Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 11:38 pm GMT

PDB ID	:	9EVX
EMDB ID	:	EMD-50019
Title	:	cryoEM structure of Photosystem II averaged across S2-S3 states at 1.71 Angstrom resolution
Authors	:	Hussein, R.; Graca, A.; Zouni, A.; Messinger, J.; Schroder, W.P.
Deposited on	:	2024-04-02
Resolution	:	1.71 Å(reported)

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

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

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

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

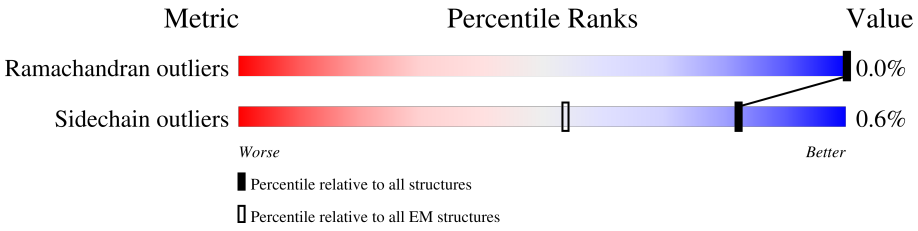
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.71 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	344	97%
1	a	344	97%
2	B	510	98%
2	b	510	98%
3	C	461	97%
3	c	461	97%
4	D	352	97%
4	d	352	97%
5	E	84	12% 98%

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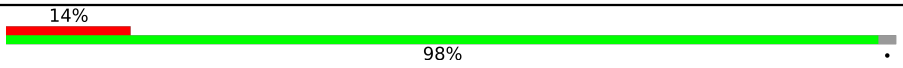
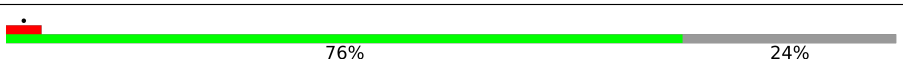
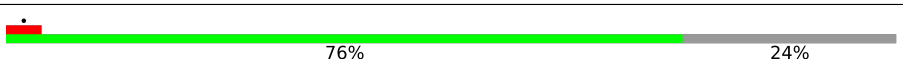
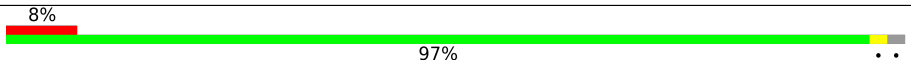
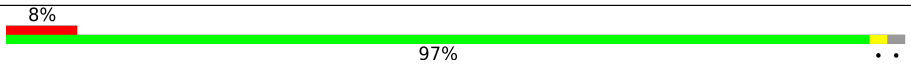
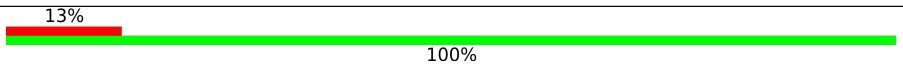
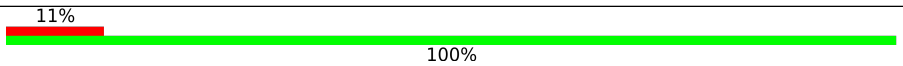
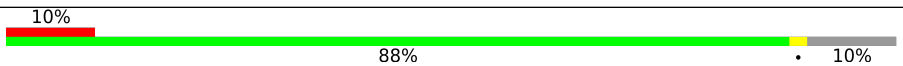
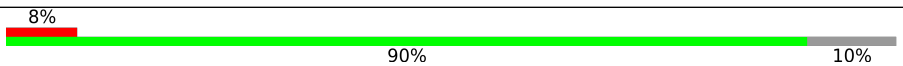
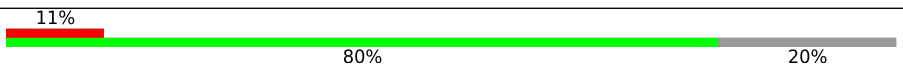
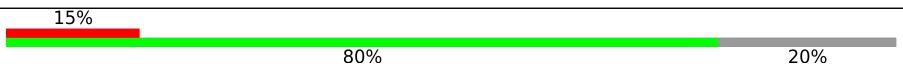
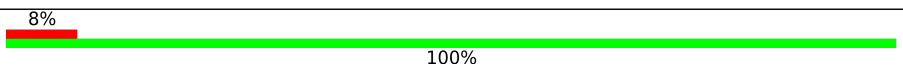
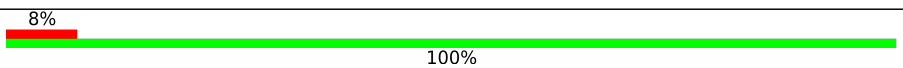
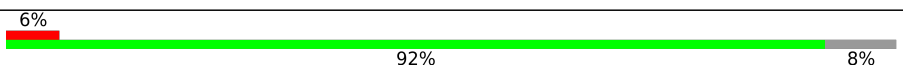
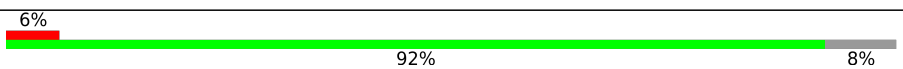
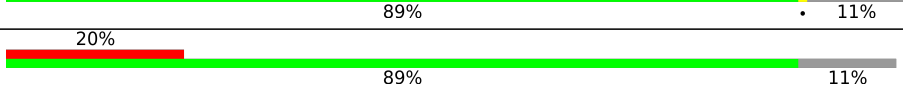
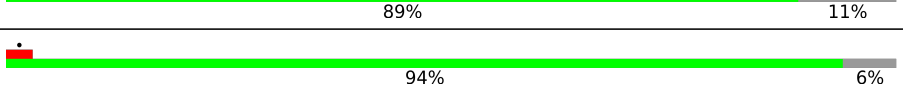
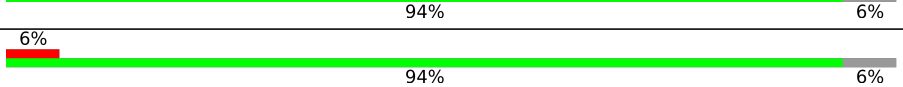
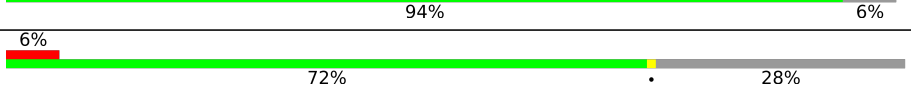
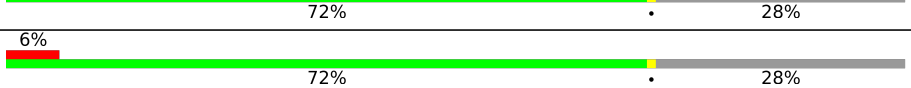
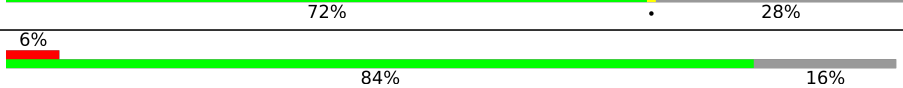
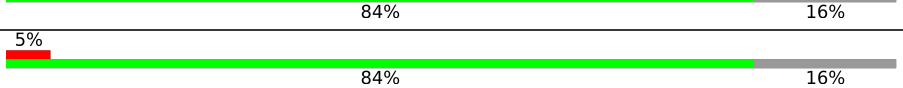
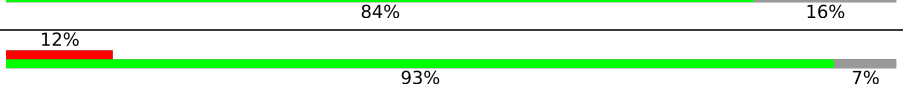
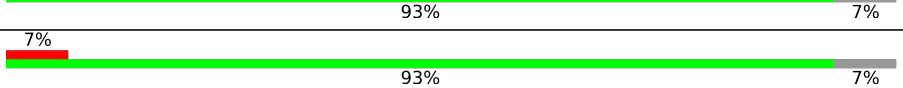
Mol	Chain	Length	Quality of chain
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	X	41	
17	x	41	

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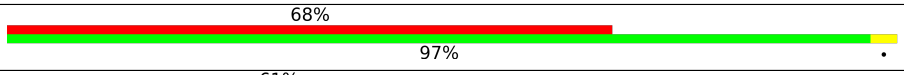
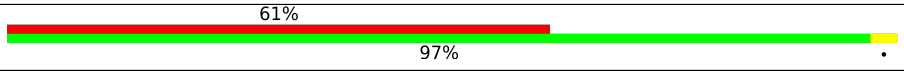
Mol	Chain	Length	Quality of chain
18	Y	46	
18	y	46	
19	Z	62	
19	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	419	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	a	406	X	-	-	-
22	CLA	a	419	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 104863 atoms, of which 52030 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 Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	334	Total	C	H	N	O	S	3	0
			5164	1723	2530	433	463	15		
1	a	334	Total	C	H	N	O	S	3	0
			5164	1723	2530	433	463	15		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	505	Total	C	H	N	O	S	3	0
			7852	2620	3858	667	694	13		
2	b	505	Total	C	H	N	O	S	3	0
			7852	2620	3858	667	694	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	451	Total	C	H	N	O	S	2	0
			6899	2283	3408	585	610	13		
3	c	451	Total	C	H	N	O	S	2	0
			6899	2283	3408	585	610	13		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0
			5338	1800	2621	444	461	12		
4	d	341	Total	C	H	N	O	S	0	0
			5338	1800	2621	444	461	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	82	Total	C	H	N	O	0	0
			1301	431	640	107	123		
5	e	82	Total	C	H	N	O	0	0
			1301	431	640	107	123		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	34	Total	C	H	N	O	S	0	0
			557	187	282	45	42	1		
6	f	34	Total	C	H	N	O	S	0	0
			557	187	282	45	42	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	65	Total	C	H	N	O	S	2	0
			1045	338	534	83	87	3		
7	h	65	Total	C	H	N	O	S	2	0
			1045	338	534	83	87	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	41	CYS	PHE	variant	UNP Q8DJ43
h	41	CYS	PHE	variant	UNP Q8DJ43

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	38	Total	C	H	N	O	S	0	0
			641	211	328	48	53	1		
8	i	38	Total	C	H	N	O	S	0	0
			641	211	328	48	53	1		

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	36	Total	C	H	N	O	S	0	0
			525	174	268	40	42	1		
9	j	36	Total	C	H	N	O	S	0	0
			525	174	268	40	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	37	Total	C	H	N	O	0	0
			598	204	305	43	46		
10	k	37	Total	C	H	N	O	0	0
			598	204	305	43	46		

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	L	37	Total	C	H	N	O	S	2	0
			640	208	328	49	54	1		
11	l	37	Total	C	H	N	O	S	2	0
			640	208	328	49	54	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	M	33	Total	C	H	N	O	S	2	0
			545	177	281	38	48	1		
12	m	33	Total	C	H	N	O	S	2	0
			545	177	281	38	48	1		

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	243	Total	C	H	N	O	S	3	0
			3710	1171	1834	313	387	5		
13	o	243	Total	C	H	N	O	S	3	0
			3710	1171	1834	313	387	5		

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	T	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		
14	t	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	97	Total	C	H	N	O	0	0
			1547	491	773	129	154		
15	u	97	Total	C	H	N	O	0	0
			1547	491	773	129	154		

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0
			2135	675	1071	177	208	4		
16	v	137	Total	C	H	N	O	S	0	0
			2135	675	1071	177	208	4		

- Molecule 17 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	38	Total	C	H	N	O	0	0
			593	188	312	45	48		
17	x	38	Total	C	H	N	O	0	0
			593	188	312	45	48		

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Y	27	Total	C	H	N	O	S	0	0
			423	131	224	35	30	3		
18	y	27	Total	C	H	N	O	S	0	0
			425	131	226	35	30	3		

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0
			995	328	516	72	77	2		
19	z	62	Total	C	H	N	O	S	0	0
			995	328	516	72	77	2		

- Molecule 20 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Fe	0
			1	1	

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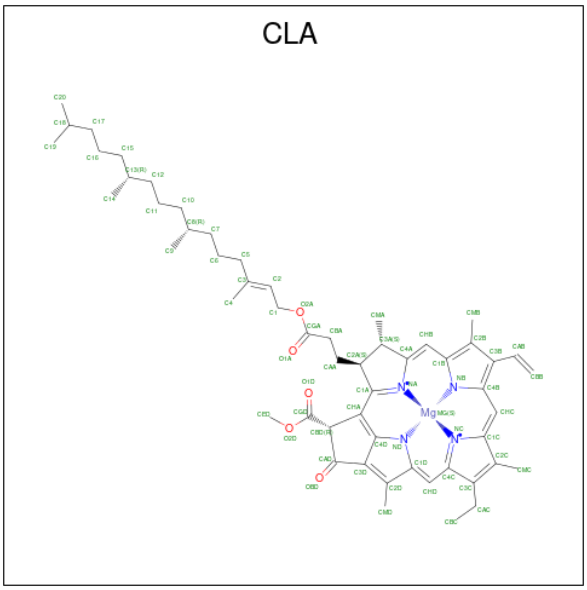
Mol	Chain	Residues	Atoms	AltConf
20	a	1	Total Fe 1 1	0

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
21	A	2	Total Cl 2 2	0
21	a	2	Total Cl 2 2	0

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



Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C H Mg N O 137 55 72 1 4 5	0
22	A	1	Total C H Mg N O 119 50 59 1 4 5	0
22	A	1	Total C H Mg N O 102 44 48 1 4 5	0
22	A	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 137 55 72 1 4 5	0
22	B	1	Total C H Mg N O 119 50 59 1 4 5	0
22	C	1	Total C H Mg N O 137 55 72 1 4 5	0
22	C	1	Total C H Mg N O 137 55 72 1 4 5	0
22	C	1	Total C H Mg N O 137 55 72 1 4 5	0
22	C	1	Total C H Mg N O 117 49 58 1 4 5	0
22	C	1	Total C H Mg N O 137 55 72 1 4 5	0
22	C	1	Total C H Mg N O 137 55 72 1 4 5	0
22	C	1	Total C H Mg N O 137 55 72 1 4 5	0

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Mol	Chain	Residues	Atoms						AltConf
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	a	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	a	1	Total 102	C 44	H 48	Mg 1	N 4	O 5	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	b	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 117	C 49	H 58	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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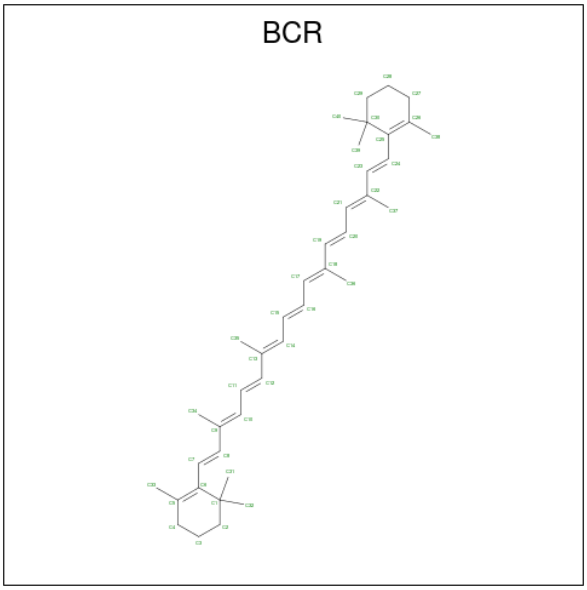
Mol	Chain	Residues	Atoms						AltConf
22	d	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	H	0
			96	40	56	
23	B	1	Total	C	H	0
			96	40	56	
23	B	1	Total	C	H	0
			96	40	56	
23	B	1	Total	C	H	0
			96	40	56	
23	C	1	Total	C	H	0
			96	40	56	
23	C	1	Total	C	H	0
			96	40	56	
23	D	1	Total	C	H	0
			96	40	56	
23	H	1	Total	C	H	0
			96	40	56	
23	K	1	Total	C	H	0
			96	40	56	
23	K	1	Total	C	H	0
			96	40	56	

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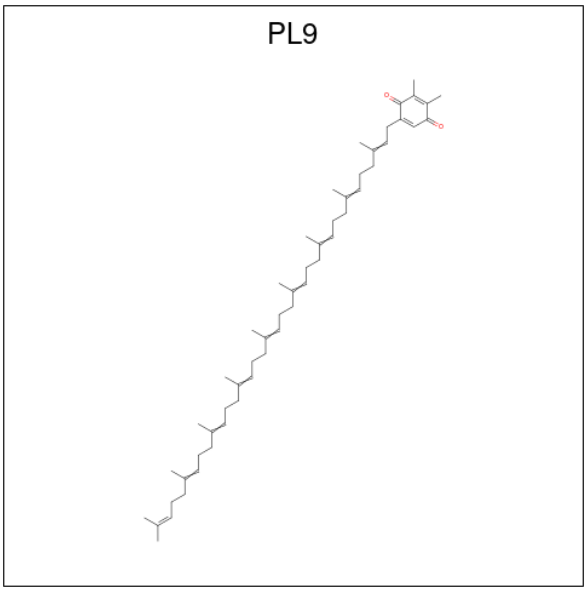
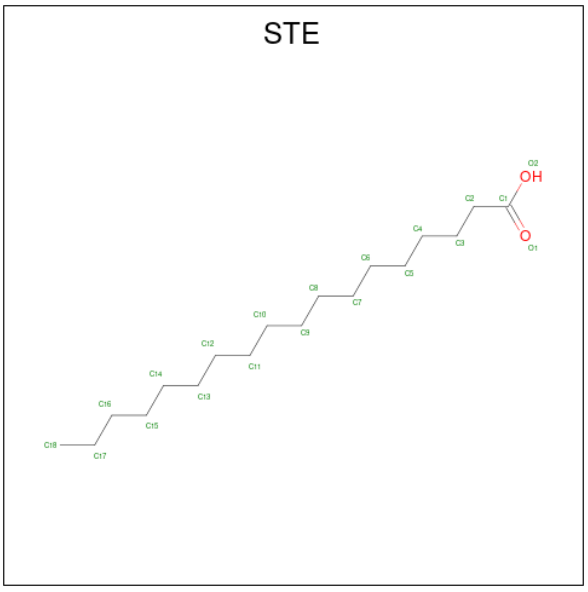
Mol	Chain	Residues	Atoms	AltConf
23	T	1	Total C H 96 40 56	0
23	a	1	Total C H 96 40 56	0
23	b	1	Total C H 96 40 56	0
23	b	1	Total C H 96 40 56	0
23	b	1	Total C H 96 40 56	0
23	c	1	Total C H 96 40 56	0
23	c	1	Total C H 96 40 56	0
23	d	1	Total C H 96 40 56	0
23	h	1	Total C H 96 40 56	0
23	k	1	Total C H 96 40 56	0
23	k	1	Total C H 96 40 56	0
23	t	1	Total C H 96 40 56	0

- Molecule 24 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 (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	H	O	0
			135	53	80	2	
24	D	1	Total	C	H	O	0
			135	53	80	2	
24	a	1	Total	C	H	O	0
			135	53	80	2	
24	d	1	Total	C	H	O	0
			135	53	80	2	

- Molecule 25 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C H 23 9 14	0
25	A	1	Total C H 23 8 15	0
25	A	1	Total C H 32 11 21	0
25	A	1	Total C H 32 11 21	0
25	A	1	Total C H O 28 10 16 2	0
25	B	1	Total C H O 43 15 26 2	0
25	B	1	Total C H O 28 10 16 2	0
25	B	1	Total C H 32 12 20	0
25	C	1	Total C H O 34 12 20 2	0
25	C	1	Total C H O 28 10 16 2	0
25	C	1	Total C H 23 8 15	0
25	D	1	Total C H O 55 18 35 2	0
25	D	1	Total C H 26 9 17	0
25	E	1	Total C H O 28 10 16 2	0
25	E	1	Total C H 35 12 23	0
25	E	1	Total C H O 55 18 35 2	0
25	I	1	Total C H 38 14 24	0
25	J	1	Total C H 32 12 20	0
25	K	1	Total C H 32 11 21	0
25	M	1	Total C H 26 10 16	0
25	T	1	Total C H 44 15 29	0
25	a	1	Total C H 23 9 14	0

