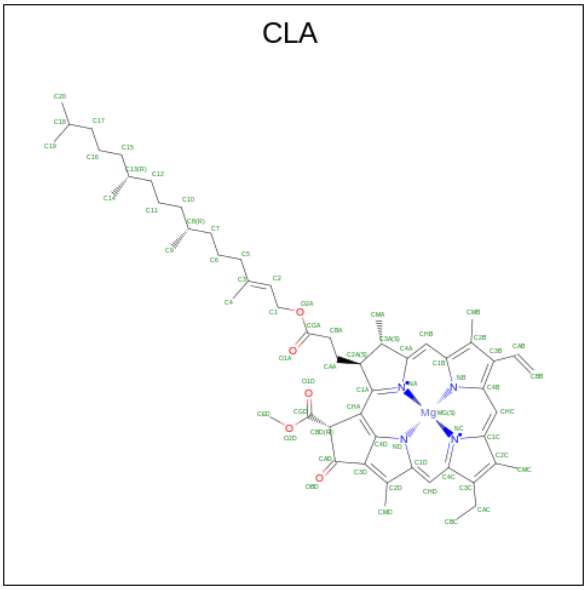
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	8	LEU	PHE	conflict	UNP A0A7S4BJL5
9	77	MET	ILE	conflict	UNP A0A7S4BJL5
3	8	LEU	PHE	conflict	UNP A0A7S4BJL5
3	77	MET	ILE	conflict	UNP A0A7S4BJL5

- Molecule 20 is a protein called Fucoxanthin chlorophyll a/c binding protein II (FCPII-4).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	4	104	822	532	140	147	3	0	0
			Total	C	N	O	S		
20	G	104	822	532	140	147	3	0	0

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	51	41	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	1	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	1	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	1	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
21	1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	43	33	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	6	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	6	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	7	1	41	33	1	4	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	7	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
21	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
21	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	61	52	1	4	4	0
			Total	C	Mg	N	O	
21	B	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	J	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
21	J	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
21	J	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	J	1	43	33	1	4	5	0
			Total	C	Mg	N	O	
21	J	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	J	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	J	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	J	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	J	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
21	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	a	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
21	a	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	61	52	1	4	4	0
			Total	C	Mg	N	O	
21	b	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	b	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	2	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	2	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	8	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
21	8	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
21	D	1	59	49	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	D	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
21	D	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	d	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
21	d	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
21	d	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
21	C	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
21	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	c	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
21	c	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	c	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
21	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	c	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
21	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	c	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
21	c	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
21	9	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
21	3	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
21	3	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

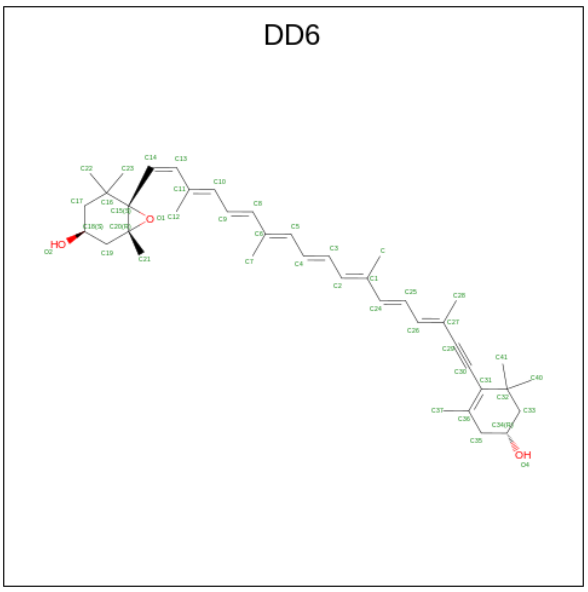
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	4	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
21	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	g	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
21	g	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
21	g	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
21	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	g	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
21	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
21	g	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
21	G	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

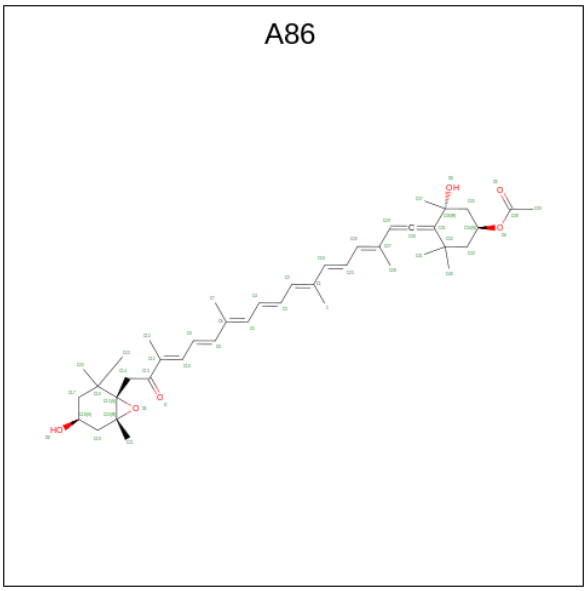
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	G	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
21	G	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
21	G	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
21	G	1	65	55	1	4	5	0

- Molecule 22 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	1	1	43	40	3	0
			Total	C	O	
22	7	1	43	40	3	0
			Total	C	O	
22	5	1	43	40	3	0
			Total	C	O	
22	g	1	43	40	3	0

- Molecule 23 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).



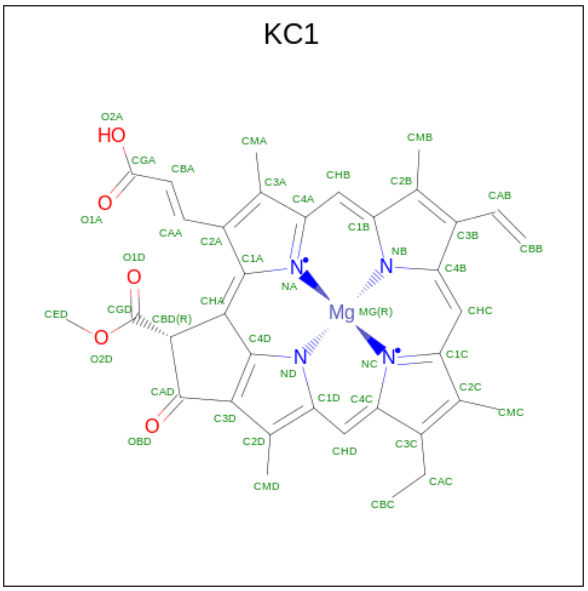
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	1	1	48	42	6	0
			Total	C	O	
23	1	1	48	42	6	0
			Total	C	O	
23	1	1	48	42	6	0
			Total	C	O	
23	6	1	48	42	6	0
			Total	C	O	
23	6	1	48	42	6	0
			Total	C	O	
23	7	1	48	42	6	0
			Total	C	O	
23	7	1	48	42	6	0
			Total	C	O	
23	7	1	44	40	4	0
			Total	C	O	
23	J	1	48	42	6	0
			Total	C	O	
23	J	1	48	42	6	0
			Total	C	O	
23	W	1	48	42	6	0
			Total	C	O	
23	2	1	48	42	6	0
			Total	C	O	
23	2	1	48	42	6	0
			Total	C	O	
23	2	1	48	42	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	2	1	48	42	6	0
			Total	C	O	
23	2	1	48	42	6	0
			Total	C	O	
23	2	1	48	42	6	0
			Total	C	O	
23	8	1	48	42	6	0
			Total	C	O	
23	8	1	48	42	6	0
			Total	C	O	
23	8	1	48	42	6	0
			Total	C	O	
23	8	1	48	42	6	0
			Total	C	O	
23	8	1	48	42	6	0
			Total	C	O	
23	4	1	48	42	6	0
			Total	C	O	
23	5	1	48	42	6	0
			Total	C	O	
23	5	1	48	42	6	0
			Total	C	O	
23	g	1	48	42	6	0
			Total	C	O	
23	g	1	48	42	6	0
			Total	C	O	
23	G	1	48	42	6	0

- Molecule 24 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	2	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

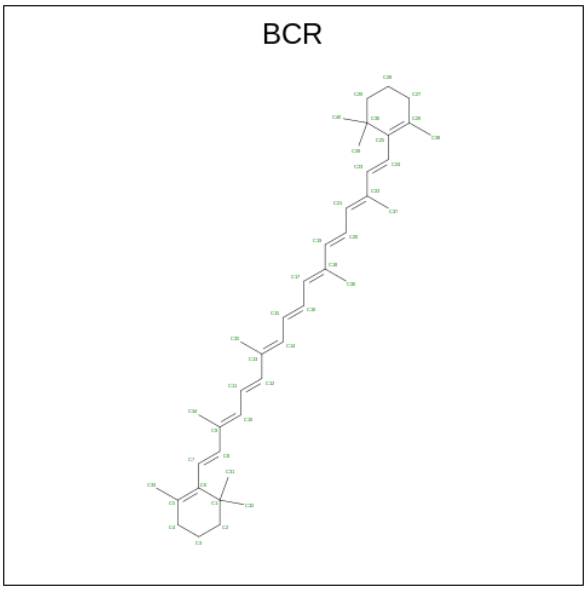
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	4	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
24	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	G	1	38	30	1	4	3	0
			Total	C	Mg	N	O	
24	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	G	1	45	35	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	G	1	45	35	1	4	5	0

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



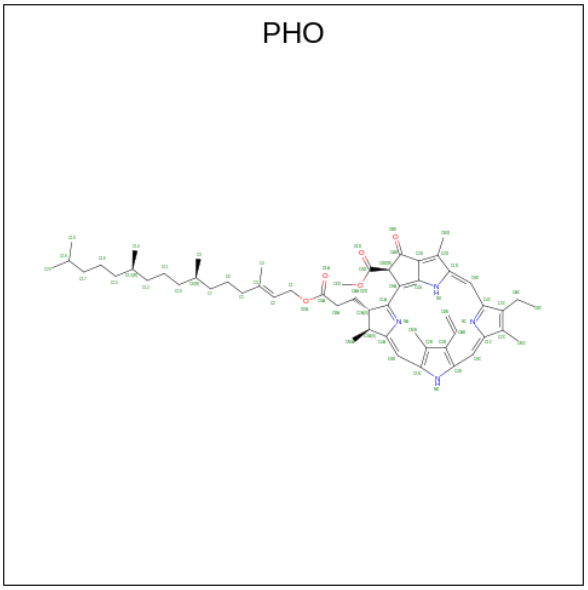
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
25	1	1	40	40	0
25	A	1	40	40	0
25	B	1	40	40	0
25	B	1	40	40	0
25	H	1	40	40	0
25	M	1	40	40	0
25	a	1	40	40	0
25	b	1	40	40	0
25	b	1	40	40	0
25	h	1	40	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	C	
25	h	1	40	40	0
			Total	C	
25	m	1	40	40	0
			Total	C	
25	D	1	40	40	0
			Total	C	
25	d	1	40	40	0
			Total	C	
25	C	1	40	40	0
			Total	C	
25	C	1	40	40	0
			Total	C	
25	c	1	40	40	0
			Total	C	
25	c	1	40	40	0

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



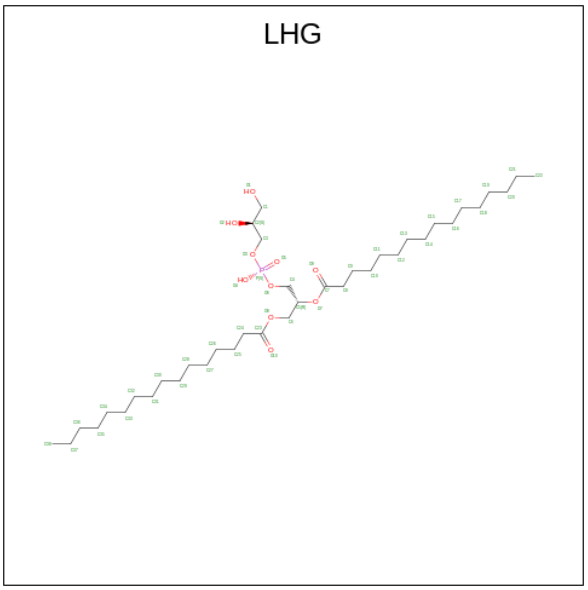
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	A	1	64	55	4	5	0
			Total	C	N	O	
26	a	1	64	55	4	5	0
			Total	C	N	O	
26	D	1	64	55	4	5	0

Continued on next page...

Continued from previous page...

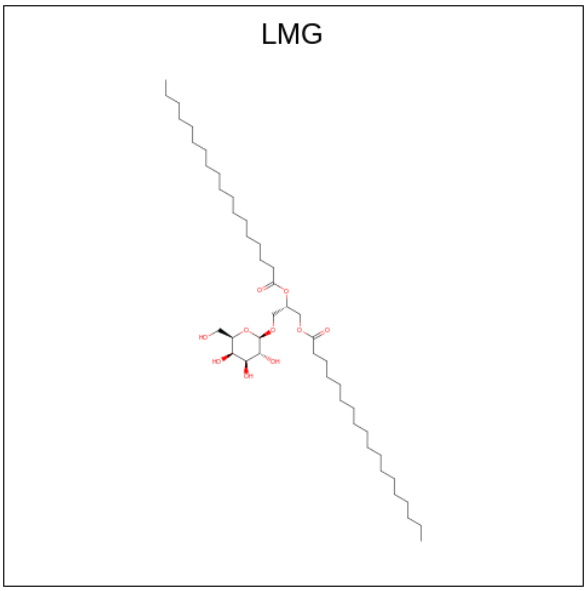
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	d	1	64	55	4	5	0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
27	A	1	49	38	10	1	0
			Total	C	O	P	
27	B	1	49	38	10	1	0
			Total	C	O	P	
27	a	1	49	38	10	1	0
			Total	C	O	P	
27	l	1	49	38	10	1	0
			Total	C	O	P	
27	D	1	43	32	10	1	0
			Total	C	O	P	
27	D	1	48	38	9	1	0
			Total	C	O	P	
27	d	1	43	32	10	1	0
			Total	C	O	P	
27	d	1	48	38	9	1	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



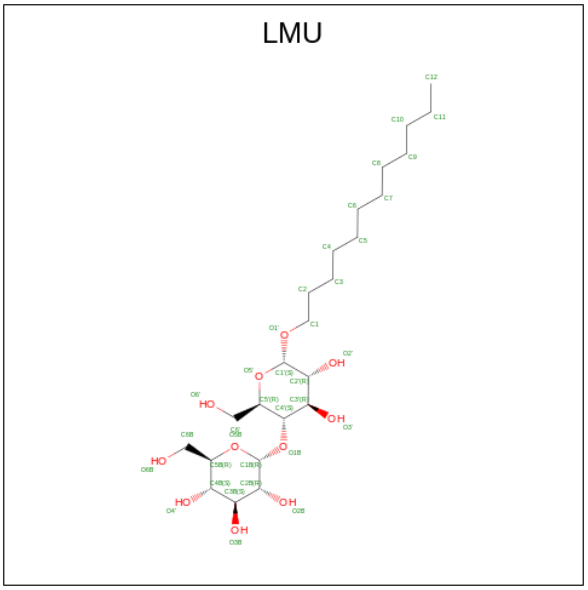
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	A	1	48	38	10	0
28	B	1	51	41	10	0
28	B	1	28	18	10	0
28	B	1	37	27	10	0
28	B	1	43	33	10	0
28	B	1	40	30	10	0
28	L	1	40	30	10	0
28	M	1	40	30	10	0
28	N	1	24	15	9	0
28	a	1	48	38	10	0
28	b	1	51	41	10	0
28	b	1	28	18	10	0
28	b	1	35	25	10	0
28	b	1	37	27	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	b	1	43	33	10	0
			Total	C	O	
28	b	1	37	27	10	0
			Total	C	O	
28	f	1	46	36	10	0
			Total	C	O	
28	2	1	46	36	10	0
			Total	C	O	
28	8	1	24	15	9	0
			Total	C	O	
28	8	1	51	41	10	0
			Total	C	O	
28	D	1	46	36	10	0

- Molecule 29 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



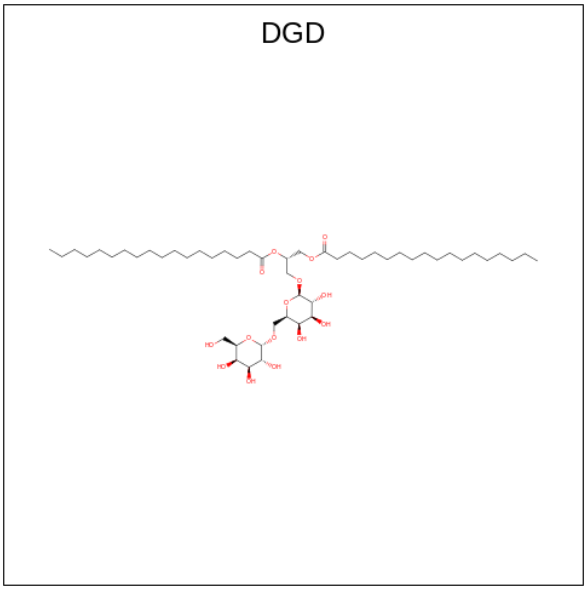
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	A	1	35	24	11	0
			Total	C	O	
29	a	1	35	24	11	0
			Total	C	O	
29	2	1	35	24	11	0
			Total	C	O	
29	8	1	35	24	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	D	1	35	24	11	0
			Total	C	O	
29	5	1	32	21	11	0
			Total	C	O	
29	5	1	23	13	10	0
			Total	C	O	
29	g	1	32	21	11	0
			Total	C	O	
29	g	1	24	13	11	0

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



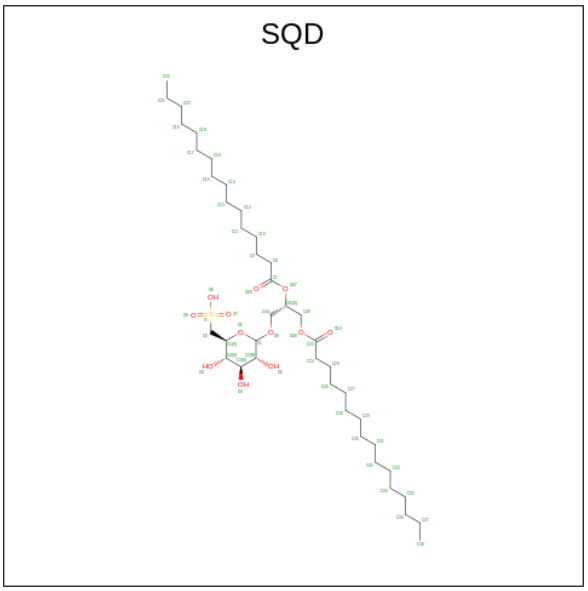
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	B	1	53	39	14	0
			Total	C	O	
30	H	1	62	47	15	0
			Total	C	O	
30	b	1	53	39	14	0
			Total	C	O	
30	h	1	62	47	15	0
			Total	C	O	
30	C	1	55	40	15	0
			Total	C	O	
30	C	1	39	26	13	0

Continued on next page...

Continued from previous page...

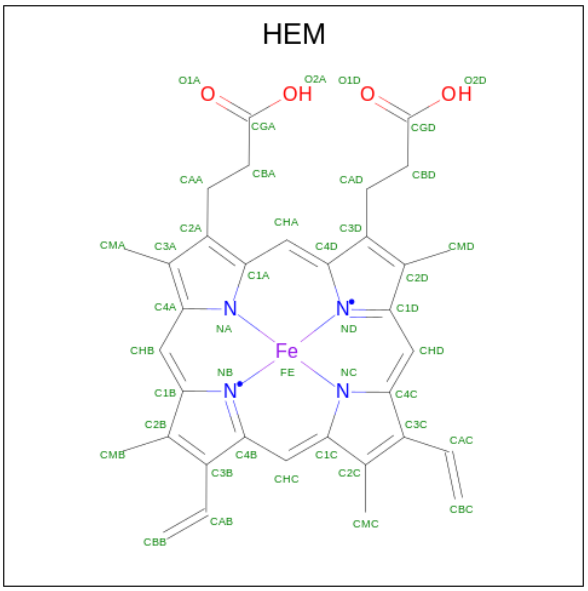
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	c	1	55	40	15	0
			Total	C	O	
30	c	1	39	26	13	0

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



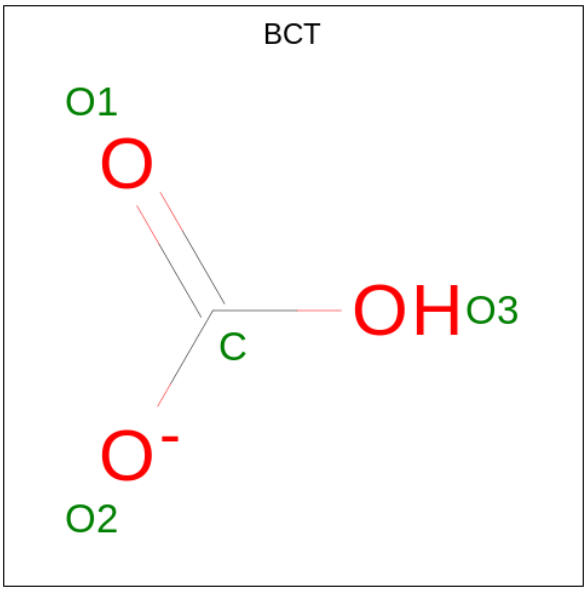
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
31	B	1	49	36	12	1	0
			Total	C	O	S	
31	B	1	54	41	12	1	0
			Total	C	O	S	
31	X	1	37	24	12	1	0
			Total	C	O	S	
31	b	1	54	41	12	1	0
			Total	C	O	S	
31	C	1	51	38	12	1	0

- Molecule 32 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
32	E	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
32	f	1	43	34	1	4	4	0

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	D	1	4	1	3	0

Continued on next page...

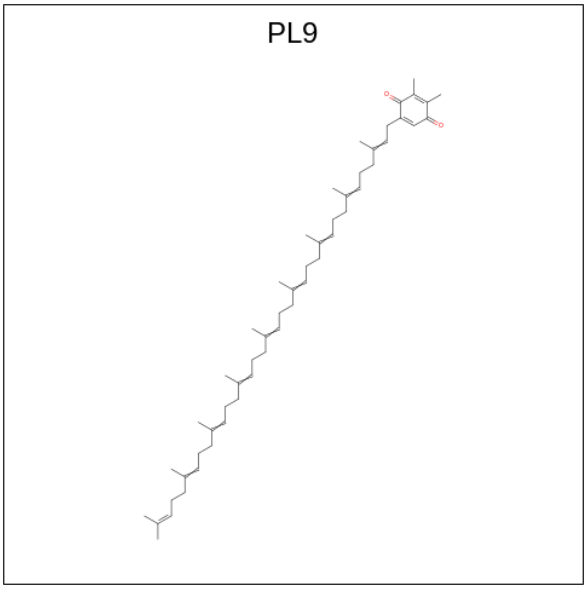
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	d	1	4	1	3	0

- Molecule 34 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
34	D	1	1	1	0
34	d	1	1	1	0

- Molecule 35 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	D	1	55	53	2	0
35	d	1	55	53	2	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
36	6	3	3	3	0
			Total	O	
36	A	15	15	15	0
			Total	O	
36	B	29	29	29	0
			Total	O	
36	E	1	1	1	0
			Total	O	
36	H	5	5	5	0
			Total	O	
36	J	1	1	1	0
			Total	O	
36	L	1	1	1	0
			Total	O	
36	M	2	2	2	0
			Total	O	
36	T	3	3	3	0
			Total	O	
36	X	2	2	2	0
			Total	O	
36	a	15	15	15	0
			Total	O	
36	b	28	28	28	0
			Total	O	
36	e	2	2	2	0
			Total	O	
36	h	5	5	5	0
			Total	O	
36	l	1	1	1	0
			Total	O	
36	m	2	2	2	0
			Total	O	
36	t	3	3	3	0
			Total	O	
36	x	2	2	2	0
			Total	O	
36	2	3	3	3	0
			Total	O	
36	D	25	25	25	0
			Total	O	
36	d	23	23	23	0
			Total	O	
36	C	5	5	5	0

Continued on next page...

Continued from previous page...

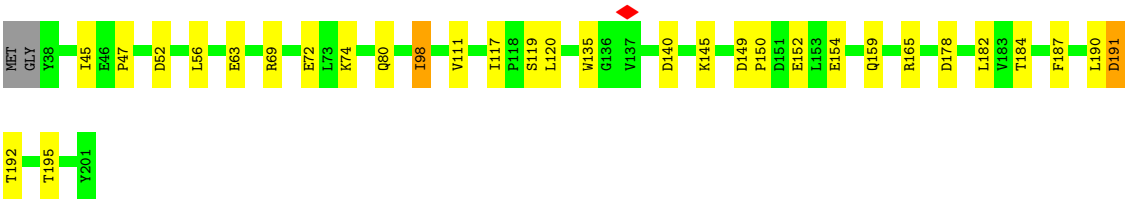
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
36	c	4	4	4	0
			Total	O	
36	5	1	1	1	0

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.

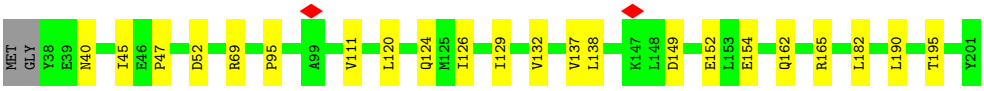
• Molecule 1: Fucoxanthin chlorophyll a/c binding protein II (FCPII-1)

Chain 1:



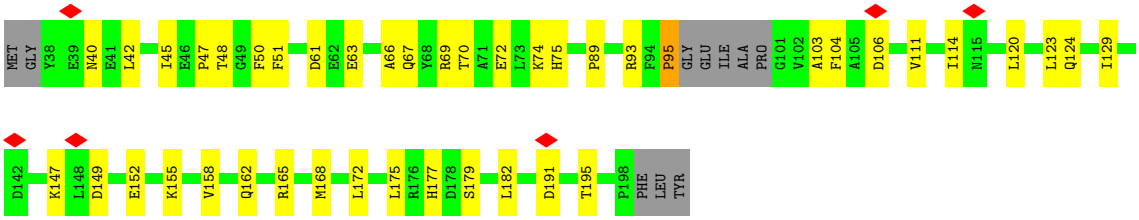
• Molecule 1: Fucoxanthin chlorophyll a/c binding protein II (FCPII-1)

Chain 7:



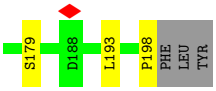
• Molecule 1: Fucoxanthin chlorophyll a/c binding protein II (FCPII-1)

Chain 5:



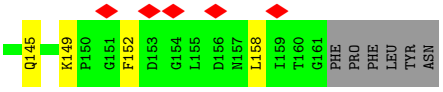
• Molecule 1: Fucoxanthin chlorophyll a/c binding protein II (FCPII-1)

Chain g:



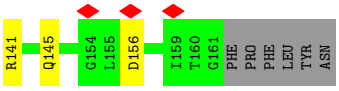
• Molecule 2: Fucoxanthin chlorophyll a/c binding protein II (FCPII-5)

Chain 6:



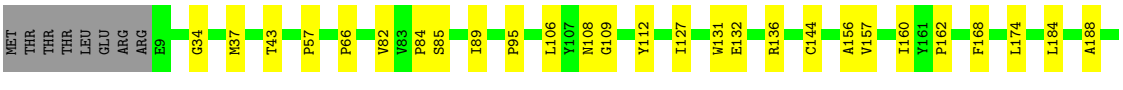
• Molecule 2: Fucoxanthin chlorophyll a/c binding protein II (FCPII-5)

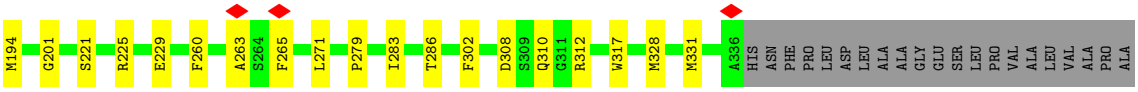
Chain J:



• Molecule 3: Photosystem II protein D1

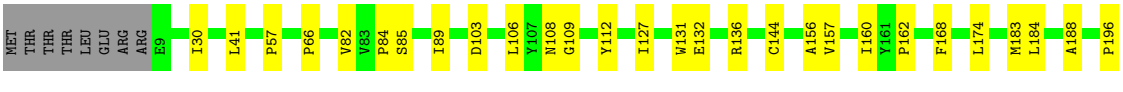
Chain A:

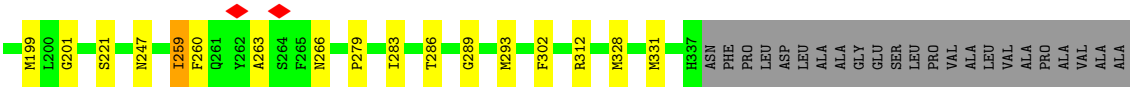




• Molecule 3: Photosystem II protein D1

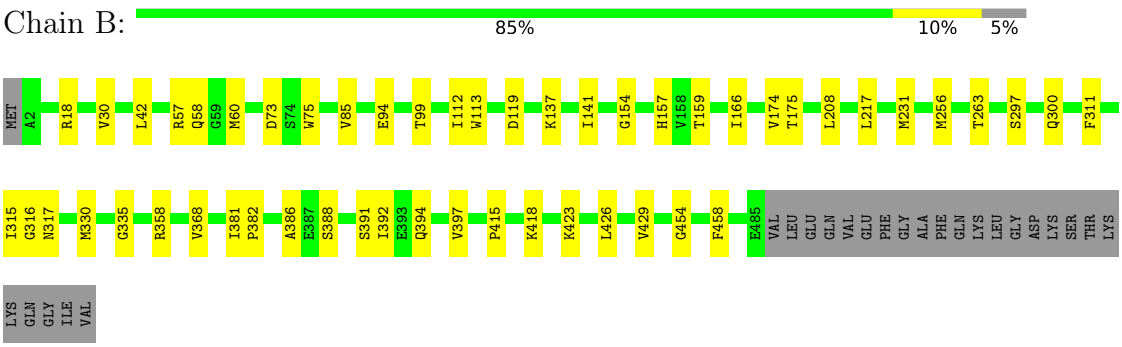
Chain a:





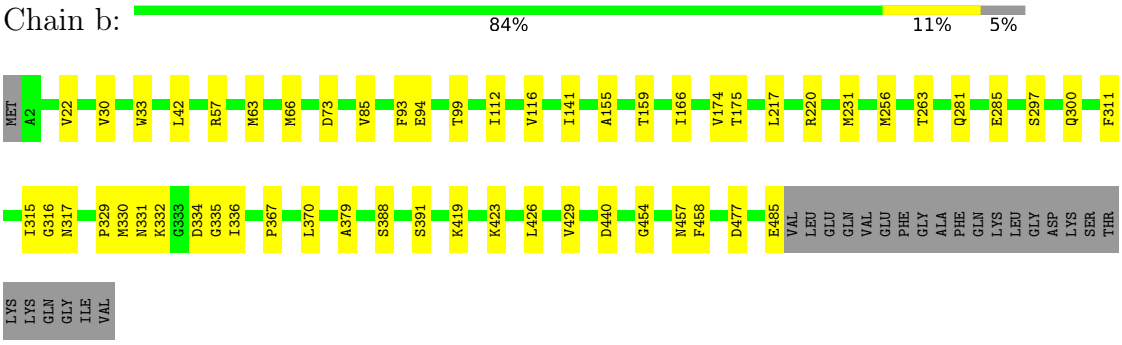
• Molecule 4: Photosystem II CP47 reaction center protein

Chain B:



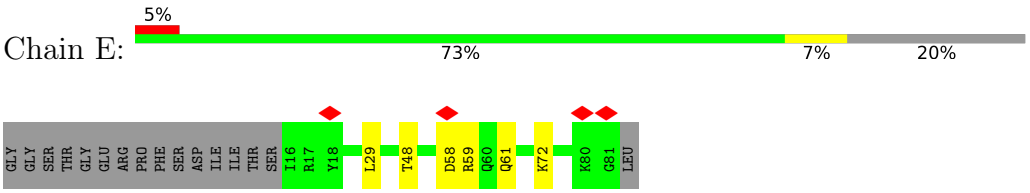
• Molecule 4: Photosystem II CP47 reaction center protein

Chain b:



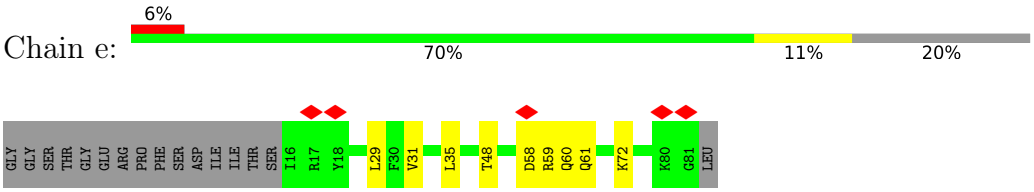
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



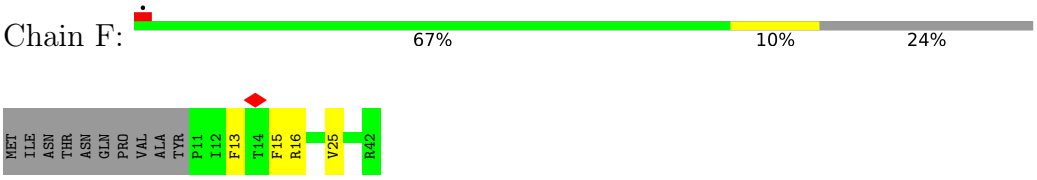
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



• Molecule 6: Cytochrome b559 subunit beta

Chain F:



• Molecule 6: Cytochrome b559 subunit beta

Chain f: 5% 74% • 24%

MET ILE ASN THR ASN GLN PRO VAL ALA TYR P11 I12 V25 R42

• Molecule 7: Photosystem II reaction center protein H (psbH)

Chain H: 80% 18% •

MET A2 I10 L11 L14 E17 K20 L55 E56 N57 V58 D61 T64 V65

• Molecule 7: Photosystem II reaction center protein H (psbH)

Chain h: 86% 12% •

MET A2 L11 L14 K20 L55 E56 N57 V58 T64 V65

• Molecule 8: Photosystem II reaction center protein I (psbI)

Chain I: 92% • 5%

M1 D27 D36 LEU GLU

• Molecule 8: Photosystem II reaction center protein I (psbI)

Chain i: • 87% 8% 5%

M1 F2 T3 L7 D27 D36 LEU GLU

• Molecule 9: Photosystem II reaction center protein K (psbK)

Chain K: 5% 80% 12% 8%

LEU LEU SER A4 L5 P6 E7 M19 P20 A21 I22 R40

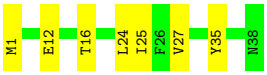
• Molecule 9: Photosystem II reaction center protein K (psbK)

Chain k: 5% 78% 12% • 8%

LEU LEU SER A4 E7 I15 M19 P20 A21 I22 L25 L28 R40

• Molecule 10: Photosystem II reaction center protein L

Chain L:

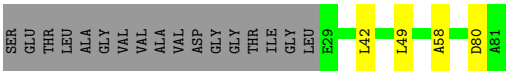


• Molecule 10: Photosystem II reaction center protein L

Chain l:

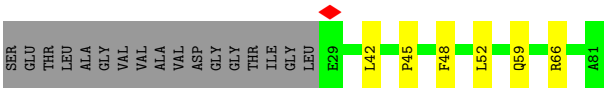
• Molecule 11: Photosystem II reaction center protein M (psbM)

Chain M:



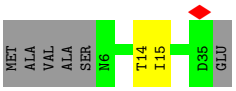
• Molecule 11: Photosystem II reaction center protein M (psbM)

Chain m:



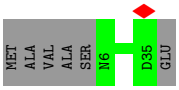
• Molecule 12: Photosystem II reaction center protein Psb36

Chain N:



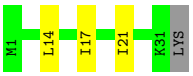
• Molecule 12: Photosystem II reaction center protein Psb36

Chain n:



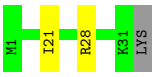
• Molecule 13: Photosystem II reaction center protein T

Chain T: 88% 9%



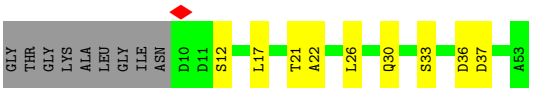
• Molecule 13: Photosystem II reaction center protein T

Chain t: 91% 6%



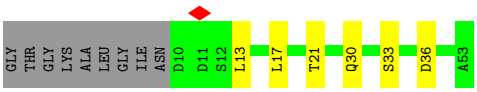
• Molecule 14: Photosystem II reaction center protein W (psbW)

Chain W: 66% 17% 17%



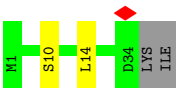
• Molecule 14: Photosystem II reaction center protein W (psbW)

Chain w: 72% 11% 17%



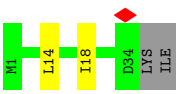
• Molecule 15: Photosystem II reaction center protein X (psbX)

Chain X: 89% 6% 6%



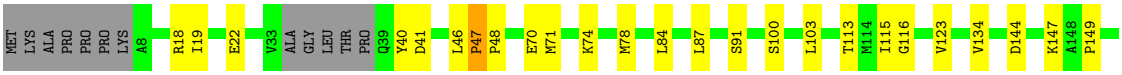
• Molecule 15: Photosystem II reaction center protein X (psbX)

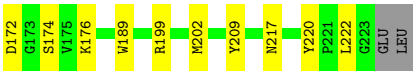
Chain x: 89% 6% 6%



• Molecule 16: Fucoxanthin chlorophyll a/c binding protein II (FCPII-2)

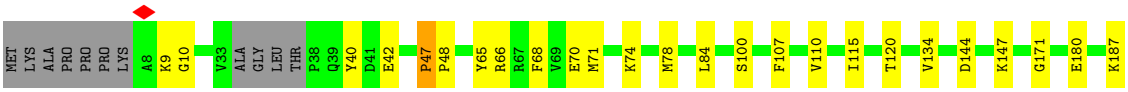
Chain 2: 78% 15% 6%

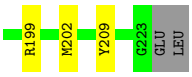




• Molecule 16: Fucoxanthin chlorophyll a/c binding protein II (FCPII-2)

Chain 8:





• Molecule 17: Photosystem II D2 protein

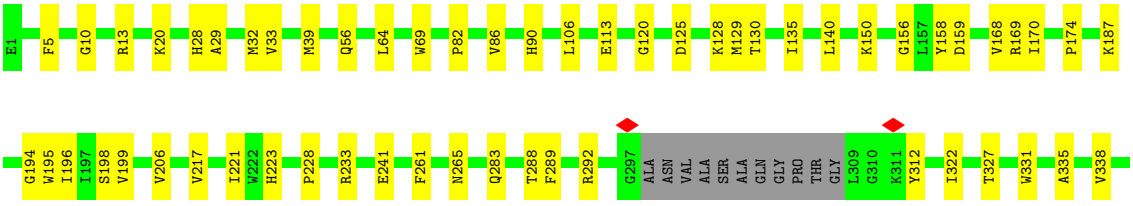
Chain D:

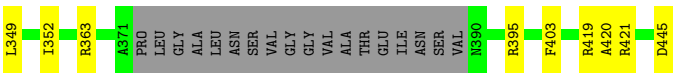
• Molecule 17: Photosystem II D2 protein

Chain d:

• Molecule 18: Photosystem II CP43 reaction center protein

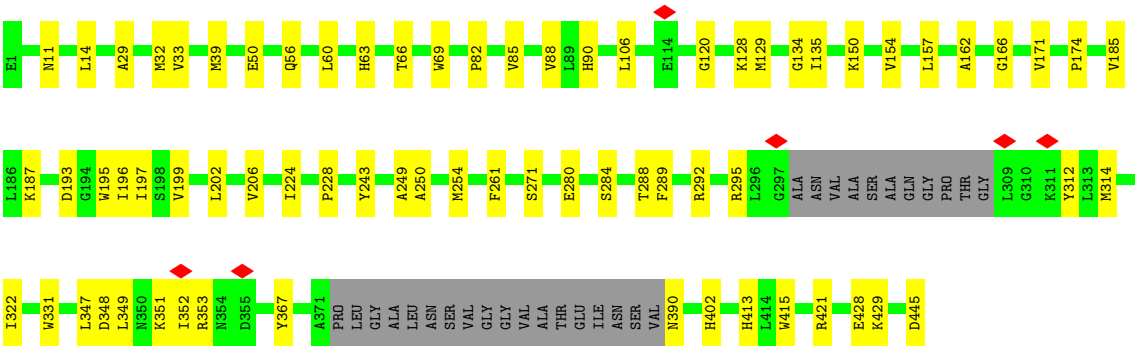
Chain C:





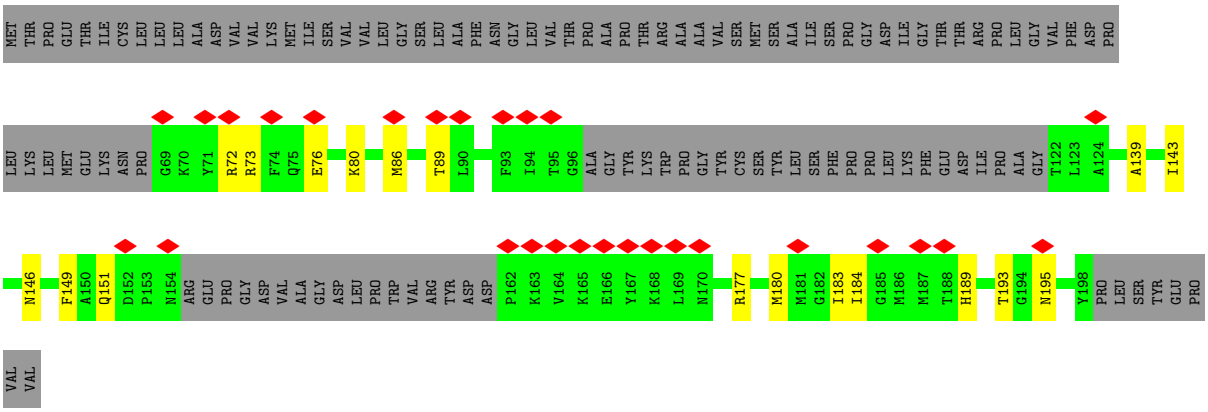
• Molecule 18: Photosystem II CP43 reaction center protein

Chain c: 78% 16% 7%



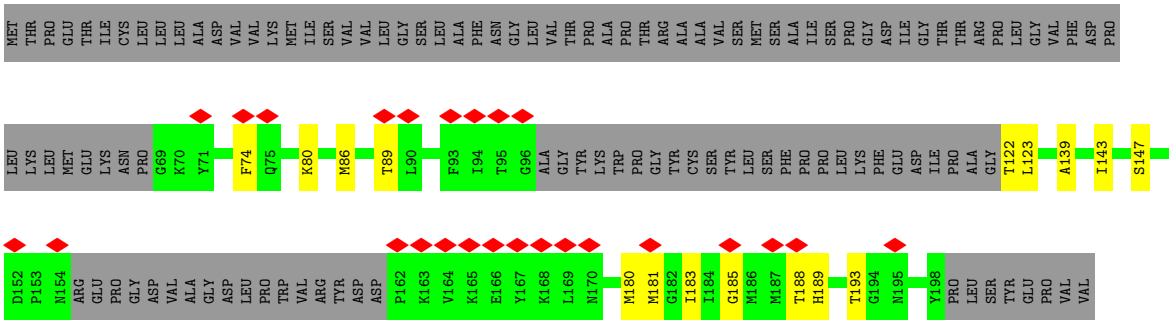
- Molecule 19: Light harvesting protein

Chain 9: 13% 37% 8% 55%



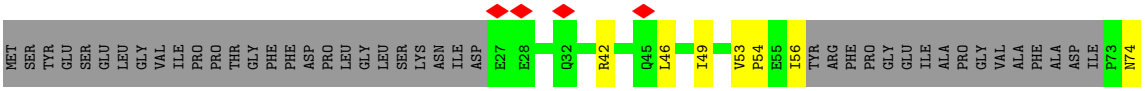
- Molecule 19: Light harvesting protein

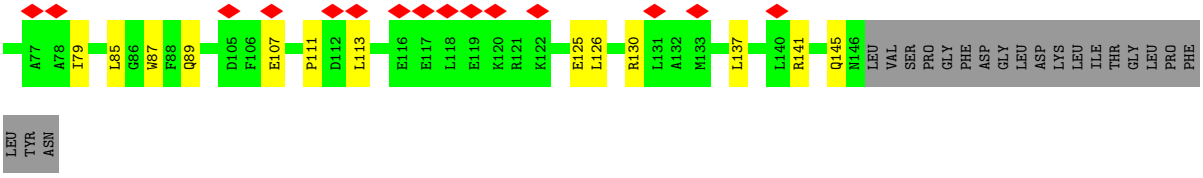
Chain 3: 12% 38% 7% 55%



- Molecule 20: Fucoxanthin chlorophyll a/c binding protein II (FCPII-4)

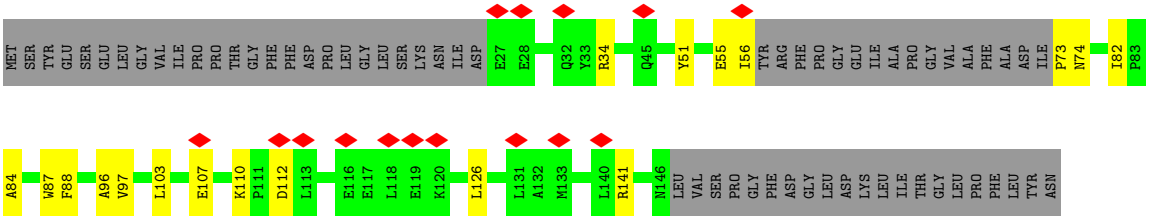
Chain 4: 11% 50% 12% 38%





• Molecule 20: Fucoxanthin chlorophyll a/c binding protein II (FCPII-4)

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	38582	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.298	Depositor
Minimum map value	-0.110	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	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: LMG, DGD, A86, DD6, HEM, PL9, BCT, CLA, SQD, PHO, KC1, FE2, LMU, LHG, BCR

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	1	0.23	0/1314	0.49	0/1791
1	5	0.57	1/1246 (0.1%)	0.71	2/1696 (0.1%)
1	7	0.29	1/1311 (0.1%)	0.49	1/1787 (0.1%)
1	g	0.65	2/1246 (0.2%)	0.77	3/1696 (0.2%)
2	6	0.29	0/1223	0.57	0/1665
2	J	0.24	0/1223	0.52	0/1665
3	A	0.21	0/2648	0.45	0/3609
3	a	0.21	0/2659	0.45	0/3624
4	B	0.23	1/3923 (0.0%)	0.38	1/5341 (0.0%)
4	b	0.17	0/3923	0.37	0/5341
5	E	0.17	0/554	0.44	0/753
5	e	0.18	0/554	0.42	0/753
6	F	0.22	0/274	0.65	0/371
6	f	0.16	0/274	0.48	0/371
7	H	0.16	0/512	0.42	0/699
7	h	0.16	0/512	0.42	0/699
8	I	0.19	0/306	0.43	0/413
8	i	0.19	0/306	0.43	0/413
9	K	0.42	0/306	0.70	1/420 (0.2%)
9	k	0.59	1/306 (0.3%)	0.61	0/420
10	L	0.20	0/322	0.35	0/438
10	l	0.17	0/322	0.31	0/438
11	M	0.20	0/406	0.45	0/555
11	m	0.18	0/406	0.44	0/555
12	N	0.17	0/205	0.46	0/280
12	n	0.20	0/205	0.56	0/280
13	T	0.16	0/265	0.33	0/359
13	t	0.15	0/265	0.30	0/359
14	W	0.13	0/350	0.39	0/477
14	w	0.13	0/350	0.45	0/477
15	X	0.21	0/243	0.54	0/334
15	x	0.21	0/243	0.48	0/334

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2	0.20	0/1702	0.46	1/2314 (0.0%)
16	8	0.18	0/1710	0.46	1/2325 (0.0%)
17	D	0.16	0/2733	0.38	0/3724
17	d	0.16	0/2684	0.39	0/3656
18	C	0.18	0/3379	0.40	0/4604
18	c	0.18	0/3379	0.39	0/4604
19	3	0.19	0/785	0.53	0/1057
19	9	0.18	0/785	0.48	0/1057
20	4	0.24	0/840	0.57	0/1136
20	G	0.22	0/840	0.50	0/1136
All	All	0.24	6/47039 (0.0%)	0.46	10/64026 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	95	PRO	N-CD	19.50	1.75	1.47
1	5	95	PRO	N-CD	17.70	1.72	1.47
4	B	415	PRO	N-CD	10.63	1.62	1.47
9	k	20	PRO	N-CD	-8.29	1.36	1.47
1	7	95	PRO	N-CD	7.15	1.57	1.47
1	g	198	PRO	N-CD	6.78	1.57	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	g	95	PRO	CA-N-CD	-17.29	87.79	112.00
1	5	95	PRO	CA-N-CD	-11.82	95.46	112.00
1	g	95	PRO	N-CD-CG	-7.59	91.82	103.20
1	5	95	PRO	N-CD-CG	-7.31	92.23	103.20
1	g	198	PRO	CA-N-CD	-7.09	102.07	112.00
4	B	415	PRO	CA-N-CD	-7.04	102.14	112.00
16	2	47	PRO	N-CA-C	6.48	118.60	110.70
9	K	6	PRO	CA-N-CD	-5.79	103.89	112.00
1	7	95	PRO	CA-N-CD	-5.39	104.46	112.00
16	8	47	PRO	N-CA-C	5.23	117.08	110.70

There are no chirality outliers.

There are no planarity outliers.

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	1	1281	0	1258	26	0
1	5	1217	0	1196	34	0
1	7	1278	0	1256	18	0
1	g	1217	0	1196	23	0
2	6	1191	0	1187	26	0
2	J	1191	0	1187	23	0
3	A	2565	0	2446	42	0
3	a	2575	0	2453	36	0
4	B	3796	0	3687	38	0
4	b	3796	0	3687	40	0
5	E	539	0	527	6	0
5	e	539	0	527	10	0
6	F	265	0	273	3	0
6	f	265	0	273	1	0
7	H	502	0	524	10	0
7	h	502	0	524	6	0
8	I	298	0	308	1	0
8	i	298	0	308	2	0
9	K	295	0	304	3	0
9	k	295	0	304	7	0
10	L	312	0	315	8	0
10	l	312	0	315	5	0
11	M	397	0	397	4	0
11	m	397	0	397	6	0
12	N	202	0	208	2	0
12	n	202	0	208	0	0
13	T	258	0	281	4	0
13	t	258	0	281	2	0
14	W	342	0	304	6	0
14	w	342	0	304	4	0
15	X	240	0	267	1	0
15	x	240	0	267	1	0
16	2	1657	0	1647	32	0
16	8	1664	0	1655	21	0
17	D	2644	0	2553	31	0
17	d	2597	0	2510	28	0
18	C	3268	0	3190	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	c	3268	0	3190	61	0
19	3	770	0	781	11	0
19	9	770	0	781	15	0
20	4	822	0	818	15	0
20	G	822	0	818	20	0
21	1	558	0	535	12	0
21	2	317	0	286	11	0
21	3	262	0	229	9	0
21	4	292	0	285	11	0
21	5	457	0	447	12	0
21	6	467	0	412	8	0
21	7	563	0	551	17	0
21	8	308	0	269	12	0
21	9	270	0	237	10	0
21	A	174	0	170	4	0
21	B	1011	0	1082	30	0
21	C	806	0	853	21	0
21	D	176	0	164	7	0
21	G	294	0	289	3	0
21	J	467	0	412	9	0
21	a	174	0	170	5	0
21	b	1002	0	1061	38	0
21	c	798	0	834	24	0
21	d	176	0	164	6	0
21	g	436	0	404	11	0
22	1	43	0	0	1	0
22	5	43	0	0	0	0
22	7	43	0	0	1	0
22	g	43	0	0	0	0
23	1	144	0	0	0	0
23	2	288	0	0	0	0
23	4	48	0	0	0	0
23	5	96	0	0	1	0
23	6	96	0	0	0	0
23	7	140	0	0	0	0
23	8	240	0	0	0	0
23	G	48	0	0	0	0
23	J	96	0	0	0	0
23	W	48	0	0	0	0
23	g	96	0	0	0	0
24	1	90	0	0	0	0
24	2	180	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	3	90	0	0	0	0
24	4	173	0	0	0	0
24	5	135	0	0	1	0
24	6	135	0	0	0	0
24	7	90	0	0	0	0
24	8	180	0	0	1	0
24	9	90	0	0	0	0
24	G	173	0	0	2	0
24	J	135	0	0	1	0
24	g	135	0	0	1	0
25	1	40	0	56	3	0
25	A	40	0	56	5	0
25	B	80	0	112	7	0
25	C	80	0	112	4	0
25	D	40	0	56	1	0
25	H	40	0	56	2	0
25	M	40	0	56	2	0
25	a	40	0	56	5	0
25	b	80	0	112	3	0
25	c	80	0	112	2	0
25	d	40	0	56	1	0
25	h	80	0	112	4	0
25	m	40	0	56	0	0
26	A	64	0	74	2	0
26	D	64	0	74	2	0
26	a	64	0	74	1	0
26	d	64	0	74	2	0
27	A	49	0	74	3	0
27	B	49	0	74	3	0
27	D	91	0	133	6	0
27	a	49	0	74	1	0
27	d	91	0	133	4	0
27	l	49	0	74	2	0
28	2	46	0	65	3	0
28	8	75	0	99	4	0
28	A	48	0	66	1	0
28	B	199	0	248	6	0
28	D	46	0	62	0	0
28	L	40	0	50	1	0
28	M	40	0	50	2	0
28	N	24	0	24	1	0
28	a	48	0	66	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	b	231	0	282	5	0
28	f	46	0	62	0	0
29	2	35	0	46	0	0
29	5	55	0	55	2	0
29	8	35	0	46	1	0
29	A	35	0	46	0	0
29	D	35	0	46	1	0
29	a	35	0	46	0	0
29	g	56	0	58	1	0
30	B	53	0	64	4	0
30	C	94	0	110	1	0
30	H	62	0	82	3	0
30	b	53	0	64	3	0
30	c	94	0	110	4	0
30	h	62	0	82	0	0
31	B	103	0	140	3	0
31	C	51	0	69	1	0
31	X	37	0	38	0	0
31	b	54	0	78	3	0
32	E	43	0	30	1	0
32	f	43	0	30	1	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	D	1	0	0	0	0
34	d	1	0	0	0	0
35	D	55	0	80	2	0
35	d	55	0	80	2	0
36	2	3	0	0	0	0
36	5	1	0	0	0	0
36	6	3	0	0	0	0
36	A	15	0	0	0	0
36	B	29	0	0	1	0
36	C	5	0	0	1	0
36	D	25	0	0	0	0
36	E	1	0	0	0	0
36	H	5	0	0	0	0
36	J	1	0	0	0	0
36	L	1	0	0	0	0
36	M	2	0	0	0	0
36	T	3	0	0	0	0
36	X	2	0	0	0	0
36	a	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	b	28	0	0	0	0
36	c	4	0	0	0	0
36	d	23	0	0	0	0
36	e	2	0	0	0	0
36	h	5	0	0	0	0
36	l	1	0	0	0	0
36	m	2	0	0	0	0
36	t	3	0	0	0	0
36	x	2	0	0	0	0
All	All	61348	0	58108	809	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 7.

All (809) 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)
20:G:82:ILE:HD11	20:G:87:TRP:CZ2	1.37	1.52
1:5:95:PRO:N	1:5:95:PRO:CD	1.72	1.39
1:g:95:PRO:CD	1:g:95:PRO:N	1.75	1.32
20:G:82:ILE:CD1	20:G:87:TRP:CZ2	2.33	1.11
20:G:82:ILE:HD11	20:G:87:TRP:CE2	1.88	1.06
1:5:120:LEU:O	1:5:124:GLN:OE1	1.82	0.97
7:H:64:THR:HG22	7:H:65:VAL:HG23	1.46	0.94
20:G:82:ILE:HD11	20:G:87:TRP:HZ2	1.28	0.90
19:3:180:MET:HE3	21:3:300:CLA:HHC	1.57	0.86
20:G:82:ILE:HG13	20:G:87:TRP:HE1	1.38	0.85
9:k:20:PRO:HB3	18:c:39:MET:HE1	1.59	0.84
16:2:71:MET:HE1	24:2:315:KC1:CBA	2.08	0.82
3:a:259:ILE:HD12	3:a:260:PHE:H	1.45	0.79
20:4:137:LEU:HD11	21:4:301:CLA:HBB2	1.65	0.79
20:G:82:ILE:CD1	20:G:87:TRP:CE2	2.62	0.77
20:G:82:ILE:HG13	20:G:87:TRP:NE1	2.00	0.75
16:2:134:VAL:HG13	21:2:302:CLA:HAB	1.69	0.74
1:7:154:GLU:OE1	16:8:10:GLY:HA2	1.86	0.73
21:c:503:CLA:HBB2	21:c:511:CLA:H151	1.69	0.73
18:c:60:LEU:HD22	21:c:504:CLA:HED3	1.71	0.73
1:1:98:ILE:HD12	1:1:117:ILE:HG13	1.70	0.73
20:G:97:VAL:HG12	20:G:103:LEU:H	1.53	0.73
4:b:297:SER:H	4:b:300:GLN:HE21	1.36	0.72
1:g:95:PRO:HD2	1:g:95:PRO:C	2.14	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:c:11:ASN:HB2	21:c:509:CLA:HBA1	1.71	0.71
1:7:45:ILE:HG23	1:7:47:PRO:HD2	1.71	0.71
9:k:25:LEU:HA	9:k:28:LEU:HD23	1.73	0.69
1:5:45:ILE:HG22	1:5:47:PRO:HD2	1.73	0.69
20:G:141:ARG:O	24:G:307:KC1:CED	2.41	0.69
18:c:171:VAL:HG21	18:c:202:LEU:HD22	1.73	0.69
3:a:289:GLY:O	3:a:293:MET:HE3	1.93	0.69
16:2:113:THR:HG22	16:2:116:GLY:H	1.58	0.69
1:1:119:SER:HG	20:4:87:TRP:CD1	2.14	0.66
19:9:80:LYS:HZ1	21:9:302:CLA:C3D	2.08	0.66
21:C:504:CLA:HBB2	21:C:512:CLA:H151	1.79	0.65
3:a:131:TRP:HZ2	18:c:421:ARG:HG2	1.62	0.65
1:1:45:ILE:HG23	1:1:47:PRO:HD2	1.77	0.65
20:4:42:ARG:HD2	21:4:302:CLA:HMA3	1.78	0.64
3:A:131:TRP:HZ2	18:C:421:ARG:HG2	1.63	0.64
1:g:95:PRO:CD	1:g:95:PRO:C	2.64	0.64
19:3:181:MET:HE3	19:3:181:MET:HA	1.80	0.64
3:A:310:GLN:NE2	3:A:312:ARG:HD3	2.13	0.64
3:a:259:ILE:CD1	3:a:260:PHE:H	2.11	0.64
4:B:119:ASP:HB3	10:L:1:MET:HG2	1.80	0.63
18:C:140:LEU:HD12	21:C:503:CLA:HMC2	1.80	0.63
18:c:428:GLU:HG2	18:c:429:LYS:HZ2	1.62	0.63
16:2:71:MET:HE1	24:2:315:KC1:CAA	2.28	0.63
21:b:610:CLA:HHD	21:8:307:CLA:HED1	1.81	0.63
9:K:20:PRO:HB3	18:C:39:MET:HE1	1.81	0.63
4:B:18:ARG:HH22	31:B:626:SQD:H61	1.63	0.63
18:C:113:GLU:HA	18:C:120:GLY:HA3	1.80	0.63
1:7:149:ASP:HB3	1:7:152:GLU:HB2	1.79	0.62
1:5:162:GLN:HA	1:5:165:ARG:HB2	1.81	0.62
13:T:21:ILE:HD11	27:D:410:LHG:H331	1.81	0.62
19:9:80:LYS:HZ1	21:9:302:CLA:C2D	2.11	0.62
1:g:107:ILE:HD12	21:g:304:CLA:HED1	1.81	0.62
3:A:310:GLN:HE21	3:A:312:ARG:CD	2.12	0.62
15:x:14:LEU:HD22	15:x:18:ILE:HD11	1.79	0.62
20:4:53:VAL:HA	20:4:56:ILE:HD12	1.82	0.62
21:b:603:CLA:HBB2	25:h:102:BCR:H351	1.81	0.62
1:5:177:HIS:NE2	1:5:191:ASP:O	2.33	0.62
1:1:165:ARG:NH2	21:1:301:CLA:O1D	2.34	0.61
7:h:55:LEU:HB2	7:h:58:VAL:HG22	1.82	0.61
3:A:310:GLN:NE2	3:A:312:ARG:CD	2.63	0.61
18:C:265:ASN:O	18:C:395:ARG:NH2	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:8:199:ARG:NH2	21:8:302:CLA:O1D	2.34	0.61
18:C:32:MET:HE3	21:C:512:CLA:HHC	1.83	0.61
1:7:129:ILE:C	1:7:129:ILE:HD12	2.26	0.61
4:B:99:THR:HG22	21:B:607:CLA:H122	1.83	0.61
1:5:165:ARG:NH2	21:5:302:CLA:O1D	2.35	0.60
16:2:199:ARG:NH2	21:2:301:CLA:O1D	2.33	0.60
28:a:407:LMG:H351	21:c:506:CLA:H101	1.83	0.60
1:g:149:ASP:HB3	1:g:152:GLU:HB3	1.83	0.60
1:5:48:THR:HB	1:5:51:PHE:HB2	1.82	0.60
1:1:98:ILE:CD1	1:1:117:ILE:HG13	2.32	0.60
16:2:47:PRO:HG2	21:2:303:CLA:HMA1	1.82	0.60
3:A:160:ILE:CD1	18:C:403:PHE:HZ	2.15	0.59
21:C:503:CLA:H202	21:C:509:CLA:HBB1	1.83	0.59
21:7:306:CLA:HBB2	25:h:101:BCR:H17C	1.83	0.59
35:d:408:PL9:H111	27:d:409:LHG:H102	1.84	0.59
1:5:168:MET:HE3	21:5:302:CLA:HMC3	1.83	0.59
18:C:289:PHE:HB3	18:C:312:TYR:HE2	1.68	0.59
3:a:160:ILE:HD11	30:c:516:DGD:HBW1	1.85	0.59
18:c:120:GLY:O	18:c:128:LYS:NZ	2.35	0.59
18:c:129:MET:HE2	18:c:243:TYR:CE2	2.38	0.59
1:5:149:ASP:HB3	1:5:152:GLU:HB2	1.83	0.59
16:8:134:VAL:HG13	21:8:303:CLA:HAB	1.84	0.59
21:B:615:CLA:H202	28:2:318:LMG:H162	1.85	0.58
16:2:87:LEU:O	16:2:91:SER:OG	2.19	0.58
18:C:187:LYS:HB3	18:C:195:TRP:HA	1.86	0.58
18:c:39:MET:HB3	18:c:60:LEU:HD12	1.85	0.58
18:C:288:THR:O	18:C:292:ARG:HD3	2.04	0.58
1:7:137:VAL:HG23	1:7:138:LEU:HD23	1.84	0.57
1:7:165:ARG:NH2	21:7:300:CLA:O1D	2.37	0.57
4:b:73:ASP:HB3	4:b:85:VAL:HG21	1.86	0.57
18:c:69:TRP:HE3	18:c:82:PRO:HB3	1.69	0.57
18:c:197:ILE:HD12	30:c:516:DGD:HG32	1.86	0.57
4:b:311:PHE:O	4:b:317:ASN:ND2	2.37	0.57
16:2:19:ILE:HD11	16:2:176:LYS:HG3	1.87	0.57
16:2:41:ASP:OD1	16:2:41:ASP:N	2.37	0.57
4:B:311:PHE:O	4:B:317:ASN:ND2	2.37	0.57
7:H:17:GLU:HG2	7:H:20:LYS:HD2	1.86	0.57
32:f:101:HEM:HHD	32:f:101:HEM:HBC2	1.86	0.57
18:C:196:ILE:HG22	18:C:261:PHE:HE2	1.70	0.57
13:t:21:ILE:HD11	27:d:409:LHG:H312	1.85	0.57
1:g:107:ILE:HG23	1:g:116:ALA:HB3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:160:ILE:HD13	18:C:403:PHE:CZ	2.40	0.56
1:g:167:ALA:O	1:g:171:THR:OG1	2.23	0.56
18:C:158:TYR:HA	18:C:168:VAL:HA	1.87	0.56
21:c:504:CLA:HBB1	21:c:513:CLA:H62	1.86	0.56
1:g:175:LEU:O	1:g:179:SER:OG	2.23	0.56
3:A:260:PHE:CE1	3:A:263:ALA:HB2	2.40	0.56
11:M:42:LEU:HD12	10:l:25:ILE:HG22	1.88	0.56
5:e:31:VAL:HG13	5:e:35:LEU:CD2	2.36	0.56
21:9:303:CLA:H51	21:9:303:CLA:HBC2	1.88	0.56
1:1:111:VAL:HG23	1:1:182:LEU:HD22	1.88	0.56
21:a:405:CLA:H3A	28:a:407:LMG:H301	1.88	0.56
2:6:27:GLU:HA	2:6:30:PHE:HB3	1.86	0.56
9:k:19:MET:HA	9:k:22:ILE:HD12	1.87	0.56
28:b:620:LMG:H171	21:b:623:CLA:H2	1.87	0.56
21:7:309:CLA:HBA1	21:7:309:CLA:HED2	1.86	0.55
5:e:72:LYS:HE3	17:d:99:ASP:HB2	1.88	0.55
4:b:99:THR:HG22	21:b:608:CLA:H122	1.88	0.55
18:C:69:TRP:HE3	18:C:82:PRO:HB3	1.70	0.55
1:g:88:VAL:HG21	21:g:304:CLA:HBC3	1.88	0.55
3:A:160:ILE:CD1	18:C:403:PHE:CZ	2.90	0.55
32:E:101:HEM:HHC	32:E:101:HEM:HBB2	1.87	0.55
30:b:601:DGD:HB32	30:b:601:DGD:HA61	1.89	0.55
16:8:110:VAL:HG13	16:8:120:THR:HB	1.88	0.55
4:B:141:ILE:HG13	4:B:217:LEU:HD21	1.88	0.55
11:M:58:ALA:HB1	11:m:59:GLN:HG3	1.89	0.55
27:A:406:LHG:HC2	18:C:419:ARG:HE	1.72	0.55
18:C:33:VAL:HG13	18:C:90:HIS:HD2	1.70	0.55
6:F:13:PHE:HD1	6:F:16:ARG:H	1.50	0.55
5:e:48:THR:HG23	17:d:55:THR:HB	1.89	0.55
18:c:280:GLU:O	18:c:284:SER:OG	2.20	0.55
7:H:55:LEU:HB2	7:H:58:VAL:HB	1.89	0.55
10:L:25:ILE:HG22	11:m:42:LEU:HD12	1.89	0.55
5:E:48:THR:HG23	17:D:55:THR:HB	1.88	0.55
27:B:601:LHG:H201	10:L:27:VAL:HG11	1.88	0.54
18:c:289:PHE:HB3	18:c:312:TYR:HE2	1.71	0.54
18:C:64:LEU:HD11	18:C:86:VAL:HG21	1.90	0.54
17:d:178:PHE:HA	17:d:181:LEU:HD12	1.89	0.54
4:B:454:GLY:HA2	28:B:619:LMG:H212	1.89	0.54
16:8:107:PHE:HD1	21:8:306:CLA:HED3	1.72	0.54
16:8:171:GLY:N	21:8:307:CLA:O1D	2.40	0.54
3:A:225:ARG:NH2	3:A:229:GLU:OE1	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:14:THR:HG23	28:N:101:LMG:H312	1.89	0.54
17:D:178:PHE:HA	17:D:181:LEU:HD12	1.89	0.54
1:1:190:LEU:HD13	1:1:195:THR:HG21	1.90	0.54
25:A:405:BCR:H392	30:b:601:DGD:HB52	1.88	0.54
21:4:300:CLA:H2A	21:4:300:CLA:HED2	1.89	0.54
18:C:150:LYS:NZ	18:C:156:GLY:O	2.41	0.54
1:5:89:PRO:O	1:5:93:ARG:NH1	2.41	0.53
21:C:506:CLA:H162	21:C:510:CLA:H121	1.90	0.53
9:K:19:MET:HA	9:K:22:ILE:HD12	1.89	0.53
4:B:391:SER:HB3	4:B:394:GLN:HG3	1.90	0.53
4:b:42:LEU:HD13	4:b:94:GLU:HG3	1.91	0.53
16:8:78:MET:HE1	21:8:303:CLA:HAC2	1.89	0.53
3:A:310:GLN:HE21	3:A:312:ARG:HG3	1.74	0.53
3:A:43:THR:HG23	25:A:405:BCR:H362	1.91	0.53
3:A:57:PRO:HB2	3:A:66:PRO:HB2	1.91	0.53
10:l:16:THR:HG21	27:d:409:LHG:HC32	1.90	0.53
17:D:171:SER:HB2	17:D:176:ALA:HB1	1.90	0.53
18:c:129:MET:HE2	18:c:243:TYR:HE2	1.73	0.53
1:g:86:TYR:O	1:g:109:ASN:ND2	2.41	0.53
17:d:171:SER:HB2	17:d:176:ALA:HB1	1.91	0.53
18:c:322:ILE:HG21	18:c:331:TRP:HB2	1.91	0.53
5:E:72:LYS:HE3	17:D:99:ASP:HB2	1.91	0.53
17:D:241:GLU:HG2	17:D:263:LYS:HZ2	1.73	0.53
18:C:135:ILE:HD13	21:C:514:CLA:HAB	1.90	0.53
16:8:199:ARG:HA	16:8:202:MET:HE3	1.91	0.52
18:c:288:THR:O	18:c:292:ARG:HG2	2.09	0.52
18:c:348:ASP:HB3	18:c:351:LYS:HB2	1.91	0.52
19:9:146:ASN:HD21	21:9:302:CLA:HHB	1.73	0.52
19:9:180:MET:HE1	19:9:184:ILE:HG13	1.91	0.52
20:4:46:LEU:HD21	21:4:302:CLA:HMA2	1.89	0.52
4:B:368:VAL:HB	4:B:381:ILE:HB	1.92	0.52
10:L:16:THR:HG21	27:D:410:LHG:HC32	1.90	0.52
2:J:34:ARG:NH1	2:J:37:GLU:OE1	2.42	0.52
2:J:124:GLN:HA	2:J:127:GLN:HB3	1.91	0.52
14:W:17:LEU:O	14:W:21:THR:HG22	2.10	0.52
18:c:33:VAL:HG13	18:c:90:HIS:HD2	1.73	0.52
4:B:256:MET:HA	4:B:263:THR:HG21	1.92	0.52
4:b:112:ILE:HG21	25:b:619:BCR:H393	1.92	0.52
17:d:78:SER:HA	17:d:171:SER:HB3	1.92	0.52
4:B:423:LYS:HE2	4:B:429:VAL:HG13	1.92	0.52
4:B:458:PHE:HB3	21:B:605:CLA:HBC2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:106:LEU:HD11	25:a:406:BCR:H292	1.91	0.52
1:7:190:LEU:HD13	1:7:195:THR:HG21	1.92	0.52
3:a:289:GLY:C	3:a:293:MET:HE3	2.34	0.52
18:c:154:VAL:HG11	21:c:503:CLA:H191	1.91	0.52
18:c:157:LEU:HB2	18:c:202:LEU:HD11	1.90	0.52
1:g:146:PRO:HG2	21:g:307:CLA:HED2	1.91	0.52
1:1:140:ASP:OD1	1:1:145:LYS:NZ	2.33	0.52
4:B:42:LEU:HD13	4:B:94:GLU:HG3	1.92	0.52
28:M:102:LMG:H292	28:M:102:LMG:H112	1.92	0.52
4:b:256:MET:HA	4:b:263:THR:HG21	1.92	0.52
16:8:84:LEU:HG	21:8:306:CLA:HBC2	1.91	0.52
20:G:141:ARG:O	24:G:307:KC1:O1D	2.28	0.52
11:M:49:LEU:HD21	27:l:101:LHG:H261	1.91	0.52
16:2:115:ILE:HD11	16:2:209:TYR:HE1	1.74	0.52
20:G:112:ASP:N	20:G:112:ASP:OD1	2.43	0.52
21:7:302:CLA:H42	20:G:96:ALA:HB2	1.91	0.51
25:B:617:BCR:HC8	21:B:621:CLA:HMC3	1.92	0.51
2:J:10:ILE:HG21	2:J:127:GLN:OE1	2.09	0.51
4:B:382:PRO:HB3	17:D:343:GLU:HB2	1.92	0.51
3:a:136:ARG:NH2	8:i:27:ASP:OD1	2.40	0.51
19:3:143:ILE:O	19:3:147:SER:OG	2.26	0.51
27:A:406:LHG:H281	27:A:406:LHG:H201	1.90	0.51
4:b:454:GLY:HA2	28:b:620:LMG:H212	1.91	0.51
17:d:262:ASN:HB3	17:d:265:TRP:HB3	1.92	0.51
1:7:162:GLN:HE21	1:7:165:ARG:HH11	1.57	0.51
17:D:278:MET:HG3	26:D:401:PHO:HBC3	1.92	0.51
1:g:138:LEU:HD13	1:g:141:PHE:HB2	1.92	0.51
2:6:121:ARG:HA	2:6:124:GLN:OE1	2.11	0.51
18:c:349:LEU:HB3	18:c:353:ARG:HH12	1.76	0.51
21:B:614:CLA:H51	31:B:626:SQD:H332	1.92	0.51
30:B:624:DGD:HB32	30:B:624:DGD:HA61	1.93	0.51
2:J:62:ILE:HA	2:J:68:PRO:HA	1.93	0.51
28:b:622:LMG:HC71	28:b:626:LMG:HC3	1.92	0.51
5:e:29:LEU:HD11	6:f:25:VAL:HG13	1.93	0.51
4:B:231:MET:HE2	21:B:610:CLA:HMC1	1.93	0.51
5:e:31:VAL:O	5:e:35:LEU:HD22	2.11	0.51
30:B:624:DGD:HB52	25:a:406:BCR:H392	1.92	0.51
2:J:156:ASP:OD1	2:J:156:ASP:N	2.44	0.51
16:8:40:TYR:CZ	16:8:47:PRO:HA	2.46	0.51
4:B:386:ALA:HA	17:D:350:ALA:HB1	1.92	0.51
4:b:30:VAL:HG12	21:b:607:CLA:HHD	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:69:ARG:NH2	21:7:300:CLA:O1D	2.44	0.50
3:A:331:MET:HE2	17:D:319:LEU:HB3	1.93	0.50
16:8:68:PHE:HA	16:8:71:MET:HE2	1.93	0.50
18:C:130:THR:HG21	18:C:228:PRO:HD3	1.92	0.50
2:6:145:GLN:HE22	21:6:303:CLA:C4D	2.24	0.50
1:7:47:PRO:HG3	21:7:304:CLA:C4B	2.41	0.50
3:a:84:PRO:HA	3:a:112:TYR:CG	2.46	0.50
4:B:112:ILE:HG21	25:B:618:BCR:H393	1.93	0.50
2:J:100:TRP:HZ3	1:g:67:GLN:OE1	1.94	0.50
17:d:154:THR:HA	17:d:158:VAL:HB	1.94	0.50
2:6:100:TRP:HZ3	1:5:67:GLN:OE1	1.94	0.50
7:H:14:LEU:HD21	28:2:318:LMG:HC92	1.93	0.50
4:b:458:PHE:HB3	21:b:606:CLA:HBC2	1.92	0.50
18:c:390:ASN:OD1	18:c:390:ASN:N	2.45	0.50
20:G:107:GLU:HA	20:G:110:LYS:HE2	1.93	0.50
2:6:85:LEU:O	2:6:89:GLN:NE2	2.44	0.50
2:6:102:VAL:HG12	2:6:103:LEU:HG	1.94	0.50
21:7:301:CLA:H62	21:7:301:CLA:HED1	1.94	0.50
21:B:612:CLA:H101	21:B:613:CLA:HAB	1.94	0.50
3:a:247:ASN:HD21	4:b:485:GLU:HB2	1.75	0.50
7:h:14:LEU:HD21	28:8:317:LMG:HC92	1.93	0.50
20:4:85:LEU:O	20:4:89:GLN:NE2	2.45	0.50
2:6:124:GLN:HG2	21:6:301:CLA:HMB2	1.93	0.50
2:J:127:GLN:HE21	21:J:307:CLA:C3D	2.25	0.50
21:8:304:CLA:H2A	21:8:304:CLA:HED3	1.94	0.50
17:D:262:ASN:HB3	17:D:265:TRP:HB3	1.93	0.50
18:C:322:ILE:HG21	18:C:331:TRP:HB2	1.92	0.50
4:B:30:VAL:HG12	21:B:606:CLA:HHD	1.93	0.50
3:A:283:ILE:HA	3:A:286:THR:HG22	1.94	0.49
35:D:409:PL9:H111	27:D:410:LHG:H102	1.94	0.49
25:C:501:BCR:H271	21:C:513:CLA:HBA1	1.93	0.49
1:5:120:LEU:HA	1:5:123:LEU:HD12	1.94	0.49
28:B:619:LMG:O5	28:B:619:LMG:O4	2.30	0.49
9:k:20:PRO:HB3	18:c:39:MET:CE	2.38	0.49
16:2:100:SER:OG	24:2:313:KC1:O2A	2.28	0.49
19:3:74:PHE:HB3	21:3:300:CLA:HHB	1.94	0.49
19:3:122:THR:OG1	19:3:123:LEU:N	2.44	0.49
20:G:82:ILE:CG1	20:G:87:TRP:NE1	2.74	0.49
3:A:84:PRO:HA	3:A:112:TYR:CG	2.46	0.49
3:A:106:LEU:HD11	25:A:405:BCR:H292	1.93	0.49
21:B:603:CLA:H71	21:B:609:CLA:H202	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:c:507:CLA:HMC1	21:c:508:CLA:H101	1.93	0.49
25:1:317:BCR:HC7	4:B:208:LEU:HD13	1.93	0.49
28:B:627:LMG:H112	17:D:31:TRP:CD1	2.48	0.49
10:l:27:VAL:HG11	27:l:101:LHG:H201	1.95	0.49
1:1:52:ASP:OD1	22:1:311:DD6:O2	2.31	0.49
1:7:120:LEU:HD13	1:7:124:GLN:NE2	2.27	0.49
3:A:279:PRO:HG2	17:D:211:ALA:HB2	1.94	0.49
2:J:114:ALA:O	2:J:117:GLU:OE1	2.31	0.49
18:c:187:LYS:HB3	18:c:195:TRP:HA	1.94	0.49
4:B:73:ASP:HB3	4:B:85:VAL:HG21	1.92	0.49
27:B:601:LHG:H321	11:m:45:PRO:HB3	1.95	0.49
3:a:162:PRO:HB3	3:a:168:PHE:HA	1.94	0.49
16:2:84:LEU:HG	21:2:305:CLA:HBC2	1.94	0.49
1:5:175:LEU:O	1:5:179:SER:OG	2.27	0.49
21:b:613:CLA:H101	21:b:614:CLA:HAB	1.95	0.49
1:5:69:ARG:HH21	1:5:72:GLU:HG2	1.78	0.49
16:2:199:ARG:HA	16:2:202:MET:HE3	1.94	0.49
17:d:20:TRP:O	17:d:25:ARG:NH1	2.40	0.49
4:B:175:THR:O	4:B:175:THR:OG1	2.30	0.49
2:J:102:VAL:HG12	2:J:103:LEU:HG	1.95	0.49
4:b:174:VAL:HG23	4:b:175:THR:HG23	1.93	0.49
16:2:71:MET:HG2	21:2:302:CLA:O2D	2.13	0.49
16:2:71:MET:CE	24:2:315:KC1:CAA	2.91	0.49
21:b:609:CLA:H12	21:b:610:CLA:H71	1.94	0.48
2:6:62:ILE:HA	2:6:68:PRO:HA	1.94	0.48
4:b:388:SER:HB2	4:b:391:SER:HB2	1.95	0.48
1:g:104:PHE:CD1	1:g:104:PHE:N	2.81	0.48
21:7:301:CLA:H2	21:7:301:CLA:HMA1	1.95	0.48
28:8:317:LMG:H391	28:8:317:LMG:H132	1.96	0.48
1:5:66:ALA:O	1:5:70:THR:OG1	2.29	0.48
21:5:307:CLA:H41	21:5:307:CLA:H61	1.62	0.48
3:a:85:SER:HA	3:a:109:GLY:HA3	1.96	0.48
2:6:10:ILE:HG22	2:6:123:LEU:HD21	1.96	0.48
1:7:111:VAL:HG23	1:7:182:LEU:HD22	1.95	0.48
21:2:301:CLA:H61	21:2:301:CLA:H41	1.50	0.48
18:c:63:HIS:O	18:c:66:THR:OG1	2.30	0.48
1:1:159:GLN:HG3	21:1:305:CLA:HED2	1.95	0.48
3:A:85:SER:HA	3:A:109:GLY:HA3	1.96	0.48
3:A:136:ARG:NH2	8:I:27:ASP:OD1	2.41	0.48
16:8:115:ILE:HD11	16:8:209:TYR:HE1	1.79	0.48
17:D:154:THR:HA	17:D:158:VAL:HB	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:C:335:ALA:HB3	18:C:338:VAL:HG23	1.96	0.48
18:c:135:ILE:HD13	21:c:513:CLA:HAB	1.96	0.48
1:1:63:GLU:OE2	1:1:63:GLU:HA	2.14	0.47
2:6:118:LEU:HG	2:6:122:LYS:HE2	1.96	0.47
18:C:10:GLY:HA3	21:C:513:CLA:HMD2	1.95	0.47
21:c:509:CLA:HBC3	21:c:511:CLA:H71	1.95	0.47
2:6:51:TYR:HE1	2:6:158:LEU:HD23	1.79	0.47
2:6:100:TRP:CZ3	1:5:67:GLN:OE1	2.67	0.47
3:A:89:ILE:HD11	3:A:108:ASN:HB3	1.95	0.47
26:A:403:PHO:H141	21:D:404:CLA:HBB1	1.96	0.47
4:B:316:GLY:O	4:B:330:MET:HE2	2.13	0.47
20:4:111:PRO:HB2	20:4:113:LEU:HG	1.96	0.47
16:2:71:MET:SD	24:2:315:KC1:CAA	3.02	0.47
16:2:144:ASP:HB3	16:2:147:LYS:HB2	1.96	0.47
3:a:279:PRO:HG2	17:d:211:ALA:HB2	1.96	0.47
18:C:174:PRO:HB3	18:C:206:VAL:HG13	1.97	0.47
21:9:300:CLA:H71	21:9:303:CLA:HBC1	1.95	0.47
1:g:147:LYS:HE3	1:g:147:LYS:HB3	1.59	0.47
21:g:306:CLA:H41	21:g:306:CLA:H61	1.59	0.47
1:1:69:ARG:NH2	21:1:301:CLA:O1D	2.47	0.47
4:B:154:GLY:O	4:B:159:THR:OG1	2.31	0.47
3:a:221:SER:HB3	17:d:137:ILE:HD12	1.96	0.47
3:a:283:ILE:HA	3:a:286:THR:HG22	1.95	0.47
18:c:193:ASP:OD1	18:c:193:ASP:N	2.47	0.47
2:6:121:ARG:NH1	21:6:301:CLA:H2	2.30	0.47
1:1:56:LEU:HD13	21:1:301:CLA:H42	1.95	0.47
3:A:34:GLY:HA2	3:A:37:MET:HB3	1.97	0.47
3:A:310:GLN:HE21	3:A:312:ARG:CG	2.27	0.47
21:B:608:CLA:H12	21:B:609:CLA:H71	1.97	0.47
5:E:58:ASP:OD1	5:E:58:ASP:N	2.44	0.47
21:b:606:CLA:HAB	21:b:612:CLA:H192	1.97	0.47
17:D:300:GLN:NE2	17:D:312:THR:OG1	2.48	0.47
17:d:278:MET:HG3	26:d:403:PHO:HBC3	1.95	0.47
21:c:508:CLA:H91	21:c:508:CLA:H111	1.79	0.47
21:B:605:CLA:HAB	21:B:611:CLA:H192	1.97	0.47
3:a:266:ASN:OD1	3:a:266:ASN:N	2.48	0.47
4:b:457:ASN:HD21	17:d:283:LEU:HA	1.79	0.47
21:b:617:CLA:H41	21:b:617:CLA:H61	1.67	0.47
10:l:35:TYR:OH	17:d:192:LEU:O	2.26	0.47
1:g:179:SER:HB2	21:g:308:CLA:HMD3	1.97	0.47
10:L:12:GLU:OE2	11:m:66:ARG:NH2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:c:134:GLY:HA3	18:c:224:ILE:HG13	1.97	0.47
27:a:401:LHG:HC5	18:c:415:TRP:HH2	1.79	0.47
17:D:78:SER:HA	17:D:171:SER:HB3	1.97	0.47
18:C:445:ASP:OD1	18:C:445:ASP:N	2.48	0.47
2:6:29:THR:HG23	2:6:33:TYR:HE1	1.79	0.46
2:J:121:ARG:NH1	21:J:301:CLA:H2	2.30	0.46
4:B:358:ARG:NH1	36:B:704:HOH:O	2.48	0.46
4:b:57:ARG:NH2	4:b:335:GLY:O	2.48	0.46
4:b:155:ALA:O	4:b:159:THR:OG1	2.32	0.46
21:b:606:CLA:H141	28:8:317:LMG:H201	1.97	0.46
16:8:100:SER:OG	24:8:313:KC1:O2A	2.30	0.46
18:C:140:LEU:HD12	21:C:503:CLA:CMC	2.44	0.46
18:c:292:ARG:HA	18:c:295:ARG:NH2	2.30	0.46
19:3:189:HIS:O	19:3:193:THR:OG1	2.33	0.46
21:4:302:CLA:H3A	21:4:302:CLA:HBA2	1.61	0.46
21:g:303:CLA:HED3	21:g:306:CLA:H2	1.97	0.46
1:1:190:LEU:O	1:1:192:THR:N	2.48	0.46
21:d:406:CLA:H41	21:d:406:CLA:H62	1.61	0.46
19:9:177:ARG:NH2	21:9:300:CLA:O1D	2.41	0.46
21:6:301:CLA:H62	21:6:301:CLA:H41	1.82	0.46
5:E:29:LEU:HD11	6:F:25:VAL:HG13	1.96	0.46
7:H:2:ALA:HA	10:L:1:MET:HE2	1.97	0.46
26:a:404:PHO:H141	21:d:404:CLA:HBB1	1.96	0.46
4:b:231:MET:HE2	21:b:611:CLA:HMC1	1.96	0.46
16:8:66:ARG:NE	16:8:70:GLU:OE1	2.47	0.46
18:c:56:GLN:HA	30:c:517:DGD:HE61	1.98	0.46
1:g:162:GLN:OE1	24:g:315:KC1:C4B	2.63	0.46
1:1:98:ILE:HD13	1:1:117:ILE:HD12	1.96	0.46
1:1:149:ASP:HB3	1:1:152:GLU:HB3	1.98	0.46
2:6:124:GLN:HA	2:6:127:GLN:HB3	1.96	0.46
21:B:606:CLA:H162	21:B:609:CLA:HBB2	1.98	0.46
25:b:618:BCR:HC8	21:b:623:CLA:HMC3	1.97	0.46
21:8:302:CLA:H62	21:8:302:CLA:H41	1.64	0.46
18:c:292:ARG:HD2	18:c:295:ARG:HH22	1.79	0.46
1:1:191:ASP:N	1:1:191:ASP:OD1	2.48	0.46
21:7:304:CLA:H111	21:7:304:CLA:H152	1.78	0.46
2:J:100:TRP:CZ3	1:g:67:GLN:OE1	2.69	0.46
15:X:10:SER:O	15:X:14:LEU:HB2	2.15	0.46
5:e:58:ASP:OD1	5:e:58:ASP:N	2.48	0.46
5:e:59:ARG:HG2	5:e:61:GLN:NE2	2.30	0.46
16:2:40:TYR:CZ	16:2:47:PRO:HA	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:8:71:MET:HG3	21:8:303:CLA:OBD	2.15	0.46
21:C:508:CLA:HBB2	21:C:509:CLA:H52	1.98	0.46
18:c:32:MET:HE3	21:c:511:CLA:HHC	1.97	0.46
18:c:60:LEU:HD22	21:c:504:CLA:CED	2.42	0.46
19:9:193:THR:OG1	19:9:195:ASN:O	2.31	0.46
2:6:112:ASP:OD1	2:6:112:ASP:N	2.40	0.46
3:A:162:PRO:HB3	3:A:168:PHE:HA	1.97	0.46
4:B:315:ILE:HG22	4:B:426:LEU:HB3	1.98	0.46
14:w:30:GLN:O	14:w:33:SER:OG	2.34	0.46
18:c:445:ASP:OD1	18:c:445:ASP:N	2.48	0.46
25:M:101:BCR:H372	28:M:102:LMG:H332	1.98	0.46
20:4:125:GLU:HA	21:4:302:CLA:HED3	1.98	0.46
20:G:55:GLU:HG2	20:G:56:ILE:HG13	1.97	0.46
21:B:611:CLA:H112	21:B:611:CLA:H72	1.76	0.46
3:a:89:ILE:HD11	3:a:108:ASN:HB3	1.98	0.46
21:b:607:CLA:H162	21:b:610:CLA:HBB2	1.98	0.46
9:k:28:LEU:HD22	9:k:28:LEU:H	1.80	0.46
16:2:18:ARG:HB2	16:2:18:ARG:HH11	1.81	0.46
18:C:223:HIS:HE1	21:C:508:CLA:NA	2.14	0.46
1:5:74:LYS:HE3	1:5:74:LYS:HB2	1.70	0.45
21:1:304:CLA:H41	21:1:304:CLA:H61	1.72	0.45
28:L:101:LMG:H132	11:m:48:PHE:HD1	1.80	0.45
16:2:48:PRO:HG3	21:2:303:CLA:C1B	2.46	0.45
2:6:145:GLN:HE21	2:6:145:GLN:HA	1.82	0.45
3:A:201:GLY:HA3	3:A:286:THR:HB	1.98	0.45
4:B:57:ARG:NH2	4:B:335:GLY:O	2.49	0.45
4:b:316:GLY:O	4:b:330:MET:HE2	2.16	0.45
9:k:15:ILE:HD11	9:k:19:MET:HE3	1.98	0.45
18:C:56:GLN:HA	30:C:518:DGD:HE61	1.98	0.45
1:5:172:LEU:HD21	21:5:303:CLA:HBB2	1.97	0.45
2:J:107:ASP:N	2:J:107:ASP:OD1	2.49	0.45
2:J:127:GLN:HE21	21:J:307:CLA:C2D	2.29	0.45
3:a:260:PHE:CE1	3:a:263:ALA:HB2	2.51	0.45
30:b:601:DGD:HB62	21:b:608:CLA:H192	1.98	0.45
28:b:620:LMG:O5	28:b:620:LMG:O4	2.27	0.45
35:d:408:PL9:H401	27:d:409:LHG:H212	1.98	0.45
21:5:308:CLA:HBA1	21:5:308:CLA:H3A	1.67	0.45
1:1:72:GLU:OE2	21:1:301:CLA:NB	2.49	0.45
21:6:302:CLA:HAB	21:6:307:CLA:H71	1.98	0.45
7:H:61:ASP:OD1	30:H:101:DGD:O4E	2.34	0.45
3:a:201:GLY:HA3	3:a:286:THR:HB	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:477:ASP:OD1	4:b:477:ASP:N	2.49	0.45
16:8:42:GLU:OE2	16:8:65:TYR:OH	2.31	0.45
21:D:407:CLA:H41	21:D:407:CLA:H62	1.64	0.45
18:C:159:ASP:OD2	18:C:169:ARG:NH2	2.49	0.45
18:C:363:ARG:NH1	36:C:601:HOH:O	2.39	0.45
21:4:301:CLA:H12	21:4:301:CLA:H2A	1.99	0.45
21:5:303:CLA:H52	21:5:303:CLA:H12	1.69	0.45
1:1:184:THR:HB	1:1:187:PHE:HB2	1.98	0.45
21:7:303:CLA:H3A	21:7:303:CLA:HBA2	1.66	0.45
21:B:606:CLA:HMC3	21:B:615:CLA:H43	1.98	0.45
21:B:607:CLA:H192	30:B:624:DGD:HB81	1.97	0.45
4:b:220:ARG:HG3	7:h:20:LYS:HD3	1.98	0.45
21:D:404:CLA:H52	35:D:409:PL9:H151	1.99	0.45
21:C:506:CLA:H41	21:C:506:CLA:H61	1.62	0.45
4:b:63:MET:HA	4:b:66:MET:HE3	1.97	0.45
7:h:64:THR:HG22	7:h:65:VAL:HG23	1.97	0.45
14:w:17:LEU:O	14:w:21:THR:HG22	2.16	0.45
20:4:74:ASN:OD1	20:4:74:ASN:N	2.49	0.45
31:B:625:SQD:H241	3:a:30:ILE:HD11	1.99	0.45
3:a:57:PRO:HB2	3:a:66:PRO:HB2	1.98	0.45
18:C:39:MET:HE2	18:C:39:MET:HA	1.97	0.45
21:4:300:CLA:H3A	21:4:300:CLA:HBA2	1.75	0.45
21:g:306:CLA:H91	21:g:306:CLA:H111	1.79	0.45
1:7:129:ILE:HD11	21:7:302:CLA:C2C	2.47	0.45
2:J:79:ILE:O	1:g:119:SER:OG	2.27	0.45
14:W:30:GLN:O	14:W:33:SER:OG	2.35	0.45
3:a:286:THR:OG1	21:a:402:CLA:O1D	2.34	0.45
4:b:141:ILE:HG13	4:b:217:LEU:HD21	1.99	0.45
21:b:607:CLA:HMC3	21:b:616:CLA:H43	1.99	0.45
18:C:106:LEU:HD11	21:C:513:CLA:H12	1.98	0.45
21:c:502:CLA:H18	21:c:508:CLA:H121	1.98	0.45
2:J:141:ARG:O	2:J:145:GLN:OE1	2.34	0.45
3:a:331:MET:HE2	17:d:319:LEU:HB3	1.99	0.45
16:2:217:ASN:HB3	16:2:220:TYR:HB2	1.98	0.45
18:C:196:ILE:HG23	25:C:516:BCR:H393	1.99	0.45
25:C:516:BCR:H20C	25:C:516:BCR:H361	1.78	0.45
18:c:106:LEU:HD11	21:c:512:CLA:H92	1.99	0.45
30:c:516:DGD:HBE2	30:c:516:DGD:HB81	1.78	0.45
19:9:189:HIS:O	19:9:193:THR:OG1	2.35	0.45
1:5:129:ILE:HG12	29:5:316:LMU:H2B	1.98	0.45
4:B:297:SER:HB3	4:B:300:GLN:HG3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:617:BCR:H15C	25:B:617:BCR:H351	1.80	0.44
25:a:406:BCR:H20C	25:a:406:BCR:H361	1.84	0.44
21:b:617:CLA:H192	21:b:617:CLA:H161	1.79	0.44
18:C:283:GLN:OE1	18:C:327:THR:HG22	2.17	0.44
21:C:504:CLA:H42	21:C:511:CLA:H41	1.99	0.44
3:A:160:ILE:HD12	18:C:403:PHE:HZ	1.82	0.44
10:L:35:TYR:OH	17:D:192:LEU:O	2.28	0.44
4:b:419:LYS:HE2	4:b:419:LYS:HB3	1.74	0.44
14:w:13:LEU:HD13	14:w:13:LEU:HA	1.84	0.44
17:D:292:LEU:HD23	17:D:292:LEU:HA	1.86	0.44
18:C:20:LYS:HB3	21:C:513:CLA:HMA1	1.99	0.44
21:g:302:CLA:HHC	21:g:302:CLA:HAB	1.78	0.44
21:6:307:CLA:H91	21:6:307:CLA:H111	1.82	0.44
3:A:188:ALA:HB2	3:A:328:MET:HE3	1.99	0.44
3:A:221:SER:HB3	17:D:137:ILE:HD12	1.98	0.44
2:J:36:ALA:O	2:J:40:HIS:ND1	2.43	0.44
3:a:131:TRP:CH2	21:c:506:CLA:HAA2	2.52	0.44
16:2:78:MET:HE1	21:2:302:CLA:HAC2	1.99	0.44
17:D:181:LEU:HA	21:D:406:CLA:HMD1	1.99	0.44
18:c:250:ALA:O	18:c:254:MET:HG3	2.18	0.44
1:7:40:ASN:HB3	16:8:9:LYS:HG3	2.00	0.44
3:A:127:ILE:HG23	3:A:144:CYS:HB2	1.99	0.44
2:J:130:ARG:NH2	21:J:300:CLA:O1D	2.36	0.44
18:C:28:HIS:O	18:C:32:MET:HG3	2.17	0.44
18:C:120:GLY:O	18:C:128:LYS:NZ	2.48	0.44
19:3:139:ALA:O	19:3:143:ILE:HD12	2.18	0.44
20:G:84:ALA:HA	20:G:87:TRP:HD1	1.82	0.44
3:A:95:PRO:HA	21:A:404:CLA:HED2	2.00	0.44
3:A:184:LEU:HD21	17:D:185:GLN:HG2	2.00	0.44
25:B:617:BCR:H20C	25:B:617:BCR:H361	1.80	0.44
31:b:602:SQD:H332	21:b:615:CLA:H51	1.99	0.44
17:d:160:PRO:HB3	17:d:169:ALA:HB2	2.00	0.44
21:c:510:CLA:HAB	21:c:510:CLA:HHC	1.80	0.44
20:4:126:LEU:HD11	20:4:130:ARG:HE	1.83	0.44
1:5:75:HIS:HB3	1:5:168:MET:SD	2.57	0.44
21:B:616:CLA:HBC3	7:H:11:LEU:HD13	1.99	0.44
29:g:301:LMU:H22	21:g:303:CLA:HED1	2.00	0.44
21:B:607:CLA:H193	21:B:607:CLA:H162	1.78	0.44
21:b:617:CLA:H141	21:b:617:CLA:H162	1.83	0.44
5:e:31:VAL:HG13	5:e:35:LEU:HD23	2.00	0.44
21:3:300:CLA:HED2	21:3:300:CLA:HAA1	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:107:ASP:OD1	2:6:107:ASP:N	2.50	0.44
1:7:154:GLU:OE2	1:7:154:GLU:C	2.61	0.44
25:B:617:BCR:H333	28:B:619:LMG:H381	1.99	0.44
21:J:307:CLA:HBA1	21:J:307:CLA:H3A	1.61	0.44
21:b:611:CLA:H203	21:b:611:CLA:H161	1.84	0.44
17:D:59:THR:HG22	17:D:81:ALA:HB2	1.99	0.44
18:c:171:VAL:HG11	18:c:206:VAL:HG11	1.99	0.44
21:c:505:CLA:H41	21:c:505:CLA:H61	1.56	0.44
21:4:300:CLA:H143	21:4:300:CLA:H112	1.86	0.44
25:1:317:BCR:H20C	25:1:317:BCR:H361	1.86	0.44
21:B:616:CLA:H12	21:B:616:CLA:H51	1.87	0.44
16:2:74:LYS:O	16:2:78:MET:HG3	2.17	0.44
21:C:504:CLA:H41	21:C:514:CLA:H11	2.00	0.44
21:7:309:CLA:HAA1	21:g:308:CLA:H11	2.00	0.43
4:B:113:TRP:HA	25:B:618:BCR:H382	2.00	0.43
25:h:101:BCR:H20C	25:h:101:BCR:H361	1.82	0.43
17:D:160:PRO:HB3	17:D:169:ALA:HB2	1.99	0.43
27:D:410:LHG:H132	27:D:410:LHG:H272	2.00	0.43
18:C:241:GLU:HG2	18:C:420:ALA:HB2	2.00	0.43
18:c:347:LEU:HB3	18:c:352:ILE:HD11	2.00	0.43
2:6:85:LEU:HB2	1:5:114:ILE:HG21	2.00	0.43
2:J:136:VAL:O	2:J:140:LEU:CD2	2.66	0.43
5:e:29:LEU:HD23	5:e:29:LEU:HA	1.89	0.43
17:d:181:LEU:HA	21:d:405:CLA:HMD1	1.99	0.43
18:c:85:VAL:HA	18:c:88:VAL:HG12	1.99	0.43
3:A:131:TRP:CH2	21:C:507:CLA:HAA2	2.52	0.43
3:A:308:ASP:OD1	3:A:312:ARG:N	2.50	0.43
21:B:616:CLA:HHC	21:B:616:CLA:HAB	1.77	0.43
2:J:120:LYS:HE3	2:J:120:LYS:HB3	1.86	0.43
18:C:125:ASP:O	18:C:129:MET:HG2	2.17	0.43
1:g:193:LEU:HD13	1:g:193:LEU:HA	1.90	0.43
3:A:302:PHE:HE2	17:D:73:LEU:HD12	1.82	0.43
4:B:388:SER:HB2	4:B:391:SER:HB2	2.01	0.43
21:b:608:CLA:H141	21:b:608:CLA:H162	1.81	0.43
21:b:616:CLA:H152	21:b:616:CLA:H112	1.74	0.43
19:9:183:ILE:HD13	19:9:183:ILE:HA	1.88	0.43
21:g:304:CLA:H41	21:g:304:CLA:H61	1.83	0.43
21:G:304:CLA:H152	21:G:304:CLA:H111	1.81	0.43
3:A:156:ALA:HA	3:A:160:ILE:HB	2.01	0.43
25:M:101:BCR:H382	21:b:615:CLA:H92	2.01	0.43
18:C:5:PHE:O	18:C:13:ARG:NH1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:301:CLA:H91	21:1:301:CLA:H112	1.86	0.43
1:7:126:ILE:HG22	21:7:302:CLA:HAB	1.99	0.43
4:B:392:ILE:HG13	4:B:418:LYS:HG2	2.01	0.43
28:B:619:LMG:H332	21:B:621:CLA:H62	2.01	0.43
14:W:12:SER:O	14:W:12:SER:OG	2.34	0.43
3:a:183:MET:HB3	21:a:402:CLA:HBC2	2.00	0.43
4:b:281:GLN:O	4:b:285:GLU:HG2	2.18	0.43
21:2:301:CLA:CHA	21:2:301:CLA:HBA1	2.49	0.43
18:c:174:PRO:HB3	18:c:206:VAL:HG13	2.00	0.43
18:c:187:LYS:HG2	18:c:193:ASP:HB3	1.99	0.43
18:c:292:ARG:HD3	18:c:295:ARG:NH2	2.34	0.43
1:5:61:ASP:OD1	1:5:61:ASP:C	2.61	0.43
4:b:334:ASP:OD1	4:b:334:ASP:N	2.49	0.43
19:9:139:ALA:O	19:9:143:ILE:HD12	2.19	0.43
1:5:40:ASN:OD1	1:5:40:ASN:N	2.44	0.43
1:5:47:PRO:HD3	24:5:315:KC1:C2D	2.48	0.43
1:1:74:LYS:HE2	21:1:303:CLA:O1D	2.19	0.43
21:A:404:CLA:H3A	28:A:407:LMG:H302	2.01	0.43
31:b:602:SQD:H242	31:b:602:SQD:H271	1.90	0.43
21:b:604:CLA:H141	21:b:604:CLA:H162	1.75	0.43
19:3:80:LYS:HZ1	21:3:302:CLA:C4D	2.31	0.43
2:6:61:GLY:HA2	16:2:103:LEU:HD21	2.00	0.43
3:A:132:GLU:O	3:A:136:ARG:HG2	2.19	0.43
4:B:137:LYS:HD2	4:B:217:LEU:HD23	2.00	0.43
21:B:603:CLA:H171	30:H:101:DGD:HBT1	2.01	0.43
4:b:175:THR:O	4:b:175:THR:OG1	2.29	0.43
16:2:172:ASP:OD1	16:2:174:SER:OG	2.29	0.43
16:8:144:ASP:HB3	16:8:147:LYS:HB2	2.01	0.43
17:D:278:MET:HE1	21:D:406:CLA:H42	2.01	0.43
25:d:407:BCR:H24C	25:d:407:BCR:H371	1.84	0.43
21:c:511:CLA:HED3	21:c:511:CLA:H2	2.01	0.43
21:3:304:CLA:H41	21:3:304:CLA:H62	1.70	0.43
20:G:34:ARG:HH22	20:G:126:LEU:HD13	1.83	0.43
1:1:98:ILE:CD1	1:1:117:ILE:CG1	2.96	0.43
2:6:36:ALA:O	2:6:40:HIS:ND1	2.46	0.43
3:A:265:PHE:HB3	3:A:271:LEU:HB2	2.01	0.43
28:B:627:LMG:H321	28:B:627:LMG:H292	1.76	0.43
4:b:370:LEU:HB2	4:b:379:ALA:HB3	2.01	0.43
2:J:39:LYS:NZ	24:J:311:KC1:O1D	2.52	0.42
21:J:303:CLA:H3A	21:J:303:CLA:HBA2	1.67	0.42
14:W:37:ASP:O	18:C:233:ARG:NH2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:184:LEU:HD21	17:d:185:GLN:HG2	2.01	0.42
3:a:302:PHE:HE2	17:d:73:LEU:HD12	1.83	0.42
4:b:166:ILE:HG21	21:b:605:CLA:HED1	2.00	0.42
4:b:329:PRO:HD2	4:b:332:LYS:HB2	2.01	0.42
21:b:617:CLA:HBC3	7:h:11:LEU:HD13	2.00	0.42
17:d:128:GLN:NE2	26:d:403:PHO:OBD	2.52	0.42
18:c:228:PRO:HA	21:c:507:CLA:HED3	2.01	0.42
1:5:42:LEU:HD23	1:5:158:VAL:HG23	2.00	0.42
21:5:306:CLA:H62	21:5:306:CLA:H41	1.63	0.42
1:7:132:VAL:HG11	21:7:305:CLA:HHB	2.00	0.42
4:b:315:ILE:HG22	4:b:426:LEU:HB3	2.01	0.42
21:b:606:CLA:HMB1	21:b:623:CLA:HHC	2.01	0.42
21:b:623:CLA:H102	21:b:623:CLA:H62	1.83	0.42
25:D:408:BCR:H20C	25:D:408:BCR:H361	1.83	0.42
21:3:301:CLA:H61	21:3:301:CLA:H41	1.65	0.42
1:7:52:ASP:OD1	22:7:310:DD6:O2	2.37	0.42
21:B:616:CLA:H192	21:B:616:CLA:H161	1.79	0.42
21:3:301:CLA:H52	21:3:304:CLA:HAB	2.00	0.42
20:4:107:GLU:H	20:4:107:GLU:HG3	1.61	0.42
29:5:301:LMU:H22	21:5:303:CLA:HED1	2.01	0.42
2:6:130:ARG:NH2	21:6:300:CLA:O1D	2.33	0.42
13:T:14:LEU:HD13	31:C:502:SQD:H382	2.01	0.42
28:2:318:LMG:H391	28:2:318:LMG:H132	2.01	0.42
16:8:74:LYS:HB2	16:8:74:LYS:HE3	1.78	0.42
21:D:407:CLA:H92	21:D:407:CLA:H61	1.91	0.42
20:G:34:ARG:HA	20:G:34:ARG:HD2	1.89	0.42
1:1:120:LEU:HD13	20:4:79:ILE:HD13	2.00	0.42
21:A:404:CLA:H112	21:A:404:CLA:H72	1.70	0.42
21:a:405:CLA:H72	21:a:405:CLA:H112	1.80	0.42
21:b:616:CLA:H71	28:8:317:LMG:H202	2.00	0.42
16:8:48:PRO:HG3	21:8:304:CLA:C2B	2.50	0.42
21:C:510:CLA:H62	21:C:510:CLA:H41	1.78	0.42
20:4:54:PRO:HB3	21:4:300:CLA:HED1	2.02	0.42
21:6:307:CLA:H3A	21:6:307:CLA:HBA1	1.71	0.42
6:F:13:PHE:HD1	6:F:15:PHE:H	1.65	0.42
3:a:188:ALA:HB2	3:a:328:MET:HE3	2.02	0.42
7:h:57:ASN:HD21	25:h:101:BCR:H292	1.84	0.42
17:D:249:ASN:O	17:D:253:SER:OG	2.33	0.42
17:d:59:THR:HG22	17:d:81:ALA:HB2	2.02	0.42
20:G:73:PRO:O	20:G:74:ASN:ND2	2.52	0.42
1:1:80:GLN:OE1	21:1:304:CLA:HAB	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:109:GLY:C	2:J:110:LYS:HD3	2.45	0.42
25:a:406:BCR:H24C	25:a:406:BCR:H371	1.80	0.42
28:b:626:LMG:O5	28:b:626:LMG:O4	2.35	0.42
21:C:511:CLA:HHC	21:C:511:CLA:HAB	1.79	0.42
18:c:199:VAL:HG21	25:c:515:BCR:H291	2.00	0.42
21:c:511:CLA:H102	21:c:511:CLA:H61	1.78	0.42
21:5:308:CLA:H92	21:5:308:CLA:H62	1.83	0.42
1:g:142:ASP:HB3	1:g:143:ILE:H	1.71	0.42
27:B:601:LHG:H172	10:L:24:LEU:HB2	2.02	0.42
17:d:22:LYS:HD2	17:d:134:LEU:HD12	2.02	0.42
18:c:50:GLU:H	18:c:50:GLU:HG3	1.67	0.42
18:c:292:ARG:CD	18:c:295:ARG:NH2	2.83	0.42
21:c:509:CLA:HHC	21:c:509:CLA:HAB	1.76	0.42
19:9:76:GLU:HG3	19:9:151:GLN:HE22	1.84	0.42
1:5:195:THR:N	23:5:311:A86:O2	2.52	0.42
27:A:406:LHG:H322	27:A:406:LHG:H291	1.93	0.42
21:J:306:CLA:H141	21:J:306:CLA:H161	1.85	0.42
13:T:17:ILE:HD11	27:D:410:LHG:H182	2.02	0.42
14:W:22:ALA:O	14:W:26:LEU:HG	2.20	0.42
3:a:127:ILE:HG23	3:a:144:CYS:HB2	2.01	0.42
4:b:440:ASP:OD1	4:b:440:ASP:N	2.50	0.42
21:b:623:CLA:H62	21:b:623:CLA:H41	1.84	0.42
17:d:209:LEU:HD23	17:d:209:LEU:HA	1.94	0.42
17:d:292:LEU:HD23	17:d:292:LEU:HA	1.85	0.42
21:9:301:CLA:H62	21:9:301:CLA:H41	1.63	0.42
21:1:308:CLA:H41	21:1:308:CLA:H61	1.64	0.42
21:7:302:CLA:H13	20:G:88:PHE:HB3	2.02	0.42
25:A:405:BCR:H371	25:A:405:BCR:H24C	1.81	0.42
21:a:402:CLA:HAB	21:a:402:CLA:HHC	1.88	0.42
4:b:331:ASN:HB3	4:b:336:ILE:HG12	2.02	0.42
21:d:405:CLA:H62	21:d:405:CLA:H41	1.85	0.42
18:c:14:LEU:HD21	21:c:512:CLA:H2A	2.02	0.42
19:9:86:MET:O	19:9:89:THR:OG1	2.28	0.42
19:9:149:PHE:HD1	19:9:149:PHE:HA	1.75	0.42
1:5:104:PHE:HE1	21:5:304:CLA:HAA1	1.85	0.42
4:B:99:THR:HG22	21:B:607:CLA:H151	2.02	0.41
5:E:59:ARG:HG3	5:E:61:GLN:HE21	1.85	0.41
7:H:10:ILE:HG12	16:2:47:PRO:HB3	2.02	0.41
3:a:196:PRO:HA	3:a:199:MET:SD	2.60	0.41
4:b:33:TRP:CD1	21:b:623:CLA:HBC2	2.55	0.41
21:b:607:CLA:HBC2	21:b:613:CLA:H111	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:189:TRP:CD2	21:2:303:CLA:HED1	2.55	0.41
17:d:188:HIS:CD2	17:d:293:ARG:HE	2.38	0.41
18:c:29:ALA:O	18:c:33:VAL:HG23	2.19	0.41
21:G:300:CLA:HBA2	21:G:300:CLA:H3A	1.89	0.41
4:B:174:VAL:HG23	4:B:175:THR:HG23	2.02	0.41
21:J:306:CLA:H2A	21:J:306:CLA:HED2	2.02	0.41
3:a:132:GLU:O	3:a:136:ARG:HG2	2.20	0.41
18:C:217:VAL:O	18:C:221:ILE:HG12	2.20	0.41
21:C:514:CLA:H203	21:C:514:CLA:H161	1.89	0.41
18:c:292:ARG:CD	18:c:295:ARG:HH22	2.33	0.41
19:9:72:ARG:HD2	19:9:72:ARG:HA	1.79	0.41
1:5:95:PRO:CD	1:5:95:PRO:C	2.86	0.41
3:A:157:VAL:HG21	21:D:404:CLA:HMC2	2.02	0.41
4:B:166:ILE:HG21	21:B:604:CLA:HED1	2.02	0.41
4:B:392:ILE:HG23	4:B:397:VAL:HG22	2.02	0.41
3:a:82:VAL:HB	3:a:174:LEU:HB2	2.02	0.41
4:b:42:LEU:HD11	4:b:93:PHE:HB3	2.00	0.41
18:C:199:VAL:HG21	25:C:516:BCR:H291	2.02	0.41
21:c:503:CLA:H2	21:c:504:CLA:H203	2.02	0.41
19:3:183:ILE:HD13	19:3:183:ILE:HA	1.86	0.41
3:A:82:VAL:HB	3:A:174:LEU:HB2	2.01	0.41
21:A:404:CLA:H51	21:A:404:CLA:H8	1.96	0.41
4:B:75:TRP:HB3	30:B:624:DGD:HG31	2.02	0.41
21:B:605:CLA:H93	21:B:605:CLA:H61	1.80	0.41
21:B:606:CLA:HBC2	21:B:612:CLA:H111	2.02	0.41
30:H:101:DGD:HB91	30:H:101:DGD:HB62	1.78	0.41
3:a:156:ALA:HA	3:a:160:ILE:HB	2.02	0.41
3:a:312:ARG:HE	3:a:312:ARG:HB3	1.73	0.41
4:b:423:LYS:HD2	4:b:429:VAL:HG13	2.03	0.41
17:D:133:ARG:HG2	29:D:412:LMU:H3'	2.02	0.41
18:c:150:LYS:HA	18:c:150:LYS:HD2	1.86	0.41
18:c:271:SER:O	18:c:367:TYR:OH	2.21	0.41
19:9:73:ARG:HD2	21:9:302:CLA:HED1	2.03	0.41
21:9:301:CLA:H93	21:9:301:CLA:H61	1.88	0.41
20:4:49:ILE:O	20:4:53:VAL:HG23	2.20	0.41
21:1:302:CLA:H111	21:1:302:CLA:H91	1.86	0.41
7:H:20:LYS:HE2	16:2:22:GLU:HB2	2.03	0.41
13:T:21:ILE:HD11	27:D:410:LHG:H312	2.02	0.41
4:b:116:VAL:HG22	31:b:602:SQD:H3	2.03	0.41
18:c:129:MET:CE	18:c:243:TYR:CE2	3.03	0.41
1:5:103:ALA:HB3	1:5:106:ASP:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:111:VAL:N	1:1:178:ASP:OD2	2.45	0.41
4:B:157:HIS:HE1	21:B:607:CLA:NA	2.19	0.41
21:B:612:CLA:HAB	21:B:612:CLA:HHC	1.78	0.41
4:b:99:THR:HG22	21:b:608:CLA:H151	2.02	0.41
11:m:52:LEU:HD23	11:m:52:LEU:HA	1.86	0.41
17:D:128:GLN:NE2	26:D:401:PHO:OBD	2.53	0.41
18:c:428:GLU:CG	18:c:429:LYS:HZ2	2.32	0.41
21:G:304:CLA:H61	21:G:304:CLA:H102	1.74	0.41
2:6:57:TYR:OH	16:2:123:VAL:HG21	2.20	0.41
25:a:406:BCR:H15C	25:a:406:BCR:H351	1.90	0.41
4:b:367:PRO:HB3	17:d:344:VAL:HB	2.03	0.41
17:D:215:ALA:O	17:D:219:ASN:ND2	2.52	0.41
18:C:349:LEU:HD23	18:C:352:ILE:HD12	2.03	0.41
21:C:510:CLA:HHC	21:C:510:CLA:HAB	1.76	0.41
18:c:185:VAL:O	18:c:195:TRP:NE1	2.51	0.41
25:1:317:BCR:H21C	25:H:100:BCR:H292	2.02	0.41
21:B:605:CLA:HMB1	21:B:621:CLA:HHC	2.02	0.41
21:J:306:CLA:H61	21:J:306:CLA:H101	1.88	0.41
14:w:36:ASP:OD1	14:w:36:ASP:N	2.39	0.41
19:3:185:GLY:O	19:3:188:THR:OG1	2.35	0.41
21:3:301:CLA:H61	21:3:301:CLA:H93	1.85	0.41
1:5:111:VAL:HG23	1:5:182:LEU:HD13	2.02	0.41
1:1:135:TRP:HZ2	21:4:304:CLA:HED2	1.85	0.41
4:B:30:VAL:HG22	21:B:613:CLA:C3C	2.51	0.41
5:E:29:LEU:HD23	5:E:29:LEU:HA	1.88	0.41
7:H:56:GLU:OE1	7:H:56:GLU:N	2.54	0.41
25:H:100:BCR:H24C	25:H:100:BCR:H371	1.92	0.41
9:K:5:LEU:HD12	9:K:5:LEU:HA	1.97	0.41
12:N:15:ILE:HD11	16:2:222:LEU:HD21	2.03	0.41
3:a:41:LEU:HD23	3:a:41:LEU:HA	1.93	0.41
3:a:157:VAL:HG21	21:d:404:CLA:HMC2	2.02	0.41
4:b:22:VAL:HG11	21:b:615:CLA:HMA1	2.03	0.41
21:b:617:CLA:H152	21:b:617:CLA:H112	1.93	0.41
10:l:5:ASN:HD21	10:l:7:ASN:HD22	1.69	0.41
16:2:70:GLU:HG3	16:2:149:PRO:HB3	2.03	0.41
29:8:318:LMU:H82	29:8:318:LMU:H111	1.77	0.41
17:D:20:TRP:HD1	17:D:23:ARG:HH21	1.69	0.41
17:d:151:VAL:HG22	21:d:405:CLA:HED1	2.02	0.41
19:9:146:ASN:ND2	21:9:302:CLA:HHB	2.35	0.41
1:5:50:PHE:HE1	21:5:302:CLA:HED2	1.86	0.41
1:5:75:HIS:HE1	21:5:303:CLA:C4D	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:283:ILE:HA	3:A:283:ILE:HD13	1.95	0.41
4:b:30:VAL:HG22	21:b:614:CLA:C3C	2.51	0.41
16:8:180:GLU:HG2	16:8:187:LYS:HB3	2.03	0.41
18:C:29:ALA:O	18:C:33:VAL:HG23	2.21	0.41
18:c:157:LEU:HD12	18:c:202:LEU:HD21	2.03	0.41
18:c:314:MET:HE3	18:c:314:MET:HB2	1.87	0.41
18:c:402:HIS:CE1	21:c:503:CLA:NA	2.89	0.41
2:J:23:LYS:HE2	2:J:23:LYS:HB2	1.86	0.40
2:J:31:ALA:O	2:J:35:THR:HG23	2.21	0.40
21:b:617:CLA:HHC	21:b:617:CLA:HAB	1.78	0.40
17:d:300:GLN:HE21	17:d:300:GLN:HB2	1.61	0.40
18:c:196:ILE:HG13	18:c:261:PHE:HE2	1.85	0.40
25:c:515:BCR:H351	25:c:515:BCR:H15C	1.82	0.40
20:4:141:ARG:HH11	20:4:145:GLN:HB3	1.86	0.40
1:g:93:ARG:HD3	1:g:93:ARG:HA	1.89	0.40
1:1:150:PRO:O	1:1:154:GLU:HG3	2.21	0.40
26:A:403:PHO:HAB	17:D:204:LEU:HD13	2.04	0.40
4:B:58:GLN:O	4:B:60:MET:HE2	2.21	0.40
25:B:618:BCR:H11C	25:B:618:BCR:H341	1.88	0.40
8:i:3:THR:O	8:i:7:LEU:HG	2.21	0.40
17:d:50:GLY:HA3	17:d:77:VAL:HG22	2.02	0.40
21:3:304:CLA:H112	21:3:304:CLA:H71	1.91	0.40
2:6:51:TYR:CE1	2:6:158:LEU:HD23	2.56	0.40
21:7:304:CLA:H92	21:7:304:CLA:H62	1.89	0.40
11:M:80:ASP:HB3	13:t:28:ARG:HD2	2.03	0.40
25:b:619:BCR:H15C	25:b:619:BCR:H351	1.87	0.40
18:c:162:ALA:HB3	18:c:166:GLY:HA2	2.03	0.40
21:1:309:CLA:HMD2	21:2:306:CLA:HBC1	2.02	0.40
2:6:149:LYS:HE2	2:6:152:PHE:CG	2.57	0.40
21:7:301:CLA:H93	21:7:302:CLA:H52	2.02	0.40
3:A:194:MET:HE3	3:A:194:MET:HB3	1.95	0.40
3:A:310:GLN:NE2	3:A:312:ARG:HG3	2.34	0.40
3:A:317:TRP:CZ3	17:D:179:ARG:HD2	2.57	0.40
25:A:405:BCR:H15C	25:A:405:BCR:H351	1.90	0.40
14:W:36:ASP:OD1	14:W:36:ASP:N	2.41	0.40
9:k:28:LEU:HD22	9:k:28:LEU:N	2.36	0.40
19:3:86:MET:O	19:3:89:THR:OG1	2.34	0.40
1:5:61:ASP:OD1	1:5:63:GLU:N	2.54	0.40
1:g:140:ASP:OD1	1:g:140:ASP:N	2.54	0.40
2:6:100:TRP:HB2	2:6:102:VAL:HG23	2.04	0.40
21:b:604:CLA:H151	21:b:604:CLA:H112	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:31:VAL:O	5:e:35:LEU:CD2	2.70	0.40
16:2:46:LEU:HB2	16:2:47:PRO:HD2	2.03	0.40
21:8:302:CLA:H121	21:8:302:CLA:H162	1.99	0.40
18:C:194:GLY:H	18:C:198:SER:HB3	1.87	0.40
18:c:249:ALA:HB2	18:c:413:HIS:CG	2.56	0.40
1:5:147:LYS:HE3	1:5:147:LYS:HB3	1.83	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	1	162/166 (98%)	159 (98%)	2 (1%)	1 (1%)	22	22
1	5	152/166 (92%)	145 (95%)	7 (5%)	0	100	100
1	7	162/166 (98%)	160 (99%)	2 (1%)	0	100	100
1	g	152/166 (92%)	140 (92%)	12 (8%)	0	100	100
2	6	152/167 (91%)	147 (97%)	5 (3%)	0	100	100
2	J	152/167 (91%)	147 (97%)	5 (3%)	0	100	100
3	A	326/360 (91%)	316 (97%)	10 (3%)	0	100	100
3	a	327/360 (91%)	321 (98%)	6 (2%)	0	100	100
4	B	482/509 (95%)	476 (99%)	6 (1%)	0	100	100
4	b	482/509 (95%)	472 (98%)	10 (2%)	0	100	100
5	E	64/82 (78%)	64 (100%)	0	0	100	100
5	e	64/82 (78%)	64 (100%)	0	0	100	100
6	F	30/42 (71%)	29 (97%)	1 (3%)	0	100	100
6	f	30/42 (71%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	h	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
8	I	34/38 (90%)	34 (100%)	0	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	K	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
9	k	35/40 (88%)	35 (100%)	0	0	100	100
10	L	36/38 (95%)	36 (100%)	0	0	100	100
10	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	M	51/130 (39%)	51 (100%)	0	0	100	100
11	m	51/130 (39%)	51 (100%)	0	0	100	100
12	N	28/36 (78%)	28 (100%)	0	0	100	100
12	n	28/36 (78%)	28 (100%)	0	0	100	100
13	T	29/32 (91%)	29 (100%)	0	0	100	100
13	t	29/32 (91%)	29 (100%)	0	0	100	100
14	W	42/53 (79%)	41 (98%)	1 (2%)	0	100	100
14	w	42/53 (79%)	41 (98%)	1 (2%)	0	100	100
15	X	32/36 (89%)	32 (100%)	0	0	100	100
15	x	32/36 (89%)	32 (100%)	0	0	100	100
16	2	207/225 (92%)	203 (98%)	4 (2%)	0	100	100
16	8	208/225 (92%)	200 (96%)	8 (4%)	0	100	100
17	D	329/351 (94%)	321 (98%)	8 (2%)	0	100	100
17	d	323/351 (92%)	318 (98%)	5 (2%)	0	100	100
18	C	410/445 (92%)	400 (98%)	10 (2%)	0	100	100
18	c	410/445 (92%)	399 (97%)	11 (3%)	0	100	100
19	3	92/216 (43%)	89 (97%)	3 (3%)	0	100	100
19	9	92/216 (43%)	89 (97%)	3 (3%)	0	100	100
20	4	100/167 (60%)	97 (97%)	3 (3%)	0	100	100
20	G	100/167 (60%)	98 (98%)	2 (2%)	0	100	100
All	All	5706/6728 (85%)	5573 (98%)	132 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	191	ASP

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	1	134/135 (99%)	133 (99%)	1 (1%)	81	89
1	5	128/135 (95%)	127 (99%)	1 (1%)	79	87
1	7	133/135 (98%)	133 (100%)	0	100	100
1	g	128/135 (95%)	127 (99%)	1 (1%)	79	87
2	6	123/135 (91%)	121 (98%)	2 (2%)	58	71
2	J	123/135 (91%)	123 (100%)	0	100	100
3	A	263/287 (92%)	263 (100%)	0	100	100
3	a	264/287 (92%)	262 (99%)	2 (1%)	79	87
4	B	384/405 (95%)	384 (100%)	0	100	100
4	b	384/405 (95%)	384 (100%)	0	100	100
5	E	58/71 (82%)	58 (100%)	0	100	100
5	e	58/71 (82%)	57 (98%)	1 (2%)	56	69
6	F	28/37 (76%)	28 (100%)	0	100	100
6	f	28/37 (76%)	28 (100%)	0	100	100
7	H	55/56 (98%)	55 (100%)	0	100	100
7	h	55/56 (98%)	55 (100%)	0	100	100
8	I	35/37 (95%)	35 (100%)	0	100	100
8	i	35/37 (95%)	35 (100%)	0	100	100
9	K	31/34 (91%)	31 (100%)	0	100	100
9	k	31/34 (91%)	31 (100%)	0	100	100
10	L	35/35 (100%)	35 (100%)	0	100	100
10	l	35/35 (100%)	35 (100%)	0	100	100
11	M	41/99 (41%)	41 (100%)	0	100	100
11	m	41/99 (41%)	41 (100%)	0	100	100
12	N	19/23 (83%)	19 (100%)	0	100	100
12	n	19/23 (83%)	19 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	T	28/29 (97%)	28 (100%)	0	100	100
13	t	28/29 (97%)	28 (100%)	0	100	100
14	W	33/38 (87%)	33 (100%)	0	100	100
14	w	33/38 (87%)	33 (100%)	0	100	100
15	X	29/31 (94%)	29 (100%)	0	100	100
15	x	29/31 (94%)	29 (100%)	0	100	100
16	2	170/181 (94%)	170 (100%)	0	100	100
16	8	171/181 (94%)	171 (100%)	0	100	100
17	D	272/284 (96%)	272 (100%)	0	100	100
17	d	266/284 (94%)	266 (100%)	0	100	100
18	C	334/353 (95%)	333 (100%)	1 (0%)	91	95
18	c	334/353 (95%)	334 (100%)	0	100	100
19	3	78/177 (44%)	78 (100%)	0	100	100
19	9	78/177 (44%)	78 (100%)	0	100	100
20	4	83/135 (62%)	83 (100%)	0	100	100
20	G	83/135 (62%)	82 (99%)	1 (1%)	67	79
All	All	4717/5434 (87%)	4707 (100%)	10 (0%)	91	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	98	ILE
2	6	51	TYR
2	6	107	ASP
3	a	103	ASP
3	a	259	ILE
5	e	60	GLN
18	C	170	ILE
1	5	155	LYS
1	g	64	THR
20	G	51	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
2	6	74	ASN
2	6	145	GLN
1	7	162	GLN
3	A	108	ASN
3	A	304	GLN
3	A	310	GLN
3	A	315	ASN
3	A	332	HIS
4	B	87	ASN
4	B	394	GLN
5	E	57	GLN
5	E	61	GLN
5	E	66	ASN
5	E	73	GLN
6	F	38	GLN
6	F	41	GLN
8	I	33	ASN
2	J	45	GLN
2	J	127	GLN
2	J	145	GLN
2	J	146	ASN
2	J	157	ASN
9	K	34	GLN
10	L	5	ASN
10	L	7	ASN
12	N	6	ASN
3	a	215	HIS
3	a	247	ASN
3	a	261	GLN
3	a	303	ASN
3	a	304	GLN
3	a	315	ASN
3	a	337	HIS
4	b	300	GLN
4	b	394	GLN
4	b	457	ASN
5	e	61	GLN
5	e	66	ASN
5	e	73	GLN
6	f	38	GLN
9	k	34	GLN
10	l	5	ASN
14	w	32	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	D	60	HIS
17	D	238	GLN
17	D	249	ASN
17	D	300	GLN
17	D	331	GLN
17	D	349	ASN
17	d	188	HIS
17	d	300	GLN
18	C	285	GLN
18	C	294	GLN
18	C	354	ASN
18	C	390	ASN
18	C	432	ASN
18	c	177	ASN
18	c	200	ASN
18	c	390	ASN
19	9	75	GLN
19	9	146	ASN
19	9	151	GLN
19	9	195	ASN
19	3	146	ASN
19	3	174	ASN
1	5	67	GLN
1	5	162	GLN
1	5	180	GLN
1	5	181	ASN
1	g	59	ASN
1	g	124	GLN
1	g	159	GLN
20	G	74	ASN
20	G	127	GLN
20	G	145	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 305 ligands modelled in this entry, 2 are monoatomic - leaving 303 for Mogul analysis.

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	$\#\|Z\| > 2$
21	CLA	C	507	18	65,73,73	2.76	18 (27%)	76,113,113	2.24	22 (28%)
23	A86	8	311	-	44,50,50	1.63	6 (13%)	51,76,76	1.58	10 (19%)
23	A86	4	305	-	44,50,50	1.61	6 (13%)	51,76,76	1.71	11 (21%)
31	SQD	b	602	-	53,54,54	0.95	5 (9%)	62,65,65	1.49	9 (14%)
21	CLA	C	509	36	65,73,73	2.45	18 (27%)	76,113,113	2.27	22 (28%)
28	LMG	8	301	-	24,24,55	0.99	0	31,31,63	1.30	5 (16%)
31	SQD	X	401	-	36,37,54	1.14	5 (13%)	45,48,65	1.67	11 (24%)
24	KC1	5	313	1	48,53,53	3.47	23 (47%)	55,89,89	3.84	31 (56%)
25	BCR	B	618	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	7 (12%)
26	PHO	d	403	-	51,69,69	0.97	3 (5%)	47,99,99	1.21	5 (10%)
27	LHG	d	409	-	46,47,48	0.63	1 (2%)	45,51,54	1.19	5 (11%)
24	KC1	J	313	2	48,53,53	3.53	26 (54%)	55,89,89	3.89	32 (58%)
21	CLA	9	304	-	56,64,73	3.92	20 (35%)	65,102,113	2.39	22 (33%)
21	CLA	5	305	-	41,49,73	3.96	19 (46%)	47,84,113	2.67	22 (46%)
24	KC1	G	309	-	48,53,53	3.52	27 (56%)	55,89,89	3.75	30 (54%)
28	LMG	8	317	-	51,51,55	0.77	1 (1%)	59,59,63	1.34	7 (11%)
35	PL9	D	409	-	55,55,55	1.17	5 (9%)	68,69,69	1.52	10 (14%)
23	A86	1	312	-	44,50,50	1.63	6 (13%)	51,76,76	1.55	9 (17%)
21	CLA	G	304	20	65,73,73	2.39	20 (30%)	76,113,113	2.17	23 (30%)
24	KC1	8	316	16	48,53,53	3.52	27 (56%)	55,89,89	3.58	30 (54%)
21	CLA	2	306	16	45,53,73	3.53	18 (40%)	52,89,113	2.60	20 (38%)
28	LMG	A	407	-	48,48,55	0.76	0	56,56,63	1.31	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
28	LMG	M	102	-	40,40,55	0.85	1 (2%)	48,48,63	1.25	5 (10%)
28	LMG	a	407	-	48,48,55	0.75	0	56,56,63	1.31	5 (8%)
23	A86	5	312	-	44,50,50	1.64	6 (13%)	51,76,76	1.53	9 (17%)
21	CLA	6	301	2	57,65,73	2.59	20 (35%)	66,103,113	2.33	23 (34%)
21	CLA	6	303	-	44,51,73	3.92	21 (47%)	54,86,113	2.59	19 (35%)
21	CLA	G	300	-	65,73,73	3.27	19 (29%)	76,113,113	2.30	24 (31%)
25	BCR	c	515	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	6 (10%)
29	LMU	g	301	-	33,33,36	1.24	2 (6%)	44,44,47	1.30	4 (9%)
21	CLA	3	302	19	47,55,73	3.64	19 (40%)	54,91,113	2.36	21 (38%)
21	CLA	1	303	1	65,73,73	2.91	20 (30%)	76,113,113	2.32	24 (31%)
21	CLA	C	508	18	45,53,73	2.94	18 (40%)	52,89,113	2.44	21 (40%)
24	KC1	G	307	20	48,53,53	3.46	25 (52%)	55,89,89	4.07	32 (58%)
25	BCR	a	406	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	6 (10%)
25	BCR	m	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	4 (7%)
21	CLA	d	404	36	59,67,73	2.62	17 (28%)	68,105,113	2.23	22 (32%)
21	CLA	D	404	36	59,67,73	2.66	18 (30%)	68,105,113	2.27	23 (33%)
21	CLA	2	305	-	65,73,73	2.54	20 (30%)	76,113,113	2.23	23 (30%)
21	CLA	7	307	-	55,63,73	2.97	18 (32%)	64,101,113	2.39	22 (34%)
21	CLA	C	512	18	65,73,73	2.29	20 (30%)	76,113,113	2.22	24 (31%)
21	CLA	B	609	4	65,73,73	2.71	18 (27%)	76,113,113	2.21	23 (30%)
21	CLA	C	515	18	49,57,73	3.31	20 (40%)	55,93,113	2.45	22 (40%)
21	CLA	6	305	-	45,53,73	3.18	19 (42%)	52,89,113	2.45	19 (36%)
21	CLA	a	405	3	60,68,73	3.63	20 (33%)	70,107,113	2.24	23 (32%)
23	A86	1	313	-	44,50,50	1.65	6 (13%)	51,76,76	1.51	7 (13%)
21	CLA	6	307	-	65,73,73	2.33	19 (29%)	76,113,113	2.12	26 (34%)
23	A86	J	310	-	44,50,50	1.63	6 (13%)	51,76,76	1.59	11 (21%)
23	A86	8	309	-	44,50,50	1.63	6 (13%)	51,76,76	1.47	8 (15%)
21	CLA	g	304	-	54,62,73	3.44	20 (37%)	62,99,113	2.26	22 (35%)
24	KC1	J	312	2	48,53,53	3.52	27 (56%)	55,89,89	3.83	32 (58%)
24	KC1	3	305	19	48,53,53	3.53	27 (56%)	55,89,89	3.84	31 (56%)
29	LMU	g	316	-	25,25,36	1.34	3 (12%)	36,36,47	1.16	3 (8%)
29	LMU	2	317	-	36,36,36	1.19	2 (5%)	47,47,47	1.05	3 (6%)
21	CLA	d	405	17	57,65,73	2.64	19 (33%)	70,103,113	2.47	26 (37%)
21	CLA	7	306	1	41,49,73	3.15	20 (48%)	47,84,113	2.52	22 (46%)
24	KC1	9	305	19	48,53,53	3.46	24 (50%)	55,89,89	3.87	31 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CLA	c	509	18	65,73,73	2.80	19 (29%)	76,113,113	2.18	24 (31%)
24	KC1	g	314	-	48,53,53	3.50	25 (52%)	55,89,89	4.01	31 (56%)
23	A86	G	305	-	44,50,50	1.67	6 (13%)	51,76,76	1.58	9 (17%)
21	CLA	1	310	1	55,63,73	3.77	19 (34%)	64,101,113	2.28	22 (34%)
21	CLA	B	608	4	65,73,73	2.55	19 (29%)	76,113,113	2.10	21 (27%)
30	DGD	b	601	-	54,54,67	1.10	5 (9%)	67,67,81	1.44	8 (11%)
23	A86	g	312	-	44,50,50	1.64	6 (13%)	51,76,76	1.88	14 (27%)
24	KC1	5	315	-	48,53,53	3.47	25 (52%)	55,89,89	3.82	31 (56%)
21	CLA	c	507	18	45,53,73	3.02	19 (42%)	52,89,113	2.47	22 (42%)
24	KC1	G	306	20	42,46,53	3.51	24 (57%)	47,79,89	4.55	29 (61%)
21	CLA	a	402	3	65,73,73	2.60	18 (27%)	76,113,113	2.20	24 (31%)
21	CLA	4	301	20	55,63,73	3.61	20 (36%)	64,101,113	2.36	21 (32%)
26	PHO	A	403	-	51,69,69	0.99	4 (7%)	47,99,99	1.13	6 (12%)
21	CLA	7	302	1	65,73,73	2.93	19 (29%)	76,113,113	2.25	23 (30%)
28	LMG	b	626	-	37,37,55	0.90	0	45,45,63	1.23	6 (13%)
23	A86	g	311	-	44,50,50	1.64	6 (13%)	51,76,76	1.50	8 (15%)
21	CLA	b	615	4	64,72,73	2.55	20 (31%)	74,111,113	2.16	23 (31%)
24	KC1	2	315	16	48,53,53	3.54	26 (54%)	55,89,89	3.87	30 (54%)
21	CLA	C	504	18	64,72,73	2.52	19 (29%)	74,111,113	2.25	19 (25%)
21	CLA	1	307	1	41,49,73	3.19	20 (48%)	47,84,113	2.51	21 (44%)
21	CLA	c	508	36	65,73,73	2.49	19 (29%)	76,113,113	2.28	21 (27%)
28	LMG	B	623	-	43,43,55	0.83	0	51,51,63	1.25	4 (7%)
21	CLA	8	306	-	58,66,73	2.67	20 (34%)	67,104,113	2.22	22 (32%)
23	A86	6	310	-	44,50,50	1.64	6 (13%)	51,76,76	1.58	10 (19%)
26	PHO	a	404	-	51,69,69	0.99	4 (7%)	47,99,99	1.13	7 (14%)
21	CLA	J	301	2	57,65,73	2.42	20 (35%)	66,103,113	2.40	23 (34%)
21	CLA	C	510	18	65,73,73	2.74	19 (29%)	76,113,113	2.18	24 (31%)
28	LMG	f	102	-	46,46,55	0.80	1 (2%)	54,54,63	1.33	7 (12%)
30	DGD	h	103	-	63,63,67	0.91	2 (3%)	77,77,81	1.38	8 (10%)
21	CLA	B	603	4	61,69,73	2.66	19 (31%)	67,106,113	2.04	18 (26%)
23	A86	1	314	-	44,50,50	1.60	6 (13%)	51,76,76	1.54	7 (13%)
28	LMG	b	620	-	51,51,55	0.79	1 (1%)	59,59,63	1.31	7 (11%)
21	CLA	1	309	1	56,64,73	3.17	20 (35%)	65,102,113	2.31	22 (33%)
28	LMG	b	621	-	28,28,55	1.00	1 (3%)	36,36,63	1.30	5 (13%)
24	KC1	4	309	20	48,53,53	3.54	26 (54%)	55,89,89	3.74	29 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	CLA	8	303	16	50,58,73	3.24	19 (38%)	58,95,113	2.47	24 (41%)
21	CLA	9	301	19	60,68,73	4.85	20 (33%)	70,107,113	2.28	22 (31%)
21	CLA	B	615	4	65,73,73	2.79	19 (29%)	76,113,113	2.12	24 (31%)
21	CLA	B	611	4	64,72,73	2.53	19 (29%)	74,111,113	2.22	22 (29%)
27	LHG	l	101	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
24	KC1	1	316	1	48,53,53	3.50	26 (54%)	55,89,89	3.84	29 (52%)
22	DD6	g	310	-	39,45,45	1.60	7 (17%)	52,67,67	1.63	10 (19%)
27	LHG	d	402	-	42,42,48	0.66	1 (2%)	45,48,54	1.20	4 (8%)
32	HEM	E	101	5	41,50,50	1.48	4 (9%)	45,82,82	1.57	9 (20%)
25	BCR	b	618	-	41,41,41	1.07	2 (4%)	56,56,56	1.23	6 (10%)
21	CLA	C	511	18	65,73,73	2.29	18 (27%)	76,113,113	2.19	23 (30%)
29	LMU	A	408	-	36,36,36	1.21	2 (5%)	47,47,47	1.08	3 (6%)
29	LMU	a	408	-	36,36,36	1.20	2 (5%)	47,47,47	1.09	3 (6%)
21	CLA	c	504	18	65,73,73	2.68	20 (30%)	76,113,113	2.15	21 (27%)
31	SQD	B	626	-	53,54,54	0.95	5 (9%)	62,65,65	1.49	9 (14%)
24	KC1	7	315	1	48,53,53	3.49	26 (54%)	55,89,89	3.81	30 (54%)
21	CLA	B	607	4	65,73,73	2.84	19 (29%)	76,113,113	2.22	23 (30%)
23	A86	8	308	-	44,50,50	1.66	6 (13%)	51,76,76	1.81	12 (23%)
28	LMG	L	101	-	40,40,55	0.82	0	48,48,63	1.24	5 (10%)
21	CLA	8	307	16	43,51,73	3.52	17 (39%)	49,86,113	2.58	19 (38%)
25	BCR	C	501	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	5 (8%)
21	CLA	b	607	4	65,73,73	2.51	20 (30%)	76,113,113	2.19	22 (28%)
27	LHG	D	403	-	42,42,48	0.67	1 (2%)	45,48,54	1.19	4 (8%)
21	CLA	5	304	-	48,56,73	3.35	20 (41%)	55,92,113	2.51	21 (38%)
21	CLA	G	301	20	57,65,73	3.37	20 (35%)	66,103,113	2.31	22 (33%)
21	CLA	5	303	1	52,60,73	3.10	19 (36%)	60,97,113	2.49	23 (38%)
21	CLA	7	305	1	41,49,73	3.59	19 (46%)	47,84,113	2.82	20 (42%)
21	CLA	7	304	-	65,73,73	2.59	19 (29%)	76,113,113	2.16	24 (31%)
21	CLA	b	604	4	61,69,73	2.62	19 (31%)	67,106,113	2.02	18 (26%)
21	CLA	2	302	16	50,58,73	3.43	21 (42%)	58,95,113	4.14	27 (46%)
30	DGD	c	516	-	56,56,67	1.01	2 (3%)	70,70,81	1.49	7 (10%)
21	CLA	6	300	2	52,60,73	3.55	20 (38%)	60,97,113	2.34	23 (38%)
21	CLA	C	506	-	64,72,73	2.48	19 (29%)	74,111,113	2.22	22 (29%)
21	CLA	4	303	-	51,59,73	4.02	19 (37%)	59,96,113	2.36	24 (40%)
23	A86	6	309	-	44,50,50	1.74	7 (15%)	51,76,76	1.87	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	CLA	b	606	4	61,69,73	2.52	19 (31%)	71,108,113	2.41	21 (29%)
21	CLA	G	303	-	51,59,73	3.77	19 (37%)	59,96,113	2.29	22 (37%)
21	CLA	A	402	36	49,57,73	3.46	19 (38%)	55,93,113	2.49	19 (34%)
21	CLA	D	407	17	60,68,73	2.98	19 (31%)	70,107,113	2.24	22 (31%)
21	CLA	1	308	-	54,62,73	3.21	19 (35%)	62,99,113	2.40	23 (37%)
21	CLA	J	306	36	65,73,73	2.75	20 (30%)	76,113,113	2.14	24 (31%)
21	CLA	b	612	4	64,72,73	2.51	18 (28%)	74,111,113	2.20	22 (29%)
22	DD6	1	311	-	39,45,45	1.58	8 (20%)	52,67,67	1.63	10 (19%)
21	CLA	b	603	-	47,55,73	3.30	18 (38%)	54,91,113	2.50	22 (40%)
25	BCR	c	501	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	6 (10%)
21	CLA	b	616	4	65,73,73	2.74	19 (29%)	76,113,113	2.13	24 (31%)
23	A86	W	101	21	44,50,50	1.56	6 (13%)	51,76,76	1.54	10 (19%)
30	DGD	H	101	-	63,63,67	0.91	2 (3%)	77,77,81	1.37	8 (10%)
27	LHG	a	401	-	48,48,48	0.61	0	51,54,54	1.26	6 (11%)
21	CLA	C	505	18	65,73,73	3.17	20 (30%)	76,113,113	2.23	22 (28%)
21	CLA	J	300	2	52,60,73	3.52	19 (36%)	60,97,113	2.36	23 (38%)
21	CLA	C	513	18	65,73,73	2.67	19 (29%)	76,113,113	2.16	20 (26%)
21	CLA	5	307	1	56,64,73	2.89	18 (32%)	65,102,113	2.20	22 (33%)
28	LMG	B	627	-	40,40,55	0.94	2 (5%)	48,48,63	1.37	7 (14%)
21	CLA	c	513	18	64,72,73	2.62	20 (31%)	74,111,113	2.11	19 (25%)
21	CLA	1	306	1	41,49,73	3.09	20 (48%)	47,84,113	2.46	21 (44%)
21	CLA	8	302	16	65,73,73	2.79	19 (29%)	76,113,113	2.13	25 (32%)
21	CLA	c	514	18	49,57,73	3.26	20 (40%)	55,93,113	2.46	22 (40%)
21	CLA	3	300	19	56,64,73	3.39	20 (35%)	65,102,113	2.34	20 (30%)
24	KC1	6	312	2	48,53,53	3.54	27 (56%)	55,89,89	3.86	32 (58%)
21	CLA	1	305	-	51,59,73	2.86	19 (37%)	59,96,113	2.37	23 (38%)
24	KC1	3	306	19	48,53,53	3.51	27 (56%)	55,89,89	3.90	30 (54%)
21	CLA	J	302	2	45,53,73	3.53	19 (42%)	52,89,113	2.47	19 (36%)
28	LMG	D	411	-	46,46,55	0.79	0	54,54,63	1.34	7 (12%)
30	DGD	c	517	-	40,40,67	1.16	1 (2%)	53,53,81	1.41	4 (7%)
24	KC1	8	313	16	48,53,53	3.51	27 (56%)	55,89,89	3.95	31 (56%)
21	CLA	b	617	4	65,73,73	2.46	18 (27%)	76,113,113	2.18	25 (32%)
21	CLA	5	306	1	65,73,73	2.38	19 (29%)	76,113,113	2.26	23 (30%)
28	LMG	B	620	-	28,28,55	1.00	1 (3%)	36,36,63	1.30	5 (13%)
25	BCR	1	317	-	41,41,41	1.01	2 (4%)	56,56,56	1.29	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CLA	J	308	2	52,60,73	2.72	20 (38%)	60,97,113	2.63	25 (41%)
21	CLA	g	303	1	50,58,73	3.01	20 (40%)	58,95,113	2.53	22 (37%)
22	DD6	5	310	-	39,45,45	1.63	8 (20%)	52,67,67	1.62	11 (21%)
25	BCR	B	617	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	5 (8%)
24	KC1	2	316	16	48,53,53	3.52	27 (56%)	55,89,89	3.57	29 (52%)
21	CLA	c	503	18	64,72,73	2.50	19 (29%)	74,111,113	2.23	20 (27%)
31	SQD	C	502	-	50,51,54	0.98	5 (10%)	59,62,65	1.59	11 (18%)
22	DD6	7	310	-	39,45,45	1.56	8 (20%)	52,67,67	1.63	10 (19%)
21	CLA	1	302	1	65,73,73	2.94	19 (29%)	76,113,113	2.21	22 (28%)
27	LHG	D	410	-	46,47,48	0.59	0	45,51,54	1.16	5 (11%)
21	CLA	c	505	-	56,64,73	2.62	19 (33%)	64,101,113	2.38	22 (34%)
28	LMG	N	101	-	24,24,55	0.98	0	31,31,63	1.27	5 (16%)
24	KC1	6	313	2	48,53,53	3.51	27 (56%)	55,89,89	3.92	32 (58%)
28	LMG	b	625	-	43,43,55	0.87	1 (2%)	51,51,63	1.22	4 (7%)
29	LMU	5	316	-	24,24,36	1.32	2 (8%)	35,35,47	1.17	2 (5%)
28	LMG	B	619	-	51,51,55	0.79	1 (1%)	59,59,63	1.33	6 (10%)
21	CLA	g	307	1	46,54,73	3.56	19 (41%)	53,90,113	2.40	22 (41%)
21	CLA	5	302	1	65,73,73	3.46	19 (29%)	76,113,113	2.25	26 (34%)
21	CLA	g	308	1	65,73,73	2.54	20 (30%)	76,113,113	2.10	22 (28%)
23	A86	2	312	-	44,50,50	1.64	6 (13%)	51,76,76	1.58	9 (17%)
28	LMG	B	622	-	37,37,55	0.88	0	45,45,63	1.27	5 (11%)
24	KC1	9	306	19	48,53,53	3.57	27 (56%)	55,89,89	3.75	30 (54%)
21	CLA	8	305	16	41,49,73	3.19	20 (48%)	47,84,113	2.59	20 (42%)
21	CLA	C	503	18	65,73,73	2.60	20 (30%)	76,113,113	2.20	22 (28%)
21	CLA	c	502	18	65,73,73	2.69	19 (29%)	76,113,113	2.21	22 (28%)
21	CLA	c	506	18	65,73,73	2.77	18 (27%)	76,113,113	2.24	21 (27%)
24	KC1	7	314	1	48,53,53	3.48	26 (54%)	55,89,89	3.81	31 (56%)
24	KC1	8	315	16	48,53,53	3.53	26 (54%)	55,89,89	3.93	31 (56%)
32	HEM	f	101	6	41,50,50	1.55	5 (12%)	45,82,82	1.42	6 (13%)
21	CLA	5	308	1	65,73,73	3.26	20 (30%)	76,113,113	2.19	22 (28%)
33	BCT	D	402	34	2,3,3	1.23	0	2,3,3	4.12	2 (100%)
24	KC1	2	313	16	48,53,53	3.49	27 (56%)	55,89,89	3.69	31 (56%)
21	CLA	d	406	17	60,68,73	2.94	19 (31%)	70,107,113	2.25	22 (31%)
24	KC1	4	307	20	48,53,53	3.47	25 (52%)	55,89,89	3.84	30 (54%)
21	CLA	8	304	23	51,59,73	2.95	19 (37%)	59,96,113	2.45	22 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	CLA	D	406	17	57,65,73	2.67	18 (31%)	70,103,113	2.46	26 (37%)
28	LMG	b	622	-	35,35,55	1.02	1 (2%)	43,43,63	1.29	3 (6%)
21	CLA	b	605	4	64,72,73	2.57	18 (28%)	74,111,113	2.15	23 (31%)
21	CLA	2	304	16	41,49,73	3.09	20 (48%)	47,84,113	2.59	20 (42%)
21	CLA	g	302	1	65,73,73	3.56	20 (30%)	76,113,113	2.16	24 (31%)
25	BCR	D	408	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	6 (10%)
21	CLA	c	511	18	65,73,73	2.32	20 (30%)	76,113,113	2.19	22 (28%)
24	KC1	1	315	-	48,53,53	3.52	27 (56%)	55,89,89	3.81	30 (54%)
21	CLA	7	300	1	65,73,73	3.45	20 (30%)	76,113,113	2.13	21 (27%)
23	A86	2	308	-	44,50,50	1.61	6 (13%)	51,76,76	1.70	11 (21%)
24	KC1	4	306	20	42,46,53	3.50	24 (57%)	47,79,89	4.51	27 (57%)
25	BCR	H	100	-	41,41,41	1.07	2 (4%)	56,56,56	1.33	6 (10%)
27	LHG	A	406	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
21	CLA	J	304	2	43,51,73	3.26	17 (39%)	49,86,113	2.60	22 (44%)
21	CLA	4	302	20	56,64,73	4.55	19 (33%)	65,102,113	2.39	24 (36%)
21	CLA	6	306	36	65,73,73	2.77	20 (30%)	76,113,113	2.13	24 (31%)
21	CLA	b	610	4	65,73,73	2.75	18 (27%)	76,113,113	2.19	22 (28%)
21	CLA	7	309	1	45,53,73	3.92	19 (42%)	52,89,113	2.44	21 (40%)
21	CLA	1	301	1	65,73,73	3.38	20 (30%)	76,113,113	2.11	22 (28%)
21	CLA	3	304	19	57,65,73	3.70	20 (35%)	66,103,113	2.30	23 (34%)
23	A86	7	312	-	44,50,50	1.64	6 (13%)	51,76,76	1.71	10 (19%)
28	LMG	2	318	-	46,46,55	0.82	2 (4%)	54,54,63	1.32	7 (12%)
21	CLA	7	303	1	65,73,73	2.96	19 (29%)	76,113,113	2.15	23 (30%)
21	CLA	g	309	1	50,58,73	4.86	20 (40%)	58,95,113	2.49	25 (43%)
21	CLA	1	304	1	65,73,73	2.94	19 (29%)	76,113,113	2.12	24 (31%)
21	CLA	c	512	18	65,73,73	2.62	20 (30%)	76,113,113	2.18	21 (27%)
21	CLA	B	616	4	65,73,73	2.52	18 (27%)	76,113,113	2.19	25 (32%)
29	LMU	D	412	-	36,36,36	1.22	2 (5%)	47,47,47	1.04	2 (4%)
30	DGD	C	518	-	40,40,67	1.17	1 (2%)	53,53,81	1.40	4 (7%)
29	LMU	5	301	-	33,33,36	1.25	2 (6%)	44,44,47	1.32	6 (13%)
21	CLA	A	401	3	65,73,73	2.61	18 (27%)	76,113,113	2.21	24 (31%)
21	CLA	a	403	36	49,57,73	3.45	19 (38%)	55,93,113	2.48	20 (36%)
25	BCR	A	405	-	41,41,41	1.11	2 (4%)	56,56,56	1.16	6 (10%)
21	CLA	b	613	4	65,73,73	2.63	20 (30%)	76,113,113	2.14	22 (28%)
23	A86	J	309	-	44,50,50	1.63	5 (11%)	51,76,76	1.64	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	KC1	J	311	2	48,53,53	3.46	26 (54%)	55,89,89	3.77	31 (56%)
21	CLA	A	404	3	60,68,73	3.13	19 (31%)	70,107,113	2.27	23 (32%)
21	CLA	6	302	2	45,53,73	3.56	20 (44%)	52,89,113	2.48	20 (38%)
23	A86	7	313	-	40,46,50	1.73	6 (15%)	45,70,76	1.75	10 (22%)
21	CLA	B	602	-	47,55,73	3.29	18 (38%)	54,91,113	2.56	21 (38%)
21	CLA	2	301	16	65,73,73	2.69	19 (29%)	76,113,113	2.21	26 (34%)
23	A86	2	307	-	44,50,50	1.64	6 (13%)	51,76,76	1.72	11 (21%)
21	CLA	B	605	4	61,69,73	2.54	19 (31%)	71,108,113	2.40	22 (30%)
24	KC1	6	311	2	48,53,53	3.46	26 (54%)	55,89,89	3.78	30 (54%)
21	CLA	3	303	19	42,50,73	4.30	19 (45%)	48,85,113	2.62	19 (39%)
24	KC1	g	313	1	48,53,53	3.47	22 (45%)	55,89,89	3.81	28 (50%)
28	LMG	b	624	-	37,37,55	0.88	1 (2%)	45,45,63	1.25	5 (11%)
21	CLA	b	608	4	65,73,73	2.82	19 (29%)	76,113,113	2.20	23 (30%)
21	CLA	6	308	2	52,60,73	2.75	20 (38%)	60,97,113	2.60	25 (41%)
21	CLA	b	614	4	65,73,73	2.96	19 (29%)	76,113,113	2.14	22 (28%)
23	A86	5	311	-	44,50,50	1.67	6 (13%)	51,76,76	1.64	10 (19%)
21	CLA	2	303	36	51,59,73	2.85	17 (33%)	59,96,113	2.43	23 (38%)
23	A86	7	311	-	44,50,50	1.63	5 (11%)	51,76,76	1.47	8 (15%)
24	KC1	2	314	16	48,53,53	3.52	26 (54%)	55,89,89	3.77	28 (50%)
24	KC1	G	308	20	48,53,53	3.58	27 (56%)	55,89,89	4.01	30 (54%)
27	LHG	B	601	-	48,48,48	0.61	1 (2%)	51,54,54	1.28	6 (11%)
21	CLA	4	300	-	65,73,73	3.16	19 (29%)	76,113,113	2.34	23 (30%)
21	CLA	J	303	2	44,51,73	8.56	21 (47%)	54,86,113	2.55	23 (42%)
21	CLA	c	510	18	65,73,73	2.33	18 (27%)	76,113,113	2.18	24 (31%)
21	CLA	9	300	19	56,64,73	3.19	20 (35%)	65,102,113	2.23	22 (33%)
23	A86	8	310	-	44,50,50	1.64	5 (11%)	51,76,76	1.71	10 (19%)
26	PHO	D	401	-	51,69,69	0.97	3 (5%)	47,99,99	1.21	6 (12%)
25	BCR	h	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	6 (10%)
30	DGD	C	517	-	56,56,67	1.00	3 (5%)	70,70,81	1.49	8 (11%)
21	CLA	B	614	4	64,72,73	2.58	20 (31%)	74,111,113	2.12	23 (31%)
21	CLA	B	612	4	65,73,73	2.68	20 (30%)	76,113,113	2.16	24 (31%)
23	A86	2	310	-	44,50,50	1.62	6 (13%)	51,76,76	1.72	11 (21%)
21	CLA	4	304	20	65,73,73	2.39	19 (29%)	76,113,113	2.16	25 (32%)
21	CLA	g	305	-	41,49,73	3.76	20 (48%)	47,84,113	2.50	23 (48%)
21	CLA	J	305	-	45,53,73	3.25	19 (42%)	52,89,113	2.45	19 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	BCR	d	407	-	41,41,41	1.05	2 (4%)	56,56,56	1.22	5 (8%)
21	CLA	J	307	-	65,73,73	2.31	20 (30%)	76,113,113	2.10	24 (31%)
30	DGD	B	624	-	54,54,67	1.09	5 (9%)	67,67,81	1.47	9 (13%)
21	CLA	9	302	19	47,55,73	3.28	20 (42%)	54,91,113	2.48	20 (37%)
23	A86	2	311	-	44,50,50	1.59	6 (13%)	51,76,76	1.74	11 (21%)
25	BCR	b	619	-	41,41,41	1.08	3 (7%)	56,56,56	1.25	6 (10%)
21	CLA	G	302	20	56,64,73	7.05	20 (35%)	65,102,113	2.28	23 (35%)
21	CLA	9	303	19	51,59,73	4.17	19 (37%)	59,96,113	2.67	23 (38%)
24	KC1	4	308	20	48,53,53	3.53	27 (56%)	55,89,89	3.90	31 (56%)
29	LMU	8	318	-	36,36,36	1.21	2 (5%)	47,47,47	0.99	1 (2%)
21	CLA	B	613	4	65,73,73	2.97	19 (29%)	76,113,113	2.14	23 (30%)
21	CLA	3	301	19	60,68,73	3.03	20 (33%)	70,107,113	2.30	24 (34%)
25	BCR	C	516	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	6 (10%)
21	CLA	B	604	4	64,72,73	2.55	18 (28%)	74,111,113	2.16	22 (29%)
21	CLA	g	306	1	65,73,73	2.37	18 (27%)	76,113,113	2.23	22 (28%)
21	CLA	6	304	2	43,51,73	3.17	17 (39%)	49,86,113	2.63	22 (44%)
24	KC1	8	314	16	48,53,53	3.52	26 (54%)	55,89,89	3.81	30 (54%)
25	BCR	h	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.31	7 (12%)
35	PL9	d	408	-	55,55,55	1.16	5 (9%)	68,69,69	1.50	11 (16%)
25	BCR	M	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	4 (7%)
33	BCT	d	401	34	2,3,3	1.28	0	2,3,3	4.07	1 (50%)
31	SQD	B	625	-	48,49,54	1.00	5 (10%)	57,60,65	1.57	8 (14%)
21	CLA	C	514	18	64,72,73	2.63	19 (29%)	74,111,113	2.12	19 (25%)
21	CLA	B	606	4	65,73,73	2.50	20 (30%)	76,113,113	2.20	22 (28%)
21	CLA	5	309	1	65,73,73	2.83	20 (30%)	76,113,113	2.51	28 (36%)
21	CLA	b	623	-	56,64,73	2.66	19 (33%)	65,102,113	2.32	22 (33%)
21	CLA	B	621	-	65,73,73	2.55	19 (29%)	76,113,113	2.15	22 (28%)
21	CLA	7	308	1	56,64,73	2.90	20 (35%)	65,102,113	2.34	22 (33%)
21	CLA	B	610	-	65,73,73	2.79	18 (27%)	76,113,113	2.18	20 (26%)
21	CLA	b	609	4	65,73,73	2.55	19 (29%)	76,113,113	2.10	21 (27%)
23	A86	2	309	-	44,50,50	1.64	6 (13%)	51,76,76	1.77	10 (19%)
23	A86	8	312	-	44,50,50	1.66	6 (13%)	51,76,76	1.66	9 (17%)
24	KC1	g	315	-	48,53,53	3.53	27 (56%)	55,89,89	3.78	30 (54%)
21	CLA	7	301	1	65,73,73	2.91	20 (30%)	76,113,113	2.18	20 (26%)
21	CLA	b	611	-	65,73,73	2.85	18 (27%)	76,113,113	2.18	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	KC1	5	314	-	48,53,53	3.50	26 (54%)	55,89,89	3.91	29 (52%)

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
21	CLA	C	507	18	-	11/37/115/115	-
23	A86	8	311	-	-	16/34/90/90	0/3/3/3
23	A86	4	305	-	-	17/34/90/90	0/3/3/3
31	SQD	b	602	-	-	26/49/69/69	0/1/1/1
21	CLA	C	509	36	1/1/15/20	15/37/115/115	-
28	LMG	8	301	-	-	8/17/37/70	0/1/1/1
31	SQD	X	401	-	-	17/32/52/69	0/1/1/1
24	KC1	5	313	1	-	8/15/71/71	-
25	BCR	B	618	-	-	8/29/63/63	0/2/2/2
26	PHO	d	403	-	-	4/37/103/103	0/5/6/6
27	LHG	d	409	-	-	21/47/51/53	-
24	KC1	J	313	2	-	8/15/71/71	-
21	CLA	9	304	-	1/1/13/20	9/27/105/115	-
21	CLA	5	305	-	1/1/10/20	2/8/86/115	-
24	KC1	G	309	-	-	9/15/71/71	-
28	LMG	8	317	-	-	22/46/66/70	0/1/1/1
35	PL9	D	409	-	-	3/53/73/73	0/1/1/1
23	A86	1	312	-	-	23/34/90/90	0/3/3/3
21	CLA	G	304	20	1/1/15/20	16/37/115/115	-
24	KC1	8	316	16	-	7/15/71/71	-
21	CLA	2	306	16	-	6/13/91/115	-
28	LMG	A	407	-	-	23/43/63/70	0/1/1/1
28	LMG	M	102	-	-	15/35/55/70	0/1/1/1
28	LMG	a	407	-	-	22/43/63/70	0/1/1/1
23	A86	5	312	-	-	24/34/90/90	0/3/3/3
21	CLA	6	301	2	1/1/13/20	14/28/106/115	-
21	CLA	6	303	-	1/1/11/20	6/13/89/115	-
21	CLA	G	300	-	1/1/15/20	9/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	c	515	-	-	9/29/63/63	0/2/2/2
29	LMU	g	301	-	-	8/18/58/61	0/2/2/2
21	CLA	3	302	19	1/1/11/20	5/16/94/115	-
21	CLA	1	303	1	1/1/15/20	15/37/115/115	-
21	CLA	C	508	18	1/1/11/20	3/13/91/115	-
24	KC1	G	307	20	-	7/15/71/71	-
25	BCR	a	406	-	-	6/29/63/63	0/2/2/2
25	BCR	m	101	-	-	5/29/63/63	0/2/2/2
21	CLA	d	404	36	1/1/13/20	7/30/108/115	-
21	CLA	D	404	36	1/1/13/20	7/30/108/115	-
21	CLA	2	305	-	1/1/15/20	19/37/115/115	-
21	CLA	7	307	-	1/1/13/20	5/25/103/115	-
21	CLA	C	512	18	1/1/15/20	9/37/115/115	-
21	CLA	B	609	4	-	5/37/115/115	-
21	CLA	C	515	18	-	3/18/96/115	-
21	CLA	6	305	-	1/1/11/20	4/13/91/115	-
21	CLA	a	405	3	-	8/31/109/115	-
23	A86	1	313	-	-	21/34/90/90	0/3/3/3
21	CLA	6	307	-	1/1/15/20	15/37/115/115	-
23	A86	J	310	-	-	19/34/90/90	0/3/3/3
23	A86	8	309	-	-	9/34/90/90	0/3/3/3
21	CLA	g	304	-	-	12/24/102/115	-
24	KC1	J	312	2	-	5/15/71/71	-
24	KC1	3	305	19	-	6/15/71/71	-
29	LMU	g	316	-	-	4/10/50/61	0/2/2/2
29	LMU	2	317	-	-	9/21/61/61	0/2/2/2
21	CLA	d	405	17	1/1/13/20	7/28/104/115	-
21	CLA	7	306	1	1/1/10/20	4/8/86/115	-
24	KC1	9	305	19	-	8/15/71/71	-
21	CLA	c	509	18	-	11/37/115/115	-
24	KC1	g	314	-	-	7/15/71/71	-
23	A86	G	305	-	-	15/34/90/90	0/3/3/3
21	CLA	1	310	1	-	10/25/103/115	-
21	CLA	B	608	4	-	10/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	b	601	-	-	24/43/79/95	0/2/2/2
23	A86	g	312	-	-	20/34/90/90	0/3/3/3
24	KC1	5	315	-	-	5/15/71/71	-
21	CLA	c	507	18	1/1/11/20	5/13/91/115	-
24	KC1	G	306	20	-	0/8/64/71	-
21	CLA	4	301	20	1/1/13/20	9/25/103/115	-
21	CLA	a	402	3	-	8/37/115/115	-
26	PHO	A	403	-	-	12/37/103/103	0/5/6/6
21	CLA	7	302	1	1/1/15/20	12/37/115/115	-
28	LMG	b	626	-	-	11/32/52/70	0/1/1/1
23	A86	g	311	-	-	20/34/90/90	0/3/3/3
21	CLA	b	615	4	1/1/14/20	13/35/113/115	-
24	KC1	2	315	16	-	7/15/71/71	-
21	CLA	C	504	18	-	8/35/113/115	-
21	CLA	1	307	1	1/1/10/20	4/8/86/115	-
21	CLA	c	508	36	1/1/15/20	14/37/115/115	-
28	LMG	B	623	-	-	15/38/58/70	0/1/1/1
21	CLA	8	306	-	1/1/13/20	12/29/107/115	-
23	A86	6	310	-	-	19/34/90/90	0/3/3/3
26	PHO	a	404	-	-	12/37/103/103	0/5/6/6
21	CLA	J	301	2	1/1/13/20	14/28/106/115	-
21	CLA	C	510	18	-	11/37/115/115	-
28	LMG	f	102	-	-	21/41/61/70	0/1/1/1
30	DGD	h	103	-	-	17/51/91/95	0/2/2/2
21	CLA	B	603	4	1/1/12/20	14/27/107/115	-
23	A86	1	314	-	-	20/34/90/90	0/3/3/3
28	LMG	b	620	-	-	19/46/66/70	0/1/1/1
21	CLA	1	309	1	1/1/13/20	8/27/105/115	-
28	LMG	b	621	-	-	3/23/43/70	0/1/1/1
24	KC1	4	309	20	-	4/15/71/71	-
21	CLA	8	303	16	1/1/12/20	4/19/97/115	-
21	CLA	9	301	19	-	11/31/109/115	-
21	CLA	B	615	4	1/1/15/20	6/37/115/115	-
21	CLA	B	611	4	-	5/35/113/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	l	101	-	-	23/53/53/53	-
24	KC1	1	316	1	-	7/15/71/71	-
22	DD6	g	310	-	-	10/26/80/80	0/3/3/3
27	LHG	d	402	-	-	15/47/47/53	-
32	HEM	E	101	5	-	6/12/54/54	-
25	BCR	b	618	-	-	7/29/63/63	0/2/2/2
21	CLA	C	511	18	1/1/15/20	8/37/115/115	-
29	LMU	A	408	-	-	7/21/61/61	0/2/2/2
29	LMU	a	408	-	-	8/21/61/61	0/2/2/2
21	CLA	c	504	18	-	14/37/115/115	-
31	SQD	B	626	-	-	27/49/69/69	0/1/1/1
24	KC1	7	315	1	-	7/15/71/71	-
21	CLA	B	607	4	-	11/37/115/115	-
23	A86	8	308	-	-	24/34/90/90	0/3/3/3
28	LMG	L	101	-	-	19/35/55/70	0/1/1/1
21	CLA	8	307	16	1/1/10/20	4/11/89/115	-
25	BCR	C	501	-	-	9/29/63/63	0/2/2/2
21	CLA	b	607	4	-	8/37/115/115	-
27	LHG	D	403	-	-	19/47/47/53	-
21	CLA	5	304	-	-	8/17/95/115	-
21	CLA	G	301	20	1/1/13/20	6/28/106/115	-
21	CLA	5	303	1	1/1/12/20	10/22/100/115	-
21	CLA	7	305	1	1/1/10/20	4/8/86/115	-
21	CLA	7	304	-	1/1/15/20	13/37/115/115	-
21	CLA	b	604	4	1/1/12/20	7/27/107/115	-
21	CLA	2	302	16	1/1/12/20	6/19/97/115	-
30	DGD	c	516	-	-	20/44/84/95	0/2/2/2
21	CLA	6	300	2	1/1/12/20	6/22/100/115	-
21	CLA	4	303	-	1/1/12/20	9/21/99/115	-
21	CLA	C	506	-	-	15/35/113/115	-
23	A86	6	309	-	-	21/34/90/90	0/3/3/3
21	CLA	b	606	4	-	13/33/111/115	-
21	CLA	G	303	-	1/1/12/20	10/21/99/115	-
21	CLA	A	402	36	-	5/18/96/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	D	407	17	-	9/31/109/115	-
21	CLA	1	308	-	-	10/24/102/115	-
21	CLA	J	306	36	1/1/15/20	13/37/115/115	-
21	CLA	b	612	4	-	6/35/113/115	-
22	DD6	1	311	-	-	5/26/80/80	0/3/3/3
21	CLA	b	603	-	1/1/11/20	6/16/94/115	-
25	BCR	c	501	-	-	7/29/63/63	0/2/2/2
21	CLA	b	616	4	1/1/15/20	7/37/115/115	-
23	A86	W	101	21	-	24/34/90/90	0/3/3/3
30	DGD	H	101	-	-	14/51/91/95	0/2/2/2
27	LHG	a	401	-	-	30/53/53/53	-
21	CLA	C	505	18	-	11/37/115/115	-
21	CLA	J	300	2	1/1/12/20	6/22/100/115	-
21	CLA	C	513	18	-	5/37/115/115	-
21	CLA	5	307	1	-	11/27/105/115	-
28	LMG	B	627	-	-	19/35/55/70	0/1/1/1
21	CLA	c	513	18	1/1/14/20	12/35/113/115	-
21	CLA	1	306	1	1/1/10/20	2/8/86/115	-
21	CLA	8	302	16	1/1/15/20	13/37/115/115	-
21	CLA	c	514	18	-	3/18/96/115	-
21	CLA	3	300	19	-	9/27/105/115	-
24	KC1	6	312	2	-	4/15/71/71	-
21	CLA	1	305	-	-	8/21/99/115	-
24	KC1	3	306	19	-	5/15/71/71	-
21	CLA	J	302	2	1/1/11/20	3/13/91/115	-
28	LMG	D	411	-	-	22/41/61/70	0/1/1/1
30	DGD	c	517	-	-	14/26/66/95	0/2/2/2
24	KC1	8	313	16	-	3/15/71/71	-
21	CLA	b	617	4	1/1/15/20	14/37/115/115	-
21	CLA	5	306	1	1/1/15/20	14/37/115/115	-
28	LMG	B	620	-	-	3/23/43/70	0/1/1/1
25	BCR	1	317	-	-	20/29/63/63	0/2/2/2
21	CLA	J	308	2	1/1/12/20	9/22/100/115	-
21	CLA	g	303	1	1/1/12/20	8/19/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	DD6	5	310	-	-	8/26/80/80	0/3/3/3
25	BCR	B	617	-	-	9/29/63/63	0/2/2/2
24	KC1	2	316	16	-	5/15/71/71	-
21	CLA	c	503	18	-	3/35/113/115	-
31	SQD	C	502	-	-	20/46/66/69	0/1/1/1
22	DD6	7	310	-	-	8/26/80/80	0/3/3/3
21	CLA	1	302	1	1/1/15/20	13/37/115/115	-
27	LHG	D	410	-	-	21/47/51/53	-
21	CLA	c	505	-	-	11/26/104/115	-
28	LMG	N	101	-	-	11/17/37/70	0/1/1/1
24	KC1	6	313	2	-	7/15/71/71	-
28	LMG	b	625	-	-	22/38/58/70	0/1/1/1
29	LMU	5	316	-	-	1/8/48/61	0/2/2/2
28	LMG	B	619	-	-	20/46/66/70	0/1/1/1
21	CLA	g	307	1	-	3/15/93/115	-
21	CLA	5	302	1	1/1/15/20	9/37/115/115	-
21	CLA	g	308	1	-	18/37/115/115	-
23	A86	2	312	-	-	19/34/90/90	0/3/3/3
28	LMG	B	622	-	-	14/32/52/70	0/1/1/1
24	KC1	9	306	19	-	6/15/71/71	-
21	CLA	C	503	18	1/1/15/20	11/37/115/115	-
21	CLA	8	305	16	-	3/8/86/115	-
21	CLA	c	502	18	1/1/15/20	11/37/115/115	-
21	CLA	c	506	18	-	11/37/115/115	-
24	KC1	7	314	1	-	6/15/71/71	-
24	KC1	8	315	16	-	4/15/71/71	-
32	HEM	f	101	6	-	5/12/54/54	-
21	CLA	5	308	1	-	11/37/115/115	-
24	KC1	2	313	16	-	8/15/71/71	-
21	CLA	d	406	17	-	9/31/109/115	-
24	KC1	4	307	20	-	8/15/71/71	-
21	CLA	8	304	23	-	9/21/99/115	-
21	CLA	D	406	17	1/1/13/20	7/28/104/115	-
28	LMG	b	622	-	-	16/30/50/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	b	605	4	1/1/14/20	9/35/113/115	-
21	CLA	2	304	16	-	3/8/86/115	-
21	CLA	g	302	1	1/1/15/20	11/37/115/115	-
25	BCR	D	408	-	-	8/29/63/63	0/2/2/2
21	CLA	c	511	18	1/1/15/20	8/37/115/115	-
24	KC1	1	315	-	-	8/15/71/71	-
21	CLA	7	300	1	1/1/15/20	12/37/115/115	-
23	A86	2	308	-	-	9/34/90/90	0/3/3/3
24	KC1	4	306	20	-	2/8/64/71	-
25	BCR	H	100	-	-	8/29/63/63	0/2/2/2
27	LHG	A	406	-	-	29/53/53/53	-
21	CLA	J	304	2	1/1/10/20	3/11/89/115	-
21	CLA	4	302	20	-	14/27/105/115	-
21	CLA	6	306	36	1/1/15/20	11/37/115/115	-
21	CLA	b	610	4	-	5/37/115/115	-
21	CLA	7	309	1	-	5/13/91/115	-
21	CLA	1	301	1	1/1/15/20	9/37/115/115	-
21	CLA	3	304	19	-	8/28/106/115	-
23	A86	7	312	-	-	21/34/90/90	0/3/3/3
28	LMG	2	318	-	-	17/41/61/70	0/1/1/1
21	CLA	7	303	1	1/1/15/20	15/37/115/115	-
21	CLA	g	309	1	1/1/12/20	8/19/97/115	-
21	CLA	1	304	1	1/1/15/20	15/37/115/115	-
21	CLA	c	512	18	1/1/15/20	6/37/115/115	-
21	CLA	B	616	4	1/1/15/20	13/37/115/115	-
29	LMU	D	412	-	-	13/21/61/61	0/2/2/2
30	DGD	C	518	-	-	16/26/66/95	0/2/2/2
29	LMU	5	301	-	-	8/18/58/61	0/2/2/2
21	CLA	A	401	3	-	8/37/115/115	-
21	CLA	a	403	36	-	5/18/96/115	-
25	BCR	A	405	-	-	5/29/63/63	0/2/2/2
21	CLA	b	613	4	1/1/15/20	10/37/115/115	-
23	A86	J	309	-	-	19/34/90/90	0/3/3/3
24	KC1	J	311	2	-	7/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	404	3	-	7/31/109/115	-
21	CLA	6	302	2	1/1/11/20	3/13/91/115	-
23	A86	7	313	-	-	14/30/84/90	0/3/3/3
21	CLA	B	602	-	1/1/11/20	5/16/94/115	-
21	CLA	2	301	16	1/1/15/20	15/37/115/115	-
23	A86	2	307	-	-	12/34/90/90	0/3/3/3
21	CLA	B	605	4	-	11/33/111/115	-
24	KC1	6	311	2	-	9/15/71/71	-
21	CLA	3	303	19	-	2/10/88/115	-
24	KC1	g	313	1	-	8/15/71/71	-
28	LMG	b	624	-	-	16/32/52/70	0/1/1/1
21	CLA	b	614	4	1/1/15/20	6/37/115/115	-
21	CLA	6	308	2	1/1/12/20	8/22/100/115	-
21	CLA	b	608	4	-	13/37/115/115	-
23	A86	5	311	-	-	10/34/90/90	0/3/3/3
21	CLA	2	303	36	1/1/12/20	8/21/99/115	-
23	A86	7	311	-	-	24/34/90/90	0/3/3/3
24	KC1	2	314	16	-	6/15/71/71	-
24	KC1	G	308	20	-	7/15/71/71	-
27	LHG	B	601	-	-	23/53/53/53	-
21	CLA	4	300	-	1/1/15/20	14/37/115/115	-
21	CLA	c	510	18	1/1/15/20	8/37/115/115	-
21	CLA	9	300	19	1/1/13/20	8/27/105/115	-
21	CLA	J	303	2	-	9/13/89/115	-
23	A86	8	310	-	-	16/34/90/90	0/3/3/3
26	PHO	D	401	-	-	0/37/103/103	0/5/6/6
25	BCR	h	101	-	-	25/29/63/63	0/2/2/2
30	DGD	C	517	-	-	19/44/84/95	0/2/2/2
21	CLA	B	614	4	1/1/14/20	14/35/113/115	-
21	CLA	B	612	4	1/1/15/20	10/37/115/115	-
23	A86	2	310	-	-	16/34/90/90	0/3/3/3
21	CLA	4	304	20	1/1/15/20	17/37/115/115	-
21	CLA	g	305	-	1/1/10/20	2/8/86/115	-
21	CLA	J	305	-	1/1/11/20	4/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	d	407	-	-	7/29/63/63	0/2/2/2
21	CLA	J	307	-	1/1/15/20	13/37/115/115	-
30	DGD	B	624	-	-	20/43/79/95	0/2/2/2
21	CLA	9	302	19	1/1/11/20	3/16/94/115	-
23	A86	2	311	-	-	23/34/90/90	0/3/3/3
25	BCR	b	619	-	-	12/29/63/63	0/2/2/2
21	CLA	G	302	20	-	10/27/105/115	-
21	CLA	9	303	19	1/1/12/20	12/21/99/115	-
24	KC1	4	308	20	-	6/15/71/71	-
29	LMU	8	318	-	-	10/21/61/61	0/2/2/2
21	CLA	B	613	4	1/1/15/20	11/37/115/115	-
21	CLA	3	301	19	1/1/14/20	12/31/109/115	-
25	BCR	C	516	-	-	10/29/63/63	0/2/2/2
21	CLA	B	604	4	1/1/14/20	10/35/113/115	-
21	CLA	g	306	1	1/1/15/20	19/37/115/115	-
21	CLA	6	304	2	1/1/10/20	3/11/89/115	-
24	KC1	8	314	16	-	6/15/71/71	-
25	BCR	h	102	-	-	7/29/63/63	0/2/2/2
35	PL9	d	408	-	-	7/53/73/73	0/1/1/1
25	BCR	M	101	-	-	4/29/63/63	0/2/2/2
31	SQD	B	625	-	-	19/44/64/69	0/1/1/1
21	CLA	C	514	18	1/1/14/20	8/35/113/115	-
21	CLA	5	309	1	1/1/15/20	18/37/115/115	-
21	CLA	B	606	4	-	9/37/115/115	-
21	CLA	b	623	-	1/1/13/20	8/27/105/115	-
21	CLA	B	621	-	-	18/37/115/115	-
21	CLA	7	308	1	1/1/13/20	9/27/105/115	-
21	CLA	B	610	-	1/1/15/20	7/37/115/115	-
21	CLA	b	609	4	-	7/37/115/115	-
23	A86	2	309	-	-	21/34/90/90	0/3/3/3
23	A86	8	312	-	-	21/34/90/90	0/3/3/3
24	KC1	g	315	-	-	9/15/71/71	-
21	CLA	7	301	1	1/1/15/20	15/37/115/115	-
21	CLA	b	611	-	1/1/15/20	7/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	KC1	5	314	-	-	7/15/71/71	-