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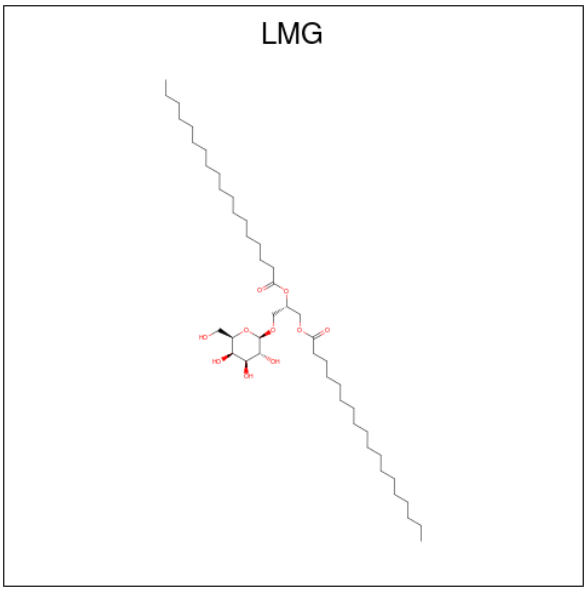
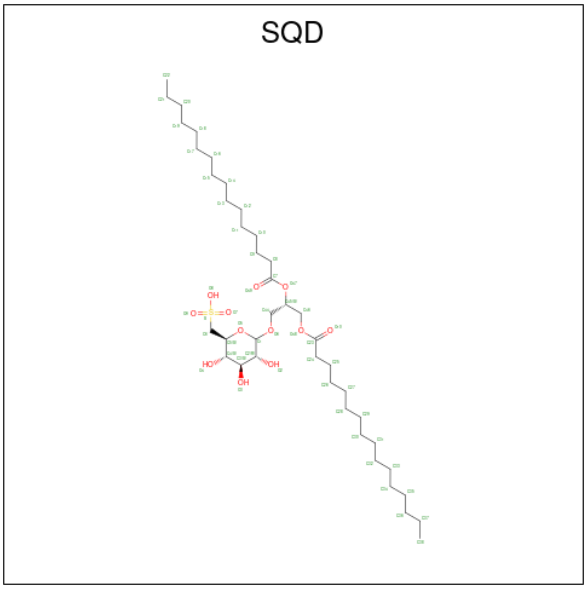
Mol	Chain	Residues	Atoms	AltConf
25	a	1	Total C H 23 8 15	0
25	a	1	Total C H 32 11 21	0
25	a	1	Total C H 32 11 21	0
25	a	1	Total C H O 28 10 16 2	0
25	b	1	Total C H 32 12 20	0
25	b	1	Total C H O 43 15 26 2	0
25	b	1	Total C H O 28 10 16 2	0
25	c	1	Total C H O 34 12 20 2	0
25	c	1	Total C H O 28 10 16 2	0
25	c	1	Total C H 23 8 15	0
25	d	1	Total C H O 55 18 35 2	0
25	d	1	Total C H 26 9 17	0
25	e	1	Total C H O 28 10 16 2	0
25	e	1	Total C H 35 12 23	0
25	e	1	Total C H O 55 18 35 2	0
25	i	1	Total C H 38 14 24	0
25	j	1	Total C H 32 12 20	0
25	k	1	Total C H 32 11 21	0
25	m	1	Total C H 26 10 16	0
25	t	1	Total C H O 46 16 28 2	0

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



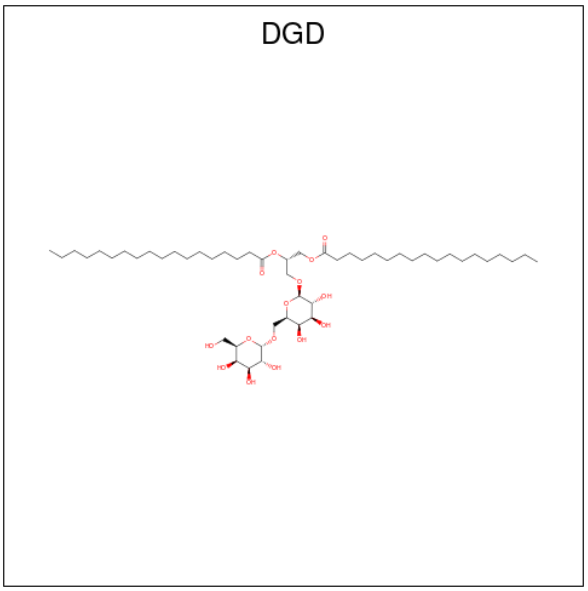
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	H	O	0
			114	38	66	10	
26	B	1	Total	C	H	O	0
			123	41	72	10	
26	C	1	Total	C	H	O	0
			114	38	66	10	
26	C	1	Total	C	H	O	0
			120	40	70	10	
26	D	1	Total	C	H	O	0
			83	29	49	5	
26	D	1	Total	C	H	O	0
			123	41	72	10	
26	H	1	Total	C	H	O	0
			98	34	59	5	
26	a	1	Total	C	H	O	0
			114	38	66	10	
26	b	1	Total	C	H	O	0
			123	41	72	10	
26	c	1	Total	C	H	O	0
			114	38	66	10	
26	c	1	Total	C	H	O	0
			120	40	70	10	
26	d	1	Total	C	H	O	0
			83	29	49	5	
26	d	1	Total	C	H	O	0
			123	41	72	10	
26	h	1	Total	C	H	O	0
			98	34	59	5	

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



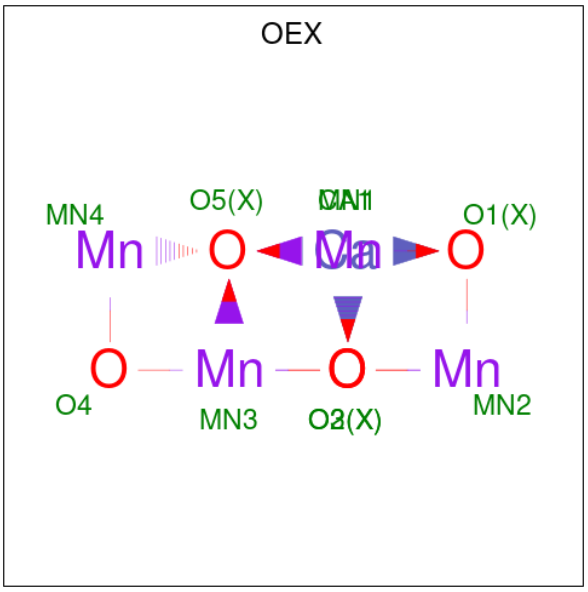
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	H	O	S	0
			122	39	70	12	1	
27	A	1	Total	C	H	O	S	0
			131	41	77	12	1	
27	B	1	Total	C	H	O	S	0
			131	41	77	12	1	
27	X	1	Total	C	H	O	S	0
			81	25	45	10	1	
27	a	1	Total	C	H	O	S	0
			122	39	70	12	1	
27	a	1	Total	C	H	O	S	0
			131	41	77	12	1	
27	b	1	Total	C	H	O	S	0
			113	36	64	12	1	
27	x	1	Total	C	H	O	S	0
			81	25	45	10	1	

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



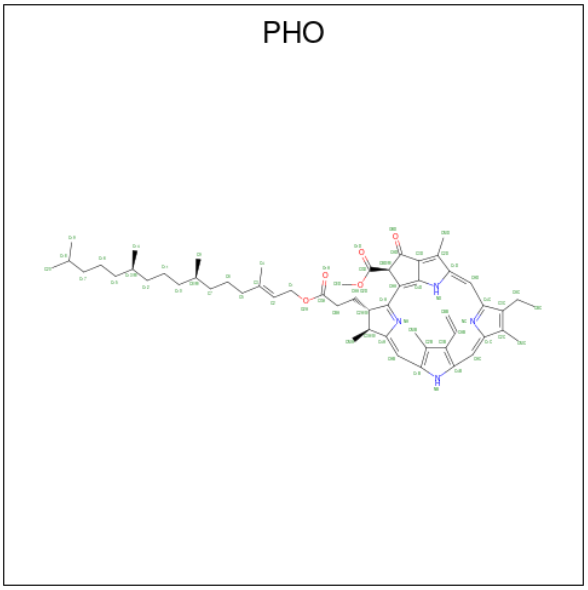
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	H	O	0
			162	51	96	15	
28	C	1	Total	C	H	O	0
			144	47	82	15	
28	C	1	Total	C	H	O	0
			129	42	72	15	
28	C	1	Total	C	H	O	0
			144	47	82	15	
28	H	1	Total	C	H	O	0
			144	47	82	15	
28	a	1	Total	C	H	O	0
			162	51	96	15	
28	c	1	Total	C	H	O	0
			144	47	82	15	
28	c	1	Total	C	H	O	0
			129	42	72	15	
28	c	1	Total	C	H	O	0
			144	47	82	15	
28	h	1	Total	C	H	O	0
			144	47	82	15	

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
29	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 30 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	H	N	O	0
			138	55	74	4	5	
30	D	1	Total	C	H	N	O	0
			138	55	74	4	5	

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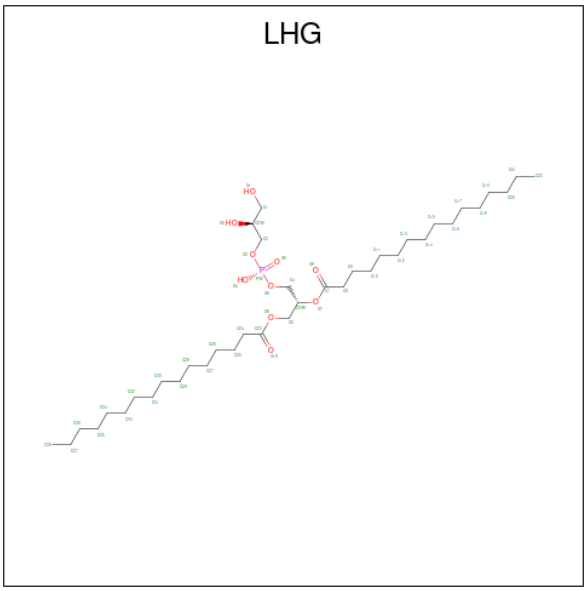
Mol	Chain	Residues	Atoms					AltConf
30	a	1	Total	C	H	N	O	0
			138	55	74	4	5	
30	d	1	Total	C	H	N	O	0
			138	55	74	4	5	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	D	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	D	1	Total	C	H	O	P	0
			114	36	67	10	1	
31	D	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	L	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	a	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	d	1	Total	C	H	O	P	0
			123	38	74	10	1	
31	d	1	Total	C	H	O	P	0
			114	36	67	10	1	
31	d	1	Total	C	H	O	P	0
			123	38	74	10	1	

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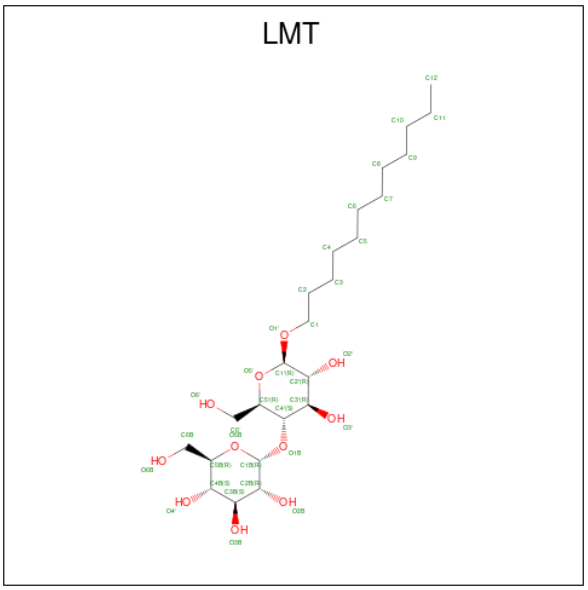
Mol	Chain	Residues	Atoms					AltConf
31	l	1	Total	C	H	O	P	0
			123	38	74	10	1	

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				AltConf
32	B	1	Total	C	H	O	0
			60	19	35	6	
32	C	1	Total	C	H	O	0
			59	18	35	6	
32	C	1	Total	C	H	O	0
			80	24	45	11	
32	E	1	Total	C	H	O	0
			57	18	33	6	
32	J	1	Total	C	H	O	0
			58	18	34	6	
32	M	1	Total	C	H	O	0
			79	24	44	11	
32	Z	1	Total	C	H	O	0
			79	24	44	11	
32	b	1	Total	C	H	O	0
			60	19	35	6	
32	c	1	Total	C	H	O	0
			59	18	35	6	
32	c	1	Total	C	H	O	0
			80	24	45	11	

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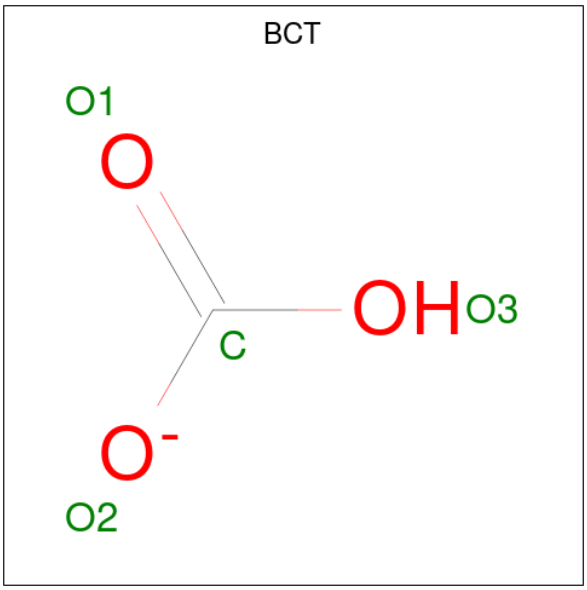
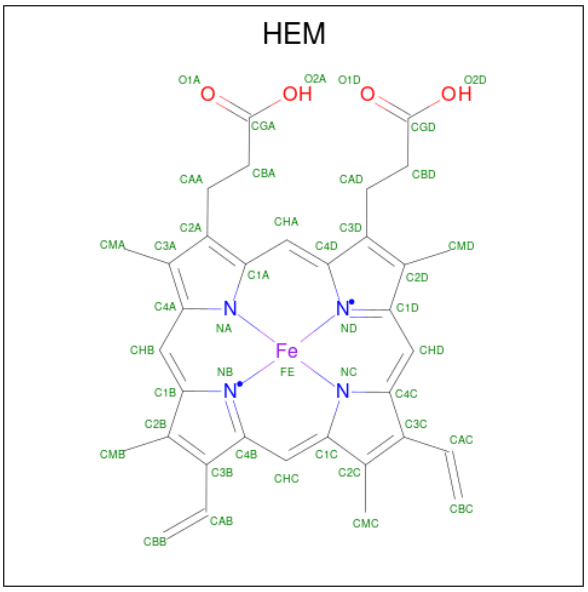
Mol	Chain	Residues	Atoms				AltConf
32	e	1	Total	C	H	O	0
			57	18	33	6	
32	j	1	Total	C	H	O	0
			58	18	34	6	
32	m	1	Total	C	H	O	0
			79	24	44	11	
32	z	1	Total	C	H	O	0
			79	24	44	11	

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



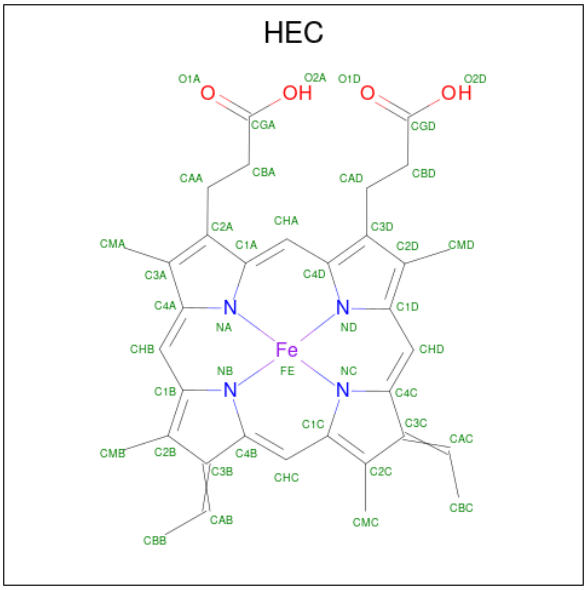
Mol	Chain	Residues	Atoms				AltConf
33	D	1	Total	C	H	O	0
			5	1	1	3	
33	d	1	Total	C	H	O	0
			5	1	1	3	

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
34	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
34	e	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
35	V	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
35	v	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	A	172	Total O 172 172	0
36	B	273	Total O 273 273	0
36	C	200	Total O 201 201	1
36	D	177	Total O 177 177	0
36	E	38	Total O 38 38	0
36	F	4	Total O 4 4	0
36	H	28	Total O 28 28	0
36	I	6	Total O 6 6	0
36	J	14	Total O 14 14	0
36	K	4	Total O 4 4	0
36	L	16	Total O 16 16	0
36	M	7	Total O 7 7	0
36	O	99	Total O 99 99	0
36	T	8	Total O 8 8	0
36	U	61	Total O 61 61	0
36	V	95	Total O 95 95	0
36	X	9	Total O 9 9	0
36	a	168	Total O 168 168	0
36	b	273	Total O 273 273	0
36	c	201	Total O 202 202	1
36	d	177	Total O 177 177	0

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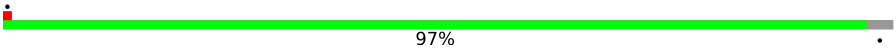
Mol	Chain	Residues	Atoms	AltConf
36	e	38	Total O 38 38	0
36	f	4	Total O 4 4	0
36	h	28	Total O 28 28	0
36	i	6	Total O 6 6	0
36	j	14	Total O 14 14	0
36	k	4	Total O 4 4	0
36	l	13	Total O 13 13	0
36	m	3	Total O 3 3	0
36	o	99	Total O 99 99	0
36	t	7	Total O 7 7	0
36	u	55	Total O 55 55	0
36	v	95	Total O 95 95	0
36	x	9	Total O 9 9	0

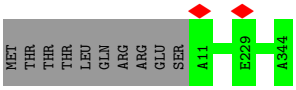
3 Residue-property plots (i)

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: Photosystem II protein D1 1

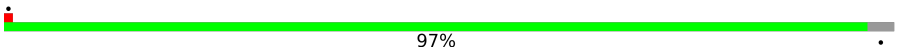
Chain A:

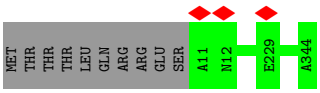




• Molecule 1: Photosystem II protein D1 1

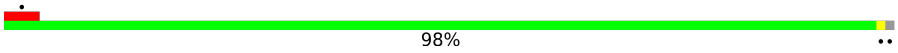
Chain a:

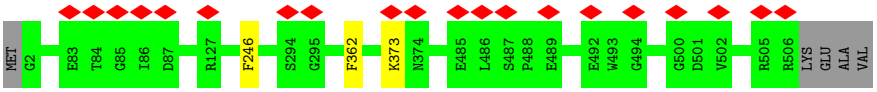




• Molecule 2: Photosystem II CP47 reaction center protein

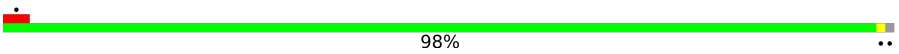
Chain B:

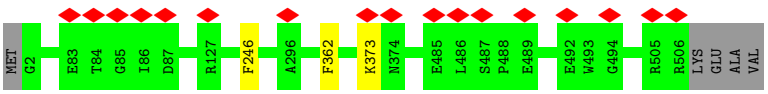




• Molecule 2: Photosystem II CP47 reaction center protein

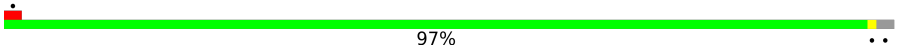
Chain b:

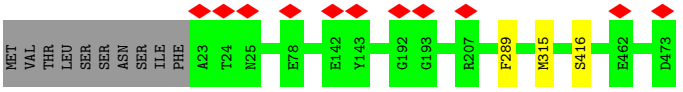




• Molecule 3: Photosystem II CP43 reaction center protein

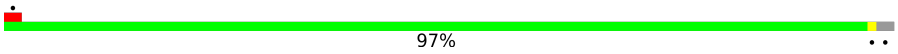
Chain C:

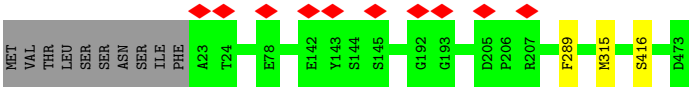




• Molecule 3: Photosystem II CP43 reaction center protein

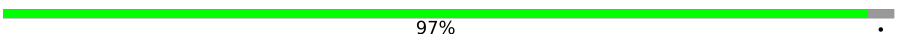
Chain c:

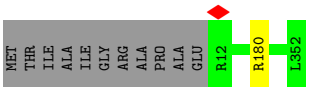




• Molecule 4: Photosystem II D2 protein

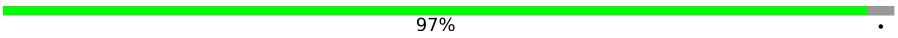
Chain D:

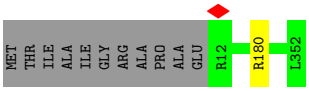




• Molecule 4: Photosystem II D2 protein

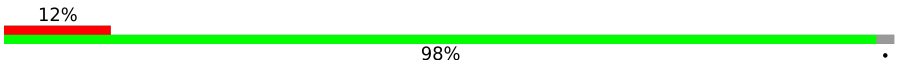
Chain d:

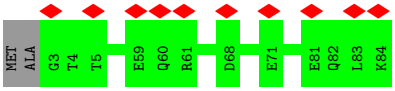




• Molecule 5: Cytochrome b559 subunit alpha

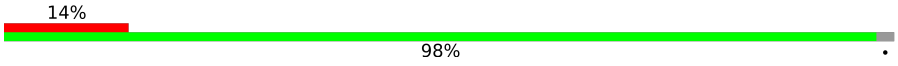
Chain E:

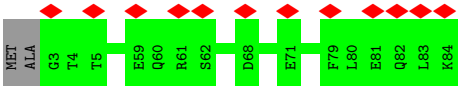




• Molecule 5: Cytochrome b559 subunit alpha

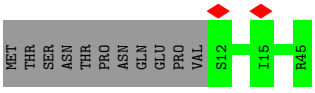
Chain e:





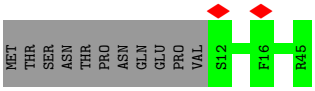
• Molecule 6: Cytochrome b559 subunit beta

Chain F:

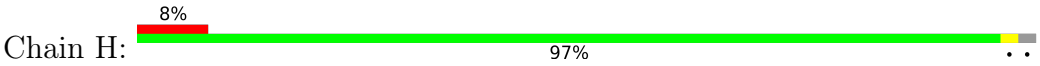


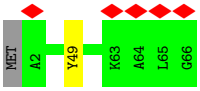
• Molecule 6: Cytochrome b559 subunit beta

Chain f:

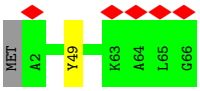


• Molecule 7: Photosystem II reaction center protein H

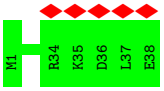




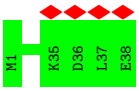
• Molecule 7: Photosystem II reaction center protein H