All (4279) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	303	CLA	MG-ND	-44.39	1.17	2.05
21	G	302	CLA	MG-ND	-34.75	1.36	2.05
21	G	302	CLA	MG-NA	29.57	2.76	2.06
21	4	302	CLA	MG-NC	27.33	2.71	2.06
21	J	303	CLA	MG-NA	26.01	2.68	2.06
21	9	301	CLA	MG-ND	25.93	2.57	2.05
21	g	309	CLA	MG-ND	23.40	2.52	2.05
21	g	302	CLA	MG-NC	21.64	2.57	2.06
21	9	304	CLA	MG-ND	21.34	2.48	2.05
21	G	302	CLA	MG-NC	20.56	2.55	2.06
21	G	303	CLA	MG-NA	20.42	2.54	2.06
21	9	301	CLA	MG-NC	19.89	2.53	2.06
21	9	303	CLA	MG-ND	-19.78	1.66	2.05
21	4	301	CLA	MG-NA	19.42	2.52	2.06
21	7	300	CLA	MG-ND	-18.84	1.68	2.05
21	5	308	CLA	MG-NC	18.83	2.51	2.06
21	g	309	CLA	MG-NC	18.72	2.50	2.06
21	4	303	CLA	MG-ND	-18.60	1.68	2.05
21	1	301	CLA	MG-ND	-18.43	1.69	2.05
21	G	301	CLA	MG-NA	18.00	2.49	2.06
21	a	405	CLA	MG-NC	17.74	2.48	2.06
21	2	306	CLA	MG-NA	17.00	2.46	2.06
21	J	300	CLA	MG-NA	16.91	2.46	2.06
21	3	302	CLA	MG-NA	16.90	2.46	2.06
21	6	300	CLA	MG-NA	16.81	2.46	2.06
21	1	310	CLA	MG-ND	16.78	2.39	2.05
21	1	302	CLA	MG-NA	16.72	2.46	2.06
21	1	308	CLA	MG-NA	16.59	2.45	2.06
21	A	402	CLA	MG-NA	16.56	2.45	2.06
21	5	302	CLA	MG-NC	16.54	2.45	2.06
21	a	403	CLA	MG-NA	16.52	2.45	2.06
21	8	307	CLA	MG-NA	16.49	2.45	2.06
21	6	303	CLA	MG-NC	16.34	2.45	2.06
21	g	307	CLA	MG-NA	16.33	2.45	2.06
21	5	305	CLA	MG-NA	16.31	2.45	2.06
21	J	302	CLA	MG-NA	16.13	2.44	2.06
21	7	301	CLA	MG-NA	16.10	2.44	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	g	305	CLA	MG-NA	16.06	2.44	2.06
21	2	302	CLA	MG-NA	16.05	2.44	2.06
21	b	603	CLA	MG-NA	15.67	2.43	2.06
21	3	303	CLA	MG-NC	15.64	2.43	2.06
21	g	304	CLA	MG-ND	15.63	2.36	2.05
21	7	309	CLA	MG-ND	15.59	2.36	2.05
21	B	602	CLA	MG-NA	15.54	2.43	2.06
21	J	303	CLA	MG-NC	15.44	2.42	2.06
21	3	304	CLA	MG-ND	-15.38	1.75	2.05
21	B	607	CLA	MG-NA	15.25	2.42	2.06
21	b	608	CLA	MG-NA	14.99	2.41	2.06
21	4	300	CLA	MG-ND	-14.97	1.76	2.05
21	5	302	CLA	MG-ND	-14.97	1.76	2.05
21	G	300	CLA	MG-NA	14.93	2.41	2.06
21	3	304	CLA	MG-NC	14.90	2.41	2.06
21	7	307	CLA	MG-NA	14.80	2.41	2.06
21	c	509	CLA	MG-NC	14.77	2.41	2.06
21	1	310	CLA	MG-NC	14.66	2.41	2.06
21	A	404	CLA	MG-NC	14.51	2.40	2.06
21	8	303	CLA	MG-NA	14.49	2.40	2.06
21	5	303	CLA	MG-NA	14.28	2.40	2.06
21	a	405	CLA	MG-ND	14.26	2.34	2.05
21	4	303	CLA	MG-NA	14.19	2.40	2.06
21	G	300	CLA	MG-ND	-14.08	1.77	2.05
21	C	505	CLA	MG-NA	13.91	2.39	2.06
21	9	303	CLA	MG-NA	13.88	2.39	2.06
21	3	303	CLA	MG-ND	13.68	2.32	2.05
21	5	307	CLA	MG-NA	13.67	2.38	2.06
21	C	507	CLA	MG-NA	13.67	2.38	2.06
21	b	611	CLA	MG-NC	13.62	2.38	2.06
21	c	506	CLA	MG-NA	13.47	2.38	2.06
21	9	302	CLA	MG-NA	13.45	2.38	2.06
21	1	309	CLA	MG-NC	13.31	2.37	2.06
21	J	305	CLA	MG-NC	13.29	2.37	2.06
21	D	407	CLA	MG-NC	13.21	2.37	2.06
21	g	303	CLA	MG-NA	13.19	2.37	2.06
21	C	510	CLA	MG-NC	13.19	2.37	2.06
21	6	302	CLA	MG-ND	-13.17	1.79	2.05
21	c	514	CLA	MG-NA	13.16	2.37	2.06
21	c	502	CLA	MG-NA	13.13	2.37	2.06
21	b	610	CLA	MG-NC	12.96	2.37	2.06
21	d	406	CLA	MG-NC	12.96	2.37	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	304	CLA	MG-NA	12.94	2.37	2.06
21	1	303	CLA	MG-NA	12.94	2.37	2.06
21	C	513	CLA	MG-NA	12.93	2.37	2.06
21	7	302	CLA	MG-NA	12.92	2.37	2.06
21	3	300	CLA	MG-NA	12.91	2.36	2.06
21	5	309	CLA	MG-NC	12.84	2.36	2.06
21	6	305	CLA	MG-NC	12.82	2.36	2.06
21	8	302	CLA	MG-NA	12.79	2.36	2.06
21	3	300	CLA	MG-ND	12.68	2.30	2.05
21	C	515	CLA	MG-NA	12.57	2.36	2.06
21	B	609	CLA	MG-NC	12.57	2.36	2.06
21	7	303	CLA	MG-ND	12.55	2.30	2.05
21	9	300	CLA	MG-ND	12.53	2.30	2.05
21	B	610	CLA	MG-NC	12.48	2.35	2.06
21	C	503	CLA	MG-NA	12.46	2.35	2.06
21	B	612	CLA	MG-NC	12.40	2.35	2.06
21	7	308	CLA	MG-NC	12.35	2.35	2.06
21	7	309	CLA	MG-NC	12.24	2.35	2.06
21	3	301	CLA	MG-NC	12.16	2.35	2.06
21	7	303	CLA	MG-NA	12.14	2.35	2.06
21	7	300	CLA	MG-NC	12.12	2.35	2.06
21	2	301	CLA	MG-NA	12.08	2.35	2.06
21	5	304	CLA	MG-ND	12.07	2.29	2.05
21	4	300	CLA	MG-NC	12.05	2.34	2.06
21	2	303	CLA	MG-NA	12.04	2.34	2.06
21	J	304	CLA	MG-NA	11.99	2.34	2.06
21	7	305	CLA	MG-NC	11.96	2.34	2.06
21	b	614	CLA	MG-NC	11.93	2.34	2.06
21	B	615	CLA	MG-NC	11.85	2.34	2.06
21	D	404	CLA	MG-NA	11.83	2.34	2.06
21	b	613	CLA	MG-NC	11.81	2.34	2.06
21	J	306	CLA	MG-ND	-11.72	1.82	2.05
21	7	304	CLA	MG-NA	11.70	2.34	2.06
21	c	504	CLA	MG-NC	11.69	2.34	2.06
21	B	616	CLA	MG-NA	11.67	2.34	2.06
21	d	404	CLA	MG-NA	11.65	2.34	2.06
21	B	613	CLA	MG-NC	11.59	2.33	2.06
21	1	307	CLA	MG-NA	11.54	2.33	2.06
21	9	300	CLA	MG-NA	11.53	2.33	2.06
21	4	302	CLA	MG-ND	11.50	2.28	2.05
21	6	304	CLA	MG-NA	11.23	2.33	2.06
21	3	301	CLA	MG-ND	-11.22	1.83	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	304	CLA	MG-ND	11.21	2.28	2.05
21	c	512	CLA	MG-NA	11.16	2.32	2.06
21	b	616	CLA	MG-NC	11.14	2.32	2.06
21	b	605	CLA	MG-NC	11.05	2.32	2.06
21	C	514	CLA	MG-NC	11.03	2.32	2.06
21	7	305	CLA	MG-ND	-10.99	1.84	2.05
21	B	603	CLA	MG-NA	10.97	2.32	2.06
21	6	306	CLA	MG-NA	10.96	2.32	2.06
21	1	301	CLA	MG-NC	10.94	2.32	2.06
21	b	609	CLA	MG-NA	10.88	2.32	2.06
21	1	309	CLA	MG-ND	-10.86	1.84	2.05
21	b	617	CLA	MG-NA	10.83	2.32	2.06
21	B	608	CLA	MG-NA	10.79	2.31	2.06
21	B	621	CLA	MG-NA	10.68	2.31	2.06
21	B	604	CLA	MG-NC	10.63	2.31	2.06
24	2	315	KC1	C1D-ND	10.62	1.44	1.35
24	G	308	KC1	C1D-ND	10.59	1.44	1.35
21	c	513	CLA	MG-NC	10.51	2.31	2.06
21	B	611	CLA	MG-NA	10.50	2.31	2.06
24	8	315	KC1	C1D-ND	10.49	1.44	1.35
21	C	505	CLA	MG-NC	10.45	2.31	2.06
21	B	613	CLA	MG-ND	-10.42	1.85	2.05
21	b	614	CLA	MG-ND	-10.41	1.85	2.05
21	5	305	CLA	MG-ND	10.41	2.26	2.05
24	9	306	KC1	C1D-ND	10.39	1.44	1.35
21	7	302	CLA	MG-ND	-10.39	1.85	2.05
24	g	314	KC1	C1D-ND	10.39	1.44	1.35
21	6	306	CLA	MG-ND	-10.38	1.85	2.05
21	A	401	CLA	MG-NC	10.37	2.30	2.06
21	1	305	CLA	MG-NA	10.37	2.30	2.06
21	8	305	CLA	MG-NA	10.37	2.30	2.06
24	4	309	KC1	C1D-ND	10.35	1.44	1.35
24	G	306	KC1	C1D-ND	10.34	1.44	1.35
21	a	402	CLA	MG-NC	10.33	2.30	2.06
21	b	612	CLA	MG-NA	10.33	2.30	2.06
24	6	312	KC1	C1D-ND	10.33	1.44	1.35
21	A	404	CLA	MG-ND	10.33	2.26	2.05
24	g	315	KC1	C1D-ND	10.33	1.44	1.35
24	J	313	KC1	C1D-ND	10.31	1.44	1.35
24	3	305	KC1	C1D-ND	10.31	1.44	1.35
24	2	313	KC1	C1D-ND	10.29	1.44	1.35
24	4	306	KC1	C1D-ND	10.26	1.44	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	312	KC1	C1D-ND	10.23	1.44	1.35
24	4	308	KC1	C1D-ND	10.20	1.44	1.35
24	5	314	KC1	C1D-ND	10.19	1.44	1.35
21	2	305	CLA	MG-NA	10.19	2.30	2.06
21	7	306	CLA	MG-NA	10.15	2.30	2.06
24	8	313	KC1	C1D-ND	10.14	1.44	1.35
24	3	306	KC1	C1D-ND	10.12	1.44	1.35
24	1	315	KC1	C1D-ND	10.11	1.44	1.35
21	6	308	CLA	MG-NC	10.11	2.30	2.06
21	8	304	CLA	MG-NA	10.11	2.30	2.06
24	G	309	KC1	C1D-ND	10.11	1.44	1.35
24	6	313	KC1	C1D-ND	10.07	1.44	1.35
24	2	316	KC1	C1D-ND	10.07	1.44	1.35
24	8	316	KC1	C1D-ND	10.04	1.44	1.35
21	6	300	CLA	MG-ND	10.02	2.25	2.05
21	9	304	CLA	MG-NC	9.99	2.30	2.06
24	1	316	KC1	C1D-ND	9.98	1.44	1.35
24	G	307	KC1	C1D-ND	9.96	1.44	1.35
24	5	313	KC1	C1D-ND	9.91	1.44	1.35
24	4	307	KC1	C1D-ND	9.91	1.44	1.35
21	B	605	CLA	MG-NA	9.91	2.29	2.06
24	7	315	KC1	C1D-ND	9.90	1.44	1.35
24	g	313	KC1	C1D-ND	9.87	1.44	1.35
24	7	314	KC1	C1D-ND	9.83	1.44	1.35
24	8	314	KC1	C1D-ND	9.81	1.44	1.35
24	2	314	KC1	C1D-ND	9.80	1.44	1.35
24	9	305	KC1	C1D-ND	9.74	1.43	1.35
24	5	315	KC1	C1D-ND	9.72	1.43	1.35
21	c	508	CLA	MG-NC	9.71	2.29	2.06
21	b	606	CLA	MG-NA	9.71	2.29	2.06
21	b	604	CLA	MG-NA	9.69	2.29	2.06
21	C	509	CLA	MG-NC	9.69	2.29	2.06
21	J	308	CLA	MG-NC	9.68	2.29	2.06
21	6	302	CLA	MG-NC	9.64	2.29	2.06
24	6	311	KC1	C1D-ND	9.60	1.43	1.35
21	1	303	CLA	MG-ND	-9.60	1.86	2.05
21	8	306	CLA	MG-NA	9.58	2.29	2.06
24	J	311	KC1	C1D-ND	9.57	1.43	1.35
21	B	610	CLA	MG-ND	-9.52	1.86	2.05
21	6	301	CLA	MG-NC	9.51	2.28	2.06
21	b	607	CLA	MG-NC	9.50	2.28	2.06
21	b	623	CLA	MG-NA	9.42	2.28	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	606	CLA	MG-NC	9.38	2.28	2.06
21	5	304	CLA	MG-NA	9.36	2.28	2.06
21	3	303	CLA	MG-NA	9.33	2.28	2.06
21	C	504	CLA	MG-NC	9.19	2.28	2.06
21	g	304	CLA	MG-NC	9.18	2.28	2.06
21	c	503	CLA	MG-NC	9.16	2.28	2.06
21	J	300	CLA	MG-ND	9.13	2.23	2.05
21	C	505	CLA	MG-ND	9.08	2.23	2.05
21	b	611	CLA	MG-ND	-9.04	1.87	2.05
21	C	506	CLA	MG-NC	9.04	2.27	2.06
21	B	614	CLA	MG-NC	8.92	2.27	2.06
21	8	302	CLA	MG-ND	8.89	2.23	2.05
21	J	303	CLA	C3B-C4B	8.84	1.49	1.39
21	g	306	CLA	MG-NC	8.80	2.27	2.06
21	5	309	CLA	MG-NA	8.74	2.27	2.06
21	g	308	CLA	MG-NA	8.74	2.27	2.06
21	6	303	CLA	C3B-C4B	8.74	1.49	1.39
21	1	306	CLA	MG-NA	8.71	2.27	2.06
21	c	507	CLA	MG-NC	8.67	2.26	2.06
21	b	616	CLA	MG-NA	8.66	2.26	2.06
21	b	615	CLA	MG-NC	8.62	2.26	2.06
21	C	515	CLA	MG-ND	8.57	2.22	2.05
21	D	406	CLA	MG-NC	8.50	2.26	2.06
21	J	304	CLA	MG-ND	8.48	2.22	2.05
21	A	401	CLA	MG-NA	8.42	2.26	2.06
21	3	302	CLA	MG-ND	-8.42	1.89	2.05
21	a	402	CLA	MG-NA	8.39	2.26	2.06
21	B	615	CLA	MG-NA	8.38	2.26	2.06
21	c	505	CLA	MG-NC	8.34	2.26	2.06
21	d	405	CLA	MG-NC	8.32	2.26	2.06
21	C	508	CLA	MG-NC	8.30	2.26	2.06
21	2	302	CLA	MG-ND	-8.27	1.89	2.05
21	D	407	CLA	MG-ND	8.18	2.22	2.05
21	D	406	CLA	MG-NA	8.10	2.25	2.06
24	4	306	KC1	C3A-C2A	8.08	1.52	1.36
21	2	304	CLA	MG-NA	8.07	2.25	2.06
21	b	610	CLA	MG-NA	8.07	2.25	2.06
21	6	303	CLA	MG-ND	8.04	2.21	2.05
21	9	301	CLA	MG-NA	8.03	2.25	2.06
21	B	609	CLA	MG-NA	8.03	2.25	2.06
24	G	306	KC1	C3A-C2A	7.99	1.52	1.36
21	B	613	CLA	MG-NA	7.99	2.25	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	304	CLA	MG-ND	7.97	2.21	2.05
21	g	308	CLA	MG-NC	7.97	2.25	2.06
21	5	308	CLA	MG-NA	7.95	2.25	2.06
21	J	306	CLA	MG-NC	7.92	2.25	2.06
21	8	303	CLA	MG-ND	-7.90	1.90	2.05
21	g	302	CLA	MG-NA	-7.89	1.87	2.06
24	2	316	KC1	C2A-C3A	7.85	1.53	1.37
21	5	306	CLA	MG-NC	7.84	2.24	2.06
24	8	316	KC1	C2A-C3A	7.80	1.53	1.37
21	8	304	CLA	MG-NC	7.73	2.24	2.06
21	G	304	CLA	MG-NA	7.72	2.24	2.06
21	d	406	CLA	MG-ND	7.69	2.21	2.05
24	8	314	KC1	C2A-C3A	7.61	1.52	1.37
21	2	301	CLA	MG-ND	7.61	2.20	2.05
21	B	614	CLA	MG-NA	7.60	2.24	2.06
24	2	314	KC1	C2A-C3A	7.59	1.52	1.37
21	g	305	CLA	MG-ND	7.55	2.20	2.05
24	2	313	KC1	C2A-C3A	7.53	1.52	1.37
21	d	405	CLA	MG-NA	7.52	2.24	2.06
24	9	306	KC1	C2A-C3A	7.43	1.52	1.37
24	2	315	KC1	C2A-C3A	7.43	1.52	1.37
24	J	311	KC1	C2A-C3A	7.41	1.52	1.37
24	G	309	KC1	C2A-C3A	7.40	1.52	1.37
21	c	504	CLA	MG-NA	7.40	2.23	2.06
24	4	309	KC1	C2A-C3A	7.40	1.52	1.37
24	4	307	KC1	C2A-C3A	7.39	1.52	1.37
21	c	514	CLA	MG-ND	7.37	2.20	2.05
21	b	614	CLA	MG-NA	7.37	2.23	2.06
21	b	615	CLA	MG-NA	7.36	2.23	2.06
24	5	314	KC1	C2A-C3A	7.35	1.52	1.37
24	6	311	KC1	C2A-C3A	7.34	1.52	1.37
24	G	308	KC1	C2A-C3A	7.34	1.52	1.37
24	8	315	KC1	C2A-C3A	7.34	1.52	1.37
24	J	313	KC1	C2A-C3A	7.34	1.52	1.37
24	6	312	KC1	C2A-C3A	7.33	1.52	1.37
24	8	313	KC1	C2A-C3A	7.32	1.52	1.37
24	6	313	KC1	C2A-C3A	7.31	1.52	1.37
24	7	314	KC1	C2A-C3A	7.30	1.52	1.37
24	J	312	KC1	C2A-C3A	7.29	1.52	1.37
24	9	305	KC1	C2A-C3A	7.29	1.52	1.37
24	G	307	KC1	C2A-C3A	7.28	1.52	1.37
24	5	315	KC1	C2A-C3A	7.28	1.52	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	315	KC1	C2A-C3A	7.26	1.52	1.37
24	3	306	KC1	C2A-C3A	7.25	1.52	1.37
24	1	315	KC1	C2A-C3A	7.25	1.52	1.37
24	g	315	KC1	C2A-C3A	7.25	1.52	1.37
24	g	314	KC1	C2A-C3A	7.24	1.51	1.37
21	C	504	CLA	MG-NA	7.23	2.23	2.06
21	C	508	CLA	MG-NA	7.22	2.23	2.06
21	B	606	CLA	MG-NA	7.21	2.23	2.06
24	5	313	KC1	C2A-C3A	7.20	1.51	1.37
24	3	305	KC1	C2A-C3A	7.20	1.51	1.37
21	4	304	CLA	MG-NA	7.18	2.23	2.06
21	b	607	CLA	MG-NA	7.17	2.23	2.06
21	c	506	CLA	MG-NC	7.15	2.23	2.06
24	g	313	KC1	C2A-C3A	7.14	1.51	1.37
21	c	503	CLA	MG-NA	7.14	2.23	2.06
24	1	316	KC1	C2A-C3A	7.13	1.51	1.37
21	c	511	CLA	MG-NC	6.98	2.22	2.06
24	4	308	KC1	C2A-C3A	6.94	1.51	1.37
21	c	507	CLA	MG-NA	6.89	2.22	2.06
21	b	604	CLA	MG-NC	6.88	2.22	2.06
24	8	316	KC1	CBA-CAA	6.82	1.53	1.33
21	1	306	CLA	MG-NC	6.82	2.22	2.06
21	C	514	CLA	MG-NA	6.81	2.22	2.06
24	2	316	KC1	CBA-CAA	6.77	1.53	1.33
21	7	308	CLA	MG-ND	-6.75	1.92	2.05
21	J	307	CLA	MG-NA	6.70	2.22	2.06
24	2	314	KC1	CBA-CAA	6.68	1.53	1.33
24	8	314	KC1	CBA-CAA	6.66	1.53	1.33
24	J	313	KC1	CBA-CAA	6.66	1.53	1.33
24	7	315	KC1	CBA-CAA	6.65	1.53	1.33
21	c	510	CLA	MG-NC	6.64	2.22	2.06
24	6	313	KC1	CBA-CAA	6.64	1.53	1.33
21	C	507	CLA	MG-NC	6.64	2.22	2.06
24	1	316	KC1	CBA-CAA	6.64	1.53	1.33
23	5	311	A86	C13-C11	-6.63	1.36	1.49
21	3	304	CLA	MG-NA	6.63	2.22	2.06
21	C	512	CLA	MG-NC	6.63	2.22	2.06
24	4	308	KC1	CBA-CAA	6.62	1.53	1.33
24	3	306	KC1	CBA-CAA	6.61	1.53	1.33
21	6	307	CLA	MG-NA	6.60	2.22	2.06
24	4	309	KC1	CBA-CAA	6.59	1.53	1.33
24	6	312	KC1	CBA-CAA	6.58	1.53	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	312	KC1	CBA-CAA	6.57	1.52	1.33
21	C	510	CLA	MG-NA	6.57	2.21	2.06
23	7	313	A86	C13-C11	-6.57	1.36	1.49
23	8	309	A86	C13-C11	-6.56	1.36	1.49
24	1	315	KC1	CBA-CAA	6.55	1.52	1.33
24	2	315	KC1	CBA-CAA	6.55	1.52	1.33
24	G	308	KC1	CBA-CAA	6.54	1.52	1.33
24	g	314	KC1	CBA-CAA	6.54	1.52	1.33
23	2	308	A86	C13-C11	-6.54	1.37	1.49
23	G	305	A86	C13-C11	-6.54	1.37	1.49
24	9	306	KC1	CBA-CAA	6.54	1.52	1.33
24	8	313	KC1	CBA-CAA	6.54	1.52	1.33
24	3	305	KC1	CBA-CAA	6.53	1.52	1.33
24	g	315	KC1	CBA-CAA	6.52	1.52	1.33
24	G	309	KC1	CBA-CAA	6.52	1.52	1.33
24	2	313	KC1	CBA-CAA	6.52	1.52	1.33
24	6	311	KC1	CBA-CAA	6.52	1.52	1.33
21	g	304	CLA	MG-NA	6.52	2.21	2.06
24	5	314	KC1	CBA-CAA	6.51	1.52	1.33
24	7	314	KC1	CBA-CAA	6.51	1.52	1.33
24	9	305	KC1	CBA-CAA	6.50	1.52	1.33
23	2	307	A86	C13-C11	-6.49	1.37	1.49
24	G	307	KC1	CBA-CAA	6.49	1.52	1.33
23	6	310	A86	C13-C11	-6.48	1.37	1.49
24	8	315	KC1	CBA-CAA	6.47	1.52	1.33
23	g	311	A86	C13-C11	-6.46	1.37	1.49
24	5	315	KC1	CBA-CAA	6.46	1.52	1.33
24	g	313	KC1	CBA-CAA	6.46	1.52	1.33
24	5	313	KC1	CBA-CAA	6.44	1.52	1.33
23	J	310	A86	C13-C11	-6.43	1.37	1.49
23	2	310	A86	C13-C11	-6.41	1.37	1.49
23	8	311	A86	C13-C11	-6.41	1.37	1.49
24	J	311	KC1	CBA-CAA	6.40	1.52	1.33
21	g	307	CLA	MG-ND	6.40	2.18	2.05
21	B	604	CLA	MG-NA	6.38	2.21	2.06
21	b	613	CLA	MG-NA	6.37	2.21	2.06
21	c	513	CLA	MG-NA	6.37	2.21	2.06
24	4	307	KC1	CBA-CAA	6.36	1.52	1.33
21	J	301	CLA	MG-NC	6.35	2.21	2.06
21	B	605	CLA	MG-NC	6.32	2.21	2.06
23	J	309	A86	C13-C11	-6.30	1.37	1.49
23	8	310	A86	C13-C11	-6.28	1.37	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	511	CLA	MG-NC	6.27	2.21	2.06
23	4	305	A86	C13-C11	-6.25	1.37	1.49
23	6	309	A86	C13-C11	-6.25	1.37	1.49
21	b	606	CLA	MG-NC	6.23	2.21	2.06
23	1	313	A86	C13-C11	-6.23	1.37	1.49
23	2	312	A86	C13-C11	-6.22	1.37	1.49
21	b	605	CLA	MG-NA	6.21	2.21	2.06
23	7	311	A86	C13-C11	-6.21	1.37	1.49
23	1	312	A86	C13-C11	-6.21	1.37	1.49
23	g	312	A86	C13-C11	-6.15	1.37	1.49
23	8	312	A86	C13-C11	-6.15	1.37	1.49
21	B	608	CLA	MG-NC	6.11	2.20	2.06
23	8	308	A86	C13-C11	-6.08	1.37	1.49
23	7	312	A86	C13-C11	-6.08	1.37	1.49
21	B	612	CLA	MG-NA	6.08	2.20	2.06
21	4	304	CLA	C3C-C2C	6.06	1.49	1.36
21	2	304	CLA	MG-NC	6.06	2.20	2.06
21	9	303	CLA	C3C-C2C	6.05	1.49	1.36
23	2	309	A86	C13-C11	-6.04	1.37	1.49
23	5	312	A86	C13-C11	-6.04	1.37	1.49
24	G	307	KC1	O2A-CGA	6.03	1.46	1.30
21	b	609	CLA	MG-NC	6.02	2.20	2.06
21	3	300	CLA	MG-NC	6.02	2.20	2.06
24	2	315	KC1	O2A-CGA	6.01	1.46	1.30
21	7	304	CLA	C3C-C2C	6.01	1.49	1.36
21	5	306	CLA	C3B-C2B	5.99	1.48	1.40
23	1	314	A86	C13-C11	-5.98	1.38	1.49
24	J	311	KC1	O2A-CGA	5.97	1.45	1.30
24	g	313	KC1	O2A-CGA	5.96	1.45	1.30
24	G	309	KC1	O2A-CGA	5.96	1.45	1.30
24	5	314	KC1	O2A-CGA	5.96	1.45	1.30
24	4	309	KC1	O2A-CGA	5.96	1.45	1.30
24	g	314	KC1	O2A-CGA	5.95	1.45	1.30
24	G	308	KC1	O2A-CGA	5.95	1.45	1.30
24	5	315	KC1	O2A-CGA	5.95	1.45	1.30
24	9	306	KC1	O2A-CGA	5.95	1.45	1.30
24	6	312	KC1	O2A-CGA	5.95	1.45	1.30
24	J	313	KC1	O2A-CGA	5.95	1.45	1.30
24	g	315	KC1	O2A-CGA	5.94	1.45	1.30
21	C	515	CLA	MG-NC	5.94	2.20	2.06
24	5	313	KC1	O2A-CGA	5.94	1.45	1.30
24	3	306	KC1	O2A-CGA	5.94	1.45	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	313	KC1	O2A-CGA	5.94	1.45	1.30
24	4	308	KC1	O2A-CGA	5.94	1.45	1.30
24	3	305	KC1	O2A-CGA	5.93	1.45	1.30
24	7	315	KC1	O2A-CGA	5.93	1.45	1.30
24	1	316	KC1	O2A-CGA	5.93	1.45	1.30
24	6	311	KC1	O2A-CGA	5.93	1.45	1.30
24	G	306	KC1	C3C-C2C	5.93	1.48	1.35
24	1	315	KC1	O2A-CGA	5.93	1.45	1.30
24	2	313	KC1	O2A-CGA	5.92	1.45	1.30
21	D	406	CLA	C3C-C2C	5.92	1.48	1.36
21	d	405	CLA	C3C-C2C	5.92	1.48	1.36
21	7	302	CLA	C3B-C2B	5.91	1.48	1.40
24	J	312	KC1	O2A-CGA	5.91	1.45	1.30
21	3	300	CLA	C3B-C2B	5.91	1.48	1.40
24	8	314	KC1	O2A-CGA	5.90	1.45	1.30
24	7	314	KC1	O2A-CGA	5.90	1.45	1.30
24	9	305	KC1	O2A-CGA	5.89	1.45	1.30
21	C	512	CLA	C3B-C2B	5.89	1.48	1.40
24	2	314	KC1	O2A-CGA	5.89	1.45	1.30
21	4	301	CLA	MG-ND	-5.89	1.94	2.05
21	c	510	CLA	MG-NA	5.88	2.20	2.06
21	1	303	CLA	C3B-C2B	5.87	1.48	1.40
24	8	313	KC1	O2A-CGA	5.86	1.45	1.30
21	6	307	CLA	MG-NC	5.85	2.20	2.06
24	8	316	KC1	O2A-CGA	5.85	1.45	1.30
24	4	306	KC1	C3C-C2C	5.85	1.48	1.35
21	g	306	CLA	C3B-C2B	5.84	1.48	1.40
23	2	311	A86	C13-C11	-5.84	1.38	1.49
21	G	304	CLA	C3B-C2B	5.83	1.48	1.40
24	2	316	KC1	O2A-CGA	5.83	1.45	1.30
24	4	307	KC1	O2A-CGA	5.83	1.45	1.30
23	W	101	A86	C13-C11	-5.82	1.38	1.49
21	5	302	CLA	C3B-C2B	5.82	1.48	1.40
21	B	603	CLA	MG-ND	-5.82	1.94	2.05
21	4	301	CLA	MG-NC	-5.82	1.92	2.06
21	2	304	CLA	MG-ND	5.79	2.17	2.05
24	G	308	KC1	C3D-C2D	5.78	1.49	1.39
21	C	511	CLA	MG-NA	5.78	2.20	2.06
21	G	302	CLA	C3B-C2B	5.77	1.48	1.40
21	g	302	CLA	MG-ND	-5.77	1.94	2.05
21	5	305	CLA	C3B-C2B	5.77	1.48	1.40
21	7	309	CLA	C3B-C2B	5.76	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	508	CLA	C3B-C2B	5.76	1.48	1.40
21	5	304	CLA	MG-NC	5.76	2.20	2.06
21	7	305	CLA	C3B-C2B	5.76	1.48	1.40
21	4	304	CLA	C3B-C2B	5.75	1.48	1.40
21	C	509	CLA	C3B-C2B	5.75	1.48	1.40
21	b	613	CLA	C3B-C2B	5.75	1.48	1.40
24	8	315	KC1	O2A-CGA	5.74	1.45	1.30
24	G	309	KC1	C3B-C2B	5.74	1.48	1.37
21	B	611	CLA	C3B-C2B	5.74	1.48	1.40
24	5	314	KC1	C3D-C2D	5.73	1.49	1.39
21	G	303	CLA	MG-NC	-5.73	1.92	2.06
24	8	314	KC1	C3D-C2D	5.72	1.49	1.39
21	4	300	CLA	C3B-C2B	5.72	1.48	1.40
24	9	306	KC1	C3B-C2B	5.72	1.48	1.37
21	9	303	CLA	C3B-C2B	5.71	1.48	1.40
24	3	306	KC1	C3D-C2D	5.71	1.49	1.39
21	A	401	CLA	C3B-C2B	5.71	1.48	1.40
21	9	304	CLA	C3B-C2B	5.70	1.48	1.40
21	4	302	CLA	C3B-C2B	5.69	1.48	1.40
21	b	612	CLA	C3B-C2B	5.68	1.48	1.40
21	9	301	CLA	C3B-C2B	5.68	1.48	1.40
21	c	511	CLA	C3B-C2B	5.68	1.48	1.40
21	1	301	CLA	C3B-C2B	5.68	1.48	1.40
21	c	505	CLA	MG-NA	5.68	2.19	2.06
21	B	612	CLA	C3B-C2B	5.68	1.48	1.40
24	4	308	KC1	C3B-C2B	5.67	1.48	1.37
24	4	308	KC1	C3D-C2D	5.67	1.49	1.39
24	3	305	KC1	C3D-C2D	5.66	1.49	1.39
24	8	315	KC1	C3D-C2D	5.66	1.49	1.39
21	B	603	CLA	C3B-C2B	5.66	1.48	1.40
24	3	305	KC1	C3B-C2B	5.65	1.48	1.37
21	4	302	CLA	C3C-C2C	5.65	1.48	1.36
21	3	300	CLA	C3C-C2C	5.65	1.48	1.36
21	C	510	CLA	C3B-C2B	5.65	1.48	1.40
24	7	315	KC1	C3D-C2D	5.65	1.49	1.39
24	G	309	KC1	C3D-C2D	5.65	1.49	1.39
21	b	617	CLA	C3B-C2B	5.64	1.48	1.40
21	5	303	CLA	C3B-C2B	5.64	1.48	1.40
24	6	311	KC1	C3D-C2D	5.64	1.49	1.39
24	2	314	KC1	C3D-C2D	5.64	1.49	1.39
24	g	313	KC1	C3B-C2B	5.64	1.48	1.37
21	5	306	CLA	C3C-C2C	5.64	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	304	CLA	C3B-C2B	5.63	1.48	1.40
24	1	316	KC1	C3D-C2D	5.63	1.49	1.39
21	a	402	CLA	C3B-C2B	5.63	1.48	1.40
21	B	614	CLA	MG-ND	5.63	2.16	2.05
21	4	303	CLA	C3B-C2B	5.63	1.48	1.40
24	2	315	KC1	C3D-C2D	5.62	1.49	1.39
24	J	311	KC1	C3D-C2D	5.62	1.49	1.39
24	9	306	KC1	C3D-C2D	5.62	1.49	1.39
21	c	510	CLA	C3B-C2B	5.62	1.48	1.40
24	4	307	KC1	C3B-C2B	5.62	1.48	1.37
21	g	302	CLA	C3B-C2B	5.62	1.48	1.40
21	g	306	CLA	C3C-C2C	5.61	1.48	1.36
24	G	308	KC1	C3B-C2B	5.61	1.48	1.37
21	B	616	CLA	C3B-C2B	5.61	1.48	1.40
24	G	306	KC1	C3B-C2B	5.61	1.48	1.37
24	8	313	KC1	C3B-C2B	5.61	1.48	1.37
24	g	315	KC1	C3B-C2B	5.61	1.48	1.37
24	4	309	KC1	C3D-C2D	5.60	1.49	1.39
24	J	311	KC1	C3B-C2B	5.60	1.48	1.37
21	5	309	CLA	C3B-C2B	5.60	1.48	1.40
21	c	509	CLA	C3B-C2B	5.60	1.48	1.40
24	5	315	KC1	C3B-C2B	5.60	1.48	1.37
21	b	604	CLA	MG-ND	-5.59	1.94	2.05
21	D	404	CLA	C3C-C2C	5.59	1.48	1.36
21	3	304	CLA	C3B-C2B	5.59	1.48	1.40
21	d	404	CLA	C3C-C2C	5.59	1.48	1.36
24	5	313	KC1	C3B-C2B	5.59	1.48	1.37
21	6	308	CLA	C3C-C2C	5.59	1.48	1.36
24	7	314	KC1	C3B-C2B	5.59	1.48	1.37
21	G	304	CLA	C3C-C2C	5.59	1.48	1.36
21	6	302	CLA	C3B-C2B	5.59	1.48	1.40
21	7	301	CLA	C3B-C2B	5.58	1.48	1.40
21	7	301	CLA	C3C-C2C	5.58	1.48	1.36
24	1	315	KC1	C3B-C2B	5.58	1.48	1.37
21	c	506	CLA	C3B-C2B	5.57	1.48	1.40
21	b	612	CLA	MG-NC	5.57	2.19	2.06
24	J	313	KC1	C3B-C2B	5.57	1.48	1.37
21	b	611	CLA	C3B-C2B	5.57	1.48	1.40
24	J	312	KC1	C3B-C2B	5.57	1.48	1.37
24	9	305	KC1	C3B-C2B	5.57	1.48	1.37
21	b	604	CLA	C3B-C2B	5.57	1.48	1.40
24	G	306	KC1	C3D-C2D	5.57	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	302	CLA	C3B-C2B	5.56	1.48	1.40
24	g	315	KC1	C3D-C2D	5.56	1.49	1.39
21	B	611	CLA	MG-NC	5.56	2.19	2.06
21	8	305	CLA	C3B-C2B	5.56	1.48	1.40
21	6	308	CLA	C3B-C2B	5.56	1.48	1.40
21	B	613	CLA	C3B-C2B	5.55	1.48	1.40
21	2	305	CLA	C3B-C2B	5.55	1.48	1.40
24	4	306	KC1	C3D-C2D	5.55	1.49	1.39
21	C	511	CLA	C3B-C2B	5.55	1.48	1.40
21	g	309	CLA	C3C-C2C	5.55	1.48	1.36
21	J	308	CLA	C3C-C2C	5.55	1.48	1.36
21	7	302	CLA	C3C-C2C	5.55	1.48	1.36
24	6	313	KC1	C3B-C2B	5.55	1.48	1.37
21	7	305	CLA	C3C-C2C	5.54	1.48	1.36
24	2	314	KC1	C3B-C2B	5.54	1.48	1.37
24	6	312	KC1	C3B-C2B	5.54	1.48	1.37
24	3	306	KC1	C3B-C2B	5.54	1.48	1.37
24	5	314	KC1	C3B-C2B	5.54	1.48	1.37
21	2	301	CLA	C3B-C2B	5.54	1.48	1.40
24	1	315	KC1	C3D-C2D	5.54	1.49	1.39
21	9	300	CLA	C3B-C2B	5.54	1.48	1.40
21	D	407	CLA	C3B-C2B	5.53	1.48	1.40
21	1	303	CLA	C3C-C2C	5.53	1.48	1.36
24	6	313	KC1	C3D-C2D	5.53	1.49	1.39
21	8	306	CLA	C3B-C2B	5.53	1.48	1.40
21	J	308	CLA	C3B-C2B	5.53	1.48	1.40
24	4	307	KC1	C3D-C2D	5.53	1.49	1.39
21	C	507	CLA	C3B-C2B	5.52	1.48	1.40
21	4	300	CLA	C3C-C2C	5.52	1.48	1.36
21	J	305	CLA	C3C-C2C	5.52	1.48	1.36
21	g	309	CLA	C3B-C2B	5.52	1.48	1.40
21	B	608	CLA	C3C-C2C	5.52	1.48	1.36
21	b	614	CLA	C3B-C2B	5.52	1.48	1.40
24	8	316	KC1	C3B-C2B	5.52	1.48	1.37
24	J	312	KC1	C3D-C2D	5.52	1.49	1.39
21	6	302	CLA	C3C-C2C	5.52	1.48	1.36
21	4	303	CLA	C3C-C2C	5.51	1.48	1.36
21	G	302	CLA	C3C-C2C	5.51	1.48	1.36
21	3	301	CLA	C3C-C2C	5.51	1.48	1.36
24	2	316	KC1	C3D-C2D	5.51	1.49	1.39
21	2	303	CLA	C3B-C2B	5.51	1.48	1.40
21	J	307	CLA	C3C-C2C	5.51	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	506	CLA	C3C-C2C	5.51	1.48	1.36
21	1	310	CLA	C3B-C2B	5.51	1.48	1.40
21	g	303	CLA	C3B-C2B	5.51	1.48	1.40
21	C	503	CLA	C3B-C2B	5.50	1.48	1.40
21	B	610	CLA	C3B-C2B	5.50	1.48	1.40
24	6	311	KC1	C3B-C2B	5.50	1.48	1.37
24	9	305	KC1	C3D-C2D	5.50	1.49	1.39
21	9	302	CLA	C3C-C2C	5.50	1.48	1.36
21	6	305	CLA	C3C-C2C	5.50	1.48	1.36
21	b	615	CLA	MG-ND	5.50	2.16	2.05
24	g	314	KC1	C3D-C2D	5.50	1.49	1.39
21	J	303	CLA	C3C-C2C	5.50	1.48	1.36
21	b	609	CLA	C3C-C2C	5.49	1.48	1.36
24	6	312	KC1	C3D-C2D	5.49	1.49	1.39
21	c	502	CLA	C3B-C2B	5.49	1.48	1.40
24	8	314	KC1	C3B-C2B	5.49	1.48	1.37
24	8	313	KC1	C3D-C2D	5.48	1.49	1.39
21	3	302	CLA	C3C-C2C	5.48	1.48	1.36
21	J	303	CLA	CHD-C1D	5.48	1.49	1.38
24	J	313	KC1	C3D-C2D	5.48	1.49	1.39
21	6	303	CLA	C3C-C2C	5.48	1.48	1.36
21	2	304	CLA	C3B-C2B	5.48	1.48	1.40
21	c	513	CLA	C3B-C2B	5.48	1.48	1.40
21	a	403	CLA	C3B-C2B	5.48	1.48	1.40
21	A	402	CLA	C3B-C2B	5.47	1.48	1.40
21	d	406	CLA	C3B-C2B	5.47	1.48	1.40
24	G	307	KC1	C3B-C2B	5.47	1.48	1.37
21	3	303	CLA	C3C-C2C	5.47	1.48	1.36
24	5	315	KC1	C3D-C2D	5.47	1.49	1.39
21	3	302	CLA	C3B-C2B	5.47	1.48	1.40
24	g	313	KC1	C3D-C2D	5.46	1.49	1.39
21	5	308	CLA	C3C-C2C	5.46	1.48	1.36
21	C	507	CLA	C3C-C2C	5.46	1.48	1.36
21	c	513	CLA	C3C-C2C	5.46	1.48	1.36
21	c	514	CLA	C3C-C2C	5.46	1.48	1.36
21	9	304	CLA	C3C-C2C	5.46	1.48	1.36
21	G	301	CLA	C3C-C2C	5.46	1.48	1.36
24	4	309	KC1	C3B-C2B	5.46	1.48	1.37
24	8	316	KC1	C3D-C2D	5.46	1.49	1.39
24	2	316	KC1	C3B-C2B	5.46	1.48	1.37
21	G	303	CLA	C3C-C2C	5.46	1.48	1.36
24	g	314	KC1	C3B-C2B	5.45	1.48	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	306	KC1	C3B-C2B	5.45	1.48	1.37
21	4	301	CLA	C3C-C2C	5.45	1.48	1.36
21	g	304	CLA	C3C-C2C	5.45	1.48	1.36
21	5	304	CLA	C3C-C2C	5.45	1.48	1.36
21	G	301	CLA	C3B-C2B	5.45	1.47	1.40
21	G	300	CLA	C3C-C2C	5.45	1.48	1.36
21	6	307	CLA	C3C-C2C	5.45	1.48	1.36
21	2	304	CLA	C3C-C2C	5.45	1.48	1.36
24	2	315	KC1	C3B-C2B	5.44	1.48	1.37
24	5	313	KC1	C3D-C2D	5.44	1.49	1.39
21	1	306	CLA	C3B-C2B	5.44	1.47	1.40
21	b	604	CLA	C3C-C2C	5.44	1.48	1.36
21	5	309	CLA	O2D-CGD	5.44	1.46	1.33
21	7	309	CLA	C3C-C2C	5.44	1.48	1.36
21	J	305	CLA	C3B-C2B	5.44	1.47	1.40
21	9	304	CLA	CHC-C1C	5.44	1.48	1.35
21	C	514	CLA	C3C-C2C	5.44	1.48	1.36
24	G	308	KC1	C3C-C2C	5.44	1.48	1.36
21	A	402	CLA	C3C-C2C	5.43	1.48	1.36
21	b	605	CLA	C3C-C2C	5.43	1.48	1.36
21	C	515	CLA	C3C-C2C	5.43	1.48	1.36
24	8	315	KC1	C3B-C2B	5.43	1.48	1.37
21	C	508	CLA	C3C-C2C	5.43	1.48	1.36
24	2	314	KC1	C3C-C2C	5.43	1.48	1.36
21	3	303	CLA	C3B-C2B	5.43	1.47	1.40
21	g	305	CLA	C3C-C2C	5.43	1.48	1.36
21	6	305	CLA	C3B-C2B	5.43	1.47	1.40
21	1	310	CLA	C3C-C2C	5.43	1.48	1.36
21	c	507	CLA	C3C-C2C	5.43	1.48	1.36
21	g	307	CLA	C3C-C2C	5.43	1.48	1.36
21	5	304	CLA	C3B-C2B	5.43	1.47	1.40
21	B	603	CLA	C3C-C2C	5.42	1.48	1.36
21	9	301	CLA	C3C-C2C	5.42	1.48	1.36
21	g	307	CLA	C3B-C2B	5.42	1.47	1.40
21	C	506	CLA	C3B-C2B	5.42	1.47	1.40
21	c	504	CLA	C3C-C2C	5.42	1.48	1.36
21	5	302	CLA	CHC-C1C	5.42	1.48	1.35
21	6	300	CLA	C3C-C2C	5.42	1.48	1.36
21	D	406	CLA	CHC-C1C	5.42	1.48	1.35
21	9	300	CLA	CHC-C1C	5.41	1.48	1.35
21	6	307	CLA	C3B-C2B	5.41	1.47	1.40
21	J	300	CLA	C3C-C2C	5.41	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	505	CLA	C3B-C2B	5.41	1.47	1.40
21	g	304	CLA	C3B-C2B	5.41	1.47	1.40
21	5	307	CLA	C3B-C2B	5.41	1.47	1.40
21	3	304	CLA	C3C-C2C	5.41	1.48	1.36
21	B	607	CLA	C3B-C2B	5.41	1.47	1.40
21	C	515	CLA	C3B-C2B	5.41	1.47	1.40
21	a	403	CLA	C3C-C2C	5.41	1.48	1.36
24	4	308	KC1	C3C-C2C	5.41	1.48	1.36
24	g	313	KC1	C3C-C2C	5.41	1.48	1.36
21	1	307	CLA	C3B-C2B	5.41	1.47	1.40
24	5	314	KC1	C3C-C2C	5.41	1.48	1.36
21	G	302	CLA	CHC-C1C	5.40	1.48	1.35
21	3	304	CLA	CHC-C1C	5.40	1.48	1.35
24	G	307	KC1	C3D-C2D	5.40	1.49	1.39
21	7	306	CLA	C3B-C2B	5.40	1.47	1.40
21	J	302	CLA	C3C-C2C	5.40	1.48	1.36
21	J	301	CLA	C3B-C2B	5.40	1.47	1.40
21	B	615	CLA	C3C-C2C	5.40	1.48	1.36
21	C	505	CLA	C3C-C2C	5.40	1.48	1.36
21	b	608	CLA	C3B-C2B	5.40	1.47	1.40
21	b	623	CLA	MG-NC	5.40	2.19	2.06
21	8	305	CLA	C3C-C2C	5.40	1.48	1.36
21	G	300	CLA	C3B-C2B	5.40	1.47	1.40
21	2	303	CLA	C3C-C2C	5.40	1.48	1.36
21	d	405	CLA	CHC-C1C	5.40	1.48	1.35
24	J	311	KC1	C3C-C2C	5.39	1.48	1.36
21	C	511	CLA	C3C-C2C	5.39	1.48	1.36
24	8	313	KC1	C3C-C2C	5.39	1.48	1.36
21	B	604	CLA	C3C-C2C	5.39	1.48	1.36
21	c	508	CLA	C3C-C2C	5.39	1.48	1.36
21	g	308	CLA	C3C-C2C	5.39	1.48	1.36
21	B	607	CLA	C3C-C2C	5.39	1.48	1.36
21	c	512	CLA	C3B-C2B	5.39	1.47	1.40
21	8	304	CLA	C3C-C2C	5.39	1.48	1.36
21	8	303	CLA	C3C-C2C	5.39	1.48	1.36
21	6	306	CLA	C3C-C2C	5.39	1.48	1.36
21	C	503	CLA	C3C-C2C	5.38	1.48	1.36
21	c	510	CLA	C3C-C2C	5.38	1.48	1.36
24	4	309	KC1	C3C-C2C	5.38	1.48	1.36
21	1	307	CLA	C3C-C2C	5.38	1.48	1.36
21	J	306	CLA	C3C-C2C	5.38	1.48	1.36
21	1	306	CLA	CHC-C1C	5.38	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	608	CLA	C3C-C2C	5.38	1.48	1.36
21	B	615	CLA	C3B-C2B	5.38	1.47	1.40
21	7	300	CLA	C3B-C2B	5.38	1.47	1.40
21	1	302	CLA	C3B-C2B	5.38	1.47	1.40
21	1	304	CLA	C3B-C2B	5.38	1.47	1.40
21	G	303	CLA	C3B-C2B	5.38	1.47	1.40
21	2	306	CLA	C3C-C2C	5.38	1.48	1.36
21	C	509	CLA	C3C-C2C	5.38	1.48	1.36
21	D	404	CLA	C3B-C2B	5.37	1.47	1.40
21	A	404	CLA	C3C-C2C	5.37	1.48	1.36
21	a	405	CLA	C3C-C2C	5.37	1.48	1.36
21	C	506	CLA	C3C-C2C	5.37	1.48	1.36
21	8	307	CLA	C3C-C2C	5.37	1.48	1.36
21	D	407	CLA	C3C-C2C	5.37	1.48	1.36
21	d	406	CLA	C3C-C2C	5.37	1.48	1.36
24	9	306	KC1	C3C-C2C	5.37	1.48	1.36
21	4	302	CLA	O2D-CGD	5.37	1.46	1.33
21	3	301	CLA	C3B-C2B	5.37	1.47	1.40
21	1	308	CLA	C3C-C2C	5.37	1.48	1.36
21	7	308	CLA	C3C-C2C	5.36	1.48	1.36
24	3	305	KC1	C3C-C2C	5.36	1.48	1.36
21	J	307	CLA	CHC-C1C	5.36	1.48	1.35
21	1	308	CLA	C3B-C2B	5.36	1.47	1.40
21	8	302	CLA	C3B-C2B	5.36	1.47	1.40
21	8	302	CLA	C3C-C2C	5.36	1.48	1.36
24	4	308	KC1	CHD-C4C	5.36	1.48	1.35
21	J	303	CLA	CHC-C1C	5.36	1.48	1.35
24	G	307	KC1	C3C-C2C	5.36	1.48	1.36
21	b	623	CLA	C3C-C2C	5.36	1.48	1.36
21	8	306	CLA	C3C-C2C	5.36	1.48	1.36
21	C	514	CLA	C3B-C2B	5.36	1.47	1.40
24	G	308	KC1	CHD-C4C	5.36	1.48	1.35
21	2	305	CLA	C3C-C2C	5.36	1.48	1.36
21	7	302	CLA	CHC-C1C	5.36	1.48	1.35
24	5	313	KC1	C3C-C2C	5.36	1.48	1.36
21	2	302	CLA	C3C-C2C	5.36	1.48	1.36
21	B	621	CLA	C3C-C2C	5.35	1.48	1.36
21	c	511	CLA	C3C-C2C	5.35	1.48	1.36
21	7	306	CLA	C3C-C2C	5.35	1.48	1.36
21	6	302	CLA	CHC-C1C	5.35	1.48	1.35
21	c	503	CLA	C3C-C2C	5.35	1.48	1.36
21	b	607	CLA	C3B-C2B	5.35	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	302	CLA	O2D-CGD	5.35	1.46	1.33
21	a	405	CLA	CHC-C1C	5.35	1.48	1.35
24	4	307	KC1	C3C-C2C	5.35	1.48	1.36
21	7	307	CLA	C3C-C2C	5.35	1.48	1.36
21	8	302	CLA	CHC-C1C	5.35	1.48	1.35
21	4	300	CLA	CHC-C1C	5.35	1.48	1.35
21	c	505	CLA	C3C-C2C	5.35	1.48	1.36
24	6	311	KC1	C3C-C2C	5.35	1.48	1.36
21	B	603	CLA	MG-NC	5.35	2.19	2.06
21	J	307	CLA	C3B-C2B	5.35	1.47	1.40
21	6	308	CLA	O2D-CGD	5.35	1.46	1.33
21	C	512	CLA	C3C-C2C	5.35	1.48	1.36
21	B	608	CLA	C3B-C2B	5.35	1.47	1.40
21	7	304	CLA	C3B-C2B	5.35	1.47	1.40
21	b	616	CLA	C3C-C2C	5.35	1.48	1.36
24	3	306	KC1	CHD-C4C	5.34	1.48	1.35
21	C	513	CLA	C3B-C2B	5.34	1.47	1.40
21	7	305	CLA	CHC-C1C	5.34	1.48	1.35
21	c	514	CLA	C3B-C2B	5.34	1.47	1.40
21	b	603	CLA	C3C-C2C	5.34	1.48	1.36
21	6	303	CLA	CHD-C1D	5.34	1.48	1.38
24	4	309	KC1	CHD-C4C	5.34	1.48	1.35
21	1	306	CLA	C3C-C2C	5.34	1.48	1.36
21	5	307	CLA	C3C-C2C	5.34	1.48	1.36
21	A	404	CLA	C3B-C2B	5.34	1.47	1.40
21	B	613	CLA	C3C-C2C	5.34	1.48	1.36
21	1	304	CLA	CHC-C1C	5.34	1.48	1.35
21	b	616	CLA	C3B-C2B	5.34	1.47	1.40
24	7	314	KC1	C3C-C2C	5.34	1.48	1.36
21	J	300	CLA	C3B-C2B	5.33	1.47	1.40
21	3	303	CLA	CHC-C1C	5.33	1.48	1.35
24	9	306	KC1	CHD-C4C	5.33	1.48	1.35
21	J	302	CLA	C3B-C2B	5.33	1.47	1.40
21	6	307	CLA	CHC-C1C	5.33	1.48	1.35
21	d	404	CLA	C3B-C2B	5.33	1.47	1.40
21	7	308	CLA	C3B-C2B	5.33	1.47	1.40
21	B	606	CLA	CHC-C1C	5.33	1.48	1.35
21	C	506	CLA	MG-NA	5.33	2.18	2.06
21	C	504	CLA	C3C-C2C	5.33	1.48	1.36
24	9	305	KC1	C3C-C2C	5.33	1.48	1.36
21	5	303	CLA	C3C-C2C	5.33	1.48	1.36
21	8	306	CLA	CHC-C1C	5.33	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	301	CLA	O2D-CGD	5.32	1.46	1.33
21	b	610	CLA	C3C-C2C	5.32	1.48	1.36
21	5	305	CLA	C3C-C2C	5.32	1.48	1.36
21	g	305	CLA	CHC-C1C	5.32	1.48	1.35
21	1	308	CLA	CHC-C1C	5.32	1.48	1.35
21	c	502	CLA	C3C-C2C	5.32	1.48	1.36
21	a	405	CLA	C3B-C2B	5.32	1.47	1.40
21	B	603	CLA	CHC-C1C	5.32	1.48	1.35
21	9	303	CLA	CHC-C1C	5.32	1.48	1.35
21	g	304	CLA	CHC-C1C	5.32	1.48	1.35
21	6	302	CLA	O2D-CGD	5.32	1.46	1.33
21	g	303	CLA	C3C-C2C	5.32	1.48	1.36
21	G	303	CLA	CHC-C1C	5.32	1.48	1.35
21	b	614	CLA	C3C-C2C	5.32	1.48	1.36
21	b	609	CLA	C3B-C2B	5.32	1.47	1.40
21	7	303	CLA	C3B-C2B	5.31	1.47	1.40
21	b	623	CLA	C3B-C2B	5.31	1.47	1.40
24	2	313	KC1	C3B-C2B	5.31	1.48	1.37
21	9	303	CLA	CHD-C1D	5.31	1.48	1.38
21	1	303	CLA	CHC-C1C	5.31	1.48	1.35
24	3	306	KC1	C3C-C2C	5.31	1.48	1.36
21	B	606	CLA	C3B-C2B	5.31	1.47	1.40
24	2	313	KC1	C3D-C2D	5.31	1.49	1.39
21	c	512	CLA	C3C-C2C	5.31	1.48	1.36
21	g	308	CLA	C3B-C2B	5.31	1.47	1.40
21	7	307	CLA	C3B-C2B	5.31	1.47	1.40
21	3	302	CLA	CHD-C1D	5.31	1.48	1.38
21	B	614	CLA	C3C-C2C	5.31	1.48	1.36
24	1	315	KC1	CHD-C4C	5.31	1.48	1.35
21	8	307	CLA	C3B-C2B	5.31	1.47	1.40
21	A	404	CLA	CHC-C1C	5.31	1.48	1.35
24	1	315	KC1	C3C-C2C	5.31	1.48	1.36
21	b	604	CLA	CHC-C1C	5.31	1.48	1.35
24	J	313	KC1	C3C-C2C	5.31	1.48	1.36
21	b	612	CLA	CHC-C1C	5.31	1.48	1.35
24	g	313	KC1	C1A-NA	-5.31	1.27	1.38
21	J	306	CLA	C3B-C2B	5.30	1.47	1.40
21	2	301	CLA	CHC-C1C	5.30	1.48	1.35
21	1	302	CLA	C3C-C2C	5.30	1.48	1.36
21	6	303	CLA	CHC-C1C	5.30	1.48	1.35
21	7	300	CLA	CHC-C1C	5.30	1.48	1.35
21	g	307	CLA	CHC-C1C	5.30	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	615	CLA	C3C-C2C	5.30	1.48	1.36
21	9	301	CLA	CHD-C1D	5.30	1.48	1.38
21	C	505	CLA	C3B-C2B	5.30	1.47	1.40
21	1	305	CLA	C3B-C2B	5.30	1.47	1.40
21	1	309	CLA	C3C-C2C	5.30	1.48	1.36
24	6	313	KC1	C3C-C2C	5.30	1.48	1.36
21	c	512	CLA	MG-NC	5.30	2.18	2.06
21	C	515	CLA	CHC-C1C	5.30	1.48	1.35
21	C	503	CLA	CHC-C1C	5.30	1.48	1.35
21	6	304	CLA	C3B-C2B	5.30	1.47	1.40
21	6	305	CLA	CHC-C1C	5.30	1.48	1.35
21	8	305	CLA	CHC-C1C	5.29	1.48	1.35
21	c	514	CLA	CHC-C1C	5.29	1.48	1.35
21	g	309	CLA	CHC-C1C	5.29	1.48	1.35
21	2	301	CLA	C3C-C2C	5.29	1.48	1.36
24	6	311	KC1	CHD-C4C	5.29	1.48	1.35
21	G	302	CLA	CHD-C1D	5.29	1.48	1.38
24	3	305	KC1	CHD-C4C	5.29	1.48	1.35
21	b	615	CLA	C3B-C2B	5.29	1.47	1.40
21	C	510	CLA	C3C-C2C	5.29	1.48	1.36
21	1	305	CLA	C3C-C2C	5.29	1.48	1.36
21	J	307	CLA	O2D-CGD	5.29	1.46	1.33
21	C	513	CLA	C3C-C2C	5.29	1.48	1.36
21	7	303	CLA	CHC-C1C	5.29	1.48	1.35
21	6	301	CLA	O2D-CGD	5.29	1.46	1.33
21	9	304	CLA	O2D-CGD	5.29	1.46	1.33
21	4	304	CLA	CHD-C1D	5.28	1.48	1.38
24	2	313	KC1	O2D-CGD	5.28	1.46	1.33
21	B	611	CLA	CHC-C1C	5.28	1.48	1.35
24	6	312	KC1	C3C-C2C	5.28	1.48	1.36
21	6	306	CLA	C3B-C2B	5.28	1.47	1.40
21	2	304	CLA	CHC-C1C	5.28	1.48	1.35
24	8	315	KC1	CHD-C4C	5.28	1.48	1.35
21	J	308	CLA	CHC-C1C	5.28	1.48	1.35
21	J	304	CLA	C3B-C2B	5.28	1.47	1.40
21	G	304	CLA	CHC-C1C	5.28	1.48	1.35
24	5	314	KC1	CHD-C4C	5.28	1.48	1.35
21	J	302	CLA	CHC-C1C	5.28	1.48	1.35
21	b	616	CLA	CHD-C1D	5.28	1.48	1.38
24	5	315	KC1	C3C-C2C	5.28	1.47	1.36
21	2	306	CLA	C3B-C2B	5.28	1.47	1.40
21	7	303	CLA	O2D-CGD	5.27	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	303	CLA	CHC-C1C	5.27	1.48	1.35
21	6	301	CLA	C3B-C2B	5.27	1.47	1.40
21	B	607	CLA	CHC-C1C	5.27	1.48	1.35
21	9	302	CLA	CHC-C1C	5.27	1.48	1.35
24	J	313	KC1	CHD-C4C	5.27	1.48	1.35
21	1	304	CLA	C3C-C2C	5.27	1.47	1.36
21	4	300	CLA	CHD-C1D	5.27	1.48	1.38
24	g	314	KC1	C3C-C2C	5.27	1.47	1.36
21	4	301	CLA	CHC-C1C	5.27	1.48	1.35
21	6	308	CLA	CHD-C1D	5.27	1.48	1.38
21	G	301	CLA	CHC-C1C	5.27	1.48	1.35
24	8	314	KC1	CHD-C4C	5.27	1.48	1.35
21	B	614	CLA	C3B-C2B	5.27	1.47	1.40
21	G	301	CLA	CHD-C1D	5.27	1.48	1.38
21	d	406	CLA	CHC-C1C	5.27	1.48	1.35
24	8	315	KC1	C3C-C2C	5.27	1.47	1.36
24	5	315	KC1	CHD-C4C	5.27	1.48	1.35
21	J	302	CLA	O2D-CGD	5.27	1.46	1.33
21	b	603	CLA	C3B-C2B	5.27	1.47	1.40
21	3	300	CLA	CHC-C1C	5.27	1.48	1.35
24	J	311	KC1	CHD-C4C	5.27	1.48	1.35
24	4	307	KC1	CHD-C4C	5.27	1.48	1.35
21	B	602	CLA	C3C-C2C	5.27	1.47	1.36
21	3	301	CLA	CHD-C1D	5.27	1.48	1.38
21	c	509	CLA	C3C-C2C	5.27	1.47	1.36
21	D	407	CLA	CHC-C1C	5.26	1.48	1.35
21	b	607	CLA	CHC-C1C	5.26	1.48	1.35
21	5	307	CLA	CHC-C1C	5.26	1.48	1.35
21	c	504	CLA	C3B-C2B	5.26	1.47	1.40
21	2	305	CLA	CHC-C1C	5.26	1.48	1.35
21	J	308	CLA	O2D-CGD	5.26	1.46	1.33
21	2	303	CLA	CHC-C1C	5.26	1.48	1.35
24	J	312	KC1	C3C-C2C	5.26	1.47	1.36
21	C	512	CLA	CHC-C1C	5.26	1.48	1.35
21	9	302	CLA	MG-NC	5.26	2.18	2.06
21	3	301	CLA	O2D-CGD	5.26	1.46	1.33
24	3	305	KC1	O2D-CGD	5.26	1.46	1.33
24	G	309	KC1	CHD-C4C	5.26	1.48	1.35
21	8	304	CLA	CHC-C1C	5.26	1.48	1.35
21	J	308	CLA	CHD-C1D	5.26	1.48	1.38
21	1	309	CLA	C3B-C2B	5.26	1.47	1.40
21	6	305	CLA	O2D-CGD	5.26	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	305	CLA	CHC-C1C	5.26	1.48	1.35
21	6	300	CLA	CHC-C1C	5.26	1.48	1.35
21	c	512	CLA	CHC-C1C	5.26	1.48	1.35
21	B	615	CLA	CHD-C1D	5.26	1.48	1.38
24	7	315	KC1	CHD-C4C	5.25	1.48	1.35
24	1	316	KC1	C3B-C2B	5.25	1.47	1.37
21	6	300	CLA	C3B-C2B	5.25	1.47	1.40
21	G	302	CLA	O2D-CGD	5.25	1.46	1.33
21	b	608	CLA	CHC-C1C	5.25	1.48	1.35
21	9	302	CLA	CHD-C1D	5.25	1.48	1.38
24	g	315	KC1	CHD-C4C	5.25	1.48	1.35
21	9	301	CLA	CHC-C1C	5.25	1.48	1.35
21	C	508	CLA	CHD-C1D	5.25	1.48	1.38
24	4	307	KC1	C1A-NA	-5.25	1.27	1.38
21	1	301	CLA	CHC-C1C	5.25	1.48	1.35
21	c	513	CLA	CHC-C1C	5.25	1.48	1.35
24	1	316	KC1	CHD-C4C	5.25	1.48	1.35
21	2	305	CLA	CHD-C1D	5.25	1.48	1.38
21	G	300	CLA	CHC-C1C	5.25	1.48	1.35
24	6	312	KC1	CHD-C4C	5.25	1.48	1.35
21	J	305	CLA	CHC-C1C	5.25	1.48	1.35
21	J	300	CLA	CHC-C1C	5.24	1.48	1.35
21	C	514	CLA	CHC-C1C	5.24	1.48	1.35
21	g	305	CLA	O2D-CGD	5.24	1.46	1.33
21	C	505	CLA	CHC-C1C	5.24	1.48	1.35
21	1	307	CLA	O2D-CGD	5.24	1.46	1.33
24	7	315	KC1	C3B-C2B	5.24	1.47	1.37
21	G	301	CLA	O2D-CGD	5.24	1.46	1.33
21	4	304	CLA	CHC-C1C	5.24	1.48	1.35
21	B	602	CLA	C3B-C2B	5.24	1.47	1.40
24	J	312	KC1	CHD-C4C	5.24	1.48	1.35
21	J	306	CLA	CHC-C1C	5.24	1.48	1.35
21	1	308	CLA	O2D-CGD	5.24	1.46	1.33
21	1	302	CLA	CHC-C1C	5.24	1.48	1.35
24	G	307	KC1	CHD-C4C	5.24	1.48	1.35
21	C	506	CLA	CHC-C1C	5.24	1.48	1.35
21	5	305	CLA	O2D-CGD	5.23	1.46	1.33
21	c	504	CLA	CHC-C1C	5.23	1.48	1.35
21	J	301	CLA	C3C-C2C	5.23	1.47	1.36
24	2	315	KC1	CHD-C4C	5.23	1.48	1.35
21	4	302	CLA	CHD-C1D	5.23	1.48	1.38
21	g	309	CLA	CHD-C1D	5.23	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	300	CLA	O2D-CGD	5.23	1.46	1.33
24	G	309	KC1	C3C-C2C	5.23	1.47	1.36
21	4	301	CLA	CHD-C1D	5.23	1.48	1.38
21	c	511	CLA	CHC-C1C	5.23	1.48	1.35
24	2	315	KC1	C3C-C2C	5.23	1.47	1.36
21	5	304	CLA	CHC-C1C	5.23	1.48	1.35
21	B	621	CLA	O2D-CGD	5.23	1.46	1.33
21	c	502	CLA	CHC-C1C	5.23	1.48	1.35
21	1	305	CLA	CHD-C1D	5.23	1.48	1.38
21	3	303	CLA	CHD-C1D	5.23	1.48	1.38
21	7	301	CLA	CHD-C1D	5.23	1.48	1.38
21	4	303	CLA	O2D-CGD	5.23	1.46	1.33
21	1	310	CLA	O2D-CGD	5.23	1.46	1.33
24	g	313	KC1	CHD-C4C	5.23	1.48	1.35
21	5	308	CLA	C3B-C2B	5.23	1.47	1.40
21	J	305	CLA	O2D-CGD	5.23	1.46	1.33
21	C	511	CLA	CHC-C1C	5.23	1.48	1.35
21	6	301	CLA	CHC-C1C	5.23	1.48	1.35
21	6	308	CLA	CHC-C1C	5.22	1.48	1.35
21	C	513	CLA	CHC-C1C	5.22	1.48	1.35
21	g	308	CLA	O2D-CGD	5.22	1.45	1.33
21	G	300	CLA	O2D-CGD	5.22	1.45	1.33
24	4	308	KC1	O2D-CGD	5.22	1.45	1.33
24	g	315	KC1	C3C-C2C	5.22	1.47	1.36
21	7	308	CLA	CHC-C1C	5.22	1.48	1.35
21	5	304	CLA	CHD-C1D	5.22	1.48	1.38
21	c	503	CLA	O2D-CGD	5.22	1.45	1.33
21	c	510	CLA	CHC-C1C	5.22	1.48	1.35
21	7	307	CLA	CHC-C1C	5.22	1.48	1.35
21	c	505	CLA	CHC-C1C	5.22	1.48	1.35
21	3	304	CLA	CHD-C1D	5.22	1.48	1.38
21	G	304	CLA	CHD-C1D	5.22	1.48	1.38
21	B	621	CLA	C3B-C2B	5.22	1.47	1.40
21	6	307	CLA	O2D-CGD	5.22	1.45	1.33
21	J	301	CLA	CHC-C1C	5.22	1.48	1.35
21	B	609	CLA	C3C-C2C	5.22	1.47	1.36
24	1	316	KC1	C3C-C2C	5.22	1.47	1.36
24	9	305	KC1	C1A-NA	-5.22	1.27	1.38
21	c	507	CLA	CHD-C1D	5.22	1.48	1.38
24	6	313	KC1	CHD-C4C	5.22	1.48	1.35
24	2	313	KC1	C3C-C2C	5.21	1.47	1.36
24	5	313	KC1	O2D-CGD	5.21	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	313	KC1	CHD-C4C	5.21	1.48	1.35
21	7	301	CLA	CHC-C1C	5.21	1.48	1.35
21	3	301	CLA	CHC-C1C	5.21	1.48	1.35
21	g	307	CLA	CHD-C1D	5.21	1.48	1.38
21	8	307	CLA	CHD-C1D	5.21	1.48	1.38
24	G	309	KC1	O2D-CGD	5.21	1.45	1.33
24	2	314	KC1	CHD-C4C	5.21	1.48	1.35
21	5	305	CLA	CHC-C1C	5.21	1.48	1.35
21	C	504	CLA	O2D-CGD	5.21	1.45	1.33
21	3	304	CLA	O2D-CGD	5.21	1.45	1.33
21	J	302	CLA	CHD-C1D	5.21	1.48	1.38
21	6	306	CLA	CHC-C1C	5.21	1.48	1.35
21	7	309	CLA	O2D-CGD	5.21	1.45	1.33
24	9	305	KC1	CHD-C4C	5.20	1.48	1.35
24	g	314	KC1	CHD-C4C	5.20	1.48	1.35
21	6	303	CLA	O2D-CGD	5.20	1.45	1.33
21	B	610	CLA	C3C-C2C	5.20	1.47	1.36
21	7	308	CLA	O2D-CGD	5.20	1.45	1.33
24	4	309	KC1	O2D-CGD	5.20	1.45	1.33
21	c	514	CLA	CHD-C1D	5.20	1.48	1.38
21	3	302	CLA	O2D-CGD	5.20	1.45	1.33
21	5	308	CLA	O2D-CGD	5.20	1.45	1.33
21	J	303	CLA	O2D-CGD	5.20	1.45	1.33
21	1	307	CLA	CHC-C1C	5.20	1.48	1.35
21	7	306	CLA	CHC-C1C	5.20	1.48	1.35
21	7	307	CLA	O2D-CGD	5.20	1.45	1.33
21	7	306	CLA	O2D-CGD	5.20	1.45	1.33
21	7	302	CLA	O2D-CGD	5.20	1.45	1.33
24	6	312	KC1	O2D-CGD	5.20	1.45	1.33
21	3	302	CLA	CHC-C1C	5.20	1.48	1.35
21	g	307	CLA	O2D-CGD	5.20	1.45	1.33
21	4	301	CLA	C3B-C2B	5.20	1.47	1.40
21	1	309	CLA	O2D-CGD	5.20	1.45	1.33
24	g	315	KC1	O2D-CGD	5.20	1.45	1.33
21	6	302	CLA	CHD-C1D	5.20	1.48	1.38
21	g	306	CLA	CHC-C1C	5.20	1.48	1.35
21	6	305	CLA	CHD-C1D	5.20	1.48	1.38
21	g	306	CLA	CHD-C1D	5.20	1.48	1.38
21	5	308	CLA	CHC-C1C	5.20	1.48	1.35
24	7	314	KC1	CHD-C4C	5.20	1.48	1.35
21	c	507	CLA	O2D-CGD	5.19	1.45	1.33
21	b	613	CLA	CHC-C1C	5.19	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	512	CLA	CHD-C1D	5.19	1.48	1.38
21	J	304	CLA	O2D-CGD	5.19	1.45	1.33
21	B	608	CLA	CHC-C1C	5.19	1.48	1.35
21	1	303	CLA	CHD-C1D	5.19	1.48	1.38
21	7	306	CLA	MG-ND	-5.19	1.95	2.05
21	5	306	CLA	CHC-C1C	5.19	1.48	1.35
21	C	505	CLA	CHD-C1D	5.19	1.48	1.38
21	7	309	CLA	CHD-C1D	5.19	1.48	1.38
21	J	305	CLA	CHD-C1D	5.19	1.48	1.38
21	7	309	CLA	CHC-C1C	5.19	1.48	1.35
21	9	304	CLA	CHD-C1D	5.19	1.48	1.38
21	C	513	CLA	O2D-CGD	5.19	1.45	1.33
24	1	315	KC1	O2D-CGD	5.19	1.45	1.33
24	G	308	KC1	O2D-CGD	5.19	1.45	1.33
21	b	609	CLA	CHC-C1C	5.19	1.48	1.35
24	4	306	KC1	O2D-CGD	5.19	1.45	1.33
24	G	306	KC1	O2D-CGD	5.19	1.45	1.33
21	1	304	CLA	O2D-CGD	5.18	1.45	1.33
21	5	307	CLA	O2D-CGD	5.18	1.45	1.33
24	5	314	KC1	O2D-CGD	5.18	1.45	1.33
21	b	605	CLA	CHD-C1D	5.18	1.48	1.38
24	7	314	KC1	O2D-CGD	5.18	1.45	1.33
24	8	316	KC1	C3C-C2C	5.18	1.47	1.36
21	1	310	CLA	CHC-C1C	5.18	1.48	1.35
21	c	502	CLA	O2D-CGD	5.18	1.45	1.33
21	B	602	CLA	O2D-CGD	5.18	1.45	1.33
21	G	303	CLA	O2D-CGD	5.18	1.45	1.33
21	C	512	CLA	O2D-CGD	5.18	1.45	1.33
21	2	304	CLA	O2D-CGD	5.18	1.45	1.33
21	C	506	CLA	CHD-C1D	5.18	1.48	1.38
24	7	314	KC1	C3D-C2D	5.18	1.48	1.39
24	J	312	KC1	O2D-CGD	5.18	1.45	1.33
21	A	402	CLA	CHC-C1C	5.18	1.48	1.35
24	5	313	KC1	CHD-C4C	5.18	1.48	1.35
21	b	607	CLA	C3C-C2C	5.18	1.47	1.36
21	C	515	CLA	O2D-CGD	5.18	1.45	1.33
21	J	306	CLA	O2D-CGD	5.18	1.45	1.33
21	c	514	CLA	O2D-CGD	5.18	1.45	1.33
21	g	305	CLA	CHD-C1D	5.18	1.48	1.38
21	G	304	CLA	O2D-CGD	5.18	1.45	1.33
21	a	403	CLA	CHC-C1C	5.18	1.48	1.35
21	8	304	CLA	CHD-C1D	5.18	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	612	CLA	C3C-C2C	5.17	1.47	1.36
24	2	316	KC1	C3C-C2C	5.17	1.47	1.36
21	4	304	CLA	O2D-CGD	5.17	1.45	1.33
21	4	303	CLA	CHD-C1D	5.17	1.48	1.38
21	B	613	CLA	CHC-C1C	5.17	1.48	1.35
21	b	603	CLA	O2D-CGD	5.17	1.45	1.33
21	5	305	CLA	CHD-C1D	5.17	1.48	1.38
21	1	303	CLA	O2D-CGD	5.17	1.45	1.33
21	B	612	CLA	CHC-C1C	5.17	1.48	1.35
21	9	300	CLA	O2D-CGD	5.17	1.45	1.33
21	B	605	CLA	CHD-C1D	5.17	1.48	1.38
21	6	304	CLA	C3C-C2C	5.17	1.47	1.36
21	2	306	CLA	CHD-C1D	5.17	1.48	1.38
21	B	606	CLA	C3C-C2C	5.17	1.47	1.36
21	6	301	CLA	C3C-C2C	5.17	1.47	1.36
21	9	300	CLA	C3C-C2C	5.17	1.47	1.36
21	8	305	CLA	O2D-CGD	5.16	1.45	1.33
21	C	506	CLA	O2D-CGD	5.16	1.45	1.33
21	c	505	CLA	O2D-CGD	5.16	1.45	1.33
24	g	314	KC1	O2D-CGD	5.16	1.45	1.33
21	g	308	CLA	CHC-C1C	5.16	1.48	1.35
21	g	302	CLA	O2D-CGD	5.16	1.45	1.33
21	5	304	CLA	O2D-CGD	5.16	1.45	1.33
21	c	512	CLA	O2D-CGD	5.16	1.45	1.33
21	J	304	CLA	C3C-C2C	5.16	1.47	1.36
21	B	610	CLA	CHC-C1C	5.16	1.48	1.35
21	B	604	CLA	CHD-C1D	5.16	1.48	1.38
24	G	307	KC1	C1A-NA	-5.16	1.27	1.38
21	5	307	CLA	CHD-C1D	5.16	1.48	1.38
21	g	305	CLA	C3B-C2B	5.16	1.47	1.40
21	C	514	CLA	O2D-CGD	5.16	1.45	1.33
21	C	515	CLA	CHD-C1D	5.16	1.48	1.38
21	c	502	CLA	MG-ND	-5.15	1.95	2.05
21	B	606	CLA	O2D-CGD	5.15	1.45	1.33
21	C	503	CLA	O2D-CGD	5.15	1.45	1.33
21	4	302	CLA	CHC-C1C	5.15	1.48	1.35
21	c	502	CLA	CHD-C1D	5.15	1.48	1.38
21	G	300	CLA	CHD-C1D	5.15	1.48	1.38
21	b	611	CLA	CHC-C1C	5.15	1.48	1.35
21	c	513	CLA	O2D-CGD	5.15	1.45	1.33
24	9	306	KC1	O2D-CGD	5.15	1.45	1.33
21	7	305	CLA	O2D-CGD	5.15	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	306	CLA	CHD-C1D	5.15	1.48	1.38
21	B	602	CLA	CHD-C1D	5.15	1.48	1.38
21	9	303	CLA	O2D-CGD	5.15	1.45	1.33
21	C	510	CLA	O2D-CGD	5.15	1.45	1.33
21	B	611	CLA	C3C-C2C	5.15	1.47	1.36
21	A	404	CLA	CHD-C1D	5.15	1.48	1.38
21	b	607	CLA	O2D-CGD	5.15	1.45	1.33
21	7	302	CLA	CHD-C1D	5.14	1.48	1.38
21	d	406	CLA	CHD-C1D	5.14	1.48	1.38
21	1	305	CLA	O2D-CGD	5.14	1.45	1.33
24	7	315	KC1	C3C-C2C	5.14	1.47	1.36
21	5	302	CLA	O2D-CGD	5.14	1.45	1.33
21	g	309	CLA	O2D-CGD	5.14	1.45	1.33
21	B	608	CLA	CHD-C1D	5.14	1.48	1.38
21	b	609	CLA	CHD-C1D	5.14	1.48	1.38
21	b	623	CLA	CHC-C1C	5.14	1.48	1.35
24	8	316	KC1	CHD-C4C	5.14	1.48	1.35
21	b	614	CLA	CHC-C1C	5.14	1.48	1.35
21	8	307	CLA	CHC-C1C	5.14	1.48	1.35
21	D	404	CLA	CHC-C1C	5.14	1.48	1.35
21	B	604	CLA	CHC-C1C	5.14	1.48	1.35
24	2	316	KC1	CHD-C4C	5.14	1.48	1.35
21	5	306	CLA	CHD-C1D	5.14	1.48	1.38
24	8	313	KC1	O2D-CGD	5.14	1.45	1.33
21	7	304	CLA	CHC-C1C	5.14	1.48	1.35
21	3	303	CLA	O2D-CGD	5.14	1.45	1.33
21	6	306	CLA	O2D-CGD	5.14	1.45	1.33
24	1	316	KC1	O2D-CGD	5.14	1.45	1.33
21	5	306	CLA	O2D-CGD	5.13	1.45	1.33
21	B	603	CLA	CHD-C1D	5.13	1.48	1.38
21	B	607	CLA	CHD-C1D	5.13	1.48	1.38
21	C	511	CLA	O2D-CGD	5.13	1.45	1.33
21	a	405	CLA	O2D-CGD	5.13	1.45	1.33
21	8	306	CLA	MG-ND	-5.13	1.95	2.05
21	B	612	CLA	O2D-CGD	5.13	1.45	1.33
21	b	617	CLA	O2D-CGD	5.13	1.45	1.33
24	8	315	KC1	O2D-CGD	5.13	1.45	1.33
21	D	404	CLA	CHD-C1D	5.13	1.48	1.38
21	B	621	CLA	CHC-C1C	5.13	1.48	1.35
21	1	310	CLA	CHD-C1D	5.13	1.48	1.38
21	c	504	CLA	CHD-C1D	5.13	1.48	1.38
21	6	300	CLA	CHD-C1D	5.13	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	609	CLA	O2D-CGD	5.13	1.45	1.33
21	c	509	CLA	O2D-CGD	5.13	1.45	1.33
21	J	300	CLA	O2D-CGD	5.13	1.45	1.33
21	c	506	CLA	CHD-C1D	5.13	1.48	1.38
21	B	602	CLA	CHC-C1C	5.13	1.48	1.35
21	b	615	CLA	CHC-C1C	5.12	1.48	1.35
24	3	306	KC1	O2D-CGD	5.12	1.45	1.33
21	A	404	CLA	O2D-CGD	5.12	1.45	1.33
21	7	300	CLA	O2D-CGD	5.12	1.45	1.33
21	7	300	CLA	C3C-C2C	5.12	1.47	1.36
21	B	605	CLA	O2D-CGD	5.12	1.45	1.33
21	g	303	CLA	CHC-C1C	5.12	1.48	1.35
21	4	301	CLA	O2D-CGD	5.12	1.45	1.33
21	C	508	CLA	O2D-CGD	5.12	1.45	1.33
21	J	300	CLA	CHD-C1D	5.12	1.48	1.38
21	5	309	CLA	CHC-C1C	5.12	1.48	1.35
24	7	315	KC1	O2D-CGD	5.12	1.45	1.33
21	c	507	CLA	C3B-C2B	5.12	1.47	1.40
21	D	407	CLA	CHD-C1D	5.12	1.48	1.38
21	B	615	CLA	CHC-C1C	5.12	1.48	1.35
21	B	616	CLA	O2D-CGD	5.12	1.45	1.33
21	5	303	CLA	CHD-C1D	5.12	1.48	1.38
21	2	302	CLA	CHC-C1C	5.12	1.48	1.35
24	2	313	KC1	CHD-C4C	5.12	1.48	1.35
21	b	616	CLA	CHC-C1C	5.12	1.48	1.35
24	G	307	KC1	O2D-CGD	5.12	1.45	1.33
21	7	305	CLA	CHD-C1D	5.12	1.48	1.38
21	5	308	CLA	CHD-C1D	5.12	1.48	1.38
21	b	605	CLA	C3B-C2B	5.12	1.47	1.40
21	b	613	CLA	C3C-C2C	5.12	1.47	1.36
21	b	603	CLA	CHC-C1C	5.12	1.48	1.35
21	B	608	CLA	O2D-CGD	5.11	1.45	1.33
21	c	508	CLA	CHC-C1C	5.11	1.48	1.35
21	1	302	CLA	CHD-C1D	5.11	1.48	1.38
21	b	608	CLA	CHD-C1D	5.11	1.48	1.38
21	2	303	CLA	CHD-C1D	5.11	1.48	1.38
21	1	309	CLA	CHC-C1C	5.11	1.48	1.35
21	c	510	CLA	O2D-CGD	5.11	1.45	1.33
21	7	308	CLA	CHD-C1D	5.11	1.48	1.38
21	B	614	CLA	CHC-C1C	5.11	1.48	1.35
21	g	302	CLA	CHC-C1C	5.11	1.48	1.35
21	b	603	CLA	CHD-C1D	5.11	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	605	CLA	CHC-C1C	5.11	1.48	1.35
21	b	606	CLA	O2D-CGD	5.11	1.45	1.33
21	7	303	CLA	C3C-C2C	5.11	1.47	1.36
21	C	509	CLA	CHC-C1C	5.11	1.48	1.35
21	B	604	CLA	C3B-C2B	5.11	1.47	1.40
21	b	604	CLA	CHD-C1D	5.11	1.48	1.38
21	c	513	CLA	CHD-C1D	5.11	1.48	1.38
24	8	314	KC1	O2D-CGD	5.11	1.45	1.33
21	B	621	CLA	CHD-C1D	5.10	1.48	1.38
21	a	402	CLA	O2D-CGD	5.10	1.45	1.33
21	5	309	CLA	C3C-C2C	5.10	1.47	1.36
21	1	301	CLA	O2D-CGD	5.10	1.45	1.33
21	G	303	CLA	CHD-C1D	5.10	1.48	1.38
21	7	301	CLA	O2D-CGD	5.10	1.45	1.33
21	C	503	CLA	CHD-C1D	5.10	1.48	1.38
21	D	404	CLA	O2D-CGD	5.10	1.45	1.33
21	5	303	CLA	CHC-C1C	5.10	1.48	1.35
21	6	300	CLA	O2D-CGD	5.10	1.45	1.33
21	C	505	CLA	O2D-CGD	5.10	1.45	1.33
24	4	307	KC1	O2D-CGD	5.10	1.45	1.33
21	A	401	CLA	O2D-CGD	5.10	1.45	1.33
21	B	609	CLA	O2D-CGD	5.10	1.45	1.33
21	b	606	CLA	CHD-C1D	5.10	1.48	1.38
21	d	404	CLA	CHC-C1C	5.09	1.48	1.35
21	g	303	CLA	CHD-C1D	5.09	1.48	1.38
21	B	616	CLA	C3C-C2C	5.09	1.47	1.36
24	9	305	KC1	O2D-CGD	5.09	1.45	1.33
24	5	313	KC1	C1A-NA	-5.09	1.28	1.38
21	B	615	CLA	O2D-CGD	5.09	1.45	1.33
21	A	401	CLA	CHC-C1C	5.09	1.48	1.35
21	1	308	CLA	CHD-C1D	5.09	1.48	1.38
21	b	611	CLA	C3C-C2C	5.09	1.47	1.36
21	8	306	CLA	CHD-C1D	5.09	1.48	1.38
21	g	308	CLA	CHD-C1D	5.09	1.48	1.38
24	8	314	KC1	C3C-C2C	5.09	1.47	1.36
21	b	610	CLA	CHD-C1D	5.09	1.48	1.38
24	2	315	KC1	O2D-CGD	5.09	1.45	1.33
21	1	306	CLA	O2D-CGD	5.09	1.45	1.33
21	8	306	CLA	MG-NC	5.09	2.18	2.06
21	J	306	CLA	CHD-C1D	5.09	1.48	1.38
21	d	404	CLA	O2D-CGD	5.08	1.45	1.33
21	C	508	CLA	C3B-C2B	5.08	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	514	CLA	CHD-C1D	5.08	1.48	1.38
21	9	301	CLA	O2D-CGD	5.08	1.45	1.33
21	B	605	CLA	C3C-C2C	5.08	1.47	1.36
21	d	405	CLA	O2D-CGD	5.08	1.45	1.33
21	b	610	CLA	O2D-CGD	5.08	1.45	1.33
21	6	306	CLA	CHD-C1D	5.08	1.48	1.38
21	7	300	CLA	CHD-C1D	5.08	1.48	1.38
21	C	509	CLA	CHD-C1D	5.08	1.48	1.38
21	4	300	CLA	O2D-CGD	5.08	1.45	1.33
21	8	305	CLA	MG-NC	5.07	2.18	2.06
21	b	606	CLA	C3C-C2C	5.07	1.47	1.36
21	g	306	CLA	O2D-CGD	5.07	1.45	1.33
21	J	306	CLA	MG-NA	5.07	2.18	2.06
21	B	616	CLA	MG-NC	5.07	2.18	2.06
21	c	506	CLA	CHC-C1C	5.07	1.48	1.35
21	c	509	CLA	CHC-C1C	5.07	1.48	1.35
21	g	302	CLA	CHD-C1D	5.07	1.48	1.38
21	D	406	CLA	O2D-CGD	5.07	1.45	1.33
21	C	510	CLA	CHC-C1C	5.07	1.48	1.35
21	B	612	CLA	C3C-C2C	5.07	1.47	1.36
21	7	304	CLA	CHD-C1D	5.07	1.48	1.38
21	a	403	CLA	CHD-C1D	5.07	1.48	1.38
21	C	507	CLA	CHD-C1D	5.07	1.48	1.38
24	5	315	KC1	O2D-CGD	5.07	1.45	1.33
21	1	301	CLA	CHD-C1D	5.07	1.48	1.38
24	g	313	KC1	O2D-CGD	5.07	1.45	1.33
21	b	616	CLA	O2D-CGD	5.07	1.45	1.33
24	5	315	KC1	C1A-NA	-5.07	1.28	1.38
21	c	506	CLA	O2D-CGD	5.07	1.45	1.33
21	8	303	CLA	CHD-C1D	5.06	1.48	1.38
21	C	508	CLA	CHC-C1C	5.06	1.47	1.35
21	b	613	CLA	O2D-CGD	5.06	1.45	1.33
21	a	402	CLA	C3C-C2C	5.06	1.47	1.36
21	8	304	CLA	O2D-CGD	5.06	1.45	1.33
24	J	311	KC1	O2D-CGD	5.06	1.45	1.33
21	2	302	CLA	O2D-CGD	5.06	1.45	1.33
21	7	307	CLA	CHD-C1D	5.06	1.48	1.38
21	C	511	CLA	CHD-C1D	5.06	1.48	1.38
21	B	613	CLA	CHD-C1D	5.06	1.48	1.38
21	J	307	CLA	CHD-C1D	5.06	1.48	1.38
21	c	503	CLA	CHC-C1C	5.06	1.47	1.35
21	a	402	CLA	CHC-C1C	5.06	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	511	CLA	O2D-CGD	5.06	1.45	1.33
21	b	608	CLA	MG-NC	5.05	2.18	2.06
21	7	304	CLA	O2D-CGD	5.05	1.45	1.33
21	B	611	CLA	O2D-CGD	5.05	1.45	1.33
21	C	504	CLA	CHC-C1C	5.05	1.47	1.35
21	1	302	CLA	O2D-CGD	5.05	1.45	1.33
21	B	610	CLA	O2D-CGD	5.05	1.45	1.33
21	c	511	CLA	MG-ND	-5.05	1.95	2.05
21	1	304	CLA	CHD-C1D	5.05	1.48	1.38
21	6	304	CLA	O2D-CGD	5.05	1.45	1.33
24	2	314	KC1	O2D-CGD	5.05	1.45	1.33
21	8	303	CLA	O2D-CGD	5.05	1.45	1.33
24	6	311	KC1	O2D-CGD	5.04	1.45	1.33
21	a	405	CLA	CHD-C1D	5.04	1.48	1.38
21	d	404	CLA	CHD-C1D	5.04	1.48	1.38
21	8	307	CLA	O2D-CGD	5.04	1.45	1.33
21	b	617	CLA	CHC-C1C	5.04	1.47	1.35
21	A	402	CLA	CHD-C1D	5.04	1.48	1.38
21	C	507	CLA	O2D-CGD	5.04	1.45	1.33
21	2	306	CLA	O2D-CGD	5.04	1.45	1.33
21	B	606	CLA	CHD-C1D	5.04	1.48	1.38
21	a	403	CLA	MG-ND	-5.04	1.95	2.05
21	1	301	CLA	C3C-C2C	5.04	1.47	1.36
21	2	302	CLA	C3B-C2B	5.04	1.47	1.40
21	A	401	CLA	C3C-C2C	5.03	1.47	1.36
21	9	304	CLA	MG-NA	5.03	2.18	2.06
21	8	303	CLA	CHC-C1C	5.03	1.47	1.35
21	C	507	CLA	CHC-C1C	5.03	1.47	1.35
21	6	304	CLA	CHC-C1C	5.03	1.47	1.35
21	b	617	CLA	C3C-C2C	5.03	1.47	1.36
21	b	612	CLA	O2D-CGD	5.03	1.45	1.33
21	B	609	CLA	C3B-C2B	5.03	1.47	1.40
21	1	309	CLA	CHD-C1D	5.03	1.48	1.38
21	6	304	CLA	CHD-C1D	5.03	1.48	1.38
21	C	513	CLA	CHD-C1D	5.03	1.48	1.38
21	B	616	CLA	CHC-C1C	5.02	1.47	1.35
21	b	614	CLA	O2D-CGD	5.02	1.45	1.33
21	b	610	CLA	C3B-C2B	5.02	1.47	1.40
21	c	507	CLA	CHC-C1C	5.02	1.47	1.35
21	B	607	CLA	O2D-CGD	5.02	1.45	1.33
21	2	305	CLA	O2D-CGD	5.02	1.45	1.33
21	C	509	CLA	O2D-CGD	5.02	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	304	CLA	CHD-C1D	5.02	1.48	1.38
21	6	302	CLA	MG-NA	5.02	2.18	2.06
21	A	402	CLA	MG-ND	-5.01	1.95	2.05
21	6	307	CLA	CHD-C1D	5.01	1.48	1.38
21	7	306	CLA	CHD-C1D	5.01	1.48	1.38
21	b	611	CLA	O2D-CGD	5.01	1.45	1.33
21	8	302	CLA	O2D-CGD	5.01	1.45	1.33
21	8	305	CLA	MG-ND	5.01	2.15	2.05
21	g	302	CLA	C3C-C2C	5.01	1.47	1.36
21	c	505	CLA	CHD-C1D	5.01	1.48	1.38
21	7	303	CLA	CHD-C1D	5.01	1.48	1.38
21	c	508	CLA	O2D-CGD	5.01	1.45	1.33
21	c	510	CLA	CHD-C1D	5.00	1.48	1.38
21	b	607	CLA	CHD-C1D	5.00	1.48	1.38
21	b	614	CLA	CHD-C1D	5.00	1.48	1.38
21	J	304	CLA	CHC-C1C	5.00	1.47	1.35
21	5	303	CLA	O2D-CGD	5.00	1.45	1.33
21	2	303	CLA	O2D-CGD	5.00	1.45	1.33
21	B	614	CLA	CHD-C1D	4.99	1.48	1.38
21	b	617	CLA	MG-NC	4.99	2.18	2.06
21	2	301	CLA	CHD-C1D	4.99	1.48	1.38
21	B	613	CLA	O2D-CGD	4.99	1.45	1.33
21	9	300	CLA	CHD-C1D	4.99	1.48	1.38
21	B	609	CLA	CHD-C1D	4.99	1.48	1.38
21	a	403	CLA	O2D-CGD	4.99	1.45	1.33
21	b	615	CLA	O2D-CGD	4.99	1.45	1.33
21	A	402	CLA	O2D-CGD	4.99	1.45	1.33
21	b	608	CLA	O2D-CGD	4.99	1.45	1.33
21	a	402	CLA	CHD-C1D	4.99	1.48	1.38
24	G	308	KC1	OBD-CAD	4.99	1.29	1.22
21	1	307	CLA	CHD-C1D	4.99	1.48	1.38
21	g	304	CLA	O2D-CGD	4.99	1.45	1.33
21	C	510	CLA	CHD-C1D	4.99	1.48	1.38
21	g	303	CLA	O2D-CGD	4.98	1.45	1.33
21	c	508	CLA	CHD-C1D	4.98	1.48	1.38
24	8	316	KC1	O2D-CGD	4.98	1.45	1.33
21	3	300	CLA	CHD-C1D	4.98	1.48	1.38
21	c	509	CLA	CHD-C1D	4.98	1.48	1.38
21	g	304	CLA	CHD-C1D	4.98	1.48	1.38
21	B	604	CLA	O2D-CGD	4.97	1.45	1.33
21	d	406	CLA	O2D-CGD	4.97	1.45	1.33
21	d	405	CLA	MG-ND	-4.97	1.95	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	605	CLA	O2D-CGD	4.97	1.45	1.33
21	b	615	CLA	CHD-C1D	4.97	1.48	1.38
21	5	303	CLA	MG-ND	4.97	2.15	2.05
21	B	609	CLA	CHC-C1C	4.97	1.47	1.35
21	2	306	CLA	CHC-C1C	4.97	1.47	1.35
21	5	302	CLA	CHD-C1D	4.97	1.48	1.38
21	b	623	CLA	CHD-C1D	4.96	1.48	1.38
21	8	303	CLA	C3B-C2B	4.96	1.47	1.40
21	A	401	CLA	CHD-C1D	4.96	1.48	1.38
24	5	314	KC1	C1A-NA	-4.95	1.28	1.38
21	5	309	CLA	CHD-C1D	4.95	1.48	1.38
21	2	302	CLA	CHD-C1D	4.95	1.48	1.38
21	c	503	CLA	CHD-C1D	4.95	1.48	1.38
21	8	302	CLA	CHD-C1D	4.94	1.48	1.38
21	B	614	CLA	O2D-CGD	4.94	1.45	1.33
21	B	615	CLA	MG-ND	4.94	2.15	2.05
21	1	305	CLA	MG-ND	4.93	2.15	2.05
24	2	316	KC1	O2D-CGD	4.93	1.45	1.33
21	8	305	CLA	CHD-C1D	4.92	1.48	1.38
24	6	311	KC1	C1A-NA	-4.92	1.28	1.38
21	8	306	CLA	O2D-CGD	4.92	1.45	1.33
21	b	610	CLA	CHC-C1C	4.92	1.47	1.35
21	D	407	CLA	O2D-CGD	4.92	1.45	1.33
21	5	302	CLA	C3C-C2C	4.92	1.47	1.36
21	b	611	CLA	CHD-C1D	4.92	1.47	1.38
24	9	306	KC1	CHC-C4B	4.91	1.47	1.38
21	G	301	CLA	MG-NC	-4.91	1.94	2.06
21	2	304	CLA	CHD-C1D	4.91	1.47	1.38
21	c	511	CLA	CHD-C1D	4.91	1.47	1.38
21	C	504	CLA	CHD-C1D	4.89	1.47	1.38
24	J	311	KC1	C1A-NA	-4.89	1.28	1.38
21	C	504	CLA	C3B-C2B	4.89	1.47	1.40
24	J	313	KC1	O2D-CGD	4.89	1.45	1.33
21	C	512	CLA	CHD-C1D	4.89	1.47	1.38
21	b	623	CLA	O2D-CGD	4.88	1.45	1.33
24	4	308	KC1	C1A-NA	-4.88	1.28	1.38
21	2	301	CLA	O2D-CGD	4.88	1.45	1.33
24	9	306	KC1	C1A-NA	-4.88	1.28	1.38
24	6	313	KC1	O2D-CGD	4.88	1.45	1.33
24	G	308	KC1	C1A-NA	-4.87	1.28	1.38
21	d	406	CLA	MG-NA	4.87	2.17	2.06
21	6	301	CLA	CHD-C1D	4.87	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	512	CLA	MG-ND	4.86	2.15	2.05
21	C	509	CLA	MG-NA	4.86	2.17	2.06
21	c	504	CLA	O2D-CGD	4.86	1.45	1.33
21	b	612	CLA	CHD-C1D	4.86	1.47	1.38
21	J	307	CLA	MG-NC	4.85	2.17	2.06
21	c	503	CLA	C3B-C2B	4.85	1.47	1.40
21	J	302	CLA	MG-ND	4.85	2.15	2.05
21	D	406	CLA	CHD-C1D	4.85	1.47	1.38
21	2	305	CLA	MG-ND	-4.83	1.96	2.05
21	b	617	CLA	CHD-C1D	4.82	1.47	1.38
21	B	610	CLA	CHD-C1D	4.82	1.47	1.38
21	B	611	CLA	CHD-C1D	4.82	1.47	1.38
24	2	313	KC1	CHB-C1B	4.81	1.47	1.38
24	8	315	KC1	C1A-NA	-4.81	1.28	1.38
21	d	405	CLA	CHD-C1D	4.81	1.47	1.38
24	g	315	KC1	CHC-C4B	4.81	1.47	1.38
24	G	306	KC1	CHC-C4B	4.80	1.47	1.38
21	B	607	CLA	MG-NC	4.80	2.17	2.06
24	4	308	KC1	CHC-C4B	4.80	1.47	1.38
24	8	313	KC1	C1A-NA	-4.80	1.28	1.38
21	J	305	CLA	MG-ND	4.79	2.15	2.05
21	B	616	CLA	CHD-C1D	4.79	1.47	1.38
21	A	402	CLA	MG-NC	-4.79	1.94	2.06
24	3	306	KC1	C1A-NA	-4.77	1.28	1.38
21	B	612	CLA	CHD-C1D	4.77	1.47	1.38
24	g	315	KC1	C1A-NA	-4.77	1.28	1.38
21	2	305	CLA	MG-NC	4.77	2.17	2.06
24	4	306	KC1	CHB-C1B	4.76	1.47	1.38
21	a	403	CLA	MG-NC	-4.76	1.95	2.06
24	4	308	KC1	C4D-ND	4.76	1.39	1.35
24	2	314	KC1	C1A-NA	-4.76	1.28	1.38
24	2	315	KC1	C1A-NA	-4.75	1.28	1.38
24	g	314	KC1	C4D-ND	4.75	1.39	1.35
24	9	306	KC1	OBD-CAD	4.75	1.28	1.22
24	1	316	KC1	C1A-NA	-4.75	1.28	1.38
24	G	309	KC1	C1A-NA	-4.75	1.28	1.38
24	1	315	KC1	OBD-CAD	4.75	1.28	1.22
24	1	315	KC1	C1A-NA	-4.74	1.28	1.38
24	6	313	KC1	CHC-C4B	4.74	1.47	1.38
24	8	314	KC1	C1A-NA	-4.74	1.28	1.38
24	7	314	KC1	CHC-C4B	4.74	1.47	1.38
24	3	305	KC1	C1A-NA	-4.73	1.28	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	312	KC1	CHC-C4B	4.73	1.47	1.38
21	b	613	CLA	CHD-C1D	4.73	1.47	1.38
24	7	315	KC1	C1A-NA	-4.73	1.28	1.38
24	3	305	KC1	OBD-CAD	4.73	1.28	1.22
21	B	605	CLA	C3B-C2B	4.73	1.46	1.40
24	8	315	KC1	CHC-C4B	4.73	1.47	1.38
24	G	306	KC1	OBD-CAD	4.72	1.28	1.22
21	b	606	CLA	C3B-C2B	4.72	1.46	1.40
24	6	312	KC1	CHC-C4B	4.72	1.47	1.38
24	8	313	KC1	CHC-C4B	4.72	1.47	1.38
24	3	306	KC1	OBD-CAD	4.72	1.28	1.22
24	4	309	KC1	OBD-CAD	4.72	1.28	1.22
24	4	306	KC1	OBD-CAD	4.71	1.28	1.22
24	4	309	KC1	CHB-C1B	4.71	1.47	1.38
24	J	312	KC1	C1A-NA	-4.70	1.28	1.38
24	6	312	KC1	OBD-CAD	4.70	1.28	1.22
24	1	315	KC1	CHC-C4B	4.70	1.47	1.38
24	7	315	KC1	OBD-CAD	4.70	1.28	1.22
24	7	314	KC1	C1A-NA	-4.70	1.28	1.38
24	4	306	KC1	CHC-C4B	4.70	1.47	1.38
24	4	308	KC1	OBD-CAD	4.69	1.28	1.22
21	G	301	CLA	MG-ND	-4.69	1.96	2.05
24	2	314	KC1	CHC-C4B	4.69	1.47	1.38
24	g	314	KC1	OBD-CAD	4.69	1.28	1.22
24	9	305	KC1	OBD-CAD	4.69	1.28	1.22
24	3	305	KC1	CHC-C4B	4.69	1.47	1.38
24	9	306	KC1	CHB-C1B	4.68	1.47	1.38
24	J	313	KC1	CHC-C4B	4.68	1.47	1.38
24	6	313	KC1	C1A-NA	-4.68	1.28	1.38
24	6	313	KC1	OBD-CAD	4.68	1.28	1.22
24	J	312	KC1	OBD-CAD	4.68	1.28	1.22
24	G	308	KC1	CHC-C4B	4.68	1.47	1.38
21	B	621	CLA	MG-NC	4.68	2.17	2.06
24	1	316	KC1	OBD-CAD	4.67	1.28	1.22
21	c	507	CLA	MG-ND	4.67	2.15	2.05
24	G	309	KC1	CHB-C1B	4.67	1.47	1.38
24	2	316	KC1	OBD-CAD	4.67	1.28	1.22
24	4	306	KC1	C1A-NA	-4.67	1.28	1.38
24	G	306	KC1	C1A-NA	-4.67	1.28	1.38
24	2	316	KC1	CHC-C4B	4.66	1.47	1.38
24	8	316	KC1	OBD-CAD	4.66	1.28	1.22
24	6	312	KC1	C1A-NA	-4.66	1.28	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	301	CLA	CHD-C1D	4.66	1.47	1.38
21	D	406	CLA	MG-ND	-4.66	1.96	2.05
24	G	309	KC1	OBD-CAD	4.66	1.28	1.22
21	B	605	CLA	CHC-C1C	4.65	1.46	1.35
24	J	313	KC1	C4D-ND	4.65	1.39	1.35
21	D	407	CLA	MG-NA	4.65	2.17	2.06
32	f	101	HEM	C3C-C2C	-4.65	1.33	1.40
24	8	314	KC1	OBD-CAD	4.65	1.28	1.22
24	5	315	KC1	OBD-CAD	4.65	1.28	1.22
24	1	316	KC1	CHC-C4B	4.65	1.47	1.38
23	8	310	A86	C2-C1	4.65	1.41	1.35
24	4	309	KC1	C1A-NA	-4.65	1.28	1.38
24	g	313	KC1	OBD-CAD	4.65	1.28	1.22
24	J	313	KC1	OBD-CAD	4.64	1.28	1.22
21	b	606	CLA	CHC-C1C	4.64	1.46	1.35
21	9	302	CLA	MG-ND	-4.64	1.96	2.05
21	6	301	CLA	MG-ND	-4.63	1.96	2.05
21	c	514	CLA	MG-NC	4.63	2.17	2.06
24	g	315	KC1	OBD-CAD	4.63	1.28	1.22
24	5	313	KC1	OBD-CAD	4.63	1.28	1.22
24	8	315	KC1	C4D-ND	4.63	1.39	1.35
24	7	314	KC1	OBD-CAD	4.62	1.28	1.22
23	6	309	A86	C26-C27	4.62	1.41	1.35
21	B	621	CLA	MG-ND	4.62	2.14	2.05
24	6	312	KC1	C4D-ND	4.62	1.39	1.35
24	J	313	KC1	C1A-NA	-4.61	1.29	1.38
24	8	316	KC1	CHC-C4B	4.61	1.47	1.38
24	8	314	KC1	CHC-C4B	4.61	1.47	1.38
24	2	314	KC1	OBD-CAD	4.60	1.28	1.22
24	4	307	KC1	OBD-CAD	4.60	1.28	1.22
24	g	314	KC1	C1A-NA	-4.60	1.29	1.38
21	7	309	CLA	MG-NA	4.60	2.17	2.06
24	5	314	KC1	OBD-CAD	4.59	1.28	1.22
24	5	315	KC1	CHC-C4B	4.59	1.47	1.38
24	2	315	KC1	C4D-ND	4.59	1.39	1.35
24	7	315	KC1	CHC-C4B	4.59	1.47	1.38
24	G	307	KC1	OBD-CAD	4.58	1.28	1.22
24	3	305	KC1	C4D-ND	4.58	1.39	1.35
21	c	508	CLA	MG-NA	4.57	2.17	2.06
24	4	307	KC1	CHB-C1B	4.57	1.47	1.38
24	g	315	KC1	CHB-C1B	4.57	1.47	1.38
24	3	305	KC1	CHB-C1B	4.57	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	311	KC1	CHC-C4B	4.57	1.47	1.38
24	g	313	KC1	CHB-C1B	4.57	1.47	1.38
24	3	306	KC1	CHC-C4B	4.56	1.47	1.38
24	5	314	KC1	CHC-C4B	4.56	1.47	1.38
24	g	314	KC1	CHC-C4B	4.56	1.47	1.38
24	g	313	KC1	CHC-C4B	4.55	1.47	1.38
24	6	313	KC1	C4D-ND	4.55	1.39	1.35
24	4	308	KC1	CHB-C1B	4.55	1.47	1.38
24	J	312	KC1	CHB-C1B	4.55	1.47	1.38
24	7	314	KC1	CHB-C1B	4.54	1.47	1.38
21	c	508	CLA	MG-ND	4.54	2.14	2.05
24	5	315	KC1	CHB-C1B	4.54	1.47	1.38
24	G	306	KC1	CHB-C1B	4.54	1.47	1.38
24	2	315	KC1	CHC-C4B	4.53	1.47	1.38
24	6	311	KC1	CHC-C4B	4.52	1.47	1.38
24	2	315	KC1	OBD-CAD	4.52	1.28	1.22
24	2	313	KC1	C1A-NA	-4.52	1.29	1.38
24	9	305	KC1	CHB-C1B	4.52	1.47	1.38
24	1	315	KC1	CHB-C1B	4.51	1.47	1.38
24	1	316	KC1	C4D-ND	4.51	1.39	1.35
24	G	306	KC1	C4D-ND	4.51	1.39	1.35
21	7	309	CLA	O2A-CGA	4.50	1.45	1.30
21	J	303	CLA	O2A-CGA	4.50	1.45	1.30
24	8	316	KC1	C1A-NA	-4.50	1.29	1.38
24	g	315	KC1	C4D-ND	4.50	1.39	1.35
24	8	315	KC1	OBD-CAD	4.49	1.28	1.22
23	6	309	A86	C5-C6	4.49	1.41	1.35
21	6	303	CLA	O2A-CGA	4.49	1.45	1.30
21	6	305	CLA	O2A-CGA	4.49	1.45	1.30
21	c	507	CLA	O2A-CGA	4.48	1.45	1.30
21	J	305	CLA	O2A-CGA	4.48	1.45	1.30
24	4	306	KC1	C4D-ND	4.48	1.39	1.35
24	6	312	KC1	CHB-C1B	4.48	1.47	1.38
21	J	302	CLA	O2A-CGA	4.47	1.45	1.30
21	C	508	CLA	O2A-CGA	4.47	1.45	1.30
21	6	302	CLA	O2A-CGA	4.47	1.45	1.30
24	1	315	KC1	C4D-ND	4.47	1.39	1.35
21	1	308	CLA	O2A-CGA	4.46	1.46	1.33
24	G	309	KC1	CHC-C4B	4.46	1.47	1.38
24	2	316	KC1	CHB-C1B	4.45	1.47	1.38
24	8	314	KC1	C4D-ND	4.44	1.39	1.35
24	2	316	KC1	C1A-NA	-4.44	1.29	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	307	KC1	CHC-C4B	4.44	1.47	1.38
24	9	305	KC1	CHC-C4B	4.44	1.47	1.38
21	2	306	CLA	O2A-CGA	4.44	1.45	1.30
24	2	313	KC1	CHC-C4B	4.43	1.47	1.38
24	8	316	KC1	CHB-C1B	4.42	1.47	1.38
21	7	306	CLA	MG-NC	4.42	2.16	2.06
23	8	308	A86	C5-C6	4.42	1.41	1.35
24	7	314	KC1	C4D-ND	4.40	1.39	1.35
24	4	309	KC1	C4D-ND	4.40	1.39	1.35
24	G	308	KC1	CHB-C1B	4.40	1.46	1.38
24	6	313	KC1	CHB-C1B	4.39	1.46	1.38
24	J	313	KC1	CHB-C1B	4.39	1.46	1.38
24	7	315	KC1	CHB-C1B	4.39	1.46	1.38
24	9	306	KC1	C4D-ND	4.39	1.39	1.35
24	7	315	KC1	C4D-ND	4.38	1.39	1.35
24	2	314	KC1	C4D-ND	4.38	1.39	1.35
21	b	623	CLA	MG-ND	4.38	2.14	2.05
24	6	311	KC1	OBD-CAD	4.38	1.28	1.22
24	5	313	KC1	CHC-C4B	4.38	1.46	1.38
24	5	313	KC1	CHB-C1B	4.38	1.46	1.38
21	J	301	CLA	MG-ND	-4.37	1.97	2.05
24	J	311	KC1	C4D-ND	4.37	1.39	1.35
24	J	312	KC1	C4D-ND	4.36	1.39	1.35
21	6	307	CLA	O2A-CGA	4.36	1.46	1.33
24	6	311	KC1	C4D-ND	4.36	1.39	1.35
23	6	309	A86	C2-C1	4.36	1.41	1.35
23	2	309	A86	C5-C6	4.35	1.41	1.35
24	5	314	KC1	CHB-C1B	4.35	1.46	1.38
24	2	313	KC1	C4D-ND	4.34	1.39	1.35
22	5	310	DD6	C10-C11	4.34	1.41	1.35
21	1	301	CLA	O2A-CGA	4.34	1.46	1.33
23	7	312	A86	C5-C6	4.34	1.41	1.35
21	9	303	CLA	O2A-CGA	4.34	1.46	1.33
21	1	309	CLA	O2A-CGA	4.33	1.46	1.33
24	3	306	KC1	CHB-C1B	4.32	1.46	1.38
21	c	510	CLA	O2A-CGA	4.32	1.46	1.33
23	7	311	A86	C2-C1	4.32	1.41	1.35
21	J	301	CLA	O2A-CGA	4.32	1.46	1.33
21	b	616	CLA	MG-ND	4.32	2.14	2.05
21	1	304	CLA	O2A-CGA	4.32	1.46	1.33
21	C	509	CLA	O2A-CGA	4.32	1.46	1.33
23	5	312	A86	C5-C6	4.31	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	304	CLA	O2A-CGA	4.31	1.45	1.33
24	1	316	KC1	CHB-C1B	4.31	1.46	1.38
21	9	301	CLA	O2A-CGA	4.30	1.45	1.33
21	7	303	CLA	O2A-CGA	4.30	1.45	1.33
24	8	314	KC1	CHB-C1B	4.30	1.46	1.38
21	B	612	CLA	MG-ND	-4.30	1.97	2.05
21	g	306	CLA	O2A-CGA	4.30	1.45	1.33
21	B	602	CLA	O2A-CGA	4.30	1.45	1.33
21	g	308	CLA	O2A-CGA	4.29	1.45	1.33
21	5	308	CLA	O2A-CGA	4.29	1.45	1.33
21	8	303	CLA	O2A-CGA	4.29	1.45	1.33
21	9	304	CLA	O2A-CGA	4.29	1.45	1.33
21	5	307	CLA	O2A-CGA	4.29	1.45	1.33
24	8	313	KC1	OBD-CAD	4.29	1.28	1.22
24	5	313	KC1	C4D-ND	4.29	1.39	1.35
24	G	307	KC1	CHC-C4B	4.29	1.46	1.38
21	3	301	CLA	O2A-CGA	4.29	1.45	1.33
23	7	312	A86	C2-C1	4.29	1.41	1.35
24	4	309	KC1	CHC-C4B	4.28	1.46	1.38
24	2	313	KC1	OBD-CAD	4.28	1.28	1.22
21	5	309	CLA	O2A-CGA	4.28	1.45	1.33
21	J	307	CLA	O2A-CGA	4.28	1.45	1.33
21	3	302	CLA	O2A-CGA	4.28	1.45	1.33
21	c	514	CLA	O2A-CGA	4.28	1.45	1.33
21	4	303	CLA	O2A-CGA	4.28	1.45	1.33
21	g	302	CLA	O2A-CGA	4.28	1.45	1.33
21	G	303	CLA	O2A-CGA	4.27	1.45	1.33
21	9	300	CLA	O2A-CGA	4.27	1.45	1.33
24	J	311	KC1	CHB-C1B	4.27	1.46	1.38
24	g	314	KC1	CHB-C1B	4.27	1.46	1.38
24	3	306	KC1	C4D-ND	4.27	1.39	1.35
21	8	306	CLA	O2A-CGA	4.27	1.45	1.33
23	8	312	A86	C2-C1	4.27	1.41	1.35
21	1	307	CLA	MG-ND	-4.26	1.97	2.05
21	5	304	CLA	O2A-CGA	4.26	1.45	1.33
21	7	301	CLA	O2A-CGA	4.26	1.45	1.33
21	g	303	CLA	O2A-CGA	4.26	1.45	1.33
21	G	302	CLA	O2A-CGA	4.26	1.45	1.33
21	C	512	CLA	O2A-CGA	4.26	1.45	1.33
23	2	309	A86	C2-C1	4.26	1.41	1.35
24	8	313	KC1	C4D-ND	4.26	1.39	1.35
21	C	511	CLA	O2A-CGA	4.26	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	304	CLA	O2A-CGA	4.26	1.45	1.33
21	2	302	CLA	O2A-CGA	4.25	1.45	1.33
21	6	301	CLA	O2A-CGA	4.25	1.45	1.33
24	G	309	KC1	C4D-ND	4.25	1.39	1.35
23	1	313	A86	C5-C6	4.25	1.41	1.35
21	C	504	CLA	O2A-CGA	4.25	1.45	1.33
21	1	305	CLA	O2A-CGA	4.25	1.45	1.33
21	4	301	CLA	O2A-CGA	4.25	1.45	1.33
21	c	511	CLA	O2A-CGA	4.25	1.45	1.33
21	5	302	CLA	O2A-CGA	4.25	1.45	1.33
21	6	300	CLA	O2A-CGA	4.24	1.45	1.33
21	G	301	CLA	O2A-CGA	4.24	1.45	1.33
21	g	304	CLA	O2A-CGA	4.24	1.45	1.33
21	1	302	CLA	O2A-CGA	4.24	1.45	1.33
21	b	603	CLA	O2A-CGA	4.23	1.45	1.33
21	C	510	CLA	O2A-CGA	4.23	1.45	1.33
21	c	503	CLA	O2A-CGA	4.23	1.45	1.33
21	D	404	CLA	O2A-CGA	4.23	1.45	1.33
21	c	509	CLA	O2A-CGA	4.23	1.45	1.33
21	7	307	CLA	O2A-CGA	4.23	1.45	1.33
21	3	304	CLA	O2A-CGA	4.23	1.45	1.33
21	9	302	CLA	O2A-CGA	4.23	1.45	1.33
21	c	512	CLA	O2A-CGA	4.22	1.45	1.33
24	G	308	KC1	C4D-ND	4.22	1.39	1.35
21	D	407	CLA	O2A-CGA	4.22	1.45	1.33
23	1	313	A86	C2-C1	4.22	1.41	1.35
21	d	404	CLA	O2A-CGA	4.22	1.45	1.33
24	J	311	KC1	OBD-CAD	4.22	1.28	1.22
21	2	305	CLA	O2A-CGA	4.22	1.45	1.33
21	1	310	CLA	O2A-CGA	4.22	1.45	1.33
21	b	614	CLA	O2A-CGA	4.22	1.45	1.33
21	B	603	CLA	O2A-CGA	4.21	1.45	1.33
21	2	301	CLA	O2A-CGA	4.21	1.45	1.33
23	5	312	A86	C2-C1	4.21	1.41	1.35
21	6	306	CLA	O2A-CGA	4.21	1.45	1.33
21	J	306	CLA	O2A-CGA	4.21	1.45	1.33
21	J	301	CLA	MG-NA	4.21	2.16	2.06
21	b	611	CLA	O2A-CGA	4.21	1.45	1.33
21	4	304	CLA	MG-NC	4.21	2.16	2.06
24	2	314	KC1	CHB-C1B	4.21	1.46	1.38
24	6	311	KC1	CHB-C1B	4.20	1.46	1.38
21	J	300	CLA	O2A-CGA	4.20	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	300	CLA	O2A-CGA	4.19	1.45	1.33
21	C	513	CLA	O2A-CGA	4.19	1.45	1.33
21	d	405	CLA	O2A-CGA	4.19	1.45	1.33
21	1	303	CLA	O2A-CGA	4.19	1.45	1.33
21	G	300	CLA	O2A-CGA	4.19	1.45	1.33
21	7	308	CLA	O2A-CGA	4.19	1.45	1.33
21	d	406	CLA	O2A-CGA	4.19	1.45	1.33
24	G	307	KC1	CHB-C1B	4.19	1.46	1.38
21	3	300	CLA	O2A-CGA	4.18	1.45	1.33
21	b	623	CLA	O2A-CGA	4.18	1.45	1.33
23	g	312	A86	C2-C1	4.18	1.41	1.35
21	c	505	CLA	O2A-CGA	4.18	1.45	1.33
21	B	616	CLA	O2A-CGA	4.18	1.45	1.33
21	a	403	CLA	O2A-CGA	4.18	1.45	1.33
21	g	309	CLA	O2A-CGA	4.18	1.45	1.33
23	8	308	A86	C2-C1	4.18	1.41	1.35
21	J	303	CLA	CHD-C4C	4.18	1.48	1.39
21	B	608	CLA	O2A-CGA	4.18	1.45	1.33
21	D	406	CLA	O2A-CGA	4.17	1.45	1.33
21	5	303	CLA	O2A-CGA	4.17	1.45	1.33
21	B	613	CLA	O2A-CGA	4.17	1.45	1.33
21	C	515	CLA	O2A-CGA	4.17	1.45	1.33
23	7	311	A86	C5-C6	4.17	1.41	1.35
24	8	316	KC1	C4D-ND	4.17	1.38	1.35
24	8	313	KC1	CHB-C1B	4.17	1.46	1.38
21	g	309	CLA	CHD-C4C	4.17	1.48	1.39
21	b	609	CLA	O2A-CGA	4.17	1.45	1.33
21	c	508	CLA	O2A-CGA	4.16	1.45	1.33
21	B	611	CLA	O2A-CGA	4.16	1.45	1.33
23	G	305	A86	C5-C6	4.16	1.41	1.35
21	5	306	CLA	O2A-CGA	4.16	1.45	1.33
21	b	612	CLA	O2A-CGA	4.16	1.45	1.33
23	1	314	A86	C2-C1	4.16	1.41	1.35
21	a	405	CLA	O2A-CGA	4.16	1.45	1.33
21	b	610	CLA	O2A-CGA	4.16	1.45	1.33
24	2	316	KC1	C4D-ND	4.16	1.38	1.35
21	B	614	CLA	O2A-CGA	4.15	1.45	1.33
21	B	615	CLA	O2A-CGA	4.15	1.45	1.33
23	J	309	A86	C2-C1	4.15	1.41	1.35
24	5	315	KC1	C4D-ND	4.15	1.38	1.35
23	2	312	A86	C2-C1	4.15	1.41	1.35
21	6	308	CLA	O2A-CGA	4.15	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	609	CLA	O2A-CGA	4.15	1.45	1.33
21	b	615	CLA	O2A-CGA	4.15	1.45	1.33
23	5	311	A86	C5-C6	4.15	1.41	1.35
21	7	304	CLA	O2A-CGA	4.15	1.45	1.33
23	8	312	A86	C5-C6	4.15	1.41	1.35
21	b	604	CLA	O2A-CGA	4.14	1.45	1.33
21	c	513	CLA	O2A-CGA	4.14	1.45	1.33
21	G	304	CLA	MG-NC	4.14	2.16	2.06
21	A	402	CLA	O2A-CGA	4.14	1.45	1.33
21	c	509	CLA	MG-NA	4.14	2.16	2.06
21	C	506	CLA	O2A-CGA	4.14	1.45	1.33
21	b	605	CLA	O2A-CGA	4.14	1.45	1.33
21	J	308	CLA	O2A-CGA	4.14	1.45	1.33
23	4	305	A86	C5-C6	4.14	1.41	1.35
21	b	617	CLA	O2A-CGA	4.14	1.45	1.33
21	J	302	CLA	CHD-C4C	4.13	1.48	1.39
23	2	312	A86	C5-C6	4.13	1.41	1.35
21	4	300	CLA	O2A-CGA	4.13	1.45	1.33
21	c	506	CLA	O2A-CGA	4.13	1.45	1.33
23	g	312	A86	C5-C6	4.13	1.41	1.35
21	9	301	CLA	CHD-C4C	4.13	1.48	1.39
21	C	507	CLA	O2A-CGA	4.12	1.45	1.33
22	5	310	DD6	C5-C6	4.12	1.41	1.35
21	C	512	CLA	MG-ND	-4.12	1.97	2.05
21	c	505	CLA	CHD-C4C	4.12	1.48	1.39
21	8	302	CLA	O2A-CGA	4.12	1.45	1.33
21	A	404	CLA	O2A-CGA	4.12	1.45	1.33
23	G	305	A86	C2-C1	4.12	1.41	1.35
21	C	503	CLA	O2A-CGA	4.12	1.45	1.33
21	5	305	CLA	CHD-C4C	4.12	1.48	1.39
21	B	610	CLA	O2A-CGA	4.11	1.45	1.33
21	1	305	CLA	CHD-C4C	4.11	1.48	1.39
21	C	514	CLA	O2A-CGA	4.11	1.45	1.33
21	b	616	CLA	O2A-CGA	4.11	1.45	1.33
21	B	604	CLA	O2A-CGA	4.11	1.45	1.33
21	b	607	CLA	O2A-CGA	4.11	1.45	1.33
21	G	302	CLA	CHD-C4C	4.11	1.48	1.39
21	B	605	CLA	O2A-CGA	4.11	1.45	1.33
21	c	504	CLA	O2A-CGA	4.11	1.45	1.33
21	8	304	CLA	O2A-CGA	4.11	1.45	1.33
21	B	615	CLA	CHD-C4C	4.11	1.48	1.39
21	6	303	CLA	CHD-C4C	4.10	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	304	CLA	CHD-C4C	4.10	1.48	1.39
21	d	404	CLA	CHD-C4C	4.10	1.48	1.39
23	1	314	A86	C5-C6	4.10	1.41	1.35
23	2	311	A86	C2-C1	4.09	1.41	1.35
21	g	307	CLA	CHD-C4C	4.09	1.48	1.39
21	4	304	CLA	CHD-C4C	4.09	1.48	1.39
23	6	310	A86	C5-C6	4.09	1.41	1.35
21	D	404	CLA	CHD-C4C	4.09	1.48	1.39
21	4	302	CLA	O2A-CGA	4.09	1.45	1.33
21	5	306	CLA	MG-ND	-4.09	1.97	2.05
21	B	606	CLA	O2A-CGA	4.09	1.45	1.33
24	2	315	KC1	C1A-CHA	4.08	1.51	1.40
23	2	307	A86	C2-C1	4.08	1.41	1.35
21	3	304	CLA	CHD-C4C	4.08	1.48	1.39
21	b	606	CLA	O2A-CGA	4.08	1.45	1.33
21	7	309	CLA	CHD-C4C	4.08	1.48	1.39
21	A	401	CLA	O2A-CGA	4.08	1.45	1.33
21	5	309	CLA	MG-ND	4.08	2.13	2.05
21	B	607	CLA	O2A-CGA	4.08	1.45	1.33
21	B	621	CLA	O2A-CGA	4.08	1.45	1.33
22	g	310	DD6	C2-C1	4.08	1.41	1.35
23	J	309	A86	C5-C6	4.08	1.41	1.35
21	C	505	CLA	O2A-CGA	4.08	1.45	1.33
23	g	311	A86	C2-C1	4.07	1.41	1.35
21	7	302	CLA	O2A-CGA	4.07	1.45	1.33
21	5	309	CLA	CHD-C4C	4.07	1.48	1.39
21	3	303	CLA	CHD-C4C	4.07	1.48	1.39
21	b	608	CLA	O2A-CGA	4.07	1.45	1.33
23	2	311	A86	C5-C6	4.07	1.41	1.35
21	g	305	CLA	CHD-C4C	4.07	1.48	1.39
21	2	303	CLA	O2A-CGA	4.07	1.45	1.33
21	a	402	CLA	O2A-CGA	4.07	1.45	1.33
21	c	502	CLA	O2A-CGA	4.07	1.45	1.33
21	9	303	CLA	CHD-C4C	4.06	1.48	1.39
21	6	302	CLA	CHD-C4C	4.06	1.48	1.39
21	G	303	CLA	CHD-C4C	4.06	1.48	1.39
21	6	304	CLA	CHD-C4C	4.06	1.48	1.39
21	4	302	CLA	CHD-C4C	4.06	1.48	1.39
23	J	310	A86	C5-C6	4.06	1.41	1.35
21	G	301	CLA	CHD-C4C	4.06	1.48	1.39
21	J	304	CLA	CHD-C4C	4.05	1.48	1.39
21	c	513	CLA	MG-ND	4.05	2.13	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	616	CLA	CHD-C4C	4.05	1.48	1.39
21	4	303	CLA	CHD-C4C	4.05	1.48	1.39
21	C	506	CLA	CHD-C4C	4.05	1.48	1.39
21	1	303	CLA	CHD-C4C	4.05	1.48	1.39
21	8	304	CLA	CHD-C4C	4.05	1.48	1.39
21	J	308	CLA	CHD-C4C	4.05	1.48	1.39
21	5	307	CLA	CHD-C4C	4.04	1.48	1.39
21	g	308	CLA	CHD-C4C	4.04	1.48	1.39
21	G	304	CLA	CHD-C4C	4.04	1.48	1.39
22	5	310	DD6	C2-C1	4.04	1.41	1.35
23	g	311	A86	C5-C6	4.04	1.41	1.35
24	8	316	KC1	C1A-CHA	4.04	1.51	1.40
21	J	300	CLA	CHD-C4C	4.04	1.48	1.39
23	2	307	A86	C5-C6	4.04	1.41	1.35
21	d	406	CLA	CHD-C4C	4.03	1.48	1.39
21	7	302	CLA	CHD-C4C	4.03	1.48	1.39
21	c	514	CLA	CHD-C4C	4.03	1.48	1.39
24	8	315	KC1	C1A-CHA	4.03	1.51	1.40
21	1	310	CLA	CHD-C4C	4.02	1.48	1.39
21	A	404	CLA	CHD-C4C	4.02	1.48	1.39
21	4	301	CLA	CHD-C4C	4.02	1.48	1.39
21	6	300	CLA	CHD-C4C	4.02	1.48	1.39
21	g	307	CLA	O2A-CGA	4.02	1.45	1.33
24	5	314	KC1	C4D-ND	4.01	1.38	1.35
23	1	312	A86	C5-C6	4.01	1.41	1.35
21	2	305	CLA	CHD-C4C	4.01	1.48	1.39
21	3	301	CLA	CHD-C4C	4.01	1.48	1.39
21	D	407	CLA	CHD-C4C	4.01	1.48	1.39
21	C	503	CLA	CHD-C4C	4.01	1.48	1.39
24	2	316	KC1	C1A-CHA	4.01	1.51	1.40
21	a	405	CLA	CHD-C4C	4.01	1.48	1.39
21	b	609	CLA	CHD-C4C	4.01	1.48	1.39
21	1	302	CLA	CHD-C4C	4.00	1.48	1.39
21	4	300	CLA	CHD-C4C	4.00	1.48	1.39
23	1	312	A86	C2-C1	4.00	1.41	1.35
21	6	308	CLA	CHD-C4C	4.00	1.48	1.39
21	9	302	CLA	CHD-C4C	4.00	1.48	1.39
21	6	305	CLA	CHD-C4C	4.00	1.48	1.39
21	J	305	CLA	CHD-C4C	4.00	1.48	1.39
24	2	313	KC1	C1A-CHA	4.00	1.51	1.40
21	9	300	CLA	CHD-C4C	4.00	1.48	1.39
21	B	603	CLA	CHD-C4C	3.99	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	612	CLA	O2A-CGA	3.99	1.45	1.33
23	5	311	A86	C2-C1	3.99	1.41	1.35
21	C	515	CLA	CHD-C4C	3.99	1.48	1.39
21	7	304	CLA	CHD-C4C	3.99	1.48	1.39
21	b	604	CLA	CHD-C4C	3.99	1.48	1.39
21	c	507	CLA	CHD-C4C	3.99	1.48	1.39
22	g	310	DD6	C10-C11	3.98	1.41	1.35
23	6	310	A86	C2-C1	3.98	1.41	1.35
21	C	508	CLA	CHD-C4C	3.98	1.48	1.39
21	5	304	CLA	CHD-C4C	3.98	1.48	1.39
21	g	304	CLA	CHD-C4C	3.98	1.48	1.39
21	a	403	CLA	CHD-C4C	3.98	1.48	1.39
21	7	301	CLA	CHD-C4C	3.98	1.48	1.39
21	J	307	CLA	CHD-C4C	3.98	1.48	1.39
21	b	613	CLA	O2A-CGA	3.98	1.45	1.33
24	J	313	KC1	C1A-CHA	3.98	1.51	1.40
21	c	502	CLA	CHD-C4C	3.98	1.48	1.39
21	c	512	CLA	CHD-C4C	3.98	1.48	1.39
21	8	306	CLA	CHD-C4C	3.98	1.48	1.39
21	1	304	CLA	CHD-C4C	3.98	1.48	1.39
21	A	402	CLA	CHD-C4C	3.97	1.48	1.39
21	g	306	CLA	CHD-C4C	3.97	1.48	1.39
21	C	505	CLA	CHD-C4C	3.97	1.48	1.39
21	c	513	CLA	CHD-C4C	3.97	1.48	1.39
21	5	306	CLA	CHD-C4C	3.97	1.48	1.39
21	J	306	CLA	CHD-C4C	3.97	1.48	1.39
21	2	306	CLA	CHD-C4C	3.97	1.48	1.39
21	7	305	CLA	CHD-C4C	3.97	1.48	1.39
21	5	308	CLA	CHD-C4C	3.97	1.48	1.39
21	6	306	CLA	CHD-C4C	3.96	1.48	1.39
21	B	607	CLA	CHD-C4C	3.96	1.48	1.39
21	B	608	CLA	CHD-C4C	3.96	1.48	1.39
21	C	513	CLA	MG-NC	3.96	2.15	2.06
24	4	309	KC1	C1A-CHA	3.96	1.51	1.40
21	7	303	CLA	CHD-C4C	3.96	1.48	1.39
21	C	511	CLA	CHD-C4C	3.96	1.48	1.39
21	c	511	CLA	CHD-C4C	3.96	1.48	1.39
23	J	310	A86	C2-C1	3.96	1.41	1.35
21	1	308	CLA	CHD-C4C	3.95	1.48	1.39
21	2	303	CLA	CHD-C4C	3.95	1.48	1.39
21	7	300	CLA	CHD-C4C	3.95	1.48	1.39
21	7	304	CLA	MG-NC	3.95	2.15	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	512	CLA	CHD-C4C	3.95	1.48	1.39
24	G	307	KC1	C4D-ND	3.95	1.38	1.35
23	8	308	A86	C26-C27	3.95	1.41	1.35
21	b	608	CLA	CHD-C4C	3.94	1.48	1.39
24	9	306	KC1	CHC-C1C	3.94	1.48	1.39
21	g	302	CLA	CHD-C4C	3.94	1.48	1.39
21	G	300	CLA	CHD-C4C	3.94	1.48	1.39
21	b	605	CLA	CHD-C4C	3.94	1.48	1.39
21	b	623	CLA	CHD-C4C	3.94	1.48	1.39
21	C	509	CLA	CHD-C4C	3.94	1.48	1.39
35	d	408	PL9	C7-C3	-3.94	1.47	1.51
24	6	313	KC1	C1A-CHA	3.94	1.51	1.40
21	B	602	CLA	CHD-C4C	3.94	1.48	1.39
21	7	308	CLA	CHD-C4C	3.94	1.48	1.39
21	b	607	CLA	CHD-C4C	3.94	1.48	1.39
21	c	504	CLA	CHD-C4C	3.94	1.48	1.39
23	8	311	A86	C2-C1	3.93	1.41	1.35
24	1	316	KC1	C1A-CHA	3.93	1.51	1.40
21	B	621	CLA	CHD-C4C	3.93	1.48	1.39
23	W	101	A86	C5-C6	3.93	1.41	1.35
21	8	307	CLA	CHD-C4C	3.93	1.48	1.39
23	2	310	A86	C2-C1	3.93	1.41	1.35
24	2	315	KC1	CHB-C1B	3.93	1.46	1.38
22	g	310	DD6	C5-C6	3.93	1.41	1.35
23	7	313	A86	C2-C1	3.93	1.41	1.35
23	8	310	A86	C5-C6	3.93	1.41	1.35
21	b	614	CLA	CHD-C4C	3.93	1.48	1.39
21	b	603	CLA	CHD-C4C	3.92	1.48	1.39
21	2	304	CLA	CHD-C4C	3.92	1.48	1.39
24	2	314	KC1	CHC-C1C	3.92	1.48	1.39
21	B	613	CLA	CHD-C4C	3.92	1.48	1.39
21	1	301	CLA	CHD-C4C	3.92	1.48	1.39
21	5	302	CLA	CHD-C4C	3.92	1.48	1.39
21	B	606	CLA	CHD-C4C	3.92	1.48	1.39
21	3	300	CLA	CHD-C4C	3.92	1.48	1.39
21	C	514	CLA	CHD-C4C	3.92	1.48	1.39
23	7	313	A86	C5-C6	3.91	1.41	1.35
21	C	507	CLA	CHD-C4C	3.91	1.48	1.39
21	8	303	CLA	CHD-C4C	3.91	1.48	1.39
23	W	101	A86	C2-C1	3.91	1.41	1.35
24	9	305	KC1	C4D-ND	3.91	1.38	1.35
23	8	311	A86	C5-C6	3.90	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	506	CLA	CHD-C4C	3.90	1.48	1.39
24	G	306	KC1	C1A-CHA	3.90	1.51	1.40
21	B	604	CLA	CHD-C4C	3.90	1.48	1.39
21	c	510	CLA	CHD-C4C	3.89	1.48	1.39
21	5	303	CLA	CHD-C4C	3.89	1.48	1.39
21	A	401	CLA	CHD-C4C	3.89	1.48	1.39
21	a	402	CLA	CHD-C4C	3.89	1.48	1.39
24	8	314	KC1	C1B-NB	-3.89	1.33	1.37
21	6	307	CLA	CHD-C4C	3.89	1.48	1.39
24	7	315	KC1	C1A-CHA	3.88	1.51	1.40
21	B	605	CLA	CHD-C4C	3.88	1.48	1.39
21	7	307	CLA	CHD-C4C	3.88	1.48	1.39
21	C	513	CLA	CHD-C4C	3.88	1.48	1.39
24	2	314	KC1	C1B-NB	-3.88	1.33	1.37
32	f	101	HEM	C3C-CAC	3.88	1.55	1.47
21	9	303	CLA	MG-NC	3.87	2.15	2.06
21	c	508	CLA	CHD-C4C	3.87	1.48	1.39
24	7	315	KC1	CHC-C1C	3.87	1.48	1.39
24	4	306	KC1	C1A-CHA	3.87	1.51	1.40
24	8	313	KC1	C1A-CHA	3.87	1.51	1.40
21	2	302	CLA	CHD-C4C	3.87	1.48	1.39
21	b	615	CLA	CHD-C4C	3.87	1.48	1.39
21	B	609	CLA	CHD-C4C	3.87	1.48	1.39
21	b	610	CLA	CHD-C4C	3.86	1.48	1.39
21	B	614	CLA	CHD-C4C	3.86	1.48	1.39
32	E	101	HEM	C3C-CAC	3.86	1.55	1.47
24	8	315	KC1	C1B-NB	-3.86	1.33	1.37
21	b	606	CLA	CHD-C4C	3.85	1.48	1.39
21	6	303	CLA	OBD-CAD	3.85	1.29	1.22
24	g	315	KC1	C1A-CHA	3.85	1.50	1.40
21	1	302	CLA	MG-ND	3.85	2.13	2.05
21	g	303	CLA	CHD-C4C	3.84	1.48	1.39
21	b	611	CLA	CHD-C4C	3.84	1.48	1.39
24	8	313	KC1	C1B-NB	-3.84	1.33	1.37
24	1	316	KC1	CHC-C1C	3.84	1.48	1.39
21	1	306	CLA	MG-ND	-3.84	1.98	2.05
23	2	310	A86	C5-C6	3.83	1.40	1.35
24	J	312	KC1	C1A-CHA	3.83	1.50	1.40
21	1	307	CLA	CHD-C4C	3.83	1.48	1.39
24	4	307	KC1	C4D-ND	3.83	1.38	1.35
24	g	313	KC1	C4D-ND	3.83	1.38	1.35
22	1	311	DD6	C5-C6	3.82	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	315	KC1	CHB-C1B	3.82	1.45	1.38
24	G	309	KC1	C1A-CHA	3.82	1.50	1.40
24	6	312	KC1	C1A-CHA	3.82	1.50	1.40
21	8	302	CLA	CHD-C4C	3.81	1.47	1.39
21	2	301	CLA	CHD-C4C	3.81	1.47	1.39
23	8	309	A86	C2-C1	3.81	1.40	1.35
21	J	303	CLA	OBD-CAD	3.80	1.29	1.22
21	8	305	CLA	CHD-C4C	3.80	1.47	1.39
21	c	505	CLA	MG-ND	-3.80	1.98	2.05
21	G	304	CLA	MG-ND	-3.80	1.98	2.05
22	7	310	DD6	C2-C1	3.80	1.40	1.35
22	7	310	DD6	C5-C6	3.79	1.40	1.35
24	8	314	KC1	CHC-C1C	3.79	1.47	1.39
24	8	314	KC1	C1A-CHA	3.79	1.50	1.40
21	8	307	CLA	MG-ND	3.79	2.13	2.05
21	g	304	CLA	OBD-CAD	3.79	1.29	1.22
21	9	301	CLA	OBD-CAD	3.79	1.29	1.22
21	1	309	CLA	CHD-C4C	3.79	1.47	1.39
21	B	610	CLA	CHD-C4C	3.78	1.47	1.39
35	D	409	PL9	C7-C3	-3.78	1.47	1.51
21	c	503	CLA	CHD-C4C	3.78	1.47	1.39
21	6	301	CLA	CHD-C4C	3.78	1.47	1.39
21	J	302	CLA	OBD-CAD	3.78	1.29	1.22
22	1	311	DD6	C2-C1	3.78	1.40	1.35
21	6	305	CLA	MG-ND	3.78	2.13	2.05
21	J	308	CLA	OBD-CAD	3.78	1.29	1.22
21	1	306	CLA	CHD-C4C	3.77	1.47	1.39
22	7	310	DD6	C10-C11	3.77	1.40	1.35
21	J	300	CLA	OBD-CAD	3.77	1.29	1.22
21	g	305	CLA	OBD-CAD	3.77	1.29	1.22
21	G	303	CLA	OBD-CAD	3.77	1.29	1.22
23	4	305	A86	C2-C1	3.77	1.40	1.35
21	9	303	CLA	OBD-CAD	3.76	1.29	1.22
21	4	302	CLA	OBD-CAD	3.76	1.29	1.22
21	c	504	CLA	MG-ND	3.76	2.13	2.05
24	7	314	KC1	C1A-CHA	3.76	1.50	1.40
24	J	311	KC1	CHC-C1C	3.76	1.47	1.39
21	C	510	CLA	CHD-C4C	3.76	1.47	1.39
21	6	302	CLA	OBD-CAD	3.76	1.29	1.22
21	4	303	CLA	OBD-CAD	3.76	1.29	1.22
24	g	313	KC1	CHC-C1C	3.76	1.47	1.39
24	8	313	KC1	CHC-C1C	3.75	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	305	KC1	CHC-C1C	3.75	1.47	1.39
24	9	306	KC1	C1A-CHA	3.75	1.50	1.40
21	5	307	CLA	OBD-CAD	3.75	1.28	1.22
24	5	315	KC1	CHC-C1C	3.75	1.47	1.39
21	7	306	CLA	CHD-C4C	3.75	1.47	1.39
21	3	300	CLA	OBD-CAD	3.75	1.28	1.22
24	6	313	KC1	CHC-C1C	3.75	1.47	1.39
24	3	305	KC1	C1A-CHA	3.75	1.50	1.40
21	3	303	CLA	OBD-CAD	3.75	1.28	1.22
24	1	315	KC1	C1A-CHA	3.75	1.50	1.40
24	g	315	KC1	CHC-C1C	3.75	1.47	1.39
21	6	308	CLA	OBD-CAD	3.75	1.28	1.22
21	6	305	CLA	OBD-CAD	3.75	1.28	1.22
21	c	509	CLA	CHD-C4C	3.75	1.47	1.39
21	J	305	CLA	OBD-CAD	3.75	1.28	1.22
21	J	307	CLA	OBD-CAD	3.74	1.28	1.22
21	C	514	CLA	OBD-CAD	3.74	1.28	1.22
21	9	300	CLA	OBD-CAD	3.74	1.28	1.22
21	7	307	CLA	OBD-CAD	3.74	1.28	1.22
21	3	304	CLA	OBD-CAD	3.74	1.28	1.22
21	2	304	CLA	OBD-CAD	3.74	1.28	1.22
21	5	306	CLA	OBD-CAD	3.74	1.28	1.22
21	C	513	CLA	MG-ND	3.74	2.13	2.05
30	C	518	DGD	O2G-C2G	-3.73	1.40	1.47
21	5	304	CLA	OBD-CAD	3.73	1.28	1.22
21	g	307	CLA	OBD-CAD	3.73	1.28	1.22
21	J	301	CLA	CHD-C4C	3.73	1.47	1.39
21	5	308	CLA	OBD-CAD	3.73	1.28	1.22
21	4	300	CLA	OBD-CAD	3.73	1.28	1.22
21	g	309	CLA	OBD-CAD	3.73	1.28	1.22
23	8	309	A86	C5-C6	3.73	1.40	1.35
29	g	316	LMU	O5'-C1'	3.73	1.51	1.41
21	5	305	CLA	OBD-CAD	3.73	1.28	1.22
21	1	301	CLA	MG-NA	3.73	2.15	2.06
24	G	308	KC1	CHC-C1C	3.73	1.47	1.39
21	J	304	CLA	OBD-CAD	3.73	1.28	1.22
21	d	405	CLA	CHD-C4C	3.73	1.47	1.39
21	c	508	CLA	OBD-CAD	3.72	1.28	1.22
21	6	306	CLA	OBD-CAD	3.72	1.28	1.22
24	3	306	KC1	C1A-CHA	3.72	1.50	1.40
21	c	513	CLA	OBD-CAD	3.72	1.28	1.22
21	7	303	CLA	OBD-CAD	3.72	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	315	KC1	C1B-NB	-3.72	1.33	1.37
24	J	313	KC1	CHC-C1C	3.72	1.47	1.39
21	8	305	CLA	OBD-CAD	3.72	1.28	1.22
24	1	315	KC1	CHC-C1C	3.72	1.47	1.39
21	1	303	CLA	OBD-CAD	3.72	1.28	1.22
21	c	511	CLA	OBD-CAD	3.72	1.28	1.22
21	3	301	CLA	OBD-CAD	3.72	1.28	1.22
21	C	504	CLA	CHD-C4C	3.72	1.47	1.39
21	b	612	CLA	CHD-C4C	3.71	1.47	1.39
21	7	302	CLA	OBD-CAD	3.71	1.28	1.22
21	c	504	CLA	OBD-CAD	3.71	1.28	1.22
21	C	512	CLA	OBD-CAD	3.71	1.28	1.22
21	6	300	CLA	OBD-CAD	3.71	1.28	1.22
21	B	606	CLA	OBD-CAD	3.71	1.28	1.22
21	B	603	CLA	OBD-CAD	3.71	1.28	1.22
21	B	611	CLA	CHD-C4C	3.71	1.47	1.39
24	6	311	KC1	CHC-C1C	3.71	1.47	1.39
21	C	515	CLA	OBD-CAD	3.71	1.28	1.22
21	C	503	CLA	OBD-CAD	3.71	1.28	1.22
21	G	300	CLA	OBD-CAD	3.71	1.28	1.22
21	8	306	CLA	OBD-CAD	3.70	1.28	1.22
21	9	304	CLA	OBD-CAD	3.70	1.28	1.22
21	4	304	CLA	OBD-CAD	3.70	1.28	1.22
21	g	306	CLA	OBD-CAD	3.70	1.28	1.22
24	8	315	KC1	CHC-C1C	3.70	1.47	1.39
21	1	306	CLA	OBD-CAD	3.70	1.28	1.22
24	G	308	KC1	C1A-CHA	3.70	1.50	1.40
21	6	307	CLA	OBD-CAD	3.70	1.28	1.22
21	7	305	CLA	OBD-CAD	3.70	1.28	1.22
21	c	506	CLA	OBD-CAD	3.70	1.28	1.22
21	d	404	CLA	OBD-CAD	3.70	1.28	1.22
21	4	301	CLA	OBD-CAD	3.70	1.28	1.22
21	C	509	CLA	OBD-CAD	3.70	1.28	1.22
24	4	308	KC1	CHC-C1C	3.69	1.47	1.39
21	c	507	CLA	OBD-CAD	3.69	1.28	1.22
21	b	613	CLA	CHD-C4C	3.69	1.47	1.39
21	7	300	CLA	OBD-CAD	3.69	1.28	1.22
21	1	309	CLA	OBD-CAD	3.69	1.28	1.22
24	g	314	KC1	C1A-CHA	3.69	1.50	1.40
21	7	308	CLA	OBD-CAD	3.69	1.28	1.22
21	A	401	CLA	OBD-CAD	3.69	1.28	1.22
21	a	403	CLA	OBD-CAD	3.69	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	304	CLA	OBD-CAD	3.69	1.28	1.22
24	4	306	KC1	CHD-C4C	3.69	1.48	1.39
21	D	406	CLA	CHD-C4C	3.69	1.47	1.39
23	2	308	A86	C5-C6	3.69	1.40	1.35
21	8	304	CLA	OBD-CAD	3.69	1.28	1.22
23	8	312	A86	C26-C27	3.69	1.40	1.35
24	6	311	KC1	C1B-NB	-3.68	1.33	1.37
21	G	304	CLA	OBD-CAD	3.68	1.28	1.22
24	8	316	KC1	CHC-C1C	3.68	1.47	1.39
21	C	513	CLA	OBD-CAD	3.68	1.28	1.22
24	J	311	KC1	C1B-NB	-3.68	1.33	1.37
21	c	503	CLA	OBD-CAD	3.68	1.28	1.22
24	G	306	KC1	CHD-C4C	3.68	1.48	1.39
21	b	610	CLA	OBD-CAD	3.68	1.28	1.22
21	c	509	CLA	OBD-CAD	3.68	1.28	1.22
21	G	301	CLA	OBD-CAD	3.68	1.28	1.22
21	9	303	CLA	C3D-C2D	3.68	1.49	1.39
21	c	514	CLA	OBD-CAD	3.67	1.28	1.22
21	A	404	CLA	OBD-CAD	3.67	1.28	1.22
21	4	304	CLA	MG-ND	-3.67	1.98	2.05
21	1	310	CLA	OBD-CAD	3.67	1.28	1.22
22	1	311	DD6	C10-C11	3.67	1.40	1.35
21	C	508	CLA	OBD-CAD	3.67	1.28	1.22
21	c	512	CLA	OBD-CAD	3.67	1.28	1.22
24	2	316	KC1	CHC-C1C	3.67	1.47	1.39
21	7	306	CLA	OBD-CAD	3.66	1.28	1.22
21	1	302	CLA	OBD-CAD	3.66	1.28	1.22
21	2	306	CLA	OBD-CAD	3.66	1.28	1.22
21	g	308	CLA	OBD-CAD	3.66	1.28	1.22
24	7	314	KC1	CHC-C1C	3.66	1.47	1.39
21	5	309	CLA	OBD-CAD	3.66	1.28	1.22
24	6	311	KC1	C1A-CHA	3.66	1.50	1.40
21	A	402	CLA	OBD-CAD	3.66	1.28	1.22
21	b	616	CLA	OBD-CAD	3.66	1.28	1.22
24	2	314	KC1	C1A-CHA	3.66	1.50	1.40
21	C	511	CLA	OBD-CAD	3.66	1.28	1.22
24	3	306	KC1	CHC-C1C	3.66	1.47	1.39
21	C	504	CLA	OBD-CAD	3.66	1.28	1.22
21	c	502	CLA	OBD-CAD	3.66	1.28	1.22
21	1	308	CLA	OBD-CAD	3.66	1.28	1.22
21	B	621	CLA	OBD-CAD	3.66	1.28	1.22
21	J	306	CLA	OBD-CAD	3.66	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	612	CLA	OBD-CAD	3.66	1.28	1.22
21	c	510	CLA	OBD-CAD	3.66	1.28	1.22
21	B	615	CLA	OBD-CAD	3.65	1.28	1.22
21	b	604	CLA	OBD-CAD	3.65	1.28	1.22
21	D	404	CLA	OBD-CAD	3.65	1.28	1.22
21	7	309	CLA	OBD-CAD	3.65	1.28	1.22
24	6	312	KC1	CHC-C1C	3.65	1.47	1.39
24	J	312	KC1	CHC-C1C	3.65	1.47	1.39
21	1	304	CLA	OBD-CAD	3.65	1.28	1.22
21	1	305	CLA	OBD-CAD	3.65	1.28	1.22
21	6	301	CLA	OBD-CAD	3.65	1.28	1.22
21	1	307	CLA	OBD-CAD	3.65	1.28	1.22
21	1	301	CLA	OBD-CAD	3.65	1.28	1.22
21	B	610	CLA	OBD-CAD	3.64	1.28	1.22
21	2	301	CLA	OBD-CAD	3.64	1.28	1.22
21	b	611	CLA	OBD-CAD	3.64	1.28	1.22
21	c	505	CLA	OBD-CAD	3.64	1.28	1.22
21	D	407	CLA	OBD-CAD	3.64	1.28	1.22
21	a	402	CLA	OBD-CAD	3.64	1.28	1.22
21	7	304	CLA	OBD-CAD	3.63	1.28	1.22
21	2	305	CLA	OBD-CAD	3.63	1.28	1.22
21	B	602	CLA	OBD-CAD	3.63	1.28	1.22
21	C	507	CLA	OBD-CAD	3.63	1.28	1.22
21	B	609	CLA	OBD-CAD	3.63	1.28	1.22
21	B	607	CLA	OBD-CAD	3.63	1.28	1.22
24	2	315	KC1	CHC-C1C	3.63	1.47	1.39
24	1	316	KC1	C1B-NB	-3.62	1.33	1.37
21	B	605	CLA	OBD-CAD	3.62	1.28	1.22
21	B	611	CLA	OBD-CAD	3.62	1.28	1.22
29	8	318	LMU	O5'-C1'	3.62	1.51	1.41
21	C	510	CLA	OBD-CAD	3.62	1.28	1.22
24	J	311	KC1	C1A-CHA	3.62	1.50	1.40
21	C	506	CLA	OBD-CAD	3.62	1.28	1.22
21	b	603	CLA	OBD-CAD	3.62	1.28	1.22
21	b	606	CLA	OBD-CAD	3.62	1.28	1.22
21	C	505	CLA	OBD-CAD	3.62	1.28	1.22
21	b	608	CLA	OBD-CAD	3.62	1.28	1.22
21	C	504	CLA	MG-ND	3.62	2.13	2.05
23	2	308	A86	C2-C1	3.62	1.40	1.35
21	b	607	CLA	OBD-CAD	3.62	1.28	1.22
21	a	405	CLA	OBD-CAD	3.62	1.28	1.22
21	8	302	CLA	OBD-CAD	3.61	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	305	KC1	CHC-C1C	3.61	1.47	1.39
29	A	408	LMU	O5'-C1'	3.61	1.51	1.41
24	4	308	KC1	C1A-CHA	3.61	1.50	1.40
21	2	303	CLA	OBD-CAD	3.61	1.28	1.22
21	8	307	CLA	OBD-CAD	3.61	1.28	1.22
21	b	623	CLA	OBD-CAD	3.61	1.28	1.22
24	g	314	KC1	CHC-C1C	3.61	1.47	1.39
29	a	408	LMU	O5'-C1'	3.61	1.51	1.41
24	5	313	KC1	C1A-CHA	3.61	1.50	1.40
21	d	406	CLA	OBD-CAD	3.60	1.28	1.22
29	g	316	LMU	O5B-C1B	3.60	1.51	1.41
21	b	609	CLA	OBD-CAD	3.60	1.28	1.22
21	B	616	CLA	CHD-C4C	3.60	1.47	1.39
24	4	307	KC1	CHC-C1C	3.60	1.47	1.39
21	B	608	CLA	OBD-CAD	3.59	1.28	1.22
21	5	302	CLA	OBD-CAD	3.58	1.28	1.22
21	5	302	CLA	MG-NA	-3.58	1.97	2.06
24	7	315	KC1	C1B-NB	-3.58	1.33	1.37
24	5	314	KC1	CHC-C1C	3.58	1.47	1.39
24	2	316	KC1	C1B-NB	-3.58	1.33	1.37
21	6	303	CLA	C3B-C2B	3.58	1.48	1.38
21	b	617	CLA	CHD-C4C	3.58	1.47	1.39
24	5	313	KC1	CHC-C1C	3.57	1.47	1.39
21	7	301	CLA	OBD-CAD	3.57	1.28	1.22
24	5	314	KC1	C1A-CHA	3.57	1.50	1.40
29	D	412	LMU	O5'-C1'	3.57	1.50	1.41
21	J	303	CLA	C3B-C2B	3.56	1.48	1.38
23	5	312	A86	C26-C27	3.56	1.40	1.35
21	B	612	CLA	CHD-C4C	3.56	1.47	1.39
23	2	312	A86	C26-C27	3.55	1.40	1.35
30	c	517	DGD	O2G-C2G	-3.55	1.41	1.47
21	4	304	CLA	C3D-C2D	3.55	1.48	1.39
24	5	315	KC1	C1A-CHA	3.55	1.50	1.40
21	7	302	CLA	C3D-C2D	3.55	1.48	1.39
21	1	305	CLA	MG-NC	3.55	2.14	2.06
24	G	307	KC1	CHC-C1C	3.54	1.47	1.39
29	5	316	LMU	O5'-C1'	3.54	1.50	1.41
21	J	303	CLA	C3D-C2D	3.54	1.48	1.39
24	8	316	KC1	C1B-NB	-3.54	1.33	1.37
21	5	303	CLA	OBD-CAD	3.53	1.28	1.22
21	9	302	CLA	OBD-CAD	3.53	1.28	1.22
24	5	313	KC1	C4B-NB	-3.53	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	315	KC1	C4B-NB	-3.52	1.33	1.37
21	d	405	CLA	OBD-CAD	3.52	1.28	1.22
21	J	301	CLA	OBD-CAD	3.52	1.28	1.22
24	J	313	KC1	C1B-NB	-3.52	1.33	1.37
21	1	303	CLA	C3D-C2D	3.52	1.48	1.39
21	D	406	CLA	OBD-CAD	3.51	1.28	1.22
21	C	506	CLA	MG-ND	-3.51	1.98	2.05
21	B	612	CLA	OBD-CAD	3.51	1.28	1.22
21	g	302	CLA	OBD-CAD	3.51	1.28	1.22
24	6	313	KC1	C1B-NB	-3.51	1.33	1.37
21	1	303	CLA	MG-NC	-3.51	1.97	2.06
21	9	304	CLA	C3D-C2D	3.50	1.48	1.39
24	J	312	KC1	C1B-NB	-3.49	1.33	1.37
21	3	304	CLA	C3D-C2D	3.49	1.48	1.39
21	4	301	CLA	C3D-C2D	3.49	1.48	1.39
23	7	312	A86	C26-C27	3.48	1.40	1.35
21	5	306	CLA	C3D-C2D	3.48	1.48	1.39
21	B	604	CLA	OBD-CAD	3.48	1.28	1.22
21	G	304	CLA	C3D-C2D	3.48	1.48	1.39
21	D	404	CLA	C3D-C2D	3.48	1.48	1.39
21	b	613	CLA	OBD-CAD	3.48	1.28	1.22
21	6	301	CLA	MG-NA	3.47	2.14	2.06
21	d	404	CLA	C3D-C2D	3.47	1.48	1.39
24	2	313	KC1	CHC-C1C	3.47	1.47	1.39
21	b	614	CLA	OBD-CAD	3.47	1.28	1.22
21	b	616	CLA	C3D-C2D	3.47	1.48	1.39
21	7	300	CLA	C3D-C2D	3.47	1.48	1.39
21	4	300	CLA	C3D-C2D	3.47	1.48	1.39
21	g	305	CLA	C3D-C2D	3.47	1.48	1.39
21	c	503	CLA	C3D-C2D	3.47	1.48	1.39
21	g	307	CLA	C3D-C2D	3.47	1.48	1.39
24	5	313	KC1	C1B-NB	-3.47	1.33	1.37
21	3	302	CLA	CHD-C4C	3.46	1.47	1.39
21	1	301	CLA	C3D-C2D	3.46	1.48	1.39
21	7	306	CLA	C3D-C2D	3.46	1.48	1.39
29	g	301	LMU	O5B-C1B	3.46	1.50	1.41
21	g	306	CLA	C3D-C2D	3.46	1.48	1.39
21	5	304	CLA	C3D-C2D	3.46	1.48	1.39
29	5	301	LMU	O5B-C1B	3.46	1.50	1.41
21	8	304	CLA	C3D-C2D	3.46	1.48	1.39
21	6	302	CLA	C3D-C2D	3.46	1.48	1.39
21	3	303	CLA	C3D-C2D	3.45	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	303	CLA	C3D-C2D	3.45	1.48	1.39
21	C	504	CLA	C3D-C2D	3.45	1.48	1.39
24	G	307	KC1	C4B-NB	-3.45	1.33	1.37
21	5	306	CLA	MG-NA	3.45	2.14	2.06
21	B	615	CLA	C3D-C2D	3.45	1.48	1.39
21	b	610	CLA	C3D-C2D	3.45	1.48	1.39
21	4	303	CLA	C3D-C2D	3.45	1.48	1.39
24	6	312	KC1	C1B-NB	-3.44	1.33	1.37
21	8	305	CLA	C3D-C2D	3.44	1.48	1.39
24	G	309	KC1	CHC-C1C	3.44	1.47	1.39
21	c	507	CLA	C3D-C2D	3.44	1.48	1.39
21	G	301	CLA	C3D-C2D	3.44	1.48	1.39
21	B	613	CLA	OBD-CAD	3.44	1.28	1.22
24	4	307	KC1	C4B-NB	-3.44	1.33	1.37
23	1	313	A86	C26-C27	3.44	1.40	1.35
24	9	305	KC1	C4B-NB	-3.43	1.33	1.37
29	5	301	LMU	O5'-C1'	3.43	1.50	1.41
21	c	514	CLA	C3D-C2D	3.43	1.48	1.39
21	b	613	CLA	MG-ND	-3.43	1.99	2.05
21	9	301	CLA	C3D-C2D	3.43	1.48	1.39
25	M	101	BCR	C1-C6	-3.43	1.49	1.53
21	4	302	CLA	C3D-C2D	3.43	1.48	1.39
21	C	508	CLA	C3D-C2D	3.43	1.48	1.39
21	B	609	CLA	C3D-C2D	3.43	1.48	1.39
29	5	316	LMU	O5B-C1B	3.43	1.50	1.41
24	9	305	KC1	C1B-NB	-3.43	1.33	1.37
21	7	305	CLA	C3D-C2D	3.43	1.48	1.39
21	c	513	CLA	C3D-C2D	3.43	1.48	1.39
21	J	308	CLA	MG-NA	3.42	2.14	2.06
24	g	313	KC1	C1B-NB	-3.42	1.33	1.37
21	C	514	CLA	C3D-C2D	3.42	1.48	1.39
32	E	101	HEM	C3C-C2C	-3.42	1.35	1.40
21	1	305	CLA	C3D-C2D	3.42	1.48	1.39
21	6	305	CLA	C3D-C2D	3.42	1.48	1.39
21	3	300	CLA	C3D-C2D	3.42	1.48	1.39
21	B	608	CLA	C3D-C2D	3.42	1.48	1.39
21	7	303	CLA	C3D-C2D	3.42	1.48	1.39
21	5	302	CLA	C3D-C2D	3.42	1.48	1.39
21	1	310	CLA	C3D-C2D	3.42	1.48	1.39
21	b	609	CLA	C3D-C2D	3.42	1.48	1.39
21	G	302	CLA	OBD-CAD	3.42	1.28	1.22
21	b	605	CLA	OBD-CAD	3.42	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	313	KC1	C1B-NB	-3.41	1.33	1.37
21	9	302	CLA	C3D-C2D	3.41	1.48	1.39
29	g	301	LMU	O5'-C1'	3.41	1.50	1.41
24	4	307	KC1	C1B-NB	-3.41	1.33	1.37
21	1	310	CLA	MG-NA	3.41	2.14	2.06
21	C	515	CLA	C3D-C2D	3.41	1.48	1.39
21	D	407	CLA	C3D-C2D	3.41	1.48	1.39
21	g	304	CLA	C3D-C2D	3.41	1.48	1.39
24	G	308	KC1	C1B-NB	-3.41	1.33	1.37
21	c	509	CLA	C3D-C2D	3.41	1.48	1.39
21	5	303	CLA	C3D-C2D	3.41	1.48	1.39
21	1	308	CLA	C3D-C2D	3.40	1.48	1.39
24	9	305	KC1	C1A-CHA	3.40	1.49	1.40
21	d	406	CLA	C3D-C2D	3.40	1.48	1.39
21	B	607	CLA	C3D-C2D	3.40	1.48	1.39
21	J	307	CLA	C3D-C2D	3.40	1.48	1.39
21	a	405	CLA	C3D-C2D	3.40	1.48	1.39
21	9	300	CLA	C3D-C2D	3.40	1.48	1.39
24	G	307	KC1	C1B-NB	-3.40	1.33	1.37
21	2	304	CLA	C3D-C2D	3.40	1.48	1.39
21	J	302	CLA	C3D-C2D	3.40	1.48	1.39
21	6	300	CLA	C3D-C2D	3.39	1.48	1.39
21	B	611	CLA	C3D-C2D	3.39	1.48	1.39
21	2	306	CLA	C3D-C2D	3.39	1.48	1.39
21	1	307	CLA	C3D-C2D	3.39	1.48	1.39
21	G	303	CLA	C3D-C2D	3.39	1.48	1.39
21	1	302	CLA	C3D-C2D	3.39	1.48	1.39
21	C	510	CLA	C3D-C2D	3.39	1.48	1.39
21	C	506	CLA	C3D-C2D	3.39	1.48	1.39
21	1	306	CLA	C3D-C2D	3.39	1.48	1.39
21	J	305	CLA	C3D-C2D	3.39	1.48	1.39
21	2	305	CLA	C3D-C2D	3.39	1.48	1.39
21	C	509	CLA	C3D-C2D	3.39	1.48	1.39
21	3	301	CLA	C3D-C2D	3.39	1.48	1.39
21	J	300	CLA	C3D-C2D	3.38	1.48	1.39
21	7	309	CLA	C3D-C2D	3.38	1.48	1.39
21	6	308	CLA	MG-NA	3.38	2.14	2.06
24	4	307	KC1	C1A-CHA	3.38	1.49	1.40
21	G	300	CLA	C3D-C2D	3.38	1.48	1.39
21	5	305	CLA	C3D-C2D	3.38	1.48	1.39
21	7	306	CLA	C3A-C2A	-3.38	1.51	1.54
21	5	307	CLA	C3D-C2D	3.38	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	301	CLA	C3D-C2D	3.37	1.48	1.39
21	J	306	CLA	C3D-C2D	3.37	1.48	1.39
24	4	308	KC1	C1B-NB	-3.37	1.33	1.37
24	G	306	KC1	C1B-NB	-3.37	1.33	1.37
21	b	612	CLA	C3D-C2D	3.37	1.48	1.39
21	A	404	CLA	C3D-C2D	3.36	1.48	1.39
21	c	505	CLA	C3D-C2D	3.36	1.48	1.39
21	2	303	CLA	C3D-C2D	3.36	1.48	1.39
21	b	603	CLA	C3D-C2D	3.36	1.48	1.39
29	D	412	LMU	O5B-C1B	3.36	1.50	1.41
21	6	306	CLA	C3D-C2D	3.36	1.48	1.39
21	1	304	CLA	C3D-C2D	3.36	1.48	1.39
21	7	301	CLA	MG-ND	3.36	2.12	2.05
24	G	307	KC1	C1A-CHA	3.36	1.49	1.40
21	g	303	CLA	OBD-CAD	3.35	1.28	1.22
24	G	309	KC1	C4B-NB	-3.35	1.33	1.37
21	B	602	CLA	C3D-C2D	3.35	1.48	1.39
21	b	608	CLA	C3D-C2D	3.35	1.48	1.39
21	C	503	CLA	C3D-C2D	3.35	1.48	1.39
21	G	302	CLA	C3D-C2D	3.35	1.48	1.39
23	G	305	A86	C26-C27	3.35	1.40	1.35
21	g	308	CLA	C3D-C2D	3.35	1.48	1.39
21	5	308	CLA	C3D-C2D	3.34	1.48	1.39
24	g	313	KC1	C1A-CHA	3.34	1.49	1.40
24	7	314	KC1	C1B-NB	-3.34	1.33	1.37
21	C	511	CLA	C3D-C2D	3.34	1.48	1.39
21	b	617	CLA	C3D-C2D	3.34	1.48	1.39
29	2	317	LMU	O5B-C1B	3.34	1.50	1.41
21	2	301	CLA	C3D-C2D	3.34	1.48	1.39
21	8	307	CLA	C3D-C2D	3.33	1.48	1.39
21	c	508	CLA	C3D-C2D	3.33	1.48	1.39
24	4	309	KC1	CHC-C1C	3.33	1.46	1.39
21	B	610	CLA	C3D-C2D	3.33	1.48	1.39
25	m	101	BCR	C1-C6	-3.33	1.49	1.53
21	5	309	CLA	C1D-ND	-3.33	1.33	1.37
22	5	310	DD6	C26-C27	3.33	1.44	1.37
21	6	307	CLA	C3D-C2D	3.33	1.48	1.39
21	b	611	CLA	C3D-C2D	3.33	1.48	1.39
21	7	307	CLA	C3D-C2D	3.33	1.48	1.39
21	b	614	CLA	C3D-C2D	3.33	1.48	1.39
21	6	308	CLA	C3D-C2D	3.32	1.48	1.39
21	8	306	CLA	C3D-C2D	3.32	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	617	CLA	OBD-CAD	3.32	1.28	1.22
24	g	313	KC1	C4B-NB	-3.32	1.33	1.37
24	1	315	KC1	C1B-NB	-3.32	1.33	1.37
21	C	505	CLA	C3D-C2D	3.31	1.48	1.39
24	5	315	KC1	C1B-NB	-3.31	1.33	1.37
21	B	621	CLA	C3D-C2D	3.31	1.48	1.39
21	A	402	CLA	C3D-C2D	3.31	1.48	1.39
24	4	309	KC1	C1B-NB	-3.31	1.33	1.37
21	g	303	CLA	C3D-C2D	3.31	1.48	1.39
21	1	309	CLA	C3D-C2D	3.31	1.48	1.39
24	6	311	KC1	C4B-NB	-3.31	1.33	1.37
21	c	510	CLA	C3D-C2D	3.31	1.48	1.39
21	6	301	CLA	C3D-C2D	3.31	1.48	1.39
21	J	308	CLA	C3D-C2D	3.31	1.48	1.39
21	C	513	CLA	C3D-C2D	3.30	1.48	1.39
21	B	614	CLA	C3D-C2D	3.30	1.48	1.39
23	7	311	A86	C26-C27	3.30	1.40	1.35
21	7	308	CLA	C3D-C2D	3.30	1.48	1.39
21	c	502	CLA	C3D-C2D	3.30	1.48	1.39
21	a	403	CLA	C3D-C2D	3.29	1.48	1.39
21	1	307	CLA	C3A-C2A	-3.29	1.51	1.54
23	g	311	A86	C26-C27	3.29	1.40	1.35
21	B	613	CLA	C3D-C2D	3.29	1.48	1.39
21	8	302	CLA	C3D-C2D	3.29	1.48	1.39
21	c	504	CLA	C3D-C2D	3.29	1.48	1.39
21	g	302	CLA	C3D-C2D	3.29	1.48	1.39
29	2	317	LMU	O5'-C1'	3.28	1.50	1.41
21	7	304	CLA	C3D-C2D	3.28	1.48	1.39
24	g	314	KC1	C1B-NB	-3.28	1.33	1.37
21	B	603	CLA	C3D-C2D	3.28	1.48	1.39
21	8	305	CLA	C3A-C2A	-3.28	1.51	1.54
21	c	512	CLA	C3D-C2D	3.28	1.48	1.39
24	G	309	KC1	C1B-NB	-3.28	1.33	1.37
23	1	312	A86	C26-C27	3.26	1.40	1.35
24	J	311	KC1	C4B-NB	-3.26	1.33	1.37
21	g	309	CLA	C3D-C2D	3.26	1.48	1.39
29	A	408	LMU	O5B-C1B	3.26	1.50	1.41
21	C	512	CLA	MG-NA	3.26	2.14	2.06
21	b	615	CLA	C3D-C2D	3.25	1.48	1.39
21	B	616	CLA	C3D-C2D	3.25	1.48	1.39
21	b	604	CLA	C3D-C2D	3.25	1.48	1.39
29	8	318	LMU	O5B-C1B	3.25	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	311	A86	C26-C27	3.25	1.40	1.35
23	2	309	A86	C26-C27	3.25	1.40	1.35
21	6	304	CLA	C3D-C2D	3.25	1.48	1.39
21	J	304	CLA	C3D-C2D	3.25	1.48	1.39
23	7	313	A86	C26-C27	3.24	1.40	1.35
21	b	623	CLA	C3D-C2D	3.24	1.48	1.39
21	D	406	CLA	C3D-C2D	3.24	1.48	1.39
21	d	405	CLA	C3D-C2D	3.24	1.48	1.39
21	B	612	CLA	C1D-ND	-3.23	1.33	1.37
24	4	306	KC1	C1B-NB	-3.23	1.33	1.37
21	B	606	CLA	C3D-C2D	3.23	1.47	1.39
21	b	607	CLA	C3D-C2D	3.23	1.47	1.39
21	c	504	CLA	C4D-CHA	3.23	1.49	1.38
21	b	613	CLA	C1D-ND	-3.22	1.33	1.37
22	g	310	DD6	C26-C27	3.21	1.43	1.37
21	J	303	CLA	C4D-CHA	3.21	1.49	1.38
24	9	306	KC1	C1B-NB	-3.21	1.33	1.37
28	b	622	LMG	C4-C5	3.21	1.59	1.53
21	2	304	CLA	C3A-C2A	-3.21	1.51	1.54
25	B	618	BCR	C1-C6	-3.21	1.49	1.53
23	g	312	A86	C26-C27	3.21	1.40	1.35
21	c	506	CLA	C3D-C2D	3.21	1.47	1.39
21	b	605	CLA	C3D-C2D	3.21	1.47	1.39
21	B	616	CLA	OBD-CAD	3.21	1.28	1.22
21	J	301	CLA	C3D-C2D	3.20	1.47	1.39
23	8	310	A86	C26-C27	3.20	1.40	1.35
21	B	616	CLA	C4D-CHA	3.20	1.49	1.38
25	b	619	BCR	C1-C6	-3.20	1.49	1.53
21	c	511	CLA	MG-NA	3.19	2.13	2.06
21	C	505	CLA	C4D-CHA	3.19	1.49	1.38
21	C	512	CLA	C1D-ND	-3.19	1.33	1.37
21	7	301	CLA	C4D-CHA	3.19	1.49	1.38
25	c	501	BCR	C1-C6	-3.18	1.49	1.53
21	3	302	CLA	C3D-C2D	3.18	1.47	1.39
23	1	314	A86	C26-C27	3.18	1.40	1.35
21	B	612	CLA	C3D-C2D	3.18	1.47	1.39
21	b	606	CLA	C3D-C2D	3.18	1.47	1.39
29	a	408	LMU	O5B-C1B	3.18	1.49	1.41
21	9	301	CLA	C4D-CHA	3.18	1.49	1.38
21	B	604	CLA	C3D-C2D	3.18	1.47	1.39
25	C	501	BCR	C1-C6	-3.17	1.49	1.53
21	B	605	CLA	C3D-C2D	3.17	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	507	CLA	C3D-C2D	3.17	1.47	1.39
25	b	618	BCR	C1-C6	-3.17	1.49	1.53
35	d	408	PL9	C3-C4	-3.17	1.44	1.49
24	g	315	KC1	C1B-NB	-3.16	1.33	1.37
21	5	303	CLA	C4D-CHA	3.16	1.49	1.38
32	f	101	HEM	CAB-C3B	3.16	1.56	1.47
21	2	302	CLA	MG-NC	-3.16	1.98	2.06
25	a	406	BCR	C1-C6	-3.16	1.49	1.53
21	b	615	CLA	OBD-CAD	3.16	1.27	1.22
25	C	516	BCR	C1-C6	-3.16	1.49	1.53
21	c	511	CLA	C1D-ND	-3.16	1.33	1.37
21	d	405	CLA	C1D-ND	-3.16	1.33	1.37
25	c	515	BCR	C1-C6	-3.16	1.49	1.53
21	G	300	CLA	C4D-CHA	3.16	1.49	1.38
21	8	303	CLA	C4D-CHA	3.16	1.49	1.38
24	3	306	KC1	C1B-NB	-3.15	1.33	1.37
23	2	311	A86	C26-C27	3.15	1.40	1.35
21	g	303	CLA	C4D-CHA	3.15	1.49	1.38
21	B	605	CLA	C4D-CHA	3.15	1.49	1.38
21	g	303	CLA	MG-NC	3.15	2.13	2.06
31	X	401	SQD	O48-C23	3.15	1.42	1.33
21	8	303	CLA	C3D-C2D	3.15	1.47	1.39
24	5	314	KC1	C1B-NB	-3.15	1.33	1.37
21	8	307	CLA	C4D-CHA	3.14	1.49	1.38
21	9	303	CLA	C1D-ND	-3.14	1.33	1.37
21	G	303	CLA	C4D-CHA	3.14	1.49	1.38
21	4	302	CLA	C4D-CHA	3.13	1.49	1.38
21	5	309	CLA	C3D-C2D	3.13	1.47	1.39
21	A	401	CLA	C3D-C2D	3.13	1.47	1.39
23	J	309	A86	C26-C27	3.13	1.39	1.35
21	2	306	CLA	C4D-CHA	3.13	1.49	1.38
31	C	502	SQD	O48-C23	3.13	1.42	1.33
21	6	305	CLA	C4D-CHA	3.13	1.49	1.38
21	D	406	CLA	C1D-ND	-3.13	1.33	1.37
21	b	606	CLA	C4D-CHA	3.13	1.49	1.38
21	2	302	CLA	C4D-CHA	3.13	1.49	1.38
21	C	509	CLA	C4D-CHA	3.13	1.49	1.38
21	a	402	CLA	C1D-ND	-3.13	1.33	1.37
31	B	625	SQD	O48-C23	3.12	1.42	1.33
35	D	409	PL9	C3-C4	-3.12	1.44	1.49
23	2	310	A86	C26-C27	3.12	1.39	1.35
21	a	402	CLA	C3D-C2D	3.12	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	303	CLA	C4D-CHA	3.12	1.49	1.38
21	7	302	CLA	C1D-ND	-3.12	1.33	1.37
21	8	305	CLA	C1D-ND	-3.12	1.33	1.37
21	c	512	CLA	C4D-CHA	3.12	1.49	1.38
21	B	615	CLA	C4D-CHA	3.12	1.49	1.38
21	4	300	CLA	C4D-CHA	3.12	1.49	1.38
21	b	616	CLA	C4D-CHA	3.12	1.49	1.38
21	b	603	CLA	C4D-CHA	3.12	1.49	1.38
21	7	308	CLA	C4D-CHA	3.11	1.49	1.38
21	G	301	CLA	C4D-CHA	3.11	1.49	1.38
31	b	602	SQD	O48-C23	3.11	1.42	1.33
21	B	614	CLA	OBD-CAD	3.11	1.27	1.22
21	2	302	CLA	C3D-C2D	3.11	1.47	1.39
21	b	617	CLA	C4D-CHA	3.11	1.49	1.38
21	C	510	CLA	C4D-CHA	3.11	1.49	1.38
21	g	304	CLA	C1D-ND	-3.11	1.34	1.37
21	c	508	CLA	C4D-CHA	3.11	1.49	1.38
25	A	405	BCR	C1-C6	-3.10	1.49	1.53
31	B	626	SQD	O48-C23	3.10	1.42	1.33
21	3	301	CLA	C4D-CHA	3.10	1.49	1.38
23	8	311	A86	C26-C27	3.10	1.39	1.35
21	J	305	CLA	C4D-CHA	3.10	1.49	1.38
21	2	305	CLA	C4D-CHA	3.10	1.49	1.38
21	7	304	CLA	C4D-CHA	3.10	1.49	1.38
25	h	101	BCR	C1-C6	-3.10	1.49	1.53
21	c	509	CLA	MG-ND	3.09	2.11	2.05
24	8	314	KC1	C4B-NB	-3.09	1.34	1.37
21	a	403	CLA	C4D-CHA	3.09	1.49	1.38
21	4	301	CLA	C4D-CHA	3.09	1.49	1.38
25	B	617	BCR	C1-C6	-3.09	1.49	1.53
21	b	610	CLA	C4D-CHA	3.09	1.49	1.38
21	5	304	CLA	C4D-CHA	3.09	1.49	1.38
21	6	302	CLA	C4D-CHA	3.09	1.49	1.38
21	C	513	CLA	C4D-CHA	3.09	1.49	1.38
21	1	302	CLA	C4D-CHA	3.08	1.49	1.38
21	C	506	CLA	C4D-CHA	3.08	1.49	1.38
21	3	303	CLA	C1D-ND	-3.08	1.34	1.37
22	1	311	DD6	C26-C27	3.08	1.43	1.37
21	8	304	CLA	MG-ND	-3.08	1.99	2.05
21	5	308	CLA	C4D-CHA	3.08	1.49	1.38
21	D	404	CLA	C1D-ND	-3.07	1.34	1.37
21	B	604	CLA	C4D-CHA	3.07	1.49	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	401	CLA	C1D-ND	-3.07	1.34	1.37
24	4	306	KC1	C4A-C3A	3.07	1.50	1.44
21	3	302	CLA	C4D-CHA	3.07	1.49	1.38
21	B	602	CLA	C4D-CHA	3.07	1.49	1.38
21	J	304	CLA	C1D-ND	-3.07	1.34	1.37
21	B	621	CLA	C4D-CHA	3.07	1.49	1.38
21	C	503	CLA	C4D-CHA	3.07	1.49	1.38
21	7	307	CLA	C4D-CHA	3.07	1.49	1.38
21	3	304	CLA	C4D-CHA	3.07	1.49	1.38
21	9	302	CLA	C4D-CHA	3.07	1.49	1.38
21	A	402	CLA	C4D-CHA	3.07	1.49	1.38
21	d	404	CLA	C1D-ND	-3.06	1.34	1.37
21	3	302	CLA	OBD-CAD	3.06	1.27	1.22
21	J	302	CLA	C4D-CHA	3.06	1.49	1.38
21	b	605	CLA	C4D-CHA	3.06	1.49	1.38
21	2	301	CLA	C1D-ND	-3.06	1.34	1.37
21	4	303	CLA	C4D-CHA	3.06	1.49	1.38
24	2	314	KC1	C4B-NB	-3.06	1.34	1.37
23	6	310	A86	C26-C27	3.06	1.39	1.35
21	C	514	CLA	C4D-CHA	3.06	1.49	1.38
21	C	507	CLA	C4D-CHA	3.06	1.49	1.38
21	b	613	CLA	C3D-C2D	3.06	1.47	1.39
21	c	511	CLA	C3D-C2D	3.05	1.47	1.39
21	1	303	CLA	C1D-ND	-3.05	1.34	1.37
21	B	609	CLA	C4D-CHA	3.05	1.49	1.38
32	E	101	HEM	CAB-C3B	3.05	1.55	1.47
21	b	611	CLA	C4D-CHA	3.05	1.49	1.38
21	B	611	CLA	C1D-ND	-3.05	1.34	1.37
24	4	309	KC1	C4B-NB	-3.05	1.34	1.37
21	c	507	CLA	C4D-CHA	3.05	1.49	1.38
21	b	623	CLA	C4D-CHA	3.05	1.49	1.38
21	7	305	CLA	C4D-CHA	3.04	1.49	1.38
21	B	613	CLA	C4D-CHA	3.04	1.49	1.38
21	C	504	CLA	C4D-CHA	3.04	1.49	1.38
21	5	305	CLA	C4D-CHA	3.04	1.49	1.38
21	c	506	CLA	C4D-CHA	3.04	1.49	1.38
21	B	614	CLA	C4D-CHA	3.04	1.49	1.38
21	G	302	CLA	C4D-CHA	3.04	1.49	1.38
21	7	303	CLA	C1D-ND	-3.04	1.34	1.37
21	c	503	CLA	C4D-CHA	3.04	1.49	1.38
21	5	307	CLA	C4D-CHA	3.04	1.49	1.38
21	c	513	CLA	C4D-CHA	3.04	1.49	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	300	CLA	C4D-CHA	3.03	1.49	1.38
21	C	508	CLA	C4D-CHA	3.03	1.49	1.38
21	D	407	CLA	C4D-CHA	3.03	1.49	1.38
21	c	514	CLA	C4D-CHA	3.03	1.49	1.38
21	b	614	CLA	C4D-CHA	3.03	1.49	1.38
21	b	615	CLA	C4D-CHA	3.03	1.49	1.38
21	J	308	CLA	C4D-CHA	3.03	1.49	1.38
24	7	315	KC1	C4B-NB	-3.03	1.34	1.37
21	J	300	CLA	C4D-CHA	3.03	1.49	1.38
21	3	303	CLA	C4D-CHA	3.03	1.49	1.38
21	d	406	CLA	C4D-CHA	3.03	1.49	1.38
21	g	309	CLA	C4D-CHA	3.03	1.49	1.38
21	C	512	CLA	C3D-C2D	3.03	1.47	1.39
24	1	315	KC1	C4B-NB	-3.03	1.34	1.37
21	c	502	CLA	C4D-CHA	3.03	1.49	1.38
21	a	405	CLA	C1D-ND	-3.03	1.34	1.37
24	1	316	KC1	C4B-NB	-3.03	1.34	1.37
21	b	612	CLA	C1D-ND	-3.03	1.34	1.37
21	1	301	CLA	C4D-CHA	3.02	1.49	1.38
21	J	301	CLA	C1D-ND	-3.02	1.34	1.37
21	2	303	CLA	C4D-CHA	3.02	1.49	1.38
21	g	308	CLA	C4D-CHA	3.02	1.49	1.38
21	c	505	CLA	C4D-CHA	3.02	1.49	1.38
21	3	300	CLA	C4D-CHA	3.02	1.49	1.38
24	g	315	KC1	C4B-NB	-3.02	1.34	1.37
21	c	510	CLA	C4D-CHA	3.02	1.49	1.38
21	C	515	CLA	C4D-CHA	3.01	1.49	1.38
21	5	302	CLA	C4D-CHA	3.01	1.49	1.38
21	1	309	CLA	C4D-CHA	3.01	1.49	1.38
21	A	404	CLA	C1D-ND	-3.01	1.34	1.37
21	6	301	CLA	C4D-CHA	3.01	1.49	1.38
21	c	505	CLA	C1D-ND	-3.01	1.34	1.37
21	c	509	CLA	C4D-CHA	3.01	1.49	1.38
21	8	306	CLA	C4D-CHA	3.01	1.49	1.38
21	9	300	CLA	C4D-CHA	3.00	1.49	1.38
21	1	310	CLA	C4D-CHA	3.00	1.49	1.38
21	B	608	CLA	C1D-ND	-3.00	1.34	1.37
21	B	610	CLA	C4D-CHA	3.00	1.49	1.38
21	B	607	CLA	C4D-CHA	3.00	1.49	1.38
23	2	307	A86	C26-C27	3.00	1.39	1.35
21	g	305	CLA	C4D-CHA	3.00	1.49	1.38
21	b	604	CLA	C4D-CHA	3.00	1.49	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	609	CLA	C1D-ND	-2.99	1.34	1.37
21	7	309	CLA	C4D-CHA	2.99	1.49	1.38
21	B	605	CLA	MG-ND	-2.99	1.99	2.05
21	6	308	CLA	C4D-CHA	2.99	1.49	1.38
21	1	304	CLA	C4D-CHA	2.99	1.49	1.38
21	9	304	CLA	C4D-CHA	2.99	1.49	1.38
21	7	306	CLA	C4D-CHA	2.99	1.49	1.38
21	b	608	CLA	C4D-CHA	2.99	1.49	1.38
24	2	316	KC1	C4A-C3A	2.99	1.50	1.44
21	1	305	CLA	C4D-CHA	2.99	1.49	1.38
21	6	300	CLA	C4D-CHA	2.99	1.49	1.38
21	B	607	CLA	C1D-ND	-2.99	1.34	1.37
21	g	302	CLA	C4D-CHA	2.99	1.49	1.38
21	B	610	CLA	C1D-ND	-2.99	1.34	1.37
21	9	300	CLA	MG-NC	2.98	2.13	2.06
21	C	504	CLA	C1D-ND	-2.98	1.34	1.37
21	g	307	CLA	C1D-ND	-2.98	1.34	1.37
21	5	307	CLA	MG-ND	2.98	2.11	2.05
21	5	305	CLA	C3A-C2A	-2.98	1.51	1.54
21	B	603	CLA	C4D-CHA	2.98	1.49	1.38
21	b	608	CLA	C1D-ND	-2.98	1.34	1.37
21	1	307	CLA	C4D-CHA	2.98	1.49	1.38
21	7	309	CLA	C4C-C3C	2.98	1.50	1.45
21	B	606	CLA	C4D-CHA	2.97	1.49	1.38
21	6	304	CLA	C1D-ND	-2.97	1.34	1.37
24	9	306	KC1	C4B-NB	-2.97	1.34	1.37
21	g	307	CLA	C4D-CHA	2.97	1.49	1.38
21	C	511	CLA	C4D-CHA	2.97	1.49	1.38
24	G	309	KC1	C4A-C3A	2.97	1.50	1.44
21	7	303	CLA	C4D-CHA	2.97	1.48	1.38
21	8	304	CLA	C4D-CHA	2.97	1.48	1.38
21	2	304	CLA	C1D-ND	-2.97	1.34	1.37
24	8	313	KC1	C4B-NB	-2.97	1.34	1.37
21	9	304	CLA	C1D-ND	-2.97	1.34	1.37
24	6	313	KC1	C4B-NB	-2.97	1.34	1.37
21	2	302	CLA	OBD-CAD	2.96	1.27	1.22
21	6	307	CLA	C4D-CHA	2.96	1.48	1.38
21	g	306	CLA	C4D-CHA	2.96	1.48	1.38
23	4	305	A86	C26-C27	2.96	1.39	1.35
21	7	306	CLA	C1D-ND	-2.96	1.34	1.37
21	1	308	CLA	C1D-ND	-2.96	1.34	1.37
21	2	306	CLA	MG-NC	-2.95	1.99	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	306	CLA	C4D-CHA	2.95	1.48	1.38
24	3	305	KC1	C1B-NB	-2.95	1.34	1.37
24	3	305	KC1	C4B-NB	-2.95	1.34	1.37
21	6	306	CLA	C4D-CHA	2.95	1.48	1.38
24	8	315	KC1	CHB-C4A	-2.95	1.32	1.39
21	b	607	CLA	C4D-CHA	2.95	1.48	1.38
21	1	308	CLA	C4D-CHA	2.95	1.48	1.38
21	8	303	CLA	OBD-CAD	2.94	1.27	1.22
21	G	304	CLA	C4D-CHA	2.94	1.48	1.38
21	6	303	CLA	MG-NA	-2.94	1.99	2.06
21	g	308	CLA	MG-ND	-2.94	2.00	2.05
21	4	304	CLA	C4D-CHA	2.94	1.48	1.38
21	2	304	CLA	C4D-CHA	2.94	1.48	1.38
21	b	612	CLA	C4D-CHA	2.94	1.48	1.38
21	B	606	CLA	C1D-ND	-2.94	1.34	1.37
21	J	306	CLA	C1D-ND	-2.94	1.34	1.37
24	J	313	KC1	C4B-NB	-2.94	1.34	1.37
21	A	404	CLA	C4D-CHA	2.93	1.48	1.38
24	4	306	KC1	C4B-NB	-2.93	1.34	1.37
25	a	406	BCR	C30-C25	-2.93	1.49	1.53
21	8	305	CLA	C4D-CHA	2.93	1.48	1.38
21	1	307	CLA	C1D-ND	-2.93	1.34	1.37
24	8	316	KC1	C4A-C3A	2.93	1.50	1.44
21	1	303	CLA	C4D-CHA	2.93	1.48	1.38
21	B	611	CLA	C4D-CHA	2.93	1.48	1.38
21	2	303	CLA	C1D-ND	-2.93	1.34	1.37
21	8	302	CLA	C4D-CHA	2.93	1.48	1.38
21	C	514	CLA	C1D-ND	-2.92	1.34	1.37
21	c	503	CLA	C1D-ND	-2.92	1.34	1.37
21	3	300	CLA	C1D-ND	-2.92	1.34	1.37
24	4	309	KC1	C4A-C3A	2.92	1.50	1.44
21	6	306	CLA	C1D-ND	-2.92	1.34	1.37
21	J	307	CLA	C1D-ND	-2.92	1.34	1.37
21	4	304	CLA	C4C-C3C	2.92	1.50	1.45
21	b	609	CLA	C4D-CHA	2.92	1.48	1.38
21	D	406	CLA	C4B-CHC	2.91	1.49	1.41
21	D	404	CLA	C4D-CHA	2.91	1.48	1.38
21	J	306	CLA	C4D-CHA	2.91	1.48	1.38
21	1	310	CLA	C4C-C3C	2.91	1.50	1.45
21	8	304	CLA	C1D-ND	-2.91	1.34	1.37
23	2	308	A86	C26-C27	2.91	1.39	1.35
21	J	301	CLA	C4D-CHA	2.91	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	304	CLA	C1D-ND	-2.91	1.34	1.37
21	g	305	CLA	C3A-C2A	-2.91	1.51	1.54
21	J	307	CLA	C4D-CHA	2.91	1.48	1.38
21	7	300	CLA	MG-NA	2.91	2.13	2.06
21	6	307	CLA	C1D-ND	-2.91	1.34	1.37
23	8	309	A86	C26-C27	2.91	1.39	1.35
21	B	603	CLA	C1D-ND	-2.91	1.34	1.37
21	8	302	CLA	C1D-ND	-2.91	1.34	1.37
21	5	306	CLA	C1D-ND	-2.91	1.34	1.37
21	G	304	CLA	C1D-ND	-2.91	1.34	1.37
21	B	608	CLA	C4D-CHA	2.91	1.48	1.38
21	G	300	CLA	C1B-CHB	2.90	1.49	1.41
24	G	308	KC1	C4C-C3C	2.90	1.50	1.45
23	J	310	A86	C26-C27	2.90	1.39	1.35
21	c	506	CLA	C1D-ND	-2.90	1.34	1.37
24	G	306	KC1	C4B-NB	-2.90	1.34	1.37
21	2	301	CLA	C4D-CHA	2.90	1.48	1.38
21	1	306	CLA	C4D-CHA	2.90	1.48	1.38
21	g	304	CLA	C4D-CHA	2.90	1.48	1.38
21	d	404	CLA	C4D-CHA	2.90	1.48	1.38
21	D	407	CLA	C1D-ND	-2.90	1.34	1.37
21	7	302	CLA	C4D-CHA	2.90	1.48	1.38
21	a	405	CLA	C4D-CHA	2.90	1.48	1.38
21	B	609	CLA	C1D-ND	-2.90	1.34	1.37
21	9	300	CLA	C4B-CHC	2.90	1.49	1.41
21	d	406	CLA	C1D-ND	-2.90	1.34	1.37
24	7	314	KC1	C4B-NB	-2.90	1.34	1.37
24	2	313	KC1	C4B-NB	-2.90	1.34	1.37
21	b	604	CLA	C1D-ND	-2.89	1.34	1.37
21	4	304	CLA	C1D-ND	-2.89	1.34	1.37
21	b	607	CLA	C1D-ND	-2.89	1.34	1.37
21	8	305	CLA	C1B-CHB	2.89	1.49	1.41
31	X	401	SQD	O47-C7	2.89	1.42	1.34
21	7	305	CLA	C1D-ND	-2.89	1.34	1.37
24	G	308	KC1	C4B-NB	-2.89	1.34	1.37
21	1	305	CLA	C1D-ND	-2.89	1.34	1.37
21	4	302	CLA	C1B-CHB	2.89	1.49	1.41
21	3	304	CLA	C1B-CHB	2.89	1.49	1.41
21	g	306	CLA	C1D-ND	-2.89	1.34	1.37
21	D	406	CLA	C1B-CHB	2.89	1.49	1.41
21	G	302	CLA	C1D-ND	-2.89	1.34	1.37
21	8	302	CLA	C4B-CHC	2.89	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	101	A86	C26-C27	2.88	1.39	1.35
21	g	308	CLA	C4C-C3C	2.88	1.50	1.45
24	2	315	KC1	CHB-C4A	-2.88	1.32	1.39
24	9	306	KC1	C4A-C3A	2.88	1.50	1.44
21	B	615	CLA	C1D-ND	-2.88	1.34	1.37
21	b	610	CLA	C1D-ND	-2.88	1.34	1.37
25	A	405	BCR	C30-C25	-2.88	1.49	1.53
24	2	316	KC1	C4B-NB	-2.88	1.34	1.37
21	9	303	CLA	C4D-CHA	2.88	1.48	1.38
21	1	305	CLA	C4C-C3C	2.88	1.50	1.45
21	1	301	CLA	C1D-ND	-2.88	1.34	1.37
21	b	616	CLA	C1D-ND	-2.88	1.34	1.37
21	g	305	CLA	C1D-ND	-2.88	1.34	1.37
21	d	405	CLA	C1B-CHB	2.87	1.49	1.41
21	9	302	CLA	C1B-CHB	2.87	1.49	1.41
21	1	308	CLA	C1B-CHB	2.87	1.49	1.41
21	9	304	CLA	C1B-CHB	2.87	1.49	1.41
21	7	309	CLA	C1D-ND	-2.87	1.34	1.37
21	d	405	CLA	C4B-CHC	2.87	1.49	1.41
21	c	512	CLA	C1B-CHB	2.87	1.49	1.41
22	7	310	DD6	C26-C27	2.87	1.43	1.37
21	c	509	CLA	C1D-ND	-2.87	1.34	1.37
21	9	301	CLA	C1B-CHB	2.87	1.49	1.41
21	G	303	CLA	C4C-C3C	2.87	1.50	1.45
21	B	614	CLA	C1D-ND	-2.87	1.34	1.37
25	h	101	BCR	C30-C25	-2.87	1.49	1.53
21	a	403	CLA	C1D-ND	-2.87	1.34	1.37
21	4	301	CLA	C1D-ND	-2.87	1.34	1.37
21	7	304	CLA	C4C-C3C	2.87	1.50	1.45
24	2	313	KC1	C4A-C3A	2.87	1.50	1.44
24	g	314	KC1	C4B-NB	-2.86	1.34	1.37
21	7	304	CLA	MG-ND	2.86	2.11	2.05
21	c	503	CLA	MG-ND	2.86	2.11	2.05
21	6	307	CLA	C4B-CHC	2.86	1.48	1.41
21	1	306	CLA	C1D-ND	-2.86	1.34	1.37
21	b	615	CLA	C1D-ND	-2.86	1.34	1.37
21	4	300	CLA	C4B-CHC	2.86	1.48	1.41
21	A	401	CLA	C4D-CHA	2.86	1.48	1.38
31	B	625	SQD	O47-C7	2.86	1.42	1.34
24	G	306	KC1	C4A-C3A	2.86	1.50	1.44
21	g	304	CLA	C4B-CHC	2.86	1.48	1.41
21	C	513	CLA	C1B-CHB	2.86	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	309	CLA	C1D-ND	-2.85	1.34	1.37
21	c	513	CLA	C1D-ND	-2.85	1.34	1.37
21	1	306	CLA	C4B-CHC	2.85	1.48	1.41
21	7	306	CLA	C1B-CHB	2.85	1.48	1.41
21	C	503	CLA	MG-ND	-2.85	2.00	2.05
21	3	302	CLA	C4B-CHC	2.85	1.48	1.41
21	g	305	CLA	C4B-CHC	2.85	1.48	1.41
21	A	402	CLA	C1D-ND	-2.85	1.34	1.37
21	c	510	CLA	C1D-ND	-2.85	1.34	1.37
24	8	313	KC1	CHB-C4A	-2.85	1.32	1.39
21	1	307	CLA	C1B-CHB	2.85	1.48	1.41
21	6	301	CLA	C1D-ND	-2.85	1.34	1.37
24	4	308	KC1	C4B-NB	-2.85	1.34	1.37
21	a	402	CLA	C4D-CHA	2.85	1.48	1.38
21	2	304	CLA	C1B-CHB	2.85	1.48	1.41
21	4	303	CLA	C4C-C3C	2.85	1.49	1.45
21	9	304	CLA	C4B-CHC	2.85	1.48	1.41
21	J	307	CLA	C4B-CHC	2.85	1.48	1.41
21	7	305	CLA	C4B-CHC	2.85	1.48	1.41
21	5	307	CLA	C1D-ND	-2.85	1.34	1.37
25	d	407	BCR	C30-C25	-2.84	1.49	1.53
21	b	611	CLA	C1D-ND	-2.84	1.34	1.37
21	b	623	CLA	C1D-ND	-2.84	1.34	1.37
21	7	305	CLA	C1B-CHB	2.84	1.48	1.41
21	c	507	CLA	C4C-C3C	2.84	1.49	1.45
24	8	316	KC1	C4B-NB	-2.84	1.34	1.37
21	B	613	CLA	C1B-CHB	2.84	1.48	1.41
21	b	612	CLA	C1B-CHB	2.84	1.48	1.41
21	9	301	CLA	C4C-C3C	2.84	1.49	1.45
21	6	303	CLA	C1B-CHB	2.84	1.48	1.41
21	3	304	CLA	C4B-CHC	2.84	1.48	1.41
21	J	302	CLA	C1B-CHB	2.84	1.48	1.41
21	G	302	CLA	C4B-CHC	2.84	1.48	1.41
21	6	300	CLA	C1D-ND	-2.84	1.34	1.37
21	J	305	CLA	C1B-CHB	2.84	1.48	1.41
24	5	315	KC1	C4A-C3A	2.84	1.50	1.44
21	1	310	CLA	C1D-ND	-2.83	1.34	1.37
21	9	300	CLA	C1D-ND	-2.83	1.34	1.37
21	3	300	CLA	C1B-CHB	2.83	1.48	1.41
24	3	306	KC1	C4B-NB	-2.83	1.34	1.37
21	8	307	CLA	C1B-CHB	2.83	1.48	1.41
35	D	409	PL9	C6-C1	-2.83	1.43	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	305	CLA	C1B-CHB	2.83	1.48	1.41
21	9	303	CLA	C4C-C3C	2.83	1.49	1.45
21	g	307	CLA	C4C-C3C	2.83	1.49	1.45
21	J	304	CLA	C1B-CHB	2.83	1.48	1.41
21	6	304	CLA	C4D-CHA	2.83	1.48	1.38
31	B	626	SQD	O47-C7	2.83	1.42	1.34
21	7	307	CLA	C1B-CHB	2.82	1.48	1.41
21	B	612	CLA	C4D-CHA	2.82	1.48	1.38
21	J	300	CLA	C1B-CHB	2.82	1.48	1.41
21	1	303	CLA	C1B-CHB	2.82	1.48	1.41
21	b	614	CLA	C1B-CHB	2.82	1.48	1.41
21	b	613	CLA	C4D-CHA	2.82	1.48	1.38
21	3	303	CLA	C4C-C3C	2.82	1.49	1.45
21	6	302	CLA	C4C-C3C	2.82	1.49	1.45
21	C	504	CLA	C1B-CHB	2.82	1.48	1.41
21	6	308	CLA	C1D-ND	-2.82	1.34	1.37
21	9	302	CLA	C4C-C3C	2.82	1.49	1.45
21	C	511	CLA	C1D-ND	-2.82	1.34	1.37
21	g	307	CLA	C4B-CHC	2.82	1.48	1.41
21	C	513	CLA	C1D-ND	-2.82	1.34	1.37
21	5	308	CLA	C1D-ND	-2.82	1.34	1.37
31	C	502	SQD	O47-C7	2.82	1.42	1.34
21	G	301	CLA	C1D-ND	-2.82	1.34	1.37
21	4	300	CLA	C4C-C3C	2.82	1.49	1.45
21	1	310	CLA	C1B-CHB	2.82	1.48	1.41
21	B	611	CLA	C1B-CHB	2.82	1.48	1.41
21	1	302	CLA	C1D-ND	-2.82	1.34	1.37
21	B	621	CLA	C4C-C3C	2.81	1.49	1.45
21	7	304	CLA	C1B-CHB	2.81	1.48	1.41
21	B	621	CLA	C1D-ND	-2.81	1.34	1.37
21	7	309	CLA	C1B-CHB	2.81	1.48	1.41
21	6	300	CLA	C1B-CHB	2.81	1.48	1.41
21	C	503	CLA	C4B-CHC	2.81	1.48	1.41
21	8	307	CLA	C4C-C3C	2.81	1.49	1.45
21	J	304	CLA	C4D-CHA	2.81	1.48	1.38
21	4	303	CLA	C1B-CHB	2.81	1.48	1.41
21	5	305	CLA	MG-NC	-2.81	1.99	2.06
24	6	312	KC1	C4A-C3A	2.81	1.50	1.44
21	c	503	CLA	C1B-CHB	2.81	1.48	1.41
21	7	300	CLA	C1D-ND	-2.81	1.34	1.37
21	5	303	CLA	C1B-CHB	2.81	1.48	1.41
21	B	602	CLA	C1D-ND	-2.81	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	305	CLA	C1D-ND	-2.81	1.34	1.37
21	1	306	CLA	C3A-C2A	-2.81	1.51	1.54
21	6	302	CLA	C4B-CHC	2.81	1.48	1.41
21	C	508	CLA	C4C-C3C	2.81	1.49	1.45
21	2	302	CLA	C1B-CHB	2.81	1.48	1.41
21	b	608	CLA	C1B-CHB	2.81	1.48	1.41
21	B	607	CLA	C1B-CHB	2.80	1.48	1.41
21	7	308	CLA	C1B-CHB	2.80	1.48	1.41
21	A	404	CLA	C4B-CHC	2.80	1.48	1.41
21	8	306	CLA	C4B-CHC	2.80	1.48	1.41
21	G	300	CLA	C4B-CHC	2.80	1.48	1.41
21	c	506	CLA	C1B-CHB	2.80	1.48	1.41
21	g	308	CLA	C1D-ND	-2.80	1.34	1.37
21	g	307	CLA	C1B-CHB	2.80	1.48	1.41
21	C	510	CLA	C1D-ND	-2.80	1.34	1.37
31	b	602	SQD	O47-C7	2.80	1.42	1.34
21	B	605	CLA	C1D-ND	-2.80	1.34	1.37
21	6	302	CLA	C1D-ND	-2.80	1.34	1.37
21	a	405	CLA	C4B-CHC	2.80	1.48	1.41
21	c	508	CLA	C1D-ND	-2.80	1.34	1.37
21	C	506	CLA	C1D-ND	-2.80	1.34	1.37
21	c	514	CLA	C1D-ND	-2.80	1.34	1.37
21	3	303	CLA	C4B-CHC	2.80	1.48	1.41
21	B	602	CLA	C1B-CHB	2.80	1.48	1.41
21	J	301	CLA	C1B-CHB	2.80	1.48	1.41
21	C	503	CLA	C1D-ND	-2.80	1.34	1.37
21	1	307	CLA	MG-NC	2.80	2.12	2.06
21	C	506	CLA	C1B-CHB	2.80	1.48	1.41
21	C	510	CLA	C1B-CHB	2.80	1.48	1.41
21	c	508	CLA	C1B-CHB	2.80	1.48	1.41
21	3	300	CLA	C4B-CHC	2.80	1.48	1.41
21	5	307	CLA	C4C-C3C	2.79	1.49	1.45
21	6	303	CLA	C4C-C3C	2.79	1.49	1.45
21	G	301	CLA	C1B-CHB	2.79	1.48	1.41
24	4	309	KC1	C4C-C3C	2.79	1.49	1.45
21	G	303	CLA	C1B-CHB	2.79	1.48	1.41
21	7	300	CLA	C1B-CHB	2.79	1.48	1.41
21	8	306	CLA	C1D-ND	-2.79	1.34	1.37
21	1	308	CLA	C4B-CHC	2.79	1.48	1.41
21	5	302	CLA	C1D-ND	-2.79	1.34	1.37
21	9	303	CLA	C4B-CHC	2.79	1.48	1.41
21	6	307	CLA	C1B-CHB	2.79	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	507	CLA	C1D-ND	-2.79	1.34	1.37
21	c	502	CLA	C1D-ND	-2.79	1.34	1.37
21	4	303	CLA	C4B-CHC	2.79	1.48	1.41
21	7	302	CLA	C1B-CHB	2.79	1.48	1.41
21	7	302	CLA	C4B-CHC	2.79	1.48	1.41
21	g	303	CLA	C1B-CHB	2.79	1.48	1.41
24	g	315	KC1	C4A-C3A	2.79	1.50	1.44
21	J	300	CLA	C4B-CHC	2.79	1.48	1.41
24	4	307	KC1	C4A-C3A	2.79	1.50	1.44
21	b	613	CLA	C4B-CHC	2.79	1.48	1.41
21	6	300	CLA	C4B-CHC	2.79	1.48	1.41
21	6	304	CLA	C1B-CHB	2.79	1.48	1.41
21	4	303	CLA	C1D-ND	-2.79	1.34	1.37
21	7	307	CLA	C4B-CHC	2.79	1.48	1.41
21	g	304	CLA	C1B-CHB	2.79	1.48	1.41
21	G	302	CLA	C4C-C3C	2.79	1.49	1.45
21	J	305	CLA	C4B-CHC	2.78	1.48	1.41
21	J	300	CLA	C1D-ND	-2.78	1.34	1.37
21	8	304	CLA	C1B-CHB	2.78	1.48	1.41
21	J	307	CLA	C1B-CHB	2.78	1.48	1.41
21	6	305	CLA	C4B-CHC	2.78	1.48	1.41
21	C	507	CLA	C1B-CHB	2.78	1.48	1.41
21	J	302	CLA	C1D-ND	-2.78	1.34	1.37
21	1	301	CLA	C1B-CHB	2.78	1.48	1.41
21	d	405	CLA	C4D-CHA	2.78	1.48	1.38
21	6	302	CLA	C1B-CHB	2.78	1.48	1.41
21	b	616	CLA	C4C-C3C	2.78	1.49	1.45
21	C	509	CLA	C1B-CHB	2.78	1.48	1.41
21	B	615	CLA	C4C-C3C	2.78	1.49	1.45
21	3	303	CLA	C1B-CHB	2.78	1.48	1.41
21	4	300	CLA	C1B-CHB	2.78	1.48	1.41
21	G	303	CLA	C4B-CHC	2.78	1.48	1.41
24	7	314	KC1	C4A-C3A	2.78	1.49	1.44
21	7	308	CLA	C1D-ND	-2.78	1.34	1.37
21	C	514	CLA	C4B-CHC	2.78	1.48	1.41
21	b	610	CLA	C1B-CHB	2.78	1.48	1.41
21	c	505	CLA	C1B-CHB	2.78	1.48	1.41
21	c	507	CLA	C1D-ND	-2.78	1.34	1.37
21	5	305	CLA	C1B-CHB	2.78	1.48	1.41
21	8	303	CLA	C1B-CHB	2.77	1.48	1.41
21	B	609	CLA	C1B-CHB	2.77	1.48	1.41
21	5	304	CLA	C1B-CHB	2.77	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	513	CLA	C4B-CHC	2.77	1.48	1.41
21	3	304	CLA	C1D-ND	-2.77	1.34	1.37
21	c	502	CLA	C1B-CHB	2.77	1.48	1.41
21	b	606	CLA	C1B-CHB	2.77	1.48	1.41
21	b	606	CLA	C1D-ND	-2.77	1.34	1.37
21	b	614	CLA	C1D-ND	-2.77	1.34	1.37
21	b	617	CLA	C1D-ND	-2.77	1.34	1.37
21	b	604	CLA	C4B-CHC	2.77	1.48	1.41
21	B	605	CLA	C1B-CHB	2.77	1.48	1.41
21	9	300	CLA	C1B-CHB	2.77	1.48	1.41
21	B	604	CLA	C1B-CHB	2.77	1.48	1.41
21	g	308	CLA	C1B-CHB	2.77	1.48	1.41
24	5	314	KC1	C4A-C3A	2.77	1.49	1.44
21	6	300	CLA	C4C-C3C	2.77	1.49	1.45
21	3	302	CLA	C1B-CHB	2.77	1.48	1.41
21	D	406	CLA	C4D-CHA	2.77	1.48	1.38
21	C	508	CLA	C1B-CHB	2.77	1.48	1.41
21	1	304	CLA	C4B-CHC	2.76	1.48	1.41
24	3	305	KC1	C4A-C3A	2.76	1.49	1.44
21	c	513	CLA	C1B-CHB	2.76	1.48	1.41
21	2	304	CLA	C4B-CHC	2.76	1.48	1.41
21	c	505	CLA	C4C-C3C	2.76	1.49	1.45
21	1	301	CLA	C4B-CHC	2.76	1.48	1.41
21	g	305	CLA	C4C-C3C	2.76	1.49	1.45
21	C	512	CLA	C1B-CHB	2.76	1.48	1.41
21	1	306	CLA	C1B-CHB	2.76	1.48	1.41
21	6	308	CLA	C1B-CHB	2.76	1.48	1.41
21	b	613	CLA	C1B-CHB	2.76	1.48	1.41
21	5	307	CLA	C4B-CHC	2.76	1.48	1.41
21	4	302	CLA	C4C-C3C	2.76	1.49	1.45
21	b	604	CLA	C1B-CHB	2.76	1.48	1.41
21	D	407	CLA	C1B-CHB	2.76	1.48	1.41
24	g	313	KC1	C4A-C3A	2.76	1.49	1.44
21	9	302	CLA	C4B-CHC	2.76	1.48	1.41
21	1	305	CLA	C1B-CHB	2.76	1.48	1.41
21	J	302	CLA	C4C-C3C	2.76	1.49	1.45
21	b	623	CLA	C4C-C3C	2.76	1.49	1.45
21	C	515	CLA	C4C-C3C	2.76	1.49	1.45
21	1	309	CLA	C1B-CHB	2.76	1.48	1.41
21	7	301	CLA	C1B-CHB	2.76	1.48	1.41
21	b	607	CLA	C1B-CHB	2.76	1.48	1.41
21	g	309	CLA	C4B-CHC	2.76	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	9	301	CLA	C1D-ND	-2.76	1.34	1.37
21	C	503	CLA	C1B-CHB	2.76	1.48	1.41
21	7	306	CLA	C4B-CHC	2.76	1.48	1.41
21	5	304	CLA	C4B-CHC	2.76	1.48	1.41
21	9	302	CLA	C1D-ND	-2.75	1.34	1.37
21	7	305	CLA	C3A-C2A	-2.75	1.52	1.54
21	2	306	CLA	C1B-CHB	2.75	1.48	1.41
21	5	307	CLA	C1B-CHB	2.75	1.48	1.41
21	g	305	CLA	C1B-CHB	2.75	1.48	1.41
21	B	603	CLA	C4B-CHC	2.75	1.48	1.41
21	B	621	CLA	C1B-CHB	2.75	1.48	1.41
21	7	300	CLA	C4B-CHC	2.75	1.48	1.41
21	7	301	CLA	C1D-ND	-2.75	1.34	1.37
21	b	605	CLA	C1B-CHB	2.75	1.48	1.41
21	3	301	CLA	C1D-ND	-2.75	1.34	1.37
24	2	315	KC1	C4B-NB	-2.75	1.34	1.37
21	B	612	CLA	C1B-CHB	2.75	1.48	1.41
24	1	315	KC1	C4A-C3A	2.75	1.49	1.44
21	2	305	CLA	C1D-ND	-2.75	1.34	1.37
21	J	302	CLA	C4B-CHC	2.75	1.48	1.41
21	G	302	CLA	C1B-CHB	2.75	1.48	1.41
21	J	303	CLA	C1B-CHB	2.75	1.48	1.41
21	b	612	CLA	C4B-CHC	2.75	1.48	1.41
21	B	616	CLA	C1D-ND	-2.75	1.34	1.37
21	8	305	CLA	C4B-CHC	2.75	1.48	1.41
21	c	514	CLA	C1B-CHB	2.75	1.48	1.41
21	J	308	CLA	C1D-ND	-2.75	1.34	1.37
21	C	515	CLA	C4B-CHC	2.75	1.48	1.41
30	B	624	DGD	C2E-C1E	2.75	1.56	1.51
24	6	311	KC1	C4A-C3A	2.75	1.49	1.44
21	B	608	CLA	C1B-CHB	2.75	1.48	1.41
21	6	303	CLA	C1D-ND	-2.75	1.34	1.37
21	b	611	CLA	C1B-CHB	2.75	1.48	1.41
25	H	100	BCR	C1-C6	-2.74	1.50	1.53
21	1	305	CLA	C4B-CHC	2.74	1.48	1.41
21	D	407	CLA	C4B-CHC	2.74	1.48	1.41
21	G	301	CLA	C4B-CHC	2.74	1.48	1.41
21	4	304	CLA	C1B-CHB	2.74	1.48	1.41
21	C	512	CLA	C4D-CHA	2.74	1.48	1.38
21	B	613	CLA	C1D-ND	-2.74	1.34	1.37
21	g	309	CLA	C1D-ND	-2.74	1.34	1.37
21	c	512	CLA	C4B-CHC	2.74	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	511	CLA	C1B-CHB	2.74	1.48	1.41
21	1	307	CLA	C4B-CHC	2.74	1.48	1.41
21	c	507	CLA	C1B-CHB	2.74	1.48	1.41
21	G	304	CLA	C1B-CHB	2.74	1.48	1.41
21	6	301	CLA	C1B-CHB	2.74	1.48	1.41
21	B	611	CLA	C4B-CHC	2.74	1.48	1.41
21	C	515	CLA	C1B-CHB	2.74	1.48	1.41
21	J	308	CLA	C4B-CHC	2.74	1.48	1.41
21	B	606	CLA	C1B-CHB	2.74	1.48	1.41
21	g	302	CLA	C1B-CHB	2.74	1.48	1.41
21	7	309	CLA	C4B-CHC	2.74	1.48	1.41
21	7	303	CLA	C4B-CHC	2.74	1.48	1.41
21	b	607	CLA	C4B-CHC	2.74	1.48	1.41
21	5	308	CLA	C1B-CHB	2.74	1.48	1.41
21	1	303	CLA	C4B-CHC	2.74	1.48	1.41
21	C	506	CLA	C4B-CHC	2.74	1.48	1.41
21	J	303	CLA	C4C-C3C	2.74	1.49	1.45
21	c	509	CLA	C1B-CHB	2.74	1.48	1.41
24	2	316	KC1	C2A-C1A	2.74	1.53	1.44
21	2	306	CLA	C1D-ND	-2.74	1.34	1.37
21	4	300	CLA	C1D-ND	-2.74	1.34	1.37
21	2	303	CLA	C1B-CHB	2.74	1.48	1.41
21	6	305	CLA	C1D-ND	-2.74	1.34	1.37
21	7	307	CLA	C1D-ND	-2.74	1.34	1.37
21	b	603	CLA	C1D-ND	-2.74	1.34	1.37
21	J	308	CLA	C1B-CHB	2.73	1.48	1.41
21	c	514	CLA	C4C-C3C	2.73	1.49	1.45
25	D	408	BCR	C30-C25	-2.73	1.50	1.53
24	2	314	KC1	CHB-C4A	-2.73	1.33	1.39
21	G	300	CLA	C4C-C3C	2.73	1.49	1.45
21	2	301	CLA	C4B-CHC	2.73	1.48	1.41
24	J	312	KC1	C4A-C3A	2.73	1.49	1.44
21	c	511	CLA	C4D-CHA	2.73	1.48	1.38
21	5	308	CLA	C4B-CHC	2.73	1.48	1.41
21	C	506	CLA	C4C-C3C	2.73	1.49	1.45
21	1	310	CLA	C4B-CHC	2.73	1.48	1.41
21	b	616	CLA	C1B-CHB	2.73	1.48	1.41
21	6	306	CLA	C1B-CHB	2.73	1.48	1.41
21	6	308	CLA	C4B-CHC	2.73	1.48	1.41
21	G	304	CLA	C4B-CHC	2.73	1.48	1.41
21	B	615	CLA	C1B-CHB	2.73	1.48	1.41
21	B	604	CLA	C1D-ND	-2.73	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	g	309	CLA	C4C-C3C	2.73	1.49	1.45
21	B	606	CLA	C4B-CHC	2.73	1.48	1.41
35	d	408	PL9	C6-C1	-2.73	1.43	1.48
21	d	406	CLA	C4B-CHC	2.73	1.48	1.41
21	C	505	CLA	C4B-CHC	2.73	1.48	1.41
21	B	610	CLA	C1B-CHB	2.72	1.48	1.41
21	c	514	CLA	C4B-CHC	2.72	1.48	1.41
21	3	301	CLA	C1B-CHB	2.72	1.48	1.41
21	7	303	CLA	C1B-CHB	2.72	1.48	1.41
21	6	306	CLA	C4B-CHC	2.72	1.48	1.41
21	5	304	CLA	C1D-ND	-2.72	1.34	1.37
21	2	305	CLA	C4B-CHC	2.72	1.48	1.41
21	C	505	CLA	C1B-CHB	2.72	1.48	1.41
21	C	514	CLA	C1B-CHB	2.72	1.48	1.41
21	g	306	CLA	C4C-C3C	2.72	1.49	1.45
21	c	504	CLA	C4B-CHC	2.72	1.48	1.41
21	B	613	CLA	C4B-CHC	2.72	1.48	1.41
21	5	302	CLA	C4B-CHC	2.72	1.48	1.41
30	b	601	DGD	C2E-C1E	2.72	1.56	1.51
21	J	301	CLA	C4B-CHC	2.72	1.48	1.41
21	1	302	CLA	C1B-CHB	2.72	1.48	1.41
21	4	302	CLA	C1D-ND	-2.72	1.34	1.37
21	5	303	CLA	C1D-ND	-2.72	1.34	1.37
24	3	306	KC1	C4A-C3A	2.72	1.49	1.44
21	a	402	CLA	C1B-CHB	2.72	1.48	1.41
21	9	301	CLA	C4B-CHC	2.72	1.48	1.41
24	J	311	KC1	C4A-C3A	2.72	1.49	1.44
21	1	304	CLA	C1B-CHB	2.71	1.48	1.41
21	b	609	CLA	C4B-CHC	2.71	1.48	1.41
21	5	306	CLA	C1B-CHB	2.71	1.48	1.41
21	g	308	CLA	C4B-CHC	2.71	1.48	1.41
21	d	406	CLA	C4C-C3C	2.71	1.49	1.45
21	b	605	CLA	C1D-ND	-2.71	1.34	1.37
21	8	307	CLA	C4B-CHC	2.71	1.48	1.41
21	g	302	CLA	C1D-ND	-2.71	1.34	1.37
21	G	300	CLA	C1D-ND	-2.71	1.34	1.37
21	B	608	CLA	C4B-CHC	2.71	1.48	1.41
21	b	614	CLA	C4B-CHC	2.71	1.48	1.41
24	8	316	KC1	C2A-C1A	2.71	1.52	1.44
21	6	308	CLA	C4C-C3C	2.71	1.49	1.45
21	C	515	CLA	C1D-ND	-2.71	1.34	1.37
21	b	623	CLA	C1B-CHB	2.71	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	609	CLA	C1B-CHB	2.71	1.48	1.41
24	G	308	KC1	C4A-C3A	2.71	1.49	1.44
21	C	508	CLA	C1D-ND	-2.71	1.34	1.37
21	b	608	CLA	C4B-CHC	2.71	1.48	1.41
21	C	509	CLA	C1D-ND	-2.71	1.34	1.37
21	6	301	CLA	C4B-CHC	2.71	1.48	1.41
21	7	308	CLA	C4B-CHC	2.71	1.48	1.41
21	J	300	CLA	C4C-C3C	2.71	1.49	1.45
21	b	606	CLA	MG-ND	-2.71	2.00	2.05
21	7	304	CLA	C1D-ND	-2.70	1.34	1.37
21	7	301	CLA	C4B-CHC	2.70	1.48	1.41
21	C	505	CLA	C4C-C3C	2.70	1.49	1.45
21	B	607	CLA	C4B-CHC	2.70	1.48	1.41
21	A	402	CLA	C1B-CHB	2.70	1.48	1.41
21	b	603	CLA	C1B-CHB	2.70	1.48	1.41
21	B	612	CLA	C4B-CHC	2.70	1.48	1.41
21	c	510	CLA	C1B-CHB	2.70	1.48	1.41
21	7	306	CLA	C4C-C3C	2.70	1.49	1.45
21	a	405	CLA	C1B-CHB	2.70	1.48	1.41
21	d	406	CLA	C1B-CHB	2.70	1.48	1.41
21	8	304	CLA	C4B-CHC	2.70	1.48	1.41
25	h	102	BCR	C1-C6	-2.70	1.50	1.53
21	B	610	CLA	C4B-CHC	2.69	1.48	1.41
21	J	306	CLA	C1B-CHB	2.69	1.48	1.41
21	J	306	CLA	C4B-CHC	2.69	1.48	1.41
21	b	605	CLA	C4C-C3C	2.69	1.49	1.45
21	A	401	CLA	C1B-CHB	2.69	1.48	1.41
21	C	513	CLA	C4B-CHC	2.69	1.48	1.41
21	9	303	CLA	C1B-CHB	2.69	1.48	1.41
21	1	302	CLA	C4B-CHC	2.69	1.48	1.41
21	B	602	CLA	C4B-CHC	2.69	1.48	1.41
21	2	303	CLA	C4B-CHC	2.69	1.48	1.41
24	G	306	KC1	C1A-C2A	2.69	1.51	1.45
21	4	301	CLA	C4B-CHC	2.69	1.48	1.41
21	c	505	CLA	C4B-CHC	2.69	1.48	1.41
21	5	305	CLA	C4B-CHC	2.69	1.48	1.41
21	b	603	CLA	C4B-CHC	2.69	1.48	1.41
21	A	404	CLA	C1B-CHB	2.69	1.48	1.41
21	C	514	CLA	C4C-C3C	2.69	1.49	1.45
21	2	305	CLA	C4C-C3C	2.69	1.49	1.45
21	2	305	CLA	C1B-CHB	2.68	1.48	1.41
21	c	502	CLA	C4B-CHC	2.68	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	307	CLA	C4C-C3C	2.68	1.49	1.45
21	D	407	CLA	C4C-C3C	2.68	1.49	1.45
21	a	403	CLA	C1B-CHB	2.68	1.48	1.41
21	g	309	CLA	C1B-CHB	2.68	1.48	1.41
21	b	615	CLA	C1B-CHB	2.68	1.48	1.41
21	4	304	CLA	C4B-CHC	2.68	1.48	1.41
21	7	304	CLA	C4B-CHC	2.68	1.48	1.41
21	5	309	CLA	C4C-C3C	2.68	1.49	1.45
21	8	306	CLA	C1B-CHB	2.68	1.48	1.41
21	8	302	CLA	C1B-CHB	2.68	1.48	1.41
21	g	302	CLA	C4C-C3C	2.67	1.49	1.45
21	7	301	CLA	C4D-ND	2.67	1.41	1.37
21	J	303	CLA	C4D-ND	2.67	1.41	1.37
24	4	306	KC1	C1A-C2A	2.67	1.51	1.45
21	J	305	CLA	C1D-ND	-2.67	1.34	1.37
21	b	608	CLA	C4C-C3C	2.67	1.49	1.45
21	B	603	CLA	C1B-CHB	2.67	1.48	1.41
21	J	304	CLA	C4B-CHC	2.67	1.48	1.41
21	C	511	CLA	C1B-CHB	2.67	1.48	1.41
21	8	307	CLA	C1D-ND	-2.67	1.34	1.37
21	B	614	CLA	C4B-CHC	2.67	1.48	1.41
21	4	301	CLA	C1B-CHB	2.67	1.48	1.41
21	5	303	CLA	C4C-C3C	2.67	1.49	1.45
21	3	302	CLA	C1C-NC	-2.67	1.33	1.37
21	c	511	CLA	C4B-CHC	2.67	1.48	1.41
21	1	309	CLA	C4B-CHC	2.66	1.48	1.41
21	b	605	CLA	C4B-CHC	2.66	1.48	1.41
21	2	301	CLA	C1B-CHB	2.66	1.48	1.41
24	G	307	KC1	CHB-C4A	-2.66	1.33	1.39
21	3	301	CLA	C4B-CHC	2.66	1.48	1.41
21	B	604	CLA	C4C-C3C	2.66	1.49	1.45
25	m	101	BCR	C30-C25	-2.66	1.50	1.53
21	G	303	CLA	C1D-ND	-2.66	1.34	1.37
21	2	302	CLA	C4B-CHC	2.66	1.48	1.41
24	6	311	KC1	CHB-C4A	-2.66	1.33	1.39
21	B	607	CLA	C4C-C3C	2.66	1.49	1.45
21	C	504	CLA	C4B-CHC	2.66	1.48	1.41
21	3	301	CLA	C4C-C3C	2.66	1.49	1.45
21	c	512	CLA	C1D-ND	-2.66	1.34	1.37
24	9	305	KC1	C4A-C3A	2.66	1.49	1.44
24	G	309	KC1	C4C-C3C	2.66	1.49	1.45
21	B	614	CLA	C1B-CHB	2.66	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	304	CLA	C4C-C3C	2.66	1.49	1.45
21	b	616	CLA	C4B-CHC	2.66	1.48	1.41
21	g	306	CLA	C1B-CHB	2.66	1.48	1.41
21	b	611	CLA	C4B-CHC	2.65	1.48	1.41
21	d	404	CLA	C1B-CHB	2.65	1.48	1.41
21	g	306	CLA	C4B-CHC	2.65	1.48	1.41
21	B	608	CLA	C4C-C3C	2.65	1.49	1.45
21	6	304	CLA	C4B-CHC	2.65	1.48	1.41
24	2	315	KC1	C4D-CHA	2.65	1.48	1.45
21	J	303	CLA	C1D-ND	-2.65	1.34	1.37
21	a	403	CLA	C4B-CHC	2.65	1.48	1.41
24	8	314	KC1	CHB-C4A	-2.65	1.33	1.39
21	c	510	CLA	C4B-CHC	2.65	1.48	1.41
21	B	605	CLA	C4D-ND	2.65	1.41	1.37
21	5	306	CLA	C4C-C3C	2.65	1.49	1.45
21	g	303	CLA	C1D-ND	-2.65	1.34	1.37
24	6	312	KC1	C4B-NB	-2.65	1.34	1.37
21	C	509	CLA	C4B-CHC	2.65	1.48	1.41
21	4	302	CLA	C4B-CHC	2.65	1.48	1.41
21	b	615	CLA	C4B-CHC	2.65	1.48	1.41
21	5	306	CLA	C4B-CHC	2.65	1.48	1.41
21	9	302	CLA	C4D-ND	2.65	1.41	1.37
21	c	504	CLA	C1D-ND	-2.64	1.34	1.37
21	c	504	CLA	C4C-C3C	2.64	1.49	1.45
21	C	512	CLA	C4B-CHC	2.64	1.48	1.41
21	A	402	CLA	C4B-CHC	2.64	1.48	1.41
21	G	304	CLA	C4C-C3C	2.64	1.49	1.45
24	g	314	KC1	C4A-C3A	2.64	1.49	1.44
21	b	617	CLA	C1C-NC	-2.64	1.33	1.37
21	5	302	CLA	C1B-CHB	2.64	1.48	1.41
21	8	307	CLA	C4D-ND	2.64	1.41	1.37
21	D	404	CLA	C1B-CHB	2.64	1.48	1.41
21	5	309	CLA	C4D-CHA	2.64	1.47	1.38
21	1	309	CLA	C4D-ND	2.64	1.41	1.37
24	4	306	KC1	C3C-C4C	2.64	1.49	1.43
21	4	301	CLA	C4C-C3C	2.64	1.49	1.45
21	6	305	CLA	C4C-C3C	2.64	1.49	1.45
21	c	513	CLA	C4C-C3C	2.63	1.49	1.45
21	g	309	CLA	MG-NA	2.63	2.12	2.06
21	g	303	CLA	C4B-CHC	2.63	1.48	1.41
24	G	306	KC1	C3C-C4C	2.63	1.49	1.43
25	M	101	BCR	C30-C25	-2.63	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	301	CLA	C4C-C3C	2.63	1.49	1.45
21	b	609	CLA	C4C-C3C	2.63	1.49	1.45
21	G	301	CLA	C4C-C3C	2.63	1.49	1.45
21	B	604	CLA	C4B-CHC	2.62	1.48	1.41
21	B	615	CLA	C4B-CHC	2.62	1.48	1.41
21	D	404	CLA	C4C-C3C	2.62	1.49	1.45
21	7	307	CLA	C4C-C3C	2.62	1.49	1.45
21	c	508	CLA	C4B-CHC	2.62	1.48	1.41
21	C	508	CLA	C4B-CHC	2.62	1.48	1.41
21	g	303	CLA	C4D-ND	2.62	1.41	1.37
21	6	306	CLA	C4C-C3C	2.62	1.49	1.45
21	8	306	CLA	C4C-C3C	2.62	1.49	1.45
21	c	504	CLA	C1B-CHB	2.62	1.48	1.41
21	J	307	CLA	C4C-C3C	2.62	1.49	1.45
21	B	616	CLA	C1B-CHB	2.62	1.48	1.41
25	b	619	BCR	C30-C25	-2.62	1.50	1.53
21	A	404	CLA	C4C-C3C	2.62	1.49	1.45
21	5	303	CLA	C4B-CHC	2.62	1.48	1.41
21	C	505	CLA	C4D-ND	2.61	1.41	1.37
21	8	303	CLA	C4B-CHC	2.61	1.48	1.41
24	5	313	KC1	C4A-C3A	2.61	1.49	1.44
21	J	305	CLA	C4C-C3C	2.61	1.49	1.45
21	J	308	CLA	C4C-C3C	2.61	1.49	1.45
21	J	307	CLA	MG-ND	-2.61	2.00	2.05
21	7	308	CLA	C4C-C3C	2.61	1.49	1.45
21	8	303	CLA	C4C-C3C	2.61	1.49	1.45
24	J	312	KC1	C4B-NB	-2.61	1.34	1.37
21	5	303	CLA	C4D-ND	2.61	1.41	1.37
21	c	503	CLA	C4B-CHC	2.61	1.48	1.41
21	5	308	CLA	MG-ND	-2.61	2.00	2.05
21	g	302	CLA	C4B-CHC	2.61	1.48	1.41
21	b	606	CLA	C4D-ND	2.61	1.41	1.37
21	J	306	CLA	C4C-C3C	2.60	1.49	1.45
25	B	618	BCR	C30-C25	-2.60	1.50	1.53
24	J	313	KC1	C4A-C3A	2.60	1.49	1.44
21	C	505	CLA	C1D-ND	-2.60	1.34	1.37
21	C	511	CLA	C4B-CHC	2.60	1.48	1.41
21	d	404	CLA	C4C-C3C	2.60	1.49	1.45
21	7	301	CLA	MG-NC	2.60	2.12	2.06
21	g	303	CLA	C4C-C3C	2.60	1.49	1.45
24	8	315	KC1	C4B-NB	-2.60	1.34	1.37
21	b	623	CLA	C4B-CHC	2.60	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	314	KC1	C4A-C3A	2.60	1.49	1.44
21	C	507	CLA	C4C-C3C	2.59	1.49	1.45
21	C	510	CLA	C4C-C3C	2.59	1.49	1.45
24	3	306	KC1	C4C-C3C	2.59	1.49	1.45
21	3	304	CLA	C4C-C3C	2.59	1.49	1.45
21	c	509	CLA	C4B-CHC	2.59	1.48	1.41
21	8	304	CLA	C4C-C3C	2.59	1.49	1.45
21	B	616	CLA	C1C-NC	-2.59	1.33	1.37
24	8	315	KC1	C4D-CHA	2.59	1.48	1.45
21	9	300	CLA	C4C-C3C	2.59	1.49	1.45
21	c	506	CLA	C4C-C3C	2.58	1.49	1.45
21	c	510	CLA	C4C-C3C	2.58	1.49	1.45
30	c	516	DGD	O1G-C1G	-2.58	1.39	1.45
21	c	512	CLA	C4C-C3C	2.58	1.49	1.45
21	B	602	CLA	C4C-C3C	2.58	1.49	1.45
25	b	618	BCR	C30-C25	-2.58	1.50	1.53
21	5	305	CLA	C4C-C3C	2.58	1.49	1.45
21	1	302	CLA	C4C-C3C	2.58	1.49	1.45
21	7	302	CLA	C4C-C3C	2.58	1.49	1.45
24	J	313	KC1	C4D-CHA	2.58	1.48	1.45
24	1	316	KC1	CHB-C4A	-2.58	1.33	1.39
21	C	510	CLA	C4B-CHC	2.58	1.48	1.41
21	2	303	CLA	C4C-C3C	2.58	1.49	1.45
21	9	304	CLA	C4C-C3C	2.58	1.49	1.45
30	B	624	DGD	O2G-C2G	-2.57	1.40	1.46
21	1	303	CLA	C4C-C3C	2.57	1.49	1.45
22	1	311	DD6	C13-C11	-2.57	1.40	1.45
21	b	603	CLA	C4C-C3C	2.57	1.49	1.45
21	1	308	CLA	C4C-C3C	2.57	1.49	1.45
24	7	315	KC1	C4A-C3A	2.57	1.49	1.44
21	c	506	CLA	C4B-CHC	2.57	1.48	1.41
21	A	401	CLA	C4B-CHC	2.57	1.48	1.41
24	8	313	KC1	C2A-C1A	2.57	1.52	1.44
26	a	404	PHO	CAC-C3C	-2.57	1.47	1.52
21	c	507	CLA	C4B-CHC	2.56	1.48	1.41
21	3	300	CLA	C4C-C3C	2.56	1.49	1.45
24	7	315	KC1	CHB-C4A	-2.56	1.33	1.39
21	7	307	CLA	C4D-ND	2.56	1.41	1.37
21	a	405	CLA	C4C-C3C	2.56	1.49	1.45
21	3	302	CLA	C4D-ND	2.56	1.41	1.37
24	J	311	KC1	CHB-C4A	-2.56	1.33	1.39
21	a	402	CLA	C4B-CHC	2.56	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	513	CLA	C4C-C3C	2.56	1.49	1.45
21	7	305	CLA	C4C-C3C	2.55	1.49	1.45
21	B	602	CLA	C4D-ND	2.55	1.41	1.37
24	5	313	KC1	CHB-C4A	-2.55	1.33	1.39
21	B	621	CLA	C4B-CHC	2.55	1.48	1.41
21	b	617	CLA	C1B-CHB	2.55	1.48	1.41
21	c	502	CLA	C4C-C3C	2.55	1.49	1.45
24	g	314	KC1	CHB-C4A	-2.55	1.33	1.39
21	b	614	CLA	C4C-C3C	2.55	1.49	1.45
26	A	403	PHO	CAC-C3C	-2.55	1.47	1.52
21	1	309	CLA	C4C-C3C	2.55	1.49	1.45
21	J	305	CLA	C4D-ND	2.55	1.41	1.37
24	8	315	KC1	C4C-C3C	2.55	1.49	1.45
21	d	404	CLA	C4B-CHC	2.55	1.48	1.41
21	6	303	CLA	C4D-ND	2.55	1.41	1.37
21	B	603	CLA	C4C-C3C	2.54	1.49	1.45
21	G	300	CLA	C4D-ND	2.54	1.41	1.37
24	8	314	KC1	C2A-C1A	2.54	1.52	1.44
21	C	511	CLA	C4C-C3C	2.54	1.49	1.45
21	B	605	CLA	C4C-C3C	2.54	1.49	1.45
21	a	403	CLA	C4C-C3C	2.54	1.49	1.45
24	2	315	KC1	C4C-C3C	2.54	1.49	1.45
21	1	304	CLA	C4C-C3C	2.54	1.49	1.45
21	C	510	CLA	C1C-NC	-2.54	1.34	1.37
24	8	314	KC1	C4A-C3A	2.54	1.49	1.44
24	5	314	KC1	C4B-NB	-2.54	1.34	1.37
22	1	311	DD6	C8-C6	-2.53	1.40	1.45
25	C	501	BCR	C30-C25	-2.53	1.50	1.53
21	3	302	CLA	C1D-ND	-2.53	1.34	1.37
21	9	303	CLA	C1C-NC	-2.53	1.34	1.37
21	g	304	CLA	C4C-C3C	2.53	1.49	1.45
24	3	306	KC1	CHB-C4A	-2.53	1.33	1.39
30	C	517	DGD	O1G-C1G	-2.53	1.39	1.45
24	8	314	KC1	C4C-C3C	2.53	1.49	1.45
24	4	308	KC1	C4C-C3C	2.53	1.49	1.45
24	G	308	KC1	CHB-C4A	-2.53	1.33	1.39
21	D	404	CLA	C4B-CHC	2.53	1.48	1.41
21	B	609	CLA	C4B-CHC	2.53	1.48	1.41
24	9	306	KC1	C4C-C3C	2.53	1.49	1.45
24	2	314	KC1	C2A-C1A	2.53	1.52	1.44
21	8	305	CLA	C4C-C3C	2.52	1.49	1.45
21	c	509	CLA	C4C-C3C	2.52	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	301	CLA	C4D-ND	2.52	1.41	1.37
21	D	404	CLA	MG-ND	2.52	2.10	2.05
24	6	313	KC1	C4A-C3A	2.52	1.49	1.44
25	B	617	BCR	C30-C25	-2.52	1.50	1.53
21	2	306	CLA	C4D-ND	2.52	1.41	1.37
21	c	506	CLA	C4D-ND	2.52	1.41	1.37
21	7	304	CLA	C1C-NC	-2.52	1.34	1.37
21	b	603	CLA	C4D-ND	2.52	1.41	1.37
21	5	309	CLA	C4B-CHC	2.52	1.48	1.41
24	3	305	KC1	C4C-C3C	2.52	1.49	1.45
24	G	308	KC1	C1C-C2C	2.52	1.49	1.44
21	G	302	CLA	C4D-ND	2.52	1.41	1.37
30	b	601	DGD	C3E-C4E	2.51	1.56	1.52
28	B	627	LMG	C7-C8	2.51	1.58	1.50
25	1	317	BCR	C30-C25	-2.51	1.50	1.53
21	B	613	CLA	C4C-C3C	2.51	1.49	1.45
21	9	301	CLA	C4D-ND	2.51	1.41	1.37
24	9	305	KC1	CHB-C4A	-2.51	1.33	1.39
21	6	307	CLA	C4C-C3C	2.51	1.49	1.45
24	8	316	KC1	CHB-C4A	-2.51	1.33	1.39
21	2	304	CLA	C4C-C3C	2.51	1.49	1.45
21	6	304	CLA	C4C-C3C	2.51	1.49	1.45
21	5	302	CLA	C1C-C2C	2.51	1.49	1.44
24	5	314	KC1	CHB-C4A	-2.51	1.33	1.39
21	2	302	CLA	C4C-C3C	2.51	1.49	1.45
21	B	621	CLA	C1C-NC	-2.51	1.34	1.37
21	c	512	CLA	C4D-ND	2.51	1.41	1.37
25	C	516	BCR	C30-C25	-2.51	1.50	1.53
21	C	507	CLA	C4D-ND	2.51	1.41	1.37
21	g	306	CLA	MG-NA	2.51	2.12	2.06
21	c	502	CLA	C4D-ND	2.51	1.41	1.37
21	G	303	CLA	C4D-ND	2.51	1.41	1.37
24	2	316	KC1	CHB-C4A	-2.51	1.33	1.39
21	C	503	CLA	C4C-C3C	2.50	1.49	1.45
21	C	514	CLA	C4D-ND	2.50	1.41	1.37
21	b	604	CLA	C4C-C3C	2.50	1.49	1.45
21	5	308	CLA	C4C-C3C	2.50	1.49	1.45
21	B	614	CLA	C4C-C3C	2.50	1.49	1.45
24	6	313	KC1	CHB-C4A	-2.50	1.33	1.39
21	c	507	CLA	C1C-NC	-2.50	1.34	1.37
21	2	306	CLA	C4B-CHC	2.50	1.47	1.41
21	8	303	CLA	C4D-ND	2.50	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	509	CLA	C4C-C3C	2.50	1.49	1.45
24	1	315	KC1	C4C-C3C	2.50	1.49	1.45
21	C	507	CLA	C4B-CHC	2.50	1.47	1.41
21	4	302	CLA	C1C-NC	-2.49	1.34	1.37
21	2	306	CLA	C4C-C3C	2.49	1.49	1.45
24	1	316	KC1	C4A-C3A	2.49	1.49	1.44
21	7	306	CLA	C4D-ND	2.49	1.41	1.37
24	8	313	KC1	C4A-C3A	2.49	1.49	1.44
21	J	308	CLA	C4D-ND	2.49	1.41	1.37
21	1	301	CLA	C4C-C3C	2.49	1.49	1.45
21	3	302	CLA	C4C-C3C	2.49	1.49	1.45
21	b	605	CLA	C4D-ND	2.49	1.41	1.37
24	J	312	KC1	CHB-C4A	-2.49	1.33	1.39
21	B	614	CLA	C1C-NC	-2.49	1.34	1.37
21	6	305	CLA	C4D-ND	2.49	1.41	1.37
21	B	615	CLA	C4D-ND	2.49	1.41	1.37
21	b	610	CLA	C4B-CHC	2.49	1.47	1.41
21	B	604	CLA	C4D-ND	2.49	1.41	1.37
25	1	317	BCR	C1-C6	-2.49	1.50	1.53
23	2	308	A86	C24-C1	-2.49	1.40	1.45
21	7	300	CLA	C4C-C3C	2.48	1.49	1.45
21	b	611	CLA	C4C-C3C	2.48	1.49	1.45
21	b	607	CLA	C4C-C3C	2.48	1.49	1.45
21	c	509	CLA	C1C-NC	-2.48	1.34	1.37
21	C	513	CLA	C4D-ND	2.48	1.41	1.37
24	g	314	KC1	C4C-C3C	2.48	1.49	1.45
24	J	313	KC1	CHB-C4A	-2.48	1.33	1.39
21	A	402	CLA	C4C-C3C	2.48	1.49	1.45
24	1	315	KC1	CHB-C4A	-2.48	1.33	1.39
24	5	314	KC1	C4C-C3C	2.48	1.49	1.45
24	6	313	KC1	C4D-CHA	2.48	1.48	1.45
21	2	305	CLA	C4D-ND	2.48	1.41	1.37
22	7	310	DD6	C8-C6	-2.47	1.40	1.45
21	C	508	CLA	C1C-NC	-2.47	1.34	1.37
24	G	306	KC1	C2C-C1C	2.47	1.49	1.43
21	8	302	CLA	C4C-C3C	2.47	1.49	1.45
21	b	610	CLA	C1C-NC	-2.47	1.34	1.37
21	c	504	CLA	C4D-ND	2.47	1.41	1.37
21	b	615	CLA	C4C-C3C	2.47	1.49	1.45
21	5	302	CLA	C4C-C3C	2.47	1.49	1.45
21	7	308	CLA	C4D-ND	2.47	1.41	1.37
24	6	312	KC1	CHB-C4A	-2.47	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	304	CLA	C4D-ND	2.47	1.41	1.37
21	b	606	CLA	C4C-C3C	2.47	1.49	1.45
21	B	612	CLA	C1C-NC	-2.47	1.34	1.37
24	4	306	KC1	C2C-C1C	2.47	1.49	1.43
24	G	307	KC1	C4A-C3A	2.47	1.49	1.44
23	8	311	A86	C24-C1	-2.47	1.40	1.45
24	g	313	KC1	C4C-C3C	2.47	1.49	1.45
30	b	601	DGD	O1G-C1G	-2.47	1.39	1.45
21	c	503	CLA	C4C-C3C	2.47	1.49	1.45
24	6	312	KC1	C3B-C4B	2.46	1.50	1.46
21	B	616	CLA	C4B-CHC	2.46	1.47	1.41
21	4	301	CLA	C4D-ND	2.46	1.41	1.37
24	8	315	KC1	C2A-C1A	2.46	1.52	1.44
21	b	623	CLA	C1C-NC	-2.46	1.34	1.37
21	b	610	CLA	C4C-C3C	2.46	1.49	1.45
21	2	302	CLA	C1D-ND	-2.46	1.34	1.37
21	b	606	CLA	C1C-NC	-2.46	1.34	1.37
21	1	310	CLA	C4D-ND	2.46	1.41	1.37
21	B	621	CLA	C4D-ND	2.46	1.41	1.37
24	2	315	KC1	C2A-C1A	2.46	1.52	1.44
21	1	302	CLA	C4D-ND	2.46	1.41	1.37
21	6	302	CLA	C4D-ND	2.46	1.41	1.37
24	6	312	KC1	C4C-C3C	2.46	1.49	1.45
21	J	304	CLA	C4C-C3C	2.46	1.49	1.45
21	2	302	CLA	C4D-ND	2.46	1.41	1.37
21	g	309	CLA	C4D-ND	2.46	1.41	1.37
21	4	304	CLA	C1C-NC	-2.46	1.34	1.37
21	c	513	CLA	C4D-ND	2.45	1.41	1.37
21	4	300	CLA	C4D-ND	2.45	1.41	1.37
21	5	308	CLA	C4D-ND	2.45	1.41	1.37
21	B	606	CLA	C4C-C3C	2.45	1.49	1.45
21	2	301	CLA	C4C-C3C	2.45	1.49	1.45
25	h	102	BCR	C30-C25	-2.45	1.50	1.53
21	c	508	CLA	C4C-C3C	2.45	1.49	1.45
21	b	616	CLA	C4D-ND	2.45	1.41	1.37
21	c	503	CLA	C1C-NC	-2.45	1.34	1.37
30	B	624	DGD	C3E-C4E	2.45	1.56	1.52
21	C	509	CLA	C4D-ND	2.45	1.41	1.37
21	3	304	CLA	C4D-ND	2.45	1.41	1.37
24	4	307	KC1	CHB-C4A	-2.45	1.33	1.39
22	7	310	DD6	C13-C11	-2.45	1.40	1.45
21	J	302	CLA	C4D-ND	2.45	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	609	CLA	C1C-NC	-2.45	1.34	1.37
21	3	301	CLA	C4D-ND	2.45	1.41	1.37
21	1	307	CLA	C4D-ND	2.44	1.41	1.37
21	g	308	CLA	C4D-ND	2.44	1.41	1.37
24	1	316	KC1	C4C-C3C	2.44	1.49	1.45
21	C	510	CLA	C4D-ND	2.44	1.41	1.37
21	4	303	CLA	C4D-ND	2.44	1.41	1.37
21	b	613	CLA	C1C-NC	-2.44	1.34	1.37
21	7	304	CLA	C4D-ND	2.44	1.41	1.37
21	4	302	CLA	C4D-ND	2.44	1.41	1.37
21	1	308	CLA	C4D-ND	2.44	1.41	1.37
21	8	303	CLA	C1D-ND	-2.44	1.34	1.37
21	7	303	CLA	C4C-C3C	2.44	1.49	1.45
24	G	306	KC1	CHB-C4A	-2.44	1.33	1.39
25	d	407	BCR	C1-C6	-2.44	1.50	1.53
24	J	312	KC1	C3B-C4B	2.44	1.50	1.46
25	H	100	BCR	C30-C25	-2.44	1.50	1.53
23	J	310	A86	C24-C1	-2.43	1.40	1.45
21	6	308	CLA	C4D-ND	2.43	1.41	1.37
21	3	301	CLA	MG-NA	2.43	2.12	2.06
21	C	503	CLA	C4D-ND	2.43	1.41	1.37
21	C	508	CLA	C4D-ND	2.43	1.41	1.37
21	7	306	CLA	C1C-NC	-2.43	1.34	1.37
21	J	303	CLA	C4B-CHC	2.43	1.48	1.43
21	b	617	CLA	C4B-CHC	2.43	1.47	1.41
21	C	506	CLA	C4D-ND	2.43	1.41	1.37
21	B	614	CLA	C4D-ND	2.43	1.41	1.37
21	5	306	CLA	C1C-NC	-2.43	1.34	1.37
24	1	316	KC1	C2A-C1A	2.43	1.52	1.44
24	J	313	KC1	C2A-C1A	2.43	1.52	1.44
23	8	309	A86	C24-C1	-2.43	1.40	1.45
24	g	313	KC1	CHB-C4A	-2.43	1.33	1.39
21	J	300	CLA	C4D-ND	2.42	1.41	1.37
24	6	313	KC1	C2A-C1A	2.42	1.52	1.44
21	g	306	CLA	C1C-NC	-2.42	1.34	1.37
24	8	313	KC1	C4C-C3C	2.42	1.49	1.45
24	8	315	KC1	C3B-C4B	2.42	1.50	1.46
21	5	307	CLA	C4D-ND	2.42	1.41	1.37
21	3	300	CLA	C1C-NC	-2.42	1.34	1.37
21	c	506	CLA	C1C-NC	-2.42	1.34	1.37
21	C	515	CLA	C4D-ND	2.42	1.41	1.37
21	1	305	CLA	C4D-ND	2.42	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	301	CLA	C4D-ND	2.42	1.41	1.37
21	B	613	CLA	C4D-ND	2.42	1.41	1.37
24	7	315	KC1	C4C-C3C	2.42	1.49	1.45
21	b	605	CLA	C1C-NC	-2.42	1.34	1.37
24	4	308	KC1	CHB-C4A	-2.41	1.33	1.39
24	7	315	KC1	C2A-C1A	2.41	1.52	1.44
21	5	309	CLA	C1B-CHB	2.41	1.47	1.41
21	C	504	CLA	C4D-ND	2.41	1.41	1.37
21	c	508	CLA	C4D-ND	2.41	1.41	1.37
24	8	313	KC1	C4D-CHA	2.41	1.48	1.45
21	b	604	CLA	C4D-ND	2.41	1.41	1.37
23	W	101	A86	C24-C1	-2.41	1.40	1.45
21	B	607	CLA	C4D-ND	2.41	1.41	1.37
24	J	312	KC1	C2A-C1A	2.41	1.52	1.44
21	c	503	CLA	C4D-ND	2.41	1.41	1.37
21	c	507	CLA	C4D-ND	2.41	1.41	1.37
21	B	608	CLA	C4D-ND	2.41	1.41	1.37
21	G	300	CLA	C1C-NC	-2.41	1.34	1.37
21	6	300	CLA	C4D-ND	2.40	1.41	1.37
21	b	608	CLA	C4D-ND	2.40	1.41	1.37
21	B	605	CLA	C1C-NC	-2.40	1.34	1.37
26	D	401	PHO	CAC-C3C	-2.40	1.48	1.52
26	d	403	PHO	CAC-C3C	-2.40	1.48	1.52
30	h	103	DGD	O1G-C1G	-2.40	1.39	1.45
24	g	315	KC1	CHB-C4A	-2.40	1.33	1.39
24	7	314	KC1	CHB-C4A	-2.40	1.33	1.39
21	b	609	CLA	C4D-ND	2.40	1.40	1.37
21	1	307	CLA	C1C-NC	-2.40	1.34	1.37
23	2	307	A86	C24-C1	-2.40	1.40	1.45
21	1	306	CLA	C1C-NC	-2.40	1.34	1.37
21	C	504	CLA	C1C-NC	-2.40	1.34	1.37
24	G	307	KC1	C4C-C3C	2.39	1.49	1.45
21	1	310	CLA	C1C-NC	-2.39	1.34	1.37
30	H	101	DGD	O1G-C1G	-2.39	1.39	1.45
21	b	615	CLA	C1C-NC	-2.39	1.34	1.37
21	5	303	CLA	C1C-NC	-2.39	1.34	1.37
21	5	305	CLA	C4D-ND	2.39	1.40	1.37
24	J	312	KC1	C4C-C3C	2.39	1.49	1.45
21	B	611	CLA	C1C-NC	-2.39	1.34	1.37
21	C	504	CLA	C4C-C3C	2.39	1.49	1.45
21	D	406	CLA	C1C-NC	-2.39	1.34	1.37
21	c	514	CLA	C4D-ND	2.39	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	306	KC1	C2A-C1A	2.39	1.51	1.44
21	B	613	CLA	C1C-NC	-2.38	1.34	1.37
21	6	303	CLA	C4B-CHC	2.38	1.48	1.43
24	6	312	KC1	C2A-C1A	2.38	1.51	1.44
21	A	401	CLA	C4C-C3C	2.38	1.49	1.45
23	2	308	A86	C8-C6	-2.38	1.40	1.45
23	G	305	A86	C8-C6	-2.38	1.40	1.45
24	2	313	KC1	C4C-C3C	2.38	1.49	1.45
24	4	309	KC1	C2A-C1A	2.38	1.51	1.44
22	g	310	DD6	C13-C11	-2.38	1.40	1.45
24	3	305	KC1	CHB-C4A	-2.38	1.33	1.39
24	5	315	KC1	CHB-C4A	-2.38	1.33	1.39
25	c	501	BCR	C30-C25	-2.38	1.50	1.53
23	2	310	A86	C24-C1	-2.38	1.40	1.45
21	1	309	CLA	C1C-NC	-2.38	1.34	1.37
21	B	616	CLA	C4D-ND	2.38	1.40	1.37
27	D	403	LHG	O7-C5	-2.38	1.40	1.46
21	b	609	CLA	C1C-NC	-2.37	1.34	1.37
27	d	402	LHG	O7-C5	-2.37	1.40	1.46
21	b	614	CLA	C4D-ND	2.37	1.40	1.37
21	3	303	CLA	C4D-ND	2.37	1.40	1.37
21	g	305	CLA	C4D-ND	2.37	1.40	1.37
24	8	316	KC1	C4C-C3C	2.37	1.49	1.45
23	4	305	A86	C8-C6	-2.37	1.40	1.45
21	8	303	CLA	C1C-NC	-2.37	1.34	1.37
23	7	313	A86	C8-C6	-2.37	1.40	1.45
21	B	604	CLA	C1C-NC	-2.37	1.34	1.37
23	8	308	A86	C25-C24	2.37	1.40	1.34
21	B	603	CLA	C4D-ND	2.37	1.40	1.37
21	B	608	CLA	C1C-NC	-2.37	1.34	1.37
21	5	304	CLA	C1C-NC	-2.37	1.34	1.37
24	2	314	KC1	C4C-C3C	2.37	1.49	1.45
25	D	408	BCR	C1-C6	-2.37	1.50	1.53
21	8	302	CLA	C4D-ND	2.36	1.40	1.37
24	4	307	KC1	C4C-C3C	2.36	1.49	1.45
21	C	507	CLA	C1C-NC	-2.36	1.34	1.37
24	7	314	KC1	C4C-C3C	2.36	1.49	1.45
21	2	301	CLA	C1C-NC	-2.36	1.34	1.37
24	4	309	KC1	C4D-CHA	2.36	1.48	1.45
23	4	305	A86	C24-C1	-2.36	1.40	1.45
21	c	508	CLA	C1C-NC	-2.36	1.34	1.37
21	C	510	CLA	MG-ND	2.36	2.10	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	d	405	CLA	C1C-NC	-2.36	1.34	1.37
21	c	510	CLA	C4D-ND	2.36	1.40	1.37
21	c	510	CLA	C1C-NC	-2.36	1.34	1.37
21	7	300	CLA	C4D-ND	2.36	1.40	1.37
21	d	406	CLA	C4D-ND	2.36	1.40	1.37
21	C	511	CLA	C1C-NC	-2.36	1.34	1.37
21	b	610	CLA	C4D-ND	2.36	1.40	1.37
24	6	311	KC1	C4C-C3C	2.35	1.49	1.45
21	b	617	CLA	C4D-ND	2.35	1.40	1.37
21	7	309	CLA	C1C-NC	-2.35	1.34	1.37
21	6	308	CLA	C1C-NC	-2.35	1.34	1.37
21	C	514	CLA	C1C-NC	-2.35	1.34	1.37
21	7	309	CLA	C4D-ND	2.35	1.40	1.37
22	7	310	DD6	C24-C1	-2.34	1.40	1.45
21	C	513	CLA	C1C-NC	-2.34	1.34	1.37
21	6	301	CLA	C4C-C3C	2.34	1.49	1.45
22	1	311	DD6	C24-C1	-2.34	1.40	1.45
21	b	603	CLA	C1C-NC	-2.34	1.34	1.37
21	g	304	CLA	C1C-NC	-2.34	1.34	1.37
24	9	306	KC1	CHB-C4A	-2.34	1.33	1.39
21	b	607	CLA	MG-ND	-2.34	2.01	2.05
24	2	316	KC1	C4C-C3C	2.34	1.49	1.45
21	G	304	CLA	C1C-NC	-2.34	1.34	1.37
21	2	301	CLA	C4D-ND	2.34	1.40	1.37
21	D	407	CLA	C4D-ND	2.34	1.40	1.37
21	b	613	CLA	C4C-C3C	2.34	1.49	1.45
24	9	306	KC1	C1C-C2C	2.34	1.49	1.44
21	B	615	CLA	C1C-NC	-2.34	1.34	1.37
21	g	307	CLA	C4D-ND	2.34	1.40	1.37
24	g	315	KC1	C4C-C3C	2.34	1.49	1.45
21	4	300	CLA	C1C-NC	-2.34	1.34	1.37
21	A	402	CLA	C4D-ND	2.34	1.40	1.37
21	b	611	CLA	C4D-ND	2.34	1.40	1.37
21	8	307	CLA	C1C-NC	-2.34	1.34	1.37
21	C	515	CLA	C1C-NC	-2.33	1.34	1.37
21	B	612	CLA	C4D-ND	2.33	1.40	1.37
24	9	305	KC1	C4C-C3C	2.33	1.49	1.45
24	5	313	KC1	C4C-C3C	2.33	1.49	1.45
21	c	513	CLA	C1C-NC	-2.33	1.34	1.37
21	a	402	CLA	C4C-C3C	2.33	1.49	1.45
21	1	308	CLA	MG-NC	-2.33	2.00	2.06
25	c	515	BCR	C30-C25	-2.33	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	g	303	CLA	C1C-NC	-2.33	1.34	1.37
23	2	309	A86	C24-C1	-2.33	1.40	1.45
21	2	302	CLA	C1C-NC	-2.33	1.34	1.37
21	b	612	CLA	C1C-NC	-2.33	1.34	1.37
21	2	304	CLA	C1C-NC	-2.32	1.34	1.37
24	2	315	KC1	C4A-C3A	2.32	1.49	1.44
24	2	313	KC1	C4D-CHA	2.32	1.47	1.45
21	g	303	CLA	MG-ND	2.32	2.10	2.05
21	c	504	CLA	C1C-NC	-2.32	1.34	1.37
21	b	615	CLA	C4D-ND	2.32	1.40	1.37
21	4	304	CLA	C4D-ND	2.32	1.40	1.37
23	8	309	A86	C8-C6	-2.32	1.41	1.45
24	8	314	KC1	C4D-CHA	2.32	1.47	1.45
21	5	307	CLA	C1C-NC	-2.32	1.34	1.37
24	2	313	KC1	C2A-C1A	2.32	1.51	1.44
21	B	607	CLA	C1C-NC	-2.32	1.34	1.37
21	C	509	CLA	C1C-NC	-2.32	1.34	1.37
21	8	305	CLA	C1C-NC	-2.32	1.34	1.37
21	C	505	CLA	C1C-NC	-2.32	1.34	1.37
24	1	315	KC1	C2A-C1A	2.32	1.51	1.44
24	g	314	KC1	C1C-C2C	2.32	1.49	1.44
24	7	314	KC1	C1C-C2C	2.32	1.49	1.44
21	8	306	CLA	C4D-ND	2.32	1.40	1.37
21	B	609	CLA	C4C-C3C	2.31	1.49	1.45
21	1	305	CLA	C1C-NC	-2.31	1.34	1.37
21	7	301	CLA	C1C-NC	-2.31	1.34	1.37
21	g	305	CLA	C1C-NC	-2.31	1.34	1.37
21	b	616	CLA	C1C-NC	-2.31	1.34	1.37
21	2	306	CLA	C1C-NC	-2.31	1.34	1.37
21	7	302	CLA	C1C-NC	-2.31	1.34	1.37
21	1	306	CLA	C4C-C3C	2.31	1.49	1.45
21	6	305	CLA	C1C-NC	-2.31	1.34	1.37
23	6	310	A86	C24-C1	-2.31	1.41	1.45
21	g	302	CLA	C4D-ND	2.31	1.40	1.37
21	6	307	CLA	C1C-NC	-2.31	1.34	1.37
23	1	314	A86	C8-C6	-2.31	1.41	1.45
21	8	304	CLA	C4D-ND	2.31	1.40	1.37
21	6	306	CLA	C4D-ND	2.30	1.40	1.37
24	G	309	KC1	C2A-C1A	2.30	1.51	1.44
21	1	303	CLA	C1C-NC	-2.30	1.34	1.37
21	B	602	CLA	C1C-NC	-2.30	1.34	1.37
21	8	302	CLA	C1C-NC	-2.30	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	314	KC1	C1C-C2C	2.30	1.49	1.44
21	b	617	CLA	C4C-C3C	2.30	1.49	1.45
21	c	505	CLA	C4D-ND	2.30	1.40	1.37
21	c	514	CLA	C1C-NC	-2.30	1.34	1.37
21	b	614	CLA	C1C-NC	-2.30	1.34	1.37
30	B	624	DGD	O1G-C1G	-2.30	1.39	1.45
21	g	308	CLA	C1C-NC	-2.30	1.34	1.37
21	9	300	CLA	C4D-ND	2.30	1.40	1.37
24	4	308	KC1	C4A-C3A	2.30	1.49	1.44
21	c	509	CLA	C4D-ND	2.30	1.40	1.37
21	B	610	CLA	C4C-C3C	2.30	1.49	1.45
24	4	309	KC1	C1D-CHD	2.30	1.47	1.41
24	8	316	KC1	C1C-C2C	2.30	1.49	1.44
21	B	606	CLA	MG-ND	-2.30	2.01	2.05
21	d	405	CLA	C1C-C2C	2.30	1.49	1.44
22	g	310	DD6	C8-C6	-2.30	1.41	1.45
21	J	307	CLA	C4D-ND	2.30	1.40	1.37
24	8	313	KC1	C1C-C2C	2.30	1.49	1.44
24	3	305	KC1	C1C-C2C	2.30	1.49	1.44
24	6	313	KC1	C4C-C3C	2.29	1.49	1.45
21	B	610	CLA	C1C-NC	-2.29	1.34	1.37
21	9	302	CLA	C1C-NC	-2.29	1.34	1.37
21	7	307	CLA	C1C-NC	-2.29	1.34	1.37
21	J	305	CLA	C1C-NC	-2.29	1.34	1.37
21	d	404	CLA	C1C-NC	-2.29	1.34	1.37
24	9	306	KC1	C2A-C1A	2.29	1.51	1.44
24	7	314	KC1	C2A-C1A	2.29	1.51	1.44
21	D	406	CLA	C1C-C2C	2.29	1.49	1.44
24	8	314	KC1	CAA-C2A	2.29	1.53	1.46
21	J	307	CLA	C1C-NC	-2.29	1.34	1.37
21	2	303	CLA	C4D-ND	2.29	1.40	1.37
21	3	300	CLA	C4D-ND	2.29	1.40	1.37
21	a	405	CLA	C1C-NC	-2.29	1.34	1.37
21	D	404	CLA	C1C-NC	-2.29	1.34	1.37
21	g	306	CLA	C4D-ND	2.29	1.40	1.37
23	8	311	A86	C8-C6	-2.28	1.41	1.45
21	A	401	CLA	C1C-NC	-2.28	1.34	1.37
23	W	101	A86	C8-C6	-2.28	1.41	1.45
23	2	311	A86	C24-C1	-2.28	1.41	1.45
21	a	402	CLA	C4D-ND	2.28	1.40	1.37
23	J	309	A86	C8-C6	-2.28	1.41	1.45
24	G	309	KC1	CHB-C4A	-2.28	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	306	CLA	C1C-NC	-2.28	1.34	1.37
24	6	313	KC1	C1C-C2C	2.28	1.49	1.44
24	4	308	KC1	C1D-CHD	2.28	1.47	1.41
21	B	609	CLA	C4D-ND	2.28	1.40	1.37
21	b	607	CLA	C4D-ND	2.28	1.40	1.37
21	b	604	CLA	C1C-NC	-2.28	1.34	1.37
21	B	612	CLA	C4C-C3C	2.28	1.49	1.45
21	6	306	CLA	C1C-NC	-2.28	1.34	1.37
23	5	311	A86	C24-C1	-2.28	1.41	1.45
30	H	101	DGD	O2G-C2G	-2.28	1.40	1.46
21	1	304	CLA	C4D-ND	2.28	1.40	1.37
21	9	304	CLA	C4D-ND	2.28	1.40	1.37
21	1	308	CLA	C1C-NC	-2.28	1.34	1.37
21	c	512	CLA	C1C-NC	-2.28	1.34	1.37
21	8	305	CLA	C4D-ND	2.28	1.40	1.37
24	g	315	KC1	C2A-C1A	2.28	1.51	1.44
21	b	608	CLA	C1C-NC	-2.28	1.34	1.37
21	a	403	CLA	C4D-ND	2.28	1.40	1.37
21	2	304	CLA	C4D-ND	2.28	1.40	1.37
21	b	612	CLA	C4C-C3C	2.28	1.49	1.45
21	J	306	CLA	C4D-ND	2.27	1.40	1.37
24	g	315	KC1	C1C-C2C	2.27	1.49	1.44
21	J	300	CLA	C1C-NC	-2.27	1.34	1.37
24	J	311	KC1	C4C-C3C	2.27	1.49	1.45
21	A	401	CLA	C4D-ND	2.27	1.40	1.37
21	6	302	CLA	C1C-NC	-2.27	1.34	1.37
24	7	315	KC1	C4D-CHA	2.27	1.47	1.45
24	J	313	KC1	C1C-C2C	2.27	1.49	1.44
21	C	511	CLA	C4D-ND	2.27	1.40	1.37
21	6	304	CLA	C4D-ND	2.27	1.40	1.37
21	7	308	CLA	C1C-NC	-2.27	1.34	1.37
21	B	616	CLA	C4C-C3C	2.27	1.48	1.45
21	C	503	CLA	C1C-NC	-2.27	1.34	1.37
21	b	607	CLA	C1C-NC	-2.27	1.34	1.37
24	g	315	KC1	C4D-CHA	2.27	1.47	1.45
21	1	301	CLA	C4D-ND	2.26	1.40	1.37
24	J	313	KC1	CAA-C2A	2.26	1.53	1.46
24	1	316	KC1	CAA-C2A	2.26	1.53	1.46
24	4	306	KC1	CHB-C4A	-2.26	1.34	1.39
21	B	611	CLA	C4C-C3C	2.26	1.48	1.45
21	2	303	CLA	C1C-NC	-2.26	1.34	1.37
21	b	611	CLA	C1C-NC	-2.26	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	313	KC1	C4C-C3C	2.26	1.48	1.45
24	2	316	KC1	C1C-C2C	2.26	1.48	1.44
21	g	309	CLA	C1C-NC	-2.26	1.34	1.37
24	2	315	KC1	C1D-CHD	2.26	1.47	1.41
24	G	308	KC1	C2A-C1A	2.26	1.51	1.44
24	8	315	KC1	C1D-CHD	2.26	1.47	1.41
24	4	308	KC1	C2A-C1A	2.26	1.51	1.44
24	G	308	KC1	CAA-C2A	2.26	1.53	1.46
27	d	409	LHG	O7-C5	-2.26	1.40	1.46
21	7	305	CLA	C4D-ND	2.26	1.40	1.37
21	G	304	CLA	C4D-ND	2.26	1.40	1.37
21	3	303	CLA	C1C-NC	-2.26	1.34	1.37
23	2	310	A86	C8-C6	-2.26	1.41	1.45
24	g	314	KC1	C2A-C1A	2.26	1.51	1.44
24	3	306	KC1	C1C-C2C	2.26	1.48	1.44
24	1	316	KC1	C4D-CHA	2.25	1.47	1.45
21	7	305	CLA	C1C-NC	-2.25	1.34	1.37
21	8	306	CLA	C1C-NC	-2.25	1.34	1.37
21	1	306	CLA	C4D-ND	2.25	1.40	1.37
23	2	307	A86	C8-C6	-2.25	1.41	1.45
21	A	402	CLA	C1C-NC	-2.25	1.34	1.37
30	b	601	DGD	O2G-C2G	-2.25	1.41	1.46
21	4	301	CLA	C1C-NC	-2.25	1.34	1.37
21	7	305	CLA	C1C-C2C	2.25	1.48	1.44
21	J	308	CLA	C1C-NC	-2.25	1.34	1.37
23	1	313	A86	C8-C6	-2.25	1.41	1.45
21	4	303	CLA	C1C-NC	-2.25	1.34	1.37
21	B	603	CLA	C1C-NC	-2.25	1.34	1.37
21	5	302	CLA	C4D-ND	2.24	1.40	1.37
21	6	301	CLA	C1C-NC	-2.24	1.34	1.37
24	1	315	KC1	C1C-C2C	2.24	1.48	1.44
21	J	304	CLA	C4D-ND	2.24	1.40	1.37
21	6	306	CLA	MG-NC	2.24	2.11	2.06
21	C	503	CLA	MG-NC	2.24	2.11	2.06
24	2	314	KC1	CAA-C2A	2.24	1.53	1.46
23	2	311	A86	C8-C6	-2.24	1.41	1.45
24	8	313	KC1	CAA-C2A	2.24	1.53	1.46
23	1	312	A86	C24-C1	-2.24	1.41	1.45
21	B	606	CLA	C1C-NC	-2.24	1.34	1.37
21	C	503	CLA	C1C-C2C	2.24	1.48	1.44
24	7	315	KC1	CAA-C2A	2.23	1.53	1.46
21	7	303	CLA	C4D-ND	2.23	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	314	KC1	C1D-CHD	2.23	1.47	1.41
21	D	404	CLA	C4D-ND	2.23	1.40	1.37
21	c	505	CLA	C1C-NC	-2.23	1.34	1.37
24	6	313	KC1	CAA-C2A	2.23	1.53	1.46
21	a	402	CLA	C1C-NC	-2.23	1.34	1.37
21	5	306	CLA	C4D-ND	2.23	1.40	1.37
24	8	315	KC1	C4A-C3A	2.23	1.48	1.44
21	a	403	CLA	C1C-NC	-2.23	1.34	1.37
21	2	305	CLA	C1C-NC	-2.23	1.34	1.37
21	3	304	CLA	C1C-NC	-2.23	1.34	1.37
24	J	312	KC1	C1C-C2C	2.23	1.48	1.44
21	7	308	CLA	MG-NA	2.23	2.11	2.06
23	G	305	A86	C24-C1	-2.23	1.41	1.45
21	6	300	CLA	C1C-NC	-2.22	1.34	1.37
21	c	502	CLA	C1C-NC	-2.22	1.34	1.37
21	G	303	CLA	C1C-NC	-2.22	1.34	1.37
24	3	305	KC1	C1D-CHD	2.22	1.47	1.41
23	5	311	A86	C8-C6	-2.22	1.41	1.45
24	G	308	KC1	C3B-C4B	2.22	1.50	1.46
21	C	512	CLA	C4D-ND	2.22	1.40	1.37
24	3	306	KC1	C1D-CHD	2.22	1.47	1.41
21	B	611	CLA	C4D-ND	2.22	1.40	1.37
21	3	304	CLA	C1C-C2C	2.22	1.48	1.44
21	C	506	CLA	C1C-NC	-2.22	1.34	1.37
21	1	303	CLA	C4D-ND	2.22	1.40	1.37
21	B	610	CLA	C4D-ND	2.22	1.40	1.37
21	3	300	CLA	C1C-C2C	2.22	1.48	1.44
21	D	407	CLA	C1C-NC	-2.22	1.34	1.37
21	g	302	CLA	C1C-NC	-2.22	1.34	1.37
24	G	306	KC1	CHC-C1C	2.22	1.47	1.40
24	1	316	KC1	C1C-C2C	2.22	1.48	1.44
24	5	314	KC1	C2A-C1A	2.22	1.51	1.44
21	1	302	CLA	C1C-NC	-2.22	1.34	1.37
24	5	315	KC1	C4C-C3C	2.22	1.48	1.45
21	9	300	CLA	C1C-NC	-2.22	1.34	1.37
21	5	308	CLA	C1C-NC	-2.22	1.34	1.37
23	1	313	A86	C24-C1	-2.22	1.41	1.45
24	1	316	KC1	C1D-CHD	2.22	1.47	1.41
24	G	309	KC1	C1D-CHD	2.22	1.47	1.41
24	G	309	KC1	C4D-CHA	2.21	1.47	1.45
21	B	606	CLA	C4D-ND	2.21	1.40	1.37
23	g	312	A86	C8-C6	-2.21	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	315	KC1	C1C-C2C	2.21	1.48	1.44
24	4	309	KC1	CAA-C2A	2.21	1.53	1.46
23	g	311	A86	C8-C6	-2.21	1.41	1.45
27	B	601	LHG	O7-C5	-2.21	1.41	1.46
24	4	309	KC1	CHB-C4A	-2.21	1.34	1.39
30	h	103	DGD	O2G-C2G	-2.21	1.41	1.46
32	f	101	HEM	CAA-C2A	2.21	1.55	1.52
21	b	623	CLA	C4D-ND	2.21	1.40	1.37
24	8	316	KC1	C4D-CHA	2.21	1.47	1.45
21	6	307	CLA	C1C-C2C	2.21	1.48	1.44
24	4	308	KC1	C1C-C2C	2.21	1.48	1.44
23	6	310	A86	C8-C6	-2.21	1.41	1.45
24	5	314	KC1	C1D-CHD	2.21	1.47	1.41
28	8	317	LMG	C4-C5	2.21	1.57	1.53
24	4	306	KC1	C1D-CHD	2.21	1.47	1.41
21	b	613	CLA	C4D-ND	2.20	1.40	1.37
24	G	306	KC1	C3B-C4B	2.20	1.50	1.46
23	g	312	A86	C24-C1	-2.20	1.41	1.45
21	6	304	CLA	C1C-NC	-2.20	1.34	1.37
21	a	405	CLA	MG-NA	-2.20	2.01	2.06
21	b	612	CLA	C4D-ND	2.20	1.40	1.37
24	7	315	KC1	C1C-C2C	2.20	1.48	1.44
24	2	316	KC1	C4D-CHA	2.20	1.47	1.45
22	5	310	DD6	C24-C1	-2.20	1.41	1.45
24	8	316	KC1	C3B-C4B	2.20	1.50	1.46
22	5	310	DD6	C13-C11	-2.20	1.41	1.45
21	g	307	CLA	C1C-NC	-2.20	1.34	1.37
21	9	304	CLA	C1C-C2C	2.19	1.48	1.44
21	c	511	CLA	C4D-ND	2.19	1.40	1.37
24	4	306	KC1	CHC-C1C	2.19	1.47	1.40
24	3	305	KC1	C2A-C1A	2.19	1.51	1.44
24	6	312	KC1	CAA-C2A	2.19	1.53	1.46
21	1	309	CLA	MG-NA	2.19	2.11	2.06
23	1	312	A86	C8-C6	-2.19	1.41	1.45
30	b	601	DGD	C4D-C5D	2.19	1.57	1.53
24	2	315	KC1	C3B-C4B	2.19	1.50	1.46
22	g	310	DD6	C24-C1	-2.19	1.41	1.45
24	1	315	KC1	C1D-CHD	2.19	1.47	1.41
23	2	309	A86	C8-C6	-2.19	1.41	1.45
23	2	312	A86	C24-C1	-2.19	1.41	1.45
21	G	302	CLA	C1C-NC	-2.19	1.34	1.37
21	6	307	CLA	C4D-ND	2.19	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	314	KC1	C1C-C2C	2.19	1.48	1.44
23	7	313	A86	C24-C1	-2.19	1.41	1.45
28	b	620	LMG	C4-C5	2.19	1.57	1.53
31	C	502	SQD	O2-C2	-2.19	1.37	1.43
24	6	312	KC1	C1C-C2C	2.18	1.48	1.44
32	E	101	HEM	CAA-C2A	2.18	1.55	1.52
21	1	301	CLA	C1C-NC	-2.18	1.34	1.37
27	l	101	LHG	O7-C5	-2.18	1.41	1.46
24	9	306	KC1	CAA-C2A	2.18	1.53	1.46
23	8	308	A86	C8-C6	-2.18	1.41	1.45
21	b	606	CLA	C4B-CHC	2.18	1.47	1.41
24	1	315	KC1	CAA-C2A	2.18	1.53	1.46
24	7	314	KC1	CAA-C2A	2.18	1.53	1.46
21	9	301	CLA	C1C-NC	-2.18	1.34	1.37
21	2	301	CLA	C1C-C2C	2.18	1.48	1.44
23	1	314	A86	C24-C1	-2.18	1.41	1.45
24	G	306	KC1	C4D-CHA	2.18	1.47	1.45
24	2	313	KC1	CHB-C4A	-2.18	1.34	1.39
21	8	304	CLA	C1C-NC	-2.18	1.34	1.37
21	G	301	CLA	C1C-NC	-2.18	1.34	1.37
24	G	308	KC1	C4D-CHA	2.18	1.47	1.45
23	2	312	A86	C8-C6	-2.18	1.41	1.45
28	b	625	LMG	C7-C8	2.18	1.57	1.50
21	a	405	CLA	C4D-ND	2.18	1.40	1.37
21	3	301	CLA	C1C-NC	-2.18	1.34	1.37
24	J	312	KC1	CAA-C2A	2.18	1.53	1.46
21	B	605	CLA	C4B-CHC	2.17	1.47	1.41
24	7	315	KC1	C1D-CHD	2.17	1.47	1.41
24	6	312	KC1	C1D-CHD	2.17	1.47	1.41
24	g	315	KC1	CAA-C2A	2.17	1.53	1.46
21	A	404	CLA	C4D-ND	2.17	1.40	1.37
35	D	409	PL9	C52-C5	-2.17	1.46	1.50
21	A	404	CLA	C1C-NC	-2.17	1.34	1.37
21	c	513	CLA	C1C-C2C	2.17	1.48	1.44
21	4	300	CLA	C1C-C2C	2.17	1.48	1.44
24	8	315	KC1	C1C-C2C	2.17	1.48	1.44
21	c	511	CLA	C4C-C3C	2.17	1.48	1.45
21	9	304	CLA	C1C-NC	-2.17	1.34	1.37
24	4	309	KC1	C1B-C2B	2.17	1.49	1.45
24	6	311	KC1	C1D-CHD	2.17	1.47	1.41
23	J	310	A86	C8-C6	-2.17	1.41	1.45
21	g	304	CLA	C1C-C2C	2.17	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	306	KC1	C1D-CHD	2.16	1.47	1.41
23	7	312	A86	C24-C1	-2.16	1.41	1.45
24	G	306	KC1	C1D-CHD	2.16	1.47	1.41
21	7	302	CLA	C1C-C2C	2.16	1.48	1.44
24	1	315	KC1	C4D-CHA	2.16	1.47	1.45
24	9	306	KC1	C3B-C4B	2.16	1.50	1.46
22	7	310	DD6	C25-C26	-2.16	1.36	1.43
21	9	300	CLA	C1C-C2C	2.16	1.48	1.44
24	5	314	KC1	C3B-C4B	2.16	1.50	1.46
24	J	313	KC1	C1D-CHD	2.16	1.47	1.41
21	g	305	CLA	C1C-C2C	2.16	1.48	1.44
21	G	300	CLA	C1C-C2C	2.16	1.48	1.44
24	4	308	KC1	C4D-CHA	2.16	1.47	1.45
21	D	406	CLA	C4D-ND	2.16	1.40	1.37
24	8	314	KC1	C1C-C2C	2.16	1.48	1.44
24	3	305	KC1	CAA-C2A	2.16	1.53	1.46
21	d	404	CLA	C4D-ND	2.16	1.40	1.37
21	6	305	CLA	C1C-C2C	2.16	1.48	1.44
24	4	306	KC1	C4D-CHA	2.15	1.47	1.45
24	4	308	KC1	CAA-C2A	2.15	1.53	1.46
24	9	305	KC1	C1C-C2C	2.15	1.48	1.44
24	G	308	KC1	C1D-CHD	2.15	1.47	1.41
24	3	306	KC1	CAA-C2A	2.15	1.53	1.46
21	d	406	CLA	C1C-NC	-2.15	1.34	1.37
31	B	626	SQD	O2-C2	-2.15	1.37	1.43
21	7	300	CLA	C1C-NC	-2.15	1.34	1.37
26	d	403	PHO	CMC-C2C	-2.15	1.46	1.51
24	4	308	KC1	C3B-C4B	2.15	1.49	1.46
21	8	306	CLA	C1C-C2C	2.15	1.48	1.44
31	b	602	SQD	O2-C2	-2.15	1.37	1.43
21	3	302	CLA	C1C-C2C	2.15	1.48	1.44
21	6	303	CLA	C1C-NC	-2.15	1.34	1.37
31	X	401	SQD	O2-C2	-2.14	1.37	1.43
21	1	306	CLA	C1C-C2C	2.14	1.48	1.44
28	2	318	LMG	C4-C5	2.14	1.57	1.53
23	6	309	A86	C25-C24	2.14	1.40	1.34
23	8	312	A86	C8-C6	-2.14	1.41	1.45
21	5	309	CLA	C3D-C4D	-2.14	1.39	1.44
23	6	309	A86	C24-C1	-2.14	1.41	1.45
21	J	307	CLA	C1C-C2C	2.14	1.48	1.44
21	4	303	CLA	C1C-C2C	2.14	1.48	1.44
22	5	310	DD6	C8-C6	-2.14	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	311	KC1	CAA-C2A	2.14	1.53	1.46
24	2	316	KC1	CAA-C2A	2.14	1.53	1.46
21	G	302	CLA	C1C-C2C	2.14	1.48	1.44
21	c	511	CLA	C1C-NC	-2.13	1.34	1.37
21	C	512	CLA	C4C-C3C	2.13	1.48	1.45
26	D	401	PHO	CMC-C2C	-2.13	1.46	1.51
24	5	315	KC1	C1B-C2B	2.13	1.49	1.45
21	5	305	CLA	C1C-NC	-2.13	1.34	1.37
24	4	306	KC1	C1B-C2B	2.13	1.49	1.45
21	2	302	CLA	C3D-C4D	-2.13	1.39	1.44
21	g	307	CLA	C1C-C2C	2.13	1.48	1.44
21	J	301	CLA	C4D-ND	2.13	1.40	1.37
21	J	305	CLA	C1C-C2C	2.13	1.48	1.44
21	C	514	CLA	C1C-C2C	2.13	1.48	1.44
21	7	302	CLA	C4D-ND	2.13	1.40	1.37
24	J	311	KC1	C1D-CHD	2.13	1.46	1.41
21	J	304	CLA	C1C-NC	-2.13	1.34	1.37
21	5	309	CLA	C4D-ND	2.13	1.40	1.37
35	D	409	PL9	C53-C6	-2.13	1.46	1.50
21	B	611	CLA	MG-ND	2.12	2.10	2.05
21	J	301	CLA	C1C-NC	-2.12	1.34	1.37
21	4	301	CLA	C1C-C2C	2.12	1.48	1.44
35	d	408	PL9	C52-C5	-2.12	1.46	1.50
24	G	309	KC1	CAA-C2A	2.12	1.53	1.46
21	d	405	CLA	C4D-ND	2.12	1.40	1.37
24	g	315	KC1	C1D-CHD	2.12	1.46	1.41
32	f	101	HEM	CMB-C2B	2.12	1.55	1.50
24	2	314	KC1	C1D-CHD	2.12	1.46	1.41
24	g	315	KC1	C3B-C4B	2.12	1.49	1.46
21	8	303	CLA	C3D-C4D	-2.12	1.39	1.44
26	a	404	PHO	CMD-C2D	-2.12	1.46	1.51
29	g	316	LMU	O5B-C5B	2.12	1.49	1.44
21	a	405	CLA	C1C-C2C	2.12	1.48	1.44
30	C	517	DGD	O2G-C2G	-2.12	1.41	1.46
24	8	316	KC1	CAA-C2A	2.12	1.53	1.46
24	J	312	KC1	C1D-CHD	2.12	1.46	1.41
35	d	408	PL9	C53-C6	-2.12	1.46	1.50
31	B	625	SQD	O2-C2	-2.12	1.38	1.43
24	J	312	KC1	C4D-CHA	2.11	1.47	1.45
21	4	302	CLA	C1C-C2C	2.11	1.48	1.44
24	G	307	KC1	C2A-C1A	2.11	1.51	1.44
21	G	301	CLA	C1C-C2C	2.11	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	g	305	CLA	MG-NC	-2.11	2.01	2.06
26	d	403	PHO	CMD-C2D	-2.11	1.46	1.51
30	B	624	DGD	C4D-C5D	2.11	1.57	1.53
24	2	313	KC1	C1C-C2C	2.11	1.48	1.44
24	8	313	KC1	C3B-C4B	2.11	1.49	1.46
26	a	404	PHO	CMC-C2C	-2.11	1.46	1.51
21	5	304	CLA	C1C-C2C	2.11	1.48	1.44
24	2	316	KC1	C3B-C4B	2.11	1.49	1.46
24	7	314	KC1	C1D-CHD	2.11	1.46	1.41
21	8	302	CLA	C1C-C2C	2.11	1.48	1.44
23	6	309	A86	C8-C6	-2.11	1.41	1.45
21	7	303	CLA	C1C-NC	-2.11	1.34	1.37
24	J	311	KC1	C1C-C2C	2.11	1.48	1.44
24	3	305	KC1	C4D-CHA	2.11	1.47	1.45
24	G	309	KC1	C1C-C2C	2.11	1.48	1.44
26	D	401	PHO	CMD-C2D	-2.10	1.46	1.51
24	6	311	KC1	C4D-CHA	2.10	1.47	1.45
24	6	312	KC1	C4D-CHA	2.10	1.47	1.45
24	g	314	KC1	CAA-C2A	2.10	1.53	1.46
23	7	311	A86	C8-C6	-2.10	1.41	1.45
21	6	303	CLA	C1C-C2C	2.10	1.48	1.44
24	2	313	KC1	C1B-C2B	2.10	1.49	1.45
21	6	302	CLA	C1C-C2C	2.10	1.48	1.44
21	6	308	CLA	MG-ND	-2.10	2.01	2.05
21	6	300	CLA	MG-NC	-2.10	2.01	2.06
21	A	404	CLA	C1C-C2C	2.10	1.48	1.44
23	5	312	A86	C24-C1	-2.10	1.41	1.45
21	J	302	CLA	C1C-NC	-2.10	1.34	1.37
26	A	403	PHO	CMC-C2C	-2.10	1.46	1.51
31	b	602	SQD	O4-C4	-2.10	1.38	1.43
31	b	602	SQD	O3-C3	-2.10	1.38	1.43
24	6	311	KC1	C2A-C1A	2.10	1.51	1.44
24	J	311	KC1	C2A-C1A	2.09	1.51	1.44
21	g	309	CLA	C1C-C2C	2.09	1.48	1.44
24	4	307	KC1	C1C-C2C	2.09	1.48	1.44
21	J	300	CLA	C1C-C2C	2.09	1.48	1.44
21	J	303	CLA	C1C-C2C	2.09	1.48	1.44
23	5	312	A86	C8-C6	-2.09	1.41	1.45
21	b	613	CLA	C1C-C2C	2.09	1.48	1.44
22	1	311	DD6	C25-C26	-2.09	1.37	1.43
24	3	306	KC1	C3B-C4B	2.09	1.49	1.46
21	J	303	CLA	C1C-NC	-2.09	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	306	KC1	C4D-CHA	2.09	1.47	1.45
24	G	309	KC1	C1B-C2B	2.09	1.49	1.45
21	J	308	CLA	C1C-C2C	2.09	1.48	1.44
24	8	313	KC1	C1D-CHD	2.09	1.46	1.41
24	6	311	KC1	C1C-C2C	2.09	1.48	1.44
21	J	301	CLA	C1C-C2C	2.08	1.48	1.44
21	9	303	CLA	C4D-ND	2.08	1.40	1.37
21	1	301	CLA	C1C-C2C	2.08	1.48	1.44
23	8	310	A86	C8-C6	-2.08	1.41	1.45
26	A	403	PHO	CMD-C2D	-2.08	1.46	1.51
21	1	304	CLA	C1C-NC	-2.08	1.34	1.37
24	J	311	KC1	C4D-CHA	2.08	1.47	1.45
24	2	315	KC1	C1C-C2C	2.08	1.48	1.44
24	8	316	KC1	C1D-CHD	2.08	1.46	1.41
21	7	306	CLA	C1C-C2C	2.08	1.48	1.44
21	9	302	CLA	C1C-C2C	2.08	1.48	1.44
21	6	308	CLA	C1C-C2C	2.08	1.48	1.44
24	6	313	KC1	C1D-CHD	2.08	1.46	1.41
21	1	308	CLA	C1C-C2C	2.08	1.48	1.44
21	d	405	CLA	C4C-C3C	2.08	1.48	1.44
21	g	304	CLA	C4D-ND	2.08	1.40	1.37
21	9	301	CLA	C1C-C2C	2.08	1.48	1.44
21	7	300	CLA	C1C-C2C	2.08	1.48	1.44
21	c	504	CLA	C1C-C2C	2.08	1.48	1.44
21	7	307	CLA	C1C-C2C	2.07	1.48	1.44
21	c	511	CLA	C1C-C2C	2.07	1.48	1.44
24	6	313	KC1	C3B-C4B	2.07	1.49	1.46
21	C	512	CLA	C1C-NC	-2.07	1.34	1.37
24	9	306	KC1	C4D-CHA	2.07	1.47	1.45
21	J	308	CLA	MG-ND	2.07	2.09	2.05
21	1	307	CLA	C1C-C2C	2.07	1.48	1.44
21	3	303	CLA	C1C-C2C	2.07	1.48	1.44
31	B	626	SQD	O4-C4	-2.07	1.38	1.43
21	1	304	CLA	C1C-C2C	2.07	1.48	1.44
21	J	302	CLA	C1C-C2C	2.07	1.48	1.44
23	g	311	A86	C24-C1	-2.06	1.41	1.45
24	1	315	KC1	C3B-C4B	2.06	1.49	1.46
21	B	614	CLA	C1C-C2C	2.06	1.48	1.44
24	5	314	KC1	CAA-C2A	2.06	1.52	1.46
21	6	300	CLA	C1C-C2C	2.06	1.48	1.44
21	5	308	CLA	C1C-C2C	2.06	1.48	1.44
21	C	505	CLA	C1C-C2C	2.06	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	624	LMG	O7-C8	-2.06	1.41	1.46
24	9	305	KC1	C1D-CHD	2.06	1.46	1.41
24	5	313	KC1	C4D-CHA	2.06	1.47	1.45
31	C	502	SQD	O4-C4	-2.06	1.38	1.43
30	c	516	DGD	O2G-C2G	-2.06	1.41	1.46
30	C	517	DGD	O5D-C6D	-2.06	1.40	1.43
24	4	307	KC1	C1D-CHD	2.06	1.46	1.41
21	B	612	CLA	C1C-C2C	2.06	1.48	1.44
21	g	302	CLA	C1C-C2C	2.06	1.48	1.44
21	1	302	CLA	C1C-C2C	2.06	1.48	1.44
24	g	314	KC1	C1D-CHD	2.05	1.46	1.41
31	B	625	SQD	O4-C4	-2.05	1.38	1.43
21	b	609	CLA	C1C-C2C	2.05	1.48	1.44
21	c	502	CLA	C1C-C2C	2.05	1.48	1.44
28	B	620	LMG	C4-C5	2.05	1.57	1.53
31	B	625	SQD	O3-C3	-2.05	1.38	1.43
31	X	401	SQD	O4-C4	-2.05	1.38	1.43
24	G	307	KC1	C1D-CHD	2.05	1.46	1.41
21	G	303	CLA	C1C-C2C	2.05	1.48	1.44
24	2	313	KC1	CAA-C2A	2.05	1.52	1.46
31	B	626	SQD	O3-C3	-2.05	1.38	1.43
21	5	309	CLA	C1C-NC	-2.05	1.34	1.37
28	b	621	LMG	C4-C5	2.05	1.57	1.53
21	b	608	CLA	C1C-C2C	2.05	1.48	1.44
24	g	313	KC1	C1C-C2C	2.05	1.48	1.44
21	1	303	CLA	C1C-C2C	2.04	1.48	1.44
28	M	102	LMG	O7-C8	-2.04	1.41	1.46
24	2	313	KC1	C1D-CHD	2.04	1.46	1.41
28	B	619	LMG	C4-C5	2.04	1.57	1.53
24	G	307	KC1	CAA-C2A	2.04	1.52	1.46
21	C	512	CLA	C1C-C2C	2.04	1.48	1.44
24	4	307	KC1	C1B-C2B	2.04	1.49	1.45
21	c	512	CLA	C1C-C2C	2.04	1.48	1.44
21	c	514	CLA	C1C-C2C	2.04	1.48	1.44
27	A	406	LHG	O7-C5	-2.04	1.41	1.46
24	2	316	KC1	C1D-CHD	2.04	1.46	1.41
23	7	312	A86	C8-C6	-2.04	1.41	1.45
24	9	305	KC1	C2A-C1A	2.04	1.50	1.44
24	7	314	KC1	C3B-C4B	2.03	1.49	1.46
31	C	502	SQD	O3-C3	-2.03	1.38	1.43
21	g	303	CLA	C1C-C2C	2.03	1.48	1.44
24	G	307	KC1	C1C-C2C	2.03	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	313	KC1	C1D-CHD	2.03	1.46	1.41
24	3	305	KC1	C3B-C4B	2.03	1.49	1.46
21	B	603	CLA	C1C-C2C	2.03	1.48	1.44
24	J	311	KC1	CAA-C2A	2.03	1.52	1.46
21	B	607	CLA	C1C-C2C	2.03	1.48	1.44
24	5	315	KC1	C1D-CHD	2.03	1.46	1.41
28	B	627	LMG	C4-C5	2.03	1.57	1.53
21	2	305	CLA	C1C-C2C	2.03	1.48	1.44
21	8	305	CLA	C1C-C2C	2.03	1.48	1.44
31	X	401	SQD	O3-C3	-2.03	1.38	1.43
21	7	303	CLA	C1C-C2C	2.03	1.48	1.44
21	J	306	CLA	C1C-C2C	2.03	1.48	1.44
21	5	303	CLA	C1C-C2C	2.03	1.48	1.44
21	b	607	CLA	C1C-C2C	2.03	1.48	1.44
22	5	310	DD6	C25-C26	-2.03	1.37	1.43
21	J	301	CLA	C4C-C3C	2.03	1.48	1.45
21	7	308	CLA	C1C-C2C	2.03	1.48	1.44
28	2	318	LMG	O7-C8	-2.03	1.41	1.46
21	2	302	CLA	C1C-C2C	2.03	1.48	1.44
21	g	308	CLA	C1C-C2C	2.03	1.48	1.44
24	2	314	KC1	C4D-CHA	2.02	1.47	1.45
21	B	608	CLA	C1C-C2C	2.02	1.48	1.44
26	A	403	PHO	CMB-C2B	-2.02	1.46	1.51
23	8	312	A86	C24-C1	-2.02	1.41	1.45
24	5	315	KC1	CAA-C2A	2.02	1.52	1.46
21	6	301	CLA	C1C-C2C	2.02	1.48	1.44
21	2	304	CLA	C1C-C2C	2.02	1.48	1.44
21	3	301	CLA	C1C-C2C	2.02	1.48	1.44
21	C	515	CLA	C1C-C2C	2.01	1.48	1.44
21	b	603	CLA	C1C-C2C	2.01	1.48	1.44
21	7	301	CLA	C1C-C2C	2.01	1.48	1.44
21	B	602	CLA	C1C-C2C	2.01	1.48	1.44
21	6	306	CLA	C1C-C2C	2.01	1.48	1.44
21	b	615	CLA	C1C-C2C	2.01	1.48	1.44
21	G	304	CLA	C1C-C2C	2.01	1.48	1.44
21	1	309	CLA	C1C-C2C	2.01	1.48	1.44
26	a	404	PHO	CMB-C2B	-2.01	1.46	1.51
21	b	604	CLA	C1C-C2C	2.01	1.48	1.44
24	4	307	KC1	CAA-C2A	2.00	1.52	1.46
28	f	102	LMG	C4-C5	2.00	1.57	1.53
25	b	619	BCR	C33-C5	-2.00	1.47	1.50
21	B	606	CLA	C1C-C2C	2.00	1.48	1.44

All (5336) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	302	CLA	C5-C3-C4	-15.68	79.97	114.60
21	2	302	CLA	C4-C3-C2	-14.73	80.08	122.65
21	2	302	CLA	C5-C3-C2	12.93	160.02	122.65
24	4	308	KC1	CMA-C3A-C4A	-12.33	106.26	125.04
24	G	307	KC1	CMA-C3A-C4A	-11.94	106.86	125.04
24	8	315	KC1	C2A-C3A-C4A	-11.63	97.86	106.49
24	2	315	KC1	C2A-C3A-C4A	-11.42	98.01	106.49
24	8	313	KC1	CMA-C3A-C4A	-11.42	107.65	125.04
24	G	308	KC1	CMA-C3A-C4A	-11.30	107.83	125.04
24	g	314	KC1	CMA-C3A-C4A	-11.20	107.98	125.04
24	9	305	KC1	CMA-C3A-C4A	-11.17	108.03	125.04
24	6	313	KC1	CMA-C3A-C4A	-11.09	108.15	125.04
24	1	316	KC1	CMA-C3A-C4A	-11.08	108.17	125.04
24	4	307	KC1	CMA-C3A-C4A	-11.08	108.17	125.04
24	7	315	KC1	CMA-C3A-C4A	-11.07	108.18	125.04
24	J	311	KC1	CMA-C3A-C4A	-11.01	108.27	125.04
24	5	313	KC1	CMA-C3A-C4A	-11.00	108.29	125.04
24	6	311	KC1	CMA-C3A-C4A	-10.95	108.36	125.04
24	g	313	KC1	CMA-C3A-C4A	-10.94	108.37	125.04
24	8	314	KC1	CMA-C3A-C4A	-10.82	108.56	125.04
24	J	313	KC1	CMA-C3A-C4A	-10.71	108.73	125.04
24	5	314	KC1	CMA-C3A-C4A	-10.60	108.90	125.04
24	1	315	KC1	CMA-C3A-C4A	-10.58	108.92	125.04
24	5	315	KC1	CMA-C3A-C4A	-10.58	108.92	125.04
24	2	314	KC1	CMA-C3A-C4A	-10.57	108.94	125.04
24	4	306	KC1	CAA-C2A-C3A	-10.56	104.84	126.75
24	G	306	KC1	CAA-C2A-C3A	-10.54	104.89	126.75
24	6	312	KC1	CMA-C3A-C4A	-10.54	108.99	125.04
24	7	314	KC1	CMA-C3A-C4A	-10.49	109.07	125.04
24	J	312	KC1	CMA-C3A-C4A	-10.48	109.08	125.04
24	3	305	KC1	CMA-C3A-C4A	-10.45	109.12	125.04
21	4	300	CLA	C4A-NA-C1A	10.43	111.39	106.71
24	9	306	KC1	CMA-C3A-C4A	-10.35	109.28	125.04
24	3	306	KC1	CMA-C3A-C4A	-10.30	109.35	125.04
24	2	313	KC1	CMA-C3A-C4A	-10.22	109.48	125.04
21	B	605	CLA	C4A-NA-C1A	10.17	111.28	106.71
24	G	308	KC1	C2A-C3A-C4A	-10.16	98.95	106.49
24	5	313	KC1	C2A-C3A-C4A	-10.10	98.99	106.49
21	b	606	CLA	C4A-NA-C1A	10.06	111.23	106.71
21	G	300	CLA	C4A-NA-C1A	10.06	111.23	106.71
24	5	314	KC1	C2A-C3A-C4A	-10.01	99.06	106.49
24	8	313	KC1	C2A-C3A-C4A	-9.99	99.08	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	307	KC1	C2A-C3A-C4A	-9.93	99.12	106.49
24	6	311	KC1	C2A-C3A-C4A	-9.90	99.14	106.49
24	8	316	KC1	C2A-C3A-C4A	-9.84	99.19	106.49
21	C	507	CLA	C4A-NA-C1A	9.84	111.13	106.71
21	6	308	CLA	C4A-NA-C1A	9.83	111.13	106.71
24	g	313	KC1	C2A-C3A-C4A	-9.83	99.19	106.49
24	4	307	KC1	C2A-C3A-C4A	-9.83	99.20	106.49
21	J	308	CLA	C4A-NA-C1A	9.82	111.12	106.71
21	C	505	CLA	C4A-NA-C1A	9.82	111.12	106.71
24	g	315	KC1	CMA-C3A-C4A	-9.81	110.09	125.04
21	J	303	CLA	C4A-NA-C1A	9.81	111.12	106.71
24	8	315	KC1	CMA-C3A-C4A	-9.78	110.14	125.04
24	9	305	KC1	C2A-C3A-C4A	-9.77	99.24	106.49
21	c	508	CLA	C4A-NA-C1A	9.76	111.10	106.71
24	3	305	KC1	C2A-C3A-C4A	-9.73	99.27	106.49
24	4	309	KC1	CMA-C3A-C4A	-9.72	110.23	125.04
21	c	506	CLA	C4A-NA-C1A	9.72	111.08	106.71
24	g	314	KC1	C2A-C3A-C4A	-9.70	99.29	106.49
24	3	306	KC1	C2A-C3A-C4A	-9.69	99.30	106.49
24	6	312	KC1	C2A-C3A-C4A	-9.65	99.32	106.49
24	9	306	KC1	C2A-C3A-C4A	-9.65	99.33	106.49
24	2	316	KC1	C2A-C3A-C4A	-9.62	99.35	106.49
24	J	311	KC1	C2A-C3A-C4A	-9.59	99.37	106.49
21	c	512	CLA	C4A-NA-C1A	9.58	111.02	106.71
24	1	315	KC1	C2A-C3A-C4A	-9.57	99.38	106.49
21	9	301	CLA	C4A-NA-C1A	9.57	111.01	106.71
24	g	315	KC1	C2A-C3A-C4A	-9.54	99.41	106.49
24	J	312	KC1	C2A-C3A-C4A	-9.54	99.41	106.49
24	2	315	KC1	CMA-C3A-C4A	-9.54	110.52	125.04
24	1	316	KC1	C2A-C3A-C4A	-9.53	99.41	106.49
24	6	313	KC1	C2A-C3A-C4A	-9.52	99.42	106.49
24	7	315	KC1	C2A-C3A-C4A	-9.51	99.43	106.49
24	G	306	KC1	CMA-C3A-C4A	-9.48	110.60	125.04
24	5	315	KC1	C2A-C3A-C4A	-9.45	99.47	106.49
24	G	309	KC1	CMA-C3A-C4A	-9.45	110.64	125.04
24	G	309	KC1	C2A-C3A-C4A	-9.44	99.48	106.49
24	J	313	KC1	C2A-C3A-C4A	-9.44	99.48	106.49
21	1	303	CLA	C4A-NA-C1A	9.43	110.95	106.71
21	C	513	CLA	C4A-NA-C1A	9.37	110.92	106.71
21	5	308	CLA	C4A-NA-C1A	9.35	110.91	106.71
24	7	314	KC1	C2A-C3A-C4A	-9.34	99.55	106.49
24	8	314	KC1	C2A-C3A-C4A	-9.34	99.56	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c	504	CLA	C4A-NA-C1A	9.34	110.91	106.71
24	2	314	KC1	C2A-C3A-C4A	-9.33	99.56	106.49
21	C	509	CLA	C4A-NA-C1A	9.31	110.89	106.71
21	8	307	CLA	C4A-NA-C1A	9.28	110.88	106.71
21	3	304	CLA	C4A-NA-C1A	9.27	110.87	106.71
24	4	309	KC1	C2A-C3A-C4A	-9.24	99.63	106.49
21	B	602	CLA	C4A-NA-C1A	9.19	110.84	106.71
21	7	301	CLA	C4A-NA-C1A	9.18	110.83	106.71
21	c	503	CLA	C4A-NA-C1A	9.18	110.83	106.71
21	C	504	CLA	C4A-NA-C1A	9.17	110.83	106.71
24	2	313	KC1	C2A-C3A-C4A	-9.16	99.69	106.49
21	B	615	CLA	C4A-NA-C1A	9.16	110.82	106.71
21	7	305	CLA	C4A-NA-C1A	9.16	110.82	106.71
21	b	608	CLA	C4A-NA-C1A	9.14	110.82	106.71
21	2	306	CLA	C4A-NA-C1A	9.12	110.81	106.71
21	5	304	CLA	C4A-NA-C1A	9.11	110.80	106.71
21	1	309	CLA	C4A-NA-C1A	9.08	110.79	106.71
21	g	303	CLA	C4A-NA-C1A	9.07	110.78	106.71
21	7	307	CLA	C4A-NA-C1A	9.06	110.78	106.71
24	G	306	KC1	CAA-C2A-C1A	-9.05	111.57	128.86
21	B	607	CLA	C4A-NA-C1A	9.04	110.77	106.71
21	b	616	CLA	C4A-NA-C1A	9.02	110.76	106.71
21	2	305	CLA	C4A-NA-C1A	8.97	110.74	106.71
21	9	302	CLA	C4A-NA-C1A	8.96	110.73	106.71
21	5	303	CLA	C4A-NA-C1A	8.94	110.73	106.71
24	4	308	KC1	C2A-C3A-C4A	-8.84	99.93	106.49
21	B	621	CLA	C4A-NA-C1A	8.81	110.67	106.71
21	9	303	CLA	C4A-NA-C1A	8.80	110.66	106.71
21	7	304	CLA	C4A-NA-C1A	8.78	110.66	106.71
24	4	306	KC1	CMA-C3A-C4A	-8.76	111.70	125.04
21	C	506	CLA	C4A-NA-C1A	8.74	110.64	106.71
21	3	301	CLA	C4A-NA-C1A	8.74	110.63	106.71
21	J	305	CLA	C4A-NA-C1A	8.72	110.62	106.71
21	b	623	CLA	C4A-NA-C1A	8.70	110.62	106.71
24	4	308	KC1	CMA-C3A-C2A	-8.70	107.01	128.30
21	7	308	CLA	C4A-NA-C1A	8.69	110.61	106.71
24	4	306	KC1	CAA-C2A-C1A	-8.67	112.29	128.86
21	6	303	CLA	C4A-NA-C1A	8.66	110.60	106.71
21	c	505	CLA	C4A-NA-C1A	8.64	110.59	106.71
21	1	302	CLA	C4A-NA-C1A	8.64	110.59	106.71
21	c	502	CLA	C4A-NA-C1A	8.63	110.59	106.71
21	6	302	CLA	C4A-NA-C1A	8.59	110.57	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	306	CLA	C4A-NA-C1A	8.58	110.56	106.71
21	3	303	CLA	C4A-NA-C1A	8.56	110.56	106.71
21	6	305	CLA	C4A-NA-C1A	8.55	110.55	106.71
24	G	307	KC1	C2B-C1B-NB	8.54	116.39	110.10
21	b	611	CLA	C4A-NA-C1A	8.52	110.54	106.71
21	C	510	CLA	C4A-NA-C1A	8.51	110.53	106.71
21	b	603	CLA	C4A-NA-C1A	8.51	110.53	106.71
24	8	315	KC1	C2B-C1B-NB	8.50	116.37	110.10
21	b	610	CLA	C4A-NA-C1A	8.49	110.52	106.71
21	D	407	CLA	C4A-NA-C1A	8.49	110.52	106.71
21	d	406	CLA	C4A-NA-C1A	8.47	110.52	106.71
21	9	304	CLA	C4A-NA-C1A	8.46	110.51	106.71
21	1	310	CLA	C4A-NA-C1A	8.44	110.50	106.71
24	G	306	KC1	C4A-C3A-C2A	-8.44	99.33	107.07
21	B	609	CLA	C4A-NA-C1A	8.42	110.49	106.71
21	c	509	CLA	C4A-NA-C1A	8.41	110.49	106.71
21	B	611	CLA	C4A-NA-C1A	8.39	110.48	106.71
21	G	301	CLA	C4A-NA-C1A	8.39	110.48	106.71
21	1	308	CLA	C4A-NA-C1A	8.35	110.46	106.71
21	3	300	CLA	C4A-NA-C1A	8.31	110.44	106.71
21	g	308	CLA	C4A-NA-C1A	8.28	110.43	106.71
21	7	302	CLA	C4A-NA-C1A	8.27	110.42	106.71
21	g	306	CLA	C4A-NA-C1A	8.26	110.42	106.71
24	4	306	KC1	C2A-C1A-NA	8.25	116.61	110.03
21	C	515	CLA	C4A-NA-C1A	8.25	110.41	106.71
21	5	309	CLA	C4D-CHA-C1A	-8.24	111.22	121.25
21	C	503	CLA	C4A-NA-C1A	8.24	110.41	106.71
21	2	304	CLA	C4A-NA-C1A	8.23	110.41	106.71
21	5	305	CLA	C4A-NA-C1A	8.21	110.40	106.71
21	8	305	CLA	C4A-NA-C1A	8.20	110.39	106.71
21	B	606	CLA	C4A-NA-C1A	8.20	110.39	106.71
21	A	402	CLA	C4A-NA-C1A	8.20	110.39	106.71
21	J	302	CLA	C4A-NA-C1A	8.19	110.39	106.71
21	4	301	CLA	C4A-NA-C1A	8.13	110.36	106.71
24	8	313	KC1	C2B-C1B-NB	8.13	116.09	110.10
24	4	306	KC1	C4A-C3A-C2A	-8.12	99.62	107.07
21	B	613	CLA	C4A-NA-C1A	8.11	110.35	106.71
21	4	303	CLA	C4A-NA-C1A	8.10	110.35	106.71
21	7	300	CLA	C4A-NA-C1A	8.09	110.34	106.71
21	b	607	CLA	C4A-NA-C1A	8.09	110.34	106.71
21	8	306	CLA	C4A-NA-C1A	8.09	110.34	106.71
21	a	403	CLA	C4A-NA-C1A	8.08	110.34	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	302	CLA	C4A-NA-C1A	8.07	110.33	106.71
21	J	300	CLA	C4A-NA-C1A	8.06	110.33	106.71
21	7	309	CLA	C4A-NA-C1A	8.05	110.33	106.71
24	2	315	KC1	C2B-C1B-NB	8.05	116.03	110.10
21	8	303	CLA	C4A-NA-C1A	8.02	110.31	106.71
21	c	514	CLA	C4A-NA-C1A	8.00	110.30	106.71
21	b	612	CLA	C4A-NA-C1A	8.00	110.30	106.71
21	A	404	CLA	C4A-NA-C1A	8.00	110.30	106.71
21	2	303	CLA	C4A-NA-C1A	7.98	110.29	106.71
24	G	308	KC1	C2B-C1B-NB	7.96	115.97	110.10
21	A	401	CLA	C4A-NA-C1A	7.95	110.28	106.71
21	2	302	CLA	C4A-NA-C1A	7.95	110.28	106.71
24	G	306	KC1	C2A-C1A-NA	7.94	116.37	110.03
21	b	614	CLA	C4A-NA-C1A	7.94	110.28	106.71
21	4	302	CLA	C4A-NA-C1A	7.91	110.26	106.71
21	7	306	CLA	C4A-NA-C1A	7.91	110.26	106.71
24	3	306	KC1	C2B-C1B-NB	7.90	115.93	110.10
21	a	402	CLA	C4A-NA-C1A	7.87	110.25	106.71
24	5	314	KC1	C2B-C1B-NB	7.86	115.90	110.10
21	C	508	CLA	C4A-NA-C1A	7.86	110.24	106.71
21	G	303	CLA	C4A-NA-C1A	7.86	110.24	106.71
24	g	314	KC1	C2B-C1B-NB	7.85	115.89	110.10
21	C	514	CLA	C4A-NA-C1A	7.81	110.22	106.71
21	J	306	CLA	C4A-NA-C1A	7.80	110.21	106.71
21	5	309	CLA	C4A-NA-C1A	7.78	110.20	106.71
21	G	304	CLA	C4A-NA-C1A	7.75	110.19	106.71
24	8	315	KC1	C3A-C4A-NA	7.74	119.02	110.57
21	8	304	CLA	C4A-NA-C1A	7.72	110.18	106.71
21	B	610	CLA	C4A-NA-C1A	7.72	110.18	106.71
21	g	302	CLA	C4A-NA-C1A	7.72	110.18	106.71
21	g	307	CLA	C4A-NA-C1A	7.70	110.17	106.71
24	8	314	KC1	C2B-C1B-NB	7.70	115.78	110.10
24	g	315	KC1	C2B-C1B-NB	7.70	115.78	110.10
21	1	307	CLA	C4A-NA-C1A	7.68	110.16	106.71
21	B	604	CLA	C4A-NA-C1A	7.68	110.16	106.71
24	8	315	KC1	CHB-C4A-C3A	-7.65	113.02	124.98
24	6	313	KC1	C2B-C1B-NB	7.64	115.74	110.10
24	4	306	KC1	CMA-C3A-C2A	-7.63	110.91	126.75
21	a	405	CLA	C4A-NA-C1A	7.63	110.14	106.71
24	8	316	KC1	C2B-C1B-NB	7.63	115.72	110.10
21	6	306	CLA	C4A-NA-C1A	7.63	110.14	106.71
21	G	302	CLA	C4A-NA-C1A	7.62	110.13	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	301	CLA	C4A-NA-C1A	7.61	110.13	106.71
21	b	613	CLA	C4A-NA-C1A	7.61	110.13	106.71
24	2	314	KC1	C2B-C1B-NB	7.61	115.71	110.10
21	c	510	CLA	C4A-NA-C1A	7.60	110.12	106.71
21	b	605	CLA	C4A-NA-C1A	7.58	110.11	106.71
21	b	609	CLA	C4A-NA-C1A	7.57	110.11	106.71
24	2	315	KC1	CHB-C4A-C3A	-7.57	113.16	124.98
24	5	315	KC1	C2B-C1B-NB	7.54	115.66	110.10
21	g	305	CLA	C4A-NA-C1A	7.53	110.09	106.71
21	9	300	CLA	C4A-NA-C1A	7.52	110.09	106.71
21	6	300	CLA	C4A-NA-C1A	7.51	110.08	106.71
21	B	612	CLA	C4A-NA-C1A	7.51	110.08	106.71
21	5	302	CLA	C4A-NA-C1A	7.50	110.08	106.71
24	5	313	KC1	C2B-C1B-NB	7.49	115.63	110.10
24	3	305	KC1	C2B-C1B-NB	7.49	115.62	110.10
21	c	507	CLA	C4A-NA-C1A	7.47	110.07	106.71
24	1	316	KC1	CMA-C3A-C2A	-7.46	110.03	128.30
21	B	608	CLA	C4A-NA-C1A	7.46	110.06	106.71
21	B	616	CLA	C4A-NA-C1A	7.46	110.06	106.71
24	J	313	KC1	C2B-C1B-NB	7.46	115.60	110.10
24	G	306	KC1	CMA-C3A-C2A	-7.46	111.28	126.75
24	g	314	KC1	CMA-C3A-C2A	-7.46	110.04	128.30
24	2	315	KC1	C3A-C4A-NA	7.45	118.71	110.57
24	2	316	KC1	C2B-C1B-NB	7.45	115.59	110.10
24	7	315	KC1	CMA-C3A-C2A	-7.44	110.08	128.30
24	6	311	KC1	C2B-C1B-NB	7.43	115.58	110.10
24	6	312	KC1	C2B-C1B-NB	7.41	115.56	110.10
24	J	312	KC1	C2B-C1B-NB	7.40	115.55	110.10
24	2	316	KC1	CMA-C3A-C4A	-7.39	113.78	125.04
24	J	311	KC1	C2B-C1B-NB	7.39	115.55	110.10
24	1	316	KC1	C2B-C1B-NB	7.36	115.53	110.10
24	2	314	KC1	C1A-C2A-C3A	-7.35	101.28	107.11
24	g	313	KC1	CMA-C3A-C2A	-7.35	110.31	128.30
24	9	305	KC1	CMA-C3A-C2A	-7.35	110.31	128.30
24	6	311	KC1	CMA-C3A-C2A	-7.33	110.35	128.30
24	J	311	KC1	CMA-C3A-C2A	-7.33	110.35	128.30
21	c	513	CLA	C4A-NA-C1A	7.32	110.00	106.71
24	5	315	KC1	CMA-C3A-C2A	-7.32	110.38	128.30
24	8	316	KC1	CMA-C3A-C4A	-7.32	113.89	125.04
24	5	313	KC1	CMA-C3A-C2A	-7.31	110.40	128.30
21	J	304	CLA	C4A-NA-C1A	7.31	109.99	106.71
24	J	312	KC1	CMA-C3A-C2A	-7.31	110.41	128.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	305	CLA	C4A-NA-C1A	7.30	109.99	106.71
24	1	315	KC1	C2B-C1B-NB	7.30	115.48	110.10
24	7	314	KC1	CMA-C3A-C2A	-7.30	110.44	128.30
24	1	315	KC1	CMA-C3A-C2A	-7.29	110.44	128.30
24	J	313	KC1	CMA-C3A-C2A	-7.29	110.46	128.30
24	7	314	KC1	C2B-C1B-NB	7.28	115.47	110.10
24	3	305	KC1	CMA-C3A-C2A	-7.28	110.47	128.30
24	6	312	KC1	CMA-C3A-C2A	-7.27	110.49	128.30
21	4	304	CLA	C4A-NA-C1A	7.27	109.97	106.71
21	6	304	CLA	C4A-NA-C1A	7.27	109.97	106.71
24	G	306	KC1	C2B-C1B-NB	7.26	115.45	110.10
24	4	309	KC1	CMA-C3A-C2A	-7.26	110.54	128.30
21	1	304	CLA	C4A-NA-C1A	7.25	109.97	106.71
21	5	307	CLA	C4A-NA-C1A	7.24	109.96	106.71
24	4	307	KC1	CMA-C3A-C2A	-7.23	110.60	128.30
21	1	301	CLA	C4A-NA-C1A	7.22	109.95	106.71
24	G	307	KC1	CMA-C3A-C2A	-7.22	110.62	128.30
24	J	313	KC1	O2D-CGD-CBD	7.20	124.07	111.27
24	9	306	KC1	CMA-C3A-C2A	-7.20	110.67	128.30
24	6	313	KC1	CMA-C3A-C2A	-7.20	110.67	128.30
24	3	306	KC1	CMA-C3A-C2A	-7.17	110.74	128.30
24	8	314	KC1	C1A-C2A-C3A	-7.17	101.42	107.11
24	g	315	KC1	CMA-C3A-C2A	-7.16	110.78	128.30
24	5	314	KC1	CMA-C3A-C2A	-7.15	110.80	128.30
24	6	313	KC1	O2D-CGD-CBD	7.13	123.94	111.27
24	4	308	KC1	C2B-C1B-NB	7.12	115.35	110.10
24	8	313	KC1	C3A-C4A-NA	7.12	118.34	110.57
24	7	315	KC1	C2B-C1B-NB	7.12	115.35	110.10
24	9	305	KC1	C2B-C1B-NB	7.11	115.34	110.10
21	B	603	CLA	C4A-NA-C1A	7.10	109.90	106.71
24	g	313	KC1	C2B-C1B-NB	7.10	115.34	110.10
24	8	313	KC1	CMA-C3A-C2A	-7.10	110.92	128.30
24	G	308	KC1	CMA-C3A-C2A	-7.10	110.92	128.30
21	C	511	CLA	C4A-NA-C1A	7.05	109.88	106.71
21	2	301	CLA	C4A-NA-C1A	7.03	109.87	106.71
24	2	313	KC1	CMA-C3A-C2A	-7.03	111.10	128.30
24	9	306	KC1	C2B-C1B-NB	7.01	115.27	110.10
24	4	308	KC1	C1A-C2A-C3A	-7.01	101.55	107.11
24	G	308	KC1	C3A-C4A-NA	7.00	118.22	110.57
24	G	309	KC1	CMA-C3A-C2A	-7.00	111.17	128.30
24	4	307	KC1	C2B-C1B-NB	6.97	115.24	110.10
24	G	309	KC1	C2B-C1B-NB	6.96	115.23	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	615	CLA	C4A-NA-C1A	6.95	109.83	106.71
21	b	617	CLA	C4A-NA-C1A	6.95	109.83	106.71
24	g	314	KC1	C3A-C4A-NA	6.90	118.10	110.57
24	8	313	KC1	CHB-C4A-C3A	-6.85	114.27	124.98
24	G	307	KC1	C1A-C2A-C3A	-6.83	101.70	107.11
21	b	604	CLA	C4A-NA-C1A	6.81	109.77	106.71
21	D	404	CLA	C4A-NA-C1A	6.79	109.76	106.71
24	G	307	KC1	C3A-C4A-NA	6.78	117.97	110.57
24	6	313	KC1	CHB-C4A-C3A	-6.77	114.40	124.98
24	2	316	KC1	C1A-C2A-C3A	-6.77	101.74	107.11
24	4	307	KC1	C1A-C2A-C3A	-6.77	101.74	107.11
24	g	314	KC1	CHB-C4A-C3A	-6.76	114.42	124.98
24	G	308	KC1	C1A-NA-C4A	-6.76	103.67	106.71
21	J	308	CLA	C4D-CHA-C1A	-6.75	113.03	121.25
24	3	306	KC1	C3A-C4A-NA	6.75	117.94	110.57
21	g	309	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	7	314	KC1	C1A-C2A-C3A	-6.75	101.76	107.11
24	2	314	KC1	C3A-C4A-NA	6.72	117.91	110.57
24	9	305	KC1	C1A-C2A-C3A	-6.72	101.78	107.11
24	g	314	KC1	C1A-C2A-C3A	-6.72	101.78	107.11
24	g	314	KC1	C1A-NA-C4A	-6.72	103.69	106.71
24	8	314	KC1	CHB-C4A-C3A	-6.69	114.53	124.98
24	1	316	KC1	CHB-C4A-C3A	-6.69	114.53	124.98
24	J	313	KC1	CHB-C4A-C3A	-6.67	114.56	124.98
24	5	314	KC1	C3A-C4A-NA	6.66	117.84	110.57
24	3	306	KC1	CHB-C4A-C3A	-6.65	114.59	124.98
24	5	315	KC1	C1A-C2A-C3A	-6.65	101.83	107.11
24	2	314	KC1	CHB-C4A-C3A	-6.65	114.59	124.98
24	3	306	KC1	C1A-C2A-C3A	-6.65	101.84	107.11
21	9	303	CLA	CHD-C1D-ND	-6.64	118.35	124.45
24	1	316	KC1	C3A-C4A-NA	6.63	117.81	110.57
24	8	314	KC1	C3A-C4A-NA	6.63	117.81	110.57
24	4	306	KC1	C2B-C1B-NB	6.62	114.98	110.10
24	7	315	KC1	CHB-C4A-C3A	-6.62	114.63	124.98
21	B	614	CLA	C4A-NA-C1A	6.61	109.68	106.71
24	7	315	KC1	C1A-C2A-C3A	-6.59	101.88	107.11
24	8	316	KC1	CHB-C4A-C3A	-6.59	114.69	124.98
24	G	307	KC1	C3B-C2B-C1B	-6.59	100.79	107.08
21	7	303	CLA	C4A-NA-C1A	6.59	109.67	106.71
24	6	312	KC1	C3A-C4A-NA	6.58	117.75	110.57
24	J	312	KC1	C1A-C2A-C3A	-6.56	101.91	107.11
24	1	315	KC1	C1A-C2A-C3A	-6.55	101.91	107.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	315	KC1	C3B-C2B-C1B	-6.55	100.82	107.08
24	6	312	KC1	C1A-C2A-C3A	-6.55	101.91	107.11
21	D	406	CLA	C4A-NA-C1A	6.55	109.65	106.71
24	3	305	KC1	C3A-C4A-NA	6.54	117.72	110.57
24	8	316	KC1	C3A-C4A-NA	6.54	117.72	110.57
24	7	315	KC1	C3A-C4A-NA	6.54	117.71	110.57
24	G	307	KC1	CHB-C4A-C3A	-6.53	114.78	124.98
24	8	313	KC1	C1A-C2A-C3A	-6.51	101.94	107.11
21	6	307	CLA	C4A-NA-C1A	6.51	109.63	106.71
24	G	309	KC1	C1A-C2A-C3A	-6.51	101.95	107.11
24	1	316	KC1	C1A-C2A-C3A	-6.50	101.95	107.11
24	G	308	KC1	C1A-C2A-C3A	-6.50	101.95	107.11
21	J	301	CLA	C4A-NA-C1A	6.50	109.63	106.71
24	J	312	KC1	C3A-C4A-NA	6.50	117.67	110.57
24	2	316	KC1	CHB-C4A-C3A	-6.50	114.83	124.98
24	6	312	KC1	CHB-C4A-C3A	-6.50	114.83	124.98
24	8	316	KC1	C1A-C2A-C3A	-6.50	101.96	107.11
24	4	309	KC1	C1A-C2A-C3A	-6.50	101.96	107.11
24	J	313	KC1	C1A-C2A-C3A	-6.49	101.96	107.11
24	2	316	KC1	C3A-C4A-NA	6.48	117.65	110.57
24	6	313	KC1	C3A-C4A-NA	6.48	117.64	110.57
24	1	315	KC1	C3A-C4A-NA	6.46	117.63	110.57
24	5	314	KC1	C1A-C2A-C3A	-6.46	101.99	107.11
21	d	405	CLA	C4A-NA-C1A	6.45	109.61	106.71
24	6	311	KC1	CHB-C4A-C3A	-6.45	114.91	124.98
24	2	313	KC1	C1A-C2A-C3A	-6.45	102.00	107.11
24	J	311	KC1	C1A-C2A-C3A	-6.44	102.00	107.11
24	J	313	KC1	C3A-C4A-NA	6.44	117.60	110.57
24	4	306	KC1	C1A-C2A-C3A	-6.43	101.91	106.93
24	J	312	KC1	CHB-C4A-C3A	-6.43	114.94	124.98
24	g	313	KC1	C1A-C2A-C3A	-6.43	102.01	107.11
24	3	305	KC1	C1A-C2A-C3A	-6.42	102.02	107.11
24	4	309	KC1	C2B-C1B-NB	6.41	114.83	110.10
24	6	313	KC1	C1A-C2A-C3A	-6.40	102.03	107.11
21	g	304	CLA	C4A-NA-C1A	6.40	109.58	106.71
24	1	315	KC1	CHB-C4A-C3A	-6.40	114.99	124.98
24	9	306	KC1	C1A-C2A-C3A	-6.39	102.04	107.11
24	4	308	KC1	CHB-C4A-C3A	-6.39	115.00	124.98
24	9	305	KC1	CHB-C4A-C3A	-6.38	115.02	124.98
21	8	302	CLA	C4A-NA-C1A	6.38	109.57	106.71
21	J	307	CLA	C4A-NA-C1A	6.37	109.57	106.71
24	J	311	KC1	CHB-C4A-C3A	-6.35	115.06	124.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	314	KC1	CHB-C4A-C3A	-6.33	115.08	124.98
21	C	512	CLA	C4A-NA-C1A	6.33	109.55	106.71
24	G	306	KC1	CHB-C4A-C3A	-6.33	115.09	124.98
24	9	305	KC1	C3A-C4A-NA	6.30	117.45	110.57
24	7	314	KC1	C3A-C4A-NA	6.30	117.45	110.57
21	g	309	CLA	C4D-CHA-C1A	-6.30	113.58	121.25
24	5	313	KC1	C3B-C2B-C1B	-6.30	101.06	107.08
24	5	313	KC1	CHB-C4A-C3A	-6.29	115.15	124.98
24	G	306	KC1	C3A-C4A-NA	6.29	117.44	110.57
21	d	404	CLA	C4A-NA-C1A	6.27	109.53	106.71
24	7	314	KC1	CHB-C4A-C3A	-6.27	115.18	124.98
24	g	315	KC1	C1A-C2A-C3A	-6.27	102.14	107.11
24	3	305	KC1	CHB-C4A-C3A	-6.25	115.22	124.98
24	9	305	KC1	C3B-C2B-C1B	-6.24	101.11	107.08
24	2	313	KC1	C2B-C1B-NB	6.23	114.69	110.10
24	5	313	KC1	C3A-C4A-NA	6.22	117.37	110.57
24	6	311	KC1	C3B-C2B-C1B	-6.22	101.14	107.08
24	G	309	KC1	C3B-C2B-C1B	-6.22	101.14	107.08
24	4	307	KC1	C3A-C4A-NA	6.21	117.35	110.57
24	g	315	KC1	CHB-C4A-C3A	-6.21	115.28	124.98
24	4	307	KC1	C3B-C2B-C1B	-6.21	101.15	107.08
24	6	311	KC1	C3A-C4A-NA	6.19	117.33	110.57
24	4	306	KC1	C2C-C1C-NC	6.19	115.69	109.97
24	g	313	KC1	C3B-C2B-C1B	-6.19	101.17	107.08
21	9	303	CLA	C1B-CHB-C4A	-6.19	117.86	130.12
21	g	304	CLA	CHD-C1D-ND	-6.19	118.77	124.45
24	g	315	KC1	C3B-C2B-C1B	-6.18	101.18	107.08
24	4	308	KC1	C3A-C4A-NA	6.17	117.31	110.57
24	3	306	KC1	C1A-NA-C4A	-6.16	103.94	106.71
24	6	311	KC1	C1A-C2A-C3A	-6.15	102.23	107.11
24	6	313	KC1	C3B-C2B-C1B	-6.15	101.21	107.08
24	g	315	KC1	C3A-C4A-NA	6.14	117.27	110.57
24	9	306	KC1	C3A-C4A-NA	6.13	117.27	110.57
24	9	306	KC1	CHB-C4A-C3A	-6.13	115.40	124.98
21	5	309	CLA	O2D-CGD-CBD	6.13	122.16	111.27
24	4	307	KC1	CHB-C4A-C3A	-6.13	115.41	124.98
24	G	308	KC1	CHB-C4A-C3A	-6.10	115.45	124.98
24	G	306	KC1	C1A-C2A-C3A	-6.10	102.17	106.93
24	J	311	KC1	C3B-C2B-C1B	-6.10	101.25	107.08
24	G	307	KC1	C1A-NA-C4A	-6.10	103.97	106.71
21	1	306	CLA	C4A-NA-C1A	6.09	109.44	106.71
24	J	313	KC1	C3B-C2B-C1B	-6.09	101.26	107.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	309	KC1	CHB-C4A-C3A	-6.09	115.47	124.98
24	5	315	KC1	CHB-C4A-C3A	-6.09	115.47	124.98
24	g	314	KC1	C3B-C2B-C1B	-6.08	101.27	107.08
21	6	303	CLA	O2D-CGD-CBD	6.08	122.07	111.27
21	B	604	CLA	O2D-CGD-CBD	6.08	122.07	111.27
21	c	511	CLA	C4A-NA-C1A	6.07	109.44	106.71
24	G	309	KC1	C3A-C4A-NA	6.07	117.20	110.57
24	G	309	KC1	CHB-C4A-C3A	-6.06	115.51	124.98
24	J	311	KC1	C3A-C4A-NA	6.05	117.17	110.57
21	7	302	CLA	CHD-C1D-ND	-6.04	118.90	124.45
24	3	305	KC1	C3B-C2B-C1B	-6.02	101.32	107.08
24	5	313	KC1	C1A-C2A-C3A	-6.02	102.33	107.11
24	8	315	KC1	C3B-C2B-C1B	-6.01	101.34	107.08
24	2	313	KC1	CHB-C4A-C3A	-6.00	115.60	124.98
24	G	308	KC1	C3B-C2B-C1B	-6.00	101.35	107.08
24	4	306	KC1	C4C-NC-C1C	-6.00	104.01	106.71
24	G	306	KC1	C2C-C1C-NC	6.00	115.50	109.97
24	g	313	KC1	C3A-C4A-NA	5.99	117.11	110.57
24	g	313	KC1	CHB-C4A-C3A	-5.99	115.62	124.98
21	1	303	CLA	O2D-CGD-CBD	5.98	121.90	111.27
24	4	309	KC1	C3A-C4A-NA	5.97	117.09	110.57
24	4	306	KC1	CHB-C4A-C3A	-5.96	115.67	124.98
21	7	302	CLA	O2D-CGD-CBD	5.96	121.86	111.27
24	3	306	KC1	C3B-C2B-C1B	-5.96	101.39	107.08
21	g	309	CLA	O2D-CGD-CBD	5.95	121.84	111.27
24	1	315	KC1	C3B-C2B-C1B	-5.94	101.40	107.08
24	1	316	KC1	C3B-C2B-C1B	-5.92	101.43	107.08
21	c	514	CLA	O2D-CGD-CBD	5.89	121.74	111.27
24	8	314	KC1	CMA-C3A-C2A	-5.89	113.87	128.30
21	6	308	CLA	C4D-CHA-C1A	-5.89	114.08	121.25
24	4	306	KC1	C3A-C4A-NA	5.89	117.00	110.57
24	2	315	KC1	C3B-C2B-C1B	-5.89	101.46	107.08
24	5	314	KC1	C3B-C2B-C1B	-5.88	101.46	107.08
24	G	308	KC1	C3C-C4C-NC	5.88	115.41	109.88
24	8	314	KC1	C3B-C2B-C1B	-5.87	101.47	107.08
24	2	313	KC1	C3A-C4A-NA	5.86	116.97	110.57
24	9	306	KC1	C3B-C2B-C1B	-5.84	101.50	107.08
24	5	315	KC1	C3A-C4A-NA	5.84	116.95	110.57
21	7	301	CLA	O2D-CGD-CBD	5.84	121.65	111.27
24	7	314	KC1	C3B-C2B-C1B	-5.84	101.50	107.08
21	1	303	CLA	CHD-C1D-ND	-5.83	119.09	124.45
24	2	314	KC1	C3B-C2B-C1B	-5.83	101.51	107.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	314	KC1	C1A-NA-C4A	-5.82	104.09	106.71
24	3	305	KC1	C1A-NA-C4A	-5.82	104.09	106.71
21	b	605	CLA	O2D-CGD-CBD	5.81	121.59	111.27
24	2	314	KC1	CMA-C3A-C2A	-5.81	114.08	128.30
21	b	606	CLA	C2C-C1C-NC	5.80	115.40	109.97
24	G	306	KC1	C3B-C2B-C1B	-5.79	101.55	107.08
24	8	316	KC1	C3B-C2B-C1B	-5.78	101.56	107.08
21	J	307	CLA	O2D-CGD-CBD	5.76	121.51	111.27
24	2	316	KC1	C3B-C2B-C1B	-5.76	101.57	107.08
23	2	307	A86	C17-C16-C15	5.76	115.04	109.16
21	b	607	CLA	O2D-CGD-CBD	5.75	121.49	111.27
24	8	314	KC1	O2D-CGD-CBD	5.74	121.46	111.27
24	G	306	KC1	C4C-NC-C1C	-5.72	104.14	106.71
21	B	605	CLA	C2C-C1C-NC	5.72	115.33	109.97
21	B	606	CLA	O2D-CGD-CBD	5.71	121.42	111.27
24	5	315	KC1	C3C-C4C-NC	5.70	115.24	109.88
24	7	315	KC1	C3B-C2B-C1B	-5.69	101.64	107.08
24	8	313	KC1	C3B-C2B-C1B	-5.69	101.64	107.08
24	6	312	KC1	CMD-C2D-C1D	5.68	137.19	128.46
24	4	306	KC1	C2A-C1A-CHA	-5.66	120.87	131.87
21	c	502	CLA	O2D-CGD-CBD	5.66	121.32	111.27
21	g	303	CLA	O2D-CGD-CBD	5.65	121.31	111.27
23	2	311	A86	C17-C16-C15	5.65	114.93	109.16
24	4	306	KC1	C3B-C2B-C1B	-5.64	101.69	107.08
21	9	303	CLA	C4D-CHA-C1A	-5.63	114.39	121.25
24	4	308	KC1	C3B-C2B-C1B	-5.63	101.70	107.08
21	1	307	CLA	O2D-CGD-CBD	5.62	121.25	111.27
24	4	309	KC1	CMD-C2D-C1D	5.59	137.06	128.46
21	5	306	CLA	CHD-C1D-ND	-5.58	119.33	124.45
21	C	515	CLA	O2D-CGD-CBD	5.58	121.18	111.27
21	5	306	CLA	O2D-CGD-CBD	5.57	121.17	111.27
24	2	316	KC1	C3C-C4C-NC	5.56	115.12	109.88
24	g	314	KC1	C3C-C4C-NC	5.56	115.11	109.88
21	3	303	CLA	CHD-C1D-ND	-5.56	119.35	124.45
21	7	306	CLA	O2D-CGD-CBD	5.55	121.13	111.27
21	G	304	CLA	O2D-CGD-CBD	5.54	121.12	111.27
21	3	300	CLA	CHD-C1D-ND	-5.54	119.36	124.45
21	J	301	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
24	8	315	KC1	CMD-C2D-C1D	5.53	136.97	128.46
21	b	603	CLA	O2D-CGD-CBD	5.53	121.10	111.27
24	2	315	KC1	CMD-C2D-C1D	5.53	136.96	128.46
21	B	608	CLA	O2D-CGD-CBD	5.52	121.08	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	316	KC1	C3C-C4C-NC	5.52	115.08	109.88
21	B	602	CLA	O2D-CGD-CBD	5.52	121.08	111.27
21	b	610	CLA	O2D-CGD-CBD	5.52	121.08	111.27
21	b	609	CLA	O2D-CGD-CBD	5.52	121.07	111.27
21	B	609	CLA	O2D-CGD-CBD	5.51	121.06	111.27
24	G	306	KC1	C2A-C1A-CHA	-5.50	121.17	131.87
21	c	507	CLA	O2D-CGD-CBD	5.49	121.02	111.27
24	2	313	KC1	CMD-C2D-C1D	5.49	136.90	128.46
21	c	503	CLA	O2D-CGD-CBD	5.46	120.97	111.27
21	2	301	CLA	O2D-CGD-CBD	5.45	120.95	111.27
24	8	313	KC1	CMD-C2D-C1D	5.44	136.83	128.46
24	7	314	KC1	CMD-C2D-C1D	5.44	136.82	128.46
24	g	315	KC1	CMD-C2D-C1D	5.43	136.81	128.46
21	C	507	CLA	O2D-CGD-CBD	5.42	120.90	111.27
21	g	306	CLA	CHD-C1D-ND	-5.42	119.47	124.45
33	d	401	BCT	O2-C-O1	5.42	133.60	119.55
24	8	313	KC1	C1A-NA-C4A	-5.42	104.27	106.71
23	g	312	A86	C17-C16-C15	5.41	114.68	109.16
21	4	304	CLA	CHD-C1D-ND	-5.41	119.48	124.45
21	g	305	CLA	O2D-CGD-CBD	5.41	120.88	111.27
21	8	305	CLA	O2D-CGD-CBD	5.40	120.86	111.27
24	G	308	KC1	CMD-C2D-C1D	5.40	136.76	128.46
24	5	314	KC1	C3C-C4C-NC	5.40	114.96	109.88
24	G	309	KC1	O2D-CGD-CBD	5.39	120.85	111.27
21	1	310	CLA	O2D-CGD-CBD	5.39	120.84	111.27
21	G	302	CLA	O2D-CGD-CBD	5.38	120.84	111.27
21	7	305	CLA	CHD-C1D-ND	-5.38	119.51	124.45
24	2	315	KC1	O2D-CGD-CBD	5.38	120.82	111.27
24	4	308	KC1	CMD-C2D-C1D	5.37	136.72	128.46
21	5	303	CLA	O2D-CGD-CBD	5.37	120.81	111.27
24	J	312	KC1	C3B-C2B-C1B	-5.37	101.95	107.08
21	5	309	CLA	C1B-CHB-C4A	-5.36	119.50	130.12
24	4	309	KC1	CHC-C1C-C2C	-5.35	116.62	124.98
21	2	304	CLA	O2D-CGD-CBD	5.35	120.78	111.27
21	d	404	CLA	CHD-C1D-ND	-5.35	119.54	124.45
21	5	308	CLA	O2D-CGD-CBD	5.35	120.77	111.27
24	4	309	KC1	C2C-C1C-NC	5.35	116.41	110.57
21	5	309	CLA	CHD-C1D-ND	-5.34	119.55	124.45
24	6	312	KC1	C3B-C2B-C1B	-5.33	101.99	107.08
21	c	506	CLA	O2D-CGD-CBD	5.32	120.72	111.27
24	G	309	KC1	CMD-C2D-C1D	5.32	136.64	128.46
33	D	402	BCT	O2-C-O1	5.32	133.34	119.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	J	312	KC1	CMD-C2D-C1D	5.32	136.63	128.46
24	4	306	KC1	CMD-C2D-C1D	5.31	136.63	128.46
24	G	307	KC1	CMD-C2D-C1D	5.31	136.63	128.46
24	2	314	KC1	C3C-C4C-NC	5.30	114.87	109.88
24	8	316	KC1	CMD-C2D-C1D	5.30	136.61	128.46
24	g	313	KC1	CMD-C2D-C1D	5.30	136.61	128.46
24	4	309	KC1	C3B-C2B-C1B	-5.30	102.01	107.08
21	B	605	CLA	O2D-CGD-CBD	5.30	120.68	111.27
21	2	306	CLA	C2C-C1C-NC	5.30	114.94	109.97
24	2	316	KC1	CMD-C2D-C1D	5.30	136.61	128.46
24	G	306	KC1	CMD-C2D-C1D	5.30	136.61	128.46
24	1	316	KC1	CMD-C2D-C1D	5.30	136.60	128.46
24	g	314	KC1	CMD-C2D-C1D	5.30	136.60	128.46
21	8	302	CLA	O2D-CGD-CBD	5.29	120.67	111.27
24	9	306	KC1	CMD-C2D-C1D	5.28	136.59	128.46
24	5	315	KC1	CMD-C2D-C1D	5.28	136.57	128.46
21	6	307	CLA	O2D-CGD-CBD	5.27	120.63	111.27
35	D	409	PL9	C7-C3-C4	5.27	121.16	116.88
21	b	606	CLA	O2D-CGD-CBD	5.26	120.62	111.27
24	7	315	KC1	CMD-C2D-C1D	5.26	136.55	128.46
21	9	303	CLA	O2D-CGD-CBD	5.26	120.62	111.27
24	g	315	KC1	O2D-CGD-CBD	5.26	120.62	111.27
24	1	316	KC1	C3C-C4C-NC	5.25	114.82	109.88
21	C	503	CLA	O2D-CGD-CBD	5.25	120.60	111.27
21	3	302	CLA	O2D-CGD-CBD	5.25	120.60	111.27
21	G	304	CLA	CHD-C1D-ND	-5.25	119.63	124.45
24	4	307	KC1	CMD-C2D-C1D	5.25	136.53	128.46
24	3	305	KC1	CMD-C2D-C1D	5.25	136.53	128.46
24	G	307	KC1	C3C-C4C-NC	5.24	114.81	109.88
21	6	300	CLA	O2D-CGD-CBD	5.24	120.58	111.27
21	7	305	CLA	C4D-CHA-C1A	-5.24	114.87	121.25
21	6	305	CLA	O2D-CGD-CBD	5.23	120.56	111.27
24	5	314	KC1	CMD-C2D-C1D	5.23	136.50	128.46
24	7	315	KC1	C3C-C4C-NC	5.23	114.80	109.88
21	J	305	CLA	O2D-CGD-CBD	5.23	120.56	111.27
21	J	302	CLA	O2D-CGD-CBD	5.22	120.55	111.27
24	1	315	KC1	CMD-C2D-C1D	5.22	136.49	128.46
21	4	302	CLA	C4D-CHA-C1A	-5.22	114.89	121.25
21	4	304	CLA	O2D-CGD-CBD	5.22	120.55	111.27
23	7	313	A86	C17-C16-C15	5.22	114.49	109.16
24	8	313	KC1	C3C-C4C-NC	5.22	114.79	109.88
24	2	313	KC1	C3C-C4C-NC	5.22	114.79	109.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	309	KC1	C3C-C4C-NC	5.22	114.79	109.88
21	6	302	CLA	O2D-CGD-CBD	5.22	120.54	111.27
24	g	315	KC1	C3C-C4C-NC	5.22	114.79	109.88
24	J	313	KC1	CMD-C2D-C1D	5.21	136.48	128.46
24	3	306	KC1	CMD-C2D-C1D	5.21	136.48	128.46
24	2	314	KC1	C1A-NA-C4A	-5.21	104.36	106.71
21	a	402	CLA	O2D-CGD-CBD	5.21	120.52	111.27
21	J	301	CLA	C2D-C1D-ND	5.20	113.94	110.10
24	9	305	KC1	C1A-NA-C4A	-5.20	104.37	106.71
21	5	305	CLA	O2D-CGD-CBD	5.20	120.51	111.27
21	g	306	CLA	O2D-CGD-CBD	5.20	120.51	111.27
24	5	313	KC1	CMD-C2D-C1D	5.20	136.45	128.46
24	9	305	KC1	CMD-C2D-C1D	5.18	136.43	128.46
21	C	504	CLA	O2D-CGD-CBD	5.18	120.47	111.27
21	8	303	CLA	O2D-CGD-CBD	5.18	120.47	111.27
21	6	308	CLA	O2D-CGD-CBD	5.17	120.45	111.27
23	8	308	A86	C4-C3-C2	5.17	134.06	123.47
35	d	408	PL9	C7-C3-C4	5.16	121.08	116.88
21	D	404	CLA	C2C-C1C-NC	5.16	114.81	109.97
24	9	306	KC1	O2D-CGD-CBD	5.15	120.42	111.27
24	6	312	KC1	C1A-NA-C4A	-5.15	104.39	106.71
24	2	314	KC1	O2D-CGD-CBD	5.14	120.40	111.27
24	G	308	KC1	C2C-C1C-NC	5.14	116.18	110.57
21	7	303	CLA	CHD-C1D-ND	-5.14	119.73	124.45
24	8	314	KC1	C3C-C4C-NC	5.13	114.71	109.88
24	3	306	KC1	C3C-C4C-NC	5.13	114.71	109.88
21	6	304	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
21	4	300	CLA	C4D-CHA-C1A	-5.13	115.01	121.25
24	7	314	KC1	O2D-CGD-CBD	5.13	120.38	111.27
21	2	306	CLA	C1C-C2C-C3C	-5.12	101.58	106.96
21	7	304	CLA	C2C-C1C-NC	5.12	114.77	109.97
21	b	615	CLA	O2D-CGD-CBD	5.11	120.35	111.27
24	3	305	KC1	C3C-C4C-NC	5.11	114.69	109.88
21	6	301	CLA	O2D-CGD-CBD	5.11	120.34	111.27
21	1	303	CLA	C4D-CHA-C1A	-5.10	115.04	121.25
21	1	304	CLA	O2D-CGD-CBD	5.10	120.34	111.27
24	6	313	KC1	C3C-C4C-NC	5.10	114.68	109.88
21	D	404	CLA	CHD-C1D-ND	-5.10	119.77	124.45
21	J	304	CLA	C1C-C2C-C3C	-5.10	101.60	106.96
23	2	309	A86	C17-C16-C15	5.09	114.36	109.16
24	G	309	KC1	C3C-C4C-NC	5.09	114.67	109.88
21	5	304	CLA	O2D-CGD-CBD	5.09	120.32	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	315	KC1	C1A-NA-C4A	-5.09	104.42	106.71
21	4	303	CLA	O2D-CGD-CBD	5.09	120.31	111.27
21	7	305	CLA	O2D-CGD-CBD	5.09	120.31	111.27
21	A	401	CLA	O2D-CGD-CBD	5.09	120.31	111.27
24	2	315	KC1	CHC-C1C-C2C	-5.09	117.03	124.98
24	5	314	KC1	O2D-CGD-CBD	5.08	120.30	111.27
21	b	606	CLA	C1C-C2C-C3C	-5.08	101.62	106.96
24	g	314	KC1	O2D-CGD-CBD	5.08	120.29	111.27
24	6	313	KC1	CMD-C2D-C1D	5.08	136.27	128.46
21	6	304	CLA	CHD-C1D-ND	-5.08	119.79	124.45
24	9	305	KC1	C3C-C4C-NC	5.07	114.65	109.88
21	2	305	CLA	O2D-CGD-O1D	-5.07	113.92	123.84
21	3	303	CLA	O2D-CGD-CBD	5.07	120.28	111.27
30	c	516	DGD	O3G-C3G-C2G	-5.07	98.67	110.90
21	6	307	CLA	CHD-C1D-ND	-5.07	119.80	124.45
21	J	308	CLA	O2D-CGD-CBD	5.06	120.27	111.27
21	J	304	CLA	CHD-C1D-ND	-5.06	119.80	124.45
24	3	306	KC1	O2D-CGD-CBD	5.06	120.25	111.27
21	B	607	CLA	O2D-CGD-O1D	-5.05	113.96	123.84
21	J	301	CLA	O2D-CGD-CBD	5.04	120.23	111.27
21	b	617	CLA	C2D-C1D-ND	5.04	113.82	110.10
21	d	404	CLA	C2C-C1C-NC	5.04	114.69	109.97
21	B	614	CLA	O2D-CGD-CBD	5.04	120.22	111.27
21	b	610	CLA	C2C-C1C-NC	5.04	114.69	109.97
24	7	314	KC1	C3C-C4C-NC	5.03	114.62	109.88
21	6	304	CLA	C2C-C1C-NC	5.03	114.69	109.97
24	g	313	KC1	C3C-C4C-NC	5.03	114.61	109.88
24	7	314	KC1	C1A-NA-C4A	-5.03	104.44	106.71
24	2	313	KC1	C3B-C2B-C1B	-5.03	102.27	107.08
24	J	313	KC1	C3C-C4C-NC	5.03	114.61	109.88
21	g	303	CLA	C4D-CHA-C1A	-5.02	115.14	121.25
21	7	309	CLA	O2D-CGD-CBD	5.02	120.19	111.27
24	8	315	KC1	O2D-CGD-CBD	5.02	120.19	111.27
24	2	315	KC1	C3C-C4C-NC	5.02	114.60	109.88
24	9	306	KC1	C3C-C4C-NC	5.02	114.60	109.88
24	J	311	KC1	C3C-C4C-NC	5.02	114.60	109.88
24	1	315	KC1	C3C-C4C-NC	5.02	114.60	109.88
21	C	512	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
21	7	302	CLA	C4D-CHA-C1A	-5.01	115.15	121.25
21	d	405	CLA	C1B-C2B-C3B	-5.01	102.26	106.92
21	J	306	CLA	O2D-CGD-CBD	5.00	120.16	111.27
21	g	307	CLA	CHD-C1D-ND	-5.00	119.86	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	J	312	KC1	C3C-C4C-NC	5.00	114.58	109.88
21	G	302	CLA	CHD-C1D-ND	-4.99	119.87	124.45
21	J	304	CLA	O2D-CGD-CBD	4.99	120.13	111.27
21	J	303	CLA	O2D-CGD-CBD	4.99	120.13	111.27
21	J	300	CLA	O2D-CGD-CBD	4.99	120.13	111.27
21	B	605	CLA	C1C-C2C-C3C	-4.99	101.71	106.96
21	J	304	CLA	C2C-C1C-NC	4.98	114.64	109.97
24	6	312	KC1	O2D-CGD-CBD	4.98	120.12	111.27
21	B	616	CLA	C2D-C1D-ND	4.98	113.77	110.10
21	b	613	CLA	O2D-CGD-CBD	4.98	120.11	111.27
24	8	315	KC1	C3C-C4C-NC	4.97	114.56	109.88
21	D	406	CLA	C4D-CHA-C1A	-4.97	115.20	121.25
24	4	307	KC1	C1A-NA-C4A	-4.96	104.47	106.71
24	6	312	KC1	C3C-C4C-NC	4.96	114.55	109.88
24	g	313	KC1	C1A-NA-C4A	-4.96	104.48	106.71
21	6	303	CLA	C4D-CHA-C1A	-4.96	115.22	121.25
21	5	303	CLA	C4D-CHA-C1A	-4.96	115.22	121.25
24	1	316	KC1	C1A-NA-C4A	-4.95	104.48	106.71
21	B	609	CLA	C2C-C1C-NC	4.95	114.61	109.97
21	9	301	CLA	O2D-CGD-CBD	4.94	120.05	111.27
24	J	312	KC1	O2D-CGD-CBD	4.94	120.05	111.27
21	d	405	CLA	C4D-CHA-C1A	-4.94	115.23	121.25
21	g	308	CLA	O2D-CGD-CBD	4.94	120.05	111.27
21	G	303	CLA	O2D-CGD-CBD	4.94	120.04	111.27
21	9	302	CLA	C4D-CHA-C1A	-4.93	115.25	121.25
21	c	511	CLA	CHD-C4C-C3C	-4.93	117.60	124.84
24	J	312	KC1	C1A-NA-C4A	-4.92	104.49	106.71
21	4	304	CLA	C2C-C1C-NC	4.92	114.58	109.97
21	B	621	CLA	O2D-CGD-CBD	4.91	120.00	111.27
21	D	406	CLA	C1B-C2B-C3B	-4.91	102.35	106.92
24	4	306	KC1	O2D-CGD-CBD	4.91	120.00	111.27
21	b	611	CLA	O2D-CGD-CBD	4.91	119.99	111.27
30	C	517	DGD	O3G-C3G-C2G	-4.91	99.06	110.90
21	c	506	CLA	C2C-C1C-NC	4.90	114.56	109.97
21	a	403	CLA	CHD-C1D-ND	-4.90	119.95	124.45
24	6	311	KC1	C3C-C4C-NC	4.90	114.49	109.88
21	8	303	CLA	C2C-C1C-NC	4.90	114.56	109.97
21	C	512	CLA	CHD-C1D-ND	-4.89	119.96	124.45
21	B	612	CLA	O2D-CGD-CBD	4.89	119.96	111.27
21	c	511	CLA	CHD-C1D-ND	-4.89	119.96	124.45
21	c	503	CLA	C2C-C1C-NC	4.89	114.55	109.97
21	A	402	CLA	CHD-C1D-ND	-4.88	119.97	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	307	KC1	C2A-C1A-NA	4.88	117.23	109.40
21	C	507	CLA	C2C-C1C-NC	4.88	114.55	109.97
24	4	307	KC1	C2A-C1A-NA	4.88	117.23	109.40
21	5	305	CLA	CHD-C1D-ND	-4.88	119.97	124.45
21	8	307	CLA	O2D-CGD-O1D	-4.88	114.30	123.84
24	G	309	KC1	C2C-C1C-NC	4.87	115.89	110.57
21	5	303	CLA	C2C-C1C-NC	4.87	114.53	109.97
21	d	405	CLA	C1C-C2C-C3C	-4.87	102.61	107.07
24	5	313	KC1	C3C-C4C-NC	4.86	114.46	109.88
21	b	612	CLA	C2D-C1D-ND	4.86	113.69	110.10
24	g	313	KC1	C2A-C1A-NA	4.86	117.19	109.40
24	G	308	KC1	C2A-C1A-NA	4.86	117.19	109.40
21	c	514	CLA	CHD-C1D-ND	-4.86	119.99	124.45
24	8	315	KC1	CHC-C1C-C2C	-4.86	117.39	124.98
21	1	309	CLA	O2D-CGD-CBD	4.85	119.88	111.27
21	4	300	CLA	CHD-C1D-ND	-4.85	120.00	124.45
24	4	307	KC1	C3C-C4C-NC	4.84	114.44	109.88
21	C	515	CLA	CHD-C1D-ND	-4.84	120.00	124.45
21	9	304	CLA	CHD-C1D-ND	-4.84	120.01	124.45
21	8	306	CLA	O2D-CGD-CBD	4.84	119.86	111.27
21	C	513	CLA	O2D-CGD-CBD	4.84	119.86	111.27
21	b	606	CLA	C4D-CHA-C1A	-4.83	115.37	121.25
21	c	507	CLA	C2C-C1C-NC	4.83	114.50	109.97
24	4	308	KC1	O2D-CGD-CBD	4.83	119.85	111.27
21	B	611	CLA	C2D-C1D-ND	4.83	113.66	110.10
21	1	309	CLA	C2C-C1C-NC	4.82	114.49	109.97
24	9	305	KC1	C2A-C1A-NA	4.82	117.13	109.40
24	2	315	KC1	C1A-C2A-C3A	-4.82	103.29	107.11
24	4	308	KC1	C1A-NA-C4A	-4.82	104.54	106.71
21	6	306	CLA	O2D-CGD-CBD	4.82	119.83	111.27
24	6	311	KC1	CMD-C2D-C1D	4.82	135.87	128.46
21	8	305	CLA	C2D-C1D-ND	4.81	113.65	110.10
24	g	314	KC1	C2A-C1A-NA	4.81	117.12	109.40
21	g	303	CLA	C2C-C1C-NC	4.81	114.48	109.97
21	J	301	CLA	CHD-C1D-ND	-4.81	120.03	124.45
21	c	511	CLA	C1C-C2C-C3C	-4.81	101.90	106.96
21	5	302	CLA	C2D-C1D-ND	4.81	113.65	110.10
21	C	508	CLA	C2C-C1C-NC	4.80	114.47	109.97
24	8	315	KC1	CMA-C3A-C2A	-4.80	116.55	128.30
24	2	316	KC1	CHD-C4C-C3C	-4.80	116.33	125.33
21	c	508	CLA	O2D-CGD-CBD	4.80	119.79	111.27
21	J	306	CLA	CHD-C1D-ND	-4.80	120.05	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	D	404	CLA	C1C-C2C-C3C	-4.79	101.92	106.96
21	3	300	CLA	O2D-CGD-CBD	4.79	119.78	111.27
24	8	316	KC1	CHD-C4C-C3C	-4.79	116.35	125.33
21	2	302	CLA	O2D-CGD-CBD	4.79	119.77	111.27
21	B	609	CLA	C1C-C2C-C3C	-4.78	101.93	106.96
21	5	304	CLA	C4D-CHA-C1A	-4.78	115.43	121.25
21	A	402	CLA	C2C-C1C-NC	4.78	114.45	109.97
24	8	315	KC1	C1A-C2A-C3A	-4.78	103.32	107.11
24	g	313	KC1	O2D-CGD-CBD	4.78	119.76	111.27
24	J	311	KC1	CMD-C2D-C1D	4.78	135.81	128.46
21	4	302	CLA	CHD-C1D-ND	-4.77	120.07	124.45
21	a	403	CLA	C2C-C1C-NC	4.77	114.44	109.97
24	G	307	KC1	O2D-CGD-CBD	4.77	119.75	111.27
21	C	511	CLA	CHD-C1D-ND	-4.77	120.07	124.45
21	C	510	CLA	C2C-C1C-NC	4.77	114.44	109.97
21	6	306	CLA	CHD-C1D-ND	-4.77	120.07	124.45
21	g	307	CLA	O2D-CGD-CBD	4.77	119.74	111.27
24	G	309	KC1	CHC-C1C-C2C	-4.76	117.54	124.98
23	6	309	A86	C26-C25-C24	4.76	138.08	123.22
21	B	610	CLA	C2D-C1D-ND	4.76	113.61	110.10
21	A	404	CLA	CHD-C1D-ND	-4.76	120.08	124.45
21	B	605	CLA	C4D-CHA-C1A	-4.76	115.45	121.25
24	4	307	KC1	O2D-CGD-CBD	4.76	119.73	111.27
21	c	508	CLA	C2C-C1C-NC	4.76	114.43	109.97
21	c	502	CLA	C4D-CHA-C1A	-4.76	115.46	121.25
21	g	306	CLA	C1B-CHB-C4A	-4.76	120.70	130.12
24	g	314	KC1	CHD-C4C-C3C	-4.76	116.40	125.33
24	5	313	KC1	O2D-CGD-CBD	4.76	119.72	111.27
21	g	309	CLA	CHD-C1D-ND	-4.76	120.08	124.45
21	C	512	CLA	C1C-C2C-C3C	-4.75	101.96	106.96
21	D	406	CLA	CHD-C4C-C3C	-4.75	117.56	124.98
21	B	602	CLA	C2C-C1C-NC	4.75	114.42	109.97
21	C	509	CLA	C2C-C1C-NC	4.75	114.42	109.97
21	3	301	CLA	O2D-CGD-CBD	4.75	119.70	111.27
21	b	610	CLA	C1C-C2C-C3C	-4.75	101.97	106.96
21	B	612	CLA	C4D-CHA-C1A	-4.75	115.47	121.25
21	c	512	CLA	O2D-CGD-CBD	4.74	119.70	111.27
24	5	314	KC1	C2A-C1A-NA	4.74	117.01	109.40
21	5	302	CLA	CMC-C2C-C1C	4.74	132.26	125.04
24	8	315	KC1	C1A-NA-C4A	-4.74	104.57	106.71
21	3	304	CLA	CHD-C1D-ND	-4.74	120.10	124.45
24	5	315	KC1	CHD-C4C-C3C	-4.74	116.44	125.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	305	KC1	O2D-CGD-CBD	4.73	119.68	111.27
21	B	606	CLA	CHD-C1D-ND	-4.73	120.11	124.45
21	D	407	CLA	O2D-CGD-CBD	4.73	119.67	111.27
21	4	302	CLA	C1C-C2C-C3C	-4.72	101.99	106.96
21	b	623	CLA	CHD-C1D-ND	-4.72	120.11	124.45
21	2	304	CLA	C2D-C1D-ND	4.72	113.58	110.10
24	3	306	KC1	C2A-C1A-NA	4.72	116.97	109.40
24	G	308	KC1	O2D-CGD-CBD	4.72	119.65	111.27
24	G	307	KC1	C2C-C1C-NC	4.72	115.72	110.57
21	8	304	CLA	CHD-C1D-ND	-4.72	120.12	124.45
21	6	301	CLA	C2D-C1D-ND	4.72	113.58	110.10
21	b	607	CLA	CHD-C1D-ND	-4.71	120.12	124.45
21	9	300	CLA	O2D-CGD-CBD	4.71	119.64	111.27
21	d	404	CLA	C1C-C2C-C3C	-4.71	102.00	106.96
21	b	603	CLA	C2C-C1C-NC	4.71	114.38	109.97
21	C	505	CLA	O2D-CGD-CBD	4.71	119.63	111.27
24	2	314	KC1	CMD-C2D-C1D	4.70	135.69	128.46
21	1	304	CLA	CHD-C1D-ND	-4.70	120.13	124.45
21	6	303	CLA	C4B-CHC-C1C	-4.70	122.38	129.64
21	c	503	CLA	C1C-C2C-C3C	-4.70	102.02	106.96
24	8	313	KC1	O2D-CGD-CBD	4.70	119.61	111.27
24	2	313	KC1	CHC-C1C-C2C	-4.70	117.64	124.98
21	9	304	CLA	O2D-CGD-CBD	4.69	119.61	111.27
21	2	306	CLA	O2D-CGD-CBD	4.69	119.61	111.27
23	2	308	A86	C17-C16-C15	4.69	113.95	109.16
24	J	313	KC1	CHD-C4C-C3C	-4.69	116.53	125.33
21	B	607	CLA	C4D-CHA-C1A	-4.69	115.55	121.25
21	8	303	CLA	C1C-C2C-C3C	-4.69	102.03	106.96
21	C	509	CLA	O2D-CGD-CBD	4.68	119.59	111.27
21	d	404	CLA	O2D-CGD-CBD	4.68	119.59	111.27
21	C	504	CLA	C2C-C1C-NC	4.68	114.36	109.97
21	b	612	CLA	O2D-CGD-CBD	4.68	119.59	111.27
24	2	313	KC1	C2C-C1C-NC	4.68	115.68	110.57
21	5	307	CLA	O2D-CGD-CBD	4.67	119.57	111.27
21	6	304	CLA	C4D-CHA-C1A	-4.67	115.56	121.25
24	3	305	KC1	C2A-C1A-NA	4.67	116.90	109.40
24	5	314	KC1	CHC-C1C-C2C	-4.67	117.68	124.98
21	8	304	CLA	O2D-CGD-CBD	4.67	119.57	111.27
21	5	302	CLA	CHD-C1D-ND	-4.67	120.16	124.45
21	5	303	CLA	C1C-C2C-C3C	-4.67	102.05	106.96
24	8	314	KC1	CMD-C2D-C1D	4.67	135.63	128.46
24	2	315	KC1	CMA-C3A-C2A	-4.66	116.88	128.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	511	CLA	C2C-C1C-NC	4.66	114.34	109.97
21	A	402	CLA	O2D-CGD-CBD	4.66	119.56	111.27
21	D	406	CLA	C1C-C2C-C3C	-4.66	102.79	107.07
21	2	302	CLA	C2C-C1C-NC	4.66	114.34	109.97
21	B	604	CLA	C2C-C1C-NC	4.66	114.34	109.97
21	B	614	CLA	C2C-C1C-NC	4.66	114.34	109.97
21	b	623	CLA	C2D-C1D-ND	4.66	113.54	110.10
21	B	603	CLA	CHD-C1D-ND	-4.66	120.17	124.45
21	G	300	CLA	O2D-CGD-O1D	-4.66	114.73	123.84
21	b	615	CLA	C2C-C1C-NC	4.66	114.34	109.97
24	2	314	KC1	C2A-C1A-NA	4.65	116.87	109.40
21	a	403	CLA	O2D-CGD-CBD	4.65	119.53	111.27
21	d	405	CLA	CHD-C4C-C3C	-4.65	117.72	124.98
21	7	301	CLA	C2C-C1C-NC	4.65	114.33	109.97
21	A	401	CLA	C4D-CHA-C1A	-4.64	115.60	121.25
21	5	305	CLA	C4D-CHA-C1A	-4.64	115.60	121.25
24	5	314	KC1	CHD-C4C-C3C	-4.64	116.61	125.33
21	c	509	CLA	C2C-C1C-NC	4.64	114.32	109.97
21	c	510	CLA	C2C-C1C-NC	4.64	114.32	109.97
21	C	509	CLA	C1C-C2C-C3C	-4.64	102.08	106.96
21	B	615	CLA	O2D-CGD-CBD	4.64	119.52	111.27
21	1	309	CLA	C1C-C2C-C3C	-4.64	102.08	106.96
21	b	605	CLA	C2C-C1C-NC	4.64	114.32	109.97
24	5	315	KC1	C2A-C1A-NA	4.63	116.83	109.40
21	a	405	CLA	CHD-C1D-ND	-4.63	120.19	124.45
24	g	315	KC1	CHD-C4C-C3C	-4.63	116.64	125.33
21	A	402	CLA	C1C-C2C-C3C	-4.63	102.09	106.96
21	B	610	CLA	O2D-CGD-CBD	4.63	119.49	111.27
21	1	309	CLA	C4D-CHA-C1A	-4.63	115.62	121.25
21	C	504	CLA	C2D-C1D-ND	4.63	113.51	110.10
21	C	512	CLA	C4D-CHA-C1A	-4.62	115.62	121.25
21	b	608	CLA	C4D-CHA-C1A	-4.62	115.62	121.25
24	8	316	KC1	CMA-C3A-C2A	-4.62	116.99	128.30
21	C	505	CLA	C2C-C1C-NC	4.62	114.30	109.97
21	8	307	CLA	C2C-C1C-NC	4.62	114.30	109.97
24	7	315	KC1	C1A-NA-C4A	-4.62	104.63	106.71
21	B	602	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
21	4	303	CLA	CHD-C1D-ND	-4.62	120.21	124.45
21	b	616	CLA	C2C-C1C-NC	4.61	114.29	109.97
24	7	314	KC1	CHD-C4C-C3C	-4.61	116.67	125.33
21	C	514	CLA	O2D-CGD-CBD	4.61	119.46	111.27
21	A	401	CLA	C2C-C1C-NC	4.61	114.29	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	621	CLA	C2C-C1C-NC	4.61	114.29	109.97
21	C	510	CLA	O2D-CGD-CBD	4.61	119.45	111.27
21	7	306	CLA	C2D-C1D-ND	4.61	113.50	110.10
21	c	513	CLA	O2D-CGD-CBD	4.61	119.45	111.27
24	5	313	KC1	CHD-C4C-C3C	-4.61	116.68	125.33
21	g	303	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
21	B	610	CLA	CHD-C1D-ND	-4.61	120.22	124.45
21	5	306	CLA	C2C-C1C-NC	4.60	114.29	109.97
21	B	615	CLA	C2C-C1C-NC	4.60	114.28	109.97
21	g	306	CLA	C2C-C1C-NC	4.60	114.28	109.97
21	8	304	CLA	C4-C3-C5	4.60	121.25	115.98
24	5	315	KC1	O2D-CGD-CBD	4.60	119.45	111.27
24	2	313	KC1	CHD-C4C-C3C	-4.60	116.69	125.33
21	6	306	CLA	C2C-C1C-NC	4.60	114.28	109.97
21	a	402	CLA	C2C-C1C-NC	4.60	114.28	109.97
21	g	304	CLA	C2D-C1D-ND	4.60	113.49	110.10
24	g	314	KC1	C2C-C1C-NC	4.60	115.59	110.57
21	b	603	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
21	a	402	CLA	C4D-CHA-C1A	-4.59	115.66	121.25
24	7	314	KC1	C2A-C1A-NA	4.59	116.77	109.40
21	5	302	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
21	a	403	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
21	c	508	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
21	3	301	CLA	C2C-C1C-NC	4.59	114.27	109.97
21	1	310	CLA	C2C-C1C-NC	4.59	114.27	109.97
21	B	612	CLA	C2D-C1D-ND	4.59	113.48	110.10
24	8	313	KC1	CHD-C4C-C3C	-4.58	116.72	125.33
21	d	406	CLA	O2D-CGD-CBD	4.58	119.41	111.27
21	5	302	CLA	O2D-CGD-CBD	4.58	119.41	111.27
24	2	315	KC1	C2C-C1C-NC	4.58	115.58	110.57
21	4	301	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
24	4	309	KC1	O2D-CGD-CBD	4.58	119.40	111.27
24	1	316	KC1	CHD-C4C-C3C	-4.58	116.74	125.33
21	5	308	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
23	4	305	A86	C17-C16-C15	4.57	113.83	109.16
21	4	304	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
21	D	406	CLA	C2D-C1D-ND	4.57	113.47	110.10
24	9	305	KC1	CHD-C4C-C3C	-4.57	116.75	125.33
21	c	503	CLA	C2D-C1D-ND	4.57	113.47	110.10
23	7	312	A86	C17-C16-C15	4.57	113.82	109.16
24	4	308	KC1	C3C-C4C-NC	4.57	114.18	109.88
24	3	305	KC1	CHD-C4C-C3C	-4.56	116.76	125.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	313	KC1	CHD-C4C-C3C	-4.56	116.77	125.33
21	B	614	CLA	C1C-C2C-C3C	-4.56	102.16	106.96
21	b	609	CLA	C2C-C1C-NC	4.56	114.25	109.97
21	C	512	CLA	C2C-C1C-NC	4.56	114.25	109.97
24	4	307	KC1	CHD-C4C-C3C	-4.56	116.77	125.33
21	1	306	CLA	CHD-C1D-ND	-4.56	120.26	124.45
21	B	610	CLA	CHD-C4C-C3C	-4.56	118.14	124.84
21	d	405	CLA	C2D-C1D-ND	4.56	113.46	110.10
21	2	302	CLA	C1C-C2C-C3C	-4.56	102.17	106.96
21	c	510	CLA	CHD-C1D-ND	-4.56	120.27	124.45
24	2	316	KC1	CMA-C3A-C2A	-4.55	117.15	128.30
21	4	301	CLA	C4D-CHA-C1A	-4.55	115.71	121.25
21	7	306	CLA	C2C-C1C-NC	4.55	114.23	109.97
24	8	314	KC1	C1A-NA-C4A	-4.55	104.66	106.71
21	c	511	CLA	C2C-C1C-NC	4.55	114.23	109.97
21	b	615	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
21	1	308	CLA	O2D-CGD-CBD	4.55	119.35	111.27
21	d	405	CLA	CAB-C3B-C4B	-4.54	121.48	128.46
21	B	608	CLA	C2C-C1C-NC	4.54	114.23	109.97
21	D	406	CLA	CAB-C3B-C4B	-4.54	121.48	128.46
21	5	305	CLA	C1C-C2C-C3C	-4.54	102.18	106.96
23	8	311	A86	C17-C16-C15	4.54	113.79	109.16
21	J	306	CLA	C2C-C1C-NC	4.54	114.22	109.97
21	5	308	CLA	C2C-C1C-NC	4.54	114.22	109.97
24	8	314	KC1	CHC-C1C-C2C	-4.53	117.90	124.98
21	6	308	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
21	c	505	CLA	C2C-C1C-NC	4.53	114.22	109.97
21	C	511	CLA	O2D-CGD-O1D	-4.53	114.98	123.84
21	1	302	CLA	C2C-C1C-NC	4.53	114.22	109.97
21	b	614	CLA	O2D-CGD-CBD	4.53	119.32	111.27
21	5	305	CLA	C2C-C1C-NC	4.53	114.22	109.97
21	J	307	CLA	CHD-C1D-ND	-4.53	120.29	124.45
21	c	502	CLA	C2C-C1C-NC	4.53	114.22	109.97
23	5	311	A86	C4-C3-C2	4.53	132.75	123.47
21	b	617	CLA	O2D-CGD-CBD	4.53	119.32	111.27
21	C	504	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
21	g	302	CLA	C2C-C1C-NC	4.53	114.21	109.97
21	2	304	CLA	CHD-C1D-ND	-4.53	120.29	124.45
24	7	315	KC1	CHD-C4C-C3C	-4.53	116.83	125.33
21	7	308	CLA	O2D-CGD-O1D	-4.53	114.99	123.84
21	B	611	CLA	CHD-C4C-C3C	-4.53	118.19	124.84
21	c	508	CLA	C2D-C1D-ND	4.53	113.44	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	610	CLA	C2C-C1C-NC	4.53	114.21	109.97
21	3	304	CLA	O2D-CGD-CBD	4.52	119.31	111.27
21	7	309	CLA	C2C-C1C-NC	4.52	114.21	109.97
24	G	308	KC1	CHD-C4C-C3C	-4.52	116.84	125.33
21	5	304	CLA	C2C-C1C-NC	4.52	114.21	109.97
21	6	301	CLA	CHD-C4C-C3C	-4.52	118.19	124.84
24	1	315	KC1	O2D-CGD-CBD	4.52	119.30	111.27
24	G	308	KC1	CHC-C1C-C2C	-4.52	117.92	124.98
21	c	507	CLA	CHD-C1D-ND	-4.52	120.30	124.45
24	J	312	KC1	CHD-C4C-C3C	-4.52	116.85	125.33
21	B	613	CLA	C2C-C1C-NC	4.52	114.20	109.97
24	1	315	KC1	C2A-C1A-NA	4.52	116.65	109.40
21	4	304	CLA	C4D-CHA-C1A	-4.51	115.75	121.25
24	3	306	KC1	CHC-C1C-C2C	-4.51	117.93	124.98
21	1	307	CLA	C2C-C1C-NC	4.51	114.20	109.97
23	2	309	A86	C4-C3-C2	4.51	132.71	123.47
21	J	305	CLA	C2C-C1C-NC	4.51	114.20	109.97
21	1	301	CLA	O2D-CGD-CBD	4.51	119.28	111.27
21	c	505	CLA	CHD-C1D-ND	-4.51	120.31	124.45
21	9	304	CLA	C4D-CHA-C1A	-4.51	115.77	121.25
21	1	302	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
21	A	404	CLA	O2D-CGD-CBD	4.51	119.28	111.27
23	8	310	A86	C4-C3-C2	4.50	132.70	123.47
21	7	307	CLA	O2D-CGD-O1D	-4.50	115.03	123.84
21	4	302	CLA	CHC-C1C-NC	-4.50	117.37	124.20
21	7	308	CLA	C2C-C1C-NC	4.50	114.19	109.97
21	B	609	CLA	C2D-C1D-ND	4.50	113.42	110.10
24	4	308	KC1	C2A-C1A-NA	4.50	116.61	109.40
21	7	304	CLA	C1C-C2C-C3C	-4.50	102.23	106.96
24	G	306	KC1	C1A-NA-C4A	-4.50	104.68	106.71
24	6	311	KC1	CHC-C1C-C2C	-4.50	117.95	124.98
21	C	508	CLA	C1C-C2C-C3C	-4.50	102.23	106.96
24	8	315	KC1	CHD-C4C-C3C	-4.50	116.89	125.33
24	6	312	KC1	C2A-C1A-NA	4.50	116.61	109.40
21	C	513	CLA	C2C-C1C-NC	4.49	114.18	109.97
21	B	613	CLA	C1C-C2C-C3C	-4.49	102.23	106.96
21	g	309	CLA	C1C-C2C-C3C	-4.49	102.23	106.96
21	b	611	CLA	CHD-C1D-ND	-4.49	120.32	124.45
21	b	611	CLA	C2C-C1C-NC	4.49	114.18	109.97
21	c	511	CLA	C4D-CHA-C1A	-4.49	115.78	121.25
21	A	401	CLA	C1C-C2C-C3C	-4.49	102.23	106.96
21	G	304	CLA	C4D-CHA-C1A	-4.49	115.78	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	309	CLA	C2C-C1C-NC	4.49	114.18	109.97
21	J	308	CLA	C1C-C2C-C3C	-4.49	102.23	106.96
21	g	305	CLA	CHD-C1D-ND	-4.49	120.33	124.45
21	b	612	CLA	CHD-C4C-C3C	-4.49	118.24	124.84
24	2	314	KC1	CHD-C4C-C3C	-4.49	116.90	125.33
21	1	305	CLA	CHD-C1D-ND	-4.49	120.33	124.45
31	B	626	SQD	O7-S-C6	4.49	112.27	106.94
21	c	510	CLA	O2D-CGD-O1D	-4.49	115.07	123.84
24	1	315	KC1	CHD-C4C-C3C	-4.48	116.91	125.33
21	1	305	CLA	C2C-C1C-NC	4.48	114.17	109.97
21	6	302	CLA	CHD-C1D-ND	-4.48	120.33	124.45
21	B	604	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
21	9	302	CLA	O2D-CGD-CBD	4.48	119.23	111.27
21	c	505	CLA	O2D-CGD-O1D	-4.48	115.08	123.84
21	B	613	CLA	O2D-CGD-CBD	4.48	119.22	111.27
21	B	616	CLA	O2D-CGD-CBD	4.48	119.22	111.27
21	7	301	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
21	C	505	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
21	B	616	CLA	C2C-C1C-NC	4.48	114.17	109.97
24	G	309	KC1	C2A-C1A-NA	4.48	116.58	109.40
21	2	303	CLA	C2C-C1C-NC	4.47	114.16	109.97
21	g	308	CLA	C2C-C1C-NC	4.47	114.16	109.97
21	c	509	CLA	O2D-CGD-CBD	4.47	119.22	111.27
21	c	506	CLA	C1C-C2C-C3C	-4.47	102.25	106.96
21	J	301	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
21	b	611	CLA	C2D-C1D-ND	4.47	113.40	110.10
21	J	304	CLA	C4D-CHA-C1A	-4.47	115.81	121.25
21	8	306	CLA	CHD-C1D-ND	-4.47	120.35	124.45
21	b	609	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
21	5	304	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
23	2	310	A86	C17-C16-C15	4.47	113.72	109.16
21	8	306	CLA	C2D-C1D-ND	4.47	113.40	110.10
21	9	300	CLA	C2D-C1D-ND	4.47	113.40	110.10
21	b	614	CLA	C2C-C1C-NC	4.47	114.16	109.97
21	c	502	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
21	C	508	CLA	CHD-C1D-ND	-4.47	120.35	124.45
21	6	305	CLA	C2C-C1C-NC	4.47	114.16	109.97
21	3	302	CLA	C4D-CHA-C1A	-4.46	115.82	121.25
21	c	509	CLA	C2D-C1D-ND	4.46	113.39	110.10
21	b	608	CLA	O2D-CGD-O1D	-4.46	115.11	123.84
21	B	615	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
21	c	513	CLA	C1C-C2C-C3C	-4.46	102.27	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	303	CLA	CHD-C1D-ND	-4.46	120.36	124.45
21	6	307	CLA	C2D-C1D-ND	4.46	113.39	110.10
21	B	614	CLA	C2D-C1D-ND	4.46	113.39	110.10
21	b	610	CLA	C2D-C1D-ND	4.46	113.39	110.10
21	3	301	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
21	1	301	CLA	CHD-C1D-ND	-4.46	120.36	124.45
24	9	306	KC1	CHD-C4C-C3C	-4.46	116.96	125.33
21	a	402	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
21	1	306	CLA	C2D-C1D-ND	4.46	113.39	110.10
24	2	316	KC1	C2C-C1C-NC	4.46	115.44	110.57
21	C	514	CLA	C2C-C1C-NC	4.45	114.14	109.97
21	4	300	CLA	O2D-CGD-O1D	-4.45	115.13	123.84
21	2	305	CLA	C2C-C1C-NC	4.45	114.14	109.97
21	C	506	CLA	C2C-C1C-NC	4.45	114.14	109.97
21	C	515	CLA	C2C-C1C-NC	4.45	114.14	109.97
21	7	307	CLA	C2C-C1C-NC	4.45	114.14	109.97
21	4	302	CLA	C2C-C1C-NC	4.45	114.14	109.97
21	b	605	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
21	b	616	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
21	8	304	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
21	8	304	CLA	C2C-C1C-NC	4.45	114.14	109.97
21	B	608	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
21	b	617	CLA	C2C-C1C-NC	4.45	114.14	109.97
21	d	406	CLA	CHD-C1D-ND	-4.45	120.37	124.45
21	D	406	CLA	CAB-C3B-C2B	4.44	133.39	124.69
21	6	308	CLA	C2C-C1C-NC	4.44	114.13	109.97
21	B	607	CLA	C2C-C1C-NC	4.44	114.13	109.97
21	4	301	CLA	C2C-C1C-NC	4.44	114.13	109.97
21	G	301	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
24	7	315	KC1	O2D-CGD-CBD	4.44	119.16	111.27
24	5	313	KC1	C2A-C1A-NA	4.44	116.53	109.40
24	2	313	KC1	C4B-C3B-C2B	-4.44	103.10	106.75
21	b	623	CLA	C2C-C1C-NC	4.44	114.13	109.97
21	6	305	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
24	J	311	KC1	CHD-C4C-C3C	-4.44	117.00	125.33
21	J	305	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
24	8	314	KC1	C2A-C1A-NA	4.44	116.52	109.40
21	c	504	CLA	C2C-C1C-NC	4.43	114.13	109.97
24	J	312	KC1	C2A-C1A-NA	4.43	116.51	109.40
21	g	302	CLA	O2D-CGD-CBD	4.43	119.15	111.27
24	J	311	KC1	CHC-C1C-C2C	-4.43	118.05	124.98
21	8	302	CLA	C2D-C1D-ND	4.43	113.37	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	d	405	CLA	CAB-C3B-C2B	4.43	133.37	124.69
24	3	306	KC1	C2C-C1C-NC	4.43	115.41	110.57
21	G	304	CLA	C2C-C1C-NC	4.43	114.12	109.97
21	g	302	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
21	6	304	CLA	O2D-CGD-CBD	4.43	119.14	111.27
21	D	407	CLA	CHD-C1D-ND	-4.43	120.38	124.45
21	J	301	CLA	C2C-C1C-NC	4.43	114.12	109.97
21	3	300	CLA	C2D-C1D-ND	4.43	113.37	110.10
24	g	313	KC1	CHD-C4C-C3C	-4.43	117.02	125.33
24	g	313	KC1	CHC-C1C-C2C	-4.43	118.06	124.98
21	2	305	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
21	B	602	CLA	C4D-CHA-C1A	-4.43	115.86	121.25
21	C	503	CLA	CHD-C1D-ND	-4.43	120.39	124.45
24	6	312	KC1	CHD-C4C-C3C	-4.42	117.02	125.33
21	c	514	CLA	C2C-C1C-NC	4.42	114.12	109.97
23	6	309	A86	C4-C3-C2	4.42	132.53	123.47
21	C	513	CLA	C2D-C1D-ND	4.42	113.36	110.10
24	8	316	KC1	C2C-C1C-NC	4.42	115.40	110.57
21	b	613	CLA	CHD-C4C-C3C	-4.42	118.34	124.84
21	c	512	CLA	C2C-C1C-NC	4.42	114.11	109.97
24	9	306	KC1	C2A-C1A-NA	4.42	116.49	109.40
21	b	615	CLA	C2D-C1D-ND	4.42	113.36	110.10
21	B	609	CLA	CHD-C1D-ND	-4.42	120.39	124.45
21	b	614	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
21	J	302	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
21	G	301	CLA	O2D-CGD-CBD	4.41	119.11	111.27
21	c	511	CLA	O2D-CGD-O1D	-4.41	115.21	123.84
24	2	315	KC1	CHD-C4C-C3C	-4.41	117.04	125.33
21	3	300	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
21	C	514	CLA	C2D-C1D-ND	4.41	113.36	110.10
21	c	505	CLA	C2D-C1D-ND	4.41	113.36	110.10
21	6	300	CLA	C2C-C1C-NC	4.41	114.11	109.97
21	1	307	CLA	C2D-C1D-ND	4.41	113.35	110.10
21	c	505	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
21	7	305	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
21	C	514	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
21	1	303	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
21	6	306	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
21	b	613	CLA	C2D-C1D-ND	4.41	113.35	110.10
21	J	308	CLA	C2C-C1C-NC	4.41	114.10	109.97
24	J	311	KC1	C2A-C1A-NA	4.40	116.47	109.40
24	J	313	KC1	C1A-NA-C4A	-4.40	104.73	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	312	KC1	C4B-C3B-C2B	-4.40	103.14	106.75
21	a	405	CLA	O2D-CGD-CBD	4.40	119.09	111.27
21	g	309	CLA	C2C-C1C-NC	4.40	114.09	109.97
21	J	300	CLA	C2C-C1C-NC	4.40	114.09	109.97
21	J	302	CLA	C2C-C1C-NC	4.40	114.09	109.97
24	5	314	KC1	C2C-C1C-NC	4.40	115.37	110.57
21	7	303	CLA	O2D-CGD-CBD	4.40	119.08	111.27
21	c	513	CLA	C2C-C1C-NC	4.40	114.09	109.97
21	C	509	CLA	O2D-CGD-O1D	-4.40	115.24	123.84
21	C	510	CLA	O2D-CGD-O1D	-4.40	115.24	123.84
24	1	316	KC1	CHC-C1C-C2C	-4.40	118.11	124.98
21	9	300	CLA	CHD-C1D-ND	-4.40	120.41	124.45
21	G	304	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
23	6	309	A86	C25-C26-C27	4.40	133.58	127.31
23	2	312	A86	C17-C16-C15	4.40	113.65	109.16
21	8	302	CLA	CHD-C4C-C3C	-4.39	118.38	124.84
21	5	302	CLA	CHD-C4C-C3C	-4.39	118.38	124.84
21	g	303	CLA	C2D-C1D-ND	4.39	113.34	110.10
21	7	307	CLA	O2D-CGD-CBD	4.39	119.07	111.27
21	b	617	CLA	O2D-CGD-O1D	-4.39	115.25	123.84
21	G	301	CLA	C2C-C1C-NC	4.39	114.08	109.97
24	5	315	KC1	C2C-C1C-NC	4.39	115.36	110.57
21	b	612	CLA	CHD-C1D-ND	-4.39	120.42	124.45
21	7	308	CLA	O2D-CGD-CBD	4.39	119.06	111.27
24	4	307	KC1	CHC-C1C-C2C	-4.39	118.13	124.98
21	7	305	CLA	O2D-CGD-O1D	-4.38	115.27	123.84
21	C	503	CLA	O2D-CGD-O1D	-4.38	115.27	123.84
24	G	307	KC1	CHD-C4C-C3C	-4.38	117.10	125.33
21	G	300	CLA	C2C-C1C-NC	4.38	114.08	109.97
21	C	506	CLA	O2D-CGD-O1D	-4.38	115.27	123.84
21	2	303	CLA	C4-C3-C5	4.38	120.99	115.98
21	3	303	CLA	C4D-CHA-C1A	-4.38	115.92	121.25
21	8	307	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
21	C	512	CLA	O2D-CGD-O1D	-4.38	115.28	123.84
24	3	305	KC1	O2D-CGD-CBD	4.38	119.05	111.27
21	C	507	CLA	C1C-C2C-C3C	-4.38	102.36	106.96
21	2	302	CLA	CHD-C1D-ND	-4.37	120.43	124.45
21	B	616	CLA	O2D-CGD-O1D	-4.37	115.29	123.84
21	G	300	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
21	b	616	CLA	O2D-CGD-CBD	4.37	119.04	111.27
21	B	607	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
21	6	303	CLA	C1C-C2C-C3C	-4.37	102.36	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	316	KC1	O2D-CGD-CBD	4.37	119.03	111.27
21	2	303	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
21	7	303	CLA	CHD-C4C-C3C	-4.37	118.42	124.84
21	c	504	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
21	4	301	CLA	O2D-CGD-O1D	-4.37	115.30	123.84
21	3	303	CLA	C2C-C1C-NC	4.36	114.06	109.97
24	6	311	KC1	O2D-CGD-CBD	4.36	119.02	111.27
21	3	302	CLA	C2C-C1C-NC	4.36	114.06	109.97
21	b	604	CLA	CHD-C1D-ND	-4.36	120.44	124.45
24	1	315	KC1	CHC-C1C-C2C	-4.36	118.16	124.98
21	2	304	CLA	CHD-C4C-C3C	-4.36	118.43	124.84
24	8	315	KC1	C2C-C1C-NC	4.36	115.33	110.57
21	6	301	CLA	C2C-C1C-NC	4.36	114.06	109.97
21	7	303	CLA	C2D-C1D-ND	4.36	113.32	110.10
24	3	306	KC1	CHD-C4C-C3C	-4.36	117.15	125.33
24	2	316	KC1	CHC-C1C-C2C	-4.36	118.17	124.98
21	g	306	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
21	8	305	CLA	CHD-C4C-C3C	-4.35	118.44	124.84
21	C	506	CLA	CHD-C1D-ND	-4.35	120.45	124.45
21	b	610	CLA	CHD-C1D-ND	-4.35	120.45	124.45
21	g	302	CLA	C2D-C1D-ND	4.35	113.31	110.10
24	9	305	KC1	CHC-C1C-C2C	-4.35	118.18	124.98
21	b	608	CLA	C2C-C1C-NC	4.35	114.05	109.97
21	b	614	CLA	C2D-C1D-ND	4.35	113.31	110.10
21	b	623	CLA	O2D-CGD-CBD	4.35	119.00	111.27
21	G	303	CLA	C2C-C1C-NC	4.35	114.04	109.97
30	C	518	DGD	O3G-C3G-C2G	-4.35	100.41	110.90
21	7	308	CLA	C1C-C2C-C3C	-4.35	102.39	106.96
21	1	306	CLA	O2D-CGD-CBD	4.35	118.99	111.27
21	J	306	CLA	C1C-C2C-C3C	-4.35	102.39	106.96
24	7	315	KC1	CHC-C1C-C2C	-4.35	118.19	124.98
21	6	308	CLA	CHD-C1D-ND	-4.35	120.46	124.45
21	C	510	CLA	C2D-C1D-ND	4.34	113.31	110.10
21	C	506	CLA	O2D-CGD-CBD	4.34	118.99	111.27
24	6	312	KC1	CHC-C1C-C2C	-4.34	118.19	124.98
21	6	304	CLA	O2D-CGD-O1D	-4.34	115.35	123.84
21	c	512	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
21	J	300	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
21	b	613	CLA	C4D-CHA-C1A	-4.34	115.97	121.25
21	2	306	CLA	O2D-CGD-O1D	-4.34	115.35	123.84
21	g	308	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
21	J	301	CLA	C4D-CHA-C1A	-4.34	115.97	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	J	312	KC1	C4B-C3B-C2B	-4.34	103.19	106.75
21	2	301	CLA	C2D-C1D-ND	4.34	113.30	110.10
24	4	309	KC1	C2A-C1A-NA	4.34	116.36	109.40
21	c	507	CLA	O2D-CGD-O1D	-4.34	115.36	123.84
24	8	313	KC1	C2A-C1A-NA	4.34	116.36	109.40
24	g	314	KC1	CHC-C1C-C2C	-4.33	118.21	124.98
21	4	302	CLA	O2D-CGD-CBD	4.33	118.97	111.27
21	C	511	CLA	C2D-C1D-ND	4.33	113.30	110.10
21	b	608	CLA	O2D-CGD-CBD	4.33	118.97	111.27
21	1	310	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
21	B	612	CLA	CHD-C4C-C3C	-4.33	118.47	124.84
24	G	306	KC1	O2D-CGD-CBD	4.33	118.96	111.27
21	1	302	CLA	O2D-CGD-O1D	-4.33	115.37	123.84
24	4	309	KC1	C4B-C3B-C2B	-4.33	103.20	106.75
21	c	514	CLA	C1C-C2C-C3C	-4.33	102.41	106.96
21	C	503	CLA	C1C-C2C-C3C	-4.33	102.41	106.96
21	c	507	CLA	C1C-C2C-C3C	-4.33	102.41	106.96
21	5	306	CLA	C1C-C2C-C3C	-4.33	102.41	106.96
21	B	613	CLA	C2D-C1D-ND	4.32	113.29	110.10
21	4	300	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
21	G	301	CLA	O2D-CGD-O1D	-4.32	115.39	123.84
21	D	407	CLA	C2C-C1C-NC	4.32	114.02	109.97
24	5	313	KC1	C1A-NA-C4A	-4.32	104.76	106.71
21	7	307	CLA	C1C-C2C-C3C	-4.32	102.42	106.96
24	8	316	KC1	CHC-C1C-C2C	-4.32	118.23	124.98
23	6	309	A86	C3-C4-C5	4.32	132.32	123.47
21	J	307	CLA	C2C-C1C-NC	4.32	114.02	109.97
21	7	302	CLA	C1C-C2C-C3C	-4.32	102.42	106.96
21	8	302	CLA	CHD-C1D-ND	-4.32	120.49	124.45
24	J	312	KC1	CHC-C1C-C2C	-4.32	118.24	124.98
21	B	607	CLA	O2D-CGD-CBD	4.32	118.94	111.27
21	1	308	CLA	C2C-C1C-NC	4.32	114.02	109.97
21	6	303	CLA	C2C-C1C-NC	4.32	114.02	109.97
21	G	301	CLA	C4D-CHA-C1A	-4.32	116.00	121.25
21	C	509	CLA	C2D-C1D-ND	4.32	113.28	110.10
21	1	304	CLA	C2D-C1D-ND	4.31	113.28	110.10
21	c	510	CLA	C2D-C1D-ND	4.31	113.28	110.10
21	B	612	CLA	C2C-C1C-NC	4.31	114.01	109.97
21	5	307	CLA	C2C-C1C-NC	4.31	114.01	109.97
21	6	300	CLA	C2D-C1D-ND	4.31	113.28	110.10
21	a	403	CLA	C2D-C1D-ND	4.31	113.28	110.10
21	a	405	CLA	C2D-C1D-ND	4.31	113.28	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	312	KC1	C2C-C1C-NC	4.31	115.28	110.57
23	8	312	A86	C17-C16-C15	4.31	113.56	109.16
24	7	315	KC1	C2A-C1A-NA	4.31	116.31	109.40
24	G	309	KC1	CHD-C4C-C3C	-4.31	117.24	125.33
21	c	504	CLA	C2D-C1D-ND	4.31	113.28	110.10
21	9	303	CLA	C2C-C1C-NC	4.30	114.00	109.97
24	1	316	KC1	C2A-C1A-NA	4.30	116.30	109.40
24	G	307	KC1	CBA-CAA-C2A	-4.30	108.87	125.27
21	1	303	CLA	C2C-C1C-NC	4.30	114.00	109.97
21	5	309	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
24	4	309	KC1	C1C-C2C-C3C	-4.30	102.43	106.96
21	2	301	CLA	C2C-C1C-NC	4.30	114.00	109.97
21	1	307	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
24	6	311	KC1	C2A-C1A-NA	4.30	116.30	109.40
21	6	300	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
21	6	302	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
21	4	303	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
21	C	508	CLA	O2D-CGD-O1D	-4.30	115.44	123.84
21	B	614	CLA	C4D-CHA-C1A	-4.30	116.02	121.25
21	7	300	CLA	CHD-C1D-ND	-4.29	120.51	124.45
21	b	611	CLA	CHD-C4C-C3C	-4.29	118.53	124.84
21	C	513	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
21	D	404	CLA	O2D-CGD-O1D	-4.29	115.44	123.84
21	1	304	CLA	CHD-C4C-C3C	-4.29	118.53	124.84
21	7	309	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
21	C	508	CLA	O2D-CGD-CBD	4.29	118.89	111.27
21	d	404	CLA	C2D-C1D-ND	4.29	113.27	110.10
21	g	305	CLA	C2C-C1C-NC	4.29	113.99	109.97
21	b	608	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
21	C	515	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
21	5	308	CLA	C2D-C1D-ND	4.29	113.26	110.10
21	9	304	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
24	5	314	KC1	CBA-CAA-C2A	-4.29	108.93	125.27
23	8	308	A86	C-C1-C2	-4.28	116.92	122.92
21	1	308	CLA	C1C-C2C-C3C	-4.28	102.45	106.96
21	A	404	CLA	C2D-C1D-ND	4.28	113.26	110.10
21	2	304	CLA	C2C-C1C-NC	4.28	113.98	109.97
21	a	405	CLA	O2D-CGD-O1D	-4.28	115.47	123.84
21	d	406	CLA	C2C-C1C-NC	4.28	113.98	109.97
21	d	405	CLA	O2D-CGD-O1D	-4.28	115.47	123.84
21	1	301	CLA	C2D-C1D-ND	4.28	113.26	110.10
21	B	606	CLA	C2D-C1D-ND	4.28	113.26	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	511	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
24	g	315	KC1	C2A-C1A-NA	4.28	116.26	109.40
24	6	313	KC1	CHC-C1C-C2C	-4.28	118.30	124.98
21	7	306	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
21	C	506	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
24	8	314	KC1	CHD-C4C-C3C	-4.27	117.30	125.33
31	B	625	SQD	O47-C7-C8	4.27	120.71	111.50
21	9	302	CLA	C1C-C2C-C3C	-4.27	102.46	106.96
21	7	303	CLA	C2C-C1C-NC	4.27	113.97	109.97
21	6	307	CLA	C2C-C1C-NC	4.27	113.97	109.97
21	c	505	CLA	O2D-CGD-CBD	4.27	118.86	111.27
21	b	604	CLA	C2C-C1C-NC	4.27	113.97	109.97
24	J	313	KC1	CHC-C1C-C2C	-4.27	118.31	124.98
21	c	510	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
21	J	304	CLA	C2D-C1D-ND	4.26	113.25	110.10
21	c	508	CLA	O2D-CGD-O1D	-4.26	115.50	123.84
24	5	313	KC1	CHC-C1C-C2C	-4.26	118.32	124.98
21	7	303	CLA	C1C-C2C-C3C	-4.26	102.47	106.96
21	3	303	CLA	C1C-C2C-C3C	-4.26	102.47	106.96
21	1	302	CLA	C2D-C1D-ND	4.26	113.25	110.10
21	J	306	CLA	C2D-C1D-ND	4.26	113.25	110.10
21	9	301	CLA	C2C-C1C-NC	4.26	113.97	109.97
21	9	302	CLA	C2C-C1C-NC	4.26	113.97	109.97
21	A	402	CLA	C2D-C1D-ND	4.26	113.25	110.10
21	D	406	CLA	O2D-CGD-O1D	-4.26	115.50	123.84
24	J	312	KC1	C2C-C1C-NC	4.26	115.22	110.57
21	9	301	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
24	6	311	KC1	CHD-C4C-C3C	-4.26	117.33	125.33
21	2	306	CLA	C2D-C1D-ND	4.26	113.24	110.10
21	A	404	CLA	C2C-C1C-NC	4.26	113.96	109.97
24	G	309	KC1	C1A-NA-C4A	-4.26	104.79	106.71
21	5	306	CLA	C4D-CHA-C1A	-4.26	116.07	121.25
24	5	313	KC1	C2C-C1C-NC	4.26	115.22	110.57
21	2	303	CLA	C2D-C1D-ND	4.26	113.24	110.10
24	g	315	KC1	C2C-C1C-NC	4.25	115.22	110.57
21	7	307	CLA	C2D-C1D-ND	4.25	113.24	110.10
21	2	302	CLA	C2D-C1D-ND	4.25	113.24	110.10
21	J	307	CLA	C1C-C2C-C3C	-4.25	102.48	106.96
21	b	613	CLA	C2C-C1C-NC	4.25	113.96	109.97
21	B	603	CLA	C1C-C2C-C3C	-4.25	102.48	106.96
21	7	303	CLA	O2D-CGD-O1D	-4.25	115.52	123.84
21	a	405	CLA	C1C-C2C-C3C	-4.25	102.49	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	313	KC1	C4B-C3B-C2B	-4.25	103.26	106.75
21	8	305	CLA	C2C-C1C-NC	4.25	113.95	109.97
24	2	313	KC1	C2A-C1A-NA	4.25	116.22	109.40
21	2	301	CLA	CHD-C1D-ND	-4.25	120.55	124.45
21	A	404	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
21	7	305	CLA	C2D-C1D-ND	4.25	113.24	110.10
21	9	304	CLA	O2D-CGD-O1D	-4.25	115.53	123.84
21	g	304	CLA	O2D-CGD-CBD	4.25	118.82	111.27
21	C	504	CLA	CHD-C4C-C3C	-4.25	118.60	124.84
30	c	517	DGD	O3G-C3G-C2G	-4.25	100.65	110.90
21	1	308	CLA	O2D-CGD-O1D	-4.25	115.54	123.84
24	6	313	KC1	C1A-NA-C4A	-4.25	104.80	106.71
21	2	301	CLA	CHD-C4C-C3C	-4.25	118.60	124.84
21	4	301	CLA	CHD-C1D-ND	-4.24	120.55	124.45
21	G	300	CLA	CHD-C1D-ND	-4.24	120.55	124.45
21	C	512	CLA	O2D-CGD-CBD	4.24	118.81	111.27
24	4	308	KC1	CHC-C1C-C2C	-4.24	118.35	124.98
21	C	503	CLA	C2D-C1D-ND	4.24	113.23	110.10
29	g	301	LMU	C1B-O1B-C4'	-4.24	107.47	117.96
24	J	313	KC1	C2A-C1A-NA	4.24	116.20	109.40
21	4	303	CLA	C2C-C1C-NC	4.24	113.94	109.97
21	b	604	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
21	g	306	CLA	C4D-CHA-C1A	-4.24	116.09	121.25
24	4	308	KC1	CHD-C4C-C3C	-4.24	117.37	125.33
21	6	307	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
21	B	621	CLA	C2D-C1D-ND	4.24	113.23	110.10
21	5	302	CLA	C2C-C1C-NC	4.24	113.94	109.97
21	G	300	CLA	C2D-C1D-ND	4.24	113.23	110.10
22	7	310	DD6	C12-C11-C10	-4.23	116.99	122.92
23	8	310	A86	C3-C4-C5	4.23	132.15	123.47
21	b	607	CLA	C2D-C1D-ND	4.23	113.22	110.10
24	5	315	KC1	CHC-C1C-C2C	-4.23	118.36	124.98
21	c	513	CLA	C2D-C1D-ND	4.23	113.22	110.10
21	1	305	CLA	O2D-CGD-O1D	-4.23	115.56	123.84
24	1	315	KC1	C2C-C1C-NC	4.23	115.19	110.57
24	3	305	KC1	C2C-C1C-NC	4.23	115.19	110.57
21	B	603	CLA	C2C-C1C-NC	4.23	113.94	109.97
21	B	611	CLA	O1D-CGD-CBD	-4.23	115.83	124.48
21	D	407	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
27	D	403	LHG	O4-P-O5	4.23	133.15	112.24
21	1	305	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
21	1	301	CLA	C1C-C2C-C3C	-4.23	102.51	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	301	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
27	d	402	LHG	O4-P-O5	4.23	133.13	112.24
21	7	300	CLA	C2D-C1D-ND	4.22	113.22	110.10
22	1	311	DD6	C12-C11-C10	-4.22	117.01	122.92
24	9	306	KC1	CHC-C1C-C2C	-4.22	118.38	124.98
30	B	624	DGD	O3G-C3G-C2G	-4.22	100.71	110.90
21	C	503	CLA	C2C-C1C-NC	4.22	113.93	109.97
21	g	305	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
21	B	610	CLA	O2D-CGD-O1D	-4.22	115.59	123.84
27	B	601	LHG	O4-P-O5	4.22	133.09	112.24
21	b	615	CLA	C4D-CHA-C1A	-4.22	116.12	121.25
21	a	405	CLA	C2C-C1C-NC	4.22	113.92	109.97
24	8	313	KC1	C2C-C1C-NC	4.22	115.17	110.57
24	4	307	KC1	C2C-C1C-NC	4.22	115.17	110.57
21	A	401	CLA	CHD-C1D-ND	-4.22	120.58	124.45
21	8	305	CLA	CHD-C1D-ND	-4.22	120.58	124.45
21	B	602	CLA	C2D-C1D-ND	4.21	113.21	110.10
21	6	300	CLA	CHD-C1D-ND	-4.21	120.58	124.45
21	6	305	CLA	C2D-C1D-ND	4.21	113.21	110.10
21	C	510	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
21	g	302	CLA	CHD-C1D-ND	-4.21	120.59	124.45
21	3	304	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
24	G	308	KC1	C1C-C2C-C3C	-4.21	102.53	106.96
21	5	303	CLA	C2D-C1D-ND	4.21	113.20	110.10
21	G	303	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
27	l	101	LHG	O4-P-O5	4.20	133.02	112.24
21	J	303	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
21	d	406	CLA	C2D-C1D-ND	4.20	113.20	110.10
31	b	602	SQD	O7-S-C6	4.20	111.93	106.94
21	G	300	CLA	O1D-CGD-CBD	-4.20	115.89	124.48
21	B	610	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
21	7	301	CLA	C4D-CHA-C1A	-4.20	116.14	121.25
21	c	512	CLA	C2D-C1D-ND	4.20	113.20	110.10
21	g	304	CLA	C1C-C2C-C3C	-4.20	102.55	106.96
24	2	316	KC1	C2A-C1A-NA	4.20	116.13	109.40
21	G	302	CLA	C4D-CHA-C1A	-4.20	116.14	121.25
21	1	306	CLA	C1C-C2C-C3C	-4.20	102.55	106.96
21	7	300	CLA	C1C-C2C-C3C	-4.20	102.55	106.96
21	c	508	CLA	CHD-C4C-C3C	-4.19	118.67	124.84
21	d	406	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
27	a	401	LHG	O4-P-O5	4.19	132.97	112.24
21	7	304	CLA	C2D-C1D-ND	4.19	113.19	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	305	CLA	C4D-CHA-C1A	-4.19	116.15	121.25
21	B	606	CLA	CHD-C4C-C3C	-4.19	118.68	124.84
21	6	302	CLA	C2C-C1C-NC	4.19	113.90	109.97
21	3	300	CLA	C2C-C1C-NC	4.19	113.90	109.97
21	J	300	CLA	C2D-C1D-ND	4.19	113.19	110.10
21	D	404	CLA	C2D-C1D-ND	4.19	113.19	110.10
24	9	305	KC1	C2C-C1C-NC	4.19	115.14	110.57
21	1	308	CLA	C2D-C1D-ND	4.18	113.19	110.10
21	a	402	CLA	CHD-C1D-ND	-4.18	120.61	124.45
27	A	406	LHG	O4-P-O5	4.18	132.92	112.24
22	g	310	DD6	C12-C11-C10	-4.18	117.06	122.92
21	c	504	CLA	O2D-CGD-O1D	-4.18	115.66	123.84
21	1	308	CLA	C4D-CHA-C1A	-4.18	116.16	121.25
21	G	300	CLA	C4D-CHA-C1A	-4.18	116.16	121.25
21	1	302	CLA	CHD-C4C-C3C	-4.18	118.69	124.84
21	5	308	CLA	CHD-C4C-C3C	-4.18	118.69	124.84
23	7	312	A86	C3-C4-C5	4.18	132.04	123.47
21	1	310	CLA	C2D-C1D-ND	4.18	113.18	110.10
21	6	306	CLA	C2D-C1D-ND	4.18	113.18	110.10
24	8	316	KC1	O2D-CGD-CBD	4.18	118.69	111.27
23	8	312	A86	C3-C4-C5	4.18	132.03	123.47
21	g	307	CLA	C2C-C1C-NC	4.18	113.89	109.97
21	2	301	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
21	G	302	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
21	B	611	CLA	CHD-C1D-ND	-4.18	120.61	124.45
21	3	302	CLA	C1C-C2C-C3C	-4.18	102.57	106.96
21	2	303	CLA	O2D-CGD-O1D	-4.17	115.68	123.84
21	1	302	CLA	C4D-CHA-C1A	-4.17	116.17	121.25
24	J	311	KC1	O2D-CGD-CBD	4.17	118.68	111.27
24	6	313	KC1	C2A-C1A-NA	4.17	116.09	109.40
21	3	301	CLA	C2D-C1D-ND	4.17	113.18	110.10
21	g	308	CLA	C2D-C1D-ND	4.17	113.18	110.10
21	8	303	CLA	CHD-C1D-ND	-4.17	120.62	124.45
21	7	300	CLA	O2D-CGD-CBD	4.17	118.67	111.27
21	g	307	CLA	C1C-C2C-C3C	-4.17	102.58	106.96
21	C	503	CLA	C4D-CHA-C1A	-4.17	116.18	121.25
21	C	514	CLA	O2D-CGD-O1D	-4.17	115.69	123.84
21	B	616	CLA	CHD-C4C-C3C	-4.17	118.72	124.84
29	5	301	LMU	C1B-O1B-C4'	-4.17	107.66	117.96
21	9	304	CLA	CHD-C4C-C3C	-4.16	118.72	124.84
24	8	314	KC1	C2C-C1C-NC	4.16	115.11	110.57
21	6	301	CLA	C4D-CHA-C1A	-4.16	116.19	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	9	302	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
21	b	607	CLA	CHD-C4C-C3C	-4.16	118.72	124.84
21	J	301	CLA	CHD-C4C-NC	4.16	130.76	124.20
21	C	507	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
24	4	309	KC1	CHD-C4C-C3C	-4.16	117.52	125.33
21	b	611	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
21	c	514	CLA	C2D-C1D-ND	4.16	113.17	110.10
21	1	301	CLA	C2C-C1C-NC	4.15	113.86	109.97
21	b	617	CLA	O1D-CGD-CBD	-4.15	115.99	124.48
24	7	314	KC1	C2C-C1C-NC	4.15	115.11	110.57
24	2	315	KC1	C1A-NA-C4A	-4.15	104.84	106.71
21	6	304	CLA	C2D-C1D-ND	4.15	113.16	110.10
21	c	506	CLA	O2D-CGD-O1D	-4.15	115.73	123.84
21	3	301	CLA	O2D-CGD-O1D	-4.15	115.73	123.84
21	C	503	CLA	CHD-C4C-C3C	-4.15	118.74	124.84
21	8	306	CLA	C1C-C2C-C3C	-4.15	102.60	106.96
21	7	307	CLA	C4D-CHA-C1A	-4.15	116.20	121.25
21	b	617	CLA	CHD-C4C-C3C	-4.15	118.75	124.84
21	7	307	CLA	O1D-CGD-CBD	-4.15	116.00	124.48
21	c	506	CLA	C4D-CHA-C1A	-4.14	116.21	121.25
21	J	300	CLA	CHD-C1D-ND	-4.14	120.65	124.45
21	9	301	CLA	CHD-C1D-ND	-4.14	120.65	124.45
21	7	309	CLA	C4D-CHA-C1A	-4.14	116.21	121.25
21	2	302	CLA	C4D-CHA-C1A	-4.14	116.21	121.25
21	G	300	CLA	O2D-CGD-CBD	4.14	118.63	111.27
21	g	304	CLA	C2C-C1C-NC	4.14	113.85	109.97
21	B	609	CLA	CHD-C4C-C3C	-4.14	118.75	124.84
21	c	504	CLA	O2D-CGD-CBD	4.14	118.62	111.27
21	C	506	CLA	C2D-C1D-ND	4.14	113.16	110.10
21	8	303	CLA	C2D-C1D-ND	4.14	113.15	110.10
21	8	303	CLA	CHA-C4D-ND	4.14	141.16	132.50
21	G	301	CLA	CHD-C1D-ND	-4.14	120.65	124.45
21	2	301	CLA	O2D-CGD-O1D	-4.14	115.75	123.84
21	9	303	CLA	C1D-CHD-C4C	-4.13	117.14	126.06
24	2	313	KC1	C1C-C2C-C3C	-4.13	102.61	106.96
21	A	401	CLA	CHD-C4C-C3C	-4.13	118.76	124.84
21	B	616	CLA	O1D-CGD-CBD	-4.13	116.03	124.48
23	G	305	A86	C4-C3-C2	4.13	131.94	123.47
24	4	306	KC1	C1A-NA-C4A	-4.13	104.85	106.71
24	7	314	KC1	CHC-C1C-C2C	-4.13	118.52	124.98
21	7	308	CLA	C2D-C1D-ND	4.13	113.15	110.10
21	B	611	CLA	O2D-CGD-O1D	-4.13	115.76	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	J	305	CLA	C2D-C1D-ND	4.13	113.15	110.10
21	C	513	CLA	CHD-C4C-C3C	-4.13	118.77	124.84
24	G	307	KC1	C1C-C2C-C3C	-4.13	102.62	106.96
21	C	507	CLA	C4D-CHA-C1A	-4.13	116.23	121.25
24	g	314	KC1	CBA-CAA-C2A	-4.13	109.54	125.27
21	7	305	CLA	C2C-C1C-NC	4.13	113.84	109.97
21	a	402	CLA	CHD-C4C-C3C	-4.13	118.78	124.84
21	b	603	CLA	C4D-CHA-C1A	-4.12	116.23	121.25
21	c	513	CLA	C4D-CHA-C1A	-4.12	116.23	121.25
21	6	303	CLA	O2D-CGD-O1D	-4.12	115.77	123.84
21	c	513	CLA	O2D-CGD-O1D	-4.12	115.77	123.84
21	B	606	CLA	C2C-C1C-NC	4.12	113.83	109.97
21	9	303	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
21	g	305	CLA	C2D-C1D-ND	4.12	113.14	110.10
21	B	612	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
21	D	407	CLA	C2D-C1D-ND	4.12	113.14	110.10
21	c	506	CLA	C2D-C1D-ND	4.12	113.14	110.10
21	7	300	CLA	O2D-CGD-O1D	-4.12	115.78	123.84
21	b	603	CLA	C2D-C1D-ND	4.12	113.14	110.10
21	7	302	CLA	C2C-C1C-NC	4.11	113.83	109.97
24	2	316	KC1	C1A-NA-C4A	-4.11	104.86	106.71
21	b	613	CLA	C1C-C2C-C3C	-4.11	102.63	106.96
21	7	304	CLA	CHD-C1D-ND	-4.11	120.68	124.45
21	2	302	CLA	CHA-C4D-ND	4.11	141.10	132.50
21	5	304	CLA	C2D-C1D-ND	4.11	113.13	110.10
21	c	510	CLA	O2D-CGD-CBD	4.11	118.57	111.27
24	G	309	KC1	C1C-C2C-C3C	-4.11	102.64	106.96
21	b	617	CLA	CHD-C1D-ND	-4.11	120.68	124.45
24	1	316	KC1	C2C-C1C-NC	4.11	115.05	110.57
23	5	311	A86	C24-C1-C2	4.10	125.24	118.94
21	9	304	CLA	C2C-C1C-NC	4.10	113.81	109.97
21	c	509	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
21	7	300	CLA	C2C-C1C-NC	4.10	113.81	109.97
21	9	301	CLA	C4D-CHA-C1A	-4.10	116.26	121.25
21	5	307	CLA	CHD-C1D-ND	-4.10	120.69	124.45
21	4	300	CLA	C2C-C1C-NC	4.10	113.81	109.97
21	5	306	CLA	C1B-CHB-C4A	-4.10	122.00	130.12
21	5	305	CLA	C2D-C1D-ND	4.10	113.12	110.10
21	B	611	CLA	O2D-CGD-CBD	4.10	118.55	111.27
24	g	315	KC1	CHC-C1C-C2C	-4.09	118.58	124.98
24	6	313	KC1	C2C-C1C-NC	4.09	115.04	110.57
21	J	307	CLA	C2D-C1D-ND	4.09	113.12	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	515	CLA	C2D-C1D-ND	4.09	113.12	110.10
24	g	313	KC1	C2C-C1C-NC	4.09	115.04	110.57
24	3	305	KC1	CHC-C1C-C2C	-4.09	118.58	124.98
21	C	512	CLA	C2D-C1D-ND	4.09	113.12	110.10
21	b	608	CLA	C2D-C1D-ND	4.09	113.12	110.10
21	d	405	CLA	O2D-CGD-CBD	4.09	118.54	111.27
24	8	316	KC1	C2A-C1A-NA	4.09	115.96	109.40
21	8	306	CLA	C2C-C1C-NC	4.09	113.80	109.97
21	G	303	CLA	C2D-C1D-ND	4.09	113.12	110.10
21	b	623	CLA	C4-C3-C5	4.09	122.15	115.27
24	9	306	KC1	C1A-NA-C4A	-4.09	104.87	106.71
21	1	304	CLA	C2C-C1C-NC	4.08	113.80	109.97
21	b	616	CLA	CHD-C1D-ND	-4.08	120.70	124.45
21	b	607	CLA	C2C-C1C-NC	4.08	113.80	109.97
21	C	511	CLA	O2D-CGD-CBD	4.08	118.52	111.27
21	c	511	CLA	C2D-C1D-ND	4.08	113.11	110.10
21	8	302	CLA	C2C-C1C-NC	4.08	113.79	109.97
21	5	304	CLA	CHD-C1D-ND	-4.08	120.71	124.45
21	B	608	CLA	C4D-CHA-C1A	-4.08	116.29	121.25
21	B	602	CLA	CHD-C4C-C3C	-4.08	118.85	124.84
21	c	509	CLA	CHD-C1D-ND	-4.08	120.71	124.45
21	C	509	CLA	CHD-C4C-C3C	-4.08	118.85	124.84
21	5	307	CLA	C2D-C1D-ND	4.07	113.11	110.10
21	5	307	CLA	C1C-C2C-C3C	-4.07	102.67	106.96
21	9	300	CLA	CHD-C4C-C3C	-4.07	118.85	124.84
24	4	308	KC1	C4B-C3B-C2B	-4.07	103.41	106.75
21	b	604	CLA	CHD-C4C-C3C	-4.07	118.86	124.84
21	1	304	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
21	8	307	CLA	O2D-CGD-CBD	4.07	118.50	111.27
21	4	300	CLA	O2D-CGD-CBD	4.07	118.50	111.27
21	2	301	CLA	C1-C2-C3	-4.07	119.01	126.04
21	4	301	CLA	O2D-CGD-CBD	4.07	118.49	111.27
21	A	404	CLA	CHD-C4C-C3C	-4.06	118.86	124.84
21	B	606	CLA	C1C-C2C-C3C	-4.06	102.68	106.96
21	7	301	CLA	C2D-C1D-ND	4.06	113.10	110.10
21	5	306	CLA	C2D-C1D-ND	4.06	113.10	110.10
21	b	609	CLA	C4D-CHA-C1A	-4.06	116.30	121.25
21	J	302	CLA	CHD-C1D-ND	-4.06	120.72	124.45
21	2	305	CLA	C2D-C1D-ND	4.06	113.10	110.10
23	1	312	A86	C3-C4-C5	4.06	131.79	123.47
24	5	315	KC1	C1A-NA-C4A	-4.06	104.88	106.71
24	g	315	KC1	C1A-NA-C4A	-4.06	104.88	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	303	CLA	CHD-C4C-C3C	-4.06	118.88	124.84
21	B	615	CLA	CHD-C1D-ND	-4.06	120.72	124.45
21	7	308	CLA	O1D-CGD-CBD	-4.06	116.18	124.48
24	8	313	KC1	CHC-C1C-C2C	-4.06	118.64	124.98
21	c	511	CLA	O2D-CGD-CBD	4.05	118.47	111.27
24	9	306	KC1	CBA-CAA-C2A	-4.05	109.83	125.27
21	3	301	CLA	CHD-C4C-C3C	-4.05	118.89	124.84
24	J	313	KC1	C2C-C1C-NC	4.05	115.00	110.57
21	1	309	CLA	C2D-C1D-ND	4.05	113.09	110.10
23	1	314	A86	C3-C4-C5	4.05	131.77	123.47
21	b	607	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
21	c	508	CLA	C4D-CHA-C1A	-4.05	116.32	121.25
21	c	507	CLA	C2D-C1D-ND	4.05	113.09	110.10
21	9	304	CLA	C2D-C1D-ND	4.05	113.09	110.10
21	1	302	CLA	CHD-C1D-ND	-4.05	120.74	124.45
21	7	301	CLA	CHD-C4C-C3C	-4.04	118.89	124.84
21	7	308	CLA	CHD-C4C-C3C	-4.04	118.89	124.84
21	b	604	CLA	C2D-C1D-ND	4.04	113.08	110.10
21	b	611	CLA	O2D-CGD-O1D	-4.04	115.94	123.84
24	7	315	KC1	C2C-C1C-NC	4.04	114.98	110.57
21	A	404	CLA	O2D-CGD-O1D	-4.04	115.94	123.84
21	B	613	CLA	O2D-CGD-O1D	-4.04	115.94	123.84
21	c	512	CLA	CHD-C4C-C3C	-4.04	118.90	124.84
21	C	507	CLA	C2D-C1D-ND	4.04	113.08	110.10
21	2	304	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
21	c	508	CLA	CHD-C1D-ND	-4.04	120.74	124.45
21	J	304	CLA	CHD-C4C-C3C	-4.04	118.91	124.84
21	1	306	CLA	O2D-CGD-O1D	-4.04	115.95	123.84
21	J	303	CLA	CHD-C1D-ND	-4.04	120.75	124.45
21	7	309	CLA	C2D-C1D-ND	4.04	113.08	110.10
21	8	304	CLA	C2D-C1D-ND	4.03	113.08	110.10
24	4	308	KC1	C2C-C1C-NC	4.03	114.97	110.57
21	d	406	CLA	O2D-CGD-O1D	-4.03	115.95	123.84
21	B	603	CLA	C2D-C1D-ND	4.03	113.08	110.10
24	8	316	KC1	C1A-NA-C4A	-4.03	104.89	106.71
21	g	307	CLA	C2D-C1D-ND	4.03	113.08	110.10
21	C	509	CLA	C4D-CHA-C1A	-4.03	116.34	121.25
21	G	302	CLA	CHA-C4D-ND	4.03	140.93	132.50
21	B	621	CLA	CHD-C1D-ND	-4.03	120.75	124.45
21	b	614	CLA	O2D-CGD-O1D	-4.03	115.97	123.84
21	D	406	CLA	O2D-CGD-CBD	4.02	118.42	111.27
21	J	306	CLA	CHD-C4C-C3C	-4.02	118.92	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	316	KC1	O2D-CGD-CBD	4.02	118.42	111.27
21	9	303	CLA	C2D-C1D-ND	4.02	113.07	110.10
21	1	308	CLA	CHD-C1D-ND	-4.02	120.76	124.45
21	4	303	CLA	C2D-C1D-ND	4.02	113.07	110.10
24	8	316	KC1	C4B-C3B-C2B	-4.02	103.45	106.75
21	b	609	CLA	CHD-C4C-C3C	-4.02	118.94	124.84
21	8	305	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
21	a	405	CLA	CHD-C4C-C3C	-4.01	118.94	124.84
21	c	503	CLA	CHD-C4C-C3C	-4.01	118.94	124.84
21	J	302	CLA	C2D-C1D-ND	4.01	113.06	110.10
21	A	402	CLA	O2D-CGD-O1D	-4.01	115.99	123.84
21	1	309	CLA	CHD-C4C-C3C	-4.01	118.94	124.84
21	a	403	CLA	CHD-C4C-C3C	-4.01	118.94	124.84
21	8	307	CLA	C2D-C1D-ND	4.01	113.06	110.10
23	g	312	A86	C3-C4-C5	4.01	131.69	123.47
23	g	312	A86	C4-C3-C2	4.01	131.69	123.47
21	a	403	CLA	C4D-CHA-C1A	-4.01	116.37	121.25
21	8	304	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
21	7	309	CLA	CHD-C1D-ND	-4.01	120.77	124.45
21	3	304	CLA	C2D-C1D-ND	4.01	113.06	110.10
21	g	308	CLA	CHD-C1D-ND	-4.00	120.78	124.45
24	6	311	KC1	C2C-C1C-NC	4.00	114.94	110.57
21	b	603	CLA	O2D-CGD-O1D	-4.00	116.02	123.84
21	G	302	CLA	C2C-C1C-NC	4.00	113.72	109.97
24	9	306	KC1	C2C-C1C-NC	4.00	114.93	110.57
21	B	604	CLA	C2D-C1D-ND	3.99	113.05	110.10
21	G	301	CLA	C2D-C1D-ND	3.99	113.05	110.10
21	6	305	CLA	CHD-C4C-C3C	-3.99	118.97	124.84
21	A	402	CLA	C4D-CHA-C1A	-3.99	116.39	121.25
21	A	402	CLA	CHD-C4C-C3C	-3.99	118.98	124.84
21	5	309	CLA	CHD-C4C-C3C	-3.99	118.98	124.84
30	b	601	DGD	O3G-C3G-C2G	-3.99	101.28	110.90
21	D	404	CLA	O1D-CGD-CBD	-3.99	116.33	124.48
24	2	315	KC1	C1C-C2C-C3C	-3.98	102.77	106.96
21	a	403	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
21	B	608	CLA	CHD-C4C-C3C	-3.98	118.98	124.84
24	8	315	KC1	CBA-CAA-C2A	-3.98	110.09	125.27
21	g	306	CLA	C2D-C1D-ND	3.98	113.04	110.10
21	1	301	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
21	B	611	CLA	C2C-C1C-NC	3.98	113.70	109.97
21	B	603	CLA	CHD-C4C-C3C	-3.98	118.99	124.84
21	b	614	CLA	CHD-C4C-C3C	-3.98	118.99	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	607	CLA	C2D-C1D-ND	3.98	113.04	110.10
21	b	605	CLA	C2D-C1D-ND	3.98	113.03	110.10
21	7	300	CLA	CHD-C4C-C3C	-3.98	119.00	124.84
21	b	615	CLA	CHD-C4C-C3C	-3.98	119.00	124.84
21	B	602	CLA	O2D-CGD-O1D	-3.97	116.07	123.84
23	g	311	A86	C4-C3-C2	3.97	131.61	123.47
21	7	307	CLA	CHD-C4C-C3C	-3.97	119.00	124.84
21	J	302	CLA	C4D-CHA-C1A	-3.97	116.42	121.25
21	B	608	CLA	C2D-C1D-ND	3.97	113.03	110.10
21	G	304	CLA	C2D-C1D-ND	3.97	113.03	110.10
24	2	316	KC1	C4B-C3B-C2B	-3.97	103.49	106.75
24	J	311	KC1	C2C-C1C-NC	3.97	114.91	110.57
21	2	302	CLA	O2D-CGD-O1D	-3.97	116.07	123.84
21	b	609	CLA	C2D-C1D-ND	3.97	113.03	110.10
21	D	407	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
21	c	510	CLA	CHD-C4C-C3C	-3.97	119.00	124.84
21	c	502	CLA	C2D-C1D-ND	3.97	113.03	110.10
24	9	305	KC1	CBA-CAA-C2A	-3.97	110.15	125.27
21	6	302	CLA	C2D-C1D-ND	3.97	113.03	110.10
21	B	614	CLA	CHD-C4C-C3C	-3.97	119.01	124.84
22	1	311	DD6	C3-C4-C5	3.97	131.60	123.47
21	3	301	CLA	CHD-C1D-ND	-3.97	120.81	124.45
21	4	301	CLA	C2D-C1D-ND	3.97	113.03	110.10
21	b	615	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
21	2	302	CLA	C1-C2-C3	-3.96	120.34	126.75
21	b	612	CLA	C2C-C1C-NC	3.96	113.69	109.97
21	C	511	CLA	CHD-C4C-C3C	-3.96	119.02	124.84
21	b	614	CLA	C4D-CHA-C1A	-3.96	116.43	121.25
21	2	305	CLA	O1D-CGD-CBD	-3.96	116.39	124.48
21	2	303	CLA	O2D-CGD-CBD	3.95	118.30	111.27
21	6	305	CLA	CHD-C1D-ND	-3.95	120.82	124.45
21	7	302	CLA	C2D-C1D-ND	3.95	113.02	110.10
21	J	308	CLA	O2D-CGD-O1D	-3.95	116.11	123.84
21	c	506	CLA	CHD-C4C-C3C	-3.95	119.03	124.84
21	1	305	CLA	C4-C3-C5	3.95	120.50	115.98
21	8	302	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
24	2	314	KC1	CHC-C1C-C2C	-3.95	118.81	124.98
24	2	315	KC1	C4B-C3B-C2B	-3.95	103.51	106.75
24	8	316	KC1	CBA-CAA-C2A	-3.95	110.21	125.27
21	b	606	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
21	G	301	CLA	CHD-C4C-C3C	-3.95	119.04	124.84
24	2	314	KC1	C2C-C1C-NC	3.95	114.88	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	605	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
30	H	101	DGD	O3G-C3G-C2G	-3.95	101.38	110.90
21	3	304	CLA	C2C-C1C-NC	3.95	113.67	109.97
21	B	621	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
21	C	512	CLA	CHD-C4C-NC	3.94	130.42	124.20
21	g	303	CLA	CHD-C4C-C3C	-3.94	119.05	124.84
21	2	306	CLA	CHD-C1D-ND	-3.94	120.83	124.45
30	h	103	DGD	O3G-C3G-C2G	-3.94	101.39	110.90
21	C	507	CLA	CHD-C4C-C3C	-3.94	119.05	124.84
24	J	312	KC1	C1C-C2C-C3C	-3.94	102.81	106.96
21	6	304	CLA	CHD-C4C-C3C	-3.93	119.06	124.84
21	B	613	CLA	C4D-CHA-C1A	-3.93	116.46	121.25
21	1	305	CLA	O2D-CGD-CBD	3.93	118.26	111.27
24	8	315	KC1	C1C-C2C-C3C	-3.93	102.82	106.96
21	9	302	CLA	C2D-C1D-ND	3.93	113.00	110.10
21	1	306	CLA	C2C-C1C-NC	3.93	113.66	109.97
24	3	306	KC1	C4B-C3B-C2B	-3.93	103.52	106.75
21	B	604	CLA	CHD-C1D-ND	-3.93	120.84	124.45
21	a	402	CLA	C2D-C1D-ND	3.93	113.00	110.10
21	C	509	CLA	CHD-C1D-ND	-3.93	120.84	124.45
24	J	312	KC1	CBA-CAA-C2A	-3.92	110.31	125.27
24	7	314	KC1	C1C-C2C-C3C	-3.92	102.83	106.96
24	8	314	KC1	CAC-C3C-C4C	3.92	129.90	124.81
21	b	603	CLA	CHD-C4C-C3C	-3.92	119.08	124.84
21	1	301	CLA	CHD-C4C-C3C	-3.92	119.08	124.84
21	C	514	CLA	O1D-CGD-CBD	-3.92	116.46	124.48
21	c	504	CLA	CHD-C1D-ND	-3.92	120.85	124.45
21	1	305	CLA	C2D-C1D-ND	3.92	112.99	110.10
21	C	505	CLA	C2D-C1D-ND	3.92	112.99	110.10
24	4	309	KC1	C1A-NA-C4A	-3.92	104.94	106.71
21	J	305	CLA	CHD-C4C-C3C	-3.92	119.08	124.84
21	B	607	CLA	CHD-C1D-ND	-3.92	120.85	124.45
24	4	307	KC1	C1C-C2C-C3C	-3.92	102.84	106.96
21	4	302	CLA	CHA-C4D-ND	3.92	140.69	132.50
23	1	313	A86	C4-C3-C2	3.92	131.50	123.47
24	g	314	KC1	C1C-C2C-C3C	-3.92	102.84	106.96
21	1	310	CLA	C4D-CHA-C1A	-3.92	116.48	121.25
21	J	303	CLA	O2D-CGD-O1D	-3.92	116.18	123.84
21	b	608	CLA	CHD-C1D-ND	-3.92	120.86	124.45
21	c	511	CLA	CHD-C4C-NC	3.91	130.37	124.20
21	J	303	CLA	C2C-C1C-NC	3.91	113.64	109.97
22	5	310	DD6	C12-C11-C10	-3.91	117.44	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	502	SQD	O7-S-C6	3.91	111.59	106.94
23	G	305	A86	C3-C4-C5	3.91	131.49	123.47
21	c	502	CLA	CHD-C1D-ND	-3.91	120.86	124.45
21	A	401	CLA	C2D-C1D-ND	3.91	112.98	110.10
21	D	404	CLA	C4D-CHA-C1A	-3.91	116.49	121.25
21	B	613	CLA	CHD-C4C-C3C	-3.91	119.10	124.84
21	1	303	CLA	C2D-C1D-ND	3.91	112.98	110.10
23	8	308	A86	C28-C27-C26	-3.91	117.45	122.92
21	6	308	CLA	O2D-CGD-O1D	-3.91	116.20	123.84
21	9	301	CLA	O2D-CGD-O1D	-3.90	116.20	123.84
23	J	309	A86	C3-C4-C5	3.90	131.47	123.47
21	3	301	CLA	C4D-CHA-C1A	-3.90	116.50	121.25
21	5	308	CLA	CHD-C1D-ND	-3.90	120.87	124.45
21	C	508	CLA	C2D-C1D-ND	3.90	112.98	110.10
24	4	308	KC1	C1C-C2C-C3C	-3.90	102.86	106.96
21	2	303	CLA	C4D-CHA-C1A	-3.90	116.50	121.25
21	c	502	CLA	CHD-C4C-C3C	-3.90	119.11	124.84
21	c	513	CLA	O1D-CGD-CBD	-3.90	116.51	124.48
21	J	302	CLA	CHD-C4C-C3C	-3.90	119.11	124.84
24	2	315	KC1	CBA-CAA-C2A	-3.90	110.41	125.27
24	6	312	KC1	C1C-C2C-C3C	-3.90	102.86	106.96
21	D	404	CLA	O2D-CGD-CBD	3.90	118.19	111.27
23	2	309	A86	C3-C4-C5	3.90	131.46	123.47
24	G	308	KC1	C4B-C3B-C2B	-3.90	103.55	106.75
24	3	306	KC1	C1C-C2C-C3C	-3.89	102.86	106.96
21	6	306	CLA	CHD-C4C-C3C	-3.89	119.12	124.84
21	C	504	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
21	G	303	CLA	CHD-C1D-ND	-3.89	120.88	124.45
21	b	610	CLA	CHD-C4C-C3C	-3.89	119.12	124.84
24	6	312	KC1	CBA-CAA-C2A	-3.89	110.46	125.27
21	B	603	CLA	C4D-CHA-C1A	-3.88	116.52	121.25
21	2	305	CLA	CHD-C4C-C3C	-3.88	119.13	124.84
21	d	406	CLA	CHD-C4C-C3C	-3.88	119.13	124.84
23	2	312	A86	C3-C4-C5	3.88	131.42	123.47
21	1	307	CLA	C4D-CHA-C1A	-3.88	116.53	121.25
21	5	308	CLA	C4D-CHA-C1A	-3.88	116.53	121.25
22	g	310	DD6	C4-C3-C2	3.88	131.42	123.47
21	5	309	CLA	C2D-C1D-ND	3.88	112.96	110.10
21	d	404	CLA	CHD-C4C-C3C	-3.88	119.14	124.84
21	2	305	CLA	CHD-C1D-ND	-3.88	120.89	124.45
24	8	314	KC1	C4B-C3B-C2B	-3.88	103.57	106.75
24	G	306	KC1	C2C-C3C-C4C	-3.88	102.57	107.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	1	314	A86	C4-C3-C2	3.88	131.41	123.47
21	J	303	CLA	C4D-CHA-C1A	-3.87	116.53	121.25
23	5	311	A86	C-C1-C2	-3.87	117.50	122.92
21	6	307	CLA	CHD-C4C-C3C	-3.87	119.15	124.84
21	7	305	CLA	O1D-CGD-CBD	-3.87	116.57	124.48
21	b	612	CLA	O2D-CGD-O1D	-3.87	116.27	123.84
21	7	304	CLA	O2D-CGD-CBD	3.87	118.14	111.27
24	8	315	KC1	C4B-C3B-C2B	-3.87	103.58	106.75
21	J	305	CLA	CHD-C1D-ND	-3.87	120.90	124.45
21	B	616	CLA	CHD-C1D-ND	-3.87	120.90	124.45
24	6	311	KC1	C1A-NA-C4A	-3.87	104.97	106.71
21	b	606	CLA	CHD-C4C-C3C	-3.87	119.16	124.84
21	b	615	CLA	CHD-C1D-ND	-3.87	120.90	124.45
23	J	309	A86	C4-C3-C2	3.86	131.39	123.47
24	J	311	KC1	C1A-NA-C4A	-3.86	104.97	106.71
21	b	614	CLA	CHD-C1D-ND	-3.86	120.90	124.45
21	1	308	CLA	CHD-C4C-C3C	-3.86	119.16	124.84
24	g	315	KC1	C1C-C2C-C3C	-3.86	102.90	106.96
21	a	405	CLA	C4D-CHA-C1A	-3.86	116.55	121.25
24	G	307	KC1	CHC-C1C-C2C	-3.86	118.95	124.98
21	3	302	CLA	CHA-C4D-ND	3.86	140.57	132.50
21	c	502	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
24	5	314	KC1	C4B-C3B-C2B	-3.86	103.58	106.75
21	1	302	CLA	O2D-CGD-CBD	3.86	118.12	111.27
24	4	306	KC1	C3C-C2C-C1C	-3.86	102.59	107.21
21	5	303	CLA	CHD-C4C-C3C	-3.86	119.17	124.84
21	b	604	CLA	C4D-CHA-C1A	-3.85	116.56	121.25
21	b	605	CLA	CHD-C1D-ND	-3.85	120.91	124.45
21	C	505	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
24	4	307	KC1	CAA-CBA-CGA	-3.85	107.47	127.26
21	8	303	CLA	C4D-CHA-C1A	-3.85	116.57	121.25
31	B	625	SQD	O7-S-C6	3.84	111.51	106.94
21	b	605	CLA	C4-C3-C5	3.84	121.74	115.27
21	D	404	CLA	CHD-C4C-C3C	-3.84	119.19	124.84
21	g	309	CLA	C2D-C1D-ND	3.84	112.94	110.10
21	B	604	CLA	C4-C3-C5	3.84	121.73	115.27
24	9	305	KC1	C1C-C2C-C3C	-3.84	102.92	106.96
24	J	313	KC1	C1C-C2C-C3C	-3.84	102.92	106.96
21	2	306	CLA	C4D-CHA-C1A	-3.84	116.58	121.25
28	b	622	LMG	O6-C5-C4	3.84	116.66	109.69
21	5	305	CLA	CHD-C4C-C3C	-3.83	119.20	124.84
21	3	300	CLA	CHC-C1C-NC	-3.83	118.39	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	313	KC1	C1C-C2C-C3C	-3.83	102.93	106.96
21	8	304	CLA	CHD-C4C-C3C	-3.83	119.21	124.84
21	8	306	CLA	CHD-C4C-C3C	-3.83	119.21	124.84
24	6	313	KC1	C1C-C2C-C3C	-3.83	102.93	106.96
21	g	309	CLA	CHA-C4D-ND	3.83	140.50	132.50
23	4	305	A86	C3-C4-C5	3.83	131.31	123.47
23	8	310	A86	C7-C6-C5	-3.83	117.56	122.92
23	2	311	A86	C4-C3-C2	3.82	131.31	123.47
21	8	304	CLA	C4D-CHA-C1A	-3.82	116.59	121.25
21	d	405	CLA	C2C-C1C-NC	3.82	113.55	109.97
21	C	510	CLA	C4D-CHA-C1A	-3.82	116.60	121.25
24	8	316	KC1	C1C-C2C-C3C	-3.82	102.94	106.96
21	B	605	CLA	CHD-C4C-C3C	-3.82	119.23	124.84
21	7	306	CLA	C4D-CHA-C1A	-3.82	116.60	121.25
24	4	306	KC1	C3C-C4C-CHD	-3.82	116.53	125.67
21	c	512	CLA	CHD-C1D-ND	-3.82	120.94	124.45
24	G	306	KC1	C3C-C4C-CHD	-3.82	116.53	125.67
21	D	407	CLA	CHD-C4C-C3C	-3.82	119.23	124.84
21	4	300	CLA	C2D-C1D-ND	3.82	112.92	110.10
24	2	314	KC1	C4B-C3B-C2B	-3.81	103.62	106.75
22	5	310	DD6	C4-C3-C2	3.81	131.28	123.47
24	2	316	KC1	CBA-CAA-C2A	-3.81	110.74	125.27
21	J	300	CLA	CHD-C4C-C3C	-3.81	119.24	124.84
21	2	306	CLA	CHD-C4C-C3C	-3.81	119.24	124.84
21	1	306	CLA	CHD-C4C-C3C	-3.81	119.24	124.84
31	X	401	SQD	O7-S-C6	3.81	111.47	106.94
21	4	302	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
21	c	505	CLA	O1D-CGD-CBD	-3.81	116.69	124.48
24	2	316	KC1	C1C-C2C-C3C	-3.81	102.95	106.96
21	c	510	CLA	O1D-CGD-CBD	-3.81	116.70	124.48
24	5	313	KC1	C1C-C2C-C3C	-3.80	102.96	106.96
24	G	308	KC1	CBA-CAA-C2A	-3.80	110.78	125.27
21	C	511	CLA	O1D-CGD-CBD	-3.80	116.70	124.48
21	b	623	CLA	CHA-C4D-ND	3.80	140.45	132.50
23	5	312	A86	C3-C4-C5	3.80	131.26	123.47
21	c	505	CLA	C4D-CHA-C1A	-3.80	116.62	121.25
24	G	306	KC1	C4B-C3B-C2B	-3.80	103.63	106.75
21	4	302	CLA	C2D-C1D-ND	3.80	112.90	110.10
23	J	310	A86	C3-C4-C5	3.80	131.25	123.47
21	b	616	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
24	2	314	KC1	CBA-CAA-C2A	-3.80	110.80	125.27
21	C	514	CLA	C4D-CHA-C1A	-3.80	116.63	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	302	CLA	CHD-C1D-ND	-3.79	120.97	124.45
21	C	510	CLA	O1D-CGD-CBD	-3.79	116.72	124.48
21	c	509	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
21	J	308	CLA	C2D-C1D-ND	3.79	112.90	110.10
21	4	300	CLA	O1D-CGD-CBD	-3.79	116.73	124.48
21	6	300	CLA	CHD-C4C-C3C	-3.79	119.27	124.84
21	B	616	CLA	CHA-C4D-ND	3.79	140.43	132.50
21	B	611	CLA	C4D-CHA-C1A	-3.79	116.64	121.25
23	1	312	A86	C4-C3-C2	3.79	131.24	123.47
22	7	310	DD6	C4-C3-C2	3.79	131.23	123.47
23	8	308	A86	C3-C4-C5	3.79	131.23	123.47
31	B	626	SQD	O9-S-O7	-3.79	100.85	113.95
24	G	307	KC1	C4B-C3B-C2B	-3.78	103.64	106.75
24	5	315	KC1	C1C-C2C-C3C	-3.78	102.98	106.96
21	b	623	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
21	B	621	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
23	8	310	A86	C-C1-C2	-3.78	117.63	122.92
24	1	315	KC1	C1C-C2C-C3C	-3.78	102.98	106.96
21	C	512	CLA	O1D-CGD-CBD	-3.78	116.75	124.48
21	9	300	CLA	C2C-C1C-NC	3.78	113.51	109.97
31	b	602	SQD	O9-S-O7	-3.78	100.88	113.95
24	2	313	KC1	O2D-CGD-CBD	3.78	117.98	111.27
24	7	314	KC1	C4B-C3B-C2B	-3.77	103.65	106.75
21	C	505	CLA	C4D-CHA-C1A	-3.77	116.66	121.25
31	X	401	SQD	O47-C7-C8	3.77	119.63	111.50
21	9	300	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
21	c	513	CLA	CHD-C4C-C3C	-3.77	119.30	124.84
21	C	514	CLA	CHD-C4C-C3C	-3.77	119.30	124.84
21	C	506	CLA	O1D-CGD-CBD	-3.77	116.77	124.48
21	B	611	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	3	305	KC1	C1C-C2C-C3C	-3.76	103.00	106.96
24	8	314	KC1	CBA-CAA-C2A	-3.76	110.94	125.27
24	5	314	KC1	C1C-C2C-C3C	-3.76	103.00	106.96
21	8	307	CLA	CHA-C4D-ND	3.76	140.36	132.50
23	6	310	A86	C3-C4-C5	3.76	131.17	123.47
21	9	302	CLA	O1D-CGD-CBD	-3.76	116.80	124.48
21	1	310	CLA	C4-C3-C5	3.75	121.59	115.27
21	1	308	CLA	O1D-CGD-CBD	-3.75	116.81	124.48
21	4	304	CLA	C2D-C1D-ND	3.75	112.87	110.10
23	1	313	A86	C3-C4-C5	3.75	131.16	123.47
23	2	307	A86	C4-C3-C2	3.75	131.15	123.47
21	9	304	CLA	O1D-CGD-CBD	-3.75	116.81	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	6	309	A86	C8-C6-C5	3.75	124.69	118.94
24	4	306	KC1	C2C-C3C-C4C	-3.74	102.73	107.21
22	5	310	DD6	C3-C4-C5	3.74	131.14	123.47
21	J	303	CLA	CHA-C4D-ND	3.74	140.33	132.50
31	C	502	SQD	O9-S-C6	3.74	111.39	106.94
21	7	303	CLA	O1D-CGD-CBD	-3.74	116.83	124.48
21	5	304	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
24	6	311	KC1	C1C-C2C-C3C	-3.74	103.03	106.96
24	J	311	KC1	C1C-C2C-C3C	-3.74	103.03	106.96
23	2	310	A86	C3-C4-C5	3.74	131.13	123.47
21	B	614	CLA	CHD-C1D-ND	-3.73	121.02	124.45
21	b	612	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
21	J	308	CLA	CHD-C1D-ND	-3.73	121.03	124.45
21	4	304	CLA	C1B-CHB-C4A	-3.73	122.73	130.12
21	B	607	CLA	CHD-C4C-C3C	-3.73	119.36	124.84
31	B	625	SQD	O9-S-C6	3.73	111.37	106.94
21	8	302	CLA	C4-C3-C5	3.73	121.54	115.27
21	A	404	CLA	C4D-CHA-C1A	-3.73	116.71	121.25
21	7	304	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
21	b	608	CLA	CHD-C4C-C3C	-3.72	119.36	124.84
21	7	308	CLA	CHD-C1D-ND	-3.72	121.03	124.45
21	8	307	CLA	O1D-CGD-CBD	-3.72	116.87	124.48
21	B	613	CLA	CHD-C1D-ND	-3.72	121.03	124.45
21	c	509	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
31	B	625	SQD	O9-S-O7	-3.72	101.08	113.95
21	6	308	CLA	C2D-C1D-ND	3.72	112.84	110.10
23	5	311	A86	C3-C4-C5	3.72	131.09	123.47
24	7	314	KC1	CBA-CAA-C2A	-3.72	111.10	125.27
24	J	311	KC1	CBA-CAA-C2A	-3.71	111.11	125.27
24	J	311	KC1	C4B-C3B-C2B	-3.71	103.70	106.75
21	4	301	CLA	O1D-CGD-CBD	-3.71	116.89	124.48
21	7	304	CLA	CHA-C4D-ND	3.71	140.27	132.50
21	1	302	CLA	O1D-CGD-CBD	-3.71	116.89	124.48
21	c	511	CLA	O1D-CGD-CBD	-3.71	116.89	124.48
21	G	301	CLA	O1D-CGD-CBD	-3.71	116.89	124.48
21	2	302	CLA	CHD-C4C-C3C	-3.71	119.39	124.84
21	J	308	CLA	CHD-C4C-C3C	-3.71	119.39	124.84
21	4	301	CLA	CHD-C4C-C3C	-3.71	119.39	124.84
21	b	612	CLA	C4D-CHA-C1A	-3.71	116.74	121.25
21	3	300	CLA	C4D-CHA-C1A	-3.71	116.74	121.25
24	G	306	KC1	C3C-C2C-C1C	-3.71	102.77	107.21
24	2	313	KC1	CAA-CBA-CGA	-3.71	108.21	127.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	306	KC1	C4B-C3B-C2B	-3.71	103.71	106.75
21	C	506	CLA	CHD-C4C-C3C	-3.70	119.39	124.84
21	c	512	CLA	CHA-C4D-ND	3.70	140.25	132.50
21	3	303	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
21	B	614	CLA	CHA-C4D-ND	3.70	140.24	132.50
21	c	504	CLA	CHA-C4D-ND	3.70	140.24	132.50
22	g	310	DD6	C3-C4-C5	3.70	131.05	123.47
21	C	505	CLA	CHD-C4C-C3C	-3.70	119.40	124.84
23	2	309	A86	C24-C1-C2	3.70	124.62	118.94
23	8	311	A86	C3-C4-C5	3.70	131.05	123.47
23	2	311	A86	C3-C4-C5	3.70	131.05	123.47
21	C	506	CLA	C4-C3-C5	3.69	121.48	115.27
21	1	307	CLA	CHD-C4C-C3C	-3.69	119.42	124.84
21	C	510	CLA	CHD-C4C-C3C	-3.69	119.42	124.84
26	d	403	PHO	CMB-C2B-C3B	3.69	131.58	124.68
21	G	304	CLA	C1B-CHB-C4A	-3.69	122.81	130.12
23	7	312	A86	C4-C3-C2	3.68	131.02	123.47
21	b	615	CLA	CHA-C4D-ND	3.68	140.20	132.50
21	B	602	CLA	CHD-C1D-ND	-3.68	121.07	124.45
21	3	303	CLA	C1B-CHB-C4A	-3.68	122.83	130.12
21	C	505	CLA	CHA-C4D-ND	3.68	140.20	132.50
21	4	300	CLA	CHC-C1C-NC	-3.68	118.62	124.20
21	A	402	CLA	CHA-C4D-ND	3.68	140.20	132.50
24	8	313	KC1	CBA-CAA-C2A	-3.68	111.25	125.27
23	g	312	A86	C28-C27-C26	-3.68	117.77	122.92
21	a	403	CLA	CHA-C4D-ND	3.68	140.19	132.50
21	C	513	CLA	C4D-CHA-C1A	-3.68	116.78	121.25
21	J	307	CLA	C4D-CHA-C1A	-3.67	116.78	121.25
21	7	306	CLA	CHD-C4C-C3C	-3.67	119.44	124.84
24	G	309	KC1	CAA-CBA-CGA	-3.67	108.38	127.26
24	2	314	KC1	C1C-C2C-C3C	-3.67	103.09	106.96
21	b	605	CLA	CHA-C4D-ND	3.67	140.18	132.50
21	6	301	CLA	CHD-C1D-ND	-3.67	121.08	124.45
31	C	502	SQD	O9-S-O7	-3.67	101.25	113.95
23	J	310	A86	C4-C3-C2	3.67	130.99	123.47
21	B	605	CLA	CHA-C4D-ND	3.66	140.16	132.50
21	g	303	CLA	CHA-C4D-ND	3.66	140.16	132.50
23	6	309	A86	C7-C6-C5	-3.66	117.80	122.92
21	b	606	CLA	CHA-C4D-ND	3.66	140.15	132.50
21	b	616	CLA	C2D-C1D-ND	3.66	112.80	110.10
21	4	300	CLA	C4-C3-C5	3.66	121.42	115.27
21	7	300	CLA	O1D-CGD-CBD	-3.66	117.00	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	315	KC1	C4B-C3B-C2B	-3.66	103.75	106.75
24	9	306	KC1	C4B-C3B-C2B	-3.65	103.75	106.75
23	8	310	A86	C24-C1-C2	3.65	124.55	118.94
21	5	308	CLA	CHA-C4D-ND	3.65	140.14	132.50
26	D	401	PHO	CMB-C2B-C3B	3.65	131.51	124.68
21	C	506	CLA	C4D-CHA-C1A	-3.65	116.81	121.25
21	B	604	CLA	CHA-C4D-ND	3.65	140.13	132.50
21	c	505	CLA	CHD-C4C-C3C	-3.65	119.48	124.84
21	g	307	CLA	CHD-C4C-C3C	-3.65	119.48	124.84
24	5	313	KC1	C4B-C3B-C2B	-3.65	103.76	106.75
31	X	401	SQD	O9-S-C6	3.65	111.27	106.94
31	X	401	SQD	O9-S-O7	-3.65	101.33	113.95
21	g	304	CLA	CHD-C4C-C3C	-3.65	119.48	124.84
21	B	608	CLA	CHD-C1D-ND	-3.65	121.10	124.45
21	5	305	CLA	CHA-C4D-ND	3.65	140.13	132.50
23	1	312	A86	C7-C6-C5	-3.65	117.82	122.92
21	J	300	CLA	CHA-C4D-ND	3.64	140.12	132.50
21	5	307	CLA	C4D-CHA-C1A	-3.64	116.81	121.25
21	8	302	CLA	O1D-CGD-CBD	-3.64	117.03	124.48
24	g	313	KC1	CAA-CBA-CGA	-3.64	108.55	127.26
23	g	311	A86	C3-C4-C5	3.64	130.93	123.47
21	b	617	CLA	CHA-C4D-ND	3.64	140.11	132.50
23	W	101	A86	C4-C3-C2	3.64	130.93	123.47
29	a	408	LMU	C1B-O1B-C4'	-3.64	108.96	117.96
21	b	606	CLA	C2D-C1D-ND	3.64	112.78	110.10
21	J	305	CLA	CHA-C4D-ND	3.64	140.10	132.50
21	d	405	CLA	O1D-CGD-CBD	-3.63	117.05	124.48
24	7	315	KC1	C4B-C3B-C2B	-3.63	103.77	106.75
21	6	301	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
24	8	315	KC1	CAA-CBA-CGA	-3.63	108.60	127.26
24	3	305	KC1	C4B-C3B-C2B	-3.63	103.77	106.75
21	D	406	CLA	O1D-CGD-CBD	-3.63	117.06	124.48
23	7	311	A86	C3-C4-C5	3.63	130.91	123.47
21	D	406	CLA	C2C-C1C-NC	3.63	113.37	109.97
21	c	514	CLA	CHA-C4D-ND	3.63	140.09	132.50
23	7	313	A86	C4-C3-C2	3.63	130.90	123.47
21	J	301	CLA	O2D-CGD-O1D	-3.63	116.75	123.84
21	A	404	CLA	O1D-CGD-CBD	-3.62	117.07	124.48
21	B	614	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
21	C	515	CLA	CHA-C4D-ND	3.62	140.08	132.50
24	g	314	KC1	C4B-C3B-C2B	-3.62	103.78	106.75
21	C	508	CLA	CHA-C4D-ND	3.62	140.07	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	g	302	CLA	CHA-C4D-ND	3.62	140.07	132.50
23	7	311	A86	C4-C3-C2	3.62	130.89	123.47
21	B	605	CLA	C2D-C1D-ND	3.62	112.77	110.10
21	6	303	CLA	CHD-C1D-ND	-3.62	121.13	124.45
21	c	508	CLA	O1D-CGD-CBD	-3.61	117.09	124.48
23	J	309	A86	C7-C6-C5	-3.61	117.86	122.92
21	5	302	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
21	2	305	CLA	CHA-C4D-ND	3.61	140.05	132.50
24	9	306	KC1	C1C-C2C-C3C	-3.61	103.16	106.96
24	2	313	KC1	CBA-CAA-C2A	-3.61	111.51	125.27
23	5	312	A86	C4-C3-C2	3.61	130.86	123.47
23	7	312	A86	C7-C6-C5	-3.61	117.87	122.92
21	G	303	CLA	CHA-C4D-ND	3.61	140.04	132.50
21	J	305	CLA	C4D-CHA-C1A	-3.60	116.86	121.25
23	2	310	A86	C4-C3-C2	3.60	130.85	123.47
23	4	305	A86	C-C1-C2	-3.60	117.88	122.92
21	6	305	CLA	C4D-CHA-C1A	-3.60	116.87	121.25
24	1	316	KC1	C1C-C2C-C3C	-3.60	103.17	106.96
21	J	307	CLA	CHD-C4C-C3C	-3.60	119.55	124.84
21	9	301	CLA	CHD-C4C-C3C	-3.60	119.55	124.84
21	4	303	CLA	C4D-CHA-C1A	-3.60	116.87	121.25
21	8	302	CLA	CHA-C4D-ND	3.60	140.02	132.50
21	B	613	CLA	CHA-C4D-ND	3.60	140.02	132.50
21	c	507	CLA	CHA-C4D-ND	3.60	140.02	132.50
21	8	305	CLA	C4D-CHA-C1A	-3.60	116.87	121.25
21	6	304	CLA	CHA-C4D-ND	3.59	140.02	132.50
23	J	309	A86	C8-C6-C5	3.59	124.45	118.94
21	c	503	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
23	2	308	A86	C4-C3-C2	3.59	130.83	123.47
21	B	615	CLA	C2D-C1D-ND	3.59	112.75	110.10
23	2	309	A86	C-C1-C2	-3.59	117.89	122.92
21	1	305	CLA	C4D-CHA-C1A	-3.59	116.88	121.25
21	7	303	CLA	C4D-CHA-C1A	-3.59	116.88	121.25
21	5	304	CLA	CHD-C4C-C3C	-3.59	119.56	124.84
21	C	508	CLA	O1D-CGD-CBD	-3.59	117.14	124.48
23	8	309	A86	C3-C4-C5	3.59	130.82	123.47
21	D	407	CLA	CHA-C4D-ND	3.59	140.00	132.50
21	c	509	CLA	CHA-C4D-ND	3.59	140.00	132.50
21	B	606	CLA	CHA-C4D-ND	3.58	140.00	132.50
21	b	603	CLA	CHA-C4D-ND	3.58	140.00	132.50
21	c	505	CLA	C4-C3-C5	3.58	121.30	115.27
22	1	311	DD6	C8-C6-C5	3.58	124.44	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	313	KC1	C1C-C2C-C3C	-3.58	103.19	106.96
21	8	302	CLA	C4D-CHA-C1A	-3.58	116.89	121.25
31	C	502	SQD	O47-C7-C8	3.58	119.21	111.50
21	6	305	CLA	CHA-C4D-ND	3.58	139.98	132.50
21	b	623	CLA	O2D-CGD-O1D	-3.58	116.85	123.84
21	C	509	CLA	O1D-CGD-CBD	-3.58	117.17	124.48
21	6	307	CLA	CHA-C4D-ND	3.58	139.98	132.50
21	7	301	CLA	CHA-C4D-ND	3.57	139.98	132.50
24	8	314	KC1	C1C-C2C-C3C	-3.57	103.20	106.96
24	3	305	KC1	CAA-CBA-CGA	-3.57	108.89	127.26
23	6	310	A86	C4-C3-C2	3.57	130.79	123.47
21	6	300	CLA	CHA-C4D-ND	3.57	139.97	132.50
21	B	609	CLA	CHA-C4D-ND	3.57	139.97	132.50
21	3	303	CLA	CHA-C4D-ND	3.57	139.97	132.50
21	9	301	CLA	C4-C3-C5	3.57	121.28	115.27
21	c	507	CLA	O1D-CGD-CBD	-3.57	117.18	124.48
23	J	309	A86	C-C1-C2	-3.57	117.92	122.92
31	B	626	SQD	O47-C7-C8	3.57	119.19	111.50
21	B	603	CLA	CHA-C4D-ND	3.57	139.97	132.50
24	g	313	KC1	CAA-C2A-C1A	-3.57	108.34	124.75
21	C	510	CLA	CHA-C4D-ND	3.57	139.96	132.50
21	b	614	CLA	CHA-C4D-ND	3.56	139.96	132.50
21	c	513	CLA	CHD-C1D-ND	-3.56	121.18	124.45
24	4	309	KC1	CBA-CAA-C2A	-3.56	111.69	125.27
21	B	609	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
21	b	604	CLA	CHA-C4D-ND	3.56	139.95	132.50
21	7	300	CLA	C4D-CHA-C1A	-3.56	116.92	121.25
21	b	610	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
21	B	621	CLA	CHA-C4D-ND	3.56	139.94	132.50
21	9	301	CLA	CHA-C4D-ND	3.56	139.94	132.50
21	G	300	CLA	CHA-C4D-ND	3.56	139.94	132.50
21	b	609	CLA	CHD-C1D-ND	-3.56	121.19	124.45
21	9	300	CLA	CHA-C4D-ND	3.56	139.94	132.50
21	6	300	CLA	C4D-CHA-C1A	-3.56	116.92	121.25
21	b	610	CLA	CHA-C4D-ND	3.56	139.94	132.50
21	d	405	CLA	CHD-C1D-ND	-3.55	121.19	124.45
21	g	303	CLA	C1-C2-C3	-3.55	121.00	126.75
21	J	302	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
23	2	312	A86	C4-C3-C2	3.55	130.75	123.47
21	5	303	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
21	3	301	CLA	CHA-C4D-ND	3.55	139.93	132.50
21	g	308	CLA	CHA-C4D-ND	3.55	139.93	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	602	SQD	O47-C7-C8	3.55	119.15	111.50
23	8	311	A86	C4-C3-C2	3.55	130.74	123.47
21	b	607	CLA	CHA-C4D-ND	3.55	139.92	132.50
23	2	308	A86	C3-C4-C5	3.55	130.74	123.47
23	1	312	A86	C-C1-C2	-3.55	117.96	122.92
23	7	313	A86	C3-C4-C5	3.54	130.73	123.47
30	c	516	DGD	O6D-C1D-O3G	-3.54	101.59	109.97
21	3	304	CLA	CHD-C4C-C3C	-3.54	119.64	124.84
23	8	312	A86	C7-C6-C5	-3.54	117.97	122.92
21	9	302	CLA	CHA-C4D-ND	3.54	139.90	132.50
21	7	304	CLA	CHD-C4C-C3C	-3.54	119.64	124.84
22	5	310	DD6	C7-C6-C5	-3.54	117.97	122.92
23	6	309	A86	C24-C1-C2	3.53	124.36	118.94
24	7	315	KC1	C1C-C2C-C3C	-3.53	103.24	106.96
21	2	306	CLA	CHA-C4D-ND	3.53	139.89	132.50
21	6	306	CLA	CHA-C4D-ND	3.53	139.89	132.50
23	8	308	A86	C7-C6-C5	-3.53	117.98	122.92
24	6	311	KC1	C4B-C3B-C2B	-3.53	103.85	106.75
21	C	513	CLA	CHA-C4D-ND	3.53	139.88	132.50
23	G	305	A86	C-C1-C2	-3.53	117.98	122.92
24	3	306	KC1	CBA-CAA-C2A	-3.53	111.82	125.27
21	G	302	CLA	C1B-CHB-C4A	-3.53	123.13	130.12
21	d	406	CLA	CHA-C4D-ND	3.53	139.88	132.50
24	5	315	KC1	CAA-CBA-CGA	-3.53	109.14	127.26
21	c	514	CLA	C4D-CHA-C1A	-3.53	116.96	121.25
23	8	312	A86	C4-C3-C2	3.52	130.69	123.47
24	2	313	KC1	C1A-NA-C4A	-3.52	105.12	106.71
21	c	510	CLA	CHA-C4D-ND	3.52	139.87	132.50
21	7	308	CLA	C4D-CHA-C1A	-3.52	116.96	121.25
21	3	304	CLA	C4D-CHA-C1A	-3.52	116.96	121.25
23	g	312	A86	C24-C1-C2	3.52	124.35	118.94
21	6	303	CLA	CHD-C4C-C3C	-3.52	119.66	124.84
21	2	301	CLA	CHA-C4D-ND	3.52	139.86	132.50
32	f	101	HEM	C4C-CHD-C1D	3.52	127.20	122.56
21	B	604	CLA	C4D-CHA-C1A	-3.52	116.97	121.25
24	J	313	KC1	C4B-C3B-C2B	-3.52	103.86	106.75
21	8	307	CLA	C4D-CHA-C1A	-3.52	116.97	121.25
21	5	307	CLA	CHA-C4D-ND	3.51	139.85	132.50
21	b	613	CLA	CHA-C4D-ND	3.51	139.85	132.50
21	B	616	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
21	J	308	CLA	C1B-CHB-C4A	-3.51	123.16	130.12
21	c	502	CLA	CHA-C4D-ND	3.51	139.85	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	302	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
24	G	309	KC1	C4B-C3B-C2B	-3.51	103.87	106.75
21	7	307	CLA	CHA-C4D-ND	3.51	139.84	132.50
25	h	102	BCR	C3-C4-C5	-3.51	107.81	114.08
24	2	315	KC1	CAC-C3C-C4C	3.51	129.37	124.81
21	2	301	CLA	C4D-CHA-C1A	-3.51	116.98	121.25
21	C	509	CLA	CHA-C4D-ND	3.51	139.84	132.50
21	1	305	CLA	O1D-CGD-CBD	-3.51	117.31	124.48
23	7	313	A86	C-C1-C2	-3.51	118.01	122.92
24	6	311	KC1	CAA-CBA-CGA	-3.51	109.23	127.26
24	1	315	KC1	CBA-CAA-C2A	-3.51	111.90	125.27
21	D	406	CLA	C4C-C3C-C2C	-3.51	103.86	107.07
21	B	610	CLA	C4D-CHA-C1A	-3.51	116.98	121.25
21	b	612	CLA	CHA-C4D-ND	3.51	139.83	132.50
23	4	305	A86	C24-C1-C2	3.50	124.32	118.94
21	5	302	CLA	CHA-C4D-ND	3.50	139.83	132.50
21	3	303	CLA	C2D-C1D-ND	3.50	112.69	110.10
21	B	602	CLA	CHA-C4D-ND	3.50	139.83	132.50
21	C	503	CLA	CHA-C4D-ND	3.50	139.83	132.50
30	C	517	DGD	O6D-C1D-O3G	-3.50	101.68	109.97
23	8	309	A86	C7-C6-C5	-3.50	118.02	122.92
24	g	313	KC1	CBA-CAA-C2A	-3.50	111.92	125.27
23	4	305	A86	C4-C3-C2	3.50	130.65	123.47
21	D	406	CLA	CHD-C4C-NC	3.50	129.72	124.20
21	C	511	CLA	CHA-C4D-ND	3.50	139.82	132.50
23	8	309	A86	C4-C3-C2	3.50	130.64	123.47
24	8	315	KC1	C2A-C1A-NA	3.50	115.01	109.40
21	5	304	CLA	CHA-C4D-ND	3.50	139.82	132.50
23	g	311	A86	C-C1-C2	-3.50	118.02	122.92
23	8	308	A86	C8-C6-C5	3.50	124.31	118.94
21	B	615	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
21	g	305	CLA	CHA-C4D-ND	3.50	139.81	132.50
23	8	308	A86	C24-C1-C2	3.50	124.31	118.94
24	g	315	KC1	CBA-CAA-C2A	-3.49	111.95	125.27
21	4	302	CLA	O1D-CGD-CBD	-3.49	117.33	124.48
28	B	627	LMG	O6-C1-O1	-3.49	101.70	109.97
21	8	306	CLA	CHA-C4D-ND	3.49	139.81	132.50
21	C	514	CLA	CHD-C1D-ND	-3.49	121.24	124.45
21	g	302	CLA	CAC-C3C-C4C	3.49	129.34	124.81
21	B	621	CLA	C4D-CHA-C1A	-3.49	117.00	121.25
21	b	623	CLA	CHD-C4C-C3C	-3.49	119.71	124.84
21	1	308	CLA	CHA-C4D-ND	3.49	139.79	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	315	KC1	CAA-CBA-CGA	-3.49	109.34	127.26
21	b	612	CLA	O1D-CGD-CBD	-3.49	117.35	124.48
21	5	307	CLA	CHD-C4C-C3C	-3.48	119.72	124.84
21	J	307	CLA	CHA-C4D-ND	3.48	139.78	132.50
21	1	304	CLA	C4D-CHA-C1A	-3.48	117.01	121.25
22	1	311	DD6	C7-C6-C5	-3.48	118.05	122.92
25	H	100	BCR	C3-C4-C5	-3.48	107.86	114.08
21	3	304	CLA	CHA-C4D-ND	3.48	139.78	132.50
21	6	302	CLA	C4D-CHA-C1A	-3.48	117.02	121.25
21	B	621	CLA	O1D-CGD-CBD	-3.48	117.37	124.48
24	5	315	KC1	CBA-CAA-C2A	-3.48	112.01	125.27
21	7	308	CLA	CHA-C4D-ND	3.48	139.77	132.50
24	4	307	KC1	C4B-C3B-C2B	-3.47	103.90	106.75
23	2	307	A86	C7-C6-C5	-3.47	118.06	122.92
21	5	302	CLA	C4D-CHA-C1A	-3.47	117.03	121.25
23	W	101	A86	C3-C4-C5	3.47	130.58	123.47
24	6	313	KC1	C4B-C3B-C2B	-3.47	103.90	106.75
21	8	307	CLA	CHD-C4C-C3C	-3.47	119.74	124.84
21	g	307	CLA	CHA-C4D-ND	3.47	139.75	132.50
22	7	310	DD6	C7-C6-C5	-3.47	118.07	122.92
21	B	612	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
21	7	305	CLA	CHD-C4C-C3C	-3.47	119.75	124.84
21	1	305	CLA	CHA-C4D-ND	3.47	139.75	132.50
21	J	308	CLA	CHA-C4D-ND	3.47	139.75	132.50
23	6	309	A86	C-C1-C2	-3.47	118.07	122.92
21	b	611	CLA	CHA-C4D-ND	3.47	139.75	132.50
21	4	303	CLA	CHA-C4D-ND	3.46	139.75	132.50
23	g	312	A86	C7-C6-C5	-3.46	118.07	122.92
21	3	301	CLA	O1D-CGD-CBD	-3.46	117.40	124.48
21	2	303	CLA	CHA-C4D-ND	3.46	139.74	132.50
24	5	314	KC1	CAA-CBA-CGA	-3.46	109.47	127.26
21	B	610	CLA	O1D-CGD-CBD	-3.46	117.40	124.48
21	J	304	CLA	CHA-C4D-ND	3.46	139.74	132.50
23	g	312	A86	C-C1-C2	-3.46	118.08	122.92
21	b	616	CLA	CHD-C4C-C3C	-3.46	119.75	124.84
24	6	311	KC1	CBA-CAA-C2A	-3.46	112.08	125.27
24	4	307	KC1	CAA-C2A-C1A	-3.46	108.84	124.75
21	G	303	CLA	CHD-C4C-C3C	-3.46	119.75	124.84
21	7	303	CLA	CHD-C4C-NC	3.46	129.65	124.20
24	g	315	KC1	C4B-C3B-C2B	-3.46	103.91	106.75
21	C	504	CLA	C4D-CHA-C1A	-3.46	117.04	121.25
21	c	506	CLA	CHA-C4D-ND	3.46	139.73	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	604	CLA	CHD-C4C-C3C	-3.46	119.76	124.84
23	2	312	A86	C7-C6-C5	-3.46	118.08	122.92
24	4	308	KC1	CBA-CAA-C2A	-3.46	112.10	125.27
21	J	303	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
23	J	310	A86	C7-C6-C5	-3.45	118.08	122.92
23	8	310	A86	C8-C6-C5	3.45	124.24	118.94
21	1	306	CLA	CHA-C4D-ND	3.45	139.72	132.50
35	d	408	PL9	C7-C3-C2	-3.45	118.76	123.30
21	d	405	CLA	CHD-C4C-NC	3.45	129.64	124.20
22	g	310	DD6	C7-C6-C5	-3.45	118.09	122.92
24	7	314	KC1	CAA-CBA-CGA	-3.45	109.53	127.26
21	1	310	CLA	CHA-C4D-ND	3.45	139.72	132.50
24	2	315	KC1	C2A-C1A-NA	3.45	114.93	109.40
21	5	302	CLA	CHD-C4C-NC	3.45	129.64	124.20
23	J	309	A86	C28-C27-C26	-3.45	118.09	122.92
21	a	405	CLA	O1D-CGD-CBD	-3.45	117.43	124.48
21	3	300	CLA	CHD-C4C-C3C	-3.45	119.77	124.84
21	C	507	CLA	CHA-C4D-ND	3.45	139.71	132.50
31	b	602	SQD	O9-S-C6	3.45	111.04	106.94
21	c	504	CLA	CHD-C4C-C3C	-3.45	119.78	124.84
21	1	301	CLA	CHA-C4D-ND	3.45	139.71	132.50
21	b	617	CLA	C1C-C2C-C3C	-3.44	103.33	106.96
23	7	311	A86	C7-C6-C5	-3.44	118.10	122.92
23	2	308	A86	C7-C6-C5	-3.44	118.10	122.92
23	8	312	A86	C-C1-C2	-3.44	118.10	122.92
21	d	404	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
21	7	302	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
21	g	309	CLA	CHD-C4C-C3C	-3.44	119.78	124.84
21	G	301	CLA	CHA-C4D-ND	3.44	139.70	132.50
21	D	406	CLA	CHD-C1D-ND	-3.44	121.29	124.45
21	6	303	CLA	C2D-C1D-ND	3.44	112.64	110.10
21	1	304	CLA	CHA-C4D-ND	3.44	139.70	132.50
21	c	508	CLA	CHA-C4D-ND	3.44	139.70	132.50
25	H	100	BCR	C2-C1-C6	3.44	115.78	110.48
21	J	306	CLA	CHA-C4D-ND	3.44	139.69	132.50
24	G	307	KC1	CAA-CBA-CGA	-3.44	109.59	127.26
21	2	301	CLA	O1D-CGD-CBD	-3.44	117.45	124.48
21	B	612	CLA	CHA-C4D-ND	3.44	139.69	132.50
21	g	308	CLA	C4D-CHA-C1A	-3.44	117.07	121.25
35	D	409	PL9	C7-C3-C2	-3.43	118.78	123.30
21	9	301	CLA	C2D-C1D-ND	3.43	112.64	110.10
21	B	621	CLA	CHD-C4C-C3C	-3.43	119.79	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	315	KC1	CAA-CBA-CGA	-3.43	109.61	127.26
21	1	306	CLA	C4D-CHA-C1A	-3.43	117.07	121.25
21	C	506	CLA	CHA-C4D-ND	3.43	139.68	132.50
24	9	305	KC1	CAA-CBA-CGA	-3.43	109.62	127.26
21	B	615	CLA	CHD-C4C-C3C	-3.43	119.80	124.84
21	7	302	CLA	C1B-CHB-C4A	-3.43	123.32	130.12
21	b	605	CLA	C4D-CHA-C1A	-3.43	117.08	121.25
21	d	406	CLA	C4D-CHA-C1A	-3.43	117.08	121.25
21	b	605	CLA	CHD-C4C-C3C	-3.43	119.80	124.84
21	6	307	CLA	C1-C2-C3	-3.43	120.11	126.04
21	1	310	CLA	CHD-C1D-ND	-3.43	121.30	124.45
21	7	300	CLA	CHA-C4D-ND	3.43	139.67	132.50
21	1	305	CLA	CHD-C4C-C3C	-3.43	119.81	124.84
21	d	406	CLA	C4-C3-C5	3.43	121.03	115.27
23	1	313	A86	C-C1-C2	-3.43	118.12	122.92
21	2	304	CLA	CHA-C4D-ND	3.42	139.66	132.50
24	3	305	KC1	CBA-CAA-C2A	-3.42	112.22	125.27
25	C	501	BCR	C15-C16-C17	-3.42	116.46	123.47
21	7	309	CLA	CHA-C4D-ND	3.42	139.66	132.50
21	2	305	CLA	O2D-CGD-CBD	3.42	117.35	111.27
21	a	402	CLA	CHA-C4D-ND	3.42	139.66	132.50
21	D	407	CLA	C4D-CHA-C1A	-3.42	117.08	121.25
21	8	303	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
21	1	308	CLA	C4-C3-C5	3.42	121.03	115.27
24	g	313	KC1	C4B-C3B-C2B	-3.42	103.94	106.75
21	B	606	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
23	1	314	A86	C7-C6-C5	-3.42	118.14	122.92
23	5	312	A86	C7-C6-C5	-3.42	118.14	122.92
21	8	304	CLA	CHA-C4D-ND	3.42	139.65	132.50
21	B	611	CLA	CHA-C4D-ND	3.42	139.64	132.50
21	g	302	CLA	CMB-C2B-C3B	3.41	131.07	124.68
21	7	305	CLA	CHA-C4D-ND	3.41	139.64	132.50
21	3	302	CLA	CHD-C4C-C3C	-3.41	119.82	124.84
23	2	309	A86	C28-C27-C26	-3.41	118.14	122.92
21	1	302	CLA	CHA-C4D-ND	3.41	139.64	132.50
24	4	306	KC1	C2C-C1C-CHC	-3.41	117.75	125.22
24	9	306	KC1	CAA-CBA-CGA	-3.41	109.73	127.26
24	J	311	KC1	CAA-CBA-CGA	-3.41	109.73	127.26
21	B	607	CLA	CHA-C4D-ND	3.41	139.63	132.50
23	G	305	A86	C24-C1-C2	3.41	124.17	118.94
21	1	306	CLA	O1D-CGD-CBD	-3.41	117.50	124.48
21	8	307	CLA	CHD-C1D-ND	-3.41	121.32	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	307	CLA	CHA-C4D-ND	3.41	139.63	132.50
24	1	316	KC1	C4B-C3B-C2B	-3.41	103.95	106.75
21	6	303	CLA	CHA-C4D-ND	3.41	139.63	132.50
21	c	511	CLA	CHA-C4D-ND	3.41	139.63	132.50
22	7	310	DD6	C-C1-C2	-3.41	118.15	122.92
22	g	310	DD6	C-C1-C2	-3.41	118.15	122.92
23	2	307	A86	C3-C4-C5	3.41	130.45	123.47
21	3	304	CLA	C4-C3-C5	3.41	121.00	115.27
21	g	302	CLA	CHD-C4C-C3C	-3.41	119.83	124.84
31	B	626	SQD	O9-S-C6	3.40	110.98	106.94
21	C	509	CLA	O2A-CGA-CBA	3.40	122.58	111.91
24	6	313	KC1	CBA-CAA-C2A	-3.40	112.31	125.27
21	g	305	CLA	CHD-C4C-C3C	-3.40	119.84	124.84
21	A	401	CLA	CHA-C4D-ND	3.40	139.61	132.50
23	2	309	A86	C7-C6-C5	-3.40	118.16	122.92
21	8	303	CLA	CHD-C4C-C3C	-3.40	119.85	124.84
21	J	300	CLA	C4D-CHA-C1A	-3.39	117.12	121.25
21	6	301	CLA	CHA-C4D-ND	3.39	139.60	132.50
21	J	301	CLA	CHA-C4D-ND	3.39	139.60	132.50
24	J	313	KC1	O2D-CGD-O1D	-3.39	117.20	123.84
21	6	302	CLA	CHA-C4D-ND	3.39	139.60	132.50
24	1	316	KC1	CAC-C3C-C4C	3.39	129.21	124.81
22	g	310	DD6	C8-C6-C5	3.39	124.14	118.94
23	1	312	A86	C24-C1-C2	3.39	124.14	118.94
23	6	310	A86	C7-C6-C5	-3.39	118.17	122.92
23	1	313	A86	C7-C6-C5	-3.39	118.18	122.92
23	1	314	A86	C-C1-C2	-3.39	118.18	122.92
21	J	302	CLA	CHA-C4D-ND	3.39	139.59	132.50
21	b	616	CLA	C4D-CHA-C1A	-3.39	117.13	121.25
21	b	608	CLA	CHA-C4D-ND	3.39	139.58	132.50
21	8	305	CLA	CHA-C4D-ND	3.39	139.58	132.50
21	g	303	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
21	B	612	CLA	CMB-C2B-C3B	3.39	131.01	124.68
21	c	513	CLA	CHA-C4D-ND	3.39	139.58	132.50
21	C	511	CLA	C1-C2-C3	-3.38	120.19	126.04
24	8	313	KC1	CAA-CBA-CGA	-3.38	109.87	127.26
21	b	616	CLA	CHA-C4D-ND	3.38	139.58	132.50
21	g	305	CLA	C4D-CHA-C1A	-3.38	117.13	121.25
29	5	316	LMU	C1B-O1B-C4'	-3.38	109.60	117.96
25	h	102	BCR	C2-C1-C6	3.38	115.69	110.48
21	6	308	CLA	CHC-C1C-NC	-3.38	119.08	124.20
21	C	515	CLA	C4D-CHA-C1A	-3.38	117.14	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	505	CLA	O1D-CGD-CBD	-3.38	117.57	124.48
24	6	313	KC1	O2D-CGD-O1D	-3.38	117.23	123.84
21	7	309	CLA	CAC-C3C-C4C	3.38	129.19	124.81
24	G	309	KC1	CAC-C3C-C4C	3.38	129.19	124.81
30	C	518	DGD	O6D-C1D-O3G	-3.38	101.97	109.97
21	d	404	CLA	CHA-C4D-ND	3.38	139.56	132.50
21	B	610	CLA	CHA-C4D-ND	3.38	139.56	132.50
21	J	304	CLA	CHD-C4C-NC	3.38	129.52	124.20
21	c	514	CLA	CHD-C4C-C3C	-3.38	119.88	124.84
21	6	301	CLA	O1D-CGD-CBD	-3.38	117.58	124.48
23	2	311	A86	C7-C6-C5	-3.38	118.19	122.92
21	A	404	CLA	CHA-C4D-ND	3.37	139.56	132.50
21	b	607	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
23	5	311	A86	C7-C6-C5	-3.37	118.20	122.92
21	5	303	CLA	CHA-C4D-ND	3.37	139.56	132.50
21	7	306	CLA	CHA-C4D-ND	3.37	139.56	132.50
23	7	312	A86	C8-C6-C5	3.37	124.12	118.94
21	5	309	CLA	O1D-CGD-CBD	-3.37	117.59	124.48
21	C	514	CLA	CHA-C4D-ND	3.37	139.55	132.50
30	B	624	DGD	C1E-O6E-C5E	3.37	118.27	113.03
21	b	607	CLA	C4-C3-C5	3.37	120.93	115.27
21	8	302	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
21	g	307	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
21	C	515	CLA	CHD-C4C-C3C	-3.36	119.89	124.84
32	E	101	HEM	C3B-C2B-C1B	3.36	108.98	106.49
23	2	311	A86	C-C1-C2	-3.36	118.21	122.92
21	c	505	CLA	CHA-C4D-ND	3.36	139.53	132.50
21	2	304	CLA	C4D-CHA-C1A	-3.36	117.16	121.25
21	D	404	CLA	CHA-C4D-ND	3.36	139.53	132.50
24	G	308	KC1	CAA-CBA-CGA	-3.36	110.00	127.26
24	4	309	KC1	CAA-CBA-CGA	-3.36	110.00	127.26
21	d	405	CLA	C4C-C3C-C2C	-3.36	103.99	107.07
21	B	615	CLA	CHA-C4D-ND	3.36	139.52	132.50
21	b	603	CLA	CHD-C1D-ND	-3.36	121.37	124.45
24	5	315	KC1	CHB-C1B-NB	-3.36	121.37	124.45
21	B	608	CLA	CHA-C4D-ND	3.35	139.52	132.50
24	g	314	KC1	CAA-CBA-CGA	-3.35	110.02	127.26
21	J	307	CLA	C1-C2-C3	-3.35	120.24	126.04
21	7	302	CLA	CHD-C4C-C3C	-3.35	119.91	124.84
24	6	312	KC1	CAA-CBA-CGA	-3.35	110.03	127.26
21	B	606	CLA	C4-C3-C5	3.35	120.91	115.27
30	c	517	DGD	O6D-C1D-O3G	-3.35	102.04	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	625	SQD	C44-O6-C1	3.35	120.28	113.74
21	C	512	CLA	CHA-C4D-ND	3.35	139.50	132.50
24	9	305	KC1	C4B-C3B-C2B	-3.35	104.00	106.75
21	4	301	CLA	CHA-C4D-ND	3.34	139.50	132.50
21	c	503	CLA	C4D-CHA-C1A	-3.34	117.18	121.25
23	g	311	A86	C7-C6-C5	-3.34	118.24	122.92
23	G	305	A86	C28-C27-C26	-3.34	118.24	122.92
24	1	315	KC1	CAA-CBA-CGA	-3.34	110.08	127.26
21	B	606	CLA	O1D-CGD-CBD	-3.34	117.65	124.48
23	7	312	A86	C-C1-C2	-3.34	118.25	122.92
23	J	310	A86	C-C1-C2	-3.34	118.25	122.92
21	1	303	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
22	5	310	DD6	C-C1-C2	-3.34	118.25	122.92
21	3	300	CLA	CHA-C4D-ND	3.34	139.48	132.50
24	4	307	KC1	CBA-CAA-C2A	-3.34	112.55	125.27
21	c	503	CLA	CHD-C1D-ND	-3.33	121.39	124.45
21	g	309	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
21	J	303	CLA	C4B-CHC-C1C	-3.33	124.50	129.64
21	9	300	CLA	C4D-CHA-C1A	-3.33	117.19	121.25
23	2	307	A86	C-C1-C2	-3.33	118.26	122.92
21	g	309	CLA	C1-C2-C3	-3.33	121.36	126.75
21	1	301	CLA	C4D-CHA-C1A	-3.33	117.20	121.25
21	B	610	CLA	CHD-C4C-NC	3.33	129.45	124.20
21	a	405	CLA	CHA-C4D-ND	3.33	139.46	132.50
21	d	405	CLA	CHA-C4D-ND	3.33	139.46	132.50
21	c	503	CLA	CHA-C4D-ND	3.33	139.46	132.50
30	b	601	DGD	C1E-O6E-C5E	3.33	118.20	113.03
21	4	300	CLA	C1-C2-C3	-3.33	120.29	126.04
24	4	309	KC1	CMB-C2B-C1B	3.33	130.57	124.71
24	7	315	KC1	CBA-CAA-C2A	-3.33	112.59	125.27
21	1	309	CLA	CHA-C4D-ND	3.33	139.46	132.50
23	8	311	A86	C7-C6-C5	-3.32	118.27	122.92
21	d	405	CLA	C1-C2-C3	-3.32	120.29	126.04
21	1	303	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
21	b	611	CLA	O1D-CGD-CBD	-3.32	117.68	124.48
21	c	512	CLA	C4D-CHA-C1A	-3.32	117.21	121.25
21	4	300	CLA	CHA-C4D-ND	3.32	139.45	132.50
21	9	303	CLA	C1-C2-C3	-3.32	120.30	126.04
23	7	311	A86	C-C1-C2	-3.32	118.27	122.92
23	2	310	A86	C7-C6-C5	-3.32	118.27	122.92
24	5	313	KC1	CAA-C2A-C1A	-3.32	109.48	124.75
21	D	406	CLA	C1-C2-C3	-3.32	120.30	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	7	315	KC1	CAC-C3C-C4C	3.32	129.12	124.81
21	b	609	CLA	CHA-C4D-ND	3.32	139.44	132.50
24	8	315	KC1	CAC-C3C-C4C	3.32	129.11	124.81
21	b	607	CLA	O1D-CGD-CBD	-3.32	117.70	124.48
21	C	504	CLA	O1D-CGD-CBD	-3.31	117.70	124.48
21	1	301	CLA	O1D-CGD-CBD	-3.31	117.70	124.48
21	6	304	CLA	CHD-C4C-NC	3.31	129.42	124.20
21	G	302	CLA	C2D-C1D-ND	3.31	112.54	110.10
23	W	101	A86	C7-C6-C5	-3.31	118.28	122.92
21	J	301	CLA	O1D-CGD-CBD	-3.31	117.72	124.48
21	4	301	CLA	C4-C3-C5	3.31	120.83	115.27
23	1	313	A86	C28-C27-C26	-3.31	118.29	122.92
21	b	613	CLA	CMB-C2B-C3B	3.31	130.87	124.68
21	J	308	CLA	O1D-CGD-CBD	-3.31	117.72	124.48
21	2	306	CLA	O1D-CGD-CBD	-3.31	117.72	124.48
24	5	315	KC1	C4B-C3B-C2B	-3.30	104.04	106.75
21	D	406	CLA	CHA-C4D-ND	3.30	139.41	132.50
23	8	312	A86	C8-C6-C5	3.30	124.01	118.94
21	2	301	CLA	O2A-CGA-CBA	3.30	122.27	111.91
23	2	312	A86	C-C1-C2	-3.30	118.30	122.92
21	6	303	CLA	C4B-C3B-C2B	-3.30	103.74	106.36
21	d	404	CLA	O1D-CGD-CBD	-3.30	117.74	124.48
21	C	504	CLA	CHA-C4D-ND	3.30	139.39	132.50
24	6	313	KC1	CAA-CBA-CGA	-3.29	110.33	127.26
21	7	303	CLA	CHA-C4D-ND	3.29	139.39	132.50
24	G	306	KC1	C2C-C1C-CHC	-3.29	118.01	125.22
21	7	307	CLA	CHD-C1D-ND	-3.29	121.43	124.45
21	g	307	CLA	C4D-CHA-C1A	-3.29	117.24	121.25
23	G	305	A86	C7-C6-C5	-3.29	118.31	122.92
21	1	309	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
23	4	305	A86	C7-C6-C5	-3.29	118.31	122.92
21	B	615	CLA	C4D-CHA-C1A	-3.29	117.24	121.25
21	6	308	CLA	C1B-CHB-C4A	-3.29	123.60	130.12
24	1	316	KC1	CBA-CAA-C2A	-3.29	112.73	125.27
23	W	101	A86	C-C1-C2	-3.29	118.32	122.92
23	1	312	A86	C8-C6-C5	3.29	123.98	118.94
23	7	313	A86	C7-C6-C5	-3.29	118.32	122.92
21	B	607	CLA	O1D-CGD-CBD	-3.29	117.76	124.48
21	7	305	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
21	6	301	CLA	CHD-C4C-NC	3.29	129.38	124.20
21	g	308	CLA	CHD-C4C-C3C	-3.28	120.02	124.84
23	J	310	A86	C28-C27-C26	-3.28	118.33	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	302	CLA	CHD-C4C-NC	3.28	129.37	124.20
32	E	101	HEM	C1B-NB-C4B	3.28	108.46	105.07
21	B	616	CLA	O2A-CGA-CBA	3.28	122.20	111.91
21	6	308	CLA	CHA-C4D-ND	3.28	139.36	132.50
21	3	300	CLA	C4-C3-C5	3.28	120.78	115.27
21	9	302	CLA	CHD-C4C-C3C	-3.28	120.02	124.84
21	5	306	CLA	CHD-C4C-C3C	-3.28	120.02	124.84
23	5	312	A86	C28-C27-C26	-3.28	118.33	122.92
21	B	613	CLA	O1D-CGD-CBD	-3.28	117.78	124.48
23	2	308	A86	C33-C32-C31	3.28	112.40	109.21
21	1	304	CLA	CHD-C4C-NC	3.28	129.37	124.20
21	g	306	CLA	CHA-C4D-ND	3.28	139.35	132.50
21	C	507	CLA	CHD-C1D-ND	-3.28	121.44	124.45
23	6	310	A86	C-C1-C2	-3.28	118.33	122.92
23	5	312	A86	C-C1-C2	-3.28	118.33	122.92
23	1	313	A86	C24-C1-C2	3.27	123.96	118.94
21	G	304	CLA	CHD-C4C-C3C	-3.27	120.03	124.84
24	5	315	KC1	CAA-C2A-C1A	-3.27	109.70	124.75
22	7	310	DD6	C8-C6-C5	3.27	123.96	118.94
21	1	310	CLA	CHD-C4C-C3C	-3.27	120.03	124.84
24	4	309	KC1	CAC-C3C-C4C	3.27	129.05	124.81
24	3	306	KC1	CAC-C3C-C4C	3.27	129.05	124.81
29	A	408	LMU	C1B-O1B-C4'	-3.27	109.87	117.96
21	C	509	CLA	C4-C3-C5	3.27	120.77	115.27
23	2	310	A86	C-C1-C2	-3.27	118.35	122.92
22	5	310	DD6	C8-C6-C5	3.27	123.95	118.94
22	7	310	DD6	C3-C4-C5	3.27	130.16	123.47
24	1	316	KC1	CAA-CBA-CGA	-3.26	110.48	127.26
21	G	304	CLA	CHA-C4D-ND	3.26	139.33	132.50
21	B	605	CLA	O1D-CGD-CBD	-3.26	117.81	124.48
21	1	304	CLA	C4-C3-C5	3.26	120.76	115.27
23	1	313	A86	C8-C6-C5	3.26	123.94	118.94
21	9	304	CLA	CHD-C4C-NC	3.26	129.34	124.20
21	c	509	CLA	C4D-CHA-C1A	-3.26	117.28	121.25
21	g	302	CLA	CMC-C2C-C1C	3.26	130.00	125.04
21	3	302	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
21	g	306	CLA	CHD-C4C-C3C	-3.26	120.05	124.84
30	B	624	DGD	O6D-C1D-O3G	-3.26	102.26	109.97
23	8	309	A86	C-C1-C2	-3.26	118.36	122.92
23	6	310	A86	C28-C27-C26	-3.25	118.36	122.92
21	A	401	CLA	CHD-C4C-NC	3.25	129.33	124.20
23	2	307	A86	C8-C6-C5	3.25	123.93	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	309	CLA	CHD-C4C-NC	3.25	129.33	124.20
24	7	315	KC1	CAA-CBA-CGA	-3.25	110.55	127.26
21	2	302	CLA	O1D-CGD-CBD	-3.25	117.83	124.48
21	7	301	CLA	CHD-C1D-ND	-3.25	121.47	124.45
24	G	306	KC1	C3C-C4C-NC	3.25	115.02	109.51
21	6	308	CLA	O1D-CGD-CBD	-3.25	117.83	124.48
21	5	306	CLA	CHA-C4D-ND	3.25	139.30	132.50
21	c	506	CLA	O1D-CGD-CBD	-3.25	117.84	124.48
21	c	513	CLA	CHC-C1C-NC	-3.24	119.28	124.20
21	d	404	CLA	C4D-CHA-C1A	-3.24	117.30	121.25
21	4	304	CLA	CHD-C4C-C3C	-3.24	120.07	124.84
24	J	312	KC1	CAA-CBA-CGA	-3.24	110.59	127.26
21	A	404	CLA	C1-C2-C3	-3.24	120.44	126.04
24	2	313	KC1	CMB-C2B-C1B	3.24	130.43	124.71
21	b	611	CLA	C4D-CHA-C1A	-3.24	117.31	121.25
24	G	309	KC1	CBA-CAA-C2A	-3.24	112.92	125.27
21	a	403	CLA	O1D-CGD-CBD	-3.24	117.86	124.48
21	4	302	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
21	9	304	CLA	CHA-C4D-ND	3.24	139.27	132.50
24	3	305	KC1	CAA-C2A-C1A	-3.24	109.87	124.75
21	g	304	CLA	CHA-C4D-ND	3.24	139.27	132.50
21	1	310	CLA	CAC-C3C-C4C	3.24	129.01	124.81
21	5	307	CLA	CAC-C3C-C4C	3.24	129.01	124.81
21	5	309	CLA	CAC-C3C-C4C	3.24	129.01	124.81
21	G	300	CLA	C1-C2-C3	-3.24	120.45	126.04
21	4	303	CLA	C1B-CHB-C4A	-3.23	123.71	130.12
24	4	306	KC1	CMB-C2B-C1B	3.23	130.41	124.71
21	7	304	CLA	O1D-CGD-CBD	-3.23	117.87	124.48
21	B	621	CLA	C4-C3-C5	3.23	120.71	115.27
21	8	306	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
21	b	606	CLA	O1D-CGD-CBD	-3.23	117.88	124.48
23	2	308	A86	C-C1-C2	-3.23	118.40	122.92
21	A	402	CLA	O1D-CGD-CBD	-3.23	117.88	124.48
24	4	306	KC1	C3C-C4C-NC	3.23	114.98	109.51
23	g	311	A86	C28-C27-C26	-3.23	118.40	122.92
23	8	311	A86	C-C1-C2	-3.23	118.40	122.92
21	7	309	CLA	CHD-C4C-C3C	-3.22	120.10	124.84
23	1	314	A86	C8-C6-C5	3.22	123.89	118.94
21	a	402	CLA	CHD-C4C-NC	3.22	129.28	124.20
21	J	302	CLA	O1D-CGD-CBD	-3.22	117.89	124.48
23	2	311	A86	C28-C27-C26	-3.22	118.41	122.92
21	2	302	CLA	C3D-C2D-C1D	-3.22	101.44	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	304	CLA	CHA-C4D-ND	3.22	139.23	132.50
21	b	610	CLA	O1D-CGD-CBD	-3.22	117.90	124.48
21	b	617	CLA	C4-C3-C5	3.22	120.69	115.27
21	d	406	CLA	C1-C2-C3	-3.22	120.48	126.04
21	B	611	CLA	CHD-C4C-NC	3.22	129.27	124.20
23	2	307	A86	C24-C1-C2	3.22	123.88	118.94
21	9	302	CLA	CHD-C1D-ND	-3.21	121.50	124.45
23	2	309	A86	C8-C6-C5	3.21	123.87	118.94
24	5	313	KC1	CBA-CAA-C2A	-3.21	113.03	125.27
21	b	614	CLA	O1D-CGD-CBD	-3.21	117.92	124.48
21	5	306	CLA	C4-C3-C5	3.21	120.67	115.27
21	C	510	CLA	CHD-C1D-ND	-3.20	121.51	124.45
21	c	506	CLA	CHD-C1D-ND	-3.20	121.51	124.45
21	3	302	CLA	O1D-CGD-CBD	-3.20	117.93	124.48
21	b	611	CLA	CHD-C4C-NC	3.20	129.25	124.20
24	5	313	KC1	CHB-C1B-NB	-3.20	121.51	124.45
31	b	602	SQD	C44-O6-C1	3.20	120.00	113.74
21	C	512	CLA	CMB-C2B-C3B	3.20	130.67	124.68
21	6	308	CLA	CHD-C4C-C3C	-3.20	120.14	124.84
21	J	303	CLA	CHD-C4C-C3C	-3.20	120.14	124.84
21	6	302	CLA	O1D-CGD-CBD	-3.20	117.94	124.48
21	3	304	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
24	1	315	KC1	CAC-C3C-C4C	3.19	128.96	124.81
21	C	507	CLA	O1D-CGD-CBD	-3.19	117.95	124.48
21	6	302	CLA	CHC-C1C-NC	-3.19	119.36	124.20
21	1	303	CLA	CHD-C4C-C3C	-3.19	120.15	124.84
21	J	303	CLA	C2D-C1D-ND	3.19	112.45	110.10
21	g	306	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
21	5	309	CLA	CHA-C4D-ND	3.18	139.16	132.50
22	1	311	DD6	C-C1-C2	-3.18	118.47	122.92
21	1	301	CLA	CMC-C2C-C1C	3.18	129.88	125.04
24	g	315	KC1	CHB-C1B-NB	-3.18	121.53	124.45
21	b	613	CLA	CHD-C1D-ND	-3.18	121.53	124.45
21	B	612	CLA	CMC-C2C-C1C	3.18	129.88	125.04
23	2	312	A86	C8-C6-C5	3.18	123.82	118.94
24	2	313	KC1	CAC-C3C-C4C	3.18	128.93	124.81
24	J	313	KC1	CAA-CBA-CGA	-3.17	110.95	127.26
21	B	609	CLA	CHD-C4C-NC	3.17	129.20	124.20
21	b	606	CLA	CHD-C1D-ND	-3.17	121.54	124.45
21	B	609	CLA	C4D-CHA-C1A	-3.17	117.39	121.25
21	C	505	CLA	CHD-C1D-ND	-3.17	121.54	124.45
21	8	303	CLA	C3D-C2D-C1D	-3.17	101.51	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	606	CLA	CHD-C4C-NC	3.17	129.19	124.20
23	G	305	A86	C8-C6-C5	3.17	123.80	118.94
23	2	311	A86	C24-C1-C2	3.16	123.80	118.94
21	C	508	CLA	C4D-CHA-C1A	-3.16	117.40	121.25
21	7	305	CLA	CHC-C1C-NC	-3.16	119.41	124.20
21	C	515	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
21	B	616	CLA	C1-C2-C3	-3.16	120.58	126.04
21	C	513	CLA	CHD-C1D-ND	-3.15	121.56	124.45
21	9	304	CLA	C1-C2-C3	-3.15	120.59	126.04
21	g	302	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
21	2	302	CLA	CMD-C2D-C1D	3.15	130.27	124.71
21	C	504	CLA	CHD-C1D-ND	-3.15	121.56	124.45
21	g	304	CLA	C1-C2-C3	-3.15	120.59	126.04
21	5	308	CLA	CHD-C4C-NC	3.15	129.17	124.20
21	D	407	CLA	C4-C3-C5	3.15	120.57	115.27
21	5	304	CLA	O1D-CGD-CBD	-3.15	118.05	124.48
21	b	607	CLA	CHD-C4C-NC	3.15	129.16	124.20
21	b	612	CLA	CHD-C4C-NC	3.15	129.16	124.20
21	7	302	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
23	g	312	A86	C8-C6-C5	3.14	123.77	118.94
21	7	309	CLA	CMB-C2B-C3B	3.14	130.56	124.68
21	b	617	CLA	CMB-C2B-C3B	3.14	130.56	124.68
24	8	316	KC1	CAC-C3C-C4C	3.14	128.89	124.81
21	5	306	CLA	CMB-C2B-C3B	3.14	130.56	124.68
21	1	303	CLA	CHA-C4D-ND	3.14	139.07	132.50
24	3	306	KC1	CAA-CBA-CGA	-3.14	111.13	127.26
21	6	302	CLA	CHD-C4C-C3C	-3.14	120.23	124.84
24	g	313	KC1	CAC-C3C-C4C	3.13	128.88	124.81
23	4	305	A86	C8-C6-C5	3.13	123.75	118.94
31	B	626	SQD	C44-O6-C1	3.13	119.85	113.74
21	J	308	CLA	CHC-C1C-NC	-3.13	119.45	124.20
23	2	310	A86	C28-C27-C26	-3.13	118.54	122.92
25	c	501	BCR	C15-C16-C17	-3.13	117.07	123.47
21	4	304	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
21	1	305	CLA	CAC-C3C-C4C	3.13	128.87	124.81
21	C	510	CLA	C4-C3-C5	3.13	120.53	115.27
23	J	310	A86	C8-C6-C5	3.13	123.74	118.94
24	2	316	KC1	CAC-C3C-C4C	3.12	128.86	124.81
21	4	301	CLA	CHC-C1C-NC	-3.12	119.46	124.20
21	J	302	CLA	CHD-C4C-NC	3.12	129.12	124.20
21	4	301	CLA	C1-C2-C3	-3.12	120.64	126.04
21	c	508	CLA	CHD-C4C-NC	3.12	129.12	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	5	306	CLA	C1D-CHD-C4C	-3.12	119.32	126.06
21	C	511	CLA	C4D-CHA-C1A	-3.12	117.45	121.25
24	2	315	KC1	CBC-CAC-C3C	-3.12	103.83	112.43
21	7	300	CLA	CMC-C2C-C1C	3.12	129.79	125.04
21	B	609	CLA	O1D-CGD-CBD	-3.12	118.10	124.48
21	4	303	CLA	CHD-C4C-C3C	-3.12	120.26	124.84
24	3	305	KC1	CAC-C3C-C4C	3.12	128.85	124.81
30	b	601	DGD	O6D-C1D-O3G	-3.12	102.59	109.97
21	8	304	CLA	O1D-CGD-CBD	-3.12	118.11	124.48
21	8	302	CLA	CHD-C4C-NC	3.12	129.11	124.20
21	c	509	CLA	C1-C2-C3	-3.11	120.66	126.04
24	g	314	KC1	CAC-C3C-C4C	3.11	128.85	124.81
21	A	404	CLA	CHD-C4C-NC	3.11	129.11	124.20
21	C	503	CLA	CHD-C4C-NC	3.11	129.11	124.20
24	6	312	KC1	CAC-C3C-C4C	3.11	128.85	124.81
21	b	623	CLA	C4D-CHA-C1A	-3.11	117.46	121.25
21	B	602	CLA	CHD-C4C-NC	3.11	129.10	124.20
21	B	605	CLA	CHD-C1D-ND	-3.11	121.60	124.45
22	1	311	DD6	C4-C3-C2	3.11	129.84	123.47
23	7	311	A86	C8-C6-C5	3.11	123.71	118.94
21	J	303	CLA	C4B-C3B-C2B	-3.11	103.89	106.36
24	g	315	KC1	CAC-C3C-C4C	3.11	128.84	124.81
25	b	618	BCR	C15-C16-C17	-3.11	117.11	123.47
21	7	302	CLA	CHA-C4D-ND	3.11	139.00	132.50
25	B	617	BCR	C15-C16-C17	-3.10	117.12	123.47
24	4	308	KC1	CAA-CBA-CGA	-3.10	111.32	127.26
21	b	613	CLA	CHD-C4C-NC	3.10	129.09	124.20
21	8	305	CLA	CHD-C4C-NC	3.10	129.09	124.20
21	J	307	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
21	2	303	CLA	CHD-C4C-NC	3.10	129.08	124.20
21	G	300	CLA	CHD-C4C-C3C	-3.10	120.29	124.84
21	2	304	CLA	CHD-C4C-NC	3.10	129.08	124.20
21	b	623	CLA	CAC-C3C-C4C	3.10	128.83	124.81
21	G	302	CLA	CMB-C2B-C3B	3.09	130.47	124.68
23	2	311	A86	C8-C6-C5	3.09	123.69	118.94
21	G	304	CLA	C1-C2-C3	-3.09	120.69	126.04
21	c	509	CLA	O1D-CGD-CBD	-3.09	118.16	124.48
21	B	608	CLA	CMB-C2B-C3B	3.09	130.46	124.68
21	c	510	CLA	C4D-CHA-C1A	-3.09	117.49	121.25
23	8	309	A86	C8-C6-C5	3.09	123.68	118.94
23	5	312	A86	C8-C6-C5	3.09	123.68	118.94
21	c	503	CLA	O1D-CGD-CBD	-3.09	118.17	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	G	303	CLA	C4-C3-C5	3.09	119.51	115.98
21	a	402	CLA	CMB-C2B-C3B	3.09	130.45	124.68
21	b	610	CLA	C1-C2-C3	-3.09	120.70	126.04
21	B	609	CLA	C1-C2-C3	-3.09	120.71	126.04
23	2	310	A86	C35-C34-C33	3.08	115.26	109.88
21	5	302	CLA	CAC-C3C-C4C	3.08	128.81	124.81
21	5	307	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
21	c	514	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
24	8	313	KC1	CAC-C3C-C4C	3.08	128.81	124.81
21	3	301	CLA	CHD-C4C-NC	3.08	129.06	124.20
21	C	514	CLA	CHC-C1C-NC	-3.08	119.53	124.20
21	6	308	CLA	C6-C5-C3	-3.08	109.58	114.62
23	1	314	A86	C28-C27-C26	-3.08	118.61	122.92
21	B	616	CLA	C3D-C2D-C1D	-3.08	101.63	105.83
21	c	512	CLA	C4-C3-C5	3.08	120.45	115.27
21	1	303	CLA	CHC-C1C-NC	-3.08	119.54	124.20
21	8	303	CLA	CMD-C2D-C1D	3.08	130.13	124.71
21	5	305	CLA	CHD-C4C-NC	3.08	129.05	124.20
21	b	605	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
30	h	103	DGD	O6D-C1D-O3G	-3.07	102.69	109.97
21	J	301	CLA	C3D-C2D-C1D	-3.07	101.64	105.83
23	4	305	A86	C20-C19-C18	-3.07	106.67	112.75
24	J	313	KC1	CHD-C4C-NC	3.07	128.86	124.20
21	b	609	CLA	CMB-C2B-C3B	3.07	130.42	124.68
24	5	313	KC1	CHD-C4C-NC	3.07	128.86	124.20
30	H	101	DGD	O6D-C1D-O3G	-3.07	102.70	109.97
23	1	314	A86	C24-C1-C2	3.07	123.65	118.94
21	b	610	CLA	C4D-CHA-C1A	-3.07	117.52	121.25
21	d	406	CLA	O1D-CGD-CBD	-3.07	118.21	124.48
21	6	301	CLA	C4-C3-C5	3.07	120.43	115.27
23	W	101	A86	C28-C27-C26	-3.07	118.63	122.92
23	5	311	A86	C8-C6-C5	3.06	123.64	118.94
21	C	509	CLA	CHD-C4C-NC	3.06	129.03	124.20
21	B	616	CLA	C1D-CHD-C4C	-3.06	119.45	126.06
21	9	300	CLA	CAC-C3C-C4C	3.06	128.78	124.81
21	G	303	CLA	C4D-CHA-C1A	-3.06	117.52	121.25
21	a	403	CLA	CHD-C4C-NC	3.06	129.03	124.20
23	J	310	A86	C24-C1-C2	3.06	123.64	118.94
21	c	512	CLA	CHD-C4C-NC	3.06	129.03	124.20
21	A	401	CLA	CMB-C2B-C3B	3.06	130.40	124.68
24	J	311	KC1	CAA-C2A-C1A	-3.06	110.68	124.75
21	J	308	CLA	C6-C5-C3	-3.06	109.62	114.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	510	CLA	CMB-C2B-C3B	3.06	130.40	124.68
21	9	300	CLA	CHD-C4C-NC	3.06	129.02	124.20
21	b	606	CLA	CHD-C4C-NC	3.06	129.02	124.20
21	a	405	CLA	CHD-C4C-NC	3.06	129.02	124.20
21	6	306	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
31	C	502	SQD	C44-O6-C1	3.05	119.71	113.74
23	2	307	A86	C28-C27-C26	-3.05	118.65	122.92
21	G	301	CLA	CHD-C4C-NC	3.05	129.01	124.20
24	9	306	KC1	CAC-C3C-C4C	3.05	128.77	124.81
21	7	300	CLA	CHD-C4C-NC	3.05	129.01	124.20
21	7	309	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
21	G	304	CLA	CMB-C2B-C3B	3.05	130.38	124.68
29	8	318	LMU	C1B-O1B-C4'	-3.05	110.42	117.96
21	d	406	CLA	CHD-C4C-NC	3.05	129.01	124.20
21	G	302	CLA	CHD-C4C-C3C	-3.05	120.36	124.84
21	1	301	CLA	CMB-C2B-C3B	3.04	130.38	124.68
23	5	311	A86	C28-C27-C26	-3.04	118.66	122.92
21	c	509	CLA	CMB-C2B-C3B	3.04	130.37	124.68
21	J	304	CLA	CMC-C2C-C1C	3.04	129.67	125.04
21	B	603	CLA	CMB-C2B-C3B	3.04	130.37	124.68
24	6	311	KC1	CAA-C2A-C1A	-3.04	110.77	124.75
21	J	300	CLA	C4-C3-C5	3.04	120.38	115.27
23	6	310	A86	C8-C6-C5	3.04	123.60	118.94
21	C	503	CLA	C1-C2-C3	-3.04	120.79	126.04
23	g	311	A86	C8-C6-C5	3.04	123.60	118.94
21	c	511	CLA	CMB-C2B-C3B	3.04	130.36	124.68
21	A	402	CLA	CHD-C4C-NC	3.04	128.99	124.20
21	5	309	CLA	CMB-C2B-C3B	3.03	130.35	124.68
23	7	312	A86	C24-C1-C2	3.03	123.59	118.94
21	J	306	CLA	C4D-CHA-C1A	-3.03	117.56	121.25
21	D	404	CLA	C1-C2-C3	-3.03	120.80	126.04
24	4	307	KC1	CHD-C4C-NC	3.03	128.80	124.20
21	b	614	CLA	CHD-C4C-NC	3.03	128.97	124.20
21	9	303	CLA	CHA-C4D-ND	3.03	138.83	132.50
35	D	409	PL9	C40-C39-C41	3.03	120.36	115.27
25	B	617	BCR	C15-C14-C13	-3.03	122.99	127.31
24	6	311	KC1	O2D-CGD-O1D	-3.03	117.92	123.84
21	g	302	CLA	C4D-CHA-C1A	-3.03	117.57	121.25
21	5	305	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
25	m	101	BCR	C15-C16-C17	-3.03	117.28	123.47
21	B	603	CLA	CHD-C4C-NC	3.02	128.97	124.20
21	c	502	CLA	C1-C2-C3	-3.02	120.81	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	101	A86	C24-C1-C2	3.02	123.58	118.94
21	6	300	CLA	C4-C3-C5	3.02	120.36	115.27
21	C	508	CLA	CHD-C4C-C3C	-3.02	120.40	124.84
24	g	315	KC1	CAA-C2A-C1A	-3.02	110.86	124.75
21	5	309	CLA	O2A-CGA-CBA	3.02	121.39	111.91
21	b	617	CLA	O2A-CGA-O1A	-3.02	115.97	123.59
21	B	621	CLA	CAC-C3C-C4C	3.02	128.73	124.81
21	1	305	CLA	O2A-CGA-CBA	3.02	121.38	111.91
21	b	617	CLA	C3D-C2D-C1D	-3.02	101.71	105.83
23	7	312	A86	C28-C27-C26	-3.02	118.70	122.92
21	b	604	CLA	CHD-C4C-NC	3.02	128.96	124.20
21	2	301	CLA	CHD-C4C-NC	3.01	128.95	124.20
21	2	305	CLA	CHD-C4C-NC	3.01	128.95	124.20
21	D	407	CLA	O1D-CGD-CBD	-3.01	118.32	124.48
21	7	308	CLA	CHD-C4C-NC	3.01	128.95	124.20
21	c	512	CLA	C1-O2A-CGA	3.01	124.35	116.44
23	2	308	A86	C8-C6-C5	3.01	123.56	118.94
21	8	304	CLA	CHD-C4C-NC	3.01	128.95	124.20
21	b	613	CLA	CMC-C2C-C1C	3.01	129.62	125.04
24	J	312	KC1	CAC-C3C-C4C	3.01	128.71	124.81
21	g	304	CLA	C1D-CHD-C4C	-3.01	119.57	126.06
21	c	511	CLA	CMD-C2D-C1D	3.01	130.01	124.71
21	G	300	CLA	C4-C3-C5	3.01	120.33	115.27
21	3	301	CLA	C1-C2-C3	-3.01	120.84	126.04
21	D	404	CLA	CHD-C4C-NC	3.01	128.94	124.20
21	g	306	CLA	C1D-CHD-C4C	-3.01	119.57	126.06
21	6	307	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
22	5	310	DD6	C24-C1-C2	3.01	123.55	118.94
21	G	303	CLA	CAC-C3C-C4C	3.01	128.71	124.81
21	B	604	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
21	J	306	CLA	CHD-C4C-NC	3.00	128.94	124.20
21	G	302	CLA	C4-C3-C5	3.00	120.32	115.27
21	3	303	CLA	CHD-C4C-C3C	-3.00	120.43	124.84
23	7	313	A86	C24-C1-C2	3.00	123.55	118.94
21	C	504	CLA	C4-C3-C5	3.00	120.32	115.27
21	J	303	CLA	O1D-CGD-CBD	-3.00	118.34	124.48
23	2	312	A86	C28-C27-C26	-3.00	118.72	122.92
21	1	307	CLA	CHD-C1D-ND	-3.00	121.70	124.45
24	J	313	KC1	CBA-CAA-C2A	-3.00	113.84	125.27
21	B	616	CLA	CMB-C2B-C3B	3.00	130.29	124.68
21	B	612	CLA	CHC-C1C-NC	-3.00	119.66	124.20
22	7	310	DD6	C24-C1-C2	3.00	123.54	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	504	CLA	CHD-C4C-NC	3.00	128.93	124.20
21	6	303	CLA	CHC-C1C-NC	-3.00	119.66	124.20
21	1	301	CLA	CHD-C4C-NC	3.00	128.92	124.20
21	3	300	CLA	CMB-C2B-C3B	3.00	130.28	124.68
26	A	403	PHO	CMB-C2B-C3B	3.00	130.28	124.68
21	2	301	CLA	C4-C3-C5	3.00	120.31	115.27
21	C	513	CLA	CHD-C4C-NC	3.00	128.92	124.20
21	D	407	CLA	CHD-C4C-NC	2.99	128.92	124.20
24	G	308	KC1	CAC-C3C-C4C	2.99	128.69	124.81
25	M	101	BCR	C15-C16-C17	-2.99	117.34	123.47
21	2	306	CLA	CHD-C4C-NC	2.99	128.92	124.20
21	1	304	CLA	O2A-CGA-CBA	2.99	121.30	111.91
21	d	404	CLA	C1-C2-C3	-2.99	120.87	126.04
21	J	300	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
21	c	507	CLA	CHD-C4C-C3C	-2.99	120.44	124.84
21	5	306	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
21	C	513	CLA	C4-C3-C5	2.99	120.30	115.27
21	9	300	CLA	CMC-C2C-C1C	2.99	129.59	125.04
21	C	512	CLA	CMD-C2D-C1D	2.99	129.98	124.71
21	g	308	CLA	C1-C2-C3	-2.99	120.88	126.04
21	4	302	CLA	C4-C3-C5	2.99	120.29	115.27
21	9	300	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
21	b	613	CLA	C4-C3-C5	2.98	120.29	115.27
23	J	309	A86	C24-C1-C2	2.98	123.52	118.94
21	5	302	CLA	O1D-CGD-CBD	-2.98	118.38	124.48
21	b	606	CLA	O2A-CGA-CBA	2.98	121.26	111.91
21	B	612	CLA	C4-C3-C5	2.98	120.28	115.27
21	6	305	CLA	CHD-C4C-NC	2.98	128.90	124.20
21	B	605	CLA	CHD-C4C-NC	2.98	128.89	124.20
28	B	623	LMG	O6-C1-O1	-2.98	102.93	109.97
23	7	313	A86	C8-C6-C5	2.97	123.51	118.94
21	7	301	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
21	B	608	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
24	7	314	KC1	CHD-C4C-NC	2.97	128.72	124.20
21	B	611	CLA	C1-C2-C3	-2.97	120.90	126.04
23	g	312	A86	C26-C25-C24	2.97	132.49	123.22
21	b	617	CLA	C1D-CHD-C4C	-2.97	119.65	126.06
23	8	312	A86	C24-C1-C2	2.97	123.50	118.94
21	C	512	CLA	C1-C2-C3	-2.97	120.90	126.04
21	g	308	CLA	CAC-C3C-C4C	2.97	128.66	124.81
21	B	608	CLA	CHD-C4C-NC	2.97	128.88	124.20
24	g	313	KC1	C4C-C3C-C2C	-2.97	102.57	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	D	406	CLA	CHC-C1C-NC	-2.97	119.70	124.20
21	B	613	CLA	CHD-C4C-NC	2.97	128.88	124.20
23	2	308	A86	C28-C27-C26	-2.97	118.77	122.92
25	b	618	BCR	C15-C14-C13	-2.97	123.08	127.31
21	c	511	CLA	C1-C2-C3	-2.97	120.91	126.04
24	5	315	KC1	C4C-C3C-C2C	-2.97	102.57	106.90
24	9	305	KC1	CAA-C2A-C1A	-2.97	111.11	124.75
21	b	609	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
29	A	408	LMU	C3B-C4B-C5B	2.96	115.53	110.24
21	b	609	CLA	CHD-C4C-NC	2.96	128.87	124.20
21	1	309	CLA	CHC-C1C-NC	-2.96	119.71	124.20
21	4	303	CLA	C4-C3-C5	2.96	119.37	115.98
21	2	303	CLA	O1D-CGD-CBD	-2.96	118.42	124.48
25	b	619	BCR	C28-C27-C26	-2.96	108.79	114.08
21	5	302	CLA	C3D-C2D-C1D	-2.96	101.79	105.83
21	g	304	CLA	C4D-CHA-C1A	-2.96	117.64	121.25
21	G	300	CLA	CHC-C1C-NC	-2.96	119.71	124.20
23	8	311	A86	C8-C6-C5	2.96	123.48	118.94
21	J	301	CLA	O2A-CGA-CBA	2.96	121.19	111.91
21	b	623	CLA	C3D-C2D-C1D	-2.96	101.79	105.83
24	G	308	KC1	C4C-C3C-C2C	-2.96	102.58	106.90
22	g	310	DD6	C24-C1-C2	2.96	123.48	118.94
21	B	614	CLA	CMB-C2B-C3B	2.96	130.21	124.68
23	W	101	A86	C8-C6-C5	2.96	123.48	118.94
21	d	404	CLA	CHD-C4C-NC	2.96	128.86	124.20
21	6	304	CLA	CMC-C2C-C1C	2.96	129.54	125.04
21	6	301	CLA	O2A-CGA-CBA	2.96	121.19	111.91
21	B	611	CLA	CMB-C2B-C3B	2.96	130.21	124.68
21	b	612	CLA	C1-C2-C3	-2.96	120.93	126.04
26	a	404	PHO	CMB-C2B-C3B	2.96	130.21	124.68
21	7	301	CLA	CMB-C2B-C3B	2.95	130.21	124.68
21	g	306	CLA	CMB-C2B-C3B	2.95	130.21	124.68
21	6	300	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
21	9	302	CLA	CHC-C1C-NC	-2.95	119.73	124.20
21	B	605	CLA	O2A-CGA-CBA	2.95	121.17	111.91
29	a	408	LMU	C3B-C4B-C5B	2.95	115.50	110.24
21	6	306	CLA	C1-C2-C3	-2.95	120.95	126.04
21	7	301	CLA	CHD-C4C-NC	2.94	128.84	124.20
21	8	303	CLA	C1-C2-C3	-2.94	121.99	126.75
31	B	625	SQD	O8-S-C6	2.94	110.43	105.74
21	9	303	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
23	g	311	A86	C24-C1-C2	2.94	123.45	118.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	d	405	CLA	C4-C3-C5	2.94	120.22	115.27
23	6	310	A86	C24-C1-C2	2.94	123.45	118.94
21	B	610	CLA	C3D-C2D-C1D	-2.94	101.82	105.83
24	5	314	KC1	C4C-C3C-C2C	-2.94	102.62	106.90
21	J	301	CLA	C4-C3-C5	2.93	120.21	115.27
23	7	313	A86	C28-C27-C26	-2.93	118.81	122.92
21	B	612	CLA	CHD-C4C-NC	2.93	128.82	124.20
21	7	304	CLA	O2A-CGA-CBA	2.93	121.11	111.91
24	G	308	KC1	CAA-C2A-C1A	-2.93	111.27	124.75
21	2	301	CLA	CMB-C2B-C3B	2.93	130.16	124.68
21	1	309	CLA	CHD-C4C-NC	2.93	128.82	124.20
21	b	617	CLA	O2A-CGA-CBA	2.93	121.10	111.91
24	J	311	KC1	O2D-CGD-O1D	-2.93	118.11	123.84
21	b	610	CLA	CHD-C4C-NC	2.93	128.82	124.20
21	c	510	CLA	O2A-CGA-CBA	2.93	121.09	111.91
24	8	315	KC1	CBC-CAC-C3C	-2.93	104.36	112.43
21	c	502	CLA	CHD-C4C-NC	2.93	128.81	124.20
21	D	406	CLA	C4-C3-C5	2.93	120.19	115.27
21	J	304	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
24	G	309	KC1	CAA-C2A-C1A	-2.92	111.31	124.75
21	J	308	CLA	C1-C2-C3	-2.92	120.99	126.04
21	b	615	CLA	CMB-C2B-C3B	2.92	130.14	124.68
31	C	502	SQD	O5-C5-C4	2.92	115.00	109.69
21	b	603	CLA	CHD-C4C-NC	2.92	128.80	124.20
24	2	314	KC1	C4C-C3C-C2C	-2.92	102.64	106.90
23	8	312	A86	C33-C32-C31	2.92	112.05	109.21
21	1	301	CLA	CAC-C3C-C4C	2.92	128.60	124.81
21	6	304	CLA	CMD-C2D-C1D	2.92	129.86	124.71
24	2	314	KC1	CAA-CBA-CGA	-2.92	112.26	127.26
21	8	302	CLA	CMB-C2B-C3B	2.92	130.14	124.68
21	c	504	CLA	C3D-C2D-C1D	-2.92	101.85	105.83
21	8	306	CLA	C4D-CHA-C1A	-2.91	117.70	121.25
21	C	511	CLA	O2A-CGA-CBA	2.91	121.05	111.91
21	b	613	CLA	CHC-C1C-NC	-2.91	119.78	124.20
21	5	308	CLA	CHC-C1C-NC	-2.91	119.78	124.20
23	J	310	A86	C35-C34-C33	2.91	114.96	109.88
21	g	307	CLA	O1D-CGD-CBD	-2.91	118.53	124.48
21	A	401	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	6	307	CLA	C1D-CHD-C4C	-2.91	119.78	126.06
24	4	308	KC1	CAC-C3C-C4C	2.91	128.59	124.81
21	d	405	CLA	CHC-C1C-NC	-2.91	119.79	124.20
21	5	304	CLA	CHC-C1C-NC	-2.91	119.79	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	615	CLA	CHD-C4C-NC	2.90	128.78	124.20
21	c	504	CLA	CHC-C1C-NC	-2.90	119.80	124.20
21	c	504	CLA	C1-C2-C3	-2.90	121.02	126.04
24	2	316	KC1	C4C-C3C-C2C	-2.90	102.67	106.90
21	A	401	CLA	C1-C2-C3	-2.90	121.03	126.04
21	J	300	CLA	C1-C2-C3	-2.90	121.03	126.04
24	4	309	KC1	CHB-C1B-NB	-2.90	121.79	124.45
23	4	305	A86	C35-C34-C33	2.90	114.94	109.88
23	2	307	A86	C23-C16-C17	-2.90	103.95	108.98
21	7	302	CLA	CHC-C1C-NC	-2.90	119.81	124.20
21	5	302	CLA	CMB-C2B-C3B	2.90	130.10	124.68
21	9	301	CLA	C1-O2A-CGA	2.90	124.05	116.44
24	9	305	KC1	CHD-C4C-NC	2.90	128.60	124.20
21	d	404	CLA	CMB-C2B-C3B	2.90	130.10	124.68
21	c	510	CLA	CMB-C2B-C3B	2.90	130.10	124.68
21	a	402	CLA	C1-C2-C3	-2.90	121.03	126.04
21	g	304	CLA	C3D-C2D-C1D	-2.90	101.88	105.83
21	C	505	CLA	CHC-C1C-NC	-2.90	119.81	124.20
21	6	304	CLA	O1D-CGD-CBD	-2.90	118.56	124.48
21	8	306	CLA	CMB-C2B-C3B	2.89	130.09	124.68
24	2	313	KC1	CHB-C1B-NB	-2.89	121.79	124.45
21	C	505	CLA	C1-C2-C3	-2.89	121.04	126.04
21	J	300	CLA	CHD-C4C-NC	2.89	128.76	124.20
24	G	307	KC1	CHB-C1B-NB	-2.89	121.80	124.45
21	J	306	CLA	C1-C2-C3	-2.89	121.04	126.04
21	c	505	CLA	CHD-C4C-NC	2.89	128.76	124.20
21	5	309	CLA	CHB-C4A-NA	-2.89	120.51	124.51
21	6	300	CLA	CHD-C4C-NC	2.89	128.76	124.20
21	D	407	CLA	C1-C2-C3	-2.89	121.05	126.04
21	7	307	CLA	C4-C3-C5	2.89	120.13	115.27
21	b	616	CLA	O1D-CGD-CBD	-2.89	118.58	124.48
21	7	306	CLA	CHC-C1C-NC	-2.89	119.82	124.20
21	5	303	CLA	CHC-C1C-NC	-2.89	119.82	124.20
23	2	310	A86	C8-C6-C5	2.89	123.37	118.94
21	D	404	CLA	O2A-CGA-CBA	2.89	120.97	111.91
21	b	612	CLA	CMB-C2B-C3B	2.89	130.08	124.68
24	4	306	KC1	CHD-C4C-NC	2.88	128.49	124.23
21	4	301	CLA	CHD-C4C-NC	2.88	128.75	124.20
21	J	305	CLA	CHD-C4C-NC	2.88	128.75	124.20
21	8	306	CLA	CHD-C4C-NC	2.88	128.75	124.20
21	B	606	CLA	C4D-CHA-C1A	-2.88	117.74	121.25
21	4	300	CLA	C1B-CHB-C4A	-2.88	124.41	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	316	KC1	CHD-C4C-NC	2.88	128.58	124.20
21	g	309	CLA	CMD-C2D-C1D	2.88	129.79	124.71
24	g	315	KC1	CHD-C4C-NC	2.88	128.57	124.20
21	8	302	CLA	O2A-CGA-CBA	2.88	120.95	111.91
21	6	306	CLA	CHD-C4C-NC	2.88	128.74	124.20
21	2	306	CLA	CHC-C1C-NC	-2.88	119.83	124.20
21	8	302	CLA	C1-C2-C3	-2.88	121.06	126.04
21	B	609	CLA	C3D-C2D-C1D	-2.88	101.90	105.83
21	b	613	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
21	4	300	CLA	C1D-CHD-C4C	-2.88	119.85	126.06
21	7	307	CLA	CHD-C4C-NC	2.88	128.74	124.20
21	B	614	CLA	CHD-C4C-NC	2.88	128.74	124.20
21	b	606	CLA	C1-C2-C3	-2.88	121.06	126.04
24	J	312	KC1	CHD-C4C-NC	2.88	128.57	124.20
21	b	615	CLA	C3D-C2D-C1D	-2.88	101.91	105.83
24	8	316	KC1	C4C-C3C-C2C	-2.88	102.70	106.90
24	g	314	KC1	C4C-C3C-C2C	-2.88	102.70	106.90
23	2	312	A86	C24-C1-C2	2.88	123.35	118.94
21	1	308	CLA	CHD-C4C-NC	2.88	128.73	124.20
21	g	306	CLA	C4-C3-C5	2.87	120.11	115.27
21	2	302	CLA	CHC-C1C-NC	-2.87	119.84	124.20
24	2	316	KC1	CHD-C4C-NC	2.87	128.56	124.20
25	C	501	BCR	C24-C23-C22	-2.87	121.90	126.23
21	b	610	CLA	C3D-C2D-C1D	-2.87	101.92	105.83
21	c	508	CLA	C3D-C2D-C1D	-2.87	101.92	105.83
24	6	313	KC1	CHD-C4C-NC	2.87	128.56	124.20
21	d	404	CLA	O2A-CGA-CBA	2.87	120.91	111.91
21	c	503	CLA	CHD-C4C-NC	2.87	128.72	124.20
24	7	315	KC1	C4C-C3C-C2C	-2.87	102.72	106.90
21	b	611	CLA	C3D-C2D-C1D	-2.87	101.92	105.83
21	C	511	CLA	CMB-C2B-C3B	2.87	130.04	124.68
21	7	304	CLA	C4-C3-C5	2.87	120.09	115.27
24	1	316	KC1	C4C-C3C-C2C	-2.87	102.72	106.90
21	B	605	CLA	C3B-C4B-NB	2.87	112.92	109.21
21	7	302	CLA	C4-C3-C5	2.87	120.09	115.27
21	b	606	CLA	C3B-C4B-NB	2.87	112.92	109.21
21	C	506	CLA	CHD-C4C-NC	2.87	128.72	124.20
21	4	303	CLA	CHC-C1C-NC	-2.87	119.86	124.20
23	2	310	A86	C24-C1-C2	2.86	123.34	118.94
21	3	302	CLA	CHC-C1C-NC	-2.86	119.86	124.20
24	8	315	KC1	CHD-C4C-NC	2.86	128.55	124.20
21	B	614	CLA	CHC-C1C-NC	-2.86	119.86	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	305	KC1	CHD-C4C-NC	2.86	128.55	124.20
21	a	403	CLA	C3D-C2D-C1D	-2.86	101.93	105.83
21	7	301	CLA	C4-C3-C5	2.86	120.08	115.27
24	8	314	KC1	CAA-CBA-CGA	-2.86	112.56	127.26
21	5	306	CLA	C1-O2A-CGA	2.86	123.95	116.44
21	7	305	CLA	C1D-CHD-C4C	-2.86	119.89	126.06
24	8	313	KC1	C4C-C3C-C2C	-2.86	102.73	106.90
21	7	302	CLA	CMB-C2B-C3B	2.86	130.03	124.68
24	5	314	KC1	CAC-C3C-C4C	2.86	128.52	124.81
24	3	305	KC1	CHB-C1B-NB	-2.86	121.83	124.45
21	B	605	CLA	C4-C3-C5	2.86	120.08	115.27
21	g	303	CLA	CHD-C4C-NC	2.86	128.70	124.20
24	G	306	KC1	CHD-C4C-NC	2.86	128.45	124.23
21	5	303	CLA	C4-C3-C5	2.85	120.07	115.27
24	5	315	KC1	CMB-C2B-C1B	2.85	129.74	124.71
23	6	310	A86	C35-C34-C33	2.85	114.85	109.88
21	1	302	CLA	O2A-CGA-CBA	2.85	120.86	111.91
21	A	402	CLA	C3D-C2D-C1D	-2.85	101.94	105.83
21	B	614	CLA	C3D-C2D-C1D	-2.85	101.94	105.83
21	1	301	CLA	C4-C3-C5	2.85	120.06	115.27
21	g	302	CLA	O1D-CGD-CBD	-2.85	118.66	124.48
24	J	313	KC1	CAA-C2A-C1A	-2.85	111.65	124.75
23	8	309	A86	C24-C1-C2	2.85	123.31	118.94
23	5	311	A86	C23-C16-C17	-2.85	104.03	108.98
22	1	311	DD6	C13-C11-C10	2.85	123.31	118.94
21	1	310	CLA	CHC-C1C-NC	-2.85	119.89	124.20
24	9	305	KC1	CAC-C3C-C4C	2.85	128.50	124.81
21	9	300	CLA	C4-C3-C5	2.85	120.06	115.27
21	b	604	CLA	CMB-C2B-C3B	2.85	130.00	124.68
32	f	101	HEM	C4D-ND-C1D	2.84	108.01	105.07
24	3	305	KC1	C4C-C3C-C2C	-2.84	102.75	106.90
31	b	602	SQD	O8-S-C6	2.84	110.27	105.74
21	B	610	CLA	C4-C3-C5	2.84	120.05	115.27
24	G	307	KC1	CAC-C3C-C4C	2.84	128.50	124.81
21	2	305	CLA	CMB-C2B-C3B	2.84	130.00	124.68
21	a	402	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
21	5	303	CLA	CHD-C4C-NC	2.84	128.68	124.20
21	D	404	CLA	CMB-C2B-C3B	2.84	129.99	124.68
24	5	313	KC1	C4C-C3C-C2C	-2.84	102.76	106.90
24	2	313	KC1	CHD-C4C-NC	2.84	128.51	124.20
21	9	301	CLA	O1D-CGD-CBD	-2.84	118.68	124.48
21	c	504	CLA	C4-C3-C5	2.84	120.04	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	304	CLA	C3D-C2D-C1D	-2.84	101.96	105.83
21	d	405	CLA	CMC-C2C-C1C	2.83	129.36	125.04
24	8	314	KC1	C4C-C3C-C2C	-2.83	102.77	106.90
23	W	101	A86	C17-C16-C15	2.83	112.05	109.16
21	b	606	CLA	C4-C3-C5	2.83	120.04	115.27
21	7	304	CLA	C4D-CHA-C1A	-2.83	117.80	121.25
21	b	612	CLA	C3D-C2D-C1D	-2.83	101.97	105.83
23	2	308	A86	C24-C1-C2	2.83	123.29	118.94
21	4	302	CLA	C1-O2A-CGA	2.83	123.88	116.44
24	9	306	KC1	C4C-C3C-C2C	-2.83	102.77	106.90
21	B	613	CLA	C3D-C2D-C1D	-2.83	101.97	105.83
21	c	510	CLA	CHD-C4C-NC	2.83	128.66	124.20
30	C	517	DGD	CDB-CCB-CBB	-2.83	100.06	114.42
21	3	300	CLA	C3D-C2D-C1D	-2.83	101.97	105.83
24	1	315	KC1	CHD-C4C-NC	2.83	128.49	124.20
21	B	605	CLA	C1-C2-C3	-2.83	121.16	126.04
21	D	406	CLA	CMC-C2C-C1C	2.82	129.34	125.04
21	b	614	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
24	8	313	KC1	CHD-C4C-NC	2.82	128.49	124.20
21	4	304	CLA	CMB-C2B-C3B	2.82	129.96	124.68
21	C	511	CLA	CHD-C4C-NC	2.82	128.65	124.20
21	5	309	CLA	CHA-C1A-NA	-2.82	119.94	126.40
21	b	605	CLA	O2A-CGA-CBA	2.82	120.76	111.91
21	g	303	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
21	G	304	CLA	CHC-C1C-NC	-2.82	119.92	124.20
21	5	308	CLA	C4-C3-C5	2.82	120.02	115.27
21	G	304	CLA	C1D-CHD-C4C	-2.82	119.97	126.06
24	J	313	KC1	O1D-CGD-CBD	-2.82	118.71	124.48
21	B	614	CLA	CMC-C2C-C1C	2.82	129.33	125.04
21	1	303	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
24	9	305	KC1	C4C-C3C-C2C	-2.82	102.79	106.90
22	7	310	DD6	C13-C11-C10	2.82	123.27	118.94
21	b	615	CLA	CHC-C1C-NC	-2.82	119.93	124.20
28	8	301	LMG	O6-C1-O1	-2.82	103.30	109.97
21	7	305	CLA	C3D-C2D-C1D	-2.82	101.99	105.83
21	B	604	CLA	O2A-CGA-CBA	2.82	120.75	111.91
21	4	302	CLA	CED-O2D-CGD	2.82	122.31	115.94
24	g	314	KC1	CHD-C4C-NC	2.82	128.48	124.20
21	1	308	CLA	O2A-CGA-CBA	2.82	120.74	111.91
24	4	309	KC1	C4C-C3C-C2C	-2.82	102.79	106.90
28	D	411	LMG	O6-C1-O1	-2.82	103.31	109.97
24	1	315	KC1	CAA-C2A-C1A	-2.82	111.81	124.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	5	312	A86	C24-C1-C2	2.81	123.26	118.94
24	J	311	KC1	C4C-C3C-C2C	-2.81	102.80	106.90
21	7	303	CLA	CMC-C2C-C1C	2.81	129.32	125.04
21	5	309	CLA	CMC-C2C-C1C	2.81	129.32	125.04
24	5	313	KC1	CAA-CBA-CGA	-2.81	112.80	127.26
23	7	311	A86	C28-C27-C26	-2.81	118.98	122.92
21	2	304	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
21	b	607	CLA	C4D-CHA-C1A	-2.81	117.83	121.25
21	5	303	CLA	CMB-C2B-C3B	2.81	129.94	124.68
21	1	307	CLA	CHC-C1C-NC	-2.81	119.94	124.20
21	g	309	CLA	CHC-C1C-NC	-2.81	119.94	124.20
21	4	304	CLA	C1D-CHD-C4C	-2.81	120.00	126.06
24	8	314	KC1	O2D-CGD-O1D	-2.81	118.34	123.84
21	3	303	CLA	O1D-CGD-CBD	-2.81	118.73	124.48
21	8	305	CLA	C3D-C2D-C1D	-2.81	102.00	105.83
28	A	407	LMG	O6-C1-O1	-2.81	103.33	109.97
24	2	316	KC1	CMB-C2B-C1B	2.81	129.66	124.71
30	c	516	DGD	O5D-C6D-C5D	-2.81	103.86	109.05
21	c	510	CLA	C1-C2-C3	-2.80	121.19	126.04
21	g	304	CLA	O2A-CGA-CBA	2.80	120.71	111.91
21	G	300	CLA	O2A-CGA-CBA	2.80	120.71	111.91
24	1	316	KC1	CAA-C2A-C1A	-2.80	111.85	124.75
21	C	503	CLA	CMB-C2B-C3B	2.80	129.92	124.68
21	7	300	CLA	CAC-C3C-C4C	2.80	128.45	124.81
21	B	606	CLA	CMC-C2C-C1C	2.80	129.31	125.04
21	B	610	CLA	O2A-CGA-CBA	2.80	120.70	111.91
23	8	309	A86	C28-C27-C26	-2.80	119.00	122.92
21	8	303	CLA	CHC-C1C-NC	-2.80	119.95	124.20
21	g	307	CLA	CAC-C3C-C4C	2.80	128.44	124.81
21	J	308	CLA	CHD-C4C-NC	2.80	128.62	124.20
21	2	302	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
30	h	103	DGD	CDB-CCB-CBB	-2.80	100.22	114.42
24	4	308	KC1	CHD-C4C-NC	2.80	128.45	124.20
21	9	301	CLA	CHD-C4C-NC	2.80	128.61	124.20
24	6	312	KC1	CHC-C4B-NB	-2.80	121.88	124.45
21	9	300	CLA	C3D-C2D-C1D	-2.80	102.01	105.83
23	1	312	A86	C28-C27-C26	-2.80	119.01	122.92
28	B	622	LMG	O6-C1-O1	-2.80	103.35	109.97
21	G	300	CLA	C3D-C2D-C1D	-2.80	102.02	105.83
24	G	307	KC1	C4C-C3C-C2C	-2.79	102.82	106.90
21	4	303	CLA	CAC-C3C-C4C	2.79	128.44	124.81
21	8	306	CLA	C4-C3-C5	2.79	119.97	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	C	505	CLA	C4-C3-C5	2.79	119.97	115.27
23	8	311	A86	C24-C1-C2	2.79	123.23	118.94
23	8	310	A86	C28-C27-C26	-2.79	119.01	122.92
21	g	307	CLA	CHD-C4C-NC	2.79	128.60	124.20
24	G	309	KC1	CHB-C1B-NB	-2.79	121.89	124.45
21	6	306	CLA	O2A-CGA-CBA	2.79	120.67	111.91
21	3	302	CLA	C2D-C1D-ND	2.79	112.16	110.10
21	b	611	CLA	O2A-CGA-CBA	2.79	120.67	111.91
21	B	607	CLA	CHD-C4C-NC	2.79	128.60	124.20
21	8	304	CLA	C1-C2-C3	-2.79	121.22	126.04
24	1	316	KC1	CHD-C4C-NC	2.79	128.44	124.20
21	6	307	CLA	O2A-CGA-CBA	2.79	120.67	111.91
21	d	404	CLA	C3D-C2D-C1D	-2.79	102.02	105.83
24	9	306	KC1	CHD-C4C-NC	2.79	128.44	124.20
21	g	302	CLA	C3D-C2D-C1D	-2.79	102.03	105.83
24	6	313	KC1	CAC-C3C-C4C	2.79	128.43	124.81
21	b	615	CLA	C4-C3-C5	2.79	119.96	115.27
21	5	307	CLA	O2A-CGA-CBA	2.79	120.66	111.91
24	5	314	KC1	CHD-C4C-NC	2.79	128.43	124.20
25	d	407	BCR	C2-C1-C6	2.79	114.77	110.48
21	A	402	CLA	O2A-CGA-CBA	2.79	120.65	111.91
21	a	403	CLA	O2A-CGA-CBA	2.79	120.65	111.91
21	c	506	CLA	CHD-C4C-NC	2.79	128.59	124.20
24	1	315	KC1	C4C-C3C-C2C	-2.79	102.84	106.90
21	3	300	CLA	C1D-CHD-C4C	-2.78	120.05	126.06
21	g	302	CLA	O2A-CGA-CBA	2.78	120.64	111.91
21	c	509	CLA	O2A-CGA-CBA	2.78	120.64	111.91
21	B	611	CLA	C3D-C2D-C1D	-2.78	102.03	105.83
24	6	311	KC1	C4C-C3C-C2C	-2.78	102.84	106.90
24	6	312	KC1	CHD-C4C-NC	2.78	128.43	124.20
25	1	317	BCR	C27-C26-C25	2.78	126.77	122.73
31	X	401	SQD	O8-S-C6	2.78	110.17	105.74
32	E	101	HEM	CMC-C2C-C3C	2.78	129.88	124.68
21	J	307	CLA	O1D-CGD-CBD	-2.78	118.80	124.48
21	b	607	CLA	CMD-C2D-C1D	2.78	129.61	124.71
21	8	305	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
21	8	306	CLA	C3D-C2D-C1D	-2.78	102.04	105.83
21	B	606	CLA	CMD-C2D-C1D	2.78	129.61	124.71
21	7	304	CLA	C3D-C2D-C1D	-2.78	102.04	105.83
21	g	303	CLA	CHC-C1C-NC	-2.78	119.99	124.20
21	4	303	CLA	O2A-CGA-CBA	2.78	120.62	111.91
21	c	513	CLA	CHD-C4C-NC	2.78	128.58	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	f	101	HEM	C4B-CHC-C1C	2.78	126.22	122.56
21	G	304	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
21	c	507	CLA	CAC-C3C-C4C	2.77	128.41	124.81
24	6	313	KC1	O1D-CGD-CBD	-2.77	118.81	124.48
24	4	307	KC1	CAC-C3C-C4C	2.77	128.41	124.81
21	3	301	CLA	O2A-CGA-CBA	2.77	120.61	111.91
21	b	607	CLA	CMC-C2C-C1C	2.77	129.26	125.04
30	b	601	DGD	CDB-CCB-CBB	-2.77	100.36	114.42
21	b	608	CLA	CHC-C1C-NC	-2.77	120.00	124.20
21	8	303	CLA	O2A-CGA-CBA	2.77	120.60	111.91
30	C	517	DGD	O5D-C6D-C5D	-2.77	103.92	109.05
23	g	311	A86	C23-C16-C17	-2.77	104.17	108.98
21	7	303	CLA	C3D-C2D-C1D	-2.77	102.05	105.83
21	C	511	CLA	C3D-C2D-C1D	-2.77	102.05	105.83
21	3	303	CLA	CAC-C3C-C4C	2.77	128.40	124.81
21	G	303	CLA	O2A-CGA-CBA	2.77	120.59	111.91
21	C	513	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
21	c	512	CLA	C3D-C2D-C1D	-2.77	102.06	105.83
24	6	311	KC1	CAC-C3C-C4C	2.77	128.40	124.81
21	b	617	CLA	C1-C2-C3	-2.77	121.26	126.04
21	1	304	CLA	C3D-C2D-C1D	-2.77	102.06	105.83
21	1	303	CLA	CMB-C2B-C3B	2.77	129.85	124.68
21	3	304	CLA	CMC-C2C-C1C	2.77	129.25	125.04
21	g	308	CLA	CHC-C1C-NC	-2.77	120.01	124.20
24	J	311	KC1	CHD-C4C-NC	2.77	128.40	124.20
21	7	303	CLA	O2A-CGA-CBA	2.77	120.58	111.91
24	g	315	KC1	CMC-C2C-C1C	2.76	129.25	125.04
21	d	405	CLA	O2A-CGA-CBA	2.76	120.58	111.91
21	d	406	CLA	CMB-C2B-C3B	2.76	129.85	124.68
24	3	306	KC1	C4C-C3C-C2C	-2.76	102.87	106.90
21	C	509	CLA	CMB-C2B-C3B	2.76	129.85	124.68
21	7	307	CLA	C1-C2-C3	-2.76	121.26	126.04
21	g	303	CLA	CHD-C1D-ND	-2.76	121.92	124.45
21	2	306	CLA	C3D-C2D-C1D	-2.76	102.06	105.83
24	8	316	KC1	CMB-C2B-C1B	2.76	129.58	124.71
24	7	315	KC1	CAA-C2A-C1A	-2.76	112.05	124.75
21	c	502	CLA	C4-C3-C5	2.76	119.92	115.27
21	3	300	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
21	b	604	CLA	CMD-C2D-C1D	2.76	129.58	124.71
32	E	101	HEM	C4B-CHC-C1C	2.76	126.20	122.56
30	B	624	DGD	CDB-CCB-CBB	-2.76	100.42	114.42
21	8	307	CLA	CHC-C1C-NC	-2.76	120.02	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c	514	CLA	O2A-CGA-CBA	2.76	120.56	111.91
21	C	514	CLA	CHD-C4C-NC	2.76	128.55	124.20
21	g	308	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
21	D	406	CLA	O2A-CGA-CBA	2.76	120.56	111.91
24	G	309	KC1	C4C-C3C-C2C	-2.76	102.88	106.90
25	D	408	BCR	C2-C1-C6	2.76	114.72	110.48
24	6	312	KC1	C4C-C3C-C2C	-2.75	102.88	106.90
26	A	403	PHO	O1D-CGD-CBD	2.75	129.33	124.74
21	J	304	CLA	CHC-C1C-NC	-2.75	120.02	124.20
21	1	301	CLA	C3D-C2D-C1D	-2.75	102.07	105.83
21	b	607	CLA	C3D-C2D-C1D	-2.75	102.07	105.83
21	1	306	CLA	C3D-C2D-C1D	-2.75	102.07	105.83
21	B	606	CLA	C3D-C2D-C1D	-2.75	102.07	105.83
21	B	603	CLA	O2A-CGA-CBA	2.75	120.55	111.91
21	6	303	CLA	CHD-C4C-NC	2.75	128.54	124.20
21	C	509	CLA	C3D-C2D-C1D	-2.75	102.07	105.83
24	6	313	KC1	C4C-C3C-C2C	-2.75	102.89	106.90
21	C	507	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	7	311	A86	C24-C1-C2	2.75	123.16	118.94
21	5	303	CLA	C1-C2-C3	-2.75	121.28	126.04
21	6	307	CLA	CHD-C4C-NC	2.75	128.54	124.20
21	b	608	CLA	CHD-C4C-NC	2.75	128.54	124.20
21	9	303	CLA	C3D-C2D-C1D	-2.75	102.08	105.83
21	C	510	CLA	CAC-C3C-C4C	2.75	128.38	124.81
21	B	603	CLA	CMD-C2D-C1D	2.75	129.56	124.71
21	1	303	CLA	C4-C3-C5	2.75	119.89	115.27
28	B	622	LMG	O1-C7-C8	-2.75	104.27	110.90
21	g	305	CLA	CAC-C3C-C4C	2.75	128.38	124.81
24	g	313	KC1	CHD-C4C-NC	2.75	128.37	124.20
21	c	510	CLA	C3D-C2D-C1D	-2.75	102.08	105.83
21	8	307	CLA	CAC-C3C-C4C	2.75	128.37	124.81
21	C	505	CLA	CHD-C4C-NC	2.75	128.53	124.20
21	c	509	CLA	C3D-C2D-C1D	-2.75	102.08	105.83
24	7	315	KC1	CHD-C4C-NC	2.75	128.37	124.20
21	6	300	CLA	C1-C2-C3	-2.75	121.30	126.04
21	5	303	CLA	C6-C5-C3	-2.75	110.13	114.62
24	g	315	KC1	C4C-C3C-C2C	-2.74	102.90	106.90
21	B	607	CLA	CHC-C1C-NC	-2.74	120.05	124.20
21	9	304	CLA	C4-C3-C5	2.74	119.88	115.27
21	C	515	CLA	O1D-CGD-CBD	-2.74	118.88	124.48
21	5	308	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
24	5	315	KC1	CAC-C3C-C4C	2.74	128.36	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	7	312	A86	C20-C19-C18	-2.74	107.33	112.75
23	4	305	A86	C28-C27-C26	-2.74	119.09	122.92
21	B	606	CLA	CAC-C3C-C4C	2.74	128.36	124.81
24	6	313	KC1	CAA-C2A-C1A	-2.74	112.16	124.75
28	f	102	LMG	O6-C1-O1	-2.74	103.49	109.97
21	6	301	CLA	C3D-C2D-C1D	-2.74	102.10	105.83
21	5	303	CLA	O2A-CGA-CBA	2.74	120.49	111.91
28	N	101	LMG	O6-C1-O1	-2.74	103.50	109.97
21	C	503	CLA	C3D-C2D-C1D	-2.74	102.10	105.83
21	3	301	CLA	C4-C3-C5	2.74	119.87	115.27
21	5	309	CLA	C1-C2-C3	-2.73	121.31	126.04
21	b	615	CLA	CMC-C2C-C1C	2.73	129.20	125.04
21	5	307	CLA	C4-C3-C5	2.73	119.87	115.27
21	J	307	CLA	CED-O2D-CGD	2.73	122.12	115.94
24	4	307	KC1	C4C-C3C-C2C	-2.73	102.91	106.90
24	4	308	KC1	CHB-C1B-NB	-2.73	121.94	124.45
28	B	620	LMG	O6-C1-O1	-2.73	103.50	109.97
21	1	302	CLA	C3D-C2D-C1D	-2.73	102.10	105.83
21	b	608	CLA	O1D-CGD-CBD	-2.73	118.89	124.48
21	c	508	CLA	CHC-C1C-NC	-2.73	120.06	124.20
21	c	505	CLA	C3D-C2D-C1D	-2.73	102.10	105.83
21	5	308	CLA	C3D-C2D-C1D	-2.73	102.10	105.83
21	b	603	CLA	CHC-C1C-NC	-2.73	120.06	124.20
28	2	318	LMG	O6-C1-O1	-2.73	103.51	109.97
21	2	303	CLA	C3D-C2D-C1D	-2.73	102.11	105.83
21	4	304	CLA	C4-C3-C5	2.73	119.86	115.27
21	g	304	CLA	CHC-C1C-NC	-2.73	120.06	124.20
24	2	315	KC1	CHD-C4C-NC	2.73	128.34	124.20
24	2	313	KC1	C4C-C3C-C2C	-2.73	102.92	106.90
21	c	508	CLA	CMB-C2B-C3B	2.73	129.78	124.68
21	6	307	CLA	C4D-CHA-C1A	-2.73	117.93	121.25
21	5	304	CLA	O2A-CGA-CBA	2.73	120.47	111.91
21	4	301	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
23	2	309	A86	C20-C19-C18	-2.73	107.35	112.75
21	c	514	CLA	C3D-C2D-C1D	-2.73	102.11	105.83
21	5	309	CLA	CED-O2D-CGD	2.73	122.10	115.94
27	B	601	LHG	O8-C23-C24	2.72	120.46	111.91
24	J	312	KC1	C4C-C3C-C2C	-2.72	102.93	106.90
21	B	614	CLA	C1-C2-C3	-2.72	121.33	126.04
21	7	308	CLA	C4-C3-C5	2.72	119.85	115.27
21	C	515	CLA	O2A-CGA-CBA	2.72	120.45	111.91
21	A	404	CLA	C3D-C2D-C1D	-2.72	102.12	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	h	101	BCR	C15-C14-C13	-2.72	123.43	127.31
21	4	301	CLA	O2A-CGA-CBA	2.72	120.45	111.91
26	a	404	PHO	O1D-CGD-CBD	2.72	129.27	124.74
21	6	307	CLA	C3D-C2D-C1D	-2.72	102.12	105.83
21	d	406	CLA	C3D-C2D-C1D	-2.72	102.12	105.83
23	g	312	A86	C35-C34-C33	2.72	114.62	109.88
31	C	502	SQD	C4-C3-C2	2.72	115.57	110.82
21	6	301	CLA	CMC-C2C-C1C	2.72	129.18	125.04
21	C	504	CLA	CHC-C1C-NC	-2.72	120.08	124.20
21	c	512	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
21	c	507	CLA	C4D-CHA-C1A	-2.72	117.94	121.25
22	7	310	DD6	C15-C14-C13	2.72	131.74	125.99
21	G	301	CLA	CHC-C1C-NC	-2.72	120.08	124.20
21	J	306	CLA	O2A-CGA-CBA	2.72	120.43	111.91
21	6	307	CLA	O1D-CGD-CBD	-2.72	118.93	124.48
24	G	307	KC1	CAA-C2A-C1A	-2.72	112.26	124.75
21	7	306	CLA	CHD-C1D-ND	-2.72	121.96	124.45
21	6	300	CLA	C3D-C2D-C1D	-2.72	102.12	105.83
21	a	402	CLA	CMC-C2C-C1C	2.72	129.17	125.04
21	b	623	CLA	CMD-C2D-C1D	2.72	129.50	124.71
24	7	314	KC1	CAA-C2A-C1A	-2.71	112.27	124.75
21	g	303	CLA	O2A-CGA-CBA	2.71	120.42	111.91
21	J	308	CLA	C4-C3-C5	2.71	119.83	115.27
21	8	306	CLA	CMC-C2C-C1C	2.71	129.17	125.04
26	A	403	PHO	O2D-CGD-O1D	-2.71	118.53	123.84
23	5	311	A86	C33-C32-C31	2.71	111.85	109.21
31	C	502	SQD	O8-S-C6	2.71	110.06	105.74
21	b	605	CLA	CHC-C1C-NC	-2.71	120.09	124.20
24	2	315	KC1	C4C-C3C-C2C	-2.71	102.94	106.90
21	1	309	CLA	O1D-CGD-CBD	-2.71	118.94	124.48
21	B	621	CLA	C3D-C2D-C1D	-2.71	102.13	105.83
30	c	516	DGD	CDB-CCB-CBB	-2.71	100.66	114.42
21	c	508	CLA	C4-C3-C5	2.71	119.83	115.27
24	5	315	KC1	CHD-C4C-NC	2.71	128.31	124.20
21	J	304	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
24	1	316	KC1	CMB-C2B-C1B	2.71	129.49	124.71
28	b	621	LMG	O6-C1-O1	-2.71	103.56	109.97
21	5	305	CLA	CMB-C2B-C3B	2.71	129.75	124.68
30	H	101	DGD	CDB-CCB-CBB	-2.71	100.68	114.42
28	B	627	LMG	O8-C28-O10	-2.71	116.76	123.59
21	D	407	CLA	C3D-C2D-C1D	-2.71	102.14	105.83
21	D	404	CLA	C3D-C2D-C1D	-2.70	102.14	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	307	CLA	CAC-C3C-C4C	2.70	128.32	124.81
23	8	311	A86	C28-C27-C26	-2.70	119.14	122.92
21	b	611	CLA	C4-C3-C5	2.70	119.82	115.27
26	d	403	PHO	O1D-CGD-CBD	2.70	129.24	124.74
21	a	405	CLA	C1-C2-C3	-2.70	121.37	126.04
25	c	515	BCR	C15-C14-C13	-2.70	123.45	127.31
21	b	616	CLA	C4-C3-C5	2.70	119.82	115.27
25	h	101	BCR	C15-C16-C17	-2.70	117.94	123.47
21	B	604	CLA	CHC-C1C-NC	-2.70	120.11	124.20
21	3	301	CLA	C3D-C2D-C1D	-2.70	102.15	105.83
21	7	300	CLA	C3D-C2D-C1D	-2.70	102.15	105.83
21	G	300	CLA	C1D-CHD-C4C	-2.70	120.23	126.06
24	2	313	KC1	CBC-CAC-C3C	-2.70	104.99	112.43
24	6	311	KC1	CHB-C1B-NB	-2.70	121.97	124.45
21	b	607	CLA	CAC-C3C-C4C	2.70	128.31	124.81
21	2	301	CLA	CMC-C2C-C1C	2.70	129.15	125.04
24	7	314	KC1	C4C-C3C-C2C	-2.70	102.97	106.90
27	D	410	LHG	O8-C23-C24	2.70	120.37	111.91
32	E	101	HEM	C4D-ND-C1D	2.70	107.86	105.07
21	6	306	CLA	C4D-CHA-C1A	-2.70	117.97	121.25
32	E	101	HEM	CHC-C4B-C3B	2.69	128.69	124.57
21	3	304	CLA	CHD-C4C-NC	2.69	128.45	124.20
21	G	300	CLA	CAC-C3C-C4C	2.69	128.30	124.81
22	1	311	DD6	C24-C1-C2	2.69	123.07	118.94
21	1	302	CLA	C1-C2-C3	-2.69	121.39	126.04
21	9	300	CLA	O2A-CGA-CBA	2.69	120.36	111.91
21	5	305	CLA	C3D-C2D-C1D	-2.69	102.16	105.83
21	5	306	CLA	C3D-C2D-C1D	-2.69	102.16	105.83
24	G	309	KC1	CMB-C2B-C1B	2.69	129.46	124.71
24	8	315	KC1	C4C-C3C-C2C	-2.69	102.97	106.90
21	g	309	CLA	CHD-C4C-NC	2.69	128.44	124.20
21	6	305	CLA	C3D-C2D-C1D	-2.69	102.16	105.83
21	7	306	CLA	CAC-C3C-C4C	2.69	128.30	124.81
21	B	602	CLA	C3D-C2D-C1D	-2.69	102.16	105.83
21	C	503	CLA	CHC-C1C-NC	-2.69	120.12	124.20
21	b	616	CLA	CHD-C4C-NC	2.69	128.44	124.20
29	g	316	LMU	C4B-C3B-C2B	2.69	115.52	110.82
21	c	507	CLA	C3D-C2D-C1D	-2.69	102.16	105.83
21	5	303	CLA	C3D-C2D-C1D	-2.69	102.16	105.83
25	B	618	BCR	C28-C27-C26	-2.69	109.28	114.08
21	J	306	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
28	B	619	LMG	O6-C1-O1	-2.69	103.61	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	G	303	CLA	C3D-C2D-C1D	-2.69	102.16	105.83
21	A	401	CLA	CMC-C2C-C1C	2.69	129.13	125.04
26	D	401	PHO	O1D-CGD-CBD	2.69	129.21	124.74
24	4	309	KC1	CAA-C2A-C1A	-2.69	112.40	124.75
21	5	302	CLA	C4-C3-C5	2.69	119.79	115.27
21	8	302	CLA	C3D-C2D-C1D	-2.69	102.17	105.83
21	8	307	CLA	C3D-C2D-C1D	-2.69	102.17	105.83
21	G	301	CLA	O2A-CGA-CBA	2.69	120.33	111.91
21	7	308	CLA	C3D-C2D-C1D	-2.68	102.17	105.83
21	C	506	CLA	C3D-C2D-C1D	-2.68	102.17	105.83
21	1	301	CLA	O2A-CGA-CBA	2.68	120.33	111.91
27	l	101	LHG	O8-C23-C24	2.68	120.33	111.91
28	8	317	LMG	O6-C1-O1	-2.68	103.62	109.97
21	c	502	CLA	CMB-C2B-C3B	2.68	129.70	124.68
21	b	615	CLA	O1D-CGD-CBD	-2.68	118.99	124.48
21	5	307	CLA	O1D-CGD-CBD	-2.68	118.99	124.48
21	c	504	CLA	CAC-C3C-C4C	2.68	128.29	124.81
35	D	409	PL9	C7-C8-C9	-2.68	122.33	126.79
28	b	624	LMG	O6-C1-O1	-2.68	103.62	109.97
21	9	300	CLA	CMB-C2B-C3B	2.68	129.70	124.68
21	g	305	CLA	CHC-C1C-NC	-2.68	120.13	124.20
21	9	301	CLA	CAC-C3C-C4C	2.68	128.29	124.81
24	4	306	KC1	CHB-C1B-NB	-2.68	121.99	124.45
21	b	603	CLA	C3D-C2D-C1D	-2.68	102.17	105.83
28	b	626	LMG	O6-C1-O1	-2.68	103.62	109.97
24	J	313	KC1	C4C-C3C-C2C	-2.68	102.99	106.90
21	c	503	CLA	CHC-C1C-NC	-2.68	120.14	124.20
21	a	405	CLA	CMC-C2C-C1C	2.68	129.12	125.04
21	4	300	CLA	CHD-C4C-C3C	-2.68	120.90	124.84
21	a	403	CLA	CMD-C2D-C1D	2.68	129.43	124.71
24	5	314	KC1	CAA-C2A-C1A	-2.68	112.44	124.75
21	b	608	CLA	C4-C3-C5	2.68	119.78	115.27
21	8	304	CLA	O2A-CGA-CBA	2.68	120.31	111.91
21	9	304	CLA	CHC-C1C-NC	-2.68	120.14	124.20
21	6	301	CLA	CHC-C1C-NC	-2.68	120.14	124.20
21	9	302	CLA	CAC-C3C-C4C	2.68	128.28	124.81
21	A	402	CLA	CMD-C2D-C1D	2.68	129.43	124.71
27	d	409	LHG	O8-C23-C24	2.68	120.31	111.91
21	b	605	CLA	CAC-C3C-C4C	2.68	128.28	124.81
21	8	303	CLA	O1D-CGD-CBD	-2.67	119.01	124.48
21	c	502	CLA	CHC-C1C-NC	-2.67	120.14	124.20
27	A	406	LHG	O8-C23-C24	2.67	120.30	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	306	CLA	CHD-C4C-NC	2.67	128.42	124.20
21	C	515	CLA	CAC-C3C-C4C	2.67	128.28	124.81
21	A	404	CLA	O2A-CGA-CBA	2.67	120.30	111.91
21	4	300	CLA	C3D-C2D-C1D	-2.67	102.18	105.83
24	2	315	KC1	O2D-CGD-O1D	-2.67	118.61	123.84
31	B	626	SQD	O8-S-C6	2.67	110.00	105.74
21	b	623	CLA	C1-O2A-CGA	2.67	123.45	116.44
21	B	602	CLA	O1D-CGD-CBD	-2.67	119.02	124.48
21	7	300	CLA	O2A-CGA-CBA	2.67	120.29	111.91
21	G	302	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
21	1	302	CLA	CMB-C2B-C3B	2.67	129.67	124.68
21	B	615	CLA	CHD-C4C-NC	2.67	128.41	124.20
21	7	301	CLA	O2A-CGA-CBA	2.67	120.28	111.91
21	C	508	CLA	CAC-C3C-C4C	2.67	128.27	124.81
21	7	307	CLA	CHC-C1C-NC	-2.67	120.16	124.20
21	C	510	CLA	C3D-C2D-C1D	-2.67	102.19	105.83
21	c	504	CLA	O2A-CGA-CBA	2.67	120.27	111.91
22	1	311	DD6	C10-C9-C8	2.67	131.53	123.22
21	6	301	CLA	C1-C2-C3	-2.66	121.43	126.04
21	J	305	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
21	b	609	CLA	CHC-C1C-NC	-2.66	120.16	124.20
21	J	304	CLA	CMD-C2D-C1D	2.66	129.41	124.71
24	6	313	KC1	CMB-C2B-C1B	2.66	129.41	124.71
21	2	302	CLA	CHD-C4C-NC	2.66	128.40	124.20
21	C	515	CLA	C3D-C2D-C1D	-2.66	102.20	105.83
24	J	311	KC1	CAC-C3C-C4C	2.66	128.26	124.81
31	X	401	SQD	O48-C23-C24	2.66	120.26	111.91
21	5	303	CLA	CHD-C1D-ND	-2.66	122.01	124.45
21	J	305	CLA	C3D-C2D-C1D	-2.66	102.20	105.83
24	G	308	KC1	CHC-C4B-NB	-2.66	122.01	124.45
21	b	603	CLA	O2A-CGA-CBA	2.66	120.25	111.91
21	5	302	CLA	O2A-CGA-CBA	2.66	120.25	111.91
25	B	618	BCR	C29-C30-C25	2.66	114.57	110.48
21	B	608	CLA	C4-C3-C5	2.66	119.74	115.27
21	C	513	CLA	CHC-C1C-NC	-2.66	120.17	124.20
21	b	604	CLA	C3D-C2D-C1D	-2.66	102.20	105.83
21	C	513	CLA	C3D-C2D-C1D	-2.66	102.20	105.83
21	C	514	CLA	C3D-C2D-C1D	-2.66	102.21	105.83
21	C	512	CLA	CHC-C1C-NC	-2.66	120.17	124.20
21	g	308	CLA	C3D-C2D-C1D	-2.66	102.21	105.83
21	D	407	CLA	CMB-C2B-C3B	2.66	129.65	124.68
21	5	309	CLA	C4-C3-C5	2.65	119.74	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	304	CLA	C3D-C2D-C1D	-2.65	102.21	105.83
21	2	302	CLA	C1D-CHD-C4C	-2.65	120.33	126.06
21	J	301	CLA	CHC-C1C-NC	-2.65	120.18	124.20
21	J	301	CLA	CMD-C2D-C1D	2.65	129.39	124.71
21	2	305	CLA	CHC-C1C-NC	-2.65	120.18	124.20
21	B	613	CLA	C4-C3-C5	2.65	119.73	115.27
24	J	313	KC1	CAC-C3C-C4C	2.65	128.25	124.81
21	c	503	CLA	C3D-C2D-C1D	-2.65	102.21	105.83
21	J	305	CLA	CHC-C1C-NC	-2.65	120.18	124.20
21	5	309	CLA	CMD-C2D-C1D	2.65	129.39	124.71
24	3	306	KC1	CMB-C2B-C1B	2.65	129.39	124.71
21	c	512	CLA	CMC-C2C-C1C	2.65	129.08	125.04
21	J	300	CLA	C3D-C2D-C1D	-2.65	102.21	105.83
21	6	304	CLA	CHC-C1C-NC	-2.65	120.18	124.20
24	2	314	KC1	CHD-C4C-NC	2.65	128.22	124.20
21	4	302	CLA	C3D-C2D-C1D	-2.65	102.22	105.83
21	g	307	CLA	C3D-C2D-C1D	-2.65	102.22	105.83
21	3	304	CLA	CHC-C1C-NC	-2.65	120.18	124.20
21	B	607	CLA	C4-C3-C5	2.65	119.73	115.27
21	c	509	CLA	CAC-C3C-C4C	2.65	128.25	124.81
26	a	404	PHO	O2D-CGD-O1D	-2.65	118.66	123.84
27	a	401	LHG	O8-C23-C24	2.65	120.22	111.91
21	B	614	CLA	C4-C3-C5	2.65	119.72	115.27
21	C	503	CLA	CMC-C2C-C1C	2.65	129.07	125.04
21	4	302	CLA	CMC-C2C-C1C	2.65	129.07	125.04
21	J	306	CLA	C3D-C2D-C1D	-2.65	102.22	105.83
21	8	306	CLA	CAC-C3C-C4C	2.65	128.24	124.81
21	b	609	CLA	C4-C3-C5	2.65	119.72	115.27
21	1	304	CLA	C1-C2-C3	-2.65	121.47	126.04
21	B	612	CLA	CAC-C3C-C4C	2.65	128.24	124.81
21	9	304	CLA	O2A-CGA-CBA	2.64	120.21	111.91
23	2	310	A86	C41-C32-C31	2.64	112.84	110.47
21	b	617	CLA	CHD-C4C-NC	2.64	128.37	124.20
21	5	304	CLA	CHD-C4C-NC	2.64	128.37	124.20
21	7	303	CLA	C4-C3-C5	2.64	119.72	115.27
24	g	315	KC1	CMB-C2B-C1B	2.64	129.37	124.71
21	B	608	CLA	CHC-C1C-NC	-2.64	120.19	124.20
21	7	302	CLA	C3D-C2D-C1D	-2.64	102.22	105.83
21	J	301	CLA	C1-C2-C3	-2.64	121.47	126.04
21	c	505	CLA	CAC-C3C-C4C	2.64	128.24	124.81
25	b	618	BCR	C27-C26-C25	2.64	126.57	122.73
21	C	504	CLA	C3D-C2D-C1D	-2.64	102.23	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	310	CLA	CMB-C2B-C3B	2.64	129.62	124.68
21	g	305	CLA	C3D-C2D-C1D	-2.64	102.23	105.83
21	C	506	CLA	CAC-C3C-C4C	2.64	128.23	124.81
21	b	614	CLA	C1-C2-C3	-2.64	121.48	126.04
21	c	514	CLA	CAC-C3C-C4C	2.64	128.23	124.81
21	B	604	CLA	C3D-C2D-C1D	-2.64	102.23	105.83
21	B	604	CLA	CMD-C2D-C1D	2.64	129.36	124.71
23	5	312	A86	C20-C19-C18	2.64	117.96	112.75
21	c	512	CLA	CMD-C2D-C1D	2.64	129.36	124.71
29	5	301	LMU	O5'-C5'-C4'	2.63	115.31	109.75
21	2	305	CLA	C3D-C2D-C1D	-2.63	102.24	105.83
21	6	305	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
35	d	408	PL9	C7-C8-C9	-2.63	122.41	126.79
21	c	513	CLA	CMB-C2B-C3B	2.63	129.60	124.68
21	C	509	CLA	CHC-C1C-NC	-2.63	120.21	124.20
21	7	309	CLA	C3D-C2D-C1D	-2.63	102.24	105.83
21	c	503	CLA	C4-C3-C5	2.63	119.70	115.27
24	J	313	KC1	CMB-C2B-C1B	2.63	129.35	124.71
24	2	313	KC1	CAA-C2A-C1A	-2.63	112.65	124.75
24	3	306	KC1	CAA-C2A-C1A	-2.63	112.65	124.75
21	a	405	CLA	C3D-C2D-C1D	-2.63	102.24	105.83
21	b	608	CLA	CAC-C3C-C4C	2.63	128.22	124.81
21	G	302	CLA	CMD-C2D-C1D	2.63	129.35	124.71
21	g	304	CLA	CHD-C4C-NC	2.63	128.35	124.20
21	1	305	CLA	CHD-C4C-NC	2.63	128.35	124.20
31	B	626	SQD	C1-O5-C5	2.63	118.85	113.69
21	b	605	CLA	C3D-C2D-C1D	-2.63	102.25	105.83
21	7	300	CLA	C4-C3-C5	2.63	119.69	115.27
21	4	301	CLA	C3D-C2D-C1D	-2.63	102.25	105.83
21	g	306	CLA	C3D-C2D-C1D	-2.63	102.25	105.83
21	c	511	CLA	O2A-CGA-CBA	2.63	120.15	111.91
21	c	506	CLA	C4-C3-C5	2.63	119.69	115.27
24	4	308	KC1	CAA-C2A-C1A	-2.63	112.68	124.75
21	9	302	CLA	O2A-CGA-CBA	2.62	120.14	111.91
21	1	303	CLA	O2A-CGA-CBA	2.62	120.14	111.91
21	8	306	CLA	O2A-CGA-CBA	2.62	120.14	111.91
27	B	601	LHG	C11-C10-C9	-2.62	101.11	114.42
21	c	512	CLA	CHC-C1C-NC	-2.62	120.22	124.20
24	J	312	KC1	CHC-C4B-NB	-2.62	122.04	124.45
21	C	508	CLA	CHC-C1C-NC	-2.62	120.22	124.20
21	6	302	CLA	CAC-C3C-C4C	2.62	128.21	124.81
21	c	507	CLA	CED-O2D-CGD	2.62	121.87	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c	506	CLA	CMB-C2B-C3B	2.62	129.58	124.68
28	2	318	LMG	C1-C2-C3	-2.62	104.54	110.00
21	c	511	CLA	CHC-C1C-NC	-2.62	120.23	124.20
28	8	317	LMG	C1-C2-C3	-2.62	104.54	110.00
24	6	311	KC1	CHD-C4C-NC	2.62	128.18	124.20
21	J	300	CLA	CAC-C3C-C4C	2.62	128.21	124.81
21	4	303	CLA	C3D-C2D-C1D	-2.62	102.26	105.83
29	g	301	LMU	O5'-C5'-C4'	2.62	115.27	109.75
21	g	309	CLA	C3D-C2D-C1D	-2.62	102.26	105.83
21	b	605	CLA	CMD-C2D-C1D	2.62	129.33	124.71
21	6	302	CLA	C3D-C2D-C1D	-2.62	102.26	105.83
21	7	301	CLA	C3D-C2D-C1D	-2.62	102.26	105.83
21	8	304	CLA	C3D-C2D-C1D	-2.62	102.26	105.83
21	6	306	CLA	C3D-C2D-C1D	-2.62	102.26	105.83
24	5	313	KC1	CMB-C2B-C1B	2.62	129.32	124.71
21	5	304	CLA	C3D-C2D-C1D	-2.61	102.26	105.83
21	9	303	CLA	CHC-C1C-NC	-2.61	120.24	124.20
21	B	607	CLA	C1-C2-C3	-2.61	121.52	126.04
21	8	305	CLA	CMB-C2B-C3B	2.61	129.57	124.68
24	G	307	KC1	CMB-C2B-C1B	2.61	129.32	124.71
21	1	310	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
21	1	303	CLA	C3D-C2D-C1D	-2.61	102.27	105.83
21	C	508	CLA	C3D-C2D-C1D	-2.61	102.27	105.83
21	c	502	CLA	CMC-C2C-C1C	2.61	129.02	125.04
21	9	301	CLA	CMB-C2B-C3B	2.61	129.56	124.68
21	B	615	CLA	C4-C3-C5	2.61	119.66	115.27
24	3	305	KC1	CMB-C2B-C1B	2.61	129.31	124.71
24	7	314	KC1	CAC-C3C-C4C	2.61	128.20	124.81
21	G	303	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
21	C	503	CLA	C4-C3-C5	2.61	119.66	115.27
21	A	401	CLA	C4-C3-C5	2.61	119.66	115.27
24	9	306	KC1	CAA-C2A-C1A	-2.61	112.75	124.75
21	B	602	CLA	CHC-C1C-NC	-2.61	120.25	124.20
21	1	306	CLA	CHC-C1C-NC	-2.61	120.25	124.20
24	6	312	KC1	CAB-C3B-C4B	2.61	131.19	124.90
21	C	513	CLA	CMC-C2C-C1C	2.61	129.01	125.04
21	9	304	CLA	C3D-C2D-C1D	-2.61	102.27	105.83
21	a	405	CLA	CMB-C2B-C3B	2.61	129.56	124.68
25	B	617	BCR	C27-C26-C25	2.61	126.52	122.73
21	7	301	CLA	CHC-C1C-NC	-2.61	120.25	124.20
21	C	515	CLA	CHC-C1C-NC	-2.61	120.25	124.20
21	6	300	CLA	C6-C5-C3	-2.61	110.36	114.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	315	KC1	O2D-CGD-O1D	-2.60	118.75	123.84
21	G	301	CLA	C3D-C2D-C1D	-2.60	102.28	105.83
21	6	301	CLA	CMB-C2B-C3B	2.60	129.55	124.68
21	B	615	CLA	O1D-CGD-CBD	-2.60	119.16	124.48
24	4	308	KC1	C4C-C3C-C2C	-2.60	103.11	106.90
21	1	304	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
21	5	304	CLA	CMB-C2B-C3B	2.60	129.54	124.68
21	d	406	CLA	CAC-C3C-C4C	2.60	128.18	124.81
21	b	616	CLA	C3D-C2D-C1D	-2.60	102.29	105.83
21	b	608	CLA	C1-C2-C3	-2.60	121.55	126.04
21	B	616	CLA	CHD-C4C-NC	2.60	128.30	124.20
21	C	507	CLA	C4-C3-C5	2.60	119.64	115.27
21	J	304	CLA	C3D-C2D-C1D	-2.60	102.29	105.83
27	l	101	LHG	C11-C10-C9	-2.59	101.25	114.42
21	g	306	CLA	CHC-C1C-NC	-2.59	120.27	124.20
21	C	503	CLA	O1D-CGD-CBD	-2.59	119.18	124.48
21	C	505	CLA	CAC-C3C-C4C	2.59	128.18	124.81
21	B	608	CLA	O2A-CGA-CBA	2.59	120.05	111.91
21	1	304	CLA	CMC-C2C-C1C	2.59	128.99	125.04
21	B	616	CLA	C4-C3-C5	2.59	119.63	115.27
21	C	512	CLA	O2A-CGA-CBA	2.59	120.04	111.91
24	3	306	KC1	CHD-C4C-NC	2.59	128.13	124.20
21	6	303	CLA	CAC-C3C-C4C	2.59	128.17	124.81
21	c	513	CLA	C3D-C2D-C1D	-2.59	102.30	105.83
21	8	306	CLA	CHC-C1C-NC	-2.59	120.27	124.20
21	B	603	CLA	C3D-C2D-C1D	-2.59	102.30	105.83
21	G	304	CLA	C3D-C2D-C1D	-2.59	102.30	105.83
21	1	309	CLA	C4-C3-C5	2.59	119.63	115.27
21	6	304	CLA	C3D-C2D-C1D	-2.59	102.30	105.83
21	6	300	CLA	CAC-C3C-C4C	2.59	128.17	124.81
21	4	300	CLA	CMB-C2B-C3B	2.59	129.52	124.68
21	c	503	CLA	O2A-CGA-CBA	2.59	120.03	111.91
21	c	513	CLA	CMC-C2C-C1C	2.59	128.98	125.04
24	7	314	KC1	CMB-C2B-C1B	2.59	129.27	124.71
21	C	505	CLA	CMC-C2C-C1C	2.59	128.98	125.04
29	2	317	LMU	C2'-C3'-C4'	2.59	115.59	109.68
21	b	617	CLA	C3B-C4B-NB	2.59	112.56	109.21
23	W	101	A86	O-C13-C14	-2.59	116.40	121.66
24	2	316	KC1	CMC-C2C-C1C	2.59	128.98	125.04
21	7	301	CLA	O1D-CGD-CBD	-2.59	119.19	124.48
21	5	307	CLA	C3D-C2D-C1D	-2.59	102.30	105.83
21	b	605	CLA	CMB-C2B-C3B	2.59	129.52	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	g	304	CLA	CMD-C2D-C1D	2.59	129.27	124.71
21	b	608	CLA	O2A-CGA-CBA	2.59	120.02	111.91
21	B	604	CLA	CMB-C2B-C3B	2.59	129.51	124.68
24	9	306	KC1	CMB-C2B-C1B	2.59	129.27	124.71
21	B	604	CLA	CAC-C3C-C4C	2.58	128.16	124.81
21	b	613	CLA	CAC-C3C-C4C	2.58	128.16	124.81
21	d	405	CLA	C3D-C2D-C1D	-2.58	102.30	105.83
21	b	603	CLA	O1D-CGD-CBD	-2.58	119.20	124.48
21	7	309	CLA	CHC-C1C-NC	-2.58	120.28	124.20
21	2	305	CLA	C1-C2-C3	-2.58	121.58	126.04
21	a	403	CLA	CMB-C2B-C3B	2.58	129.51	124.68
21	B	607	CLA	CAC-C3C-C4C	2.58	128.16	124.81
21	D	407	CLA	CAC-C3C-C4C	2.58	128.16	124.81
21	1	302	CLA	CMC-C2C-C1C	2.58	128.97	125.04
21	A	404	CLA	CMC-C2C-C1C	2.58	128.97	125.04
21	1	308	CLA	CHC-C1C-NC	-2.58	120.28	124.20
21	b	609	CLA	O2A-CGA-CBA	2.58	120.01	111.91
23	8	308	A86	C25-C26-C27	2.58	130.99	127.31
31	X	401	SQD	C44-O6-C1	2.58	118.78	113.74
21	6	305	CLA	CHC-C1C-NC	-2.58	120.29	124.20
21	J	303	CLA	CAC-C3C-C4C	2.58	128.16	124.81
21	1	310	CLA	C3D-C2D-C1D	-2.58	102.31	105.83
21	b	603	CLA	CMC-C2C-C1C	2.58	128.97	125.04
21	C	507	CLA	CMB-C2B-C3B	2.58	129.50	124.68
24	5	313	KC1	CAC-C3C-C4C	2.58	128.16	124.81
21	9	303	CLA	CHD-C4C-C3C	-2.58	121.05	124.84
21	C	505	CLA	O2A-CGA-CBA	2.58	120.00	111.91
24	9	305	KC1	CMB-C2B-C1B	2.58	129.26	124.71
24	5	314	KC1	CMB-C2B-C1B	2.58	129.26	124.71
21	C	513	CLA	CAC-C3C-C4C	2.58	128.16	124.81
21	1	305	CLA	C3D-C2D-C1D	-2.58	102.31	105.83
21	7	300	CLA	CHC-C1C-NC	-2.58	120.29	124.20
21	g	302	CLA	CHD-C4C-NC	2.58	128.27	124.20
24	g	315	KC1	O2D-CGD-O1D	-2.58	118.80	123.84
21	b	615	CLA	C1-O2A-CGA	2.58	123.21	116.44
31	C	502	SQD	O48-C23-C24	2.58	120.00	111.91
21	G	302	CLA	CAC-C3C-C4C	2.58	128.15	124.81
24	4	308	KC1	CMB-C2B-C1B	2.58	129.25	124.71
21	c	504	CLA	C4D-CHA-C1A	-2.58	118.11	121.25
21	B	602	CLA	CMC-C2C-C1C	2.58	128.96	125.04
21	J	302	CLA	C3D-C2D-C1D	-2.58	102.32	105.83
21	4	304	CLA	CHC-C1C-NC	-2.58	120.30	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	619	BCR	C11-C10-C9	-2.58	123.64	127.31
21	g	307	CLA	CMC-C2C-C1C	2.57	128.96	125.04
23	2	308	A86	C23-C16-C17	-2.57	104.51	108.98
21	B	615	CLA	C3D-C2D-C1D	-2.57	102.32	105.83
21	1	307	CLA	CHD-C4C-NC	2.57	128.26	124.20
21	G	303	CLA	CHD-C4C-NC	2.57	128.25	124.20
21	c	512	CLA	CAC-C3C-C4C	2.57	128.15	124.81
21	J	300	CLA	C6-C5-C3	-2.57	110.42	114.62
21	c	504	CLA	CMB-C2B-C3B	2.57	129.49	124.68
21	g	305	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
21	c	507	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
21	c	514	CLA	CHC-C1C-NC	-2.57	120.30	124.20
21	a	405	CLA	CAC-C3C-C4C	2.57	128.14	124.81
21	G	302	CLA	C1D-CHD-C4C	-2.57	120.52	126.06
21	9	304	CLA	CMB-C2B-C3B	2.57	129.48	124.68
21	g	306	CLA	O2A-CGA-CBA	2.57	119.96	111.91
21	J	307	CLA	CHD-C4C-NC	2.57	128.25	124.20
21	g	303	CLA	CMC-C2C-C1C	2.57	128.95	125.04
24	4	307	KC1	CMB-C2B-C1B	2.57	129.23	124.71
21	J	307	CLA	O2A-CGA-CBA	2.56	119.96	111.91
21	B	607	CLA	O2A-CGA-CBA	2.56	119.95	111.91
21	5	303	CLA	O1D-CGD-CBD	-2.56	119.24	124.48
24	G	309	KC1	O2D-CGD-O1D	-2.56	118.83	123.84
21	9	304	CLA	CMC-C2C-C1C	2.56	128.94	125.04
24	1	315	KC1	CMB-C2B-C1B	2.56	129.23	124.71
21	3	304	CLA	O1D-CGD-CBD	-2.56	119.24	124.48
21	B	613	CLA	CMC-C2C-C1C	2.56	128.94	125.04
21	2	301	CLA	C3D-C2D-C1D	-2.56	102.33	105.83
21	D	406	CLA	C3D-C2D-C1D	-2.56	102.33	105.83
21	A	402	CLA	CMB-C2B-C3B	2.56	129.47	124.68
21	b	617	CLA	C4D-CHA-C1A	-2.56	118.13	121.25
31	b	602	SQD	C1-O5-C5	2.56	118.72	113.69
28	b	620	LMG	O6-C1-O1	-2.56	103.91	109.97
24	G	309	KC1	CHD-C4C-NC	2.56	128.09	124.20
21	c	509	CLA	C1D-CHD-C4C	-2.56	120.53	126.06
23	8	310	A86	C26-C25-C24	2.56	131.21	123.22
24	J	312	KC1	CMB-C2B-C1B	2.56	129.22	124.71
21	6	304	CLA	CBC-CAC-C3C	-2.56	105.38	112.43
24	7	315	KC1	CMB-C2B-C1B	2.56	129.22	124.71
21	7	306	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
21	1	308	CLA	C3D-C2D-C1D	-2.56	102.34	105.83
21	b	608	CLA	C3D-C2D-C1D	-2.56	102.34	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	616	CLA	CAC-C3C-C4C	2.56	128.13	124.81
24	G	307	KC1	CHD-C4C-NC	2.56	128.09	124.20
21	B	616	CLA	C3B-C4B-NB	2.56	112.52	109.21
26	d	403	PHO	O2D-CGD-O1D	-2.56	118.84	123.84
21	2	302	CLA	CMC-C2C-C1C	2.56	128.93	125.04
25	B	618	BCR	C11-C10-C9	-2.56	123.66	127.31
21	C	505	CLA	C3D-C2D-C1D	-2.56	102.34	105.83
21	4	304	CLA	C3D-C2D-C1D	-2.56	102.34	105.83
21	b	611	CLA	CAC-C3C-C4C	2.56	128.13	124.81
21	a	405	CLA	O2A-CGA-CBA	2.56	119.93	111.91
24	G	306	KC1	CMB-C2B-C1B	2.56	129.22	124.71
21	g	309	CLA	O2A-CGA-CBA	2.55	119.92	111.91
21	1	304	CLA	CMB-C2B-C3B	2.55	129.46	124.68
21	1	307	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
21	J	301	CLA	CMC-C2C-C1C	2.55	128.93	125.04
21	g	302	CLA	C1-C2-C3	-2.55	121.63	126.04
29	A	408	LMU	O5B-C5B-C4B	2.55	114.33	109.69
21	c	504	CLA	CMC-C2C-C1C	2.55	128.92	125.04
21	1	309	CLA	O2A-CGA-CBA	2.55	119.91	111.91
21	B	616	CLA	C4C-C3C-C2C	-2.55	103.18	106.90
21	c	509	CLA	CHD-C4C-NC	2.55	128.22	124.20
21	5	307	CLA	CHD-C4C-NC	2.55	128.22	124.20
21	5	305	CLA	CAA-C2A-C3A	-2.55	110.15	116.10
21	5	303	CLA	CMC-C2C-C1C	2.55	128.92	125.04
21	J	300	CLA	O2A-CGA-CBA	2.55	119.91	111.91
21	J	303	CLA	CHD-C4C-NC	2.55	128.22	124.20
21	4	300	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	8	310	A86	C33-C32-C31	2.55	111.69	109.21
24	4	307	KC1	CHB-C1B-NB	-2.55	122.11	124.45
21	a	402	CLA	CAC-C3C-C4C	2.55	128.12	124.81
21	3	303	CLA	CMD-C2D-C1D	2.55	129.20	124.71
21	G	302	CLA	CHC-C1C-NC	-2.55	120.34	124.20
21	7	303	CLA	CMB-C2B-C3B	2.55	129.44	124.68
28	B	619	LMG	C40-C39-C38	-2.55	101.50	114.42
21	a	402	CLA	C4-C3-C5	2.55	119.56	115.27
26	D	401	PHO	O2D-CGD-O1D	-2.55	118.86	123.84
21	1	309	CLA	CMC-C2C-C1C	2.55	128.92	125.04
21	8	303	CLA	C1D-CHD-C4C	-2.55	120.57	126.06
21	4	301	CLA	CMC-C2C-C1C	2.54	128.91	125.04
21	2	303	CLA	C1-C2-C3	-2.54	121.64	126.04
31	X	401	SQD	O6-C1-C2	2.54	112.27	108.30
25	h	101	BCR	C27-C26-C25	2.54	126.42	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	304	CLA	C1-C2-C3	-2.54	121.65	126.04
21	7	308	CLA	O2A-CGA-CBA	2.54	119.88	111.91
21	g	302	CLA	C4-C3-C5	2.54	119.55	115.27
21	c	502	CLA	C3D-C2D-C1D	-2.54	102.36	105.83
31	X	401	SQD	O5-C5-C4	2.54	114.31	109.69
21	J	301	CLA	CMB-C2B-C3B	2.54	129.43	124.68
21	B	611	CLA	CMC-C2C-C1C	2.54	128.90	125.04
21	g	303	CLA	CMB-C2B-C3B	2.54	129.43	124.68
23	1	312	A86	C35-C34-C33	2.54	114.30	109.88
24	G	307	KC1	O2D-CGD-O1D	-2.54	118.88	123.84
21	J	300	CLA	CHC-C1C-NC	-2.54	120.36	124.20
21	7	305	CLA	CHD-C4C-NC	2.53	128.20	124.20
25	C	501	BCR	C15-C14-C13	-2.53	123.69	127.31
23	8	311	A86	C20-C19-C18	-2.53	107.74	112.75
21	C	514	CLA	CMC-C2C-C1C	2.53	128.90	125.04
24	g	314	KC1	CAA-C2A-C1A	-2.53	113.11	124.75
21	b	617	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
21	8	304	CLA	CMB-C2B-C3B	2.53	129.41	124.68
21	8	307	CLA	CHD-C4C-NC	2.53	128.19	124.20
21	4	300	CLA	O2A-CGA-CBA	2.53	119.85	111.91
21	7	307	CLA	C3D-C2D-C1D	-2.53	102.38	105.83
24	2	314	KC1	O2D-CGD-O1D	-2.53	118.89	123.84
24	G	307	KC1	CHC-C4B-NB	-2.53	122.13	124.45
21	2	305	CLA	C4-C3-C5	2.53	119.52	115.27
21	c	514	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
24	6	313	KC1	CBC-CAC-C3C	-2.53	105.47	112.43
21	7	302	CLA	O2A-CGA-CBA	2.53	119.83	111.91
31	B	625	SQD	C1-O5-C5	2.53	118.65	113.69
21	9	301	CLA	C3D-C2D-C1D	-2.53	102.38	105.83
21	a	405	CLA	C4-C3-C5	2.53	119.52	115.27
21	9	302	CLA	C3D-C2D-C1D	-2.52	102.39	105.83
24	6	312	KC1	CMB-C2B-C1B	2.52	129.16	124.71
21	4	300	CLA	CMC-C2C-C1C	2.52	128.88	125.04
27	d	402	LHG	C11-C10-C9	-2.52	101.62	114.42
31	B	625	SQD	O48-C23-C24	2.52	119.82	111.91
21	6	300	CLA	CHC-C1C-NC	-2.52	120.38	124.20
21	6	300	CLA	O2A-CGA-CBA	2.52	119.82	111.91
24	J	312	KC1	CAB-C3B-C4B	2.52	130.99	124.90
21	C	506	CLA	CMB-C2B-C3B	2.52	129.40	124.68
21	1	308	CLA	CAC-C3C-C4C	2.52	128.08	124.81
25	M	101	BCR	C33-C5-C6	-2.52	121.70	124.53
21	3	304	CLA	CAC-C3C-C4C	2.52	128.08	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	302	CLA	O2A-CGA-CBA	2.52	119.81	111.91
21	C	515	CLA	C1D-CHD-C4C	-2.52	120.62	126.06
29	g	316	LMU	O5B-C5B-C4B	2.52	114.27	109.69
21	B	615	CLA	CMB-C2B-C3B	2.52	129.39	124.68
21	3	303	CLA	C1D-CHD-C4C	-2.52	120.63	126.06
21	1	304	CLA	CAC-C3C-C4C	2.52	128.08	124.81
28	a	407	LMG	O6-C1-O1	-2.52	104.02	109.97
21	3	303	CLA	C3D-C2D-C1D	-2.51	102.40	105.83
24	8	316	KC1	CMC-C2C-C1C	2.51	128.87	125.04
21	B	604	CLA	CHD-C4C-NC	2.51	128.16	124.20
21	1	301	CLA	CHC-C1C-NC	-2.51	120.39	124.20
24	1	316	KC1	CMC-C2C-C1C	2.51	128.87	125.04
21	A	401	CLA	CAC-C3C-C4C	2.51	128.07	124.81
27	a	401	LHG	C11-C10-C9	-2.51	101.67	114.42
24	8	314	KC1	CMC-C2C-C1C	2.51	128.87	125.04
23	8	309	A86	C23-C16-C17	-2.51	104.62	108.98
21	A	401	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
29	5	316	LMU	O5B-C5B-C4B	2.51	114.03	109.52
21	7	308	CLA	C1-C2-C3	-2.51	121.70	126.04
27	D	403	LHG	C11-C10-C9	-2.51	101.68	114.42
21	9	303	CLA	C4-C3-C5	2.51	118.85	115.98
21	b	617	CLA	CAC-C3C-C4C	2.51	128.07	124.81
21	1	302	CLA	C4-C3-C5	2.51	119.50	115.27
24	G	309	KC1	CBC-CAC-C3C	-2.51	105.51	112.43
21	6	308	CLA	C4-C3-C5	2.51	119.49	115.27
21	7	305	CLA	CMB-C2B-C3B	2.51	129.37	124.68
24	8	313	KC1	OBD-CAD-C3D	-2.51	123.81	127.98
21	G	301	CLA	CMC-C2C-C1C	2.51	128.86	125.04
21	7	307	CLA	CAC-C3C-C4C	2.51	128.06	124.81
35	D	409	PL9	C22-C23-C24	-2.51	121.62	127.66
24	G	307	KC1	CBC-CAC-C3C	-2.51	105.52	112.43
21	G	300	CLA	CMC-C2C-C1C	2.51	128.86	125.04
21	a	402	CLA	CMD-C2D-C1D	2.51	129.13	124.71
21	6	308	CLA	C1D-CHD-C4C	-2.51	120.65	126.06
21	g	303	CLA	O1D-CGD-CBD	-2.51	119.36	124.48
21	6	302	CLA	CMC-C2C-C1C	2.51	128.85	125.04
22	g	310	DD6	C13-C11-C10	2.50	122.78	118.94
21	c	504	CLA	CHD-C4C-NC	2.50	128.15	124.20
27	d	402	LHG	O8-C23-C24	2.50	119.75	111.91
30	c	516	DGD	C3G-C2G-C1G	-2.50	105.88	111.79
21	2	303	CLA	O2A-CGA-CBA	2.50	119.75	111.91
21	c	507	CLA	C1D-CHD-C4C	-2.50	120.67	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	302	CLA	O2A-CGA-CBA	2.50	119.75	111.91
25	1	317	BCR	C15-C14-C13	-2.50	123.75	127.31
21	b	614	CLA	CMC-C2C-C1C	2.50	128.84	125.04
23	7	313	A86	C23-C16-C17	-2.50	104.64	108.98
21	A	401	CLA	CMD-C2D-C1D	2.50	129.11	124.71
21	9	301	CLA	C4-C3-C2	-2.50	117.27	123.68
21	A	404	CLA	CAC-C3C-C4C	2.50	128.05	124.81
21	9	303	CLA	CMB-C2B-C3B	2.50	129.35	124.68
24	8	314	KC1	CHD-C4C-NC	2.50	127.99	124.20
28	B	620	LMG	O1-C7-C8	-2.49	104.88	110.90
21	C	514	CLA	CMB-C2B-C3B	2.49	129.34	124.68
21	c	505	CLA	CMB-C2B-C3B	2.49	129.34	124.68
25	d	407	BCR	C27-C26-C25	2.49	126.35	122.73
21	B	615	CLA	CAC-C3C-C4C	2.49	128.04	124.81
21	b	614	CLA	CMB-C2B-C3B	2.49	129.34	124.68
25	C	516	BCR	C15-C14-C13	-2.49	123.75	127.31
21	4	303	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
21	B	613	CLA	CHC-C1C-NC	-2.49	120.42	124.20
35	d	408	PL9	C22-C23-C24	-2.49	121.66	127.66
27	A	406	LHG	C11-C10-C9	-2.49	101.79	114.42
21	g	308	CLA	C4-C3-C5	2.49	119.46	115.27
21	9	300	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
21	6	303	CLA	CMC-C2C-C1C	2.49	128.83	125.04
21	C	511	CLA	CMD-C2D-C1D	2.49	129.10	124.71
21	g	305	CLA	CHD-C4C-NC	2.49	128.12	124.20
21	g	306	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
21	5	306	CLA	CHC-C1C-NC	-2.49	120.43	124.20
21	b	612	CLA	CMC-C2C-C1C	2.49	128.83	125.04
28	B	619	LMG	C38-C37-C36	-2.49	101.80	114.42
21	B	607	CLA	C3D-C2D-C1D	-2.49	102.44	105.83
24	g	314	KC1	CMB-C2B-C1B	2.49	129.09	124.71
24	8	315	KC1	CHB-C1B-C2B	-2.49	120.27	125.48
28	D	411	LMG	O1-C7-C8	-2.49	104.90	110.90
21	7	307	CLA	CMC-C2C-C1C	2.49	128.82	125.04
21	5	305	CLA	CHC-C1C-NC	-2.49	120.43	124.20
21	g	306	CLA	C1-O2A-CGA	2.49	122.97	116.44
21	c	514	CLA	CHD-C4C-NC	2.48	128.12	124.20
21	g	309	CLA	CMB-C2B-C3B	2.48	129.33	124.68
21	C	515	CLA	CHD-C4C-NC	2.48	128.12	124.20
21	A	404	CLA	C4-C3-C5	2.48	119.45	115.27
21	g	304	CLA	C4-C3-C5	2.48	119.45	115.27
21	c	514	CLA	CED-O2D-CGD	2.48	121.55	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	6	303	CLA	C3D-C2D-C1D	-2.48	102.44	105.83
21	J	302	CLA	CHC-C1C-NC	-2.48	120.44	124.20
21	b	616	CLA	CMB-C2B-C3B	2.48	129.32	124.68
21	b	614	CLA	O2A-CGA-CBA	2.48	119.69	111.91
24	2	315	KC1	CHB-C4A-NA	2.48	128.11	124.20
21	J	302	CLA	CAC-C3C-C4C	2.48	128.03	124.81
28	b	626	LMG	O1-C7-C8	-2.48	104.92	110.90
21	7	304	CLA	CMD-C2D-C1D	2.48	129.08	124.71
21	5	303	CLA	CAC-C3C-C4C	2.48	128.03	124.81
21	9	304	CLA	CED-O2D-CGD	2.48	121.54	115.94
27	d	409	LHG	C11-C10-C9	-2.48	101.85	114.42
25	m	101	BCR	C33-C5-C6	-2.48	121.75	124.53
21	c	514	CLA	C1D-CHD-C4C	-2.48	120.72	126.06
24	g	313	KC1	CMB-C2B-C1B	2.47	129.07	124.71
21	1	307	CLA	C3D-C2D-C1D	-2.47	102.45	105.83
21	b	616	CLA	CAC-C3C-C4C	2.47	128.02	124.81
21	c	504	CLA	CMD-C2D-C1D	2.47	129.07	124.71
24	J	313	KC1	CBC-CAC-C3C	-2.47	105.62	112.43
21	7	306	CLA	C3D-C2D-C1D	-2.47	102.46	105.83
21	2	305	CLA	CMC-C2C-C1C	2.47	128.80	125.04
21	a	405	CLA	CHC-C1C-NC	-2.47	120.45	124.20
21	1	308	CLA	CMC-C2C-C1C	2.47	128.80	125.04
21	J	307	CLA	CMB-C2B-C3B	2.47	129.30	124.68
21	9	302	CLA	CMC-C2C-C1C	2.47	128.80	125.04
21	7	306	CLA	CHD-C4C-NC	2.47	128.10	124.20
21	c	502	CLA	CAC-C3C-C4C	2.47	128.01	124.81
21	G	301	CLA	C4-C3-C5	2.47	119.42	115.27
21	B	607	CLA	CMC-C2C-C1C	2.47	128.80	125.04
21	C	512	CLA	C4-C3-C5	2.47	119.42	115.27
21	2	304	CLA	CMB-C2B-C3B	2.47	129.30	124.68
21	B	616	CLA	C4D-CHA-C1A	-2.47	118.25	121.25
21	b	603	CLA	CMB-C2B-C3B	2.47	129.30	124.68
21	J	307	CLA	C3D-C2D-C1D	-2.47	102.46	105.83
25	c	515	BCR	C20-C21-C22	-2.47	123.79	127.31
21	b	615	CLA	C1-C2-C3	-2.47	121.78	126.04
21	c	511	CLA	CMC-C2C-C1C	2.47	128.80	125.04
21	g	308	CLA	CMD-C2D-C1D	2.47	129.06	124.71
21	b	605	CLA	CHD-C4C-NC	2.47	128.09	124.20
21	B	613	CLA	O2A-CGA-CBA	2.47	119.65	111.91
21	g	308	CLA	CHD-C4C-NC	2.47	128.09	124.20
21	g	307	CLA	CMB-C2B-C3B	2.47	129.29	124.68
21	c	508	CLA	O2A-CGA-CBA	2.46	119.64	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	J	311	KC1	CHB-C1B-NB	-2.46	122.19	124.45
21	1	306	CLA	CED-O2D-CGD	2.46	121.51	115.94
21	1	302	CLA	CHC-C1C-NC	-2.46	120.47	124.20
21	9	304	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
25	c	515	BCR	C15-C16-C17	-2.46	118.43	123.47
27	A	406	LHG	C20-C19-C18	-2.46	101.93	114.42
21	G	302	CLA	C3D-C2D-C1D	-2.46	102.47	105.83
21	B	613	CLA	CMB-C2B-C3B	2.46	129.28	124.68
24	6	313	KC1	CHB-C1B-NB	-2.46	122.19	124.45
21	7	303	CLA	CAC-C3C-C4C	2.46	128.00	124.81
21	J	303	CLA	C3D-C2D-C1D	-2.46	102.47	105.83
21	g	302	CLA	CMD-C2D-C1D	2.46	129.05	124.71
21	3	302	CLA	CMB-C2B-C3B	2.46	129.28	124.68
21	b	615	CLA	CMD-C2D-C1D	2.46	129.05	124.71
21	g	303	CLA	CAC-C3C-C4C	2.46	128.00	124.81
21	A	404	CLA	CMB-C2B-C3B	2.46	129.28	124.68
21	C	512	CLA	CMC-C2C-C1C	2.46	128.78	125.04
21	J	307	CLA	CAC-C3C-C4C	2.46	128.00	124.81
21	7	302	CLA	CHD-C4C-NC	2.46	128.08	124.20
23	2	310	A86	C20-C19-C18	-2.46	107.89	112.75
28	B	622	LMG	O1-C1-C2	-2.46	104.47	108.30
21	5	305	CLA	CMD-C2D-C1D	2.46	129.04	124.71
21	7	305	CLA	CMC-C2C-C1C	2.46	128.78	125.04
21	C	508	CLA	C1D-CHD-C4C	-2.46	120.76	126.06
21	4	303	CLA	C1-C2-C3	-2.46	121.80	126.04
25	b	619	BCR	C29-C30-C25	2.45	114.26	110.48
21	J	308	CLA	C3D-C2D-C1D	-2.45	102.48	105.83
21	J	302	CLA	CMC-C2C-C1C	2.45	128.78	125.04
21	J	307	CLA	C1D-CHD-C4C	-2.45	120.77	126.06
21	8	306	CLA	CMD-C2D-C1D	2.45	129.03	124.71
21	1	307	CLA	CMC-C2C-C1C	2.45	128.77	125.04
24	8	313	KC1	CHC-C4B-NB	-2.45	122.20	124.45
21	6	308	CLA	C3D-C2D-C1D	-2.45	102.49	105.83
28	a	407	LMG	C40-C39-C38	-2.45	101.98	114.42
28	L	101	LMG	O6-C1-O1	-2.45	104.17	109.97
24	1	315	KC1	CHB-C1B-NB	-2.45	122.20	124.45
25	1	317	BCR	C15-C16-C17	-2.45	118.45	123.47
21	g	305	CLA	CMC-C2C-C1C	2.45	128.77	125.04
21	1	307	CLA	CMB-C2B-C3B	2.45	129.26	124.68
21	c	510	CLA	CMD-C2D-C1D	2.45	129.03	124.71
21	g	304	CLA	CMC-C2C-C1C	2.45	128.77	125.04
25	c	501	BCR	C24-C23-C22	-2.45	122.54	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	310	DD6	C23-C16-C17	-2.45	104.73	108.98
27	D	410	LHG	C11-C10-C9	-2.45	102.00	114.42
21	8	303	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
21	7	309	CLA	CHD-C4C-NC	2.44	128.06	124.20
21	7	308	CLA	CHC-C1C-NC	-2.44	120.49	124.20
25	d	407	BCR	C15-C16-C17	-2.44	118.47	123.47
24	8	316	KC1	CAA-CBA-CGA	-2.44	114.70	127.26
24	2	314	KC1	CAC-C3C-C4C	2.44	127.98	124.81
28	L	101	LMG	O1-C7-C8	-2.44	105.01	110.90
21	1	308	CLA	C4-C3-C2	-2.44	117.41	123.68
21	7	306	CLA	CMC-C2C-C1C	2.44	128.76	125.04
21	J	307	CLA	CHC-C1C-NC	-2.44	120.50	124.20
30	H	101	DGD	C1D-C2D-C3D	-2.44	104.91	110.00
21	c	510	CLA	C4-C3-C5	2.44	119.38	115.27
21	3	300	CLA	CHD-C4C-NC	2.44	128.05	124.20
21	9	301	CLA	CMD-C2D-C1D	2.44	129.01	124.71
21	1	305	CLA	CMC-C2C-C1C	2.44	128.75	125.04
21	8	307	CLA	CMD-C2D-C1D	2.44	129.01	124.71
27	a	401	LHG	C20-C19-C18	-2.44	102.05	114.42
21	b	623	CLA	CMB-C2B-C3B	2.44	129.24	124.68
25	D	408	BCR	C27-C26-C25	2.44	126.27	122.73
21	b	614	CLA	CHC-C1C-NC	-2.44	120.51	124.20
21	C	510	CLA	CHD-C4C-NC	2.44	128.04	124.20
21	c	514	CLA	CMD-C2D-C1D	2.44	129.01	124.71
24	7	315	KC1	CMC-C2C-C1C	2.43	128.75	125.04
24	1	315	KC1	CBC-CAC-C3C	-2.43	105.72	112.43
23	8	308	A86	C26-C25-C24	2.43	130.81	123.22
21	3	301	CLA	CHC-C1C-NC	-2.43	120.51	124.20
32	E	101	HEM	C4C-CHD-C1D	2.43	125.77	122.56
21	C	503	CLA	CMD-C2D-C1D	2.43	129.00	124.71
21	G	300	CLA	CMD-C2D-C1D	2.43	129.00	124.71
30	c	517	DGD	O5D-C6D-C5D	-2.43	104.55	109.05
21	B	612	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
21	B	621	CLA	CHD-C4C-NC	2.43	128.03	124.20
21	1	306	CLA	CMB-C2B-C3B	2.43	129.22	124.68
24	J	313	KC1	CHB-C1B-NB	-2.43	122.22	124.45
21	B	613	CLA	CMD-C2D-C1D	2.43	128.99	124.71
21	8	303	CLA	CHD-C4C-NC	2.43	128.03	124.20
21	1	306	CLA	CMC-C2C-C1C	2.43	128.74	125.04
28	M	102	LMG	O6-C1-O1	-2.43	104.23	109.97
21	D	407	CLA	O2A-CGA-CBA	2.43	119.52	111.91
21	c	506	CLA	C3D-C2D-C1D	-2.43	102.52	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	607	CLA	CMB-C2B-C3B	2.43	129.22	124.68
21	1	310	CLA	CHD-C4C-NC	2.42	128.02	124.20
21	G	304	CLA	O2A-CGA-CBA	2.42	119.52	111.91
28	f	102	LMG	O1-C7-C8	-2.42	105.05	110.90
27	d	409	LHG	C20-C19-C18	-2.42	102.12	114.42
21	B	606	CLA	CMB-C2B-C3B	2.42	129.21	124.68
21	b	614	CLA	CMD-C2D-C1D	2.42	128.98	124.71
21	B	621	CLA	CMD-C2D-C1D	2.42	128.98	124.71
35	d	408	PL9	C20-C19-C21	2.42	119.34	115.27
27	B	601	LHG	C20-C19-C18	-2.42	102.14	114.42
27	l	101	LHG	C20-C19-C18	-2.42	102.14	114.42
21	J	300	CLA	CMC-C2C-C1C	2.42	128.72	125.04
21	5	304	CLA	CMC-C2C-C1C	2.42	128.72	125.04
21	B	621	CLA	C4-C3-C2	-2.42	117.48	123.68
28	b	621	LMG	O1-C7-C8	-2.42	105.07	110.90
24	6	311	KC1	CMB-C2B-C1B	2.42	128.97	124.71
21	d	406	CLA	O2A-CGA-CBA	2.42	119.49	111.91
21	7	306	CLA	CMB-C2B-C3B	2.42	129.20	124.68
21	8	302	CLA	CHC-C1C-NC	-2.42	120.54	124.20
21	a	402	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
21	5	308	CLA	CMB-C2B-C3B	2.42	129.20	124.68
21	b	608	CLA	CMC-C2C-C1C	2.42	128.72	125.04
21	3	304	CLA	CMB-C2B-C3B	2.41	129.20	124.68
21	A	404	CLA	CMD-C2D-C1D	2.41	128.97	124.71
21	c	505	CLA	CMD-C2D-C1D	2.41	128.97	124.71
21	J	307	CLA	CMC-C2C-C1C	2.41	128.71	125.04
21	6	304	CLA	C3D-C4D-CHA	-2.41	107.20	112.72
21	1	304	CLA	CMD-C2D-C1D	2.41	128.97	124.71
24	G	308	KC1	CMB-C2B-C1B	2.41	128.97	124.71
21	8	302	CLA	CMC-C2C-C1C	2.41	128.71	125.04
23	8	308	A86	C17-C16-C15	2.41	111.62	109.16
21	2	301	CLA	CHC-C1C-NC	-2.41	120.55	124.20
21	3	301	CLA	CMD-C2D-C1D	2.41	128.96	124.71
21	B	611	CLA	CAC-C3C-C4C	2.41	127.94	124.81
21	6	302	CLA	CHD-C4C-NC	2.41	128.00	124.20
21	2	303	CLA	CMD-C2D-C1D	2.41	128.96	124.71
30	h	103	DGD	C1D-C2D-C3D	-2.41	104.98	110.00
21	c	508	CLA	C1-C2-C3	-2.41	121.88	126.04
21	g	308	CLA	O2A-CGA-CBA	2.41	119.47	111.91
21	6	306	CLA	CMD-C2D-C1D	2.41	128.96	124.71
21	C	514	CLA	CAC-C3C-C4C	2.41	127.93	124.81
21	3	300	CLA	CMC-C2C-C1C	2.41	128.71	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	621	CLA	CED-O2D-CGD	2.41	121.38	115.94
21	6	308	CLA	C1-C2-C3	-2.41	121.88	126.04
21	g	308	CLA	CMB-C2B-C3B	2.41	129.18	124.68
21	b	612	CLA	CAC-C3C-C4C	2.41	127.93	124.81
21	C	515	CLA	CMD-C2D-C1D	2.41	128.95	124.71
25	D	408	BCR	C3-C4-C5	-2.40	109.78	114.08
21	7	305	CLA	CMD-C2D-C1D	2.40	128.95	124.71
21	C	504	CLA	O2A-CGA-CBA	2.40	119.45	111.91
21	C	515	CLA	CMB-C2B-C3B	2.40	129.17	124.68
21	6	308	CLA	CED-O2D-CGD	2.40	121.37	115.94
21	9	302	CLA	CHD-C4C-NC	2.40	127.99	124.20
30	b	601	DGD	C3G-C2G-C1G	-2.40	106.11	111.79
21	b	623	CLA	CHD-C4C-NC	2.40	127.99	124.20
21	5	307	CLA	CMC-C2C-C1C	2.40	128.70	125.04
21	8	307	CLA	CMC-C2C-C1C	2.40	128.69	125.04
31	X	401	SQD	C4-C3-C2	2.40	115.01	110.82
27	D	403	LHG	O8-C23-C24	2.40	119.44	111.91
21	1	303	CLA	CED-O2D-CGD	2.40	121.36	115.94
21	6	306	CLA	CMB-C2B-C3B	2.40	129.17	124.68
24	J	312	KC1	CAA-C2A-C1A	-2.40	113.72	124.75
21	1	309	CLA	CHB-C4A-NA	2.40	127.83	124.51
28	b	620	LMG	C38-C37-C36	-2.40	102.25	114.42
21	G	302	CLA	C3D-C4D-CHA	-2.40	107.23	112.72
24	4	308	KC1	CBC-CAC-C3C	-2.40	105.82	112.43
29	a	408	LMU	O5B-C5B-C4B	2.40	114.05	109.69
30	H	101	DGD	C3G-C2G-C1G	-2.40	106.12	111.79
21	7	309	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
21	J	308	CLA	CMB-C2B-C3B	2.40	129.16	124.68
23	8	308	A86	C10-C9-C8	2.40	130.70	123.22
21	b	614	CLA	C4-C3-C5	2.40	119.30	115.27
21	c	511	CLA	C3D-C2D-C1D	-2.40	102.56	105.83
24	g	314	KC1	CMC-C2C-C1C	2.40	128.69	125.04
21	g	305	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
21	6	308	CLA	CMD-C2D-C1D	2.40	128.93	124.71
21	J	308	CLA	CMD-C2D-C1D	2.40	128.93	124.71
21	6	307	CLA	CMB-C2B-C3B	2.40	129.16	124.68
21	J	306	CLA	CMB-C2B-C3B	2.40	129.16	124.68
21	C	504	CLA	CMC-C2C-C1C	2.39	128.69	125.04
21	G	303	CLA	CHC-C1C-NC	-2.39	120.57	124.20
21	C	507	CLA	C3D-C2D-C1D	-2.39	102.56	105.83
21	9	300	CLA	C1-C2-C3	-2.39	121.90	126.04
35	D	409	PL9	C20-C19-C21	2.39	119.30	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	D	406	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
28	a	407	LMG	C38-C37-C36	-2.39	102.28	114.42
21	2	305	CLA	CAC-C3C-C4C	2.39	127.91	124.81
21	g	304	CLA	CMB-C2B-C3B	2.39	129.15	124.68
21	B	614	CLA	CMD-C2D-C1D	2.39	128.93	124.71
21	b	612	CLA	C1D-CHD-C4C	-2.39	120.90	126.06
24	2	316	KC1	CAA-CBA-CGA	-2.39	114.97	127.26
21	B	610	CLA	CMB-C2B-C3B	2.39	129.15	124.68
21	C	510	CLA	CHC-C1C-NC	-2.39	120.58	124.20
21	6	302	CLA	CMD-C2D-C1D	2.39	128.93	124.71
28	A	407	LMG	C40-C39-C38	-2.39	102.29	114.42
21	2	303	CLA	CMB-C2B-C3B	2.39	129.15	124.68
21	g	309	CLA	O1D-CGD-CBD	-2.39	119.60	124.48
21	7	302	CLA	CMC-C2C-C1C	2.39	128.68	125.04
21	C	507	CLA	C3B-C4B-NB	2.39	112.30	109.21
25	h	101	BCR	C33-C5-C6	-2.39	121.85	124.53
33	D	402	BCT	O3-C-O1	-2.39	113.35	119.55
21	c	508	CLA	CMD-C2D-C1D	2.39	128.92	124.71
27	D	410	LHG	C20-C19-C18	-2.39	102.30	114.42
28	B	627	LMG	O3-C3-C2	-2.39	104.83	110.35
24	2	315	KC1	CMB-C2B-C1B	2.39	128.92	124.71
28	b	624	LMG	O1-C7-C8	-2.39	105.14	110.90
25	a	406	BCR	C15-C16-C17	-2.39	118.58	123.47
21	g	307	CLA	CMD-C2D-C1D	2.39	128.92	124.71
21	4	303	CLA	CMB-C2B-C3B	2.39	129.14	124.68
21	9	301	CLA	CMC-C2C-C1C	2.39	128.67	125.04
25	d	407	BCR	C3-C4-C5	-2.39	109.82	114.08
21	b	603	CLA	CAC-C3C-C4C	2.39	127.91	124.81
21	c	514	CLA	CMB-C2B-C3B	2.39	129.14	124.68
21	J	306	CLA	C4-C3-C5	2.38	119.28	115.27
21	d	405	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
24	6	313	KC1	CHB-C4A-NA	2.38	127.96	124.20
21	1	310	CLA	CMC-C2C-C1C	2.38	128.67	125.04
21	C	513	CLA	C1-O2A-CGA	2.38	122.69	116.44
21	4	303	CLA	CMC-C2C-C1C	2.38	128.67	125.04
21	7	303	CLA	CED-O2D-CGD	2.38	121.32	115.94
21	4	300	CLA	CMD-C2D-C1D	2.38	128.91	124.71
21	B	615	CLA	CHC-C1C-NC	-2.38	120.59	124.20
21	7	307	CLA	O2A-CGA-CBA	2.38	119.37	111.91
21	g	309	CLA	C5-C3-C4	2.38	119.86	114.60
32	f	101	HEM	C1B-NB-C4B	2.38	107.53	105.07
21	c	514	CLA	CMC-C2C-C1C	2.38	128.66	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	616	CLA	CHC-C1C-NC	-2.38	120.59	124.20
24	6	312	KC1	CAA-C2A-C1A	-2.38	113.81	124.75
21	5	306	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
22	1	311	DD6	C15-C14-C13	2.38	131.02	125.99
21	b	605	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
31	B	626	SQD	O48-C23-C24	2.38	119.37	111.91
21	5	306	CLA	CMD-C2D-C1D	2.38	128.90	124.71
21	1	303	CLA	CHD-C4C-NC	2.38	127.95	124.20
21	B	614	CLA	CAC-C3C-C4C	2.38	127.89	124.81
21	J	306	CLA	CMC-C2C-C1C	2.38	128.66	125.04
28	2	318	LMG	C40-C39-C38	-2.37	102.37	114.42
21	5	304	CLA	CAC-C3C-C4C	2.37	127.89	124.81
21	7	303	CLA	CMD-C2D-C1D	2.37	128.90	124.71
21	d	406	CLA	CMD-C2D-C1D	2.37	128.90	124.71
21	J	300	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
21	6	305	CLA	CMD-C2D-C1D	2.37	128.90	124.71
21	3	300	CLA	CMD-C2D-C1D	2.37	128.90	124.71
23	W	101	A86	O-C13-C11	-2.37	115.91	121.15
21	7	306	CLA	CAA-C2A-C3A	-2.37	110.56	116.10
21	g	309	CLA	CMC-C2C-C1C	2.37	128.65	125.04
21	C	505	CLA	CMB-C2B-C3B	2.37	129.12	124.68
21	c	511	CLA	C4-C3-C5	2.37	119.26	115.27
21	C	504	CLA	CED-O2D-CGD	2.37	121.30	115.94
21	1	307	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
21	B	621	CLA	CMB-C2B-C3B	2.37	129.12	124.68
21	g	304	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
21	g	302	CLA	CHC-C1C-NC	-2.37	120.61	124.20
21	c	506	CLA	C3B-C4B-NB	2.37	112.28	109.21
21	8	303	CLA	CAC-C3C-C4C	2.37	127.89	124.81
21	B	602	CLA	CMD-C2D-C1D	2.37	128.89	124.71
21	b	613	CLA	O2A-CGA-CBA	2.37	119.35	111.91
25	M	101	BCR	C27-C26-C25	2.37	126.17	122.73
21	B	612	CLA	CHD-C1D-ND	-2.37	122.28	124.45
21	J	305	CLA	CMB-C2B-C3B	2.37	129.11	124.68
24	7	314	KC1	CBC-CAC-C3C	-2.37	105.90	112.43
21	c	513	CLA	O2A-CGA-CBA	2.37	119.34	111.91
21	6	307	CLA	CMC-C2C-C1C	2.37	128.65	125.04
24	9	305	KC1	CHB-C1B-NB	-2.37	122.28	124.45
21	6	308	CLA	CMB-C2B-C3B	2.37	129.11	124.68
21	G	303	CLA	CMC-C2C-C1C	2.37	128.65	125.04
28	B	627	LMG	O7-C10-O9	-2.37	117.98	123.70
21	J	302	CLA	CMD-C2D-C1D	2.37	128.89	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	304	CLA	C4C-C3C-C2C	-2.37	103.45	106.90
28	b	620	LMG	C1-C2-C3	-2.37	105.07	110.00
21	5	305	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
31	B	626	SQD	O5-C5-C4	2.37	113.99	109.69
21	6	300	CLA	CMC-C2C-C1C	2.37	128.64	125.04
24	9	305	KC1	CBC-CAC-C3C	-2.37	105.91	112.43
21	B	612	CLA	O2A-CGA-CBA	2.37	119.33	111.91
21	2	301	CLA	CAC-C3C-C4C	2.37	127.88	124.81
28	B	620	LMG	C1-C2-C3	-2.37	105.07	110.00
21	g	309	CLA	C3D-C4D-CHA	-2.36	107.31	112.72
25	H	100	BCR	C7-C8-C9	-2.36	122.66	126.23
21	B	613	CLA	C1-C2-C3	-2.36	121.95	126.04
30	C	518	DGD	C1G-C2G-C3G	-2.36	105.84	112.63
24	8	313	KC1	CMC-C2C-C1C	2.36	128.64	125.04
21	G	303	CLA	CMD-C2D-C1D	2.36	128.88	124.71
24	J	312	KC1	CBC-CAC-C3C	-2.36	105.92	112.43
21	G	304	CLA	CHD-C4C-NC	2.36	127.93	124.20
21	9	302	CLA	CED-O2D-CGD	2.36	121.28	115.94
24	9	306	KC1	O2D-CGD-O1D	-2.36	119.22	123.84
24	8	315	KC1	CHB-C4A-NA	2.36	127.93	124.20
21	c	505	CLA	CHC-C1C-NC	-2.36	120.62	124.20
21	D	407	CLA	CMD-C2D-C1D	2.36	128.87	124.71
28	8	317	LMG	C40-C39-C38	-2.36	102.44	114.42
24	7	314	KC1	CMC-C2C-C1C	2.36	128.63	125.04
21	b	614	CLA	CAC-C3C-C4C	2.36	127.87	124.81
21	b	615	CLA	CAC-C3C-C4C	2.36	127.87	124.81
21	8	304	CLA	CMD-C2D-C1D	2.36	128.87	124.71
28	b	620	LMG	C40-C39-C38	-2.36	102.46	114.42
21	d	404	CLA	CMD-C2D-C1D	2.36	128.87	124.71
23	2	311	A86	O-C13-C14	-2.36	116.87	121.66
21	3	301	CLA	CED-O2D-CGD	2.36	121.27	115.94
28	B	620	LMG	O1-C1-C2	-2.36	104.62	108.30
21	c	513	CLA	CAC-C3C-C4C	2.36	127.87	124.81
32	f	101	HEM	CMA-C3A-C4A	-2.36	124.84	128.46
24	3	306	KC1	CBC-CAC-C3C	-2.36	105.94	112.43
21	8	305	CLA	CHC-C1C-NC	-2.36	120.63	124.20
21	3	303	CLA	CMB-C2B-C3B	2.35	129.08	124.68
30	h	103	DGD	C3G-C2G-C1G	-2.35	106.22	111.79
21	B	608	CLA	C3D-C2D-C1D	-2.35	102.62	105.83
21	g	305	CLA	CMB-C2B-C3B	2.35	129.08	124.68
21	A	404	CLA	CHC-C1C-NC	-2.35	120.63	124.20
21	B	608	CLA	O1D-CGD-CBD	-2.35	119.67	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	G	302	CLA	CMC-C2C-C1C	2.35	128.62	125.04
21	b	611	CLA	CMD-C2D-C1D	2.35	128.86	124.71
21	g	304	CLA	CAC-C3C-C4C	2.35	127.86	124.81
21	D	404	CLA	CMD-C2D-C1D	2.35	128.86	124.71
24	6	313	KC1	CMC-C2C-C1C	2.35	128.62	125.04
21	6	303	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
21	6	306	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
21	c	502	CLA	CMD-C2D-C1D	2.35	128.86	124.71
24	8	315	KC1	CMB-C2B-C1B	2.35	128.86	124.71
25	C	501	BCR	C27-C26-C25	2.35	126.14	122.73
21	c	505	CLA	CMC-C2C-C1C	2.35	128.62	125.04
21	6	307	CLA	CHC-C1C-NC	-2.35	120.64	124.20
24	3	306	KC1	O2D-CGD-O1D	-2.35	119.25	123.84
21	C	514	CLA	O2A-CGA-CBA	2.35	119.28	111.91
21	5	307	CLA	CHC-C1C-NC	-2.35	120.64	124.20
21	1	306	CLA	CAC-C3C-C4C	2.35	127.86	124.81
21	G	303	CLA	CMB-C2B-C3B	2.35	129.07	124.68
21	4	302	CLA	CHD-C4C-C3C	-2.35	121.39	124.84
24	4	307	KC1	CBC-CAC-C3C	-2.35	105.96	112.43
28	b	621	LMG	O1-C1-C2	-2.35	104.64	108.30
21	C	511	CLA	C4-C3-C5	2.35	119.22	115.27
21	b	609	CLA	C3D-C2D-C1D	-2.34	102.63	105.83
21	6	300	CLA	CMB-C2B-C3B	2.34	129.06	124.68
21	B	607	CLA	CMB-C2B-C3B	2.34	129.06	124.68
21	C	511	CLA	C1D-CHD-C4C	-2.34	121.00	126.06
24	6	312	KC1	CBC-CAC-C3C	-2.34	105.97	112.43
28	B	623	LMG	C38-C37-C36	-2.34	102.53	114.42
21	C	504	CLA	C1-C2-C3	-2.34	121.99	126.04
29	2	317	LMU	C1B-O1B-C4'	-2.34	112.17	117.96
21	J	303	CLA	CMC-C2C-C1C	2.34	128.61	125.04
21	5	308	CLA	CMC-C2C-C1C	2.34	128.61	125.04
21	3	304	CLA	C1D-CHD-C4C	-2.34	121.00	126.06
21	7	300	CLA	CMB-C2B-C3B	2.34	129.06	124.68
21	B	605	CLA	CMD-C2D-C1D	2.34	128.84	124.71
24	8	316	KC1	CBC-CAC-C3C	-2.34	105.98	112.43
21	5	307	CLA	CMB-C2B-C3B	2.34	129.06	124.68
25	c	515	BCR	C11-C10-C9	-2.34	123.97	127.31
21	G	302	CLA	CHD-C4C-NC	2.34	127.89	124.20
21	3	301	CLA	CMB-C2B-C3B	2.34	129.06	124.68
24	5	313	KC1	CBC-CAC-C3C	-2.34	105.98	112.43
21	9	300	CLA	CMD-C2D-C1D	2.34	128.83	124.71
31	b	602	SQD	O5-C5-C4	2.34	113.94	109.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	g	306	CLA	CMD-C2D-C1D	2.34	128.83	124.71
21	a	402	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
21	A	401	CLA	C3B-C4B-NB	2.34	112.23	109.21
21	5	302	CLA	C1D-CHD-C4C	-2.34	121.02	126.06
23	G	305	A86	C35-C34-C33	2.34	113.95	109.88
21	3	302	CLA	C4C-C3C-C2C	-2.34	103.49	106.90
21	B	610	CLA	CMD-C2D-C1D	2.34	128.83	124.71
25	D	408	BCR	C15-C16-C17	-2.34	118.69	123.47
21	A	401	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
21	B	604	CLA	CMC-C2C-C1C	2.34	128.60	125.04
21	J	300	CLA	CMD-C2D-C1D	2.34	128.83	124.71
21	a	402	CLA	O2A-CGA-CBA	2.34	119.24	111.91
21	b	610	CLA	C3B-C4B-NB	2.34	112.23	109.21
30	B	624	DGD	C3G-C2G-C1G	-2.34	106.27	111.79
21	J	308	CLA	CMC-C2C-C1C	2.34	128.59	125.04
21	6	308	CLA	CHD-C4C-NC	2.33	127.88	124.20
21	b	608	CLA	CMB-C2B-C3B	2.33	129.05	124.68
21	7	309	CLA	CMC-C2C-C1C	2.33	128.59	125.04
24	8	313	KC1	CAA-C2A-C1A	-2.33	114.02	124.75
21	b	606	CLA	CMD-C2D-C1D	2.33	128.82	124.71
21	7	308	CLA	CMC-C2C-C1C	2.33	128.59	125.04
21	B	613	CLA	CAC-C3C-C4C	2.33	127.84	124.81
21	2	303	CLA	CMC-C2C-C1C	2.33	128.59	125.04
24	2	316	KC1	CBC-CAC-C3C	-2.33	106.00	112.43
21	B	609	CLA	O2A-CGA-CBA	2.33	119.23	111.91
21	g	303	CLA	C5-C3-C4	2.33	119.75	114.60
21	B	611	CLA	CHC-C1C-NC	-2.33	120.67	124.20
21	C	515	CLA	CMC-C2C-C1C	2.33	128.59	125.04
21	1	306	CLA	CMD-C2D-C1D	2.33	128.82	124.71
21	6	305	CLA	CMB-C2B-C3B	2.33	129.04	124.68
28	A	407	LMG	C38-C37-C36	-2.33	102.59	114.42
21	c	510	CLA	C1D-CHD-C4C	-2.33	121.03	126.06
24	J	312	KC1	CMC-C2C-C1C	2.33	128.59	125.04
21	1	303	CLA	CMD-C2D-C1D	2.33	128.82	124.71
21	1	308	CLA	C1-O2A-CGA	2.33	122.56	116.44
21	J	303	CLA	CMD-C2D-C1D	2.33	128.82	124.71
24	6	311	KC1	CBC-CAC-C3C	-2.33	106.01	112.43
25	c	501	BCR	C15-C14-C13	-2.33	123.99	127.31
21	6	301	CLA	CED-O2D-CGD	2.33	121.20	115.94
21	J	301	CLA	CED-O2D-CGD	2.33	121.20	115.94
25	1	317	BCR	C2-C1-C6	2.33	114.06	110.48
21	3	304	CLA	O2A-CGA-CBA	2.33	119.21	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	402	CLA	C3B-C4B-NB	2.33	112.22	109.21
21	3	304	CLA	CMD-C2D-C1D	2.33	128.81	124.71
21	d	404	CLA	C1D-CHD-C4C	-2.33	121.04	126.06
25	a	406	BCR	C24-C23-C22	-2.33	122.72	126.23
21	1	305	CLA	CMB-C2B-C3B	2.33	129.03	124.68
21	b	612	CLA	O2A-CGA-CBA	2.33	119.21	111.91
24	J	313	KC1	CMC-C2C-C1C	2.33	128.58	125.04
21	1	305	CLA	CMD-C2D-C1D	2.33	128.81	124.71
21	D	407	CLA	CMC-C2C-C1C	2.33	128.58	125.04
21	6	307	CLA	CED-O2D-CGD	2.33	121.20	115.94
25	m	101	BCR	C27-C26-C25	2.32	126.11	122.73
21	8	304	CLA	CMC-C2C-C1C	2.32	128.58	125.04
28	b	625	LMG	C38-C37-C36	-2.32	102.63	114.42
21	9	302	CLA	CMB-C2B-C3B	2.32	129.03	124.68
24	7	314	KC1	CHB-C1B-NB	-2.32	122.32	124.45
24	5	314	KC1	O2D-CGD-O1D	-2.32	119.30	123.84
21	7	304	CLA	CMB-C2B-C3B	2.32	129.02	124.68
21	8	303	CLA	CMC-C2C-C1C	2.32	128.57	125.04
21	b	606	CLA	C3D-C2D-C1D	-2.32	102.66	105.83
21	9	304	CLA	CMD-C2D-C1D	2.32	128.80	124.71
21	C	510	CLA	C3B-C4B-NB	2.32	112.21	109.21
21	6	302	CLA	CMB-C2B-C3B	2.32	129.02	124.68
24	G	308	KC1	CHD-C4C-NC	2.32	127.72	124.20
21	J	304	CLA	C3D-C4D-CHA	-2.32	107.42	112.72
25	a	406	BCR	C15-C14-C13	-2.32	124.00	127.31
21	7	308	CLA	CMD-C2D-C1D	2.32	128.80	124.71
21	J	305	CLA	CMD-C2D-C1D	2.32	128.80	124.71
21	C	512	CLA	C3D-C2D-C1D	-2.32	102.67	105.83
25	b	619	BCR	C24-C23-C22	-2.32	122.73	126.23
21	1	302	CLA	CAC-C3C-C4C	2.32	127.82	124.81
21	C	506	CLA	CMD-C2D-C1D	2.32	128.80	124.71
21	3	300	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
21	J	306	CLA	CMD-C2D-C1D	2.32	128.79	124.71
21	d	406	CLA	CMC-C2C-C1C	2.32	128.56	125.04
21	C	510	CLA	O2A-CGA-CBA	2.32	119.17	111.91
21	C	506	CLA	CMC-C2C-C1C	2.31	128.56	125.04
21	4	303	CLA	CHD-C4C-NC	2.31	127.85	124.20
21	B	609	CLA	CHC-C1C-NC	-2.31	120.69	124.20
21	C	506	CLA	CHC-C1C-NC	-2.31	120.69	124.20
24	3	306	KC1	CHB-C1B-NB	-2.31	122.33	124.45
24	g	313	KC1	CHB-C1B-NB	-2.31	122.33	124.45
21	7	304	CLA	CHC-C1C-NC	-2.31	120.69	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	315	KC1	O2D-CGD-O1D	-2.31	119.32	123.84
24	g	314	KC1	O2D-CGD-O1D	-2.31	119.32	123.84
21	4	304	CLA	O2A-CGA-CBA	2.31	119.16	111.91
21	C	509	CLA	CMD-C2D-C1D	2.31	128.79	124.71
23	6	310	A86	C17-C16-C15	-2.31	106.81	109.16
24	g	315	KC1	CBC-CAC-C3C	-2.31	106.06	112.43
21	b	613	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
21	b	611	CLA	CMB-C2B-C3B	2.31	129.00	124.68
21	b	603	CLA	CMD-C2D-C1D	2.31	128.79	124.71
21	4	303	CLA	CMD-C2D-C1D	2.31	128.78	124.71
21	9	300	CLA	CHC-C1C-NC	-2.31	120.70	124.20
21	6	306	CLA	C4-C3-C5	2.31	119.16	115.27
24	J	313	KC1	CHB-C4A-NA	2.31	127.84	124.20
21	g	308	CLA	CMC-C2C-C1C	2.31	128.55	125.04
21	C	508	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
28	8	301	LMG	O1-C1-C2	-2.31	104.70	108.30
21	C	508	CLA	CMD-C2D-C1D	2.31	128.78	124.71
21	B	608	CLA	C1-C2-C3	-2.31	122.05	126.04
21	C	511	CLA	CAA-CBA-CGA	-2.31	106.52	113.25
21	1	307	CLA	CAA-C2A-C3A	-2.31	110.72	116.10
21	1	309	CLA	CAC-C3C-C4C	2.30	127.80	124.81
21	g	305	CLA	CMD-C2D-C1D	2.30	128.77	124.71
24	7	314	KC1	O2D-CGD-O1D	-2.30	119.33	123.84
21	J	300	CLA	CMB-C2B-C3B	2.30	128.99	124.68
21	B	609	CLA	C3B-C4B-NB	2.30	112.19	109.21
21	2	305	CLA	CMD-C2D-C1D	2.30	128.77	124.71
21	5	308	CLA	CMD-C2D-C1D	2.30	128.77	124.71
21	g	307	CLA	CHC-C1C-NC	-2.30	120.71	124.20
21	c	509	CLA	C4-C3-C5	2.30	119.14	115.27
21	1	303	CLA	CMC-C2C-C1C	2.30	128.54	125.04
21	7	308	CLA	CMB-C2B-C3B	2.30	128.98	124.68
21	J	304	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
21	J	306	CLA	CAC-C3C-C4C	2.30	127.80	124.81
21	g	302	CLA	C3B-C4B-NB	2.30	112.19	109.21
21	g	309	CLA	C1D-CHD-C4C	-2.30	121.09	126.06
21	4	304	CLA	CMD-C2D-C1D	2.30	128.77	124.71
25	h	102	BCR	C7-C8-C9	-2.30	122.76	126.23
29	2	317	LMU	O5B-C5B-C4B	2.30	113.87	109.69
24	9	306	KC1	CHB-C1B-NB	-2.30	122.34	124.45
21	b	616	CLA	O2A-CGA-CBA	2.30	119.12	111.91
25	c	515	BCR	C27-C26-C25	2.30	126.07	122.73
21	b	604	CLA	CHC-C1C-NC	-2.30	120.72	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	605	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
24	5	313	KC1	O2D-CGD-O1D	-2.30	119.35	123.84
24	4	306	KC1	O2D-CGD-O1D	-2.30	119.35	123.84
21	6	302	CLA	CED-O2D-CGD	2.30	121.13	115.94
21	7	309	CLA	CMD-C2D-C1D	2.30	128.76	124.71
24	8	315	KC1	CHC-C4B-NB	-2.30	122.34	124.45
21	5	309	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
21	C	505	CLA	CMD-C2D-C1D	2.30	128.76	124.71
30	C	517	DGD	C3G-C2G-C1G	-2.30	106.36	111.79
24	J	311	KC1	CBC-CAC-C3C	-2.30	106.10	112.43
24	5	315	KC1	CBC-CAC-C3C	-2.30	106.10	112.43
23	2	307	A86	C20-C19-C18	-2.30	108.21	112.75
24	4	309	KC1	CHD-C4C-NC	2.30	127.69	124.20
31	b	602	SQD	O48-C23-C24	2.29	119.11	111.91
21	b	605	CLA	CMC-C2C-C1C	2.29	128.53	125.04
25	1	317	BCR	C30-C25-C26	-2.29	119.38	122.61
21	B	612	CLA	C3D-C4D-CHA	-2.29	107.47	112.72
21	9	303	CLA	O2A-CGA-CBA	2.29	119.11	111.91
21	9	303	CLA	C4C-C3C-C2C	-2.29	103.55	106.90
21	c	511	CLA	C3D-C4D-CHA	-2.29	107.48	112.72
24	J	312	KC1	O2D-CGD-O1D	-2.29	119.36	123.84
21	c	503	CLA	C1-C2-C3	-2.29	122.08	126.04
21	9	301	CLA	CHC-C1C-NC	-2.29	120.72	124.20
21	b	610	CLA	CMD-C2D-C1D	2.29	128.75	124.71
28	8	301	LMG	O3-C3-C2	-2.29	105.05	110.35
21	A	401	CLA	O2A-CGA-CBA	2.29	119.10	111.91
21	2	302	CLA	OBD-CAD-C3D	-2.29	123.01	128.52
27	d	409	LHG	C18-C17-C16	-2.29	102.79	114.42
21	G	301	CLA	CMB-C2B-C3B	2.29	128.96	124.68
21	b	610	CLA	O2A-CGA-CBA	2.29	119.10	111.91
21	b	606	CLA	CAA-CBA-CGA	-2.29	106.56	113.25
21	b	613	CLA	C3D-C4D-CHA	-2.29	107.49	112.72
28	b	621	LMG	C1-C2-C3	-2.29	105.23	110.00
21	8	303	CLA	C5-C3-C4	2.29	119.66	114.60
21	9	303	CLA	CMC-C2C-C3C	2.29	132.33	126.12
21	4	302	CLA	CAC-C3C-C4C	2.29	127.78	124.81
21	c	509	CLA	C3B-C4B-NB	2.29	112.17	109.21
21	6	300	CLA	CMD-C2D-C1D	2.29	128.74	124.71
21	d	405	CLA	CMB-C2B-C3B	2.29	129.16	124.69
21	6	306	CLA	CMC-C2C-C1C	2.29	128.52	125.04
21	7	302	CLA	CED-O2D-CGD	2.28	121.11	115.94
25	C	516	BCR	C11-C10-C9	-2.28	124.05	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	312	KC1	O2D-CGD-O1D	-2.28	119.37	123.84
21	7	308	CLA	CAC-C3C-C4C	2.28	127.77	124.81
21	9	301	CLA	O2A-CGA-CBA	2.28	119.07	111.91
28	D	411	LMG	O3-C3-C2	-2.28	105.07	110.35
21	c	507	CLA	CMD-C2D-C1D	2.28	128.74	124.71
25	m	101	BCR	C15-C14-C13	-2.28	124.05	127.31
21	4	302	CLA	C3D-C4D-CHA	-2.28	107.50	112.72
24	6	312	KC1	CMC-C2C-C1C	2.28	128.51	125.04
21	6	304	CLA	CMB-C2B-C3B	2.28	128.95	124.68
21	b	609	CLA	C1-C2-C3	-2.28	122.10	126.04
23	J	309	A86	O4-C34-C33	2.28	113.27	107.59
21	6	308	CLA	CMC-C2C-C1C	2.28	128.51	125.04
24	3	306	KC1	CMC-C2C-C1C	2.28	128.51	125.04
21	4	302	CLA	CMB-C2B-C3B	2.28	128.94	124.68
21	B	609	CLA	CMD-C2D-C1D	2.28	128.73	124.71
21	7	307	CLA	CMB-C2B-C3B	2.28	128.94	124.68
28	8	317	LMG	O3-C3-C2	-2.28	105.08	110.35
21	6	303	CLA	CMD-C2D-C1D	2.28	128.73	124.71
24	8	313	KC1	CHB-C1B-C2B	-2.28	120.70	125.48
21	9	303	CLA	CED-O2D-CGD	2.28	121.09	115.94
28	2	318	LMG	C38-C37-C36	-2.28	102.86	114.42
21	3	300	CLA	O2A-CGA-CBA	2.28	119.05	111.91
21	9	303	CLA	O1D-CGD-CBD	-2.28	119.83	124.48
21	1	309	CLA	CMB-C2B-C3B	2.28	128.94	124.68
21	5	305	CLA	CMC-C2C-C1C	2.28	128.50	125.04
21	4	300	CLA	C6-C7-C8	-2.28	108.56	115.92
21	5	307	CLA	CMD-C2D-C1D	2.27	128.72	124.71
21	B	609	CLA	CMC-C2C-C1C	2.27	128.50	125.04
21	J	307	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
21	2	306	CLA	C3B-C4B-NB	2.27	112.15	109.21
23	2	311	A86	O-C13-C11	-2.27	116.13	121.15
21	8	306	CLA	O2A-C1-C2	2.27	114.61	108.64
25	h	101	BCR	C11-C10-C9	-2.27	124.07	127.31
28	f	102	LMG	O3-C3-C2	-2.27	105.10	110.35
21	2	306	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
25	H	100	BCR	C16-C15-C14	-2.27	118.83	123.47
28	B	622	LMG	O2-C2-C1	-2.27	104.53	110.05
25	1	317	BCR	C40-C30-C25	2.27	113.98	110.30
21	b	612	CLA	CHC-C1C-NC	-2.27	120.76	124.20
24	3	305	KC1	CMC-C2C-C1C	2.27	128.50	125.04
21	G	301	CLA	C1-C2-C3	-2.27	122.12	126.04
21	B	611	CLA	O2A-CGA-CBA	2.27	119.03	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	412	LMU	O1B-C4'-C3'	2.27	113.31	107.28
21	6	301	CLA	CAC-C3C-C4C	2.27	127.75	124.81
25	B	617	BCR	C11-C10-C9	-2.27	124.08	127.31
21	b	623	CLA	C4C-C3C-C2C	-2.27	103.59	106.90
21	6	307	CLA	CMD-C2D-C1D	2.27	128.71	124.71
24	1	315	KC1	CMC-C2C-C1C	2.27	128.49	125.04
21	c	510	CLA	CAA-CBA-CGA	-2.27	106.63	113.25
21	c	512	CLA	CMB-C2B-C3B	2.26	128.91	124.68
21	5	309	CLA	C3D-C4D-CHA	-2.26	107.54	112.72
21	2	303	CLA	CHC-C1C-NC	-2.26	120.77	124.20
21	C	503	CLA	CAC-C3C-C4C	2.26	127.75	124.81
28	N	101	LMG	O3-C3-C2	-2.26	105.12	110.35
21	6	305	CLA	CMC-C2C-C1C	2.26	128.48	125.04
21	b	623	CLA	C1D-CHD-C4C	-2.26	121.18	126.06
21	B	602	CLA	CAC-C3C-C4C	2.26	127.74	124.81
21	7	302	CLA	CMD-C2D-C1D	2.26	128.70	124.71
21	8	302	CLA	CMD-C2D-C1D	2.26	128.70	124.71
21	D	406	CLA	CMB-C2B-C3B	2.26	129.12	124.69
21	J	304	CLA	CMB-C2B-C3B	2.26	128.91	124.68
21	1	308	CLA	CED-O2D-CGD	2.26	121.05	115.94
21	B	611	CLA	C1D-CHD-C4C	-2.26	121.18	126.06
24	7	315	KC1	CBC-CAC-C3C	-2.26	106.20	112.43
21	b	623	CLA	C3D-C4D-CHA	-2.26	107.56	112.72
27	D	410	LHG	C18-C17-C16	-2.26	102.96	114.42
24	4	308	KC1	O2D-CGD-O1D	-2.26	119.42	123.84
21	G	302	CLA	O2A-CGA-CBA	2.26	118.99	111.91
21	1	310	CLA	C4-C3-C2	-2.26	117.89	123.68
30	c	517	DGD	C1G-C2G-C3G	-2.26	106.14	112.63
21	C	509	CLA	CMC-C2C-C1C	2.26	128.48	125.04
21	5	306	CLA	CHD-C4C-NC	2.26	127.76	124.20
21	B	602	CLA	CED-O2D-CGD	2.25	121.04	115.94
21	g	306	CLA	CHD-C4C-NC	2.25	127.76	124.20
24	J	311	KC1	CHB-C4A-NA	2.25	127.76	124.20
21	b	611	CLA	CMC-C2C-C1C	2.25	128.47	125.04
21	5	305	CLA	C3D-C4D-CHA	-2.25	107.57	112.72
21	b	605	CLA	C1D-CHD-C4C	-2.25	121.19	126.06
21	G	301	CLA	CED-O2D-CGD	2.25	121.03	115.94
21	J	302	CLA	CMB-C2B-C3B	2.25	128.90	124.68
24	6	311	KC1	CHB-C4A-NA	2.25	127.75	124.20
21	8	302	CLA	C3D-C4D-CHA	-2.25	107.57	112.72
21	B	615	CLA	CMD-C2D-C1D	2.25	128.68	124.71
21	c	503	CLA	CED-O2D-CGD	2.25	121.03	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	303	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
24	2	313	KC1	CMC-C2C-C1C	2.25	128.47	125.04
21	8	304	CLA	CAC-C3C-C4C	2.25	127.73	124.81
28	a	407	LMG	C1-C2-C3	-2.25	105.31	110.00
28	D	411	LMG	C6-C5-C4	-2.25	107.73	113.00
21	J	302	CLA	CED-O2D-CGD	2.25	121.03	115.94
21	C	513	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
21	B	615	CLA	O2A-CGA-CBA	2.25	118.96	111.91
23	7	313	A86	C20-C19-C18	-2.25	108.30	112.75
25	1	317	BCR	C7-C8-C9	-2.25	122.84	126.23
29	g	301	LMU	C3'-C4'-C5'	2.25	116.08	110.93
28	8	317	LMG	C38-C37-C36	-2.25	103.02	114.42
21	7	304	CLA	CMC-C2C-C3C	2.25	132.22	126.12
25	A	405	BCR	C27-C26-C25	2.25	125.99	122.73
21	G	304	CLA	CMD-C2D-C1D	2.24	128.67	124.71
25	b	619	BCR	C37-C22-C21	-2.24	119.78	122.92
21	G	304	CLA	C4-C3-C5	2.24	119.05	115.27
21	J	300	CLA	C3D-C4D-CHA	-2.24	107.59	112.72
21	b	604	CLA	C1-O2A-CGA	2.24	122.33	116.44
21	J	305	CLA	CMC-C2C-C1C	2.24	128.46	125.04
21	B	614	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
21	b	617	CLA	CED-O2D-CGD	2.24	121.01	115.94
24	g	314	KC1	CBC-CAC-C3C	-2.24	106.25	112.43
21	A	401	CLA	CBA-CAA-C2A	-2.24	107.25	113.86
21	2	305	CLA	CHB-C4A-NA	2.24	127.61	124.51
28	B	622	LMG	O3-C3-C2	-2.24	105.17	110.35
25	C	516	BCR	C15-C16-C17	-2.24	118.89	123.47
21	5	302	CLA	CMD-C2D-C1D	2.24	128.66	124.71
24	4	308	KC1	CHC-C4B-NB	-2.24	122.40	124.45
21	J	307	CLA	C3D-C4D-CHA	-2.24	107.60	112.72
28	2	318	LMG	O3-C3-C2	-2.24	105.17	110.35
25	a	406	BCR	C27-C26-C25	2.24	125.98	122.73
30	C	517	DGD	C1D-C2D-C3D	-2.24	105.34	110.00
21	C	506	CLA	CED-O2D-CGD	2.24	120.99	115.94
21	1	308	CLA	CMB-C2B-C3B	2.24	128.86	124.68
24	9	306	KC1	CBC-CAC-C3C	-2.23	106.28	112.43
21	1	306	CLA	C3D-C4D-CHA	-2.23	107.62	112.72
21	C	512	CLA	C3D-C4D-CHA	-2.23	107.62	112.72
27	A	406	LHG	C18-C17-C16	-2.23	103.09	114.42
21	6	306	CLA	CAC-C3C-C4C	2.23	127.71	124.81
21	1	304	CLA	CHC-C1C-NC	-2.23	120.82	124.20
25	c	501	BCR	C33-C5-C6	-2.23	122.02	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	301	CLA	C3D-C4D-CHA	-2.23	107.62	112.72
21	2	303	CLA	CAC-C3C-C4C	2.23	127.70	124.81
21	G	300	CLA	CED-O2D-CGD	2.23	120.98	115.94
24	4	308	KC1	CMC-C2C-C1C	2.23	128.44	125.04
21	5	308	CLA	CED-O2D-CGD	2.23	120.98	115.94
21	5	307	CLA	C1-C2-C3	-2.23	122.19	126.04
21	D	404	CLA	CED-O2D-CGD	2.23	120.98	115.94
23	6	309	A86	C17-C16-C15	2.23	111.44	109.16
24	4	307	KC1	C2A-C1A-CHA	-2.23	120.07	127.44
21	C	514	CLA	CBA-CAA-C2A	-2.23	107.28	113.86
21	2	304	CLA	CHC-C1C-NC	-2.23	120.82	124.20
21	6	304	CLA	CAC-C3C-C4C	2.23	127.70	124.81
28	b	626	LMG	O3-C3-C2	-2.23	105.20	110.35
21	C	506	CLA	C1-C2-C3	-2.23	122.19	126.04
21	5	305	CLA	CED-O2D-CGD	2.23	120.97	115.94
24	g	313	KC1	C2A-C1A-CHA	-2.23	120.08	127.44
25	A	405	BCR	C24-C23-C22	-2.23	122.87	126.23
21	7	307	CLA	CED-O2D-CGD	2.23	120.97	115.94
21	c	506	CLA	CMD-C2D-C1D	2.23	128.64	124.71
24	1	316	KC1	CBC-CAC-C3C	-2.23	106.30	112.43
21	2	306	CLA	CMD-C2D-C1D	2.22	128.63	124.71
21	b	610	CLA	CHC-C1C-NC	-2.22	120.83	124.20
21	b	604	CLA	CMC-C2C-C1C	2.22	128.43	125.04
25	B	618	BCR	C20-C21-C22	-2.22	124.14	127.31
21	7	304	CLA	C1D-CHD-C4C	-2.22	121.26	126.06
21	c	512	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
29	g	301	LMU	C2'-C3'-C4'	2.22	114.76	109.68
21	3	301	CLA	CHB-C4A-NA	2.22	127.58	124.51
28	b	624	LMG	O1-C1-C2	-2.22	104.83	108.30
24	4	309	KC1	O2D-CGD-O1D	-2.22	119.49	123.84
21	B	612	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
21	J	308	CLA	CED-O2D-CGD	2.22	120.96	115.94
28	f	102	LMG	C1-C2-C3	-2.22	105.37	110.00
25	C	501	BCR	C33-C5-C6	-2.22	122.03	124.53
24	9	306	KC1	CMC-C2C-C1C	2.22	128.42	125.04
24	5	315	KC1	CMC-C2C-C1C	2.22	128.42	125.04
21	6	307	CLA	C3D-C4D-CHA	-2.22	107.65	112.72
24	G	306	KC1	CHB-C1B-NB	-2.22	122.42	124.45
28	D	411	LMG	O1-C1-C2	-2.22	104.84	108.30
21	a	402	CLA	CHC-C1C-NC	-2.22	120.84	124.20
27	d	402	LHG	C27-C26-C25	-2.22	103.16	114.42
24	J	311	KC1	CMB-C2B-C1B	2.22	128.62	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	401	LHG	C18-C17-C16	-2.22	103.16	114.42
27	d	409	LHG	C27-C26-C25	-2.22	103.17	114.42
21	G	300	CLA	CMB-C2B-C3B	2.22	128.83	124.68
21	d	405	CLA	C3D-C4D-CHA	-2.22	107.65	112.72
21	G	301	CLA	CMD-C2D-C1D	2.22	128.62	124.71
21	1	307	CLA	CED-O2D-CGD	2.22	120.95	115.94
21	5	308	CLA	CAA-CBA-CGA	-2.22	106.78	113.25
21	D	404	CLA	C3B-C4B-NB	2.22	112.08	109.21
35	d	408	PL9	C27-C28-C29	-2.22	122.32	127.66
21	7	300	CLA	CMD-C2D-C1D	2.22	128.62	124.71
24	7	315	KC1	O2D-CGD-O1D	-2.22	119.51	123.84
21	b	612	CLA	C3D-C4D-CHA	-2.22	107.65	112.72
21	B	603	CLA	CMC-C2C-C1C	2.22	128.41	125.04
21	5	302	CLA	CHC-C1C-NC	-2.21	120.84	124.20
27	l	101	LHG	C27-C26-C25	-2.21	103.18	114.42
28	B	619	LMG	C1-C2-C3	-2.21	105.39	110.00
21	7	306	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
21	c	507	CLA	CHC-C1C-NC	-2.21	120.84	124.20
21	c	507	CLA	CMB-C2B-C3B	2.21	128.82	124.68
35	d	408	PL9	C37-C38-C39	-2.21	122.33	127.66
21	6	300	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
21	c	503	CLA	CMC-C2C-C1C	2.21	128.41	125.04
25	M	101	BCR	C15-C14-C13	-2.21	124.15	127.31
35	D	409	PL9	C27-C28-C29	-2.21	122.33	127.66
24	2	313	KC1	O2D-CGD-O1D	-2.21	119.51	123.84
30	C	517	DGD	CBB-CAB-C9B	-2.21	103.19	114.42
21	8	302	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
28	B	627	LMG	O7-C10-C11	2.21	116.27	111.50
21	B	604	CLA	C1D-CHD-C4C	-2.21	121.29	126.06
24	8	315	KC1	CMC-C2C-C1C	2.21	128.41	125.04
21	B	603	CLA	CAA-CBA-CGA	-2.21	106.80	113.25
21	1	309	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
29	5	301	LMU	C3'-C4'-C5'	2.21	115.99	110.93
35	D	409	PL9	O1-C4-C3	-2.21	118.29	120.72
21	B	604	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
25	H	100	BCR	C24-C23-C22	-2.21	122.90	126.23
21	8	304	CLA	CHC-C1C-NC	-2.21	120.85	124.20
21	5	309	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
21	B	602	CLA	O2A-CGA-CBA	2.21	118.84	111.91
29	5	301	LMU	C2'-C3'-C4'	2.21	114.72	109.68
21	c	506	CLA	CHC-C1C-NC	-2.21	120.85	124.20
21	2	302	CLA	C3D-C4D-CHA	-2.21	107.67	112.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	304	CLA	C1-C2-C3	-2.21	122.23	126.04
21	6	300	CLA	C3D-C4D-CHA	-2.21	107.67	112.72
21	g	303	CLA	CHB-C4A-NA	2.21	127.56	124.51
28	D	411	LMG	C1-C2-C3	-2.21	105.40	110.00
28	b	624	LMG	O3-C3-C2	-2.21	105.25	110.35
28	8	301	LMG	O2-C2-C1	-2.20	104.69	110.05
21	B	605	CLA	CAA-CBA-CGA	-2.20	106.82	113.25
22	5	310	DD6	C13-C11-C10	2.20	122.32	118.94
24	5	315	KC1	C2A-C1A-CHA	-2.20	120.16	127.44
24	4	308	KC1	CHB-C4A-NA	2.20	127.67	124.20
21	B	603	CLA	CHC-C1C-NC	-2.20	120.86	124.20
27	B	601	LHG	C18-C17-C16	-2.20	103.25	114.42
21	c	514	CLA	C3D-C4D-CHA	-2.20	107.69	112.72
21	3	302	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
21	C	507	CLA	CMD-C2D-C1D	2.20	128.59	124.71
28	2	318	LMG	C42-C41-C40	-2.20	103.27	114.42
21	b	610	CLA	C4-C3-C5	2.20	118.97	115.27
21	C	513	CLA	CMB-C2B-C3B	2.20	128.79	124.68
23	2	308	A86	C20-C19-C18	-2.20	108.41	112.75
25	C	516	BCR	C7-C8-C9	-2.20	122.92	126.23
21	8	303	CLA	OBD-CAD-C3D	-2.19	123.24	128.52
24	8	314	KC1	CHB-C4A-NA	2.19	127.66	124.20
21	6	306	CLA	C3D-C4D-CHA	-2.19	107.70	112.72
21	6	306	CLA	CHC-C1C-NC	-2.19	120.87	124.20
21	2	302	CLA	CAC-C3C-C4C	2.19	127.66	124.81
21	d	404	CLA	C4-C3-C5	2.19	118.96	115.27
28	b	622	LMG	C1-O6-C5	2.19	117.99	113.69
27	D	410	LHG	C27-C26-C25	-2.19	103.29	114.42
24	7	315	KC1	CHB-C4A-NA	2.19	127.66	124.20
25	D	408	BCR	C24-C23-C22	-2.19	122.92	126.23
21	4	304	CLA	CMC-C2C-C3C	2.19	132.07	126.12
21	5	305	CLA	CAC-C3C-C4C	2.19	127.65	124.81
21	A	401	CLA	CHC-C1C-NC	-2.19	120.88	124.20
21	b	616	CLA	CMD-C2D-C1D	2.19	128.57	124.71
30	c	516	DGD	C1D-C2D-C3D	-2.19	105.43	110.00
24	1	316	KC1	CHB-C4A-NA	2.19	127.66	124.20
21	B	616	CLA	CMD-C2D-C1D	2.19	128.57	124.71
21	C	508	CLA	CMB-C2B-C3B	2.19	128.78	124.68
31	C	502	SQD	C1-O5-C5	2.19	117.98	113.69
21	C	509	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
28	B	623	LMG	O3-C3-C2	-2.19	105.29	110.35
24	3	305	KC1	O2D-CGD-O1D	-2.19	119.56	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	l	101	LHG	C18-C17-C16	-2.19	103.32	114.42
30	B	624	DGD	O5D-C6D-C5D	-2.19	105.00	109.05
21	b	623	CLA	C5-C3-C2	-2.19	116.69	121.12
28	A	407	LMG	O3-C3-C2	-2.19	105.30	110.35
21	B	606	CLA	CHC-C1C-NC	-2.19	120.89	124.20
21	2	304	CLA	CAA-C2A-C3A	-2.18	111.00	116.10
24	G	307	KC1	C4B-CHC-C1C	-2.18	121.35	126.06
24	8	313	KC1	CBC-CAC-C3C	-2.18	106.41	112.43
21	7	301	CLA	CMD-C2D-C1D	2.18	128.56	124.71
21	7	303	CLA	C1-C2-C3	-2.18	122.27	126.04
21	C	515	CLA	C3D-C4D-CHA	-2.18	107.73	112.72
21	b	609	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
23	2	309	A86	C26-C25-C24	2.18	130.03	123.22
21	2	305	CLA	O2A-CGA-CBA	2.18	118.76	111.91
31	X	401	SQD	C1-O5-C5	2.18	117.97	113.69
21	D	406	CLA	C3D-C4D-CHA	-2.18	107.73	112.72
26	a	404	PHO	O2A-CGA-O1A	-2.18	118.09	123.59
21	G	303	CLA	C1-C2-C3	-2.18	122.27	126.04
21	g	305	CLA	CED-O2D-CGD	2.18	120.87	115.94
21	9	300	CLA	C3D-C4D-CHA	-2.18	107.73	112.72
21	a	402	CLA	CBA-CAA-C2A	-2.18	107.43	113.86
21	B	616	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
21	B	621	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
21	4	304	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
24	J	313	KC1	CBD-CHA-C1A	2.18	132.94	128.88
28	B	627	LMG	O2-C2-C1	-2.18	104.76	110.05
21	B	609	CLA	C4-C3-C5	2.18	118.93	115.27
24	9	305	KC1	O2D-CGD-O1D	-2.18	119.58	123.84
21	J	306	CLA	CHC-C1C-NC	-2.18	120.90	124.20
21	g	309	CLA	CAC-C3C-C4C	2.17	127.63	124.81
21	J	304	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
21	8	307	CLA	CMB-C2B-C3B	2.17	128.75	124.68
25	h	102	BCR	C16-C15-C14	-2.17	119.02	123.47
30	B	624	DGD	CBB-CAB-C9B	-2.17	103.39	114.42
21	C	508	CLA	CHD-C4C-NC	2.17	127.63	124.20
21	4	301	CLA	CMB-C2B-C3B	2.17	128.74	124.68
21	1	302	CLA	CMD-C2D-C1D	2.17	128.54	124.71
21	1	310	CLA	CED-O2D-CGD	2.17	120.85	115.94
21	g	302	CLA	C6-C5-C3	-2.17	107.76	113.45
28	B	619	LMG	O2-C2-C1	-2.17	104.77	110.05
27	B	601	LHG	C27-C26-C25	-2.17	103.39	114.42
21	J	303	CLA	CHC-C1C-NC	-2.17	120.91	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	601	DGD	O5D-C6D-C5D	-2.17	105.03	109.05
21	C	506	CLA	O2A-CGA-CBA	2.17	118.72	111.91
21	1	310	CLA	O2A-CGA-CBA	2.17	118.72	111.91
28	b	626	LMG	O2-C2-C1	-2.17	104.77	110.05
21	8	303	CLA	C3D-C4D-CHA	-2.17	107.76	112.72
21	B	612	CLA	CED-O2D-CGD	2.17	120.84	115.94
25	A	405	BCR	C16-C15-C14	-2.17	119.03	123.47
24	G	309	KC1	CMC-C2C-C1C	2.17	128.34	125.04
23	8	308	A86	C23-C16-C17	-2.17	105.22	108.98
21	4	304	CLA	CAC-C3C-C2C	2.17	131.24	127.53
21	6	306	CLA	C1D-CHD-C4C	-2.17	121.38	126.06
24	4	307	KC1	O2D-CGD-O1D	-2.17	119.60	123.84
24	8	313	KC1	O1D-CGD-CBD	-2.17	120.05	124.48
35	d	408	PL9	O1-C4-C3	-2.17	118.33	120.72
22	5	310	DD6	C37-C36-C31	-2.17	121.40	124.35
21	4	302	CLA	CMD-C2D-C1D	2.17	128.53	124.71
21	d	404	CLA	C3B-C4B-NB	2.17	112.01	109.21
30	b	601	DGD	CBB-CAB-C9B	-2.17	103.43	114.42
21	A	401	CLA	C3D-C4D-CHA	-2.16	107.77	112.72
21	8	306	CLA	C1-C2-C3	-2.16	122.30	126.04
21	b	612	CLA	C4C-C3C-C2C	-2.16	103.74	106.90
21	B	614	CLA	C3D-C4D-CHA	-2.16	107.77	112.72
21	c	508	CLA	CMC-C2C-C1C	2.16	128.34	125.04
28	8	317	LMG	C42-C41-C40	-2.16	103.44	114.42
21	5	308	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
21	8	302	CLA	C1D-CHD-C4C	-2.16	121.39	126.06
21	G	301	CLA	CAC-C3C-C4C	2.16	127.62	124.81
21	G	300	CLA	CHD-C4C-NC	2.16	127.61	124.20
21	b	603	CLA	CED-O2D-CGD	2.16	120.83	115.94
21	3	301	CLA	CMC-C2C-C1C	2.16	128.33	125.04
25	b	618	BCR	C11-C10-C9	-2.16	124.23	127.31
23	g	312	A86	C20-C19-C18	-2.16	108.47	112.75
21	a	402	CLA	C3D-C4D-CHA	-2.16	107.78	112.72
21	3	302	CLA	C3D-C4D-CHA	-2.16	107.79	112.72
23	J	310	A86	C17-C16-C15	-2.16	106.96	109.16
21	c	505	CLA	O2A-CGA-CBA	2.16	118.68	111.91
21	4	303	CLA	C1D-CHD-C4C	-2.16	121.41	126.06
21	C	511	CLA	CAC-C3C-C4C	2.16	127.61	124.81
29	g	316	LMU	C1B-C2B-C3B	2.16	114.48	110.00
21	C	515	CLA	CED-O2D-CGD	2.16	120.81	115.94
22	g	310	DD6	C10-C9-C8	2.15	129.94	123.22
24	8	316	KC1	CHB-C1B-NB	-2.15	122.47	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	306	CLA	C2A-C1A-CHA	-2.15	120.09	123.85
24	1	316	KC1	O2D-CGD-O1D	-2.15	119.63	123.84
21	B	614	CLA	C1-O2A-CGA	2.15	122.10	116.44
21	6	307	CLA	C2A-C1A-CHA	-2.15	120.09	123.86
21	C	507	CLA	CHB-C4A-NA	2.15	127.49	124.51
21	2	306	CLA	CMB-C2B-C3B	2.15	128.71	124.68
21	a	405	CLA	C2A-C1A-CHA	-2.15	120.09	123.86
23	5	311	A86	C26-C25-C24	2.15	129.93	123.22
24	J	312	KC1	CHB-C1B-NB	-2.15	122.48	124.45
21	G	303	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
21	8	305	CLA	CED-O2D-CGD	2.15	120.80	115.94
21	B	616	CLA	C3C-C4C-NC	2.15	112.98	110.57
21	2	304	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
25	c	515	BCR	C7-C8-C9	-2.15	122.98	126.23
21	b	607	CLA	CHC-C1C-NC	-2.15	120.94	124.20
21	1	308	CLA	C3D-C4D-CHA	-2.15	107.80	112.72
24	G	307	KC1	C2A-C1A-CHA	-2.15	120.33	127.44
28	b	621	LMG	O3-C3-C2	-2.15	105.38	110.35
35	D	409	PL9	C31-C32-C33	-2.15	104.82	111.88
21	5	303	CLA	C3B-C4B-NB	2.15	111.99	109.21
21	B	612	CLA	C1-C2-C3	-2.15	122.33	126.04
21	8	305	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
21	5	308	CLA	C3D-C4D-CHA	-2.15	107.81	112.72
24	G	308	KC1	CMC-C2C-C1C	2.15	128.31	125.04
21	B	603	CLA	C3D-C4D-CHA	-2.15	107.81	112.72
21	C	510	CLA	C4C-C3C-C2C	-2.15	103.77	106.90
24	8	315	KC1	CGD-CBD-CAD	-2.15	103.78	110.73
21	1	305	CLA	CHC-C1C-NC	-2.15	120.95	124.20
21	c	509	CLA	CHC-C1C-NC	-2.15	120.95	124.20
25	B	618	BCR	C33-C5-C6	-2.15	122.12	124.53
21	B	602	CLA	CMB-C2B-C3B	2.15	128.69	124.68
24	G	307	KC1	CMC-C2C-C1C	2.15	128.31	125.04
21	C	508	CLA	C3D-C4D-CHA	-2.15	107.81	112.72
21	7	304	CLA	CHD-C4C-NC	2.15	127.58	124.20
24	8	316	KC1	CHB-C4A-NA	2.15	127.58	124.20
21	g	304	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
21	g	302	CLA	C3D-C4D-CHA	-2.14	107.82	112.72
21	J	306	CLA	CBA-CAA-C2A	2.14	120.19	113.86
21	c	509	CLA	C3D-C4D-CHA	-2.14	107.82	112.72
29	D	412	LMU	O5B-C5B-C4B	2.14	113.59	109.69
24	2	316	KC1	CHB-C1B-NB	-2.14	122.48	124.45
28	B	627	LMG	C8-O7-C10	2.14	123.07	117.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	624	LMG	O2-C2-C1	-2.14	104.84	110.05
28	b	622	LMG	O1-C7-C8	-2.14	105.73	110.90
21	b	615	CLA	C3D-C4D-CHA	-2.14	107.82	112.72
21	4	302	CLA	O2A-CGA-CBA	2.14	118.63	111.91
21	G	302	CLA	CED-O2D-CGD	2.14	120.78	115.94
21	a	403	CLA	C1D-CHD-C4C	-2.14	121.44	126.06
21	c	509	CLA	C4C-C3C-C2C	-2.14	103.78	106.90
21	b	606	CLA	CHB-C4A-NA	2.14	127.47	124.51
24	5	315	KC1	CHB-C4A-NA	2.14	127.58	124.20
21	1	303	CLA	CAC-C3C-C4C	2.14	127.59	124.81
21	B	611	CLA	C4C-C3C-C2C	-2.14	103.78	106.90
28	f	102	LMG	C6-C5-C4	-2.14	108.00	113.00
23	8	312	A86	C28-C27-C26	-2.14	119.93	122.92
27	D	403	LHG	C27-C26-C25	-2.14	103.57	114.42
21	2	306	CLA	CMC-C2C-C1C	2.14	128.29	125.04
21	g	305	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
21	D	404	CLA	C4-C3-C5	2.14	118.87	115.27
21	J	306	CLA	C3D-C4D-CHA	-2.14	107.83	112.72
25	B	618	BCR	C30-C25-C26	-2.14	119.60	122.61
21	C	507	CLA	CHC-C1C-NC	-2.14	120.96	124.20
21	2	301	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
21	4	304	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
21	b	616	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
24	9	305	KC1	C2A-C1A-CHA	-2.14	120.38	127.44
21	a	405	CLA	CMD-C2D-C1D	2.14	128.48	124.71
21	J	305	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
21	b	607	CLA	C1-C2-C3	-2.13	122.35	126.04
21	b	604	CLA	CAC-C3C-C4C	2.13	127.58	124.81
30	C	517	DGD	O6E-C5E-C4E	2.13	113.57	109.69
24	8	314	KC1	CBC-CAC-C3C	-2.13	106.56	112.43
21	B	608	CLA	C3D-C4D-CHA	-2.13	107.85	112.72
21	4	304	CLA	C1-C2-C3	-2.13	122.36	126.04
27	A	406	LHG	C27-C26-C25	-2.13	103.61	114.42
26	a	404	PHO	CMC-C2C-C3C	2.13	128.96	124.94
21	6	302	CLA	C1D-CHD-C4C	-2.13	121.46	126.06
21	b	608	CLA	CMD-C2D-C1D	2.13	128.47	124.71
21	3	303	CLA	C3D-C4D-CHA	-2.13	107.85	112.72
23	2	307	A86	C10-C9-C8	2.13	129.86	123.22
24	g	313	KC1	O2D-CGD-O1D	-2.13	119.67	123.84
21	D	407	CLA	CHC-C1C-NC	-2.13	120.97	124.20
21	d	406	CLA	CHC-C1C-NC	-2.13	120.97	124.20
21	B	616	CLA	CED-O2D-CGD	2.13	120.75	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	305	KC1	CBC-CAC-C3C	-2.13	106.56	112.43
21	J	304	CLA	CAC-C3C-C4C	2.13	127.57	124.81
23	6	309	A86	O4-C34-C33	2.13	112.89	107.59
23	7	312	A86	C10-C9-C8	2.13	129.85	123.22
21	4	304	CLA	CHD-C4C-NC	2.13	127.56	124.20
24	2	314	KC1	CAA-C2A-C1A	-2.13	114.97	124.75
24	9	305	KC1	CMC-C2C-C1C	2.13	128.28	125.04
21	c	505	CLA	CED-O2D-CGD	2.13	120.75	115.94
21	A	402	CLA	C1D-CHD-C4C	-2.13	121.47	126.06
24	2	314	KC1	CMC-C2C-C1C	2.13	128.28	125.04
23	G	305	A86	C26-C25-C24	2.13	129.85	123.22
28	N	101	LMG	O1-C1-C2	-2.13	104.98	108.30
21	D	407	CLA	C3D-C4D-CHA	-2.13	107.86	112.72
21	B	605	CLA	CAC-C3C-C4C	2.12	127.57	124.81
24	6	313	KC1	CBD-CHA-C1A	2.12	132.84	128.88
21	1	301	CLA	CMD-C2D-C1D	2.12	128.46	124.71
23	6	310	A86	C19-C18-C17	2.12	114.87	110.77
32	E	101	HEM	C4A-C3A-C2A	2.12	108.47	107.00
28	b	625	LMG	O3-C3-C2	-2.12	105.44	110.35
21	b	609	CLA	C3D-C4D-CHA	-2.12	107.87	112.72
25	b	618	BCR	C40-C30-C25	2.12	113.74	110.30
21	6	308	CLA	CAC-C3C-C4C	2.12	127.56	124.81
28	A	407	LMG	O2-C2-C1	-2.12	104.89	110.05
21	B	606	CLA	C1D-CHD-C4C	-2.12	121.48	126.06
32	f	101	HEM	CMB-C2B-C1B	-2.12	121.81	125.04
21	2	304	CLA	CED-O2D-CGD	2.12	120.74	115.94
21	2	304	CLA	CMD-C2D-C1D	2.12	128.45	124.71
21	B	610	CLA	C1D-CHD-C4C	-2.12	121.48	126.06
21	B	607	CLA	CMD-C2D-C1D	2.12	128.45	124.71
21	1	310	CLA	CMD-C2D-C1D	2.12	128.45	124.71
30	b	601	DGD	CAB-C9B-C8B	-2.12	103.66	114.42
21	1	304	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
21	B	605	CLA	CHB-C4A-NA	2.12	127.44	124.51
21	b	616	CLA	CHB-C4A-NA	2.12	127.44	124.51
21	C	511	CLA	C3B-C4B-NB	2.12	111.95	109.21
21	B	606	CLA	C1-C2-C3	-2.12	122.38	126.04
30	B	624	DGD	CAB-C9B-C8B	-2.12	103.67	114.42
21	2	304	CLA	C4C-C3C-C2C	-2.12	103.81	106.90
21	g	309	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
28	f	102	LMG	O2-C2-C1	-2.12	104.90	110.05
21	c	507	CLA	C3D-C4D-CHA	-2.12	107.88	112.72
24	3	305	KC1	CED-O2D-CGD	2.12	120.72	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	403	CLA	C3D-C4D-CHA	-2.12	107.88	112.72
21	7	306	CLA	CED-O2D-CGD	2.12	120.72	115.94
28	B	619	LMG	O3-C3-C2	-2.11	105.46	110.35
21	c	510	CLA	CAC-C3C-C4C	2.11	127.55	124.81
21	8	302	CLA	C4C-C3C-C2C	-2.11	103.82	106.90
23	J	309	A86	C17-C16-C15	2.11	111.32	109.16
26	A	403	PHO	CMC-C2C-C3C	2.11	128.93	124.94
21	b	607	CLA	C1D-CHD-C4C	-2.11	121.50	126.06
21	g	307	CLA	C3D-C4D-CHA	-2.11	107.89	112.72
21	6	305	CLA	CED-O2D-CGD	2.11	120.71	115.94
25	h	102	BCR	C11-C10-C9	-2.11	124.30	127.31
23	1	312	A86	C26-C25-C24	2.11	129.81	123.22
21	8	307	CLA	C3D-C4D-CHA	-2.11	107.89	112.72
25	A	405	BCR	C33-C5-C6	-2.11	122.16	124.53
21	c	502	CLA	C3D-C4D-CHA	-2.11	107.89	112.72
27	a	401	LHG	C27-C26-C25	-2.11	103.71	114.42
28	L	101	LMG	O3-C3-C2	-2.11	105.47	110.35
21	c	506	CLA	O2A-CGA-CBA	2.11	118.53	111.91
21	c	513	CLA	CBA-CAA-C2A	-2.11	107.63	113.86
28	D	411	LMG	O2-C2-C1	-2.11	104.92	110.05
21	1	309	CLA	CHD-C1D-ND	-2.11	122.52	124.45
21	g	305	CLA	C3D-C4D-CHA	-2.11	107.90	112.72
24	2	315	KC1	CHB-C1B-C2B	-2.11	121.06	125.48
26	A	403	PHO	O2A-CGA-O1A	-2.11	118.27	123.59
21	5	307	CLA	C3D-C4D-CHA	-2.11	107.90	112.72
21	b	613	CLA	C1-C2-C3	-2.11	122.39	126.04
21	a	405	CLA	C3D-C4D-CHA	-2.11	107.90	112.72
21	C	510	CLA	C1D-CHD-C4C	-2.11	121.51	126.06
28	b	625	LMG	O6-C1-O1	-2.11	104.98	109.97
28	N	101	LMG	O2-C2-C1	-2.11	104.92	110.05
21	1	309	CLA	C1-O2A-CGA	2.11	121.98	116.44
25	h	102	BCR	C24-C23-C22	-2.11	123.05	126.23
24	6	312	KC1	CHB-C1B-NB	-2.11	122.52	124.45
24	9	305	KC1	CHB-C4A-NA	2.11	127.53	124.20
21	C	510	CLA	C1-C2-C3	-2.11	122.40	126.04
28	B	620	LMG	O3-C3-C2	-2.11	105.48	110.35
28	M	102	LMG	O3-C3-C2	-2.11	105.48	110.35
21	8	305	CLA	C4C-C3C-C2C	-2.11	103.83	106.90
26	d	403	PHO	CMC-C2C-C3C	2.11	128.91	124.94
30	C	518	DGD	O5D-C6D-C5D	-2.11	105.15	109.05
21	1	302	CLA	CHB-C4A-NA	2.11	127.42	124.51
21	1	307	CLA	C3D-C4D-CHA	-2.11	107.91	112.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c	506	CLA	CHB-C4A-NA	2.10	127.42	124.51
28	8	301	LMG	O1-C7-C8	-2.10	104.73	108.76
24	G	308	KC1	O2D-CGD-O1D	-2.10	119.72	123.84
26	a	404	PHO	C1B-NB-C4B	2.10	111.41	107.09
26	D	401	PHO	C1B-NB-C4B	2.10	111.41	107.09
21	3	303	CLA	CHD-C4C-NC	2.10	127.52	124.20
21	b	609	CLA	CMC-C2C-C1C	2.10	128.24	125.04
21	2	305	CLA	C3D-C4D-CHA	-2.10	107.91	112.72
21	5	302	CLA	C1-C2-C3	-2.10	122.41	126.04
26	d	403	PHO	C1B-NB-C4B	2.10	111.41	107.09
21	3	302	CLA	CAC-C3C-C4C	2.10	127.54	124.81
24	8	316	KC1	O2D-CGD-O1D	-2.10	119.73	123.84
28	b	626	LMG	O1-C1-C2	-2.10	105.02	108.30
21	1	310	CLA	C3D-C4D-CHA	-2.10	107.92	112.72
21	4	303	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
21	7	303	CLA	C1D-CHD-C4C	-2.10	121.53	126.06
21	9	303	CLA	CMD-C2D-C1D	2.10	128.41	124.71
23	J	310	A86	C19-C18-C17	2.10	114.83	110.77
24	5	313	KC1	CED-O2D-CGD	2.10	120.69	115.94
24	2	316	KC1	CHB-C4A-NA	2.10	127.51	124.20
35	d	408	PL9	C40-C39-C41	2.10	118.80	115.27
28	M	102	LMG	O2-C2-C1	-2.10	104.95	110.05
25	B	618	BCR	C37-C22-C21	-2.10	119.98	122.92
21	g	307	CLA	C1D-CHD-C4C	-2.10	121.53	126.06
24	8	314	KC1	O1D-CGD-CBD	-2.10	120.19	124.48
26	a	404	PHO	C1-C2-C3	-2.10	122.42	126.04
21	J	305	CLA	C3D-C4D-CHA	-2.10	107.93	112.72
21	8	305	CLA	CAA-C2A-C3A	-2.10	111.21	116.10
21	g	309	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
21	B	621	CLA	C3B-C4B-NB	2.10	111.92	109.21
21	C	507	CLA	O2A-CGA-CBA	2.10	118.48	111.91
21	b	611	CLA	C1D-CHD-C4C	-2.10	121.54	126.06
21	A	402	CLA	C3D-C4D-CHA	-2.09	107.93	112.72
24	2	315	KC1	CMC-C2C-C1C	2.09	128.23	125.04
24	G	306	KC1	O2D-CGD-O1D	-2.09	119.74	123.84
21	6	304	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
21	8	305	CLA	C3D-C4D-CHA	-2.09	107.93	112.72
21	d	404	CLA	C3D-C4D-CHA	-2.09	107.93	112.72
28	A	407	LMG	O1-C7-C8	-2.09	105.85	110.90
21	d	404	CLA	CED-O2D-CGD	2.09	120.67	115.94
21	J	305	CLA	CED-O2D-CGD	2.09	120.67	115.94
21	5	306	CLA	CED-O2D-CGD	2.09	120.67	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	103	DGD	CBB-CAB-C9B	-2.09	103.81	114.42
28	L	101	LMG	O7-C10-O9	-2.09	118.65	123.70
21	B	615	CLA	C6-C5-C3	-2.09	107.97	113.45
21	6	305	CLA	C3D-C4D-CHA	-2.09	107.94	112.72
21	B	610	CLA	CMC-C2C-C1C	2.09	128.22	125.04
21	b	615	CLA	C3B-C4B-NB	2.09	111.91	109.21
21	6	306	CLA	CBA-CAA-C2A	2.09	120.03	113.86
21	c	507	CLA	CHD-C4C-NC	2.09	127.50	124.20
30	H	101	DGD	O5D-C6D-C5D	-2.09	105.18	109.05
21	b	604	CLA	O2A-CGA-CBA	2.09	118.46	111.91
21	7	306	CLA	C3D-C4D-CHA	-2.09	107.94	112.72
26	D	401	PHO	CMC-C2C-C3C	2.09	128.88	124.94
24	4	309	KC1	CBC-CAC-C3C	-2.09	106.67	112.43
24	2	314	KC1	CHB-C4A-NA	2.09	127.49	124.20
21	5	308	CLA	O2A-CGA-CBA	2.09	118.46	111.91
21	J	306	CLA	C1D-CHD-C4C	-2.09	121.55	126.06
21	B	611	CLA	C3D-C4D-CHA	-2.09	107.95	112.72
21	d	406	CLA	C3D-C4D-CHA	-2.09	107.95	112.72
21	c	510	CLA	C3B-C4B-NB	2.09	111.91	109.21
25	H	100	BCR	C28-C27-C26	-2.09	110.35	114.08
21	7	306	CLA	CMA-C3A-C2A	-2.09	111.23	116.10
21	6	307	CLA	CAC-C3C-C4C	2.09	127.52	124.81
32	E	101	HEM	CAA-CBA-CGA	-2.09	107.91	113.76
29	5	301	LMU	O1'-C1'-C2'	2.08	111.56	108.30
24	g	314	KC1	C2A-C1A-CHA	-2.08	120.55	127.44
21	2	303	CLA	C4-C3-C2	-2.08	118.33	123.68
21	2	301	CLA	C1D-CHD-C4C	-2.08	121.56	126.06
21	b	608	CLA	C6-C5-C3	-2.08	107.99	113.45
35	d	408	PL9	C31-C32-C33	-2.08	105.04	111.88
21	B	612	CLA	C1D-CHD-C4C	-2.08	121.57	126.06
24	J	311	KC1	CBD-CHA-C1A	2.08	132.76	128.88
21	5	302	CLA	C3D-C4D-CHA	-2.08	107.96	112.72
30	h	103	DGD	O5D-C6D-C5D	-2.08	105.20	109.05
21	g	308	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
21	1	304	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
24	5	313	KC1	CHB-C4A-NA	2.08	127.48	124.20
21	8	304	CLA	C3D-C4D-CHA	-2.08	107.97	112.72
21	6	305	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
23	g	312	A86	C34-O4-C38	2.08	121.77	117.90
28	N	101	LMG	O1-C7-C8	-2.08	104.78	108.76
21	B	606	CLA	C3D-C4D-CHA	-2.08	107.97	112.72
21	7	301	CLA	CHB-C4A-NA	2.08	127.39	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	c	508	CLA	C3B-C4B-NB	2.08	111.90	109.21
21	B	608	CLA	CMC-C2C-C1C	2.08	128.20	125.04
25	c	501	BCR	C27-C26-C25	2.08	125.75	122.73
21	1	304	CLA	C3D-C4D-CHA	-2.08	107.97	112.72
24	G	308	KC1	CHB-C1B-C2B	-2.08	121.12	125.48
21	7	309	CLA	C3D-C4D-CHA	-2.08	107.97	112.72
21	5	302	CLA	C6-C5-C3	-2.08	108.01	113.45
21	B	615	CLA	CMC-C2C-C1C	2.08	128.20	125.04
21	g	305	CLA	CAA-C2A-C3A	-2.08	111.25	116.10
21	5	305	CLA	C1D-CHD-C4C	-2.08	121.58	126.06
21	7	301	CLA	C3B-C4B-NB	2.08	111.89	109.21
25	a	406	BCR	C33-C5-C6	-2.08	122.20	124.53
24	g	314	KC1	CHB-C4A-NA	2.08	127.48	124.20
24	5	313	KC1	O2A-CGA-O1A	-2.08	118.36	122.67
21	g	308	CLA	C3D-C4D-CHA	-2.08	107.97	112.72
31	C	502	SQD	O6-C1-C2	2.08	111.54	108.30
21	G	304	CLA	CED-O2D-CGD	2.08	120.63	115.94
21	1	305	CLA	C1-C2-C3	-2.08	122.45	126.04
21	3	302	CLA	C3C-C4C-NC	2.07	112.90	110.57
21	b	604	CLA	C3D-C4D-CHA	-2.07	107.98	112.72
25	C	516	BCR	C20-C21-C22	-2.07	124.35	127.31
21	B	609	CLA	CMB-C2B-C3B	2.07	128.56	124.68
21	5	306	CLA	C3B-C4B-NB	2.07	111.89	109.21
24	8	314	KC1	CAA-C2A-C1A	-2.07	115.21	124.75
21	2	304	CLA	C3D-C4D-CHA	-2.07	107.98	112.72
24	G	306	KC1	CHB-C4A-NA	2.07	127.47	124.20
30	B	624	DGD	O3G-C1D-C2D	-2.07	105.07	108.30
21	6	301	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
21	A	404	CLA	C3D-C4D-CHA	-2.07	107.98	112.72
21	7	303	CLA	CHC-C1C-NC	-2.07	121.06	124.20
21	c	506	CLA	C1-C2-C3	-2.07	122.46	126.04
21	b	616	CLA	CMC-C2C-C1C	2.07	128.19	125.04
21	c	510	CLA	CHC-C1C-NC	-2.07	121.06	124.20
24	3	306	KC1	CHB-C4A-NA	2.07	127.47	124.20
21	J	301	CLA	C1D-CHD-C4C	-2.07	121.59	126.06
21	6	301	CLA	CMD-C2D-C1D	2.07	128.36	124.71
26	A	403	PHO	C1B-NB-C4B	2.07	111.34	107.09
21	C	507	CLA	C1-C2-C3	-2.07	122.47	126.04
21	1	301	CLA	C1D-CHD-C4C	-2.07	121.59	126.06
21	G	300	CLA	C6-C7-C8	-2.07	109.23	115.92
21	C	509	CLA	C3B-C4B-NB	2.07	111.88	109.21
21	5	309	CLA	CHC-C1C-NC	-2.07	121.07	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	615	CLA	CHB-C4A-NA	2.07	127.37	124.51
21	D	404	CLA	C1D-CHD-C4C	-2.07	121.60	126.06
21	c	512	CLA	C3D-C4D-CHA	-2.07	108.00	112.72
21	8	305	CLA	CMA-C3A-C2A	-2.07	111.28	116.10
22	7	310	DD6	O1-C20-C19	-2.06	111.83	113.38
24	G	306	KC1	CED-O2D-CGD	2.06	120.61	115.94
21	7	304	CLA	C3D-C4D-CHA	-2.06	108.00	112.72
21	C	511	CLA	C3D-C4D-CHA	-2.06	108.00	112.72
21	2	302	CLA	CMB-C2B-C3B	2.06	128.54	124.68
23	5	312	A86	C19-C18-C17	2.06	114.76	110.77
25	b	618	BCR	C30-C25-C26	-2.06	119.71	122.61
25	C	516	BCR	C27-C26-C25	2.06	125.72	122.73
21	c	507	CLA	C3B-C4B-NB	2.06	111.88	109.21
21	B	607	CLA	C6-C5-C3	-2.06	108.05	113.45
28	b	626	LMG	O7-C10-O9	-2.06	118.72	123.70
21	B	603	CLA	CAC-C3C-C4C	2.06	127.48	124.81
23	g	312	A86	C23-C16-C17	-2.06	105.40	108.98
21	5	304	CLA	C1D-CHD-C4C	-2.06	121.61	126.06
24	7	315	KC1	CHB-C1B-NB	-2.06	122.56	124.45
21	b	617	CLA	C3C-C4C-NC	2.06	112.88	110.57
21	b	607	CLA	C3D-C4D-CHA	-2.06	108.01	112.72
23	2	311	A86	C26-C25-C24	2.06	129.64	123.22
21	b	605	CLA	C3D-C4D-CHA	-2.06	108.01	112.72
21	7	306	CLA	C4C-C3C-C2C	-2.06	103.90	106.90
24	2	314	KC1	CHB-C1B-C2B	-2.06	121.16	125.48
24	g	315	KC1	CHB-C4A-NA	2.06	127.45	124.20
23	2	312	A86	C23-C16-C17	-2.06	105.41	108.98
21	B	621	CLA	O2A-CGA-CBA	2.06	118.37	111.91
25	h	102	BCR	C27-C26-C25	2.06	125.72	122.73
21	7	309	CLA	CED-O2D-CGD	2.06	120.59	115.94
21	B	605	CLA	C3D-C4D-CHA	-2.06	108.02	112.72
21	b	616	CLA	C6-C5-C3	-2.06	108.06	113.45
23	8	310	A86	C23-C16-C17	-2.06	105.41	108.98
21	J	308	CLA	C3D-C4D-CHA	-2.06	108.02	112.72
21	C	503	CLA	O2A-CGA-CBA	2.06	118.36	111.91
21	c	509	CLA	C6-C5-C3	-2.05	108.07	113.45
21	B	609	CLA	C3D-C4D-CHA	-2.05	108.02	112.72
25	A	405	BCR	C15-C16-C17	-2.05	119.27	123.47
21	5	309	CLA	C2A-C1A-CHA	2.05	127.45	123.86
21	C	512	CLA	C3B-C4B-NB	2.05	111.86	109.21
21	5	303	CLA	C1-O2A-CGA	2.05	121.83	116.44
21	g	307	CLA	O2A-CGA-CBA	2.05	120.34	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1	305	CLA	CED-O2D-CGD	2.05	120.58	115.94
25	a	406	BCR	C11-C10-C9	-2.05	124.38	127.31
21	7	307	CLA	C3D-C4D-CHA	-2.05	108.03	112.72
21	B	612	CLA	C4C-C3C-C2C	-2.05	103.91	106.90
21	C	512	CLA	CED-O2D-CGD	2.05	120.58	115.94
24	4	309	KC1	CHB-C4A-NA	2.05	127.44	124.20
30	H	101	DGD	C5B-C4B-C3B	-2.05	104.01	114.42
21	1	307	CLA	CMA-C3A-C2A	-2.05	111.31	116.10
21	C	505	CLA	CHB-C4A-NA	2.05	127.35	124.51
28	b	620	LMG	O7-C10-O9	-2.05	118.74	123.70
28	b	620	LMG	O2-C2-C1	-2.05	105.06	110.05
21	g	305	CLA	C1D-CHD-C4C	-2.05	121.63	126.06
21	c	510	CLA	C3D-C4D-CHA	-2.05	108.03	112.72
21	2	306	CLA	CHB-C4A-NA	2.05	127.35	124.51
21	C	510	CLA	C1-O2A-CGA	2.05	121.82	116.44
21	a	403	CLA	C3B-C4B-NB	2.05	111.86	109.21
21	C	503	CLA	C3D-C4D-CHA	-2.05	108.03	112.72
25	D	408	BCR	C16-C15-C14	-2.05	119.28	123.47
24	7	314	KC1	O1D-CGD-CBD	-2.05	120.29	124.48
25	h	101	BCR	C35-C13-C14	-2.05	120.05	122.92
21	5	304	CLA	C3D-C4D-CHA	-2.05	108.04	112.72
21	1	303	CLA	C1-C2-C3	-2.05	122.50	126.04
21	g	303	CLA	C3B-C4B-NB	2.05	111.86	109.21
21	1	305	CLA	C3D-C4D-CHA	-2.05	108.04	112.72
21	B	604	CLA	C3D-C4D-CHA	-2.05	108.04	112.72
24	2	313	KC1	CHB-C4A-NA	2.05	127.43	124.20
21	J	306	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
21	G	304	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
24	1	315	KC1	O2D-CGD-O1D	-2.05	119.84	123.84
21	3	302	CLA	CMC-C2C-C1C	2.05	128.16	125.04
21	4	302	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
28	a	407	LMG	O3-C3-C2	-2.05	105.62	110.35
24	5	314	KC1	CHB-C1B-C2B	-2.04	121.19	125.48
21	b	610	CLA	C3D-C4D-CHA	-2.04	108.05	112.72
23	4	305	A86	C23-C16-C17	-2.04	105.43	108.98
21	C	509	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
24	3	305	KC1	C2A-C1A-CHA	-2.04	120.68	127.44
21	b	616	CLA	C3B-C4B-NB	2.04	111.85	109.21
21	b	609	CLA	CED-O2D-CGD	2.04	120.56	115.94
21	7	305	CLA	C3D-C4D-CHA	-2.04	108.05	112.72
24	2	316	KC1	O2D-CGD-O1D	-2.04	119.84	123.84
21	G	303	CLA	C3D-C4D-CHA	-2.04	108.05	112.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	7	311	A86	C17-C16-C15	2.04	111.25	109.16
21	B	615	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
21	1	309	CLA	CED-O2D-CGD	2.04	120.56	115.94
24	6	311	KC1	CBD-CHA-C1A	2.04	132.69	128.88
21	b	623	CLA	C3B-C4B-NB	2.04	111.85	109.21
28	8	317	LMG	O7-C10-O9	-2.04	118.77	123.70
28	f	102	LMG	O1-C1-C2	-2.04	105.12	108.30
21	B	609	CLA	CAC-C3C-C4C	2.04	127.46	124.81
21	D	404	CLA	C3D-C4D-CHA	-2.04	108.06	112.72
24	6	312	KC1	CHB-C4A-NA	2.04	127.42	124.20
30	H	101	DGD	CBB-CAB-C9B	-2.04	104.07	114.42
21	7	309	CLA	C3B-C4B-NB	2.04	111.85	109.21
21	6	308	CLA	O2A-CGA-CBA	2.04	118.31	111.91
25	c	501	BCR	C11-C10-C9	-2.04	124.40	127.31
25	B	617	BCR	C40-C30-C25	2.04	113.61	110.30
21	3	304	CLA	C3D-C4D-CHA	-2.04	108.06	112.72
21	c	504	CLA	C1D-CHD-C4C	-2.04	121.66	126.06
21	5	309	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
35	d	408	PL9	O2-C1-C2	-2.04	117.11	121.78
28	b	620	LMG	O3-C3-C2	-2.04	105.64	110.35
23	8	311	A86	C23-C16-C17	-2.04	105.44	108.98
21	J	307	CLA	C4-C3-C5	2.04	118.70	115.27
21	A	402	CLA	C3B-C4B-NB	2.04	111.84	109.21
21	J	301	CLA	C3D-C4D-CHA	-2.04	108.07	112.72
21	A	404	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
21	6	307	CLA	C4-C3-C5	2.03	118.69	115.27
21	3	302	CLA	C1D-CHD-C4C	-2.03	121.67	126.06
25	d	407	BCR	C24-C23-C22	-2.03	123.16	126.23
24	5	314	KC1	CMC-C2C-C1C	2.03	128.14	125.04
21	b	606	CLA	C3D-C4D-CHA	-2.03	108.07	112.72
21	7	308	CLA	CED-O2D-CGD	2.03	120.54	115.94
21	C	510	CLA	C3D-C4D-CHA	-2.03	108.07	112.72
24	G	309	KC1	O1D-CGD-CBD	-2.03	120.32	124.48
21	J	303	CLA	CMB-C2B-C3B	2.03	128.65	124.93
21	2	301	CLA	O2A-C1-C2	2.03	113.98	108.64
21	c	511	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
21	2	301	CLA	CMD-C2D-C1D	2.03	128.29	124.71
21	B	613	CLA	C3D-C4D-CHA	-2.03	108.08	112.72
21	D	404	CLA	CMC-C2C-C3C	2.03	131.63	126.12
28	L	101	LMG	C1-C2-C3	-2.03	105.77	110.00
21	C	507	CLA	C4C-C3C-C2C	-2.03	103.94	106.90
21	b	610	CLA	CMB-C2B-C3B	2.03	128.47	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	M	102	LMG	O7-C10-O9	-2.03	118.80	123.70
21	B	608	CLA	CED-O2D-CGD	2.03	120.53	115.94
24	8	316	KC1	O2A-CGA-O1A	-2.03	118.46	122.67
21	B	613	CLA	C1-O2A-CGA	2.03	121.77	116.44
25	A	405	BCR	C15-C14-C13	-2.03	124.42	127.31
21	B	607	CLA	C3D-C4D-CHA	-2.03	108.09	112.72
21	C	508	CLA	CMC-C2C-C1C	2.03	128.12	125.04
21	b	603	CLA	CHB-C4A-NA	2.03	127.31	124.51
21	1	304	CLA	CED-O2D-CGD	2.03	120.52	115.94
21	b	613	CLA	C1D-CHD-C4C	-2.03	121.69	126.06
24	9	306	KC1	O1D-CGD-CBD	-2.03	120.34	124.48
21	8	306	CLA	C3D-C4D-CHA	-2.03	108.09	112.72
23	g	312	A86	C40-C32-C31	2.02	112.28	110.47
21	B	610	CLA	CAC-C3C-C4C	2.02	127.44	124.81
21	J	303	CLA	C3D-C4D-CHA	-2.02	108.09	112.72
24	J	312	KC1	CHB-C4A-NA	2.02	127.39	124.20
21	5	304	CLA	CMD-C2D-C1D	2.02	128.28	124.71
21	5	306	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
21	6	307	CLA	CAA-CBA-CGA	-2.02	107.34	113.25
21	D	406	CLA	CMD-C2D-C1D	2.02	128.28	124.71
24	2	315	KC1	CHC-C1C-NC	2.02	127.39	124.20
21	c	502	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
28	B	623	LMG	O1-C1-C2	-2.02	105.14	108.30
21	b	614	CLA	C3D-C4D-CHA	-2.02	108.10	112.72
22	g	310	DD6	C15-C14-C13	2.02	130.27	125.99
21	7	304	CLA	CAC-C3C-C2C	2.02	130.99	127.53
21	C	513	CLA	C3D-C4D-CHA	-2.02	108.10	112.72
21	8	302	CLA	CAC-C3C-C4C	2.02	127.43	124.81
30	h	103	DGD	C5B-C4B-C3B	-2.02	104.17	114.42
21	B	615	CLA	C3B-C4B-NB	2.02	111.82	109.21
30	c	516	DGD	O6E-C5E-C4E	2.02	113.36	109.69
21	2	303	CLA	C3D-C4D-CHA	-2.02	108.10	112.72
21	B	614	CLA	C3B-C4B-NB	2.02	111.82	109.21
25	b	619	BCR	C30-C25-C26	-2.02	119.77	122.61
28	M	102	LMG	C1-C2-C3	-2.02	105.79	110.00
21	3	301	CLA	C3D-C4D-CHA	-2.02	108.10	112.72
21	g	307	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
21	J	304	CLA	CED-O2D-CGD	2.02	120.50	115.94
21	1	301	CLA	C3D-C4D-CHA	-2.02	108.11	112.72
21	b	603	CLA	C3D-C4D-CHA	-2.02	108.11	112.72
24	1	315	KC1	CHB-C4A-NA	2.02	127.38	124.20
21	c	505	CLA	C1-O2A-CGA	2.02	121.74	116.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	b	610	CLA	CAC-C3C-C4C	2.02	127.43	124.81
24	8	313	KC1	CHB-C4A-NA	2.02	127.38	124.20
21	b	605	CLA	C3B-C4B-NB	2.02	111.82	109.21
24	J	311	KC1	C2A-C1A-CHA	-2.02	120.78	127.44
35	D	409	PL9	O2-C1-C2	-2.02	117.16	121.78
21	B	602	CLA	CHB-C4A-NA	2.02	127.30	124.51
24	5	314	KC1	CBC-CAC-C3C	-2.01	106.88	112.43
21	4	304	CLA	CED-O2D-CGD	2.01	120.49	115.94
21	J	308	CLA	O2A-CGA-CBA	2.01	118.23	111.91
21	7	302	CLA	CAC-C3C-C4C	2.01	127.42	124.81
21	b	613	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
21	4	301	CLA	CAC-C3C-C4C	2.01	127.42	124.81
24	G	308	KC1	CBC-CAC-C3C	-2.01	106.89	112.43
21	b	608	CLA	C3D-C4D-CHA	-2.01	108.12	112.72
21	c	503	CLA	C3B-C4B-NB	2.01	111.81	109.21
21	C	512	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
21	4	303	CLA	C3D-C4D-CHA	-2.01	108.12	112.72
21	3	301	CLA	CAC-C3C-C4C	2.01	127.42	124.81
24	2	313	KC1	CBD-CHA-C1A	2.01	132.63	128.88
21	7	300	CLA	C3D-C4D-CHA	-2.01	108.12	112.72
21	c	502	CLA	O2A-CGA-CBA	2.01	118.21	111.91
21	2	301	CLA	C3B-C4B-NB	2.01	111.81	109.21
21	7	302	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
21	a	403	CLA	CHC-C1C-NC	-2.01	121.16	124.20
28	2	318	LMG	O1-C7-C8	-2.01	106.05	110.90
24	7	314	KC1	CHB-C4A-NA	2.01	127.37	124.20
26	D	401	PHO	C1-C2-C3	-2.01	122.57	126.04
22	5	310	DD6	C15-C14-C13	2.01	130.23	125.99
24	4	307	KC1	CMC-C2C-C1C	2.00	128.09	125.04
21	J	303	CLA	C1D-CHD-C4C	-2.00	121.73	126.06
21	5	302	CLA	C3B-C4B-NB	2.00	111.80	109.21
28	b	625	LMG	O2-C2-C1	-2.00	105.18	110.05
24	8	314	KC1	CHB-C1B-NB	-2.00	122.61	124.45
21	J	308	CLA	CAC-C3C-C4C	2.00	127.41	124.81
21	d	405	CLA	CMD-C2D-C1D	2.00	128.24	124.71
21	9	302	CLA	C3D-C4D-CHA	-2.00	108.14	112.72
21	b	617	CLA	CMD-C2D-C1D	2.00	128.24	124.71
21	6	304	CLA	C3B-C4B-NB	2.00	111.80	109.21
21	5	302	CLA	CED-O2D-CGD	2.00	120.46	115.94
21	G	304	CLA	C3D-C4D-CHA	-2.00	108.14	112.72
21	g	306	CLA	C4C-C3C-C2C	-2.00	103.98	106.90
29	5	301	LMU	O5B-C1B-C2B	2.00	114.58	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	314	KC1	O1D-CGD-CBD	-2.00	120.39	124.48
23	J	310	A86	C20-C19-C18	2.00	116.71	112.75