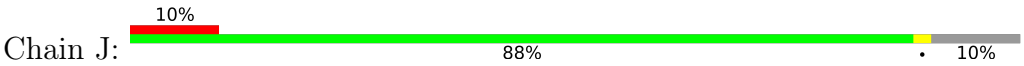
• Molecule 8: Photosystem II reaction center protein I

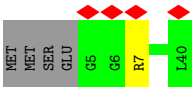


• Molecule 8: Photosystem II reaction center protein I

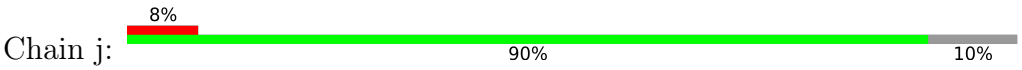


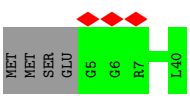
• Molecule 9: Photosystem II reaction center protein J





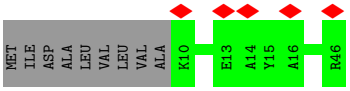
• Molecule 9: Photosystem II reaction center protein J





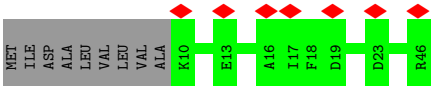
• Molecule 10: Photosystem II reaction center protein K

Chain K:



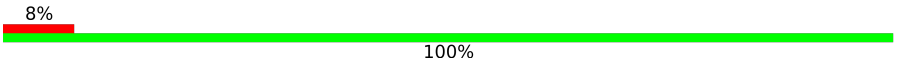
• Molecule 10: Photosystem II reaction center protein K

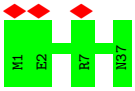
Chain k:



• Molecule 11: Photosystem II reaction center protein L

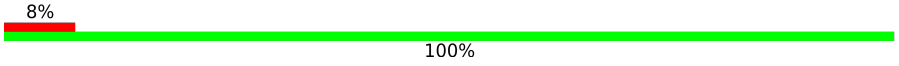
Chain L:

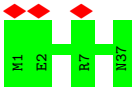




• Molecule 11: Photosystem II reaction center protein L

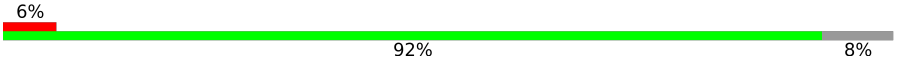
Chain l:

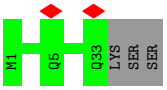




• Molecule 12: Photosystem II reaction center protein M

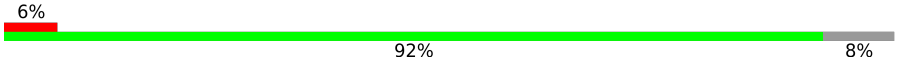
Chain M:

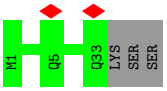




• Molecule 12: Photosystem II reaction center protein M

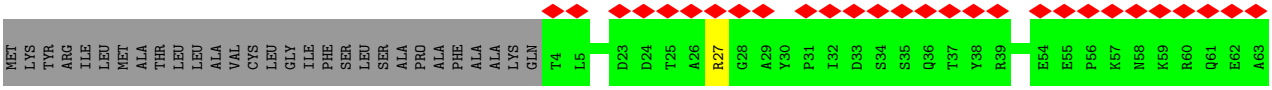
Chain m:

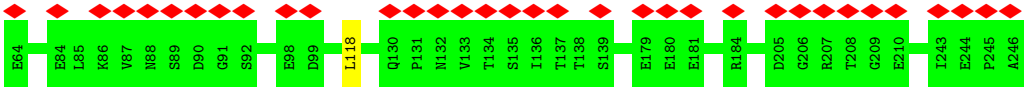




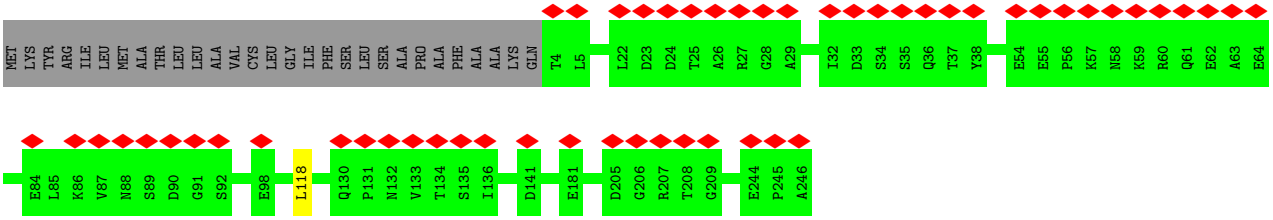
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

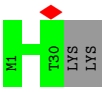




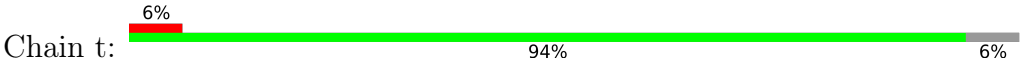
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

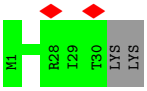


• Molecule 14: Photosystem II reaction center protein T

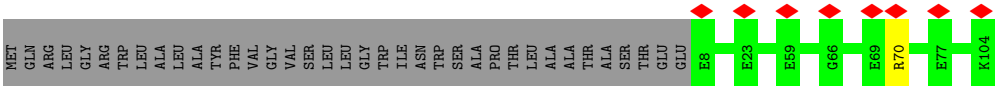


• Molecule 14: Photosystem II reaction center protein T

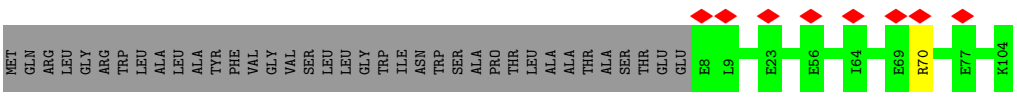




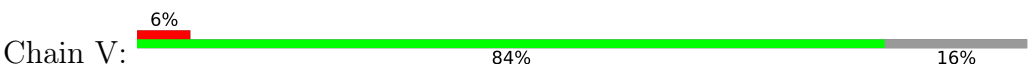
• Molecule 15: Photosystem II 12 kDa extrinsic protein

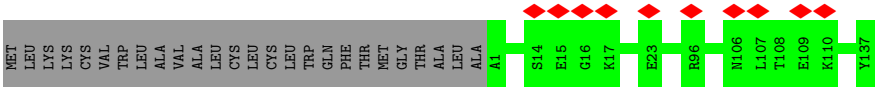


• Molecule 15: Photosystem II 12 kDa extrinsic protein

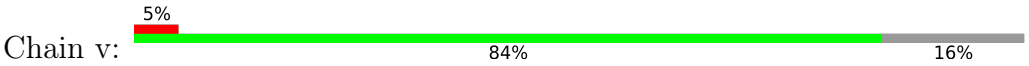


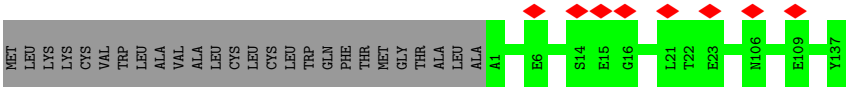
• Molecule 16: Cytochrome c-550



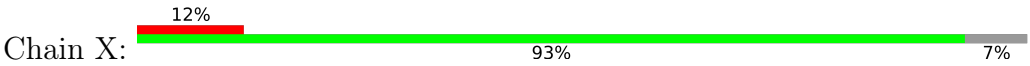


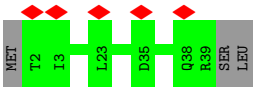
• Molecule 16: Cytochrome c-550



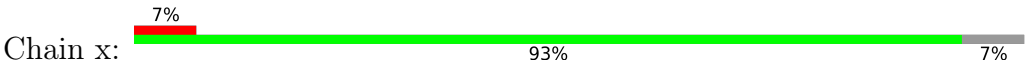


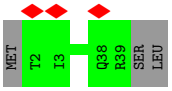
• Molecule 17: Photosystem II reaction center X protein



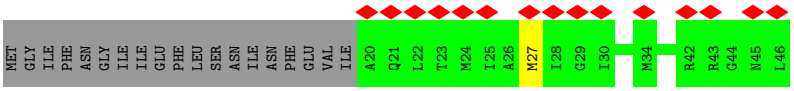


• Molecule 17: Photosystem II reaction center X protein

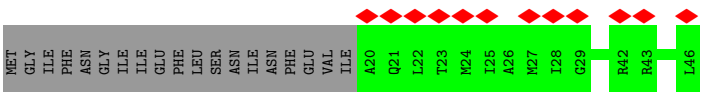




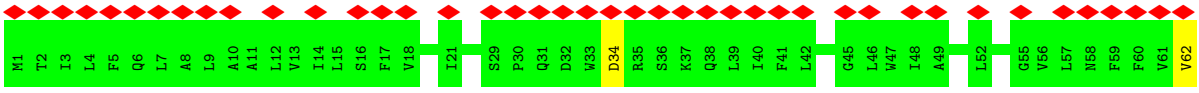
• Molecule 18: Photosystem II reaction center protein Ycf12



• Molecule 18: Photosystem II reaction center protein Ycf12

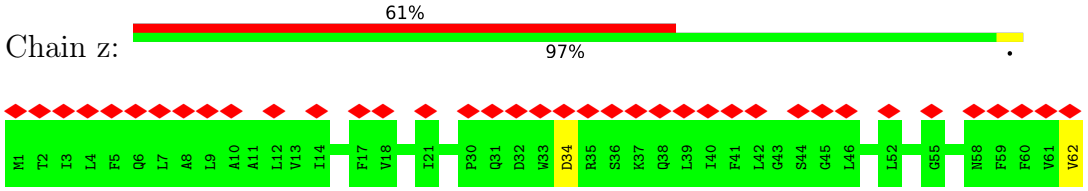


• Molecule 19: Photosystem II reaction center protein Z



• Molecule 19: Photosystem II reaction center protein Z

Chain z:


61%
97%
M1
T2
I3
L4
F5
Q6
L7
A8
L9
A10
A11
L12
V13
I14
F17
V18
I21
P30
Q31
D32
W33
D34
R35
S36
K37
Q38
L39
T40
F41
L42
G43
S44
G45
L46
L52
G55
M58
F59
F60
V61
V62

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	631270	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.426	Depositor
Minimum map value	-0.651	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	413.28, 413.28, 413.28	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.574, 0.574, 0.574	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: OEX, STE, DGD, PHO, LMG, PL9, HEM, FE2, HEC, BCT, SQD, LHG, LMT, CL, FME, CLA, 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	A	0.26	0/2723	0.49	0/3713
1	a	0.26	0/2723	0.49	0/3713
2	B	0.26	0/4140	0.49	0/5641
2	b	0.26	0/4140	0.49	0/5641
3	C	0.26	0/3612	0.47	0/4917
3	c	0.26	0/3612	0.47	0/4917
4	D	0.26	0/2812	0.50	0/3832
4	d	0.26	0/2812	0.50	0/3832
5	E	0.25	0/680	0.48	0/929
5	e	0.25	0/680	0.48	0/929
6	F	0.29	0/284	0.45	0/387
6	f	0.29	0/284	0.45	0/387
7	H	0.25	0/539	0.46	0/736
7	h	0.25	0/539	0.47	0/736
8	I	0.26	0/310	0.48	0/419
8	i	0.26	0/310	0.49	0/419
9	J	0.27	0/263	0.47	0/356
9	j	0.27	0/263	0.47	0/356
10	K	0.28	0/303	0.44	0/416
10	k	0.28	0/303	0.44	0/416
11	L	0.25	0/327	0.45	0/444
11	l	0.25	0/327	0.45	0/444
12	M	0.26	0/264	0.40	0/363
12	m	0.26	0/264	0.40	0/363
13	O	0.25	0/1910	0.52	0/2594
13	o	0.25	0/1910	0.52	0/2594
14	T	0.28	0/257	0.48	0/349
14	t	0.27	0/257	0.48	0/349
15	U	0.24	0/785	0.47	0/1064
15	u	0.24	0/785	0.47	0/1064
16	V	0.24	0/1085	0.46	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.24	0/1085	0.46	0/1473
17	X	0.25	0/284	0.42	0/384
17	x	0.25	0/284	0.42	0/384
18	Y	0.25	0/200	0.48	0/268
18	y	0.26	0/200	0.50	0/268
19	Z	0.26	0/490	0.40	0/669
19	z	0.26	0/490	0.40	0/669
All	All	0.26	0/42536	0.48	0/57908

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	328 (98%)	7 (2%)	0	100	100
1	a	335/344 (97%)	328 (98%)	7 (2%)	0	100	100
2	B	506/510 (99%)	499 (99%)	7 (1%)	0	100	100
2	b	506/510 (99%)	499 (99%)	7 (1%)	0	100	100
3	C	451/461 (98%)	440 (98%)	10 (2%)	1 (0%)	44	29
3	c	451/461 (98%)	440 (98%)	10 (2%)	1 (0%)	44	29
4	D	339/352 (96%)	333 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	339/352 (96%)	333 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	80 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	65/66 (98%)	64 (98%)	1 (2%)	0	100	100
7	h	65/66 (98%)	64 (98%)	1 (2%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	37/37 (100%)	37 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	33/36 (92%)	33 (100%)	0	0	100	100
13	O	244/272 (90%)	233 (96%)	11 (4%)	0	100	100
13	o	244/272 (90%)	235 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	V	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
16	v	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
17	X	36/41 (88%)	36 (100%)	0	0	100	100
17	x	36/41 (88%)	36 (100%)	0	0	100	100
18	Y	25/46 (54%)	25 (100%)	0	0	100	100
18	y	25/46 (54%)	24 (96%)	1 (4%)	0	100	100
19	Z	60/62 (97%)	60 (100%)	0	0	100	100
19	z	60/62 (97%)	60 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5212/5618 (93%)	5109 (98%)	101 (2%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	272/280 (97%)	272 (100%)	0	100 100
1	a	272/280 (97%)	272 (100%)	0	100 100
2	B	406/407 (100%)	403 (99%)	3 (1%)	81 74
2	b	406/407 (100%)	403 (99%)	3 (1%)	81 74
3	C	354/362 (98%)	352 (99%)	2 (1%)	84 78
3	c	354/362 (98%)	352 (99%)	2 (1%)	84 78
4	D	276/283 (98%)	275 (100%)	1 (0%)	89 85
4	d	276/283 (98%)	275 (100%)	1 (0%)	89 85
5	E	71/73 (97%)	71 (100%)	0	100 100
5	e	71/73 (97%)	71 (100%)	0	100 100
6	F	28/39 (72%)	28 (100%)	0	100 100
6	f	28/39 (72%)	28 (100%)	0	100 100
7	H	56/55 (102%)	55 (98%)	1 (2%)	54 37
7	h	56/55 (102%)	55 (98%)	1 (2%)	54 37
8	I	34/34 (100%)	34 (100%)	0	100 100
8	i	34/34 (100%)	34 (100%)	0	100 100
9	J	24/28 (86%)	23 (96%)	1 (4%)	25 9
9	j	24/28 (86%)	24 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	K	30/37 (81%)	30 (100%)	0	100 100
10	k	30/37 (81%)	30 (100%)	0	100 100
11	L	37/35 (106%)	37 (100%)	0	100 100
11	l	37/35 (106%)	37 (100%)	0	100 100
12	M	30/32 (94%)	30 (100%)	0	100 100
12	m	30/32 (94%)	30 (100%)	0	100 100
13	O	207/228 (91%)	205 (99%)	2 (1%)	73 63
13	o	207/228 (91%)	206 (100%)	1 (0%)	86 82
14	T	26/28 (93%)	26 (100%)	0	100 100
14	t	26/28 (93%)	26 (100%)	0	100 100
15	U	84/112 (75%)	83 (99%)	1 (1%)	67 55
15	u	84/112 (75%)	83 (99%)	1 (1%)	67 55
16	V	117/138 (85%)	117 (100%)	0	100 100
16	v	117/138 (85%)	117 (100%)	0	100 100
17	X	31/34 (91%)	31 (100%)	0	100 100
17	x	31/34 (91%)	31 (100%)	0	100 100
18	Y	20/37 (54%)	19 (95%)	1 (5%)	20 6
18	y	20/37 (54%)	20 (100%)	0	100 100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	28 11
19	z	52/52 (100%)	50 (96%)	2 (4%)	28 11
All	All	4310/4588 (94%)	4285 (99%)	25 (1%)	82 78

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	246	PHE
2	B	362	PHE
2	B	373	LYS
3	C	289	PHE
3	C	315	MET
4	D	180	ARG
7	H	49	TYR
9	J	7	ARG
13	O	27	ARG
13	O	118	LEU

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Mol	Chain	Res	Type
15	U	70	ARG
18	Y	27	MET
19	Z	34	ASP
19	Z	62	VAL
2	b	246	PHE
2	b	362	PHE
2	b	373	LYS
3	c	289	PHE
3	c	315	MET
4	d	180	ARG
7	h	49	TYR
13	o	118	LEU
15	u	70	ARG
19	z	34	ASP
19	z	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	343	HIS
2	b	343	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	I	1	8	8,9,10	0.93	0	7,9,11	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	FME	T	1	14	8,9,10	0.93	0	7,9,11	0.99	0
14	FME	t	1	14	8,9,10	0.93	0	7,9,11	1.00	0
12	FME	M	1	12	8,9,10	0.93	0	7,9,11	0.70	0
12	FME	m	1	12	8,9,10	0.92	0	7,9,11	0.70	0
8	FME	i	1	8	8,9,10	0.93	0	7,9,11	0.80	0