All (101) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	1	301	CLA	ND
21	1	302	CLA	ND
21	1	303	CLA	ND
21	1	304	CLA	ND
21	1	306	CLA	ND
21	1	307	CLA	ND
21	1	309	CLA	ND
21	6	300	CLA	ND
21	6	301	CLA	ND
21	6	302	CLA	ND
21	6	303	CLA	ND
21	6	304	CLA	ND
21	6	305	CLA	ND
21	6	306	CLA	ND
21	6	307	CLA	ND
21	6	308	CLA	ND
21	7	300	CLA	ND
21	7	301	CLA	ND
21	7	302	CLA	ND
21	7	303	CLA	ND
21	7	304	CLA	ND
21	7	305	CLA	ND
21	7	306	CLA	ND
21	7	307	CLA	ND
21	7	308	CLA	ND
21	B	602	CLA	ND
21	B	603	CLA	ND
21	B	604	CLA	ND
21	B	610	CLA	ND
21	B	612	CLA	ND
21	B	613	CLA	ND
21	B	614	CLA	ND
21	B	615	CLA	ND
21	B	616	CLA	ND
21	J	300	CLA	ND
21	J	301	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	J	302	CLA	ND
21	J	304	CLA	ND
21	J	305	CLA	ND
21	J	306	CLA	ND
21	J	307	CLA	ND
21	J	308	CLA	ND
21	b	603	CLA	ND
21	b	604	CLA	ND
21	b	605	CLA	ND
21	b	611	CLA	ND
21	b	613	CLA	ND
21	b	614	CLA	ND
21	b	615	CLA	ND
21	b	616	CLA	ND
21	b	617	CLA	ND
21	b	623	CLA	ND
21	2	301	CLA	ND
21	2	302	CLA	ND
21	2	303	CLA	ND
21	2	305	CLA	ND
21	8	302	CLA	ND
21	8	303	CLA	ND
21	8	306	CLA	ND
21	8	307	CLA	ND
21	D	404	CLA	ND
21	D	406	CLA	ND
21	d	404	CLA	ND
21	d	405	CLA	ND
21	C	503	CLA	ND
21	C	508	CLA	ND
21	C	509	CLA	ND
21	C	511	CLA	ND
21	C	512	CLA	ND
21	C	514	CLA	ND
21	c	502	CLA	ND
21	c	507	CLA	ND
21	c	508	CLA	ND
21	c	510	CLA	ND
21	c	511	CLA	ND
21	c	512	CLA	ND
21	c	513	CLA	ND
21	9	300	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	9	302	CLA	ND
21	9	303	CLA	ND
21	9	304	CLA	ND
21	3	301	CLA	ND
21	3	302	CLA	ND
21	4	300	CLA	ND
21	4	301	CLA	ND
21	4	303	CLA	ND
21	4	304	CLA	ND
21	5	302	CLA	ND
21	5	303	CLA	ND
21	5	305	CLA	ND
21	5	306	CLA	ND
21	5	309	CLA	ND
21	g	302	CLA	ND
21	g	303	CLA	ND
21	g	305	CLA	ND
21	g	306	CLA	ND
21	g	309	CLA	ND
21	G	300	CLA	ND
21	G	301	CLA	ND
21	G	303	CLA	ND
21	G	304	CLA	ND

All (3240) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1	301	CLA	CBD-CGD-O2D-CED
21	1	303	CLA	C1A-C2A-CAA-CBA
21	1	303	CLA	CBD-CGD-O2D-CED
21	1	303	CLA	O1D-CGD-O2D-CED
21	1	304	CLA	CBD-CGD-O2D-CED
21	1	304	CLA	O1D-CGD-O2D-CED
21	1	304	CLA	C2-C3-C5-C6
21	1	304	CLA	C4-C3-C5-C6
21	1	305	CLA	CHA-CBD-CGD-O2D
21	1	305	CLA	C2-C3-C5-C6
21	1	305	CLA	C4-C3-C5-C6
21	1	306	CLA	CBD-CGD-O2D-CED
21	1	307	CLA	CHA-CBD-CGD-O1D
21	1	307	CLA	CBD-CGD-O2D-CED
21	1	307	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	308	CLA	C1A-C2A-CAA-CBA
21	1	308	CLA	CBD-CGD-O2D-CED
21	1	309	CLA	CBD-CGD-O2D-CED
21	1	310	CLA	CBD-CGD-O2D-CED
21	1	310	CLA	O1D-CGD-O2D-CED
21	1	310	CLA	C2-C3-C5-C6
21	1	310	CLA	C4-C3-C5-C6
21	6	300	CLA	CBD-CGD-O2D-CED
21	6	301	CLA	CHA-CBD-CGD-O2D
21	6	301	CLA	CAD-CBD-CGD-O2D
21	6	301	CLA	CBD-CGD-O2D-CED
21	6	301	CLA	C2-C3-C5-C6
21	6	301	CLA	C4-C3-C5-C6
21	6	302	CLA	CHA-CBD-CGD-O2D
21	6	302	CLA	CBD-CGD-O2D-CED
21	6	303	CLA	C1A-C2A-CAA-CBA
21	6	303	CLA	CHA-CBD-CGD-O2D
21	6	304	CLA	CHA-CBD-CGD-O1D
21	6	304	CLA	CBD-CGD-O2D-CED
21	6	305	CLA	CBD-CGD-O2D-CED
21	6	306	CLA	C1A-C2A-CAA-CBA
21	6	306	CLA	CHA-CBD-CGD-O2D
21	6	306	CLA	CBD-CGD-O2D-CED
21	6	306	CLA	O1D-CGD-O2D-CED
21	6	307	CLA	C1A-C2A-CAA-CBA
21	6	307	CLA	C3A-C2A-CAA-CBA
21	6	307	CLA	CBD-CGD-O2D-CED
21	6	308	CLA	CHA-CBD-CGD-O1D
21	6	308	CLA	CAD-CBD-CGD-O1D
21	7	300	CLA	O1D-CGD-O2D-CED
21	7	301	CLA	CBD-CGD-O2D-CED
21	7	302	CLA	CBD-CGD-O2D-CED
21	7	303	CLA	C1A-C2A-CAA-CBA
21	7	303	CLA	C3A-C2A-CAA-CBA
21	7	303	CLA	CBD-CGD-O2D-CED
21	7	306	CLA	CHA-CBD-CGD-O1D
21	7	306	CLA	CBD-CGD-O2D-CED
21	7	306	CLA	O1D-CGD-O2D-CED
21	7	307	CLA	CBD-CGD-O2D-CED
21	7	307	CLA	O1D-CGD-O2D-CED
21	7	309	CLA	CHA-CBD-CGD-O2D
21	7	309	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	401	CLA	C1A-C2A-CAA-CBA
21	A	401	CLA	C3A-C2A-CAA-CBA
21	A	401	CLA	CBD-CGD-O2D-CED
21	A	404	CLA	CBD-CGD-O2D-CED
21	B	602	CLA	CHA-CBD-CGD-O1D
21	B	602	CLA	CAD-CBD-CGD-O1D
21	B	603	CLA	C1A-C2A-CAA-CBA
21	B	606	CLA	CBD-CGD-O2D-CED
21	B	608	CLA	CBD-CGD-O2D-CED
21	B	608	CLA	O1D-CGD-O2D-CED
21	B	609	CLA	CBD-CGD-O2D-CED
21	B	611	CLA	CHA-CBD-CGD-O2D
21	B	612	CLA	CHA-CBD-CGD-O1D
21	B	612	CLA	CBD-CGD-O2D-CED
21	B	613	CLA	CBD-CGD-O2D-CED
21	B	613	CLA	O1D-CGD-O2D-CED
21	B	614	CLA	CHA-CBD-CGD-O1D
21	B	614	CLA	CAD-CBD-CGD-O1D
21	B	616	CLA	O1D-CGD-O2D-CED
21	B	621	CLA	CHA-CBD-CGD-O2D
21	B	621	CLA	CAD-CBD-CGD-O2D
21	B	621	CLA	CBD-CGD-O2D-CED
21	J	300	CLA	CBD-CGD-O2D-CED
21	J	301	CLA	CHA-CBD-CGD-O2D
21	J	301	CLA	CAD-CBD-CGD-O2D
21	J	301	CLA	CBD-CGD-O2D-CED
21	J	301	CLA	C2-C3-C5-C6
21	J	301	CLA	C4-C3-C5-C6
21	J	302	CLA	CHA-CBD-CGD-O2D
21	J	302	CLA	CBD-CGD-O2D-CED
21	J	303	CLA	C1A-C2A-CAA-CBA
21	J	303	CLA	C3A-C2A-CAA-CBA
21	J	304	CLA	CBD-CGD-O2D-CED
21	J	304	CLA	O1D-CGD-O2D-CED
21	J	305	CLA	CBD-CGD-O2D-CED
21	J	306	CLA	C1A-C2A-CAA-CBA
21	J	306	CLA	CBD-CGD-O2D-CED
21	J	306	CLA	O1D-CGD-O2D-CED
21	J	307	CLA	C3A-C2A-CAA-CBA
21	J	307	CLA	CBD-CGD-O2D-CED
21	J	308	CLA	CHA-CBD-CGD-O1D
21	J	308	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	J	308	CLA	CBD-CGD-O2D-CED
21	a	402	CLA	O1A-CGA-O2A-C1
21	a	402	CLA	CBD-CGD-O2D-CED
21	a	405	CLA	CBD-CGD-O2D-CED
21	b	603	CLA	CHA-CBD-CGD-O1D
21	b	603	CLA	CAD-CBD-CGD-O1D
21	b	605	CLA	CHA-CBD-CGD-O2D
21	b	607	CLA	CBD-CGD-O2D-CED
21	b	609	CLA	CBD-CGD-O2D-CED
21	b	609	CLA	O1D-CGD-O2D-CED
21	b	610	CLA	CBD-CGD-O2D-CED
21	b	612	CLA	CBD-CGD-O2D-CED
21	b	613	CLA	CBD-CGD-O2D-CED
21	b	613	CLA	O1D-CGD-O2D-CED
21	b	614	CLA	CBD-CGD-O2D-CED
21	b	614	CLA	O1D-CGD-O2D-CED
21	b	615	CLA	CHA-CBD-CGD-O1D
21	b	617	CLA	C1A-C2A-CAA-CBA
21	b	617	CLA	C3A-C2A-CAA-CBA
21	b	617	CLA	CBD-CGD-O2D-CED
21	b	617	CLA	O1D-CGD-O2D-CED
21	b	617	CLA	C2-C3-C5-C6
21	b	617	CLA	C4-C3-C5-C6
21	b	623	CLA	CBD-CGD-O2D-CED
21	b	623	CLA	O1D-CGD-O2D-CED
21	2	301	CLA	C1A-C2A-CAA-CBA
21	2	301	CLA	CHA-CBD-CGD-O1D
21	2	303	CLA	CHA-CBD-CGD-O2D
21	2	303	CLA	C2-C3-C5-C6
21	2	303	CLA	C4-C3-C5-C6
21	2	304	CLA	CBD-CGD-O2D-CED
21	2	304	CLA	O1D-CGD-O2D-CED
21	2	305	CLA	C1A-C2A-CAA-CBA
21	2	305	CLA	O1D-CGD-O2D-CED
21	2	306	CLA	CHA-CBD-CGD-O2D
21	8	302	CLA	C1A-C2A-CAA-CBA
21	8	303	CLA	CBD-CGD-O2D-CED
21	8	304	CLA	CHA-CBD-CGD-O1D
21	8	304	CLA	C2-C3-C5-C6
21	8	305	CLA	CBD-CGD-O2D-CED
21	8	305	CLA	O1D-CGD-O2D-CED
21	8	306	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	8	307	CLA	CBD-CGD-O2D-CED
21	D	406	CLA	CBD-CGD-O2D-CED
21	D	407	CLA	C2-C3-C5-C6
21	D	407	CLA	C4-C3-C5-C6
21	d	404	CLA	CHA-CBD-CGD-O1D
21	d	404	CLA	CBD-CGD-O2D-CED
21	d	405	CLA	CBD-CGD-O2D-CED
21	C	503	CLA	CBD-CGD-O2D-CED
21	C	503	CLA	O1D-CGD-O2D-CED
21	C	504	CLA	CBD-CGD-O2D-CED
21	C	506	CLA	O1D-CGD-O2D-CED
21	C	507	CLA	CHA-CBD-CGD-O1D
21	C	509	CLA	CHA-CBD-CGD-O1D
21	C	510	CLA	CHA-CBD-CGD-O1D
21	C	512	CLA	CBD-CGD-O2D-CED
21	C	512	CLA	O1D-CGD-O2D-CED
21	C	513	CLA	CBD-CGD-O2D-CED
21	C	513	CLA	O1D-CGD-O2D-CED
21	C	514	CLA	C1A-C2A-CAA-CBA
21	C	514	CLA	C3A-C2A-CAA-CBA
21	C	515	CLA	CBD-CGD-O2D-CED
21	c	502	CLA	CAD-CBD-CGD-O1D
21	c	502	CLA	CAD-CBD-CGD-O2D
21	c	503	CLA	CHA-CBD-CGD-O2D
21	c	503	CLA	CBD-CGD-O2D-CED
21	c	504	CLA	CBD-CGD-O2D-CED
21	c	505	CLA	O1D-CGD-O2D-CED
21	c	506	CLA	CHA-CBD-CGD-O1D
21	c	508	CLA	CHA-CBD-CGD-O1D
21	c	509	CLA	CHA-CBD-CGD-O1D
21	c	509	CLA	CBD-CGD-O2D-CED
21	c	511	CLA	CBD-CGD-O2D-CED
21	c	512	CLA	CBD-CGD-O2D-CED
21	c	512	CLA	O1D-CGD-O2D-CED
21	c	514	CLA	CBD-CGD-O2D-CED
21	9	300	CLA	CHA-CBD-CGD-O2D
21	9	300	CLA	CBD-CGD-O2D-CED
21	9	300	CLA	O1D-CGD-O2D-CED
21	9	302	CLA	CHA-CBD-CGD-O1D
21	9	302	CLA	CBD-CGD-O2D-CED
21	9	303	CLA	C1A-C2A-CAA-CBA
21	9	303	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	9	303	CLA	O1A-CGA-O2A-C1
21	9	303	CLA	CBD-CGD-O2D-CED
21	9	303	CLA	O1D-CGD-O2D-CED
21	9	303	CLA	C2-C3-C5-C6
21	9	303	CLA	C4-C3-C5-C6
21	9	304	CLA	CBD-CGD-O2D-CED
21	3	300	CLA	CHA-CBD-CGD-O2D
21	3	300	CLA	CBD-CGD-O2D-CED
21	3	300	CLA	O1D-CGD-O2D-CED
21	3	301	CLA	CHA-CBD-CGD-O1D
21	3	301	CLA	CAD-CBD-CGD-O1D
21	3	302	CLA	C1A-C2A-CAA-CBA
21	3	302	CLA	CBD-CGD-O2D-CED
21	3	303	CLA	CBD-CGD-O2D-CED
21	3	304	CLA	CHA-CBD-CGD-O2D
21	3	304	CLA	CBD-CGD-O2D-CED
21	3	304	CLA	O1D-CGD-O2D-CED
21	3	304	CLA	C2-C3-C5-C6
21	3	304	CLA	C4-C3-C5-C6
21	4	300	CLA	C1A-C2A-CAA-CBA
21	4	300	CLA	C3A-C2A-CAA-CBA
21	4	300	CLA	CHA-CBD-CGD-O1D
21	4	300	CLA	CBD-CGD-O2D-CED
21	4	301	CLA	C2-C3-C5-C6
21	4	301	CLA	C4-C3-C5-C6
21	4	302	CLA	C1A-C2A-CAA-CBA
21	4	302	CLA	C3A-C2A-CAA-CBA
21	4	302	CLA	CHA-CBD-CGD-O1D
21	4	302	CLA	CAD-CBD-CGD-O1D
21	4	303	CLA	CBD-CGD-O2D-CED
21	4	303	CLA	O1D-CGD-O2D-CED
21	4	304	CLA	CBD-CGD-O2D-CED
21	4	304	CLA	O1D-CGD-O2D-CED
21	5	302	CLA	CHA-CBD-CGD-O2D
21	5	302	CLA	CBD-CGD-O2D-CED
21	5	303	CLA	CBA-CGA-O2A-C1
21	5	303	CLA	O1A-CGA-O2A-C1
21	5	303	CLA	CBD-CGD-O2D-CED
21	5	303	CLA	O1D-CGD-O2D-CED
21	5	304	CLA	CBD-CGD-O2D-CED
21	5	305	CLA	CBD-CGD-O2D-CED
21	5	305	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	5	306	CLA	CBD-CGD-O2D-CED
21	5	306	CLA	O1D-CGD-O2D-CED
21	5	306	CLA	C2-C3-C5-C6
21	5	306	CLA	C4-C3-C5-C6
21	5	307	CLA	CBD-CGD-O2D-CED
21	5	307	CLA	C4-C3-C5-C6
21	5	308	CLA	C1A-C2A-CAA-CBA
21	5	308	CLA	CBD-CGD-O2D-CED
21	5	308	CLA	O1D-CGD-O2D-CED
21	5	309	CLA	C6-C7-C8-C9
21	5	309	CLA	C14-C13-C15-C16
21	g	302	CLA	CBD-CGD-O2D-CED
21	g	302	CLA	O1D-CGD-O2D-CED
21	g	303	CLA	CBD-CGD-O2D-CED
21	g	303	CLA	O1D-CGD-O2D-CED
21	g	304	CLA	C1A-C2A-CAA-CBA
21	g	304	CLA	CBD-CGD-O2D-CED
21	g	304	CLA	O1D-CGD-O2D-CED
21	g	305	CLA	CBD-CGD-O2D-CED
21	g	305	CLA	O1D-CGD-O2D-CED
21	g	306	CLA	CBD-CGD-O2D-CED
21	g	306	CLA	C2-C3-C5-C6
21	g	306	CLA	C4-C3-C5-C6
21	g	306	CLA	C6-C7-C8-C9
21	g	307	CLA	CBD-CGD-O2D-CED
21	g	308	CLA	CBD-CGD-O2D-CED
21	g	308	CLA	O1D-CGD-O2D-CED
21	g	309	CLA	CHA-CBD-CGD-O2D
21	G	300	CLA	C1A-C2A-CAA-CBA
21	G	300	CLA	O1D-CGD-O2D-CED
21	G	301	CLA	CBD-CGD-O2D-CED
21	G	302	CLA	CBD-CGD-O2D-CED
21	G	302	CLA	O1D-CGD-O2D-CED
21	G	303	CLA	CBD-CGD-O2D-CED
21	G	303	CLA	O1D-CGD-O2D-CED
21	G	304	CLA	CBD-CGD-O2D-CED
21	G	304	CLA	O1D-CGD-O2D-CED
22	1	311	DD6	C10-C11-C13-C14
22	1	311	DD6	C12-C11-C13-C14
22	1	311	DD6	C2-C3-C4-C5
22	7	310	DD6	C-C1-C24-C25
22	7	310	DD6	C2-C1-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	5	310	DD6	C10-C11-C13-C14
22	5	310	DD6	C12-C11-C13-C14
22	g	310	DD6	C10-C11-C13-C14
22	g	310	DD6	C12-C11-C13-C14
22	g	310	DD6	C3-C4-C5-C6
23	1	312	A86	C10-C11-C13-O
23	1	312	A86	C12-C11-C13-O
23	1	312	A86	C1-C24-C25-C26
23	1	312	A86	C25-C26-C27-C28
23	1	312	A86	C25-C26-C27-C29
23	1	312	A86	C2-C3-C4-C5
23	1	312	A86	C6-C8-C9-C10
23	1	313	A86	C-C1-C2-C3
23	1	313	A86	C24-C1-C2-C3
23	1	313	A86	C9-C10-C11-C12
23	1	313	A86	C9-C10-C11-C13
23	1	313	A86	C10-C11-C13-O
23	1	313	A86	C12-C11-C13-O
23	1	313	A86	C1-C24-C25-C26
23	1	313	A86	C2-C3-C4-C5
23	1	313	A86	C39-C38-O4-C34
23	1	313	A86	C4-C5-C6-C7
23	1	313	A86	C4-C5-C6-C8
23	1	313	A86	C5-C6-C8-C9
23	1	313	A86	C7-C6-C8-C9
23	1	313	A86	C6-C8-C9-C10
23	1	314	A86	C9-C10-C11-C12
23	1	314	A86	C9-C10-C11-C13
23	1	314	A86	C11-C10-C9-C8
23	1	314	A86	C10-C11-C13-O
23	1	314	A86	C10-C11-C13-C14
23	1	314	A86	C12-C11-C13-O
23	1	314	A86	C2-C3-C4-C5
23	1	314	A86	C39-C38-O4-C34
23	1	314	A86	O5-C38-O4-C34
23	1	314	A86	C4-C5-C6-C7
23	1	314	A86	C4-C5-C6-C8
23	1	314	A86	C5-C6-C8-C9
23	1	314	A86	C7-C6-C8-C9
23	1	314	A86	C6-C8-C9-C10
23	6	309	A86	C-C1-C2-C3
23	6	309	A86	C24-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	6	309	A86	C-C1-C24-C25
23	6	309	A86	C2-C1-C24-C25
23	6	309	A86	C9-C10-C11-C12
23	6	309	A86	C9-C10-C11-C13
23	6	309	A86	C10-C11-C13-O
23	6	309	A86	C10-C11-C13-C14
23	6	309	A86	C12-C11-C13-O
23	6	309	A86	C1-C24-C25-C26
23	6	309	A86	C3-C4-C5-C6
23	6	309	A86	C6-C8-C9-C10
23	6	310	A86	C-C1-C2-C3
23	6	310	A86	C24-C1-C2-C3
23	6	310	A86	C-C1-C24-C25
23	6	310	A86	C2-C1-C24-C25
23	6	310	A86	C9-C10-C11-C12
23	6	310	A86	C9-C10-C11-C13
23	6	310	A86	C11-C10-C9-C8
23	6	310	A86	C1-C24-C25-C26
23	6	310	A86	C2-C3-C4-C5
23	6	310	A86	C3-C4-C5-C6
23	6	310	A86	C4-C5-C6-C7
23	6	310	A86	C4-C5-C6-C8
23	6	310	A86	C5-C6-C8-C9
23	6	310	A86	C7-C6-C8-C9
23	7	311	A86	C-C1-C2-C3
23	7	311	A86	C24-C1-C2-C3
23	7	311	A86	C-C1-C24-C25
23	7	311	A86	C2-C1-C24-C25
23	7	311	A86	C10-C11-C13-O
23	7	311	A86	C10-C11-C13-C14
23	7	311	A86	C12-C11-C13-O
23	7	311	A86	C1-C2-C3-C4
23	7	311	A86	C1-C24-C25-C26
23	7	311	A86	C28-C27-C29-C30
23	7	311	A86	C2-C3-C4-C5
23	7	311	A86	C4-C5-C6-C7
23	7	311	A86	C4-C5-C6-C8
23	7	311	A86	C6-C8-C9-C10
23	7	312	A86	C-C1-C2-C3
23	7	312	A86	C24-C1-C2-C3
23	7	312	A86	C9-C10-C11-C12
23	7	312	A86	C9-C10-C11-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	7	312	A86	C10-C11-C13-O
23	7	312	A86	C12-C11-C13-O
23	7	312	A86	C1-C24-C25-C26
23	7	312	A86	C2-C3-C4-C5
23	7	312	A86	C39-C38-O4-C34
23	7	312	A86	C5-C6-C8-C9
23	7	312	A86	C7-C6-C8-C9
23	7	312	A86	C6-C8-C9-C10
23	7	313	A86	C-C1-C2-C3
23	7	313	A86	C24-C1-C2-C3
23	7	313	A86	C1-C24-C25-C26
23	7	313	A86	C2-C3-C4-C5
23	7	313	A86	C5-C6-C8-C9
23	7	313	A86	C7-C6-C8-C9
23	J	309	A86	C-C1-C2-C3
23	J	309	A86	C9-C10-C11-C12
23	J	309	A86	C9-C10-C11-C13
23	J	309	A86	C10-C11-C13-O
23	J	309	A86	C10-C11-C13-C14
23	J	309	A86	C12-C11-C13-O
23	J	309	A86	C1-C24-C25-C26
23	J	309	A86	C6-C8-C9-C10
23	J	310	A86	C-C1-C2-C3
23	J	310	A86	C24-C1-C2-C3
23	J	310	A86	C-C1-C24-C25
23	J	310	A86	C2-C1-C24-C25
23	J	310	A86	C9-C10-C11-C12
23	J	310	A86	C9-C10-C11-C13
23	J	310	A86	C11-C10-C9-C8
23	J	310	A86	C1-C24-C25-C26
23	J	310	A86	C2-C3-C4-C5
23	J	310	A86	C39-C38-O4-C34
23	J	310	A86	C3-C4-C5-C6
23	J	310	A86	C4-C5-C6-C7
23	J	310	A86	C4-C5-C6-C8
23	J	310	A86	C5-C6-C8-C9
23	J	310	A86	C7-C6-C8-C9
23	W	101	A86	C-C1-C2-C3
23	W	101	A86	C24-C1-C2-C3
23	W	101	A86	C9-C10-C11-C12
23	W	101	A86	C9-C10-C11-C13
23	W	101	A86	C10-C11-C13-O

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	W	101	A86	C12-C11-C13-O
23	W	101	A86	O-C13-C14-C15
23	W	101	A86	C11-C13-C14-C15
23	W	101	A86	C13-C14-C15-C20
23	W	101	A86	C13-C14-C15-O1
23	W	101	A86	C2-C3-C4-C5
23	W	101	A86	C35-C34-O4-C38
23	W	101	A86	C39-C38-O4-C34
23	W	101	A86	C4-C5-C6-C7
23	W	101	A86	C4-C5-C6-C8
23	W	101	A86	C6-C8-C9-C10
23	2	307	A86	C9-C10-C11-C12
23	2	307	A86	C9-C10-C11-C13
23	2	307	A86	C11-C10-C9-C8
23	2	307	A86	C2-C3-C4-C5
23	2	307	A86	C39-C38-O4-C34
23	2	307	A86	O5-C38-O4-C34
23	2	307	A86	C4-C5-C6-C7
23	2	307	A86	C4-C5-C6-C8
23	2	307	A86	C5-C6-C8-C9
23	2	307	A86	C7-C6-C8-C9
23	2	307	A86	C6-C8-C9-C10
23	2	308	A86	C-C1-C24-C25
23	2	308	A86	C2-C1-C24-C25
23	2	309	A86	C-C1-C24-C25
23	2	309	A86	C2-C1-C24-C25
23	2	309	A86	C10-C11-C13-O
23	2	309	A86	C12-C11-C13-O
23	2	309	A86	C1-C24-C25-C26
23	2	309	A86	C26-C27-C29-C30
23	2	309	A86	C39-C38-O4-C34
23	2	309	A86	C3-C4-C5-C6
23	2	309	A86	C4-C5-C6-C7
23	2	309	A86	C4-C5-C6-C8
23	2	309	A86	C5-C6-C8-C9
23	2	309	A86	C7-C6-C8-C9
23	2	310	A86	C9-C10-C11-C12
23	2	310	A86	C9-C10-C11-C13
23	2	310	A86	C10-C11-C13-O
23	2	310	A86	C10-C11-C13-C14
23	2	310	A86	C12-C11-C13-O
23	2	310	A86	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	2	310	A86	C3-C4-C5-C6
23	2	310	A86	C4-C5-C6-C7
23	2	310	A86	C4-C5-C6-C8
23	2	310	A86	C5-C6-C8-C9
23	2	310	A86	C6-C8-C9-C10
23	2	311	A86	C-C1-C2-C3
23	2	311	A86	C24-C1-C2-C3
23	2	311	A86	C9-C10-C11-C12
23	2	311	A86	C9-C10-C11-C13
23	2	311	A86	C10-C11-C13-O
23	2	311	A86	C12-C11-C13-O
23	2	311	A86	O-C13-C14-C15
23	2	311	A86	C11-C13-C14-C15
23	2	311	A86	C13-C14-C15-C20
23	2	311	A86	C2-C3-C4-C5
23	2	311	A86	C35-C34-O4-C38
23	2	311	A86	C39-C38-O4-C34
23	2	311	A86	C4-C5-C6-C7
23	2	311	A86	C4-C5-C6-C8
23	2	311	A86	C6-C8-C9-C10
23	2	312	A86	C-C1-C24-C25
23	2	312	A86	C2-C1-C24-C25
23	2	312	A86	C9-C10-C11-C12
23	2	312	A86	C9-C10-C11-C13
23	2	312	A86	C10-C11-C13-O
23	2	312	A86	C10-C11-C13-C14
23	2	312	A86	C12-C11-C13-O
23	2	312	A86	C2-C3-C4-C5
23	2	312	A86	C6-C8-C9-C10
23	8	308	A86	C-C1-C2-C3
23	8	308	A86	C24-C1-C2-C3
23	8	308	A86	C-C1-C24-C25
23	8	308	A86	C2-C1-C24-C25
23	8	308	A86	C10-C11-C13-O
23	8	308	A86	C12-C11-C13-O
23	8	308	A86	C13-C14-C15-O1
23	8	308	A86	C1-C2-C3-C4
23	8	308	A86	C1-C24-C25-C26
23	8	308	A86	C2-C3-C4-C5
23	8	308	A86	C4-C5-C6-C7
23	8	308	A86	C4-C5-C6-C8
23	8	308	A86	C5-C6-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	8	308	A86	C7-C6-C8-C9
23	8	308	A86	C6-C8-C9-C10
23	8	309	A86	C-C1-C2-C3
23	8	309	A86	C24-C1-C2-C3
23	8	309	A86	C-C1-C24-C25
23	8	309	A86	C2-C1-C24-C25
23	8	309	A86	C9-C10-C11-C13
23	8	309	A86	C6-C8-C9-C10
23	8	310	A86	C-C1-C2-C3
23	8	310	A86	C24-C1-C2-C3
23	8	310	A86	C9-C10-C11-C12
23	8	310	A86	C9-C10-C11-C13
23	8	310	A86	C10-C11-C13-O
23	8	310	A86	C12-C11-C13-O
23	8	310	A86	C1-C2-C3-C4
23	8	310	A86	C1-C24-C25-C26
23	8	310	A86	C39-C38-O4-C34
23	8	310	A86	C6-C8-C9-C10
23	8	311	A86	C10-C11-C13-O
23	8	311	A86	C10-C11-C13-C14
23	8	311	A86	C12-C11-C13-O
23	8	311	A86	C2-C3-C4-C5
23	8	311	A86	C3-C4-C5-C6
23	8	311	A86	C5-C6-C8-C9
23	8	311	A86	C7-C6-C8-C9
23	8	311	A86	C6-C8-C9-C10
23	8	312	A86	C-C1-C2-C3
23	8	312	A86	C24-C1-C2-C3
23	8	312	A86	C9-C10-C11-C12
23	8	312	A86	C9-C10-C11-C13
23	8	312	A86	C10-C11-C13-O
23	8	312	A86	C10-C11-C13-C14
23	8	312	A86	C12-C11-C13-O
23	8	312	A86	C1-C24-C25-C26
23	8	312	A86	C5-C6-C8-C9
23	8	312	A86	C7-C6-C8-C9
23	8	312	A86	C6-C8-C9-C10
23	4	305	A86	C10-C11-C13-O
23	4	305	A86	C12-C11-C13-O
23	4	305	A86	C1-C24-C25-C26
23	4	305	A86	C2-C3-C4-C5
23	4	305	A86	C39-C38-O4-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	4	305	A86	O5-C38-O4-C34
23	4	305	A86	C3-C4-C5-C6
23	4	305	A86	C5-C6-C8-C9
23	4	305	A86	C7-C6-C8-C9
23	5	311	A86	C9-C10-C11-C12
23	5	311	A86	C9-C10-C11-C13
23	5	311	A86	C1-C24-C25-C26
23	5	311	A86	C2-C3-C4-C5
23	5	311	A86	C4-C5-C6-C7
23	5	311	A86	C4-C5-C6-C8
23	5	312	A86	C-C1-C24-C25
23	5	312	A86	C2-C1-C24-C25
23	5	312	A86	C9-C10-C11-C13
23	5	312	A86	C10-C11-C13-O
23	5	312	A86	C10-C11-C13-C14
23	5	312	A86	C12-C11-C13-O
23	5	312	A86	C13-C14-C15-C16
23	5	312	A86	C13-C14-C15-O1
23	5	312	A86	C1-C24-C25-C26
23	5	312	A86	C28-C27-C29-C30
23	5	312	A86	C2-C3-C4-C5
23	5	312	A86	C39-C38-O4-C34
23	5	312	A86	O5-C38-O4-C34
23	5	312	A86	C4-C5-C6-C7
23	5	312	A86	C4-C5-C6-C8
23	5	312	A86	C6-C8-C9-C10
23	g	311	A86	C-C1-C2-C3
23	g	311	A86	C24-C1-C2-C3
23	g	311	A86	C-C1-C24-C25
23	g	311	A86	C2-C1-C24-C25
23	g	311	A86	C9-C10-C11-C12
23	g	311	A86	C9-C10-C11-C13
23	g	311	A86	C1-C2-C3-C4
23	g	311	A86	C1-C24-C25-C26
23	g	311	A86	C39-C38-O4-C34
23	g	311	A86	C3-C4-C5-C6
23	g	311	A86	C4-C5-C6-C7
23	g	311	A86	C4-C5-C6-C8
23	g	312	A86	C9-C10-C11-C12
23	g	312	A86	C9-C10-C11-C13
23	g	312	A86	C10-C11-C13-O
23	g	312	A86	C10-C11-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	g	312	A86	C12-C11-C13-O
23	g	312	A86	C2-C3-C4-C5
23	g	312	A86	C35-C34-O4-C38
23	g	312	A86	C39-C38-O4-C34
23	g	312	A86	C5-C6-C8-C9
23	g	312	A86	C7-C6-C8-C9
23	G	305	A86	C-C1-C2-C3
23	G	305	A86	C24-C1-C2-C3
23	G	305	A86	C9-C10-C11-C12
23	G	305	A86	C9-C10-C11-C13
23	G	305	A86	C11-C10-C9-C8
23	G	305	A86	C1-C24-C25-C26
23	G	305	A86	C2-C3-C4-C5
23	G	305	A86	C3-C4-C5-C6
23	G	305	A86	C4-C5-C6-C7
23	G	305	A86	C4-C5-C6-C8
24	1	315	KC1	C2A-CAA-CBA-CGA
24	1	316	KC1	C2B-C3B-CAB-CBB
24	1	316	KC1	C4B-C3B-CAB-CBB
24	1	316	KC1	C2A-CAA-CBA-CGA
24	6	311	KC1	C1A-C2A-CAA-CBA
24	6	311	KC1	C2A-CAA-CBA-CGA
24	6	312	KC1	C3A-C2A-CAA-CBA
24	6	312	KC1	C2A-CAA-CBA-CGA
24	6	313	KC1	C2A-CAA-CBA-CGA
24	7	314	KC1	C3A-C2A-CAA-CBA
24	7	314	KC1	C2A-CAA-CBA-CGA
24	7	315	KC1	C2B-C3B-CAB-CBB
24	7	315	KC1	C4B-C3B-CAB-CBB
24	7	315	KC1	C2A-CAA-CBA-CGA
24	J	311	KC1	C1A-C2A-CAA-CBA
24	J	312	KC1	C3A-C2A-CAA-CBA
24	J	312	KC1	C2A-CAA-CBA-CGA
24	J	313	KC1	C2A-CAA-CBA-CGA
24	2	313	KC1	C3A-C2A-CAA-CBA
24	2	313	KC1	CBD-CGD-O2D-CED
24	2	314	KC1	C2B-C3B-CAB-CBB
24	2	314	KC1	C4B-C3B-CAB-CBB
24	2	314	KC1	C2A-CAA-CBA-CGA
24	2	315	KC1	C3A-C2A-CAA-CBA
24	2	315	KC1	C2A-CAA-CBA-CGA
24	2	316	KC1	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	2	316	KC1	C3A-C2A-CAA-CBA
24	2	316	KC1	C2A-CAA-CBA-CGA
24	8	313	KC1	C2A-CAA-CBA-CGA
24	8	314	KC1	C2B-C3B-CAB-CBB
24	8	314	KC1	C2A-CAA-CBA-CGA
24	8	315	KC1	C3A-C2A-CAA-CBA
24	8	315	KC1	C2A-CAA-CBA-CGA
24	8	316	KC1	C1A-C2A-CAA-CBA
24	8	316	KC1	C3A-C2A-CAA-CBA
24	8	316	KC1	C2A-CAA-CBA-CGA
24	9	305	KC1	C3A-C2A-CAA-CBA
24	9	305	KC1	C2B-C3B-CAB-CBB
24	9	305	KC1	C4B-C3B-CAB-CBB
24	9	305	KC1	CBD-CGD-O2D-CED
24	9	306	KC1	C3A-C2A-CAA-CBA
24	3	305	KC1	C3A-C2A-CAA-CBA
24	3	305	KC1	C2A-CAA-CBA-CGA
24	3	306	KC1	C3A-C2A-CAA-CBA
24	3	306	KC1	C2A-CAA-CBA-CGA
24	4	307	KC1	C2B-C3B-CAB-CBB
24	4	307	KC1	C4B-C3B-CAB-CBB
24	4	307	KC1	C2A-CAA-CBA-CGA
24	4	307	KC1	CBD-CGD-O2D-CED
24	4	308	KC1	C3A-C2A-CAA-CBA
24	4	308	KC1	C2A-CAA-CBA-CGA
24	4	309	KC1	C3A-C2A-CAA-CBA
24	4	309	KC1	C2A-CAA-CBA-CGA
24	5	313	KC1	C3A-C2A-CAA-CBA
24	5	313	KC1	C2B-C3B-CAB-CBB
24	5	313	KC1	C4B-C3B-CAB-CBB
24	5	313	KC1	C2A-CAA-CBA-CGA
24	5	313	KC1	CBD-CGD-O2D-CED
24	5	313	KC1	O1D-CGD-O2D-CED
24	5	314	KC1	C3A-C2A-CAA-CBA
24	5	314	KC1	C2A-CAA-CBA-CGA
24	5	315	KC1	C2B-C3B-CAB-CBB
24	5	315	KC1	C4B-C3B-CAB-CBB
24	5	315	KC1	CBD-CGD-O2D-CED
24	g	313	KC1	C3A-C2A-CAA-CBA
24	g	313	KC1	C2B-C3B-CAB-CBB
24	g	313	KC1	C4B-C3B-CAB-CBB
24	g	313	KC1	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	g	314	KC1	C2A-CAA-CBA-CGA
24	g	315	KC1	C2A-CAA-CBA-CGA
24	G	307	KC1	C3A-C2A-CAA-CBA
24	G	307	KC1	C2B-C3B-CAB-CBB
24	G	307	KC1	C4B-C3B-CAB-CBB
24	G	307	KC1	C2A-CAA-CBA-CGA
24	G	308	KC1	C3A-C2A-CAA-CBA
24	G	308	KC1	C2A-CAA-CBA-CGA
24	G	309	KC1	C3A-C2A-CAA-CBA
24	G	309	KC1	C4B-C3B-CAB-CBB
24	G	309	KC1	CHA-CBD-CGD-O1D
24	G	309	KC1	CHA-CBD-CGD-O2D
25	1	317	BCR	C6-C7-C8-C9
25	1	317	BCR	C11-C10-C9-C8
25	1	317	BCR	C11-C10-C9-C34
25	1	317	BCR	C13-C14-C15-C16
25	1	317	BCR	C15-C16-C17-C18
25	1	317	BCR	C20-C21-C22-C23
25	1	317	BCR	C20-C21-C22-C37
25	1	317	BCR	C21-C22-C23-C24
25	1	317	BCR	C22-C23-C24-C25
25	A	405	BCR	C1-C6-C7-C8
25	A	405	BCR	C7-C8-C9-C34
25	B	617	BCR	C7-C8-C9-C34
25	B	618	BCR	C1-C6-C7-C8
25	B	618	BCR	C7-C8-C9-C10
25	B	618	BCR	C7-C8-C9-C34
25	B	618	BCR	C21-C22-C23-C24
25	B	618	BCR	C22-C23-C24-C25
25	H	100	BCR	C1-C6-C7-C8
25	H	100	BCR	C7-C8-C9-C34
25	a	406	BCR	C1-C6-C7-C8
25	a	406	BCR	C7-C8-C9-C34
25	b	618	BCR	C7-C8-C9-C34
25	b	619	BCR	C7-C8-C9-C10
25	b	619	BCR	C7-C8-C9-C34
25	b	619	BCR	C20-C21-C22-C37
25	b	619	BCR	C21-C22-C23-C24
25	b	619	BCR	C22-C23-C24-C25
25	h	101	BCR	C6-C7-C8-C9
25	h	101	BCR	C7-C8-C9-C34
25	h	101	BCR	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	h	101	BCR	C10-C11-C12-C13
25	h	101	BCR	C11-C12-C13-C35
25	h	101	BCR	C14-C15-C16-C17
25	h	101	BCR	C16-C17-C18-C19
25	h	101	BCR	C16-C17-C18-C36
25	h	101	BCR	C19-C20-C21-C22
25	h	101	BCR	C20-C21-C22-C23
25	h	101	BCR	C20-C21-C22-C37
25	h	101	BCR	C21-C22-C23-C24
25	h	102	BCR	C1-C6-C7-C8
25	h	102	BCR	C7-C8-C9-C34
25	D	408	BCR	C7-C8-C9-C34
25	d	407	BCR	C7-C8-C9-C34
25	d	407	BCR	C23-C24-C25-C30
25	C	501	BCR	C1-C6-C7-C8
25	C	501	BCR	C22-C23-C24-C25
25	C	516	BCR	C7-C8-C9-C10
25	C	516	BCR	C7-C8-C9-C34
25	c	501	BCR	C1-C6-C7-C8
25	c	501	BCR	C11-C12-C13-C35
25	c	515	BCR	C7-C8-C9-C10
25	c	515	BCR	C7-C8-C9-C34
26	a	404	PHO	O1A-CGA-O2A-C1
27	A	406	LHG	C4-O6-P-O5
27	A	406	LHG	C8-C7-O7-C5
27	B	601	LHG	C3-O3-P-O4
27	B	601	LHG	C3-O3-P-O5
27	B	601	LHG	C3-O3-P-O6
27	a	401	LHG	O1-C1-C2-C3
27	a	401	LHG	C8-C7-O7-C5
27	D	410	LHG	C1-C2-C3-O3
27	d	409	LHG	C1-C2-C3-O3
28	A	407	LMG	O7-C8-C9-O8
28	B	623	LMG	C2-C1-O1-C7
28	B	623	LMG	O6-C1-O1-C7
28	B	627	LMG	C2-C1-O1-C7
28	B	627	LMG	O6-C1-O1-C7
28	B	627	LMG	O9-C10-O7-C8
28	B	627	LMG	C11-C10-O7-C8
28	B	627	LMG	O10-C28-O8-C9
28	B	627	LMG	C29-C28-O8-C9
28	M	102	LMG	O7-C8-C9-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	N	101	LMG	O1-C7-C8-C9
28	N	101	LMG	O1-C7-C8-O7
28	N	101	LMG	O7-C8-C9-O8
28	b	622	LMG	C2-C1-O1-C7
28	b	622	LMG	O6-C1-O1-C7
28	b	625	LMG	C11-C10-O7-C8
28	b	626	LMG	C11-C10-O7-C8
28	2	318	LMG	O7-C8-C9-O8
28	8	317	LMG	O7-C8-C9-O8
29	8	318	LMU	O5'-C1'-O1'-C1
29	D	412	LMU	C2'-C1'-O1'-C1
29	D	412	LMU	O5'-C1'-O1'-C1
29	D	412	LMU	C2-C1-O1'-C1'
29	g	316	LMU	O5B-C1B-O1B-C4'
30	B	624	DGD	C2B-C1B-O2G-C2G
30	B	624	DGD	C2E-C1E-O5D-C6D
30	B	624	DGD	O6E-C1E-O5D-C6D
30	b	601	DGD	C2B-C1B-O2G-C2G
30	b	601	DGD	C2E-C1E-O5D-C6D
30	b	601	DGD	O6E-C1E-O5D-C6D
30	C	518	DGD	C1G-C2G-C3G-O3G
30	C	518	DGD	O2G-C2G-C3G-O3G
30	c	517	DGD	C1G-C2G-C3G-O3G
30	c	517	DGD	O2G-C2G-C3G-O3G
31	B	625	SQD	O5-C5-C6-S
31	B	625	SQD	C5-C6-S-O7
31	B	625	SQD	C5-C6-S-O8
31	B	625	SQD	C5-C6-S-O9
31	B	626	SQD	O5-C1-O6-C44
31	B	626	SQD	O49-C7-O47-C45
31	B	626	SQD	C8-C7-O47-C45
31	B	626	SQD	O5-C5-C6-S
31	X	401	SQD	C2-C1-O6-C44
31	X	401	SQD	O5-C1-O6-C44
31	X	401	SQD	O49-C7-O47-C45
31	X	401	SQD	C8-C7-O47-C45
31	X	401	SQD	O5-C5-C6-S
31	b	602	SQD	O5-C1-O6-C44
31	b	602	SQD	O49-C7-O47-C45
31	b	602	SQD	C8-C7-O47-C45
31	b	602	SQD	O5-C5-C6-S
31	C	502	SQD	C5-C6-S-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	E	101	HEM	C2A-CAA-CBA-CGA
35	d	408	PL9	C37-C38-C39-C41
23	1	313	A86	O5-C38-O4-C34
23	6	309	A86	C39-C38-O4-C34
23	W	101	A86	O5-C38-O4-C34
23	5	311	A86	C39-C38-O4-C34
23	g	311	A86	O5-C38-O4-C34
23	g	312	A86	O5-C38-O4-C34
21	1	306	CLA	O1D-CGD-O2D-CED
21	1	308	CLA	O1D-CGD-O2D-CED
21	6	300	CLA	O1D-CGD-O2D-CED
21	6	301	CLA	O1D-CGD-O2D-CED
21	6	304	CLA	O1D-CGD-O2D-CED
21	7	303	CLA	O1D-CGD-O2D-CED
21	7	308	CLA	O1D-CGD-O2D-CED
21	B	606	CLA	O1D-CGD-O2D-CED
21	B	609	CLA	O1D-CGD-O2D-CED
21	B	621	CLA	O1D-CGD-O2D-CED
21	J	301	CLA	O1D-CGD-O2D-CED
21	J	302	CLA	O1D-CGD-O2D-CED
21	J	308	CLA	O1D-CGD-O2D-CED
21	b	607	CLA	O1D-CGD-O2D-CED
21	b	610	CLA	O1D-CGD-O2D-CED
21	b	612	CLA	O1D-CGD-O2D-CED
21	8	307	CLA	O1D-CGD-O2D-CED
21	D	406	CLA	O1D-CGD-O2D-CED
21	d	404	CLA	O1D-CGD-O2D-CED
21	d	405	CLA	O1D-CGD-O2D-CED
21	c	503	CLA	O1D-CGD-O2D-CED
21	c	507	CLA	O1D-CGD-O2D-CED
21	c	509	CLA	O1D-CGD-O2D-CED
21	c	513	CLA	O1D-CGD-O2D-CED
21	9	302	CLA	O1D-CGD-O2D-CED
21	3	301	CLA	O1D-CGD-O2D-CED
21	3	303	CLA	O1D-CGD-O2D-CED
21	4	302	CLA	O1D-CGD-O2D-CED
21	5	302	CLA	O1D-CGD-O2D-CED
21	5	304	CLA	O1D-CGD-O2D-CED
21	G	301	CLA	O1D-CGD-O2D-CED
23	6	310	A86	C39-C38-O4-C34
23	7	312	A86	O5-C38-O4-C34
23	2	308	A86	C39-C38-O4-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	2	309	A86	O5-C38-O4-C34
23	2	311	A86	O5-C38-O4-C34
23	8	312	A86	C39-C38-O4-C34
21	1	301	CLA	O1D-CGD-O2D-CED
21	1	309	CLA	O1D-CGD-O2D-CED
21	6	302	CLA	O1D-CGD-O2D-CED
21	6	307	CLA	O1D-CGD-O2D-CED
21	6	308	CLA	O1D-CGD-O2D-CED
21	A	401	CLA	O1D-CGD-O2D-CED
21	A	404	CLA	O1D-CGD-O2D-CED
21	B	602	CLA	O1D-CGD-O2D-CED
21	B	605	CLA	O1D-CGD-O2D-CED
21	B	610	CLA	O1D-CGD-O2D-CED
21	B	611	CLA	O1D-CGD-O2D-CED
21	J	303	CLA	O1D-CGD-O2D-CED
21	a	402	CLA	O1D-CGD-O2D-CED
21	a	405	CLA	O1D-CGD-O2D-CED
21	b	603	CLA	O1D-CGD-O2D-CED
21	b	606	CLA	O1D-CGD-O2D-CED
21	b	611	CLA	O1D-CGD-O2D-CED
21	b	616	CLA	O1D-CGD-O2D-CED
21	2	302	CLA	O1D-CGD-O2D-CED
21	8	303	CLA	O1D-CGD-O2D-CED
21	C	504	CLA	O1D-CGD-O2D-CED
21	C	505	CLA	O1D-CGD-O2D-CED
21	C	508	CLA	O1D-CGD-O2D-CED
21	C	510	CLA	O1D-CGD-O2D-CED
21	C	514	CLA	O1D-CGD-O2D-CED
21	C	515	CLA	O1D-CGD-O2D-CED
21	c	508	CLA	O1D-CGD-O2D-CED
21	9	301	CLA	O1D-CGD-O2D-CED
21	9	304	CLA	O1D-CGD-O2D-CED
21	3	302	CLA	O1D-CGD-O2D-CED
21	4	300	CLA	O1D-CGD-O2D-CED
21	4	301	CLA	O1D-CGD-O2D-CED
21	5	309	CLA	O1D-CGD-O2D-CED
24	2	313	KC1	O1D-CGD-O2D-CED
24	5	315	KC1	O1D-CGD-O2D-CED
21	6	303	CLA	CBD-CGD-O2D-CED
21	6	308	CLA	CBD-CGD-O2D-CED
21	7	300	CLA	CBD-CGD-O2D-CED
21	7	305	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	7	308	CLA	CBD-CGD-O2D-CED
21	B	602	CLA	CBD-CGD-O2D-CED
21	B	605	CLA	CBD-CGD-O2D-CED
21	B	610	CLA	CBD-CGD-O2D-CED
21	B	611	CLA	CBD-CGD-O2D-CED
21	B	616	CLA	CBD-CGD-O2D-CED
21	J	303	CLA	CBD-CGD-O2D-CED
21	b	603	CLA	CBD-CGD-O2D-CED
21	b	606	CLA	CBD-CGD-O2D-CED
21	b	611	CLA	CBD-CGD-O2D-CED
21	b	615	CLA	CBD-CGD-O2D-CED
21	b	616	CLA	CBD-CGD-O2D-CED
21	2	302	CLA	CBD-CGD-O2D-CED
21	2	305	CLA	CBD-CGD-O2D-CED
21	8	304	CLA	CBD-CGD-O2D-CED
21	D	407	CLA	CBD-CGD-O2D-CED
21	d	406	CLA	CBD-CGD-O2D-CED
21	C	505	CLA	CBD-CGD-O2D-CED
21	C	506	CLA	CBD-CGD-O2D-CED
21	C	508	CLA	CBD-CGD-O2D-CED
21	C	510	CLA	CBD-CGD-O2D-CED
21	C	514	CLA	CBD-CGD-O2D-CED
21	c	502	CLA	CBD-CGD-O2D-CED
21	c	505	CLA	CBD-CGD-O2D-CED
21	c	507	CLA	CBD-CGD-O2D-CED
21	c	508	CLA	CBD-CGD-O2D-CED
21	c	513	CLA	CBD-CGD-O2D-CED
21	9	301	CLA	CBD-CGD-O2D-CED
21	3	301	CLA	CBD-CGD-O2D-CED
21	4	301	CLA	CBD-CGD-O2D-CED
21	4	302	CLA	CBD-CGD-O2D-CED
21	5	309	CLA	CBD-CGD-O2D-CED
21	g	309	CLA	CBD-CGD-O2D-CED
21	G	300	CLA	CBD-CGD-O2D-CED
24	6	311	KC1	CBD-CGD-O2D-CED
24	J	311	KC1	CBD-CGD-O2D-CED
21	A	401	CLA	O1A-CGA-O2A-C1
27	A	406	LHG	O10-C23-O8-C6
28	M	102	LMG	O10-C28-O8-C9
28	2	318	LMG	O10-C28-O8-C9
28	8	317	LMG	O10-C28-O8-C9
21	1	302	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	6	303	CLA	O1D-CGD-O2D-CED
21	6	305	CLA	O1D-CGD-O2D-CED
21	7	301	CLA	O1D-CGD-O2D-CED
21	7	302	CLA	O1D-CGD-O2D-CED
21	7	304	CLA	O1D-CGD-O2D-CED
21	7	305	CLA	O1D-CGD-O2D-CED
21	7	309	CLA	O1D-CGD-O2D-CED
21	B	612	CLA	O1D-CGD-O2D-CED
21	J	300	CLA	O1D-CGD-O2D-CED
21	J	305	CLA	O1D-CGD-O2D-CED
21	8	304	CLA	O1D-CGD-O2D-CED
21	8	306	CLA	O1D-CGD-O2D-CED
21	D	407	CLA	O1D-CGD-O2D-CED
21	d	406	CLA	O1D-CGD-O2D-CED
21	c	502	CLA	O1D-CGD-O2D-CED
21	c	504	CLA	O1D-CGD-O2D-CED
21	c	511	CLA	O1D-CGD-O2D-CED
21	5	307	CLA	O1D-CGD-O2D-CED
21	g	306	CLA	O1D-CGD-O2D-CED
24	4	307	KC1	O1D-CGD-O2D-CED
24	g	313	KC1	O1D-CGD-O2D-CED
21	1	305	CLA	O1D-CGD-O2D-CED
21	B	607	CLA	O1D-CGD-O2D-CED
21	B	615	CLA	O1D-CGD-O2D-CED
21	J	307	CLA	O1D-CGD-O2D-CED
21	b	615	CLA	O1D-CGD-O2D-CED
21	2	306	CLA	O1D-CGD-O2D-CED
21	D	404	CLA	O1D-CGD-O2D-CED
21	C	509	CLA	O1D-CGD-O2D-CED
21	C	511	CLA	O1D-CGD-O2D-CED
21	c	510	CLA	O1D-CGD-O2D-CED
21	c	514	CLA	O1D-CGD-O2D-CED
21	g	307	CLA	O1D-CGD-O2D-CED
21	g	309	CLA	O1D-CGD-O2D-CED
24	9	305	KC1	O1D-CGD-O2D-CED
31	b	602	SQD	C24-C23-O48-C46
21	7	304	CLA	CBD-CGD-O2D-CED
21	B	614	CLA	CBD-CGD-O2D-CED
21	B	615	CLA	CBD-CGD-O2D-CED
21	2	301	CLA	CBD-CGD-O2D-CED
21	2	306	CLA	CBD-CGD-O2D-CED
24	1	316	KC1	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	7	315	KC1	CBD-CGD-O2D-CED
21	6	307	CLA	O1A-CGA-O2A-C1
21	J	307	CLA	O1A-CGA-O2A-C1
21	4	301	CLA	O1A-CGA-O2A-C1
21	5	309	CLA	O1A-CGA-O2A-C1
21	g	303	CLA	O1A-CGA-O2A-C1
26	A	403	PHO	O1A-CGA-O2A-C1
27	a	401	LHG	O10-C23-O8-C6
28	b	622	LMG	O10-C28-O8-C9
28	b	624	LMG	O10-C28-O8-C9
28	b	625	LMG	O10-C28-O8-C9
28	b	626	LMG	O10-C28-O8-C9
28	8	301	LMG	O10-C28-O8-C9
31	B	626	SQD	O10-C23-O48-C46
31	b	602	SQD	O10-C23-O48-C46
21	B	614	CLA	O1D-CGD-O2D-CED
23	6	309	A86	O5-C38-O4-C34
23	5	311	A86	O5-C38-O4-C34
23	8	309	A86	C39-C38-O4-C34
21	C	509	CLA	CBD-CGD-O2D-CED
27	A	406	LHG	O9-C7-O7-C5
27	a	401	LHG	O9-C7-O7-C5
28	L	101	LMG	O9-C10-O7-C8
28	M	102	LMG	O9-C10-O7-C8
28	b	622	LMG	O9-C10-O7-C8
30	b	601	DGD	O1B-C1B-O2G-C2G
28	A	407	LMG	O10-C28-O8-C9
23	J	310	A86	O5-C38-O4-C34
23	G	305	A86	C39-C38-O4-C34
21	7	303	CLA	C3-C5-C6-C7
21	b	617	CLA	C3-C5-C6-C7
21	2	301	CLA	C3-C5-C6-C7
21	2	305	CLA	C3-C5-C6-C7
21	D	407	CLA	C3-C5-C6-C7
21	5	308	CLA	C3-C5-C6-C7
21	1	302	CLA	CBA-CGA-O2A-C1
21	6	307	CLA	CBA-CGA-O2A-C1
21	A	401	CLA	CBA-CGA-O2A-C1
21	J	307	CLA	CBA-CGA-O2A-C1
21	a	402	CLA	CBA-CGA-O2A-C1
21	C	505	CLA	CBA-CGA-O2A-C1
21	9	304	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	5	309	CLA	CBA-CGA-O2A-C1
21	g	303	CLA	CBA-CGA-O2A-C1
26	a	404	PHO	CBA-CGA-O2A-C1
28	b	622	LMG	C29-C28-O8-C9
28	b	625	LMG	C29-C28-O8-C9
28	b	626	LMG	C29-C28-O8-C9
28	8	301	LMG	C29-C28-O8-C9
28	8	317	LMG	C29-C28-O8-C9
31	B	626	SQD	C24-C23-O48-C46
30	C	518	DGD	C2B-C1B-O2G-C2G
21	c	506	CLA	O1D-CGD-O2D-CED
21	1	302	CLA	CBD-CGD-O2D-CED
21	7	304	CLA	C2C-C3C-CAC-CBC
21	4	304	CLA	C2C-C3C-CAC-CBC
23	8	310	A86	O5-C38-O4-C34
29	2	317	LMU	O5B-C5B-C6B-O6B
24	G	308	KC1	CAA-CBA-CGA-O1A
24	G	308	KC1	CAA-CBA-CGA-O2A
23	J	309	A86	C39-C38-O4-C34
21	7	307	CLA	C4-C3-C5-C6
21	B	606	CLA	C4-C3-C5-C6
21	b	607	CLA	C4-C3-C5-C6
21	C	510	CLA	C4-C3-C5-C6
21	3	301	CLA	C4-C3-C5-C6
21	3	301	CLA	C2-C3-C5-C6
21	5	307	CLA	C2-C3-C5-C6
21	B	607	CLA	C2A-CAA-CBA-CGA
21	b	608	CLA	C2A-CAA-CBA-CGA
21	b	611	CLA	C2A-CAA-CBA-CGA
21	c	508	CLA	C2A-CAA-CBA-CGA
21	c	505	CLA	C3-C5-C6-C7
21	g	306	CLA	C3-C5-C6-C7
26	A	403	PHO	C3-C5-C6-C7
26	a	404	PHO	C3-C5-C6-C7
21	1	304	CLA	CBA-CGA-O2A-C1
21	6	301	CLA	CBA-CGA-O2A-C1
21	c	504	CLA	CBA-CGA-O2A-C1
21	c	510	CLA	CBA-CGA-O2A-C1
21	4	301	CLA	CBA-CGA-O2A-C1
21	G	301	CLA	CBA-CGA-O2A-C1
26	A	403	PHO	CBA-CGA-O2A-C1
27	A	406	LHG	C24-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	401	LHG	C24-C23-O8-C6
28	A	407	LMG	C29-C28-O8-C9
28	b	624	LMG	C29-C28-O8-C9
28	2	318	LMG	C29-C28-O8-C9
23	8	312	A86	O5-C38-O4-C34
21	C	507	CLA	O1D-CGD-O2D-CED
30	C	518	DGD	C4D-C5D-C6D-O5D
21	B	607	CLA	CBD-CGD-O2D-CED
21	D	404	CLA	CBD-CGD-O2D-CED
30	H	101	DGD	O6E-C5E-C6E-O5E
28	b	625	LMG	O9-C10-O7-C8
30	C	518	DGD	O1B-C1B-O2G-C2G
21	1	302	CLA	O1A-CGA-O2A-C1
21	1	304	CLA	O1A-CGA-O2A-C1
21	C	505	CLA	O1A-CGA-O2A-C1
21	c	510	CLA	O1A-CGA-O2A-C1
28	N	101	LMG	O10-C28-O8-C9
21	9	303	CLA	C2C-C3C-CAC-CBC
24	J	311	KC1	O1D-CGD-O2D-CED
23	1	312	A86	C1-C2-C3-C4
23	1	313	A86	C1-C2-C3-C4
23	6	309	A86	C24-C25-C26-C27
23	7	312	A86	C11-C10-C9-C8
23	J	309	A86	C3-C4-C5-C6
23	2	311	A86	C11-C10-C9-C8
23	2	312	A86	C11-C10-C9-C8
23	2	312	A86	C1-C2-C3-C4
23	8	312	A86	C11-C10-C9-C8
23	4	305	A86	C11-C10-C9-C8
23	5	312	A86	C11-C10-C9-C8
23	g	312	A86	C1-C2-C3-C4
25	h	101	BCR	C9-C10-C11-C12
25	h	101	BCR	C15-C16-C17-C18
27	d	409	LHG	C23-C24-C25-C26
21	7	304	CLA	C4C-C3C-CAC-CBC
23	6	310	A86	O5-C38-O4-C34
24	2	316	KC1	CBD-CGD-O2D-CED
24	6	311	KC1	O1D-CGD-O2D-CED
27	l	101	LHG	O2-C2-C3-O3
21	1	310	CLA	C3-C5-C6-C7
21	B	616	CLA	C3-C5-C6-C7
21	g	302	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	1	308	CLA	CBA-CGA-O2A-C1
21	J	301	CLA	CBA-CGA-O2A-C1
21	8	306	CLA	CBA-CGA-O2A-C1
21	C	511	CLA	CBA-CGA-O2A-C1
21	C	514	CLA	CBA-CGA-O2A-C1
21	g	304	CLA	CBA-CGA-O2A-C1
21	g	308	CLA	CBA-CGA-O2A-C1
28	N	101	LMG	C29-C28-O8-C9
21	C	511	CLA	O1A-CGA-O2A-C1
21	9	304	CLA	O1A-CGA-O2A-C1
21	G	301	CLA	O1A-CGA-O2A-C1
28	2	318	LMG	O6-C5-C6-O5
30	h	103	DGD	O6E-C5E-C6E-O5E
28	L	101	LMG	C11-C10-O7-C8
28	M	102	LMG	C11-C10-O7-C8
28	b	622	LMG	C11-C10-O7-C8
21	8	302	CLA	CBD-CGD-O2D-CED
21	4	304	CLA	C4C-C3C-CAC-CBC
23	7	312	A86	C33-C34-O4-C38
21	6	301	CLA	O1A-CGA-O2A-C1
21	8	306	CLA	O1A-CGA-O2A-C1
28	B	622	LMG	O6-C5-C6-O5
30	c	516	DGD	O6E-C5E-C6E-O5E
29	2	317	LMU	C4B-C5B-C6B-O6B
21	1	308	CLA	C3-C5-C6-C7
21	g	308	CLA	C3-C5-C6-C7
28	M	102	LMG	C29-C28-O8-C9
28	f	102	LMG	O6-C5-C6-O5
24	1	315	KC1	CAA-CBA-CGA-O2A
24	7	315	KC1	CAA-CBA-CGA-O1A
29	g	316	LMU	C4'-C5'-C6'-O6'
21	J	301	CLA	O1A-CGA-O2A-C1
21	c	504	CLA	O1A-CGA-O2A-C1
21	g	308	CLA	O1A-CGA-O2A-C1
23	2	308	A86	O5-C38-O4-C34
28	N	101	LMG	O6-C5-C6-O5
29	2	317	LMU	O5'-C5'-C6'-O6'
29	D	412	LMU	O5B-C5B-C6B-O6B
21	1	308	CLA	C4-C3-C5-C6
21	B	604	CLA	C4-C3-C5-C6
21	b	605	CLA	C4-C3-C5-C6
21	b	623	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	301	CLA	C4-C3-C5-C6
21	8	302	CLA	C4-C3-C5-C6
21	d	406	CLA	C4-C3-C5-C6
21	C	506	CLA	C4-C3-C5-C6
21	c	505	CLA	C4-C3-C5-C6
21	9	301	CLA	C4-C3-C5-C6
21	4	300	CLA	C4-C3-C5-C6
21	1	308	CLA	C2-C3-C5-C6
21	B	604	CLA	C2-C3-C5-C6
21	b	605	CLA	C2-C3-C5-C6
21	b	623	CLA	C2-C3-C5-C6
21	2	301	CLA	C2-C3-C5-C6
21	8	302	CLA	C2-C3-C5-C6
21	d	406	CLA	C2-C3-C5-C6
21	C	506	CLA	C2-C3-C5-C6
21	C	510	CLA	C2-C3-C5-C6
21	c	505	CLA	C2-C3-C5-C6
21	9	301	CLA	C2-C3-C5-C6
21	4	300	CLA	C2-C3-C5-C6
21	7	303	CLA	C2A-CAA-CBA-CGA
21	B	603	CLA	C2A-CAA-CBA-CGA
23	1	312	A86	C39-C38-O4-C34
28	B	623	LMG	O6-C5-C6-O5
28	b	624	LMG	O6-C5-C6-O5
21	1	308	CLA	O1A-CGA-O2A-C1
21	2	305	CLA	O1A-CGA-O2A-C1
21	C	514	CLA	O1A-CGA-O2A-C1
21	g	304	CLA	O1A-CGA-O2A-C1
30	C	518	DGD	O6D-C1D-O3G-C3G
31	C	502	SQD	O5-C1-O6-C44
21	9	303	CLA	C4C-C3C-CAC-CBC
21	C	505	CLA	C3-C5-C6-C7
21	2	305	CLA	CBA-CGA-O2A-C1
21	C	506	CLA	CBA-CGA-O2A-C1
27	D	410	LHG	C23-C24-C25-C26
24	1	315	KC1	CAA-CBA-CGA-O1A
24	1	316	KC1	CAA-CBA-CGA-O1A
24	6	312	KC1	CAA-CBA-CGA-O2A
24	7	314	KC1	CAA-CBA-CGA-O1A
24	J	312	KC1	CAA-CBA-CGA-O1A
24	8	315	KC1	CAA-CBA-CGA-O1A
24	g	314	KC1	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	g	315	KC1	CAA-CBA-CGA-O1A
29	A	408	LMU	O5B-C1B-O1B-C4'
29	5	316	LMU	O5B-C1B-O1B-C4'
28	b	624	LMG	C4-C5-C6-O5
29	D	412	LMU	C3'-C4'-O1B-C1B
21	b	608	CLA	O1D-CGD-O2D-CED
28	B	622	LMG	C4-C5-C6-O5
28	2	318	LMG	C4-C5-C6-O5
21	7	301	CLA	C3-C5-C6-C7
21	d	406	CLA	C3-C5-C6-C7
21	3	301	CLA	C3-C5-C6-C7
21	B	621	CLA	CBA-CGA-O2A-C1
21	J	306	CLA	CBA-CGA-O2A-C1
21	c	505	CLA	CBA-CGA-O2A-C1
21	c	513	CLA	CBA-CGA-O2A-C1
21	4	302	CLA	CBA-CGA-O2A-C1
21	b	608	CLA	C10-C11-C12-C13
24	8	316	KC1	CBD-CGD-O2D-CED
22	5	310	DD6	C3-C4-C5-C6
23	6	309	A86	C1-C2-C3-C4
23	W	101	A86	C1-C2-C3-C4
23	2	310	A86	C11-C10-C9-C8
23	2	311	A86	C3-C4-C5-C6
23	2	312	A86	C3-C4-C5-C6
23	8	311	A86	C11-C10-C9-C8
27	a	401	LHG	C23-C24-C25-C26
21	b	615	CLA	C8-C10-C11-C12
28	B	623	LMG	C4-C5-C6-O5
28	N	101	LMG	C4-C5-C6-O5
28	8	301	LMG	C7-C8-C9-O8
24	1	316	KC1	CAA-CBA-CGA-O2A
24	6	313	KC1	CAA-CBA-CGA-O1A
24	7	314	KC1	CAA-CBA-CGA-O2A
24	7	315	KC1	CAA-CBA-CGA-O2A
24	J	312	KC1	CAA-CBA-CGA-O2A
24	J	313	KC1	CAA-CBA-CGA-O2A
24	2	315	KC1	CAA-CBA-CGA-O2A
24	4	308	KC1	CAA-CBA-CGA-O2A
24	5	314	KC1	CAA-CBA-CGA-O1A
24	g	313	KC1	CAA-CBA-CGA-O1A
24	g	315	KC1	CAA-CBA-CGA-O2A
24	G	309	KC1	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	D	412	LMU	C4'-C5'-C6'-O6'
21	2	301	CLA	C5-C6-C7-C8
21	g	308	CLA	C5-C6-C7-C8
27	D	410	LHG	O2-C2-C3-O3
27	d	409	LHG	O2-C2-C3-O3
27	B	601	LHG	C23-C24-C25-C26
27	d	409	LHG	C7-C8-C9-C10
30	b	601	DGD	O1G-C1G-C2G-O2G
21	c	513	CLA	O1A-CGA-O2A-C1
28	B	622	LMG	O10-C28-O8-C9
29	g	316	LMU	O5'-C5'-C6'-O6'
21	B	606	CLA	C2-C3-C5-C6
21	b	607	CLA	C2-C3-C5-C6
21	7	302	CLA	C11-C12-C13-C14
21	7	304	CLA	C11-C10-C8-C9
21	B	603	CLA	C14-C13-C15-C16
21	B	613	CLA	C14-C13-C15-C16
21	b	604	CLA	C14-C13-C15-C16
21	b	608	CLA	C11-C10-C8-C9
21	g	308	CLA	C13-C15-C16-C17
21	6	308	CLA	C2A-CAA-CBA-CGA
21	J	301	CLA	C2A-CAA-CBA-CGA
21	5	303	CLA	C2A-CAA-CBA-CGA
22	7	310	DD6	C12-C11-C13-C14
22	5	310	DD6	C-C1-C24-C25
23	1	312	A86	C7-C6-C8-C9
23	1	313	A86	C-C1-C24-C25
23	1	314	A86	C-C1-C24-C25
23	7	311	A86	C7-C6-C8-C9
23	2	310	A86	C7-C6-C8-C9
23	2	312	A86	C7-C6-C8-C9
23	8	310	A86	C7-C6-C8-C9
23	g	311	A86	C7-C6-C8-C9
25	h	101	BCR	C37-C22-C23-C24
25	c	515	BCR	C37-C22-C23-C24
22	7	310	DD6	C10-C11-C13-C14
22	5	310	DD6	C2-C1-C24-C25
23	1	312	A86	C5-C6-C8-C9
23	1	313	A86	C2-C1-C24-C25
23	7	311	A86	C5-C6-C8-C9
23	2	312	A86	C5-C6-C8-C9
23	g	311	A86	C5-C6-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	h	101	BCR	C11-C12-C13-C14
25	c	515	BCR	C21-C22-C23-C24
27	D	410	LHG	C7-C8-C9-C10
28	8	301	LMG	C28-C29-C30-C31
30	c	517	DGD	C1B-C2B-C3B-C4B
21	B	621	CLA	O1A-CGA-O2A-C1
21	4	302	CLA	O1A-CGA-O2A-C1
21	d	406	CLA	C10-C11-C12-C13
21	C	506	CLA	C10-C11-C12-C13
21	4	304	CLA	C8-C10-C11-C12
21	g	306	CLA	C10-C11-C12-C13
21	1	305	CLA	CBD-CGD-O2D-CED
29	2	317	LMU	C4'-C5'-C6'-O6'
24	6	313	KC1	CAA-CBA-CGA-O2A
24	J	313	KC1	CAA-CBA-CGA-O1A
24	8	315	KC1	CAA-CBA-CGA-O2A
24	4	308	KC1	CAA-CBA-CGA-O1A
24	5	313	KC1	CAA-CBA-CGA-O1A
24	5	314	KC1	CAA-CBA-CGA-O2A
24	g	313	KC1	CAA-CBA-CGA-O2A
24	G	307	KC1	CAA-CBA-CGA-O1A
23	8	309	A86	O5-C38-O4-C34
21	c	504	CLA	C3-C5-C6-C7
21	J	308	CLA	CBA-CGA-O2A-C1
21	G	302	CLA	CBA-CGA-O2A-C1
21	1	302	CLA	C8-C10-C11-C12
21	1	302	CLA	C10-C11-C12-C13
21	1	303	CLA	C8-C10-C11-C12
21	6	307	CLA	C10-C11-C12-C13
21	7	303	CLA	C5-C6-C7-C8
21	B	613	CLA	C10-C11-C12-C13
21	J	307	CLA	C10-C11-C12-C13
21	C	511	CLA	C13-C15-C16-C17
21	G	304	CLA	C8-C10-C11-C12
27	d	402	LHG	C32-C33-C34-C35
23	2	309	A86	C2-C3-C4-C5
21	1	304	CLA	C13-C15-C16-C17
21	b	604	CLA	C13-C15-C16-C17
21	b	614	CLA	C10-C11-C12-C13
21	2	305	CLA	C13-C15-C16-C17
21	C	506	CLA	C15-C16-C17-C18
21	c	504	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	G	300	CLA	C10-C11-C12-C13
28	a	407	LMG	C28-C29-C30-C31
28	b	620	LMG	C28-C29-C30-C31
28	b	622	LMG	C10-C11-C12-C13
28	b	625	LMG	C10-C11-C12-C13
28	f	102	LMG	C10-C11-C12-C13
28	f	102	LMG	C28-C29-C30-C31
28	8	317	LMG	C28-C29-C30-C31
28	D	411	LMG	C28-C29-C30-C31
30	h	103	DGD	C1A-C2A-C3A-C4A
30	C	517	DGD	O6E-C5E-C6E-O5E
21	B	604	CLA	CBD-CGD-O2D-CED
21	B	603	CLA	C10-C11-C12-C13
21	B	612	CLA	C8-C10-C11-C12
21	B	614	CLA	C15-C16-C17-C18
21	b	613	CLA	C8-C10-C11-C12
21	9	301	CLA	C5-C6-C7-C8
21	g	302	CLA	C5-C6-C7-C8
21	6	306	CLA	CBA-CGA-O2A-C1
28	B	622	LMG	C29-C28-O8-C9
23	G	305	A86	O5-C38-O4-C34
27	d	402	LHG	C29-C30-C31-C32
30	B	624	DGD	O1B-C1B-O2G-C2G
24	2	315	KC1	CAA-CBA-CGA-O1A
24	5	313	KC1	CAA-CBA-CGA-O2A
24	g	314	KC1	CAA-CBA-CGA-O2A
24	G	307	KC1	CAA-CBA-CGA-O2A
24	G	309	KC1	CAA-CBA-CGA-O1A
30	H	101	DGD	C4E-C5E-C6E-O5E
21	B	606	CLA	C5-C6-C7-C8
21	B	621	CLA	C10-C11-C12-C13
21	b	607	CLA	C5-C6-C7-C8
28	2	318	LMG	C28-C29-C30-C31
30	H	101	DGD	C1A-C2A-C3A-C4A
29	8	318	LMU	O1'-C1-C2-C3
21	C	505	CLA	C15-C16-C17-C18
21	J	300	CLA	C4-C3-C5-C6
21	5	306	CLA	C12-C13-C15-C16
21	9	301	CLA	C3-C5-C6-C7
21	c	505	CLA	O1A-CGA-O2A-C1
30	C	517	DGD	O1A-C1A-O1G-C1G
22	5	310	DD6	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	g	310	DD6	C1-C2-C3-C4
23	1	312	A86	C24-C25-C26-C27
23	6	310	A86	C1-C2-C3-C4
23	7	311	A86	C3-C4-C5-C6
23	J	310	A86	C1-C2-C3-C4
23	W	101	A86	C11-C10-C9-C8
23	2	309	A86	C11-C10-C9-C8
23	8	308	A86	C3-C4-C5-C6
23	g	312	A86	C11-C10-C9-C8
23	g	312	A86	C3-C4-C5-C6
23	G	305	A86	C1-C2-C3-C4
25	h	101	BCR	C13-C14-C15-C16
21	B	610	CLA	C2A-CAA-CBA-CGA
21	C	509	CLA	C2A-CAA-CBA-CGA
21	c	509	CLA	C2A-CAA-CBA-CGA
21	G	302	CLA	C2A-CAA-CBA-CGA
24	7	315	KC1	O1D-CGD-O2D-CED
21	B	610	CLA	C15-C16-C17-C18
21	b	604	CLA	C15-C16-C17-C18
21	5	308	CLA	C10-C11-C12-C13
21	g	306	CLA	C5-C6-C7-C8
21	G	300	CLA	C13-C15-C16-C17
21	G	302	CLA	C5-C6-C7-C8
29	D	412	LMU	C4B-C5B-C6B-O6B
24	6	312	KC1	CAA-CBA-CGA-O1A
24	8	313	KC1	CAA-CBA-CGA-O2A
25	h	101	BCR	C22-C23-C24-C25
21	J	306	CLA	O1A-CGA-O2A-C1
21	C	506	CLA	O1A-CGA-O2A-C1
30	c	516	DGD	O1A-C1A-O1G-C1G
29	8	318	LMU	C4'-C5'-C6'-O6'
21	J	306	CLA	C13-C15-C16-C17
21	c	511	CLA	C8-C10-C11-C12
21	5	306	CLA	C8-C10-C11-C12
24	1	316	KC1	O1D-CGD-O2D-CED
35	d	408	PL9	C39-C41-C42-C43
22	g	310	DD6	C1-C24-C25-C26
23	1	314	A86	C1-C24-C25-C26
23	6	310	A86	C6-C8-C9-C10
23	7	313	A86	C6-C8-C9-C10
23	2	308	A86	C6-C8-C9-C10
23	2	309	A86	C6-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	4	305	A86	C6-C8-C9-C10
23	g	312	A86	C6-C8-C9-C10
23	G	305	A86	C6-C8-C9-C10
25	C	501	BCR	C10-C11-C12-C13
25	c	501	BCR	C10-C11-C12-C13
21	B	621	CLA	C3-C5-C6-C7
21	c	510	CLA	C3-C5-C6-C7
21	5	306	CLA	C3-C5-C6-C7
21	6	307	CLA	C8-C10-C11-C12
21	B	621	CLA	C8-C10-C11-C12
21	4	300	CLA	C8-C10-C11-C12
21	4	302	CLA	C5-C6-C7-C8
21	G	302	CLA	O1A-CGA-O2A-C1
30	h	103	DGD	C4E-C5E-C6E-O5E
21	b	606	CLA	C10-C11-C12-C13
21	b	608	CLA	C15-C16-C17-C18
21	8	306	CLA	C5-C6-C7-C8
21	C	514	CLA	C10-C11-C12-C13
21	6	306	CLA	O1A-CGA-O2A-C1
21	B	607	CLA	C15-C16-C17-C18
21	B	613	CLA	C13-C15-C16-C17
21	c	508	CLA	C8-C10-C11-C12
21	4	300	CLA	C10-C11-C12-C13
21	5	309	CLA	C10-C11-C12-C13
27	A	406	LHG	C3-O3-P-O6
21	6	308	CLA	CBA-CGA-O2A-C1
21	d	406	CLA	CBA-CGA-O2A-C1
26	A	403	PHO	CBD-CGD-O2D-CED
27	l	101	LHG	C23-C24-C25-C26
28	B	622	LMG	C10-C11-C12-C13
28	b	626	LMG	O9-C10-O7-C8
21	C	509	CLA	C4-C3-C5-C6
21	7	307	CLA	C2-C3-C5-C6
21	6	301	CLA	C2A-CAA-CBA-CGA
21	J	308	CLA	C2A-CAA-CBA-CGA
21	2	301	CLA	C2A-CAA-CBA-CGA
21	2	305	CLA	C16-C17-C18-C20
21	C	506	CLA	C3-C5-C6-C7
21	1	303	CLA	CBA-CGA-O2A-C1
21	1	305	CLA	CBA-CGA-O2A-C1
21	1	310	CLA	CBA-CGA-O2A-C1
23	8	312	A86	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	g	301	LMU	O1'-C1-C2-C3
22	7	310	DD6	C24-C25-C26-C27
23	1	312	A86	C11-C10-C9-C8
23	7	311	A86	C11-C10-C9-C8
23	J	309	A86	C1-C2-C3-C4
23	W	101	A86	C3-C4-C5-C6
23	2	311	A86	C1-C2-C3-C4
23	8	312	A86	C1-C2-C3-C4
23	4	305	A86	C1-C2-C3-C4
23	7	312	A86	C35-C34-O4-C38
28	b	622	LMG	C28-C29-C30-C31
31	C	502	SQD	C23-C24-C25-C26
27	D	403	LHG	C28-C29-C30-C31
29	5	301	LMU	O1'-C1-C2-C3
21	5	309	CLA	C8-C10-C11-C12
22	1	311	DD6	C4-C5-C6-C7
22	7	310	DD6	C4-C5-C6-C7
23	6	309	A86	C4-C5-C6-C7
23	2	308	A86	C-C1-C2-C3
23	2	310	A86	C-C1-C2-C3
23	2	312	A86	C-C1-C2-C3
23	8	311	A86	C-C1-C2-C3
23	8	311	A86	C4-C5-C6-C7
23	8	312	A86	C4-C5-C6-C7
23	g	312	A86	C4-C5-C6-C7
25	1	317	BCR	C35-C13-C14-C15
25	1	317	BCR	C16-C17-C18-C36
25	B	617	BCR	C16-C17-C18-C36
25	B	617	BCR	C20-C21-C22-C37
25	h	101	BCR	C11-C10-C9-C34
25	C	501	BCR	C16-C17-C18-C36
25	C	501	BCR	C20-C21-C22-C37
30	c	517	DGD	O6D-C5D-C6D-O5D
21	C	504	CLA	C6-C7-C8-C10
27	D	410	LHG	C15-C16-C17-C18
27	d	409	LHG	C15-C16-C17-C18
28	b	620	LMG	C15-C16-C17-C18
28	b	624	LMG	C17-C18-C19-C20
30	B	624	DGD	C6B-C7B-C8B-C9B
31	B	626	SQD	C16-C17-C18-C19
23	8	309	A86	C9-C10-C11-C12
23	8	311	A86	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	5	312	A86	C9-C10-C11-C12
24	J	311	KC1	C2A-CAA-CBA-CGA
24	2	313	KC1	C2A-CAA-CBA-CGA
24	9	305	KC1	C2A-CAA-CBA-CGA
24	9	306	KC1	C2A-CAA-CBA-CGA
24	5	315	KC1	C2A-CAA-CBA-CGA
21	C	510	CLA	CBA-CGA-O2A-C1
27	l	101	LHG	C28-C29-C30-C31
28	A	407	LMG	C30-C31-C32-C33
28	B	627	LMG	C31-C32-C33-C34
28	b	626	LMG	C11-C12-C13-C14
28	f	102	LMG	C11-C12-C13-C14
28	f	102	LMG	C33-C34-C35-C36
30	c	516	DGD	C5B-C6B-C7B-C8B
24	9	305	KC1	CAA-CBA-CGA-O2A
28	B	627	LMG	C10-C11-C12-C13
27	a	401	LHG	C28-C29-C30-C31
27	d	409	LHG	C28-C29-C30-C31
28	f	102	LMG	C32-C33-C34-C35
28	2	318	LMG	C13-C14-C15-C16
31	b	602	SQD	C18-C19-C20-C21
31	b	602	SQD	C29-C30-C31-C32
28	B	623	LMG	C15-C16-C17-C18
28	L	101	LMG	C13-C14-C15-C16
30	B	624	DGD	C4A-C5A-C6A-C7A
30	h	103	DGD	C6A-C7A-C8A-C9A
28	f	102	LMG	C4-C5-C6-O5
21	7	304	CLA	C8-C10-C11-C12
21	B	616	CLA	C10-C11-C12-C13
27	a	401	LHG	C32-C33-C34-C35
27	d	409	LHG	C27-C28-C29-C30
28	B	623	LMG	C13-C14-C15-C16
28	M	102	LMG	C31-C32-C33-C34
28	2	318	LMG	C40-C41-C42-C43
28	8	317	LMG	C41-C42-C43-C44
31	b	602	SQD	C30-C31-C32-C33
22	1	311	DD6	C4-C5-C6-C8
22	7	310	DD6	C4-C5-C6-C8
23	6	309	A86	C4-C5-C6-C8
23	J	309	A86	C24-C1-C2-C3
23	2	308	A86	C24-C1-C2-C3
23	2	310	A86	C24-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	2	312	A86	C24-C1-C2-C3
23	8	311	A86	C24-C1-C2-C3
23	8	311	A86	C4-C5-C6-C8
23	8	312	A86	C4-C5-C6-C8
23	g	312	A86	C4-C5-C6-C8
25	1	317	BCR	C12-C13-C14-C15
25	h	101	BCR	C12-C13-C14-C15
29	5	301	LMU	C2'-C1'-O1'-C1
29	g	301	LMU	C2'-C1'-O1'-C1
30	C	518	DGD	C2D-C1D-O3G-C3G
30	c	517	DGD	C2E-C1E-O5D-C6D
31	B	625	SQD	C2-C1-O6-C44
31	B	626	SQD	C2-C1-O6-C44
31	b	602	SQD	C2-C1-O6-C44
29	8	318	LMU	C4B-C5B-C6B-O6B
23	J	309	A86	O5-C38-O4-C34
27	A	406	LHG	C26-C27-C28-C29
27	A	406	LHG	C34-C35-C36-C37
27	D	403	LHG	C32-C33-C34-C35
27	D	410	LHG	C14-C15-C16-C17
27	D	410	LHG	C28-C29-C30-C31
29	A	408	LMU	C3-C4-C5-C6
31	C	502	SQD	C9-C10-C11-C12
21	B	616	CLA	C15-C16-C17-C18
21	4	304	CLA	C10-C11-C12-C13
21	6	308	CLA	O1A-CGA-O2A-C1
21	a	405	CLA	C11-C12-C13-C14
35	d	408	PL9	C37-C38-C39-C40
35	d	408	PL9	C40-C39-C41-C42
27	A	406	LHG	C31-C32-C33-C34
28	B	619	LMG	C36-C37-C38-C39
28	L	101	LMG	C14-C15-C16-C17
28	b	625	LMG	C37-C38-C39-C40
28	b	626	LMG	C32-C33-C34-C35
28	8	317	LMG	C16-C17-C18-C19
21	A	404	CLA	C6-C7-C8-C9
21	B	621	CLA	C11-C12-C13-C14
21	b	613	CLA	C11-C12-C13-C14
21	C	509	CLA	C14-C13-C15-C16
21	C	512	CLA	C6-C7-C8-C9
21	C	506	CLA	C8-C10-C11-C12
28	B	619	LMG	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	M	102	LMG	C32-C33-C34-C35
28	a	407	LMG	C33-C34-C35-C36
30	b	601	DGD	C4A-C5A-C6A-C7A
30	h	103	DGD	CAB-CBB-CCB-CDB
21	a	405	CLA	C10-C11-C12-C13
24	8	313	KC1	CAA-CBA-CGA-O1A
24	9	305	KC1	CAA-CBA-CGA-O1A
24	3	305	KC1	CAA-CBA-CGA-O1A
24	3	305	KC1	CAA-CBA-CGA-O2A
21	1	304	CLA	C2A-CAA-CBA-CGA
21	7	301	CLA	C2A-CAA-CBA-CGA
21	J	307	CLA	C2A-CAA-CBA-CGA
21	9	304	CLA	C2A-CAA-CBA-CGA
21	J	308	CLA	O1A-CGA-O2A-C1
22	g	310	DD6	C-C1-C24-C25
25	b	619	BCR	C37-C22-C23-C24
27	a	401	LHG	C14-C15-C16-C17
28	b	626	LMG	C31-C32-C33-C34
30	H	101	DGD	C6A-C7A-C8A-C9A
27	A	406	LHG	O1-C1-C2-C3
27	D	403	LHG	O1-C1-C2-C3
27	D	410	LHG	O1-C1-C2-C3
27	d	402	LHG	O1-C1-C2-C3
27	d	409	LHG	O1-C1-C2-C3
22	g	310	DD6	C2-C1-C24-C25
28	8	301	LMG	O7-C8-C9-O8
21	b	617	CLA	C10-C11-C12-C13
28	D	411	LMG	C11-C10-O7-C8
27	D	410	LHG	C29-C30-C31-C32
28	B	623	LMG	C30-C31-C32-C33
30	b	601	DGD	C6B-C7B-C8B-C9B
30	C	517	DGD	C5A-C6A-C7A-C8A
31	B	626	SQD	C29-C30-C31-C32
31	X	401	SQD	C9-C10-C11-C12
28	L	101	LMG	C29-C28-O8-C9
31	X	401	SQD	C23-C24-C25-C26
27	B	601	LHG	C15-C16-C17-C18
27	l	101	LHG	C15-C16-C17-C18
28	A	407	LMG	C32-C33-C34-C35
28	B	619	LMG	C38-C39-C40-C41
28	B	623	LMG	C14-C15-C16-C17
28	D	411	LMG	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	b	602	SQD	C12-C13-C14-C15
28	8	317	LMG	O6-C5-C6-O5
21	a	405	CLA	C11-C12-C13-C15
21	2	305	CLA	C16-C17-C18-C19
21	G	304	CLA	C16-C17-C18-C19
21	G	304	CLA	C16-C17-C18-C20
29	5	301	LMU	O5'-C1'-O1'-C1
29	g	301	LMU	O5'-C1'-O1'-C1
30	c	517	DGD	O6E-C1E-O5D-C6D
21	B	614	CLA	C8-C10-C11-C12
21	b	617	CLA	C15-C16-C17-C18
27	A	406	LHG	C14-C15-C16-C17
27	B	601	LHG	C24-C25-C26-C27
27	D	410	LHG	C13-C14-C15-C16
28	b	622	LMG	C30-C31-C32-C33
30	h	103	DGD	CBB-CCB-CDB-CEB
30	c	516	DGD	C5A-C6A-C7A-C8A
31	B	626	SQD	C17-C18-C19-C20
31	b	602	SQD	C17-C18-C19-C20
27	B	601	LHG	C12-C13-C14-C15
27	B	601	LHG	C30-C31-C32-C33
28	b	625	LMG	C30-C31-C32-C33
30	B	624	DGD	C4B-C5B-C6B-C7B
30	h	103	DGD	C6B-C7B-C8B-C9B
31	B	626	SQD	C12-C13-C14-C15
31	X	401	SQD	C11-C10-C9-C8
21	1	310	CLA	O1A-CGA-O2A-C1
27	l	101	LHG	C12-C13-C14-C15
28	a	407	LMG	C32-C33-C34-C35
28	b	620	LMG	C34-C35-C36-C37
28	2	318	LMG	C41-C42-C43-C44
21	4	304	CLA	C3-C5-C6-C7
21	g	306	CLA	CBA-CGA-O2A-C1
28	D	411	LMG	C13-C14-C15-C16
31	b	602	SQD	C9-C10-C11-C12
21	1	302	CLA	C3A-C2A-CAA-CBA
21	1	308	CLA	C3A-C2A-CAA-CBA
21	6	306	CLA	C3A-C2A-CAA-CBA
21	7	301	CLA	C3A-C2A-CAA-CBA
21	7	308	CLA	C3A-C2A-CAA-CBA
21	7	309	CLA	C3A-C2A-CAA-CBA
21	B	603	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	616	CLA	C3A-C2A-CAA-CBA
21	J	306	CLA	C3A-C2A-CAA-CBA
21	a	402	CLA	C3A-C2A-CAA-CBA
21	2	301	CLA	C3A-C2A-CAA-CBA
21	2	305	CLA	C3A-C2A-CAA-CBA
21	8	302	CLA	C3A-C2A-CAA-CBA
21	C	509	CLA	C3A-C2A-CAA-CBA
21	9	303	CLA	C3A-C2A-CAA-CBA
21	3	302	CLA	C3A-C2A-CAA-CBA
21	4	301	CLA	C3A-C2A-CAA-CBA
21	4	303	CLA	C3A-C2A-CAA-CBA
21	5	303	CLA	C3A-C2A-CAA-CBA
21	5	308	CLA	C3A-C2A-CAA-CBA
21	g	303	CLA	C3A-C2A-CAA-CBA
21	g	304	CLA	C3A-C2A-CAA-CBA
21	G	301	CLA	C3A-C2A-CAA-CBA
26	d	403	PHO	C3A-C2A-CAA-CBA
21	C	510	CLA	C10-C11-C12-C13
28	L	101	LMG	O6-C5-C6-O5
23	7	311	A86	C24-C25-C26-C27
29	2	317	LMU	C2-C1-O1'-C1'
29	8	318	LMU	C2-C1-O1'-C1'
27	A	406	LHG	C33-C34-C35-C36
28	B	619	LMG	C31-C32-C33-C34
28	B	619	LMG	C37-C38-C39-C40
28	8	317	LMG	C40-C41-C42-C43
31	B	625	SQD	C25-C26-C27-C28
24	2	316	KC1	O1D-CGD-O2D-CED
21	d	406	CLA	O1A-CGA-O2A-C1
27	A	406	LHG	C15-C16-C17-C18
28	b	620	LMG	C13-C14-C15-C16
31	B	626	SQD	C30-C31-C32-C33
31	C	502	SQD	C10-C11-C12-C13
21	b	615	CLA	C12-C13-C15-C16
30	H	101	DGD	CBB-CCB-CDB-CEB
30	B	624	DGD	O6D-C5D-C6D-O5D
30	b	601	DGD	O6D-C5D-C6D-O5D
21	1	301	CLA	C3-C5-C6-C7
23	8	311	A86	C9-C10-C11-C13
27	D	403	LHG	C31-C32-C33-C34
21	C	510	CLA	O1A-CGA-O2A-C1
35	D	409	PL9	C13-C14-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	d	408	PL9	C13-C14-C16-C17
27	d	409	LHG	O1-C1-C2-O2
21	6	306	CLA	C13-C15-C16-C17
28	B	627	LMG	C11-C12-C13-C14
28	b	620	LMG	C38-C39-C40-C41
30	c	517	DGD	C7B-C8B-C9B-CAB
21	8	307	CLA	C2A-CAA-CBA-CGA
21	2	303	CLA	O1D-CGD-O2D-CED
21	1	303	CLA	O1A-CGA-O2A-C1
23	8	308	A86	C39-C38-O4-C34
28	a	407	LMG	C34-C35-C36-C37
28	8	317	LMG	C18-C19-C20-C21
27	d	409	LHG	C30-C31-C32-C33
30	h	103	DGD	C5B-C6B-C7B-C8B
21	8	302	CLA	C3-C5-C6-C7
28	a	407	LMG	O6-C5-C6-O5
21	2	303	CLA	CBA-CGA-O2A-C1
21	5	308	CLA	CBA-CGA-O2A-C1
27	d	402	LHG	C30-C31-C32-C33
28	b	620	LMG	C31-C32-C33-C34
28	2	318	LMG	C31-C32-C33-C34
28	D	411	LMG	C20-C21-C22-C23
21	1	305	CLA	O1A-CGA-O2A-C1
27	l	101	LHG	C1-C2-C3-O3
27	A	406	LHG	C32-C33-C34-C35
30	b	601	DGD	C5A-C6A-C7A-C8A
24	8	314	KC1	CAA-CBA-CGA-O1A
21	C	511	CLA	C2-C1-O2A-CGA
21	c	510	CLA	C2-C1-O2A-CGA
23	1	312	A86	O5-C38-O4-C34
27	d	409	LHG	C14-C15-C16-C17
28	B	627	LMG	C33-C34-C35-C36
30	C	518	DGD	C7B-C8B-C9B-CAB
31	b	602	SQD	C16-C17-C18-C19
29	8	318	LMU	C1-C2-C3-C4
28	b	625	LMG	C32-C33-C34-C35
31	C	502	SQD	C33-C34-C35-C36
21	C	511	CLA	C3-C5-C6-C7
25	A	405	BCR	C5-C6-C7-C8
25	A	405	BCR	C23-C24-C25-C26
25	A	405	BCR	C23-C24-C25-C30
25	B	618	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	H	100	BCR	C5-C6-C7-C8
25	M	101	BCR	C1-C6-C7-C8
25	M	101	BCR	C5-C6-C7-C8
25	a	406	BCR	C5-C6-C7-C8
25	a	406	BCR	C23-C24-C25-C26
25	a	406	BCR	C23-C24-C25-C30
25	b	619	BCR	C1-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
25	b	619	BCR	C23-C24-C25-C30
25	h	101	BCR	C1-C6-C7-C8
25	h	101	BCR	C5-C6-C7-C8
25	h	101	BCR	C23-C24-C25-C26
25	h	101	BCR	C23-C24-C25-C30
25	h	102	BCR	C5-C6-C7-C8
25	m	101	BCR	C1-C6-C7-C8
25	m	101	BCR	C5-C6-C7-C8
25	d	407	BCR	C23-C24-C25-C26
25	C	501	BCR	C5-C6-C7-C8
25	c	501	BCR	C5-C6-C7-C8
28	M	102	LMG	C30-C31-C32-C33
32	E	101	HEM	C3D-CAD-CBD-CGD
31	C	502	SQD	C8-C7-O47-C45
27	a	401	LHG	C11-C10-C9-C8
27	a	401	LHG	C15-C16-C17-C18
29	2	317	LMU	C7-C8-C9-C10
30	C	517	DGD	C5B-C6B-C7B-C8B
31	C	502	SQD	C13-C14-C15-C16
21	g	306	CLA	O1A-CGA-O2A-C1
28	D	411	LMG	C10-C11-C12-C13
30	B	624	DGD	C1A-C2A-C3A-C4A
27	l	101	LHG	C27-C28-C29-C30
21	c	502	CLA	C10-C11-C12-C13
29	D	412	LMU	O5'-C5'-C6'-O6'
21	B	609	CLA	C4-C3-C5-C6
21	b	610	CLA	C4-C3-C5-C6
21	7	302	CLA	C11-C12-C13-C15
21	A	404	CLA	C6-C7-C8-C10
21	B	609	CLA	C2-C3-C5-C6
21	B	621	CLA	C11-C12-C13-C15
21	b	608	CLA	C11-C10-C8-C7
21	b	610	CLA	C2-C3-C5-C6
21	b	613	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	C	509	CLA	C12-C13-C15-C16
21	C	512	CLA	C6-C7-C8-C10
21	g	308	CLA	C11-C10-C8-C7
21	G	304	CLA	C6-C7-C8-C10
21	9	300	CLA	C3-C5-C6-C7
21	G	304	CLA	C3-C5-C6-C7
21	2	303	CLA	O1A-CGA-O2A-C1
23	g	311	A86	C11-C10-C9-C8
30	C	518	DGD	C1B-C2B-C3B-C4B
21	5	307	CLA	CBA-CGA-O2A-C1
27	d	409	LHG	C32-C33-C34-C35
21	1	303	CLA	C2A-CAA-CBA-CGA
21	8	306	CLA	C2A-CAA-CBA-CGA
21	C	503	CLA	C2A-CAA-CBA-CGA
21	C	505	CLA	C2A-CAA-CBA-CGA
21	c	502	CLA	C2A-CAA-CBA-CGA
21	c	504	CLA	C2A-CAA-CBA-CGA
21	5	307	CLA	C2A-CAA-CBA-CGA
21	B	614	CLA	C12-C13-C15-C16
27	a	401	LHG	C18-C19-C20-C21
28	A	407	LMG	C18-C19-C20-C21
28	B	623	LMG	C29-C30-C31-C32
28	a	407	LMG	C31-C32-C33-C34
28	f	102	LMG	C29-C30-C31-C32
28	f	102	LMG	C31-C32-C33-C34
29	D	412	LMU	C2-C3-C4-C5
30	c	516	DGD	C2B-C3B-C4B-C5B
31	b	602	SQD	C10-C11-C12-C13
28	B	627	LMG	C32-C33-C34-C35
28	b	620	LMG	C39-C40-C41-C42
31	B	626	SQD	C9-C10-C11-C12
31	C	502	SQD	C31-C32-C33-C34
21	B	613	CLA	C5-C6-C7-C8
26	A	403	PHO	C5-C6-C7-C8
28	A	407	LMG	C14-C15-C16-C17
28	B	619	LMG	C17-C18-C19-C20
28	B	619	LMG	C33-C34-C35-C36
28	a	407	LMG	C18-C19-C20-C21
29	a	408	LMU	C3-C4-C5-C6
24	1	315	KC1	C2B-C3B-CAB-CBB
24	6	311	KC1	C2B-C3B-CAB-CBB
24	6	313	KC1	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	7	314	KC1	C2B-C3B-CAB-CBB
24	J	313	KC1	C2B-C3B-CAB-CBB
24	2	313	KC1	C2B-C3B-CAB-CBB
24	2	315	KC1	C2B-C3B-CAB-CBB
24	9	306	KC1	C2B-C3B-CAB-CBB
24	3	305	KC1	C2B-C3B-CAB-CBB
24	3	306	KC1	C2B-C3B-CAB-CBB
24	4	306	KC1	C2B-C3B-CAB-CBB
24	5	314	KC1	C2B-C3B-CAB-CBB
24	g	314	KC1	C2B-C3B-CAB-CBB
24	g	315	KC1	C2B-C3B-CAB-CBB
24	G	308	KC1	C2B-C3B-CAB-CBB
24	G	309	KC1	C2B-C3B-CAB-CBB
24	2	314	KC1	CAA-CBA-CGA-O1A
24	8	314	KC1	CAA-CBA-CGA-O2A
31	C	502	SQD	C14-C15-C16-C17
25	C	516	BCR	C22-C23-C24-C25
30	c	517	DGD	C4D-C5D-C6D-O5D
21	c	509	CLA	C16-C17-C18-C20
28	a	407	LMG	O6-C1-O1-C7
30	C	517	DGD	O6D-C1D-O3G-C3G
30	c	516	DGD	O6D-C1D-O3G-C3G
21	b	615	CLA	C15-C16-C17-C18
21	C	503	CLA	C10-C11-C12-C13
28	N	101	LMG	C29-C30-C31-C32
28	a	407	LMG	C29-C30-C31-C32
28	D	411	LMG	C15-C16-C17-C18
28	B	622	LMG	C11-C10-O7-C8
28	b	624	LMG	C11-C10-O7-C8
28	f	102	LMG	C11-C10-O7-C8
31	B	625	SQD	C8-C7-O47-C45
29	a	408	LMU	O5'-C5'-C6'-O6'
25	1	317	BCR	C10-C11-C12-C13
27	d	409	LHG	C31-C32-C33-C34
28	B	619	LMG	C13-C14-C15-C16
28	b	620	LMG	C17-C18-C19-C20
24	1	315	KC1	C4B-C3B-CAB-CBB
24	6	313	KC1	C4B-C3B-CAB-CBB
24	7	314	KC1	C4B-C3B-CAB-CBB
24	J	313	KC1	C4B-C3B-CAB-CBB
24	2	315	KC1	C4B-C3B-CAB-CBB
24	8	314	KC1	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	9	306	KC1	C4B-C3B-CAB-CBB
24	3	305	KC1	C4B-C3B-CAB-CBB
24	3	306	KC1	C4B-C3B-CAB-CBB
24	4	306	KC1	C4B-C3B-CAB-CBB
24	g	314	KC1	C4B-C3B-CAB-CBB
24	G	308	KC1	C4B-C3B-CAB-CBB
21	7	300	CLA	C10-C11-C12-C13
21	c	508	CLA	C13-C15-C16-C17
27	l	101	LHG	C25-C26-C27-C28
30	B	624	DGD	C4D-C5D-C6D-O5D
30	b	601	DGD	C4D-C5D-C6D-O5D
30	b	601	DGD	C5B-C6B-C7B-C8B
28	B	619	LMG	O7-C8-C9-O8
28	B	622	LMG	O7-C8-C9-O8
30	B	624	DGD	O1G-C1G-C2G-O2G
28	a	407	LMG	C37-C38-C39-C40
30	B	624	DGD	C5B-C6B-C7B-C8B
24	6	311	KC1	CAA-CBA-CGA-O1A
21	5	308	CLA	O1A-CGA-O2A-C1
30	c	517	DGD	C2B-C3B-C4B-C5B
29	5	301	LMU	O5B-C5B-C6B-O6B
21	g	306	CLA	C15-C16-C17-C18
21	C	505	CLA	C4-C3-C5-C6
21	J	300	CLA	C2-C3-C5-C6
21	C	505	CLA	C2-C3-C5-C6
21	C	509	CLA	C2-C3-C5-C6
22	g	310	DD6	C27-C29-C30-C31
28	B	619	LMG	C11-C12-C13-C14
28	B	619	LMG	C34-C35-C36-C37
21	7	303	CLA	C14-C13-C15-C16
21	B	607	CLA	C11-C12-C13-C14
21	B	612	CLA	C11-C12-C13-C14
21	b	617	CLA	C11-C10-C8-C9
21	C	506	CLA	C11-C12-C13-C14
21	c	508	CLA	C14-C13-C15-C16
21	5	306	CLA	C14-C13-C15-C16
26	a	404	PHO	CBD-CGD-O2D-CED
31	B	626	SQD	C10-C11-C12-C13
21	7	300	CLA	C2A-CAA-CBA-CGA
21	B	616	CLA	C2A-CAA-CBA-CGA
30	c	516	DGD	C4A-C5A-C6A-C7A
30	C	517	DGD	C2A-C1A-O1G-C1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	516	BCR	C37-C22-C23-C24
30	C	518	DGD	O6D-C5D-C6D-O5D
21	8	302	CLA	C8-C10-C11-C12
21	4	300	CLA	C15-C16-C17-C18
26	A	403	PHO	C15-C16-C17-C18
26	a	404	PHO	C15-C16-C17-C18
28	8	317	LMG	C31-C32-C33-C34
30	C	518	DGD	C2B-C3B-C4B-C5B
21	1	302	CLA	C1A-C2A-CAA-CBA
21	1	304	CLA	C1A-C2A-CAA-CBA
21	6	300	CLA	C1A-C2A-CAA-CBA
21	6	301	CLA	C1A-C2A-CAA-CBA
21	7	300	CLA	C1A-C2A-CAA-CBA
21	7	301	CLA	C1A-C2A-CAA-CBA
21	7	304	CLA	C1A-C2A-CAA-CBA
21	7	308	CLA	C1A-C2A-CAA-CBA
21	7	309	CLA	C1A-C2A-CAA-CBA
21	B	614	CLA	C1A-C2A-CAA-CBA
21	B	616	CLA	C1A-C2A-CAA-CBA
21	J	300	CLA	C1A-C2A-CAA-CBA
21	J	301	CLA	C1A-C2A-CAA-CBA
21	J	307	CLA	C1A-C2A-CAA-CBA
21	a	402	CLA	C1A-C2A-CAA-CBA
21	b	615	CLA	C1A-C2A-CAA-CBA
21	8	307	CLA	C1A-C2A-CAA-CBA
21	C	509	CLA	C1A-C2A-CAA-CBA
21	9	300	CLA	C1A-C2A-CAA-CBA
21	3	300	CLA	C1A-C2A-CAA-CBA
21	4	301	CLA	C1A-C2A-CAA-CBA
21	4	303	CLA	C1A-C2A-CAA-CBA
21	4	304	CLA	C1A-C2A-CAA-CBA
21	5	302	CLA	C1A-C2A-CAA-CBA
21	5	303	CLA	C1A-C2A-CAA-CBA
21	5	307	CLA	C1A-C2A-CAA-CBA
21	g	302	CLA	C1A-C2A-CAA-CBA
21	g	303	CLA	C1A-C2A-CAA-CBA
21	G	301	CLA	C1A-C2A-CAA-CBA
29	g	301	LMU	O5B-C5B-C6B-O6B
28	2	318	LMG	C11-C10-O7-C8
28	8	317	LMG	C38-C39-C40-C41
29	a	408	LMU	O5B-C1B-O1B-C4'
23	1	313	A86	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	619	BCR	C19-C20-C21-C22
21	B	614	CLA	C5-C6-C7-C8
28	a	407	LMG	C17-C18-C19-C20
28	B	623	LMG	C28-C29-C30-C31
28	a	407	LMG	C10-C11-C12-C13
21	B	604	CLA	O1D-CGD-O2D-CED
28	b	620	LMG	C35-C36-C37-C38
28	b	624	LMG	C14-C15-C16-C17
28	f	102	LMG	C15-C16-C17-C18
27	d	402	LHG	C7-C8-C9-C10
27	l	101	LHG	C29-C30-C31-C32
31	C	502	SQD	C28-C29-C30-C31
28	D	411	LMG	O6-C5-C6-O5
28	A	407	LMG	C39-C40-C41-C42
30	H	101	DGD	C5B-C6B-C7B-C8B
30	b	601	DGD	C4B-C5B-C6B-C7B
24	6	311	KC1	CAA-CBA-CGA-O2A
24	2	314	KC1	CAA-CBA-CGA-O2A
28	B	627	LMG	C13-C14-C15-C16
21	7	302	CLA	C3-C5-C6-C7
26	a	404	PHO	C5-C6-C7-C8
28	b	625	LMG	C31-C32-C33-C34
30	B	624	DGD	C7B-C8B-C9B-CAB
21	B	608	CLA	CBA-CGA-O2A-C1
27	d	402	LHG	C1-C2-C3-O3
35	D	409	PL9	C15-C14-C16-C17
28	D	411	LMG	C11-C12-C13-C14
21	b	608	CLA	C5-C6-C7-C8
27	D	403	LHG	C7-C8-C9-C10
28	A	407	LMG	C11-C10-O7-C8
21	5	307	CLA	O1A-CGA-O2A-C1
27	a	401	LHG	C29-C30-C31-C32
28	2	318	LMG	C11-C12-C13-C14
28	8	317	LMG	C32-C33-C34-C35
21	g	307	CLA	C2A-CAA-CBA-CGA
27	A	406	LHG	C4-C5-C6-O8
28	A	407	LMG	C7-C8-C9-O8
28	A	407	LMG	C12-C13-C14-C15
28	B	619	LMG	C7-C8-C9-O8
28	L	101	LMG	O1-C7-C8-C9
28	b	626	LMG	O1-C7-C8-C9
28	8	317	LMG	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	D	411	LMG	O1-C7-C8-C9
31	B	625	SQD	C44-C45-C46-O48
28	A	407	LMG	O6-C5-C6-O5
27	B	601	LHG	C28-C29-C30-C31
30	C	517	DGD	C4A-C5A-C6A-C7A
28	b	622	LMG	C8-C7-O1-C1
31	X	401	SQD	C45-C44-O6-C1
28	8	301	LMG	O6-C5-C6-O5
21	7	303	CLA	C10-C11-C12-C13
28	A	407	LMG	C17-C18-C19-C20
28	b	620	LMG	C36-C37-C38-C39
31	X	401	SQD	C27-C28-C29-C30
31	b	602	SQD	C25-C26-C27-C28
28	N	101	LMG	C30-C31-C32-C33
21	B	614	CLA	C3-C5-C6-C7
28	2	318	LMG	C37-C38-C39-C40
21	D	407	CLA	CBA-CGA-O2A-C1
30	c	516	DGD	C2A-C1A-O1G-C1G
29	A	408	LMU	O5'-C5'-C6'-O6'
29	g	316	LMU	O5B-C5B-C6B-O6B
27	a	401	LHG	O1-C1-C2-O2
21	5	304	CLA	O2A-C1-C2-C3
29	D	412	LMU	O1'-C1-C2-C3
23	5	312	A86	C33-C34-O4-C38
21	B	603	CLA	C3-C5-C6-C7
27	A	406	LHG	C7-C8-C9-C10
28	b	625	LMG	C34-C35-C36-C37
28	8	317	LMG	C11-C10-O7-C8
29	2	317	LMU	O1'-C1-C2-C3
30	b	601	DGD	C7B-C8B-C9B-CAB
25	b	618	BCR	C20-C21-C22-C37
29	5	301	LMU	O5'-C5'-C6'-O6'
29	g	301	LMU	O5'-C5'-C6'-O6'
21	B	614	CLA	C4-C3-C5-C6
21	C	507	CLA	C4-C3-C5-C6
21	c	506	CLA	C4-C3-C5-C6
26	a	404	PHO	C4-C3-C5-C6
28	f	102	LMG	C18-C19-C20-C21
28	8	317	LMG	C19-C20-C21-C22
26	a	404	PHO	C2-C3-C5-C6
24	g	313	KC1	C2A-CAA-CBA-CGA
28	b	625	LMG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	626	SQD	C7-C8-C9-C10
21	3	301	CLA	C11-C12-C13-C14
21	5	309	CLA	C16-C17-C18-C19
28	M	102	LMG	O6-C5-C6-O5
28	b	625	LMG	O6-C5-C6-O5
29	A	408	LMU	O1'-C1-C2-C3
21	b	606	CLA	C8-C10-C11-C12
28	N	101	LMG	C7-C8-C9-O8
28	b	626	LMG	C33-C34-C35-C36
28	b	622	LMG	C9-C8-O7-C10
21	a	402	CLA	C2A-CAA-CBA-CGA
21	a	405	CLA	C2A-CAA-CBA-CGA
21	g	304	CLA	C2A-CAA-CBA-CGA
21	J	307	CLA	C2-C1-O2A-CGA
21	g	309	CLA	C2-C1-O2A-CGA
27	a	401	LHG	C24-C25-C26-C27
27	D	403	LHG	C25-C26-C27-C28
28	a	407	LMG	C12-C13-C14-C15
29	5	301	LMU	C6-C7-C8-C9
28	8	301	LMG	C4-C5-C6-O5
31	B	625	SQD	C12-C13-C14-C15
31	B	626	SQD	C25-C26-C27-C28
21	b	609	CLA	CBA-CGA-O2A-C1
21	8	304	CLA	CBA-CGA-O2A-C1
21	4	303	CLA	CBA-CGA-O2A-C1
21	c	509	CLA	C16-C17-C18-C19
21	c	510	CLA	CBD-CGD-O2D-CED
21	B	611	CLA	C8-C10-C11-C12
28	b	624	LMG	C12-C13-C14-C15
30	b	601	DGD	C3A-C4A-C5A-C6A
21	B	608	CLA	O1A-CGA-O2A-C1
21	b	611	CLA	C15-C16-C17-C18
21	8	302	CLA	C13-C15-C16-C17
21	c	513	CLA	C15-C16-C17-C18
21	3	301	CLA	C10-C11-C12-C13
25	b	619	BCR	C20-C21-C22-C23
28	b	625	LMG	C2-C1-O1-C7
28	B	622	LMG	O1-C7-C8-O7
28	B	623	LMG	O7-C8-C9-O8
28	B	627	LMG	O7-C8-C9-O8
30	C	517	DGD	O2G-C2G-C3G-O3G
28	B	619	LMG	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	612	CLA	C8-C10-C11-C12
21	D	407	CLA	O1A-CGA-O2A-C1
30	C	517	DGD	C2B-C3B-C4B-C5B
21	6	300	CLA	C4-C3-C5-C6
21	b	615	CLA	C4-C3-C5-C6
21	C	513	CLA	C4-C3-C5-C6
21	c	504	CLA	C4-C3-C5-C6
35	d	408	PL9	C15-C14-C16-C17
21	7	303	CLA	C12-C13-C15-C16
21	B	607	CLA	C11-C12-C13-C15
21	B	608	CLA	C11-C12-C13-C15
21	B	612	CLA	C11-C12-C13-C15
21	B	614	CLA	C2-C3-C5-C6
21	B	621	CLA	C12-C13-C15-C16
21	b	615	CLA	C2-C3-C5-C6
21	b	617	CLA	C11-C10-C8-C7
21	C	504	CLA	C11-C12-C13-C15
21	C	507	CLA	C2-C3-C5-C6
21	C	509	CLA	C6-C7-C8-C10
21	c	508	CLA	C12-C13-C15-C16
21	c	509	CLA	C11-C12-C13-C15
21	5	309	CLA	C11-C12-C13-C15
21	5	309	CLA	C12-C13-C15-C16
21	B	608	CLA	C11-C12-C13-C14
21	2	301	CLA	C11-C12-C13-C14
21	D	406	CLA	C6-C7-C8-C9
21	d	405	CLA	C6-C7-C8-C9
21	C	504	CLA	C11-C12-C13-C14
21	C	509	CLA	C6-C7-C8-C9
21	C	509	CLA	C11-C10-C8-C9
21	c	508	CLA	C11-C10-C8-C9
21	c	509	CLA	C11-C12-C13-C14
21	5	309	CLA	C11-C12-C13-C14
25	a	406	BCR	C14-C15-C16-C17
31	X	401	SQD	C25-C26-C27-C28
21	b	613	CLA	CBA-CGA-O2A-C1
21	G	303	CLA	CBA-CGA-O2A-C1
21	2	305	CLA	C15-C16-C17-C18
30	c	516	DGD	CDB-CEB-CFB-CGB
21	b	609	CLA	O1A-CGA-O2A-C1
25	B	618	BCR	C37-C22-C23-C24
27	d	409	LHG	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	h	103	DGD	C2B-C3B-C4B-C5B
24	8	316	KC1	O1D-CGD-O2D-CED
28	a	407	LMG	C19-C20-C21-C22
27	D	403	LHG	C1-C2-C3-O3
27	D	410	LHG	C27-C28-C29-C30
21	7	302	CLA	CBA-CGA-O2A-C1
21	B	612	CLA	CBA-CGA-O2A-C1
21	b	623	CLA	CBA-CGA-O2A-C1
21	3	300	CLA	CBA-CGA-O2A-C1
21	7	301	CLA	C5-C6-C7-C8
21	B	603	CLA	C11-C10-C8-C7
24	1	315	KC1	CBD-CGD-O2D-CED
21	g	306	CLA	C8-C10-C11-C12
27	D	410	LHG	O6-C4-C5-C6
21	5	307	CLA	C3-C5-C6-C7
28	A	407	LMG	C34-C35-C36-C37
21	7	301	CLA	C8-C10-C11-C12
21	3	300	CLA	C4-C3-C5-C6
21	G	302	CLA	C4-C3-C5-C6
21	C	513	CLA	C2-C3-C5-C6
21	c	504	CLA	C2-C3-C5-C6
21	c	506	CLA	C2-C3-C5-C6
21	G	302	CLA	C2-C3-C5-C6
27	D	410	LHG	C25-C26-C27-C28
21	D	404	CLA	C2C-C3C-CAC-CBC
21	g	304	CLA	C5-C6-C7-C8
27	l	101	LHG	C32-C33-C34-C35
28	L	101	LMG	C32-C33-C34-C35
21	C	507	CLA	CBA-CGA-O2A-C1
28	b	620	LMG	O8-C28-C29-C30
29	D	412	LMU	C5'-C4'-O1B-C1B
30	c	516	DGD	C6B-C7B-C8B-C9B
26	A	403	PHO	O1D-CGD-O2D-CED
21	1	303	CLA	C3A-C2A-CAA-CBA
21	6	303	CLA	C3A-C2A-CAA-CBA
21	G	300	CLA	C3A-C2A-CAA-CBA
21	d	404	CLA	C2C-C3C-CAC-CBC
28	a	407	LMG	C39-C40-C41-C42
28	8	301	LMG	C30-C31-C32-C33
31	B	625	SQD	C16-C17-C18-C19
23	1	312	A86	O-C13-C14-C15
23	6	309	A86	O-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	6	310	A86	O-C13-C14-C15
23	7	311	A86	O-C13-C14-C15
23	7	312	A86	O-C13-C14-C15
23	J	309	A86	O-C13-C14-C15
23	J	310	A86	O-C13-C14-C15
23	5	311	A86	O-C13-C14-C15
23	5	312	A86	O-C13-C14-C15
23	g	311	A86	O-C13-C14-C15
28	8	317	LMG	C12-C13-C14-C15
31	B	626	SQD	C14-C15-C16-C17
28	f	102	LMG	C13-C14-C15-C16
30	H	101	DGD	C9A-CAA-CBA-CCA
29	a	408	LMU	O5B-C5B-C6B-O6B
21	2	302	CLA	CBA-CGA-O2A-C1
27	d	409	LHG	C33-C34-C35-C36
28	M	102	LMG	C29-C30-C31-C32
21	D	407	CLA	C8-C10-C11-C12
27	B	601	LHG	C4-C5-C6-O8
28	A	407	LMG	O1-C7-C8-C9
28	B	622	LMG	O1-C7-C8-C9
28	a	407	LMG	O1-C7-C8-C9
28	f	102	LMG	O1-C7-C8-C9
28	f	102	LMG	C7-C8-C9-O8
28	8	317	LMG	C7-C8-C9-O8
30	B	624	DGD	O1G-C1G-C2G-C3G
30	b	601	DGD	O1G-C1G-C2G-C3G
30	c	516	DGD	C1G-C2G-C3G-O3G
31	B	625	SQD	O6-C44-C45-C46
21	c	506	CLA	CBD-CGD-O2D-CED
21	D	404	CLA	C11-C12-C13-C14
28	A	407	LMG	C19-C20-C21-C22
28	B	619	LMG	C16-C17-C18-C19
29	a	408	LMU	C7-C8-C9-C10
28	L	101	LMG	C33-C34-C35-C36
23	2	309	A86	C9-C10-C11-C13
27	B	601	LHG	C32-C33-C34-C35
27	D	403	LHG	C29-C30-C31-C32
21	8	304	CLA	O1A-CGA-O2A-C1
21	B	621	CLA	C5-C6-C7-C8
27	D	410	LHG	C31-C32-C33-C34
28	b	625	LMG	C16-C17-C18-C19
21	g	308	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	4	303	CLA	O1A-CGA-O2A-C1
28	B	619	LMG	C30-C31-C32-C33
30	c	516	DGD	C4E-C5E-C6E-O5E
21	A	401	CLA	C2A-CAA-CBA-CGA
21	A	404	CLA	C2A-CAA-CBA-CGA
21	d	406	CLA	C5-C6-C7-C8
21	c	504	CLA	C15-C16-C17-C18
21	c	506	CLA	C13-C15-C16-C17
23	8	308	A86	O5-C38-O4-C34
27	B	601	LHG	C16-C17-C18-C19
29	A	408	LMU	C7-C8-C9-C10
27	a	401	LHG	O6-C4-C5-O7
29	g	301	LMU	C1-C2-C3-C4
28	b	624	LMG	C28-C29-C30-C31
21	3	301	CLA	C11-C12-C13-C15
28	8	317	LMG	C37-C38-C39-C40
28	b	622	LMG	C15-C16-C17-C18
21	b	613	CLA	O1A-CGA-O2A-C1
21	G	303	CLA	O1A-CGA-O2A-C1
28	2	318	LMG	C32-C33-C34-C35
27	A	406	LHG	O7-C5-C6-O8
27	l	101	LHG	O7-C5-C6-O8
28	A	407	LMG	O1-C7-C8-O7
28	B	623	LMG	O1-C7-C8-O7
31	X	401	SQD	O6-C44-C45-O47
21	C	511	CLA	CBD-CGD-O2D-CED
21	2	301	CLA	C10-C11-C12-C13
27	l	101	LHG	C30-C31-C32-C33
28	B	622	LMG	C13-C14-C15-C16
27	a	401	LHG	C27-C28-C29-C30
28	D	411	LMG	C30-C31-C32-C33
21	C	505	CLA	C8-C10-C11-C12
23	1	312	A86	C10-C11-C13-C14
23	1	313	A86	C10-C11-C13-C14
23	7	312	A86	C10-C11-C13-C14
23	W	101	A86	C10-C11-C13-C14
23	2	309	A86	C10-C11-C13-C14
23	2	311	A86	C10-C11-C13-C14
23	8	308	A86	C10-C11-C13-C14
23	8	310	A86	C10-C11-C13-C14
23	4	305	A86	C10-C11-C13-C14
27	A	406	LHG	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	A	407	LMG	C40-C41-C42-C43
28	f	102	LMG	O9-C10-O7-C8
28	D	411	LMG	O9-C10-O7-C8
26	A	403	PHO	C4-C3-C5-C6
21	B	621	CLA	C2-C1-O2A-CGA
21	J	306	CLA	C2-C1-O2A-CGA
21	8	302	CLA	C2-C1-O2A-CGA
21	4	304	CLA	C2-C1-O2A-CGA
21	3	300	CLA	C2-C3-C5-C6
21	B	615	CLA	C10-C11-C12-C13
21	B	607	CLA	C14-C13-C15-C16
21	B	614	CLA	C11-C10-C8-C9
21	B	621	CLA	C14-C13-C15-C16
21	b	606	CLA	C11-C12-C13-C14
21	2	301	CLA	C11-C10-C8-C9
21	8	306	CLA	C11-C10-C8-C9
21	4	304	CLA	C6-C7-C8-C9
27	d	402	LHG	C26-C27-C28-C29
30	H	101	DGD	CAB-CBB-CCB-CDB
29	D	412	LMU	C9-C10-C11-C12
21	b	608	CLA	C8-C10-C11-C12
21	c	509	CLA	C10-C11-C12-C13
21	G	304	CLA	C5-C6-C7-C8
21	8	304	CLA	C4-C3-C5-C6
26	d	403	PHO	C1A-C2A-CAA-CBA
21	b	623	CLA	O1A-CGA-O2A-C1
27	B	601	LHG	C27-C28-C29-C30
28	A	407	LMG	C31-C32-C33-C34
28	B	619	LMG	C32-C33-C34-C35
31	B	625	SQD	C14-C15-C16-C17
21	b	616	CLA	C16-C17-C18-C19
21	5	309	CLA	C16-C17-C18-C20
21	b	605	CLA	CBD-CGD-O2D-CED
25	1	317	BCR	C5-C6-C7-C8
25	1	317	BCR	C23-C24-C25-C26
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C23-C24-C25-C26
25	H	100	BCR	C23-C24-C25-C26
25	H	100	BCR	C23-C24-C25-C30
25	b	618	BCR	C1-C6-C7-C8
25	b	619	BCR	C23-C24-C25-C26
25	h	102	BCR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	h	102	BCR	C23-C24-C25-C30
25	D	408	BCR	C5-C6-C7-C8
25	D	408	BCR	C23-C24-C25-C26
25	D	408	BCR	C23-C24-C25-C30
25	d	407	BCR	C5-C6-C7-C8
25	C	501	BCR	C23-C24-C25-C26
25	C	501	BCR	C23-C24-C25-C30
25	C	516	BCR	C1-C6-C7-C8
25	C	516	BCR	C5-C6-C7-C8
25	c	501	BCR	C23-C24-C25-C26
25	c	501	BCR	C23-C24-C25-C30
25	c	515	BCR	C1-C6-C7-C8
25	c	515	BCR	C5-C6-C7-C8
25	c	515	BCR	C23-C24-C25-C26
25	c	515	BCR	C23-C24-C25-C30
23	7	312	A86	C-C1-C24-C25
23	1	314	A86	C2-C1-C24-C25
23	8	310	A86	C5-C6-C8-C9
21	7	304	CLA	C5-C6-C7-C8
21	A	401	CLA	C15-C16-C17-C18
29	g	301	LMU	C6-C7-C8-C9
31	X	401	SQD	C7-C8-C9-C10
23	8	310	A86	C2-C3-C4-C5
21	b	615	CLA	C5-C6-C7-C8
28	f	102	LMG	C30-C31-C32-C33
30	h	103	DGD	CDB-CEB-CFB-CGB
21	4	302	CLA	C11-C10-C8-C9
27	B	601	LHG	C33-C34-C35-C36
21	B	612	CLA	O1A-CGA-O2A-C1
28	a	407	LMG	C14-C15-C16-C17
21	B	621	CLA	C15-C16-C17-C18
27	d	409	LHG	O6-C4-C5-C6
21	9	304	CLA	C4-C3-C5-C6
21	A	402	CLA	O1D-CGD-O2D-CED
27	l	101	LHG	C17-C18-C19-C20
28	b	625	LMG	C33-C34-C35-C36
21	1	303	CLA	C12-C13-C15-C16
21	7	301	CLA	C11-C10-C8-C7
21	7	304	CLA	C11-C10-C8-C7
21	B	603	CLA	C12-C13-C15-C16
21	2	301	CLA	C11-C10-C8-C7
21	2	301	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	C	506	CLA	C11-C12-C13-C15
21	5	309	CLA	C6-C7-C8-C10
21	g	306	CLA	C6-C7-C8-C10
26	A	403	PHO	C2-C3-C5-C6
23	7	313	A86	C1-C2-C3-C4
28	B	622	LMG	C11-C12-C13-C14
30	h	103	DGD	CDA-CEA-CFA-CGA
21	8	303	CLA	CBA-CGA-O2A-C1
21	B	608	CLA	C5-C6-C7-C8
23	1	312	A86	C4-C5-C6-C7
23	7	313	A86	C4-C5-C6-C7
23	J	309	A86	C4-C5-C6-C7
23	4	305	A86	C-C1-C2-C3
23	g	312	A86	C-C1-C2-C3
25	b	618	BCR	C16-C17-C18-C36
25	c	501	BCR	C20-C21-C22-C37
28	N	101	LMG	C28-C29-C30-C31
23	2	309	A86	C9-C10-C11-C12
24	G	309	KC1	C2A-CAA-CBA-CGA
21	c	508	CLA	CBA-CGA-O2A-C1
21	4	302	CLA	C11-C10-C8-C7
28	a	407	LMG	C38-C39-C40-C41
31	b	602	SQD	C14-C15-C16-C17
26	A	403	PHO	C13-C15-C16-C17
26	a	404	PHO	C13-C15-C16-C17
21	7	302	CLA	O1A-CGA-O2A-C1
21	1	302	CLA	CAD-CBD-CGD-O2D
21	7	302	CLA	CAD-CBD-CGD-O2D
21	7	305	CLA	CAD-CBD-CGD-O2D
21	B	605	CLA	CAD-CBD-CGD-O2D
21	B	616	CLA	CAD-CBD-CGD-O2D
21	b	606	CLA	CAD-CBD-CGD-O2D
21	C	510	CLA	CAD-CBD-CGD-O2D
21	4	300	CLA	CAD-CBD-CGD-O2D
21	g	306	CLA	CAD-CBD-CGD-O2D
21	g	309	CLA	CAD-CBD-CGD-O2D
21	G	300	CLA	CAD-CBD-CGD-O2D
23	1	312	A86	C28-C27-C29-C30
23	6	309	A86	C28-C27-C29-C30
23	W	101	A86	C28-C27-C29-C30
23	2	311	A86	C28-C27-C29-C30
23	2	312	A86	C28-C27-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	5	311	A86	C28-C27-C29-C30
23	g	311	A86	C28-C27-C29-C30
24	J	311	KC1	C2B-C3B-CAB-CBB
24	2	315	KC1	CAD-CBD-CGD-O2D
24	8	314	KC1	CAD-CBD-CGD-O2D
24	4	309	KC1	C2B-C3B-CAB-CBB
24	G	307	KC1	CAD-CBD-CGD-O2D
31	B	626	SQD	C46-C45-O47-C7
31	b	602	SQD	C46-C45-O47-C7
29	8	318	LMU	O5'-C5'-C6'-O6'
21	d	404	CLA	C11-C12-C13-C14
27	B	601	LHG	C29-C30-C31-C32
21	D	407	CLA	C5-C6-C7-C8
21	c	506	CLA	CBA-CGA-O2A-C1
21	7	300	CLA	C4-C3-C5-C6
21	7	304	CLA	C4-C3-C5-C6
21	d	405	CLA	C4-C3-C5-C6
21	9	301	CLA	C11-C12-C13-C15
28	L	101	LMG	O6-C1-O1-C7
35	d	408	PL9	C38-C39-C41-C42
27	A	406	LHG	C2-C3-O3-P
27	l	101	LHG	C4-C5-C6-O8
27	D	403	LHG	C4-C5-C6-O8
28	M	102	LMG	C7-C8-C9-O8
30	C	517	DGD	C1G-C2G-C3G-O3G
21	3	300	CLA	O1A-CGA-O2A-C1
30	c	517	DGD	C8B-C9B-CAB-CBB
29	8	318	LMU	O5B-C5B-C6B-O6B
28	D	411	LMG	C32-C33-C34-C35
24	6	311	KC1	C4B-C3B-CAB-CBB
24	2	313	KC1	C4B-C3B-CAB-CBB
32	E	101	HEM	C4B-C3B-CAB-CBB
24	4	307	KC1	CAA-CBA-CGA-O1A
30	b	601	DGD	C2A-C1A-O1G-C1G
25	1	317	BCR	C14-C15-C16-C17
27	A	406	LHG	C13-C14-C15-C16
21	a	403	CLA	O1D-CGD-O2D-CED
21	1	302	CLA	CHA-CBD-CGD-O1D
21	6	301	CLA	CHA-CBD-CGD-O1D
21	6	308	CLA	CHA-CBD-CGD-O2D
21	7	300	CLA	CHA-CBD-CGD-O2D
21	7	304	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	7	305	CLA	CHA-CBD-CGD-O1D
21	7	308	CLA	CHA-CBD-CGD-O1D
21	A	402	CLA	CHA-CBD-CGD-O1D
21	B	604	CLA	CHA-CBD-CGD-O1D
21	B	604	CLA	CHA-CBD-CGD-O2D
21	B	605	CLA	CHA-CBD-CGD-O1D
21	B	609	CLA	CHA-CBD-CGD-O2D
21	J	301	CLA	CHA-CBD-CGD-O1D
21	J	303	CLA	CHA-CBD-CGD-O1D
21	J	303	CLA	CHA-CBD-CGD-O2D
21	a	403	CLA	CHA-CBD-CGD-O1D
21	b	605	CLA	CHA-CBD-CGD-O1D
21	b	606	CLA	CHA-CBD-CGD-O1D
21	b	610	CLA	CHA-CBD-CGD-O2D
21	2	301	CLA	CHA-CBD-CGD-O2D
21	8	302	CLA	CHA-CBD-CGD-O2D
21	D	404	CLA	CHA-CBD-CGD-O2D
21	C	504	CLA	CHA-CBD-CGD-O2D
21	C	505	CLA	CHA-CBD-CGD-O2D
21	C	506	CLA	CHA-CBD-CGD-O1D
21	c	505	CLA	CHA-CBD-CGD-O1D
21	c	507	CLA	CHA-CBD-CGD-O1D
21	9	301	CLA	CHA-CBD-CGD-O1D
21	9	301	CLA	CHA-CBD-CGD-O2D
21	4	301	CLA	CHA-CBD-CGD-O2D
21	5	304	CLA	CHA-CBD-CGD-O2D
21	g	309	CLA	CHA-CBD-CGD-O1D
21	G	300	CLA	CHA-CBD-CGD-O1D
24	6	313	KC1	CHA-CBD-CGD-O1D
24	6	313	KC1	CHA-CBD-CGD-O2D
24	J	313	KC1	CHA-CBD-CGD-O1D
24	4	308	KC1	CHA-CBD-CGD-O1D
24	g	315	KC1	CHA-CBD-CGD-O1D
24	g	315	KC1	CHA-CBD-CGD-O2D
21	B	607	CLA	C5-C6-C7-C8
21	C	507	CLA	O1A-CGA-O2A-C1
27	A	406	LHG	C11-C10-C9-C8
31	b	602	SQD	C11-C12-C13-C14
23	4	305	A86	C24-C1-C2-C3
25	1	317	BCR	C16-C17-C18-C19
25	H	100	BCR	C11-C10-C9-C8
27	a	401	LHG	O7-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	B	627	LMG	O1-C7-C8-O7
28	a	407	LMG	O1-C7-C8-O7
28	b	625	LMG	O1-C7-C8-O7
28	f	102	LMG	O7-C8-C9-O8
28	D	411	LMG	O1-C7-C8-O7
30	c	516	DGD	O2G-C2G-C3G-O3G
31	B	626	SQD	O6-C44-C45-O47
31	b	602	SQD	O6-C44-C45-O47
29	8	318	LMU	C3-C4-C5-C6
24	4	307	KC1	CAA-CBA-CGA-O2A
21	b	605	CLA	C15-C16-C17-C18
21	2	302	CLA	O1A-CGA-O2A-C1
30	b	601	DGD	C2B-C3B-C4B-C5B
31	B	625	SQD	C10-C11-C12-C13
23	1	312	A86	C13-C14-C15-O1
23	1	313	A86	C13-C14-C15-O1
23	7	311	A86	C13-C14-C15-O1
23	J	309	A86	C13-C14-C15-O1
23	8	310	A86	C13-C14-C15-O1
27	A	406	LHG	O1-C1-C2-O2
27	D	403	LHG	O1-C1-C2-O2
27	D	410	LHG	O1-C1-C2-O2
27	d	402	LHG	O1-C1-C2-O2
27	a	401	LHG	C33-C34-C35-C36
21	g	304	CLA	C3-C5-C6-C7
21	1	303	CLA	C4-C3-C5-C6
28	b	624	LMG	C30-C31-C32-C33
21	8	303	CLA	O1A-CGA-O2A-C1
21	7	300	CLA	C2-C3-C5-C6
22	5	310	DD6	C27-C29-C30-C31
21	7	301	CLA	C11-C10-C8-C9
26	a	404	PHO	O1D-CGD-O2D-CED
21	c	508	CLA	O1A-CGA-O2A-C1
21	B	607	CLA	C10-C11-C12-C13
31	B	625	SQD	C4-C5-C6-S
31	B	626	SQD	C4-C5-C6-S
31	X	401	SQD	C4-C5-C6-S
31	C	502	SQD	C5-C6-S-O8
21	1	301	CLA	C2A-CAA-CBA-CGA
28	b	620	LMG	C19-C20-C21-C22
21	c	506	CLA	O1A-CGA-O2A-C1
21	7	303	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	1	312	A86	C-C1-C24-C25
23	7	313	A86	C-C1-C24-C25
25	m	101	BCR	C37-C22-C23-C24
21	B	604	CLA	C15-C16-C17-C18
25	C	516	BCR	C21-C22-C23-C24
28	b	620	LMG	C16-C17-C18-C19
30	c	517	DGD	C4B-C5B-C6B-C7B
21	1	301	CLA	C1A-C2A-CAA-CBA
21	B	604	CLA	C1A-C2A-CAA-CBA
21	b	605	CLA	C1A-C2A-CAA-CBA
21	d	404	CLA	C1A-C2A-CAA-CBA
21	c	502	CLA	C1A-C2A-CAA-CBA
21	g	306	CLA	C1A-C2A-CAA-CBA
21	G	304	CLA	C1A-C2A-CAA-CBA
21	C	509	CLA	C13-C15-C16-C17
21	B	616	CLA	CBA-CGA-O2A-C1
31	B	626	SQD	C18-C19-C20-C21
21	B	616	CLA	O1A-CGA-O2A-C1
27	l	101	LHG	C3-O3-P-O6
28	b	625	LMG	C13-C14-C15-C16
21	B	612	CLA	C4-C3-C5-C6
21	b	613	CLA	C4-C3-C5-C6
21	D	406	CLA	C4-C3-C5-C6
21	4	304	CLA	C5-C6-C7-C8
27	a	401	LHG	C2-C3-O3-P
30	C	517	DGD	C4D-C5D-C6D-O5D
21	7	303	CLA	O1A-CGA-O2A-C1
27	A	406	LHG	C3-O3-P-O5
27	a	401	LHG	C3-O3-P-O4
27	l	101	LHG	C3-O3-P-O4
31	B	625	SQD	O5-C1-O6-C44
21	8	302	CLA	CBA-CGA-O2A-C1
27	a	401	LHG	O6-C4-C5-C6
30	C	518	DGD	C4B-C5B-C6B-C7B
21	b	612	CLA	C12-C13-C15-C16
21	7	300	CLA	C16-C17-C18-C20
21	6	301	CLA	CAD-CBD-CGD-O1D
21	A	402	CLA	CAD-CBD-CGD-O1D
21	B	604	CLA	CAD-CBD-CGD-O1D
21	B	605	CLA	CAD-CBD-CGD-O1D
21	J	301	CLA	CAD-CBD-CGD-O1D
21	a	403	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	b	605	CLA	CAD-CBD-CGD-O1D
21	b	606	CLA	CAD-CBD-CGD-O1D
21	b	615	CLA	CAD-CBD-CGD-O1D
21	C	506	CLA	CAD-CBD-CGD-O1D
21	C	507	CLA	CAD-CBD-CGD-O1D
21	c	505	CLA	CAD-CBD-CGD-O1D
21	c	506	CLA	CAD-CBD-CGD-O1D
21	g	309	CLA	CAD-CBD-CGD-O1D
23	1	312	A86	C26-C27-C29-C30
23	6	309	A86	C26-C27-C29-C30
23	7	311	A86	C26-C27-C29-C30
23	W	101	A86	C26-C27-C29-C30
23	2	312	A86	C26-C27-C29-C30
23	5	312	A86	C26-C27-C29-C30
24	g	315	KC1	CAD-CBD-CGD-O1D
30	c	516	DGD	C4D-C5D-C6D-O5D
29	a	408	LMU	C4-C5-C6-C7
28	L	101	LMG	O10-C28-O8-C9
21	1	309	CLA	CBA-CGA-O2A-C1
31	C	502	SQD	C12-C13-C14-C15
21	7	302	CLA	C6-C7-C8-C10
21	7	304	CLA	C2-C3-C5-C6
21	2	305	CLA	C11-C12-C13-C15
21	C	503	CLA	C11-C12-C13-C15
21	c	502	CLA	C11-C12-C13-C15
21	4	304	CLA	C12-C13-C15-C16
21	G	304	CLA	C11-C10-C8-C7
27	D	410	LHG	O6-C4-C5-O7
27	d	409	LHG	O6-C4-C5-O7
31	b	602	SQD	C7-C8-C9-C10
21	B	611	CLA	C12-C13-C15-C16
28	B	619	LMG	C19-C20-C21-C22
30	C	517	DGD	O6D-C5D-C6D-O5D
30	B	624	DGD	C3A-C4A-C5A-C6A
21	B	603	CLA	C15-C16-C17-C18
21	5	309	CLA	C13-C15-C16-C17
30	b	601	DGD	C1A-C2A-C3A-C4A
30	c	516	DGD	CAB-CBB-CCB-CDB
27	A	406	LHG	O2-C2-C3-O3
27	D	403	LHG	O2-C2-C3-O3
27	d	402	LHG	O2-C2-C3-O3
28	B	619	LMG	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	B	627	LMG	C12-C13-C14-C15
21	4	302	CLA	C2A-CAA-CBA-CGA
21	g	308	CLA	C2A-CAA-CBA-CGA
30	H	101	DGD	CDA-CEA-CFA-CGA
30	C	518	DGD	C8B-C9B-CAB-CBB
21	B	605	CLA	C3-C5-C6-C7
27	a	401	LHG	C4-C5-C6-O8
28	B	622	LMG	C7-C8-C9-O8
28	B	623	LMG	O1-C7-C8-C9
28	B	627	LMG	O1-C7-C8-C9
28	b	625	LMG	O1-C7-C8-C9
28	2	318	LMG	C7-C8-C9-O8
28	8	317	LMG	O1-C7-C8-C9
31	X	401	SQD	O6-C44-C45-C46
27	B	601	LHG	O7-C5-C6-O8
28	b	626	LMG	O1-C7-C8-O7
28	D	411	LMG	O7-C8-C9-O8
31	C	502	SQD	O6-C44-C45-O47
28	b	624	LMG	C16-C17-C18-C19
29	A	408	LMU	C1-C2-C3-C4
27	a	401	LHG	C30-C31-C32-C33
30	c	516	DGD	O6D-C5D-C6D-O5D
21	b	616	CLA	C16-C17-C18-C20
21	b	609	CLA	C8-C10-C11-C12
23	2	308	A86	C9-C10-C11-C13
21	5	309	CLA	C4-C3-C5-C6
28	L	101	LMG	C29-C30-C31-C32
29	A	408	LMU	C4-C5-C6-C7
21	1	303	CLA	C2-C3-C5-C6
23	8	308	A86	C13-C14-C15-C20
29	5	301	LMU	C1-C2-C3-C4
28	B	619	LMG	C35-C36-C37-C38
21	7	303	CLA	C13-C15-C16-C17
21	4	304	CLA	C15-C16-C17-C18
21	5	306	CLA	C10-C11-C12-C13
21	1	303	CLA	C14-C13-C15-C16
21	b	608	CLA	C11-C12-C13-C14
21	4	302	CLA	C6-C7-C8-C9
21	1	309	CLA	O1A-CGA-O2A-C1
21	8	302	CLA	O1A-CGA-O2A-C1
27	B	601	LHG	C17-C18-C19-C20
21	9	301	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	2	317	LMU	C5-C6-C7-C8
28	A	407	LMG	C38-C39-C40-C41
21	b	616	CLA	C10-C11-C12-C13
27	A	406	LHG	C28-C29-C30-C31
25	D	408	BCR	C21-C22-C23-C24
21	C	507	CLA	C13-C15-C16-C17
27	a	401	LHG	C16-C17-C18-C19
21	4	300	CLA	C3-C5-C6-C7
21	G	304	CLA	C4-C3-C5-C6
30	H	101	DGD	O2G-C1B-C2B-C3B
28	M	102	LMG	C35-C36-C37-C38
21	6	300	CLA	C2-C3-C5-C6
21	B	612	CLA	C2-C3-C5-C6
21	d	405	CLA	C2-C3-C5-C6
23	2	308	A86	C9-C10-C11-C12
23	8	308	A86	C9-C10-C11-C12
27	d	409	LHG	C25-C26-C27-C28
21	A	402	CLA	C1-C2-C3-C4
21	a	403	CLA	C1-C2-C3-C4
21	C	515	CLA	C1-C2-C3-C4
21	c	514	CLA	C1-C2-C3-C4
27	D	410	LHG	C19-C20-C21-C22
30	B	624	DGD	C2A-C3A-C4A-C5A
28	L	101	LMG	C7-C8-O7-C10
21	3	300	CLA	C2A-CAA-CBA-CGA
21	g	302	CLA	C2A-CAA-CBA-CGA
21	1	308	CLA	C2-C1-O2A-CGA
21	B	603	CLA	C2-C1-O2A-CGA
21	B	613	CLA	C2-C1-O2A-CGA
21	B	616	CLA	C2-C1-O2A-CGA
21	J	308	CLA	C2-C1-O2A-CGA
21	a	405	CLA	C2-C1-O2A-CGA
21	b	614	CLA	C2-C1-O2A-CGA
21	b	623	CLA	C2-C1-O2A-CGA
21	G	302	CLA	C2-C1-O2A-CGA
22	g	310	DD6	C2-C3-C4-C5
28	2	318	LMG	C38-C39-C40-C41
23	7	312	A86	C12-C11-C13-C14
28	D	411	LMG	C19-C20-C21-C22
28	D	411	LMG	C34-C35-C36-C37
21	b	606	CLA	O1A-CGA-O2A-C1
23	5	312	A86	C35-C34-O4-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	625	SQD	C26-C27-C28-C29
21	b	608	CLA	C16-C17-C18-C19
21	1	309	CLA	C4-C3-C5-C6
21	5	308	CLA	C4-C3-C5-C6
25	1	317	BCR	C1-C6-C7-C8
25	1	317	BCR	C23-C24-C25-C30
25	B	617	BCR	C5-C6-C7-C8
25	B	617	BCR	C23-C24-C25-C30
25	M	101	BCR	C23-C24-C25-C26
25	M	101	BCR	C23-C24-C25-C30
25	b	618	BCR	C5-C6-C7-C8
25	b	618	BCR	C23-C24-C25-C26
25	D	408	BCR	C1-C6-C7-C8
25	d	407	BCR	C1-C6-C7-C8
25	C	516	BCR	C23-C24-C25-C26
21	b	613	CLA	C2-C3-C5-C6
21	B	605	CLA	O1A-CGA-O2A-C1
30	h	103	DGD	C3B-C4B-C5B-C6B
21	D	404	CLA	C4C-C3C-CAC-CBC
21	d	404	CLA	C4C-C3C-CAC-CBC
21	g	308	CLA	CAA-CBA-CGA-O2A
21	g	308	CLA	C16-C17-C18-C20
23	1	312	A86	C4-C5-C6-C8
23	J	309	A86	C4-C5-C6-C8
28	a	407	LMG	C2-C1-O1-C7
30	C	517	DGD	C2D-C1D-O3G-C3G
30	c	516	DGD	C2D-C1D-O3G-C3G
27	D	403	LHG	O7-C5-C6-O8
28	L	101	LMG	O1-C7-C8-O7
28	f	102	LMG	O1-C7-C8-O7
27	a	401	LHG	C3-O3-P-O6
30	c	516	DGD	C1B-C2B-C3B-C4B
21	B	603	CLA	C8-C10-C11-C12
28	A	407	LMG	C15-C16-C17-C18
31	b	602	SQD	C28-C29-C30-C31
30	C	517	DGD	C8B-C9B-CAB-CBB
28	D	411	LMG	C7-C8-C9-O8
21	6	307	CLA	C4-C3-C5-C6
21	C	512	CLA	C4-C3-C5-C6
28	b	620	LMG	C33-C34-C35-C36
21	b	606	CLA	C11-C12-C13-C15
21	b	608	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	D	406	CLA	C2-C3-C5-C6
21	C	509	CLA	C11-C10-C8-C7
27	l	101	LHG	C16-C17-C18-C19
21	1	304	CLA	C3-C5-C6-C7
29	2	317	LMU	C3-C4-C5-C6
30	C	518	DGD	C5B-C6B-C7B-C8B
30	c	516	DGD	CCB-CDB-CEB-CFB
21	7	302	CLA	C6-C7-C8-C9
21	C	503	CLA	C11-C12-C13-C14
21	c	502	CLA	C11-C12-C13-C14
21	4	304	CLA	C14-C13-C15-C16
21	g	308	CLA	C11-C10-C8-C9
21	G	304	CLA	C6-C7-C8-C9
23	8	311	A86	C1-C2-C3-C4
30	C	517	DGD	C7B-C8B-C9B-CAB
21	9	300	CLA	C2A-CAA-CBA-CGA
27	B	601	LHG	C26-C27-C28-C29
31	C	502	SQD	C11-C10-C9-C8
25	H	100	BCR	C37-C22-C23-C24
21	B	615	CLA	C16-C17-C18-C19
21	5	306	CLA	C2C-C3C-CAC-CBC
21	B	605	CLA	C8-C10-C11-C12
23	7	312	A86	C2-C1-C24-C25
25	h	102	BCR	C7-C8-C9-C10
27	l	101	LHG	C7-C8-C9-C10
21	b	608	CLA	C16-C17-C18-C20
21	B	605	CLA	CBA-CGA-O2A-C1
21	b	606	CLA	CBA-CGA-O2A-C1
31	B	626	SQD	C11-C12-C13-C14
28	D	411	LMG	C31-C32-C33-C34
21	G	304	CLA	CBA-CGA-O2A-C1
21	B	604	CLA	C2A-CAA-CBA-CGA
21	b	605	CLA	C2A-CAA-CBA-CGA
30	b	601	DGD	O6D-C1D-O3G-C3G
23	1	314	A86	C1-C2-C3-C4
23	2	310	A86	C1-C2-C3-C4
31	C	502	SQD	C29-C30-C31-C32
29	a	408	LMU	C1-C2-C3-C4
21	B	605	CLA	C5-C6-C7-C8
21	4	300	CLA	C5-C6-C7-C8
22	5	310	DD6	C1-C24-C25-C26
23	J	310	A86	C6-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	515	BCR	C18-C19-C20-C21
30	b	601	DGD	O1G-C1A-C2A-C3A
24	5	314	KC1	C4B-C3B-CAB-CBB
24	g	315	KC1	C4B-C3B-CAB-CBB
21	C	507	CLA	CBD-CGD-O2D-CED
21	G	304	CLA	O1A-CGA-O2A-C1
28	B	622	LMG	C31-C32-C33-C34
21	6	306	CLA	C2-C1-O2A-CGA
21	A	404	CLA	C2-C1-O2A-CGA
21	D	406	CLA	C2-C1-O2A-CGA
21	d	405	CLA	C2-C1-O2A-CGA
21	c	509	CLA	C2-C1-O2A-CGA
21	5	306	CLA	C2-C1-O2A-CGA
21	g	308	CLA	C2-C1-O2A-CGA
21	G	303	CLA	C2-C1-O2A-CGA
28	b	624	LMG	C11-C12-C13-C14
28	b	625	LMG	C35-C36-C37-C38
21	2	306	CLA	C2A-CAA-CBA-CGA
21	5	302	CLA	C2A-CAA-CBA-CGA
21	g	309	CLA	C2A-CAA-CBA-CGA
28	b	622	LMG	O7-C8-C9-O8
28	b	624	LMG	C18-C19-C20-C21
27	d	402	LHG	C11-C12-C13-C14
28	8	317	LMG	C17-C18-C19-C20
21	5	304	CLA	C3A-C2A-CAA-CBA
21	J	303	CLA	CAA-CBA-CGA-O1A
32	E	101	HEM	CAD-CBD-CGD-O2D
32	f	101	HEM	CAA-CBA-CGA-O1A
21	B	607	CLA	C16-C17-C18-C19
28	a	407	LMG	C15-C16-C17-C18
31	C	502	SQD	C26-C27-C28-C29
21	c	505	CLA	C5-C6-C7-C8
21	g	308	CLA	C6-C7-C8-C9
21	2	306	CLA	CAA-CBA-CGA-O1A
27	D	403	LHG	C11-C12-C13-C14
30	c	517	DGD	C5B-C6B-C7B-C8B
28	B	622	LMG	C33-C34-C35-C36
22	7	310	DD6	C9-C10-C11-C12
23	7	311	A86	C25-C26-C27-C28
23	7	313	A86	C25-C26-C27-C28
23	J	309	A86	C25-C26-C27-C28
23	8	308	A86	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	4	305	A86	C25-C26-C27-C28
23	5	312	A86	C25-C26-C27-C28
23	g	311	A86	C25-C26-C27-C28
27	A	406	LHG	C1-C2-C3-O3
27	d	402	LHG	C4-C5-C6-O8
28	b	620	LMG	C7-C8-C9-O8
28	b	625	LMG	C7-C8-C9-O8
21	6	305	CLA	CAA-CBA-CGA-O1A
21	7	300	CLA	C16-C17-C18-C19
21	B	607	CLA	C16-C17-C18-C20
25	B	617	BCR	C37-C22-C23-C24
25	C	501	BCR	C7-C8-C9-C34
32	E	101	HEM	CAD-CBD-CGD-O1D
23	8	308	A86	C9-C10-C11-C13
21	J	307	CLA	C4-C3-C5-C6
21	b	603	CLA	C1A-C2A-CAA-CBA
21	D	404	CLA	C1A-C2A-CAA-CBA
21	C	503	CLA	C1A-C2A-CAA-CBA
21	c	504	CLA	C1A-C2A-CAA-CBA
21	c	507	CLA	C1A-C2A-CAA-CBA
21	c	513	CLA	C1A-C2A-CAA-CBA
21	5	304	CLA	C1A-C2A-CAA-CBA
21	G	303	CLA	C1A-C2A-CAA-CBA
21	c	506	CLA	C12-C13-C15-C16
21	c	513	CLA	C12-C13-C15-C16
21	5	302	CLA	C11-C12-C13-C15
21	9	300	CLA	C5-C6-C7-C8
21	J	305	CLA	CAA-CBA-CGA-O1A
28	D	411	LMG	C29-C30-C31-C32
23	1	314	A86	C3-C4-C5-C6
21	J	303	CLA	CAA-CBA-CGA-O2A
29	g	301	LMU	C4-C5-C6-C7
21	J	303	CLA	C2A-CAA-CBA-CGA
21	3	304	CLA	C2A-CAA-CBA-CGA
21	4	303	CLA	C2A-CAA-CBA-CGA
27	D	403	LHG	C33-C34-C35-C36
28	b	620	LMG	C30-C31-C32-C33
21	B	613	CLA	C15-C16-C17-C18
27	D	410	LHG	C32-C33-C34-C35
24	1	315	KC1	C3A-C2A-CAA-CBA
24	2	314	KC1	C3A-C2A-CAA-CBA
24	g	314	KC1	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	g	315	KC1	C3A-C2A-CAA-CBA
21	2	306	CLA	CAA-CBA-CGA-O2A
21	c	512	CLA	C4-C3-C5-C6
28	A	407	LMG	C37-C38-C39-C40
21	6	307	CLA	C2-C3-C5-C6
21	5	309	CLA	C2-C3-C5-C6
31	B	625	SQD	C13-C14-C15-C16
21	G	302	CLA	C3-C5-C6-C7
23	7	311	A86	C25-C26-C27-C29
23	7	313	A86	C25-C26-C27-C29
23	J	309	A86	C25-C26-C27-C29
23	W	101	A86	C13-C14-C15-C16
23	8	308	A86	C25-C26-C27-C29
23	4	305	A86	C25-C26-C27-C29
23	5	312	A86	C25-C26-C27-C29
23	g	311	A86	C25-C26-C27-C29
28	B	627	LMG	C15-C16-C17-C18
27	d	402	LHG	O7-C5-C6-O8
28	b	625	LMG	O7-C8-C9-O8
28	8	317	LMG	O1-C7-C8-O7
30	b	601	DGD	CCB-CDB-CEB-CFB
24	1	315	KC1	O1D-CGD-O2D-CED
27	a	401	LHG	C1-C2-C3-O3
21	J	305	CLA	CAA-CBA-CGA-O2A
21	b	616	CLA	C4-C3-C5-C6
21	4	304	CLA	C4-C3-C5-C6
21	C	512	CLA	C2-C3-C5-C6
21	5	308	CLA	C2-C3-C5-C6
21	5	306	CLA	C4C-C3C-CAC-CBC
21	6	305	CLA	CAA-CBA-CGA-O2A
29	5	301	LMU	C4-C5-C6-C7
21	1	304	CLA	C14-C13-C15-C16
21	B	610	CLA	C11-C12-C13-C14
23	2	311	A86	C33-C34-O4-C38
24	J	312	KC1	C1A-C2A-CAA-CBA
24	2	313	KC1	C1A-C2A-CAA-CBA
24	3	306	KC1	C1A-C2A-CAA-CBA
24	4	309	KC1	C1A-C2A-CAA-CBA
24	G	308	KC1	C1A-C2A-CAA-CBA
24	G	309	KC1	C1A-C2A-CAA-CBA
25	B	618	BCR	C23-C24-C25-C30
25	b	618	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	m	101	BCR	C23-C24-C25-C26
25	m	101	BCR	C23-C24-C25-C30
25	C	516	BCR	C23-C24-C25-C30
28	M	102	LMG	C36-C37-C38-C39
27	d	402	LHG	C12-C13-C14-C15
28	b	622	LMG	C7-C8-C9-O8
28	2	318	LMG	O1-C7-C8-C9
31	B	626	SQD	O6-C44-C45-C46
32	f	101	HEM	CAA-CBA-CGA-O2A
21	5	306	CLA	C13-C15-C16-C17
27	l	101	LHG	O1-C1-C2-C3
31	B	625	SQD	C24-C25-C26-C27
21	7	301	CLA	C4-C3-C5-C6
21	g	302	CLA	C4-C3-C5-C6
23	1	312	A86	C2-C1-C24-C25
25	H	100	BCR	C7-C8-C9-C10
27	d	402	LHG	C10-C11-C12-C13
21	1	309	CLA	C2-C3-C5-C6
21	G	304	CLA	C2-C3-C5-C6
30	B	624	DGD	O1A-C1A-O1G-C1G
28	M	102	LMG	C8-C7-O1-C1
28	D	411	LMG	C8-C7-O1-C1
30	c	517	DGD	C5D-C6D-O5D-C1E
27	A	406	LHG	C29-C30-C31-C32
31	B	626	SQD	C28-C29-C30-C31
29	D	412	LMU	C5-C6-C7-C8
32	f	101	HEM	CAD-CBD-CGD-O1D
24	8	316	KC1	CAA-CBA-CGA-O1A
24	8	316	KC1	CAA-CBA-CGA-O2A
27	d	409	LHG	C12-C13-C14-C15
27	D	403	LHG	C12-C13-C14-C15
28	B	623	LMG	C29-C28-O8-C9
27	a	401	LHG	C31-C32-C33-C34
21	g	306	CLA	C2C-C3C-CAC-CBC
21	1	303	CLA	C5-C6-C7-C8
21	c	504	CLA	C8-C10-C11-C12
21	3	301	CLA	C8-C10-C11-C12
21	g	308	CLA	C4-C3-C5-C6
21	7	301	CLA	C2-C3-C5-C6
21	B	614	CLA	C11-C10-C8-C7
21	b	612	CLA	C2-C3-C5-C6
21	C	507	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	9	304	CLA	C2-C3-C5-C6
21	4	302	CLA	C6-C7-C8-C10
21	5	309	CLA	C11-C10-C8-C7
21	g	302	CLA	C2-C3-C5-C6
28	a	407	LMG	C29-C28-O8-C9
27	l	101	LHG	O1-C1-C2-O2
21	b	604	CLA	O1A-CGA-O2A-C1
22	g	310	DD6	C24-C25-C26-C27
27	D	403	LHG	C24-C25-C26-C27
31	B	626	SQD	C19-C20-C21-C22
28	f	102	LMG	C35-C36-C37-C38
21	c	509	CLA	C5-C6-C7-C8
27	A	406	LHG	C30-C31-C32-C33
21	B	615	CLA	C16-C17-C18-C20
21	2	303	CLA	CAA-CBA-CGA-O2A
21	4	303	CLA	CAA-CBA-CGA-O2A
28	b	624	LMG	O8-C28-C29-C30
30	B	624	DGD	CCB-CDB-CEB-CFB
21	2	305	CLA	C4-C3-C5-C6
21	c	511	CLA	C4-C3-C5-C6
21	9	300	CLA	C4-C3-C5-C6
21	5	302	CLA	C4-C3-C5-C6
21	1	301	CLA	C10-C11-C12-C13
21	c	511	CLA	C13-C15-C16-C17
21	J	307	CLA	C2-C3-C5-C6
21	1	309	CLA	CAA-CBA-CGA-O2A
21	7	300	CLA	CAA-CBA-CGA-O2A
31	C	502	SQD	O47-C7-C8-C9
28	b	622	LMG	C31-C32-C33-C34
21	b	611	CLA	C11-C12-C13-C14
21	b	615	CLA	C11-C10-C8-C9
21	2	305	CLA	C11-C12-C13-C14
21	C	507	CLA	C14-C13-C15-C16
21	c	506	CLA	C14-C13-C15-C16
21	c	513	CLA	C14-C13-C15-C16
21	9	301	CLA	C11-C10-C8-C9
21	3	301	CLA	C11-C10-C8-C9
21	5	302	CLA	C11-C12-C13-C14
26	A	403	PHO	C14-C13-C15-C16
26	a	404	PHO	C14-C13-C15-C16
21	a	405	CLA	C3-C5-C6-C7
21	c	504	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	c	513	CLA	C3A-C2A-CAA-CBA
21	G	303	CLA	C3A-C2A-CAA-CBA
21	4	304	CLA	O1A-CGA-O2A-C1
21	c	502	CLA	CAA-CBA-CGA-O2A
30	h	103	DGD	O2G-C1B-C2B-C3B
21	B	603	CLA	C2-C3-C5-C6
21	7	308	CLA	CAD-CBD-CGD-O2D
21	A	402	CLA	CAD-CBD-CGD-O2D
21	J	308	CLA	CAD-CBD-CGD-O2D
21	a	403	CLA	CAD-CBD-CGD-O2D
21	b	615	CLA	CAD-CBD-CGD-O2D
21	b	617	CLA	CAD-CBD-CGD-O2D
21	C	503	CLA	CAD-CBD-CGD-O2D
21	C	506	CLA	CAD-CBD-CGD-O2D
21	C	508	CLA	CAD-CBD-CGD-O2D
21	c	505	CLA	CAD-CBD-CGD-O2D
21	c	507	CLA	CAD-CBD-CGD-O2D
21	5	306	CLA	CAD-CBD-CGD-O2D
23	2	309	A86	C28-C27-C29-C30
24	6	311	KC1	CAD-CBD-CGD-O2D
24	J	311	KC1	CAD-CBD-CGD-O2D
24	J	313	KC1	CAD-CBD-CGD-O2D
24	2	313	KC1	CAD-CBD-CGD-O2D
24	g	314	KC1	CAD-CBD-CGD-O2D
26	A	403	PHO	CAD-CBD-CGD-O2D
26	a	404	PHO	CAD-CBD-CGD-O2D
28	8	317	LMG	C15-C16-C17-C18
27	d	402	LHG	C34-C35-C36-C37
30	C	517	DGD	C1B-C2B-C3B-C4B
21	B	603	CLA	CAA-CBA-CGA-O2A
21	c	513	CLA	CAA-CBA-CGA-O2A
28	B	620	LMG	O7-C10-C11-C12
27	B	601	LHG	C11-C10-C9-C8
21	7	308	CLA	C4-C3-C5-C6
21	B	608	CLA	C4-C3-C5-C6
21	b	606	CLA	C4-C3-C5-C6
21	b	609	CLA	C4-C3-C5-C6
21	g	306	CLA	C4C-C3C-CAC-CBC
30	b	601	DGD	O1A-C1A-C2A-C3A
21	5	308	CLA	C5-C6-C7-C8
21	c	512	CLA	C2-C3-C5-C6
21	5	304	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	g	306	CLA	CAA-CBA-CGA-O2A
28	B	627	LMG	O8-C28-C29-C30
23	7	313	A86	C2-C1-C24-C25
25	1	317	BCR	C7-C8-C9-C10
25	D	408	BCR	C7-C8-C9-C10
25	d	407	BCR	C7-C8-C9-C10
21	C	510	CLA	C13-C15-C16-C17
26	d	403	PHO	C2C-C3C-CAC-CBC
28	B	623	LMG	C7-C8-C9-O8
28	B	627	LMG	C7-C8-C9-O8
28	M	102	LMG	O1-C7-C8-C9
28	b	624	LMG	O1-C7-C8-C9
30	B	624	DGD	C1G-C2G-C3G-O3G
31	b	602	SQD	O6-C44-C45-C46
30	C	517	DGD	C6B-C7B-C8B-C9B
21	7	301	CLA	CAA-CBA-CGA-O2A
21	8	304	CLA	CAA-CBA-CGA-O2A
21	c	508	CLA	CAA-CBA-CGA-O2A
27	d	409	LHG	O8-C23-C24-C25
28	b	620	LMG	O7-C10-C11-C12
28	b	621	LMG	O7-C10-C11-C12
25	h	102	BCR	C10-C11-C12-C13
30	H	101	DGD	C3B-C4B-C5B-C6B
21	8	306	CLA	O2A-C1-C2-C3
29	a	408	LMU	C2B-C1B-O1B-C4'
28	A	407	LMG	C35-C36-C37-C38
24	J	311	KC1	C4B-C3B-CAB-CBB
21	4	304	CLA	CBA-CGA-O2A-C1
21	C	512	CLA	C8-C10-C11-C12
21	1	305	CLA	CAA-CBA-CGA-O2A
21	7	303	CLA	CAA-CBA-CGA-O2A
21	g	308	CLA	C16-C17-C18-C19
30	H	101	DGD	C5A-C6A-C7A-C8A
21	1	301	CLA	CHA-CBD-CGD-O2D
21	1	302	CLA	CHA-CBD-CGD-O2D
21	1	304	CLA	CHA-CBD-CGD-O2D
21	1	307	CLA	CHA-CBD-CGD-O2D
21	1	310	CLA	CHA-CBD-CGD-O1D
21	1	310	CLA	CHA-CBD-CGD-O2D
21	6	300	CLA	CHA-CBD-CGD-O2D
21	6	303	CLA	CHA-CBD-CGD-O1D
21	6	307	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	7	304	CLA	CHA-CBD-CGD-O2D
21	7	306	CLA	CHA-CBD-CGD-O2D
21	A	404	CLA	CHA-CBD-CGD-O2D
21	B	602	CLA	CHA-CBD-CGD-O2D
21	B	606	CLA	CHA-CBD-CGD-O2D
21	B	616	CLA	CHA-CBD-CGD-O1D
21	B	621	CLA	CHA-CBD-CGD-O1D
21	J	300	CLA	CHA-CBD-CGD-O2D
21	J	304	CLA	CHA-CBD-CGD-O1D
21	J	306	CLA	CHA-CBD-CGD-O2D
21	J	307	CLA	CHA-CBD-CGD-O1D
21	b	603	CLA	CHA-CBD-CGD-O2D
21	b	607	CLA	CHA-CBD-CGD-O2D
21	b	613	CLA	CHA-CBD-CGD-O1D
21	b	617	CLA	CHA-CBD-CGD-O1D
21	b	623	CLA	CHA-CBD-CGD-O1D
21	2	302	CLA	CHA-CBD-CGD-O1D
21	2	304	CLA	CHA-CBD-CGD-O2D
21	2	305	CLA	CHA-CBD-CGD-O1D
21	2	305	CLA	CHA-CBD-CGD-O2D
21	8	302	CLA	CHA-CBD-CGD-O1D
21	8	305	CLA	CHA-CBD-CGD-O2D
21	D	406	CLA	CHA-CBD-CGD-O2D
21	d	405	CLA	CHA-CBD-CGD-O2D
21	C	511	CLA	CHA-CBD-CGD-O1D
21	C	513	CLA	CHA-CBD-CGD-O2D
21	C	514	CLA	CHA-CBD-CGD-O1D
21	c	510	CLA	CHA-CBD-CGD-O1D
21	c	511	CLA	CHA-CBD-CGD-O1D
21	c	513	CLA	CHA-CBD-CGD-O1D
21	9	303	CLA	CHA-CBD-CGD-O2D
21	5	303	CLA	CHA-CBD-CGD-O2D
21	g	302	CLA	CHA-CBD-CGD-O2D
21	g	303	CLA	CHA-CBD-CGD-O2D
21	G	300	CLA	CHA-CBD-CGD-O2D
24	J	313	KC1	CHA-CBD-CGD-O2D
24	4	308	KC1	CHA-CBD-CGD-O2D
21	B	615	CLA	C4-C3-C5-C6
21	C	503	CLA	CAA-CBA-CGA-O2A
21	g	302	CLA	CAA-CBA-CGA-O2A
28	D	411	LMG	O7-C10-C11-C12
21	g	304	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	2	305	CLA	C2-C3-C5-C6
27	D	403	LHG	C10-C11-C12-C13
24	9	306	KC1	CAA-CBA-CGA-O1A
27	a	401	LHG	C25-C26-C27-C28
23	7	313	A86	C4-C5-C6-C8
23	g	312	A86	C24-C1-C2-C3
21	1	301	CLA	CAA-CBA-CGA-O2A
21	6	306	CLA	CAA-CBA-CGA-O2A
21	c	511	CLA	CAA-CBA-CGA-O2A
28	b	620	LMG	O7-C8-C9-O8
21	C	504	CLA	O1A-CGA-O2A-C1
31	B	625	SQD	C24-C23-O48-C46
21	9	304	CLA	CAA-CBA-CGA-O2A
31	X	401	SQD	O47-C7-C8-C9
23	1	314	A86	C13-C14-C15-O1
23	2	307	A86	C13-C14-C15-O1
23	2	312	A86	C13-C14-C15-O1
23	8	312	A86	C13-C14-C15-O1
23	g	312	A86	C13-C14-C15-O1
26	d	403	PHO	CHA-CBD-CGD-O2D
31	C	502	SQD	C30-C31-C32-C33
21	b	604	CLA	CBA-CGA-O2A-C1
21	b	611	CLA	CBA-CGA-O2A-C1
30	H	101	DGD	C2B-C3B-C4B-C5B
21	6	307	CLA	CAA-CBA-CGA-O2A
21	B	613	CLA	CAA-CBA-CGA-O2A
21	C	512	CLA	CAA-CBA-CGA-O2A
21	5	307	CLA	CAA-CBA-CGA-O2A
21	g	304	CLA	CAA-CBA-CGA-O2A
27	l	101	LHG	C11-C10-C9-C8
28	L	101	LMG	C31-C32-C33-C34
21	B	605	CLA	C4-C3-C5-C6
27	B	601	LHG	C14-C15-C16-C17
30	H	101	DGD	CBA-CCA-CDA-CEA
30	h	103	DGD	C4A-C5A-C6A-C7A
30	h	103	DGD	C9A-CAA-CBA-CCA
21	a	402	CLA	C15-C16-C17-C18
21	1	304	CLA	C12-C13-C15-C16
21	B	608	CLA	C2-C3-C5-C6
21	B	613	CLA	C12-C13-C15-C16
21	b	604	CLA	C2-C3-C5-C6
21	1	304	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	6	301	CLA	CAA-CBA-CGA-O2A
27	D	410	LHG	O8-C23-C24-C25
21	1	302	CLA	C11-C12-C13-C14
21	B	606	CLA	C11-C12-C13-C14
21	G	304	CLA	C11-C10-C8-C9
25	D	408	BCR	C9-C10-C11-C12
25	d	407	BCR	C9-C10-C11-C12
25	C	516	BCR	C9-C10-C11-C12
27	D	403	LHG	C24-C23-O8-C6
21	G	303	CLA	CAA-CBA-CGA-O2A
31	b	602	SQD	C4-C5-C6-S
21	b	606	CLA	C3-C5-C6-C7
28	b	625	LMG	C15-C16-C17-C18
32	f	101	HEM	C2A-CAA-CBA-CGA
21	J	301	CLA	CAA-CBA-CGA-O2A
21	C	510	CLA	C5-C6-C7-C8
23	8	312	A86	C-C1-C24-C25
21	5	304	CLA	CAA-CBA-CGA-O1A
21	b	616	CLA	C2-C3-C5-C6
21	g	308	CLA	C2-C3-C5-C6
35	D	409	PL9	C43-C44-C46-C47
21	7	302	CLA	CAA-CBA-CGA-O2A
30	C	517	DGD	CDB-CEB-CFB-CGB
21	7	300	CLA	CAA-CBA-CGA-O1A
23	8	312	A86	C2-C1-C24-C25
25	h	101	BCR	C7-C8-C9-C10
21	C	504	CLA	CBA-CGA-O2A-C1
21	B	608	CLA	C1A-C2A-CAA-CBA
21	b	609	CLA	C1A-C2A-CAA-CBA
28	L	101	LMG	C36-C37-C38-C39
21	6	301	CLA	CAA-CBA-CGA-O1A
21	4	303	CLA	CAA-CBA-CGA-O1A
21	g	306	CLA	CAA-CBA-CGA-O1A
28	B	620	LMG	O9-C10-C11-C12
30	C	518	DGD	O1B-C1B-C2B-C3B
27	B	601	LHG	C7-C8-C9-C10
21	7	303	CLA	CAA-CBA-CGA-O1A
21	c	508	CLA	CAA-CBA-CGA-O1A
21	g	302	CLA	CAA-CBA-CGA-O1A
28	L	101	LMG	O9-C10-C11-C12
31	B	626	SQD	O49-C7-C8-C9
31	b	602	SQD	O49-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	h	103	DGD	C5A-C6A-C7A-C8A
32	f	101	HEM	CAD-CBD-CGD-O2D
28	b	626	LMG	C7-C8-C9-O8
30	b	601	DGD	C1G-C2G-C3G-O3G
21	7	308	CLA	CAA-CBA-CGA-O2A
31	B	626	SQD	O47-C7-C8-C9
27	a	401	LHG	O2-C2-C3-O3
21	b	617	CLA	C16-C17-C18-C19
21	c	510	CLA	C16-C17-C18-C19
21	1	309	CLA	CAA-CBA-CGA-O1A
21	J	301	CLA	CAA-CBA-CGA-O1A
21	2	303	CLA	CAA-CBA-CGA-O1A
21	c	513	CLA	CAA-CBA-CGA-O1A
28	b	621	LMG	O9-C10-C11-C12
21	b	612	CLA	C4-C3-C5-C6
21	J	306	CLA	CAA-CBA-CGA-O2A
21	b	614	CLA	CAA-CBA-CGA-O2A
21	5	303	CLA	CAA-CBA-CGA-O2A
21	6	306	CLA	CAA-CBA-CGA-O1A
21	B	603	CLA	CAA-CBA-CGA-O1A
32	E	101	HEM	CAA-CBA-CGA-O2A
28	L	101	LMG	C2-C1-O1-C7
30	C	517	DGD	C6A-C7A-C8A-C9A
28	b	620	LMG	C18-C19-C20-C21
21	7	301	CLA	CAA-CBA-CGA-O1A
21	8	304	CLA	CAA-CBA-CGA-O1A
21	C	503	CLA	CAA-CBA-CGA-O1A
30	c	517	DGD	O1B-C1B-C2B-C3B
21	c	508	CLA	C10-C11-C12-C13
21	1	301	CLA	CAA-CBA-CGA-O1A
21	1	304	CLA	CAA-CBA-CGA-O1A
21	c	502	CLA	CAA-CBA-CGA-O1A
27	D	410	LHG	O9-C7-C8-C9
31	C	502	SQD	O49-C7-C8-C9
21	3	302	CLA	C4C-C3C-CAC-CBC
27	A	406	LHG	C12-C13-C14-C15
21	b	611	CLA	O1A-CGA-O2A-C1
21	1	303	CLA	CAA-CBA-CGA-O2A
21	c	512	CLA	C8-C10-C11-C12
28	L	101	LMG	C11-C12-C13-C14
24	5	314	KC1	CBD-CGD-O2D-CED
21	B	613	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	l	101	LHG	O7-C7-C8-C9
21	7	301	CLA	C13-C15-C16-C17
31	X	401	SQD	O49-C7-C8-C9
21	1	310	CLA	CAD-CBD-CGD-O1D
21	6	307	CLA	CAD-CBD-CGD-O1D
21	B	621	CLA	CAD-CBD-CGD-O1D
21	J	306	CLA	CAD-CBD-CGD-O1D
21	2	302	CLA	CAD-CBD-CGD-O1D
21	2	305	CLA	CAD-CBD-CGD-O1D
21	C	503	CLA	CAD-CBD-CGD-O1D
21	9	303	CLA	CAD-CBD-CGD-O1D
23	2	311	A86	C26-C27-C29-C30
24	4	307	KC1	CAD-CBD-CGD-O1D
21	C	512	CLA	CAA-CBA-CGA-O1A
21	9	304	CLA	CAA-CBA-CGA-O1A
21	g	304	CLA	CAA-CBA-CGA-O1A
28	b	624	LMG	O10-C28-C29-C30
31	b	602	SQD	O47-C7-C8-C9
21	J	306	CLA	C11-C12-C13-C14
21	b	607	CLA	C11-C12-C13-C14
21	c	512	CLA	C15-C16-C17-C18
21	6	307	CLA	CAA-CBA-CGA-O1A
21	5	307	CLA	CAA-CBA-CGA-O1A
29	8	318	LMU	C11-C10-C9-C8
21	b	607	CLA	C13-C15-C16-C17
21	c	504	CLA	C5-C6-C7-C8
21	g	303	CLA	C2A-CAA-CBA-CGA
21	G	303	CLA	C2A-CAA-CBA-CGA
24	9	306	KC1	CAA-CBA-CGA-O2A
21	J	307	CLA	CAA-CBA-CGA-O2A
21	2	305	CLA	CAA-CBA-CGA-O2A
21	3	304	CLA	CAA-CBA-CGA-O2A
27	B	601	LHG	O7-C7-C8-C9
28	f	102	LMG	O7-C10-C11-C12
30	C	518	DGD	O2G-C1B-C2B-C3B
27	D	403	LHG	O9-C7-O7-C5
21	b	608	CLA	C4-C3-C5-C6
21	8	306	CLA	C4-C3-C5-C6
21	1	302	CLA	C11-C12-C13-C15
21	B	606	CLA	C11-C12-C13-C15
21	b	604	CLA	C12-C13-C15-C16
21	8	306	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	7	302	CLA	CAA-CBA-CGA-O1A
27	D	410	LHG	O10-C23-C24-C25
28	b	621	LMG	O10-C28-C29-C30
21	7	307	CLA	CAA-CBA-CGA-O2A
21	B	610	CLA	CAA-CBA-CGA-O2A
21	8	306	CLA	CAA-CBA-CGA-O2A
30	h	103	DGD	CBA-CCA-CDA-CEA
21	4	300	CLA	C13-C15-C16-C17
23	G	305	A86	C5-C6-C8-C9
25	B	617	BCR	C7-C8-C9-C10
21	G	303	CLA	CAA-CBA-CGA-O1A
27	l	101	LHG	O9-C7-C8-C9
30	B	624	DGD	O1B-C1B-C2B-C3B
30	b	601	DGD	O1B-C1B-C2B-C3B
23	2	309	A86	C1-C2-C3-C4
30	c	516	DGD	C6A-C7A-C8A-C9A
21	1	303	CLA	CAA-CBA-CGA-O1A
21	7	308	CLA	CAA-CBA-CGA-O1A
21	b	614	CLA	CAA-CBA-CGA-O1A
21	8	306	CLA	CAA-CBA-CGA-O1A
21	c	511	CLA	CAA-CBA-CGA-O1A
21	3	304	CLA	CAA-CBA-CGA-O1A
21	5	303	CLA	CAA-CBA-CGA-O1A
27	B	601	LHG	O9-C7-C8-C9
27	d	409	LHG	O10-C23-C24-C25
28	B	620	LMG	O10-C28-C29-C30
21	B	606	CLA	C13-C15-C16-C17
21	5	302	CLA	CAA-CBA-CGA-O2A
28	b	622	LMG	C12-C13-C14-C15
21	B	610	CLA	CAA-CBA-CGA-O1A
28	B	619	LMG	O9-C10-C11-C12
21	6	307	CLA	C2A-CAA-CBA-CGA
21	J	306	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

191 monomers are involved in 362 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	C	507	CLA	1	0
31	b	602	SQD	3	0
21	C	509	CLA	2	0
25	B	618	BCR	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	d	403	PHO	2	0
27	d	409	LHG	4	0
28	8	317	LMG	4	0
35	D	409	PL9	2	0
21	G	304	CLA	2	0
21	2	306	CLA	1	0
28	A	407	LMG	1	0
28	M	102	LMG	2	0
28	a	407	LMG	2	0
21	6	301	CLA	3	0
21	6	303	CLA	1	0
21	G	300	CLA	1	0
25	c	515	BCR	2	0
29	g	301	LMU	1	0
21	3	302	CLA	1	0
21	1	303	CLA	1	0
21	C	508	CLA	2	0
24	G	307	KC1	2	0
25	a	406	BCR	5	0
21	d	404	CLA	2	0
21	D	404	CLA	3	0
21	2	305	CLA	1	0
21	C	512	CLA	2	0
21	B	609	CLA	3	0
21	a	405	CLA	2	0
21	6	307	CLA	3	0
21	g	304	CLA	3	0
21	d	405	CLA	3	0
21	7	306	CLA	1	0
21	c	509	CLA	3	0
21	B	608	CLA	1	0
30	b	601	DGD	3	0
24	5	315	KC1	1	0
21	c	507	CLA	2	0
21	a	402	CLA	3	0
21	4	301	CLA	2	0
26	A	403	PHO	2	0
21	7	302	CLA	5	0
28	b	626	LMG	2	0
21	b	615	CLA	3	0
24	2	315	KC1	4	0
21	C	504	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	c	508	CLA	3	0
21	8	306	CLA	2	0
26	a	404	PHO	1	0
21	J	301	CLA	1	0
21	C	510	CLA	3	0
21	B	603	CLA	2	0
28	b	620	LMG	3	0
21	1	309	CLA	1	0
21	8	303	CLA	3	0
21	9	301	CLA	2	0
21	B	615	CLA	2	0
21	B	611	CLA	2	0
27	l	101	LHG	2	0
32	E	101	HEM	1	0
25	b	618	BCR	1	0
21	C	511	CLA	2	0
21	c	504	CLA	4	0
31	B	626	SQD	2	0
21	B	607	CLA	5	0
28	L	101	LMG	1	0
21	8	307	CLA	2	0
25	C	501	BCR	1	0
21	b	607	CLA	4	0
21	5	304	CLA	1	0
21	5	303	CLA	4	0
21	7	305	CLA	1	0
21	7	304	CLA	3	0
21	b	604	CLA	2	0
21	2	302	CLA	3	0
30	c	516	DGD	3	0
21	6	300	CLA	1	0
21	C	506	CLA	2	0
21	b	606	CLA	4	0
21	D	407	CLA	2	0
21	1	308	CLA	1	0
21	J	306	CLA	3	0
21	b	612	CLA	1	0
22	1	311	DD6	1	0
21	b	603	CLA	1	0
21	b	616	CLA	3	0
30	H	101	DGD	3	0
27	a	401	LHG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	J	300	CLA	1	0
21	C	513	CLA	4	0
21	5	307	CLA	1	0
28	B	627	LMG	2	0
21	c	513	CLA	2	0
21	8	302	CLA	3	0
21	3	300	CLA	3	0
21	1	305	CLA	1	0
30	c	517	DGD	1	0
24	8	313	KC1	1	0
21	b	617	CLA	6	0
21	5	306	CLA	1	0
25	1	317	BCR	3	0
21	g	303	CLA	2	0
25	B	617	BCR	4	0
21	c	503	CLA	4	0
31	C	502	SQD	1	0
22	7	310	DD6	1	0
21	1	302	CLA	1	0
27	D	410	LHG	6	0
21	c	505	CLA	1	0
28	N	101	LMG	1	0
29	5	316	LMU	1	0
28	B	619	LMG	4	0
21	g	307	CLA	1	0
21	5	302	CLA	3	0
21	g	308	CLA	2	0
21	C	503	CLA	3	0
21	c	502	CLA	1	0
21	c	506	CLA	2	0
32	f	101	HEM	1	0
21	5	308	CLA	2	0
24	2	313	KC1	1	0
21	d	406	CLA	1	0
21	8	304	CLA	2	0
21	D	406	CLA	2	0
28	b	622	LMG	1	0
21	b	605	CLA	1	0
21	g	302	CLA	1	0
25	D	408	BCR	1	0
21	c	511	CLA	5	0
21	7	300	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	H	100	BCR	2	0
27	A	406	LHG	3	0
21	4	302	CLA	4	0
21	b	610	CLA	3	0
21	7	309	CLA	2	0
21	1	301	CLA	5	0
21	3	304	CLA	3	0
28	2	318	LMG	3	0
21	7	303	CLA	1	0
21	1	304	CLA	2	0
21	c	512	CLA	2	0
21	B	616	CLA	4	0
29	D	412	LMU	1	0
30	C	518	DGD	1	0
29	5	301	LMU	1	0
25	A	405	BCR	5	0
21	b	613	CLA	2	0
24	J	311	KC1	1	0
21	A	404	CLA	4	0
21	6	302	CLA	1	0
21	2	301	CLA	3	0
21	B	605	CLA	4	0
21	b	608	CLA	4	0
21	b	614	CLA	2	0
23	5	311	A86	1	0
21	2	303	CLA	3	0
27	B	601	LHG	3	0
21	4	300	CLA	4	0
21	J	303	CLA	1	0
21	c	510	CLA	1	0
21	9	300	CLA	2	0
26	D	401	PHO	2	0
25	h	101	BCR	3	0
21	B	614	CLA	1	0
21	B	612	CLA	3	0
21	4	304	CLA	1	0
25	d	407	BCR	1	0
21	J	307	CLA	3	0
30	B	624	DGD	4	0
21	9	302	CLA	5	0
25	b	619	BCR	2	0
21	9	303	CLA	2	0

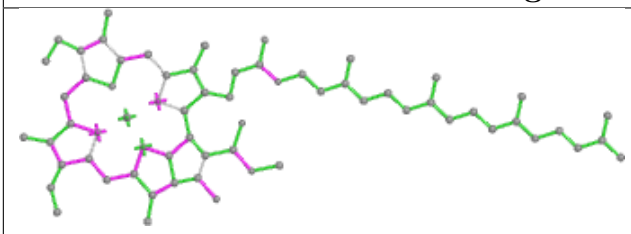
Continued on next page...

Continued from previous page...

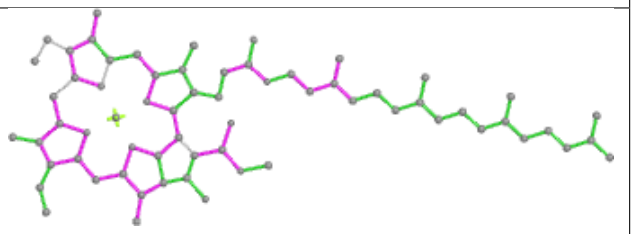
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	8	318	LMU	1	0
21	B	613	CLA	2	0
21	3	301	CLA	3	0
25	C	516	BCR	3	0
21	B	604	CLA	1	0
21	g	306	CLA	3	0
25	h	102	BCR	1	0
35	d	408	PL9	2	0
25	M	101	BCR	2	0
31	B	625	SQD	1	0
21	C	514	CLA	3	0
21	B	606	CLA	4	0
21	b	623	CLA	6	0
21	B	621	CLA	3	0
21	B	610	CLA	1	0
21	b	609	CLA	1	0
24	g	315	KC1	1	0
21	7	301	CLA	3	0
21	b	611	CLA	2	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.

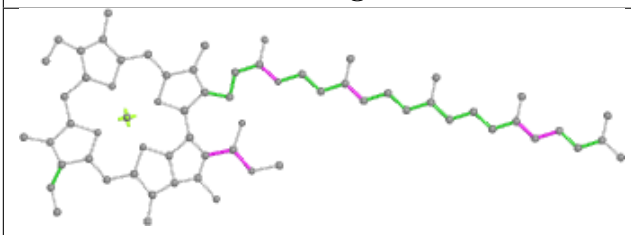
Ligand CLA C 507



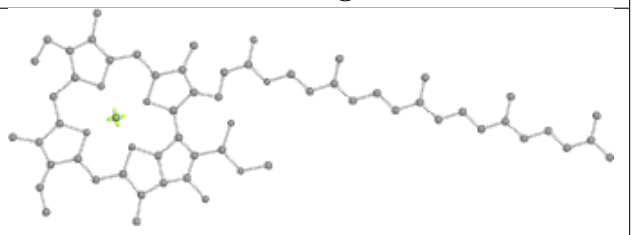
Bond lengths



Bond angles

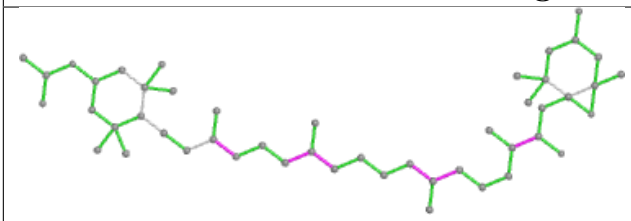


Torsions

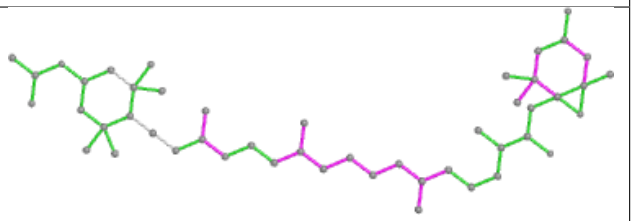


Rings

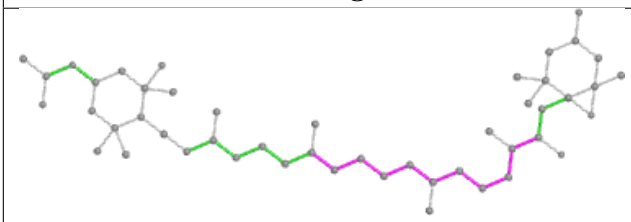
Ligand A86 8 311



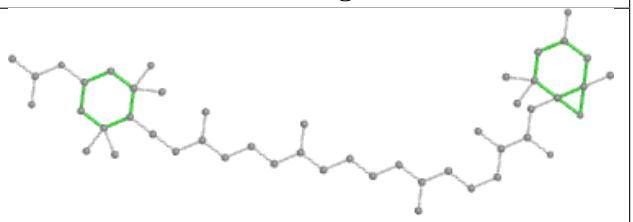
Bond lengths



Bond angles

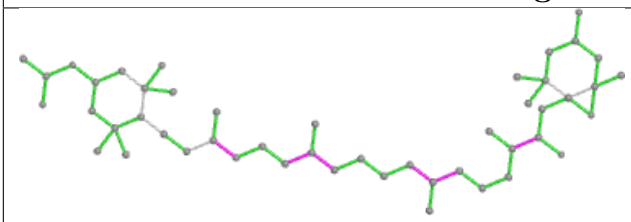


Torsions

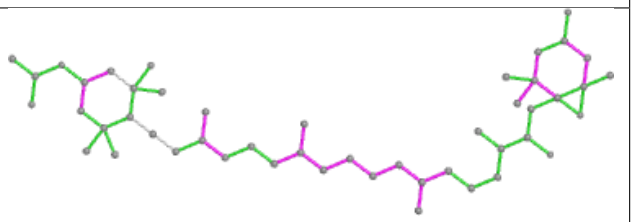


Rings

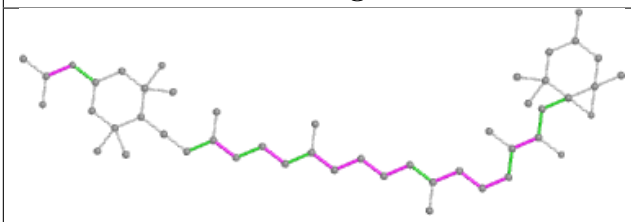
Ligand A86 4 305



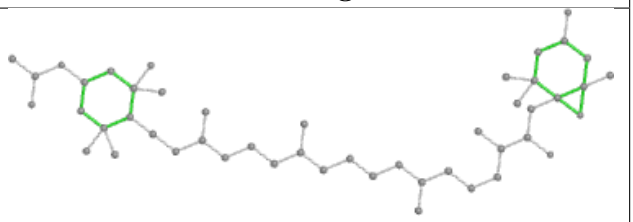
Bond lengths



Bond angles

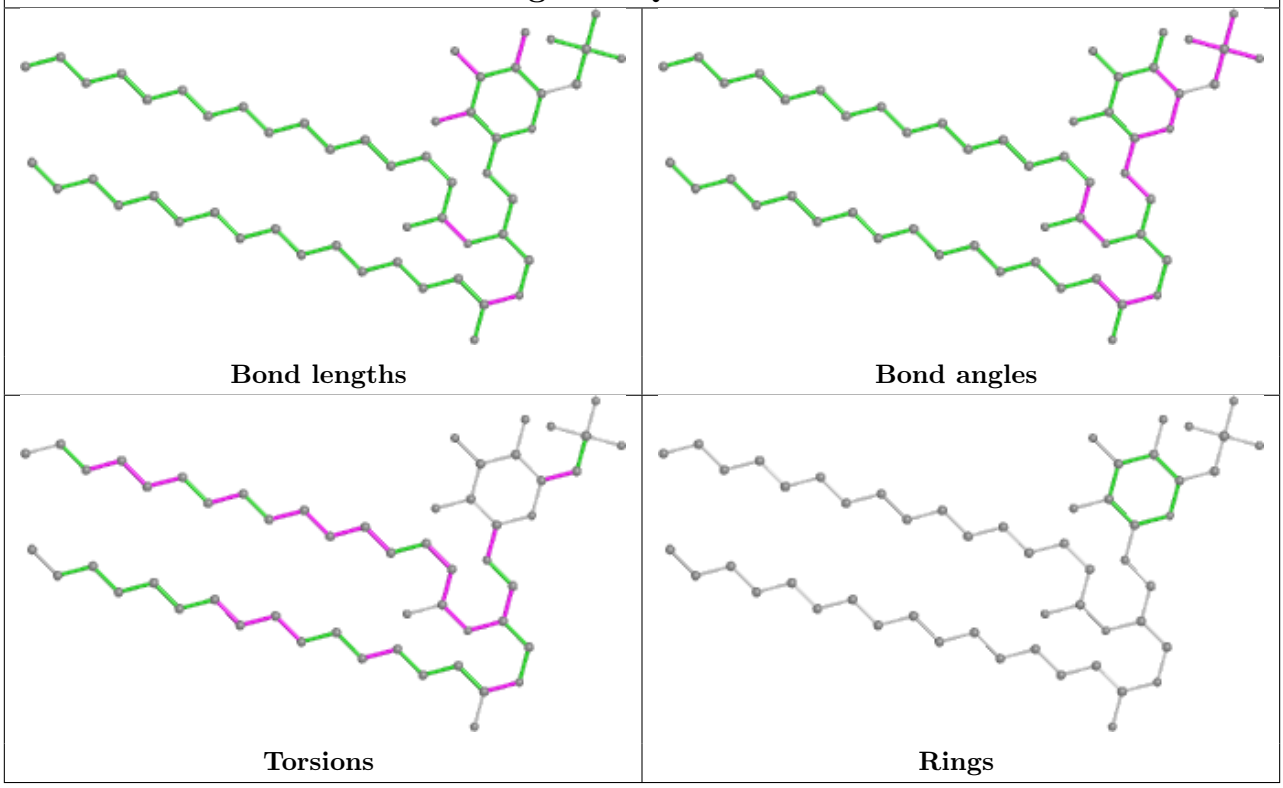


Torsions

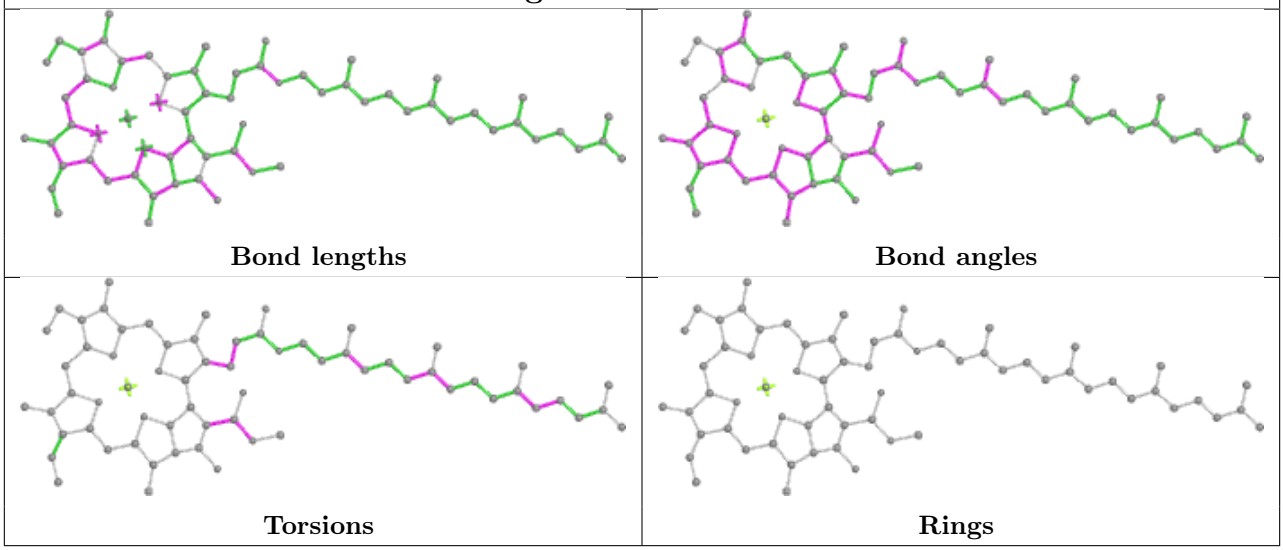


Rings

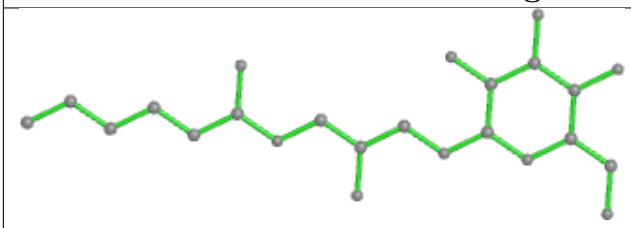
Ligand SQD b 602



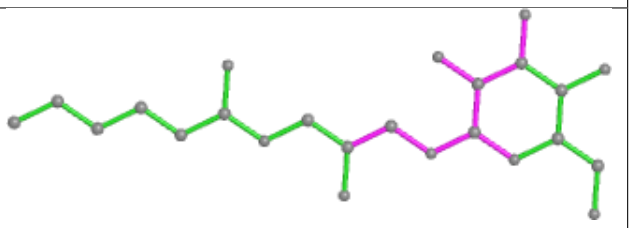
Ligand CLA C 509



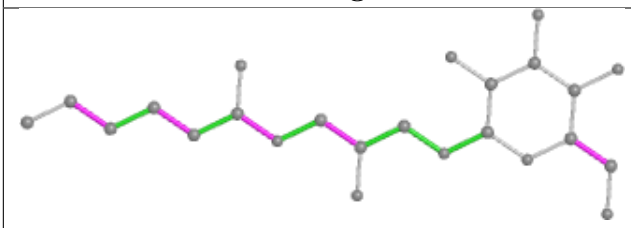
Ligand LMG 8 301



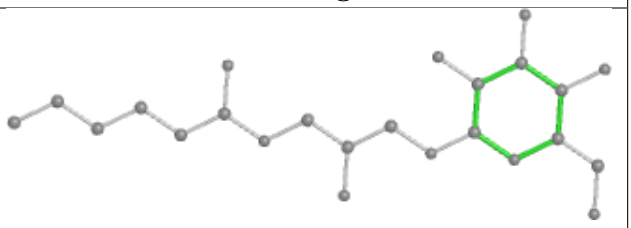
Bond lengths



Bond angles

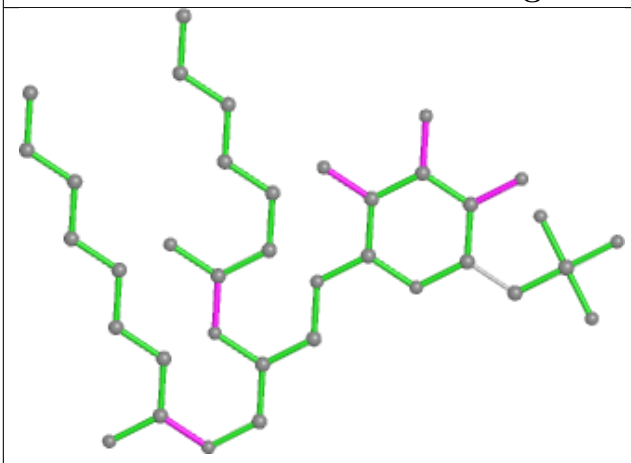


Torsions

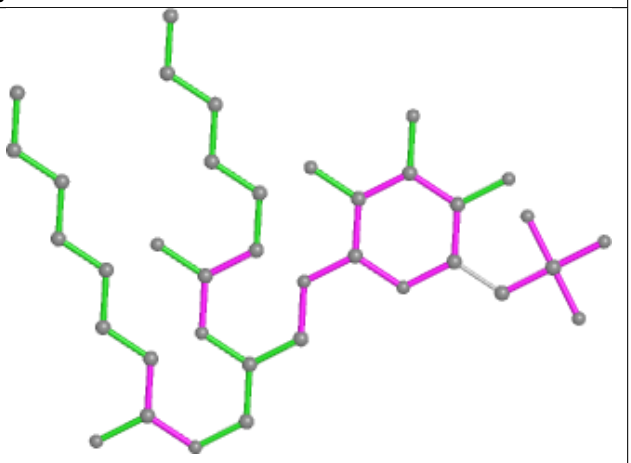


Rings

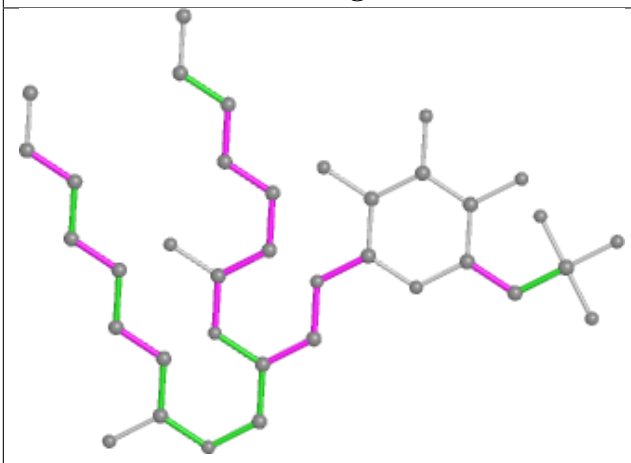
Ligand SQD X 401



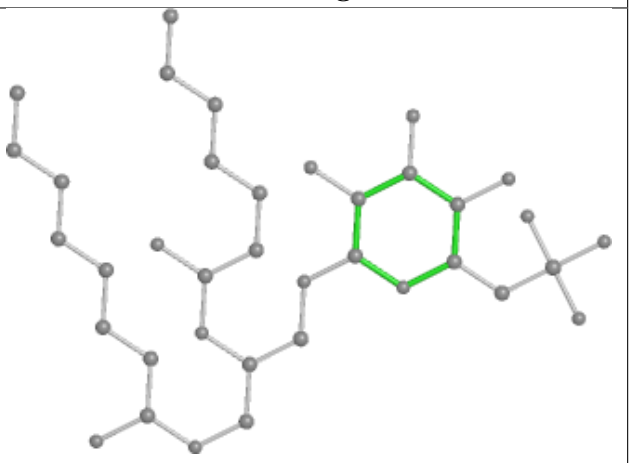
Bond lengths



Bond angles

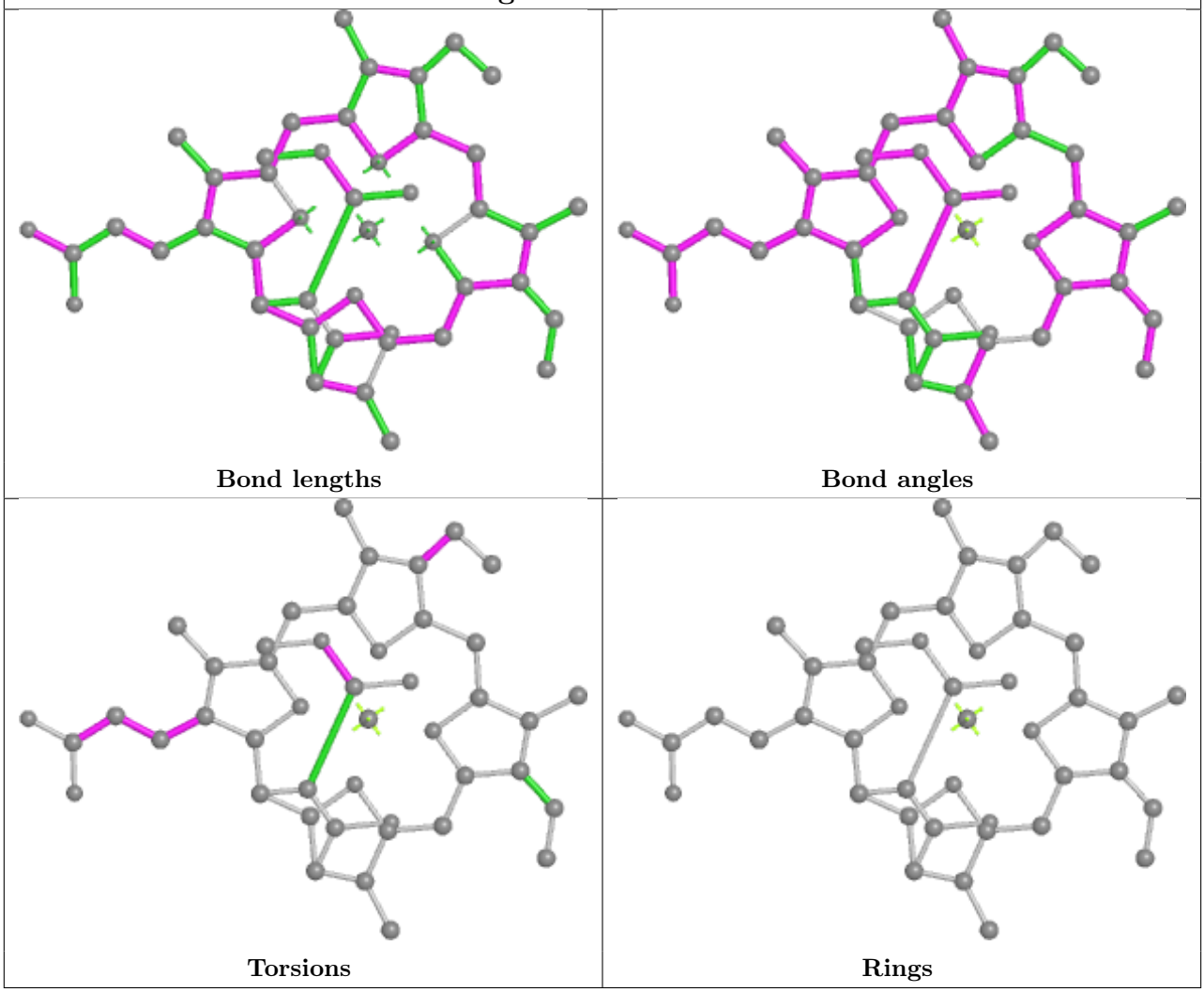


Torsions

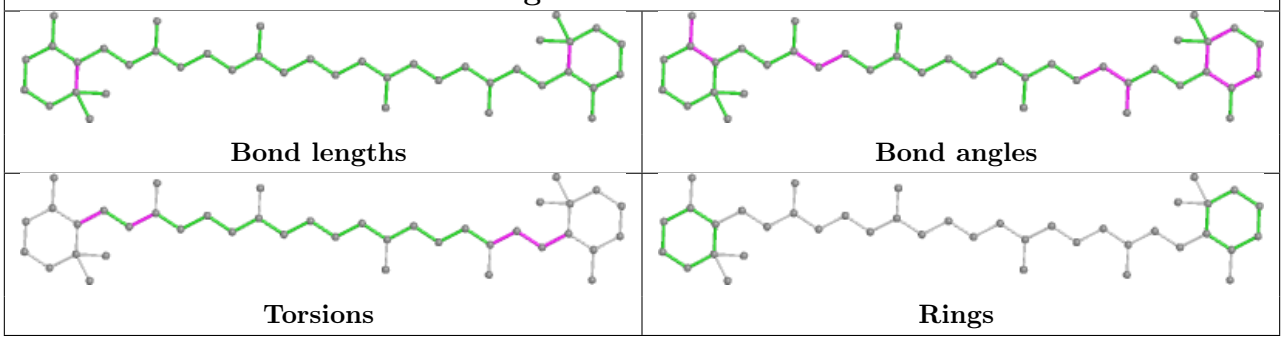


Rings

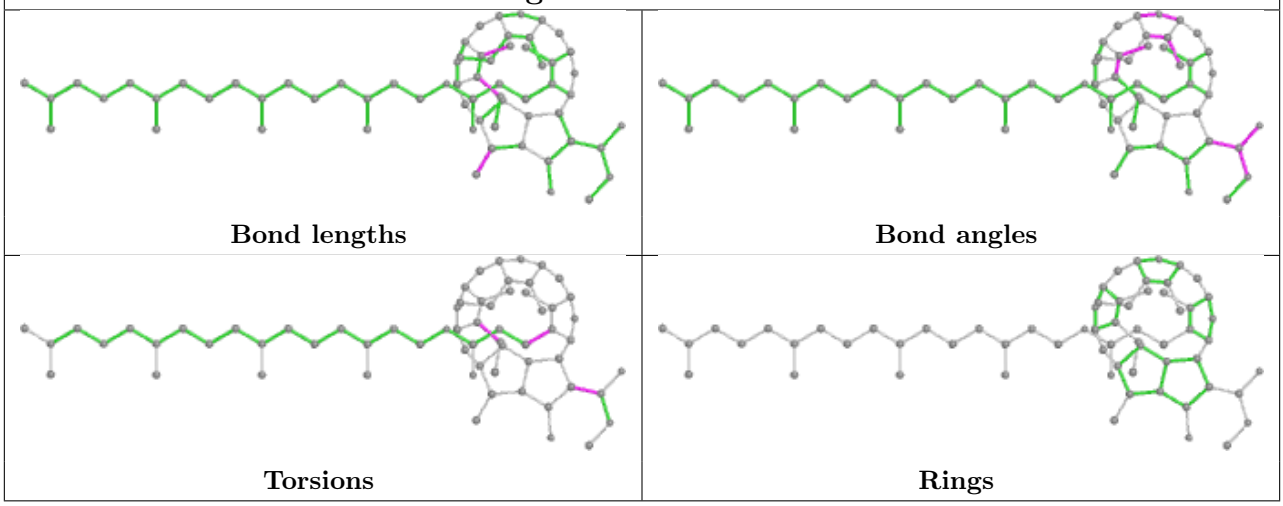
Ligand KC1 5 313



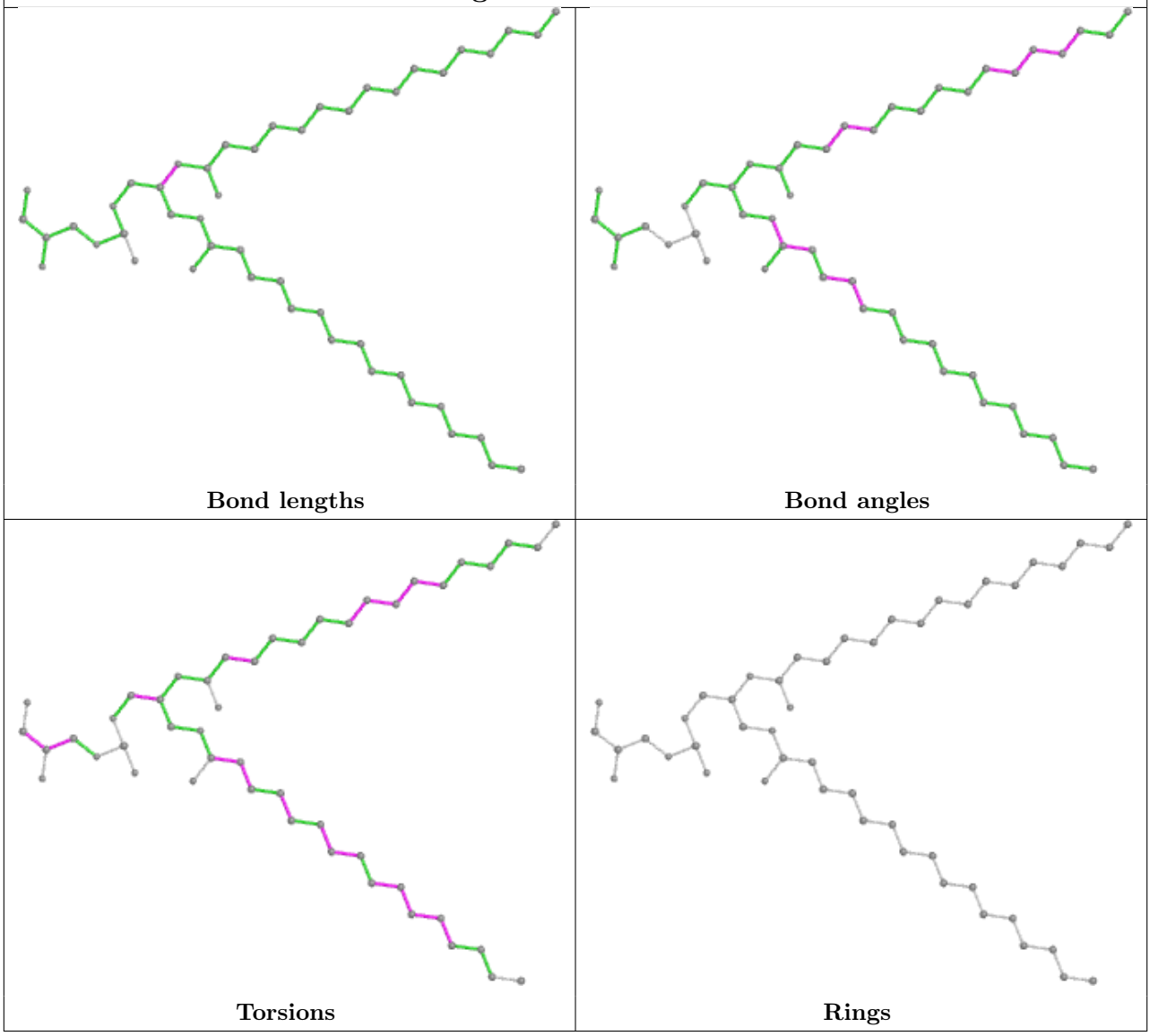
Ligand BCR B 618



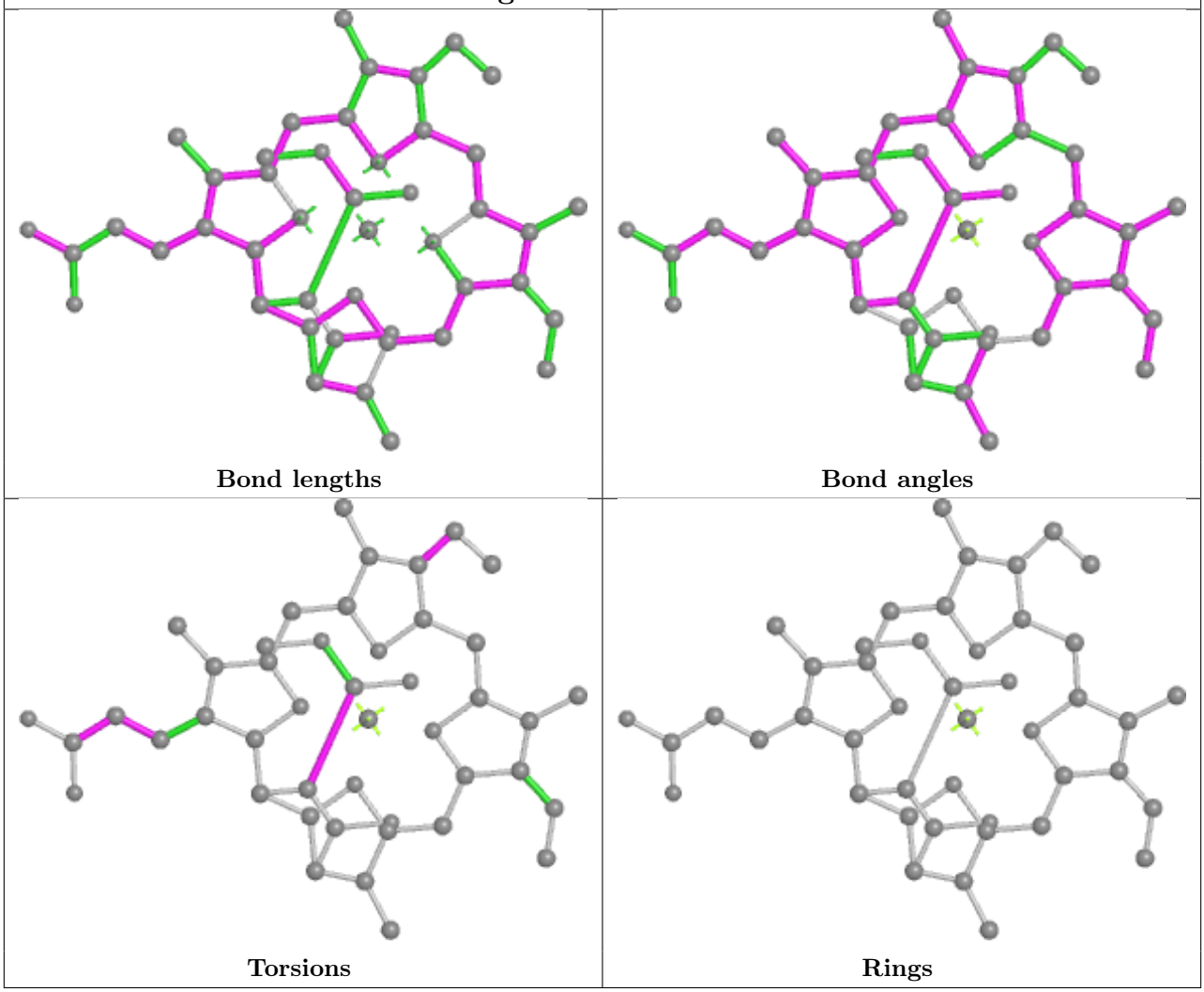
Ligand PHO d 403

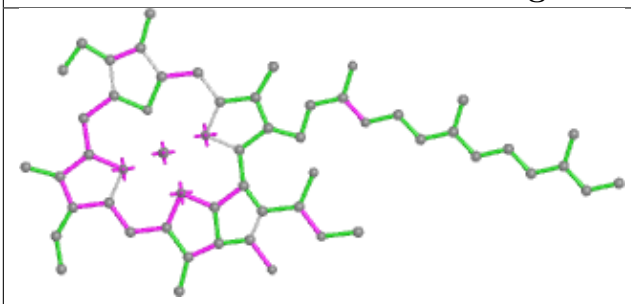
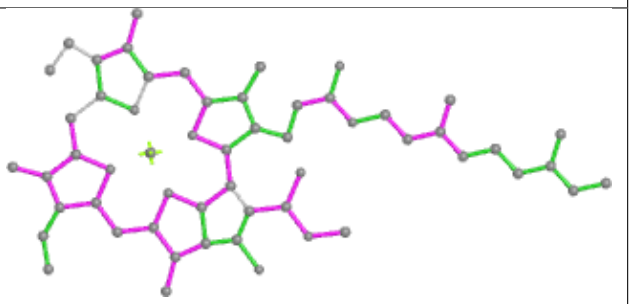
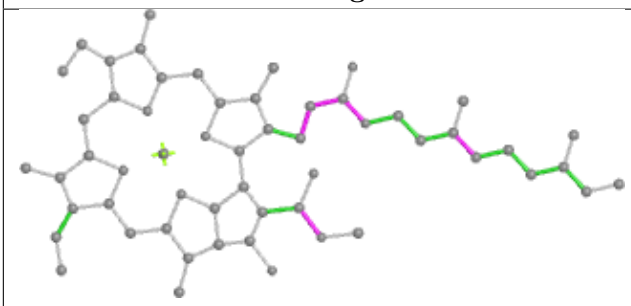
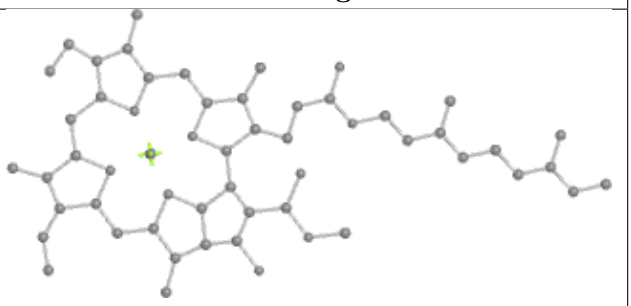


Ligand LHG d 409

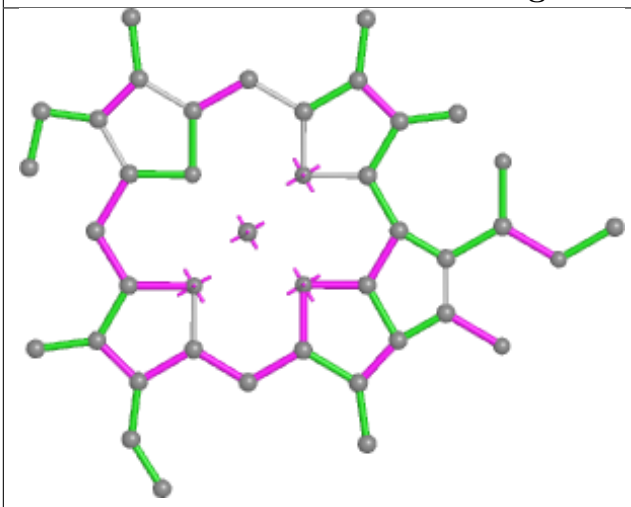


Ligand KC1 J 313

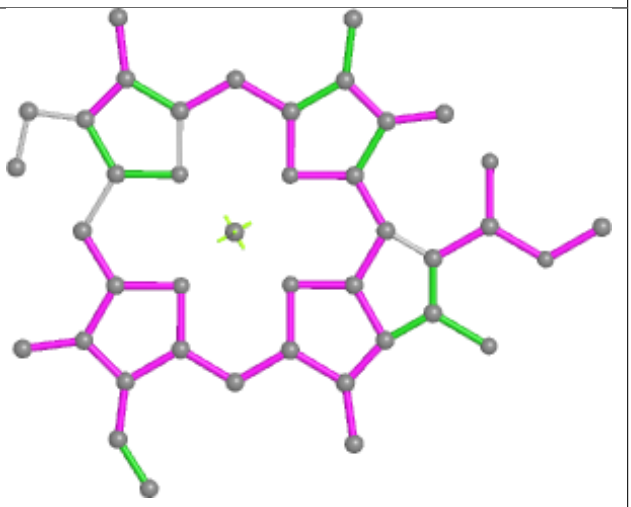


Ligand CLA 9 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

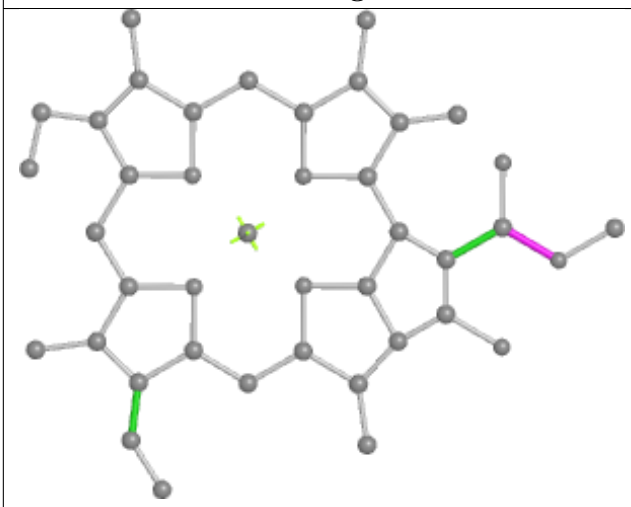
Ligand CLA 5 305



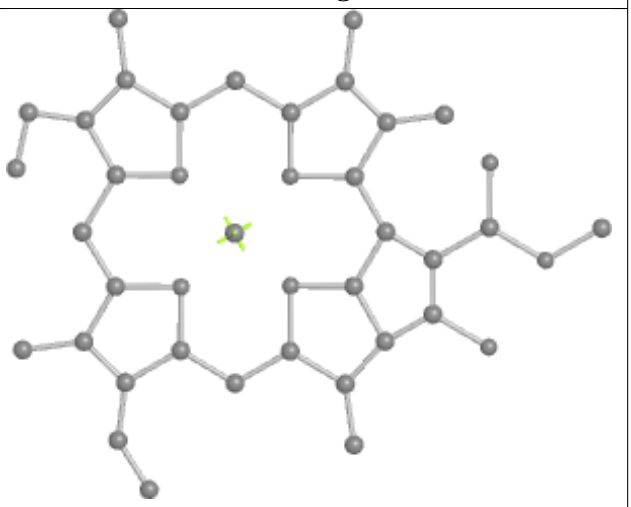
Bond lengths



Bond angles

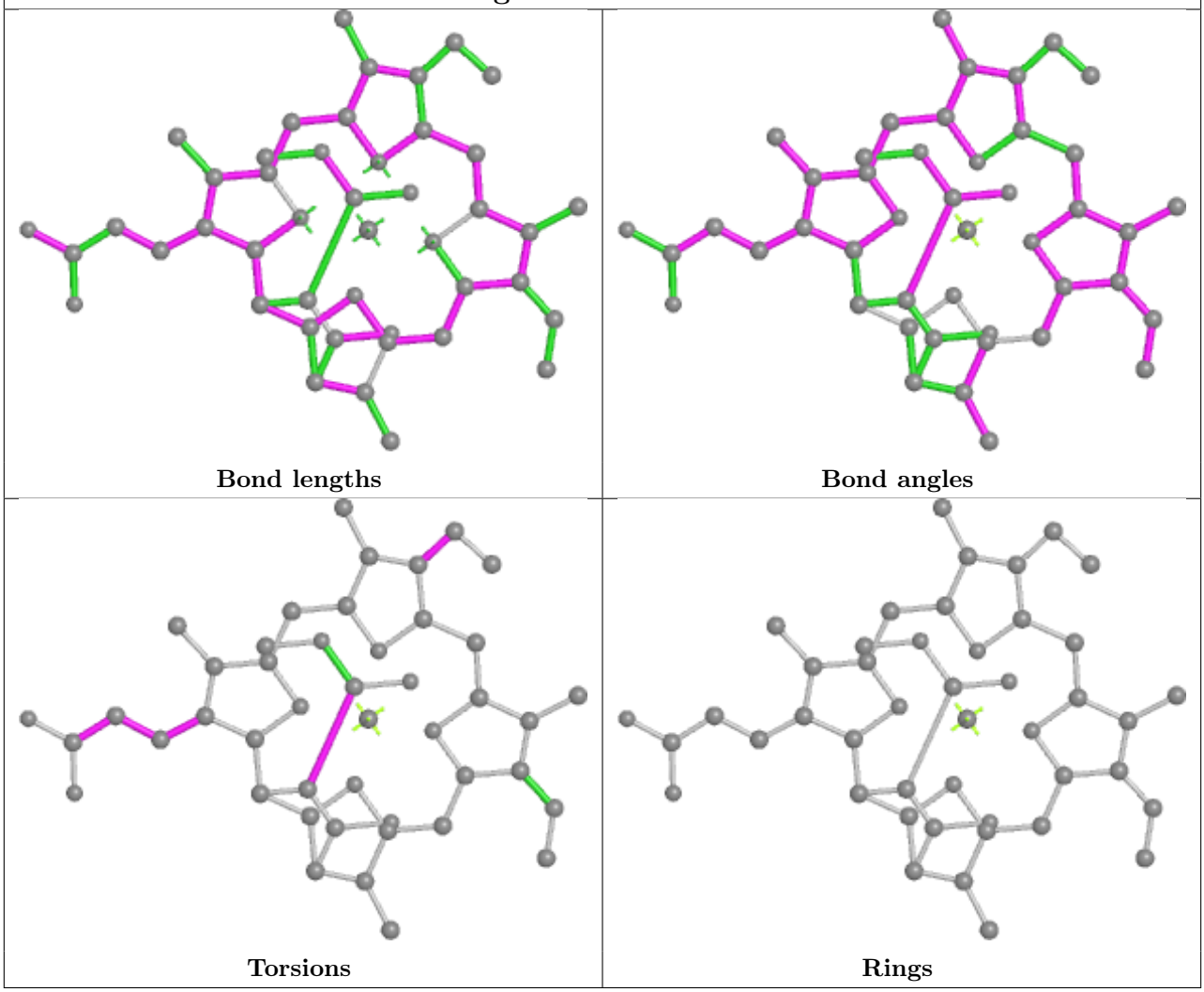


Torsions

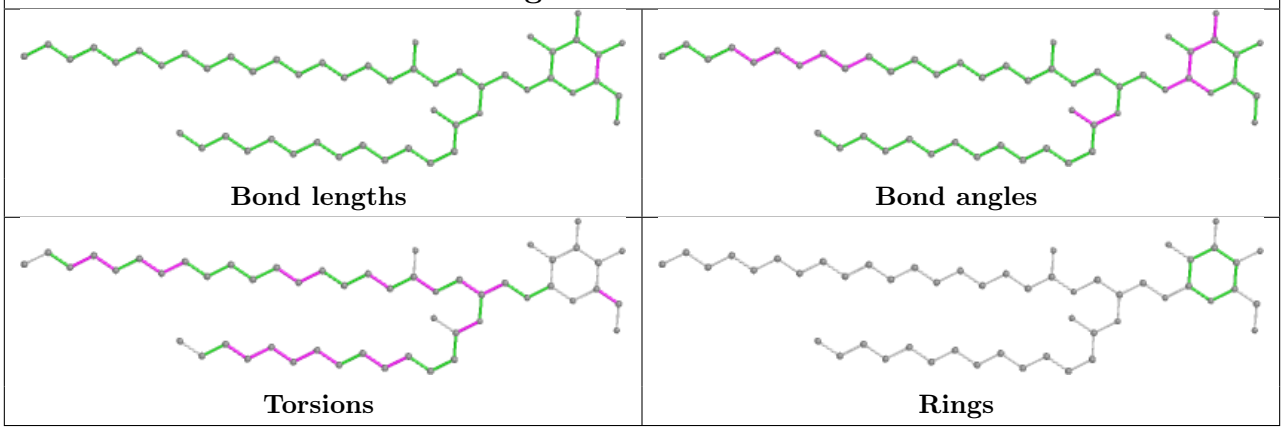


Rings

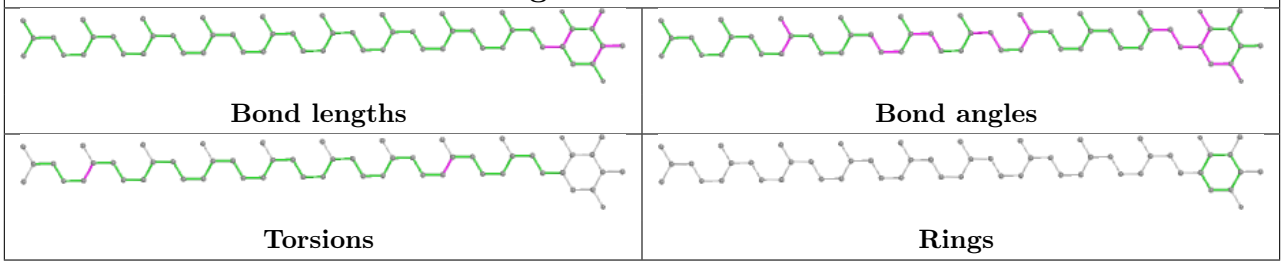
Ligand KC1 G 309



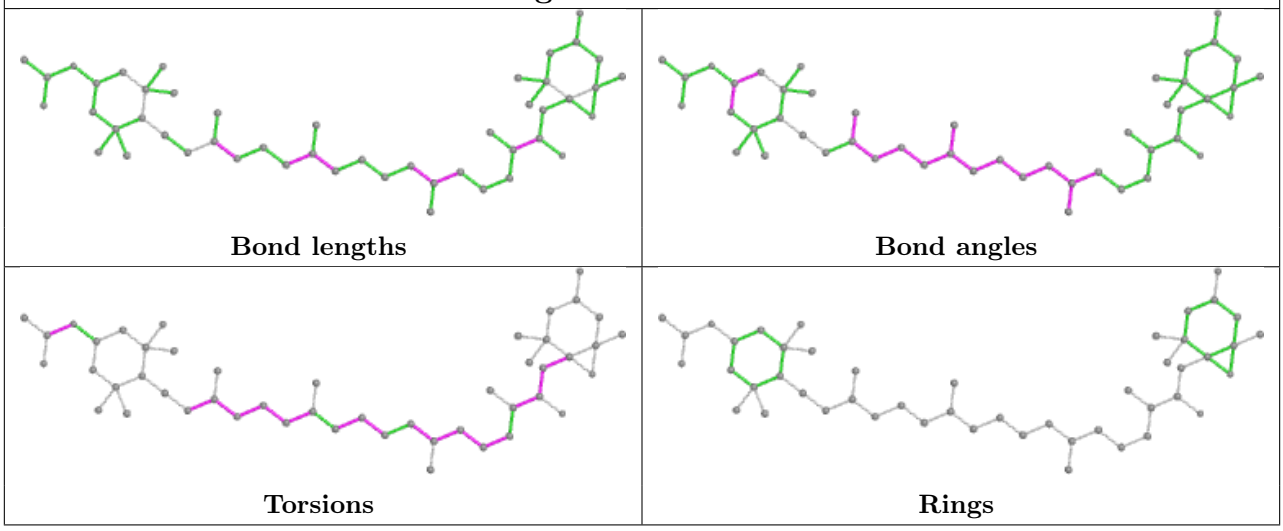
Ligand LMG 8 317



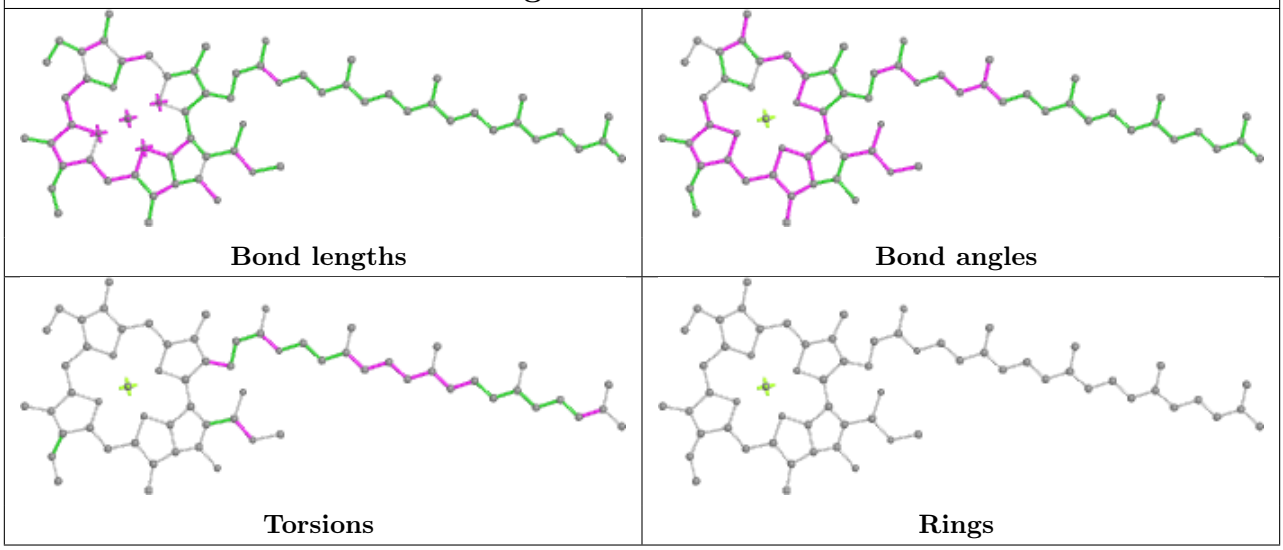
Ligand PL9 D 409



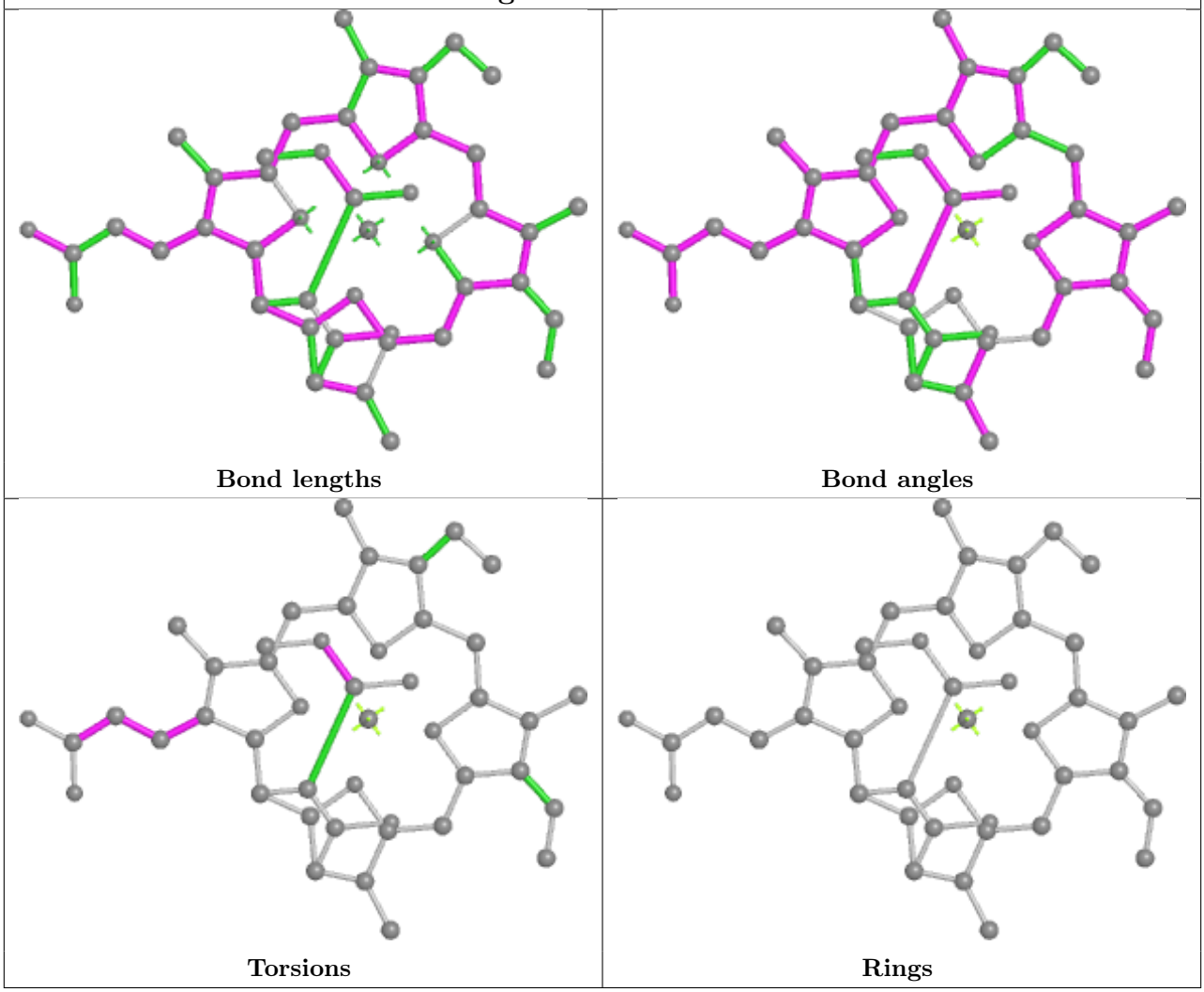
Ligand A86 1 312



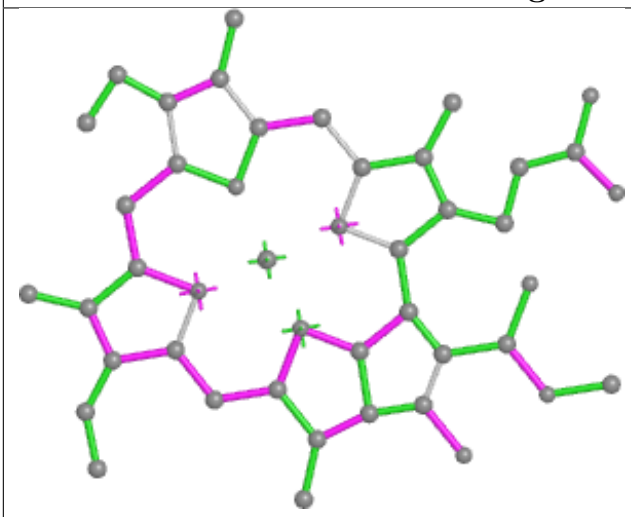
Ligand CLA G 304



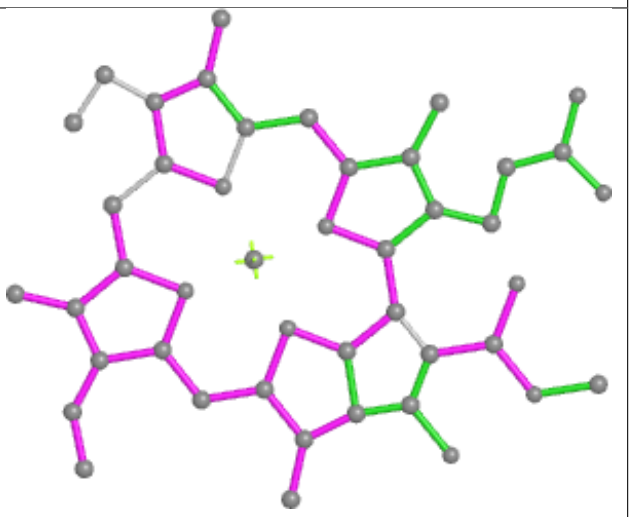
Ligand KC1 8 316



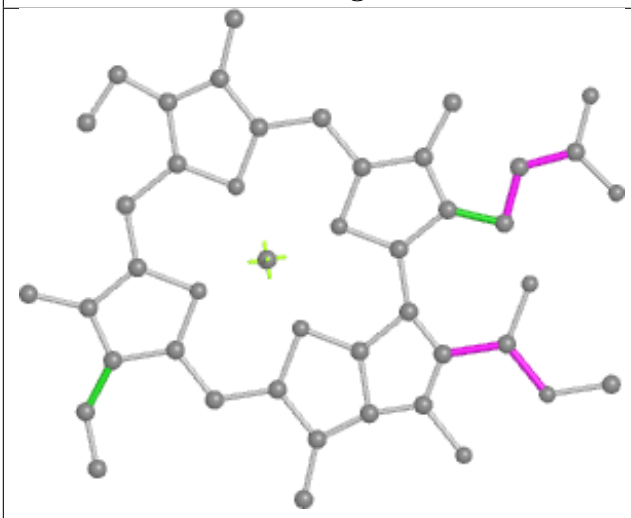
Ligand CLA 2 306



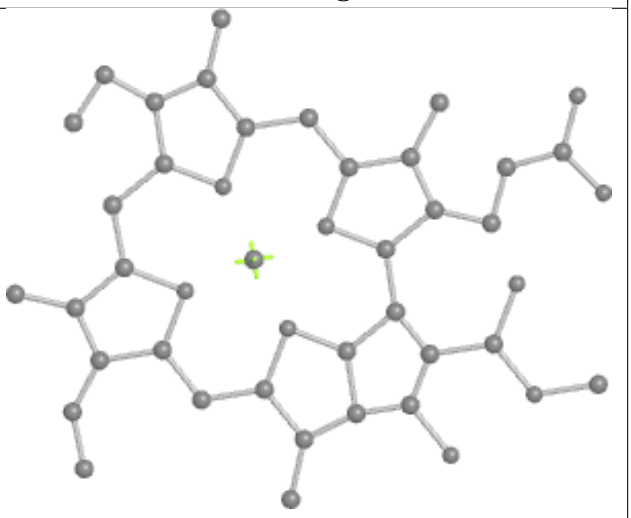
Bond lengths



Bond angles

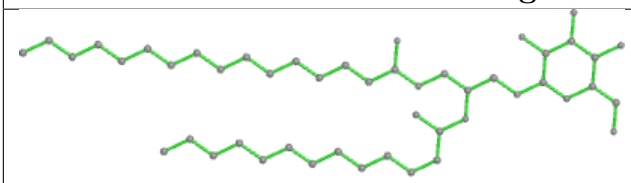


Torsions

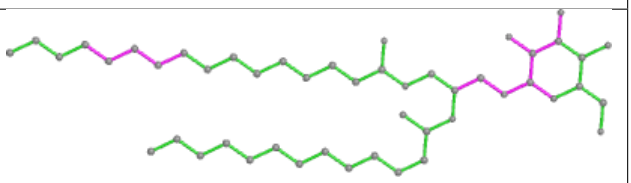


Rings

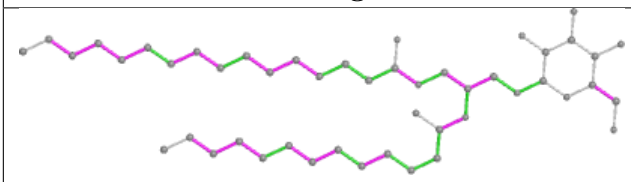
Ligand LMG A 407



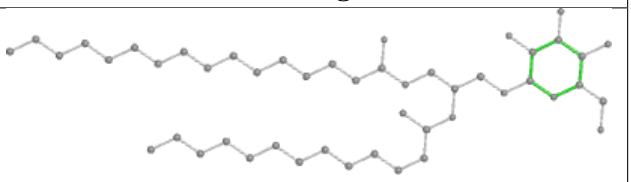
Bond lengths



Bond angles

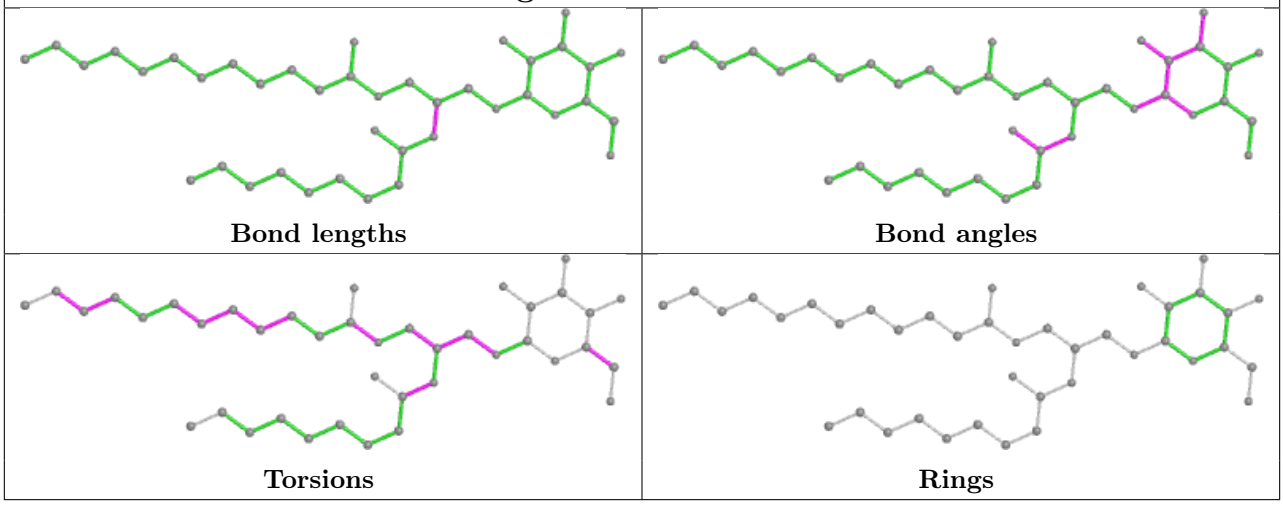


Torsions

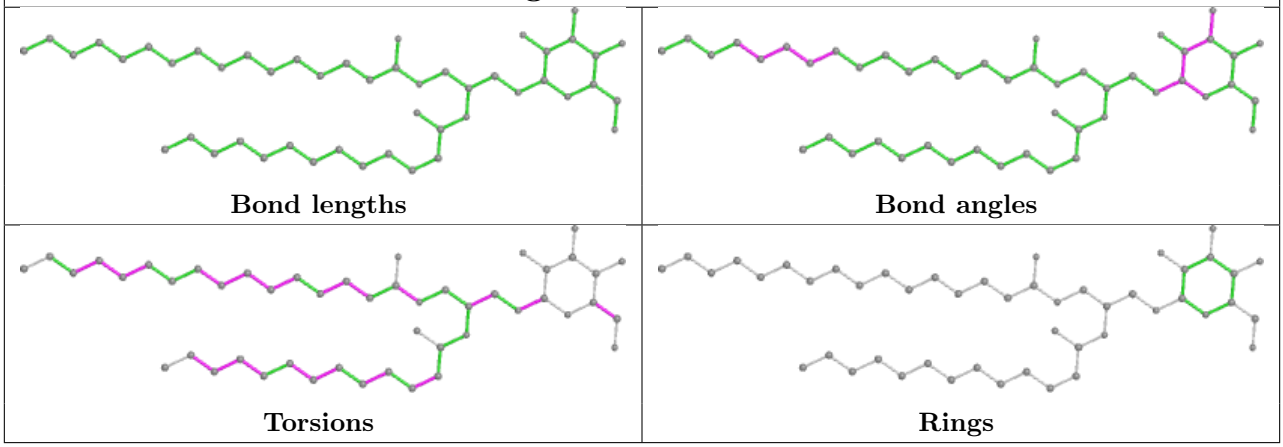


Rings

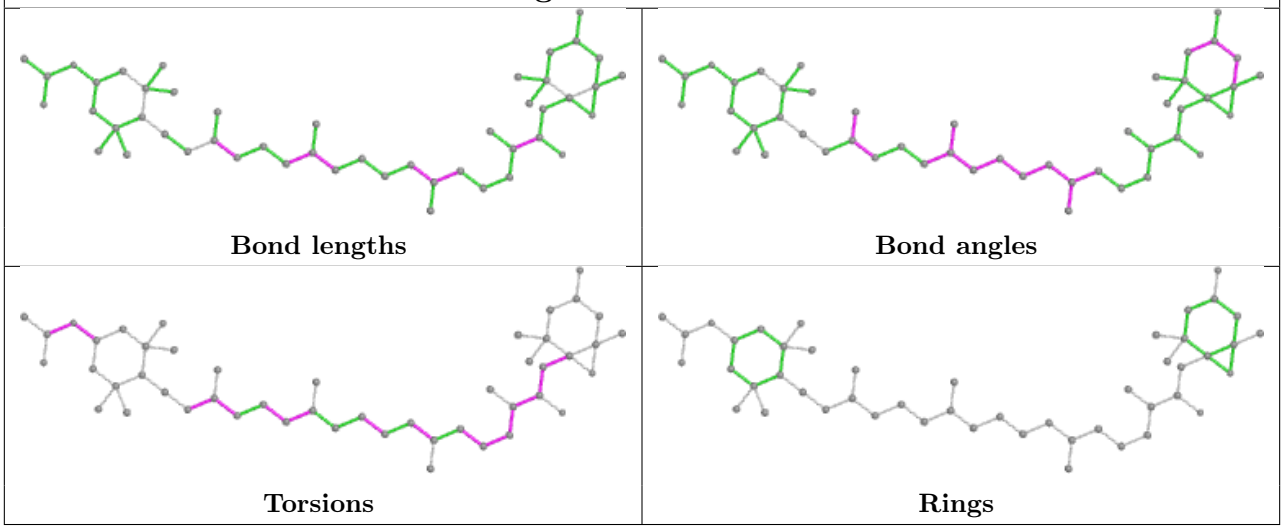
Ligand LMG M 102

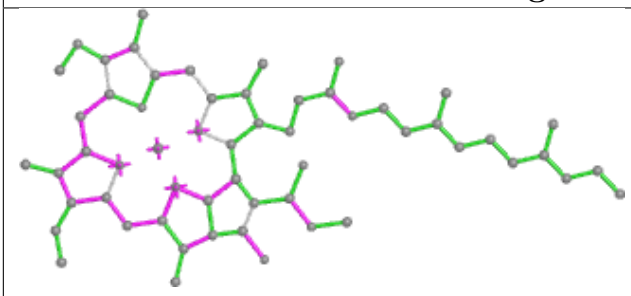
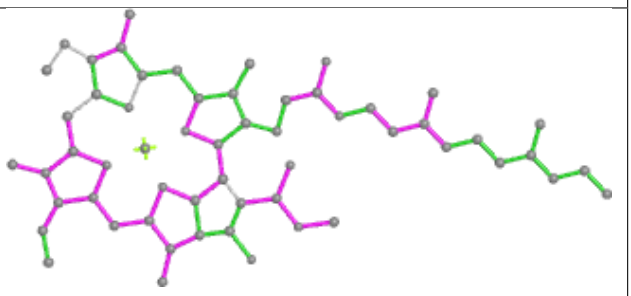
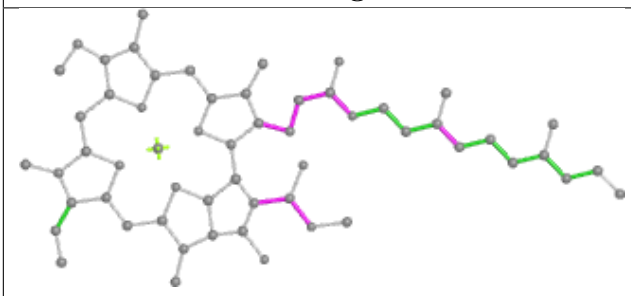
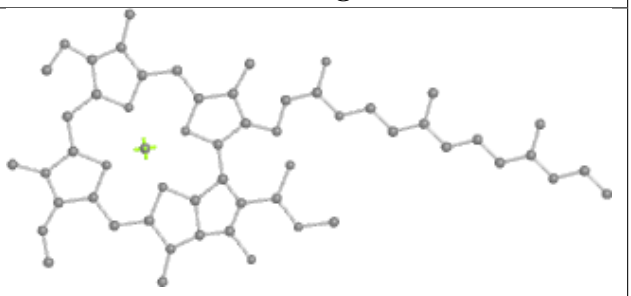


Ligand LMG a 407

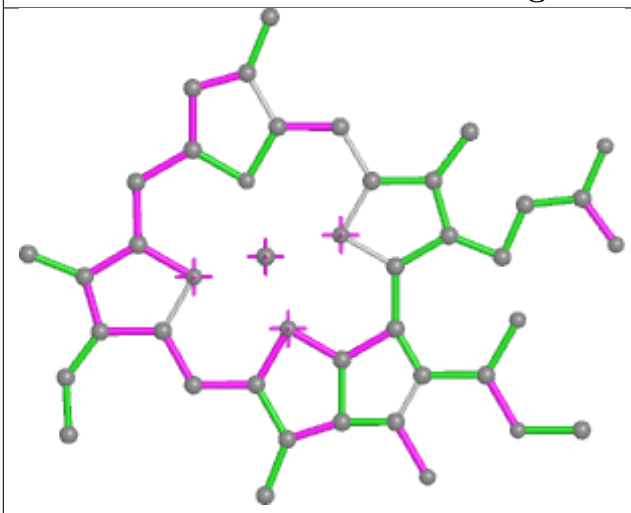


Ligand A86 5 312

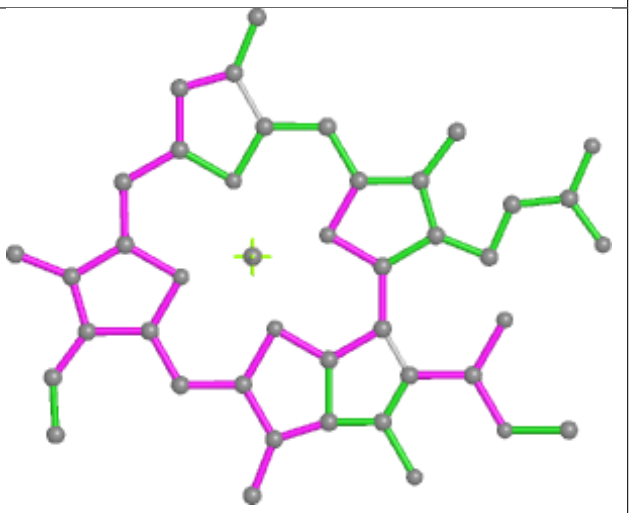


Ligand CLA 6 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

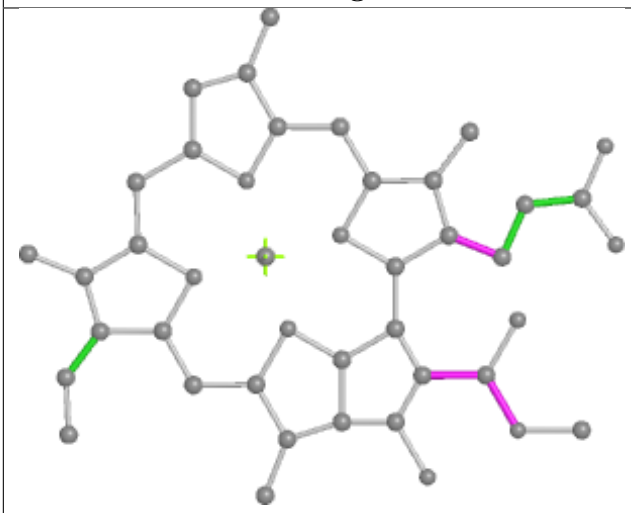
Ligand CLA 6 303



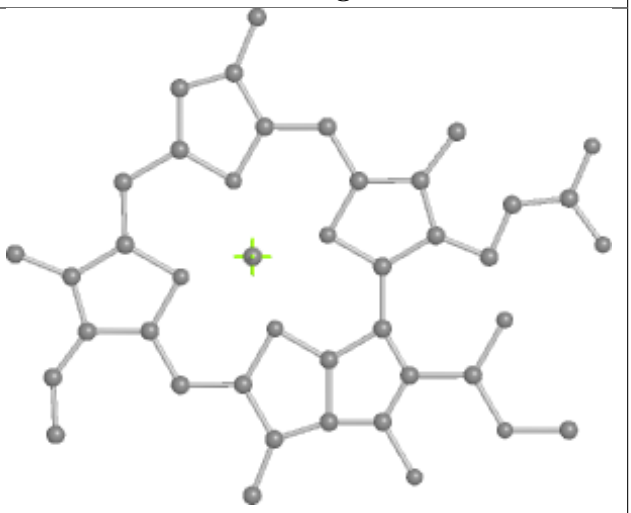
Bond lengths



Bond angles

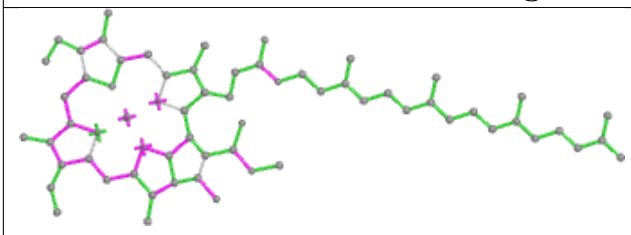


Torsions

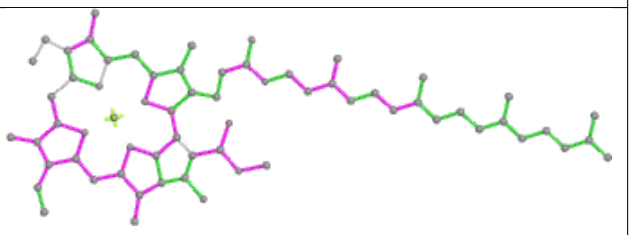


Rings

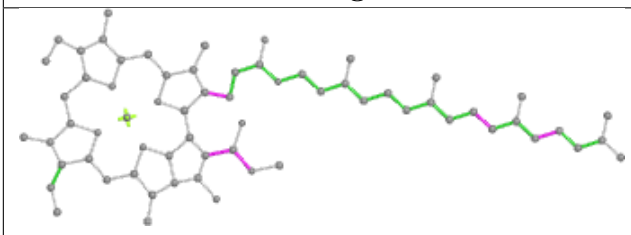
Ligand CLA G 300



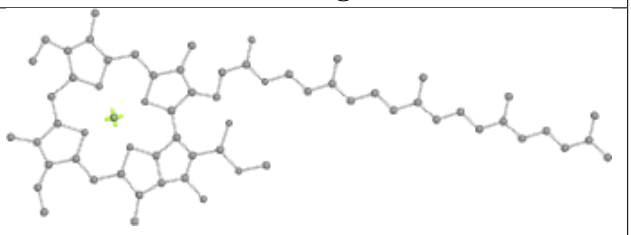
Bond lengths



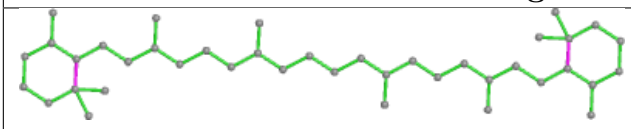
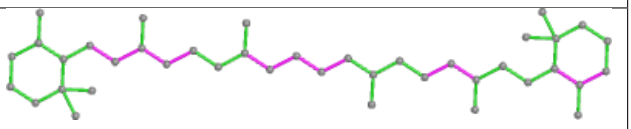
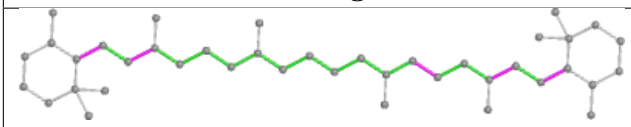
Bond angles

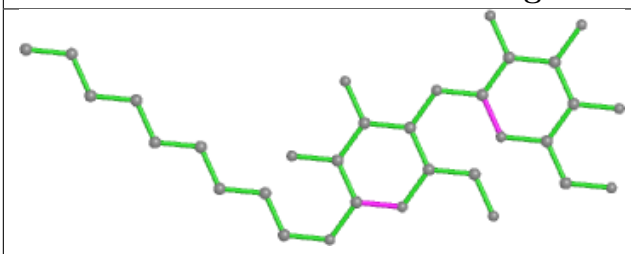
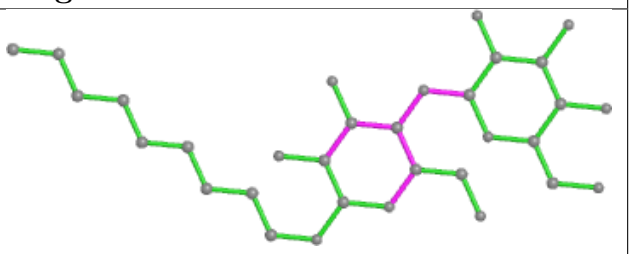
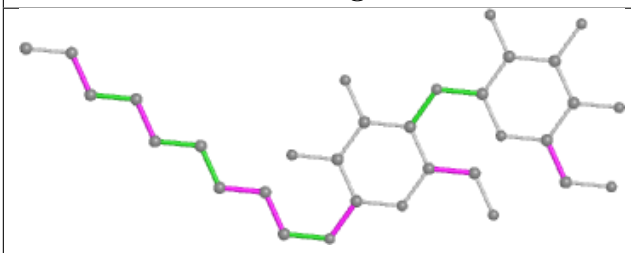
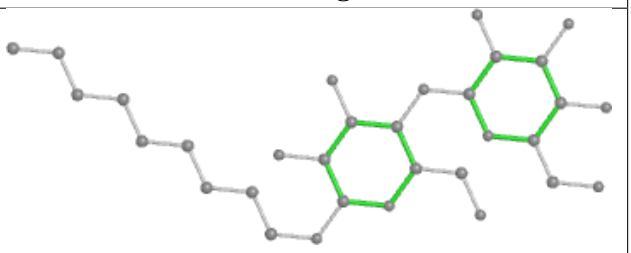


Torsions

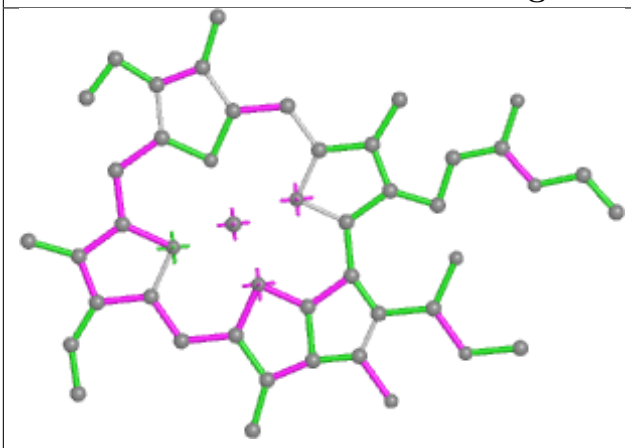


Rings

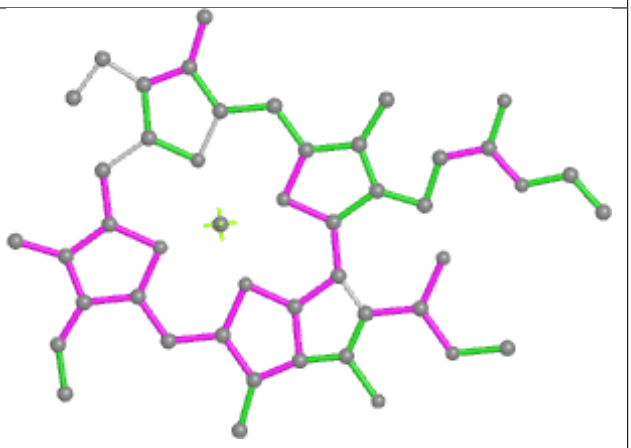
Ligand BCR c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMU g 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

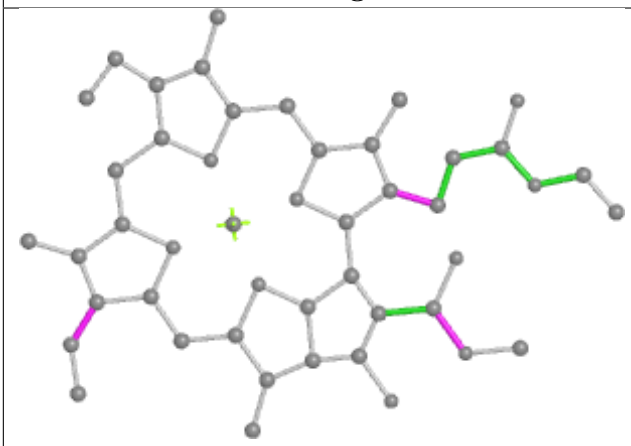
Ligand CLA 3 302



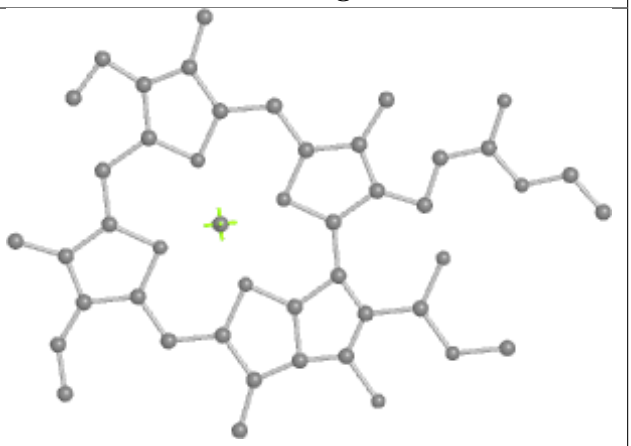
Bond lengths



Bond angles

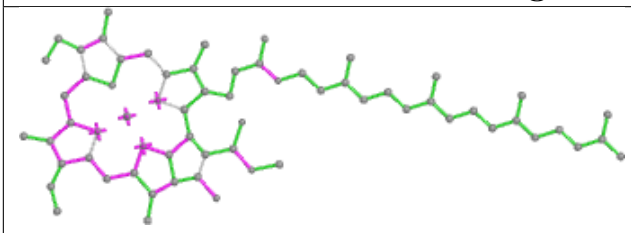


Torsions

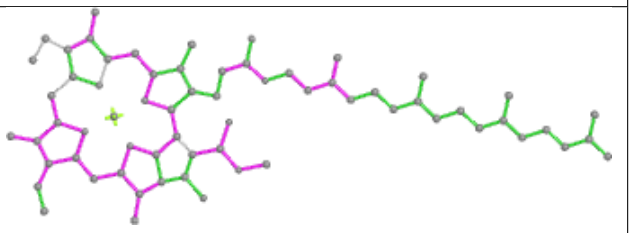


Rings

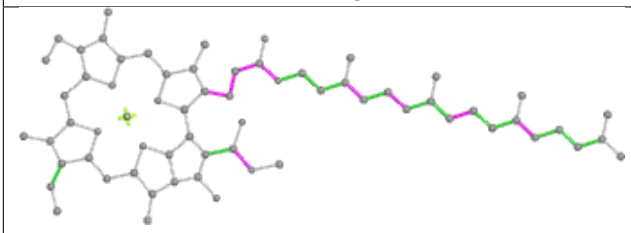
Ligand CLA 1 303



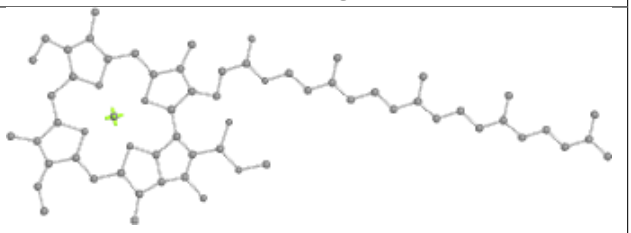
Bond lengths



Bond angles

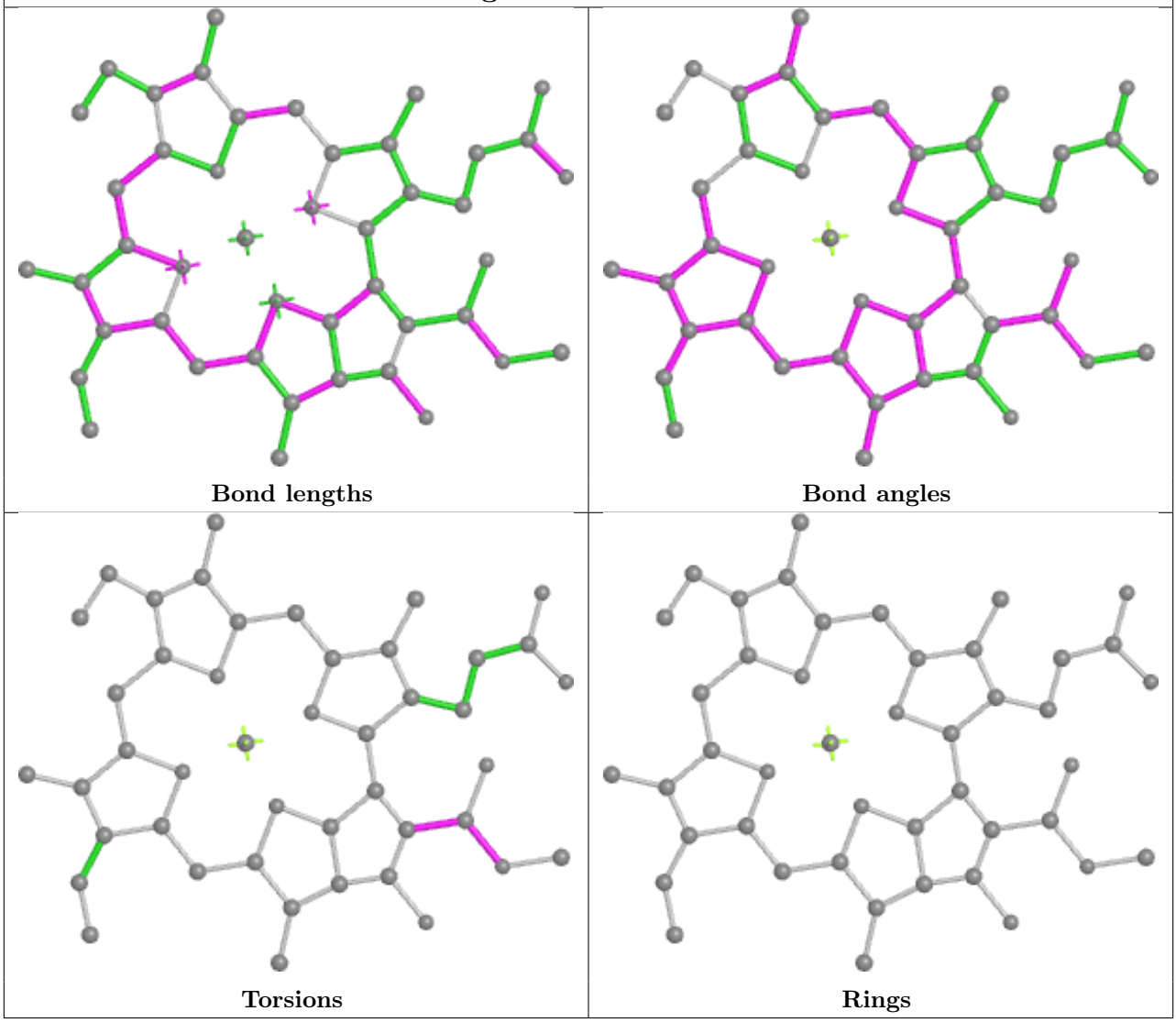


Torsions

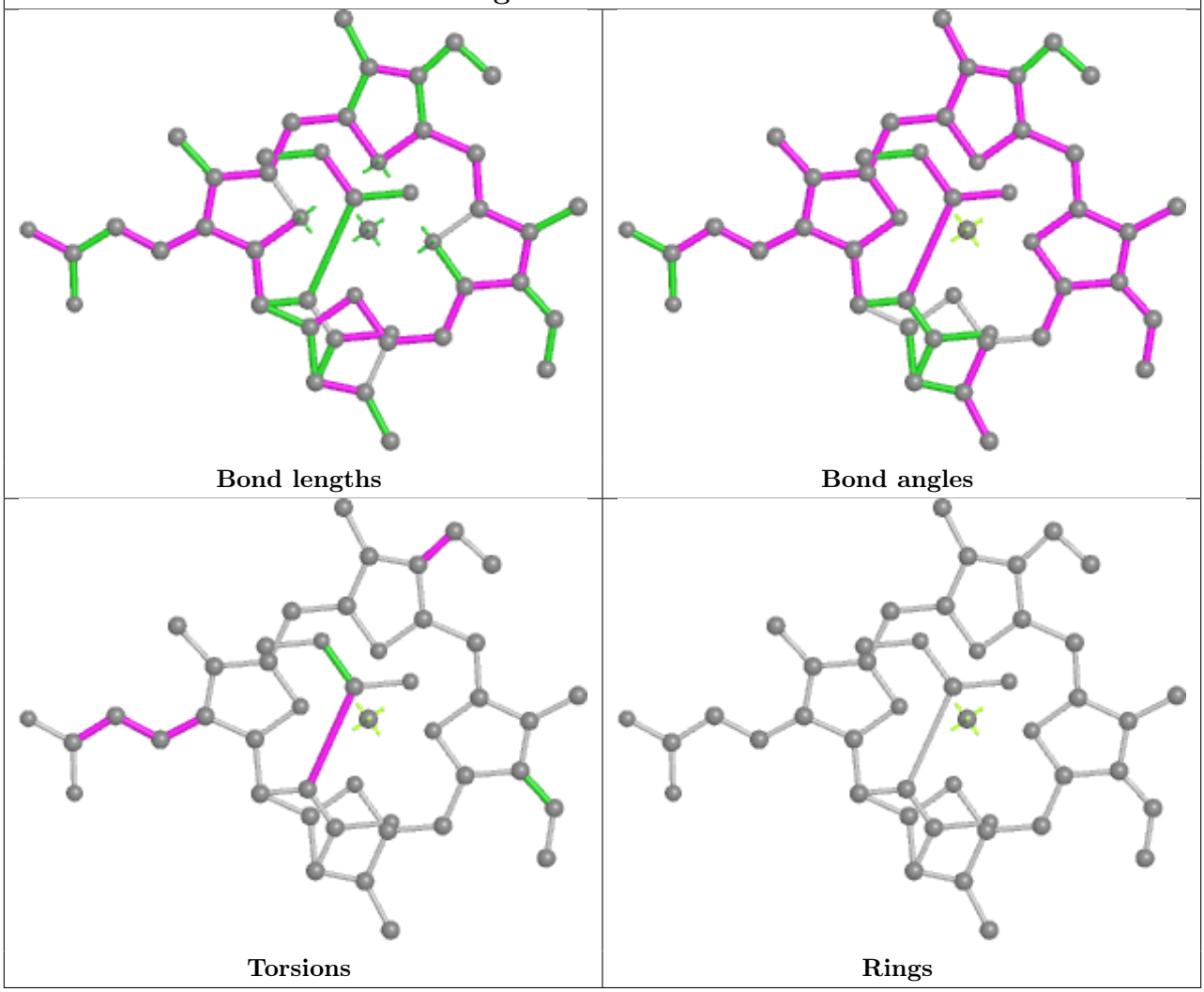


Rings

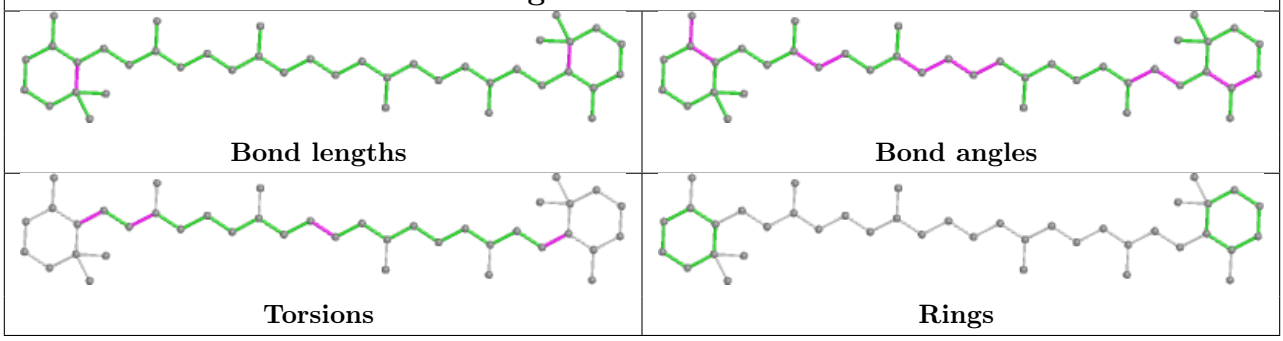
Ligand CLA C 508



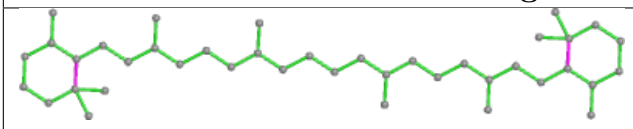
Ligand KC1 G 307



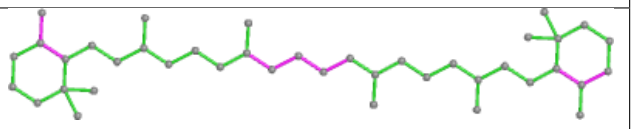
Ligand BCR a 406



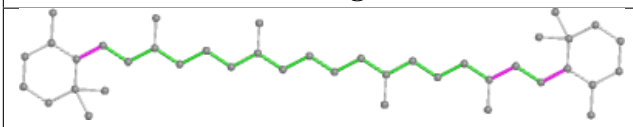
Ligand BCR m 101



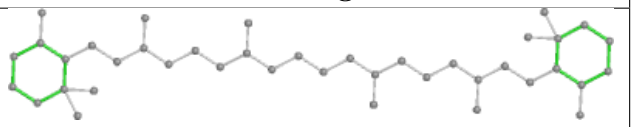
Bond lengths



Bond angles

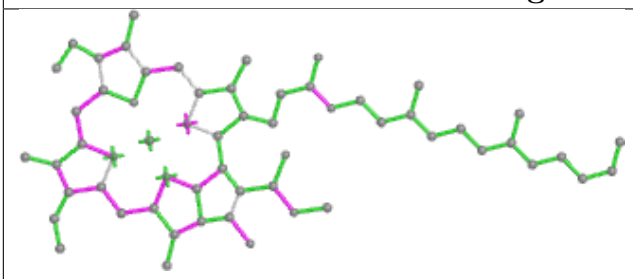


Torsions

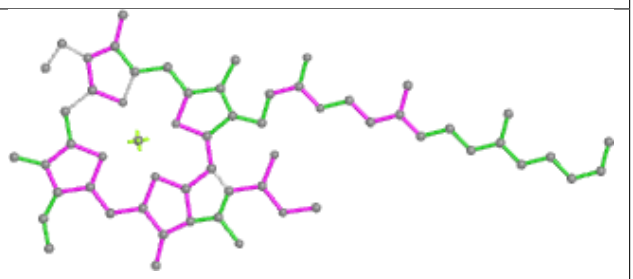


Rings

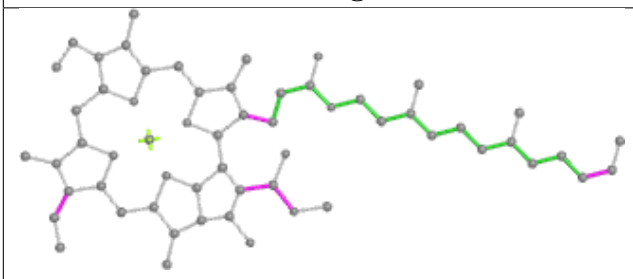
Ligand CLA d 404



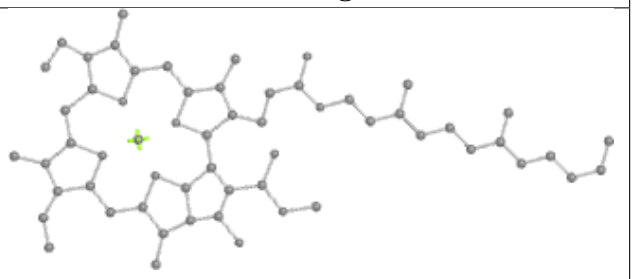
Bond lengths



Bond angles

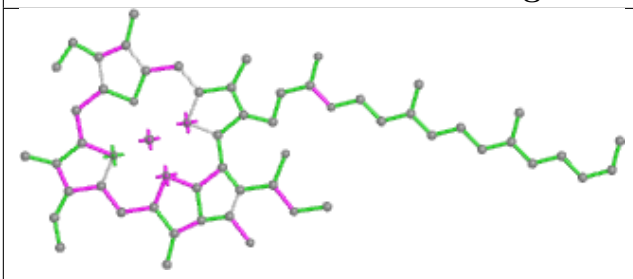


Torsions

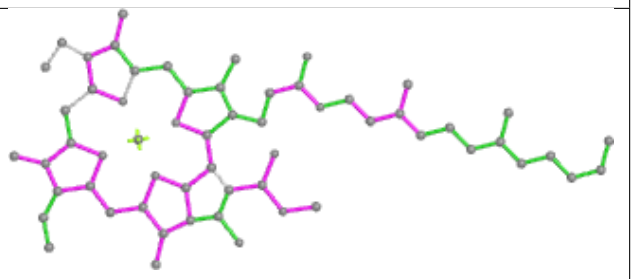


Rings

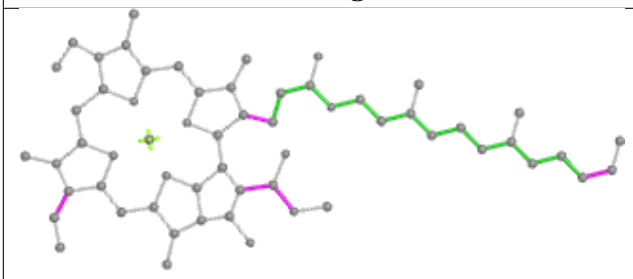
Ligand CLA D 404



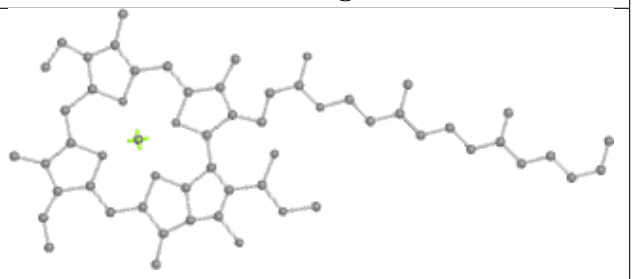
Bond lengths



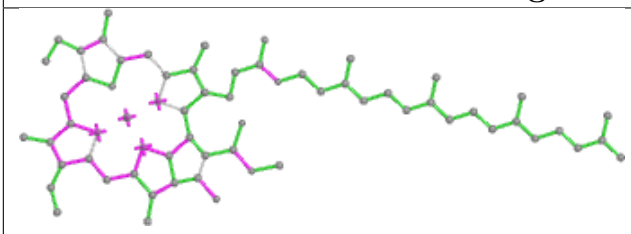
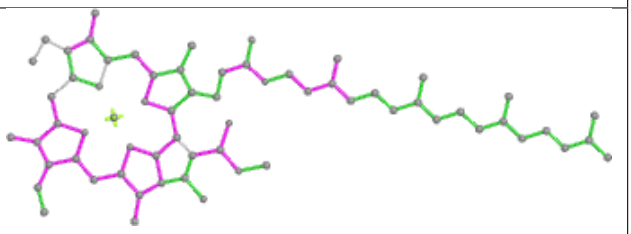
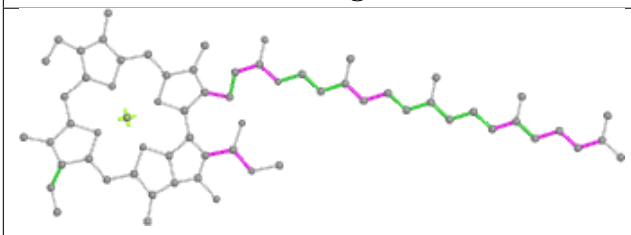
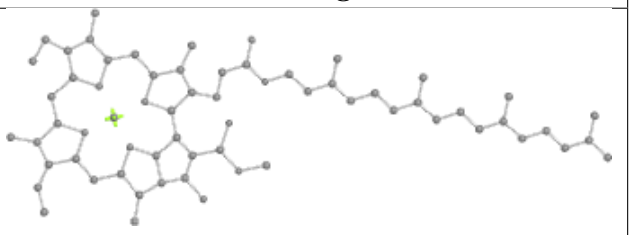
Bond angles

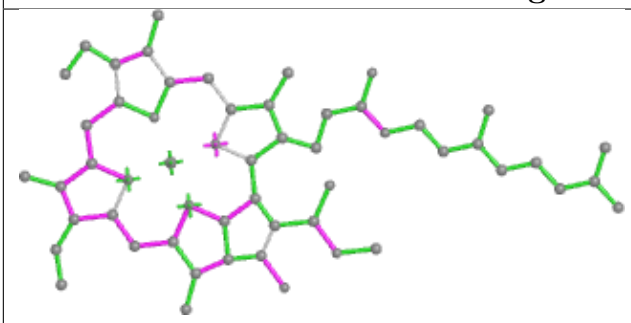
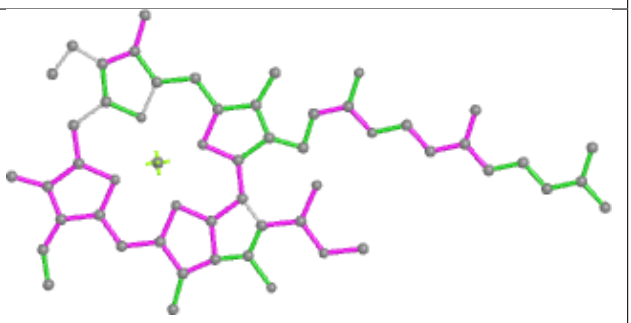
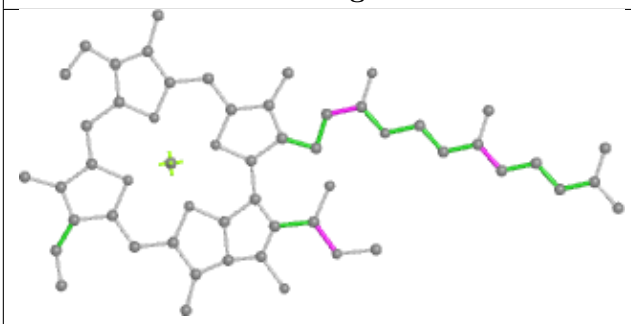
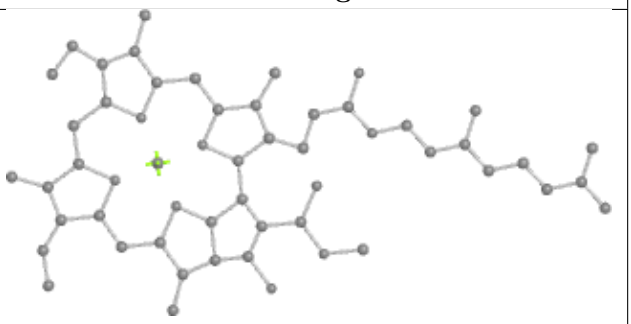


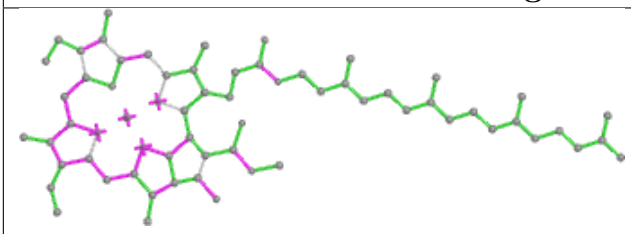
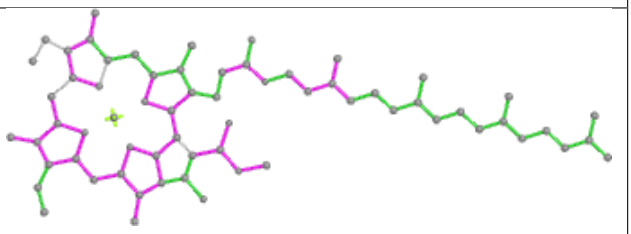
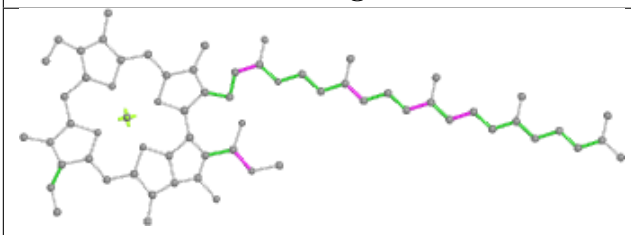
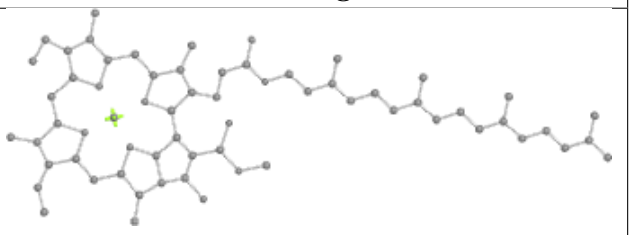
Torsions

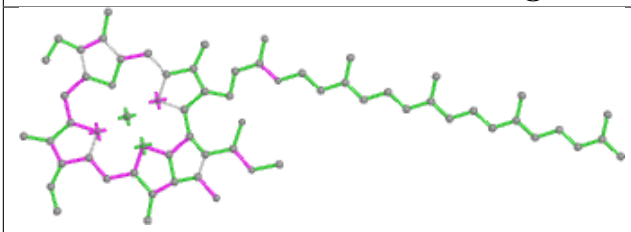
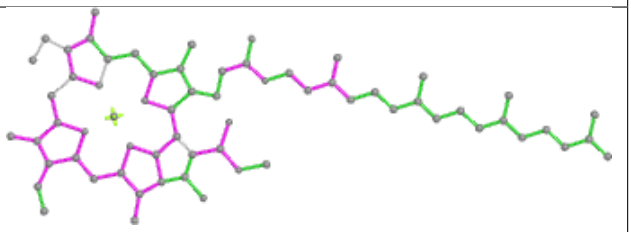
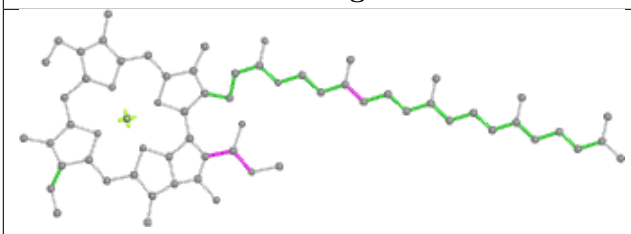
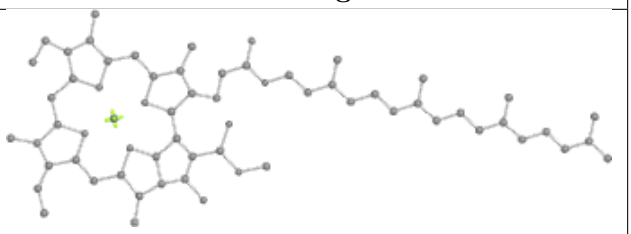


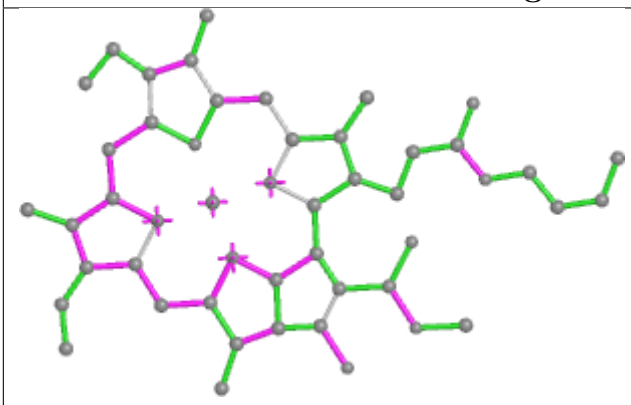
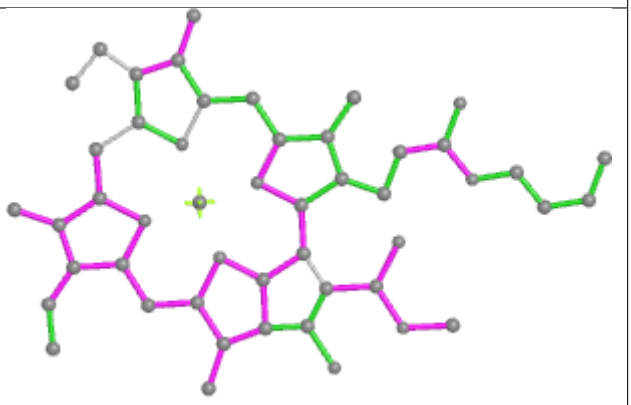
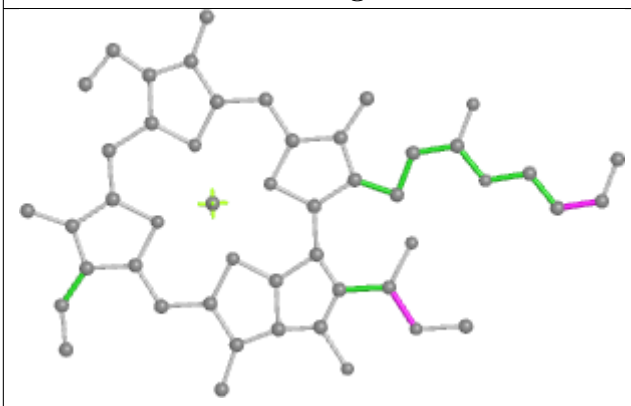
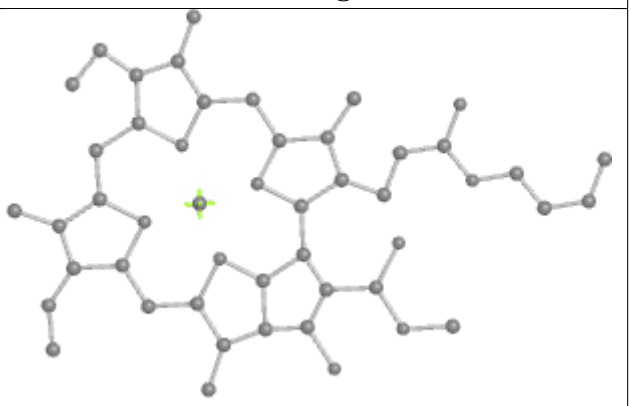
Rings

Ligand CLA 2 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

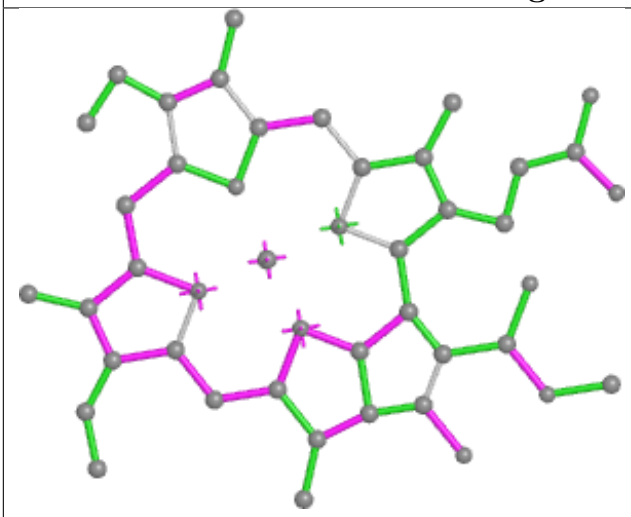
Ligand CLA 7 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

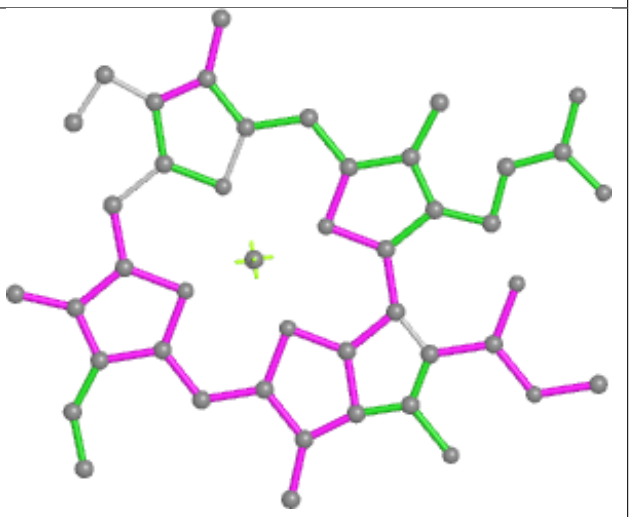
Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