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
8	FME	I	1	8	-	2/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
8	i	1	FME	O-C-CA-CB
12	M	1	FME	CB-CA-N-CN
12	m	1	FME	CB-CA-N-CN
8	I	1	FME	CB-CG-SD-CE
8	i	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 212 ligands modelled in this entry, 6 are monoatomic - leaving 206 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	$\#\|Z\| > 2$
28	DGD	c	517	-	63,63,67	0.86	1 (1%)	77,77,81	1.34	7 (9%)
25	STE	a	415	-	10,10,19	0.31	0	9,9,19	0.72	0
26	LMG	A	410	-	48,48,55	0.79	0	56,56,63	1.25	5 (8%)
27	SQD	a	412	-	53,54,54	1.51	7 (13%)	62,65,65	1.34	6 (9%)
25	STE	E	103	-	19,19,19	0.55	0	19,19,19	1.06	0
22	CLA	d	405	-	65,73,73	1.66	9 (13%)	76,113,113	1.37	8 (10%)
28	DGD	a	413	-	67,67,67	0.91	2 (2%)	81,81,81	1.35	12 (14%)
31	LHG	d	410	-	46,46,48	0.68	1 (2%)	49,52,54	1.18	4 (8%)
32	LMT	C	525	-	36,36,36	1.16	5 (13%)	47,47,47	0.91	1 (2%)
22	CLA	C	506	-	65,73,73	1.50	7 (10%)	76,113,113	1.33	8 (10%)
25	STE	k	102	-	10,10,19	0.29	0	9,9,19	0.78	0
22	CLA	b	615	-	65,73,73	1.51	7 (10%)	76,113,113	1.29	7 (9%)
22	CLA	A	406	-	54,62,73	1.79	6 (11%)	62,99,113	1.44	8 (12%)
22	CLA	b	609	-	65,73,73	1.61	8 (12%)	76,113,113	1.32	7 (9%)
22	CLA	D	405	-	65,73,73	1.66	9 (13%)	76,113,113	1.37	8 (10%)
22	CLA	a	405	36	60,68,73	1.54	6 (10%)	70,107,113	1.46	9 (12%)
22	CLA	c	508	-	65,73,73	1.58	8 (12%)	76,113,113	1.36	9 (11%)
25	STE	e	102	-	11,11,19	0.29	0	10,10,19	0.81	0
22	CLA	c	513	-	65,73,73	1.46	7 (10%)	76,113,113	1.30	9 (11%)
27	SQD	a	411	-	51,52,54	1.53	5 (9%)	60,63,65	1.47	9 (15%)
32	LMT	Z	101	-	36,36,36	1.20	5 (13%)	47,47,47	0.97	1 (2%)
33	BCT	d	403	20	2,3,3	1.17	0	2,3,3	4.48	2 (100%)
23	BCR	b	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.11	3 (5%)
26	LMG	b	625	-	51,51,55	0.72	0	59,59,63	1.34	6 (10%)
35	HEC	V	201	16	32,50,50	2.22	3 (9%)	24,82,82	1.45	3 (12%)
32	LMT	j	102	-	24,24,36	1.05	2 (8%)	29,29,47	1.10	2 (6%)
23	BCR	C	515	-	41,41,41	1.07	2 (4%)	56,56,56	1.14	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	d	406	-	41,41,41	1.09	2 (4%)	56,56,56	1.12	4 (7%)
31	LHG	D	410	-	46,46,48	0.67	1 (2%)	49,52,54	1.17	4 (8%)
25	STE	I	101	-	13,13,19	0.26	0	12,12,19	0.86	0
22	CLA	b	604	-	65,73,73	1.55	8 (12%)	76,113,113	1.23	7 (9%)
23	BCR	b	620	-	41,41,41	1.05	2 (4%)	56,56,56	1.13	5 (8%)
22	CLA	d	404	-	65,73,73	1.69	7 (10%)	76,113,113	1.36	9 (11%)
23	BCR	T	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	5 (8%)
32	LMT	m	101	-	36,36,36	1.15	5 (13%)	47,47,47	0.97	2 (4%)
22	CLA	C	505	-	65,73,73	1.63	8 (12%)	76,113,113	1.34	7 (9%)
24	PL9	A	408	-	55,55,55	1.00	3 (5%)	68,69,69	1.52	12 (17%)
26	LMG	D	402	-	33,33,55	0.59	0	35,35,63	1.21	2 (5%)
22	CLA	a	404	-	65,73,73	1.60	7 (10%)	76,113,113	1.27	6 (7%)
32	LMT	e	104	-	24,24,36	1.02	2 (8%)	29,29,47	1.08	2 (6%)
25	STE	e	101	-	11,11,19	0.70	0	11,11,19	1.14	0
23	BCR	h	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	6 (10%)
22	CLA	B	615	-	65,73,73	1.68	9 (13%)	76,113,113	1.32	6 (7%)
35	HEC	v	201	16	32,50,50	2.23	3 (9%)	24,82,82	1.46	3 (12%)
22	CLA	B	614	-	65,73,73	1.51	7 (10%)	76,113,113	1.30	7 (9%)
27	SQD	A	412	-	53,54,54	1.51	7 (13%)	62,65,65	1.34	6 (9%)
34	HEM	E	105	6,5	41,50,50	1.47	4 (9%)	45,82,82	1.42	5 (11%)
31	LHG	D	409	-	48,48,48	0.62	0	51,54,54	1.16	5 (9%)
22	CLA	B	602	-	65,73,73	1.56	8 (12%)	76,113,113	1.32	10 (13%)
22	CLA	c	512	-	65,73,73	1.55	7 (10%)	76,113,113	1.38	8 (10%)
23	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
22	CLA	C	511	3	65,73,73	1.52	6 (9%)	76,113,113	1.35	7 (9%)
22	CLA	b	611	36	65,73,73	1.51	7 (10%)	76,113,113	1.41	7 (9%)
24	PL9	a	408	-	55,55,55	1.00	3 (5%)	68,69,69	1.52	12 (17%)
25	STE	t	101	-	17,17,19	0.58	0	17,17,19	1.08	1 (5%)
22	CLA	C	504	36	59,67,73	1.56	7 (11%)	68,105,113	1.41	7 (10%)
32	LMT	b	624	-	25,25,36	1.00	2 (8%)	30,30,47	1.09	2 (6%)
22	CLA	B	606	-	65,73,73	1.51	7 (10%)	76,113,113	1.36	6 (7%)
27	SQD	b	621	-	48,49,54	1.60	9 (18%)	57,60,65	1.38	6 (10%)
26	LMG	D	408	-	51,51,55	0.78	0	59,59,63	1.29	5 (8%)
22	CLA	b	603	-	65,73,73	1.55	8 (12%)	76,113,113	1.32	10 (13%)
28	DGD	A	413	-	67,67,67	0.92	2 (2%)	81,81,81	1.35	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	STE	K	102	-	10,10,19	0.30	0	9,9,19	0.79	0
23	BCR	B	619	-	41,41,41	1.05	2 (4%)	56,56,56	1.13	5 (8%)
22	CLA	B	608	-	65,73,73	1.61	8 (12%)	76,113,113	1.32	8 (10%)
23	BCR	k	103	-	41,41,41	1.12	2 (4%)	56,56,56	1.13	3 (5%)
32	LMT	c	525	-	36,36,36	1.16	5 (13%)	47,47,47	0.91	1 (2%)
28	DGD	c	518	-	58,58,67	0.95	3 (5%)	72,72,81	1.31	5 (6%)
25	STE	j	101	-	11,11,19	0.28	0	10,10,19	0.83	0
27	SQD	A	411	-	51,52,54	1.52	5 (9%)	60,63,65	1.48	9 (15%)
28	DGD	H	103	-	63,63,67	0.94	1 (1%)	77,77,81	1.29	6 (7%)
22	CLA	C	513	-	65,73,73	1.46	7 (10%)	76,113,113	1.30	9 (11%)
22	CLA	B	603	-	65,73,73	1.56	8 (12%)	76,113,113	1.23	7 (9%)
22	CLA	b	602	36	65,73,73	1.47	5 (7%)	76,113,113	1.31	9 (11%)
29	OEX	a	417	3,1,36	0,15,15	-	-	-		
31	LHG	l	101	-	48,48,48	0.62	1 (2%)	51,54,54	1.20	5 (9%)
22	CLA	A	404	-	65,73,73	1.60	7 (10%)	76,113,113	1.27	6 (7%)
22	CLA	c	507	36	65,73,73	1.52	7 (10%)	76,113,113	1.38	7 (9%)
22	CLA	a	406	-	54,62,73	1.78	6 (11%)	62,99,113	1.44	8 (12%)
22	CLA	B	616	-	60,68,73	1.67	8 (13%)	70,107,113	1.44	7 (10%)
23	BCR	B	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.11	4 (7%)
22	CLA	C	501	-	65,73,73	1.50	7 (10%)	76,113,113	1.32	8 (10%)
25	STE	J	101	-	11,11,19	0.28	0	10,10,19	0.83	0
25	STE	a	421	-	11,11,19	0.69	0	11,11,19	1.17	0
22	CLA	b	617	-	60,68,73	1.68	8 (13%)	70,107,113	1.44	6 (8%)
26	LMG	c	520	-	48,48,55	0.81	1 (2%)	56,56,63	1.30	6 (10%)
22	CLA	b	608	36	65,73,73	1.50	6 (9%)	76,113,113	1.33	7 (9%)
23	BCR	a	407	-	41,41,41	1.06	2 (4%)	56,56,56	1.11	3 (5%)
22	CLA	B	613	-	65,73,73	1.60	8 (12%)	76,113,113	1.40	8 (10%)
25	STE	D	413	-	8,8,19	0.30	0	7,7,19	0.74	0
31	LHG	A	420	-	48,48,48	0.66	2 (4%)	51,54,54	1.28	7 (13%)
25	STE	B	625	-	11,11,19	0.29	0	10,10,19	0.79	0
22	CLA	a	419	36	65,73,73	1.48	7 (10%)	76,113,113	1.33	9 (11%)
32	LMT	c	523	-	24,24,36	1.13	4 (16%)	29,29,47	1.29	2 (6%)
27	SQD	B	620	-	53,54,54	1.52	8 (15%)	62,65,65	1.39	6 (9%)
23	BCR	k	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	5 (8%)
28	DGD	C	518	-	58,58,67	0.95	3 (5%)	72,72,81	1.31	5 (6%)
22	CLA	c	511	3	65,73,73	1.51	7 (10%)	76,113,113	1.34	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	C	512	-	65,73,73	1.55	7 (10%)	76,113,113	1.37	8 (10%)
23	BCR	C	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
32	LMT	J	102	-	24,24,36	1.05	2 (8%)	29,29,47	1.10	2 (6%)
34	HEM	e	105	6,5	41,50,50	1.47	4 (9%)	45,82,82	1.41	5 (11%)
31	LHG	d	409	-	48,48,48	0.63	1 (2%)	51,54,54	1.16	5 (9%)
32	LMT	E	104	-	24,24,36	1.02	2 (8%)	29,29,47	1.08	2 (6%)
22	CLA	B	605	-	65,73,73	1.64	7 (10%)	76,113,113	1.29	10 (13%)
22	CLA	b	605	-	65,73,73	1.62	8 (12%)	76,113,113	1.45	7 (9%)
32	LMT	B	623	-	25,25,36	1.01	2 (8%)	30,30,47	1.09	2 (6%)
25	STE	b	623	-	11,11,19	0.68	0	11,11,19	1.22	1 (9%)
25	STE	c	516	-	13,13,19	0.63	0	13,13,19	1.14	1 (7%)
25	STE	a	414	-	7,7,19	0.29	0	6,6,19	0.67	0
22	CLA	A	419	36	65,73,73	1.48	7 (10%)	76,113,113	1.33	9 (11%)
24	PL9	d	407	-	55,55,55	0.97	4 (7%)	68,69,69	1.46	8 (11%)
25	STE	C	521	-	11,11,19	0.70	0	11,11,19	1.14	0
26	LMG	c	524	-	50,50,55	0.75	1 (2%)	58,58,63	1.33	7 (12%)
22	CLA	b	614	-	65,73,73	1.59	8 (12%)	76,113,113	1.40	9 (11%)
24	PL9	D	407	-	55,55,55	0.97	4 (7%)	68,69,69	1.46	8 (11%)
26	LMG	h	101	-	38,38,55	0.51	0	40,40,63	1.31	2 (5%)
25	STE	C	516	-	13,13,19	0.63	0	13,13,19	1.13	1 (7%)
25	STE	b	601	-	11,11,19	0.29	0	10,10,19	0.79	0
23	BCR	A	407	-	41,41,41	1.06	2 (4%)	56,56,56	1.10	3 (5%)
31	LHG	a	420	-	48,48,48	0.65	2 (4%)	51,54,54	1.26	6 (11%)
22	CLA	B	610	36	65,73,73	1.52	7 (10%)	76,113,113	1.41	7 (9%)
22	CLA	b	613	-	65,73,73	1.59	8 (12%)	76,113,113	1.42	8 (10%)
22	CLA	c	510	-	65,73,73	1.50	6 (9%)	76,113,113	1.32	7 (9%)
22	CLA	B	609	-	65,73,73	1.63	8 (12%)	76,113,113	1.35	9 (11%)
22	CLA	C	503	-	65,73,73	1.73	9 (13%)	76,113,113	1.26	7 (9%)
23	BCR	D	406	-	41,41,41	1.09	2 (4%)	56,56,56	1.12	4 (7%)
25	STE	E	102	-	11,11,19	0.29	0	10,10,19	0.82	0
27	SQD	X	101	-	35,36,54	1.46	5 (14%)	42,45,65	1.56	7 (16%)
25	STE	a	409	-	8,8,19	0.30	0	7,7,19	0.72	0
26	LMG	d	408	-	51,51,55	0.78	0	59,59,63	1.29	5 (8%)
23	BCR	H	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	6 (10%)
26	LMG	B	624	-	51,51,55	0.72	0	59,59,63	1.33	6 (10%)
23	BCR	t	102	-	41,41,41	1.06	2 (4%)	56,56,56	1.17	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	B	617	-	41,41,41	1.08	2 (4%)	56,56,56	1.17	6 (10%)
25	STE	D	412	-	19,19,19	0.56	0	19,19,19	1.01	0
33	BCT	D	403	20	2,3,3	1.17	0	2,3,3	4.47	2 (100%)
32	LMT	M	102	-	36,36,36	1.15	5 (13%)	47,47,47	0.97	2 (4%)
27	SQD	x	101	-	35,36,54	1.47	5 (14%)	42,45,65	1.57	7 (16%)
22	CLA	c	506	-	65,73,73	1.51	7 (10%)	76,113,113	1.33	8 (10%)
25	STE	B	621	-	16,16,19	0.58	0	16,16,19	1.09	0
25	STE	A	414	-	7,7,19	0.29	0	6,6,19	0.66	0
25	STE	a	416	-	10,10,19	0.29	0	9,9,19	0.76	0
25	STE	c	522	-	7,7,19	0.29	0	6,6,19	0.70	0
22	CLA	c	509	-	65,73,73	1.53	7 (10%)	76,113,113	1.40	7 (9%)
28	DGD	h	103	-	63,63,67	0.94	1 (1%)	77,77,81	1.29	6 (7%)
23	BCR	K	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.16	5 (8%)
25	STE	M	101	-	9,9,19	0.28	0	8,8,19	0.83	0
26	LMG	C	524	-	50,50,55	0.75	1 (2%)	58,58,63	1.33	7 (12%)
22	CLA	C	502	-	65,73,73	1.62	9 (13%)	76,113,113	1.33	6 (7%)
28	DGD	c	519	-	63,63,67	0.89	0	77,77,81	1.26	5 (6%)
31	LHG	L	101	-	48,48,48	0.62	1 (2%)	51,54,54	1.20	5 (9%)
22	CLA	b	607	-	65,73,73	1.52	7 (10%)	76,113,113	1.36	6 (7%)
30	PHO	D	401	-	51,69,69	1.00	4 (7%)	47,99,99	1.12	5 (10%)
22	CLA	B	611	-	65,73,73	1.63	8 (12%)	76,113,113	1.41	9 (11%)
22	CLA	A	405	36	60,68,73	1.57	7 (11%)	70,107,113	1.51	10 (14%)
25	STE	A	409	-	8,8,19	0.31	0	7,7,19	0.73	0
32	LMT	z	101	-	36,36,36	1.20	5 (13%)	47,47,47	0.97	1 (2%)
25	STE	T	102	-	14,14,19	0.29	0	13,13,19	0.82	0
23	BCR	b	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	6 (10%)
25	STE	A	416	-	10,10,19	0.30	0	9,9,19	0.77	0
25	STE	m	102	-	9,9,19	0.28	0	8,8,19	0.83	0
28	DGD	C	517	-	63,63,67	0.86	1 (1%)	77,77,81	1.34	7 (9%)
31	LHG	d	411	-	48,48,48	0.64	1 (2%)	51,54,54	1.21	6 (11%)
25	STE	E	101	-	11,11,19	0.69	0	11,11,19	1.14	0
25	STE	b	622	-	16,16,19	0.58	0	16,16,19	1.10	0
30	PHO	a	418	-	51,69,69	1.03	4 (7%)	47,99,99	1.05	5 (10%)
25	STE	B	622	-	11,11,19	0.67	0	11,11,19	1.22	1 (9%)
22	CLA	b	616	-	65,73,73	1.66	9 (13%)	76,113,113	1.31	6 (7%)
26	LMG	a	410	-	48,48,55	0.80	0	56,56,63	1.26	5 (8%)
30	PHO	A	418	-	51,69,69	1.03	4 (7%)	47,99,99	1.05	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	C	507	36	65,73,73	1.52	7 (10%)	76,113,113	1.38	7 (9%)
31	LHG	D	411	-	48,48,48	0.64	1 (2%)	51,54,54	1.21	6 (11%)
23	BCR	c	515	-	41,41,41	1.07	2 (4%)	56,56,56	1.14	5 (8%)
22	CLA	C	510	-	65,73,73	1.50	6 (9%)	76,113,113	1.32	7 (9%)
22	CLA	c	503	-	65,73,73	1.73	9 (13%)	76,113,113	1.26	7 (9%)
26	LMG	C	520	-	48,48,55	0.81	1 (2%)	56,56,63	1.30	6 (10%)
25	STE	A	415	-	10,10,19	0.31	0	9,9,19	0.73	0
25	STE	c	521	-	11,11,19	0.71	0	11,11,19	1.15	0
22	CLA	c	504	36	59,67,73	1.56	7 (11%)	68,105,113	1.41	7 (10%)
25	STE	i	101	-	13,13,19	0.27	0	12,12,19	0.86	0
22	CLA	C	509	-	65,73,73	1.54	7 (10%)	76,113,113	1.40	8 (10%)
22	CLA	D	404	-	65,73,73	1.69	7 (10%)	76,113,113	1.36	9 (11%)
22	CLA	b	612	-	65,73,73	1.65	8 (12%)	76,113,113	1.41	9 (11%)
25	STE	d	413	-	8,8,19	0.30	0	7,7,19	0.74	0
25	STE	d	412	-	19,19,19	0.55	0	19,19,19	1.01	0
22	CLA	B	601	36	65,73,73	1.47	5 (7%)	76,113,113	1.31	9 (11%)
22	CLA	B	607	36	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
26	LMG	d	402	-	33,33,55	0.59	0	35,35,63	1.21	2 (5%)
22	CLA	B	612	-	65,73,73	1.59	8 (12%)	76,113,113	1.42	8 (10%)
22	CLA	b	606	-	65,73,73	1.64	7 (10%)	76,113,113	1.28	10 (13%)
30	PHO	d	401	-	51,69,69	1.00	5 (9%)	47,99,99	1.13	5 (10%)
32	LMT	C	523	-	24,24,36	1.13	4 (16%)	29,29,47	1.25	2 (6%)
29	OEX	A	417	3,1,36	0,15,15	-	-	-		
22	CLA	b	610	-	65,73,73	1.62	8 (12%)	76,113,113	1.34	9 (11%)
26	LMG	H	101	-	38,38,55	0.51	0	40,40,63	1.31	2 (5%)
22	CLA	c	502	-	65,73,73	1.62	9 (13%)	76,113,113	1.32	6 (7%)
23	BCR	K	103	-	41,41,41	1.12	2 (4%)	56,56,56	1.14	3 (5%)
25	STE	e	103	-	19,19,19	0.56	0	19,19,19	1.06	0
25	STE	A	421	-	11,11,19	0.68	0	11,11,19	1.16	0
22	CLA	c	501	-	65,73,73	1.49	7 (10%)	76,113,113	1.32	8 (10%)
28	DGD	C	519	-	63,63,67	0.89	0	77,77,81	1.26	5 (6%)
22	CLA	B	604	-	65,73,73	1.63	8 (12%)	76,113,113	1.45	7 (9%)
25	STE	C	522	-	7,7,19	0.30	0	6,6,19	0.70	0
22	CLA	c	505	-	65,73,73	1.63	8 (12%)	76,113,113	1.34	7 (9%)
22	CLA	C	508	-	65,73,73	1.59	8 (12%)	76,113,113	1.37	9 (11%)

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
28	DGD	c	517	-	-	18/51/91/95	0/2/2/2
25	STE	a	415	-	-	5/8/8/17	-
26	LMG	A	410	-	-	25/43/63/70	0/1/1/1
27	SQD	a	412	-	-	19/49/69/69	0/1/1/1
25	STE	E	103	-	-	8/17/17/17	-
22	CLA	d	405	-	-	6/37/115/115	-
28	DGD	a	413	-	-	25/55/95/95	0/2/2/2
31	LHG	d	410	-	-	12/51/51/53	-
32	LMT	C	525	-	-	8/21/61/61	0/2/2/2
22	CLA	C	506	-	1/1/20/20	13/37/115/115	-
25	STE	k	102	-	-	5/8/8/17	-
22	CLA	b	615	-	1/1/20/20	14/37/115/115	-
22	CLA	A	406	-	1/1/17/20	5/24/102/115	-
22	CLA	b	609	-	1/1/20/20	5/37/115/115	-
22	CLA	a	405	36	1/1/19/20	6/31/109/115	-
22	CLA	D	405	-	-	6/37/115/115	-
22	CLA	c	508	-	-	5/37/115/115	-
25	STE	e	102	-	-	6/9/9/17	-
22	CLA	c	513	-	1/1/20/20	8/37/115/115	-
27	SQD	a	411	-	-	18/47/67/69	0/1/1/1
32	LMT	Z	101	-	-	12/21/61/61	0/2/2/2
23	BCR	b	619	-	-	4/29/63/63	0/2/2/2
26	LMG	b	625	-	-	16/46/66/70	0/1/1/1
35	HEC	V	201	16	-	2/10/54/54	-
32	LMT	j	102	-	-	10/15/35/61	0/1/1/2
23	BCR	C	515	-	-	0/29/63/63	0/2/2/2
23	BCR	d	406	-	-	3/29/63/63	0/2/2/2
31	LHG	D	410	-	-	10/51/51/53	-
25	STE	I	101	-	-	6/11/11/17	-
22	CLA	b	604	-	1/1/20/20	8/37/115/115	-
23	BCR	b	620	-	-	1/29/63/63	0/2/2/2
22	CLA	d	404	-	-	4/37/115/115	-
23	BCR	T	101	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	m	101	-	-	3/21/61/61	0/2/2/2
22	CLA	C	505	-	1/1/20/20	6/37/115/115	-
24	PL9	A	408	-	-	20/53/73/73	0/1/1/1
26	LMG	D	402	-	-	8/35/35/70	-
22	CLA	a	404	-	1/1/20/20	2/37/115/115	-
32	LMT	e	104	-	-	9/15/35/61	0/1/1/2
25	STE	e	101	-	-	4/9/9/17	-
23	BCR	h	102	-	-	6/29/63/63	0/2/2/2
22	CLA	B	615	-	1/1/20/20	7/37/115/115	-
35	HEC	v	201	16	-	2/10/54/54	-
22	CLA	B	614	-	1/1/20/20	13/37/115/115	-
27	SQD	A	412	-	-	19/49/69/69	0/1/1/1
34	HEM	E	105	6,5	-	0/12/54/54	-
31	LHG	D	409	-	-	12/53/53/53	-
22	CLA	B	602	-	1/1/20/20	5/37/115/115	-
22	CLA	c	512	-	1/1/20/20	13/37/115/115	-
23	BCR	c	514	-	-	0/29/63/63	0/2/2/2
22	CLA	C	511	3	1/1/20/20	1/37/115/115	-
22	CLA	b	611	36	1/1/20/20	0/37/115/115	-
24	PL9	a	408	-	-	20/53/73/73	0/1/1/1
25	STE	t	101	-	-	10/15/15/17	-
22	CLA	C	504	36	1/1/18/20	5/30/108/115	-
32	LMT	b	624	-	-	6/17/37/61	0/1/1/2
22	CLA	B	606	-	1/1/20/20	10/37/115/115	-
27	SQD	b	621	-	-	21/44/64/69	0/1/1/1
26	LMG	D	408	-	-	16/46/66/70	0/1/1/1
22	CLA	b	603	-	1/1/20/20	5/37/115/115	-
28	DGD	A	413	-	-	27/55/95/95	0/2/2/2
25	STE	K	102	-	-	5/8/8/17	-
23	BCR	B	619	-	-	1/29/63/63	0/2/2/2
22	CLA	B	608	-	1/1/20/20	5/37/115/115	-
23	BCR	k	103	-	-	2/29/63/63	0/2/2/2
32	LMT	c	525	-	-	8/21/61/61	0/2/2/2
28	DGD	c	518	-	-	15/46/86/95	0/2/2/2
25	STE	j	101	-	-	2/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	A	411	-	-	18/47/67/69	0/1/1/1
28	DGD	H	103	-	-	14/51/91/95	0/2/2/2
22	CLA	C	513	-	1/1/20/20	8/37/115/115	-
22	CLA	B	603	-	1/1/20/20	8/37/115/115	-
22	CLA	b	602	36	1/1/20/20	24/37/115/115	-
31	LHG	l	101	-	-	17/53/53/53	-
22	CLA	A	404	-	1/1/20/20	2/37/115/115	-
22	CLA	c	507	36	1/1/20/20	8/37/115/115	-
22	CLA	a	406	-	1/1/17/20	5/24/102/115	-
22	CLA	B	616	-	1/1/19/20	8/31/109/115	-
23	BCR	B	618	-	-	2/29/63/63	0/2/2/2
22	CLA	C	501	-	1/1/20/20	2/37/115/115	-
25	STE	J	101	-	-	2/9/9/17	-
25	STE	a	421	-	-	5/9/9/17	-
22	CLA	b	617	-	1/1/19/20	8/31/109/115	-
26	LMG	c	520	-	-	20/43/63/70	0/1/1/1
22	CLA	b	608	36	1/1/20/20	3/37/115/115	-
23	BCR	a	407	-	-	0/29/63/63	0/2/2/2
22	CLA	B	613	-	1/1/20/20	6/37/115/115	-
25	STE	D	413	-	-	1/6/6/17	-
31	LHG	A	420	-	-	24/53/53/53	-
25	STE	B	625	-	-	4/9/9/17	-
22	CLA	a	419	36	1/1/20/20	4/37/115/115	-
32	LMT	c	523	-	-	2/15/35/61	0/1/1/2
27	SQD	B	620	-	-	29/49/69/69	0/1/1/1
23	BCR	k	101	-	-	0/29/63/63	0/2/2/2
28	DGD	C	518	-	-	15/46/86/95	0/2/2/2
22	CLA	c	511	3	1/1/20/20	1/37/115/115	-
22	CLA	C	512	-	1/1/20/20	14/37/115/115	-
23	BCR	C	514	-	-	0/29/63/63	0/2/2/2
32	LMT	J	102	-	-	10/15/35/61	0/1/1/2
34	HEM	e	105	6,5	-	0/12/54/54	-
31	LHG	d	409	-	-	12/53/53/53	-
32	LMT	E	104	-	-	9/15/35/61	0/1/1/2
22	CLA	B	605	-	-	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	605	-	1/1/20/20	9/37/115/115	-
32	LMT	B	623	-	-	6/17/37/61	0/1/1/2
25	STE	b	623	-	-	5/9/9/17	-
25	STE	c	516	-	-	8/11/11/17	-
25	STE	a	414	-	-	1/5/5/17	-
22	CLA	A	419	36	1/1/20/20	4/37/115/115	-
24	PL9	d	407	-	-	7/53/73/73	0/1/1/1
25	STE	C	521	-	-	7/9/9/17	-
26	LMG	c	524	-	-	20/45/65/70	0/1/1/1
22	CLA	b	614	-	1/1/20/20	6/37/115/115	-
24	PL9	D	407	-	-	7/53/73/73	0/1/1/1
26	LMG	h	101	-	-	17/40/40/70	-
25	STE	C	516	-	-	8/11/11/17	-
25	STE	b	601	-	-	3/9/9/17	-
23	BCR	A	407	-	-	0/29/63/63	0/2/2/2
31	LHG	a	420	-	-	25/53/53/53	-
22	CLA	B	610	36	1/1/20/20	0/37/115/115	-
22	CLA	b	613	-	1/1/20/20	5/37/115/115	-
22	CLA	c	510	-	1/1/20/20	8/37/115/115	-
22	CLA	B	609	-	-	5/37/115/115	-
22	CLA	C	503	-	-	6/37/115/115	-
23	BCR	D	406	-	-	3/29/63/63	0/2/2/2
25	STE	E	102	-	-	5/9/9/17	-
27	SQD	X	101	-	-	11/28/48/69	0/1/1/1
25	STE	a	409	-	-	5/6/6/17	-
26	LMG	d	408	-	-	16/46/66/70	0/1/1/1
23	BCR	H	102	-	-	7/29/63/63	0/2/2/2
26	LMG	B	624	-	-	16/46/66/70	0/1/1/1
23	BCR	t	102	-	-	3/29/63/63	0/2/2/2
23	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	STE	D	412	-	-	6/17/17/17	-
32	LMT	M	102	-	-	3/21/61/61	0/2/2/2
27	SQD	x	101	-	-	11/28/48/69	0/1/1/1
22	CLA	c	506	-	1/1/20/20	13/37/115/115	-
25	STE	B	621	-	-	5/14/14/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	STE	A	414	-	-	1/5/5/17	-
25	STE	a	416	-	-	5/8/8/17	-
25	STE	c	522	-	-	1/5/5/17	-
22	CLA	c	509	-	1/1/20/20	7/37/115/115	-
28	DGD	h	103	-	-	14/51/91/95	0/2/2/2
23	BCR	K	101	-	-	0/29/63/63	0/2/2/2
25	STE	M	101	-	-	3/7/7/17	-
26	LMG	C	524	-	-	20/45/65/70	0/1/1/1
22	CLA	C	502	-	-	5/37/115/115	-
28	DGD	c	519	-	-	15/51/91/95	0/2/2/2
31	LHG	L	101	-	-	17/53/53/53	-
22	CLA	b	607	-	1/1/20/20	10/37/115/115	-
30	PHO	D	401	-	-	0/37/103/103	0/5/6/6
22	CLA	B	611	-	1/1/20/20	4/37/115/115	-
22	CLA	A	405	36	1/1/19/20	9/31/109/115	-
25	STE	A	409	-	-	5/6/6/17	-
32	LMT	z	101	-	-	12/21/61/61	0/2/2/2
25	STE	T	102	-	-	5/12/12/17	-
23	BCR	b	618	-	-	2/29/63/63	0/2/2/2
25	STE	A	416	-	-	5/8/8/17	-
25	STE	m	102	-	-	3/7/7/17	-
28	DGD	C	517	-	-	19/51/91/95	0/2/2/2
31	LHG	d	411	-	-	9/53/53/53	-
25	STE	E	101	-	-	4/9/9/17	-
25	STE	b	622	-	-	5/14/14/17	-
30	PHO	a	418	-	-	3/37/103/103	0/5/6/6
25	STE	B	622	-	-	5/9/9/17	-
22	CLA	b	616	-	1/1/20/20	7/37/115/115	-
26	LMG	a	410	-	-	25/43/63/70	0/1/1/1
30	PHO	A	418	-	-	3/37/103/103	0/5/6/6
22	CLA	C	507	36	1/1/20/20	8/37/115/115	-
31	LHG	D	411	-	-	9/53/53/53	-
23	BCR	c	515	-	-	0/29/63/63	0/2/2/2
22	CLA	C	510	-	1/1/20/20	7/37/115/115	-
22	CLA	c	503	-	-	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMG	C	520	-	-	21/43/63/70	0/1/1/1
25	STE	A	415	-	-	3/8/8/17	-
25	STE	c	521	-	-	7/9/9/17	-
22	CLA	c	504	36	1/1/18/20	5/30/108/115	-
25	STE	i	101	-	-	6/11/11/17	-
22	CLA	C	509	-	1/1/20/20	7/37/115/115	-
22	CLA	D	404	-	-	4/37/115/115	-
22	CLA	b	612	-	1/1/20/20	4/37/115/115	-
25	STE	d	413	-	-	1/6/6/17	-
25	STE	d	412	-	-	6/17/17/17	-
22	CLA	B	601	36	1/1/20/20	24/37/115/115	-
22	CLA	B	607	36	1/1/20/20	3/37/115/115	-
26	LMG	d	402	-	-	8/35/35/70	-
22	CLA	B	612	-	1/1/20/20	5/37/115/115	-
22	CLA	b	606	-	-	7/37/115/115	-
30	PHO	d	401	-	-	0/37/103/103	0/5/6/6
32	LMT	C	523	-	-	2/15/35/61	0/1/1/2
22	CLA	b	610	-	-	5/37/115/115	-
26	LMG	H	101	-	-	18/40/40/70	-
22	CLA	c	502	-	-	5/37/115/115	-
23	BCR	K	103	-	-	2/29/63/63	0/2/2/2
25	STE	e	103	-	-	8/17/17/17	-
25	STE	A	421	-	-	5/9/9/17	-
22	CLA	c	501	-	1/1/20/20	2/37/115/115	-
28	DGD	C	519	-	-	15/51/91/95	0/2/2/2
22	CLA	B	604	-	1/1/20/20	9/37/115/115	-
25	STE	C	522	-	-	1/5/5/17	-
22	CLA	c	505	-	1/1/20/20	6/37/115/115	-
22	CLA	C	508	-	-	5/37/115/115	-