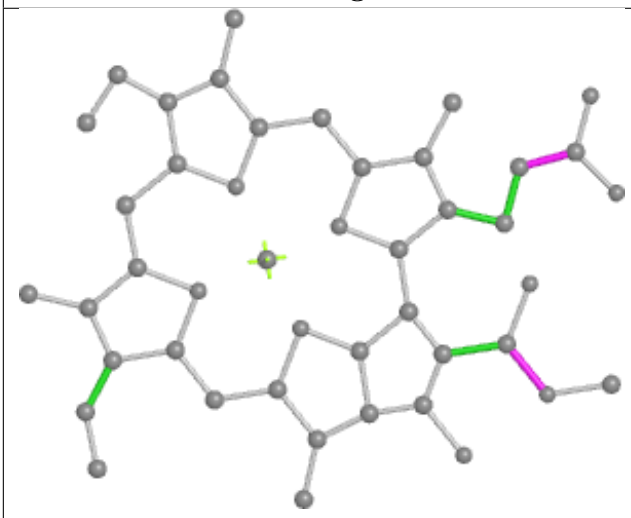
Ligand CLA 6 305



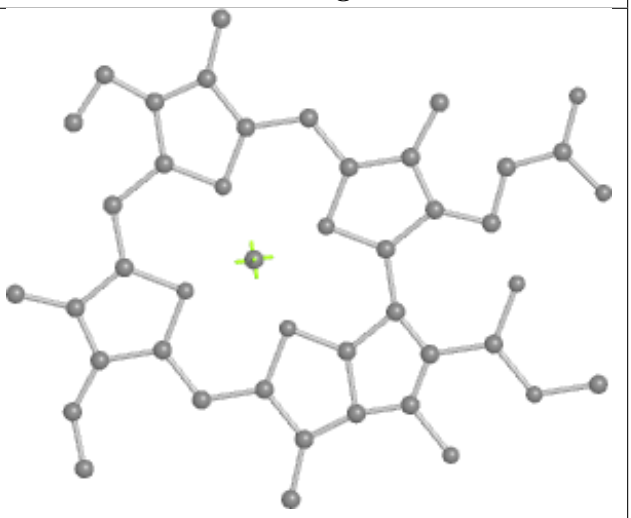
Bond lengths



Bond angles

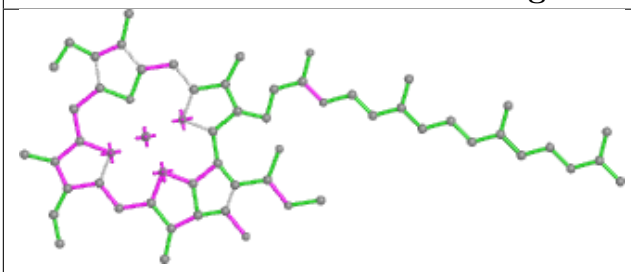


Torsions

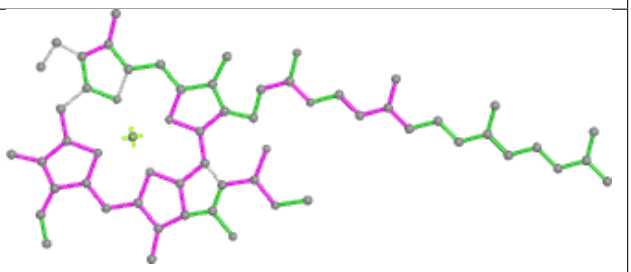


Rings

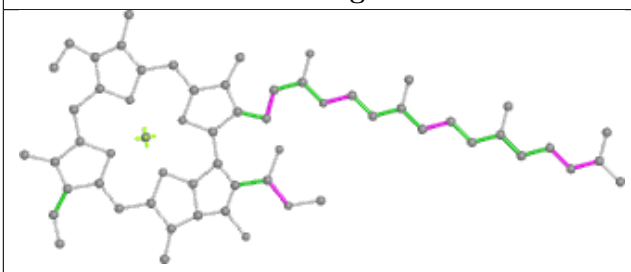
Ligand CLA a 405



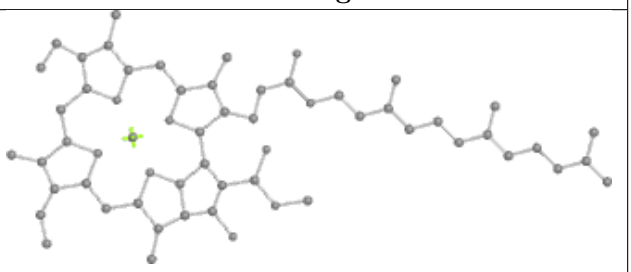
Bond lengths



Bond angles

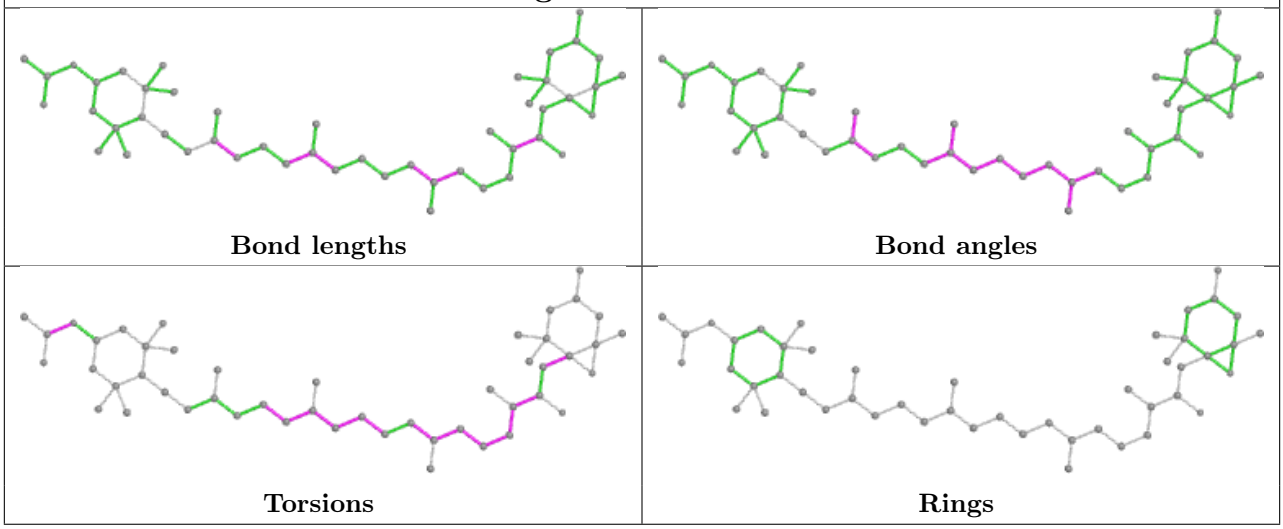


Torsions

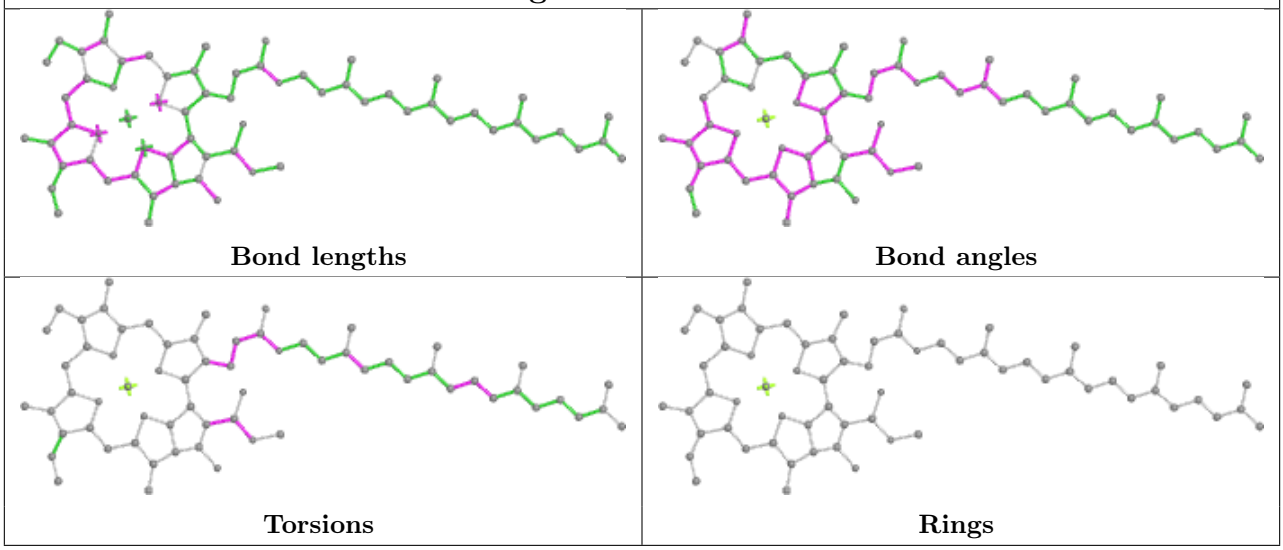


Rings

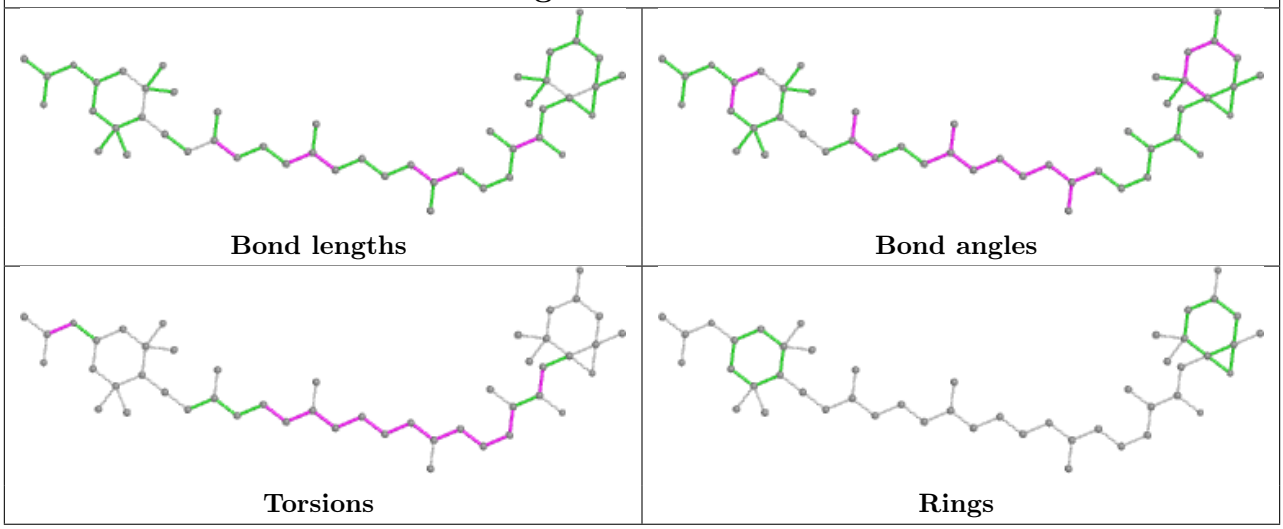
Ligand A86 1 313



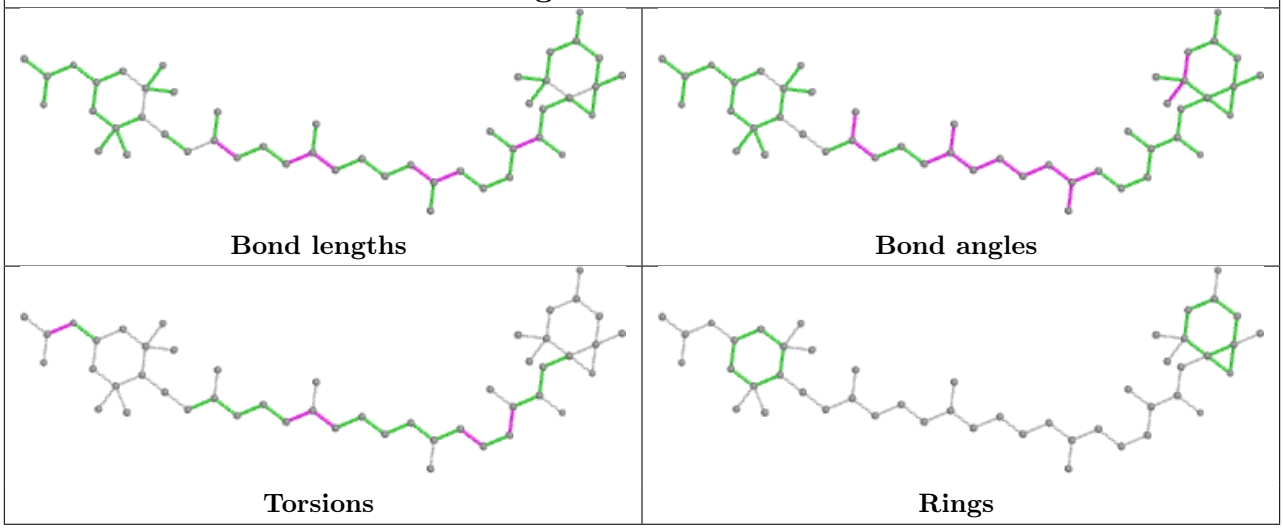
Ligand CLA 6 307



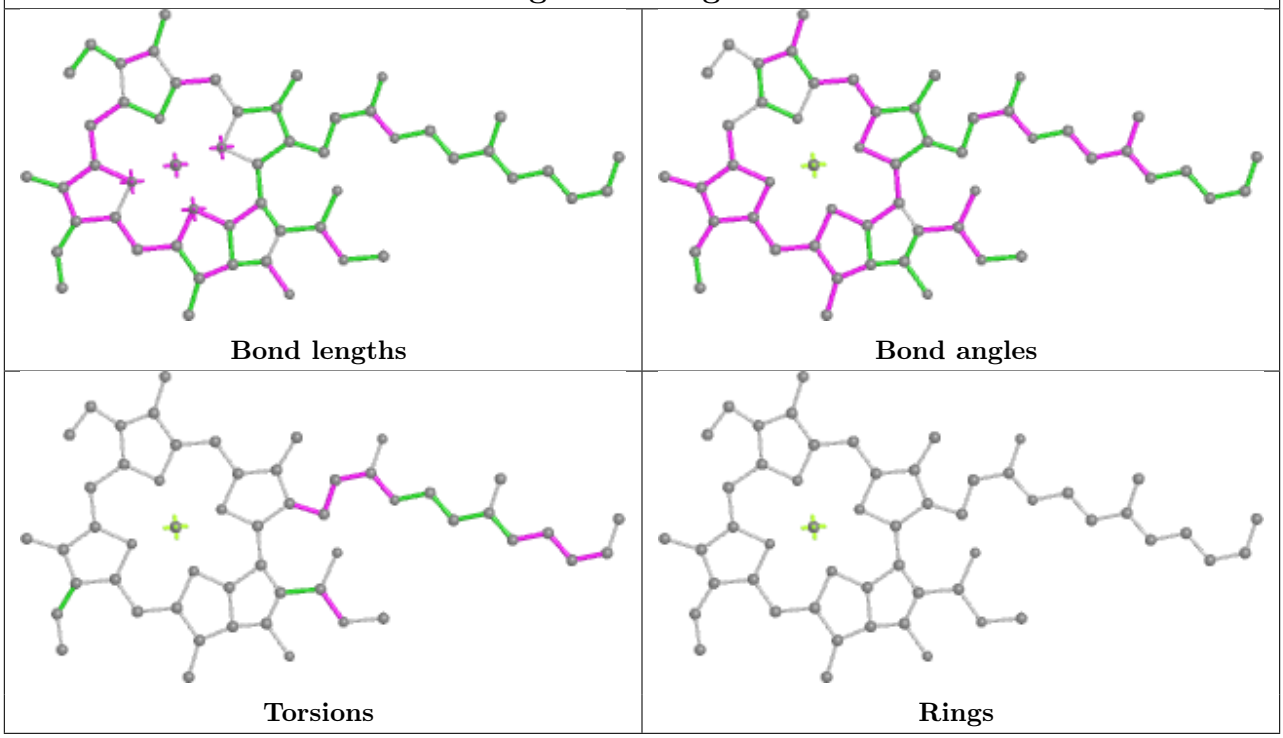
Ligand A86 J 310



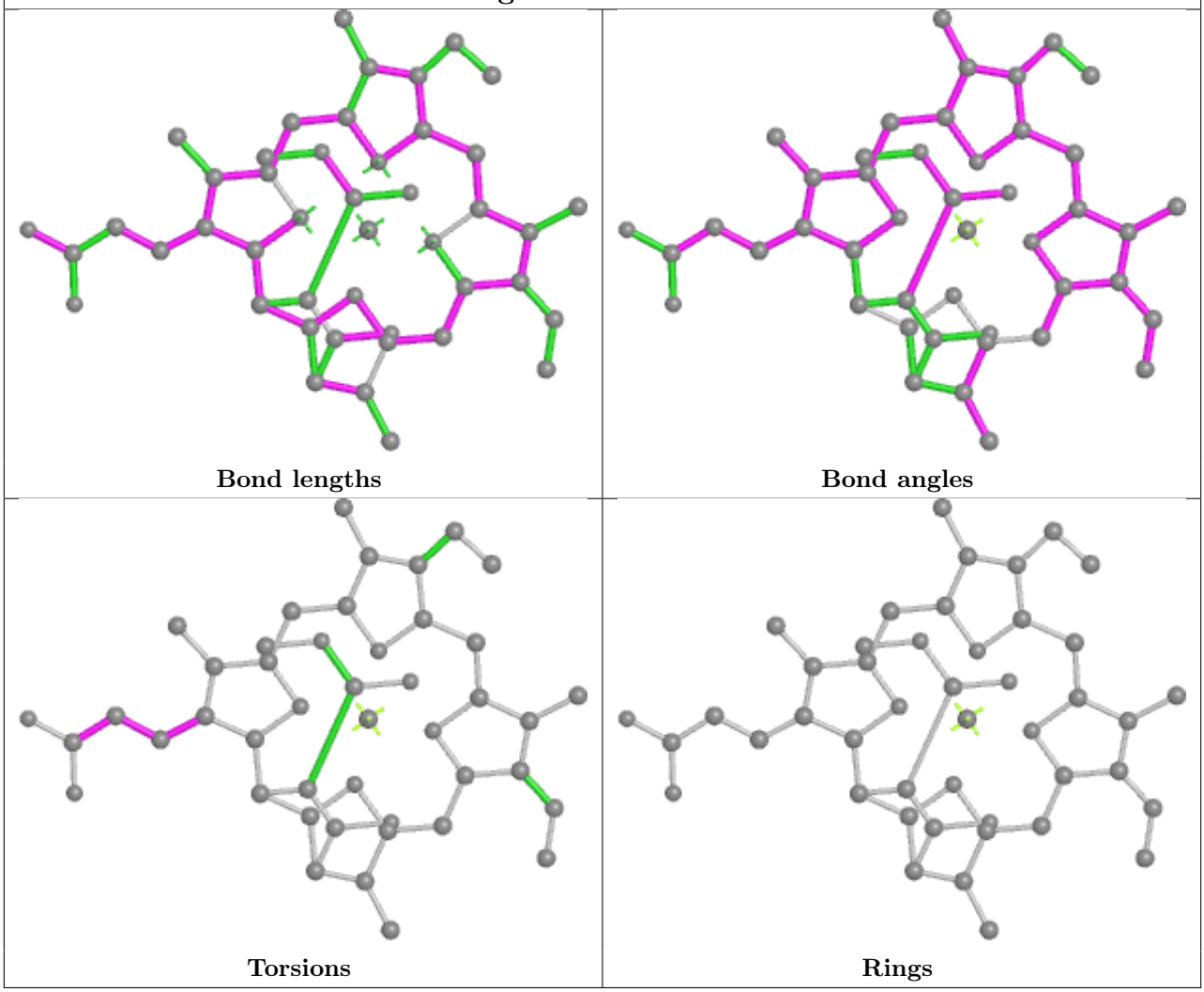
Ligand A86 8 309



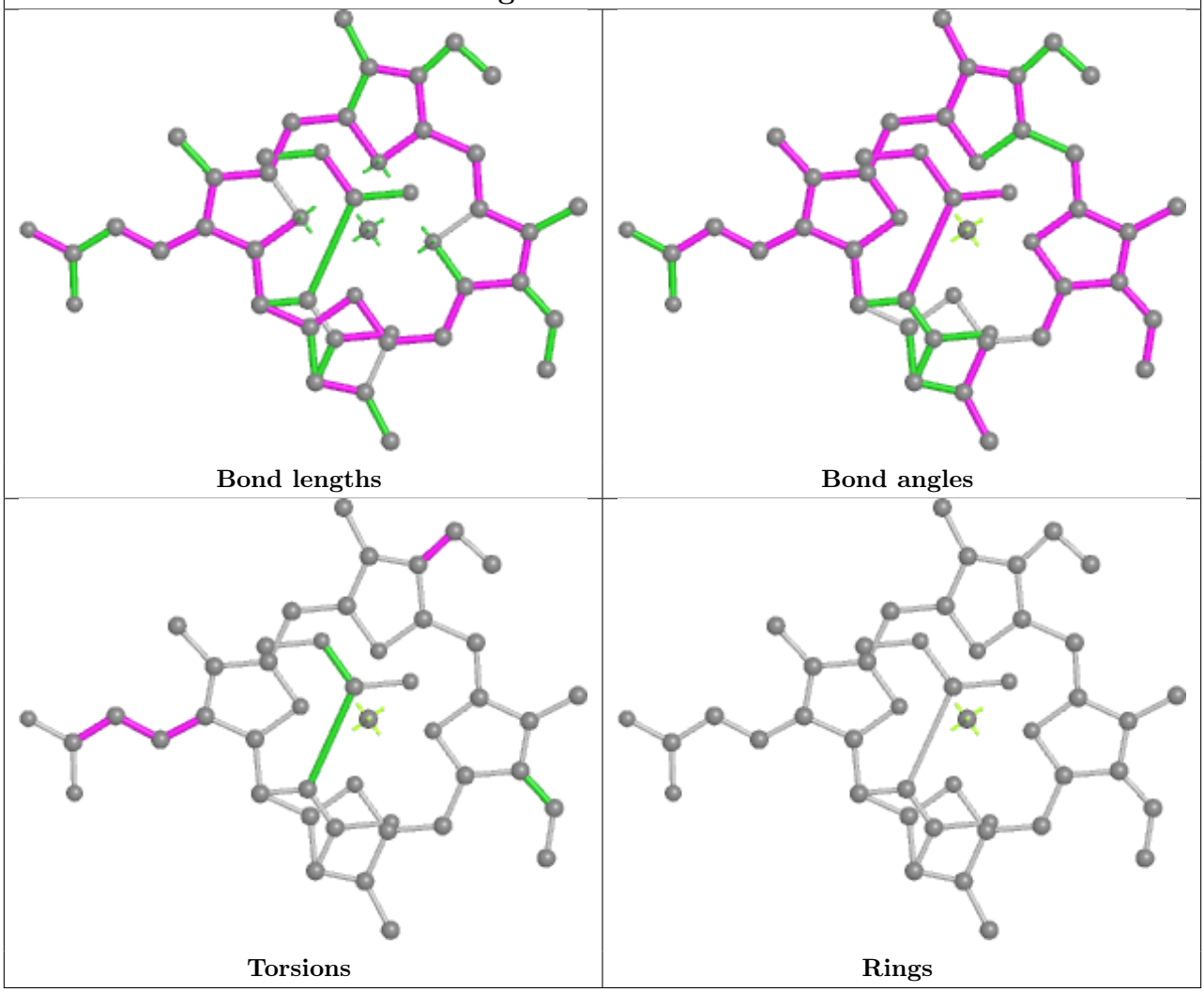
Ligand CLA g 304



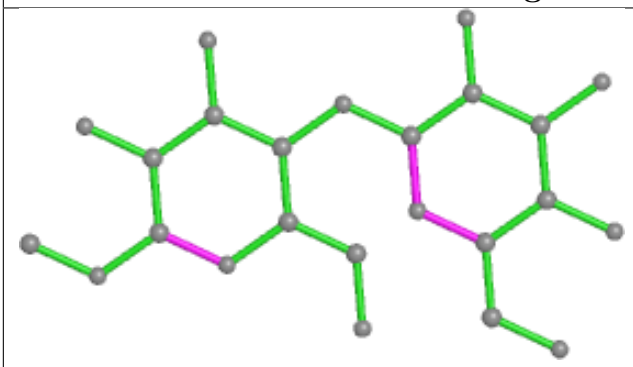
Ligand KC1 J 312



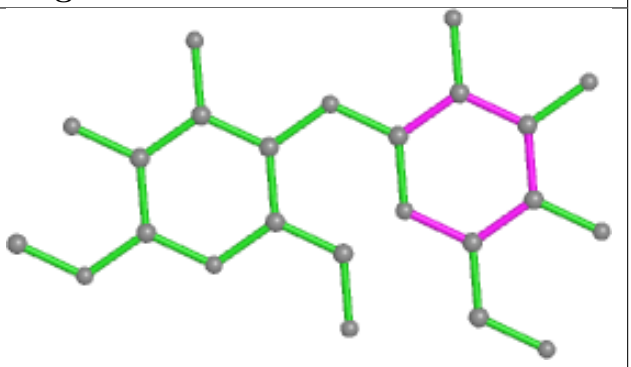
Ligand KC1 3 305



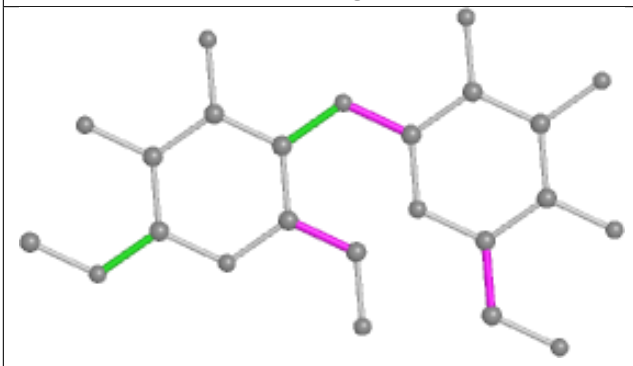
Ligand LMU g 316



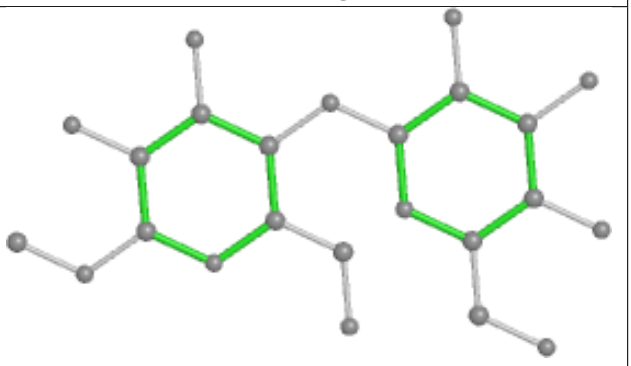
Bond lengths



Bond angles

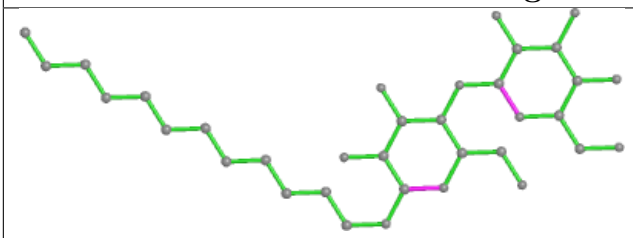


Torsions

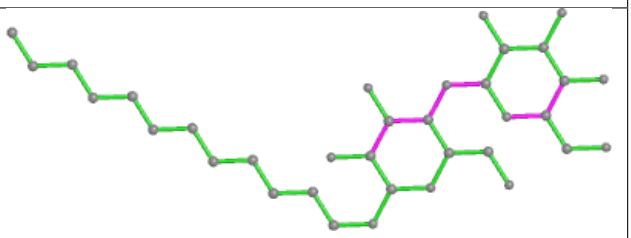


Rings

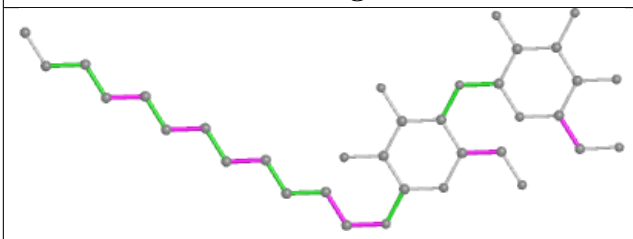
Ligand LMU 2 317



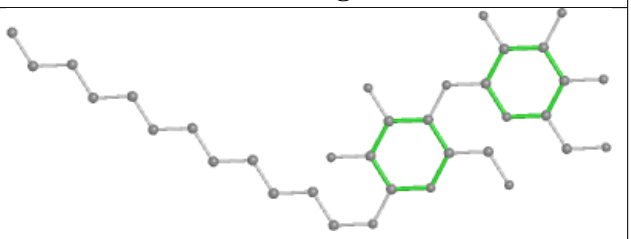
Bond lengths



Bond angles

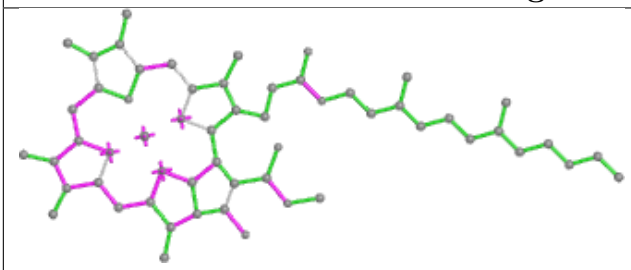


Torsions

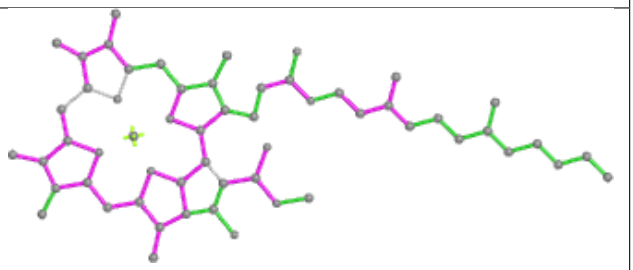


Rings

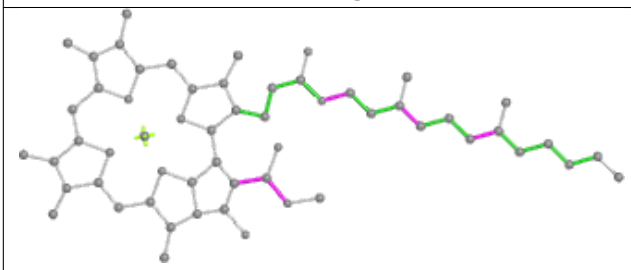
Ligand CLA d 405



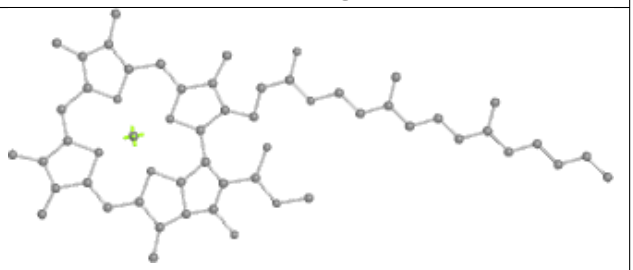
Bond lengths



Bond angles

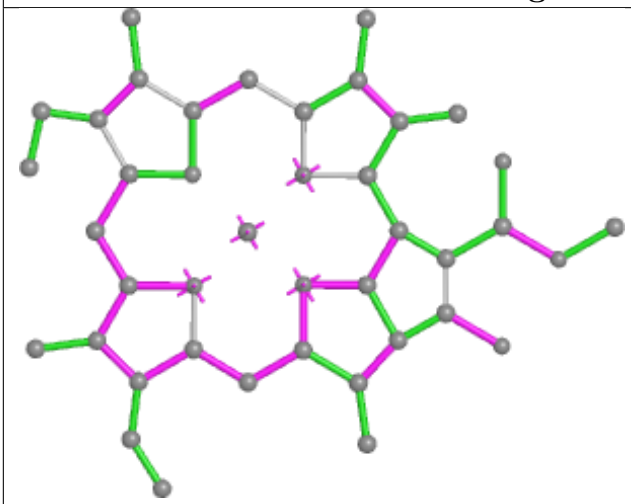


Torsions

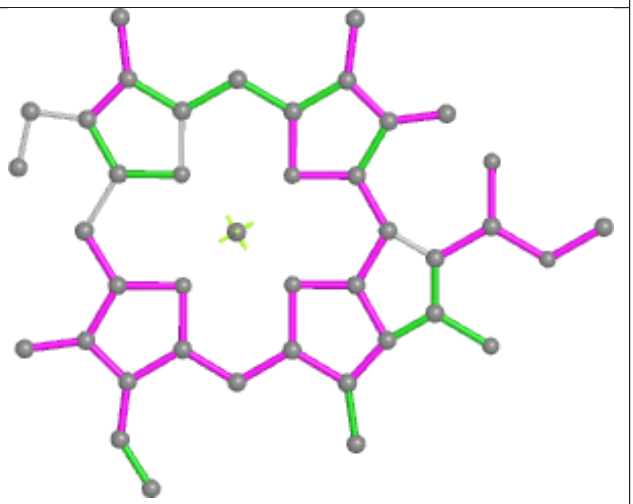


Rings

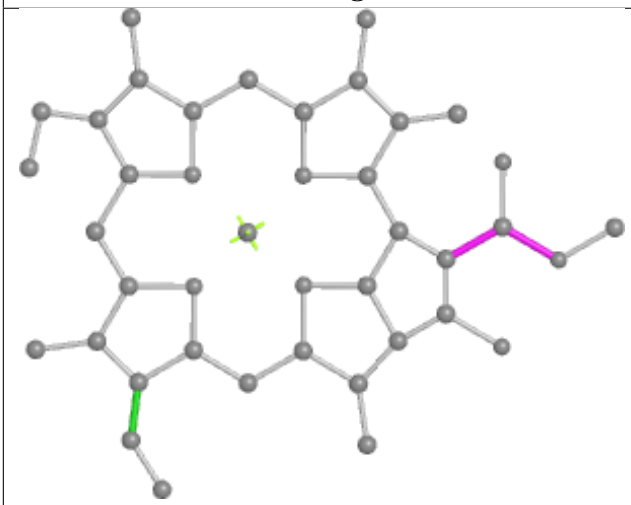
Ligand CLA 7 306



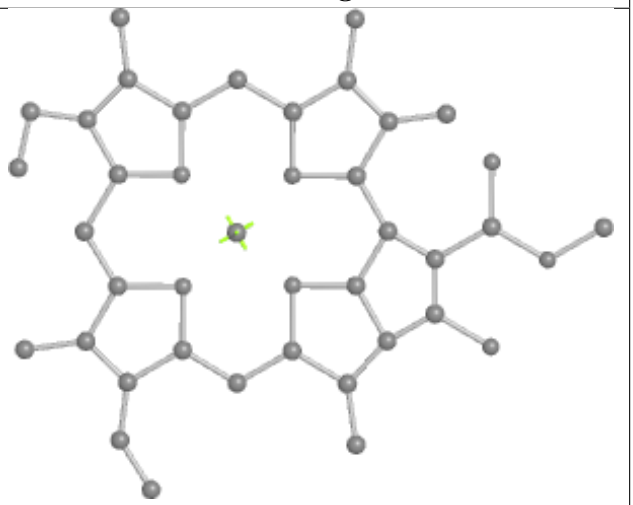
Bond lengths



Bond angles

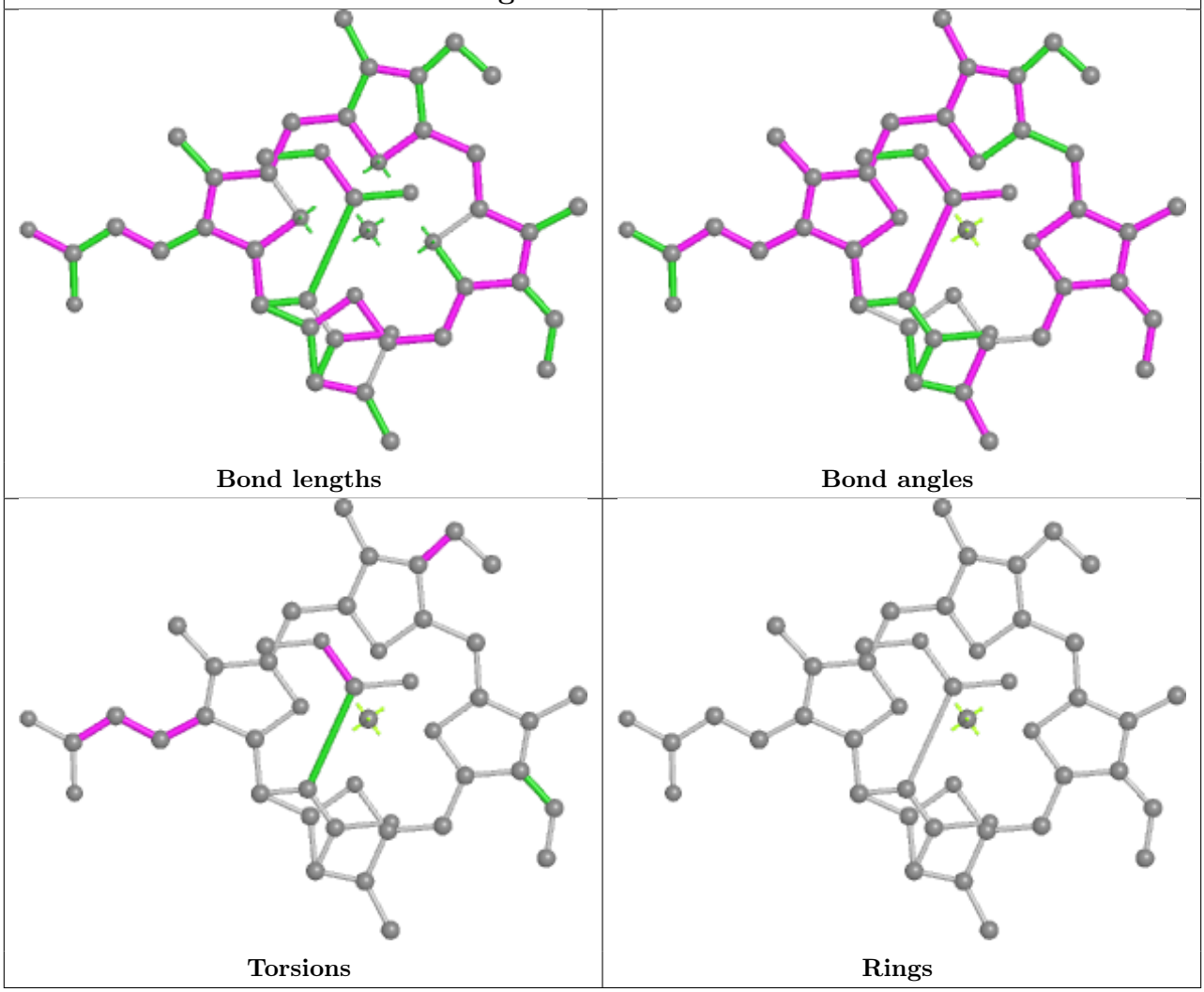


Torsions

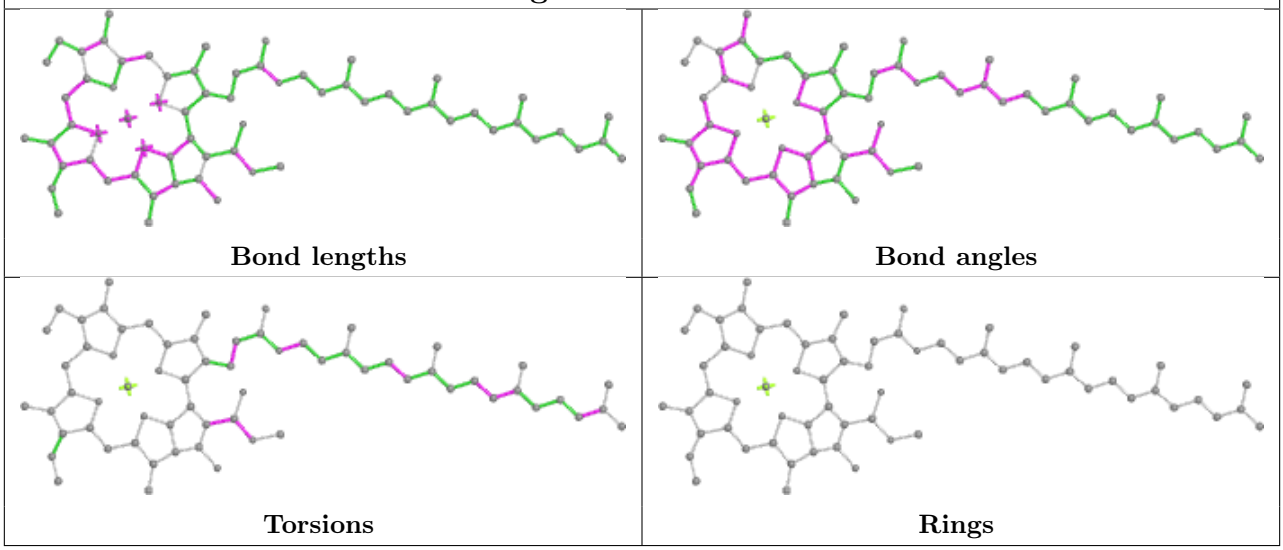


Rings

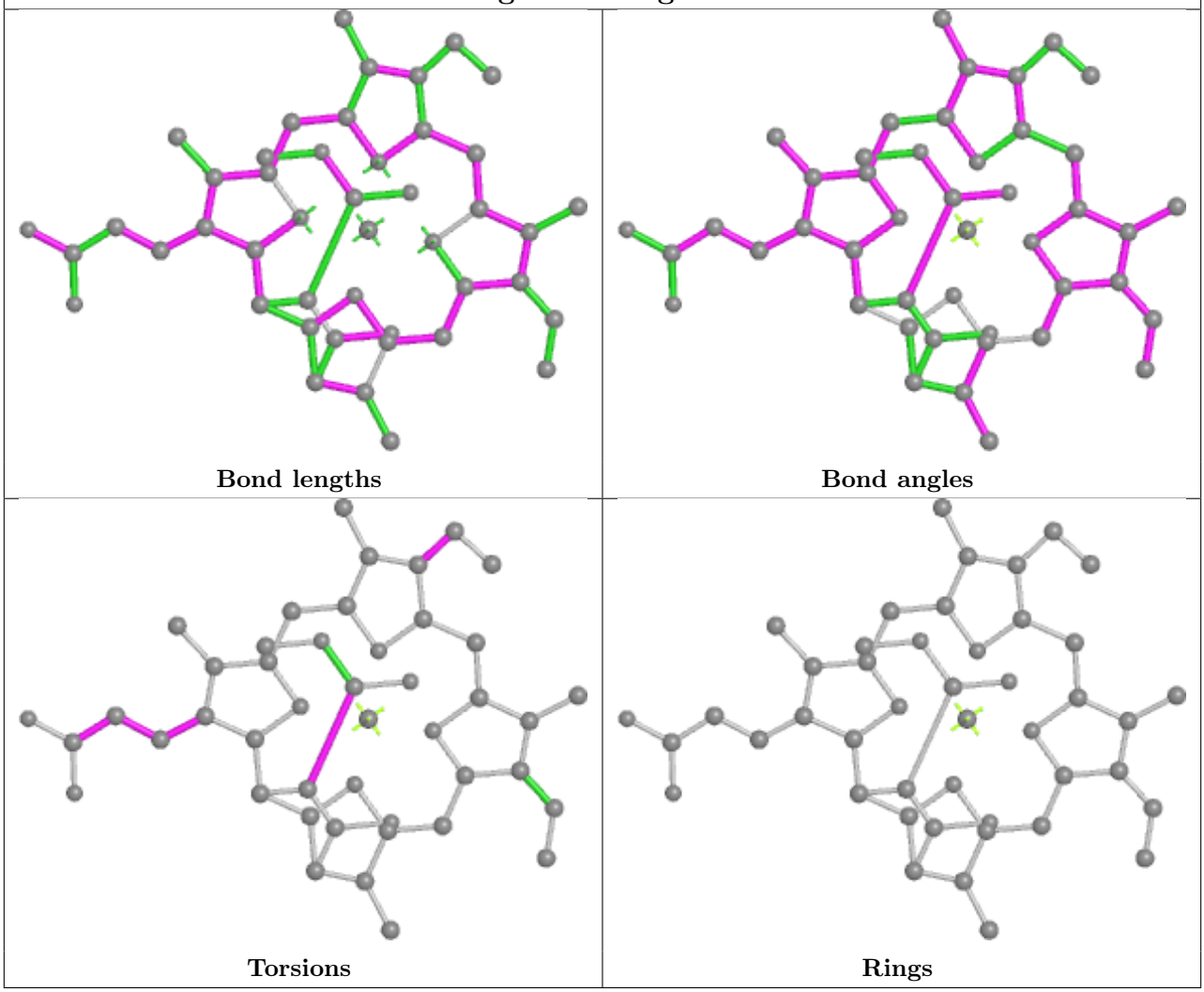
Ligand KC1 9 305



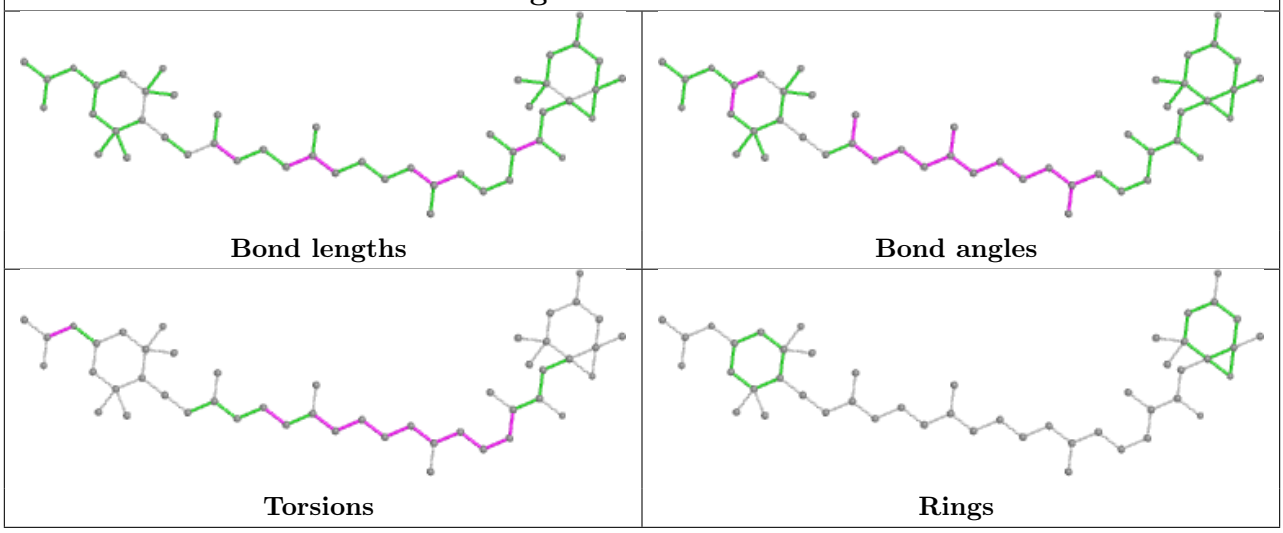
Ligand CLA c 509

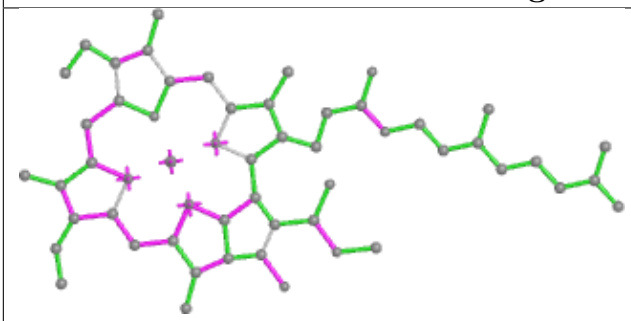
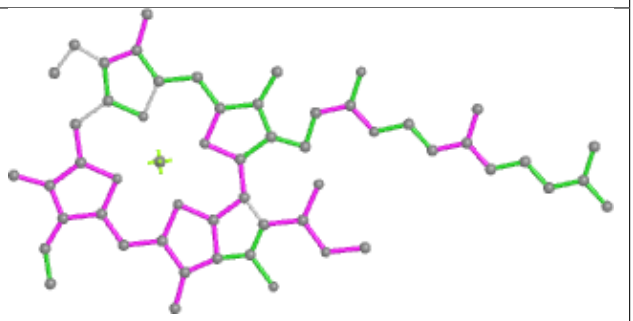
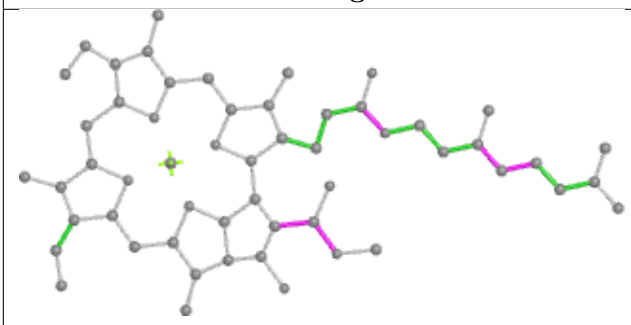
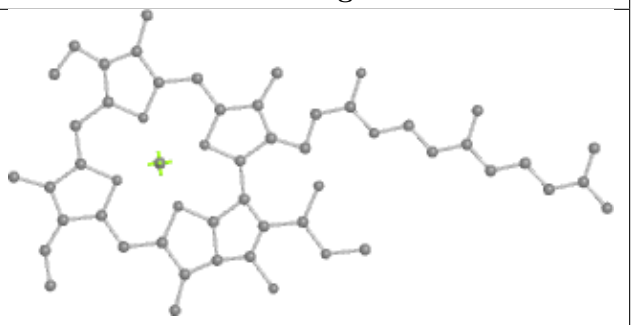


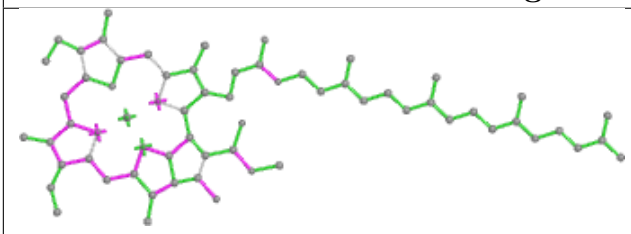
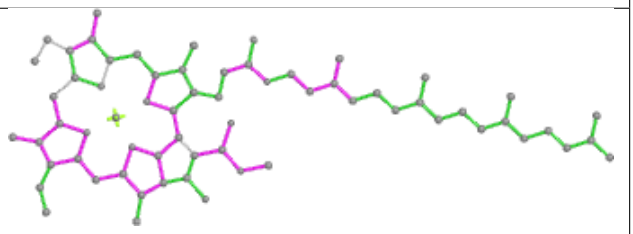
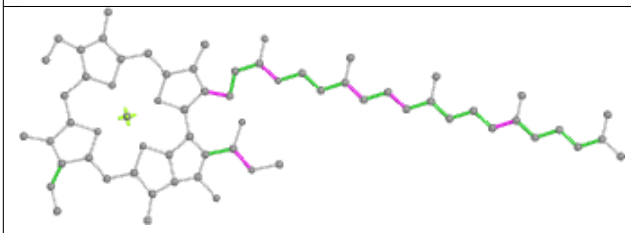
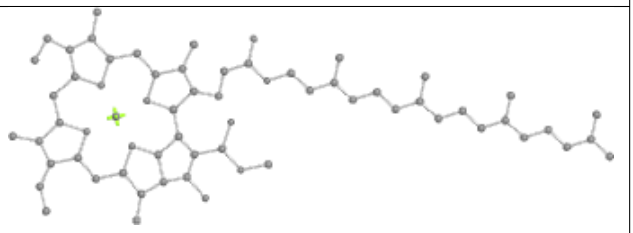
Ligand KC1 g 314

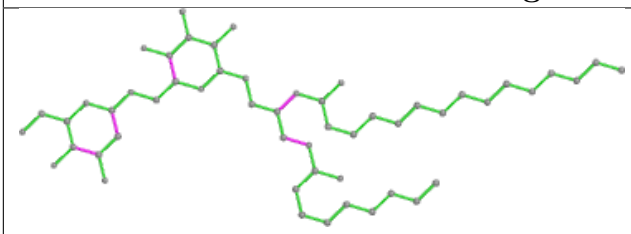
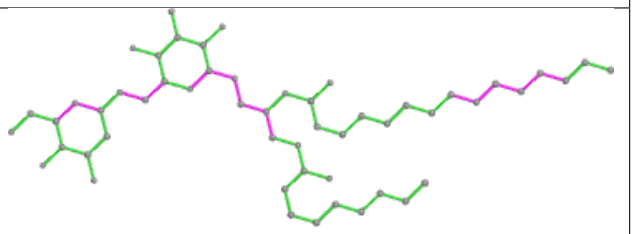
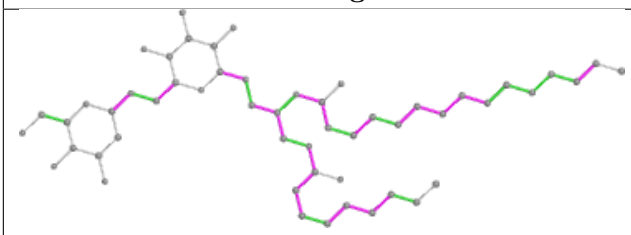
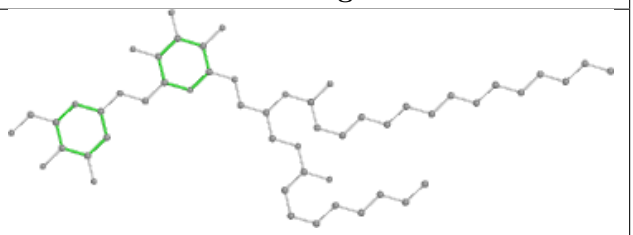


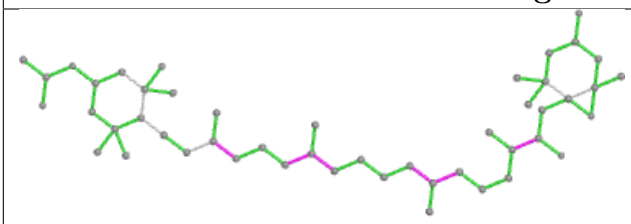
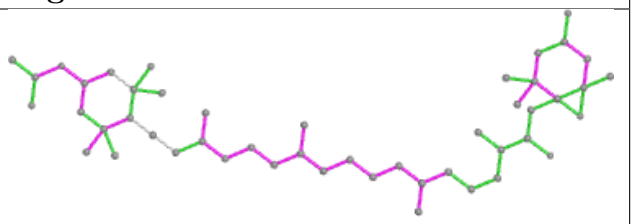
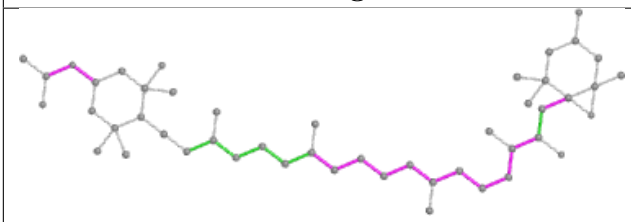
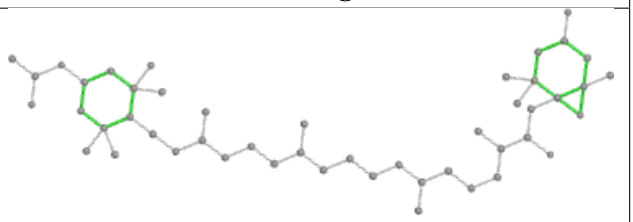
Ligand A86 G 305



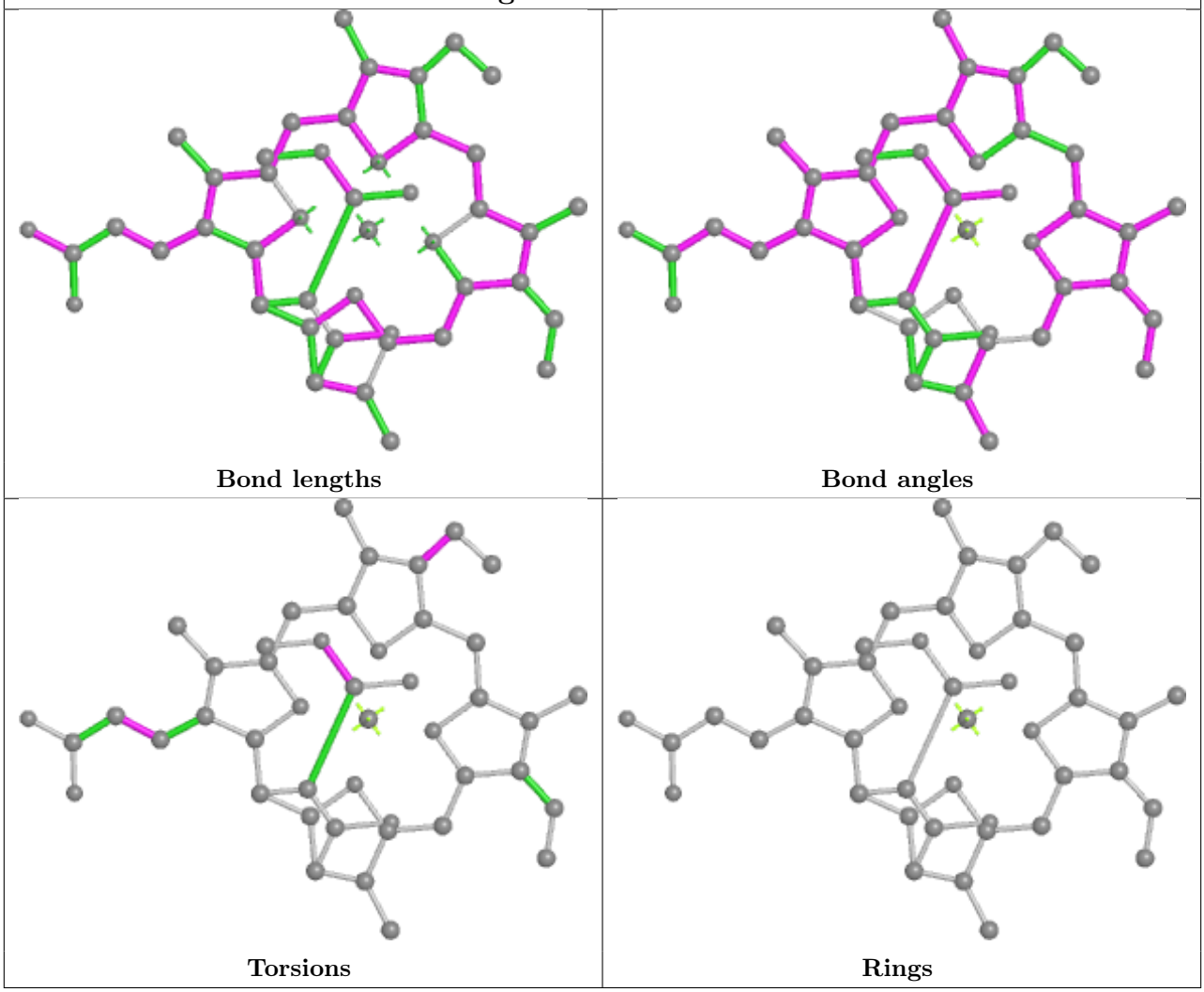
Ligand CLA 1 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

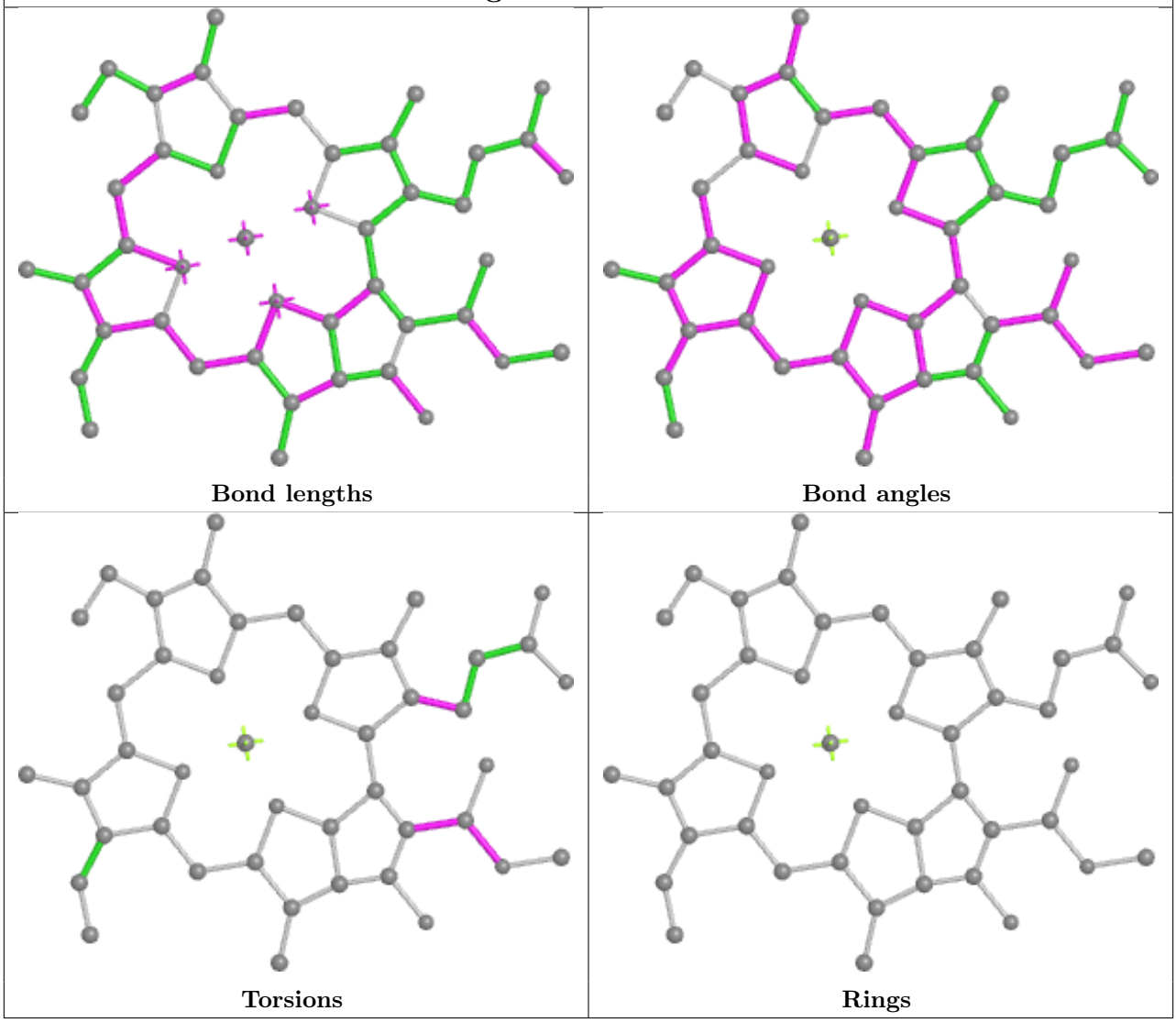
Ligand DGD b 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 g 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

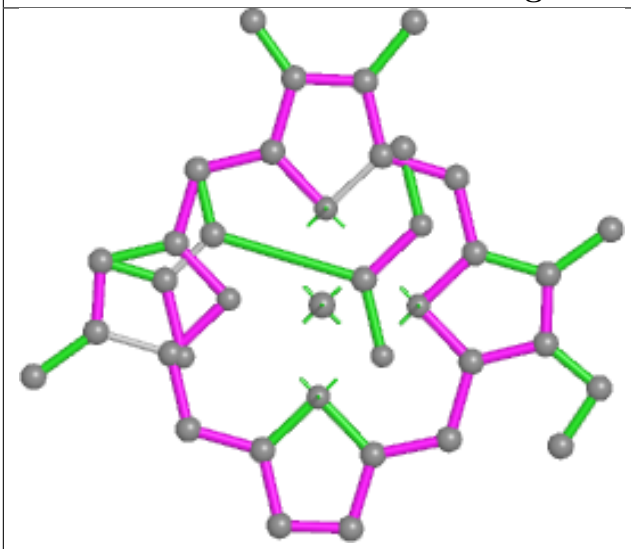
Ligand KC1 5 315



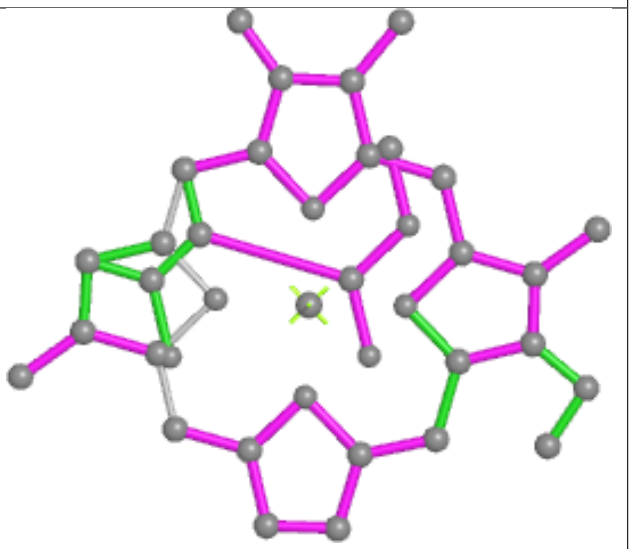
Ligand CLA c 507



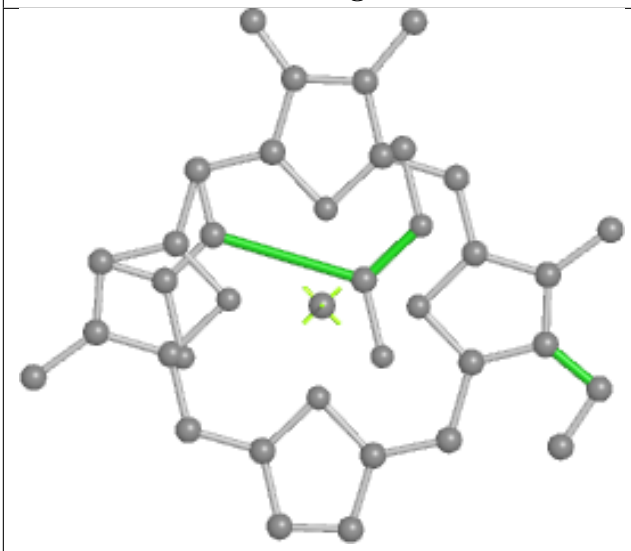
Ligand KC1 G 306



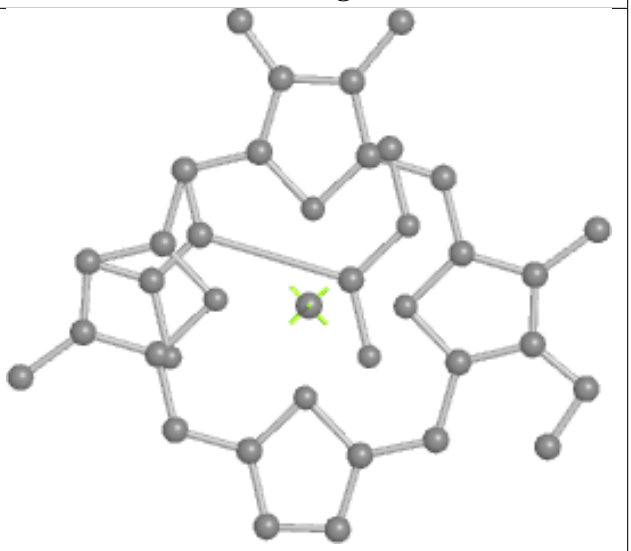
Bond lengths



Bond angles

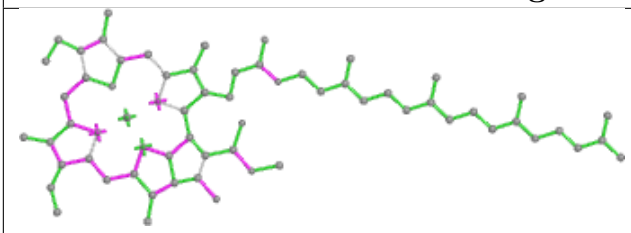


Torsions

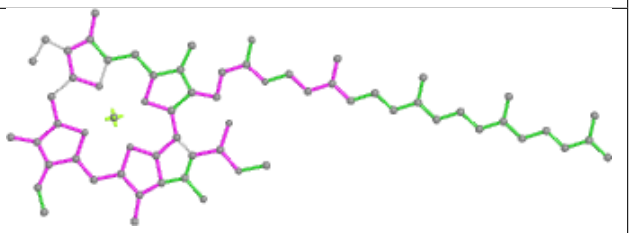


Rings

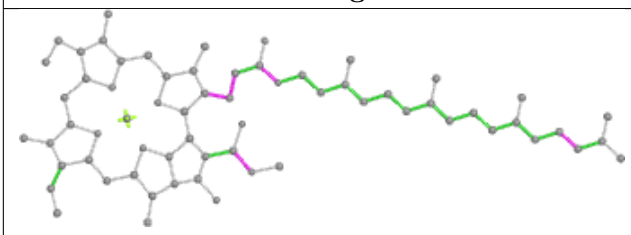
Ligand CLA a 402



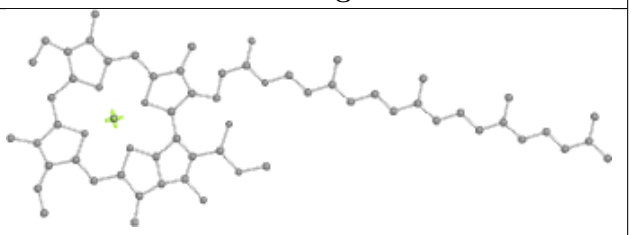
Bond lengths



Bond angles

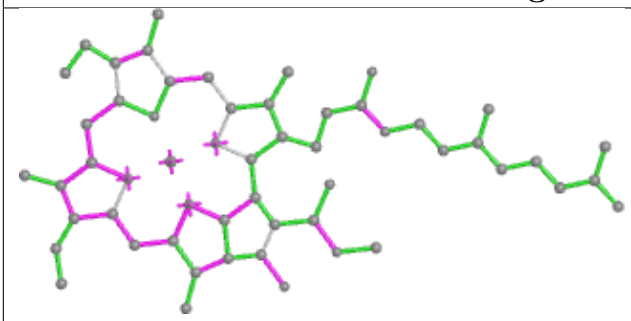


Torsions

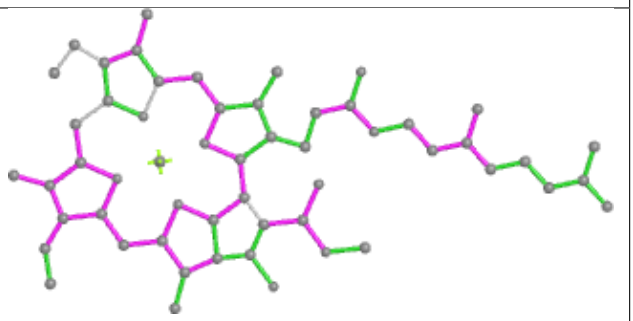


Rings

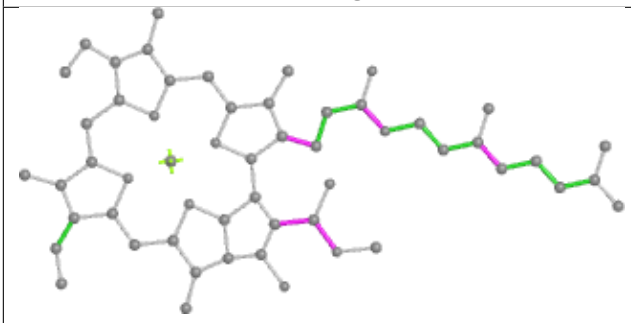
Ligand CLA 4 301



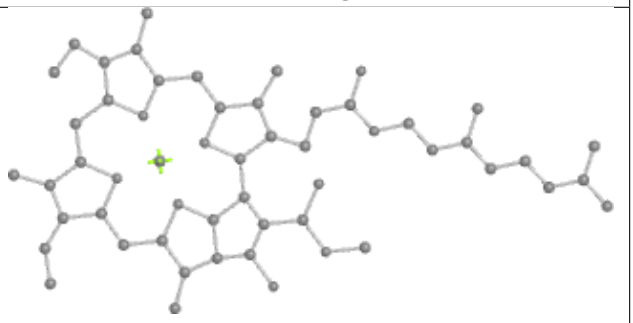
Bond lengths



Bond angles

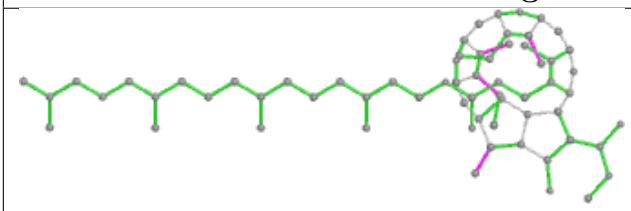


Torsions

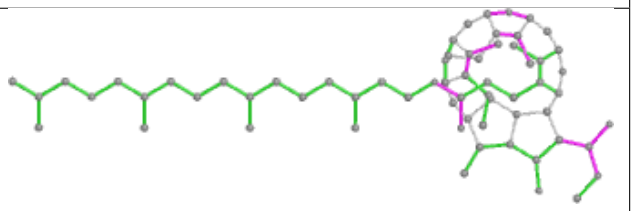


Rings

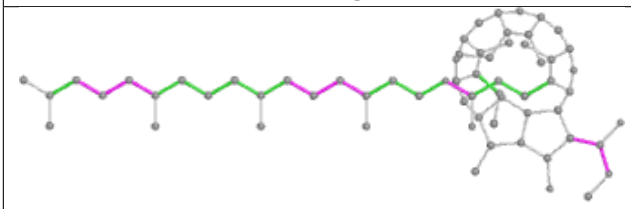
Ligand PHO A 403



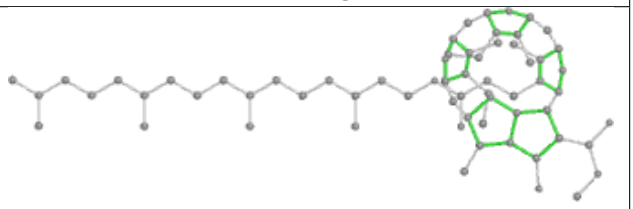
Bond lengths



Bond angles

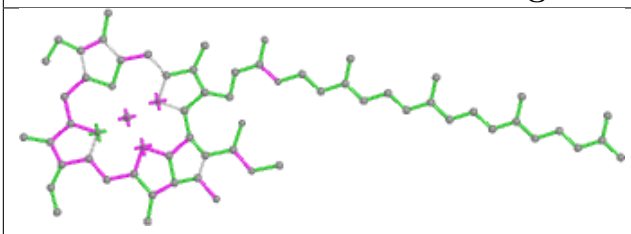


Torsions

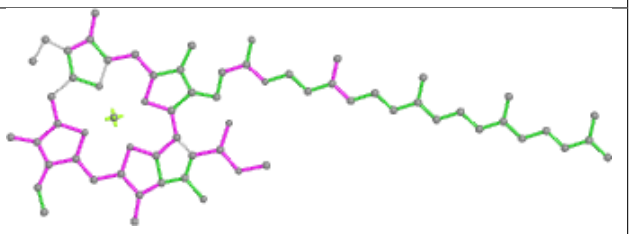


Rings

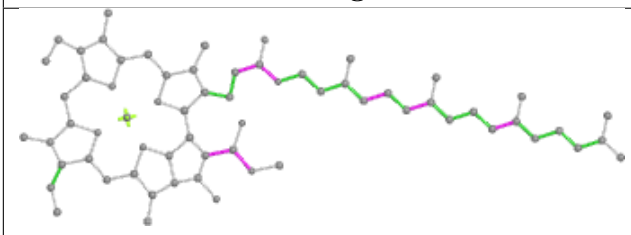
Ligand CLA 7 302



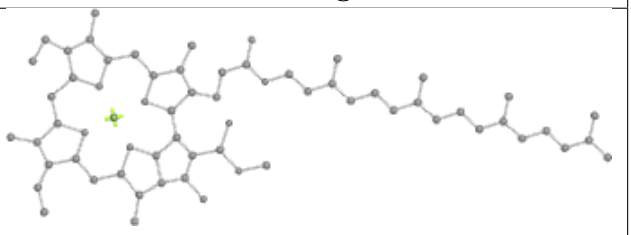
Bond lengths



Bond angles

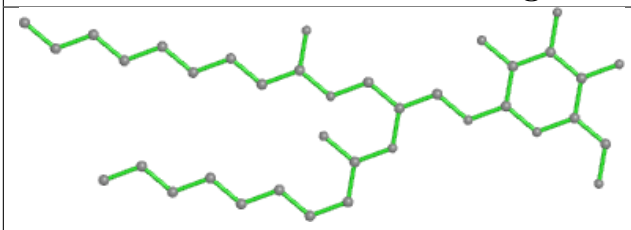


Torsions

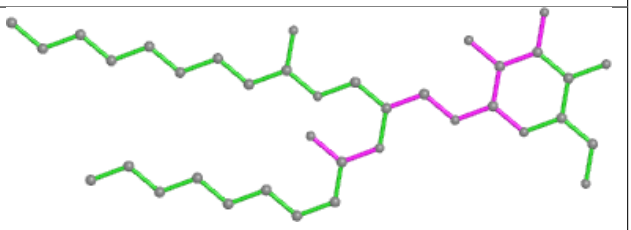


Rings

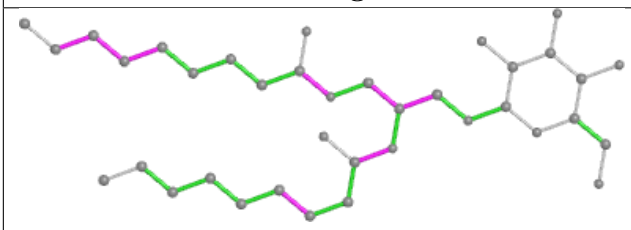
Ligand LMG b 626



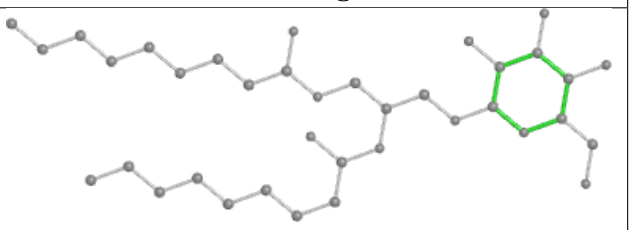
Bond lengths



Bond angles

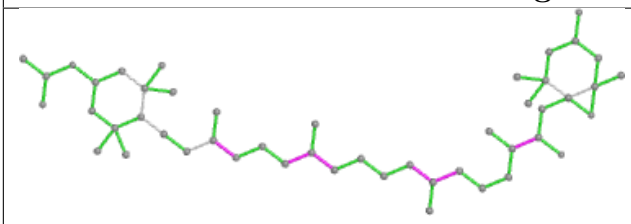


Torsions

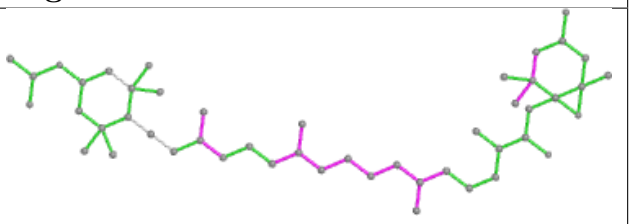


Rings

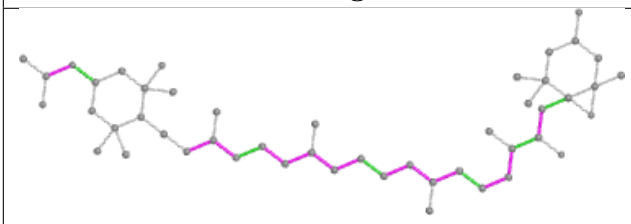
Ligand A86 g 311



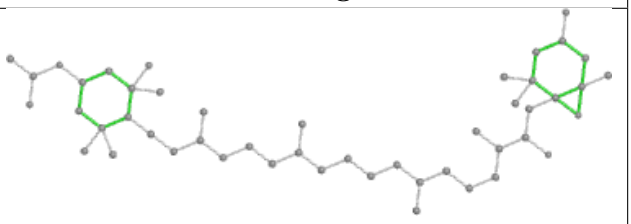
Bond lengths



Bond angles

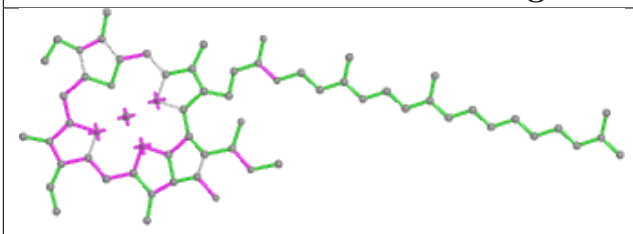


Torsions

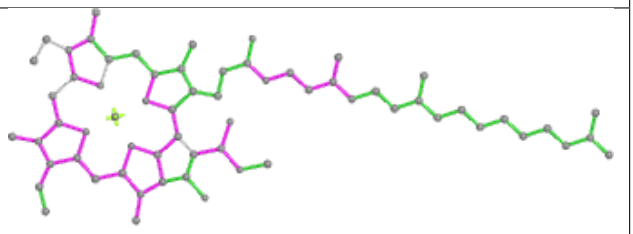


Rings

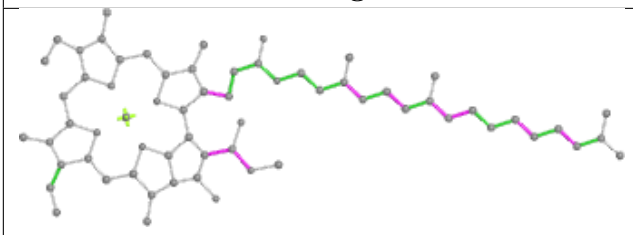
Ligand CLA b 615



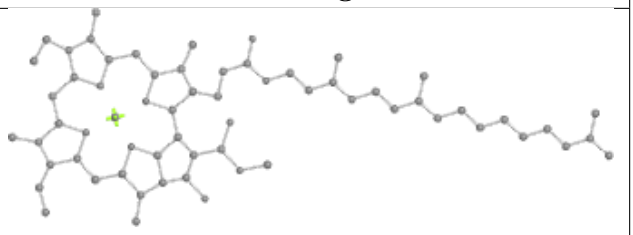
Bond lengths



Bond angles

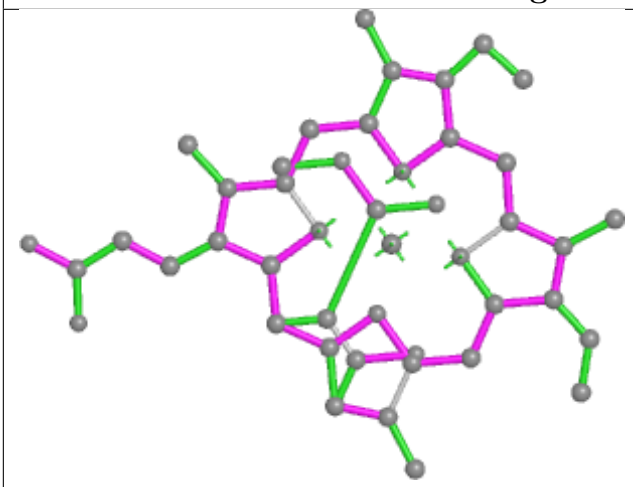


Torsions

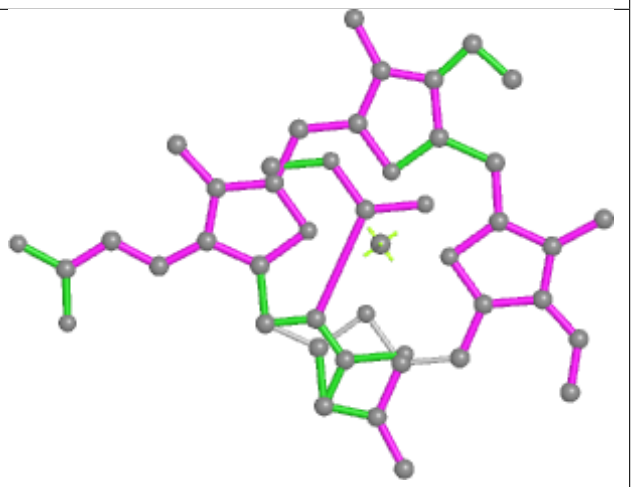


Rings

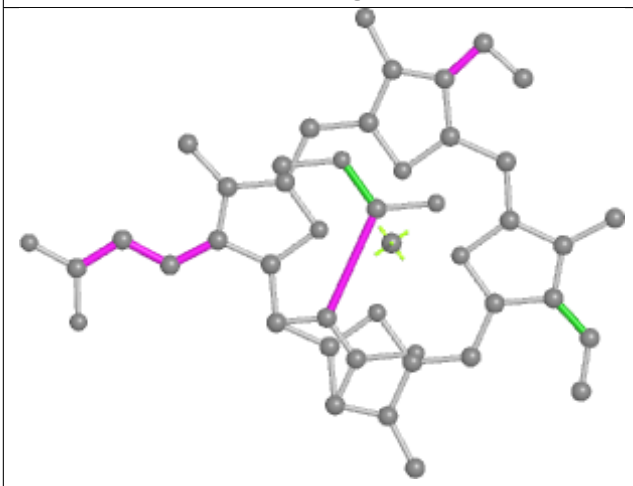
Ligand KC1 2 315



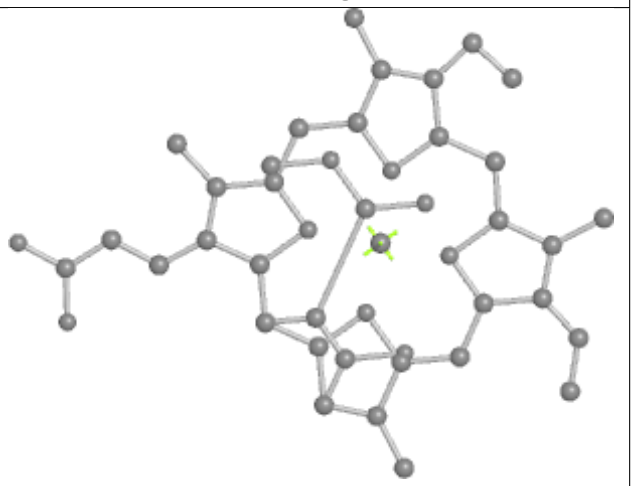
Bond lengths



Bond angles

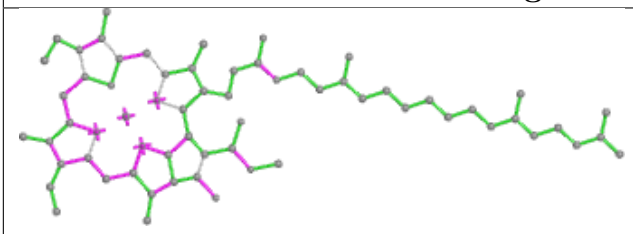


Torsions

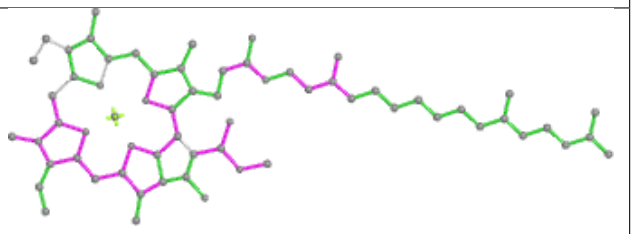


Rings

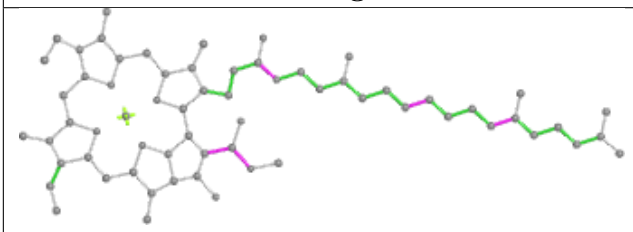
Ligand CLA C 504



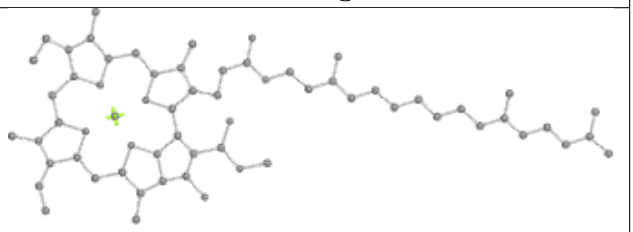
Bond lengths



Bond angles

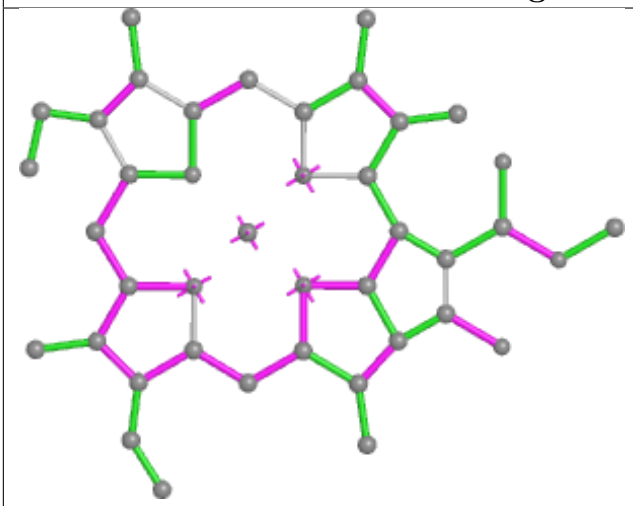


Torsions

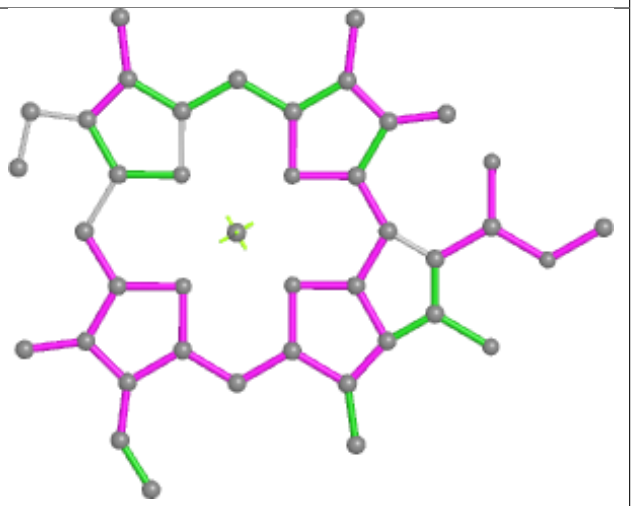


Rings

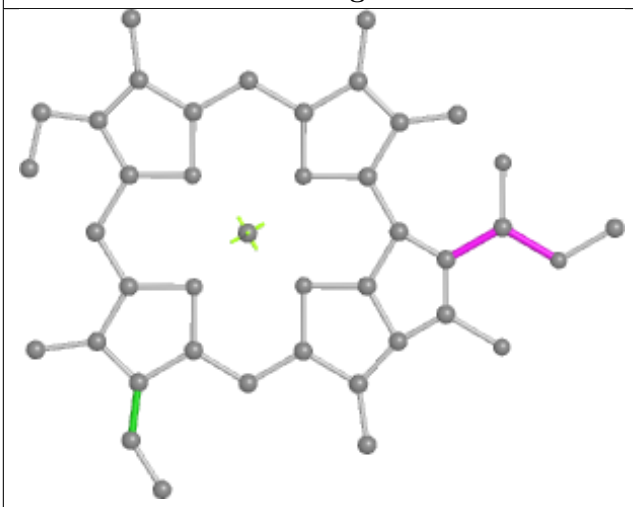
Ligand CLA 1 307



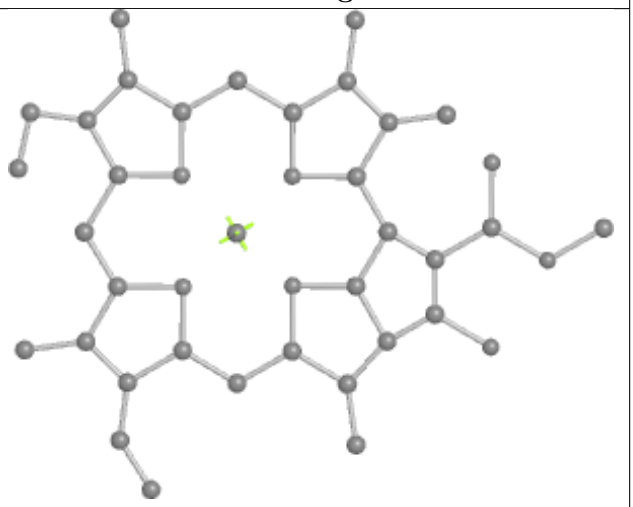
Bond lengths



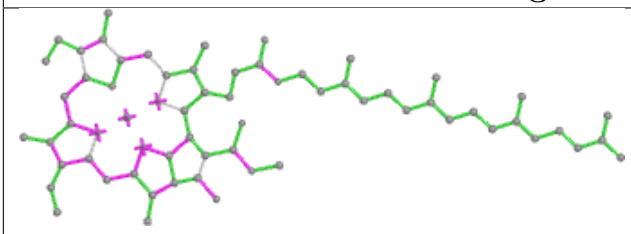
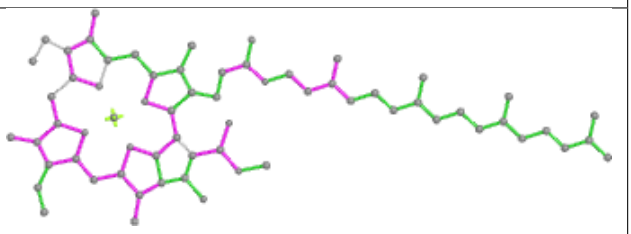
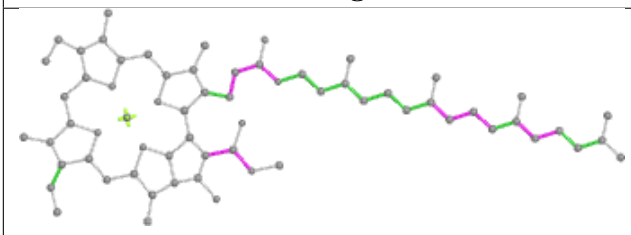
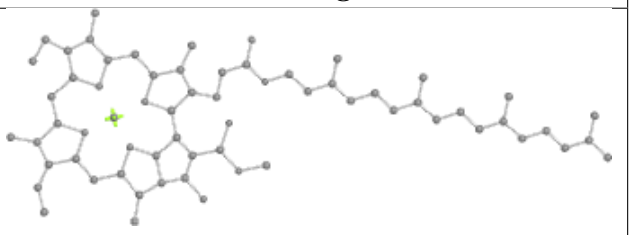
Bond angles

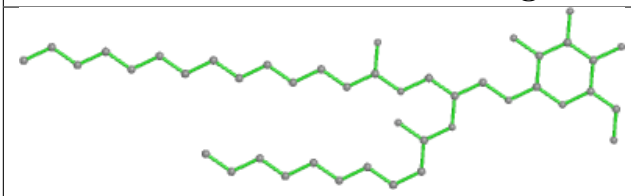
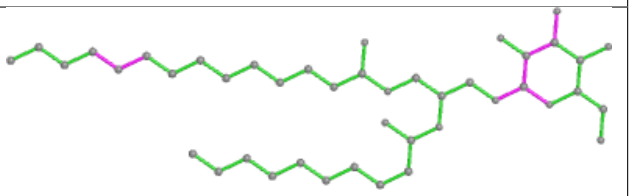
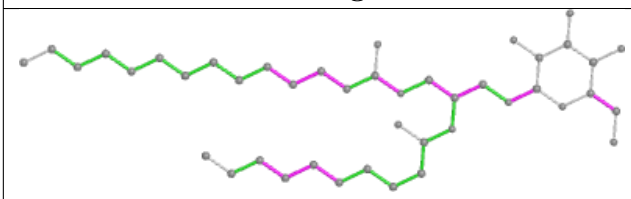
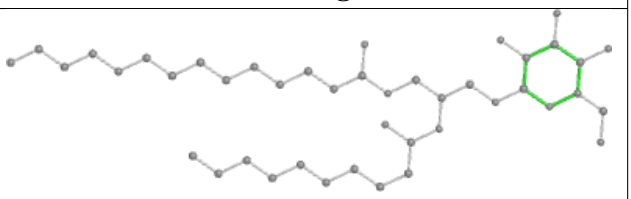


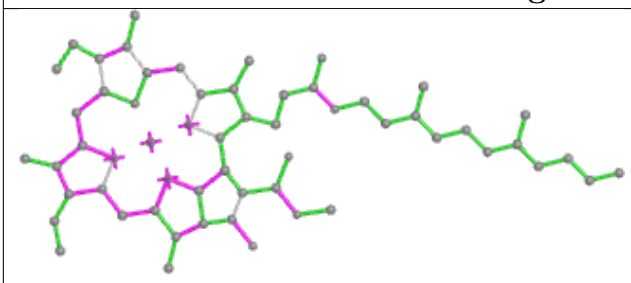
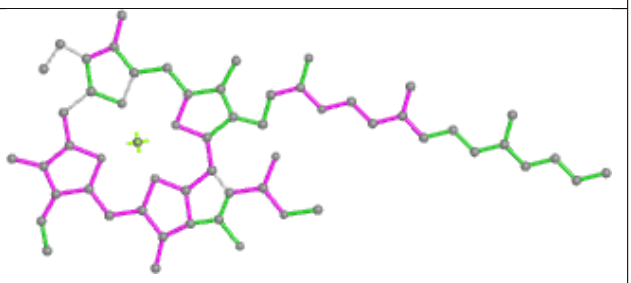
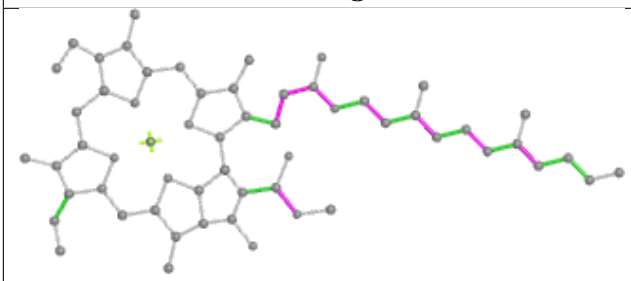
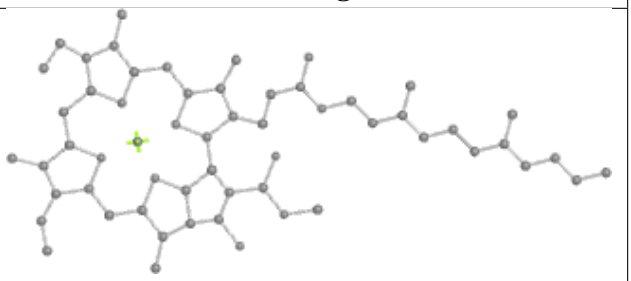
Torsions



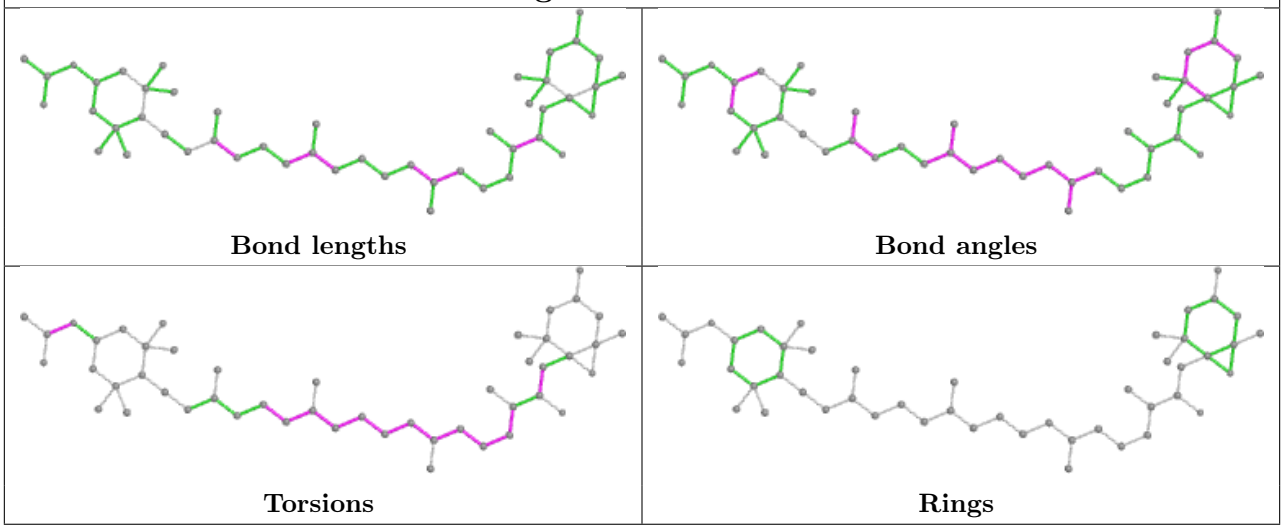
Rings

Ligand CLA c 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

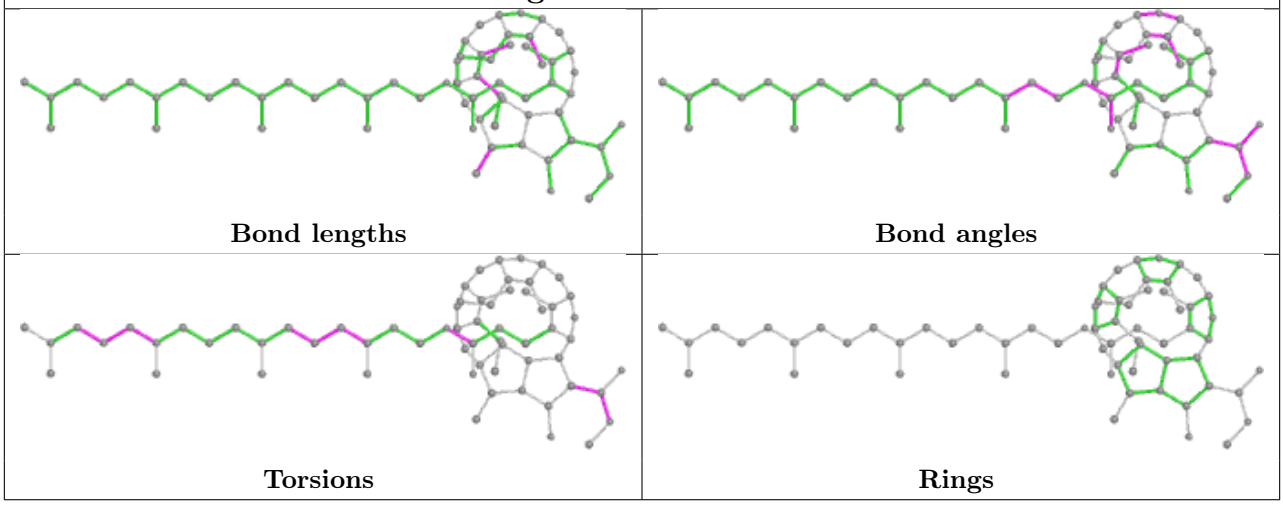
Ligand LMG B 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

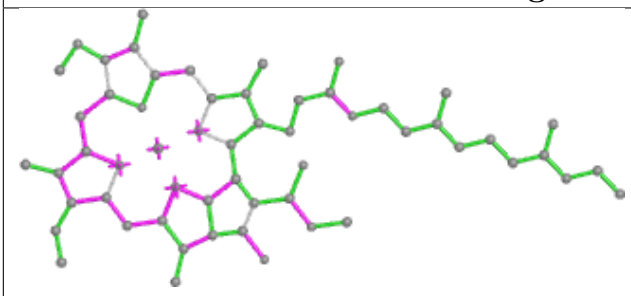
Ligand A86 6 310



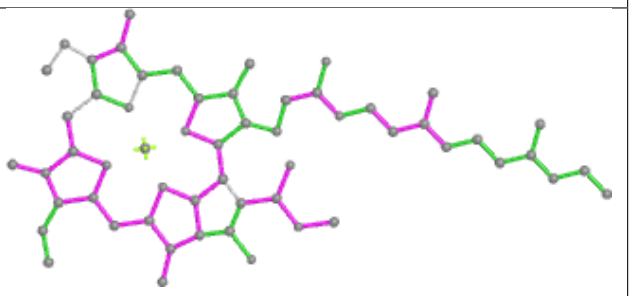
Ligand PHO a 404



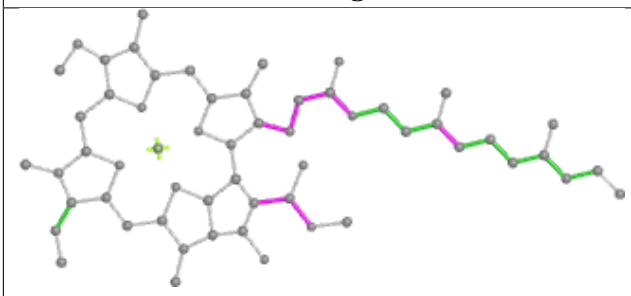
Ligand CLA J 301



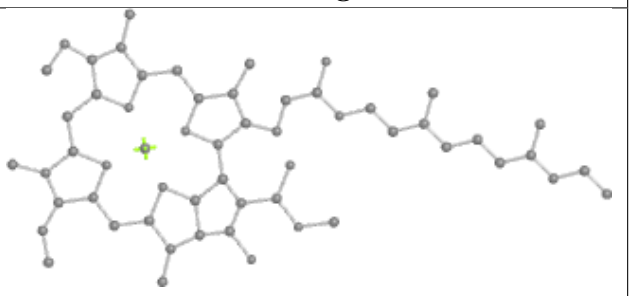
Bond lengths



Bond angles

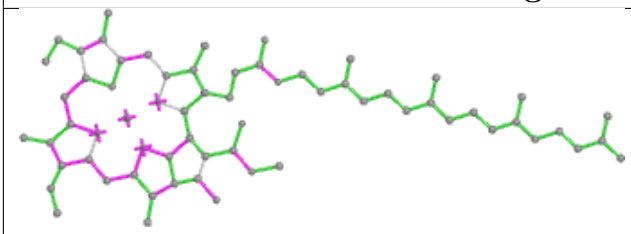


Torsions

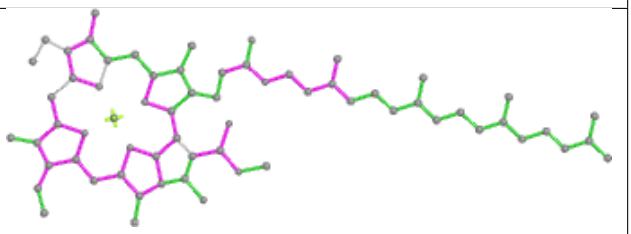


Rings

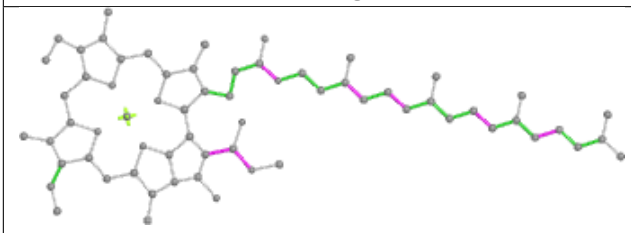
Ligand CLA C 510



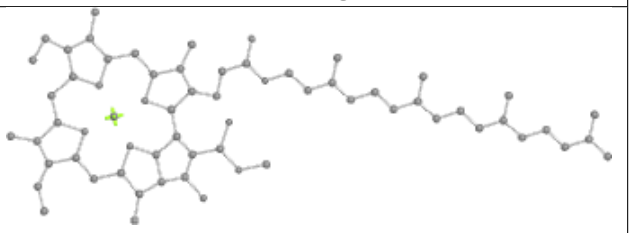
Bond lengths



Bond angles

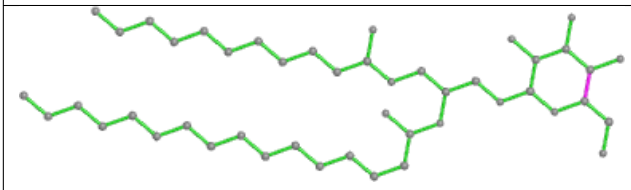


Torsions

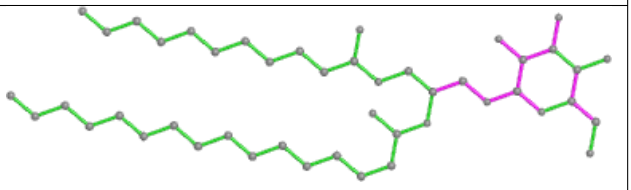


Rings

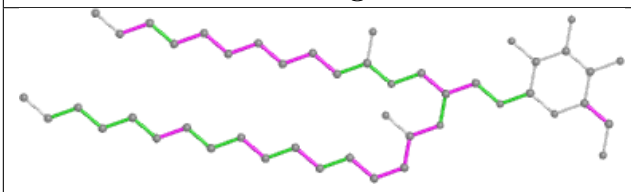
Ligand LMG f 102



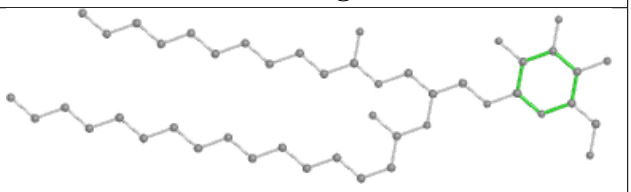
Bond lengths



Bond angles

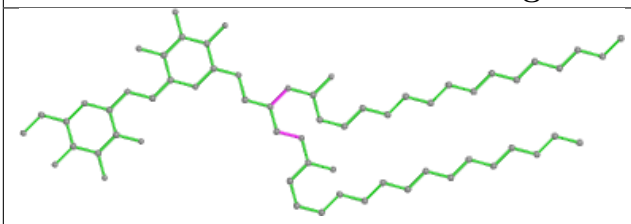


Torsions

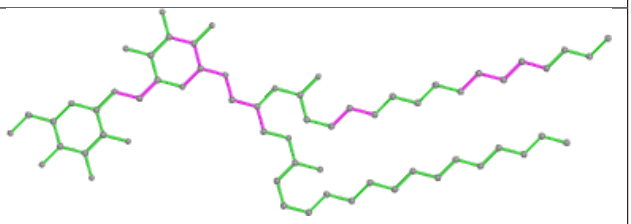


Rings

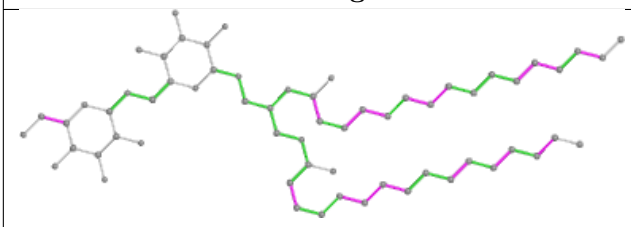
Ligand DGD h 103



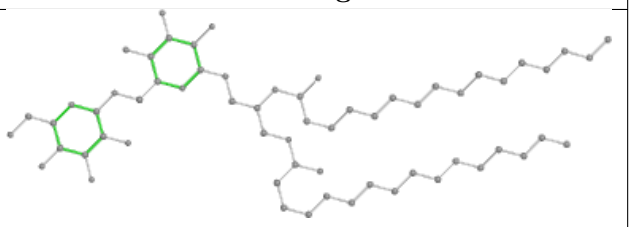
Bond lengths



Bond angles

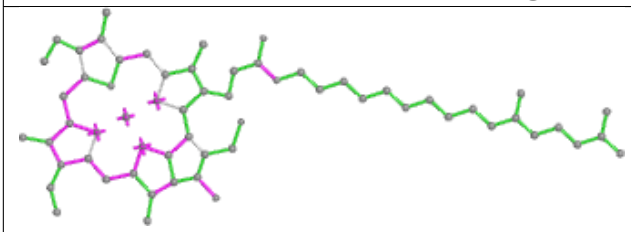


Torsions

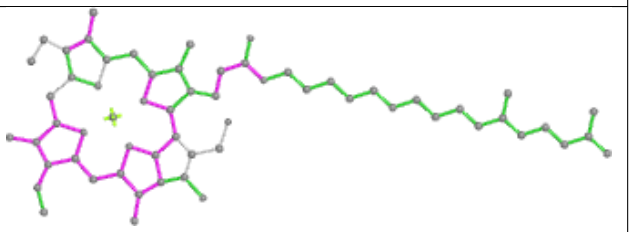


Rings

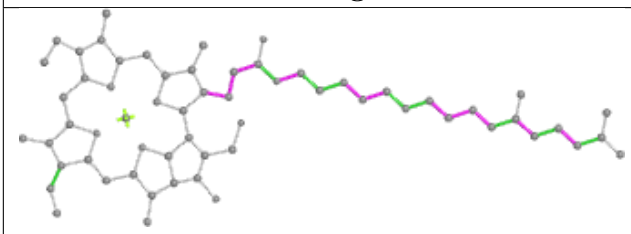
Ligand CLA B 603



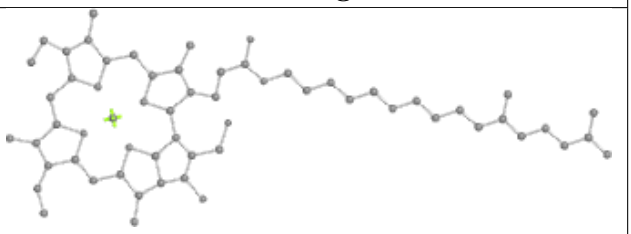
Bond lengths



Bond angles

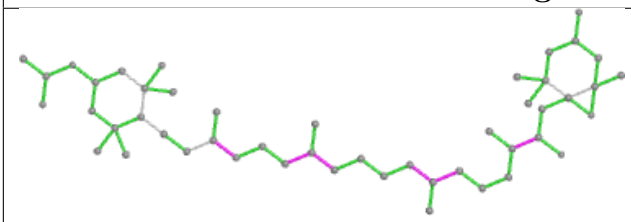


Torsions

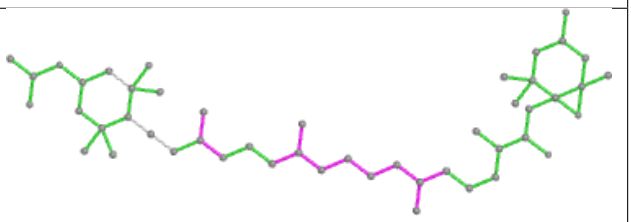


Rings

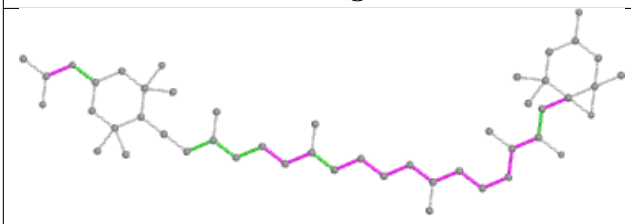
Ligand A86 1 314



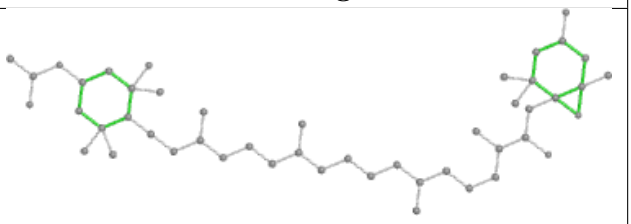
Bond lengths



Bond angles

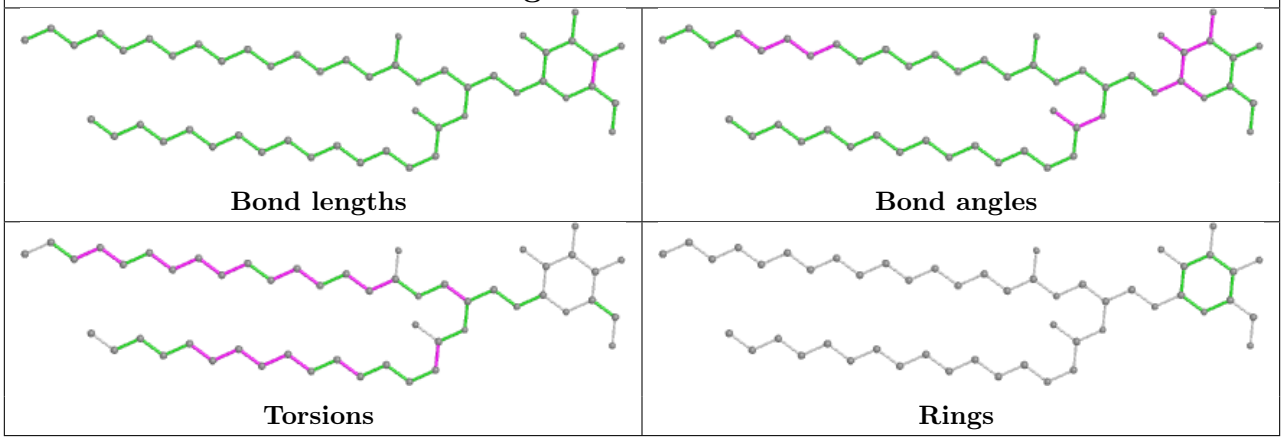


Torsions

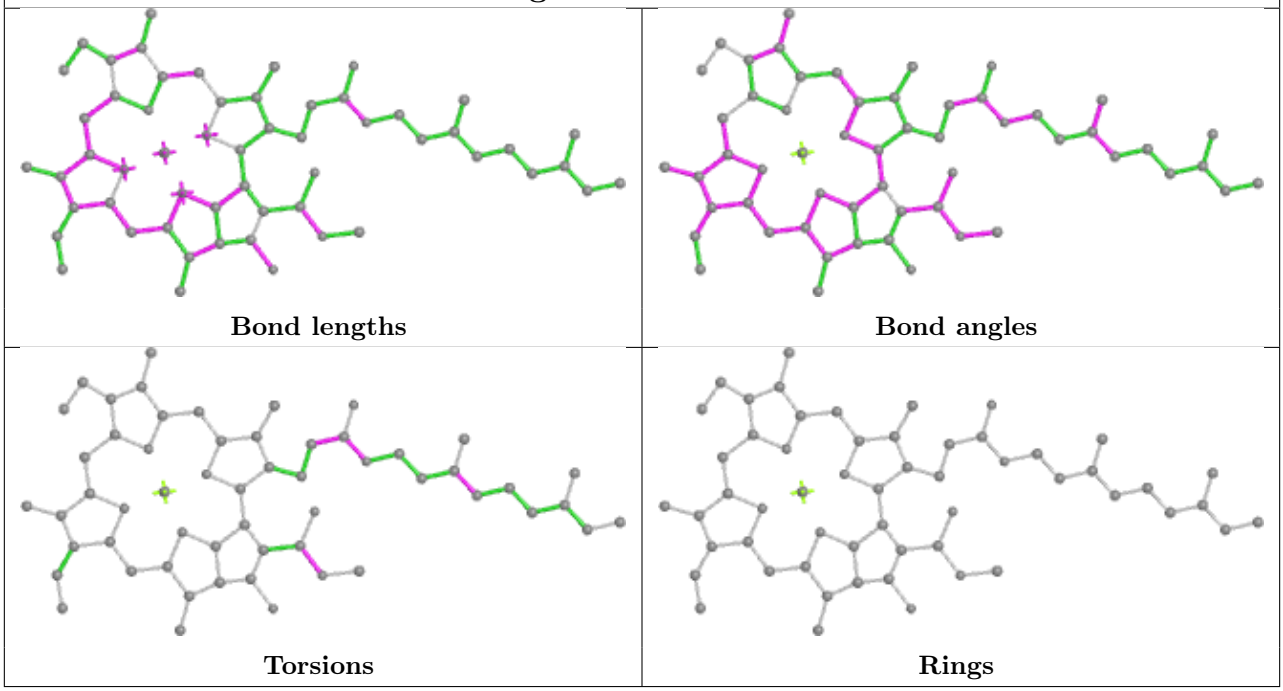


Rings

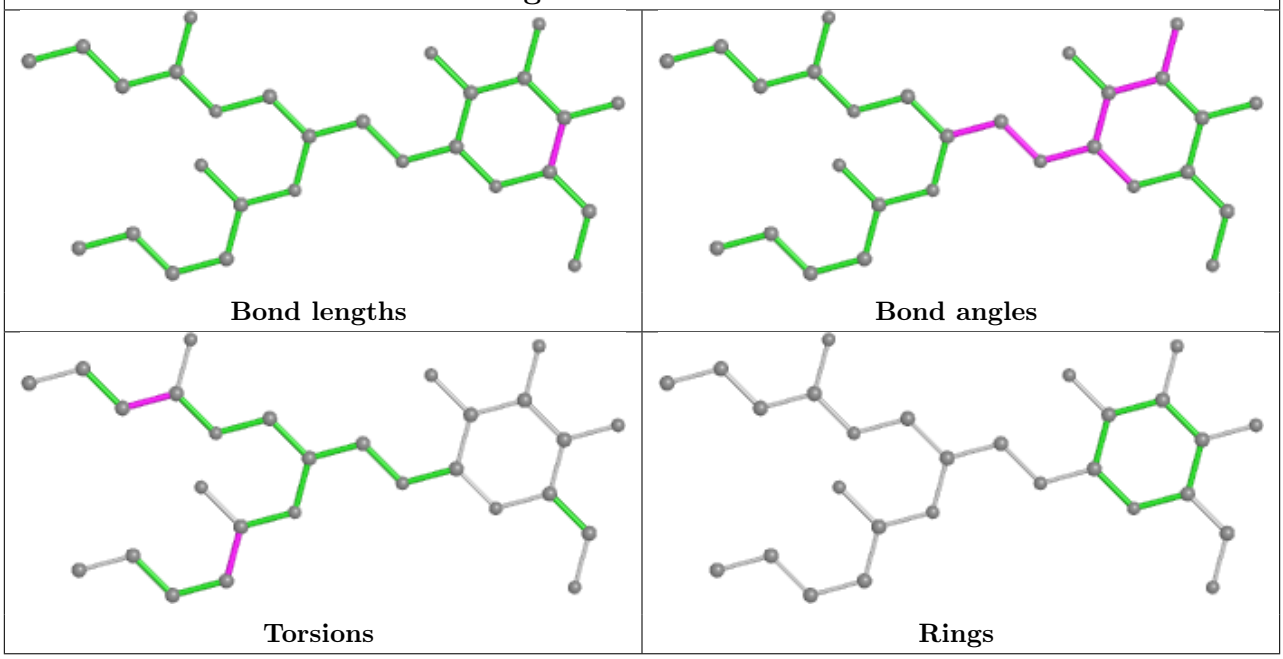
Ligand LMG b 620



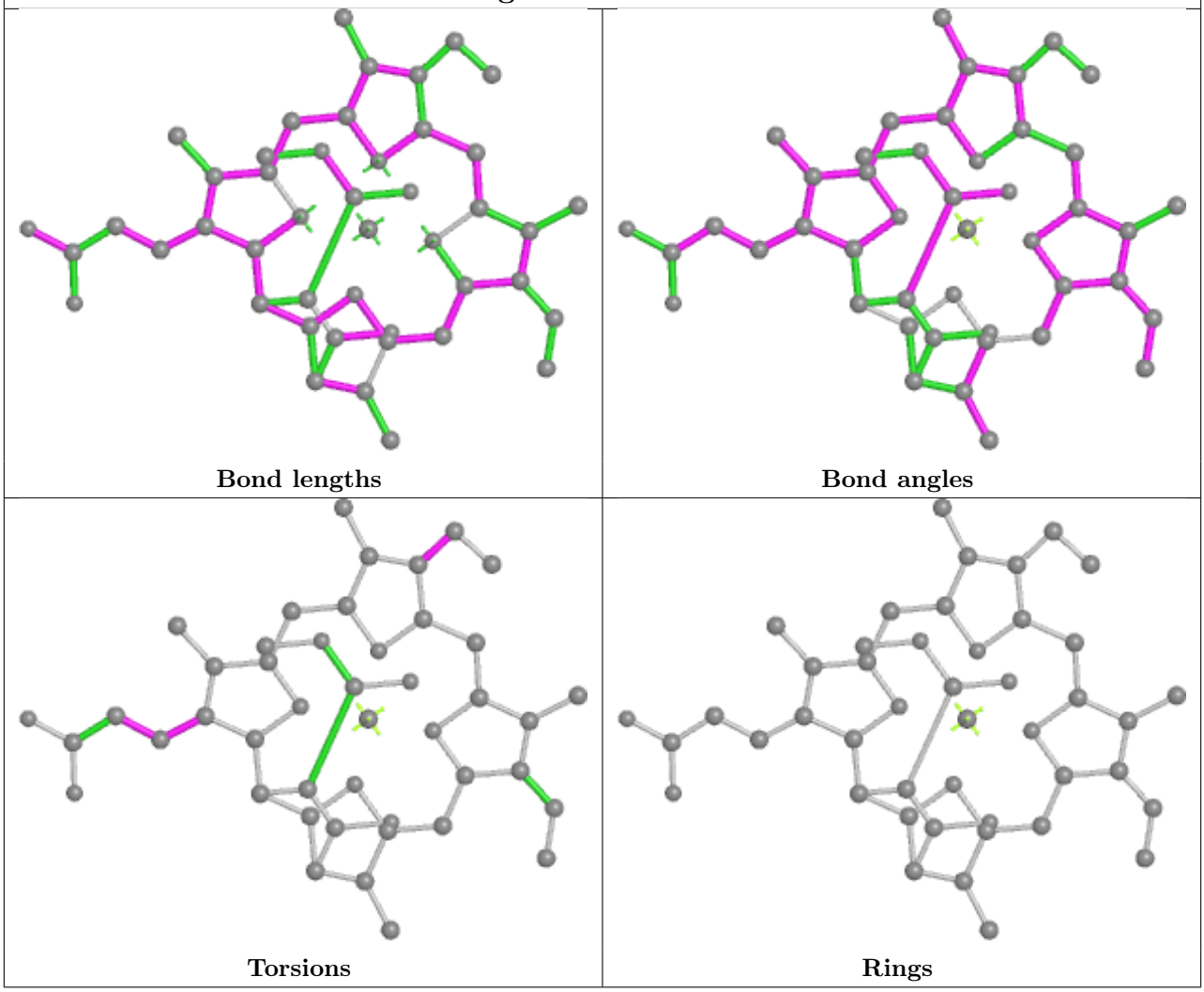
Ligand CLA 1 309



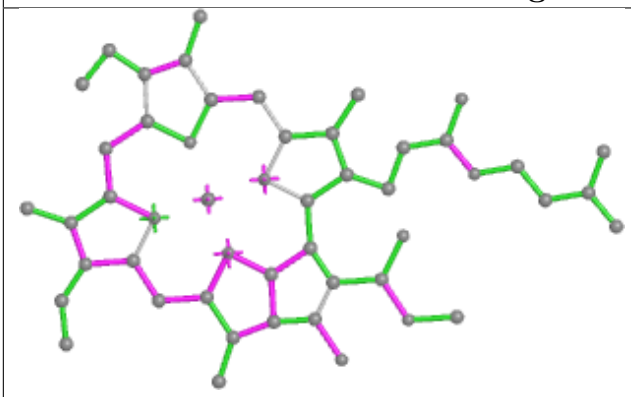
Ligand LMG b 621



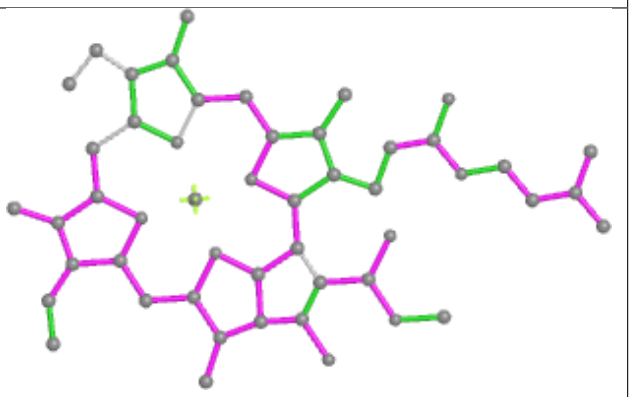
Ligand KC1 4 309



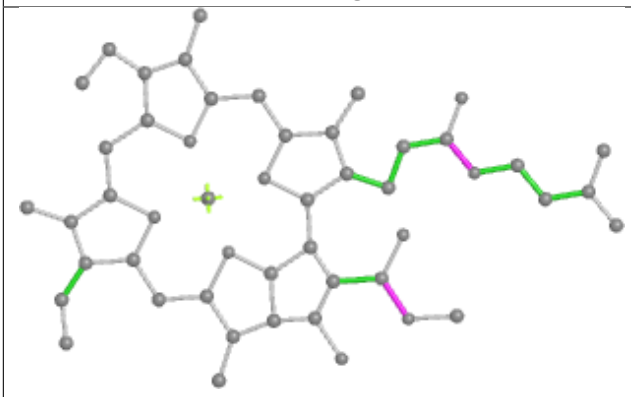
Ligand CLA 8 303



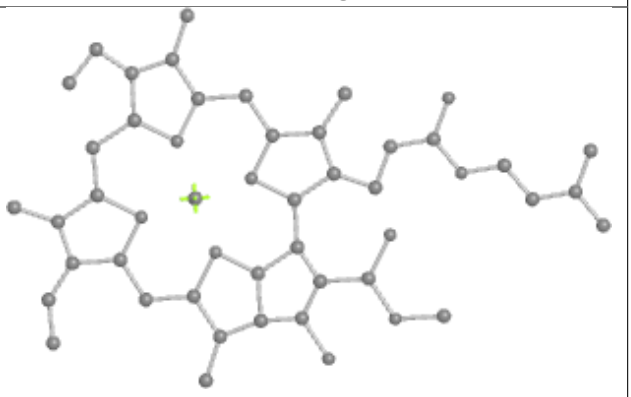
Bond lengths



Bond angles

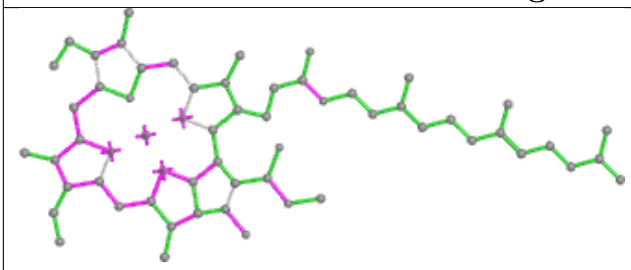


Torsions

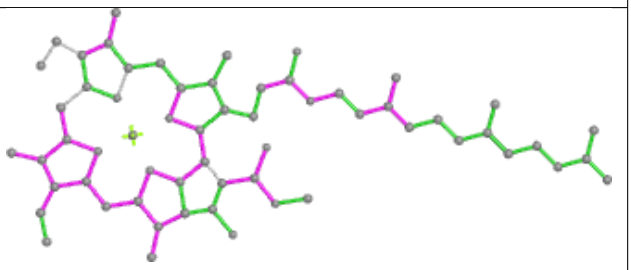


Rings

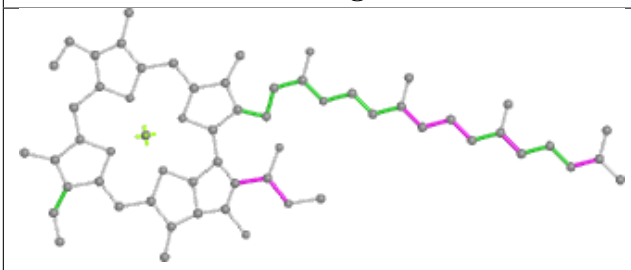
Ligand CLA 9 301



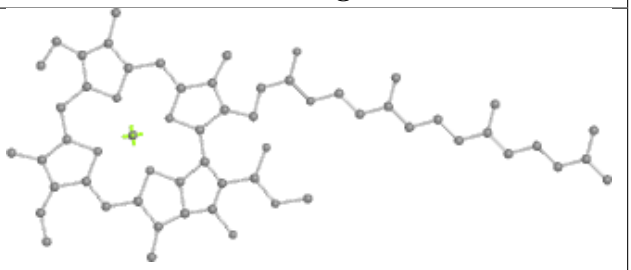
Bond lengths



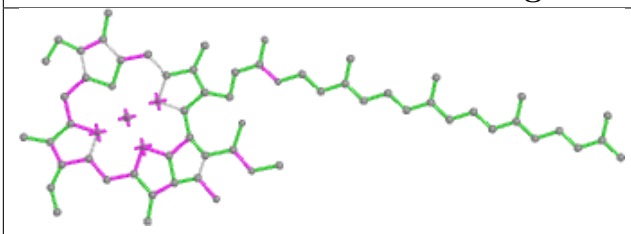
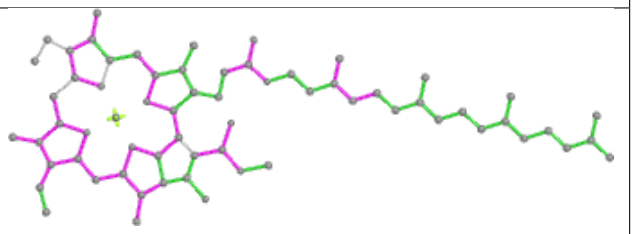
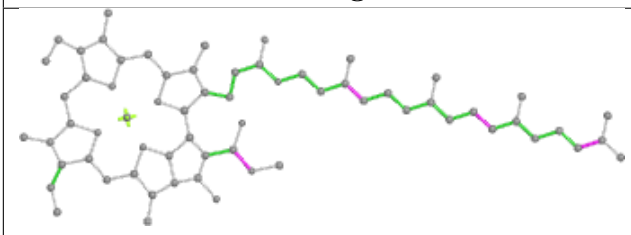
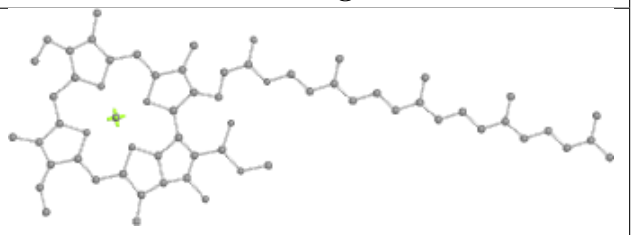
Bond angles

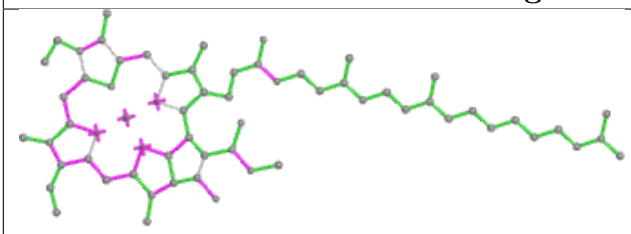
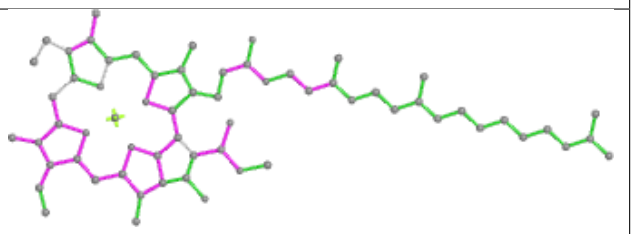
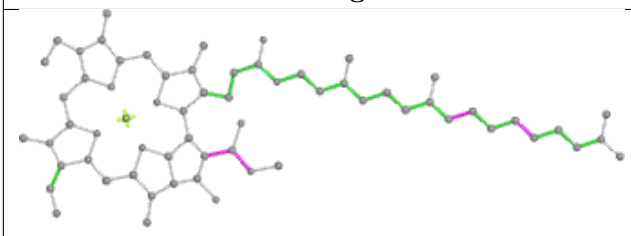
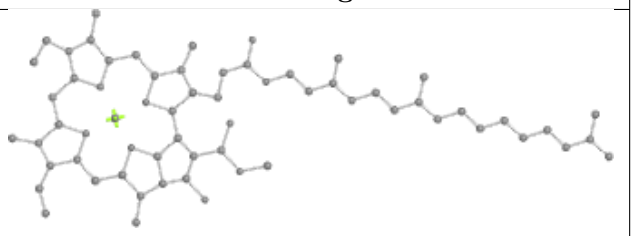


Torsions

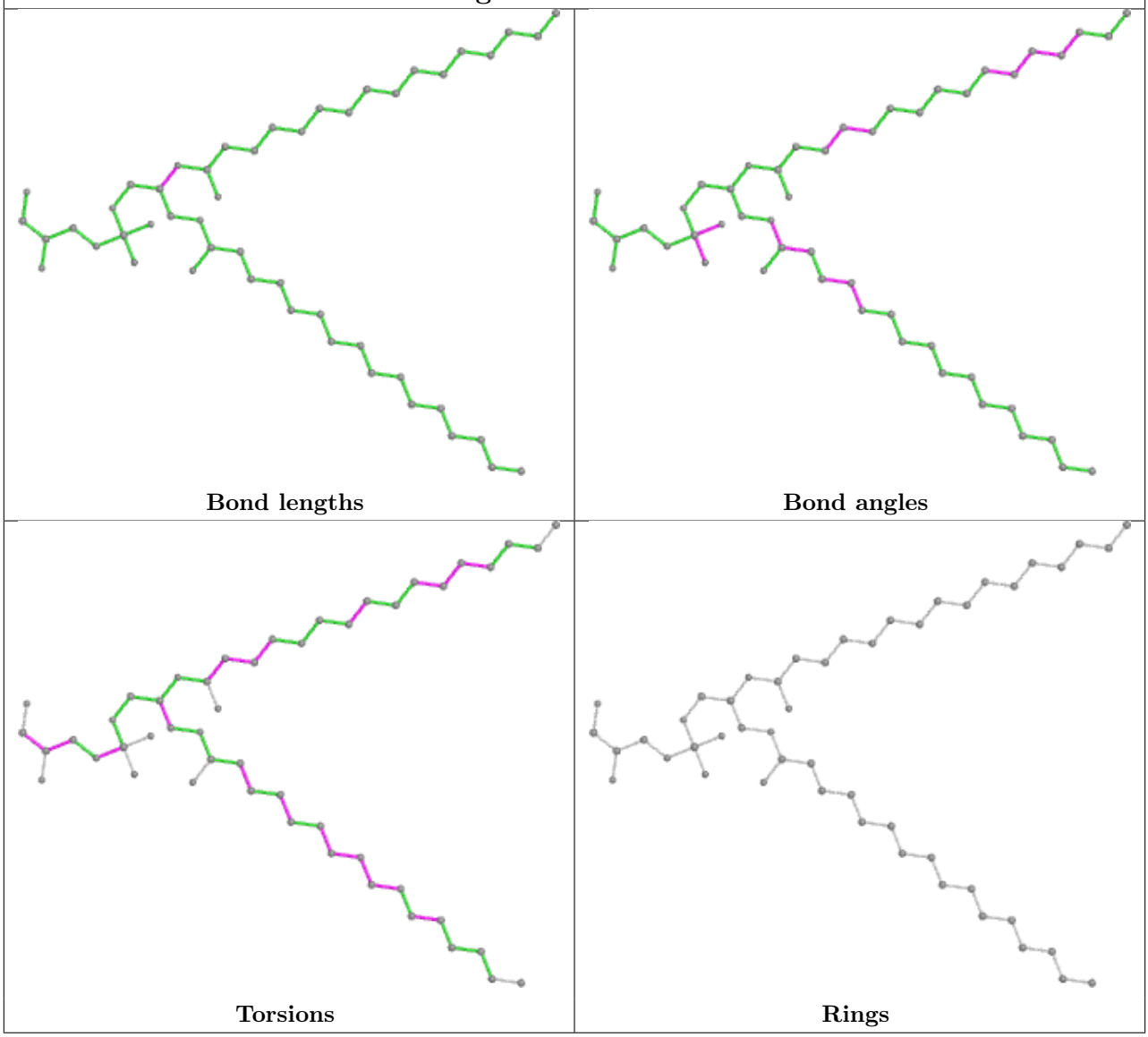


Rings

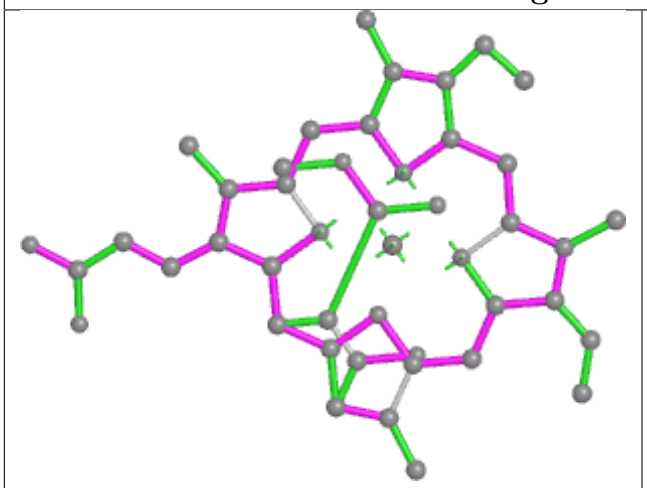
Ligand CLA B 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

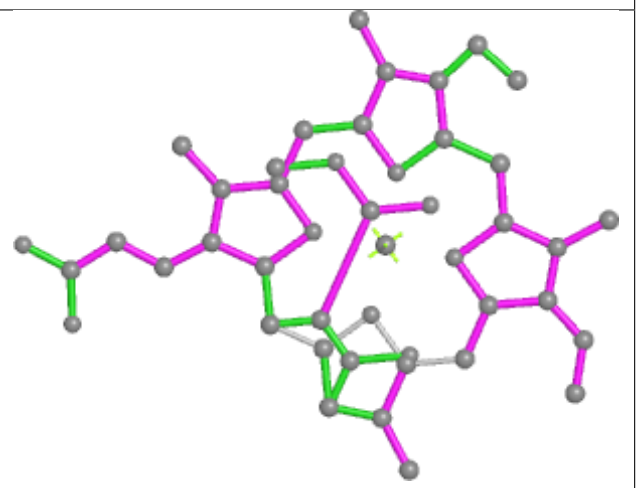
Ligand LHG l 101



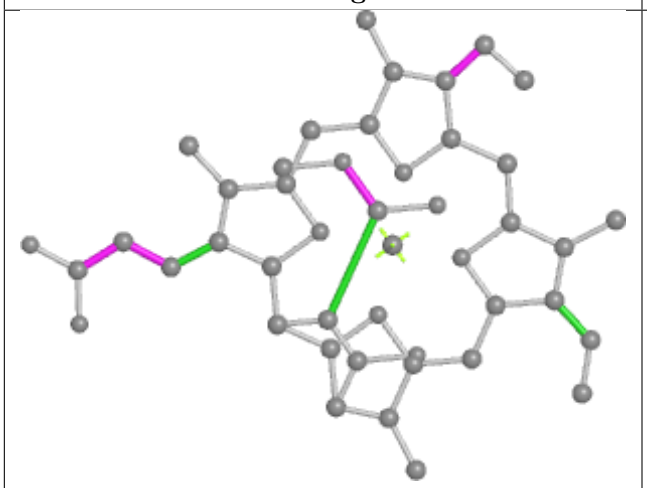
Ligand KC1 1 316



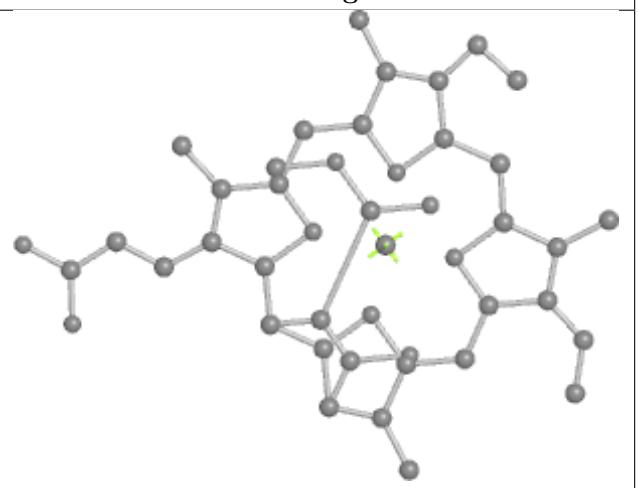
Bond lengths



Bond angles

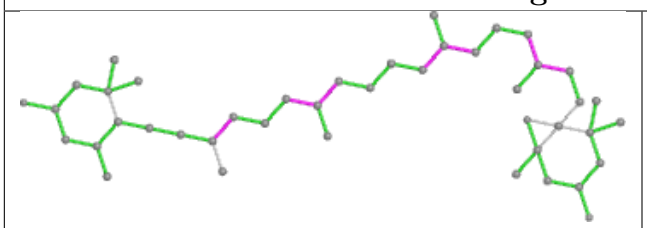


Torsions

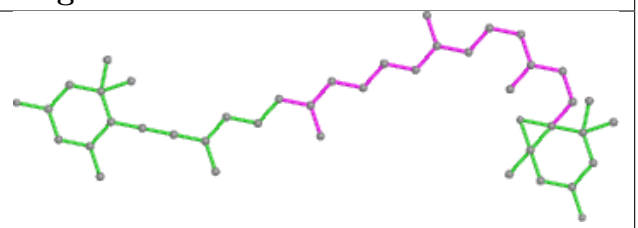


Rings

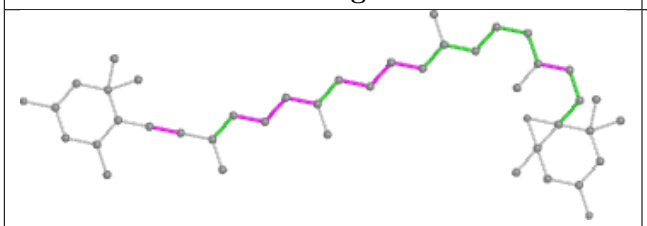
Ligand DD6 g 310



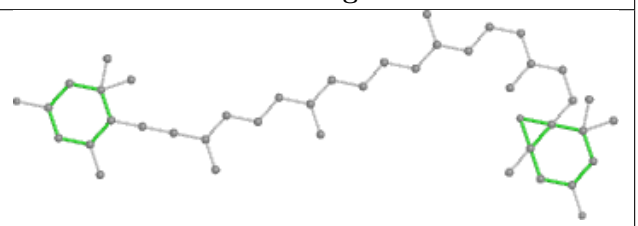
Bond lengths



Bond angles

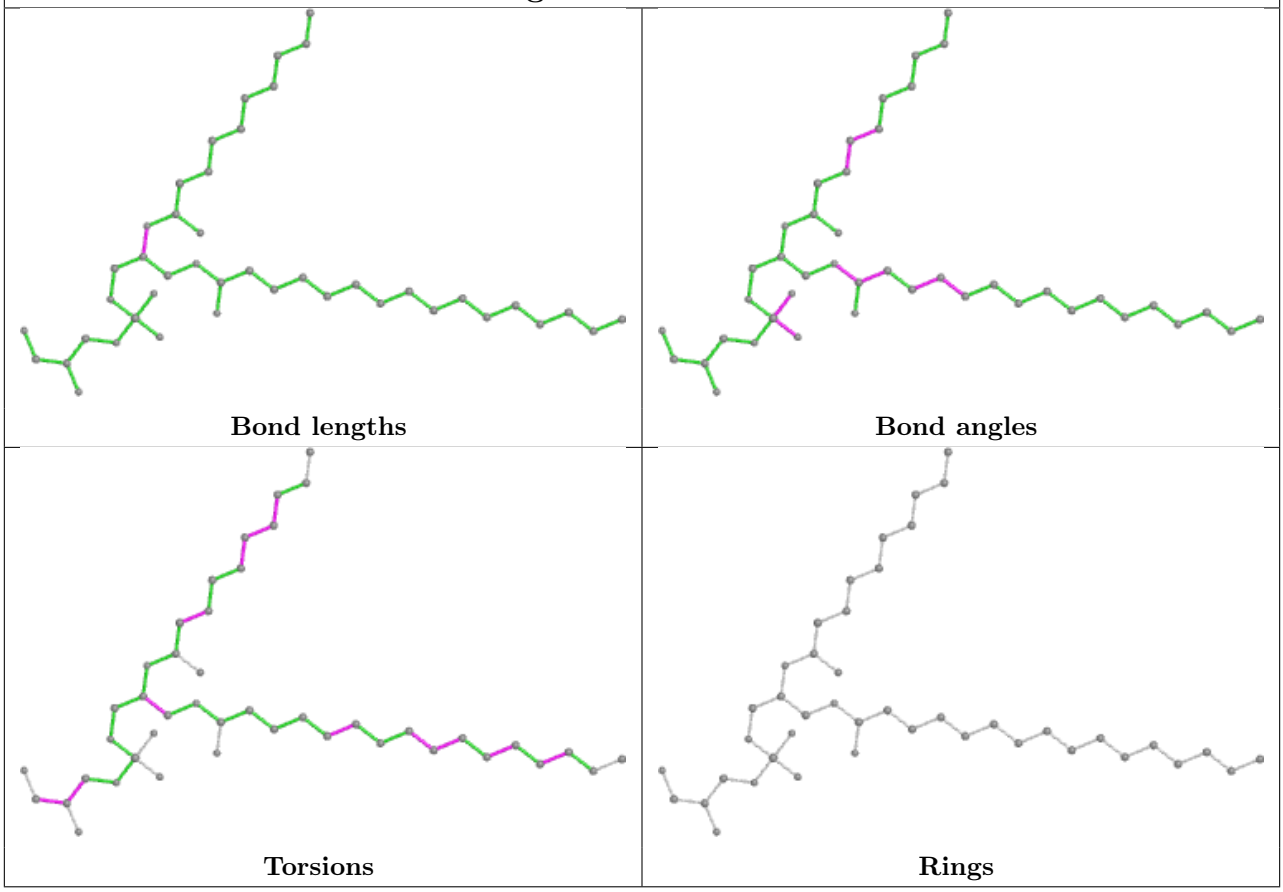


Torsions

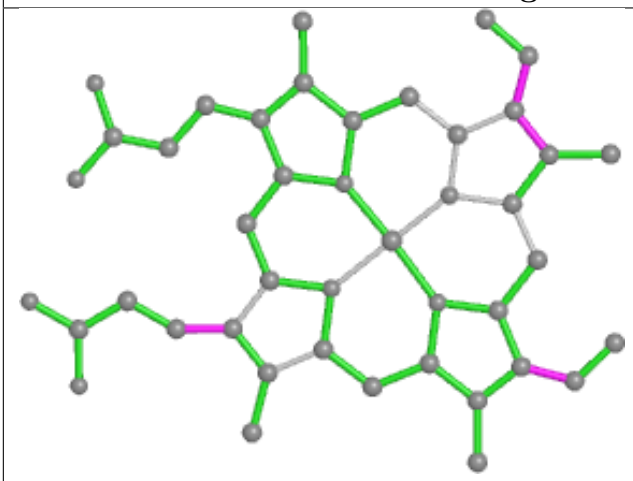


Rings

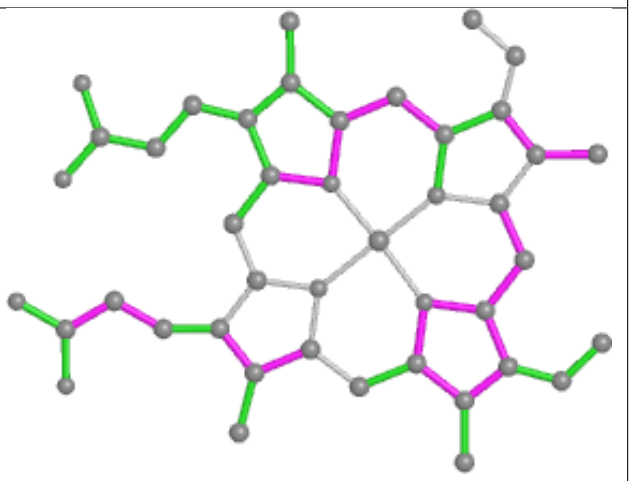
Ligand LHG d 402



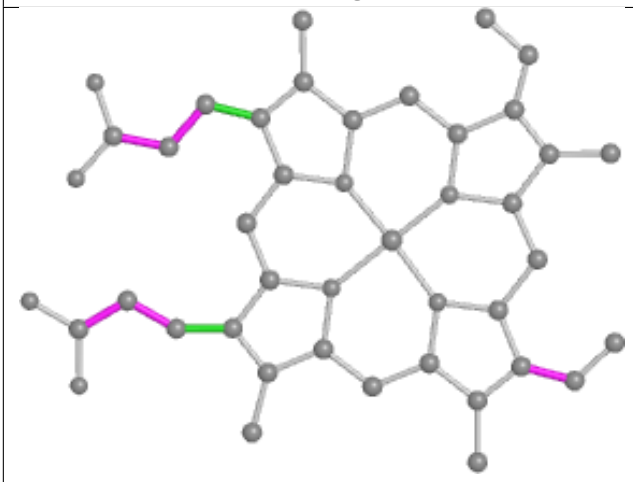
Ligand HEM E 101



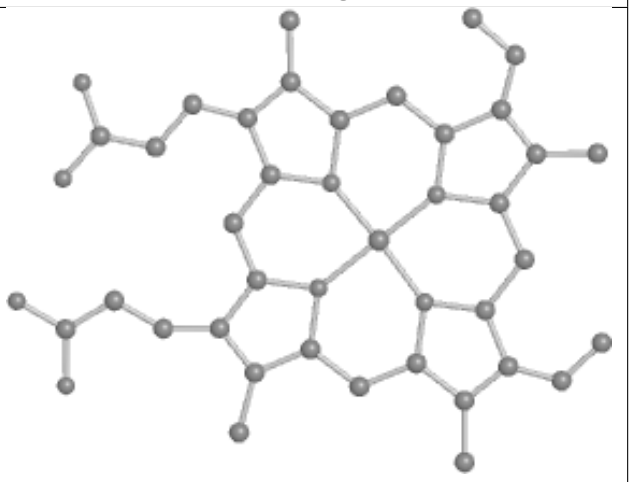
Bond lengths



Bond angles

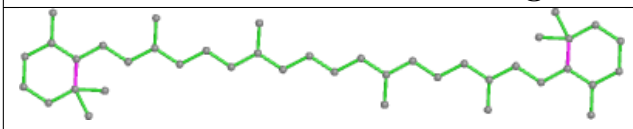


Torsions

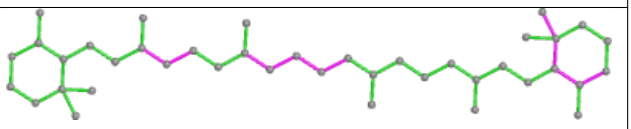


Rings

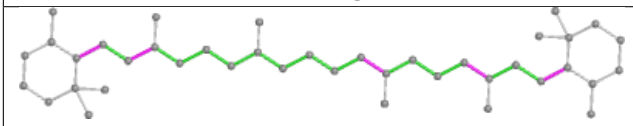
Ligand BCR b 618



Bond lengths



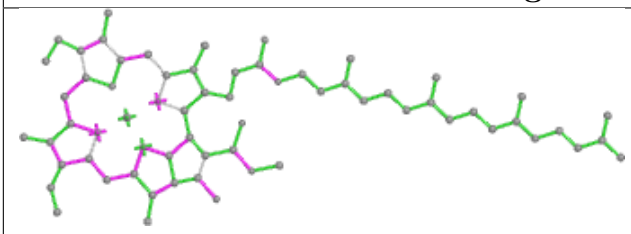
Bond angles



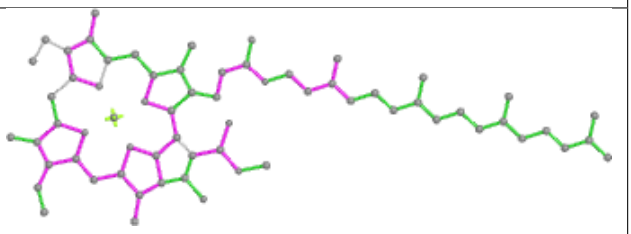
Torsions

Rings

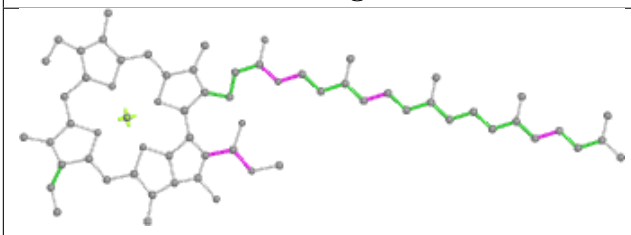
Ligand CLA C 511



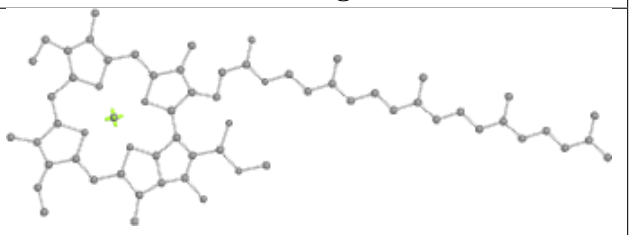
Bond lengths



Bond angles

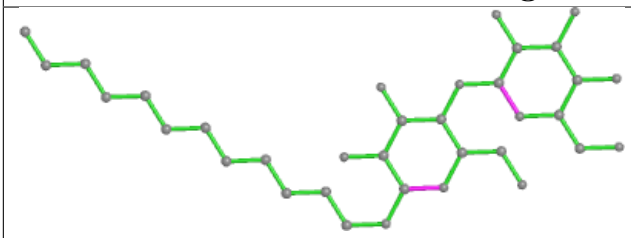


Torsions

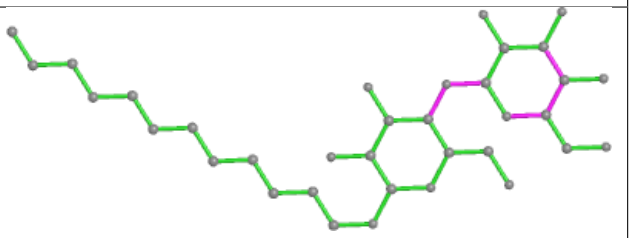


Rings

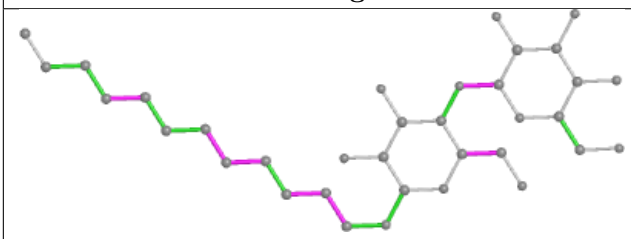
Ligand LMU A 408



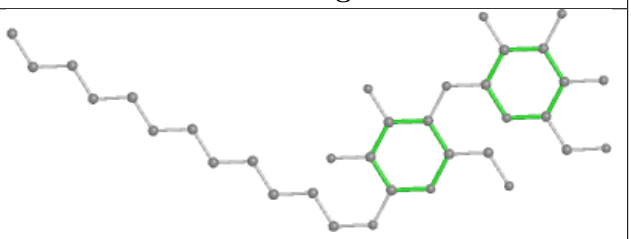
Bond lengths



Bond angles

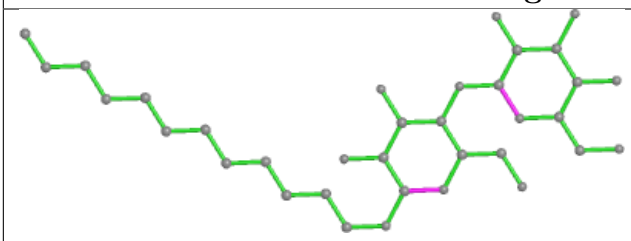


Torsions

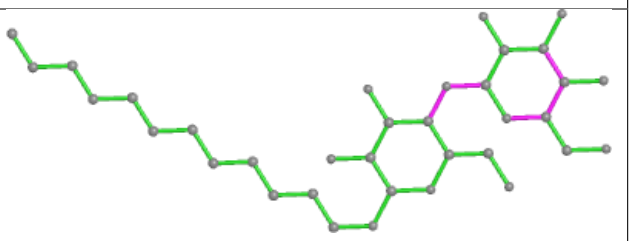


Rings

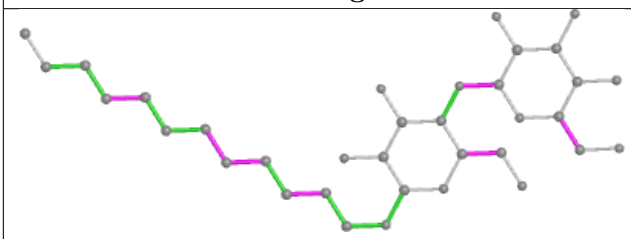
Ligand LMU a 408



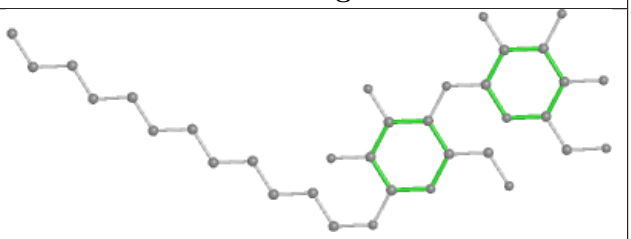
Bond lengths



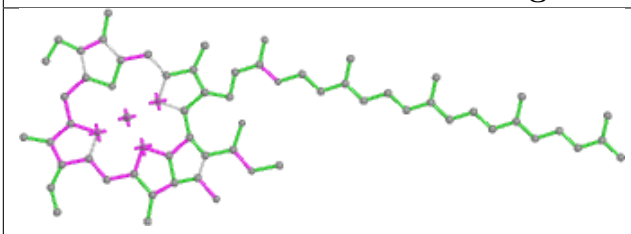
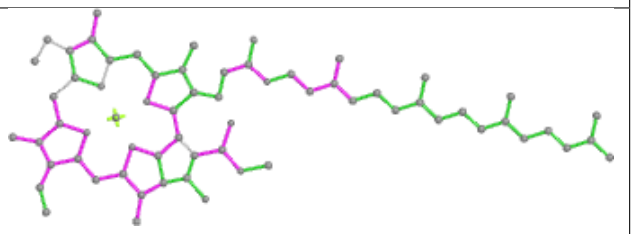
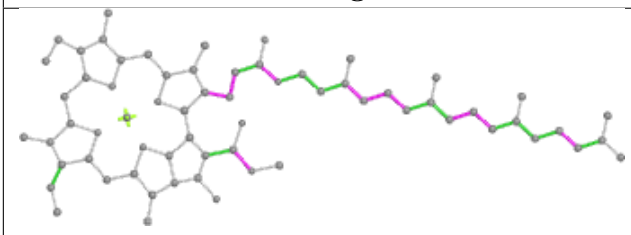
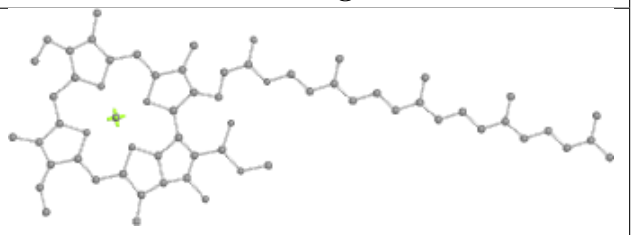
Bond angles

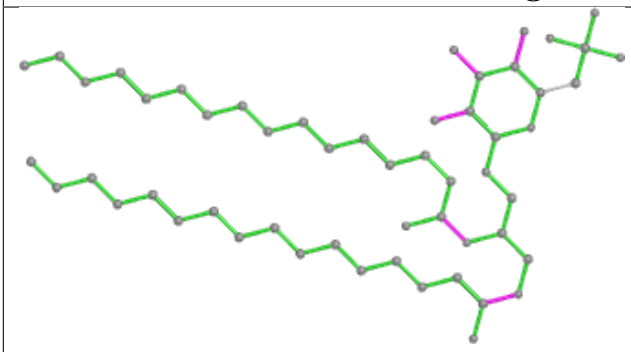
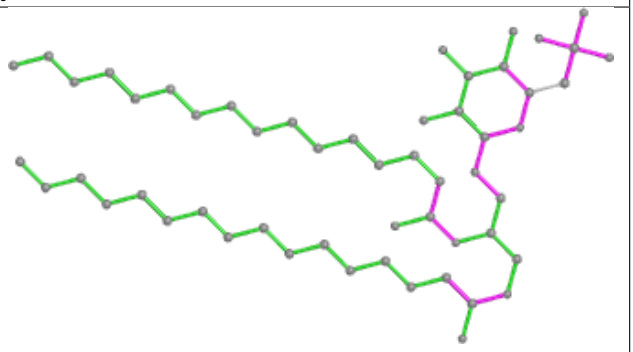
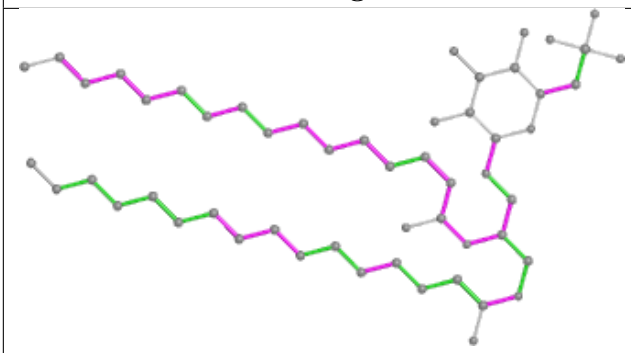
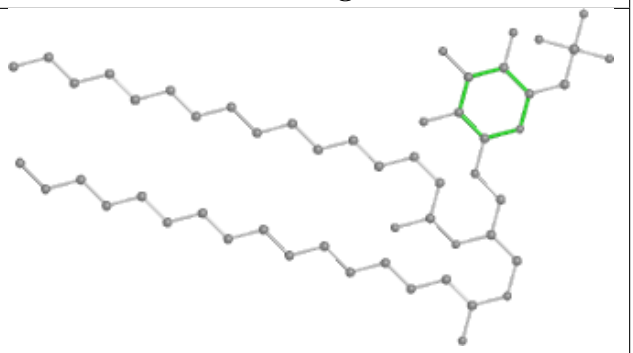


Torsions

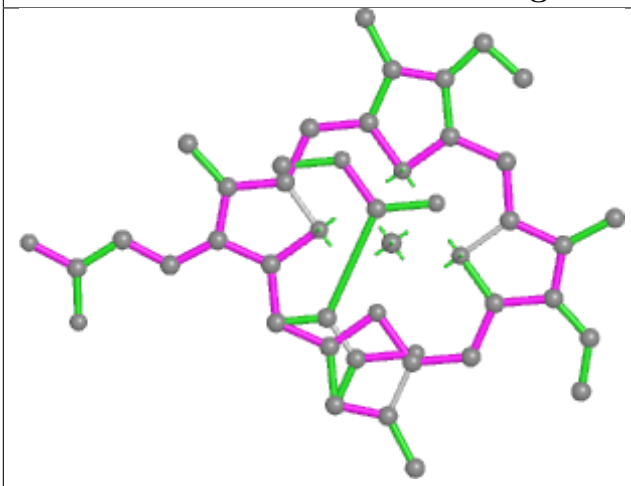


Rings

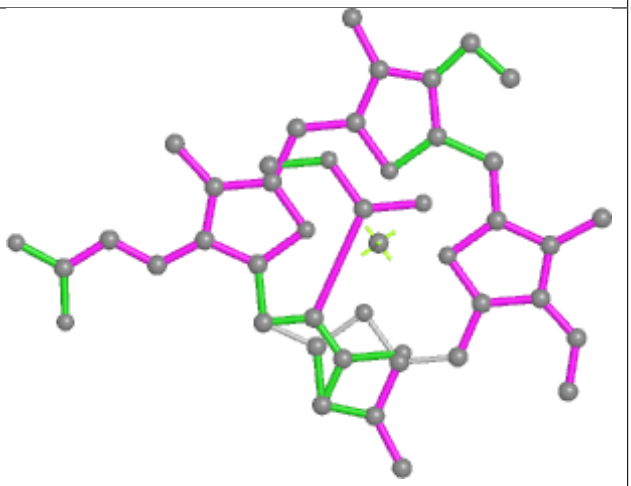
Ligand CLA c 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD B 626	
 Bond lengths	 Bond angles
 Torsions	 Rings

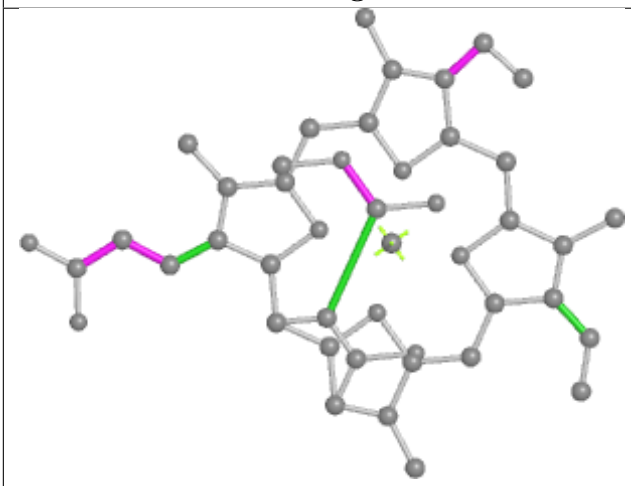
Ligand KC1 7 315



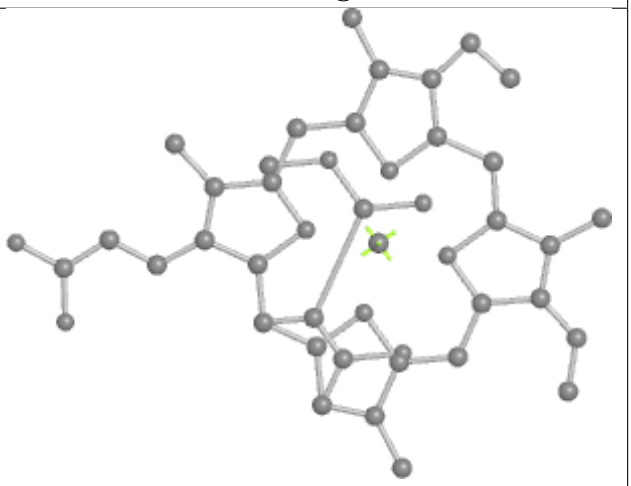
Bond lengths



Bond angles

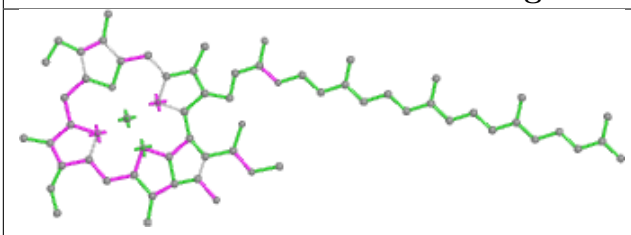


Torsions

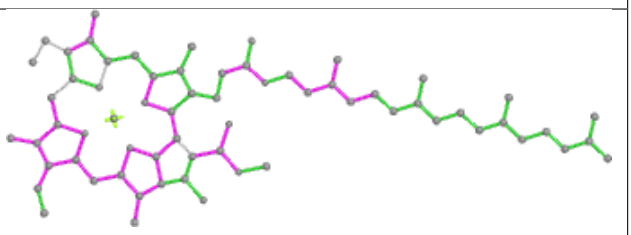


Rings

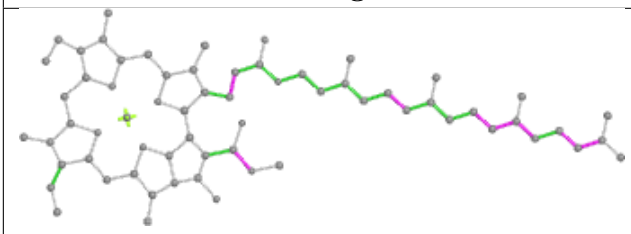
Ligand CLA B 607



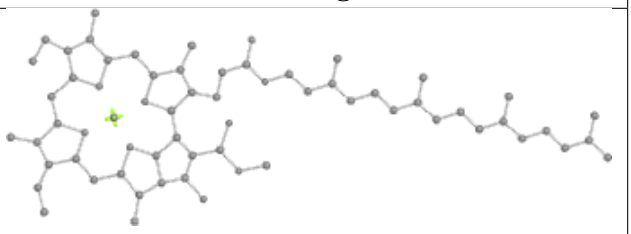
Bond lengths



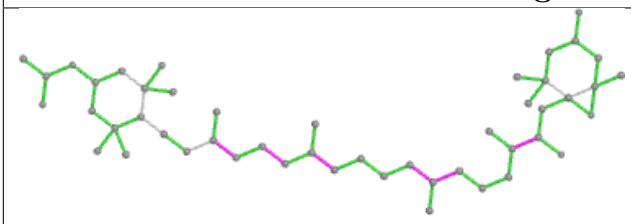
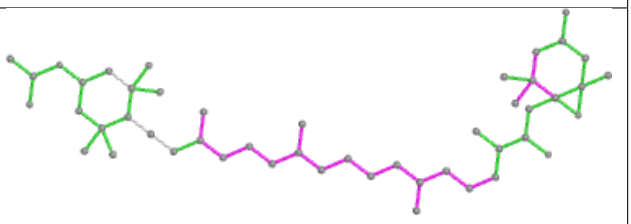
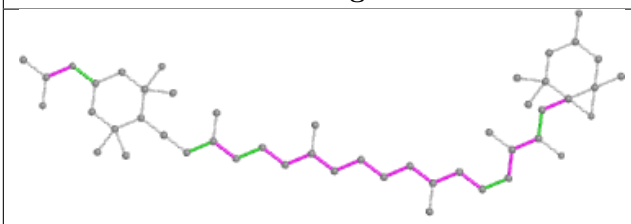
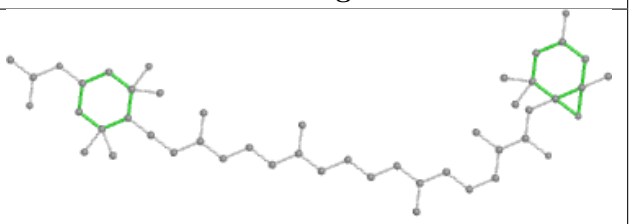
Bond angles

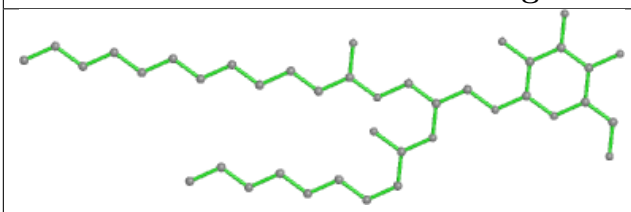
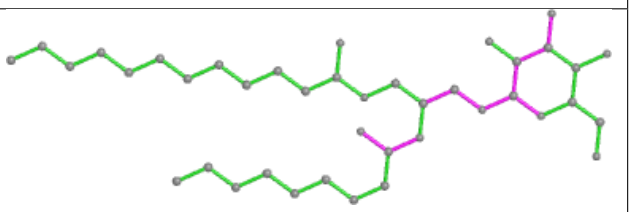
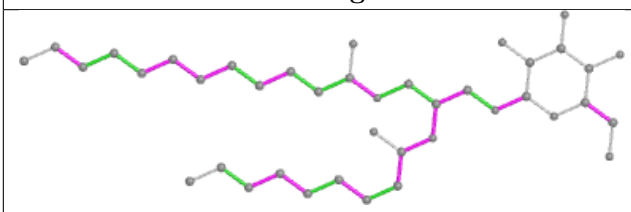
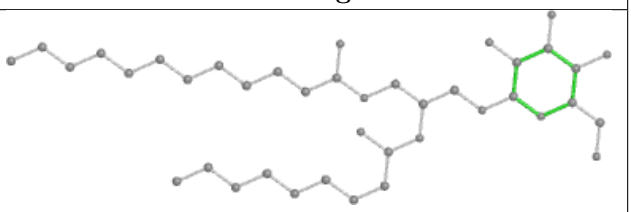


Torsions

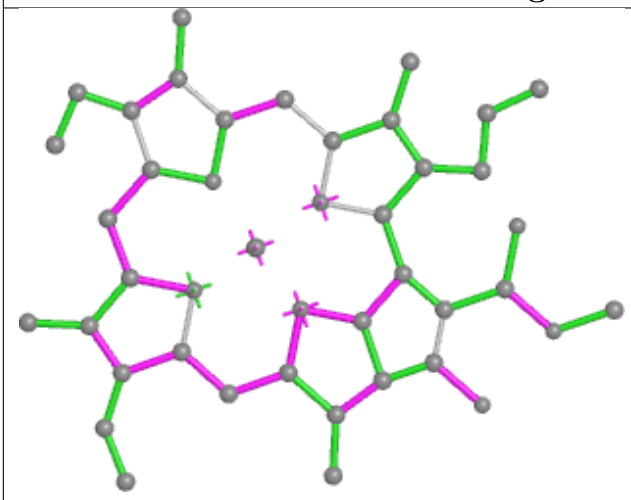


Rings

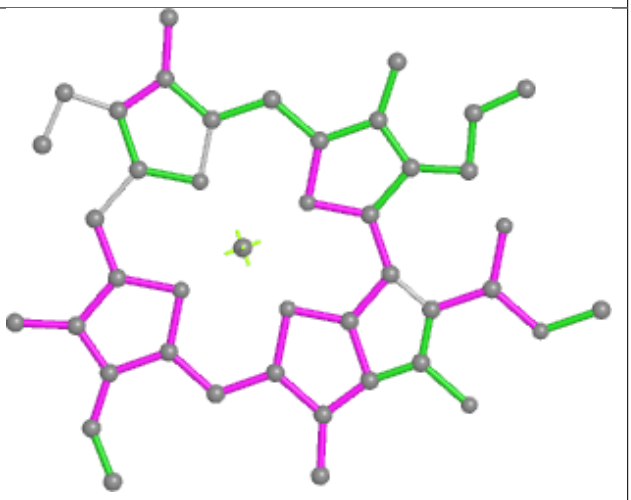
Ligand A86 8 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG L 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

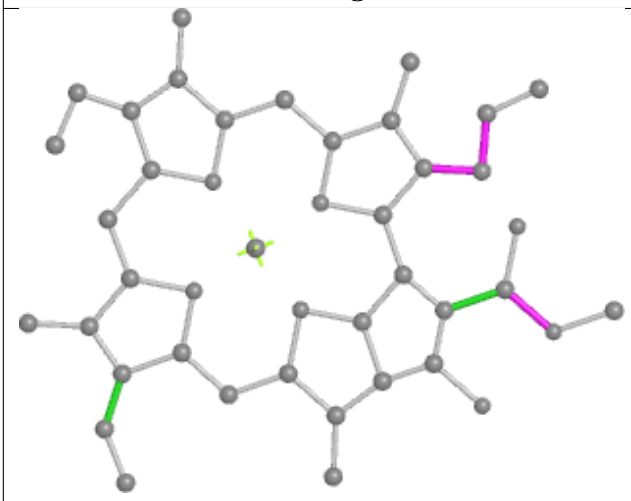
Ligand CLA 8 307



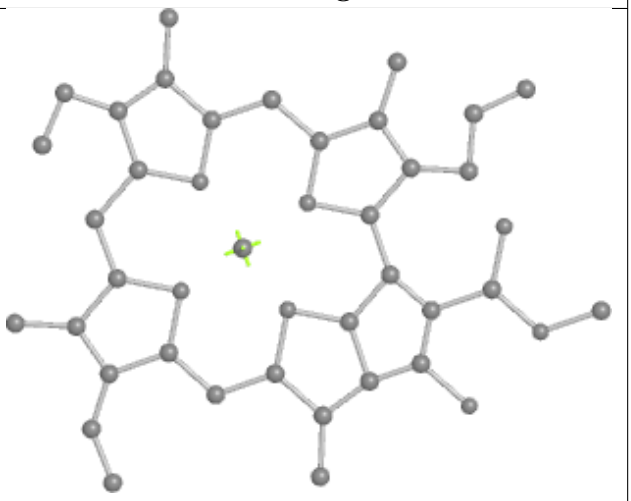
Bond lengths



Bond angles

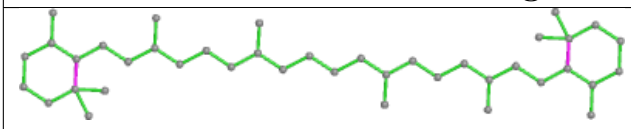


Torsions

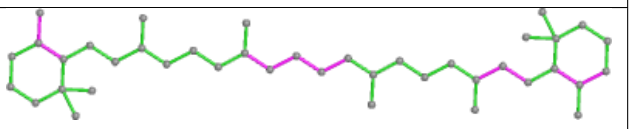


Rings

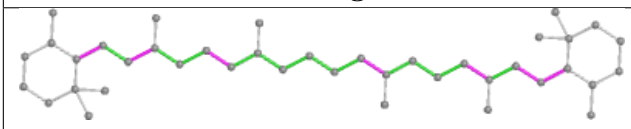
Ligand BCR C 501



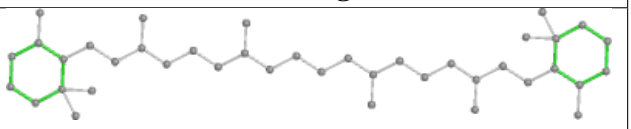
Bond lengths



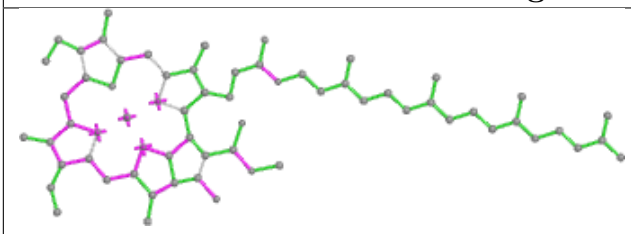
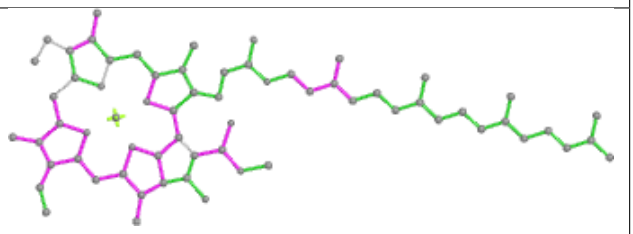
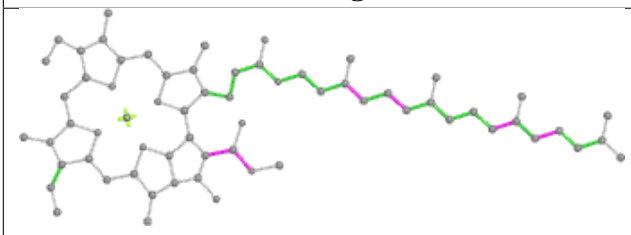
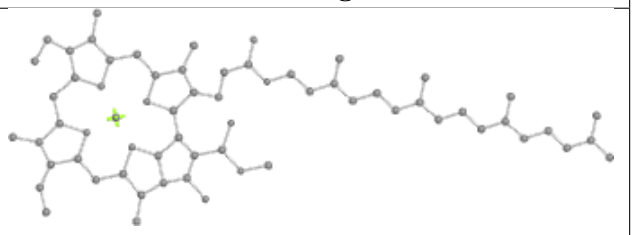
Bond angles

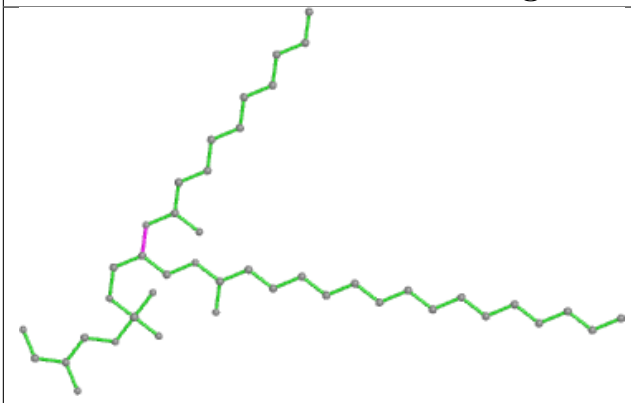
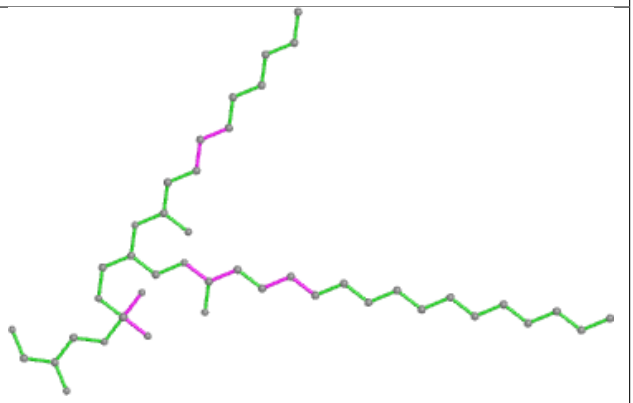
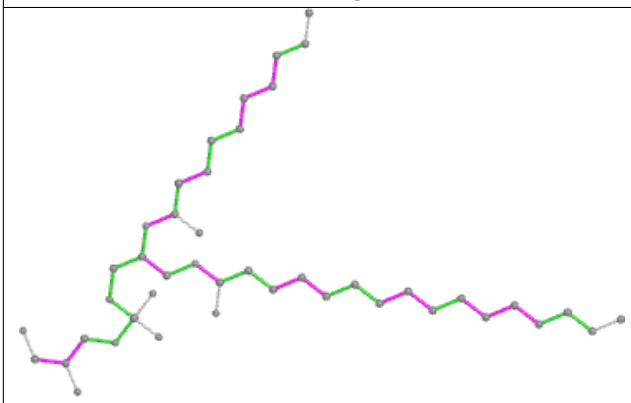
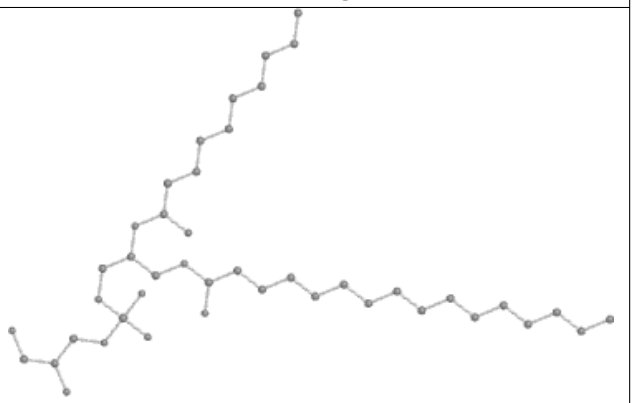


Torsions

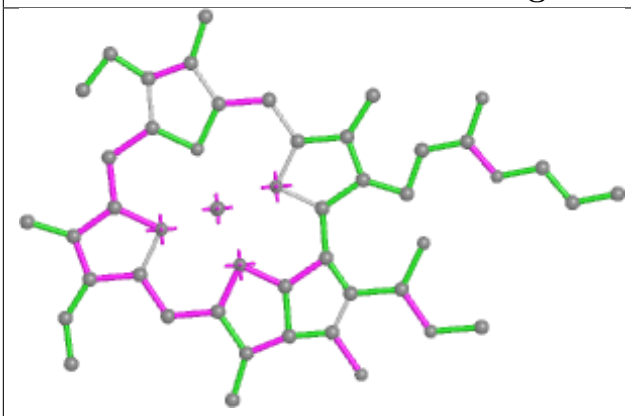


Rings

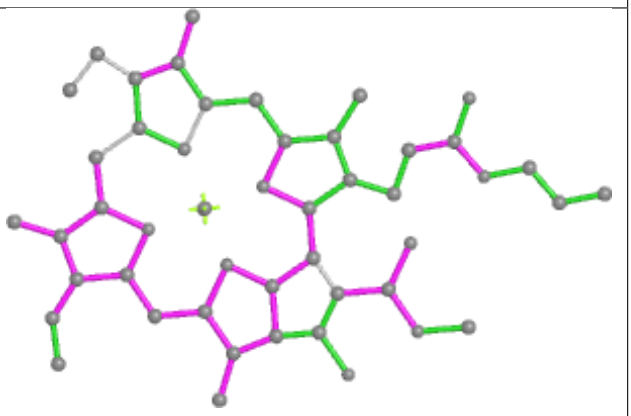
Ligand CLA b 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG D 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

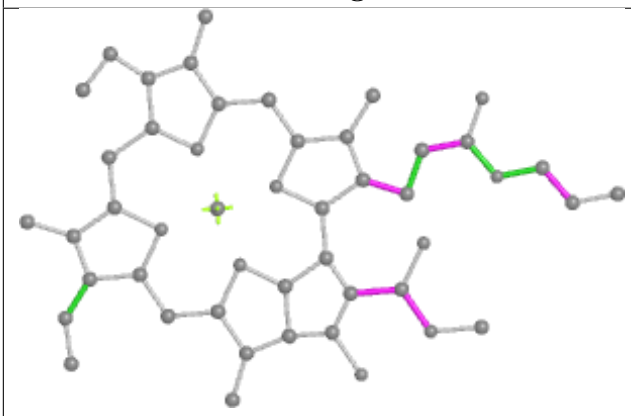
Ligand CLA 5 304



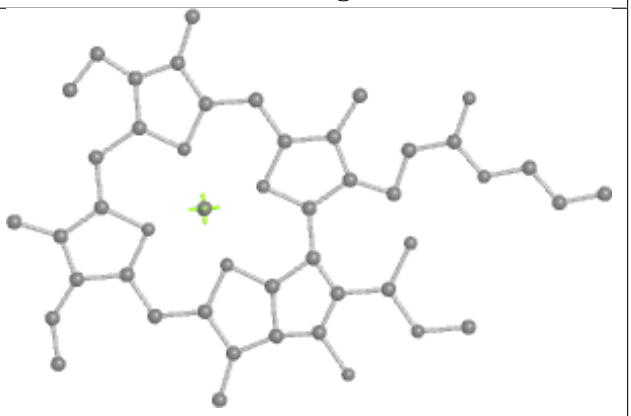
Bond lengths



Bond angles

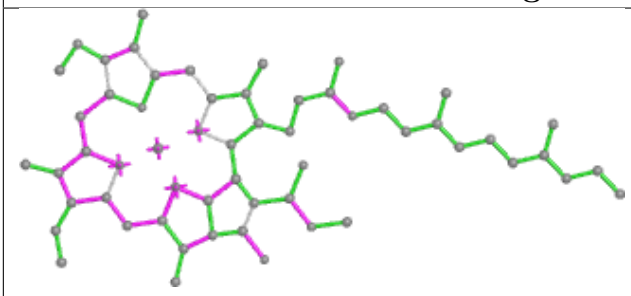


Torsions

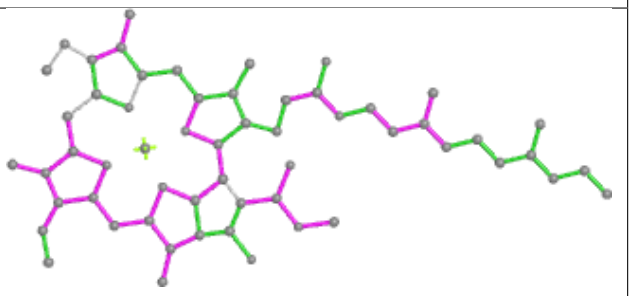


Rings

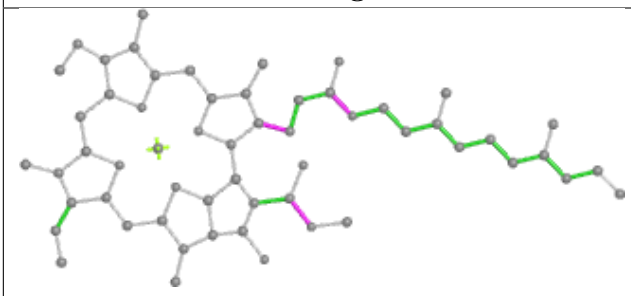
Ligand CLA G 301



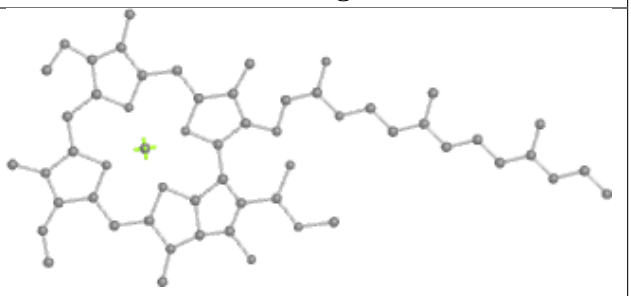
Bond lengths



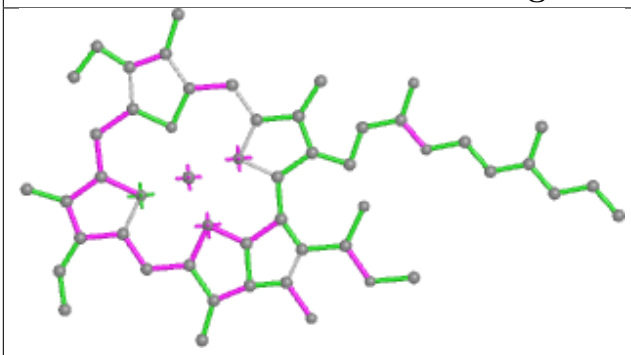
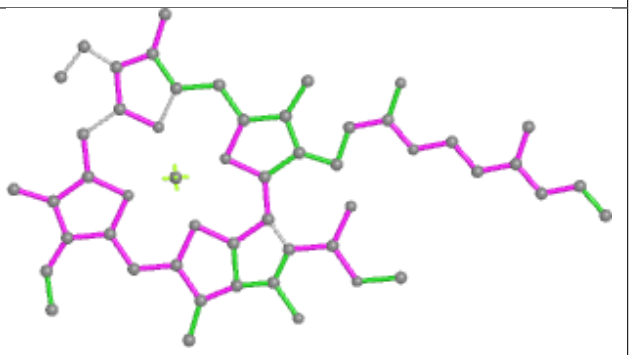
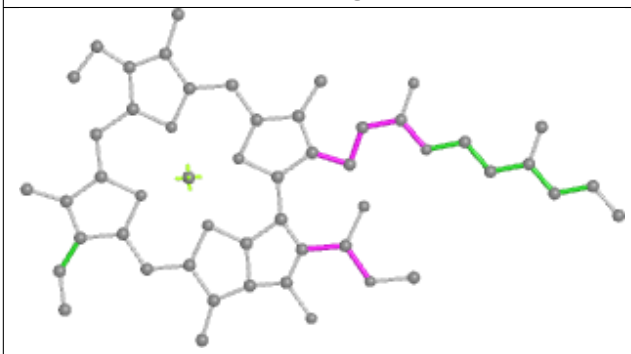
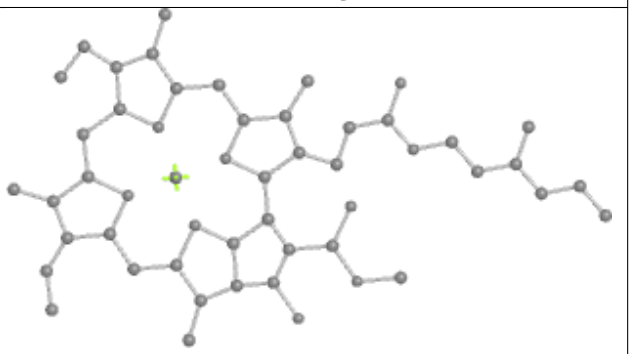
Bond angles



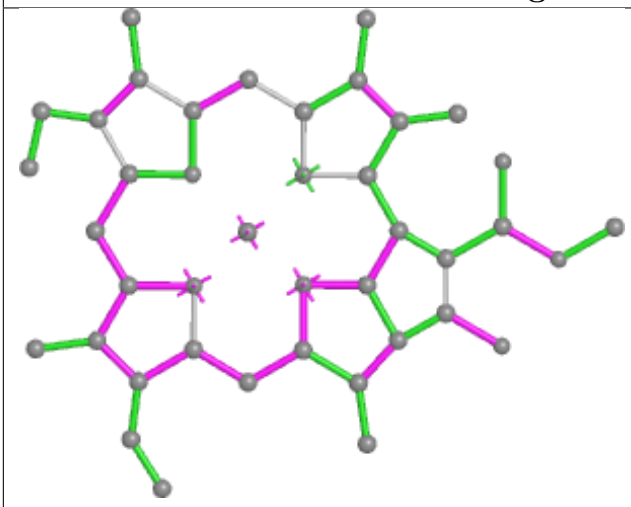
Torsions



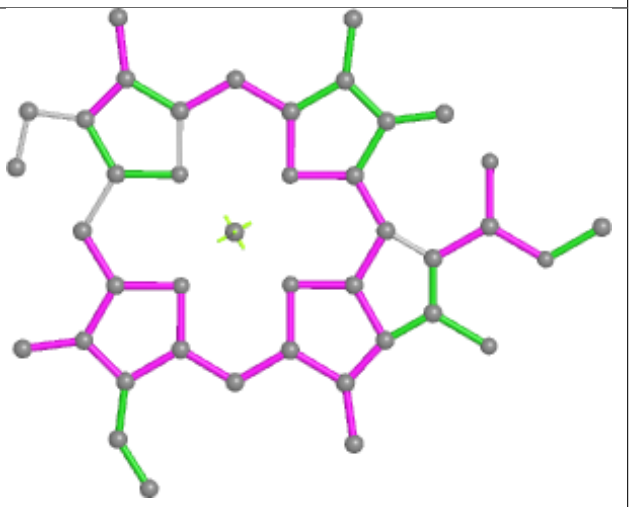
Rings

Ligand CLA 5 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

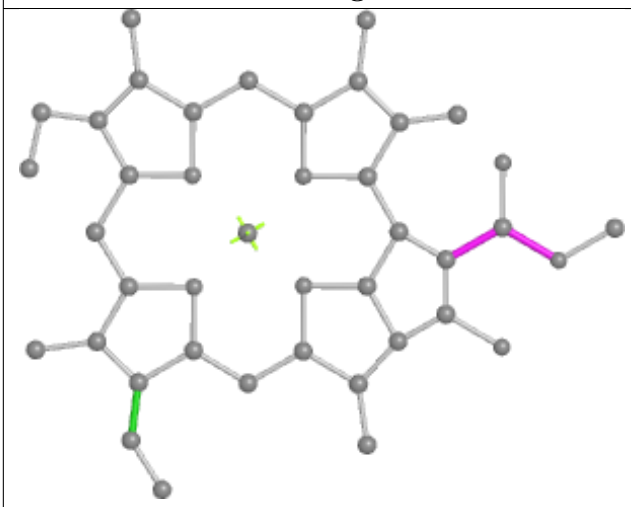
Ligand CLA 7 305



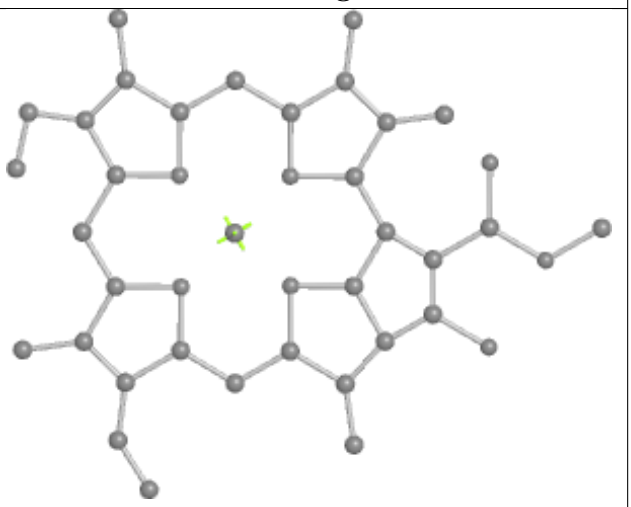
Bond lengths



Bond angles

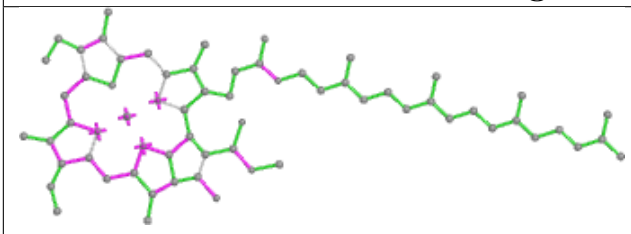


Torsions

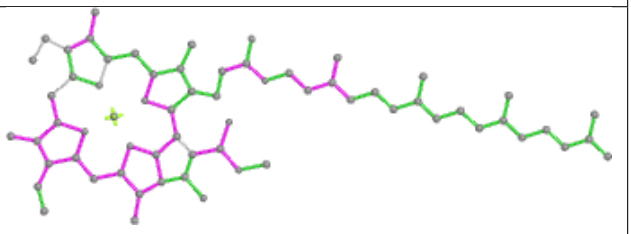


Rings

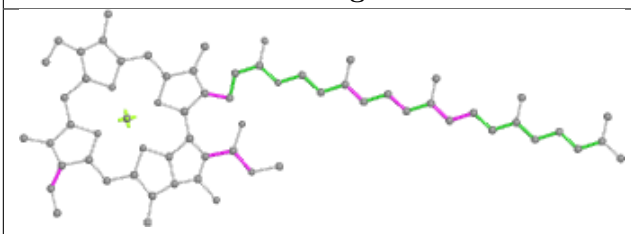
Ligand CLA 7 304



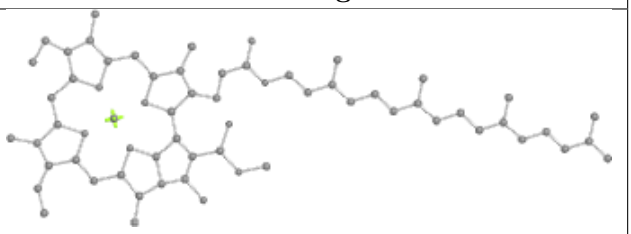
Bond lengths



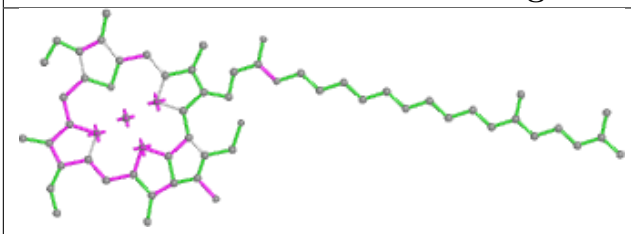
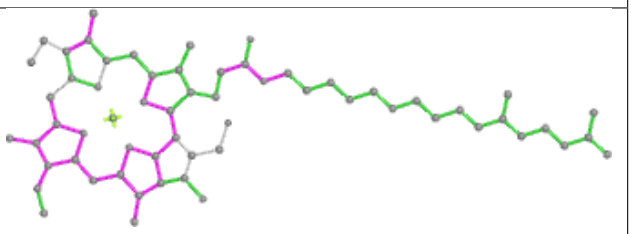
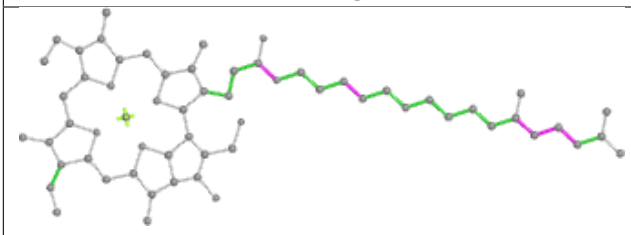
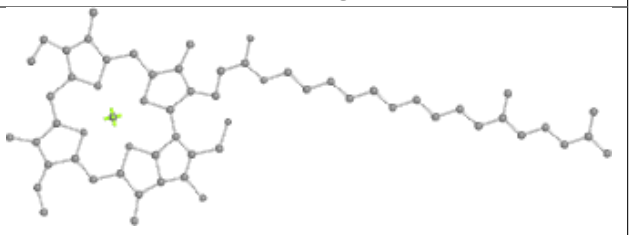
Bond angles

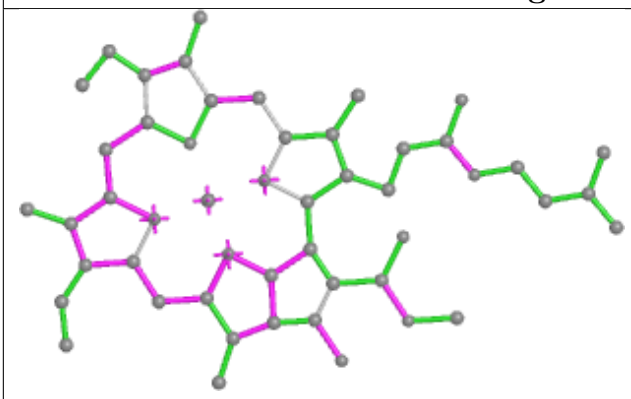
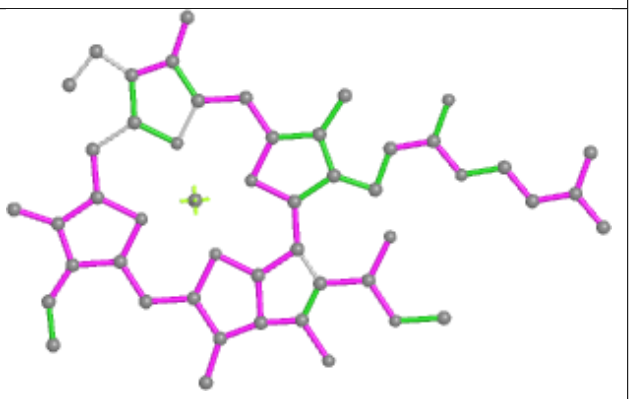
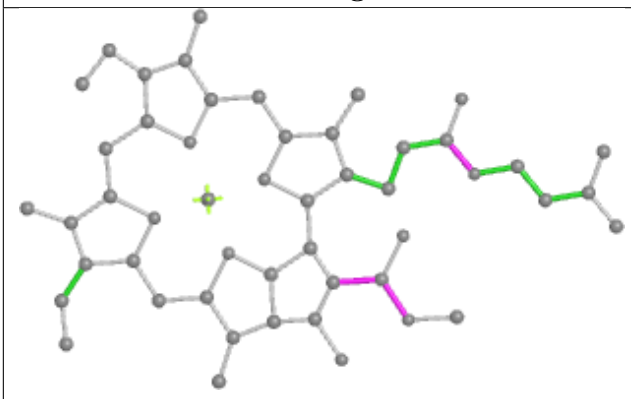
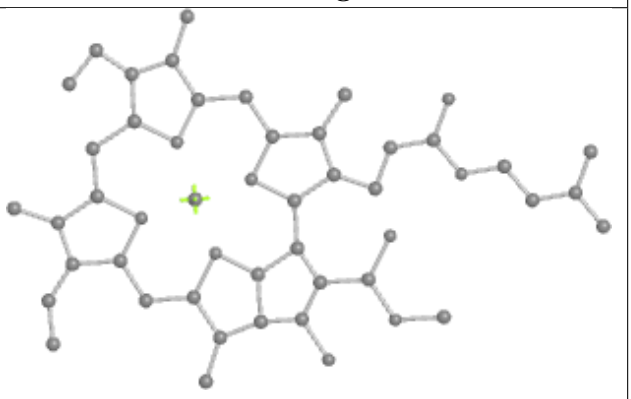


Torsions

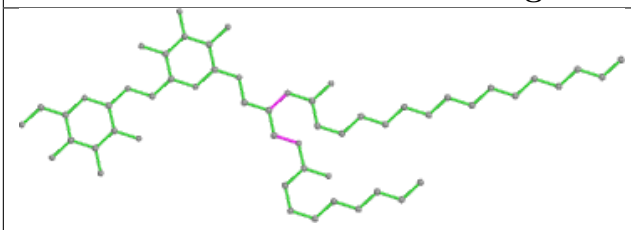


Rings

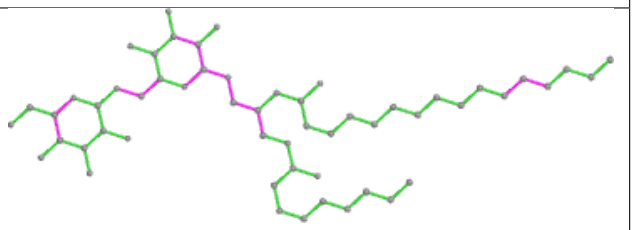
Ligand CLA b 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

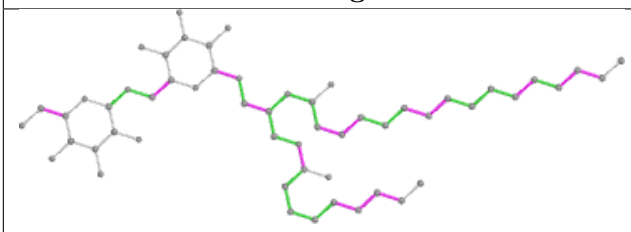
Ligand DGD c 516



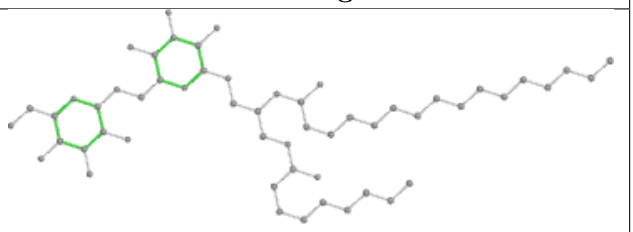
Bond lengths



Bond angles

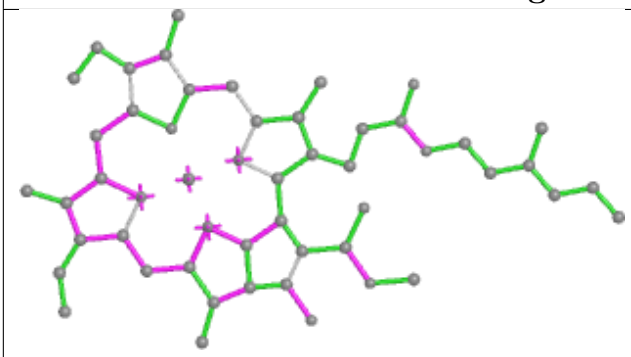


Torsions

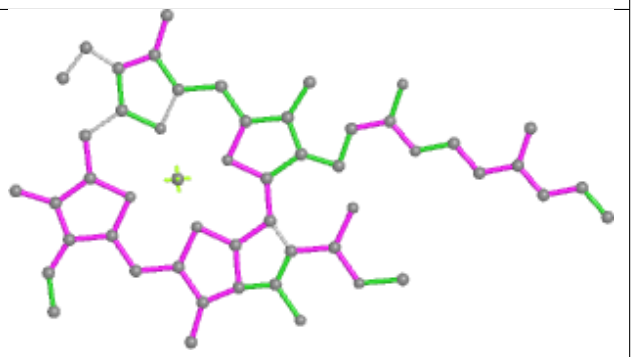


Rings

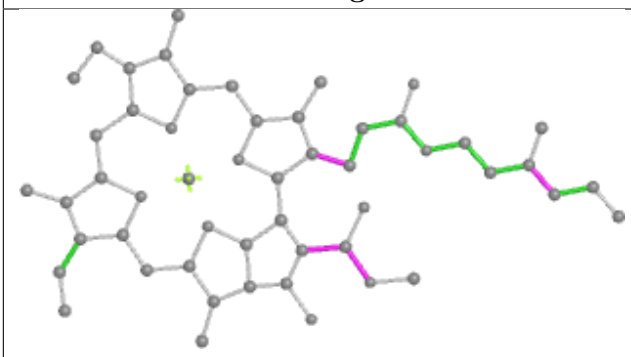
Ligand CLA 6 300



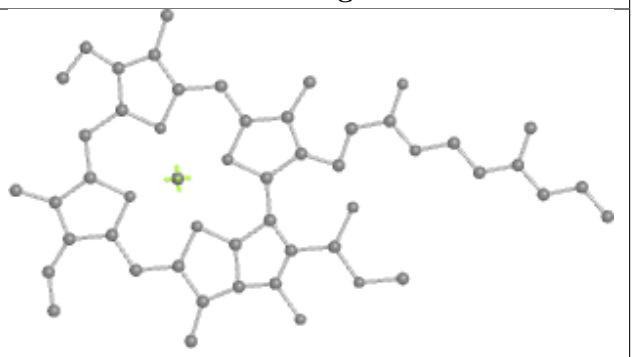
Bond lengths



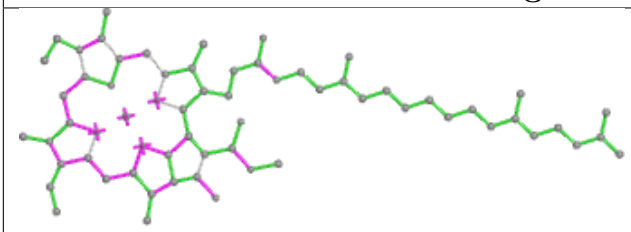
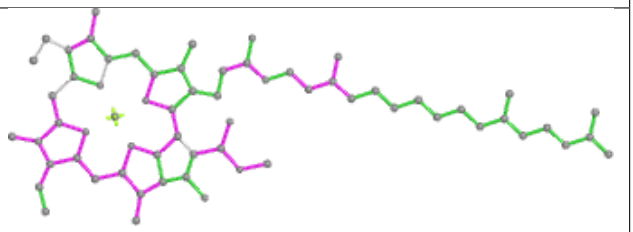
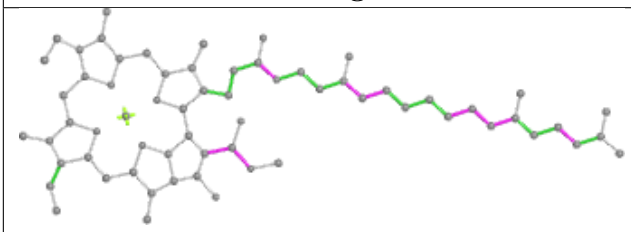
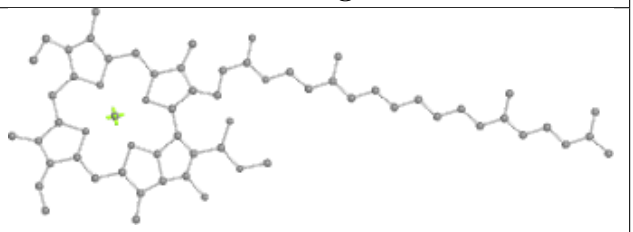
Bond angles

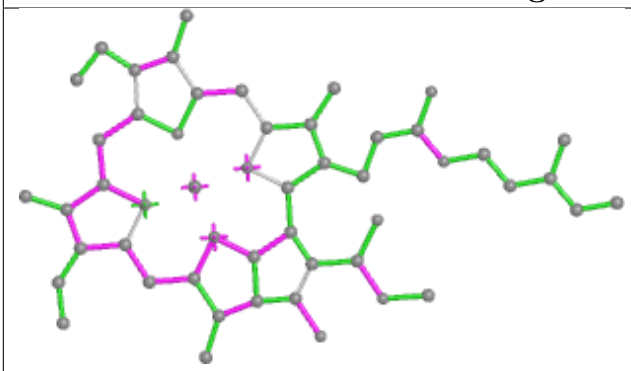
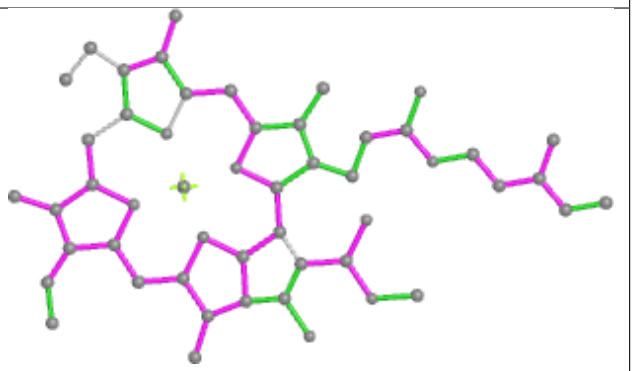
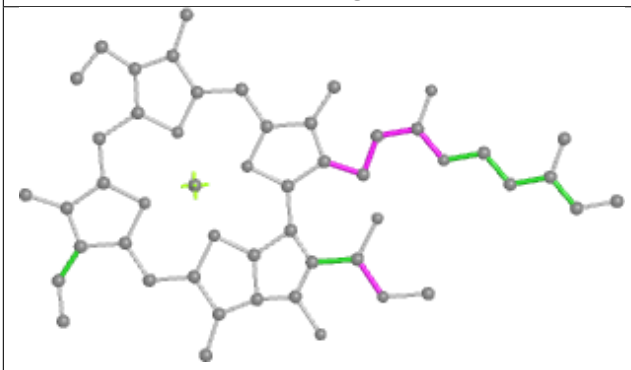
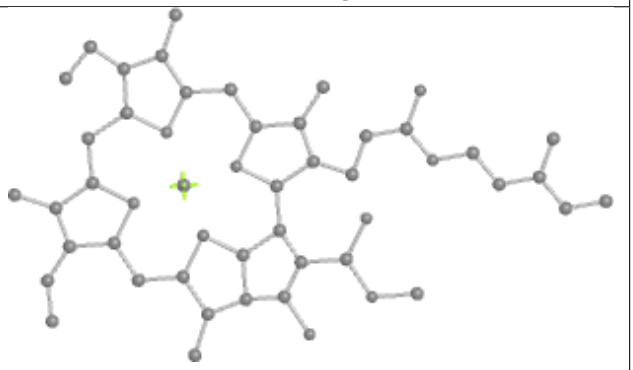


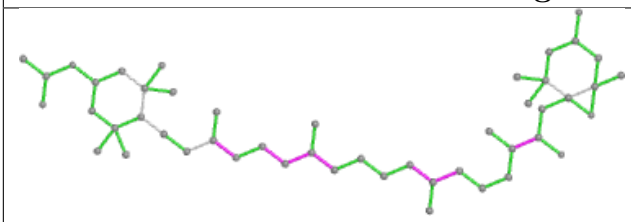
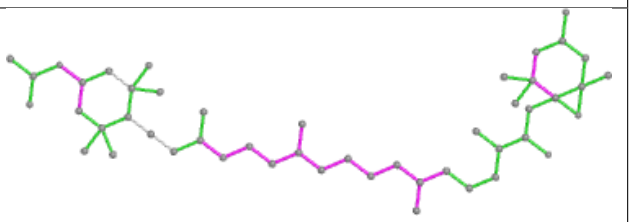
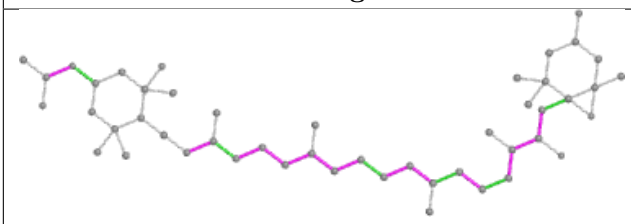
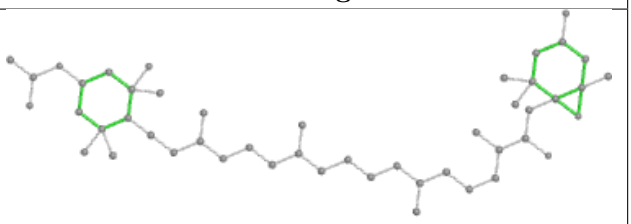
Torsions

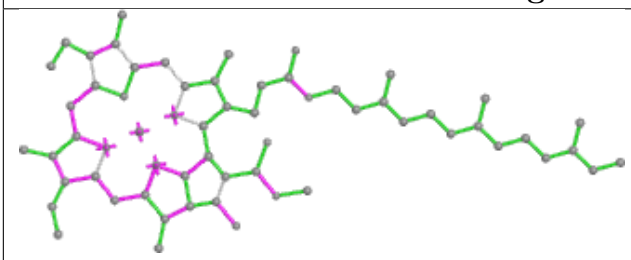
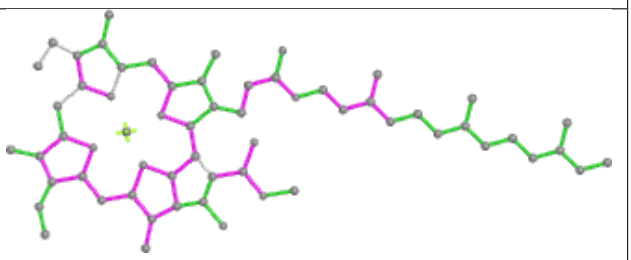
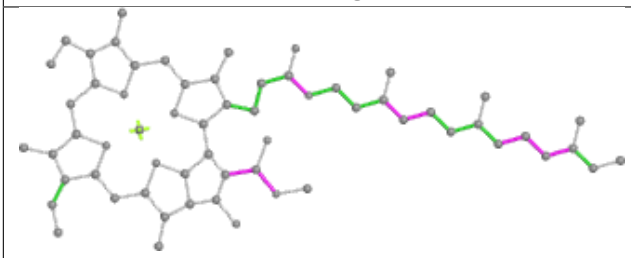
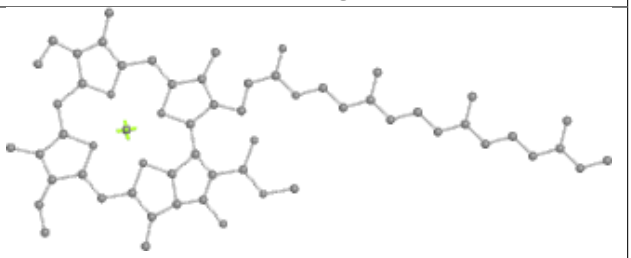


Rings

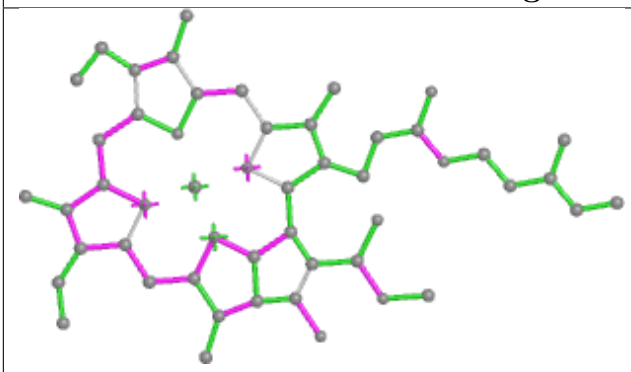
Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

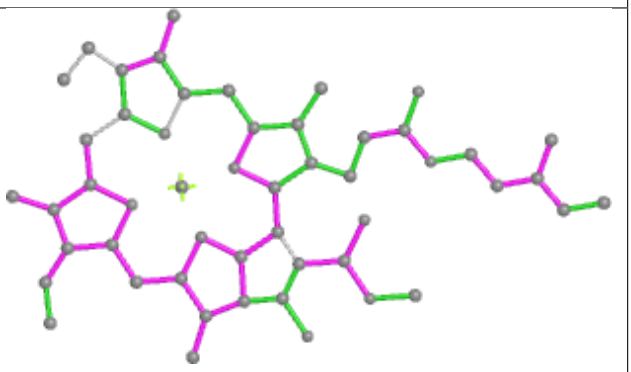
Ligand A86 6 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

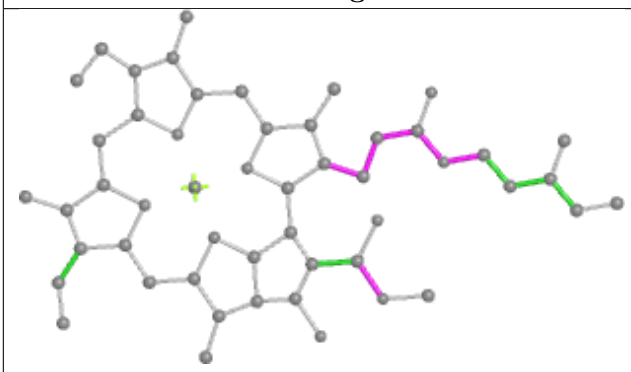
Ligand CLA G 303



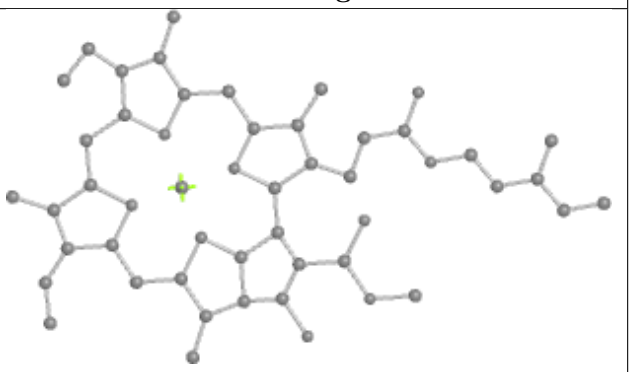
Bond lengths



Bond angles

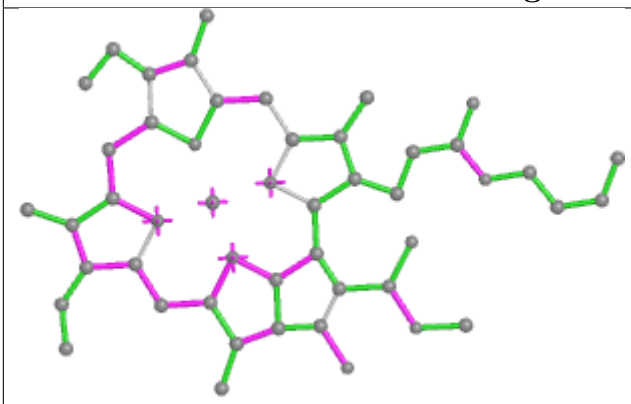


Torsions

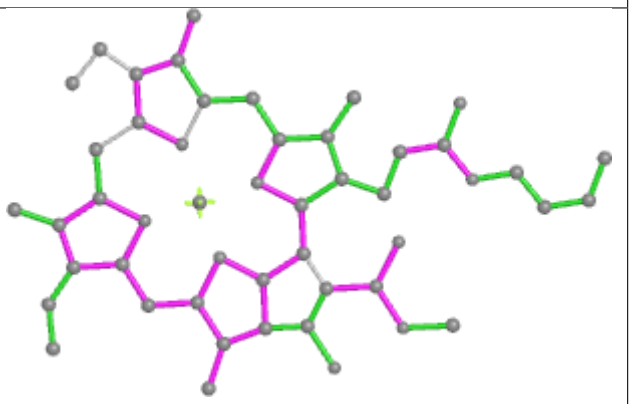


Rings

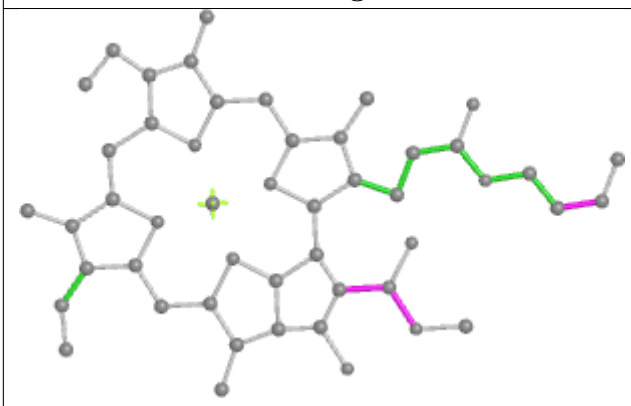
Ligand CLA A 402



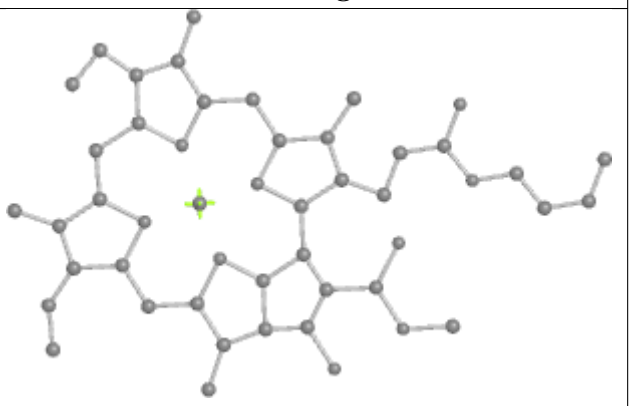
Bond lengths



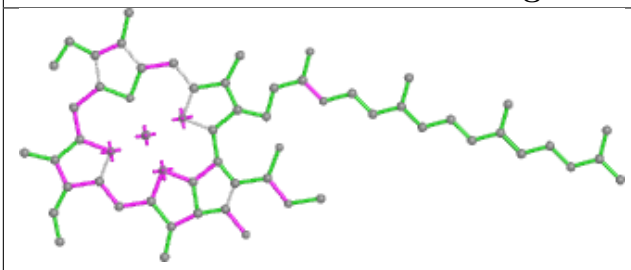
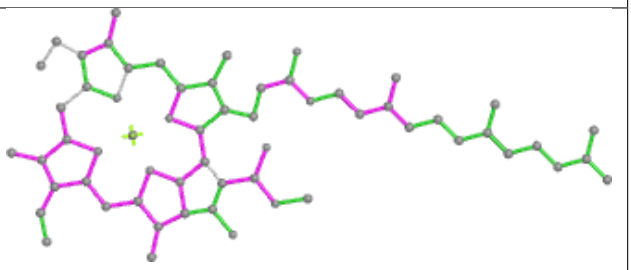
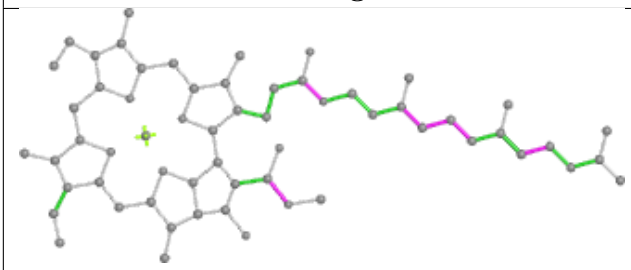
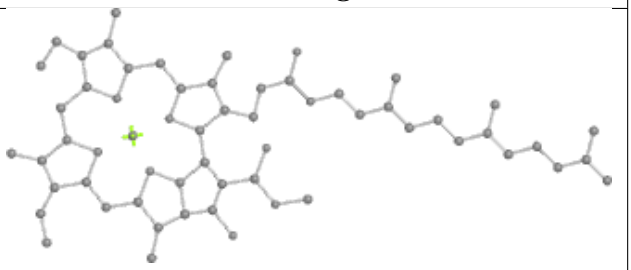
Bond angles

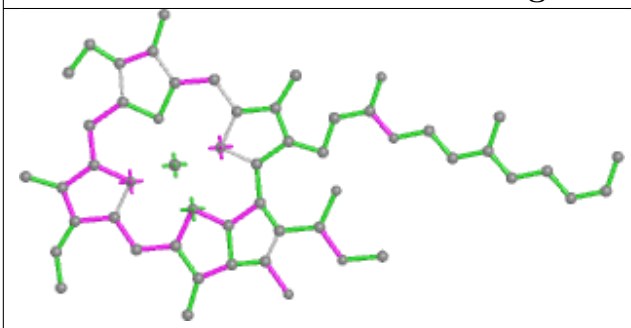
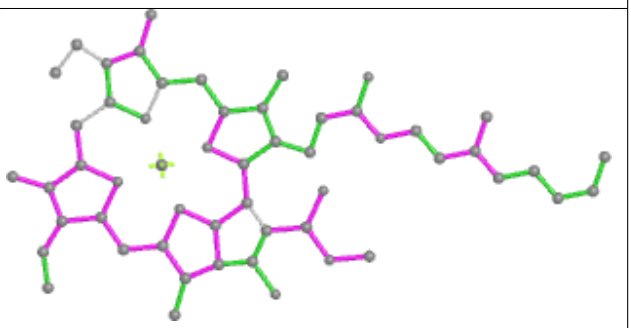
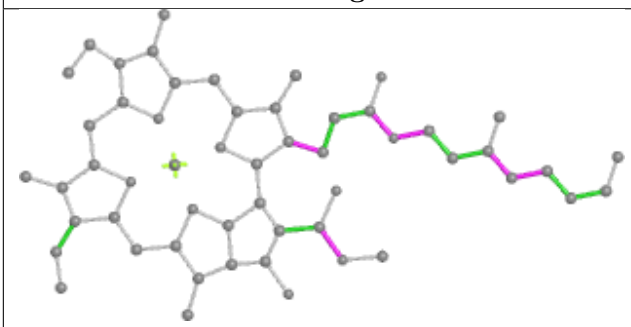
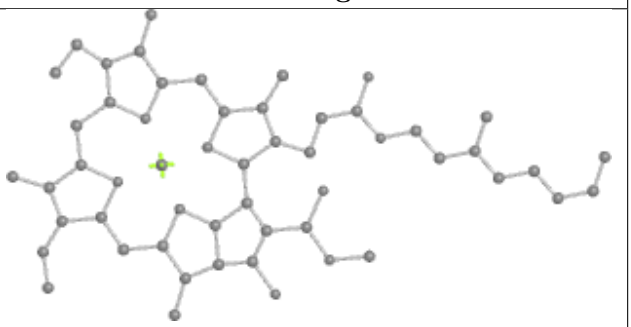


Torsions

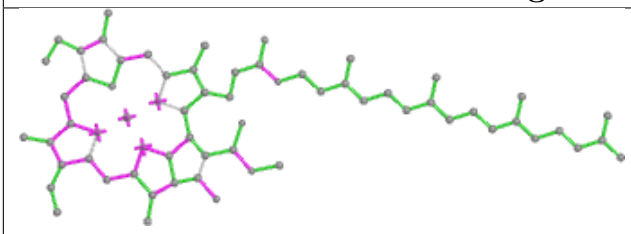


Rings

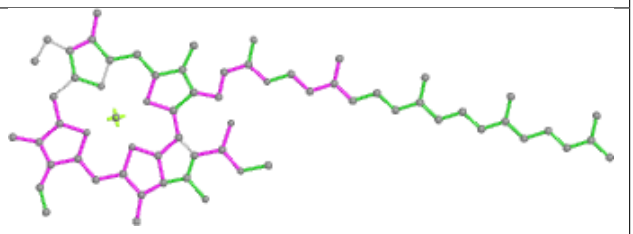
Ligand CLA D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

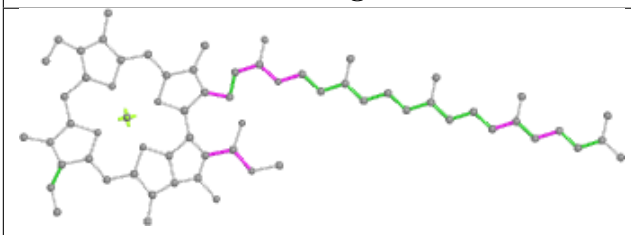
Ligand CLA J 306



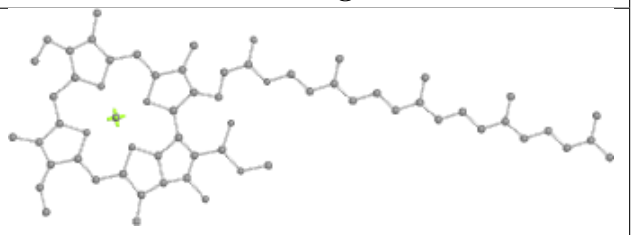
Bond lengths



Bond angles

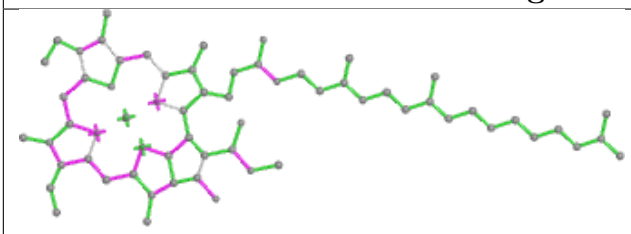


Torsions

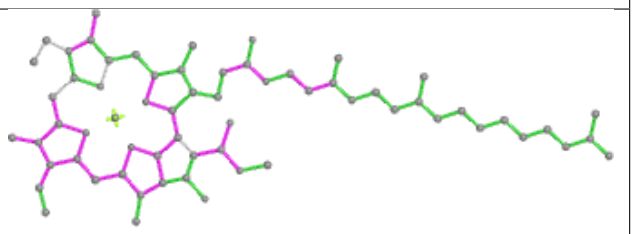


Rings

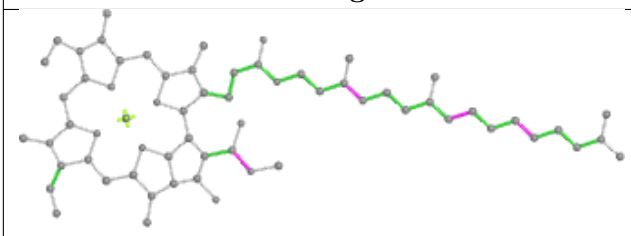
Ligand CLA b 612



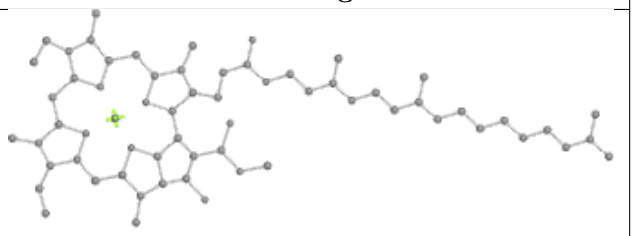
Bond lengths



Bond angles

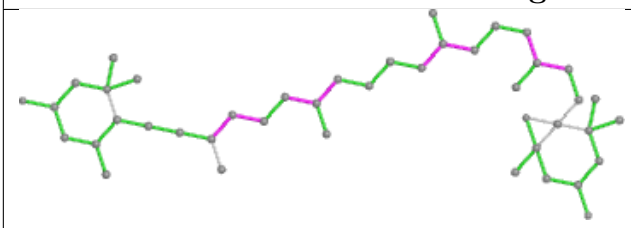


Torsions

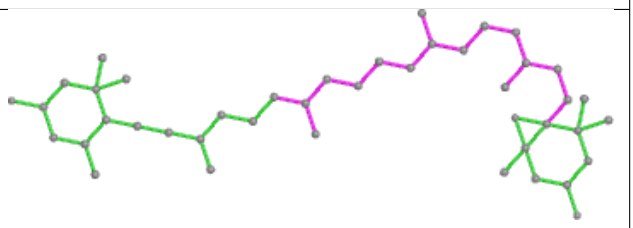


Rings

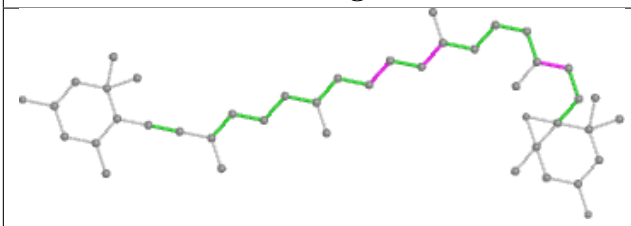
Ligand DD6 1 311



Bond lengths

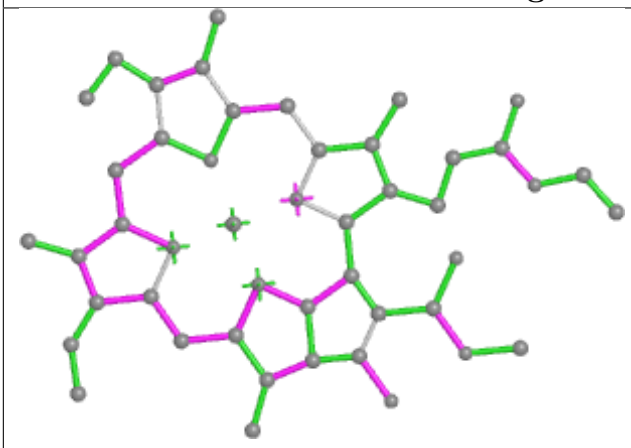
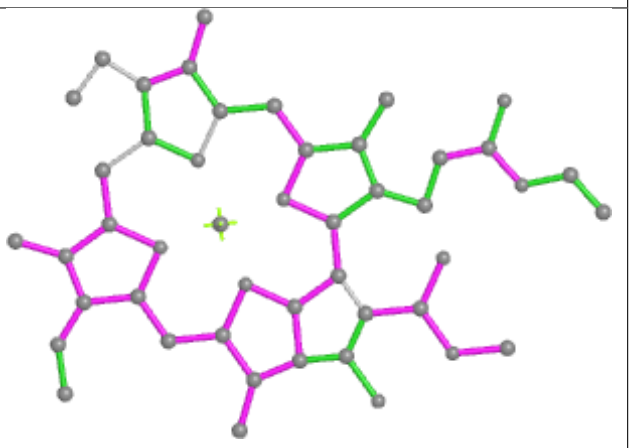
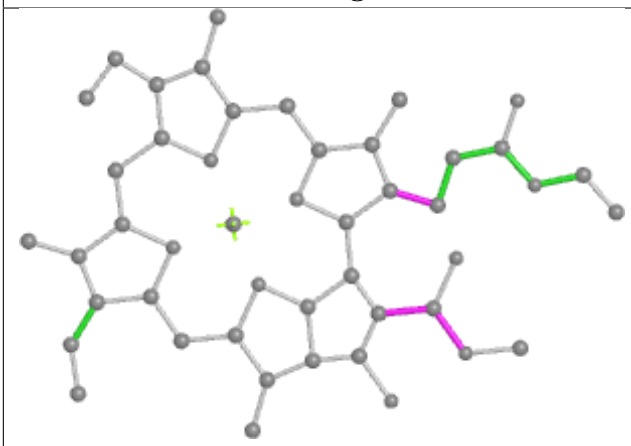
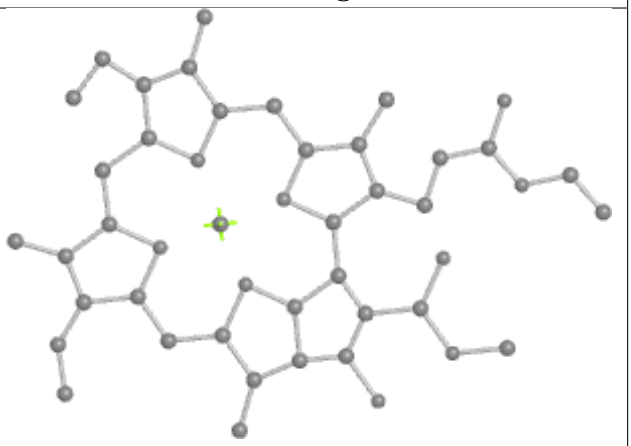


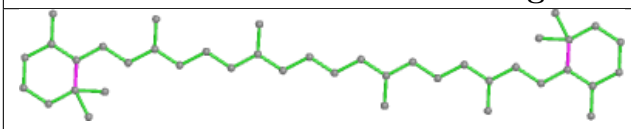
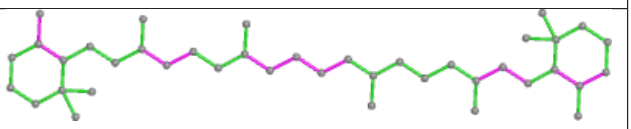
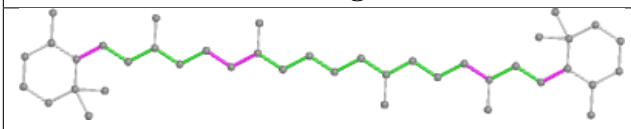
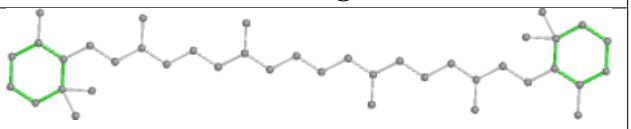
Bond angles



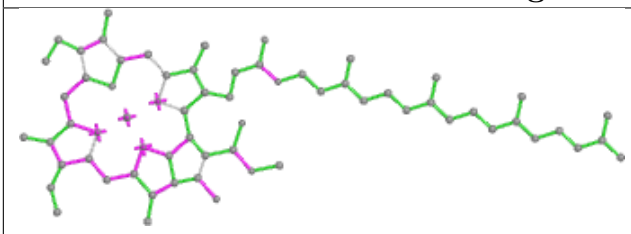
Torsions

Rings

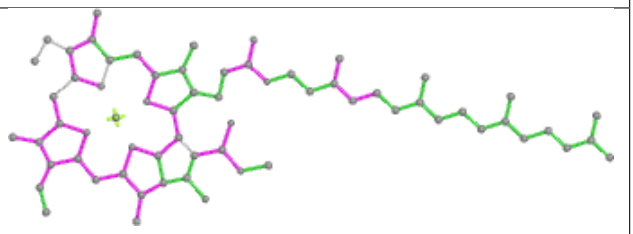
Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR c 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

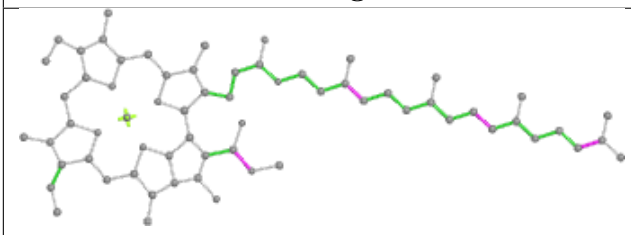
Ligand CLA b 616



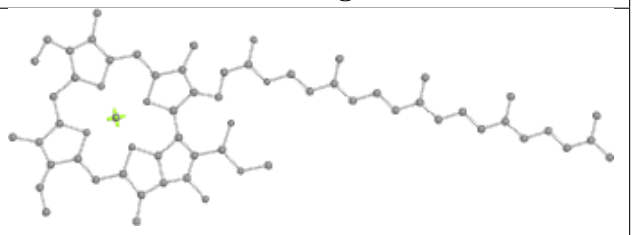
Bond lengths



Bond angles

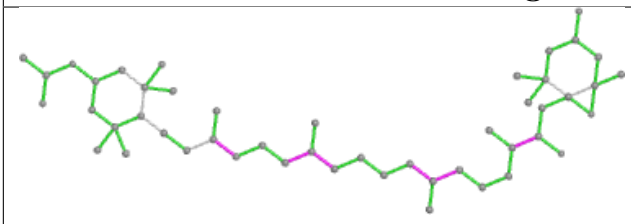


Torsions

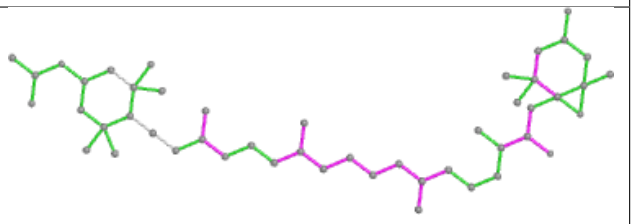


Rings

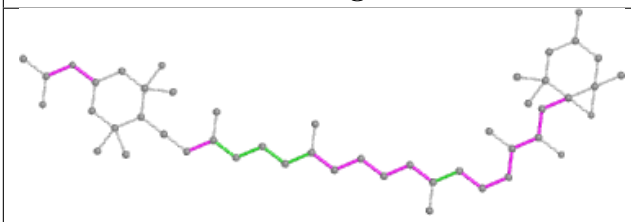
Ligand A86 W 101



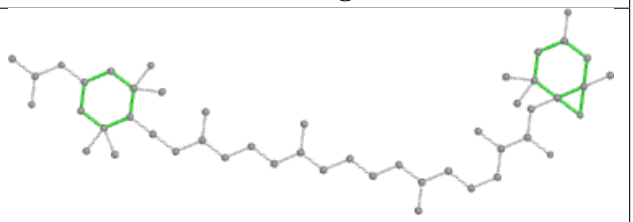
Bond lengths



Bond angles

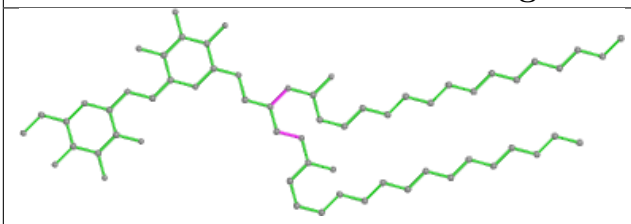


Torsions

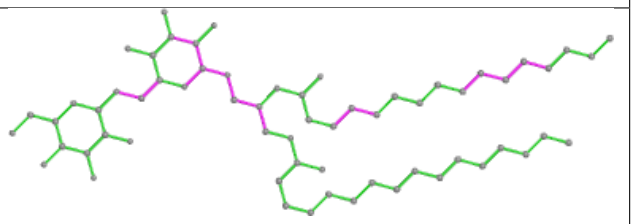


Rings

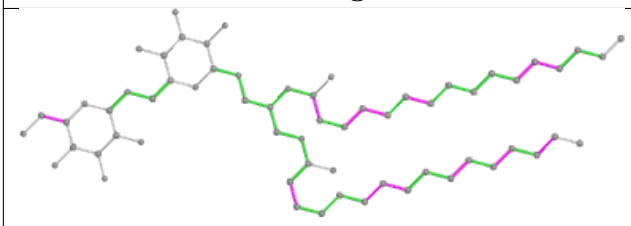
Ligand DGD H 101



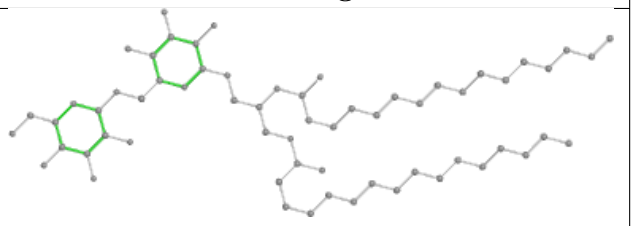
Bond lengths



Bond angles

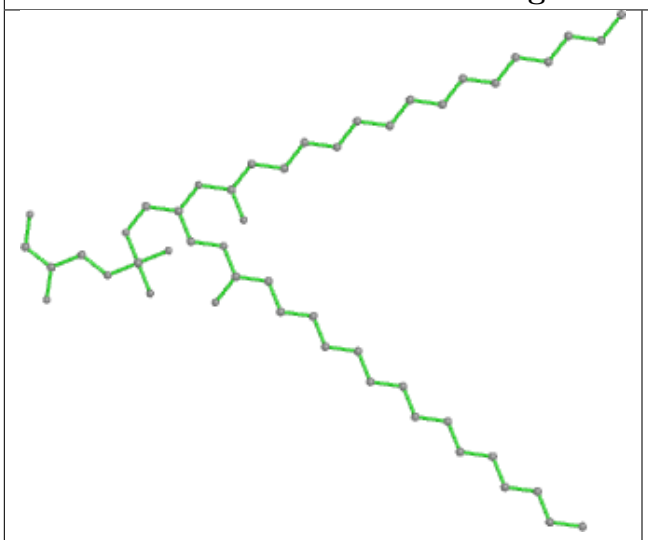


Torsions

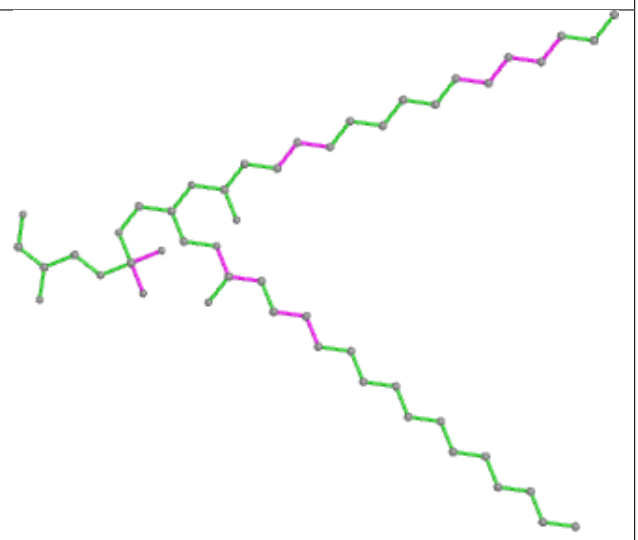


Rings

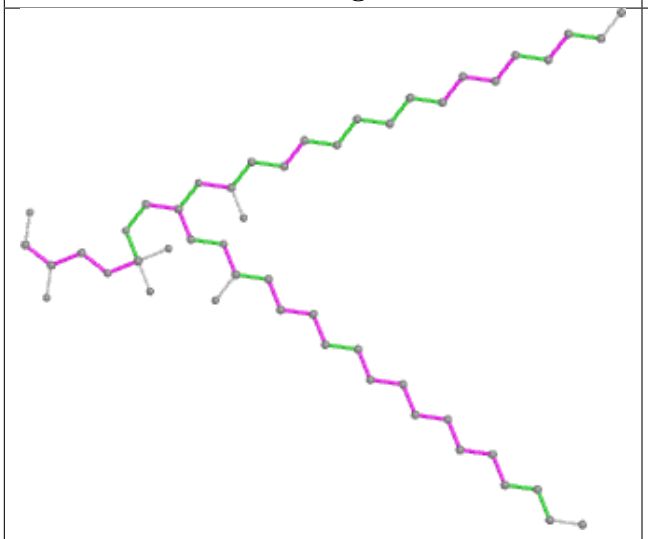
Ligand LHG a 401



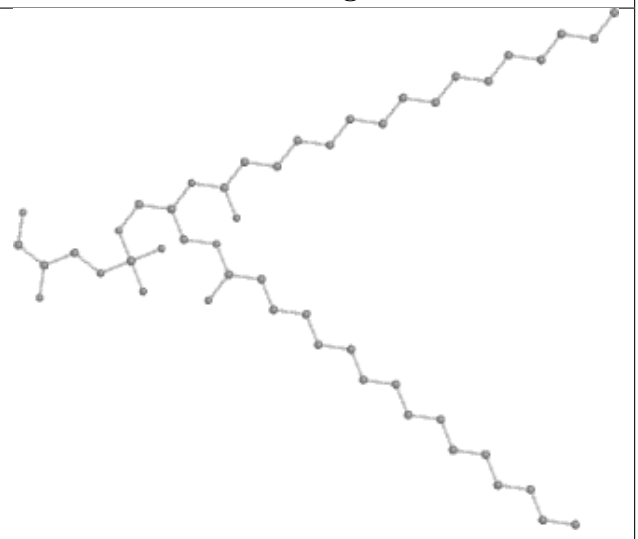
Bond lengths



Bond angles

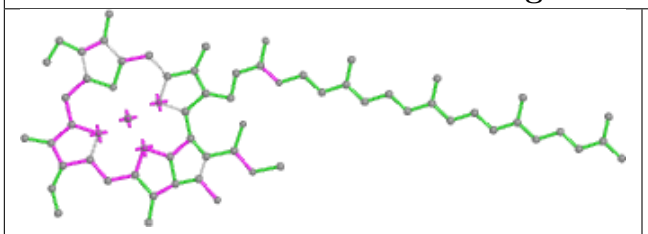


Torsions

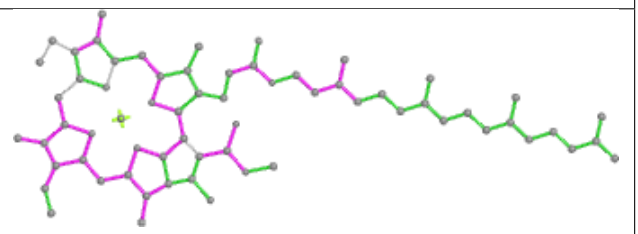


Rings

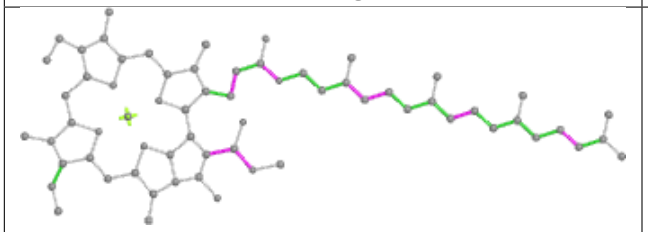
Ligand CLA C 505



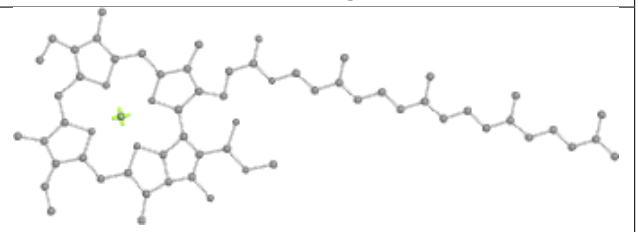
Bond lengths



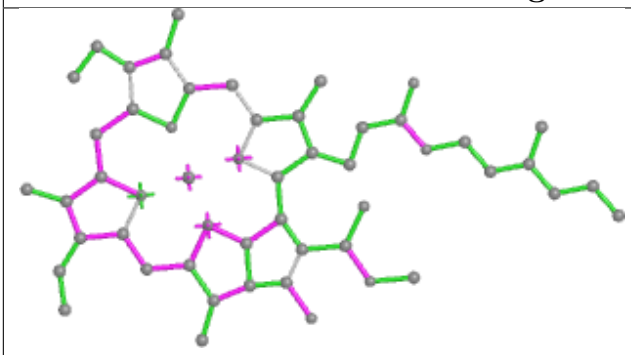
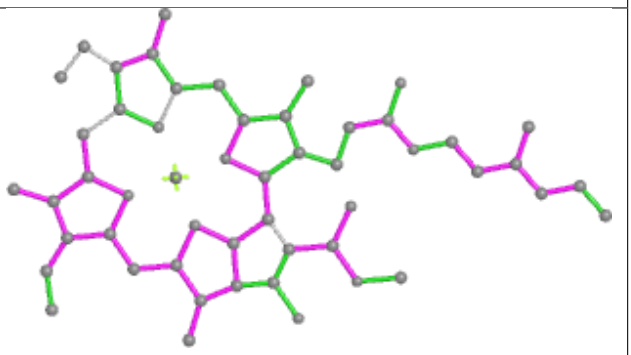
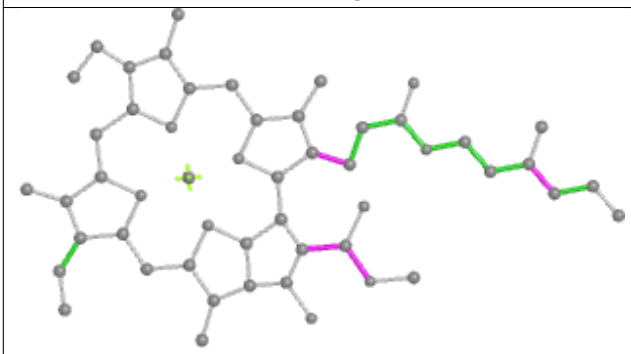
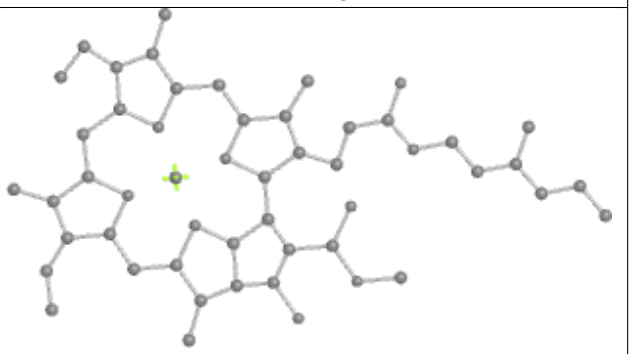
Bond angles

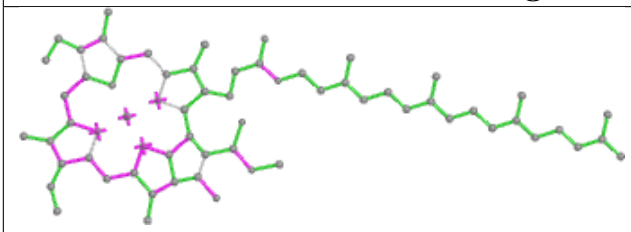
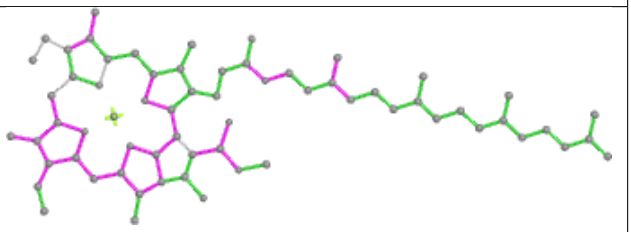
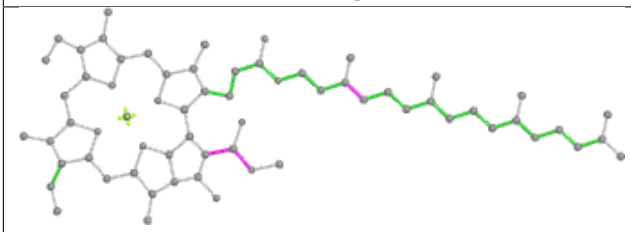
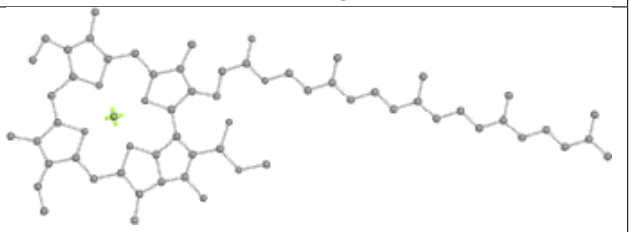


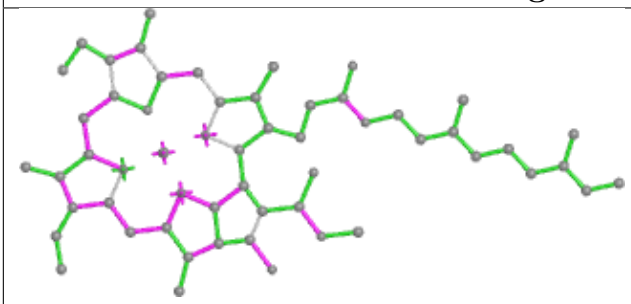
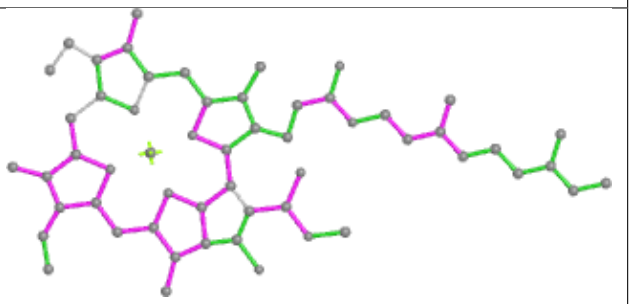
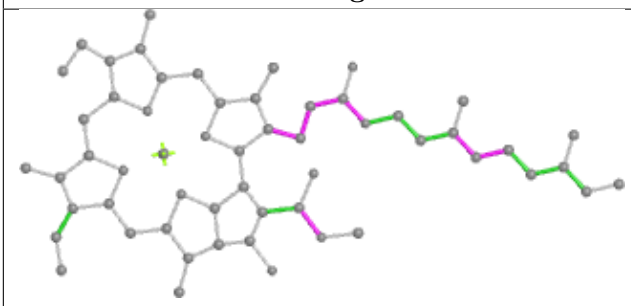
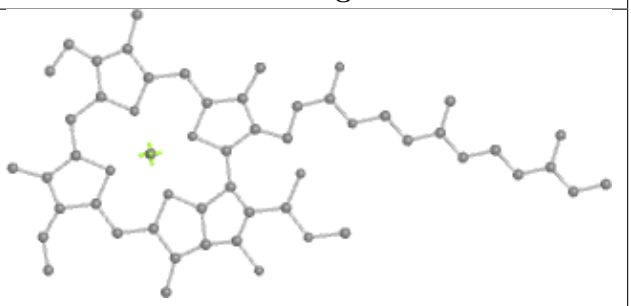
Torsions

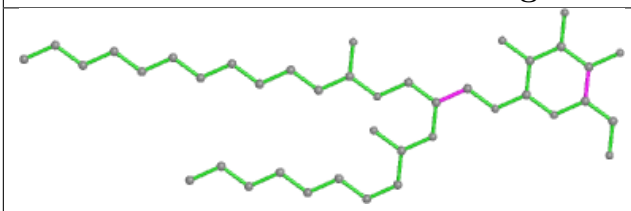
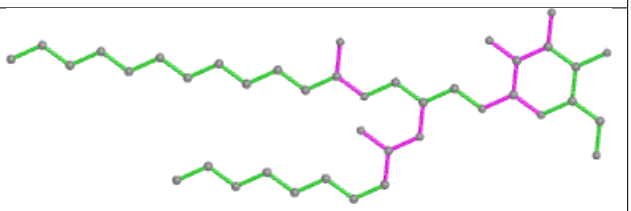
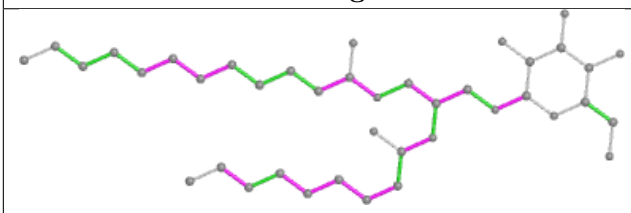
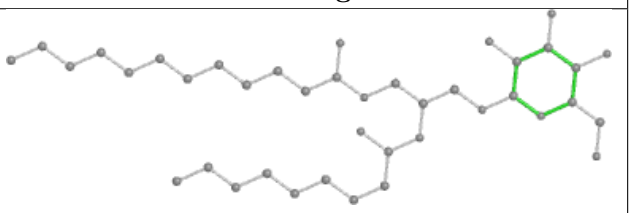


Rings

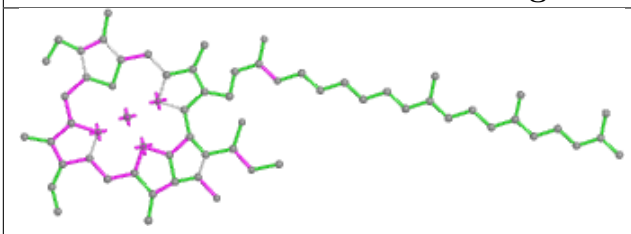
Ligand CLA J 300	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

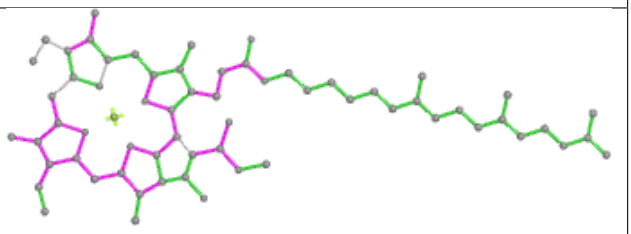
Ligand CLA 5 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG B 627	
 Bond lengths	 Bond angles
 Torsions	 Rings

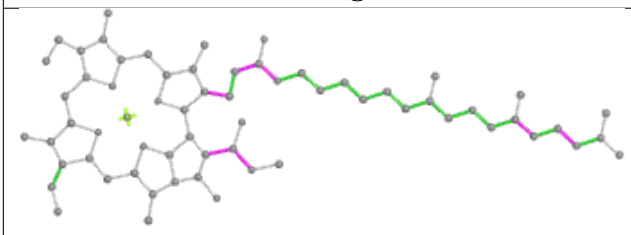
Ligand CLA c 513



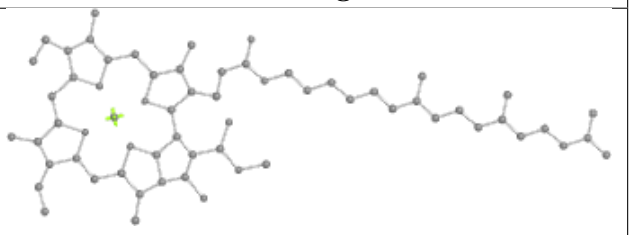
Bond lengths



Bond angles

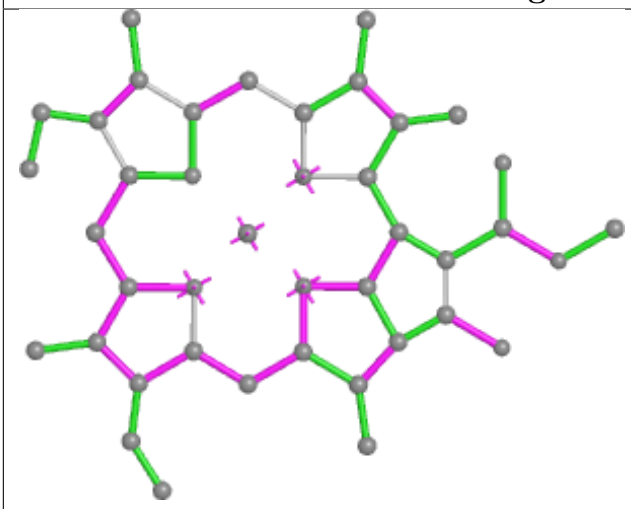


Torsions

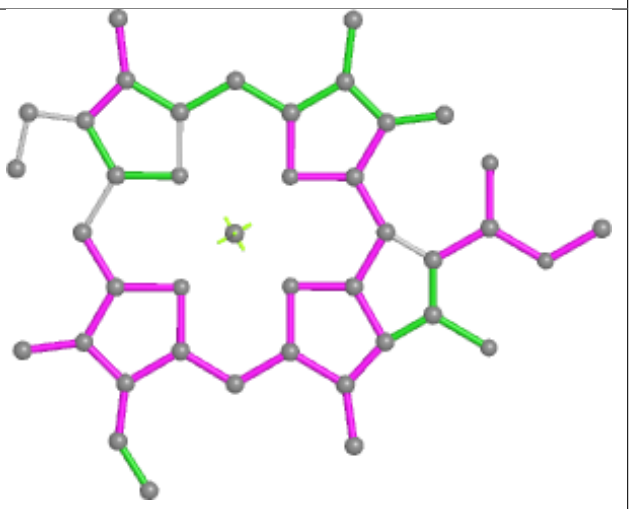


Rings

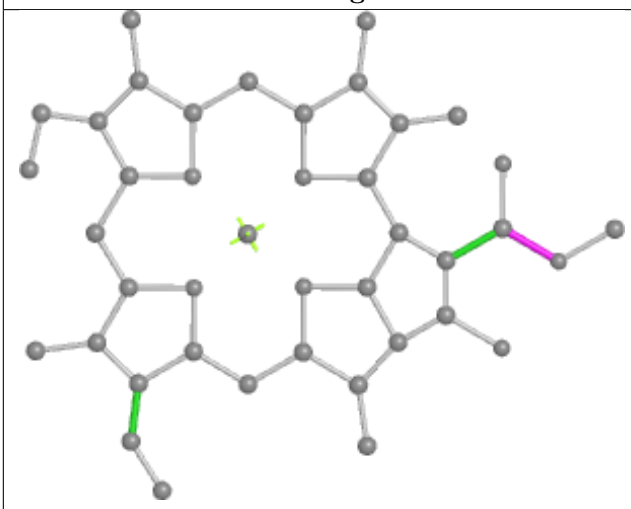
Ligand CLA 1 306



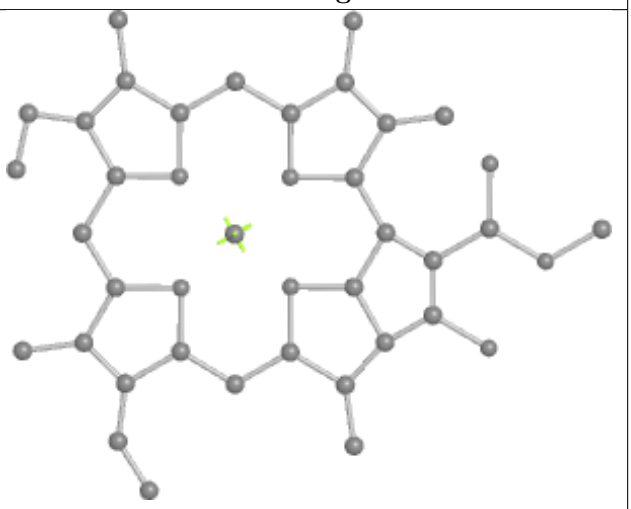
Bond lengths



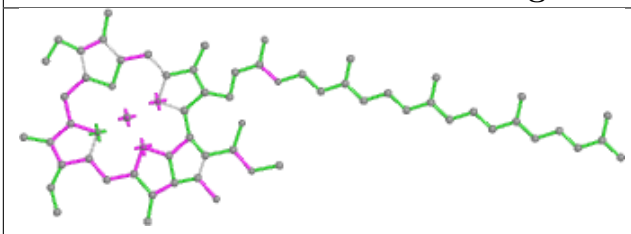
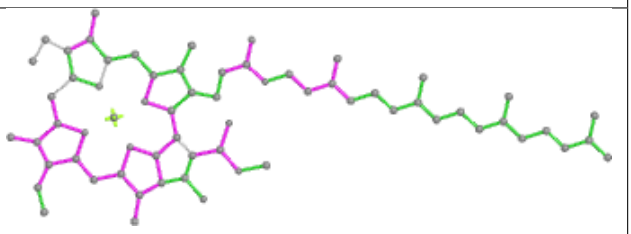
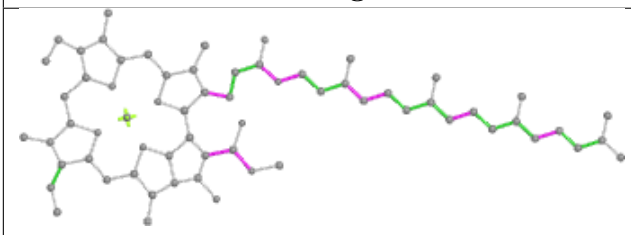
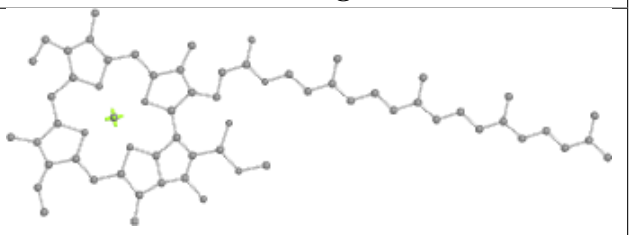
Bond angles

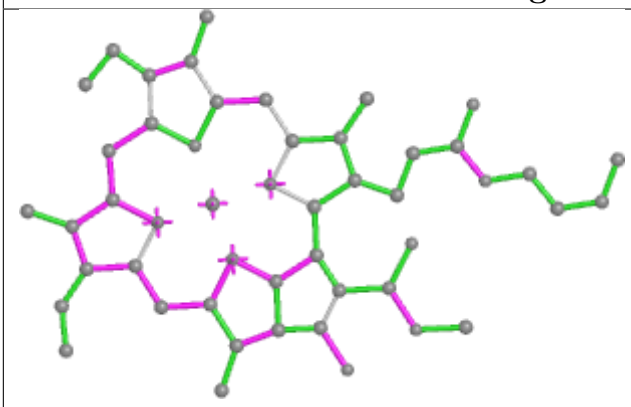
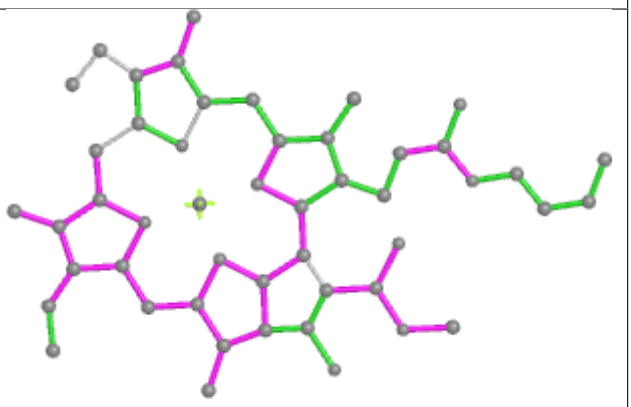
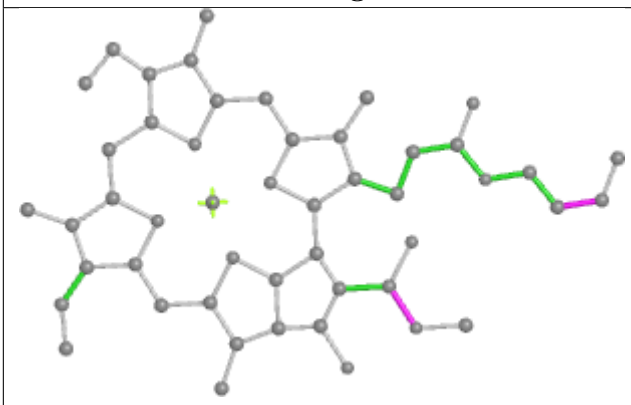
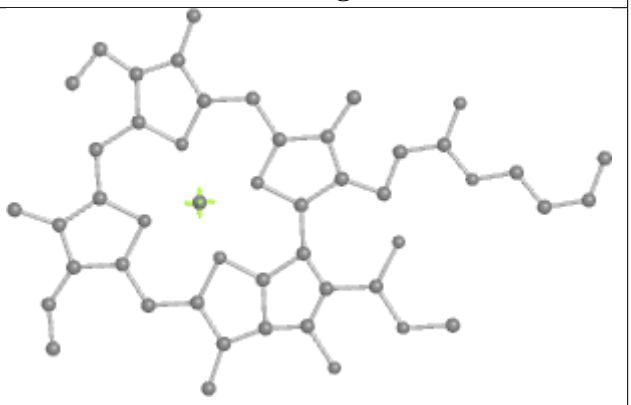


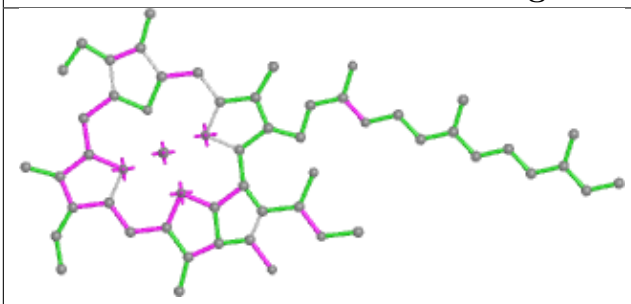
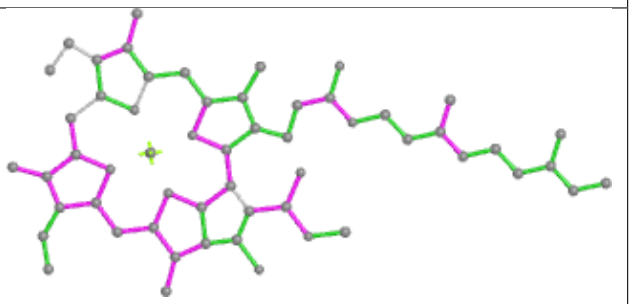
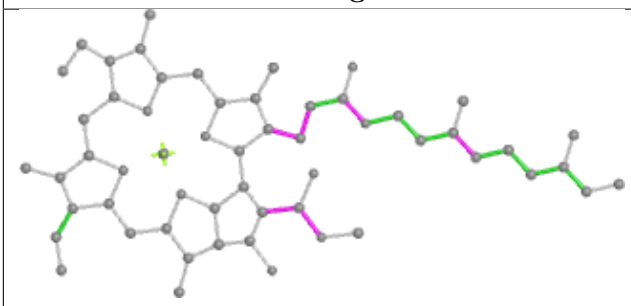
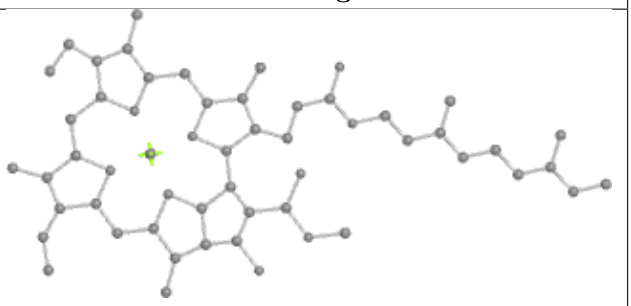
Torsions



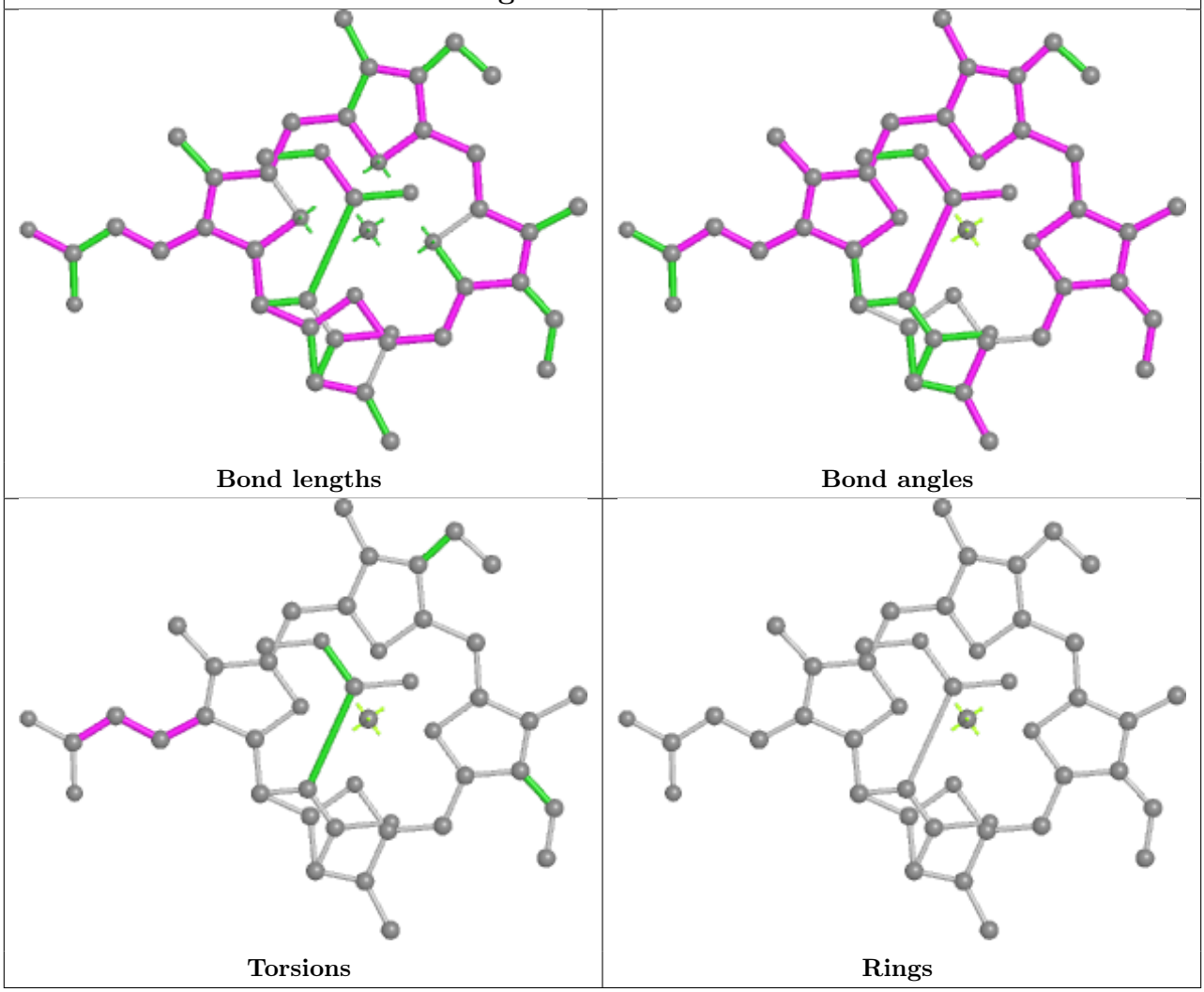
Rings

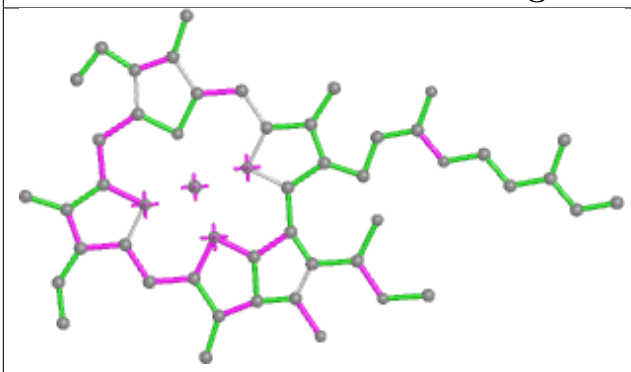
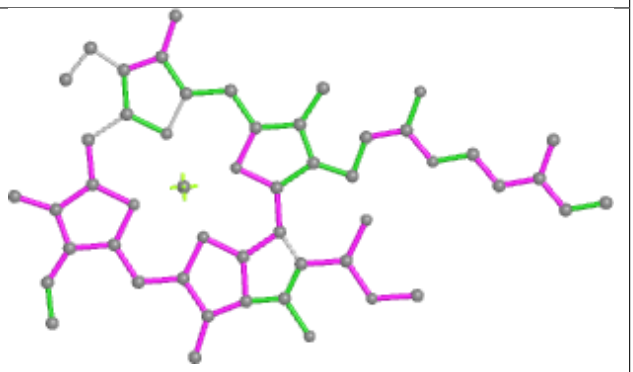
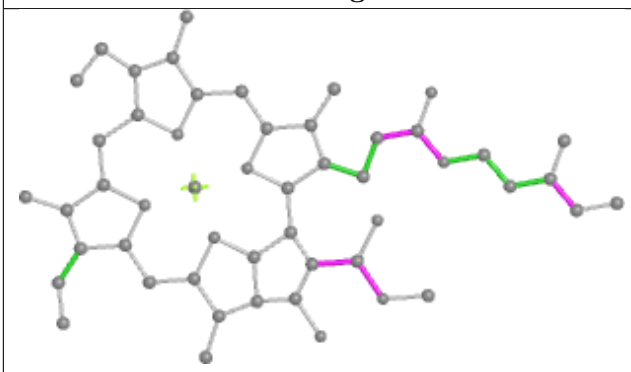
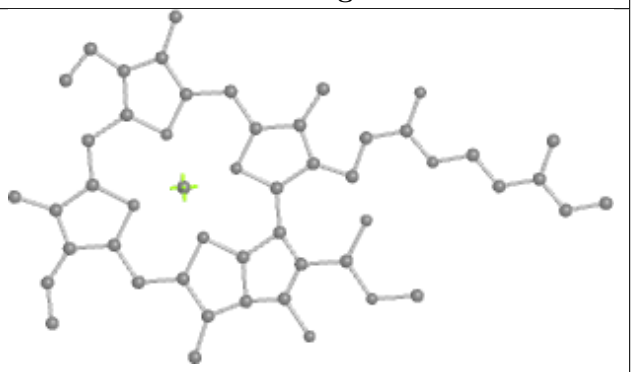
Ligand CLA 8 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

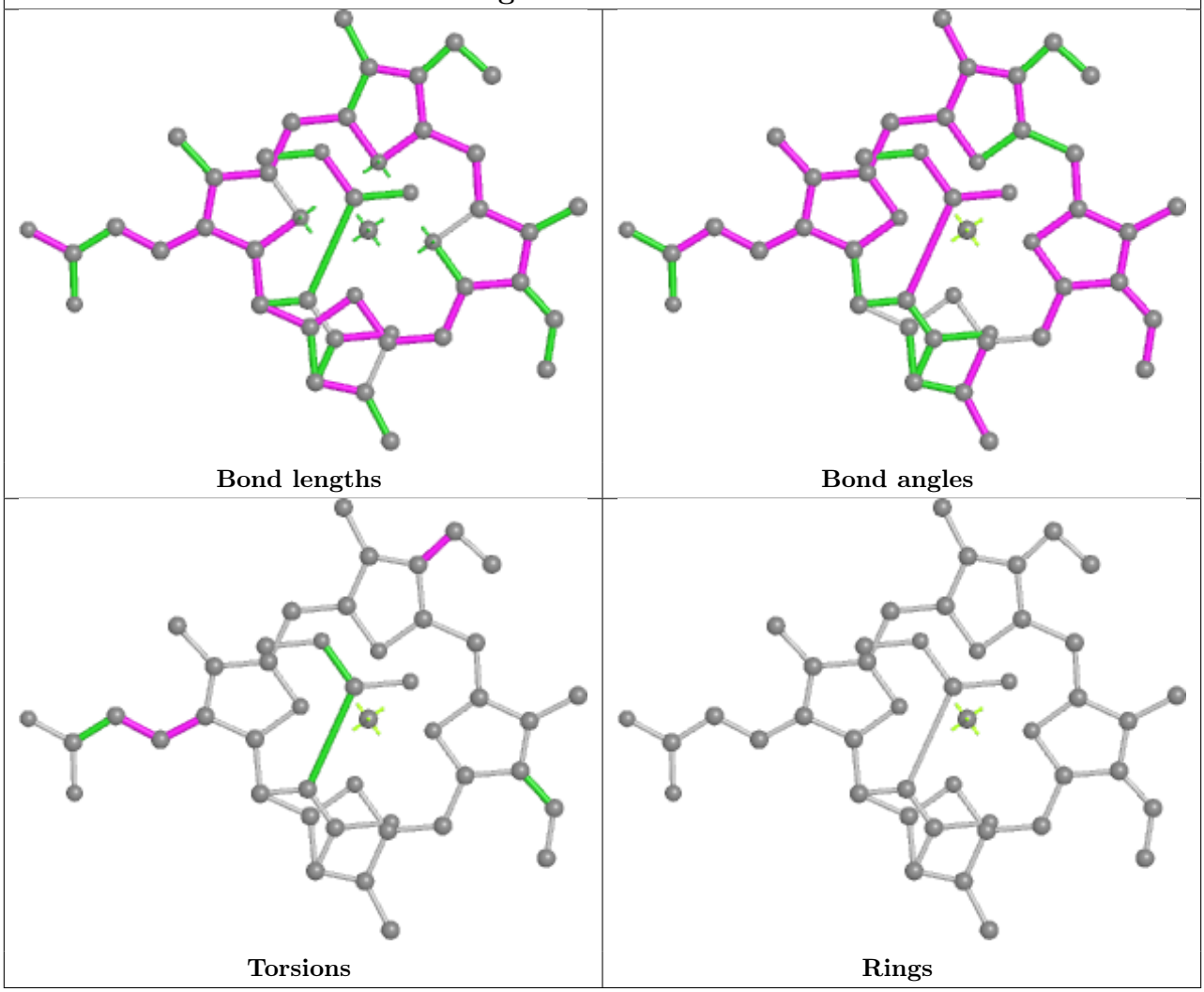
Ligand CLA 3 300	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 6 312

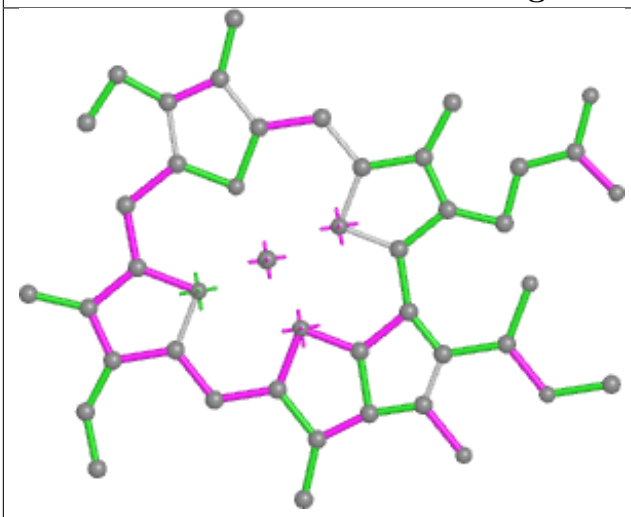


Ligand CLA 1 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

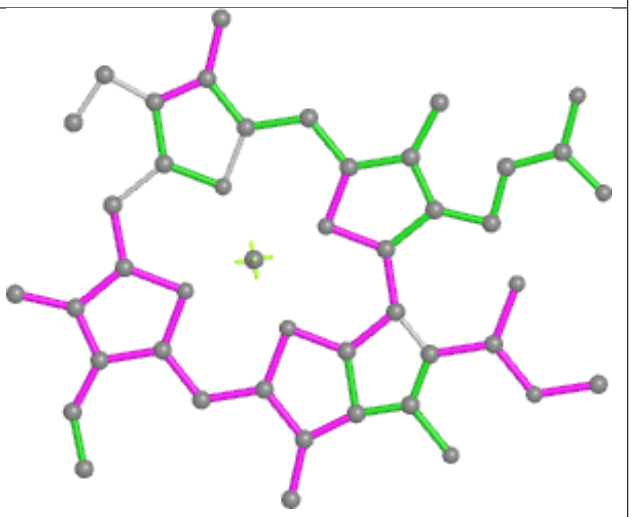
Ligand KC1 3 306



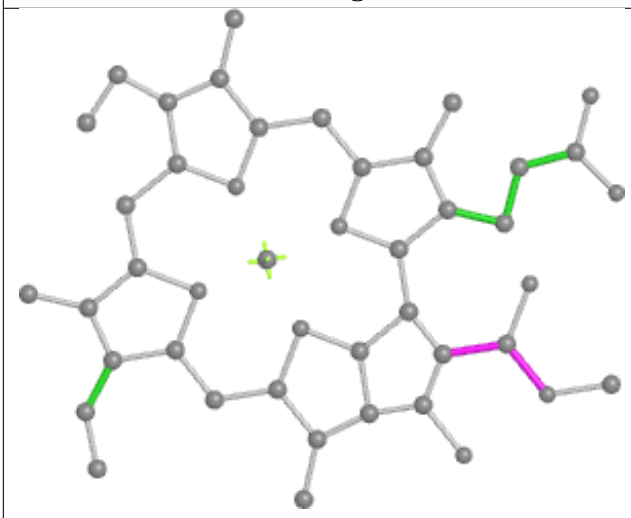
Ligand CLA J 302



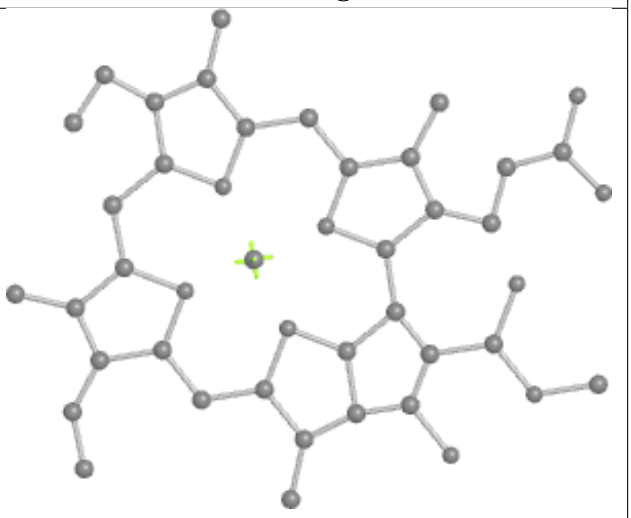
Bond lengths



Bond angles

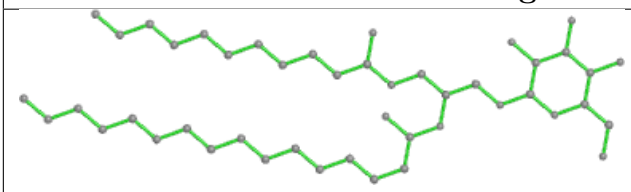


Torsions

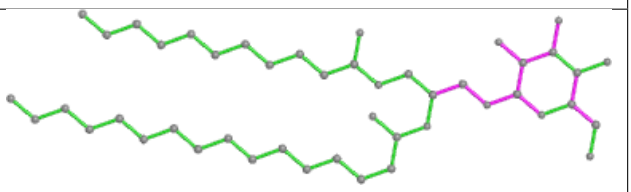


Rings

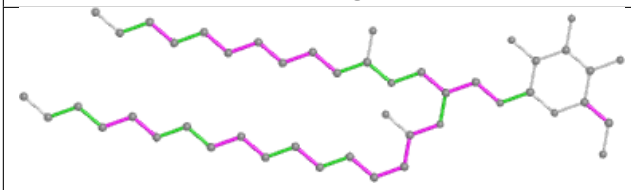
Ligand LMG D 411



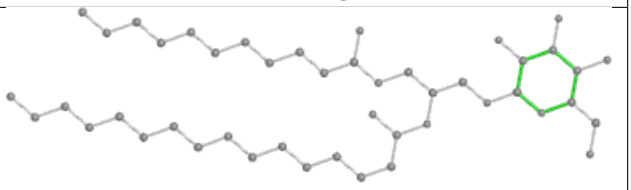
Bond lengths



Bond angles

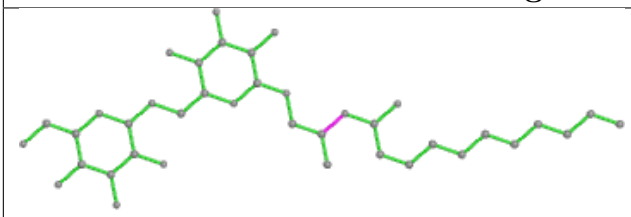


Torsions

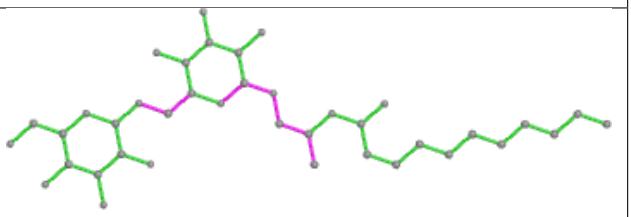


Rings

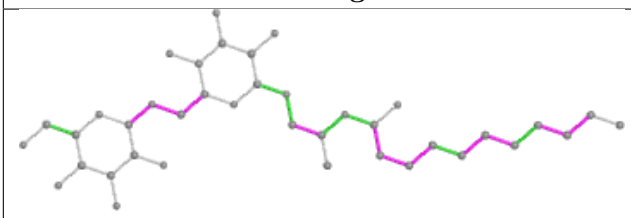
Ligand DGD c 517



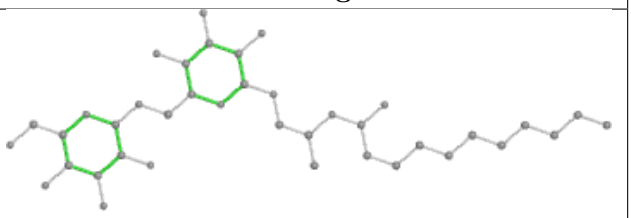
Bond lengths



Bond angles

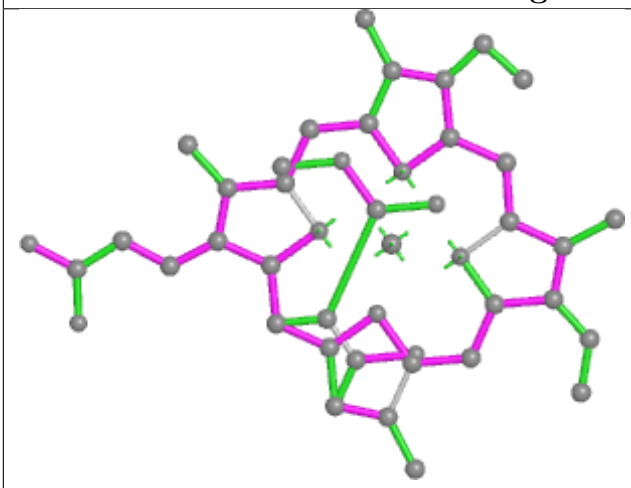


Torsions

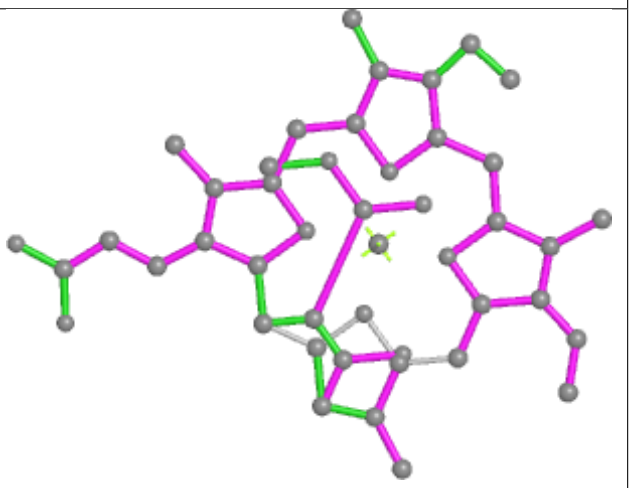


Rings

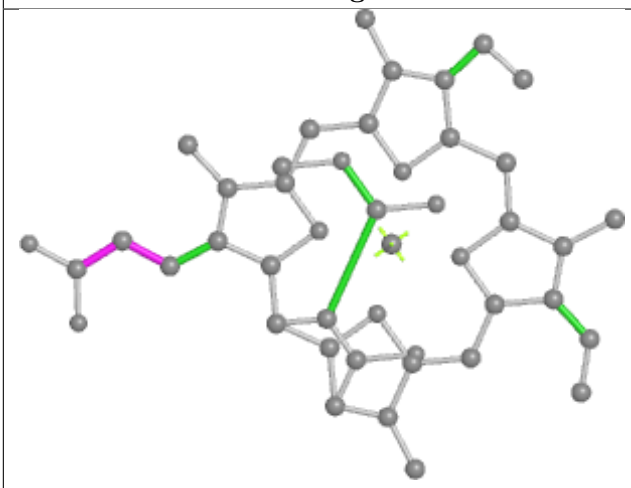
Ligand KC1 8 313



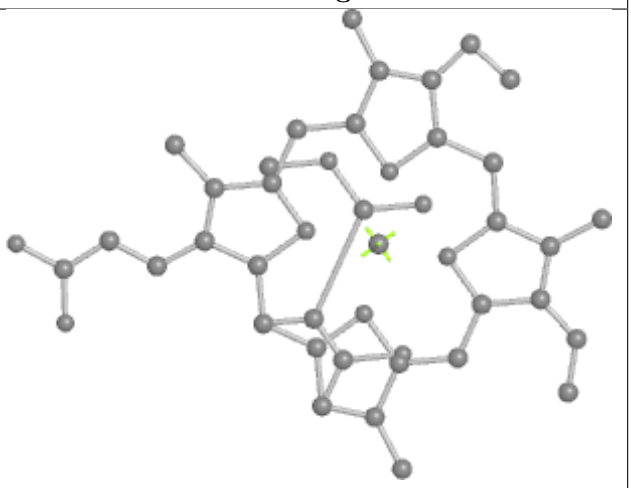
Bond lengths



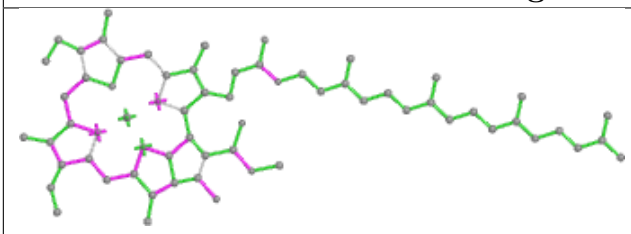
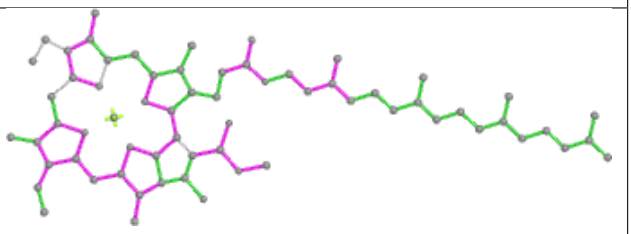
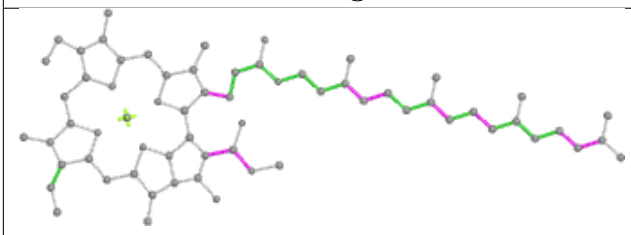
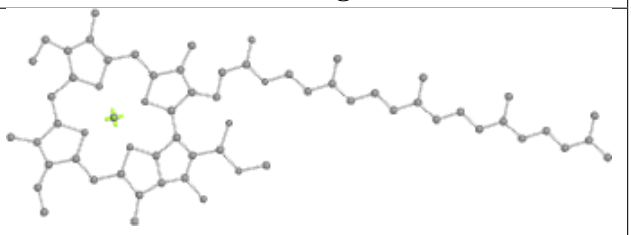
Bond angles

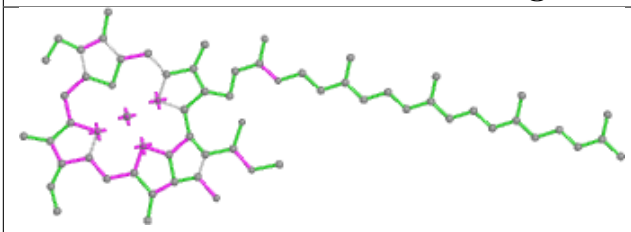
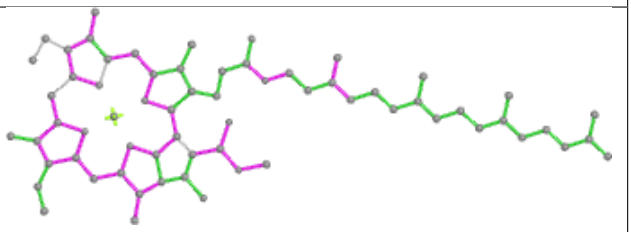
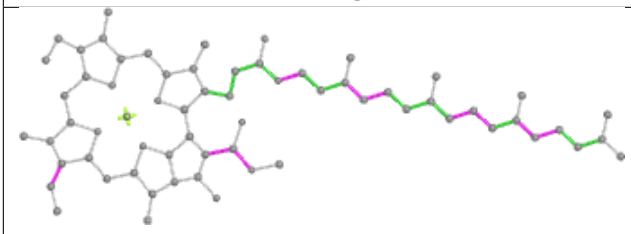
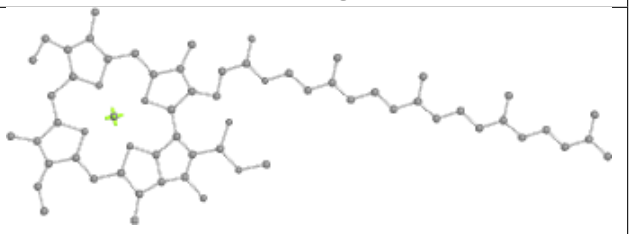


Torsions

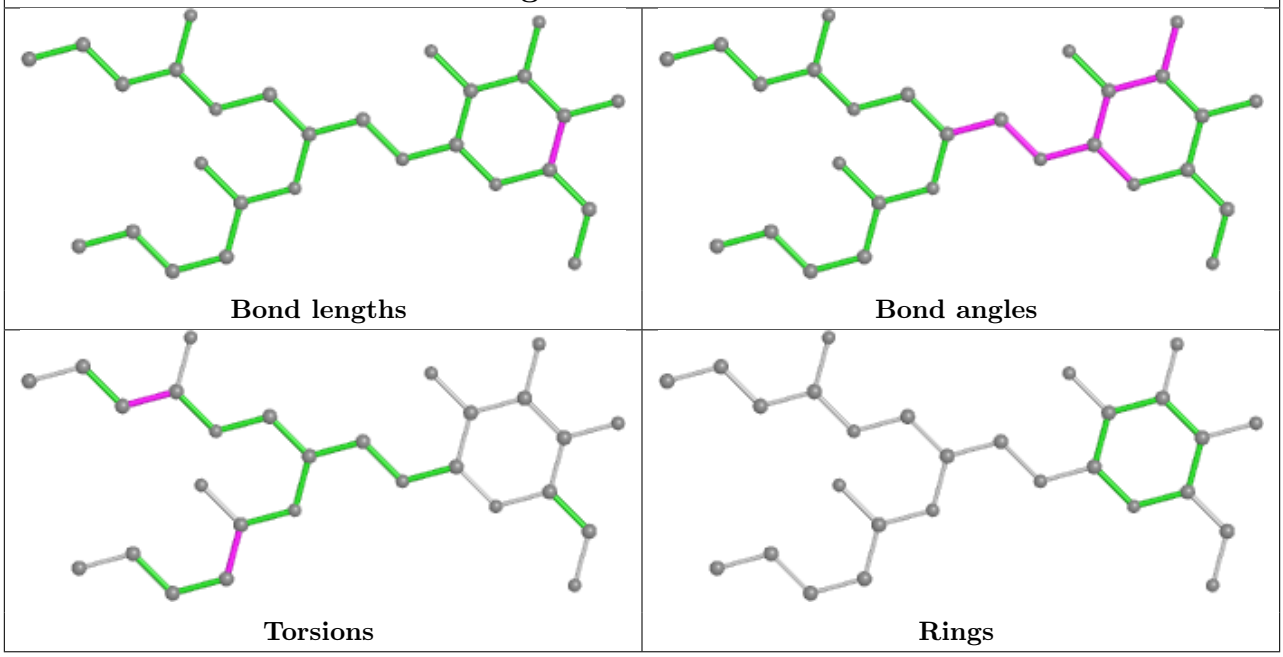


Rings

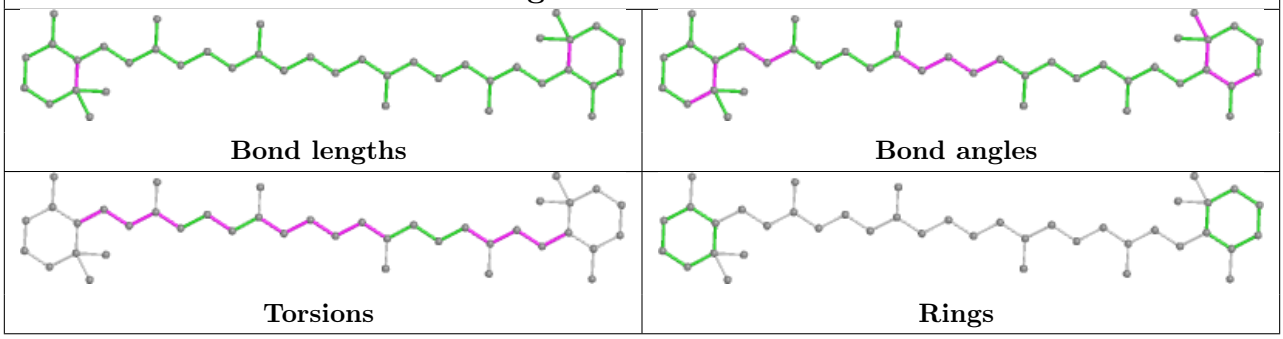
Ligand CLA b 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

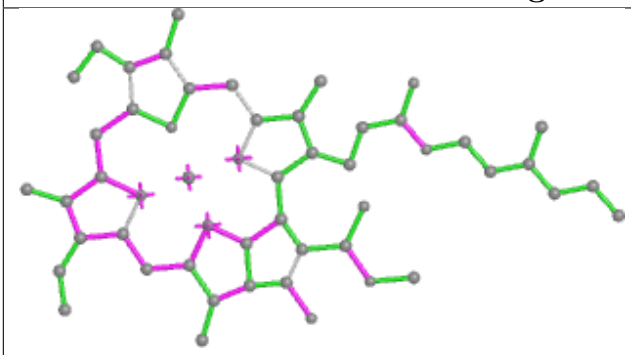
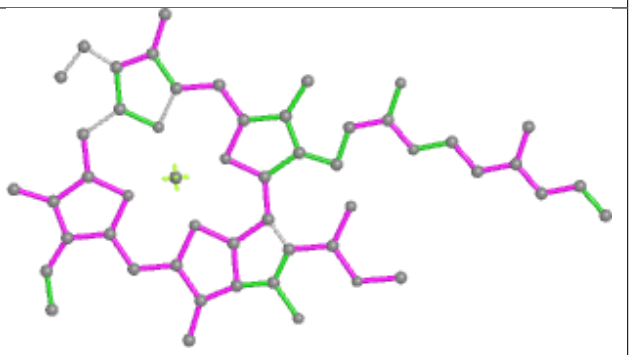
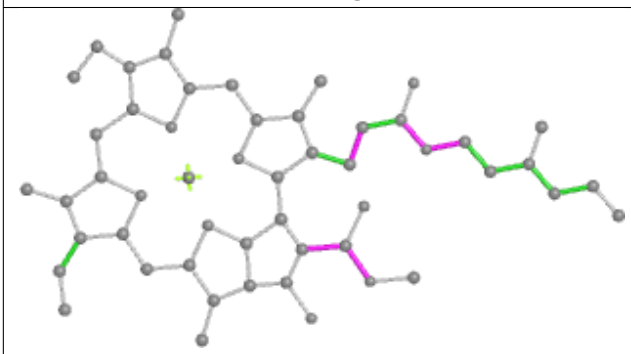
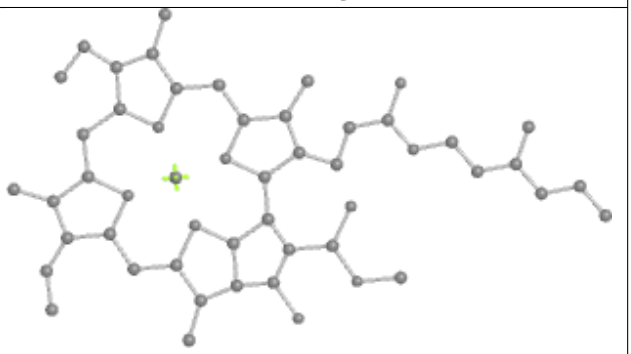
Ligand CLA 5 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

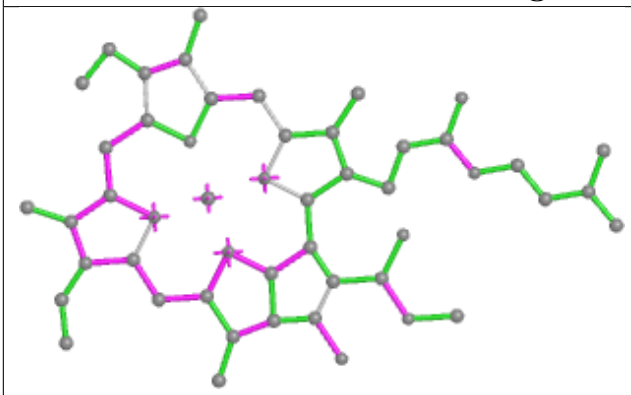
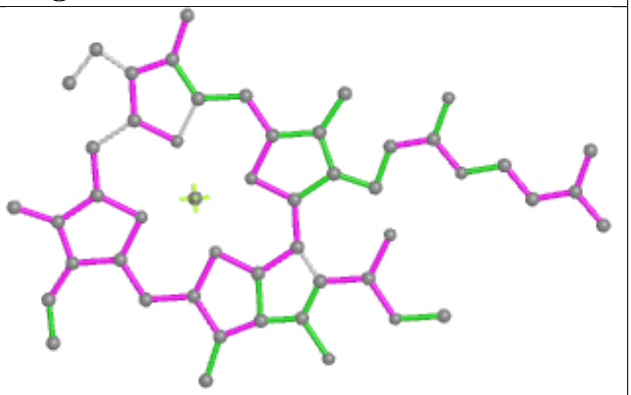
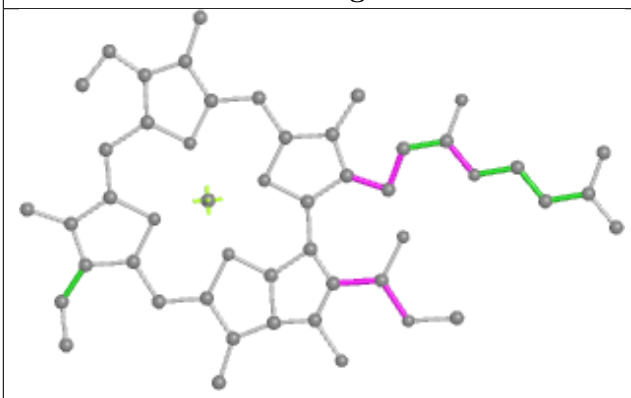
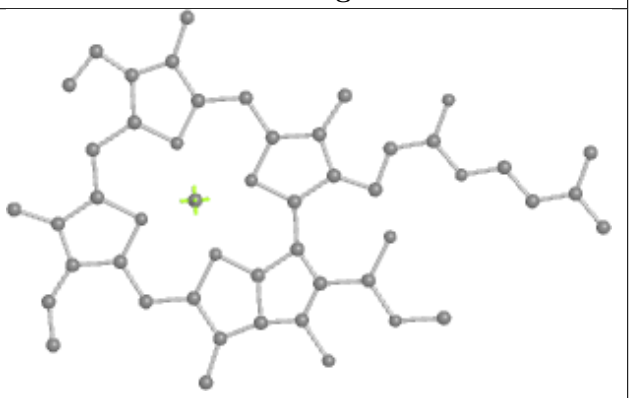
Ligand LMG B 620

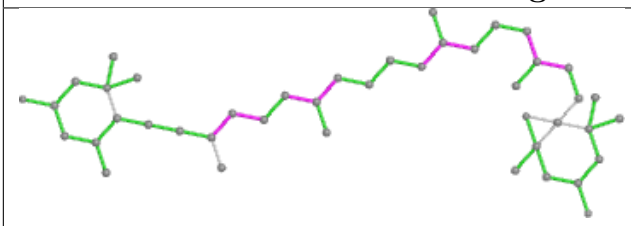
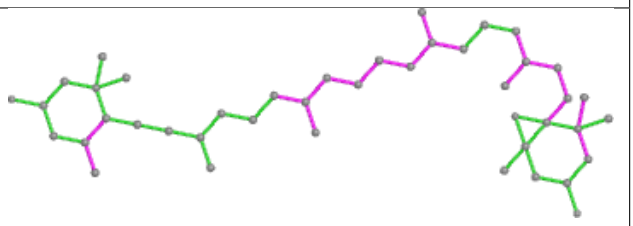
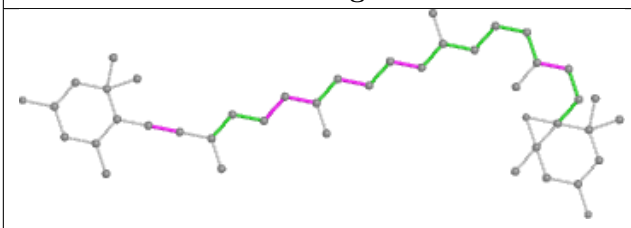
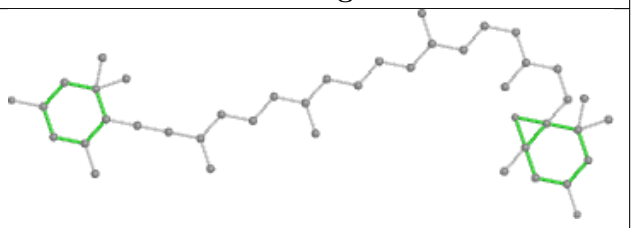


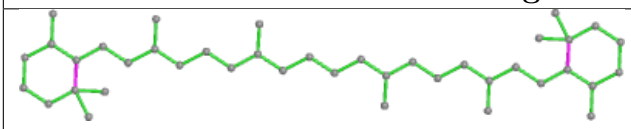
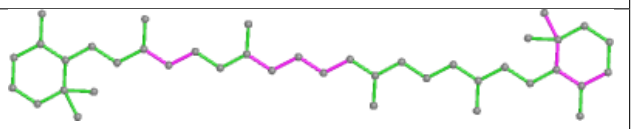
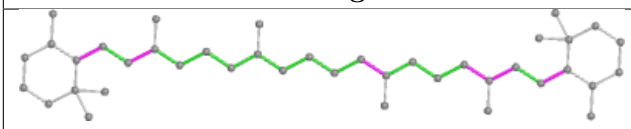
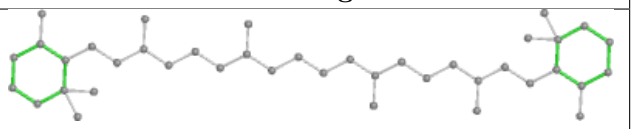
Ligand BCR 1 317



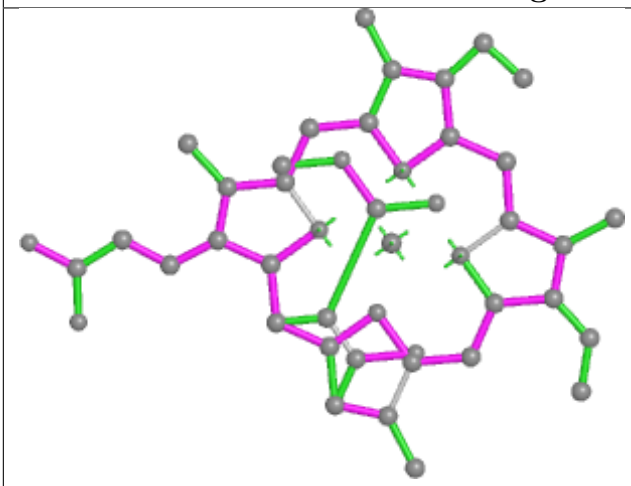
Ligand CLA J 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

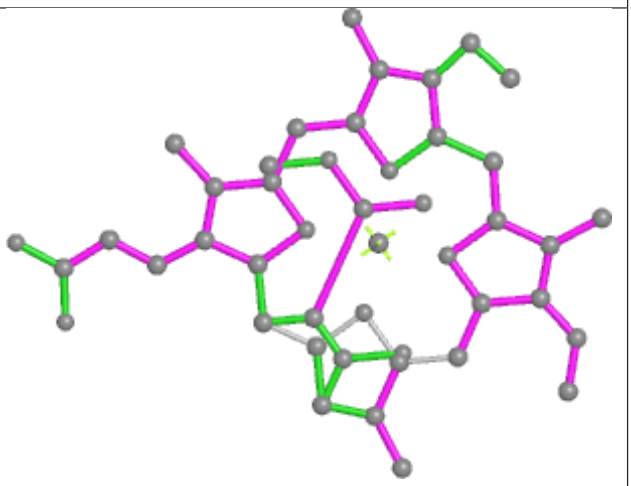
Ligand DD6 5 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

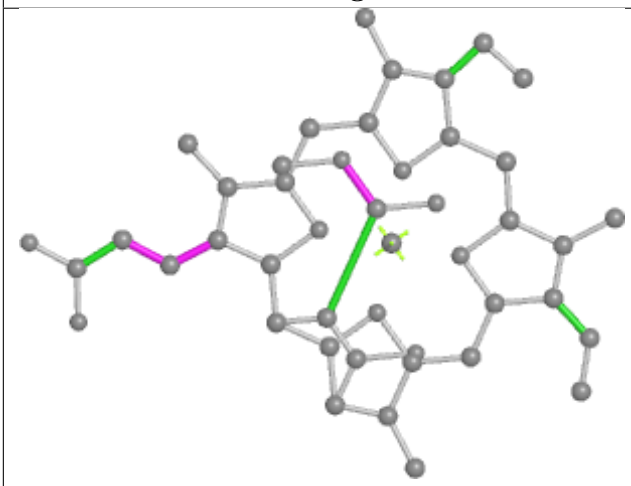
Ligand KC1 2 316



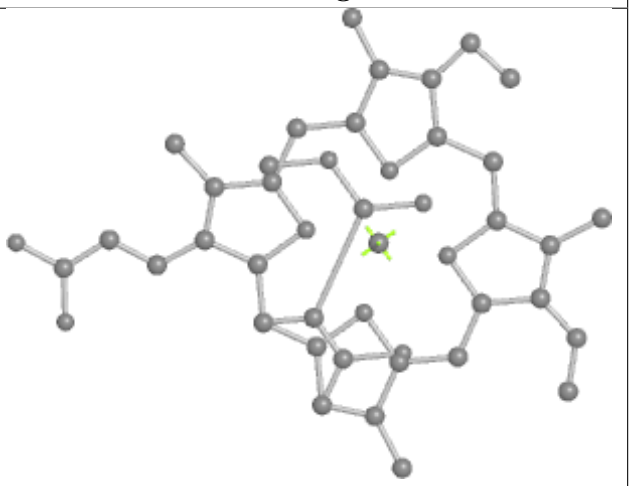
Bond lengths



Bond angles

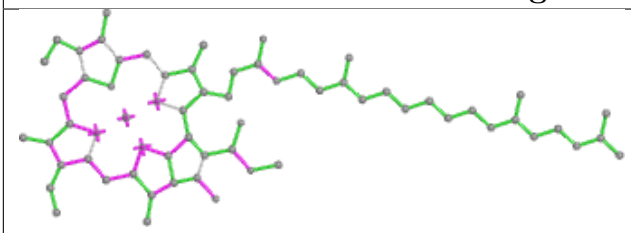


Torsions

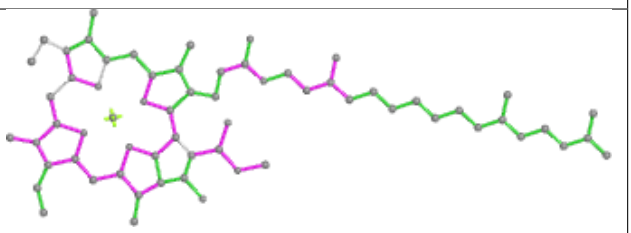


Rings

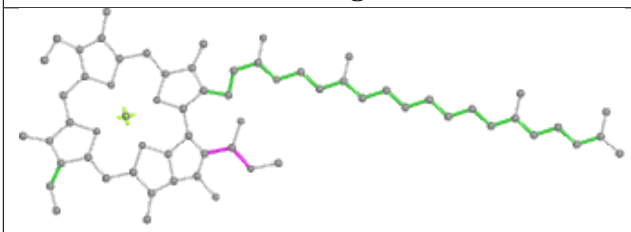
Ligand CLA c 503



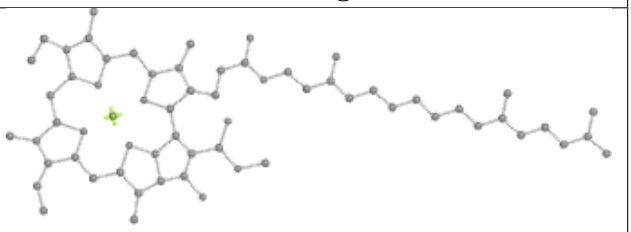
Bond lengths



Bond angles

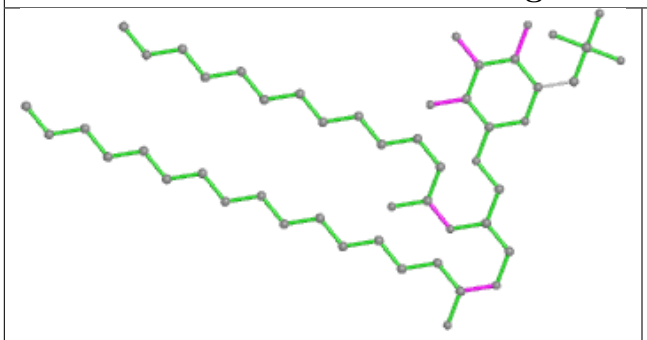


Torsions

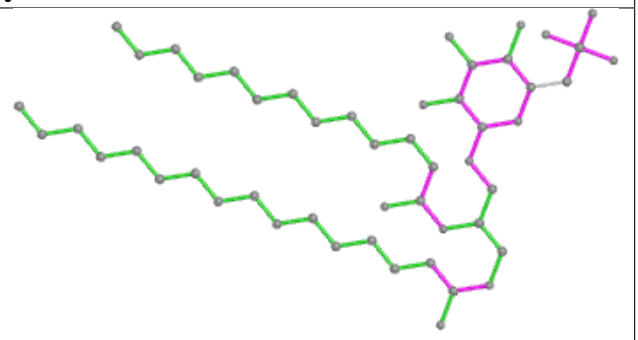


Rings

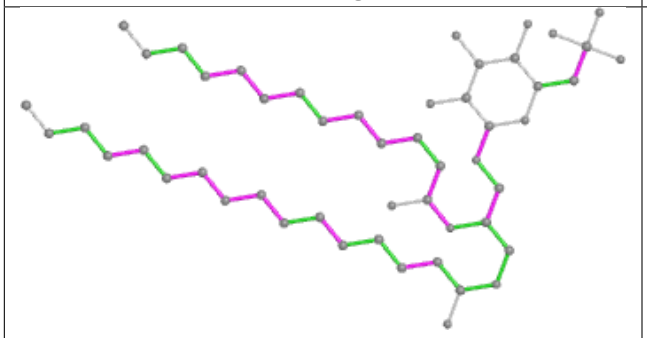
Ligand SQD C 502



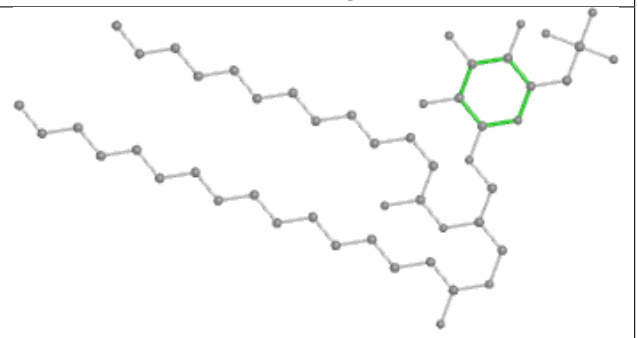
Bond lengths



Bond angles

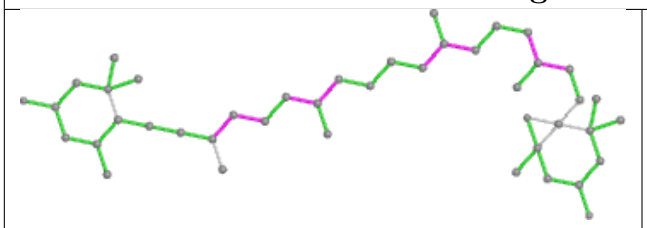


Torsions

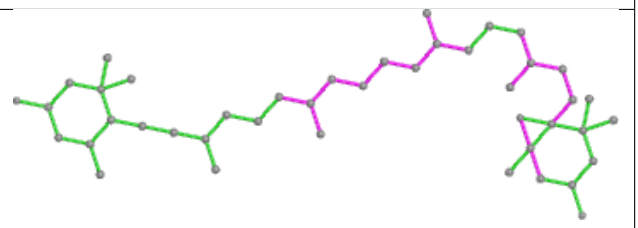


Rings

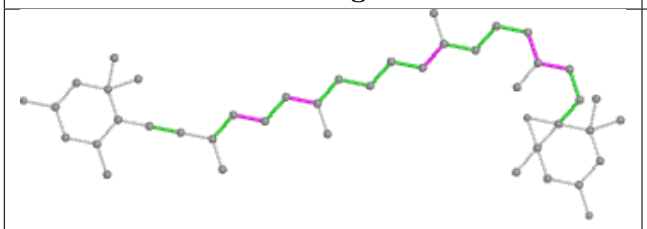
Ligand DD6 7 310



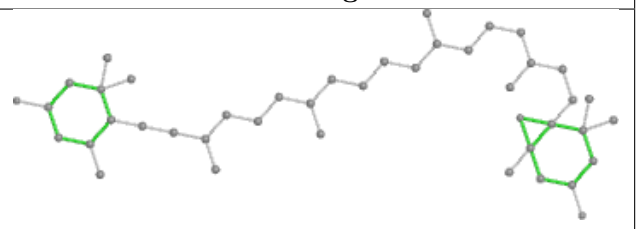
Bond lengths



Bond angles

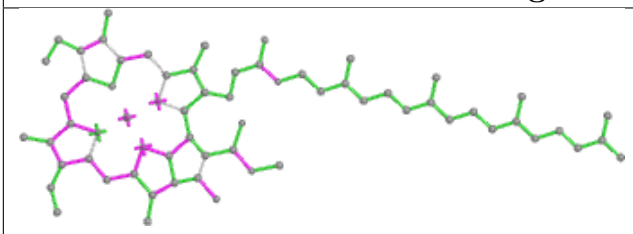


Torsions

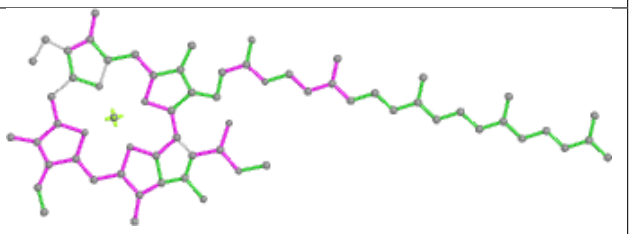


Rings

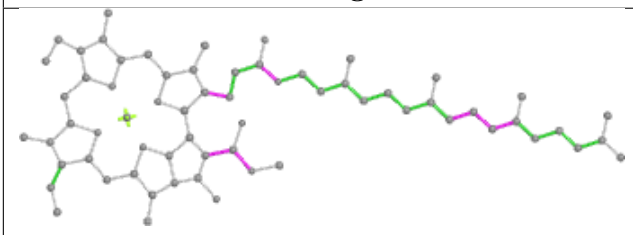
Ligand CLA 1 302



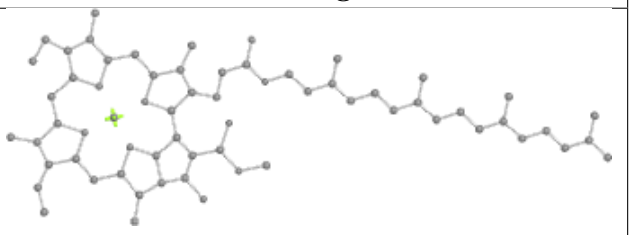
Bond lengths



Bond angles

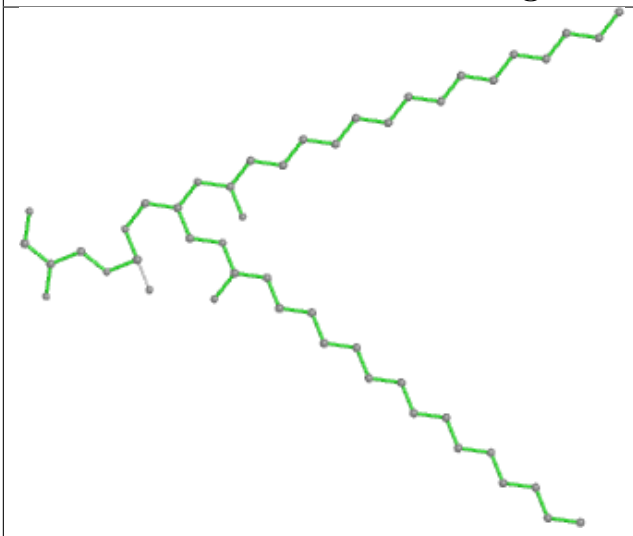


Torsions

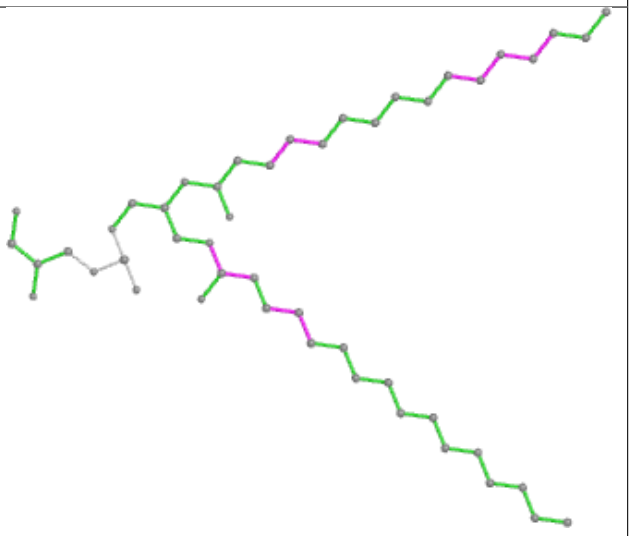


Rings

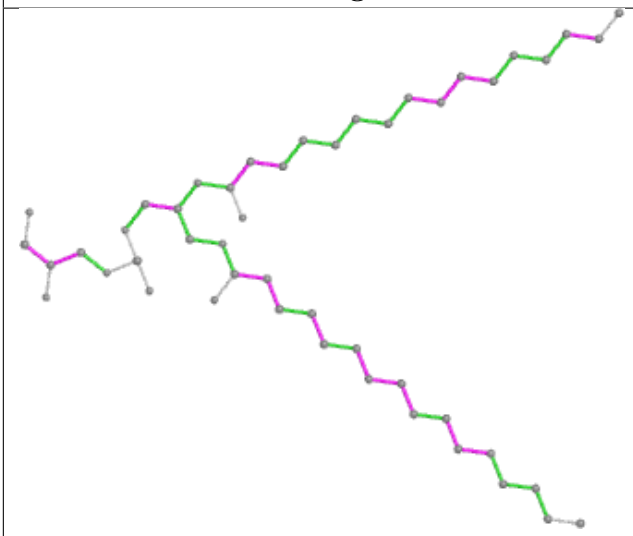
Ligand LHG D 410



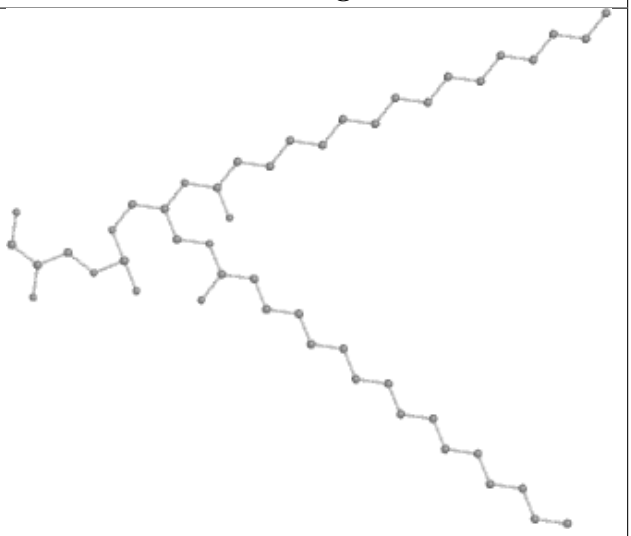
Bond lengths



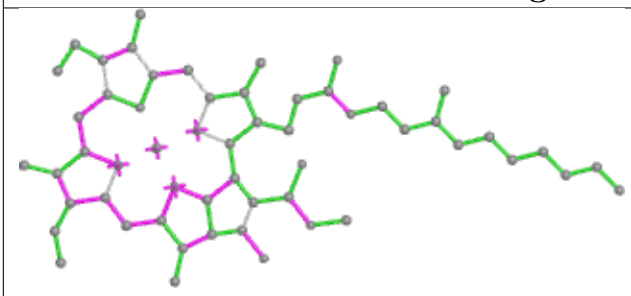
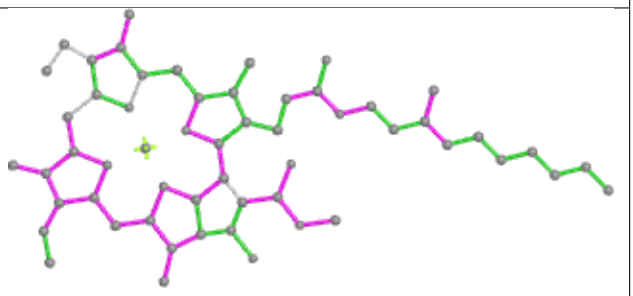
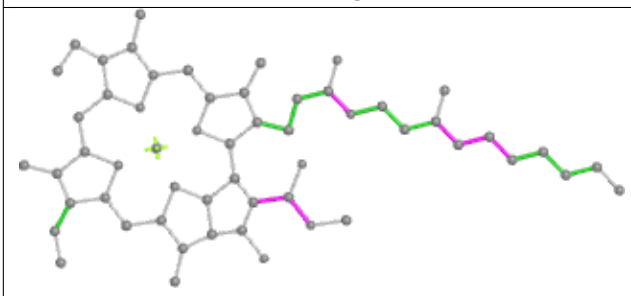
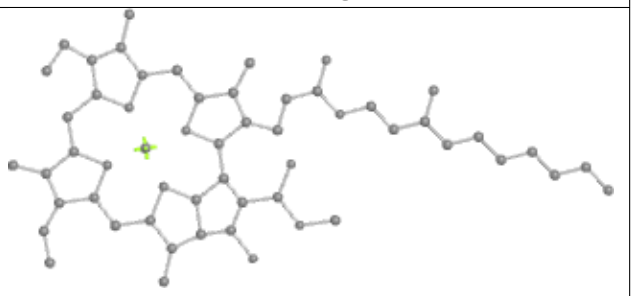
Bond angles

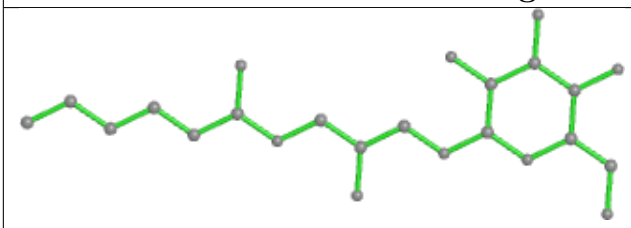
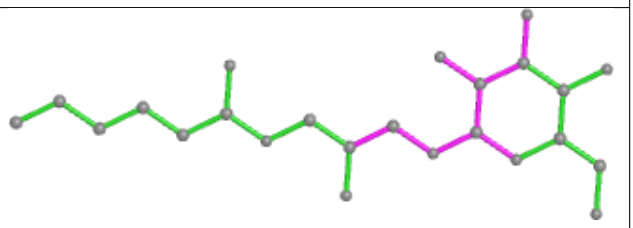
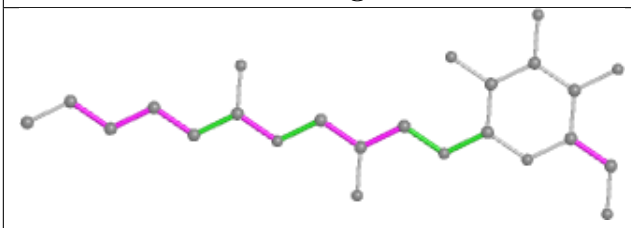
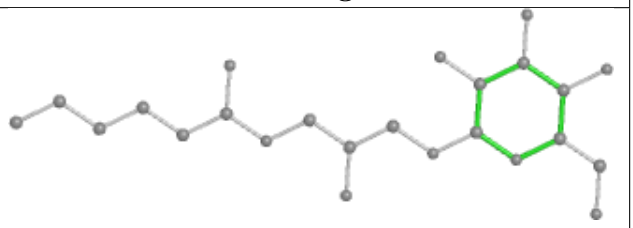


Torsions

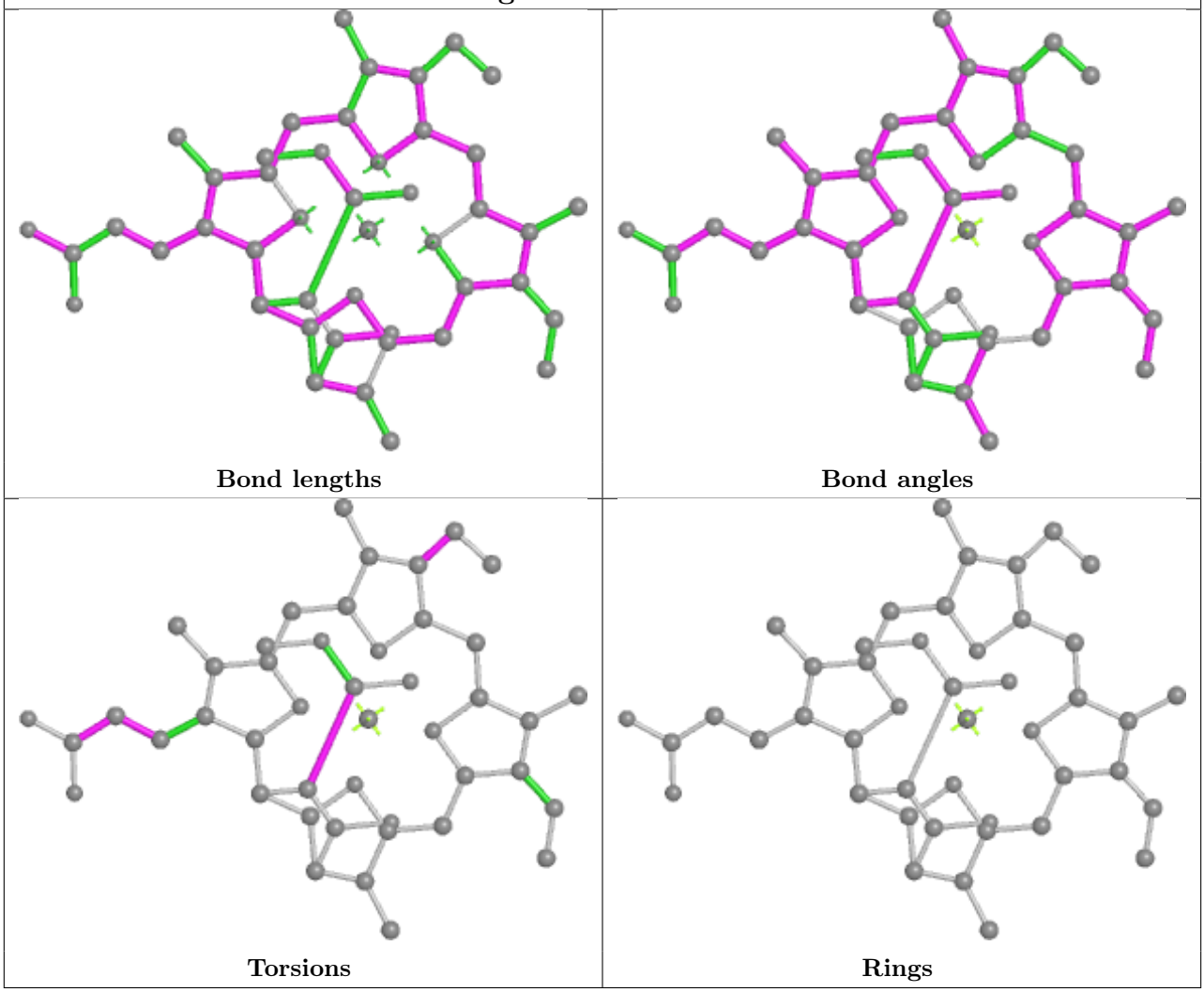


Rings

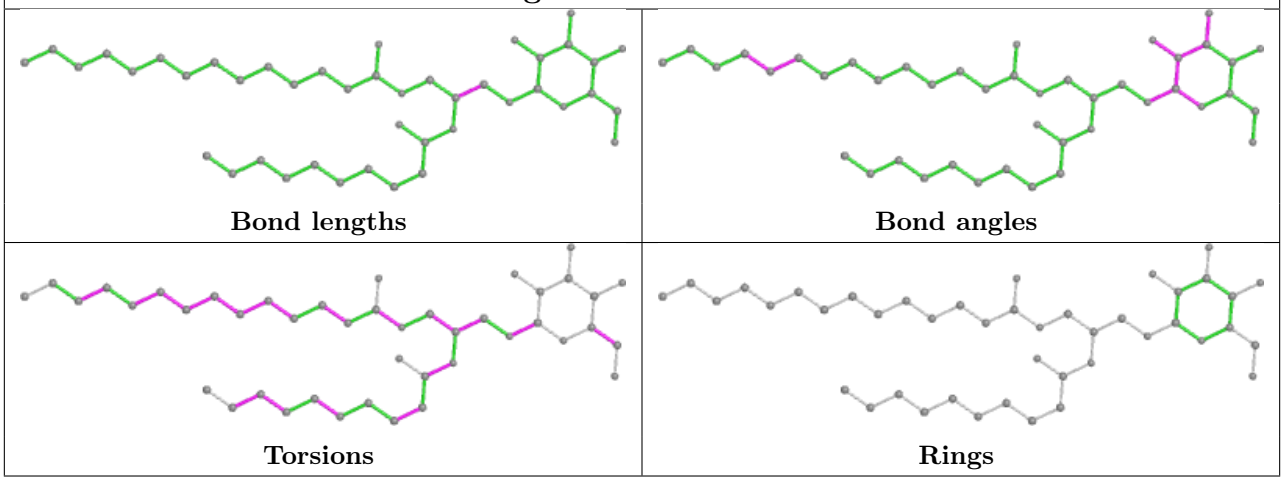
Ligand CLA c 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG N 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

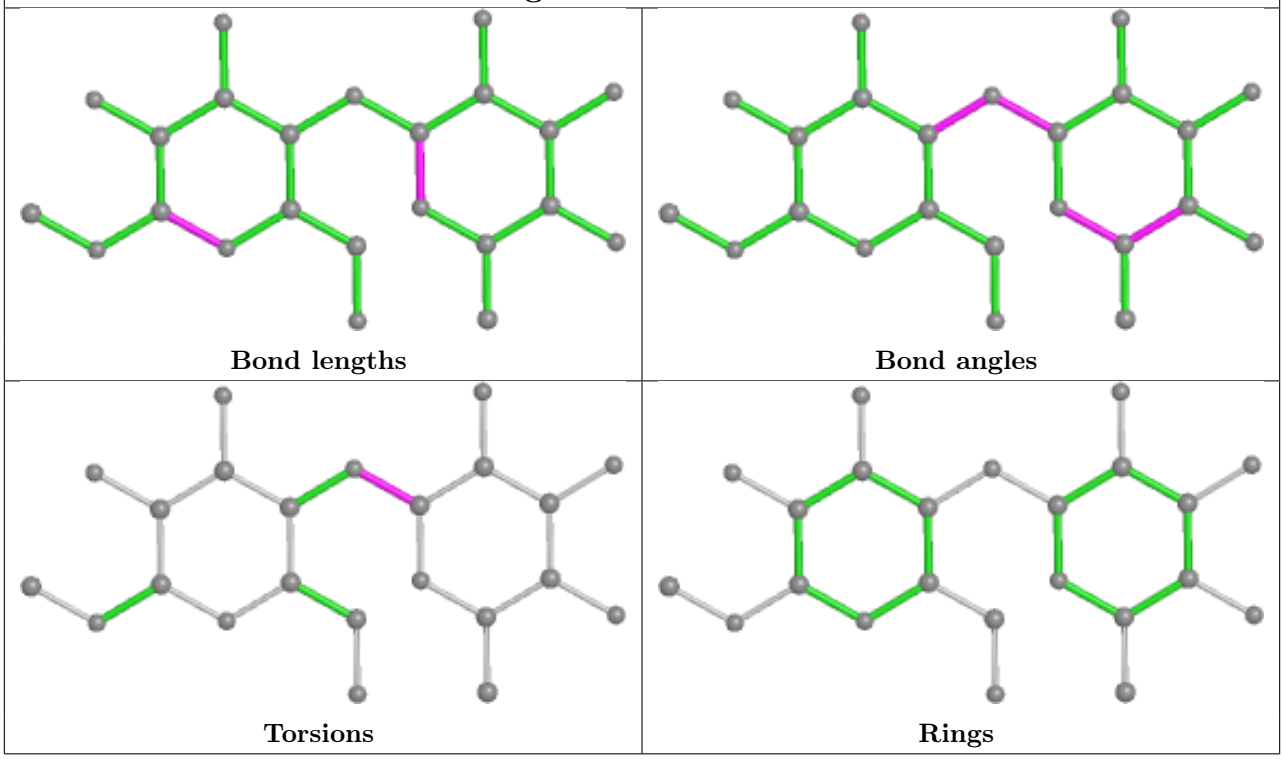
Ligand KC1 6 313



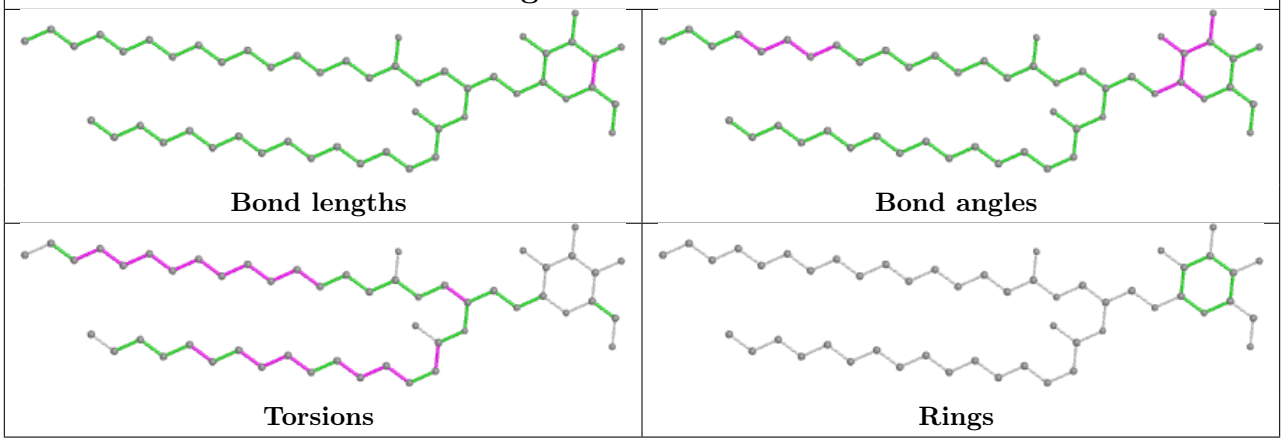
Ligand LMG b 625



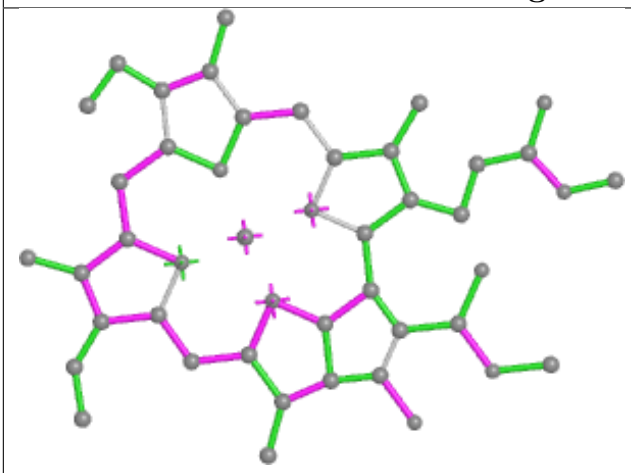
Ligand LMU 5 316



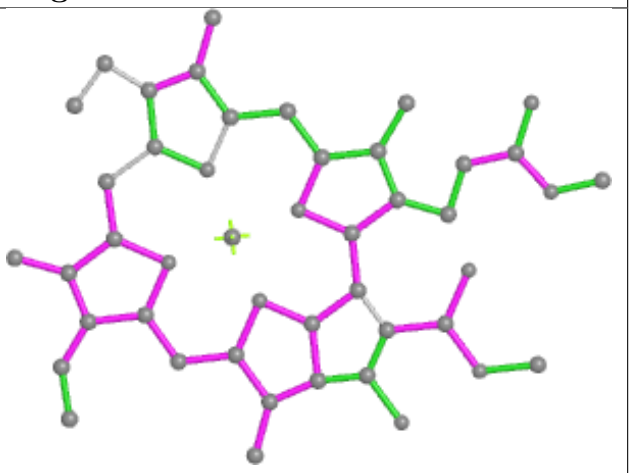
Ligand LMG B 619



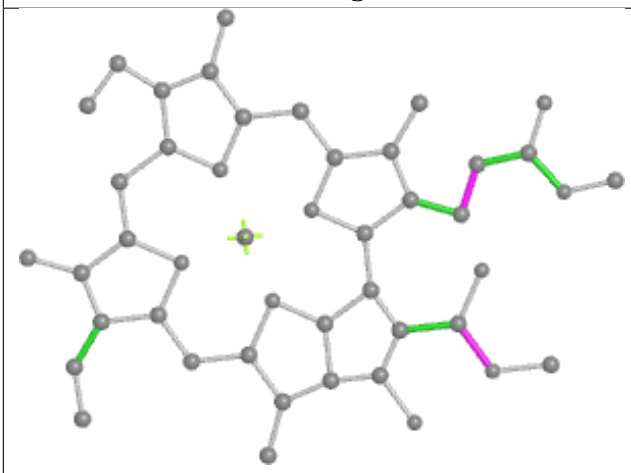
Ligand CLA g 307



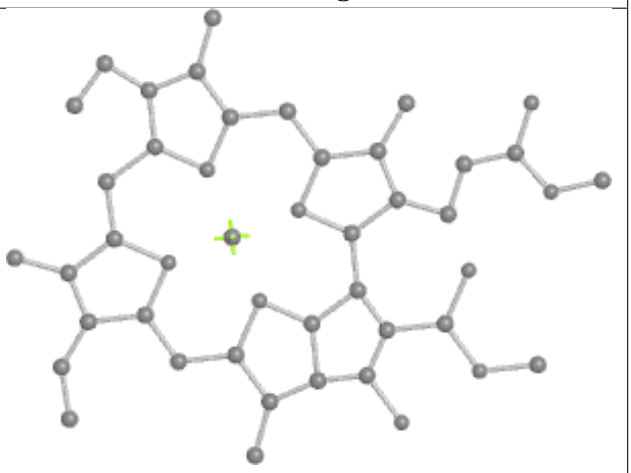
Bond lengths



Bond angles

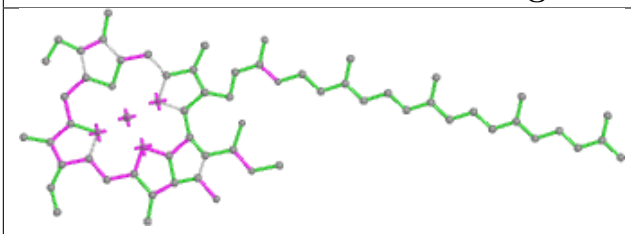


Torsions

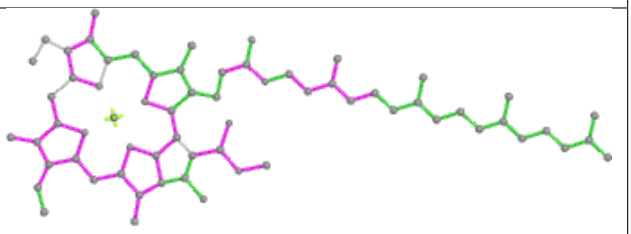


Rings

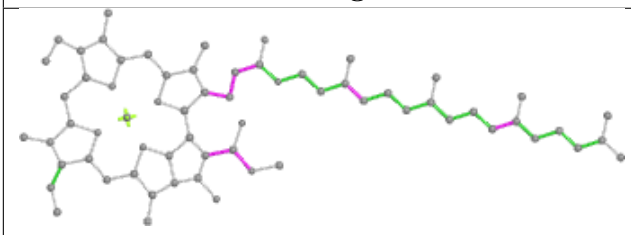
Ligand CLA 5 302



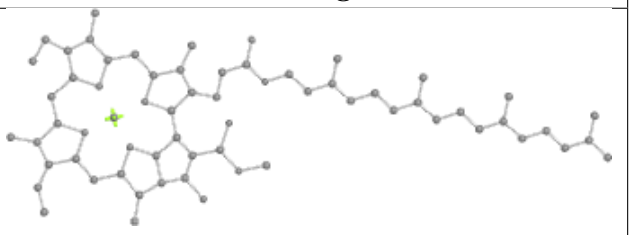
Bond lengths



Bond angles

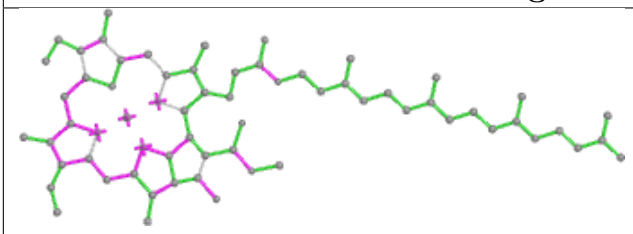


Torsions

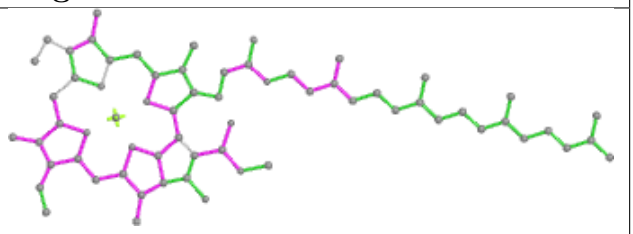


Rings

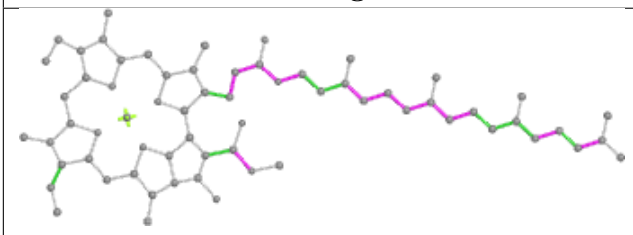
Ligand CLA g 308



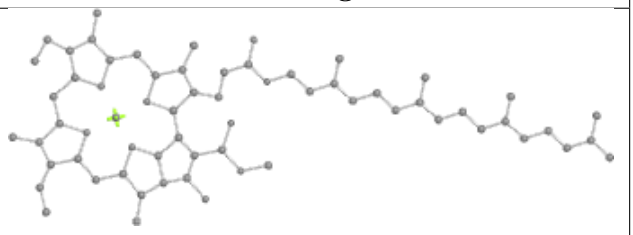
Bond lengths



Bond angles

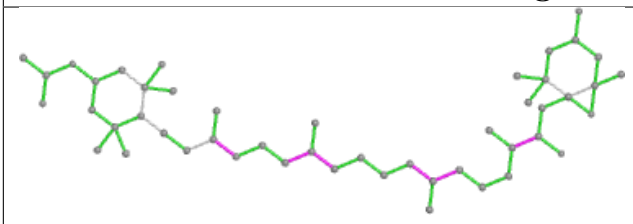


Torsions

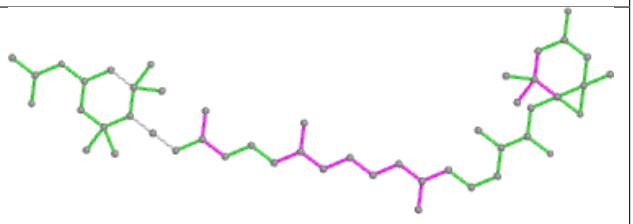


Rings

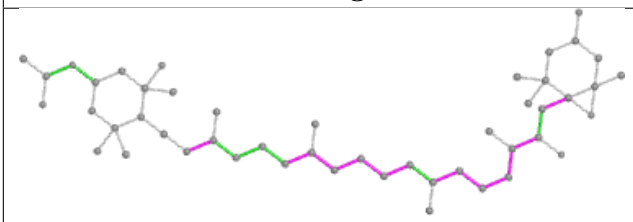
Ligand A86 2 312



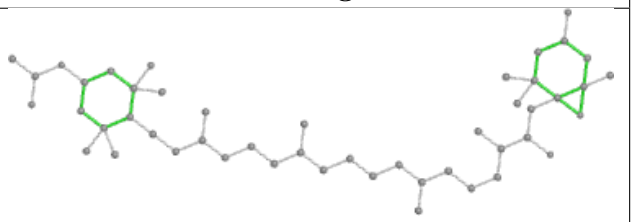
Bond lengths



Bond angles

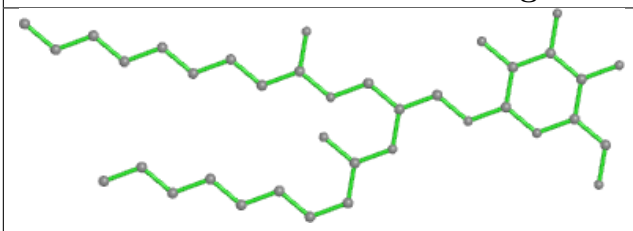


Torsions

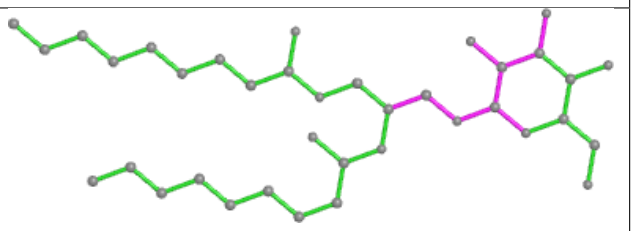


Rings

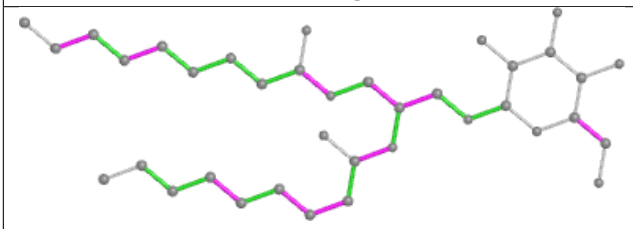
Ligand LMG B 622



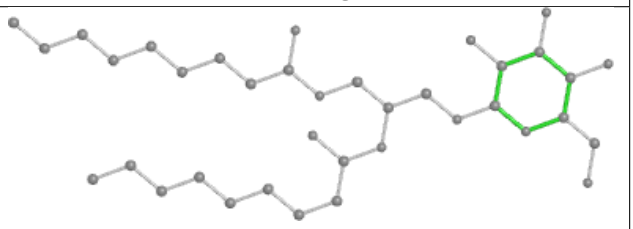
Bond lengths



Bond angles

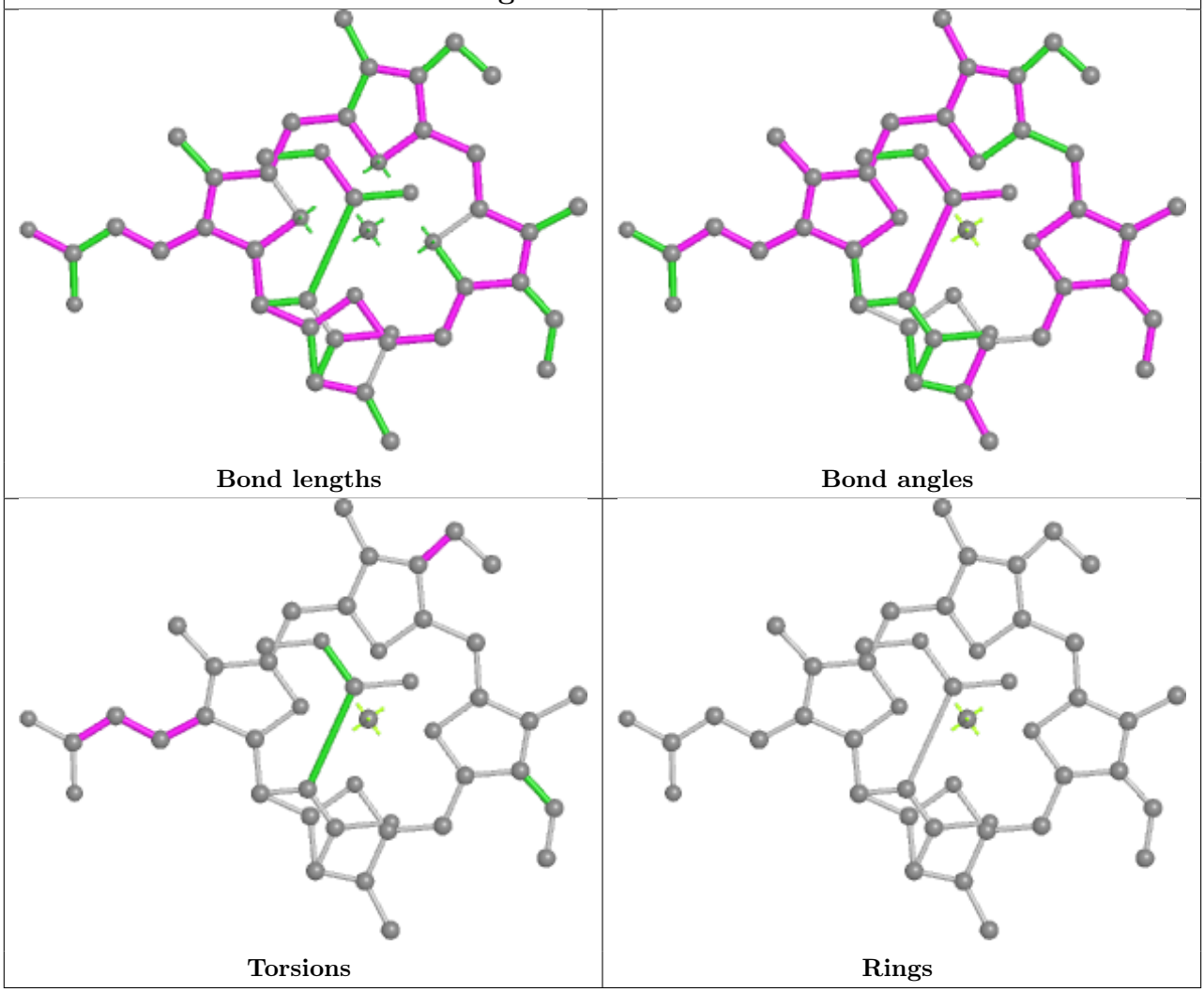


Torsions

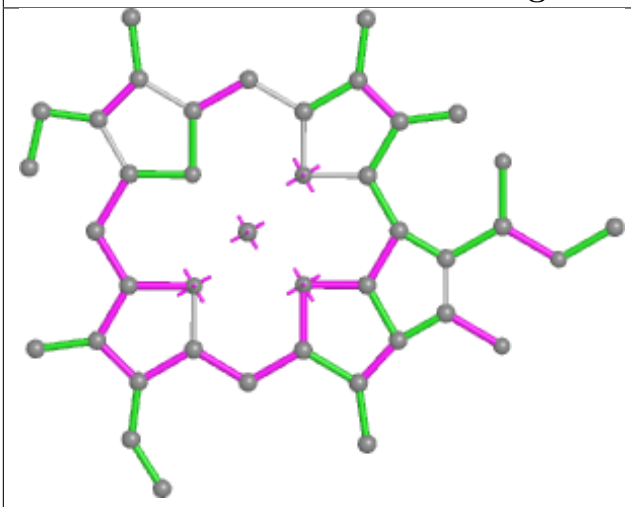


Rings

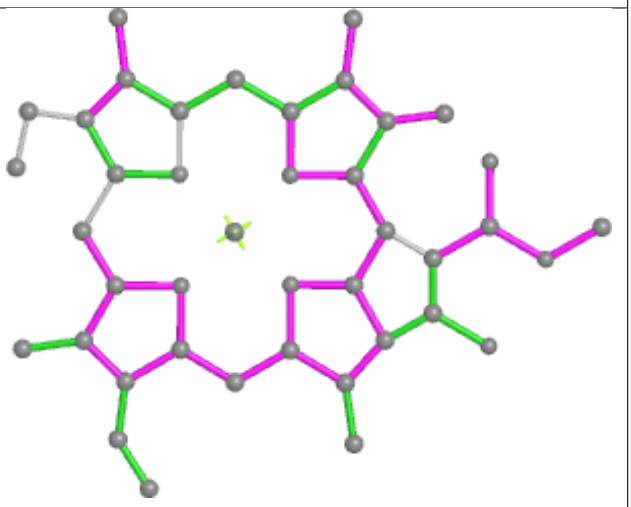
Ligand KC1 9 306



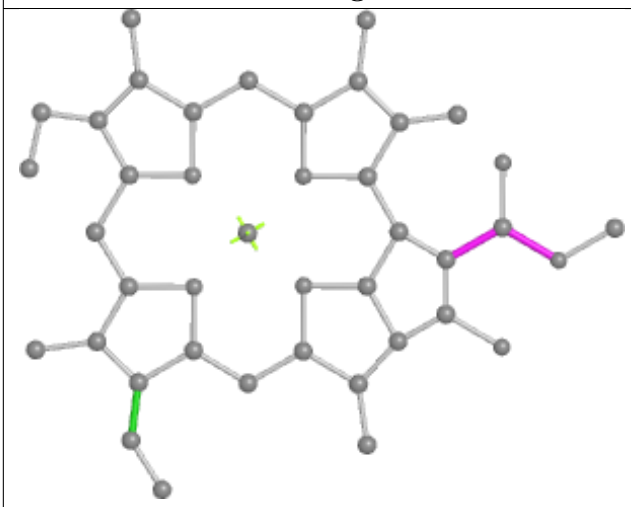
Ligand CLA 8 305



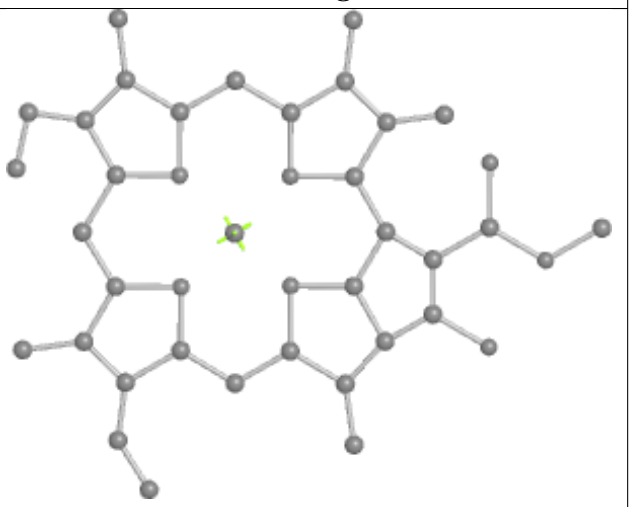
Bond lengths



Bond angles

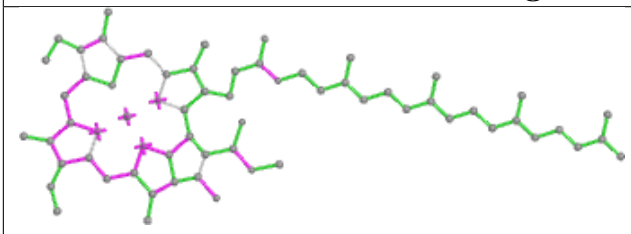


Torsions

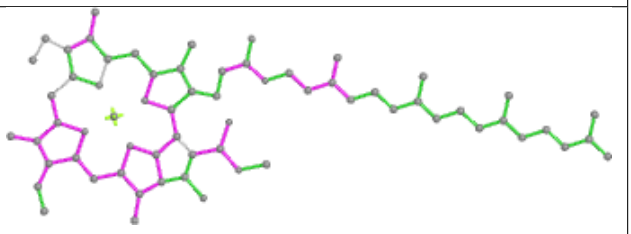


Rings

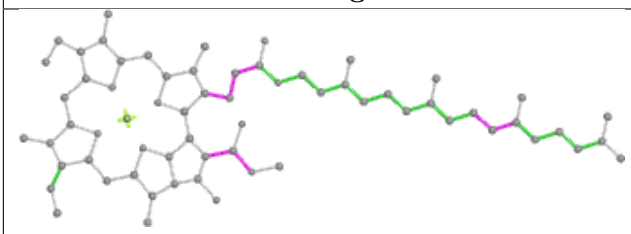
Ligand CLA C 503



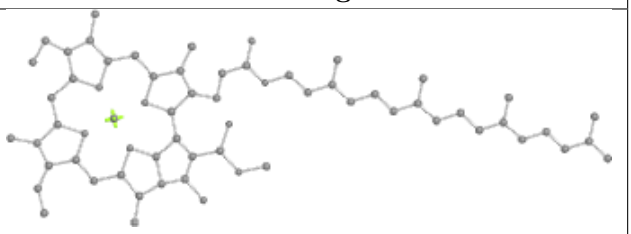
Bond lengths



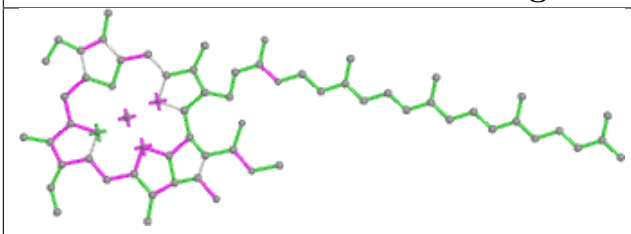
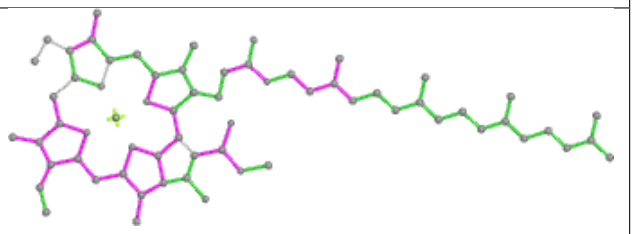
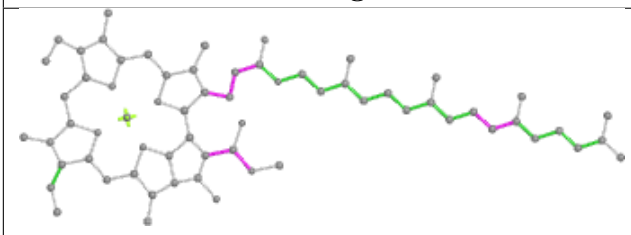
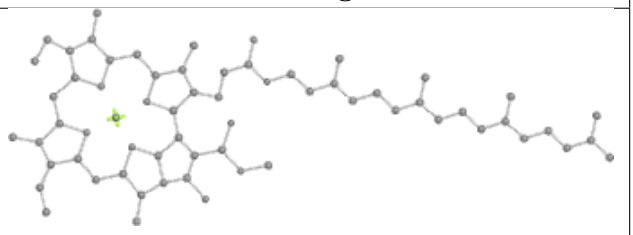
Bond angles

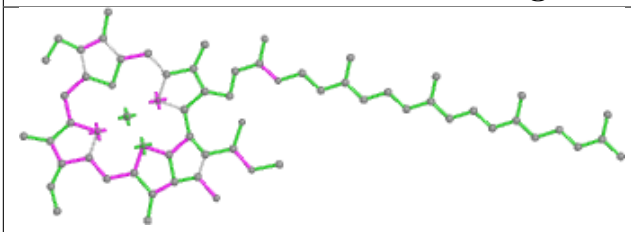
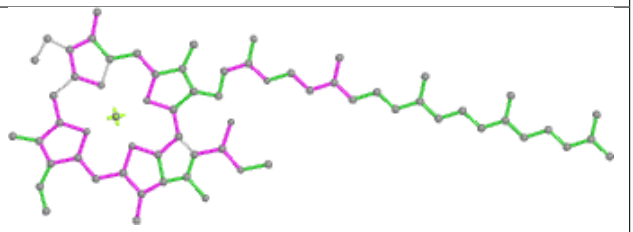
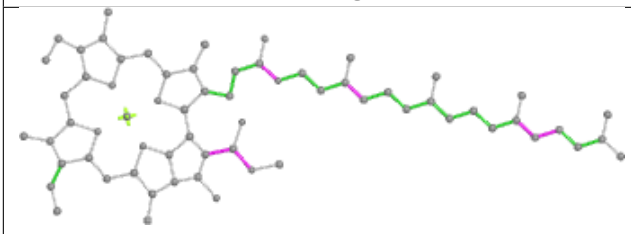
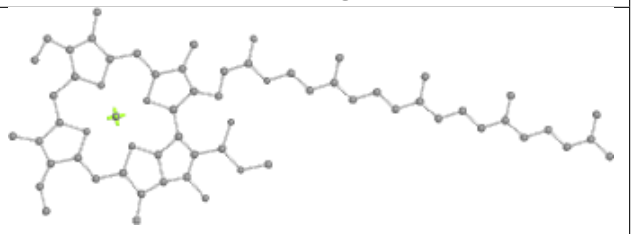


Torsions

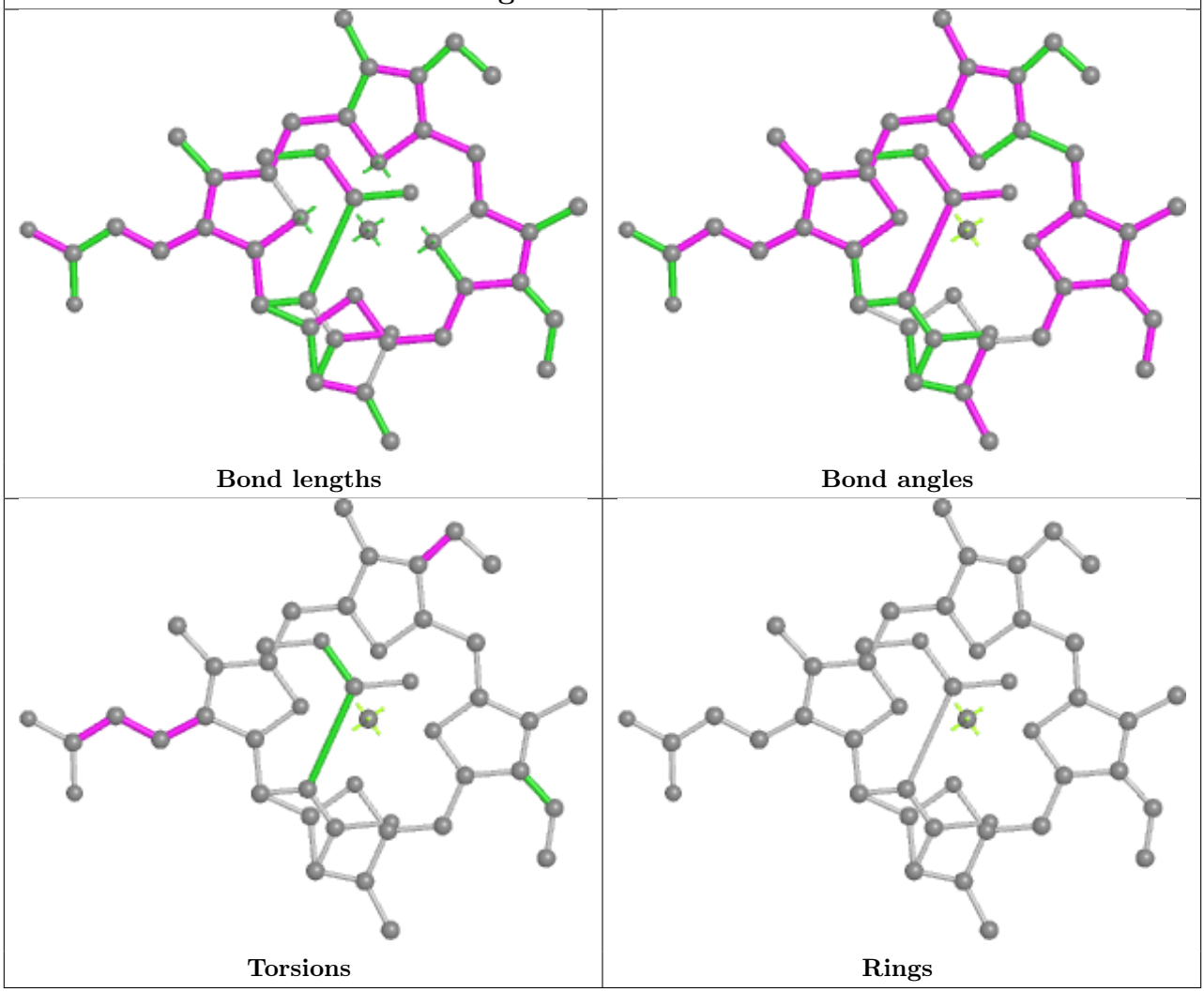


Rings

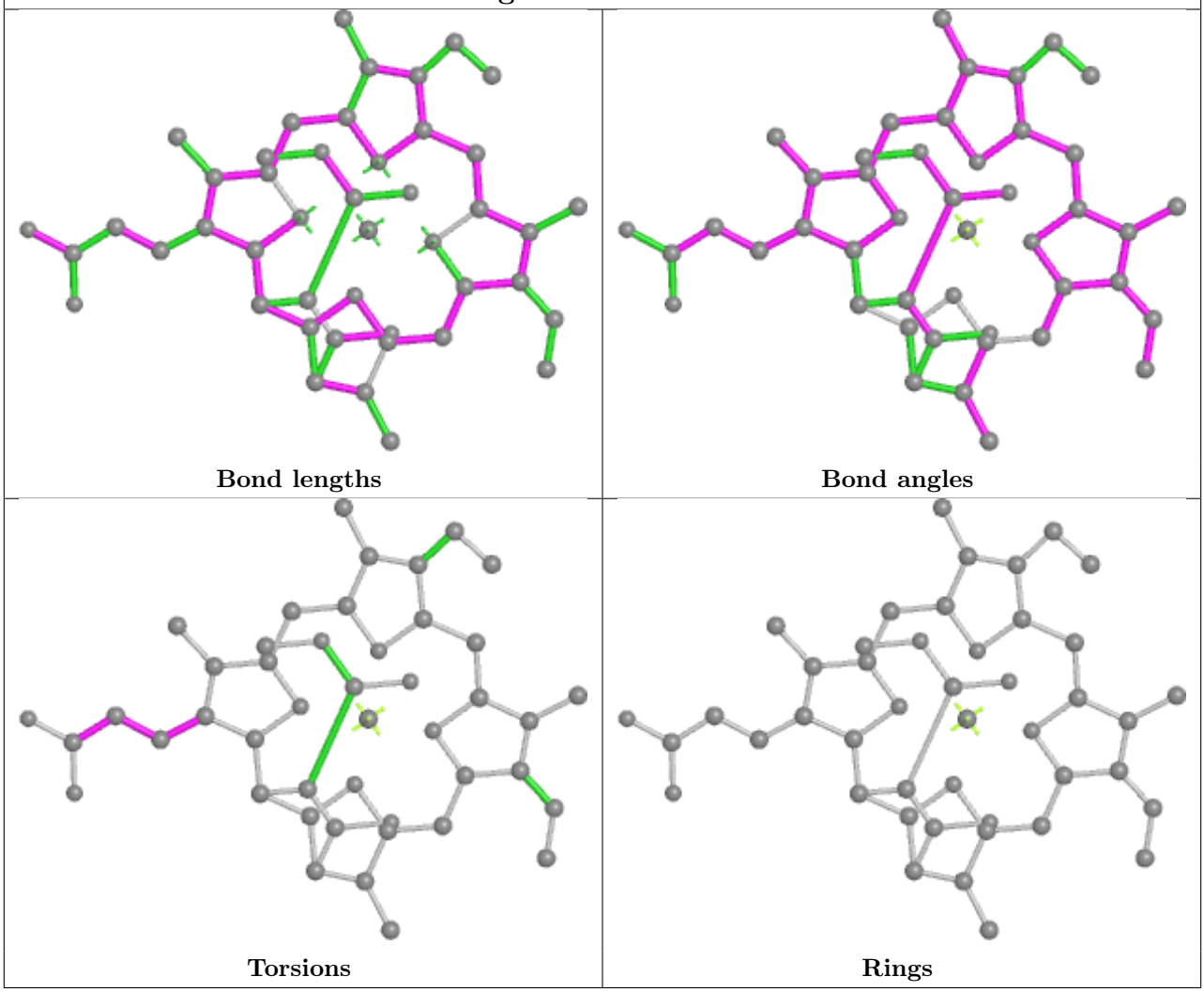
Ligand CLA c 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

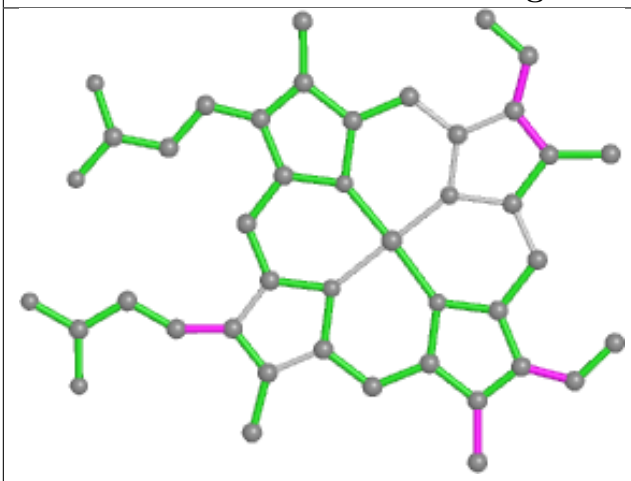
Ligand KC1 7 314



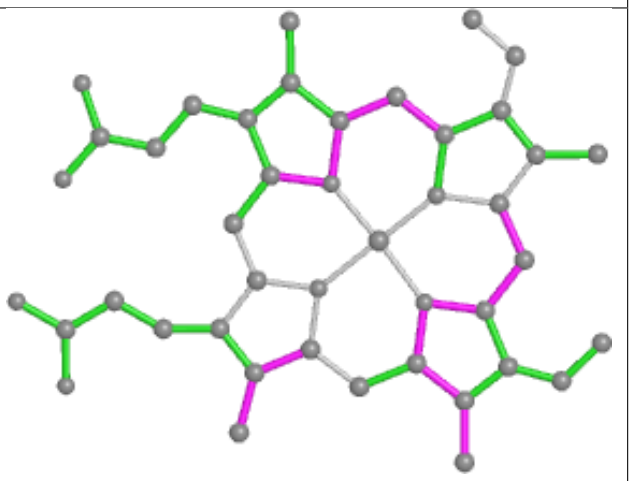
Ligand KC1 8 315



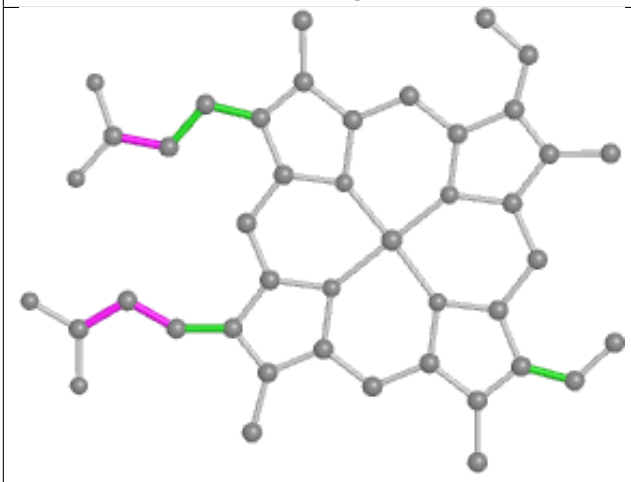
Ligand HEM f 101



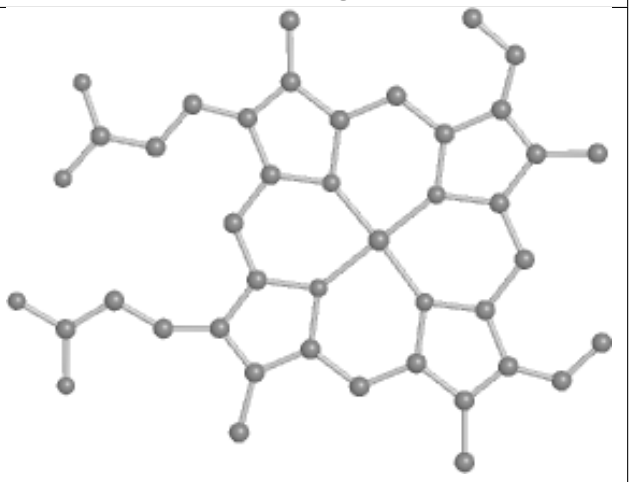
Bond lengths



Bond angles

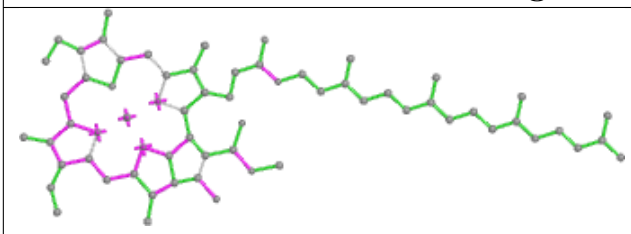


Torsions

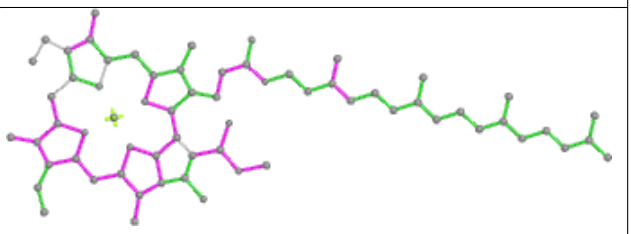


Rings

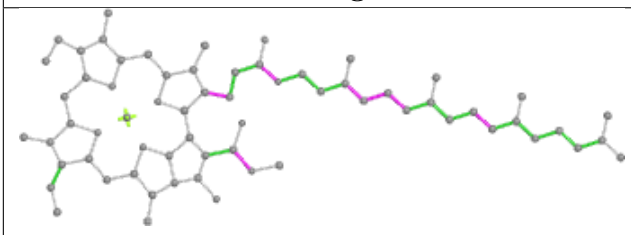
Ligand CLA 5 308



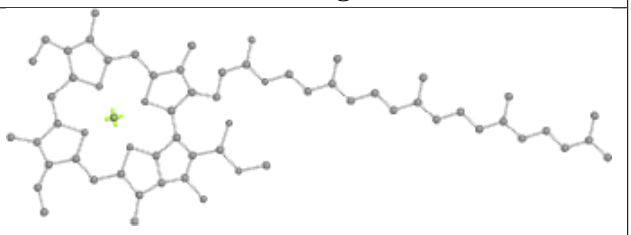
Bond lengths



Bond angles

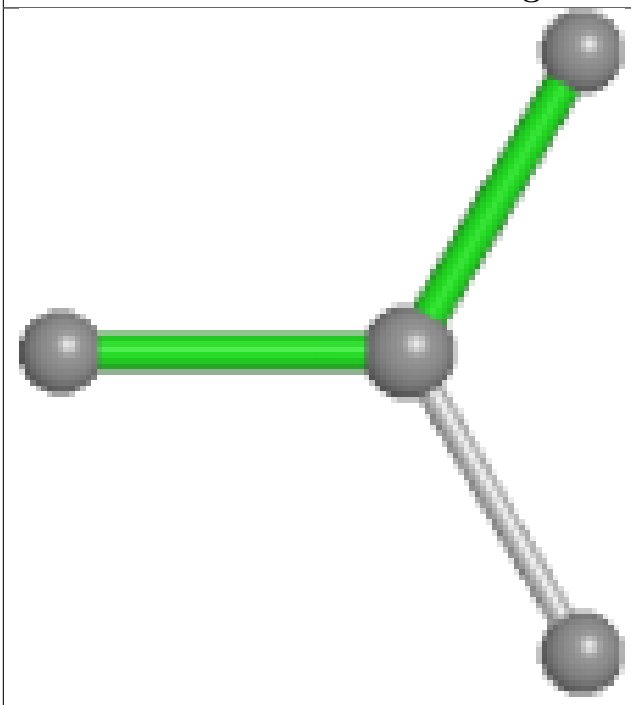


Torsions

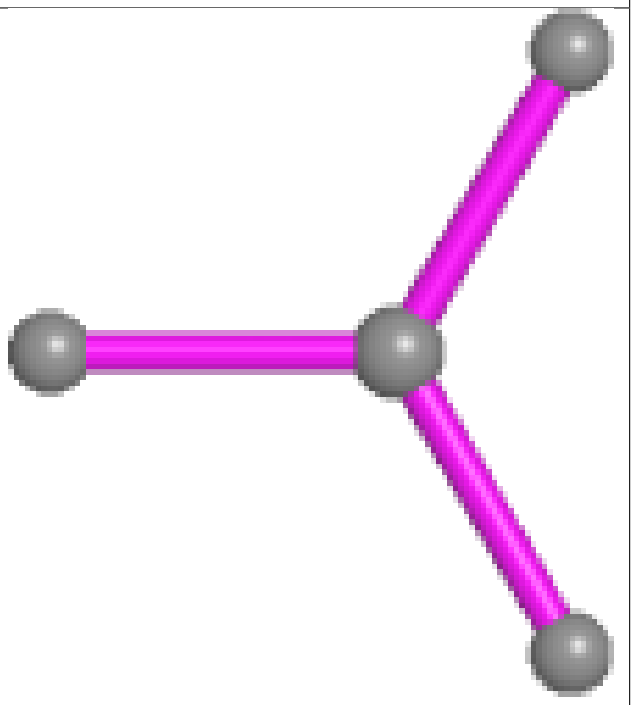


Rings

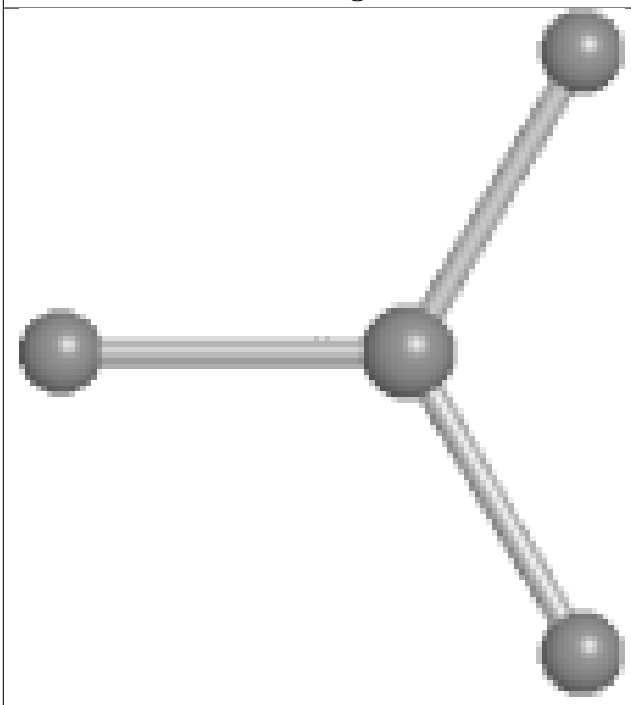
Ligand BCT D 402



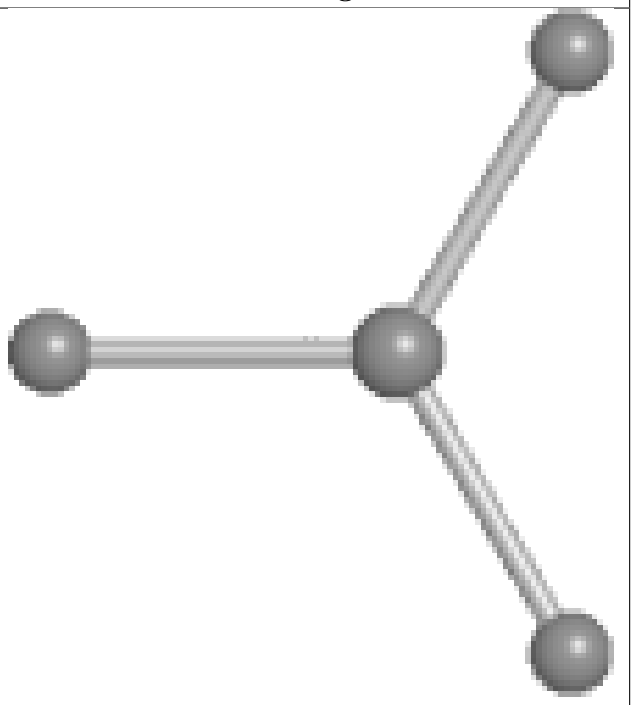
Bond lengths



Bond angles

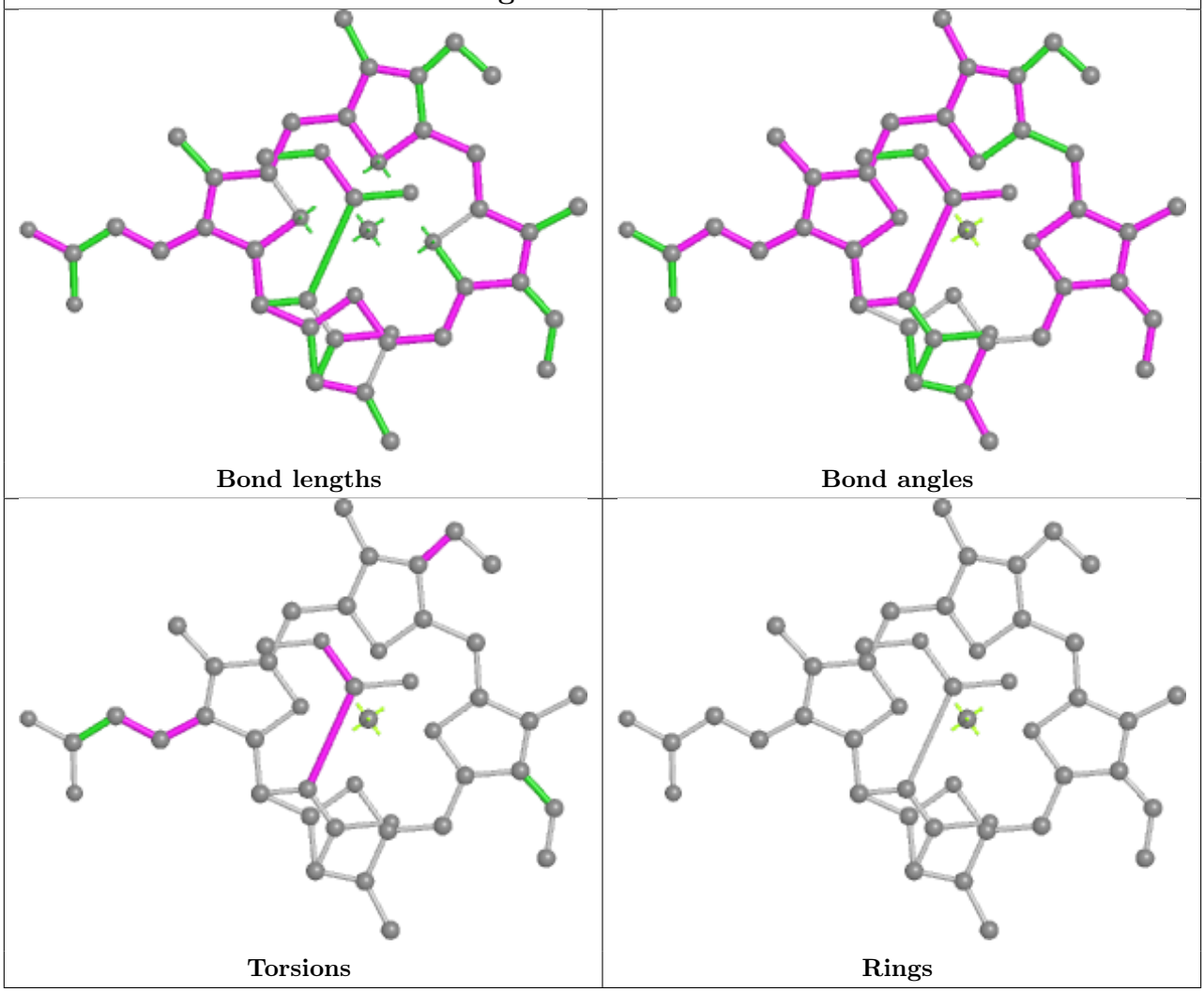


Torsions

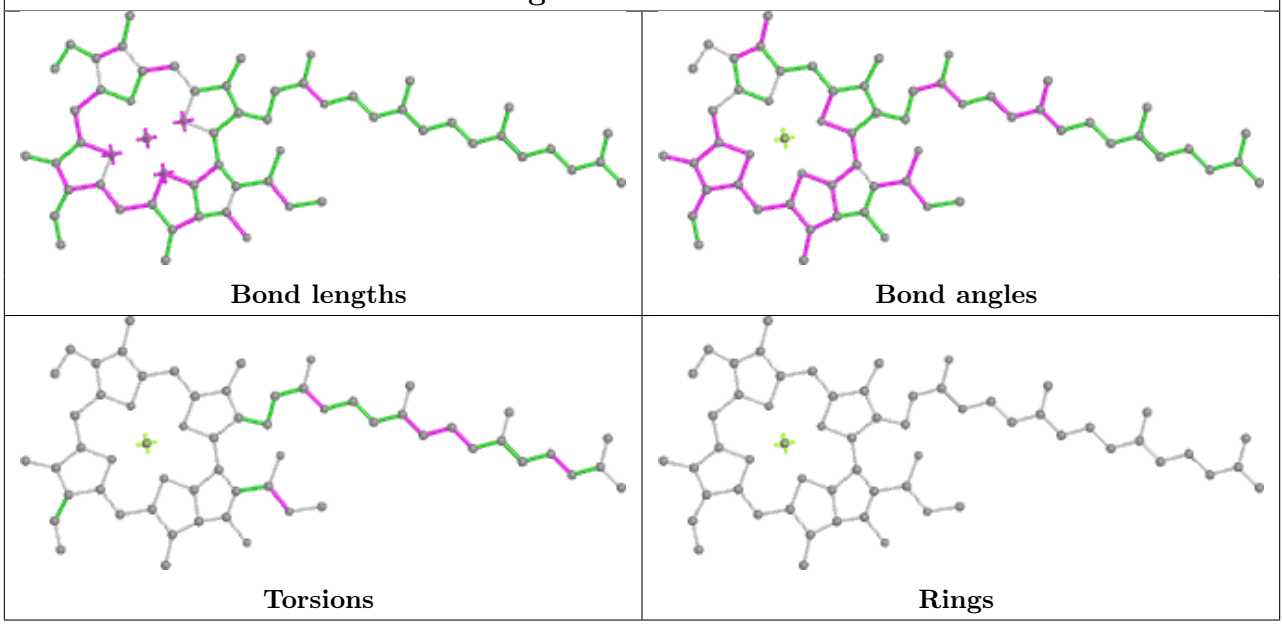


Rings

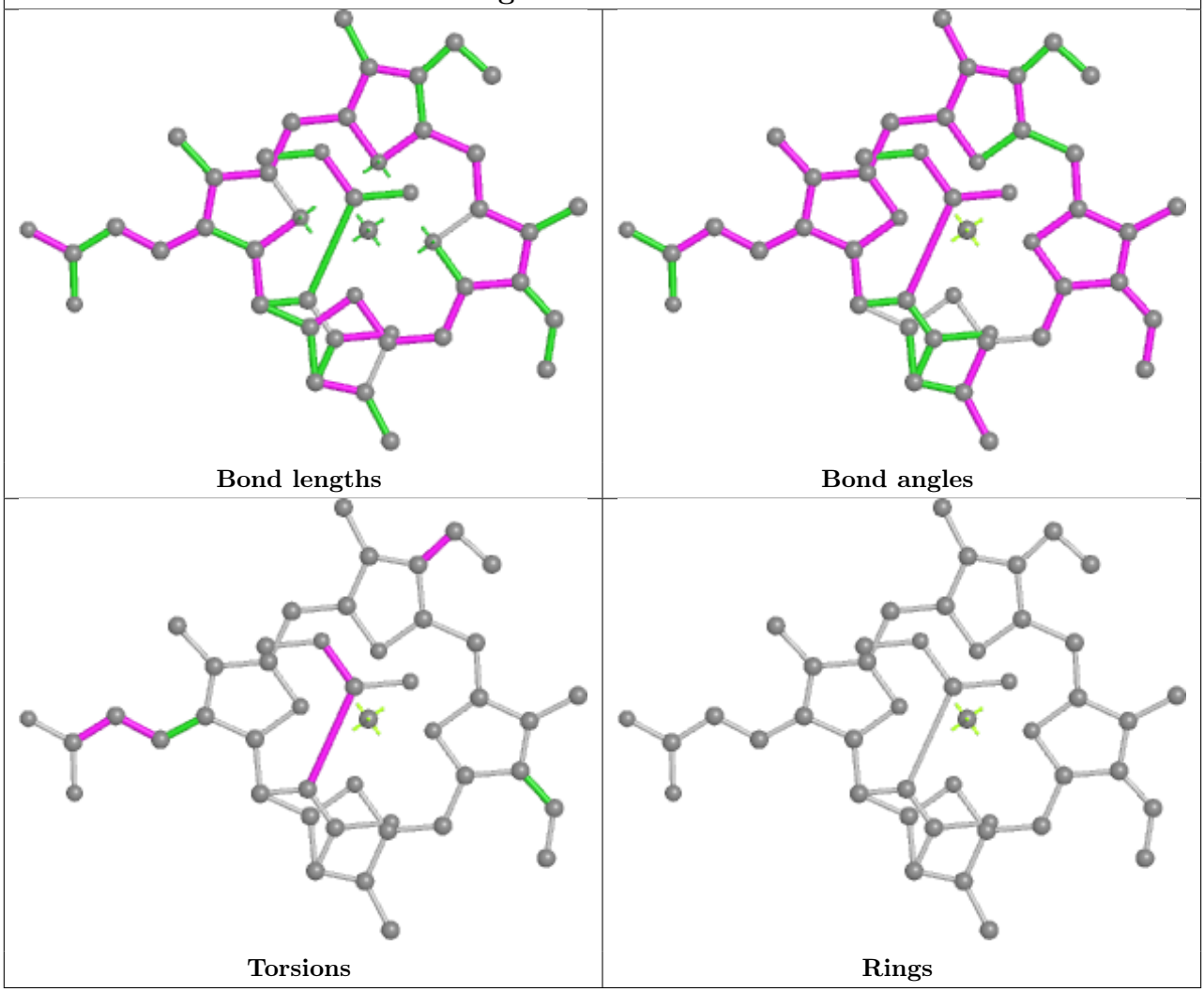
Ligand KC1 2 313

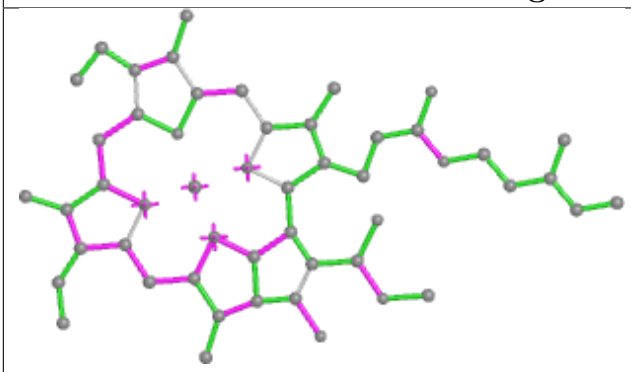
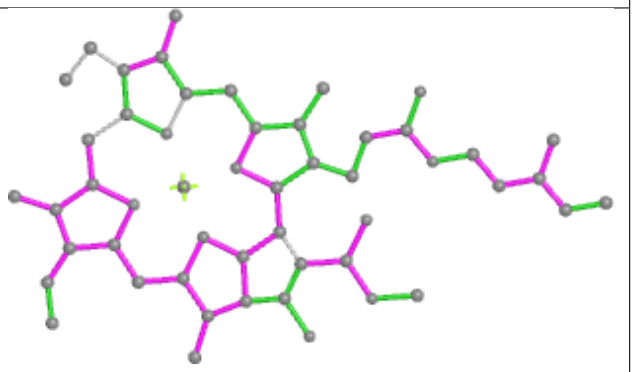
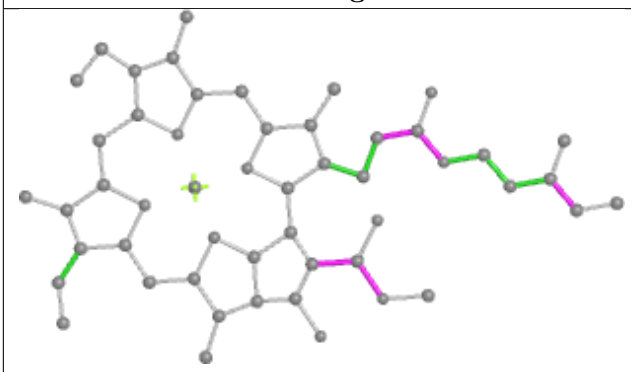
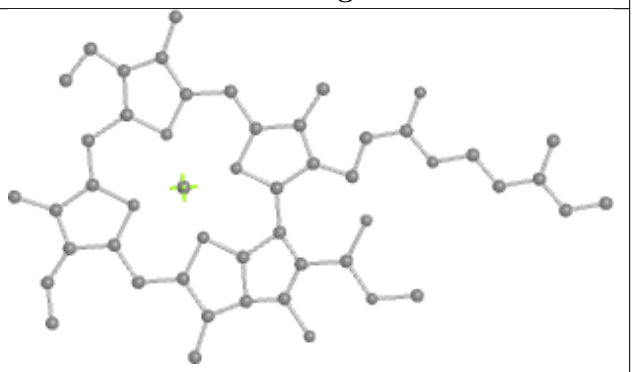


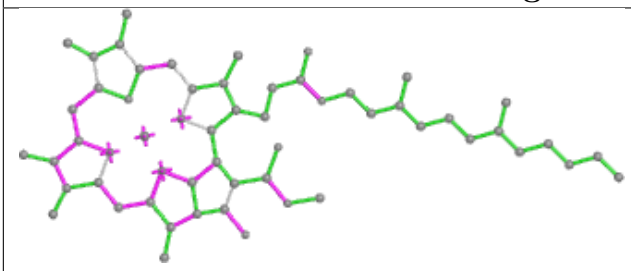
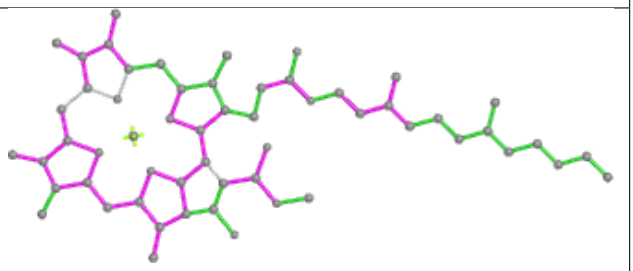
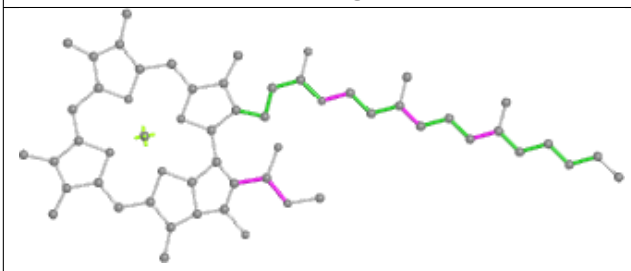
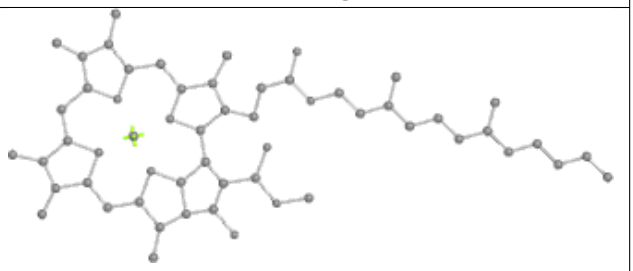
Ligand CLA d 406

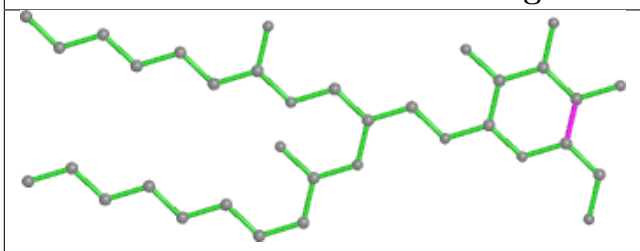
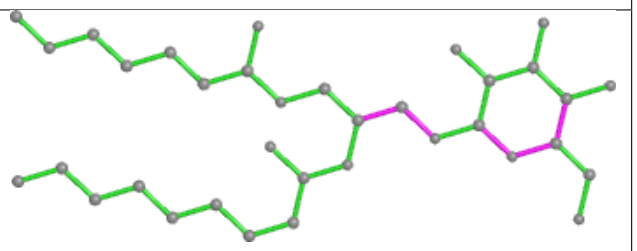
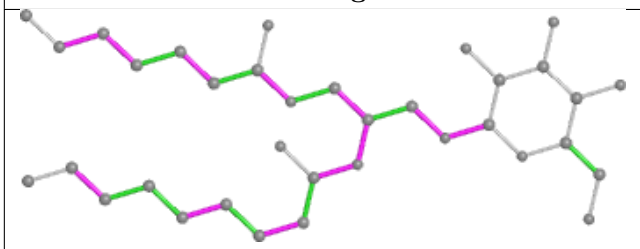
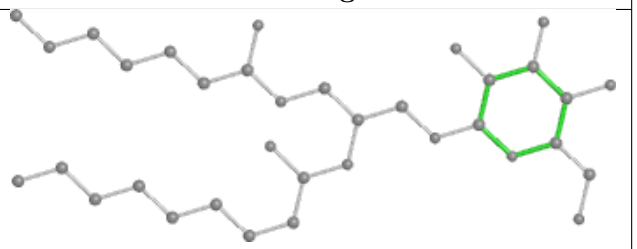


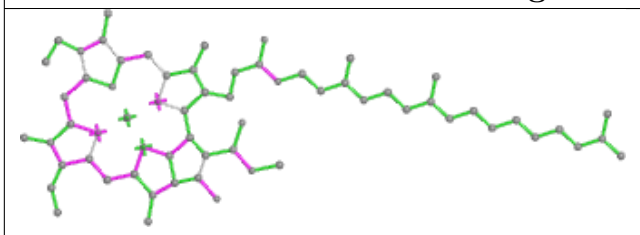
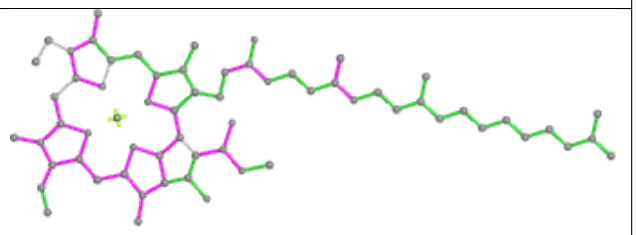
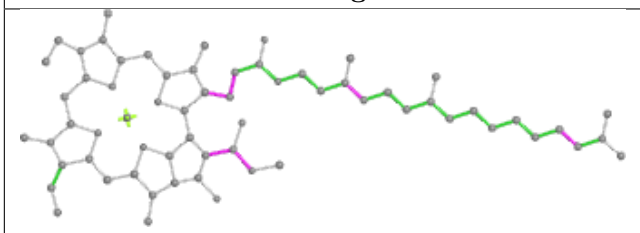
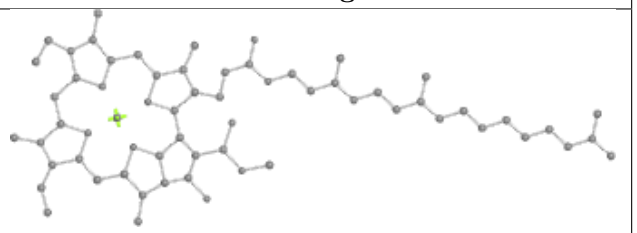
Ligand KC1 4 307



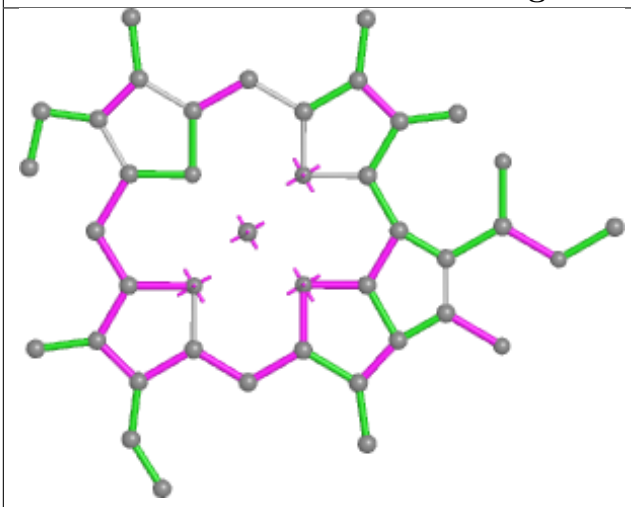
Ligand CLA 8 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

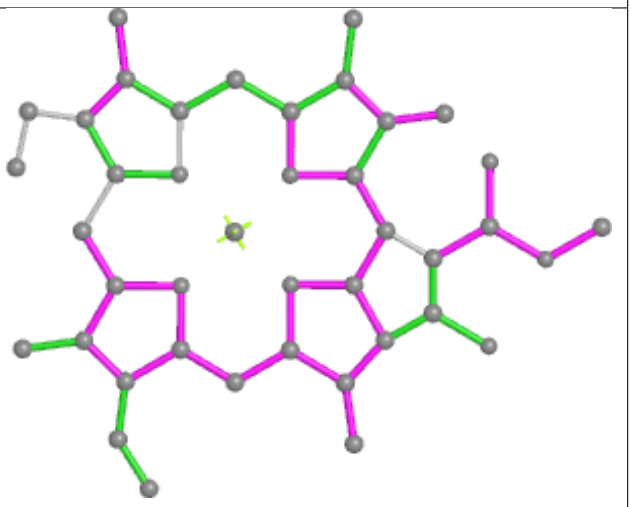
Ligand LMG b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

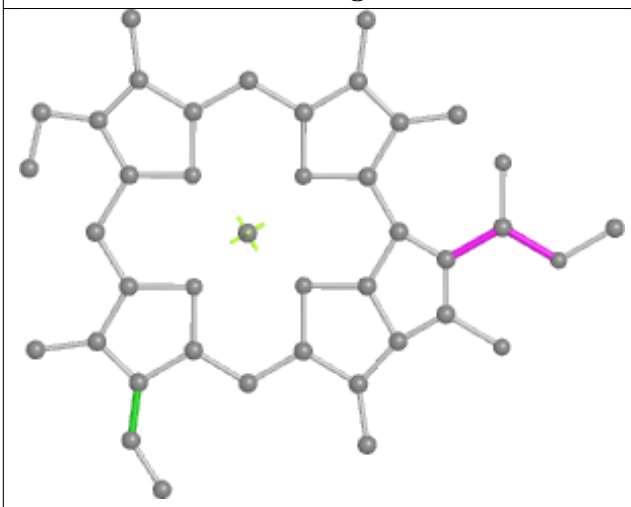
Ligand CLA 2 304



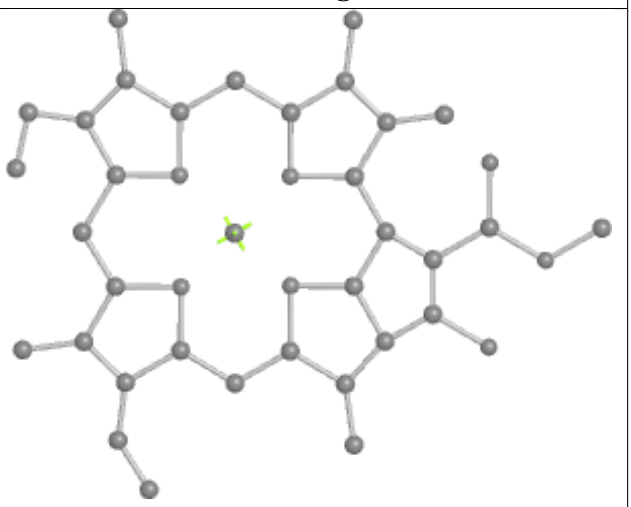
Bond lengths



Bond angles

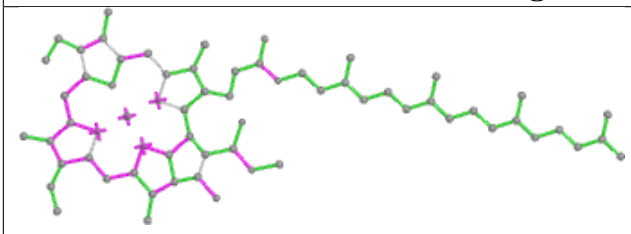


Torsions

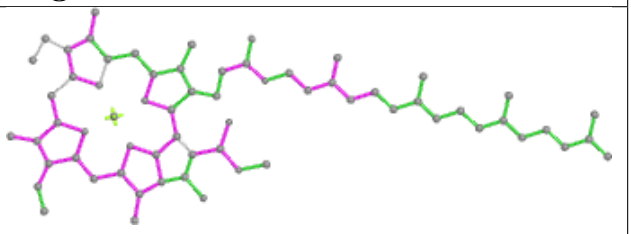


Rings

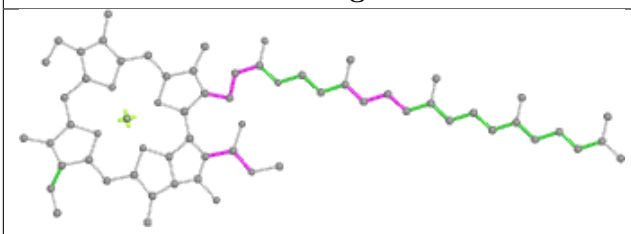
Ligand CLA g 302



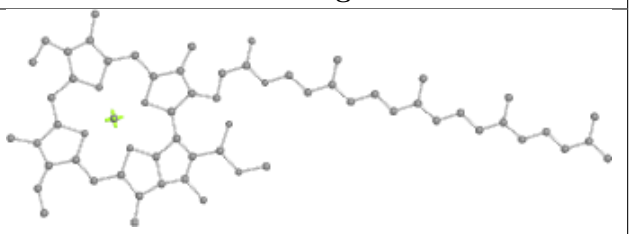
Bond lengths



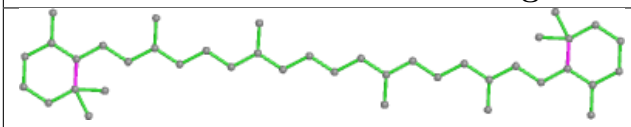
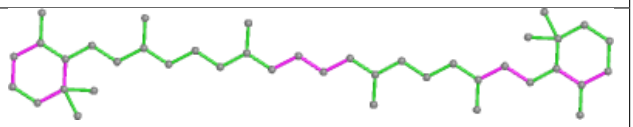
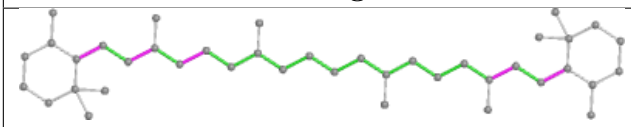
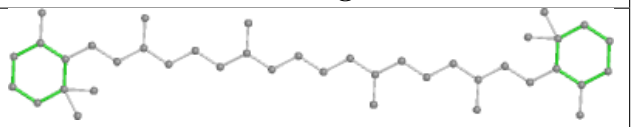
Bond angles

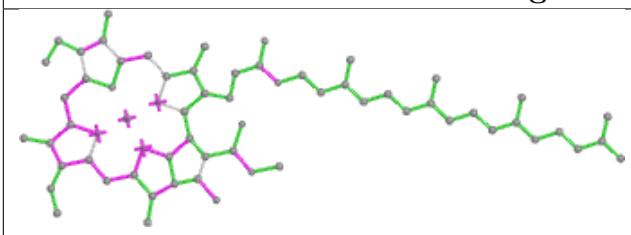
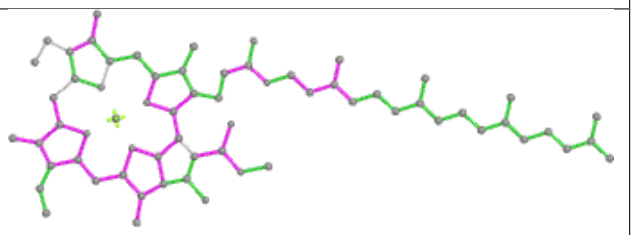
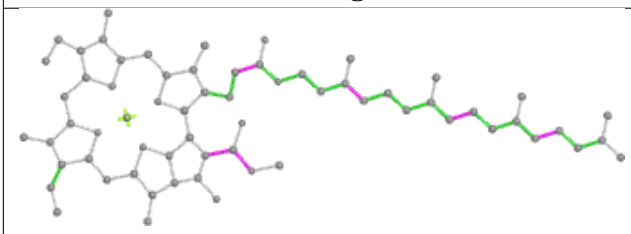
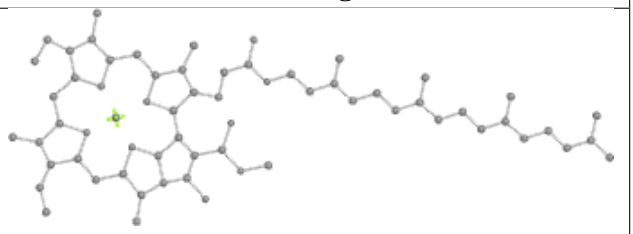


Torsions

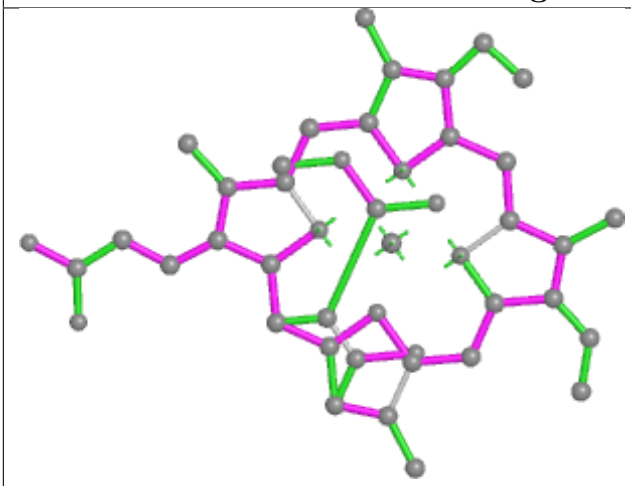


Rings

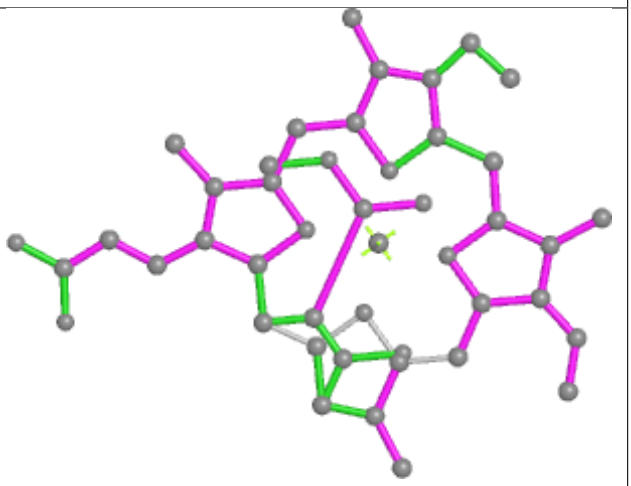
Ligand BCR D 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

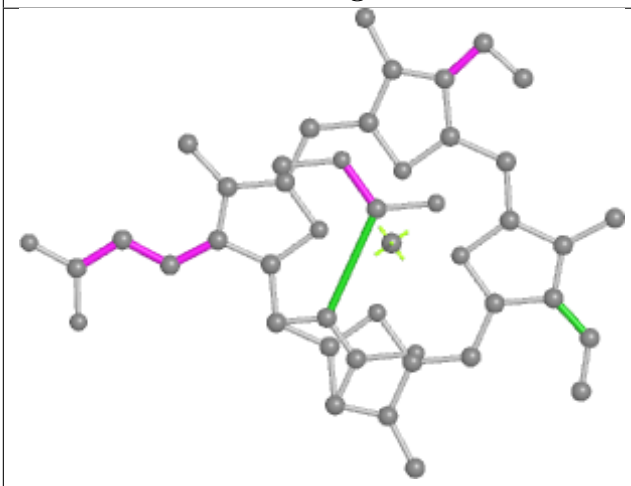
Ligand KC1 1 315



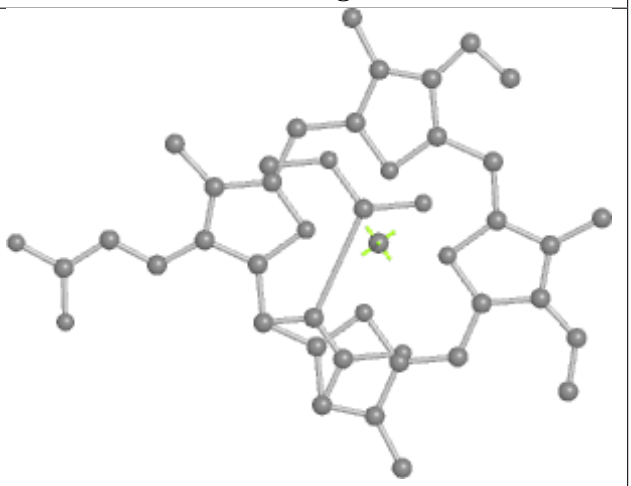
Bond lengths



Bond angles

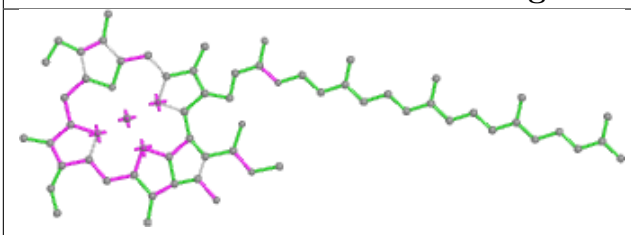


Torsions

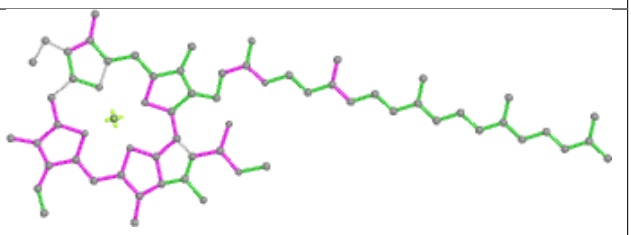


Rings

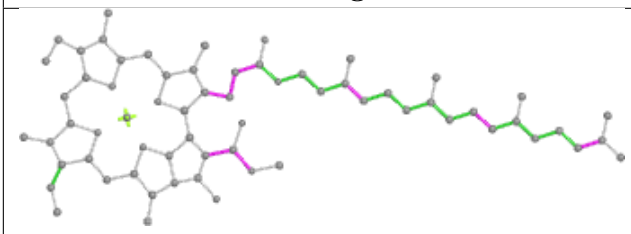
Ligand CLA 7 300



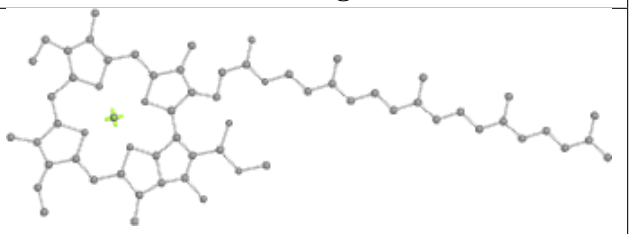
Bond lengths



Bond angles

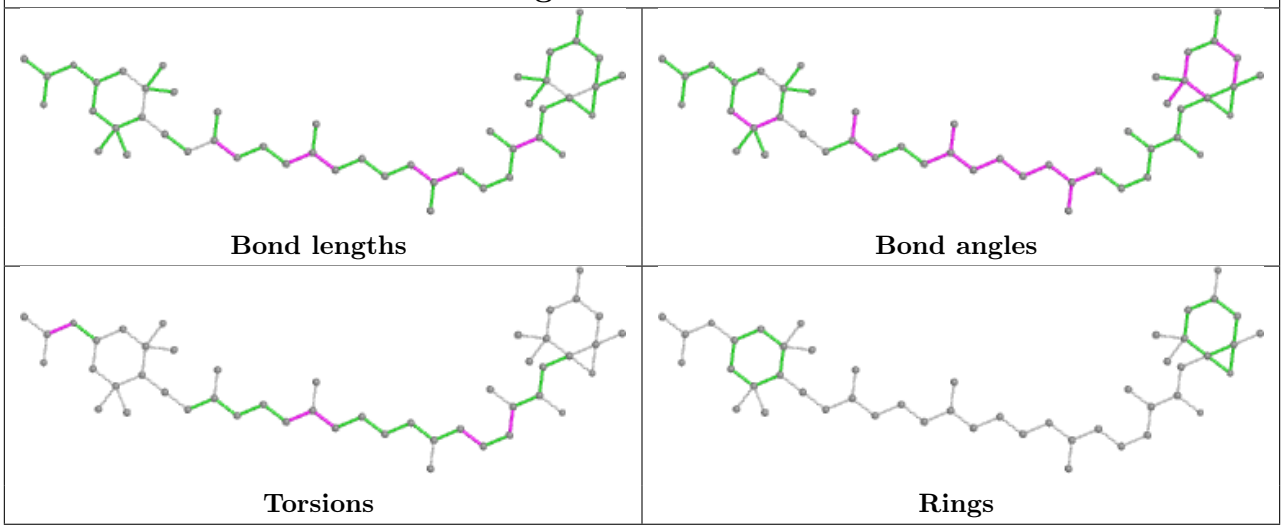


Torsions

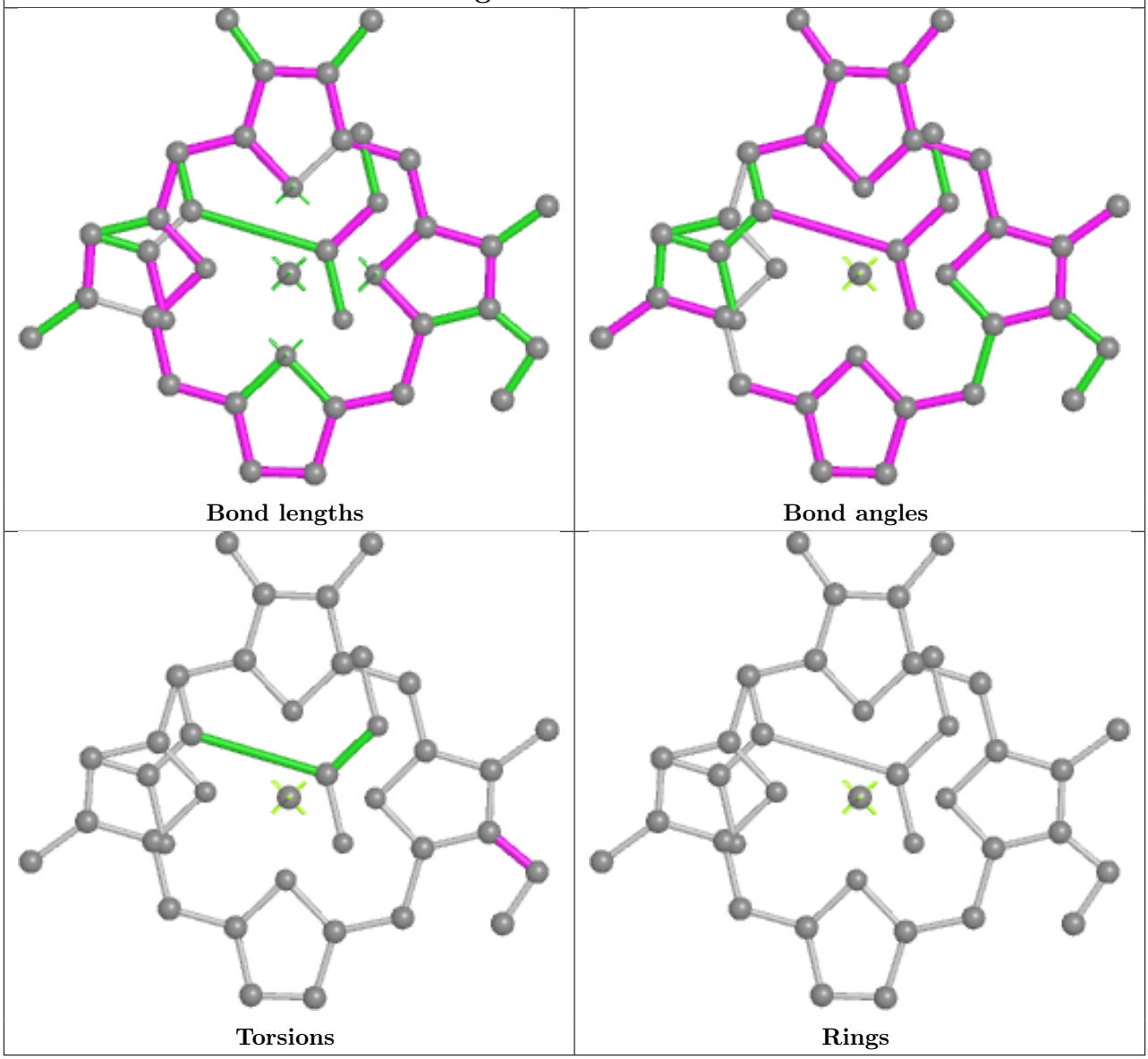


Rings

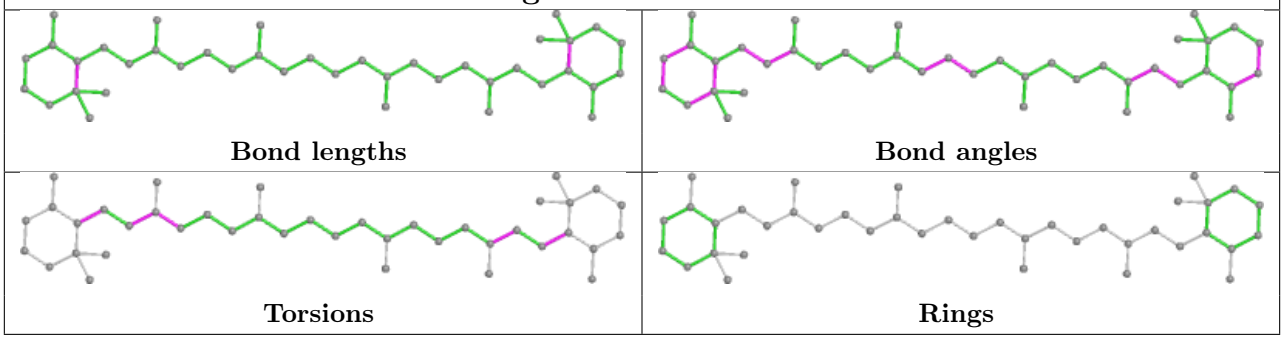
Ligand A86 2 308



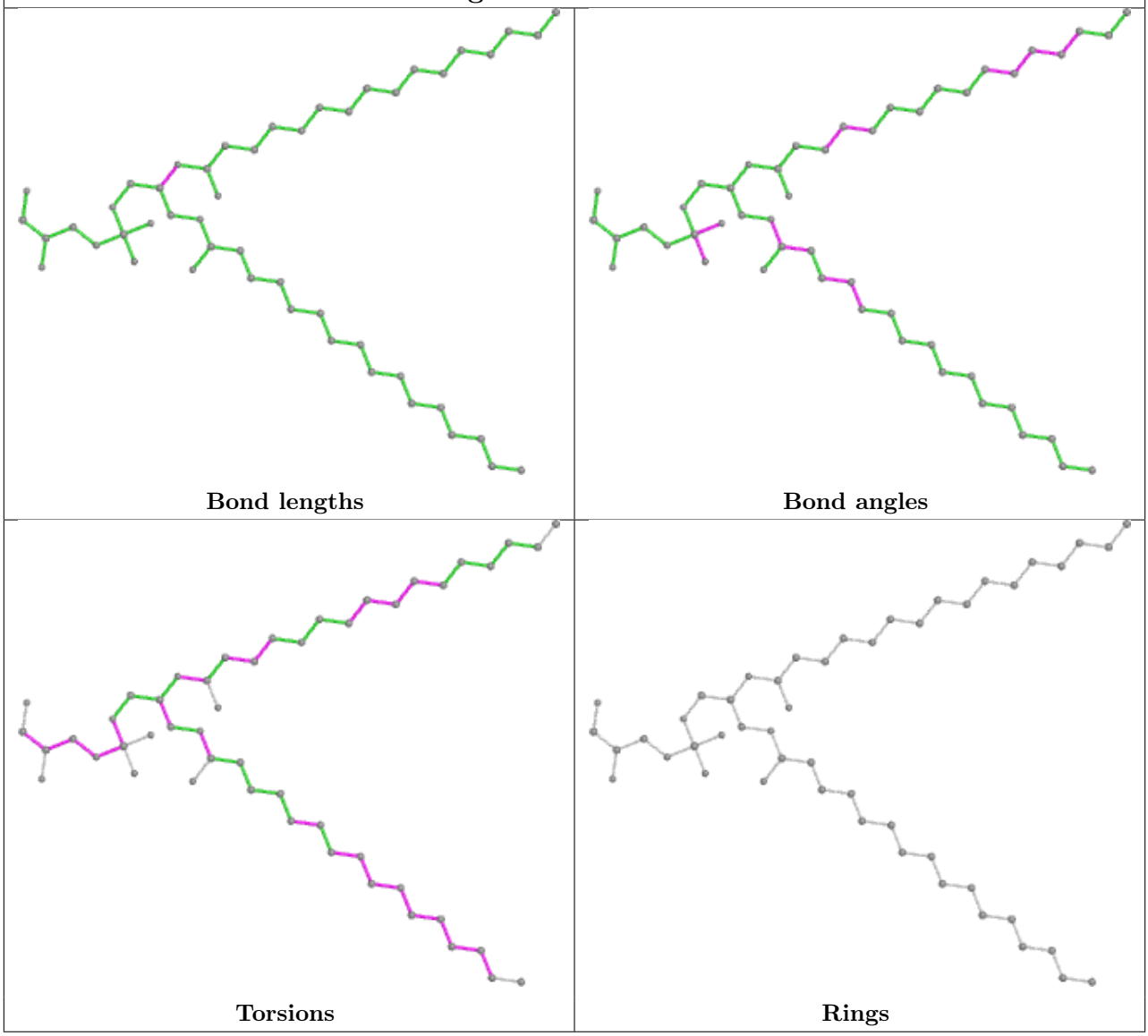
Ligand KC1 4 306



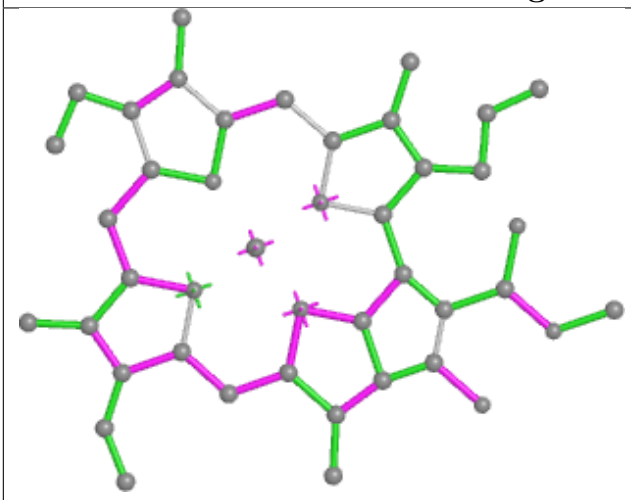
Ligand BCR H 100



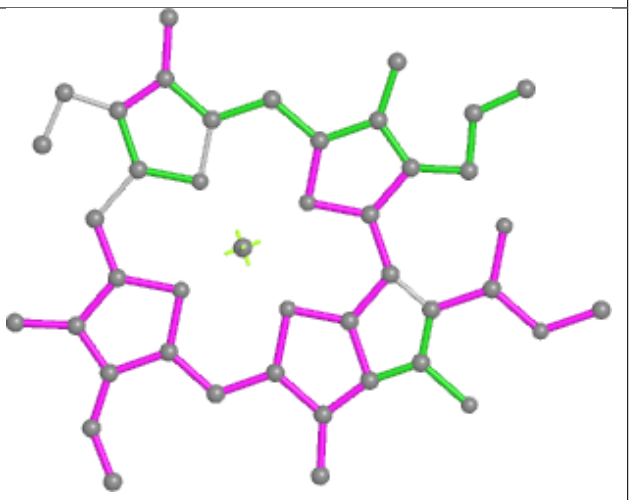
Ligand LHG A 406



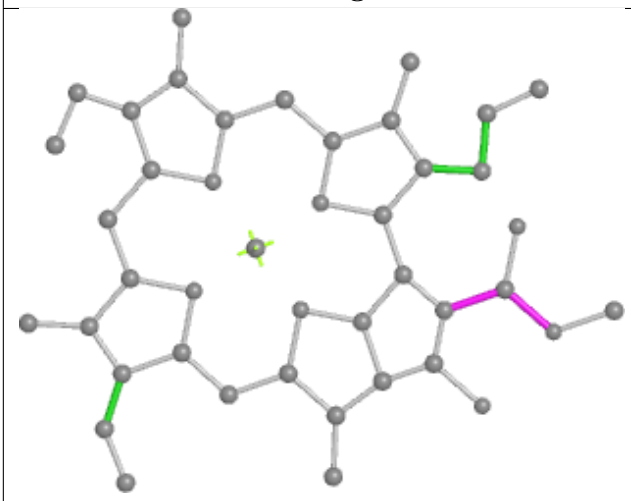
Ligand CLA J 304



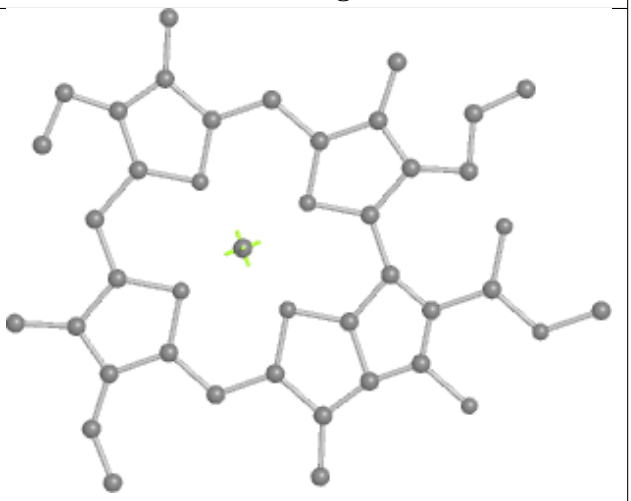
Bond lengths



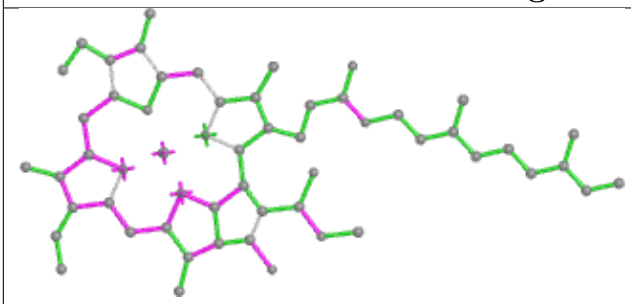
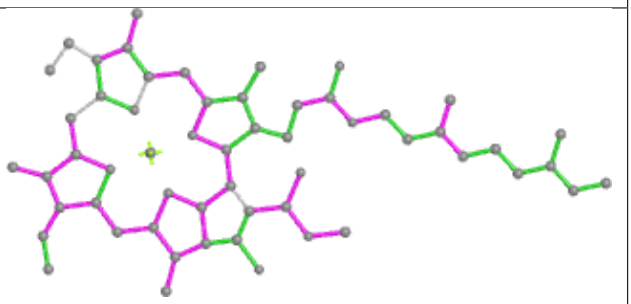
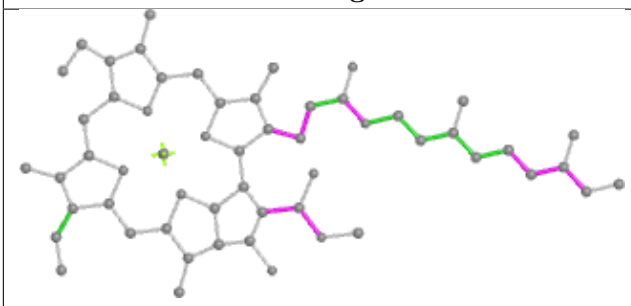
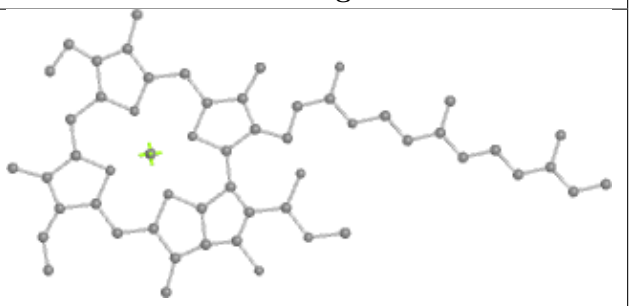
Bond angles

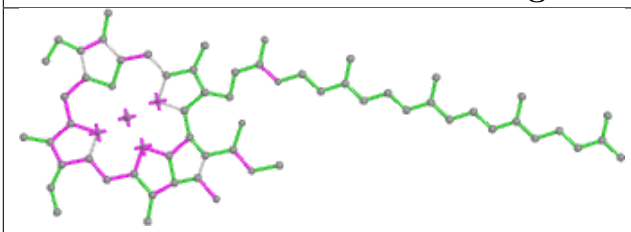
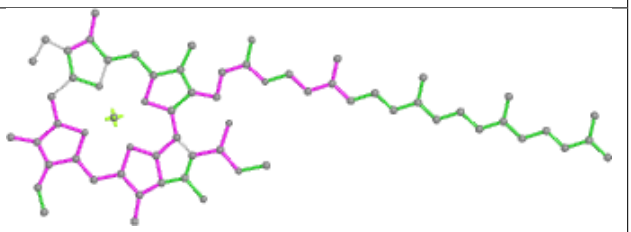
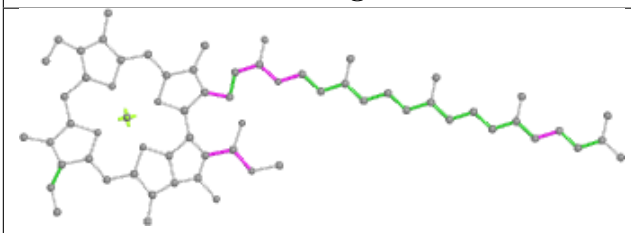
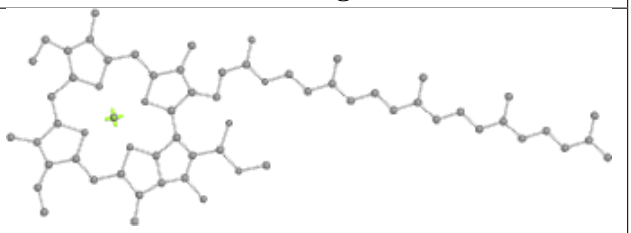


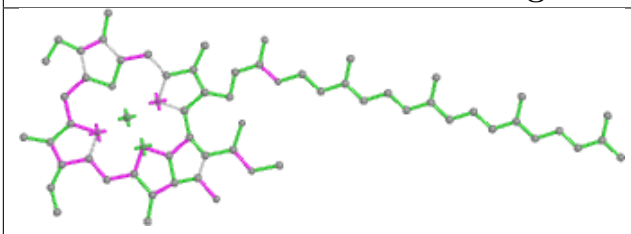
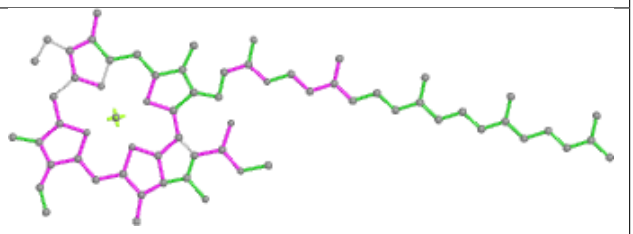
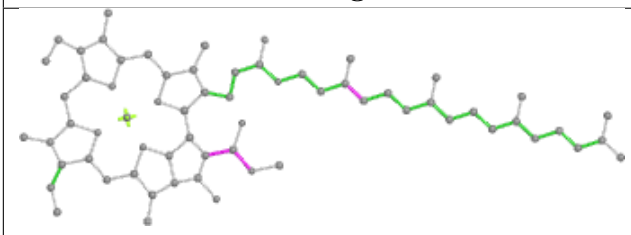
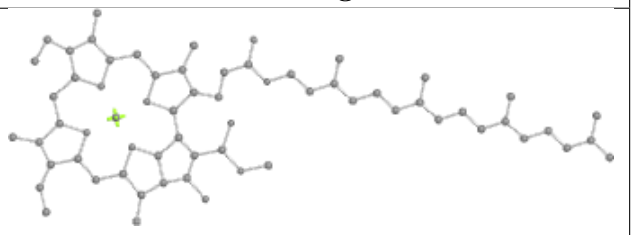
Torsions

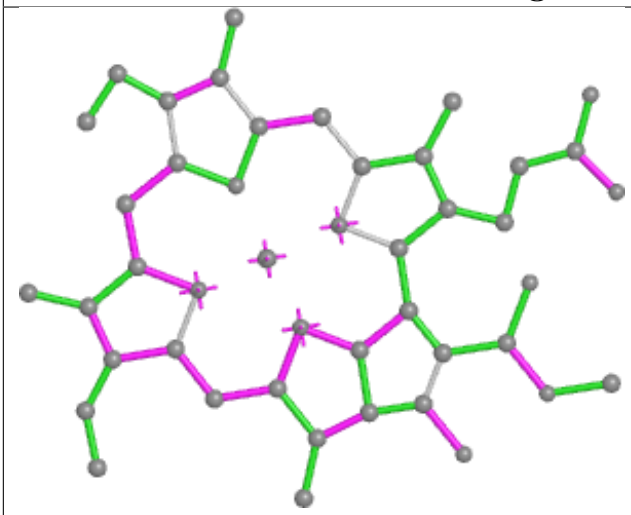
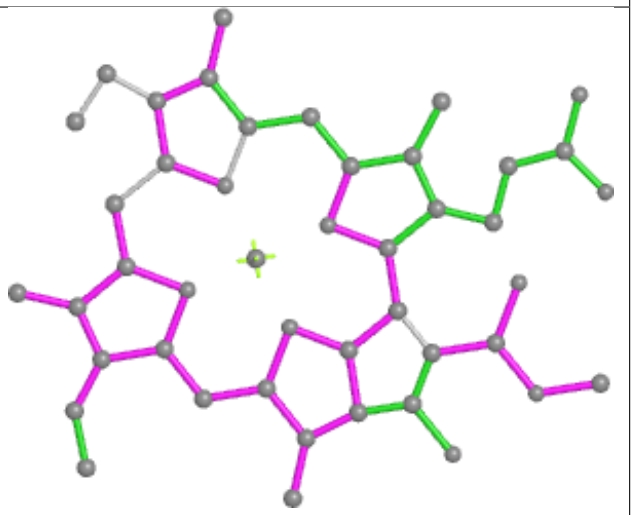
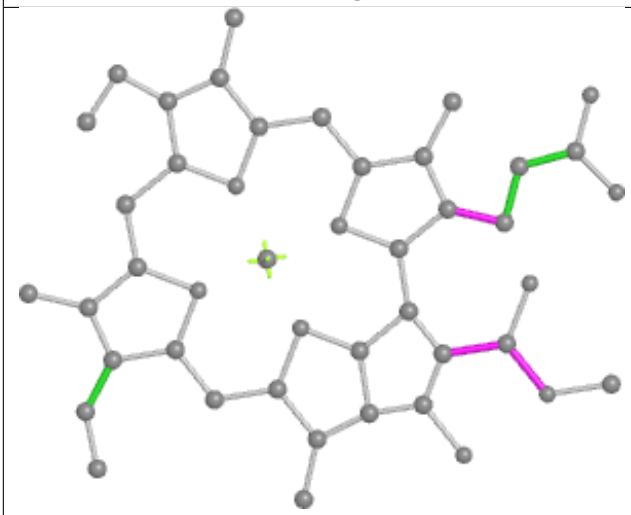
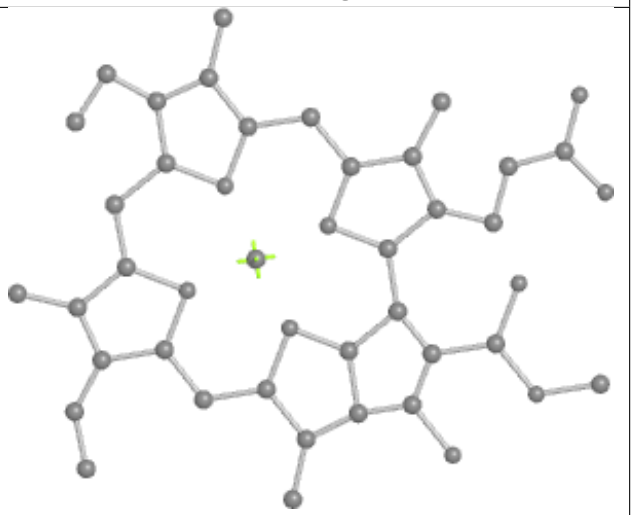


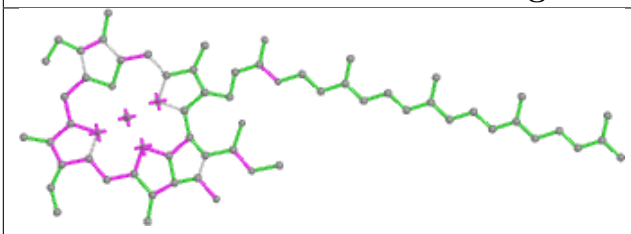
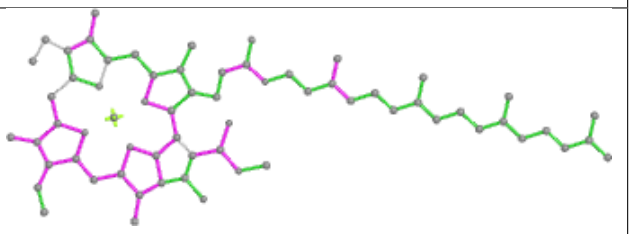
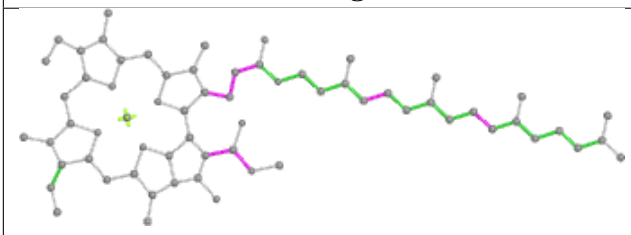
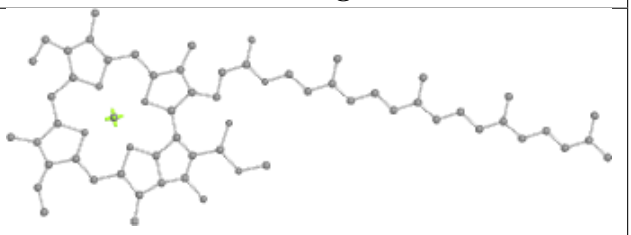
Rings

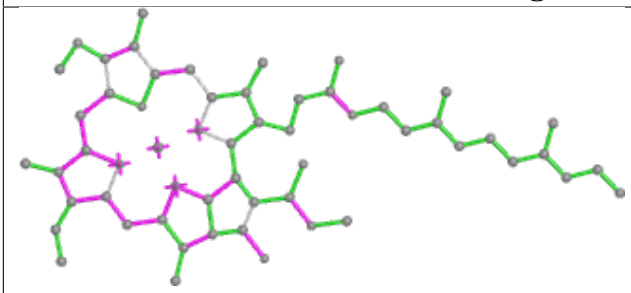
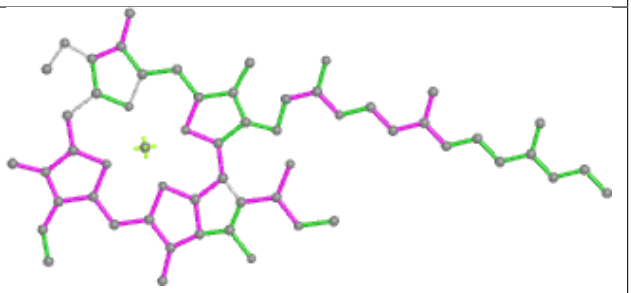
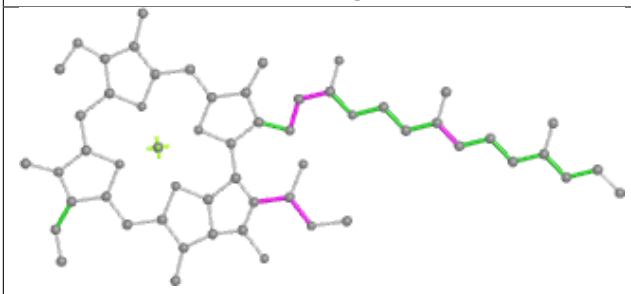
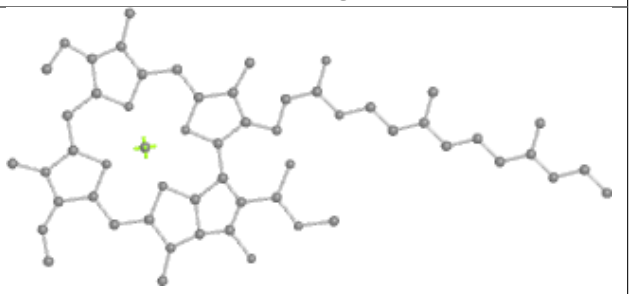
Ligand CLA 4 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

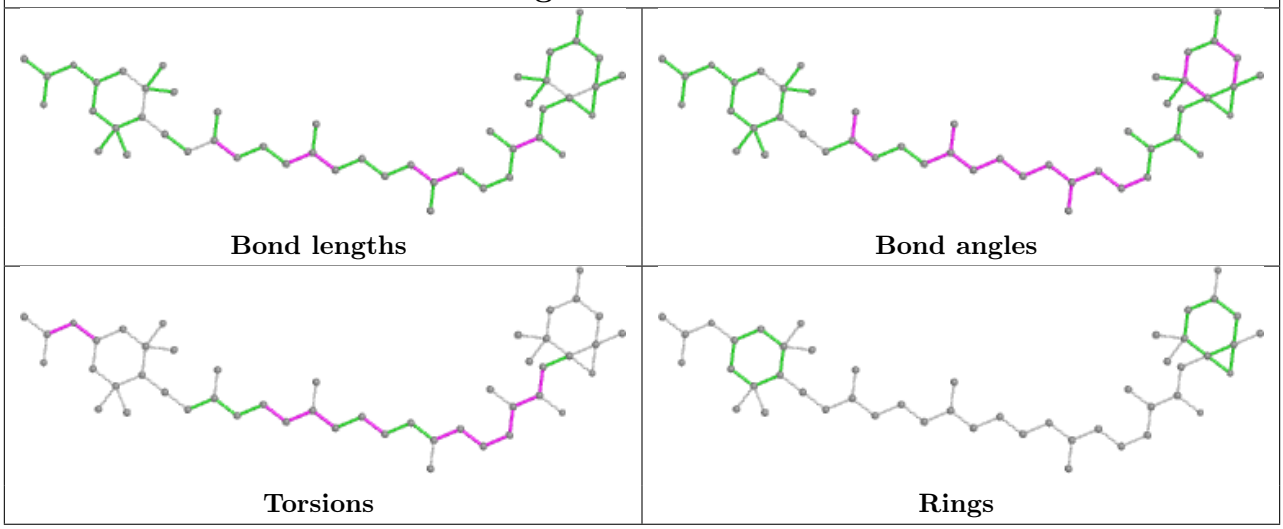
Ligand CLA b 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

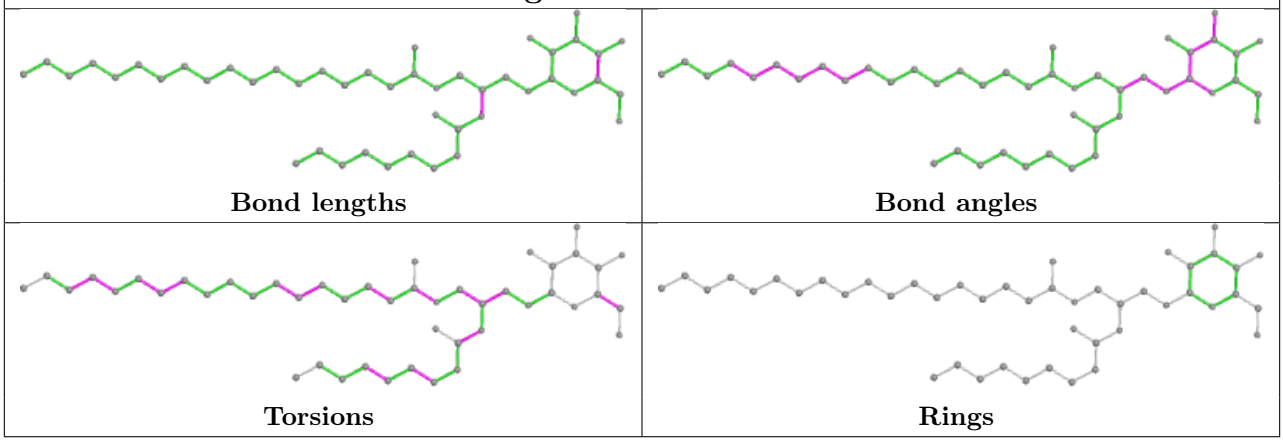
Ligand CLA 1 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

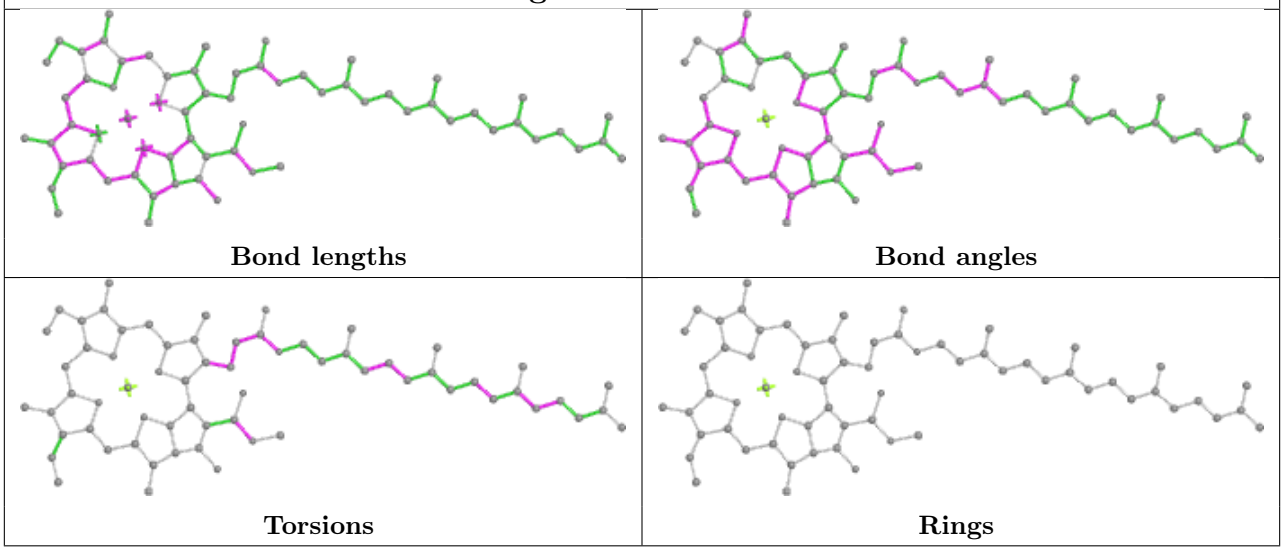
Ligand A86 7 312

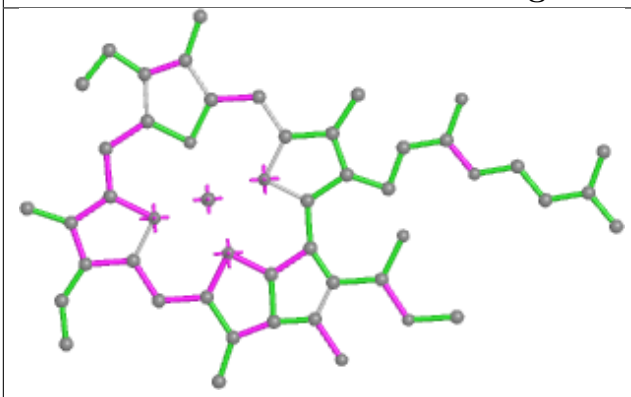
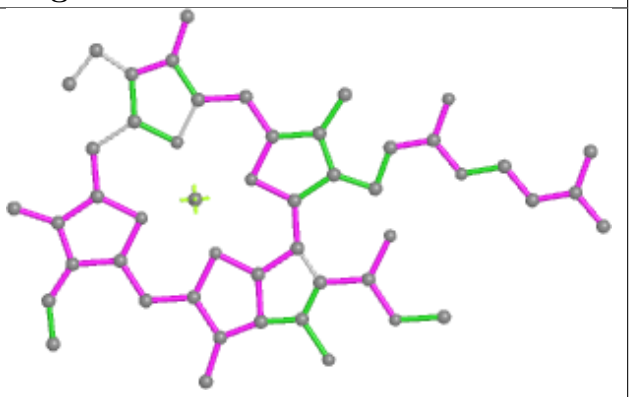
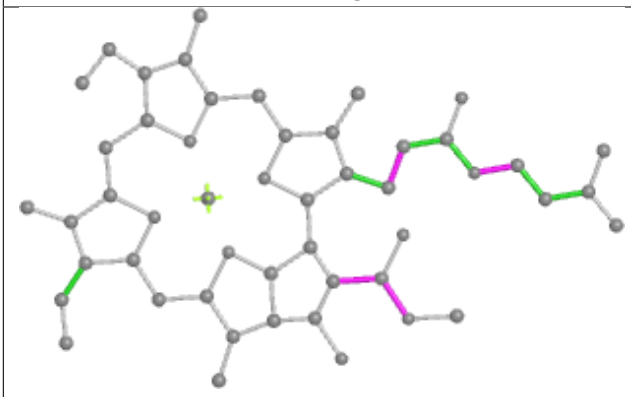
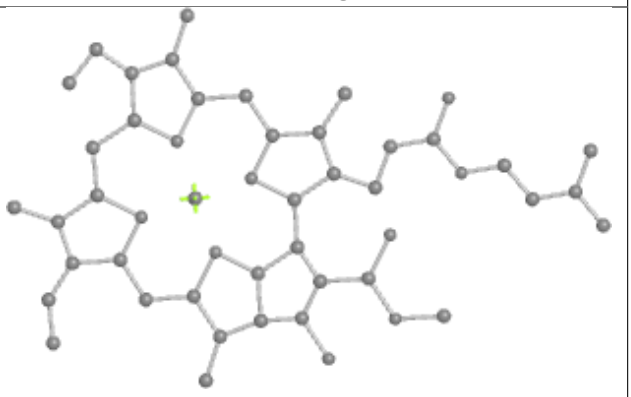


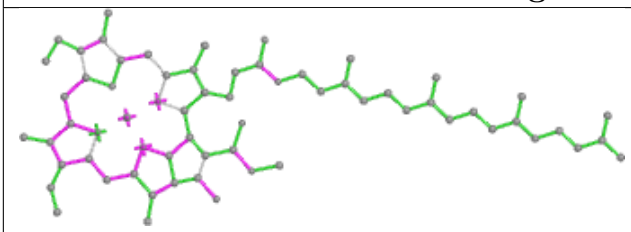
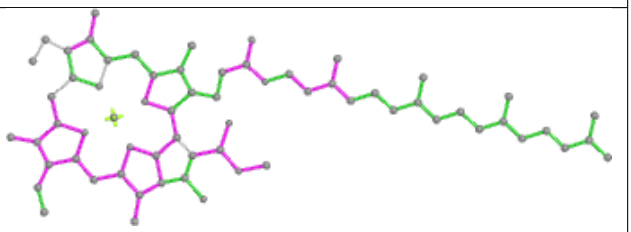
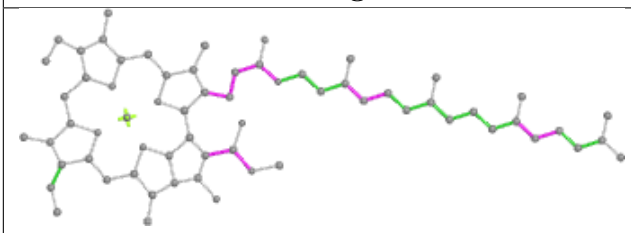
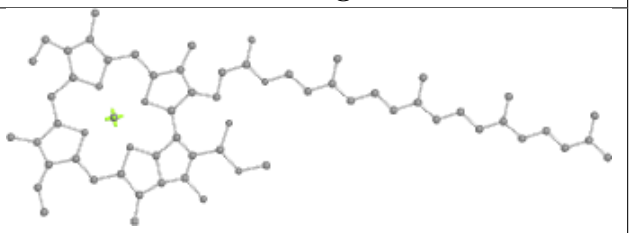
Ligand LMG 2 318



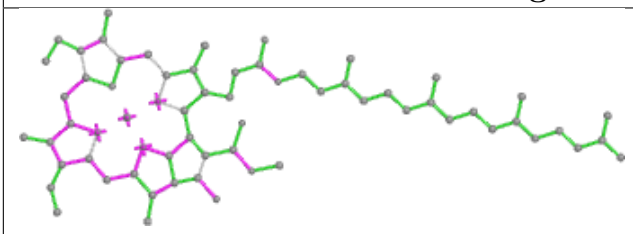
Ligand CLA 7 303



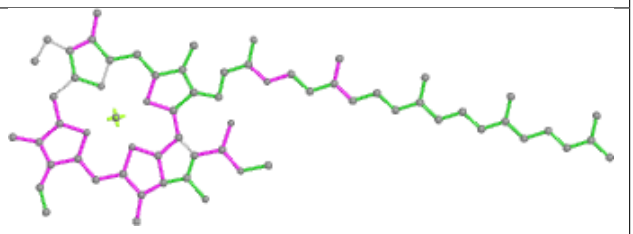
Ligand CLA g 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