All (736) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	404	CLA	C4B-NB	7.89	1.42	1.35
22	d	404	CLA	C4B-NB	7.89	1.42	1.35
22	B	615	CLA	C4B-NB	7.87	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	C4B-NB	7.86	1.42	1.35
22	c	502	CLA	C4B-NB	7.86	1.42	1.35
22	b	616	CLA	C4B-NB	7.77	1.42	1.35
22	B	602	CLA	C4B-NB	7.63	1.42	1.35
22	C	511	CLA	C4B-NB	7.59	1.42	1.35
22	b	603	CLA	C4B-NB	7.58	1.42	1.35
22	C	512	CLA	C4B-NB	7.57	1.42	1.35
22	B	605	CLA	C4B-NB	7.55	1.41	1.35
22	b	606	CLA	C4B-NB	7.55	1.41	1.35
22	C	507	CLA	C4B-NB	7.55	1.41	1.35
22	c	507	CLA	C4B-NB	7.55	1.41	1.35
22	C	509	CLA	C4B-NB	7.54	1.41	1.35
22	c	512	CLA	C4B-NB	7.52	1.41	1.35
22	c	511	CLA	C4B-NB	7.49	1.41	1.35
22	B	607	CLA	C4B-NB	7.49	1.41	1.35
22	c	509	CLA	C4B-NB	7.48	1.41	1.35
22	B	608	CLA	C4B-NB	7.47	1.41	1.35
22	b	609	CLA	C4B-NB	7.47	1.41	1.35
22	A	406	CLA	C4B-NB	7.46	1.41	1.35
22	b	607	CLA	C4B-NB	7.42	1.41	1.35
22	a	406	CLA	C4B-NB	7.41	1.41	1.35
22	B	603	CLA	C4B-NB	7.41	1.41	1.35
22	C	505	CLA	C4B-NB	7.40	1.41	1.35
22	b	608	CLA	C4B-NB	7.40	1.41	1.35
22	c	505	CLA	C4B-NB	7.40	1.41	1.35
22	B	613	CLA	C4B-NB	7.39	1.41	1.35
22	C	503	CLA	C4B-NB	7.38	1.41	1.35
22	c	503	CLA	C4B-NB	7.38	1.41	1.35
22	C	508	CLA	C4B-NB	7.35	1.41	1.35
22	c	508	CLA	C4B-NB	7.35	1.41	1.35
22	B	604	CLA	C4B-NB	7.33	1.41	1.35
22	B	606	CLA	C4B-NB	7.33	1.41	1.35
22	B	610	CLA	C4B-NB	7.32	1.41	1.35
22	b	611	CLA	C4B-NB	7.32	1.41	1.35
22	B	601	CLA	C4B-NB	7.32	1.41	1.35
22	B	609	CLA	C4B-NB	7.30	1.41	1.35
22	b	610	CLA	C4B-NB	7.30	1.41	1.35
22	C	501	CLA	C4B-NB	7.30	1.41	1.35
22	D	405	CLA	C4B-NB	7.30	1.41	1.35
22	d	405	CLA	C4B-NB	7.30	1.41	1.35
22	B	612	CLA	C4B-NB	7.30	1.41	1.35
22	b	613	CLA	C4B-NB	7.30	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	C4B-NB	7.30	1.41	1.35
22	b	612	CLA	C4B-NB	7.29	1.41	1.35
22	b	605	CLA	C4B-NB	7.27	1.41	1.35
22	C	504	CLA	C4B-NB	7.27	1.41	1.35
22	c	504	CLA	C4B-NB	7.27	1.41	1.35
22	b	602	CLA	C4B-NB	7.27	1.41	1.35
22	b	604	CLA	C4B-NB	7.27	1.41	1.35
22	C	506	CLA	C4B-NB	7.27	1.41	1.35
22	c	506	CLA	C4B-NB	7.27	1.41	1.35
22	B	614	CLA	C4B-NB	7.25	1.41	1.35
22	b	615	CLA	C4B-NB	7.25	1.41	1.35
22	A	405	CLA	C4B-NB	7.24	1.41	1.35
22	c	501	CLA	C4B-NB	7.20	1.41	1.35
22	B	611	CLA	C4B-NB	7.19	1.41	1.35
22	a	404	CLA	C4B-NB	7.18	1.41	1.35
22	a	405	CLA	C4B-NB	7.15	1.41	1.35
22	A	419	CLA	C4B-NB	7.12	1.41	1.35
22	a	419	CLA	C4B-NB	7.12	1.41	1.35
22	C	510	CLA	C4B-NB	7.10	1.41	1.35
22	c	510	CLA	C4B-NB	7.10	1.41	1.35
22	A	404	CLA	C4B-NB	7.09	1.41	1.35
22	B	616	CLA	C4B-NB	7.03	1.41	1.35
22	b	617	CLA	C4B-NB	7.03	1.41	1.35
22	C	513	CLA	C4B-NB	7.02	1.41	1.35
22	c	513	CLA	C4B-NB	7.02	1.41	1.35
35	v	201	HEC	C2B-C3B	-6.66	1.33	1.40
35	V	201	HEC	C2B-C3B	-6.60	1.33	1.40
35	v	201	HEC	C3C-C2C	-6.46	1.34	1.40
35	V	201	HEC	C3C-C2C	-6.40	1.34	1.40
22	A	406	CLA	MG-NC	5.54	2.19	2.06
22	a	406	CLA	MG-NC	5.48	2.19	2.06
22	C	503	CLA	MG-NA	5.45	2.19	2.06
22	c	503	CLA	MG-NA	5.45	2.19	2.06
35	V	201	HEC	C3D-C2D	5.43	1.53	1.37
35	v	201	HEC	C3D-C2D	5.40	1.53	1.37
22	D	405	CLA	MG-NC	5.38	2.19	2.06
22	d	405	CLA	MG-NC	5.38	2.19	2.06
22	C	505	CLA	MG-NA	5.28	2.18	2.06
22	c	505	CLA	MG-NA	5.28	2.18	2.06
22	B	616	CLA	MG-NA	4.98	2.18	2.06
22	b	617	CLA	MG-NA	4.98	2.18	2.06
22	A	404	CLA	MG-NC	4.83	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	404	CLA	MG-NC	4.83	2.17	2.06
22	b	605	CLA	MG-NA	4.83	2.17	2.06
22	B	604	CLA	MG-NA	4.80	2.17	2.06
22	b	610	CLA	MG-NC	4.74	2.17	2.06
22	B	609	CLA	MG-NC	4.74	2.17	2.06
22	D	404	CLA	MG-NA	4.73	2.17	2.06
22	d	404	CLA	MG-NA	4.73	2.17	2.06
27	A	411	SQD	O48-C23	4.65	1.46	1.33
27	a	411	SQD	O48-C23	4.65	1.46	1.33
27	x	101	SQD	O48-C23	4.65	1.46	1.33
27	A	412	SQD	O48-C23	4.65	1.46	1.33
27	X	101	SQD	O48-C23	4.64	1.46	1.33
27	a	412	SQD	O48-C23	4.62	1.46	1.33
22	B	605	CLA	MG-NA	4.62	2.17	2.06
22	b	606	CLA	MG-NA	4.62	2.17	2.06
27	b	621	SQD	O48-C23	4.61	1.46	1.33
27	B	620	SQD	O48-C23	4.60	1.46	1.33
22	B	608	CLA	MG-NC	4.48	2.16	2.06
22	b	609	CLA	MG-NC	4.48	2.16	2.06
22	B	611	CLA	MG-NC	4.42	2.16	2.06
22	b	612	CLA	MG-NC	4.42	2.16	2.06
22	b	613	CLA	MG-NC	4.38	2.16	2.06
22	B	612	CLA	MG-NC	4.37	2.16	2.06
22	B	615	CLA	MG-NC	4.35	2.16	2.06
22	b	616	CLA	MG-NC	4.35	2.16	2.06
34	E	105	HEM	C3C-C2C	-4.27	1.34	1.40
34	e	105	HEM	C3C-C2C	-4.21	1.34	1.40
22	B	610	CLA	C1D-ND	4.14	1.42	1.37
22	a	404	CLA	C1D-ND	4.09	1.42	1.37
22	A	404	CLA	C1D-ND	4.07	1.42	1.37
22	B	604	CLA	C1D-ND	4.07	1.42	1.37
22	b	605	CLA	C1D-ND	4.07	1.42	1.37
22	b	611	CLA	C1D-ND	4.06	1.42	1.37
22	C	503	CLA	MG-NC	4.03	2.15	2.06
22	c	503	CLA	MG-NC	4.03	2.15	2.06
22	c	509	CLA	C1D-ND	3.94	1.42	1.37
22	d	404	CLA	C1D-ND	3.93	1.42	1.37
22	B	612	CLA	C1D-ND	3.92	1.42	1.37
22	b	613	CLA	C1D-ND	3.92	1.42	1.37
22	B	613	CLA	C1D-ND	3.92	1.42	1.37
22	b	614	CLA	C1D-ND	3.92	1.42	1.37
22	C	509	CLA	C1D-ND	3.89	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	MG-NA	3.87	2.15	2.06
22	D	404	CLA	C1D-ND	3.85	1.42	1.37
22	C	510	CLA	C1D-ND	3.85	1.42	1.37
22	c	510	CLA	C1D-ND	3.85	1.42	1.37
22	C	506	CLA	C1D-ND	3.84	1.42	1.37
22	c	506	CLA	C1D-ND	3.84	1.42	1.37
22	b	614	CLA	MG-NA	3.84	2.15	2.06
22	B	602	CLA	C1D-ND	3.83	1.42	1.37
22	b	603	CLA	C1D-ND	3.83	1.42	1.37
22	A	405	CLA	C1D-ND	3.82	1.42	1.37
22	B	616	CLA	C1D-ND	3.82	1.42	1.37
22	b	617	CLA	C1D-ND	3.82	1.42	1.37
22	B	609	CLA	C1D-ND	3.82	1.42	1.37
22	b	610	CLA	C1D-ND	3.82	1.42	1.37
22	c	502	CLA	C1D-ND	3.79	1.42	1.37
22	b	602	CLA	C1D-ND	3.76	1.42	1.37
22	C	508	CLA	MG-NC	3.76	2.15	2.06
22	C	502	CLA	C1D-ND	3.76	1.42	1.37
22	B	601	CLA	C1D-ND	3.75	1.42	1.37
22	B	605	CLA	C1D-ND	3.75	1.42	1.37
22	b	606	CLA	C1D-ND	3.75	1.42	1.37
22	C	505	CLA	C1D-ND	3.75	1.42	1.37
22	c	505	CLA	C1D-ND	3.75	1.42	1.37
22	B	611	CLA	C1D-ND	3.75	1.42	1.37
22	b	612	CLA	C1D-ND	3.75	1.42	1.37
22	a	406	CLA	C1D-ND	3.74	1.42	1.37
22	A	406	CLA	C1D-ND	3.74	1.42	1.37
22	B	615	CLA	C1D-ND	3.72	1.42	1.37
22	C	507	CLA	C1D-ND	3.71	1.42	1.37
22	c	507	CLA	C1D-ND	3.71	1.42	1.37
22	B	606	CLA	C1D-ND	3.71	1.42	1.37
22	B	608	CLA	C1D-ND	3.70	1.42	1.37
22	b	609	CLA	C1D-ND	3.70	1.42	1.37
22	C	504	CLA	C1D-ND	3.70	1.42	1.37
22	c	504	CLA	C1D-ND	3.70	1.42	1.37
22	c	508	CLA	MG-NC	3.68	2.15	2.06
22	b	607	CLA	C1D-ND	3.67	1.42	1.37
22	a	405	CLA	C1D-ND	3.67	1.42	1.37
22	B	615	CLA	MG-NA	3.67	2.15	2.06
22	b	616	CLA	MG-NA	3.67	2.15	2.06
22	B	603	CLA	C1D-ND	3.66	1.42	1.37
22	b	604	CLA	C1D-ND	3.66	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	C1D-ND	3.66	1.42	1.37
22	b	608	CLA	C1D-ND	3.66	1.42	1.37
22	D	405	CLA	C1D-ND	3.66	1.42	1.37
22	b	616	CLA	C1D-ND	3.65	1.42	1.37
22	C	508	CLA	C1D-ND	3.65	1.42	1.37
22	c	508	CLA	C1D-ND	3.65	1.42	1.37
22	C	513	CLA	C1D-ND	3.64	1.42	1.37
22	c	513	CLA	C1D-ND	3.64	1.42	1.37
22	d	405	CLA	C1D-ND	3.64	1.42	1.37
22	c	511	CLA	C1D-ND	3.63	1.42	1.37
27	a	411	SQD	O47-C45	-3.62	1.37	1.46
22	C	512	CLA	C1D-ND	3.62	1.42	1.37
27	A	411	SQD	O47-C45	-3.61	1.37	1.46
23	K	103	BCR	C1-C6	-3.60	1.48	1.53
23	k	103	BCR	C1-C6	-3.60	1.48	1.53
22	c	512	CLA	C1D-ND	3.58	1.42	1.37
22	B	614	CLA	C1D-ND	3.58	1.42	1.37
22	C	503	CLA	C1D-ND	3.58	1.42	1.37
22	c	503	CLA	C1D-ND	3.58	1.42	1.37
22	C	511	CLA	C1D-ND	3.58	1.42	1.37
23	H	102	BCR	C1-C6	-3.58	1.48	1.53
23	h	102	BCR	C1-C6	-3.58	1.48	1.53
23	B	617	BCR	C1-C6	-3.57	1.48	1.53
23	b	618	BCR	C1-C6	-3.57	1.48	1.53
27	a	412	SQD	O47-C45	-3.57	1.37	1.46
24	A	408	PL9	C7-C3	-3.55	1.47	1.51
24	a	408	PL9	C7-C3	-3.55	1.47	1.51
22	C	501	CLA	C1D-ND	3.55	1.42	1.37
22	c	501	CLA	C1D-ND	3.55	1.42	1.37
27	A	412	SQD	O47-C45	-3.52	1.37	1.46
22	b	615	CLA	C1D-ND	3.52	1.42	1.37
34	E	105	HEM	C3C-CAC	3.50	1.55	1.47
22	A	405	CLA	C4D-ND	-3.46	1.32	1.37
34	e	105	HEM	C3C-CAC	3.46	1.54	1.47
27	b	621	SQD	O47-C45	-3.44	1.38	1.46
22	A	419	CLA	C4D-ND	-3.44	1.33	1.37
22	b	614	CLA	MG-NC	3.43	2.14	2.06
22	a	419	CLA	C4D-ND	-3.42	1.33	1.37
22	d	405	CLA	C4D-ND	-3.41	1.33	1.37
27	b	621	SQD	O5-C1	3.41	1.50	1.41
22	a	405	CLA	C4D-ND	-3.39	1.33	1.37
23	d	406	BCR	C1-C6	-3.38	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	MG-NC	3.38	2.14	2.06
23	D	406	BCR	C1-C6	-3.38	1.49	1.53
22	c	502	CLA	C4D-ND	-3.38	1.33	1.37
23	c	514	BCR	C1-C6	-3.38	1.49	1.53
22	D	405	CLA	C4D-ND	-3.35	1.33	1.37
23	K	101	BCR	C1-C6	-3.34	1.49	1.53
22	B	603	CLA	MG-NC	3.34	2.14	2.06
22	b	604	CLA	MG-NC	3.34	2.14	2.06
22	b	612	CLA	C4D-ND	-3.34	1.33	1.37
22	B	614	CLA	C4D-ND	-3.32	1.33	1.37
22	B	611	CLA	MG-NA	3.32	2.14	2.06
22	b	612	CLA	MG-NA	3.32	2.14	2.06
27	B	620	SQD	O5-C1	3.31	1.50	1.41
23	C	515	BCR	C1-C6	-3.31	1.49	1.53
23	c	515	BCR	C1-C6	-3.31	1.49	1.53
22	A	406	CLA	C4D-ND	-3.31	1.33	1.37
22	a	406	CLA	C4D-ND	-3.31	1.33	1.37
22	B	602	CLA	MG-NC	3.30	2.14	2.06
22	b	603	CLA	MG-NC	3.30	2.14	2.06
23	b	619	BCR	C30-C25	-3.30	1.49	1.53
23	C	514	BCR	C1-C6	-3.30	1.49	1.53
22	b	615	CLA	C4D-ND	-3.30	1.33	1.37
22	C	502	CLA	C4D-ND	-3.29	1.33	1.37
27	B	620	SQD	O47-C45	-3.29	1.38	1.46
22	B	611	CLA	C4D-ND	-3.29	1.33	1.37
27	b	621	SQD	O47-C7	3.28	1.43	1.34
22	C	512	CLA	MG-NC	3.27	2.14	2.06
22	B	614	CLA	MG-NC	3.27	2.14	2.06
27	B	620	SQD	O47-C7	3.27	1.43	1.34
22	A	419	CLA	C1D-ND	3.27	1.41	1.37
22	a	419	CLA	C1D-ND	3.27	1.41	1.37
23	B	618	BCR	C30-C25	-3.26	1.49	1.53
22	B	609	CLA	C4D-ND	-3.26	1.33	1.37
22	b	610	CLA	C4D-ND	-3.26	1.33	1.37
22	B	616	CLA	MG-NC	3.26	2.14	2.06
22	b	617	CLA	MG-NC	3.26	2.14	2.06
23	k	101	BCR	C1-C6	-3.26	1.49	1.53
22	B	607	CLA	CHC-C1C	3.25	1.43	1.35
22	b	615	CLA	MG-NC	3.25	2.14	2.06
22	D	404	CLA	MG-NC	3.24	2.14	2.06
22	d	404	CLA	MG-NC	3.24	2.14	2.06
22	C	503	CLA	MG-ND	3.23	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	503	CLA	MG-ND	3.23	2.12	2.05
22	c	512	CLA	MG-NC	3.23	2.13	2.06
22	B	603	CLA	MG-NA	3.23	2.13	2.06
22	b	604	CLA	MG-NA	3.23	2.13	2.06
22	D	404	CLA	C4D-ND	-3.23	1.33	1.37
22	d	404	CLA	C4D-ND	-3.23	1.33	1.37
22	C	503	CLA	C4D-ND	-3.21	1.33	1.37
22	c	503	CLA	C4D-ND	-3.21	1.33	1.37
22	C	511	CLA	CHC-C1C	3.21	1.43	1.35
22	a	405	CLA	CHC-C1C	3.21	1.43	1.35
23	A	407	BCR	C1-C6	-3.20	1.49	1.53
22	B	610	CLA	CHC-C1C	3.20	1.43	1.35
22	b	611	CLA	CHC-C1C	3.20	1.43	1.35
22	C	508	CLA	C4D-ND	-3.20	1.33	1.37
22	c	508	CLA	C4D-ND	-3.20	1.33	1.37
22	B	615	CLA	CHC-C1C	3.20	1.43	1.35
22	b	608	CLA	CHC-C1C	3.19	1.43	1.35
23	a	407	BCR	C1-C6	-3.19	1.49	1.53
22	B	608	CLA	C4D-ND	-3.19	1.33	1.37
22	b	609	CLA	C4D-ND	-3.19	1.33	1.37
22	c	511	CLA	CHC-C1C	3.19	1.43	1.35
22	c	507	CLA	CHC-C1C	3.18	1.43	1.35
27	A	412	SQD	O5-C1	3.18	1.50	1.41
27	a	412	SQD	O5-C1	3.18	1.50	1.41
22	B	605	CLA	MG-NC	3.18	2.13	2.06
22	b	616	CLA	CHC-C1C	3.18	1.43	1.35
22	C	510	CLA	CHC-C1C	3.17	1.43	1.35
22	C	501	CLA	CHC-C1C	3.17	1.43	1.35
22	c	501	CLA	CHC-C1C	3.17	1.43	1.35
22	C	501	CLA	C4D-ND	-3.17	1.33	1.37
22	c	501	CLA	C4D-ND	-3.17	1.33	1.37
22	B	608	CLA	CHC-C1C	3.17	1.43	1.35
22	b	609	CLA	CHC-C1C	3.17	1.43	1.35
22	B	615	CLA	C4D-ND	-3.17	1.33	1.37
22	d	405	CLA	MG-ND	3.17	2.12	2.05
22	c	510	CLA	CHC-C1C	3.16	1.43	1.35
22	A	405	CLA	CHC-C1C	3.15	1.43	1.35
22	B	605	CLA	CHC-C1C	3.15	1.43	1.35
22	b	606	CLA	CHC-C1C	3.15	1.43	1.35
22	A	406	CLA	CHC-C1C	3.15	1.43	1.35
22	a	406	CLA	CHC-C1C	3.15	1.43	1.35
22	C	508	CLA	MG-NA	3.15	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	508	CLA	MG-NA	3.15	2.13	2.06
22	C	503	CLA	CHC-C1C	3.15	1.43	1.35
22	c	502	CLA	CHC-C1C	3.15	1.43	1.35
22	c	503	CLA	CHC-C1C	3.15	1.43	1.35
22	b	606	CLA	MG-NC	3.14	2.13	2.06
22	B	607	CLA	C4D-ND	-3.14	1.33	1.37
22	b	608	CLA	C4D-ND	-3.14	1.33	1.37
22	c	513	CLA	CHC-C1C	3.14	1.43	1.35
27	A	412	SQD	O47-C7	3.13	1.43	1.34
22	C	502	CLA	CHC-C1C	3.13	1.43	1.35
22	C	507	CLA	CHC-C1C	3.13	1.43	1.35
22	D	405	CLA	MG-ND	3.13	2.12	2.05
22	b	613	CLA	CHC-C1C	3.13	1.43	1.35
27	a	412	SQD	O47-C7	3.13	1.43	1.34
22	B	609	CLA	CHC-C1C	3.13	1.43	1.35
22	b	610	CLA	CHC-C1C	3.13	1.43	1.35
22	C	505	CLA	CHC-C1C	3.12	1.43	1.35
22	c	505	CLA	CHC-C1C	3.12	1.43	1.35
23	b	619	BCR	C1-C6	-3.12	1.49	1.53
22	B	612	CLA	C4D-ND	-3.12	1.33	1.37
22	b	613	CLA	C4D-ND	-3.12	1.33	1.37
22	C	512	CLA	C4D-ND	-3.12	1.33	1.37
22	c	512	CLA	C4D-ND	-3.12	1.33	1.37
24	D	407	PL9	C3-C4	-3.12	1.44	1.49
24	d	407	PL9	C3-C4	-3.12	1.44	1.49
27	a	411	SQD	O47-C7	3.11	1.43	1.34
23	D	406	BCR	C30-C25	-3.11	1.49	1.53
23	d	406	BCR	C30-C25	-3.11	1.49	1.53
22	C	513	CLA	CHC-C1C	3.11	1.42	1.35
22	b	616	CLA	C4D-ND	-3.11	1.33	1.37
22	B	612	CLA	CHC-C1C	3.11	1.42	1.35
22	B	604	CLA	CHC-C1C	3.11	1.42	1.35
22	C	504	CLA	C4D-ND	-3.10	1.33	1.37
22	c	504	CLA	C4D-ND	-3.10	1.33	1.37
22	C	512	CLA	CHC-C1C	3.10	1.42	1.35
23	B	618	BCR	C1-C6	-3.10	1.49	1.53
22	B	602	CLA	CHC-C1C	3.10	1.42	1.35
22	b	603	CLA	CHC-C1C	3.10	1.42	1.35
22	b	605	CLA	CHC-C1C	3.10	1.42	1.35
22	b	610	CLA	MG-NA	3.10	2.13	2.06
22	C	510	CLA	C4D-ND	-3.09	1.33	1.37
22	c	510	CLA	C4D-ND	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	102	BCR	C30-C25	-3.09	1.49	1.53
22	b	614	CLA	CHC-C1C	3.09	1.42	1.35
22	D	404	CLA	CHC-C1C	3.09	1.42	1.35
22	d	404	CLA	CHC-C1C	3.09	1.42	1.35
27	A	411	SQD	O47-C7	3.08	1.43	1.34
22	c	512	CLA	CHC-C1C	3.08	1.42	1.35
22	B	601	CLA	CHC-C1C	3.08	1.42	1.35
22	b	602	CLA	CHC-C1C	3.08	1.42	1.35
22	B	604	CLA	MG-NC	3.08	2.13	2.06
22	B	609	CLA	MG-NA	3.08	2.13	2.06
22	C	506	CLA	C4D-ND	-3.08	1.33	1.37
22	c	506	CLA	C4D-ND	-3.08	1.33	1.37
22	B	611	CLA	CHC-C1C	3.07	1.42	1.35
22	b	612	CLA	CHC-C1C	3.07	1.42	1.35
22	B	605	CLA	C4D-ND	-3.07	1.33	1.37
22	b	606	CLA	C4D-ND	-3.07	1.33	1.37
23	k	103	BCR	C30-C25	-3.07	1.49	1.53
22	C	506	CLA	CHC-C1C	3.07	1.42	1.35
22	c	506	CLA	CHC-C1C	3.07	1.42	1.35
22	c	511	CLA	C4D-ND	-3.07	1.33	1.37
27	x	101	SQD	O5-C1	3.07	1.49	1.41
23	T	101	BCR	C1-C6	-3.07	1.49	1.53
22	B	603	CLA	C4D-ND	-3.06	1.33	1.37
22	b	604	CLA	C4D-ND	-3.06	1.33	1.37
22	b	605	CLA	MG-NC	3.06	2.13	2.06
22	B	613	CLA	CHC-C1C	3.06	1.42	1.35
22	C	507	CLA	C4D-ND	-3.06	1.33	1.37
22	c	507	CLA	C4D-ND	-3.06	1.33	1.37
23	K	103	BCR	C30-C25	-3.06	1.49	1.53
22	A	419	CLA	CHC-C1C	3.06	1.42	1.35
22	a	419	CLA	CHC-C1C	3.06	1.42	1.35
22	C	511	CLA	C4D-ND	-3.06	1.33	1.37
23	c	514	BCR	C30-C25	-3.06	1.49	1.53
22	C	509	CLA	CHC-C1C	3.06	1.42	1.35
22	c	509	CLA	CHC-C1C	3.06	1.42	1.35
22	C	509	CLA	C4D-ND	-3.05	1.33	1.37
27	b	621	SQD	C24-C23	3.05	1.59	1.50
23	b	620	BCR	C1-C6	-3.05	1.49	1.53
22	B	603	CLA	CHC-C1C	3.05	1.42	1.35
22	b	604	CLA	CHC-C1C	3.05	1.42	1.35
22	B	606	CLA	CHC-C1C	3.05	1.42	1.35
22	b	607	CLA	CHC-C1C	3.05	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	T	101	BCR	C30-C25	-3.04	1.49	1.53
23	t	102	BCR	C30-C25	-3.04	1.49	1.53
22	B	606	CLA	C4D-ND	-3.04	1.33	1.37
22	b	607	CLA	C4D-ND	-3.04	1.33	1.37
23	t	102	BCR	C1-C6	-3.04	1.49	1.53
27	X	101	SQD	O5-C1	3.04	1.49	1.41
22	D	405	CLA	CHC-C1C	3.03	1.42	1.35
22	d	405	CLA	CHC-C1C	3.03	1.42	1.35
22	C	504	CLA	CHC-C1C	3.03	1.42	1.35
22	c	504	CLA	CHC-C1C	3.03	1.42	1.35
22	B	614	CLA	CHC-C1C	3.02	1.42	1.35
23	h	102	BCR	C30-C25	-3.02	1.49	1.53
27	a	411	SQD	C24-C23	3.02	1.59	1.50
22	c	509	CLA	C4D-ND	-3.02	1.33	1.37
23	B	619	BCR	C1-C6	-3.01	1.49	1.53
22	B	610	CLA	C4D-ND	-3.01	1.33	1.37
22	b	615	CLA	CHC-C1C	3.01	1.42	1.35
27	a	412	SQD	C24-C23	3.00	1.59	1.50
23	C	514	BCR	C30-C25	-3.00	1.49	1.53
27	A	411	SQD	C24-C23	3.00	1.59	1.50
22	A	404	CLA	C4D-ND	-2.99	1.33	1.37
22	C	508	CLA	CHC-C1C	2.99	1.42	1.35
22	c	508	CLA	CHC-C1C	2.99	1.42	1.35
22	C	513	CLA	C4D-ND	-2.98	1.33	1.37
22	a	404	CLA	C4D-ND	-2.98	1.33	1.37
22	c	513	CLA	C4D-ND	-2.98	1.33	1.37
22	B	602	CLA	C4D-ND	-2.97	1.33	1.37
22	b	603	CLA	C4D-ND	-2.97	1.33	1.37
22	a	404	CLA	CHC-C1C	2.97	1.42	1.35
27	A	412	SQD	C24-C23	2.97	1.59	1.50
22	b	611	CLA	C4D-ND	-2.96	1.33	1.37
23	C	515	BCR	C30-C25	-2.96	1.49	1.53
23	c	515	BCR	C30-C25	-2.96	1.49	1.53
22	b	602	CLA	C4D-ND	-2.96	1.33	1.37
22	A	404	CLA	CHC-C1C	2.96	1.42	1.35
27	A	411	SQD	O5-C1	2.96	1.49	1.41
22	B	601	CLA	C4D-ND	-2.95	1.33	1.37
27	x	101	SQD	C24-C23	2.94	1.59	1.50
22	B	604	CLA	C4D-ND	-2.94	1.33	1.37
22	b	605	CLA	C4D-ND	-2.94	1.33	1.37
23	A	407	BCR	C30-C25	-2.94	1.49	1.53
23	a	407	BCR	C30-C25	-2.94	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	620	SQD	C24-C23	2.94	1.59	1.50
32	Z	101	LMT	O3'-C3'	-2.93	1.36	1.43
27	a	411	SQD	O5-C1	2.93	1.49	1.41
22	b	617	CLA	CHC-C1C	2.93	1.42	1.35
22	B	613	CLA	C4D-ND	-2.92	1.33	1.37
22	b	614	CLA	C4D-ND	-2.92	1.33	1.37
22	B	616	CLA	CHC-C1C	2.92	1.42	1.35
23	b	620	BCR	C30-C25	-2.92	1.49	1.53
32	C	525	LMT	O3'-C3'	-2.91	1.36	1.43
32	z	101	LMT	O3'-C3'	-2.91	1.36	1.43
27	X	101	SQD	C24-C23	2.91	1.59	1.50
22	C	510	CLA	MG-NA	2.90	2.13	2.06
32	c	525	LMT	O3'-C3'	-2.89	1.36	1.43
22	B	616	CLA	C4D-ND	-2.88	1.33	1.37
22	b	617	CLA	C4D-ND	-2.88	1.33	1.37
22	c	510	CLA	MG-NA	2.87	2.13	2.06
22	C	505	CLA	C4D-ND	-2.86	1.33	1.37
22	c	505	CLA	C4D-ND	-2.86	1.33	1.37
23	K	101	BCR	C30-C25	-2.86	1.49	1.53
23	k	101	BCR	C30-C25	-2.86	1.49	1.53
22	c	502	CLA	MG-NC	2.85	2.13	2.06
23	B	619	BCR	C30-C25	-2.84	1.49	1.53
30	A	418	PHO	CAC-C3C	-2.84	1.47	1.52
30	a	418	PHO	CAC-C3C	-2.84	1.47	1.52
22	C	502	CLA	MG-NC	2.83	2.13	2.06
22	C	511	CLA	MG-NA	2.80	2.12	2.06
22	c	511	CLA	MG-NA	2.80	2.12	2.06
34	E	105	HEM	CAB-C3B	2.78	1.55	1.47
34	e	105	HEM	CAB-C3B	2.78	1.55	1.47
22	C	509	CLA	MG-NA	2.77	2.12	2.06
22	c	509	CLA	MG-NA	2.77	2.12	2.06
32	j	102	LMT	O3'-C3'	-2.75	1.36	1.43
32	m	101	LMT	O3'-C3'	-2.74	1.36	1.43
28	A	413	DGD	O1G-C1G	-2.74	1.38	1.45
32	J	102	LMT	O3'-C3'	-2.73	1.36	1.43
23	b	618	BCR	C30-C25	-2.73	1.50	1.53
23	B	617	BCR	C30-C25	-2.72	1.50	1.53
32	E	104	LMT	O3'-C3'	-2.72	1.36	1.43
32	e	104	LMT	O3'-C3'	-2.72	1.36	1.43
32	M	102	LMT	O3'-C3'	-2.71	1.36	1.43
22	C	502	CLA	MG-NA	2.65	2.12	2.06
22	c	502	CLA	MG-NA	2.65	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	623	LMT	O3'-C3'	-2.63	1.36	1.43
22	B	607	CLA	MG-NA	2.61	2.12	2.06
22	b	608	CLA	MG-NA	2.61	2.12	2.06
32	b	624	LMT	O3'-C3'	-2.61	1.36	1.43
32	C	523	LMT	O3'-C3'	-2.60	1.36	1.43
28	c	518	DGD	O1G-C1G	-2.59	1.39	1.45
28	a	413	DGD	O1G-C1G	-2.58	1.39	1.45
22	C	505	CLA	CMB-C2B	-2.57	1.46	1.51
22	c	505	CLA	CMB-C2B	-2.57	1.46	1.51
24	D	407	PL9	C7-C3	-2.57	1.48	1.51
22	b	605	CLA	CMB-C2B	-2.56	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.56	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.56	1.46	1.51
28	C	518	DGD	O1G-C1G	-2.56	1.39	1.45
32	c	523	LMT	O3'-C3'	-2.55	1.37	1.43
32	M	102	LMT	O2B-C2B	-2.55	1.37	1.43
22	C	512	CLA	CMB-C2B	-2.54	1.46	1.51
32	m	101	LMT	O2B-C2B	-2.54	1.37	1.43
22	B	604	CLA	CMB-C2B	-2.54	1.46	1.51
22	b	612	CLA	MG-ND	2.54	2.10	2.05
28	A	413	DGD	O2G-C2G	-2.53	1.40	1.46
22	B	612	CLA	CMB-C2B	-2.53	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.53	1.46	1.51
22	C	502	CLA	CMB-C2B	-2.53	1.46	1.51
24	d	407	PL9	C7-C3	-2.53	1.48	1.51
22	A	406	CLA	CMB-C2B	-2.52	1.46	1.51
28	a	413	DGD	O2G-C2G	-2.51	1.40	1.46
22	C	513	CLA	MG-NA	2.51	2.12	2.06
22	c	512	CLA	CMB-C2B	-2.50	1.46	1.51
22	C	501	CLA	CMB-C2B	-2.50	1.46	1.51
22	c	501	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.50	1.46	1.51
22	C	510	CLA	CMB-C2B	-2.50	1.46	1.51
22	b	607	CLA	CMB-C2B	-2.50	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	611	CLA	MG-ND	2.50	2.10	2.05
22	c	502	CLA	CMB-C2B	-2.49	1.46	1.51
22	C	505	CLA	MG-NC	2.49	2.12	2.06
22	c	505	CLA	MG-NC	2.49	2.12	2.06
22	A	404	CLA	MG-NA	2.49	2.12	2.06
22	a	404	CLA	MG-NA	2.49	2.12	2.06
22	d	404	CLA	CMB-C2B	-2.48	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	504	CLA	CMB-C2B	-2.48	1.46	1.51
22	c	504	CLA	CMB-C2B	-2.48	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.48	1.46	1.51
22	c	506	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	405	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	612	CLA	MG-NA	2.47	2.12	2.06
22	a	406	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	513	CLA	MG-NA	2.47	2.12	2.06
22	b	613	CLA	MG-NA	2.47	2.12	2.06
22	B	609	CLA	CMB-C2B	-2.46	1.46	1.51
22	D	405	CLA	CMB-C2B	-2.46	1.46	1.51
22	d	405	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	609	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.46	1.46	1.51
30	D	401	PHO	CAC-C3C	-2.46	1.47	1.52
30	d	401	PHO	CAC-C3C	-2.46	1.47	1.52
22	B	611	CLA	CMB-C2B	-2.45	1.46	1.51
22	b	612	CLA	CMB-C2B	-2.45	1.46	1.51
22	a	419	CLA	MG-NA	2.45	2.12	2.06
22	B	605	CLA	CMB-C2B	-2.45	1.46	1.51
22	b	606	CLA	CMB-C2B	-2.45	1.46	1.51
22	D	404	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	616	CLA	CMB-C2B	-2.44	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	614	CLA	CMB-C2B	-2.44	1.46	1.51
22	A	419	CLA	MG-NA	2.43	2.12	2.06
22	c	511	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	610	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	611	CLA	CMB-C2B	-2.43	1.46	1.51
22	C	509	CLA	CMB-C2B	-2.43	1.46	1.51
22	c	509	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	603	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	604	CLA	CMB-C2B	-2.43	1.46	1.51
22	C	507	CLA	CMB-C2B	-2.42	1.46	1.51
22	c	507	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	601	CLA	CMB-C2B	-2.42	1.46	1.51
22	C	513	CLA	CMB-C2B	-2.42	1.46	1.51
22	c	513	CLA	CMB-C2B	-2.42	1.46	1.51
26	C	520	LMG	O7-C8	-2.42	1.40	1.46
31	d	410	LHG	P-O6	2.42	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	CMB-C2B	-2.41	1.46	1.51
22	b	615	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	503	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	503	CLA	CMB-C2B	-2.41	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.41	1.46	1.51
22	b	603	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	511	CLA	CMB-C2B	-2.41	1.46	1.51
22	a	419	CLA	CMB-C2B	-2.40	1.46	1.51
31	D	410	LHG	P-O6	2.39	1.69	1.59
22	a	405	CLA	CMB-C2B	-2.39	1.46	1.51
32	C	525	LMT	O2'-C2'	-2.39	1.37	1.43
22	B	616	CLA	CMB-C2B	-2.39	1.46	1.51
22	b	602	CLA	CMB-C2B	-2.38	1.46	1.51
32	z	101	LMT	O2'-C2'	-2.37	1.37	1.43
32	Z	101	LMT	O2'-C2'	-2.37	1.37	1.43
22	C	501	CLA	MG-NA	2.37	2.11	2.06
22	c	501	CLA	MG-NA	2.37	2.11	2.06
22	A	419	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	617	CLA	CMB-C2B	-2.37	1.46	1.51
22	B	606	CLA	MG-NA	2.37	2.11	2.06
22	b	607	CLA	MG-NA	2.37	2.11	2.06
26	c	520	LMG	O7-C8	-2.36	1.40	1.46
32	c	525	LMT	O2'-C2'	-2.36	1.37	1.43
31	A	420	LHG	O7-C5	-2.35	1.40	1.46
31	a	420	LHG	O7-C5	-2.35	1.40	1.46
31	D	411	LHG	O7-C5	-2.33	1.40	1.46
31	d	411	LHG	O7-C5	-2.33	1.40	1.46
24	D	407	PL9	C6-C1	-2.33	1.44	1.48
24	d	407	PL9	C6-C1	-2.33	1.44	1.48
24	A	408	PL9	C6-C1	-2.33	1.44	1.48
24	a	408	PL9	C6-C1	-2.33	1.44	1.48
22	B	608	CLA	MG-NA	2.33	2.11	2.06
22	b	609	CLA	MG-NA	2.33	2.11	2.06
32	c	525	LMT	O3B-C3B	-2.33	1.37	1.43
32	z	101	LMT	O2B-C2B	-2.33	1.37	1.43
22	B	607	CLA	CMB-C2B	-2.33	1.46	1.51
22	b	608	CLA	CMB-C2B	-2.33	1.46	1.51
32	B	623	LMT	O2'-C2'	-2.32	1.37	1.43
32	b	624	LMT	O2'-C2'	-2.32	1.37	1.43
32	C	523	LMT	O2'-C2'	-2.32	1.37	1.43
32	C	525	LMT	O3B-C3B	-2.32	1.37	1.43
32	Z	101	LMT	O2B-C2B	-2.32	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	404	CLA	CMB-C2B	-2.32	1.46	1.51
22	b	611	CLA	MG-NC	2.32	2.11	2.06
22	B	610	CLA	MG-NC	2.30	2.11	2.06
22	a	404	CLA	CMB-C2B	-2.29	1.46	1.51
22	c	506	CLA	MG-NC	2.29	2.11	2.06
32	c	523	LMT	O2'-C2'	-2.28	1.37	1.43
22	B	606	CLA	MG-ND	-2.27	2.01	2.05
22	b	607	CLA	MG-ND	-2.27	2.01	2.05
22	C	506	CLA	MG-NC	2.25	2.11	2.06
32	z	101	LMT	O3B-C3B	-2.25	1.37	1.43
22	C	509	CLA	MG-NC	2.24	2.11	2.06
24	D	407	PL9	C53-C6	-2.24	1.46	1.50
24	d	407	PL9	C53-C6	-2.24	1.46	1.50
22	C	506	CLA	MG-NA	2.24	2.11	2.06
22	c	506	CLA	MG-NA	2.24	2.11	2.06
32	j	102	LMT	O2'-C2'	-2.23	1.37	1.43
32	c	525	LMT	O2B-C2B	-2.23	1.37	1.43
28	C	517	DGD	O1G-C1G	-2.23	1.40	1.45
28	c	517	DGD	O1G-C1G	-2.23	1.40	1.45
32	Z	101	LMT	O3B-C3B	-2.22	1.37	1.43
32	z	101	LMT	O4'-C4B	-2.22	1.37	1.43
32	E	104	LMT	O2'-C2'	-2.21	1.37	1.43
32	e	104	LMT	O2'-C2'	-2.21	1.37	1.43
32	Z	101	LMT	O4'-C4B	-2.21	1.37	1.43
32	C	525	LMT	O2B-C2B	-2.21	1.37	1.43
22	c	509	CLA	MG-NC	2.20	2.11	2.06
32	J	102	LMT	O2'-C2'	-2.20	1.37	1.43
32	M	102	LMT	O2'-C2'	-2.18	1.37	1.43
32	M	102	LMT	O3B-C3B	-2.17	1.37	1.43
32	m	101	LMT	O3B-C3B	-2.17	1.37	1.43
22	B	615	CLA	MG-ND	2.17	2.10	2.05
22	b	616	CLA	MG-ND	2.17	2.10	2.05
22	a	405	CLA	CMD-C2D	-2.17	1.46	1.50
31	L	101	LHG	O7-C5	-2.17	1.41	1.46
31	l	101	LHG	O7-C5	-2.17	1.41	1.46
22	C	507	CLA	MG-NC	2.16	2.11	2.06
22	c	507	CLA	MG-NC	2.16	2.11	2.06
32	m	101	LMT	O2'-C2'	-2.16	1.37	1.43
32	C	525	LMT	O4'-C4B	-2.15	1.37	1.43
30	A	418	PHO	CMC-C2C	-2.15	1.46	1.51
32	c	525	LMT	O4'-C4B	-2.15	1.37	1.43
22	A	405	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	418	PHO	CMC-C2C	-2.14	1.46	1.51
27	b	621	SQD	O9-S	2.14	1.51	1.45
22	B	602	CLA	MG-NA	2.14	2.11	2.06
22	b	603	CLA	MG-NA	2.14	2.11	2.06
32	C	523	LMT	O1'-C1'	-2.14	1.36	1.40
30	a	418	PHO	CMD-C2D	-2.14	1.46	1.51
27	B	620	SQD	O9-S	2.14	1.51	1.45
30	d	401	PHO	CMC-C2C	-2.13	1.46	1.51
30	D	401	PHO	CMC-C2C	-2.13	1.46	1.51
27	A	412	SQD	O9-S	2.13	1.51	1.45
27	b	621	SQD	O7-S	2.12	1.51	1.45
24	A	408	PL9	C3-C4	-2.12	1.46	1.49
26	C	524	LMG	C7-C8	2.12	1.57	1.50
32	M	102	LMT	O4'-C4B	-2.12	1.38	1.43
22	C	502	CLA	MG-ND	-2.12	2.01	2.05
22	C	503	CLA	CMD-C2D	-2.12	1.46	1.50
22	c	503	CLA	CMD-C2D	-2.12	1.46	1.50
32	c	523	LMT	O1'-C1'	-2.12	1.36	1.40
34	E	105	HEM	FE-ND	2.11	2.07	1.96
32	c	523	LMT	O5'-C5'	-2.11	1.39	1.44
22	B	610	CLA	MG-NA	2.11	2.11	2.06
22	c	502	CLA	MG-ND	-2.11	2.01	2.05
26	c	524	LMG	C7-C8	2.11	1.57	1.50
30	A	418	PHO	CMD-C2D	-2.11	1.46	1.51
22	B	613	CLA	CMD-C2D	-2.10	1.46	1.50
22	b	614	CLA	CMD-C2D	-2.10	1.46	1.50
27	a	412	SQD	O9-S	2.10	1.51	1.45
22	D	405	CLA	MG-NA	2.10	2.11	2.06
22	d	405	CLA	MG-NA	2.10	2.11	2.06
22	b	611	CLA	MG-NA	2.10	2.11	2.06
34	e	105	HEM	FE-ND	2.09	2.07	1.96
22	B	612	CLA	CMD-C2D	-2.09	1.46	1.50
22	b	613	CLA	CMD-C2D	-2.09	1.46	1.50
22	C	512	CLA	CMD-C2D	-2.09	1.46	1.50
22	B	603	CLA	CMD-C2D	-2.09	1.46	1.50
22	b	604	CLA	CMD-C2D	-2.09	1.46	1.50
24	a	408	PL9	C3-C4	-2.08	1.46	1.49
30	a	418	PHO	CMB-C2B	-2.08	1.46	1.51
22	B	608	CLA	CMD-C2D	-2.08	1.46	1.50
22	b	609	CLA	CMD-C2D	-2.08	1.46	1.50
32	m	101	LMT	O4'-C4B	-2.07	1.38	1.43
22	A	419	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	419	CLA	CMD-C2D	-2.07	1.46	1.50
22	C	508	CLA	CMD-C2D	-2.07	1.46	1.50
22	c	508	CLA	CMD-C2D	-2.07	1.46	1.50
22	c	504	CLA	MG-NA	2.07	2.11	2.06
22	C	501	CLA	CMD-C2D	-2.07	1.46	1.50
22	c	501	CLA	CMD-C2D	-2.07	1.46	1.50
28	C	518	DGD	O2G-C2G	-2.07	1.41	1.46
31	A	420	LHG	P-O6	2.06	1.67	1.59
28	H	103	DGD	O2G-C2G	-2.06	1.41	1.46
30	A	418	PHO	CMB-C2B	-2.06	1.46	1.51
22	C	504	CLA	MG-NA	2.05	2.11	2.06
30	D	401	PHO	CMB-C2B	-2.05	1.46	1.51
27	B	620	SQD	O7-S	2.05	1.51	1.45
27	A	412	SQD	O7-S	2.05	1.51	1.45
27	a	412	SQD	O7-S	2.05	1.51	1.45
22	C	513	CLA	CMD-C2D	-2.05	1.46	1.50
22	c	513	CLA	CMD-C2D	-2.05	1.46	1.50
22	C	504	CLA	CMD-C2D	-2.05	1.46	1.50
22	c	504	CLA	CMD-C2D	-2.05	1.46	1.50
22	A	405	CLA	MG-NC	2.05	2.11	2.06
27	B	620	SQD	C8-C7	2.04	1.56	1.50
22	B	602	CLA	CMD-C2D	-2.04	1.46	1.50
22	b	603	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	616	CLA	CMD-C2D	-2.04	1.46	1.50
28	c	518	DGD	O2G-C2G	-2.04	1.41	1.46
22	B	604	CLA	CMD-C2D	-2.04	1.46	1.50
30	d	401	PHO	CMB-C2B	-2.04	1.46	1.51
22	B	615	CLA	CMD-C2D	-2.04	1.46	1.50
22	b	616	CLA	CMD-C2D	-2.04	1.46	1.50
27	b	621	SQD	C6-S	2.04	1.84	1.77
22	b	615	CLA	CMD-C2D	-2.04	1.46	1.50
22	C	502	CLA	CMD-C2D	-2.04	1.46	1.50
22	c	502	CLA	CMD-C2D	-2.04	1.46	1.50
22	c	512	CLA	CMD-C2D	-2.03	1.46	1.50
30	D	401	PHO	CMD-C2D	-2.03	1.46	1.51
22	b	617	CLA	CMD-C2D	-2.03	1.46	1.50
28	h	103	DGD	O2G-C2G	-2.03	1.41	1.46
22	c	511	CLA	CMD-C2D	-2.03	1.46	1.50
32	C	523	LMT	O5'-C5'	-2.03	1.39	1.44
22	C	507	CLA	CMC-C2C	-2.03	1.46	1.50
22	c	507	CLA	CMC-C2C	-2.03	1.46	1.50
31	a	420	LHG	P-O6	2.03	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	401	PHO	C3B-C2B	-2.02	1.37	1.40
30	d	401	PHO	CMD-C2D	-2.02	1.46	1.51
22	B	614	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	609	CLA	CMD-C2D	-2.01	1.46	1.50
27	X	101	SQD	O9-S	2.01	1.51	1.45
22	D	405	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	605	CLA	CMD-C2D	-2.01	1.46	1.50
22	d	405	CLA	CMD-C2D	-2.01	1.46	1.50
27	x	101	SQD	O7-S	2.01	1.51	1.45
27	x	101	SQD	O9-S	2.01	1.51	1.45
22	C	505	CLA	CMD-C2D	-2.01	1.46	1.50
22	c	505	CLA	CMD-C2D	-2.01	1.46	1.50
23	K	101	BCR	C33-C5	-2.01	1.47	1.50
28	C	518	DGD	C4D-C3D	2.01	1.57	1.52
28	c	518	DGD	C4D-C3D	2.01	1.57	1.52
31	d	409	LHG	P-O6	2.01	1.67	1.59
27	b	621	SQD	C8-C7	2.00	1.56	1.50
27	X	101	SQD	O7-S	2.00	1.50	1.45
22	b	610	CLA	CMD-C2D	-2.00	1.46	1.50