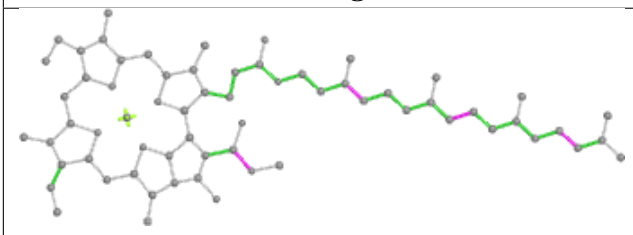
Ligand CLA c 512



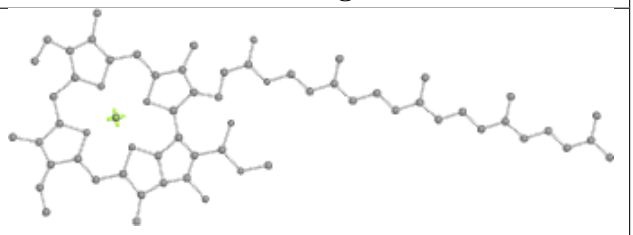
Bond lengths



Bond angles

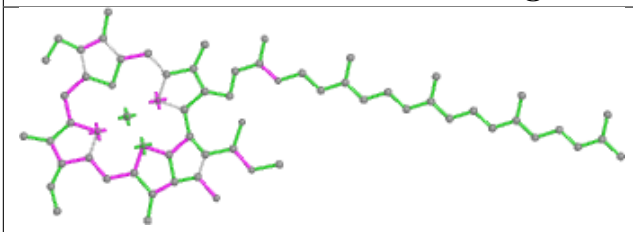


Torsions

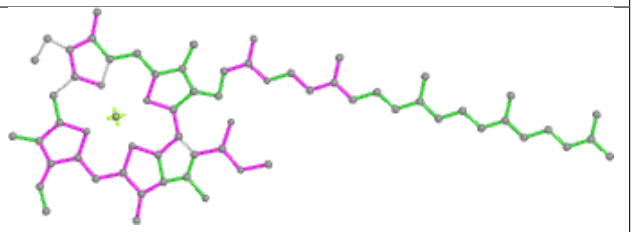


Rings

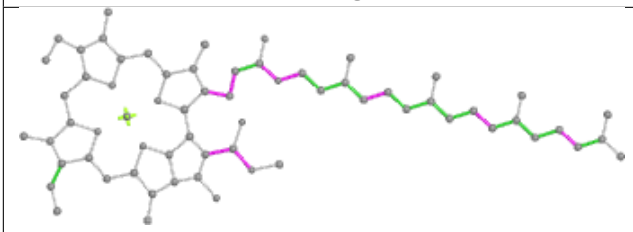
Ligand CLA B 616



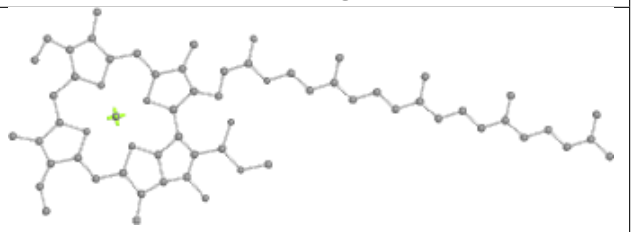
Bond lengths



Bond angles

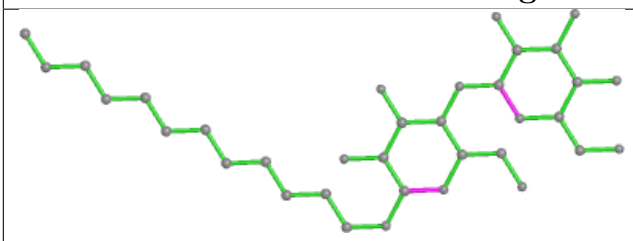


Torsions

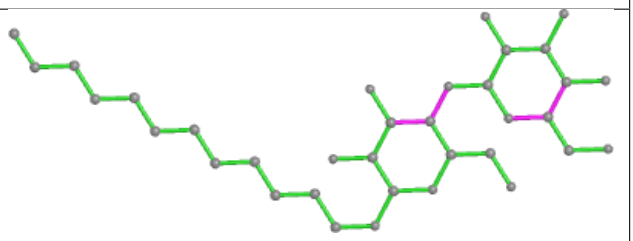


Rings

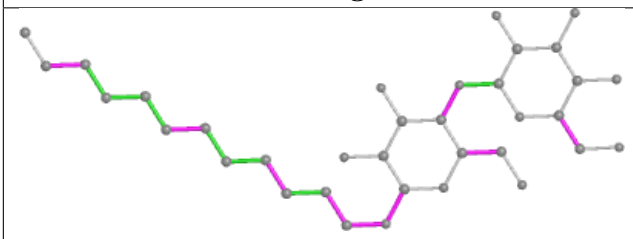
Ligand LMU D 412



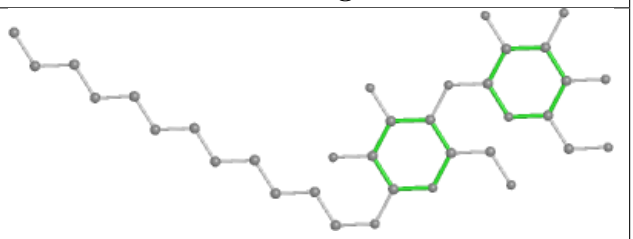
Bond lengths



Bond angles

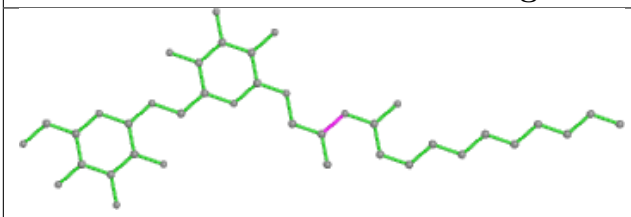


Torsions

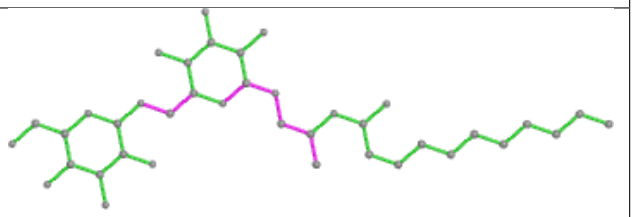


Rings

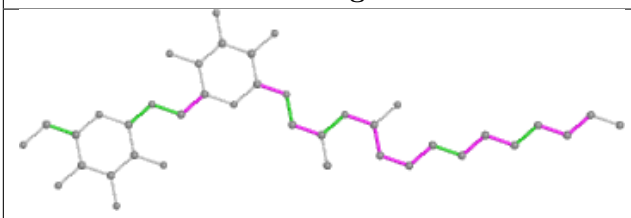
Ligand DGD C 518



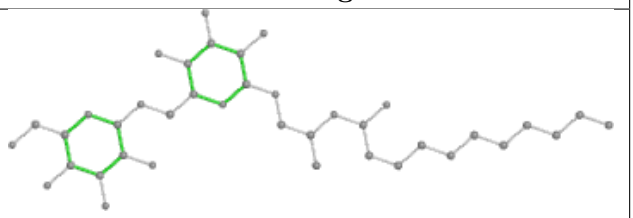
Bond lengths



Bond angles

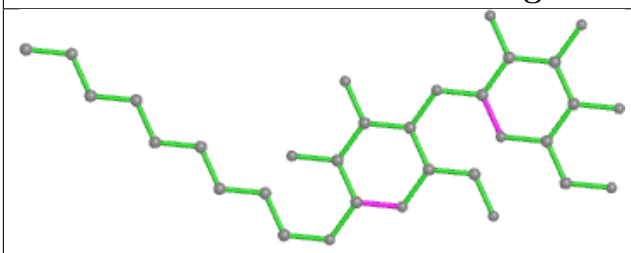


Torsions

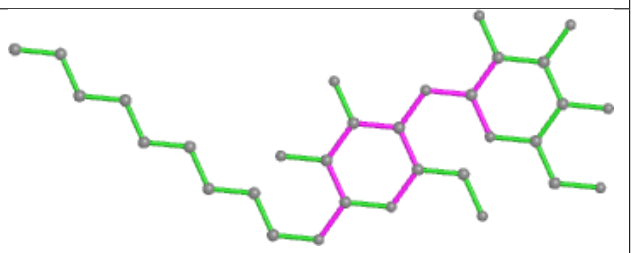


Rings

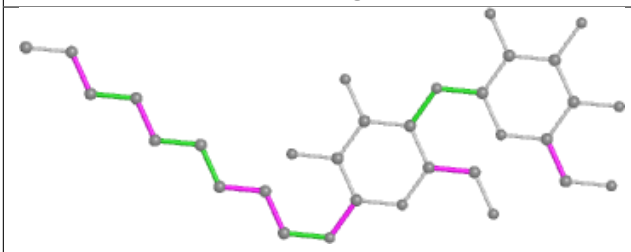
Ligand LMU 5 301



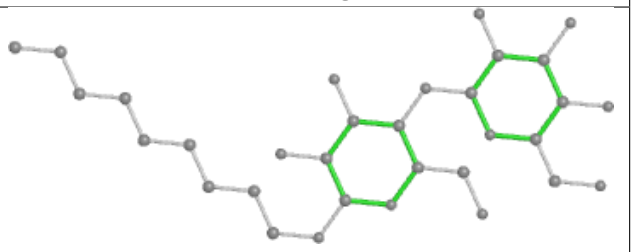
Bond lengths



Bond angles

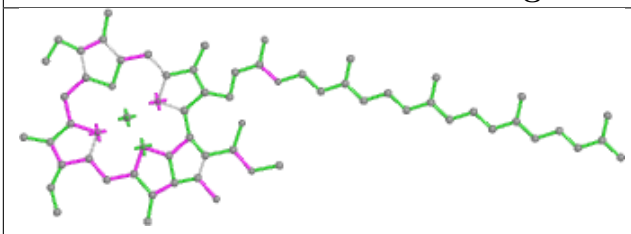


Torsions

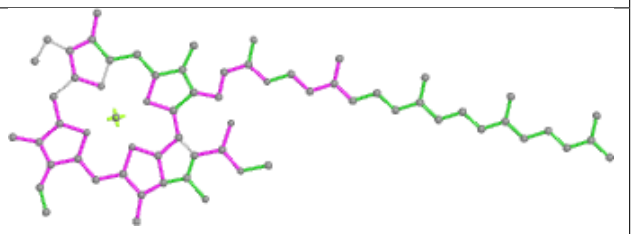


Rings

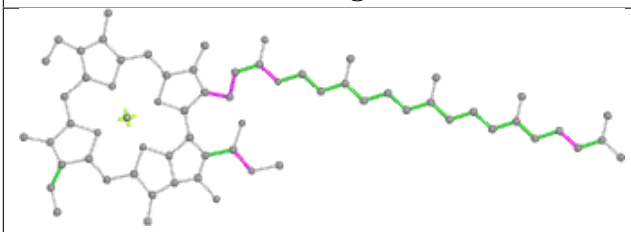
Ligand CLA A 401



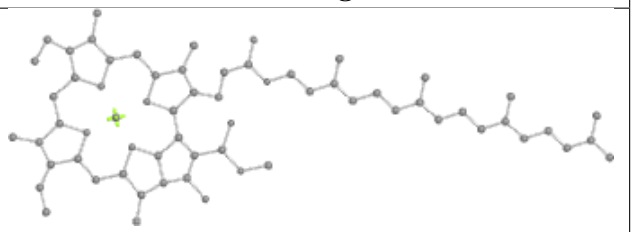
Bond lengths



Bond angles

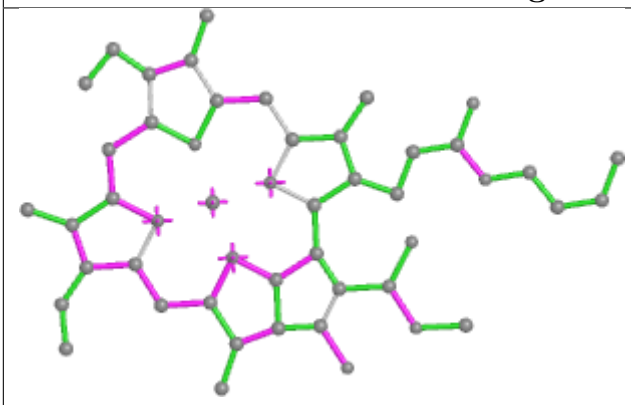


Torsions

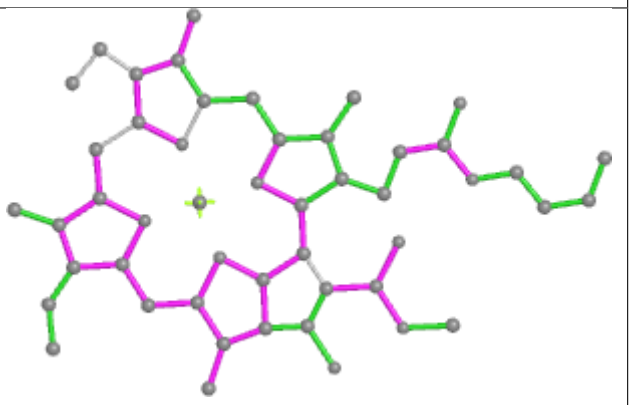


Rings

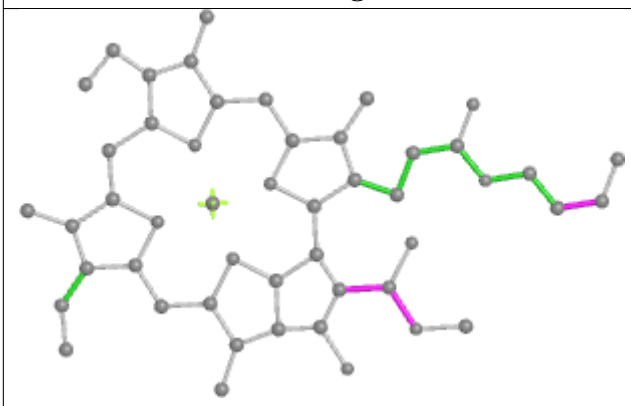
Ligand CLA a 403



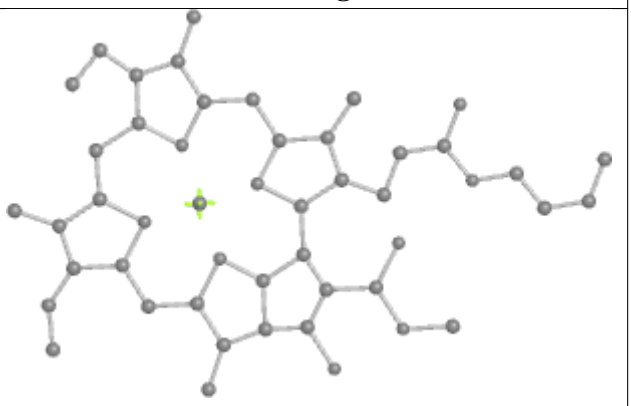
Bond lengths



Bond angles

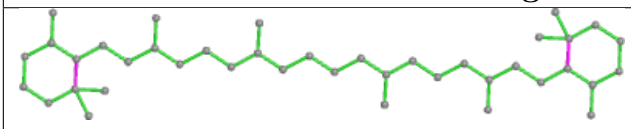


Torsions

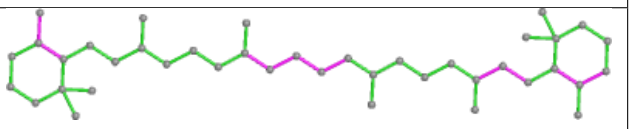


Rings

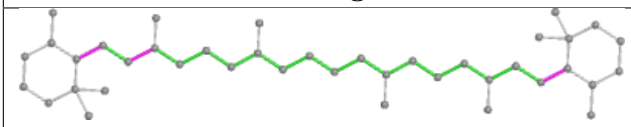
Ligand BCR A 405



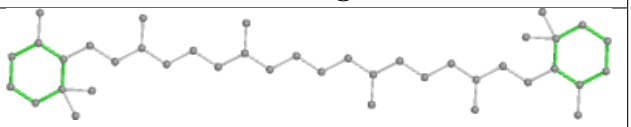
Bond lengths



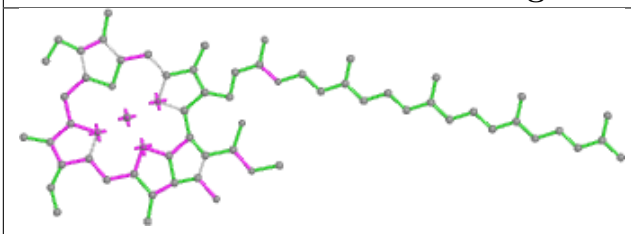
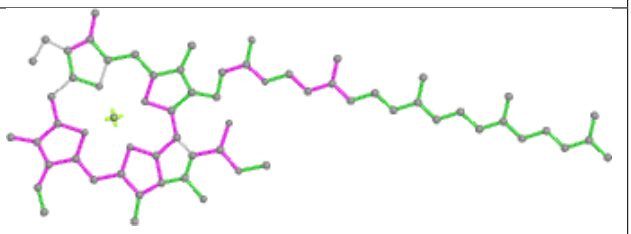
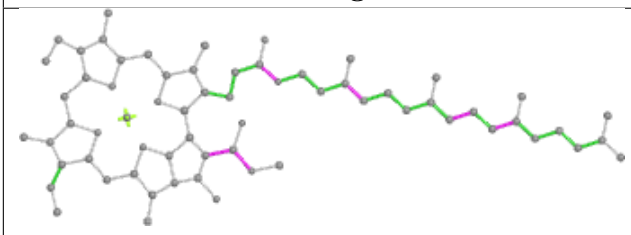
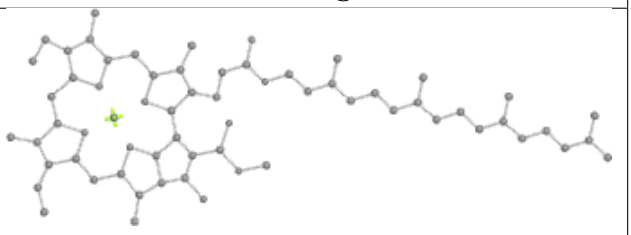
Bond angles

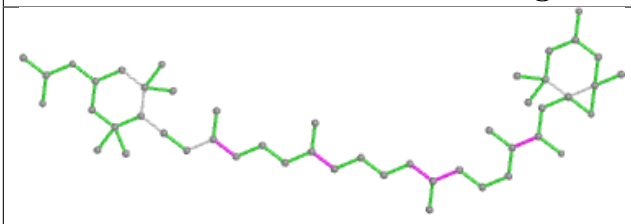
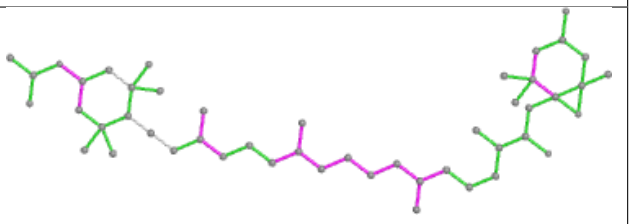
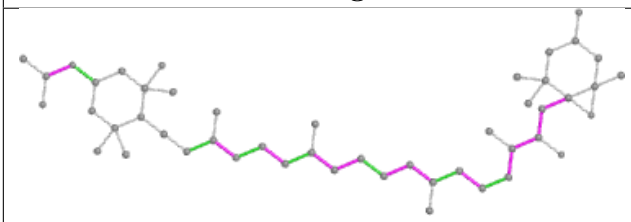
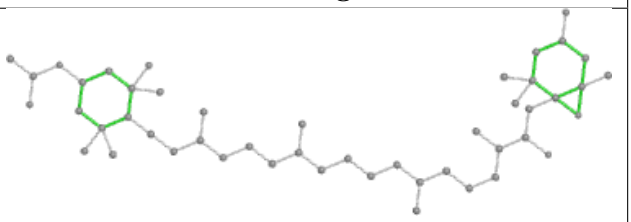


Torsions

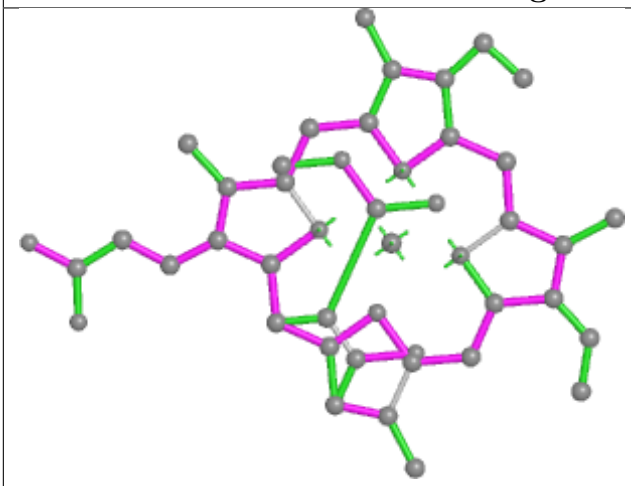


Rings

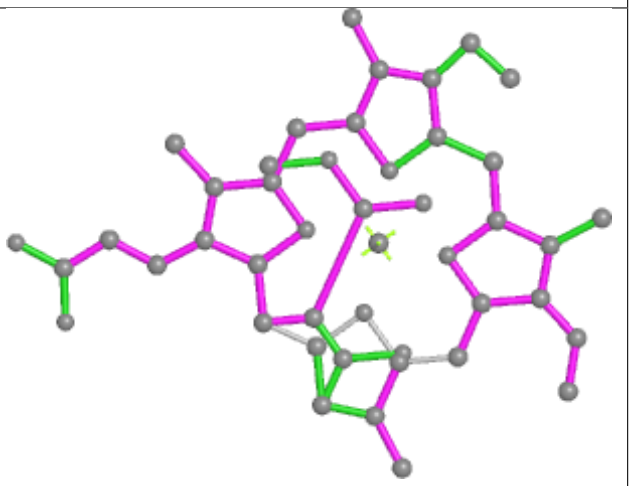
Ligand CLA b 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 J 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

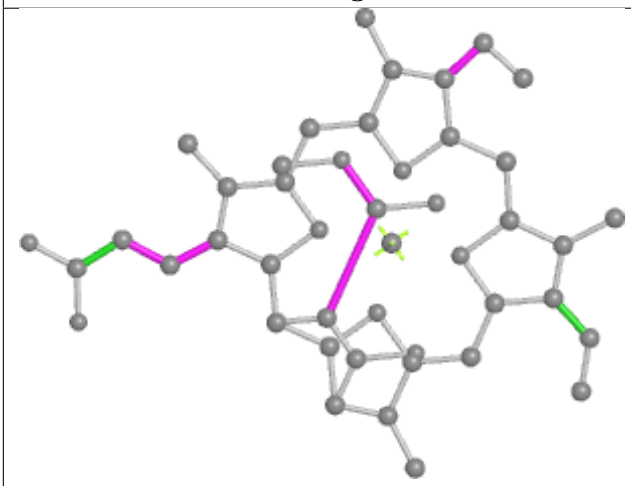
Ligand KC1 J 311



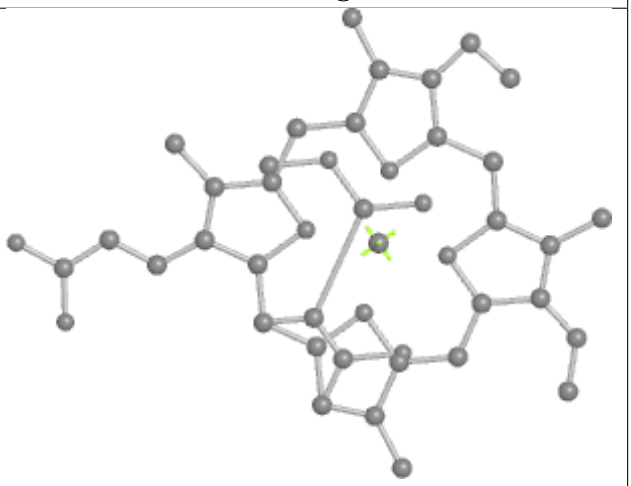
Bond lengths



Bond angles

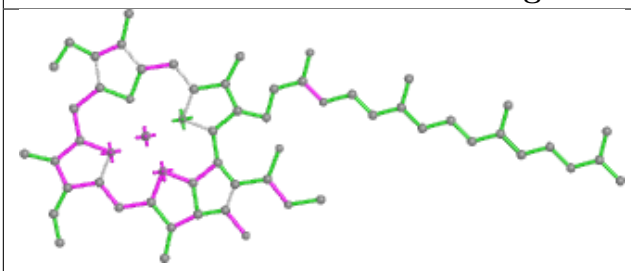


Torsions

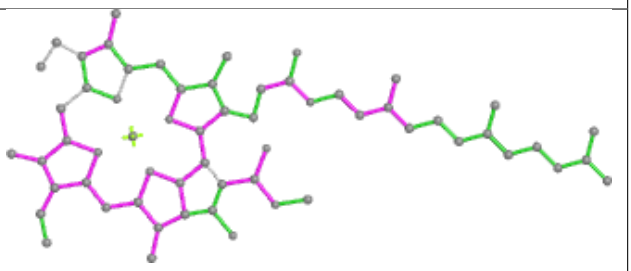


Rings

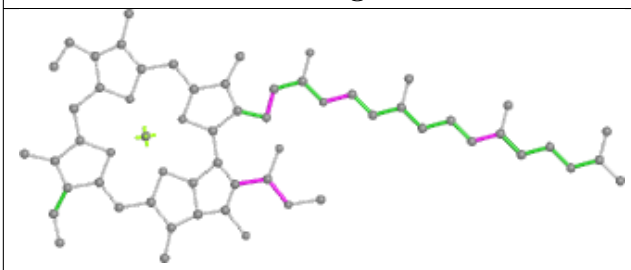
Ligand CLA A 404



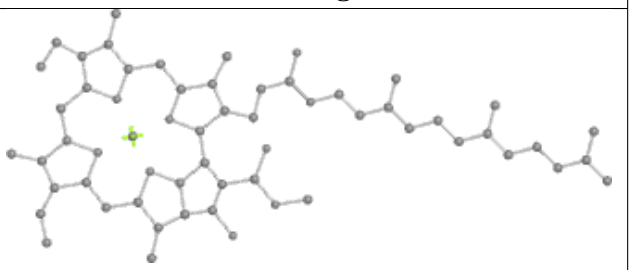
Bond lengths



Bond angles

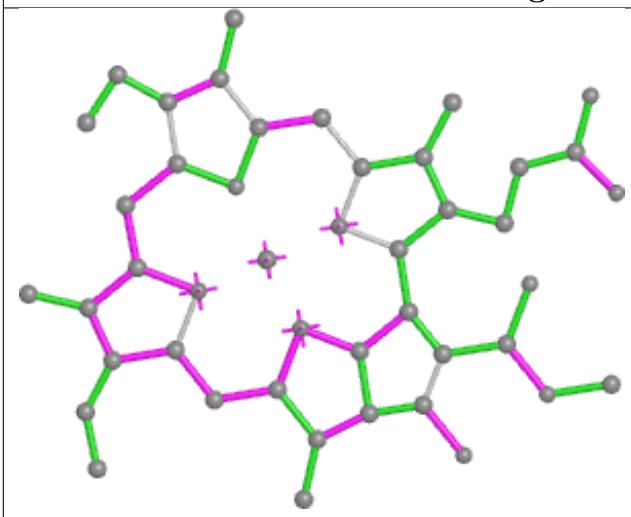


Torsions

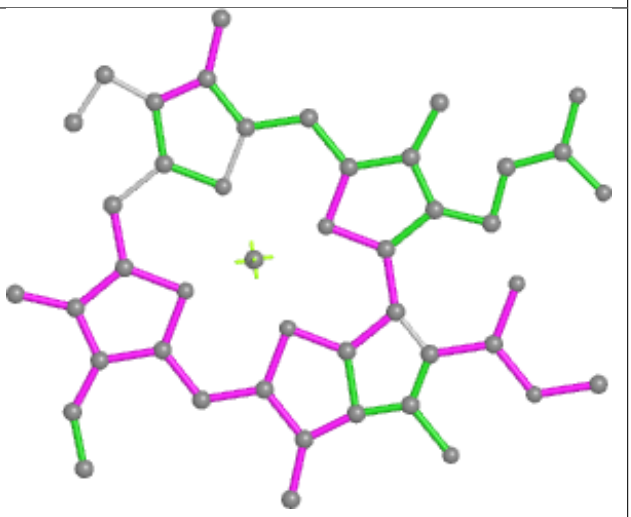


Rings

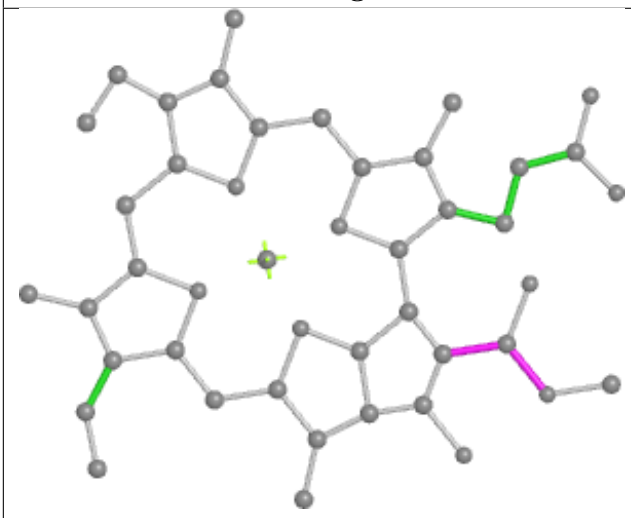
Ligand CLA 6 302



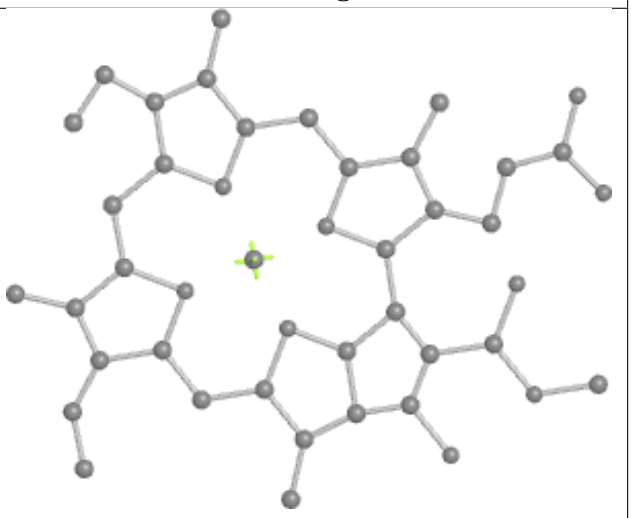
Bond lengths



Bond angles

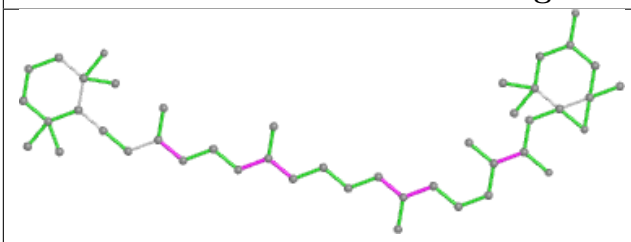


Torsions

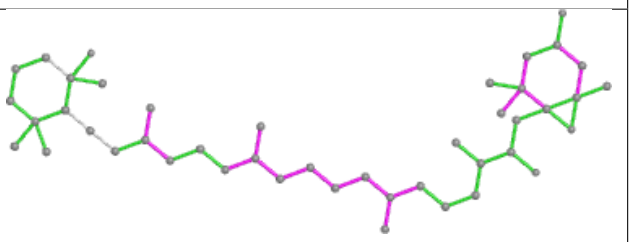


Rings

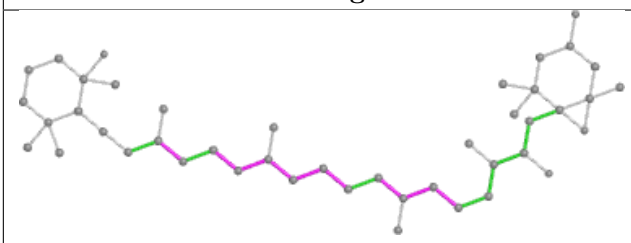
Ligand A86 7 313



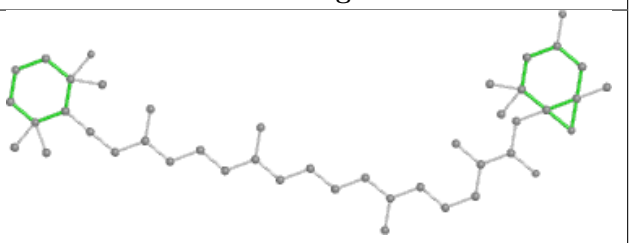
Bond lengths



Bond angles

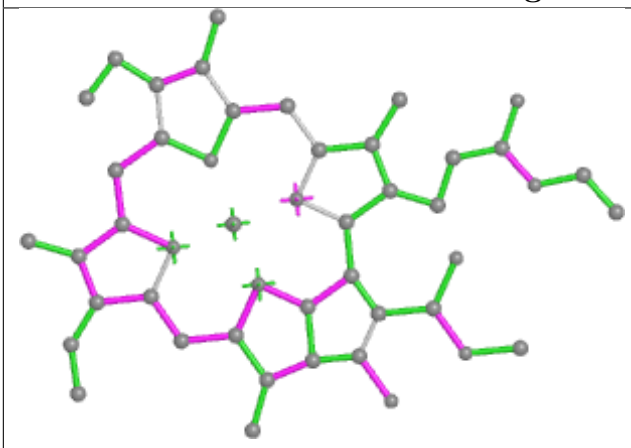


Torsions

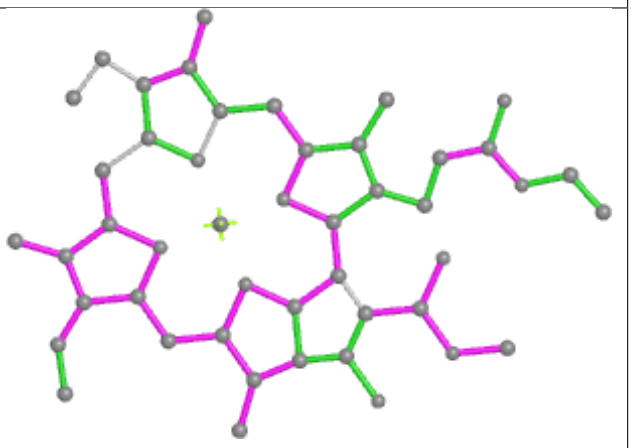


Rings

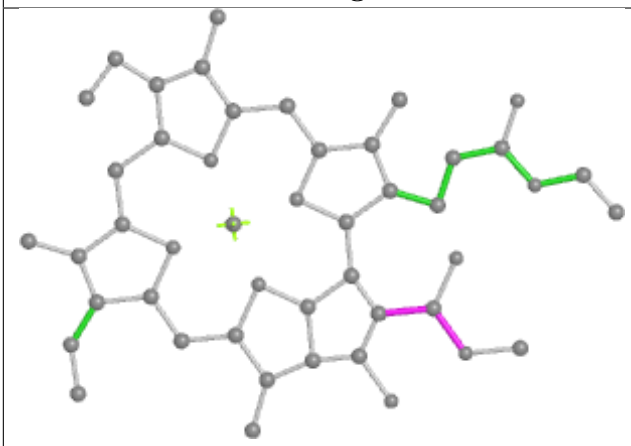
Ligand CLA B 602



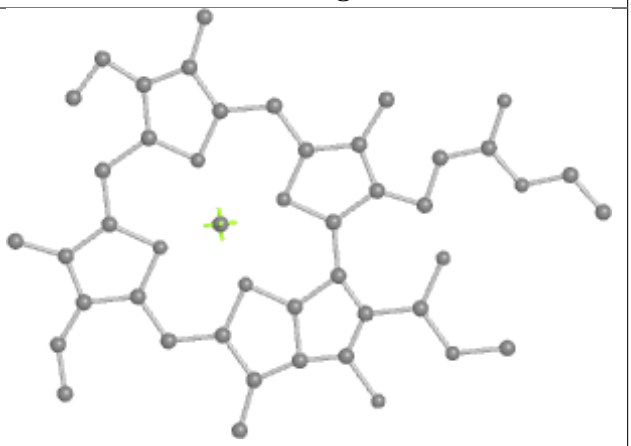
Bond lengths



Bond angles

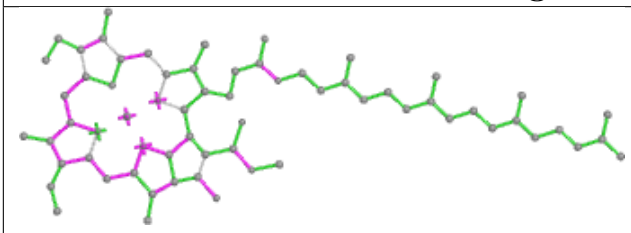


Torsions

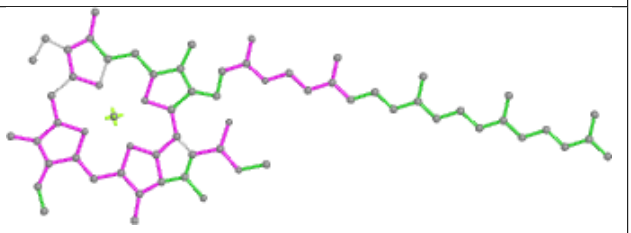


Rings

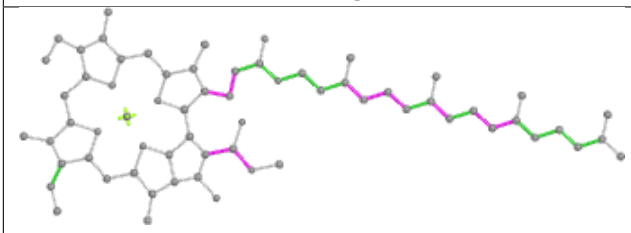
Ligand CLA 2 301



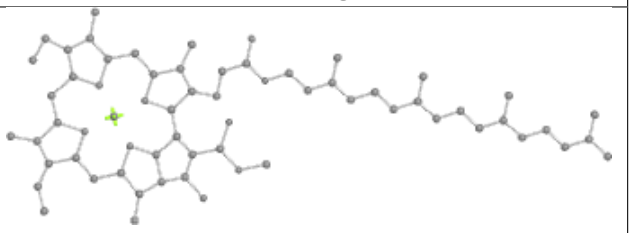
Bond lengths



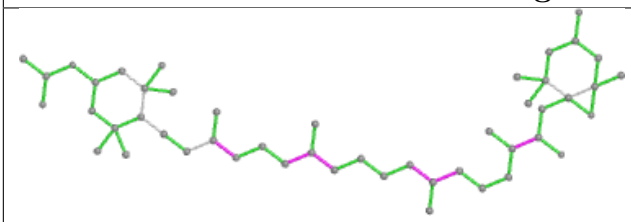
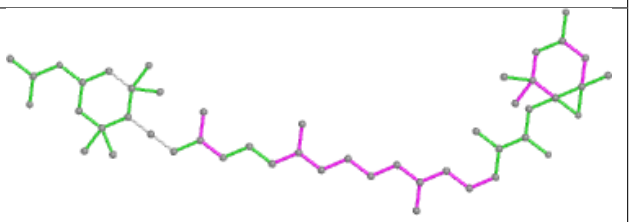
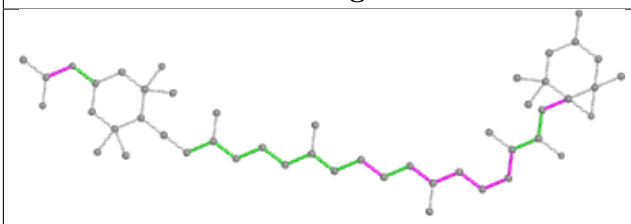
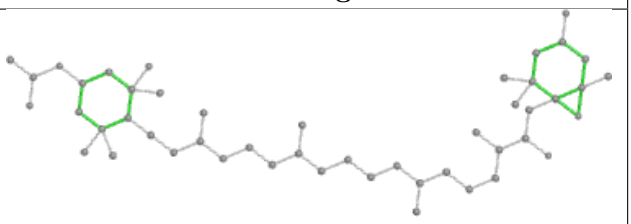
Bond angles

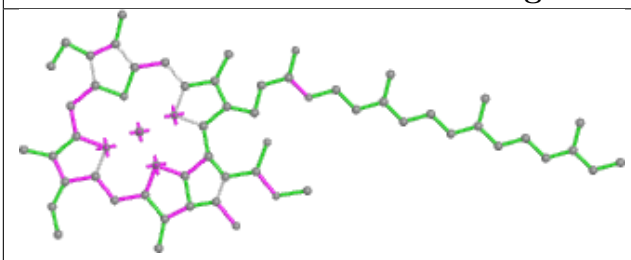
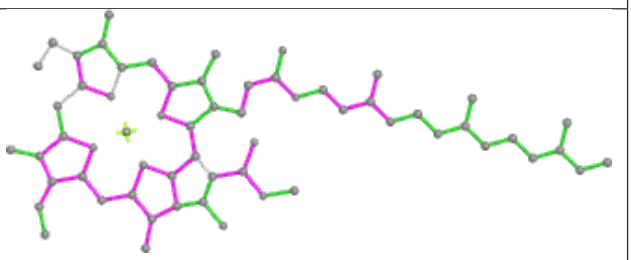
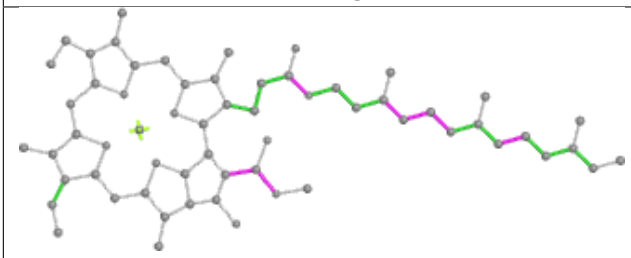
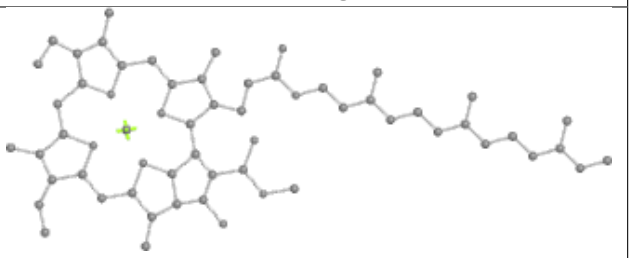


Torsions

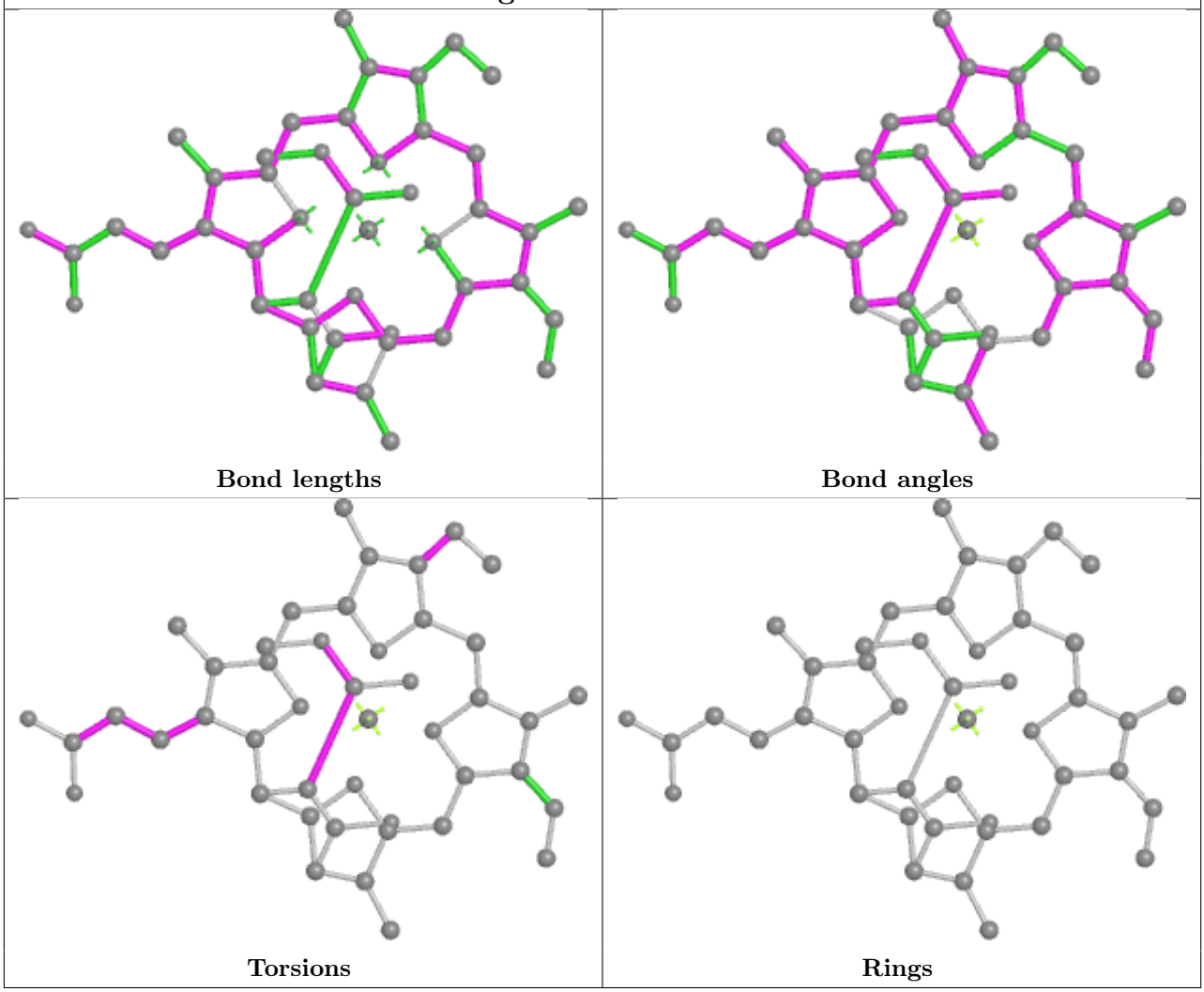


Rings

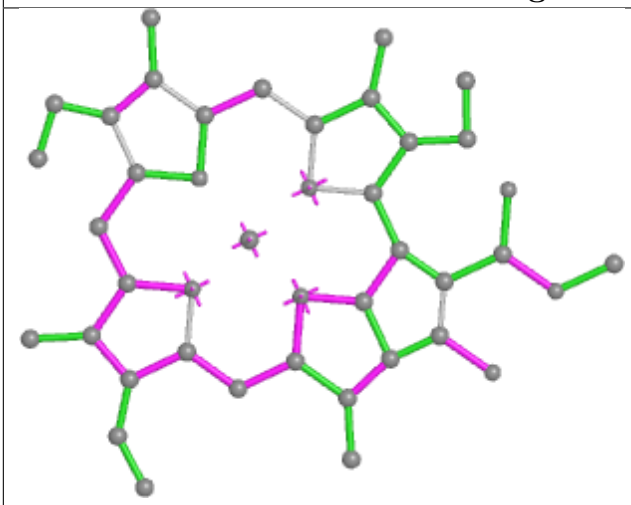
Ligand A86 2 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

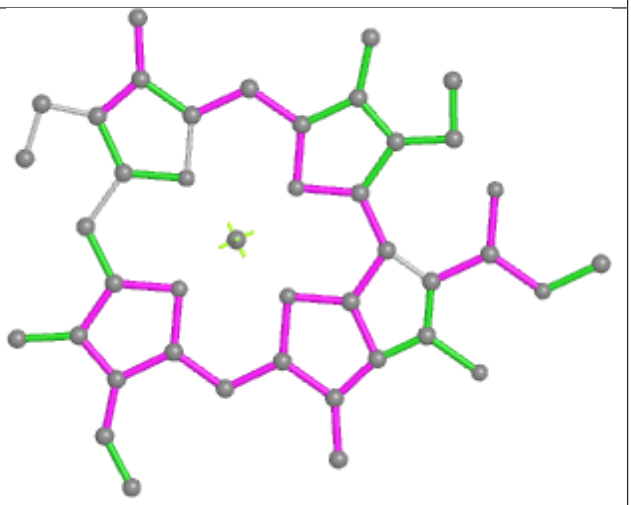
Ligand KC1 6 311



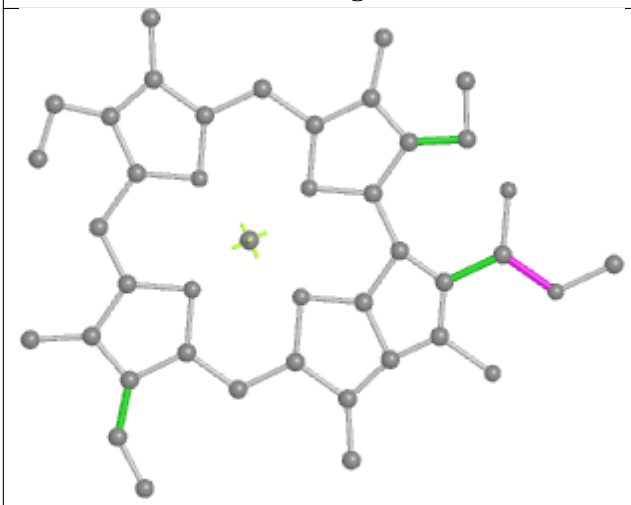
Ligand CLA 3 303



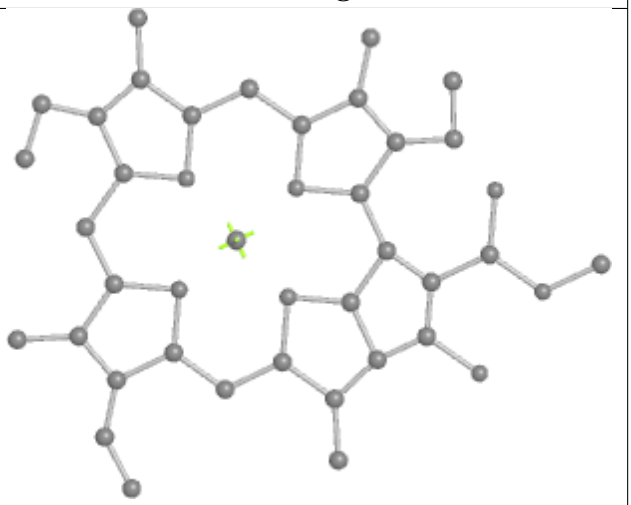
Bond lengths



Bond angles

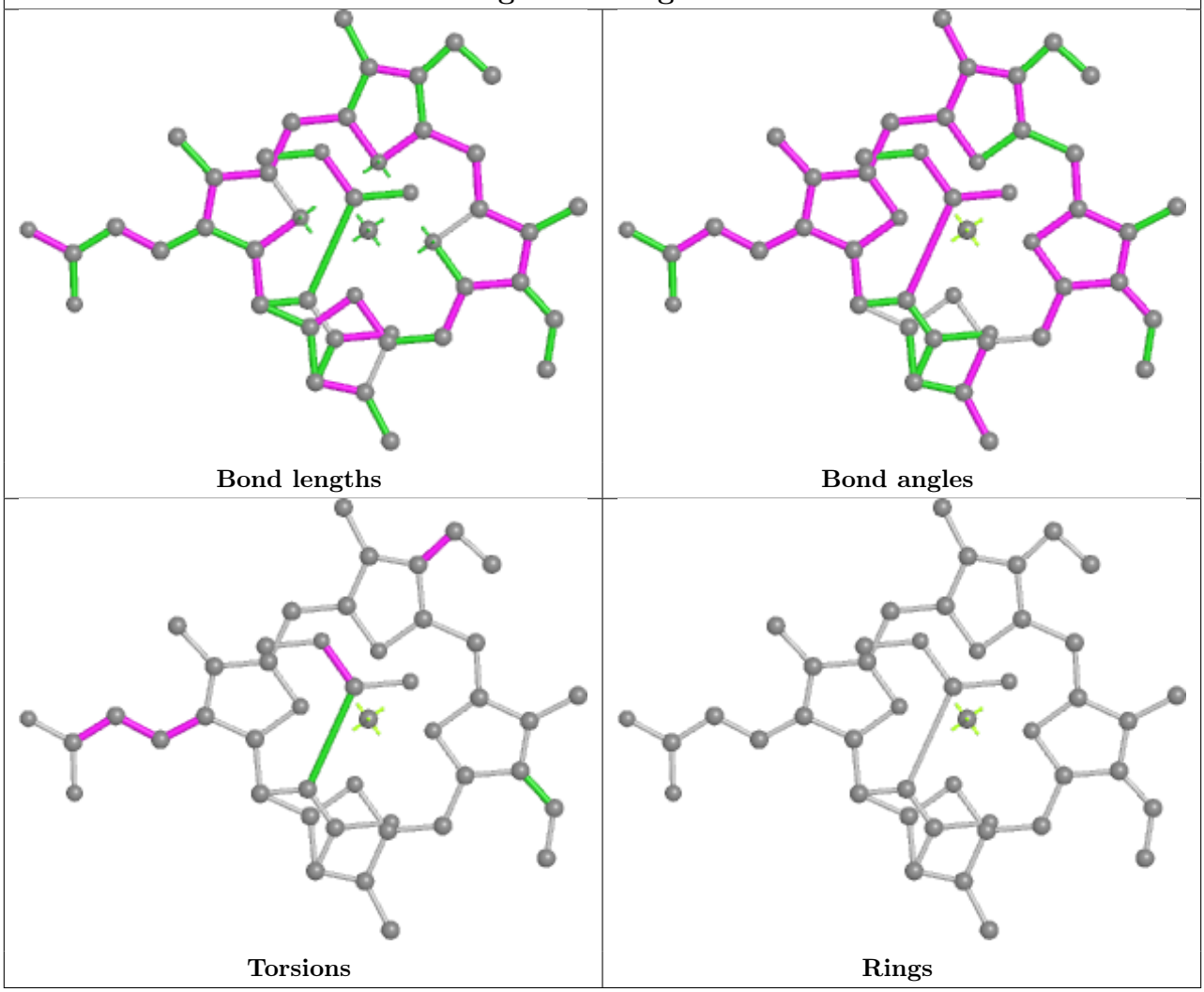


Torsions

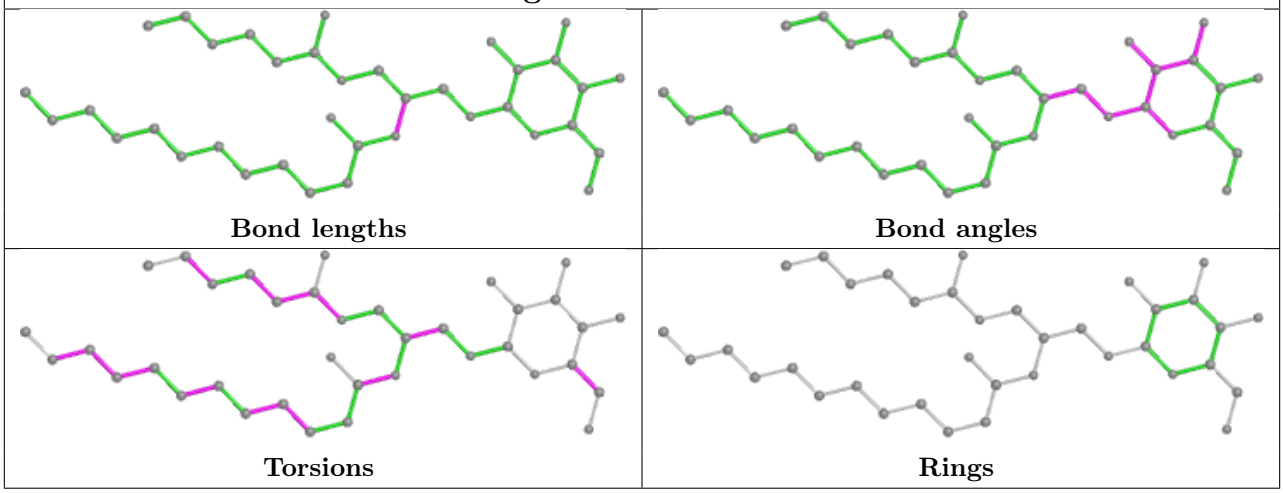


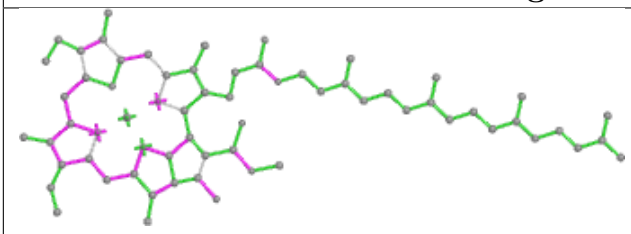
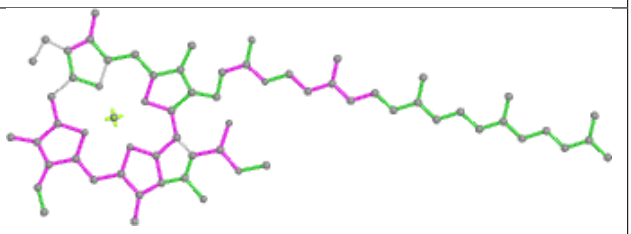
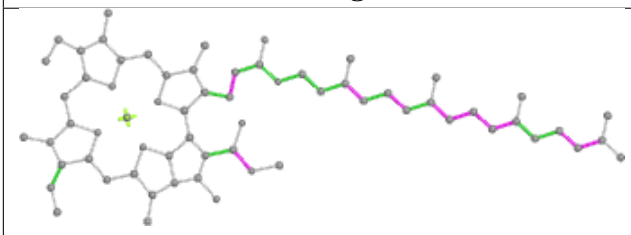
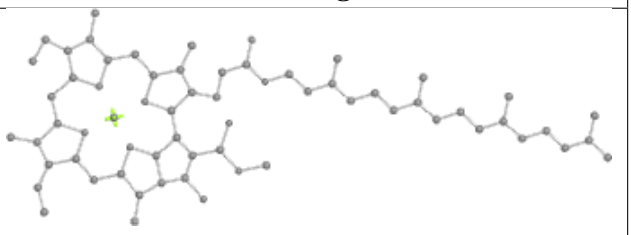
Rings

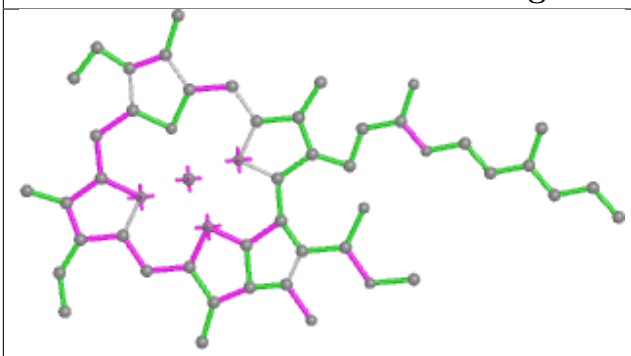
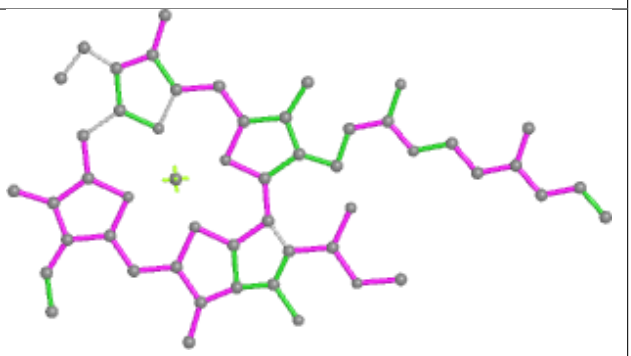
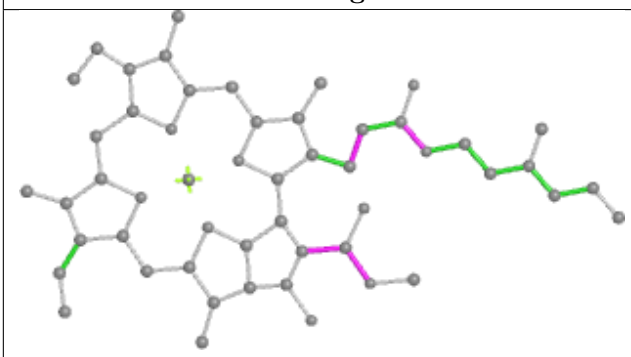
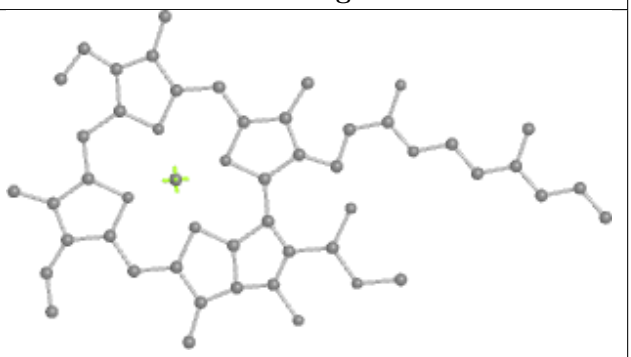
Ligand KC1 g 313

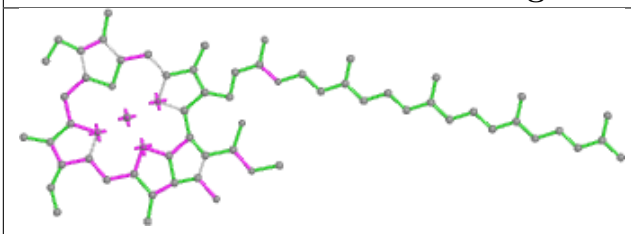
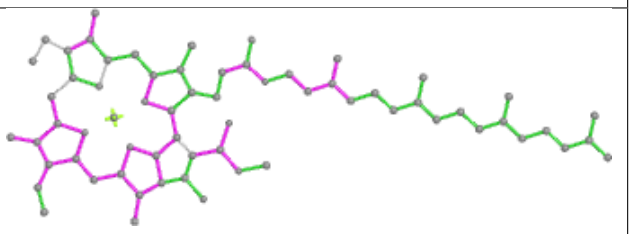
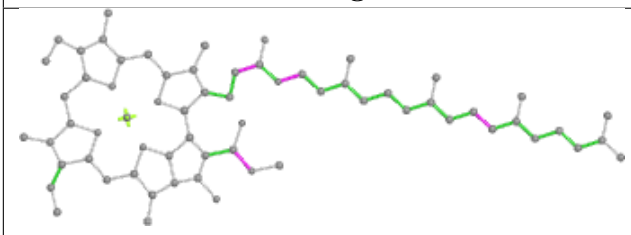
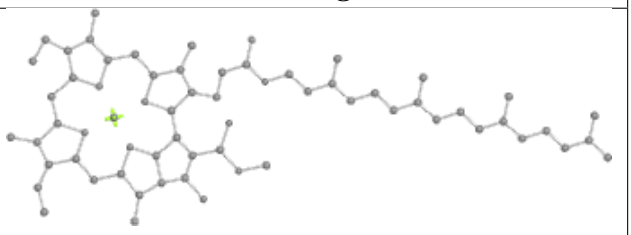


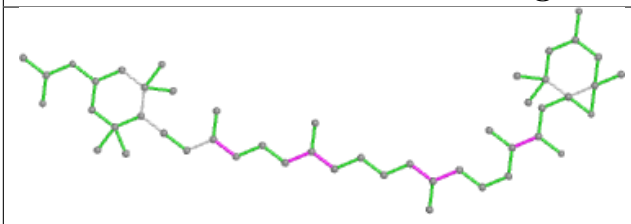
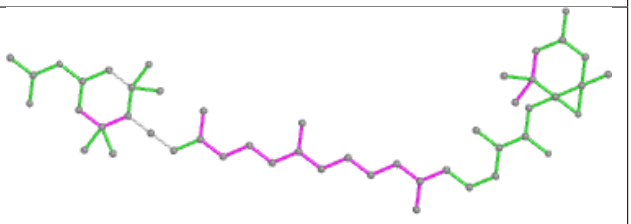
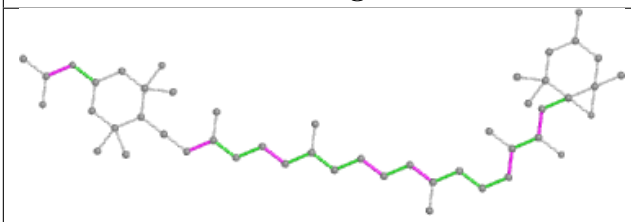
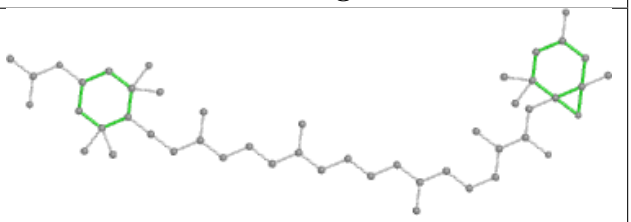
Ligand LMG b 624

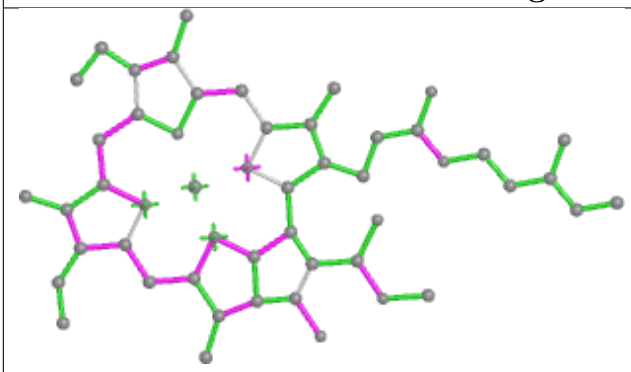
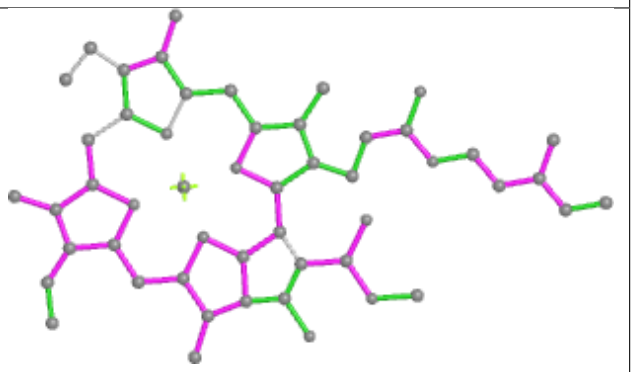
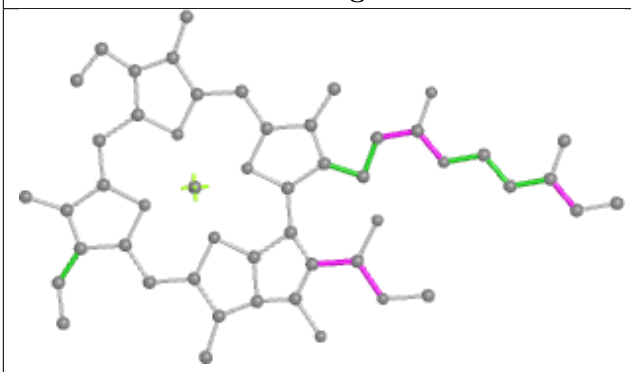
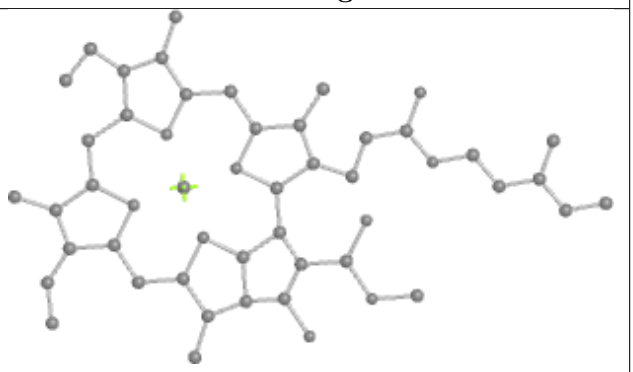


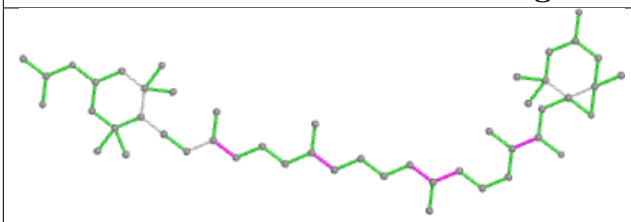
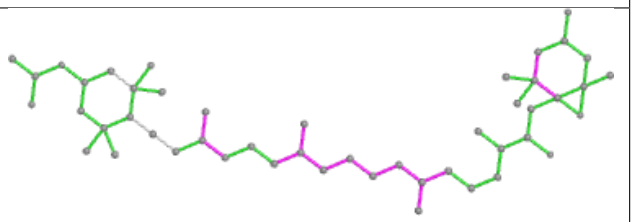
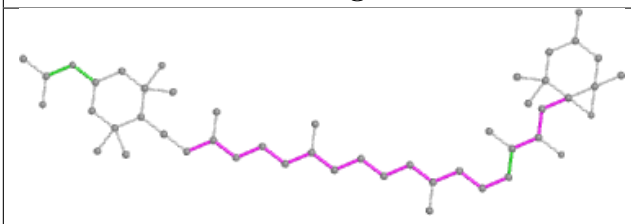
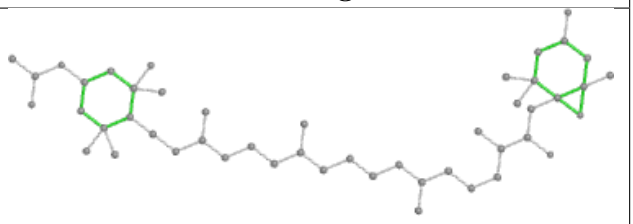
Ligand CLA b 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

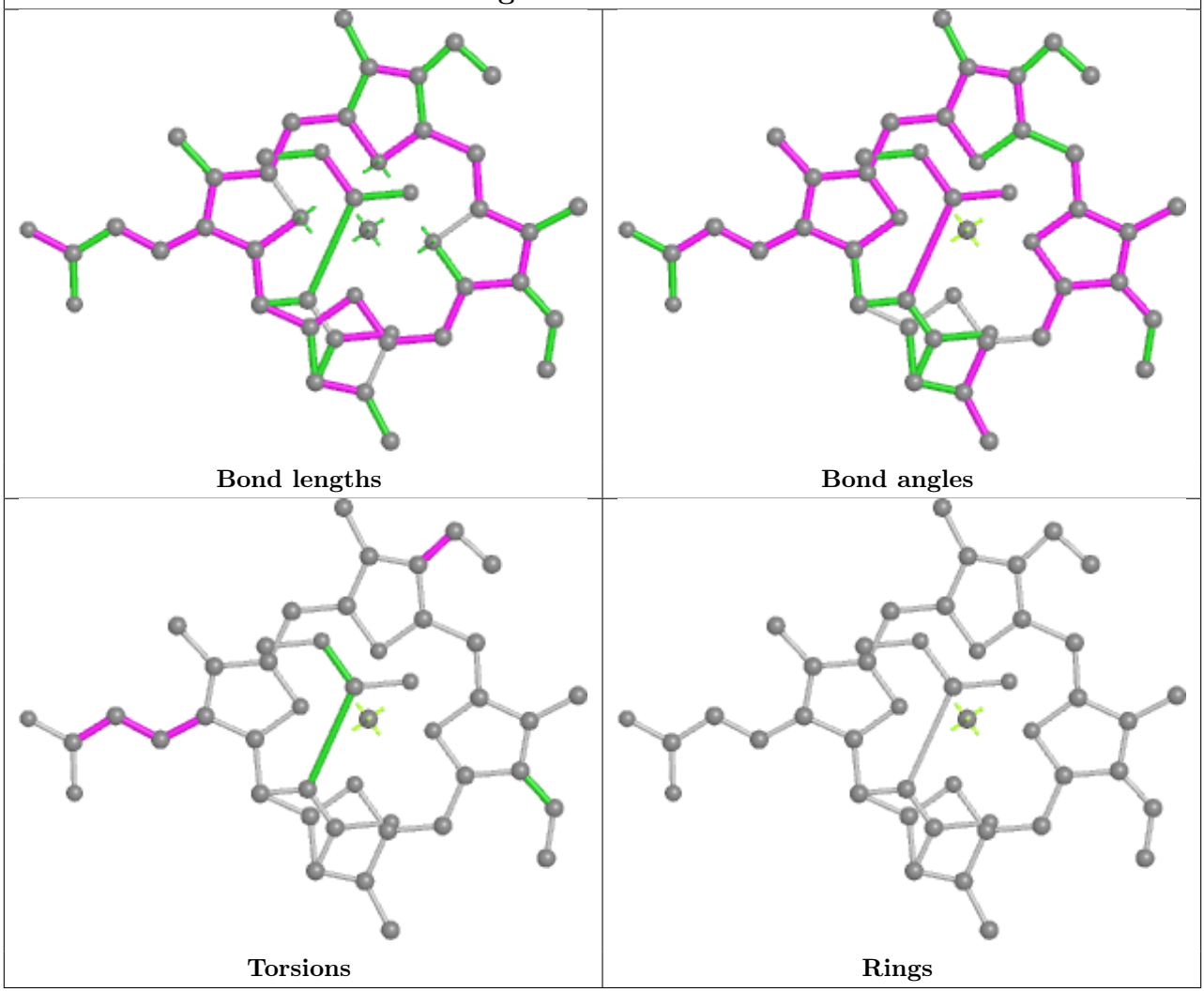
Ligand CLA b 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 5 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

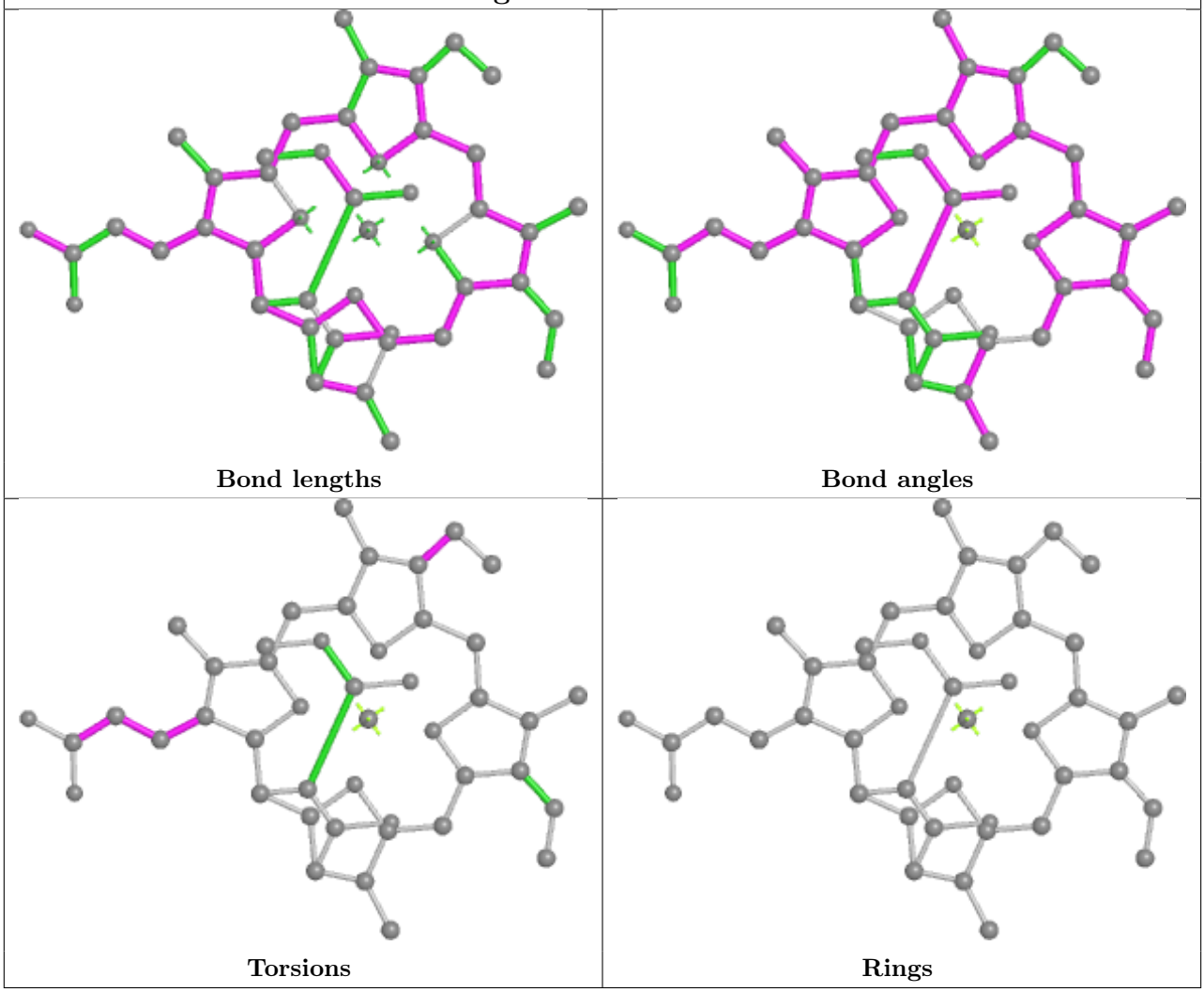
Ligand CLA 2 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 7 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

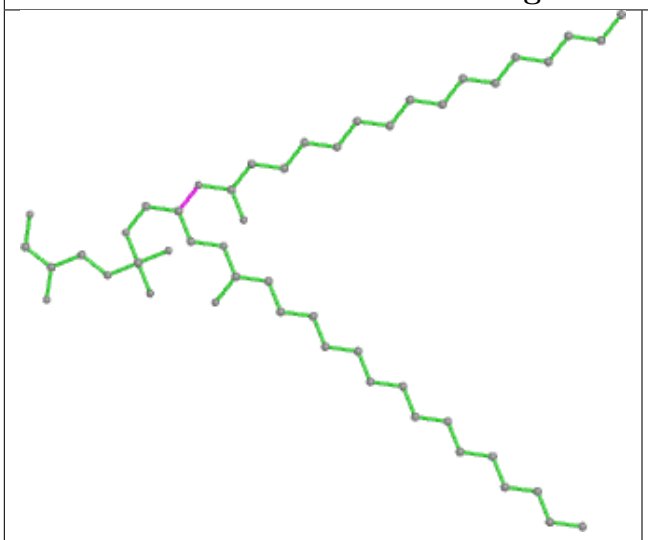
Ligand KC1 2 314



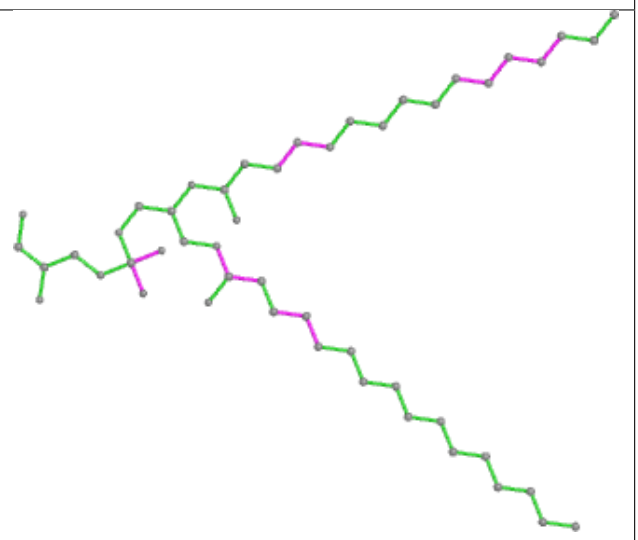
Ligand KC1 G 308



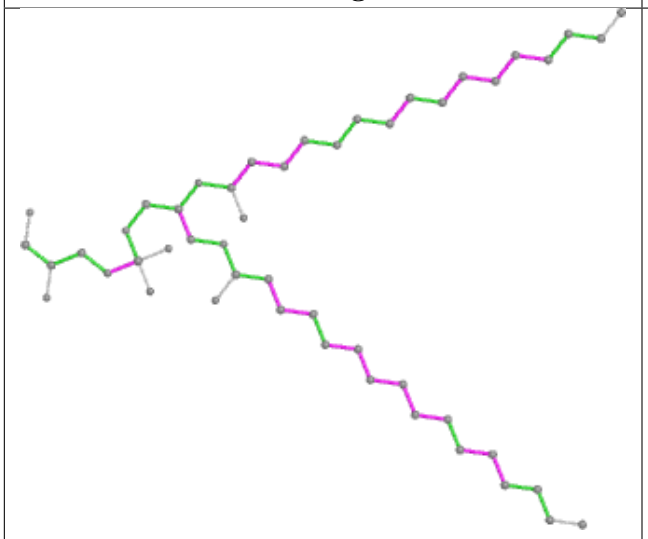
Ligand LHG B 601



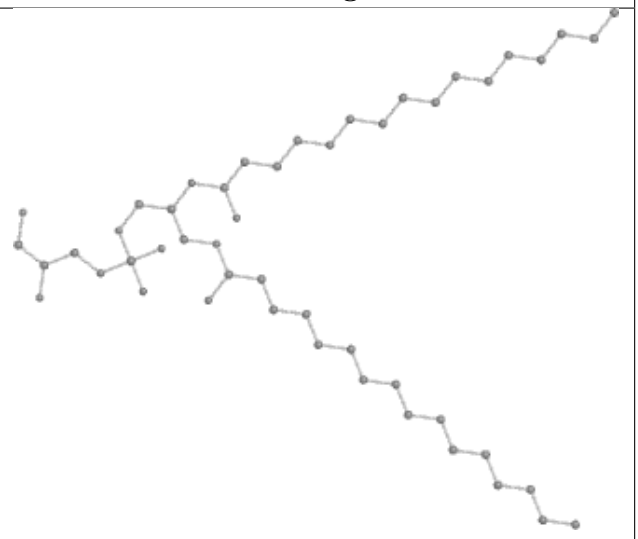
Bond lengths



Bond angles

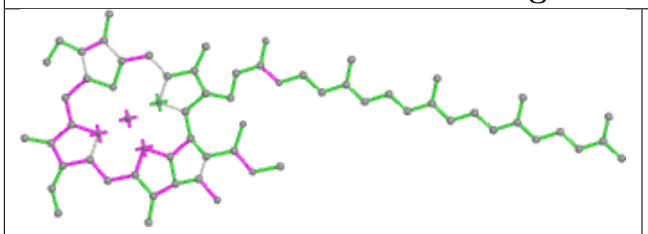


Torsions

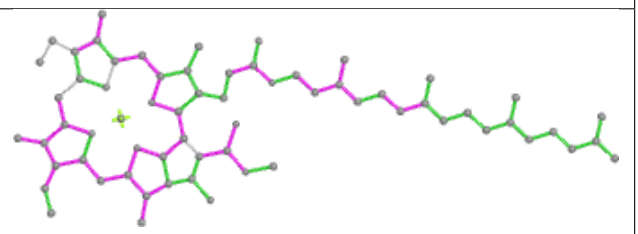


Rings

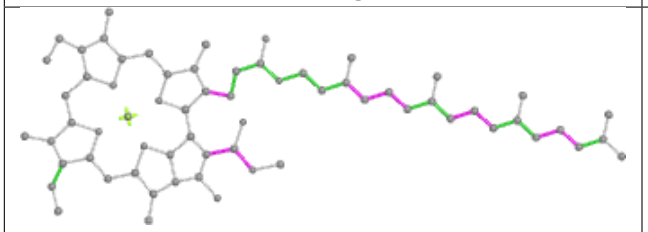
Ligand CLA 4 300



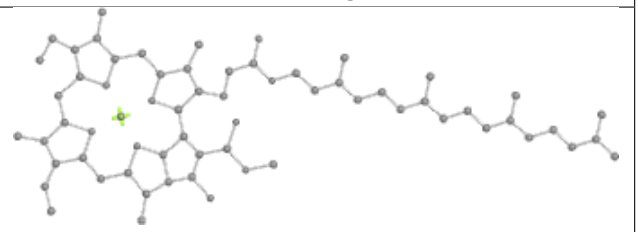
Bond lengths



Bond angles

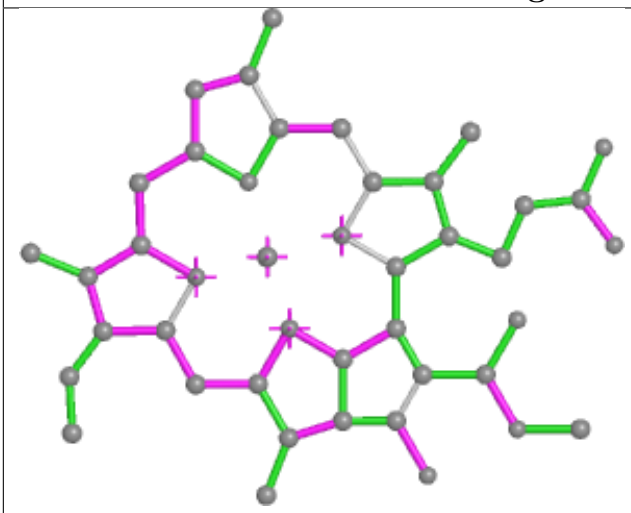


Torsions

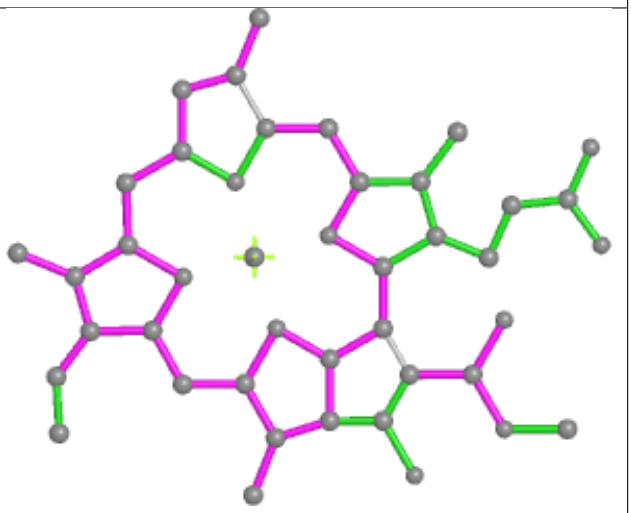


Rings

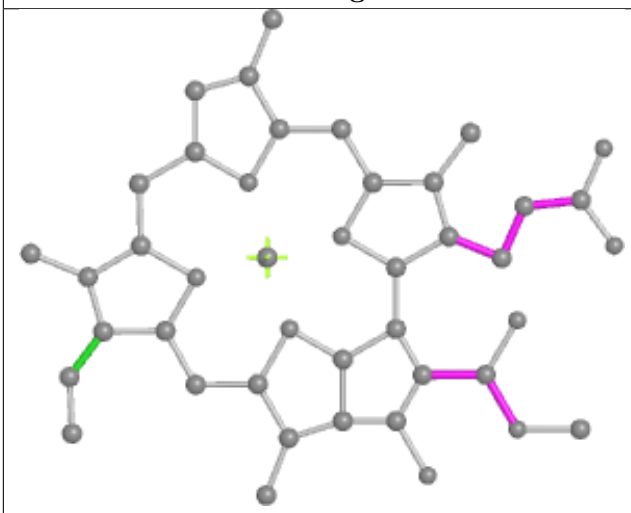
Ligand CLA J 303



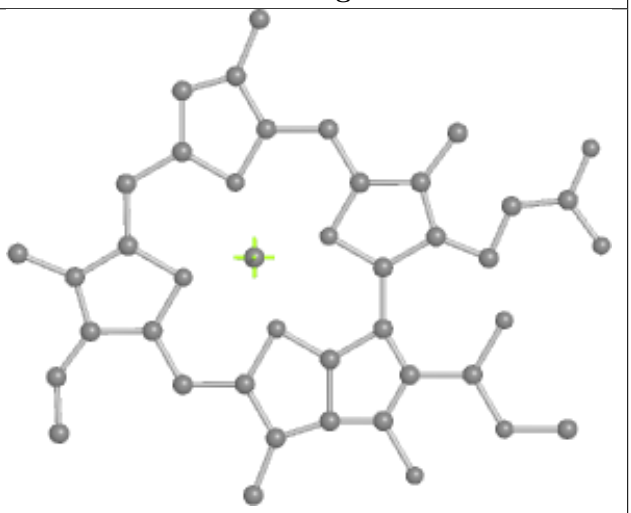
Bond lengths



Bond angles

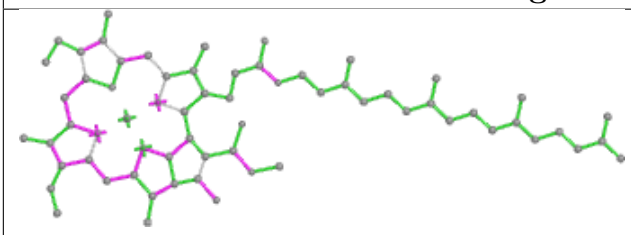


Torsions

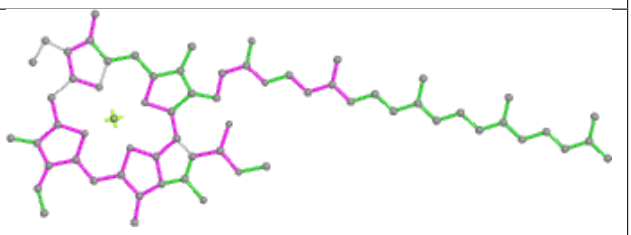


Rings

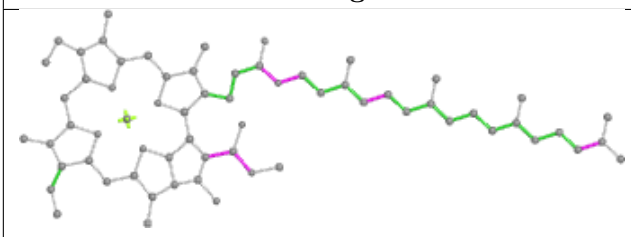
Ligand CLA c 510



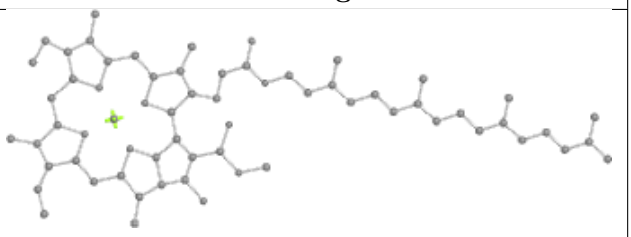
Bond lengths



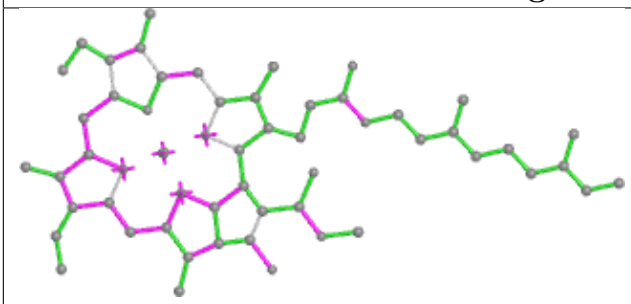
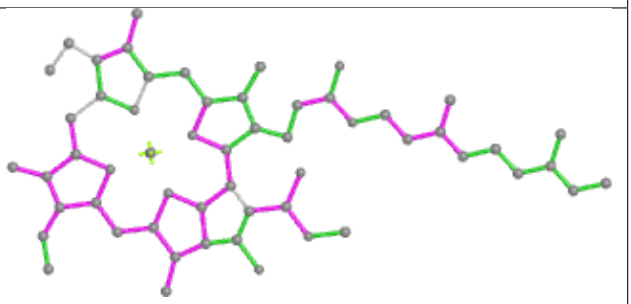
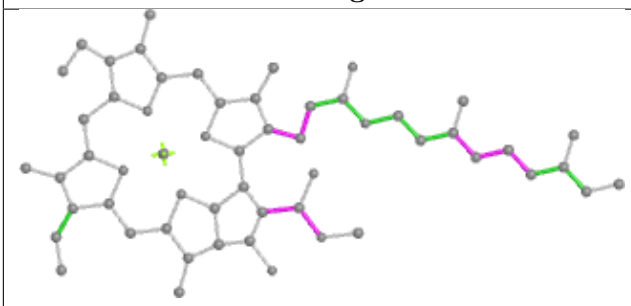
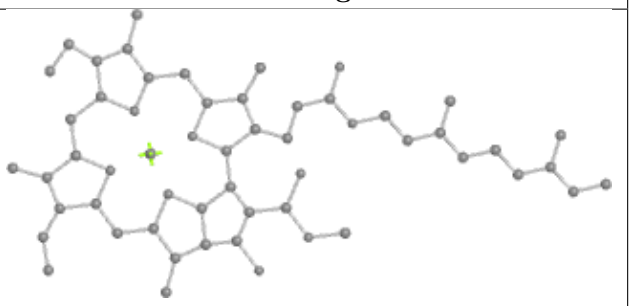
Bond angles

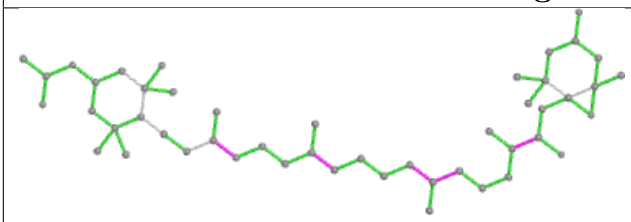
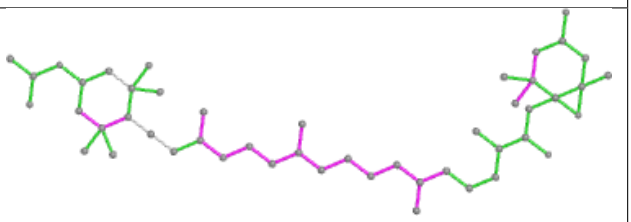
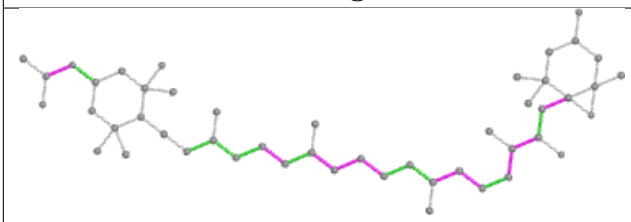
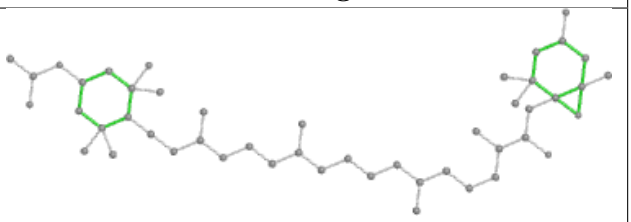


Torsions

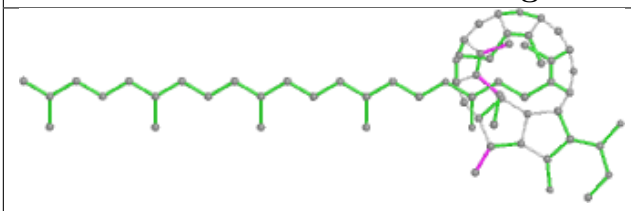


Rings

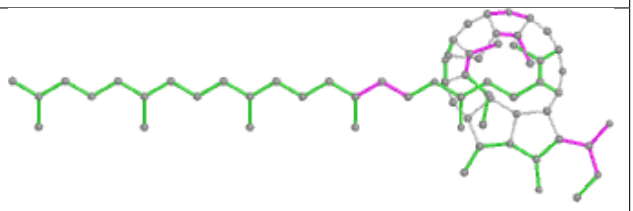
Ligand CLA 9 300	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 8 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

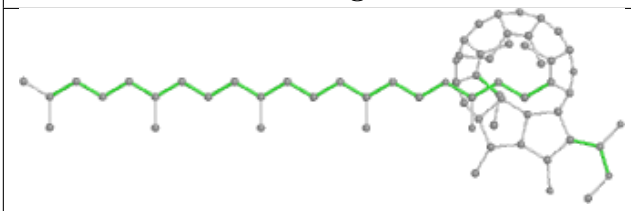
Ligand PHO D 401



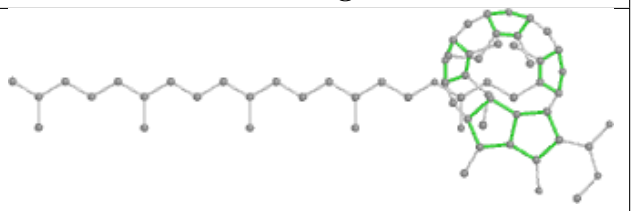
Bond lengths



Bond angles



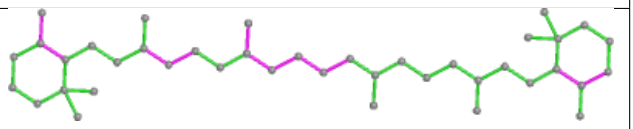
Torsions



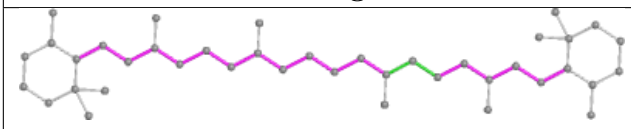
Rings

Ligand BCR h 101

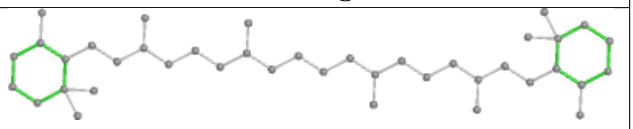
Bond lengths



Bond angles

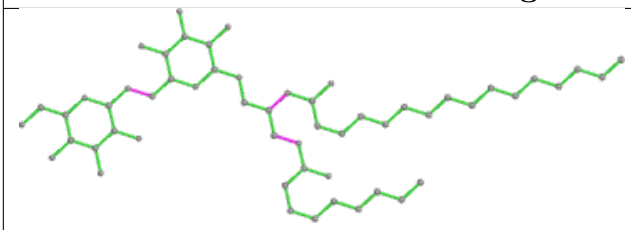


Torsions

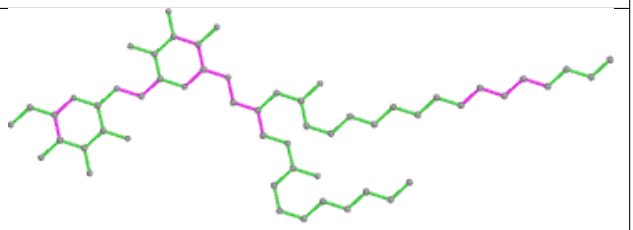


Rings

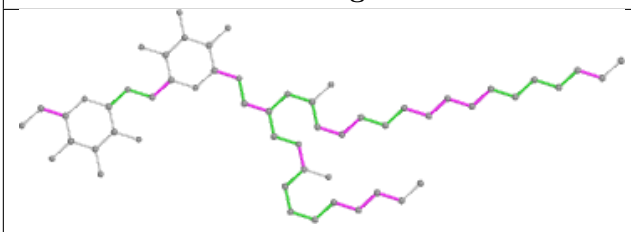
Ligand DGD C 517



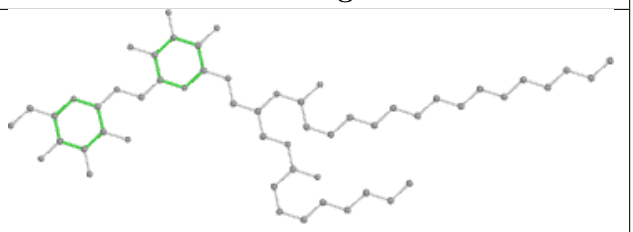
Bond lengths



Bond angles

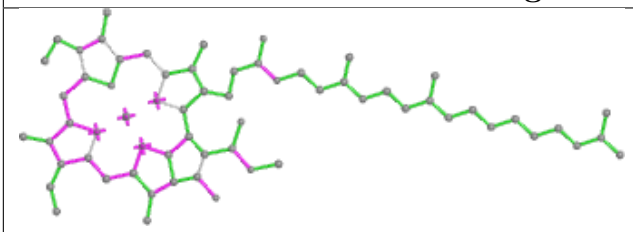


Torsions

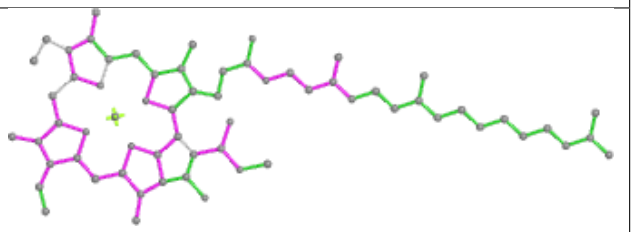


Rings

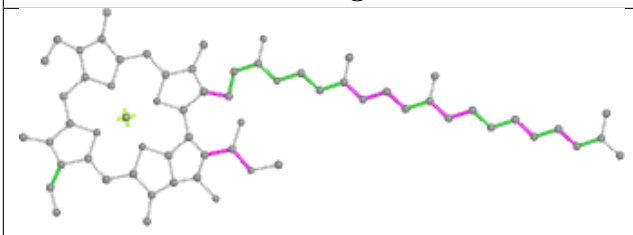
Ligand CLA B 614



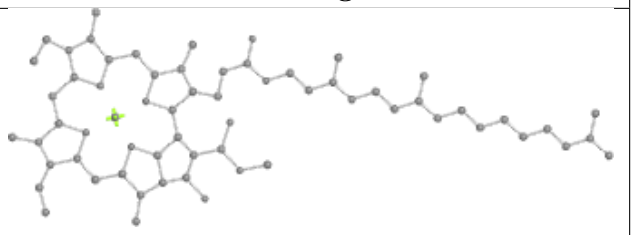
Bond lengths



Bond angles

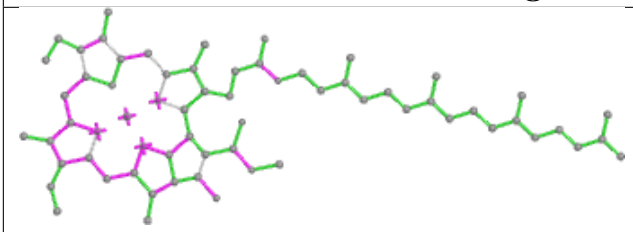


Torsions

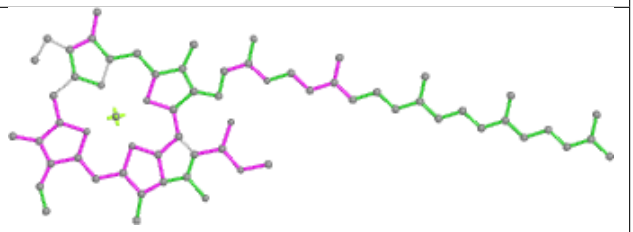


Rings

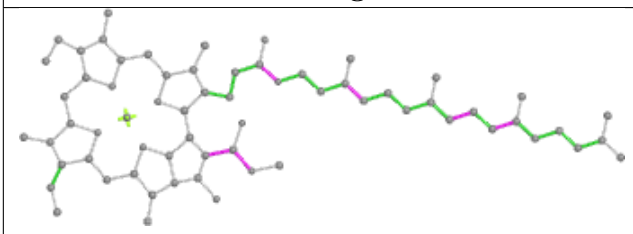
Ligand CLA B 612



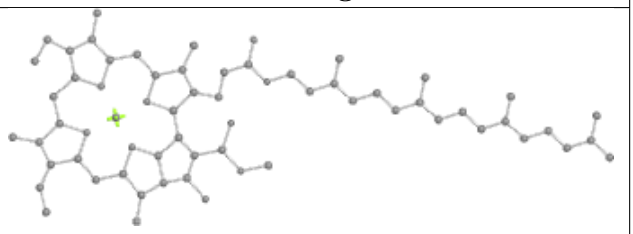
Bond lengths



Bond angles

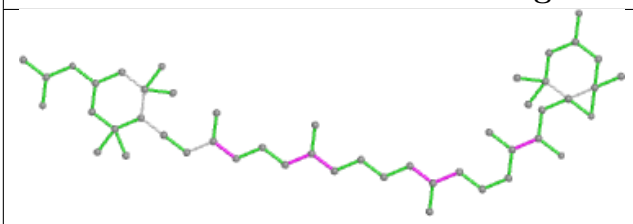


Torsions

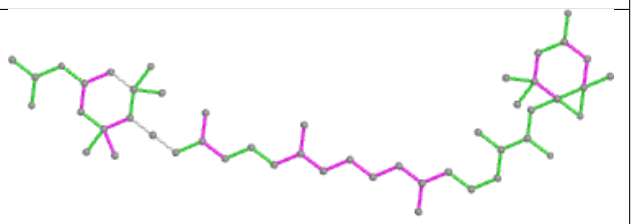


Rings

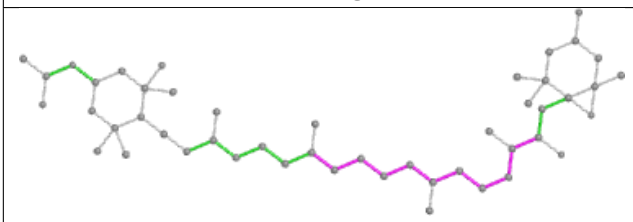
Ligand A86 2 310



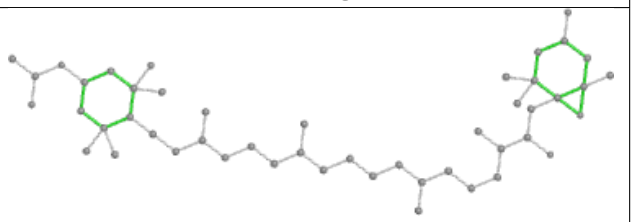
Bond lengths



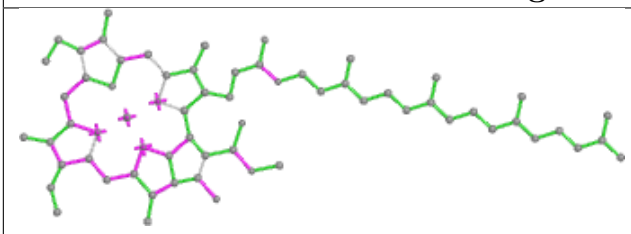
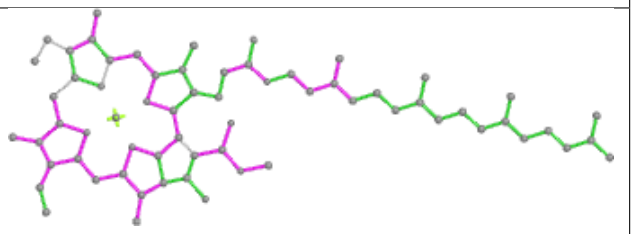
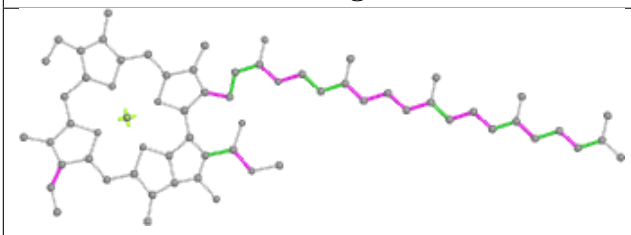
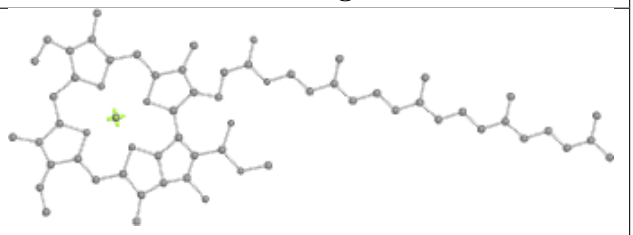
Bond angles

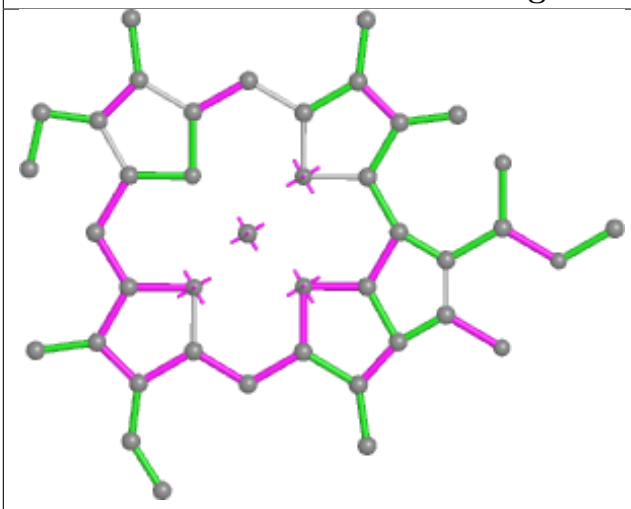
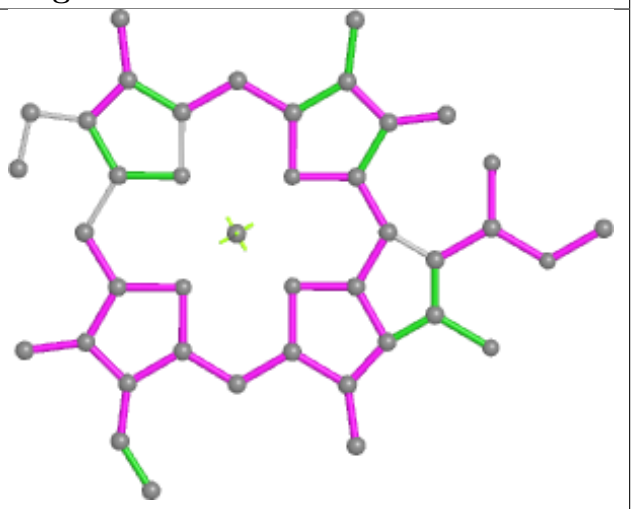
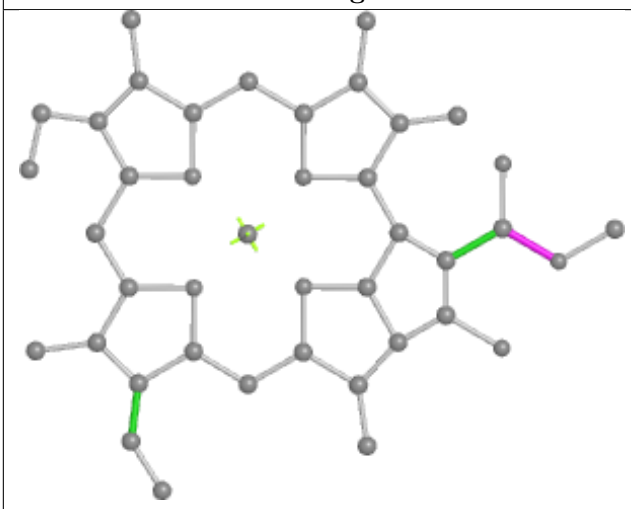
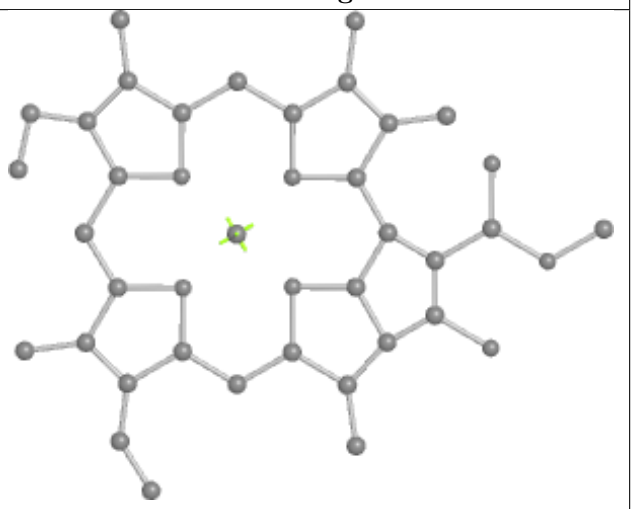


Torsions

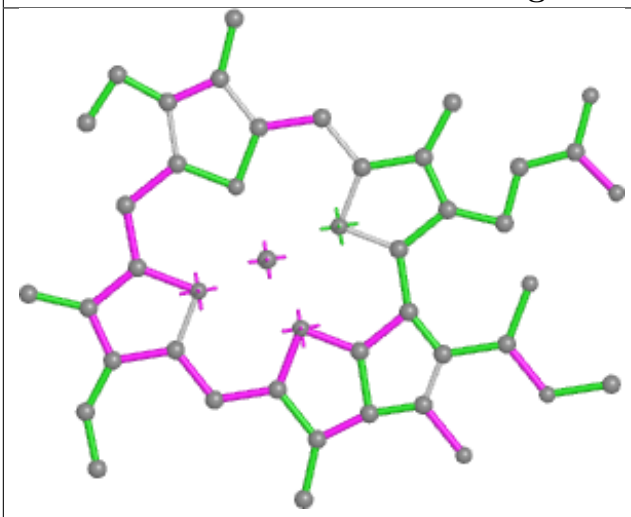


Rings

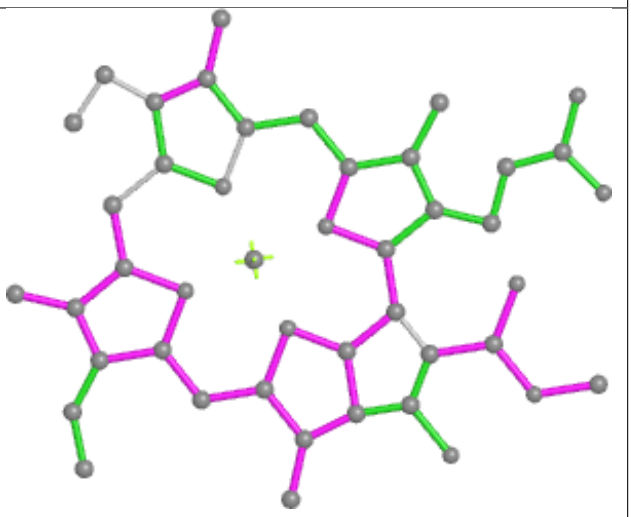
Ligand CLA 4 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

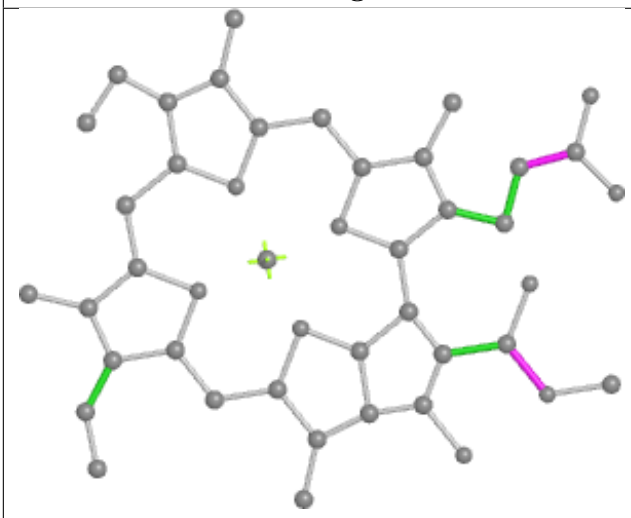
Ligand CLA J 305



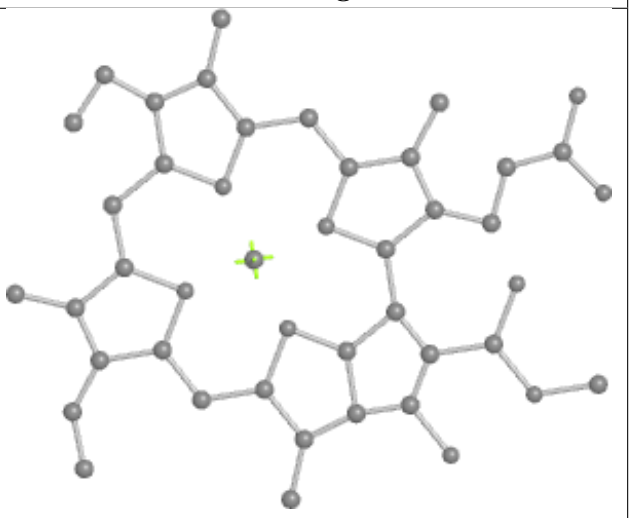
Bond lengths



Bond angles

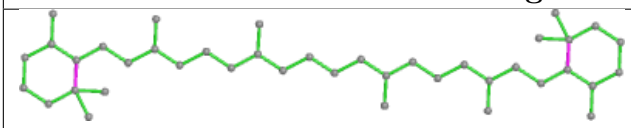


Torsions

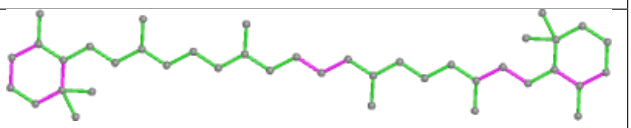


Rings

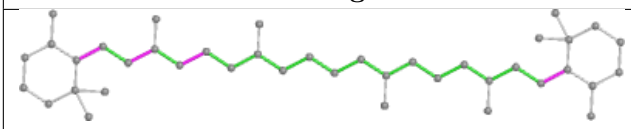
Ligand BCR d 407



Bond lengths

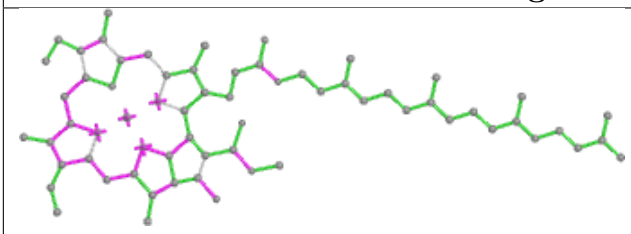
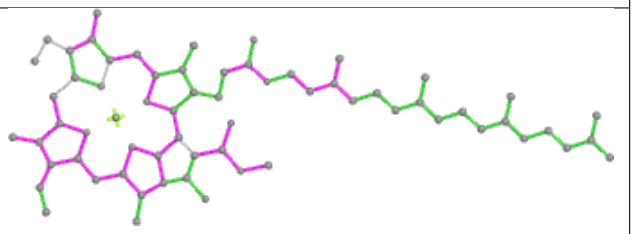
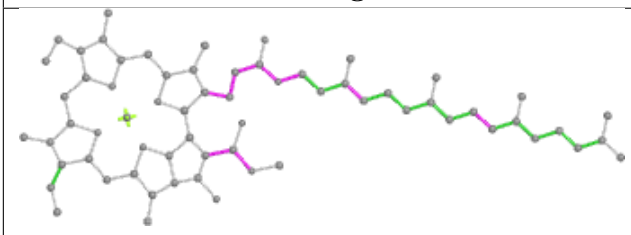
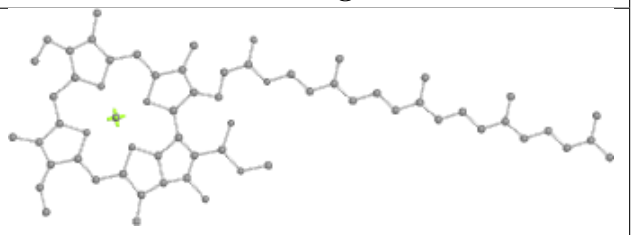


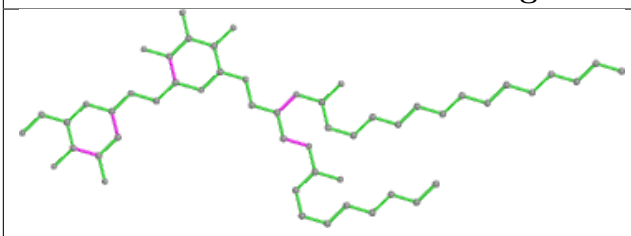
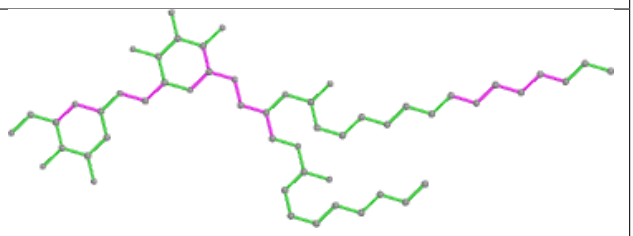
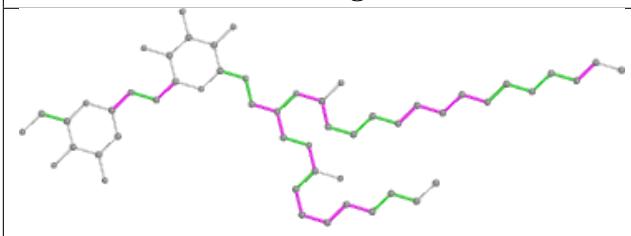
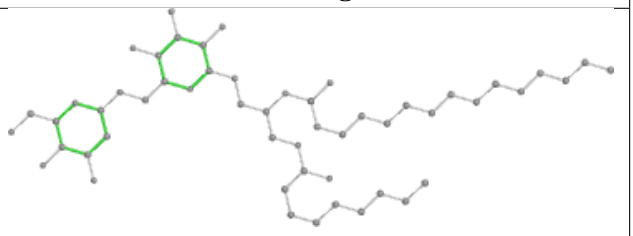
Bond angles



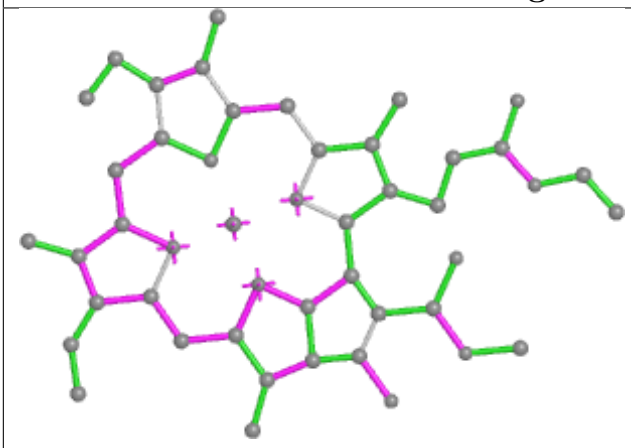
Torsions

Rings

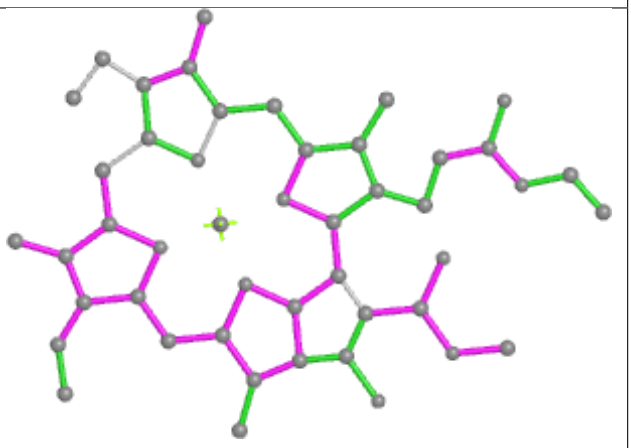
Ligand CLA J 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD B 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

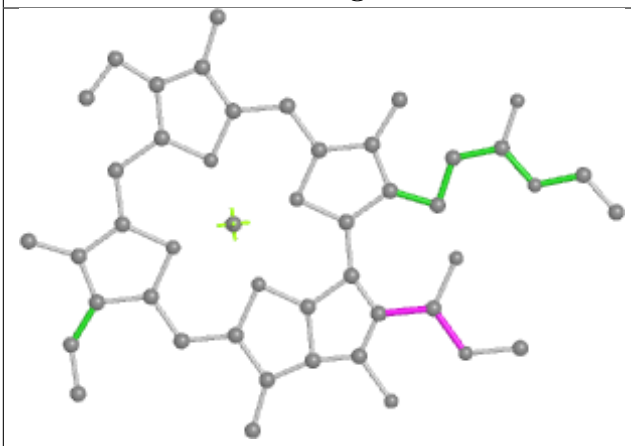
Ligand CLA 9 302



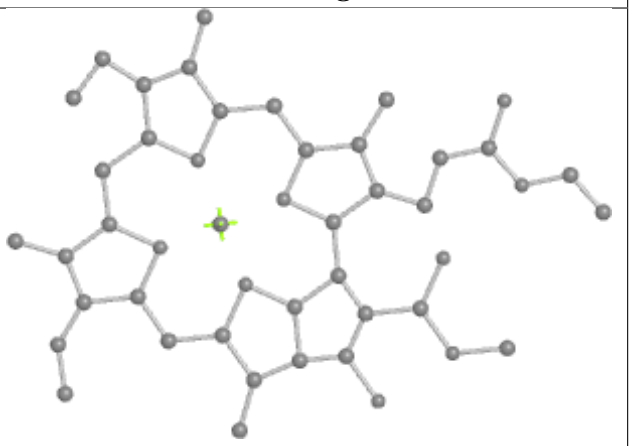
Bond lengths



Bond angles

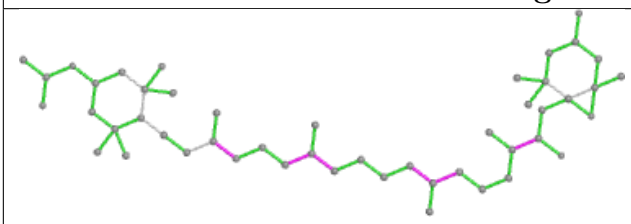


Torsions

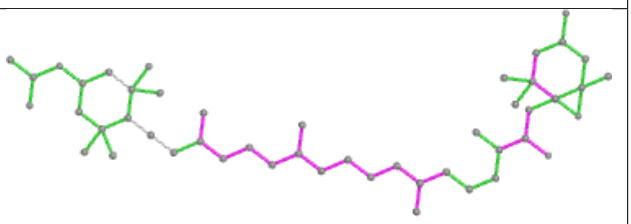


Rings

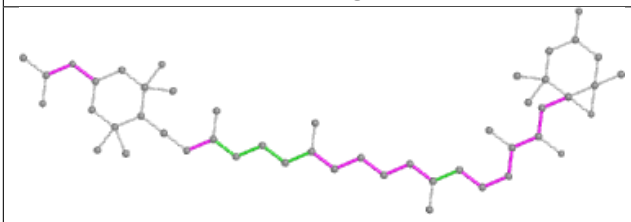
Ligand A86 2 311



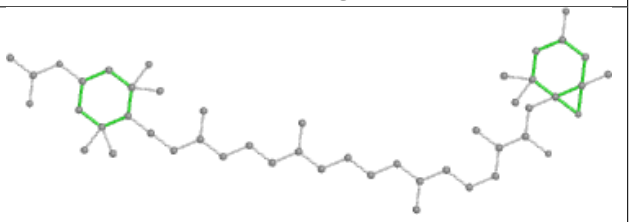
Bond lengths



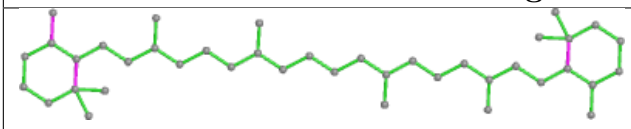
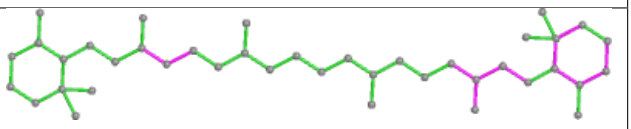
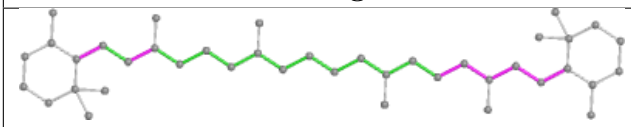
Bond angles

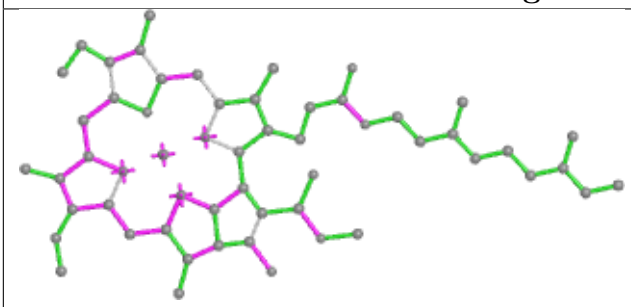
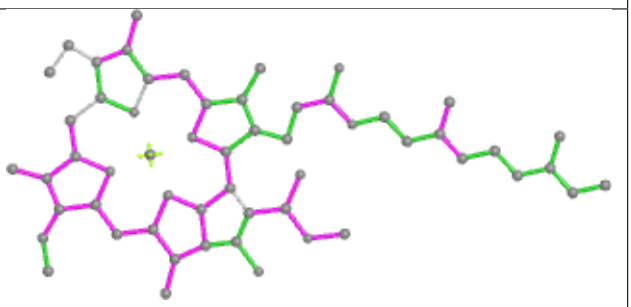
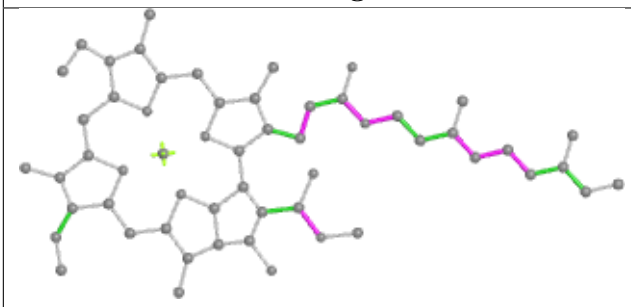
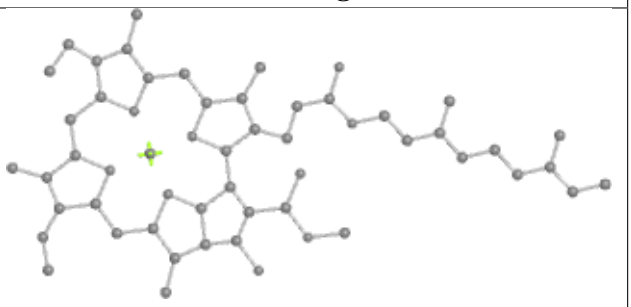


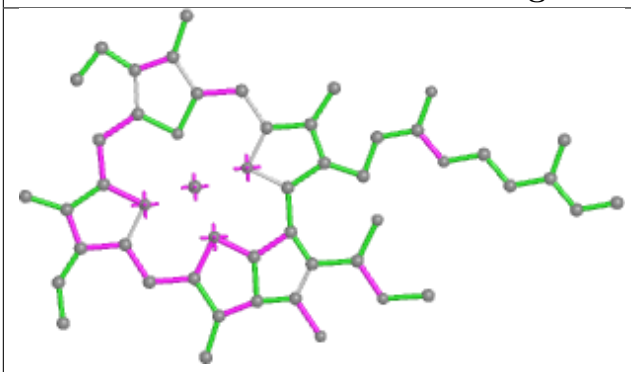
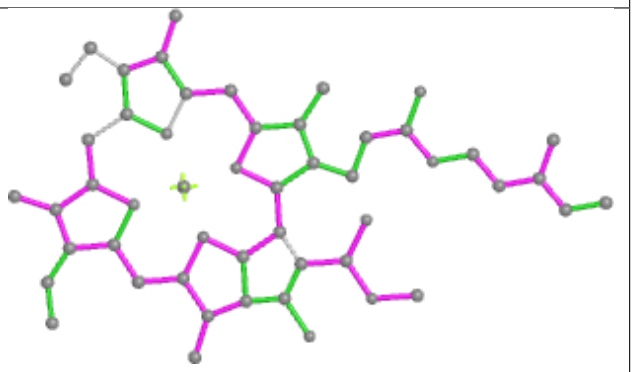
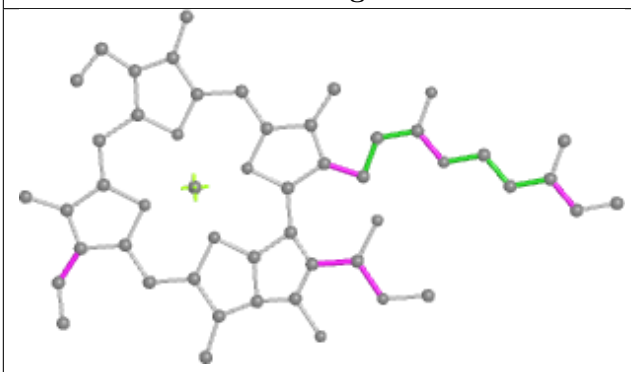
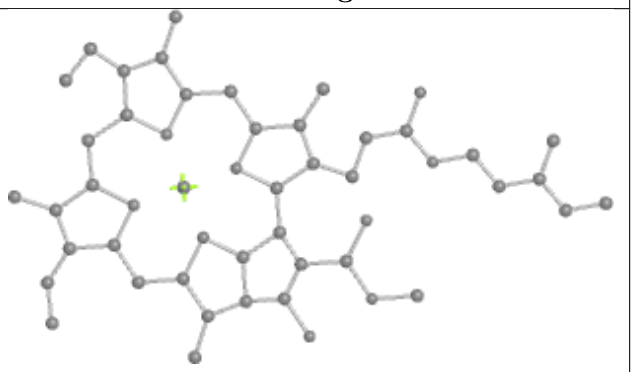
Torsions



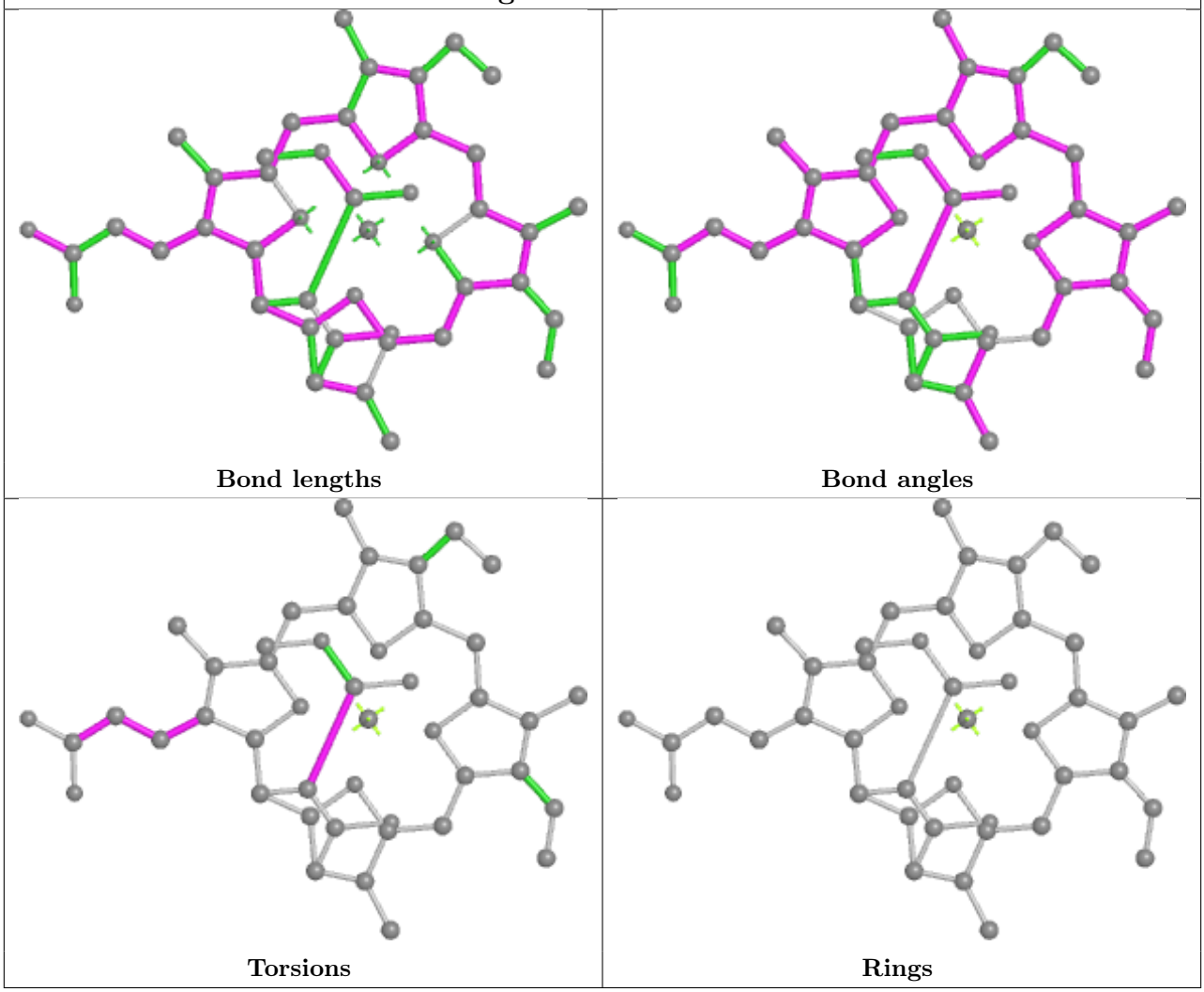
Rings

Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

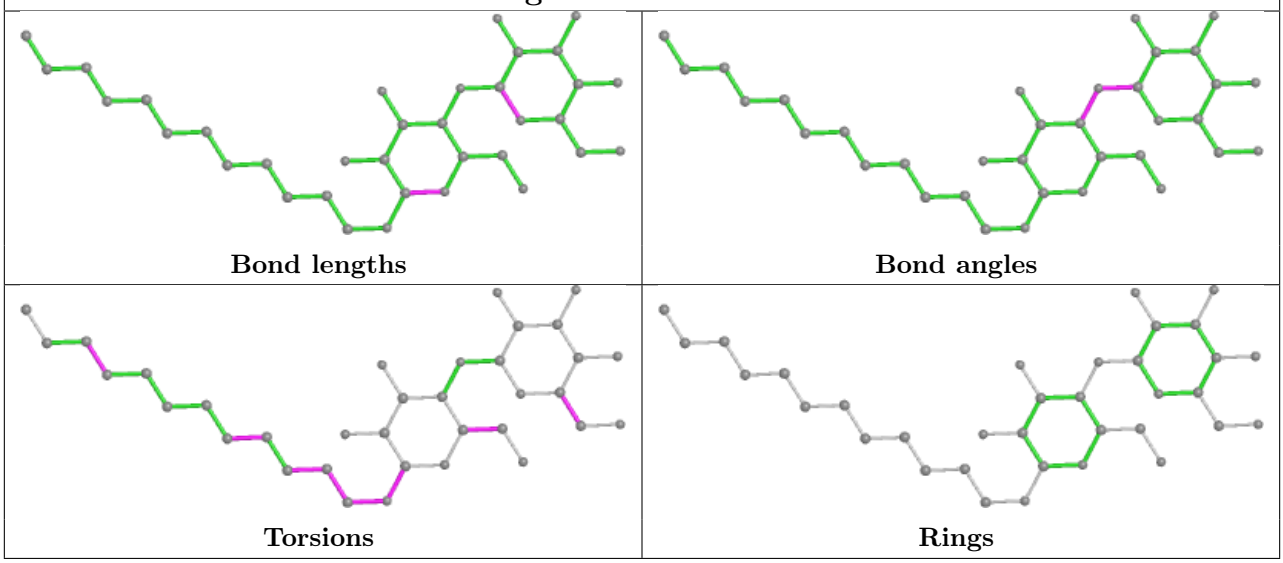
Ligand CLA G 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

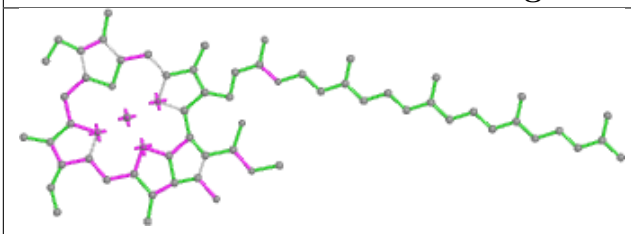
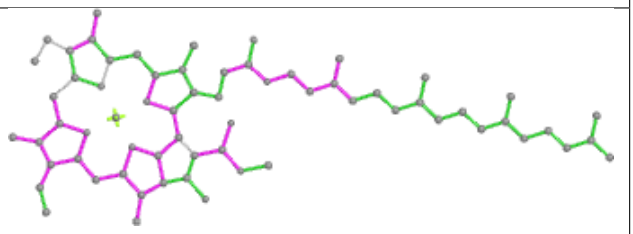
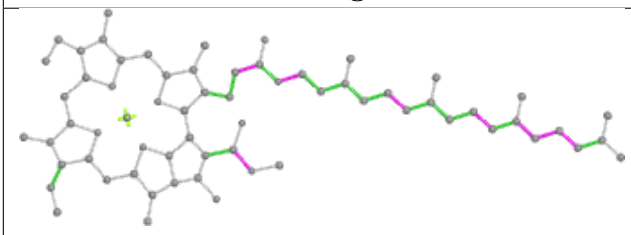
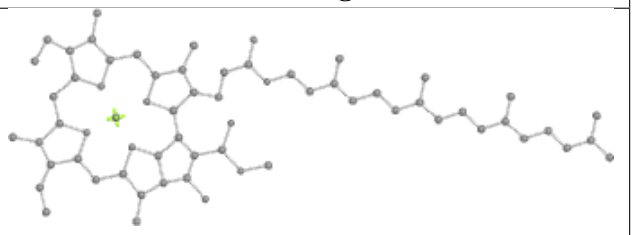
Ligand CLA 9 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

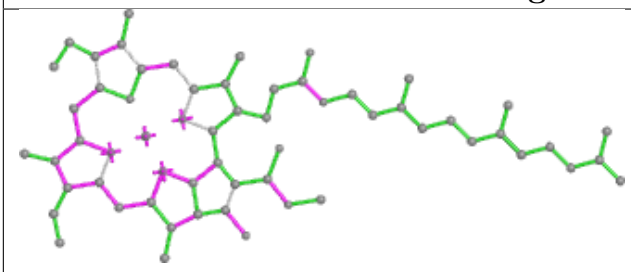
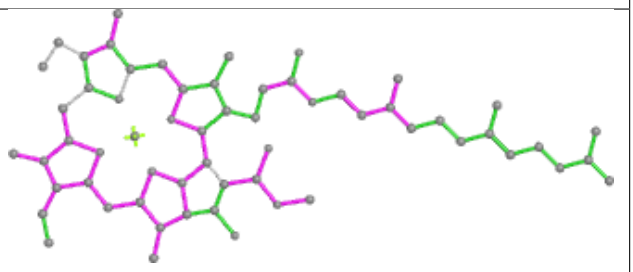
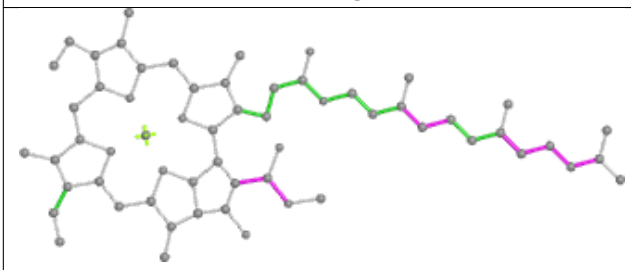
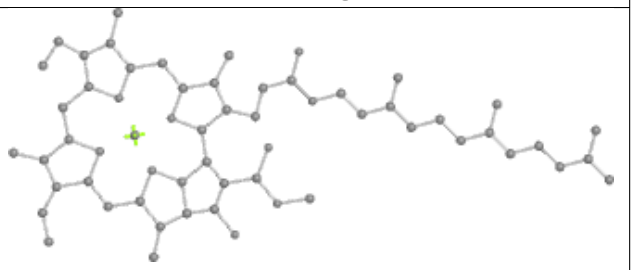
Ligand KC1 4 308

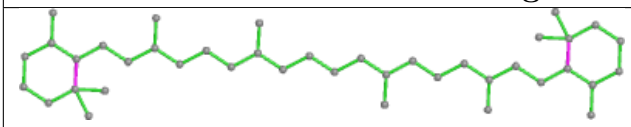
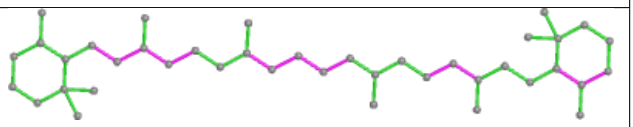
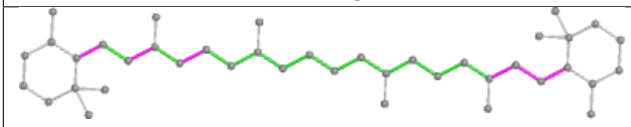
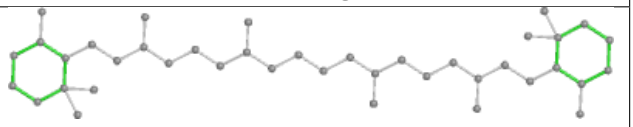


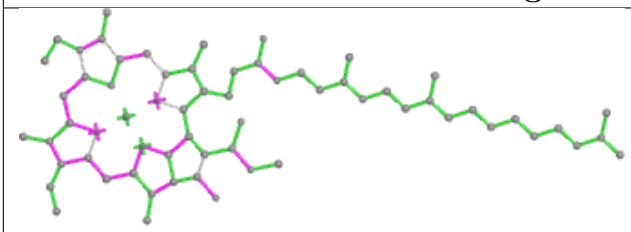
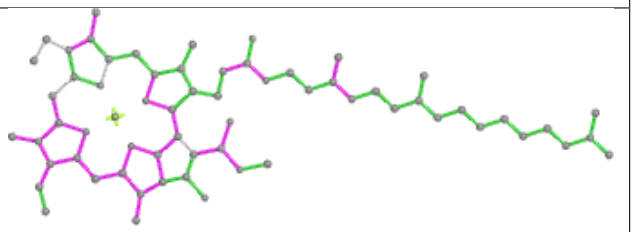
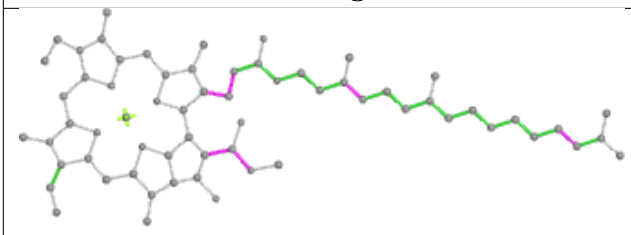
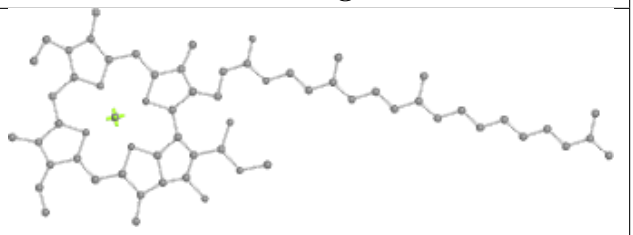
Ligand LMU 8 318

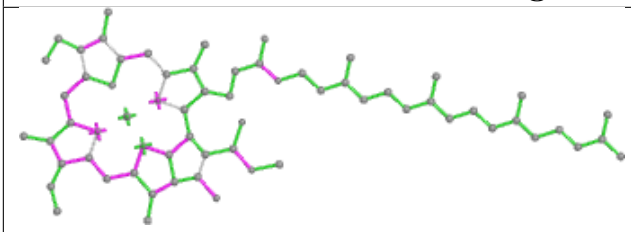
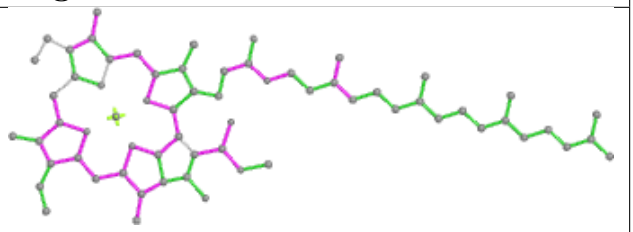
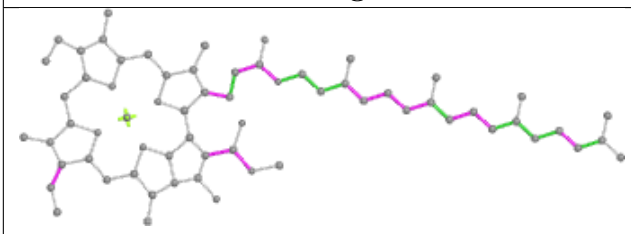
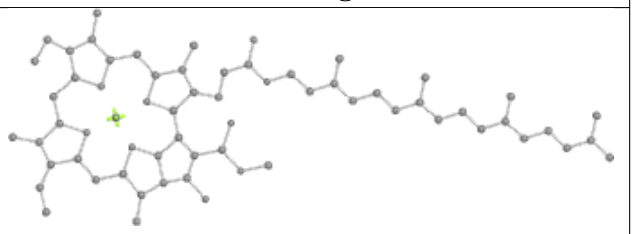


Ligand CLA B 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

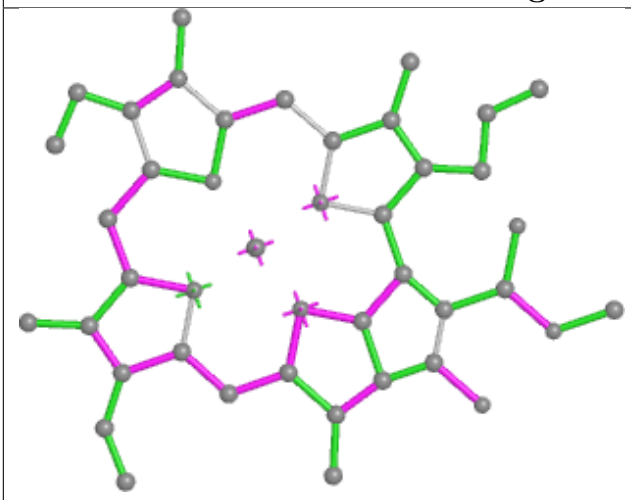
Ligand CLA 3 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR C 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

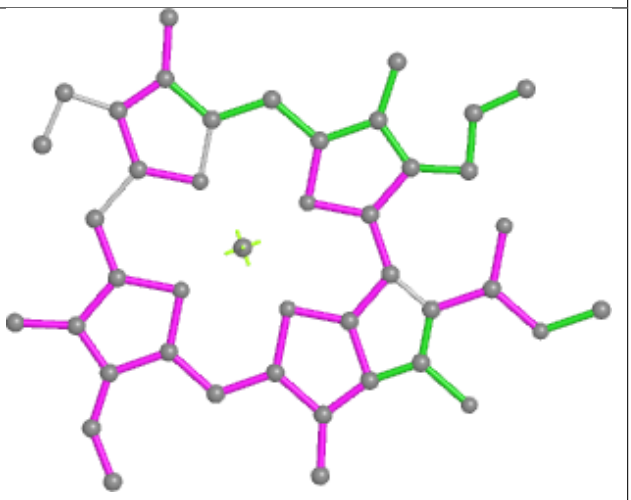
Ligand CLA B 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

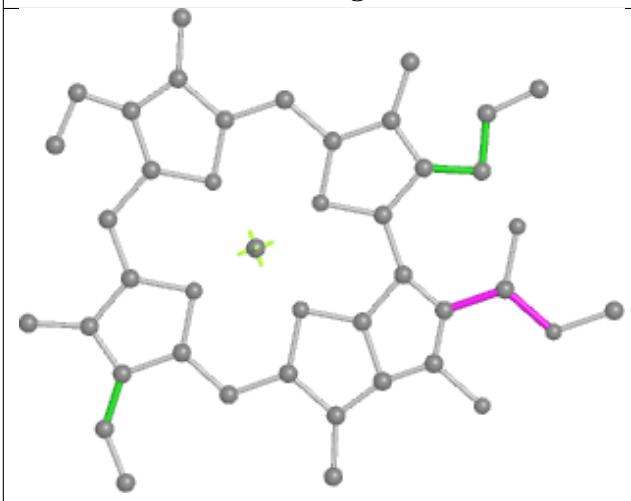
Ligand CLA 6 304



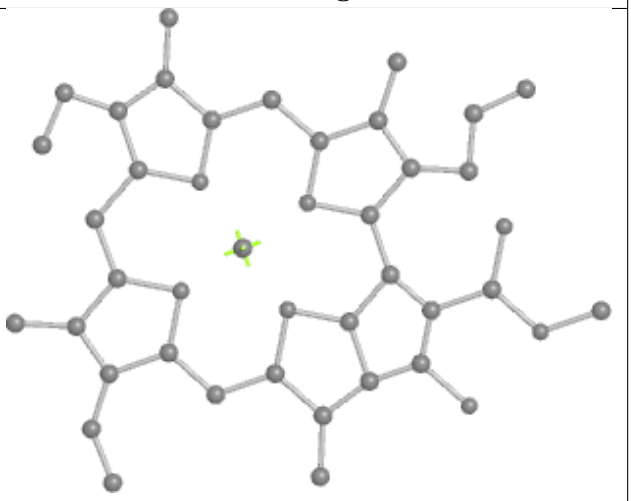
Bond lengths



Bond angles

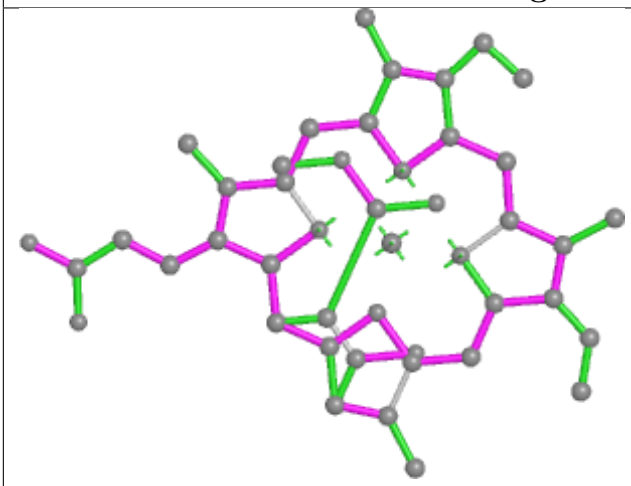


Torsions

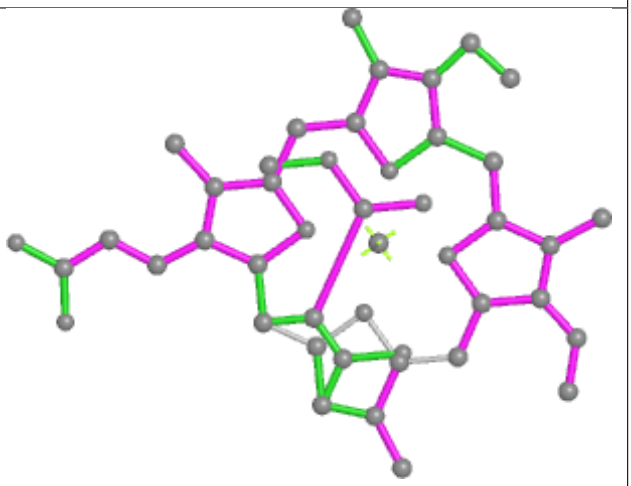


Rings

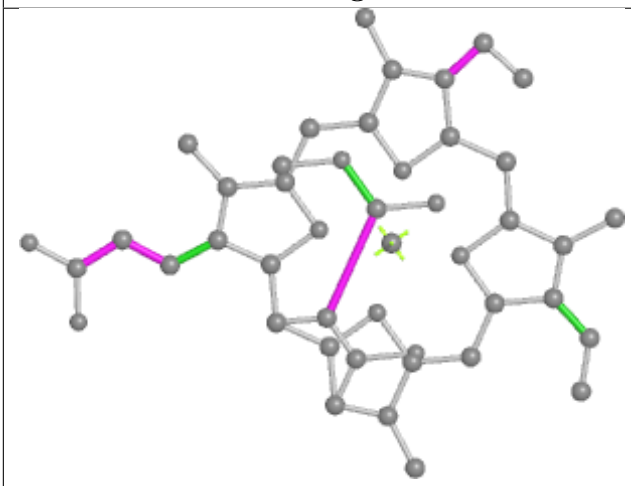
Ligand KC1 8 314



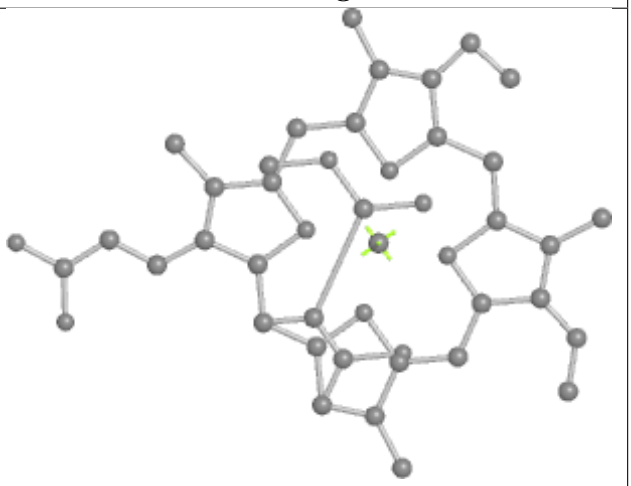
Bond lengths



Bond angles

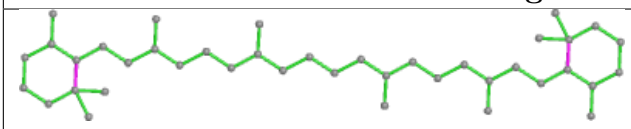


Torsions

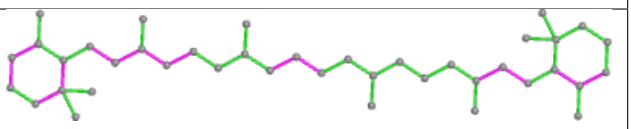


Rings

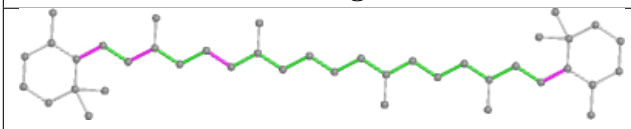
Ligand BCR h 102



Bond lengths



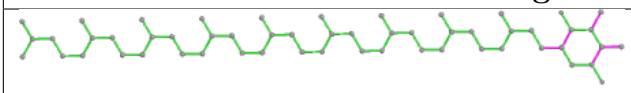
Bond angles



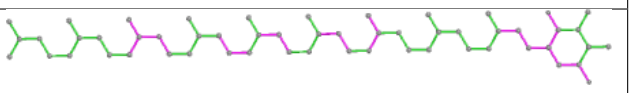
Torsions

Rings

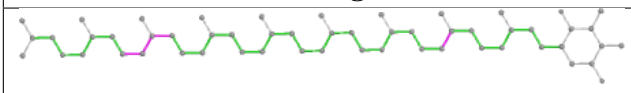
Ligand PL9 d 408



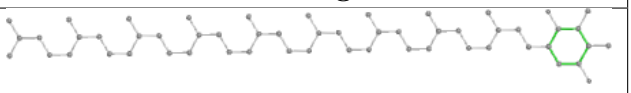
Bond lengths



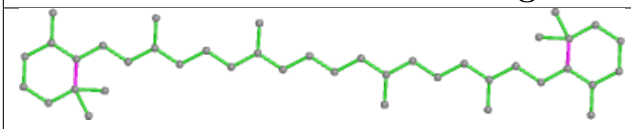
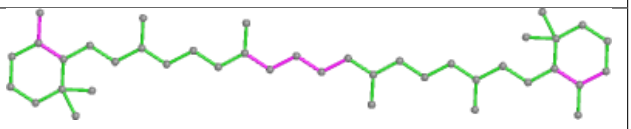
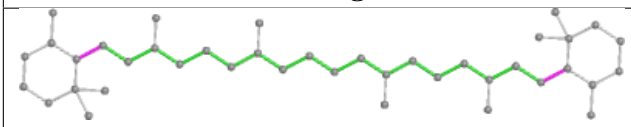
Bond angles



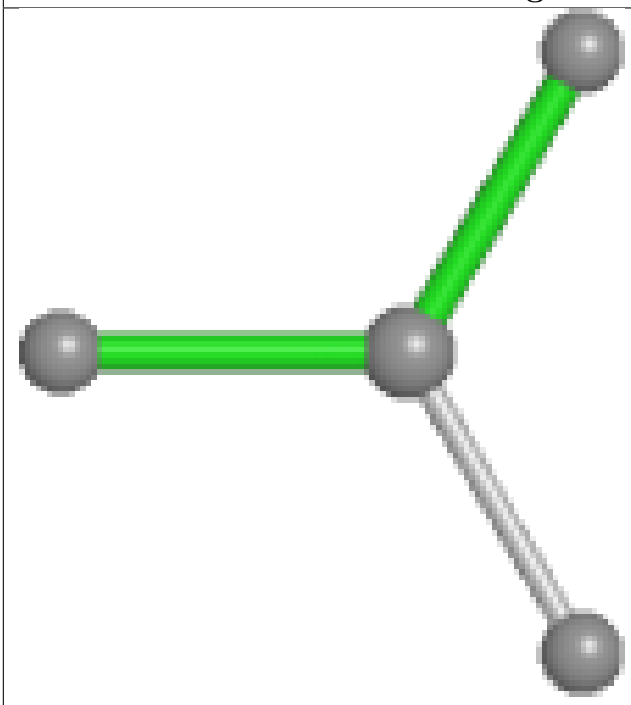
Torsions



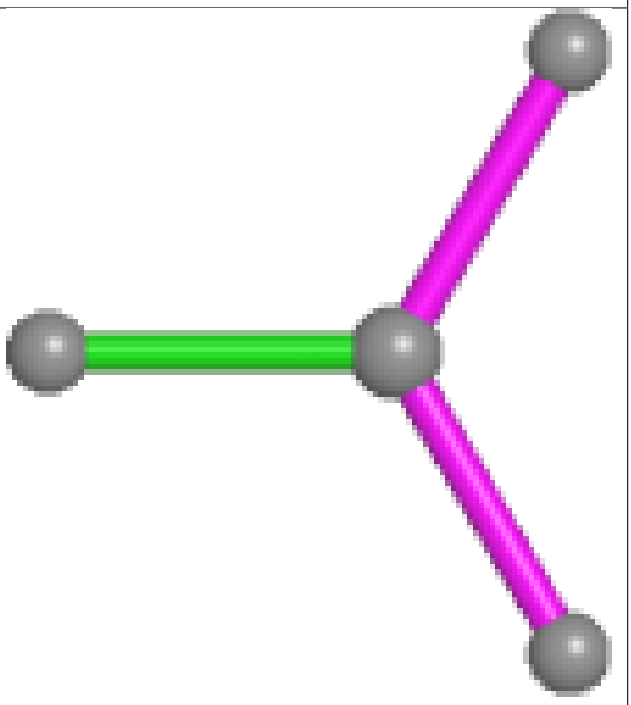
Rings

Ligand BCR M 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

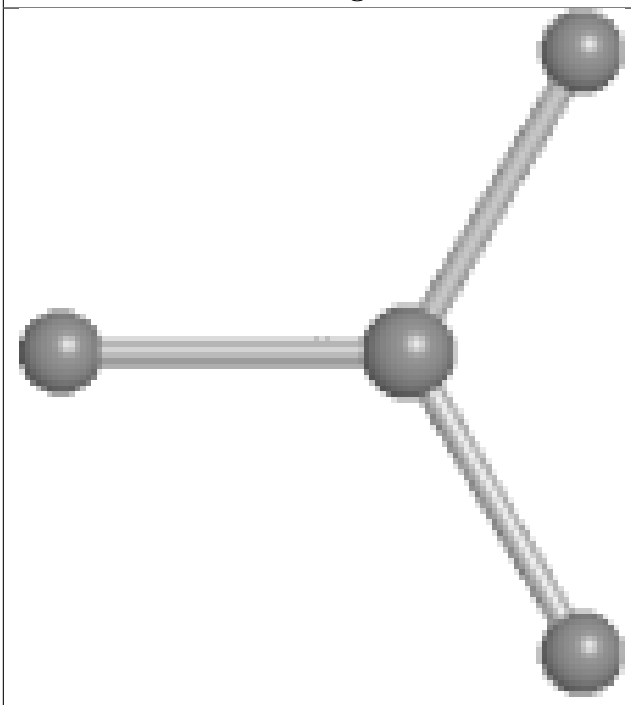
Ligand BCT d 401



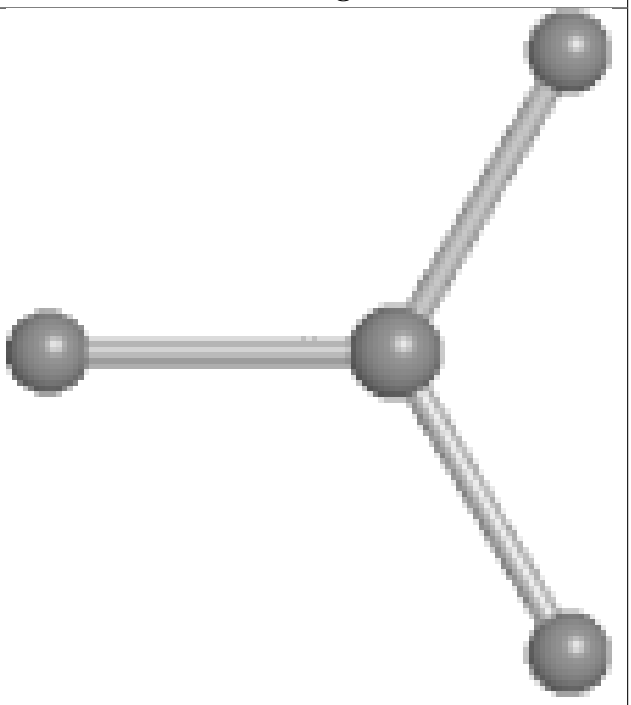
Bond lengths



Bond angles

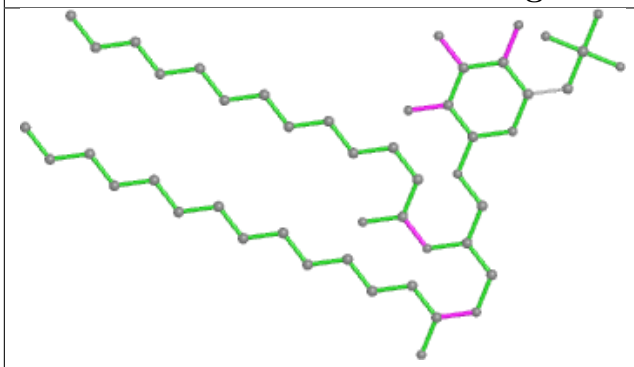


Torsions

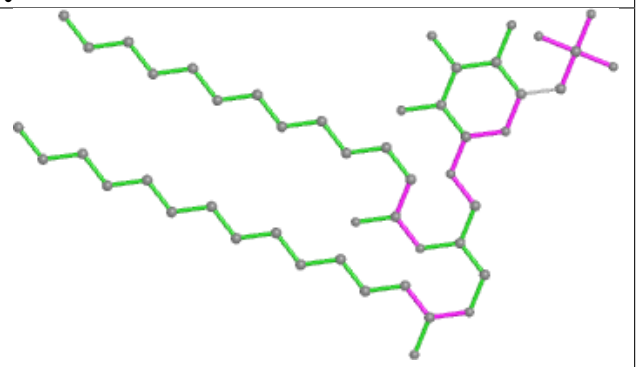


Rings

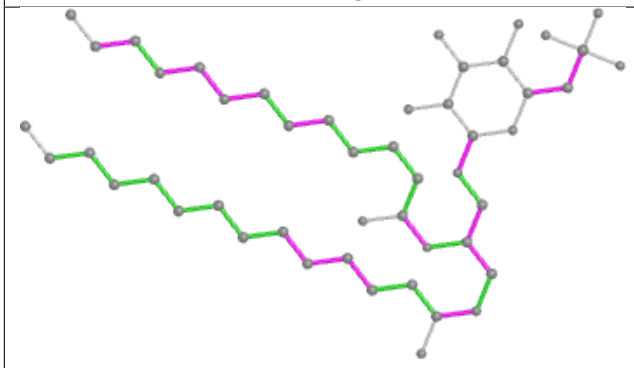
Ligand SQD B 625



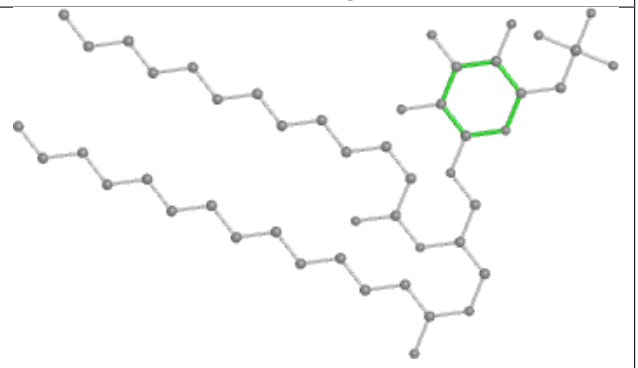
Bond lengths



Bond angles

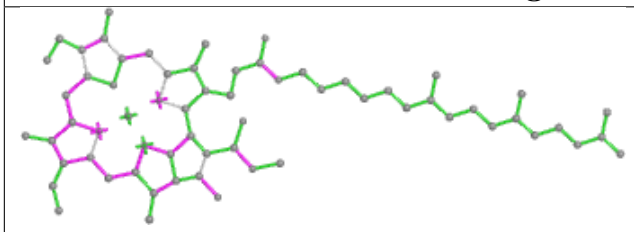


Torsions

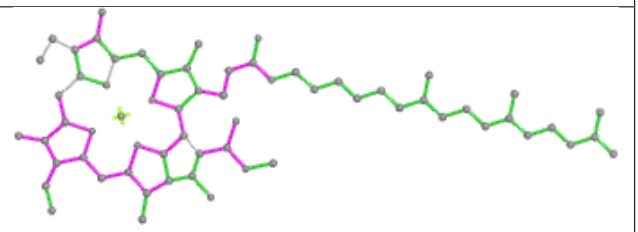


Rings

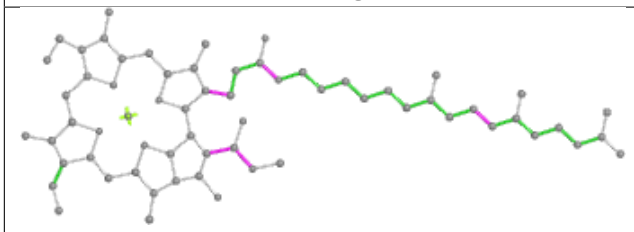
Ligand CLA C 514



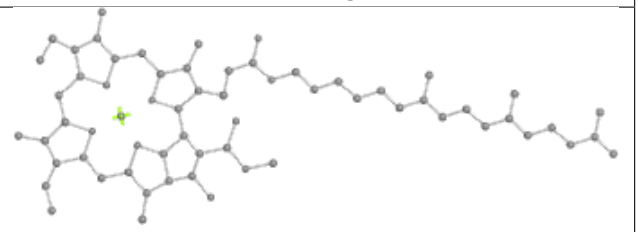
Bond lengths



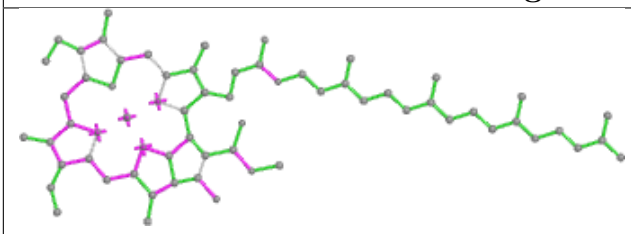
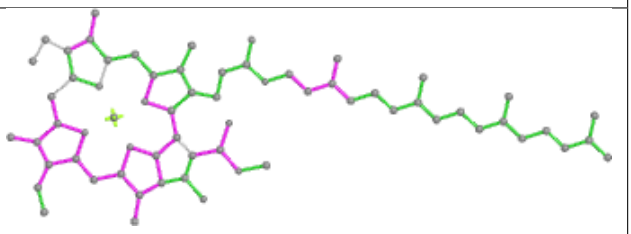
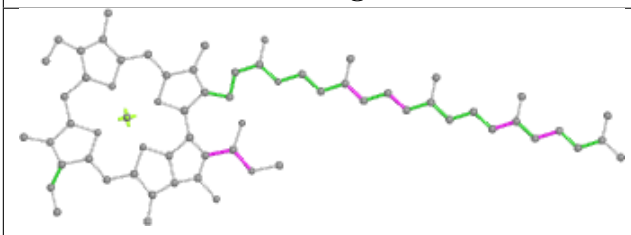
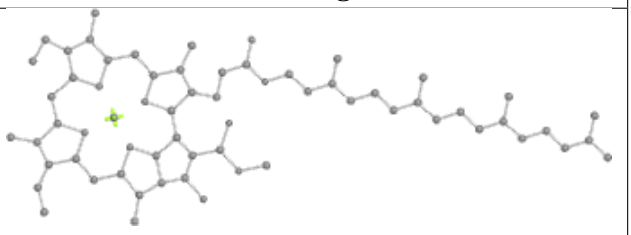
Bond angles

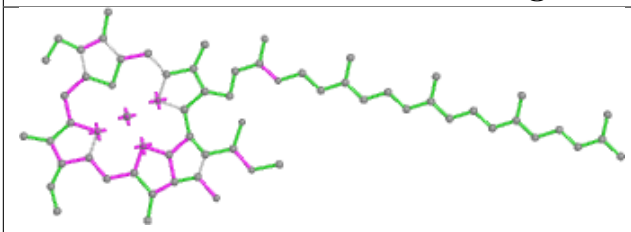
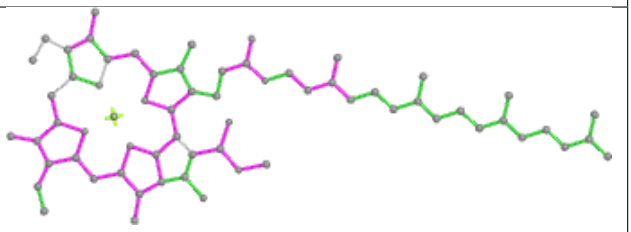
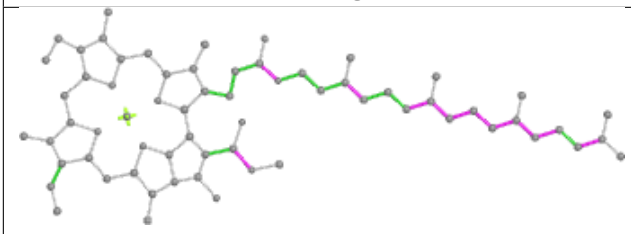
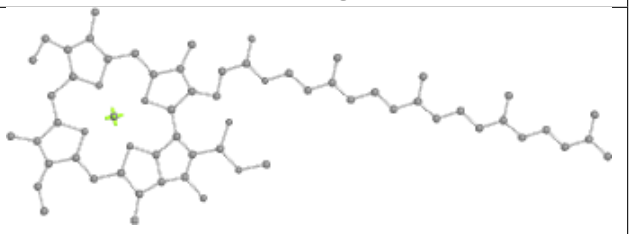


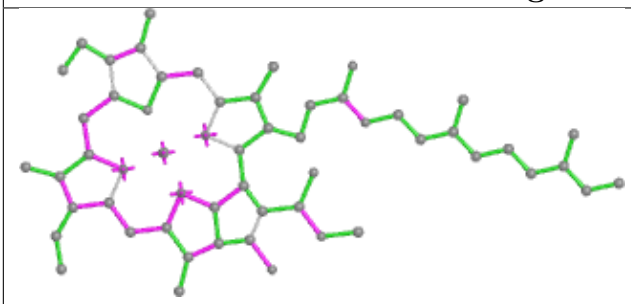
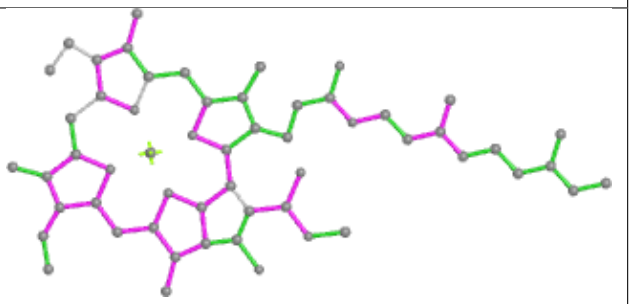
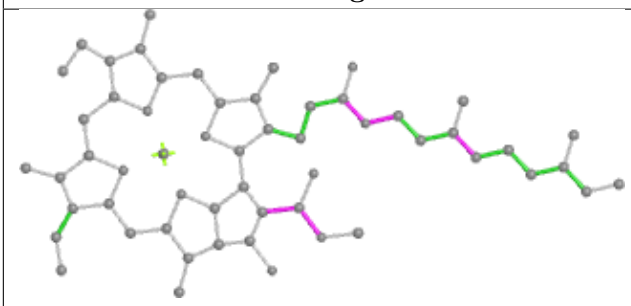
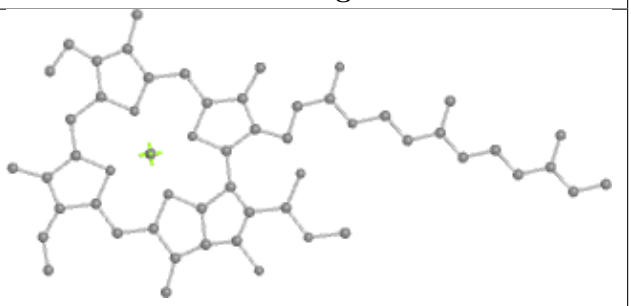
Torsions

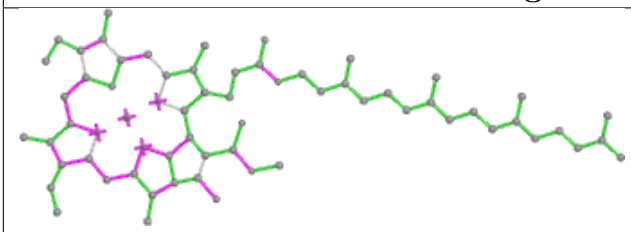
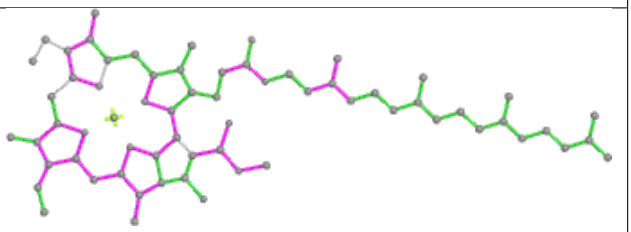
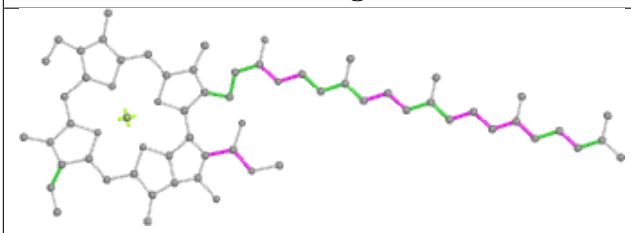
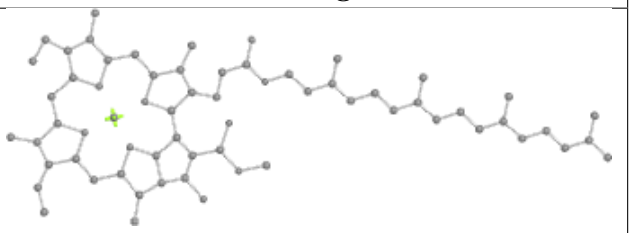


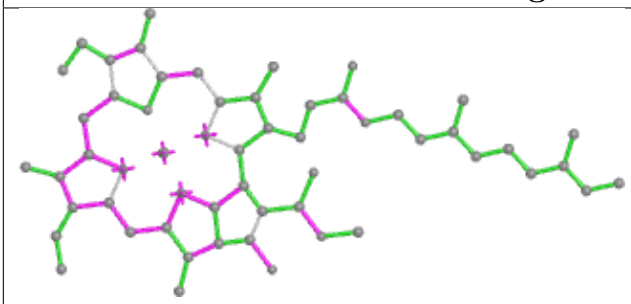
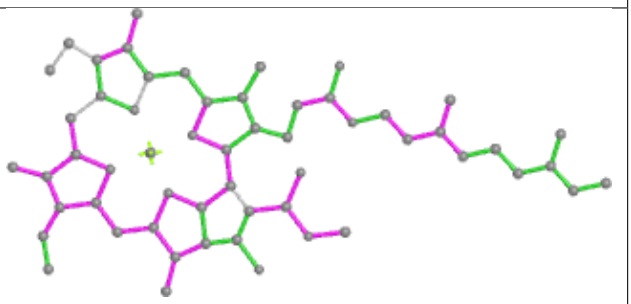
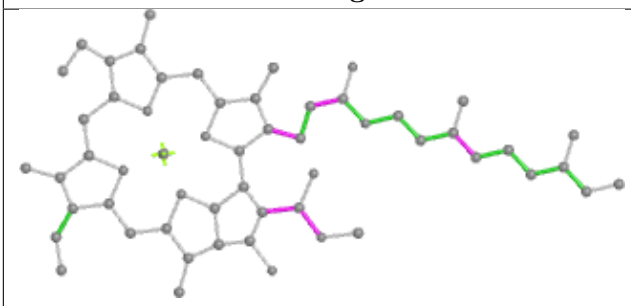
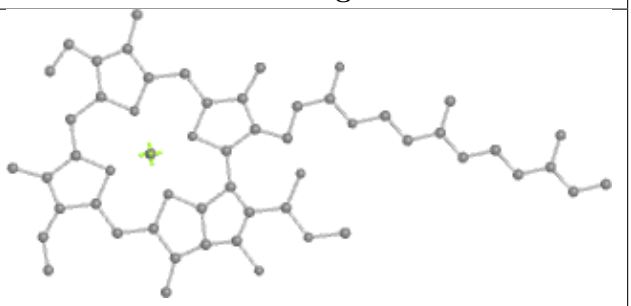
Rings

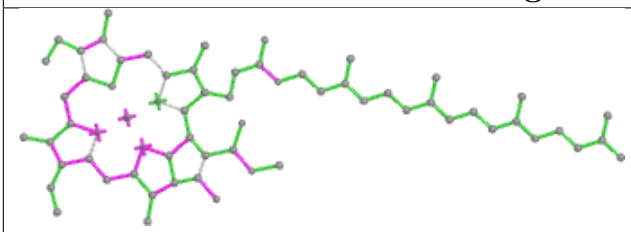
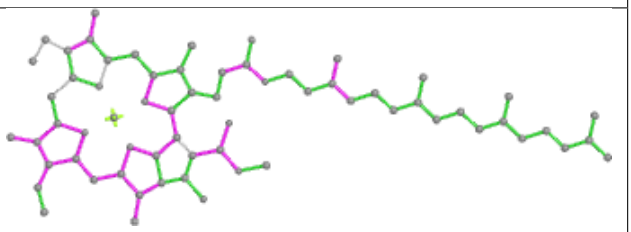
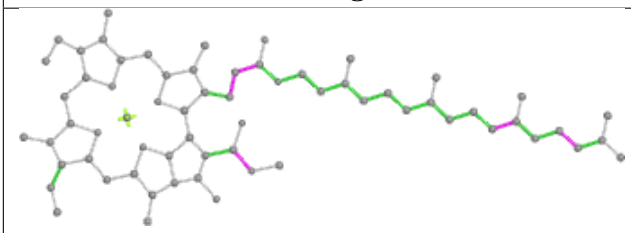
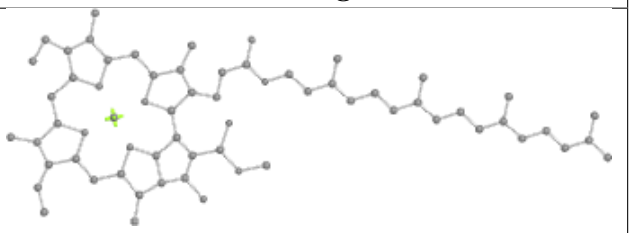
Ligand CLA B 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

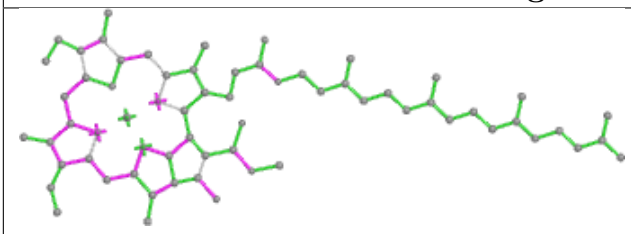
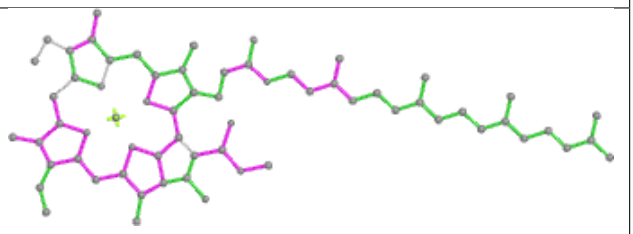
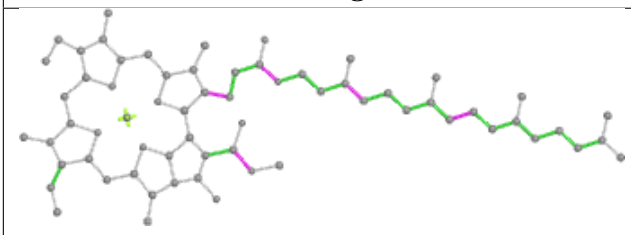
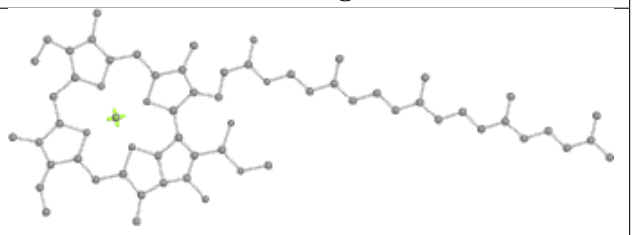
Ligand CLA 5 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

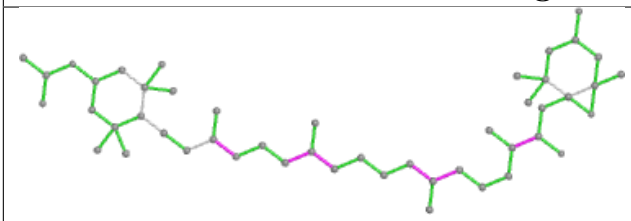
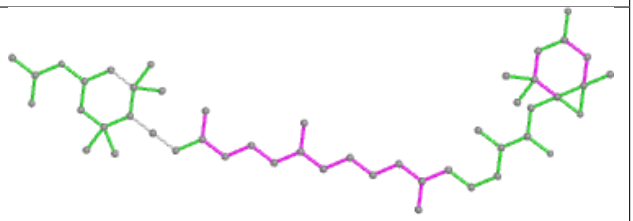
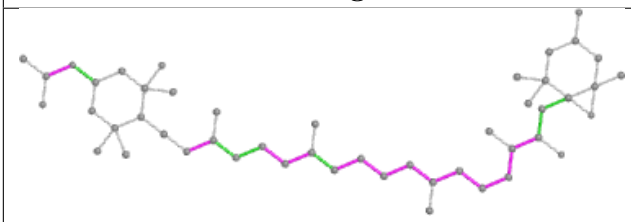
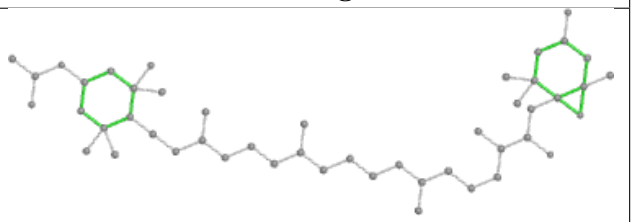
Ligand CLA b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

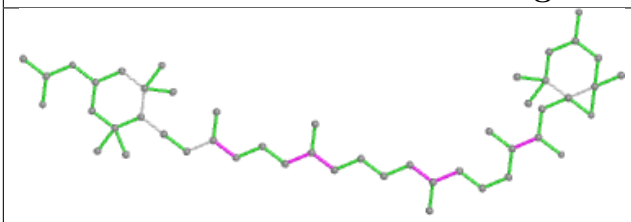
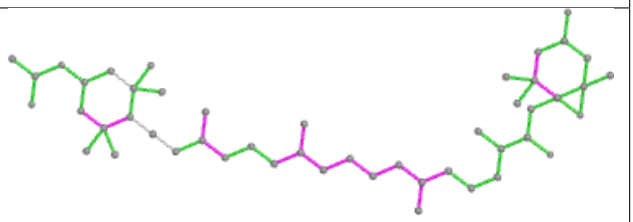
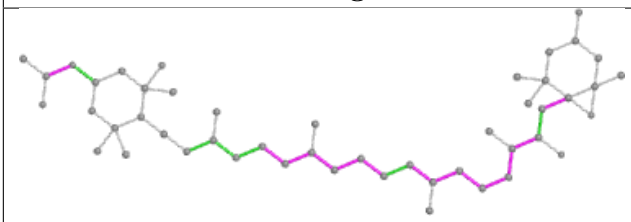
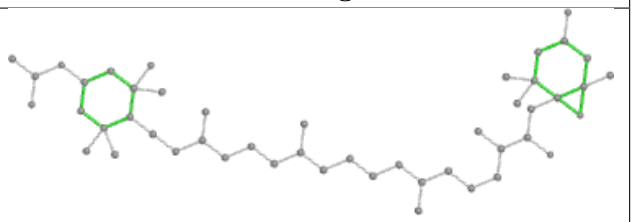
Ligand CLA B 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

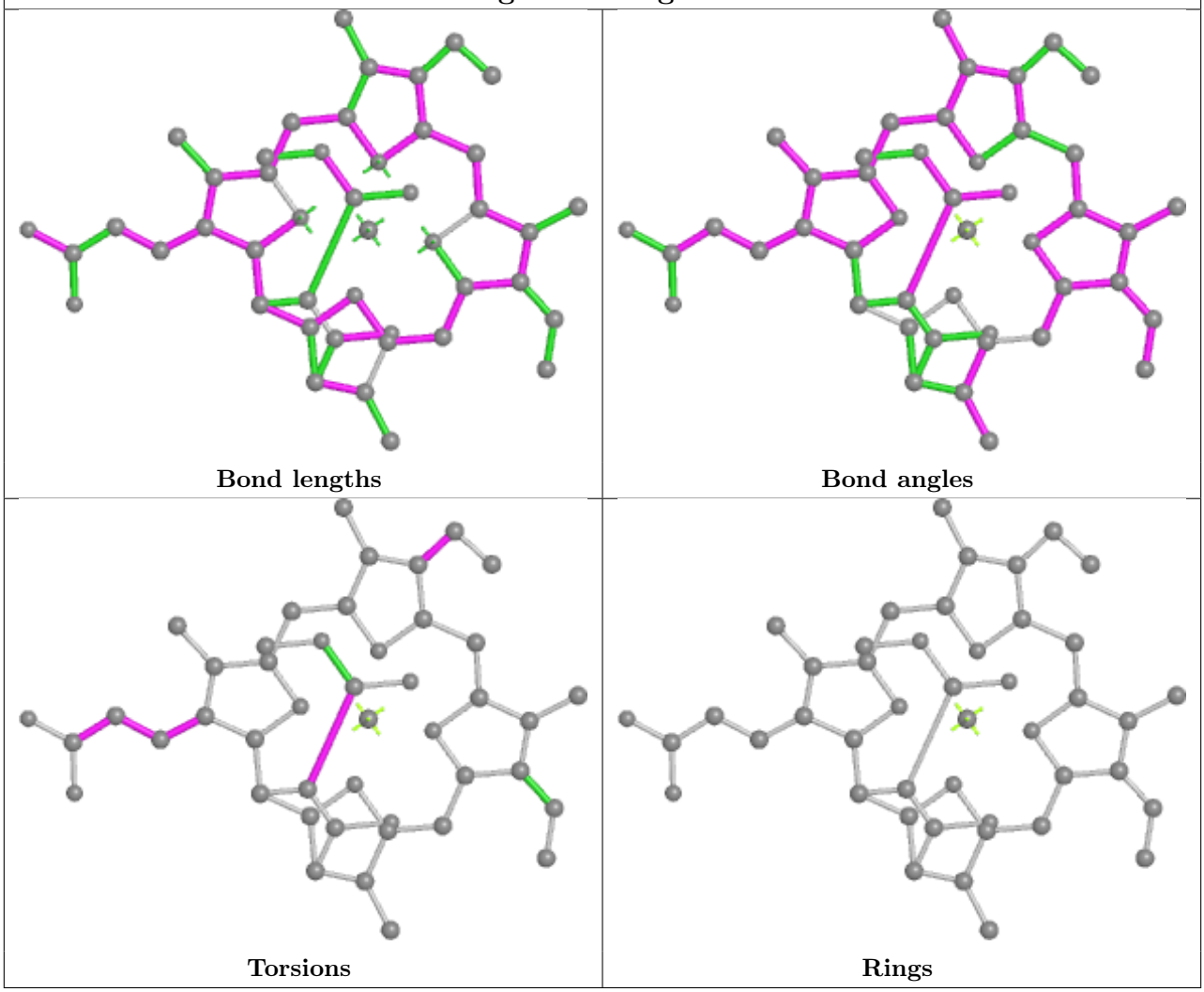
Ligand CLA B 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

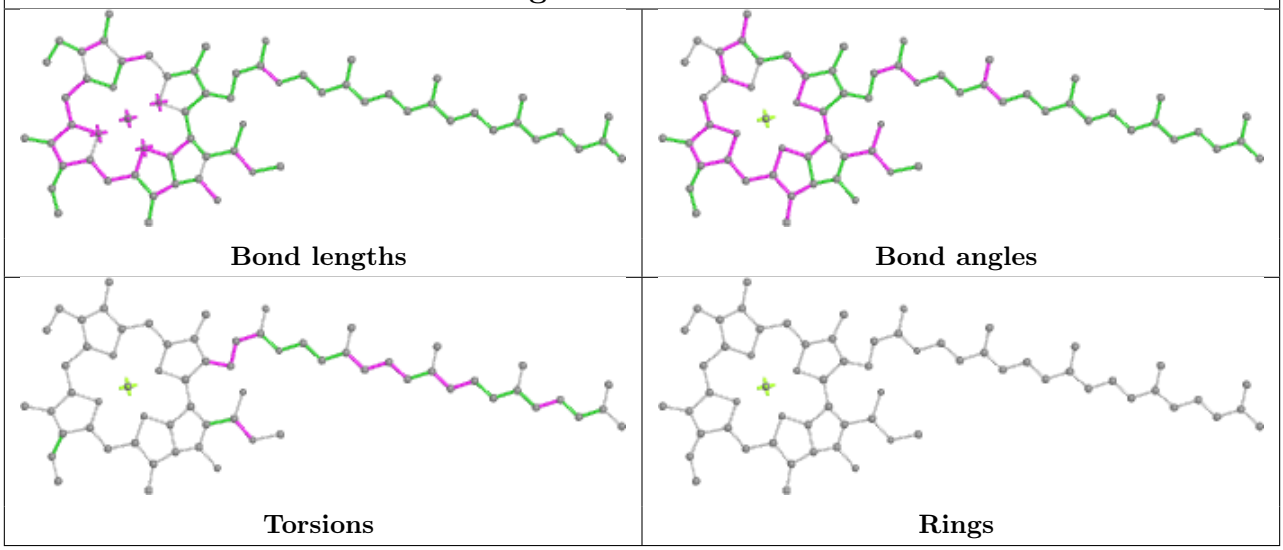
Ligand A86 2 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 8 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

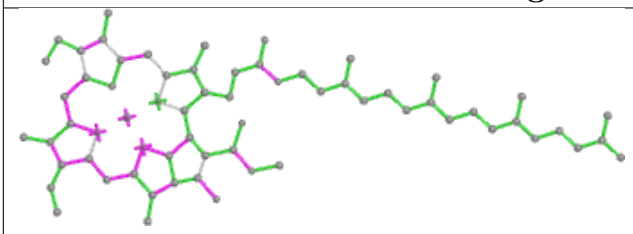
Ligand KC1 g 315



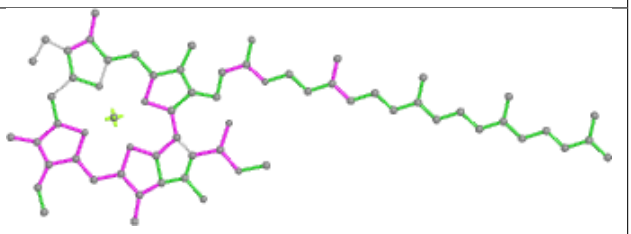
Ligand CLA 7 301



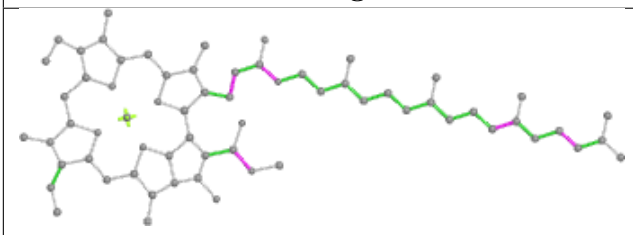
Ligand CLA b 611



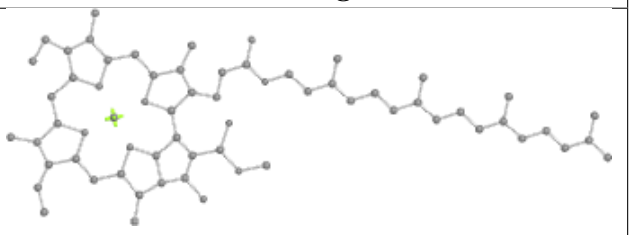
Bond lengths



Bond angles

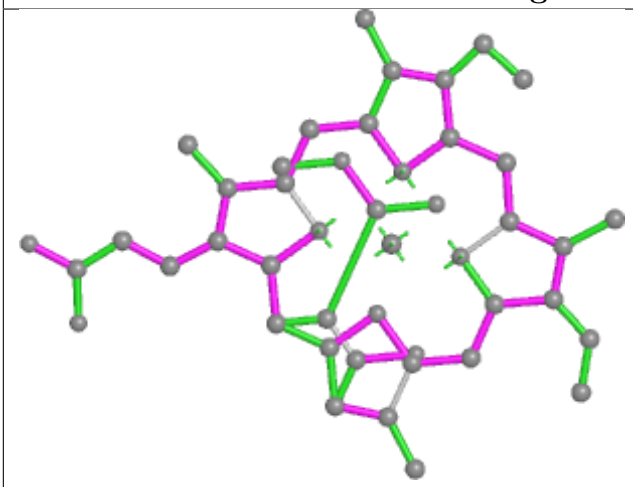


Torsions

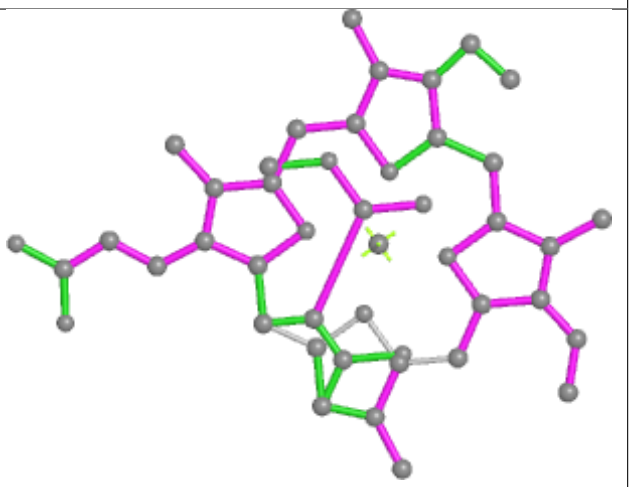


Rings

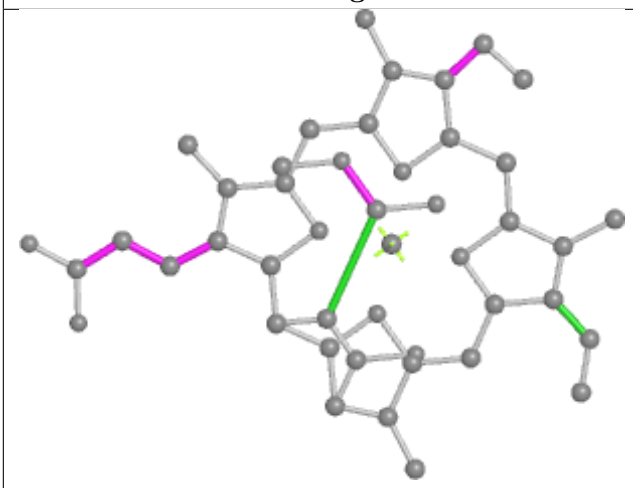
Ligand KC1 5 314



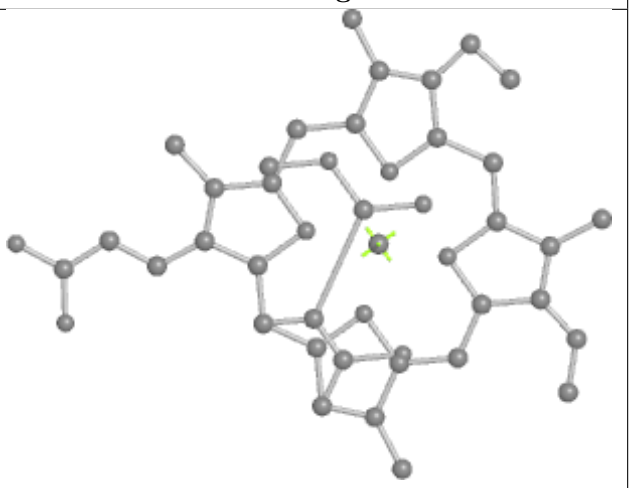
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

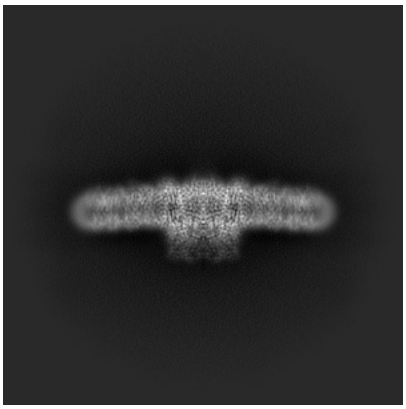
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-62499. These allow visual inspection of the internal detail of the map and identification of artifacts.

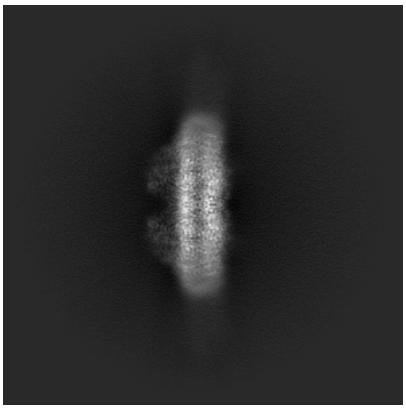
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

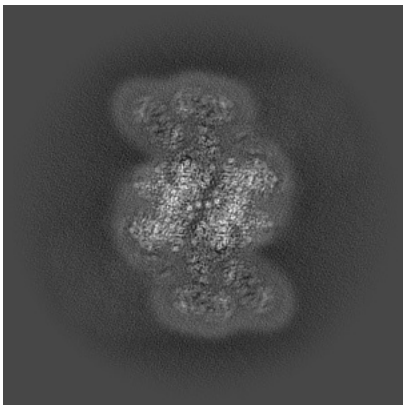
6.1.1 Primary map



X

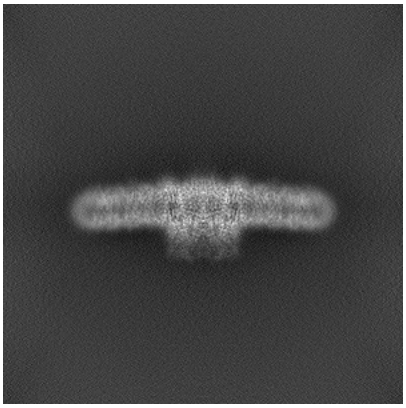


Y

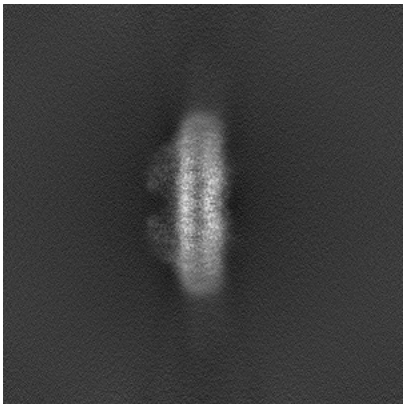


Z

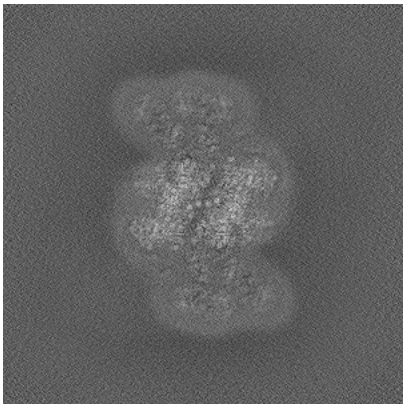
6.1.2 Raw map



X



Y

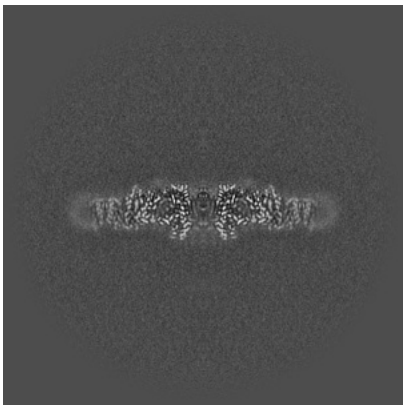


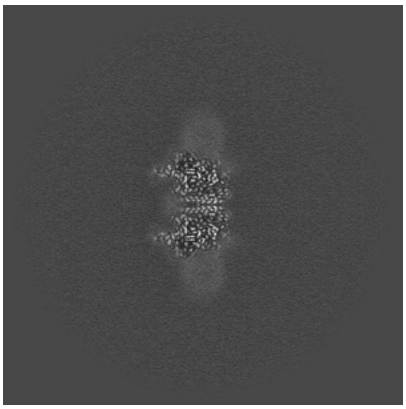
Z

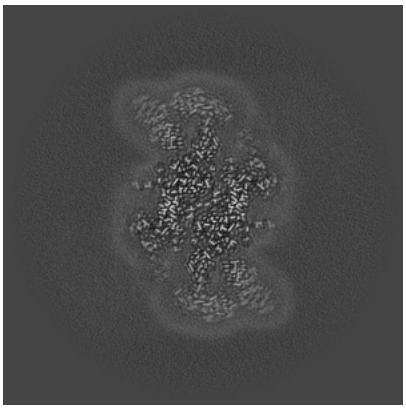
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

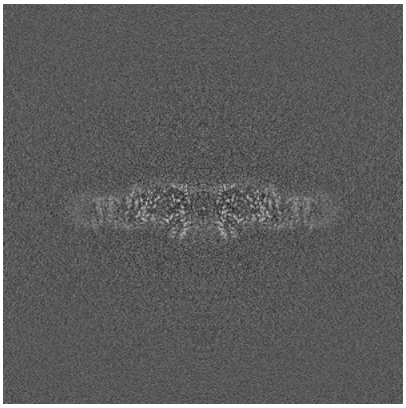
6.2.1 Primary map

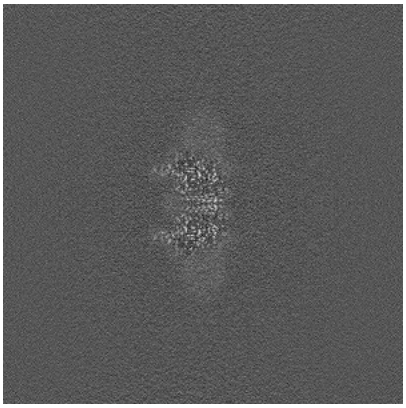

X Index: 300

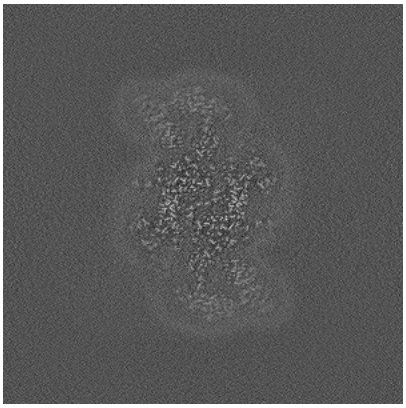

Y Index: 300


Z Index: 300

6.2.2 Raw map


X Index: 300

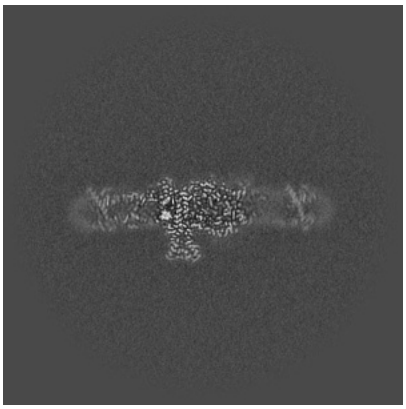

Y Index: 300

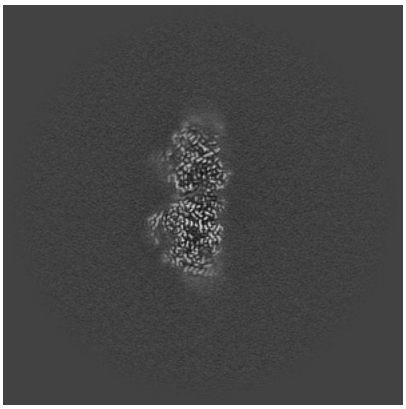

Z Index: 300

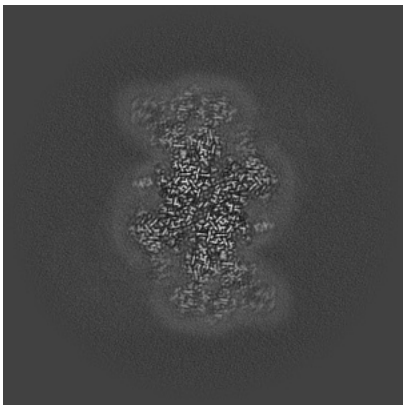
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

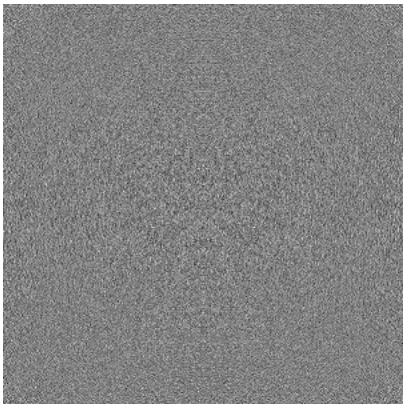
6.3.1 Primary map

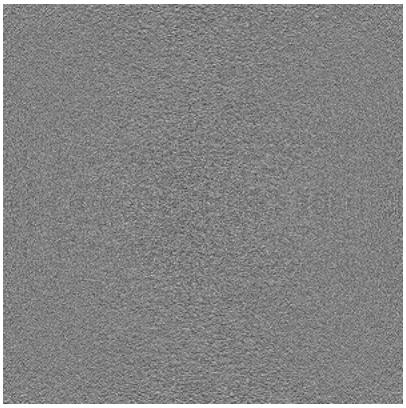

X Index: 332

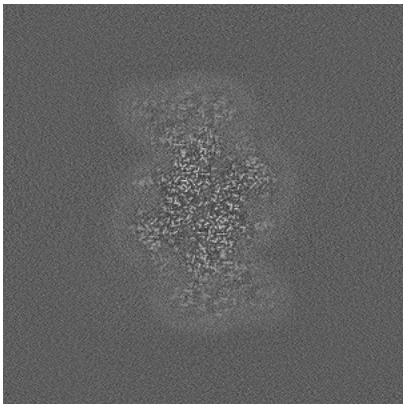

Y Index: 328


Z Index: 308

6.3.2 Raw map


X Index: 0

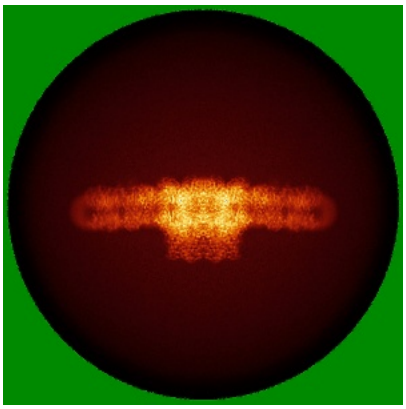

Y Index: 0

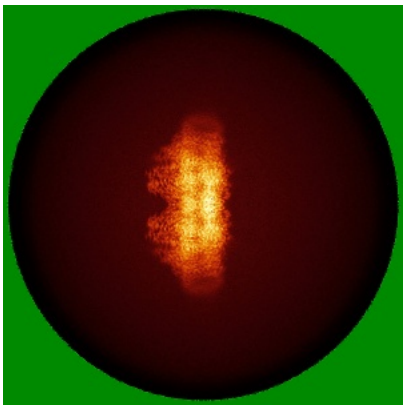

Z Index: 308

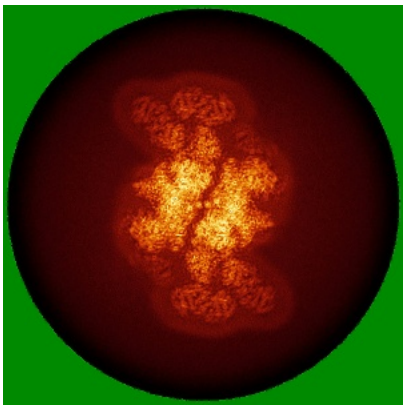
The images above show the largest variance slices of the map in three orthogonal directions.

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

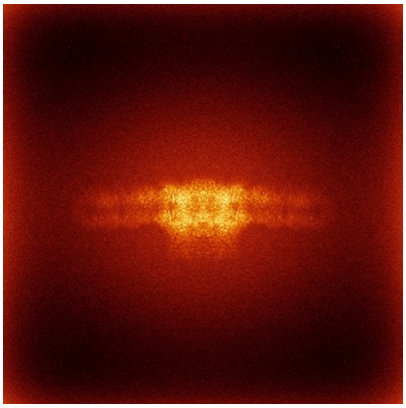
6.4.1 Primary map

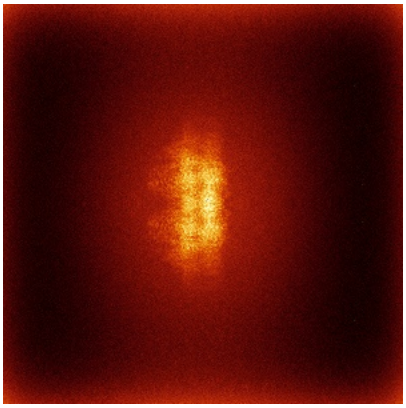

X

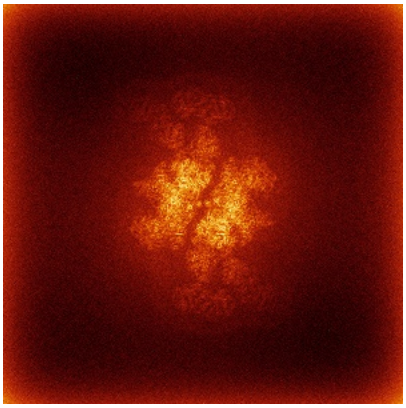

Y


Z

6.4.2 Raw 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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

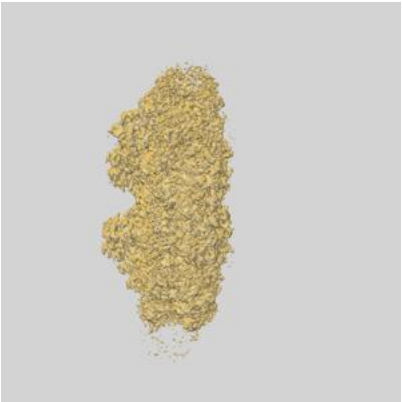
This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

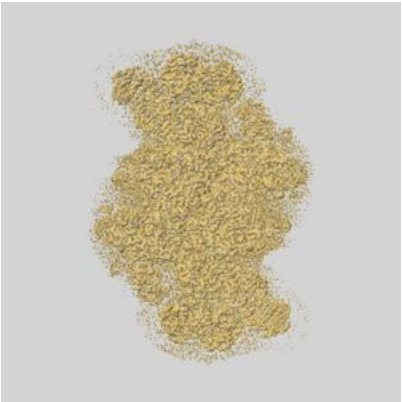
- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_62499_msk_1.map (i)

X



Y

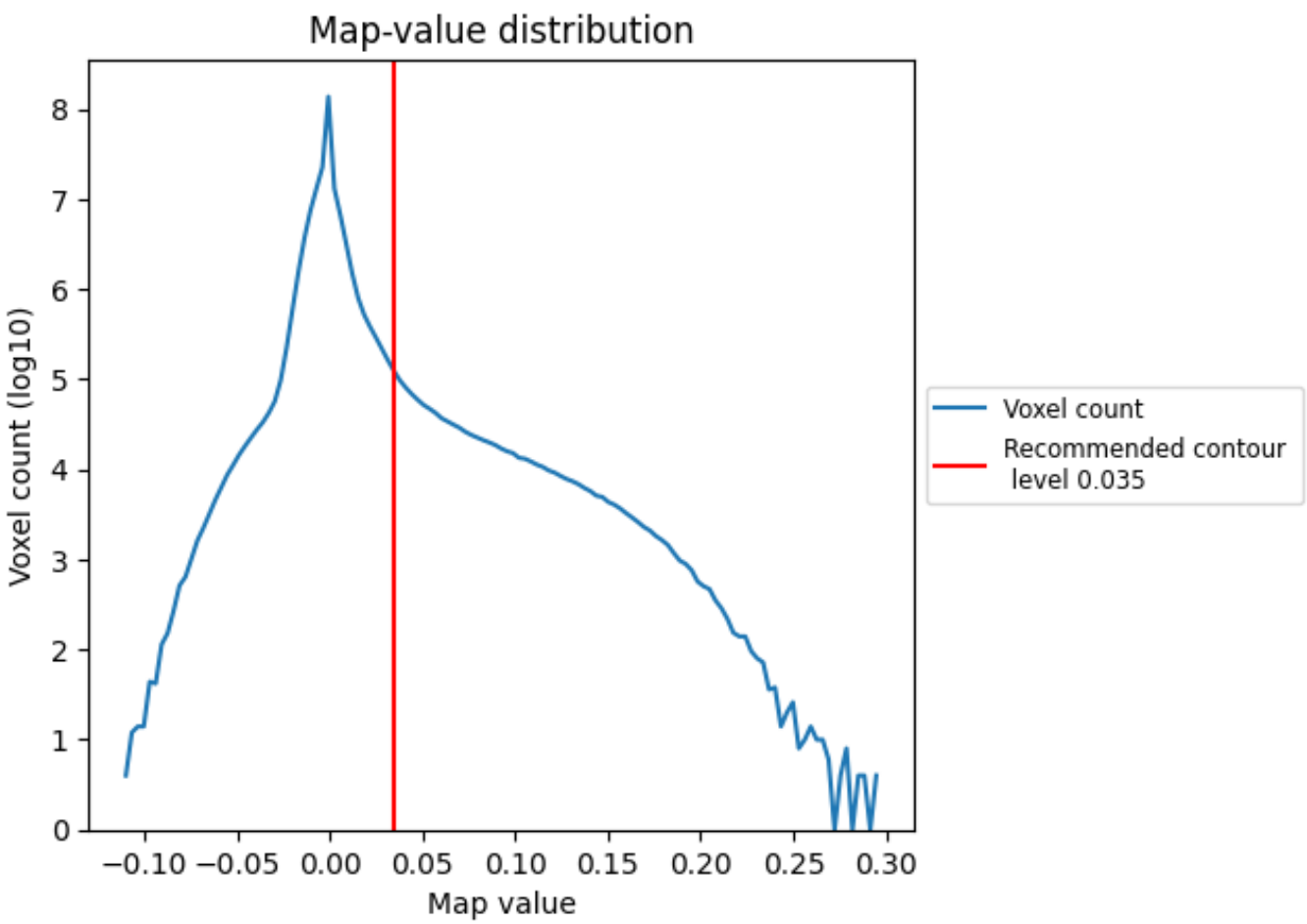


Z

7 Map analysis (i)

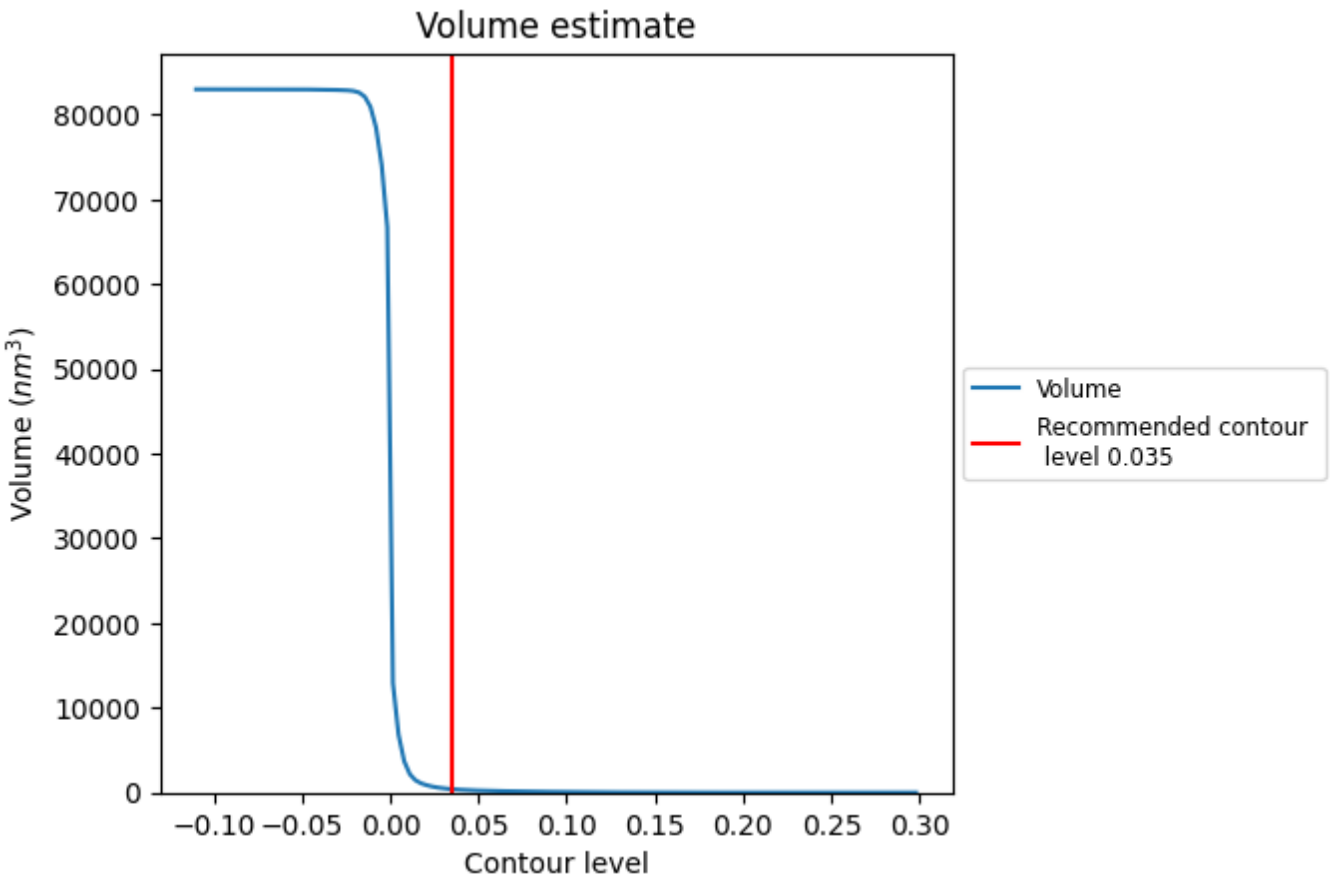
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

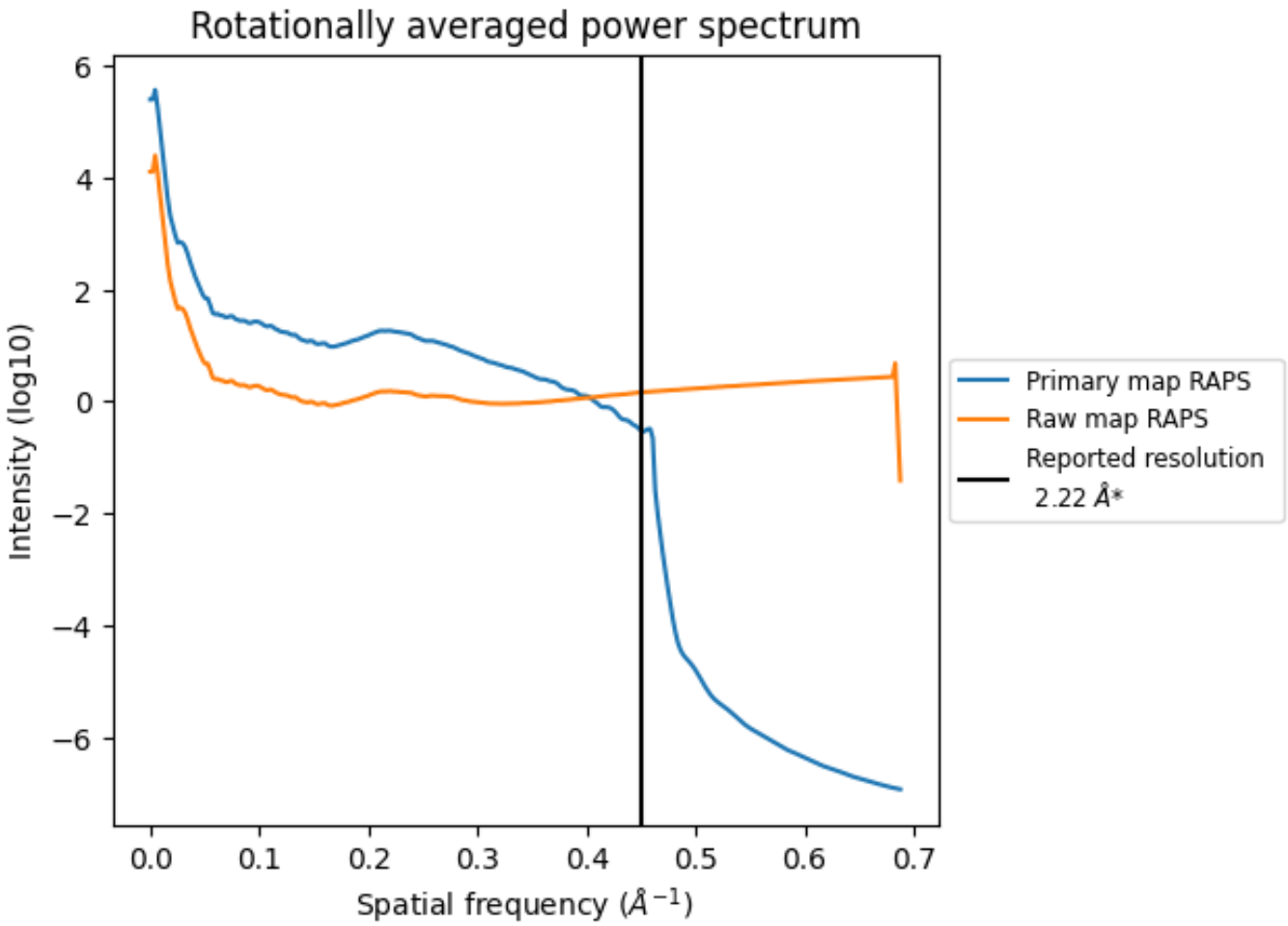
7.2 Volume estimate (i)



The volume at the recommended contour level is 402 nm^3; this corresponds to an approximate mass of 363 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)

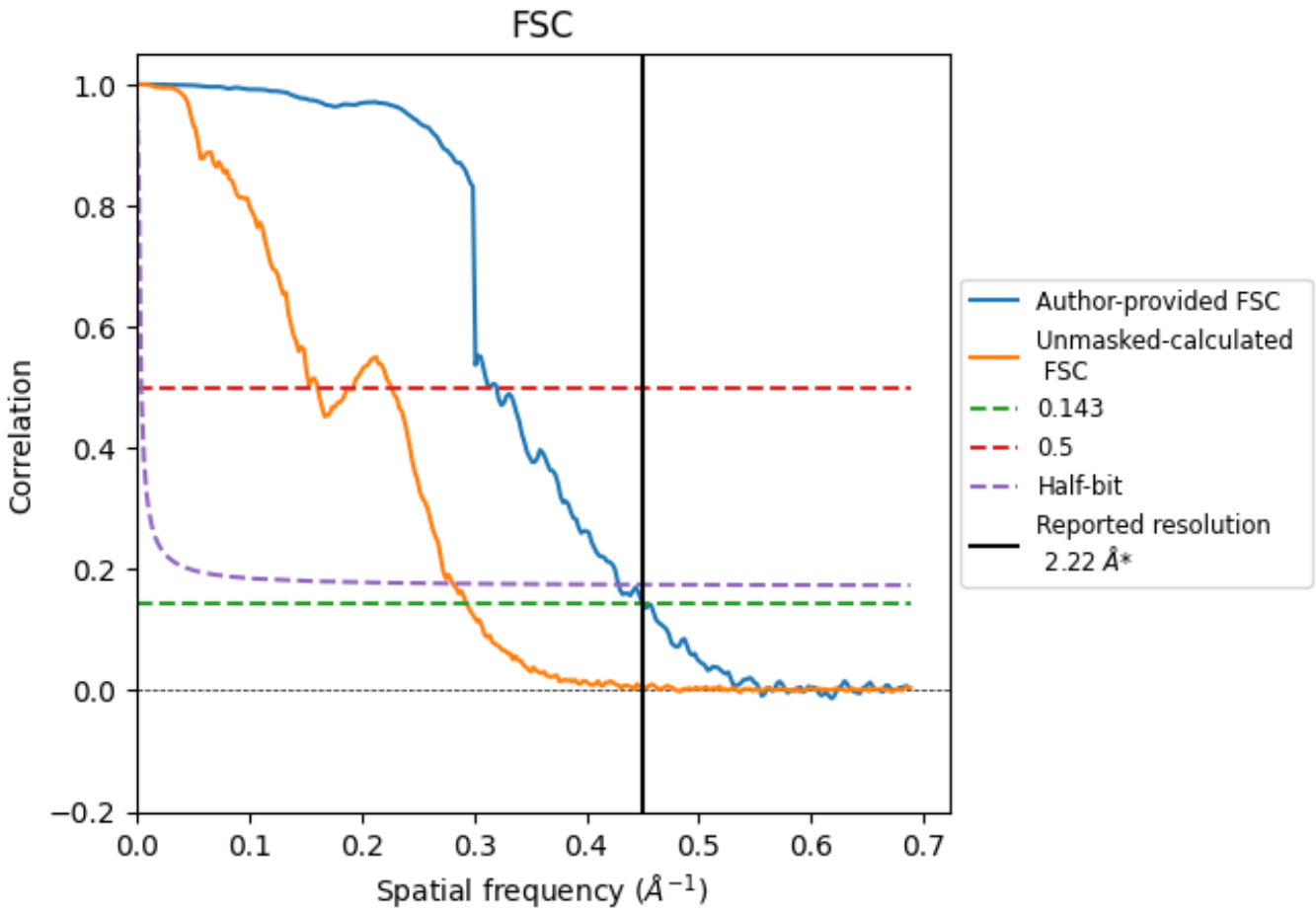


*Reported resolution corresponds to spatial frequency of 0.450 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.450 Å^{-1}

8.2 Resolution estimates (i)

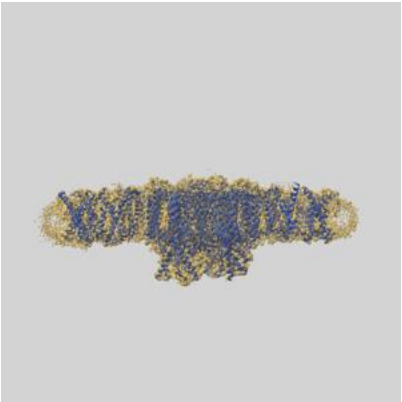
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.22	-	-
Author-provided FSC curve	2.22	3.12	2.33
Unmasked-calculated*	3.41	6.21	3.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.41 differs from the reported value 2.22 by more than 10 %

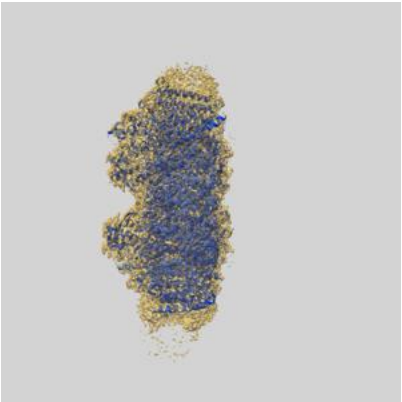
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-62499 and PDB model 9KQB. Per-residue inclusion information can be found in section 3 on page 36.

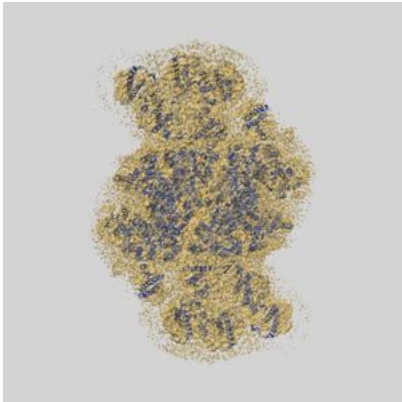
9.1 Map-model overlay (i)



X



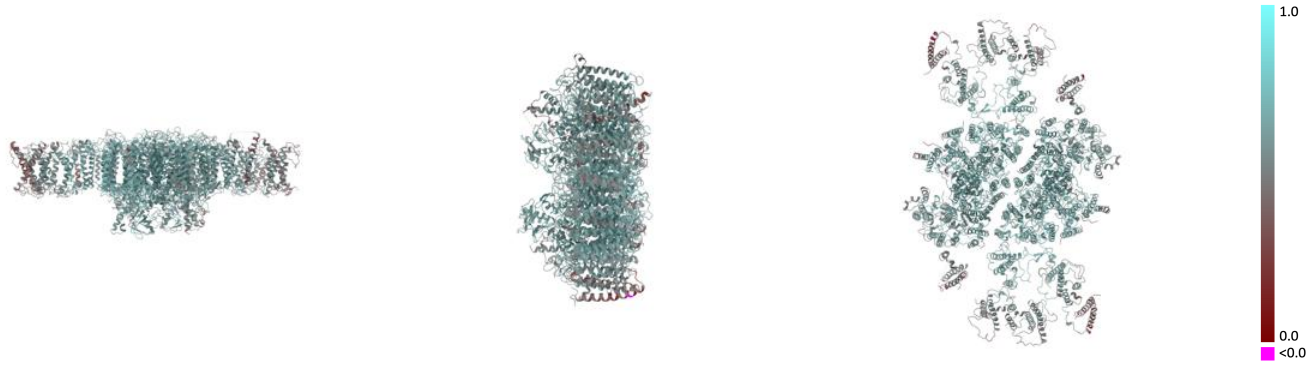
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

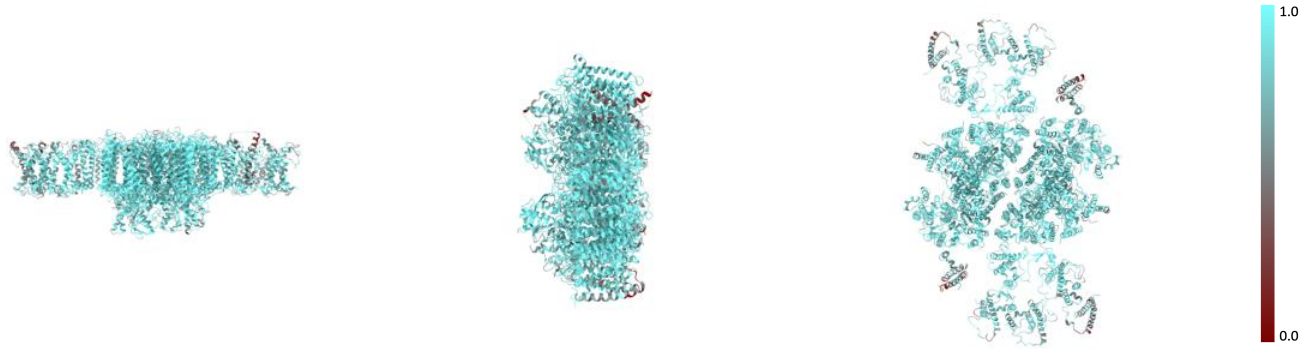
9.2 Q-score mapped to coordinate model (i)



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.

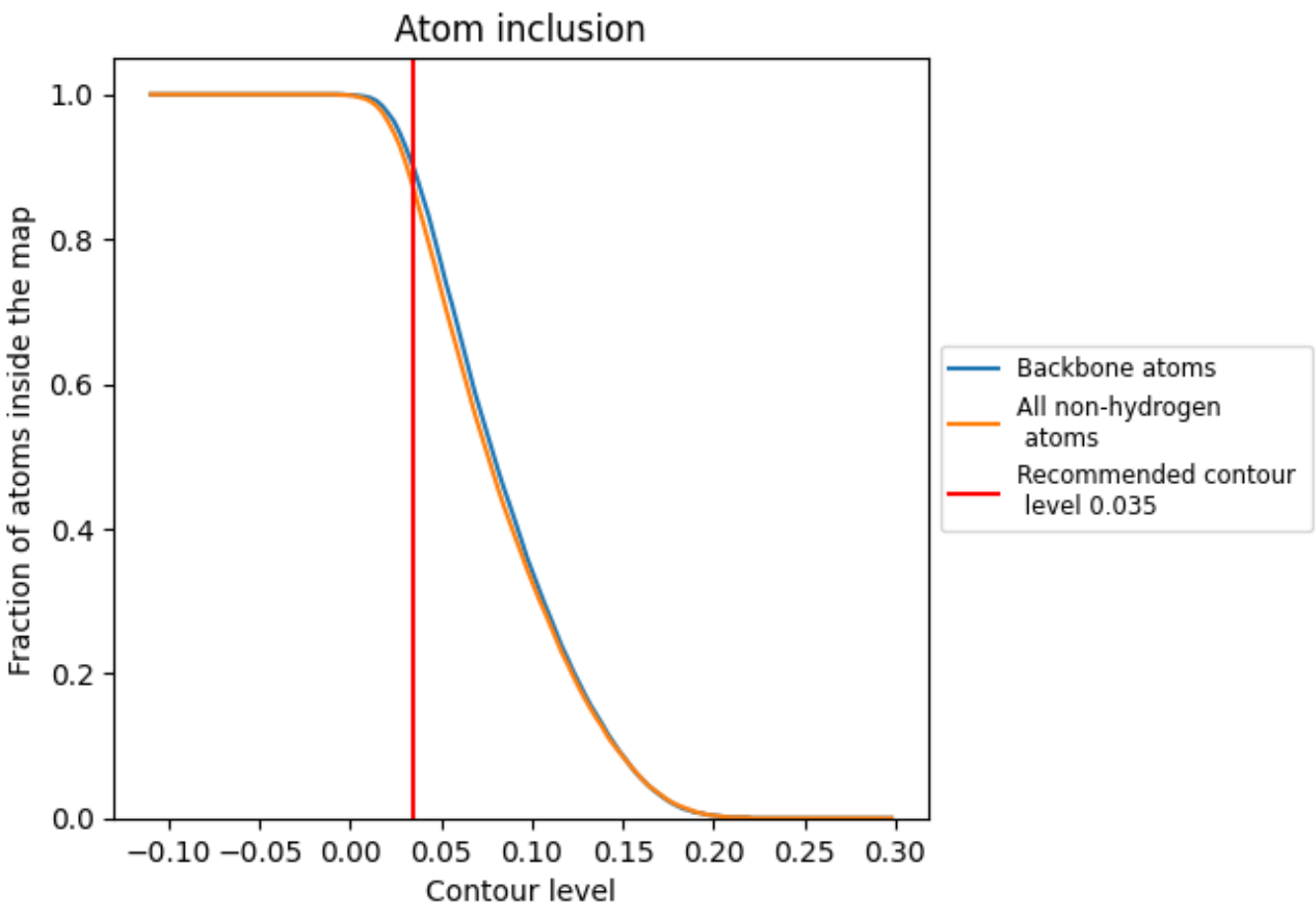
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.5890
1	0.8120	0.5590
2	0.9190	0.6140
3	0.5640	0.4510
4	0.6030	0.3970
5	0.7310	0.4840
6	0.7480	0.4860
7	0.8190	0.5580
8	0.9180	0.6110
9	0.5510	0.4530
A	0.9370	0.6400
B	0.9510	0.6520
C	0.8820	0.5840
D	0.9510	0.6650
E	0.8340	0.5730
F	0.8420	0.5610
G	0.6060	0.3930
H	0.9820	0.6700
I	0.9520	0.6410
J	0.7550	0.4840
K	0.7990	0.5050
L	0.9370	0.6450
M	0.9260	0.6350
N	0.9160	0.6200
T	0.9530	0.6600
W	0.8900	0.5810
X	0.9350	0.6080
a	0.9340	0.6440
b	0.9530	0.6530
c	0.8870	0.5870
d	0.9750	0.6730
e	0.8440	0.5730
f	0.8090	0.5570
g	0.7280	0.4800
h	0.9460	0.6490

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.9420	0.6340
k	0.8100	0.5140
l	0.9640	0.6710
m	0.9420	0.6450
n	0.9300	0.6330
t	0.9450	0.6540
w	0.8950	0.5800
x	0.9460	0.6130