All (996) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	C4A-NA-C1A	8.17	110.38	106.71
22	b	605	CLA	C4A-NA-C1A	8.17	110.38	106.71
22	B	612	CLA	C4A-NA-C1A	7.73	110.18	106.71
22	b	613	CLA	C4A-NA-C1A	7.73	110.18	106.71
22	b	614	CLA	C4A-NA-C1A	7.43	110.05	106.71
22	B	613	CLA	C4A-NA-C1A	7.42	110.04	106.71
22	C	509	CLA	C4A-NA-C1A	7.37	110.02	106.71
22	c	509	CLA	C4A-NA-C1A	7.37	110.02	106.71
22	A	405	CLA	C4A-NA-C1A	7.19	109.94	106.71
22	B	616	CLA	C4A-NA-C1A	7.17	109.93	106.71
22	b	617	CLA	C4A-NA-C1A	7.17	109.93	106.71
22	a	405	CLA	C4A-NA-C1A	7.11	109.90	106.71
22	C	511	CLA	C4A-NA-C1A	7.04	109.87	106.71
22	B	610	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	D	404	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	b	611	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	d	404	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	c	511	CLA	C4A-NA-C1A	6.92	109.81	106.71
22	C	507	CLA	C4A-NA-C1A	6.79	109.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	507	CLA	C4A-NA-C1A	6.79	109.76	106.71
22	C	505	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	c	505	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	B	611	CLA	C4A-NA-C1A	6.58	109.67	106.71
22	b	612	CLA	C4A-NA-C1A	6.58	109.67	106.71
22	C	502	CLA	C4A-NA-C1A	6.58	109.66	106.71
22	C	508	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	c	502	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	C	504	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	c	504	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	d	405	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	B	615	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	B	606	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	b	607	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	D	405	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	b	616	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	C	506	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	c	506	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	c	508	CLA	C4A-NA-C1A	6.33	109.55	106.71
22	B	609	CLA	C4A-NA-C1A	6.28	109.53	106.71
22	b	610	CLA	C4A-NA-C1A	6.26	109.52	106.71
22	c	512	CLA	C4A-NA-C1A	6.21	109.50	106.71
22	B	614	CLA	C4A-NA-C1A	6.18	109.48	106.71
22	b	615	CLA	C4A-NA-C1A	6.15	109.47	106.71
22	a	406	CLA	C4A-NA-C1A	6.10	109.45	106.71
22	A	406	CLA	C4A-NA-C1A	6.08	109.44	106.71
22	B	607	CLA	C4A-NA-C1A	6.04	109.42	106.71
22	b	608	CLA	C4A-NA-C1A	6.04	109.42	106.71
22	C	512	CLA	C4A-NA-C1A	6.02	109.41	106.71
22	c	510	CLA	C4A-NA-C1A	5.99	109.40	106.71
22	C	510	CLA	C4A-NA-C1A	5.96	109.38	106.71
22	C	501	CLA	C4A-NA-C1A	5.83	109.33	106.71
22	c	501	CLA	C4A-NA-C1A	5.83	109.33	106.71
22	a	404	CLA	C4A-NA-C1A	5.82	109.32	106.71
22	A	404	CLA	C4A-NA-C1A	5.82	109.32	106.71
22	B	602	CLA	C4A-NA-C1A	5.74	109.29	106.71
22	C	513	CLA	C4A-NA-C1A	5.74	109.29	106.71
22	b	603	CLA	C4A-NA-C1A	5.74	109.29	106.71
22	c	513	CLA	C4A-NA-C1A	5.74	109.29	106.71
22	C	503	CLA	C4A-NA-C1A	5.73	109.28	106.71
22	c	503	CLA	C4A-NA-C1A	5.73	109.28	106.71
22	B	608	CLA	C4A-NA-C1A	5.70	109.27	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	609	CLA	C4A-NA-C1A	5.70	109.27	106.71
24	a	408	PL9	C7-C3-C4	5.65	121.47	116.88
24	A	408	PL9	C7-C3-C4	5.62	121.44	116.88
22	A	419	CLA	C4A-NA-C1A	5.59	109.22	106.71
22	a	419	CLA	C4A-NA-C1A	5.59	109.22	106.71
33	d	403	BCT	O2-C-O1	5.55	133.95	119.55
33	D	403	BCT	O2-C-O1	5.54	133.91	119.55
22	B	605	CLA	C4A-NA-C1A	5.25	109.06	106.71
22	b	606	CLA	C4A-NA-C1A	5.25	109.06	106.71
24	D	407	PL9	C7-C3-C4	5.04	120.97	116.88
24	d	407	PL9	C7-C3-C4	5.01	120.95	116.88
22	B	601	CLA	C4A-NA-C1A	4.76	108.85	106.71
22	b	602	CLA	C4A-NA-C1A	4.71	108.82	106.71
31	a	420	LHG	O4-P-O5	4.18	132.91	112.24
31	A	420	LHG	O4-P-O5	4.18	132.88	112.24
31	l	101	LHG	O4-P-O5	4.14	132.70	112.24
22	B	603	CLA	C4A-NA-C1A	4.13	108.56	106.71
22	b	604	CLA	C4A-NA-C1A	4.13	108.56	106.71
31	L	101	LHG	O4-P-O5	4.12	132.61	112.24
31	d	410	LHG	O4-P-O5	4.12	132.60	112.24
27	B	620	SQD	O7-S-C6	4.12	111.83	106.94
31	D	410	LHG	O4-P-O5	4.11	132.56	112.24
28	a	413	DGD	O3G-C3G-C2G	-4.10	101.01	110.90
28	A	413	DGD	O3G-C3G-C2G	-4.09	101.02	110.90
31	D	411	LHG	O4-P-O5	4.06	132.30	112.24
31	d	411	LHG	O4-P-O5	4.05	132.28	112.24
31	d	409	LHG	O4-P-O5	4.00	132.00	112.24
31	D	409	LHG	O4-P-O5	3.99	131.98	112.24
27	b	621	SQD	O7-S-C6	3.98	111.67	106.94
27	B	620	SQD	O47-C7-C8	3.95	120.00	111.50
28	C	518	DGD	O3G-C3G-C2G	-3.92	101.43	110.90
28	c	518	DGD	O3G-C3G-C2G	-3.91	101.46	110.90
27	b	621	SQD	O9-S-O7	-3.87	100.54	113.95
22	B	603	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
22	b	604	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
27	B	620	SQD	O9-S-O7	-3.84	100.67	113.95
22	C	505	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
22	c	505	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
28	C	517	DGD	O3G-C3G-C2G	-3.82	101.69	110.90
27	A	411	SQD	O9-S-O7	-3.81	100.75	113.95
27	a	411	SQD	O9-S-O7	-3.80	100.78	113.95
27	a	412	SQD	O47-C7-C8	3.80	119.68	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	517	DGD	O3G-C3G-C2G	-3.79	101.74	110.90
27	A	412	SQD	O47-C7-C8	3.78	119.64	111.50
27	b	621	SQD	O47-C7-C8	3.77	119.62	111.50
32	c	523	LMT	C1'-O5'-C5'	-3.74	106.34	113.69
27	x	101	SQD	O9-S-O7	-3.72	101.07	113.95
22	D	405	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
22	d	405	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
27	X	101	SQD	O9-S-O7	-3.71	101.10	113.95
27	A	411	SQD	O9-S-C6	3.71	111.35	106.94
27	a	411	SQD	O9-S-C6	3.68	111.32	106.94
27	A	412	SQD	O9-S-O7	-3.66	101.30	113.95
27	A	412	SQD	O7-S-C6	3.65	111.27	106.94
27	a	412	SQD	O9-S-O7	-3.64	101.34	113.95
32	C	523	LMT	C1'-O5'-C5'	-3.63	106.55	113.69
24	A	408	PL9	C7-C3-C2	-3.61	118.56	123.30
24	a	408	PL9	C7-C3-C2	-3.61	118.56	123.30
27	b	621	SQD	O9-S-C6	3.60	111.22	106.94
27	a	412	SQD	O7-S-C6	3.58	111.20	106.94
22	C	504	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	c	504	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	B	607	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
22	b	608	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
27	a	412	SQD	O9-S-C6	3.56	111.17	106.94
22	B	601	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
27	A	411	SQD	O47-C7-C8	3.54	119.13	111.50
27	a	411	SQD	O47-C7-C8	3.54	119.12	111.50
22	b	602	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
22	a	405	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
27	x	101	SQD	O7-S-C6	3.53	111.13	106.94
27	A	412	SQD	O9-S-C6	3.52	111.13	106.94
22	B	609	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
22	B	611	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
22	b	612	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
22	c	512	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
22	a	419	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
22	B	610	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
22	b	611	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
22	c	513	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
22	A	419	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
22	C	513	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
27	X	101	SQD	O9-S-C6	3.49	111.09	106.94
27	X	101	SQD	O7-S-C6	3.49	111.08	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	610	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
22	a	406	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
27	x	101	SQD	O9-S-C6	3.47	111.07	106.94
22	B	606	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	b	607	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	A	406	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
27	X	101	SQD	C3-C4-C5	3.47	116.42	110.24
22	C	507	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
22	c	507	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
22	C	512	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
27	x	101	SQD	C3-C4-C5	3.44	116.38	110.24
22	B	602	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
22	b	603	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
28	H	103	DGD	O3G-C3G-C2G	-3.42	102.65	110.90
28	h	103	DGD	O3G-C3G-C2G	-3.41	102.66	110.90
34	E	105	HEM	CBA-CAA-C2A	-3.41	106.80	112.62
22	A	405	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
34	e	105	HEM	CBA-CAA-C2A	-3.39	106.83	112.62
24	D	407	PL9	C7-C3-C2	-3.39	118.84	123.30
28	C	519	DGD	O3G-C3G-C2G	-3.38	102.73	110.90
28	c	519	DGD	O3G-C3G-C2G	-3.38	102.75	110.90
24	d	407	PL9	C7-C3-C2	-3.37	118.86	123.30
22	B	608	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
22	b	609	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
27	a	411	SQD	O7-S-C6	3.37	110.94	106.94
22	b	617	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
27	A	411	SQD	O7-S-C6	3.36	110.93	106.94
22	D	404	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
22	C	511	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
22	c	511	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	d	404	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	C	506	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
22	c	506	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
22	b	616	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
22	B	616	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	B	615	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	B	604	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
22	C	503	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
22	c	503	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
22	C	510	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
22	c	510	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
22	b	605	CLA	CMB-C2B-C1B	-3.30	123.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	612	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
22	b	613	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
22	c	512	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
22	C	508	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
22	c	508	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
27	A	411	SQD	O6-C1-C2	3.26	113.39	108.30
27	a	411	SQD	C1-O5-C5	-3.25	107.30	113.69
22	C	512	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
27	a	411	SQD	O6-C1-C2	3.24	113.37	108.30
27	A	411	SQD	C1-O5-C5	-3.24	107.33	113.69
28	c	518	DGD	O6D-C1D-O3G	-3.24	102.31	109.97
28	C	518	DGD	O6D-C1D-O3G	-3.23	102.32	109.97
22	B	602	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
22	b	603	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	B	603	CLA	CMB-C2B-C3B	3.19	130.65	124.68
22	b	604	CLA	CMB-C2B-C3B	3.19	130.65	124.68
22	C	501	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
22	c	501	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
22	A	419	CLA	CHB-C4A-NA	3.17	128.90	124.51
22	a	419	CLA	CHB-C4A-NA	3.17	128.90	124.51
22	c	502	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
22	B	614	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
22	c	504	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
22	B	615	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
22	b	616	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
22	b	615	CLA	CMB-C2B-C1B	-3.15	123.63	128.46
22	D	405	CLA	CMB-C2B-C3B	3.14	130.56	124.68
22	d	405	CLA	CMB-C2B-C3B	3.14	130.56	124.68
22	C	502	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
22	C	504	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
28	c	519	DGD	O6D-C1D-O3G	-3.12	102.58	109.97
32	e	104	LMT	C3'-C4'-C5'	-3.12	104.68	110.24
22	b	612	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
28	C	519	DGD	O6D-C1D-O3G	-3.12	102.60	109.97
22	B	611	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
22	B	613	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
32	E	104	LMT	C3'-C4'-C5'	-3.10	104.71	110.24
27	B	620	SQD	O9-S-C6	3.09	110.62	106.94
22	b	614	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
22	c	501	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
22	C	505	CLA	CMB-C2B-C3B	3.07	130.43	124.68
22	c	505	CLA	CMB-C2B-C3B	3.07	130.43	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	509	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
22	c	509	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
22	C	501	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
22	A	404	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
33	d	403	BCT	O3-C-O1	-3.04	111.65	119.55
33	D	403	BCT	O3-C-O1	-3.04	111.66	119.55
22	c	512	CLA	CHB-C4A-NA	3.04	128.71	124.51
22	d	404	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
22	D	404	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
22	C	507	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
22	c	507	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
27	b	621	SQD	O8-S-C6	3.03	110.57	105.74
22	a	404	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
32	J	102	LMT	C3'-C4'-C5'	-3.02	104.84	110.24
22	C	512	CLA	CHB-C4A-NA	3.02	128.68	124.51
32	j	102	LMT	C3'-C4'-C5'	-3.01	104.86	110.24
30	d	401	PHO	O1D-CGD-CBD	3.01	129.75	124.74
22	C	509	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
27	X	101	SQD	O8-S-C6	3.00	110.52	105.74
22	a	419	CLA	CMB-C2B-C3B	3.00	130.29	124.68
22	B	601	CLA	CMB-C2B-C3B	3.00	130.29	124.68
22	b	602	CLA	CMB-C2B-C3B	3.00	130.29	124.68
22	c	509	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
22	C	508	CLA	CHB-C4A-NA	2.99	128.65	124.51
22	A	419	CLA	CMB-C2B-C3B	2.99	130.27	124.68
22	B	614	CLA	CHB-C4A-NA	2.99	128.64	124.51
22	b	615	CLA	CHB-C4A-NA	2.98	128.64	124.51
22	B	605	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
27	x	101	SQD	O8-S-C6	2.98	110.48	105.74
22	C	504	CLA	CMB-C2B-C3B	2.97	130.24	124.68
22	c	504	CLA	CMB-C2B-C3B	2.97	130.24	124.68
30	d	401	PHO	CMB-C2B-C3B	2.97	130.23	124.68
22	b	606	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
22	B	610	CLA	CHB-C4A-NA	2.97	128.62	124.51
22	b	611	CLA	CHB-C4A-NA	2.97	128.62	124.51
22	c	508	CLA	CHB-C4A-NA	2.96	128.61	124.51
22	B	603	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
30	D	401	PHO	O1D-CGD-CBD	2.96	129.66	124.74
22	C	508	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
22	c	508	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
22	B	609	CLA	CMB-C2B-C3B	2.95	130.21	124.68
27	a	411	SQD	O8-S-C6	2.95	110.44	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	D	401	PHO	CMB-C2B-C3B	2.95	130.19	124.68
27	A	411	SQD	O8-S-C6	2.94	110.43	105.74
22	C	507	CLA	CHB-C4A-NA	2.94	128.58	124.51
22	c	507	CLA	CHB-C4A-NA	2.94	128.58	124.51
22	a	405	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	A	405	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	b	604	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
30	a	418	PHO	CMB-C2B-C3B	2.93	130.16	124.68
22	b	617	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
22	A	419	CLA	CHD-C1D-ND	-2.92	121.77	124.45
22	b	610	CLA	CMB-C2B-C3B	2.92	130.14	124.68
22	b	617	CLA	CMB-C2B-C3B	2.91	130.13	124.68
22	B	616	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
30	A	418	PHO	CMB-C2B-C3B	2.91	130.12	124.68
22	a	419	CLA	CHD-C1D-ND	-2.90	121.79	124.45
22	B	612	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	b	608	CLA	CMB-C2B-C3B	2.90	130.10	124.68
22	a	405	CLA	O2D-CGD-CBD	2.89	116.41	111.27
22	B	616	CLA	CMB-C2B-C3B	2.89	130.09	124.68
22	c	512	CLA	CMB-C2B-C3B	2.89	130.09	124.68
35	v	201	HEC	CBD-CAD-C3D	-2.89	107.69	112.62
22	B	607	CLA	CMB-C2B-C3B	2.89	130.08	124.68
24	a	408	PL9	C40-C39-C41	2.89	120.13	115.27
34	e	105	HEM	C4B-CHC-C1C	2.88	126.36	122.56
22	A	406	CLA	CMB-C2B-C3B	2.88	130.07	124.68
22	A	405	CLA	O2D-CGD-CBD	2.88	116.39	111.27
22	a	406	CLA	CMB-C2B-C3B	2.88	130.07	124.68
34	E	105	HEM	C1B-NB-C4B	2.88	108.05	105.07
22	C	513	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
34	e	105	HEM	C1B-NB-C4B	2.88	108.05	105.07
22	B	605	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	B	608	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	b	618	BCR	C33-C5-C6	-2.88	121.30	124.53
22	c	513	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
22	b	613	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	x	101	SQD	O5-C5-C4	2.87	114.91	109.69
24	A	408	PL9	C40-C39-C41	2.86	120.09	115.27
22	a	405	CLA	CMB-C2B-C3B	2.86	130.04	124.68
22	B	602	CLA	CMB-C2B-C3B	2.86	130.03	124.68
22	b	603	CLA	CMB-C2B-C3B	2.86	130.03	124.68
22	a	404	CLA	CHB-C4A-NA	2.86	128.47	124.51
22	C	513	CLA	CMB-C2B-C3B	2.86	130.03	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	513	CLA	CMB-C2B-C3B	2.86	130.03	124.68
34	E	105	HEM	C4B-CHC-C1C	2.86	126.33	122.56
31	A	420	LHG	O8-C23-C24	2.85	120.86	111.91
22	b	609	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	A	404	CLA	CHB-C4A-NA	2.85	128.45	124.51
22	C	512	CLA	CMB-C2B-C3B	2.85	130.00	124.68
22	b	614	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	B	613	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	B	604	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	b	605	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
31	a	420	LHG	O8-C23-C24	2.82	120.77	111.91
22	b	606	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	B	611	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	b	612	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	C	510	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	c	510	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	C	501	CLA	CHD-C1D-ND	-2.82	121.86	124.45
22	c	501	CLA	CHD-C1D-ND	-2.82	121.86	124.45
27	X	101	SQD	O5-C5-C4	2.82	114.82	109.69
22	b	613	CLA	CHB-C4A-NA	2.81	128.40	124.51
24	A	408	PL9	C27-C28-C29	-2.80	120.91	127.66
22	B	612	CLA	CHB-C4A-NA	2.80	128.39	124.51
35	V	201	HEC	CBD-CAD-C3D	-2.80	107.84	112.62
22	B	610	CLA	CMB-C2B-C3B	2.80	129.92	124.68
22	b	611	CLA	CMB-C2B-C3B	2.80	129.92	124.68
32	b	624	LMT	C1'-O5'-C5'	-2.80	108.20	113.69
32	Z	101	LMT	C1'-O5'-C5'	-2.79	108.21	113.69
24	a	408	PL9	C27-C28-C29	-2.79	120.94	127.66
23	B	619	BCR	C2-C1-C6	2.79	114.78	110.48
22	B	605	CLA	C4-C3-C5	2.79	119.96	115.27
23	b	620	BCR	C2-C1-C6	2.79	114.77	110.48
32	B	623	LMT	C1'-O5'-C5'	-2.78	108.23	113.69
23	B	617	BCR	C33-C5-C6	-2.78	121.41	124.53
22	B	606	CLA	CMB-C2B-C3B	2.78	129.88	124.68
22	b	607	CLA	CMB-C2B-C3B	2.78	129.88	124.68
22	B	607	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
22	b	606	CLA	C4-C3-C5	2.78	119.94	115.27
22	A	405	CLA	C9-C8-C10	2.78	121.34	111.29
32	z	101	LMT	C1'-O5'-C5'	-2.77	108.25	113.69
28	a	413	DGD	O6D-C1D-O3G	-2.77	103.42	109.97
22	C	506	CLA	CMB-C2B-C3B	2.77	129.85	124.68
22	c	506	CLA	CMB-C2B-C3B	2.77	129.85	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	608	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	B	608	CLA	CMB-C2B-C3B	2.76	129.85	124.68
22	b	609	CLA	CMB-C2B-C3B	2.76	129.85	124.68
22	C	507	CLA	CMB-C2B-C3B	2.76	129.83	124.68
22	c	507	CLA	CMB-C2B-C3B	2.76	129.83	124.68
22	C	513	CLA	CHB-C4A-NA	2.76	128.32	124.51
22	c	513	CLA	CHB-C4A-NA	2.76	128.32	124.51
23	K	101	BCR	C27-C26-C25	2.75	126.73	122.73
23	k	101	BCR	C27-C26-C25	2.75	126.73	122.73
22	C	511	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	c	511	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
26	c	520	LMG	O6-C1-O1	-2.75	103.46	109.97
32	c	523	LMT	C4'-C3'-C2'	2.75	115.62	110.82
28	A	413	DGD	O6D-C1D-O3G	-2.75	103.46	109.97
26	C	520	LMG	O6-C1-O1	-2.74	103.48	109.97
22	b	612	CLA	CHD-C1D-ND	-2.74	121.94	124.45
28	a	413	DGD	C3G-C2G-C1G	-2.73	105.33	111.79
32	c	525	LMT	C3'-C4'-C5'	-2.73	104.67	110.93
26	c	524	LMG	C1-O6-C5	-2.73	108.34	113.69
27	B	620	SQD	O48-C23-C24	2.72	120.45	111.91
34	E	105	HEM	C4D-ND-C1D	2.72	107.88	105.07
22	B	606	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	b	607	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	A	405	CLA	CMB-C2B-C3B	2.72	129.76	124.68
23	T	101	BCR	C33-C5-C6	-2.71	121.48	124.53
22	d	405	CLA	CHB-C4A-NA	2.71	128.26	124.51
22	C	503	CLA	CMB-C2B-C3B	2.71	129.75	124.68
22	c	503	CLA	CMB-C2B-C3B	2.71	129.75	124.68
27	B	620	SQD	O8-S-C6	2.71	110.05	105.74
23	t	102	BCR	C7-C8-C9	-2.70	122.15	126.23
32	C	525	LMT	C3'-C4'-C5'	-2.70	104.73	110.93
22	D	405	CLA	CHD-C1D-ND	-2.70	121.97	124.45
23	T	101	BCR	C7-C8-C9	-2.70	122.16	126.23
28	h	103	DGD	CDB-CCB-CBB	-2.70	100.72	114.42
23	t	102	BCR	C33-C5-C6	-2.70	121.50	124.53
28	H	103	DGD	CDB-CCB-CBB	-2.70	100.74	114.42
22	b	607	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
22	D	405	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	C	524	LMG	C1-O6-C5	-2.68	108.42	113.69
22	B	611	CLA	CHD-C1D-ND	-2.68	121.99	124.45
22	B	610	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
22	b	611	CLA	O2D-CGD-O1D	-2.68	118.59	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	h	102	BCR	C24-C23-C22	-2.68	122.18	126.23
22	B	614	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
34	e	105	HEM	C4D-ND-C1D	2.68	107.84	105.07
22	c	510	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
28	c	517	DGD	O6D-C1D-O3G	-2.68	103.64	109.97
23	H	102	BCR	C24-C23-C22	-2.67	122.19	126.23
22	C	510	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
22	a	405	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	d	405	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
22	B	612	CLA	CMB-C2B-C3B	2.67	129.68	124.68
22	b	613	CLA	CMB-C2B-C3B	2.67	129.68	124.68
32	m	101	LMT	C3'-C4'-C5'	-2.67	104.80	110.93
28	C	517	DGD	O6D-C1D-O3G	-2.67	103.65	109.97
32	M	102	LMT	C3'-C4'-C5'	-2.67	104.81	110.93
22	B	606	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
28	C	517	DGD	CDB-CCB-CBB	-2.67	100.89	114.42
22	C	508	CLA	CMB-C2B-C3B	2.66	129.66	124.68
22	c	508	CLA	CMB-C2B-C3B	2.66	129.66	124.68
22	d	405	CLA	CHD-C1D-ND	-2.66	122.01	124.45
28	c	517	DGD	CDB-CCB-CBB	-2.66	100.94	114.42
22	C	501	CLA	CMB-C2B-C3B	2.65	129.64	124.68
22	c	501	CLA	CMB-C2B-C3B	2.65	129.64	124.68
22	D	405	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
22	A	405	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	b	615	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
22	b	602	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
24	A	408	PL9	C22-C23-C24	-2.65	121.29	127.66
22	C	505	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	c	505	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
22	B	601	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
22	A	404	CLA	CMB-C2B-C3B	2.64	129.61	124.68
23	C	514	BCR	C33-C5-C6	-2.63	121.58	124.53
28	A	413	DGD	C3G-C2G-C1G	-2.63	105.57	111.79
22	b	602	CLA	CHB-C4A-NA	2.63	128.14	124.51
23	c	514	BCR	C33-C5-C6	-2.62	121.58	124.53
23	k	103	BCR	C33-C5-C6	-2.62	121.59	124.53
22	B	601	CLA	CHB-C4A-NA	2.62	128.13	124.51
23	b	619	BCR	C27-C26-C25	2.61	126.53	122.73
22	c	510	CLA	CHB-C4A-NA	2.61	128.13	124.51
30	d	401	PHO	O2D-CGD-O1D	-2.61	118.73	123.84
22	C	510	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	D	408	LMG	O6-C1-O1	-2.61	103.79	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	406	BCR	C27-C26-C25	2.61	126.52	122.73
22	c	502	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
22	b	603	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
24	a	408	PL9	C7-C8-C9	-2.60	122.46	126.79
22	B	607	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	b	608	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	K	103	BCR	C33-C5-C6	-2.60	121.61	124.53
22	C	502	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
26	d	408	LMG	O6-C1-O1	-2.60	103.83	109.97
22	B	607	CLA	CHD-C1D-ND	-2.60	122.07	124.45
22	b	608	CLA	CHD-C1D-ND	-2.60	122.07	124.45
22	C	506	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	c	506	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	B	602	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
22	b	602	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
31	a	420	LHG	C11-C10-C9	-2.59	101.29	114.42
22	B	605	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
22	b	606	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
22	c	511	CLA	CMB-C2B-C3B	2.59	129.52	124.68
22	B	614	CLA	CMB-C2B-C3B	2.58	129.51	124.68
22	B	601	CLA	O2A-CGA-O1A	-2.58	117.07	123.59
22	D	404	CLA	CMB-C2B-C3B	2.58	129.51	124.68
22	a	404	CLA	CMB-C2B-C3B	2.58	129.51	124.68
22	C	511	CLA	CMB-C2B-C3B	2.58	129.51	124.68
23	A	407	BCR	C27-C26-C25	2.58	126.48	122.73
23	a	407	BCR	C27-C26-C25	2.58	126.48	122.73
31	A	420	LHG	C11-C10-C9	-2.58	101.33	114.42
22	B	615	CLA	CMB-C2B-C3B	2.58	129.50	124.68
28	H	103	DGD	O6D-C1D-O3G	-2.58	103.87	109.97
28	h	103	DGD	O6D-C1D-O3G	-2.58	103.87	109.97
24	a	408	PL9	C22-C23-C24	-2.58	121.45	127.66
22	B	604	CLA	CMB-C2B-C3B	2.58	129.50	124.68
23	d	406	BCR	C27-C26-C25	2.58	126.47	122.73
22	b	615	CLA	CMB-C2B-C3B	2.58	129.50	124.68
31	d	409	LHG	O8-C23-C24	2.57	119.99	111.91
22	b	616	CLA	CMB-C2B-C3B	2.57	129.49	124.68
30	D	401	PHO	O2D-CGD-O1D	-2.57	118.82	123.84
22	A	419	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
22	a	419	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
31	D	409	LHG	O8-C23-C24	2.57	119.96	111.91
22	b	605	CLA	CMB-C2B-C3B	2.57	129.48	124.68
35	v	201	HEC	C1D-C2D-C3D	-2.56	105.21	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	618	BCR	C27-C26-C25	2.56	126.44	122.73
28	c	517	DGD	O5D-C6D-C5D	-2.56	104.31	109.05
24	d	407	PL9	C20-C19-C21	2.56	119.57	115.27
22	d	404	CLA	CMB-C2B-C3B	2.56	129.46	124.68
24	A	408	PL9	C7-C8-C9	-2.56	122.54	126.79
23	b	620	BCR	C27-C26-C25	2.55	126.44	122.73
23	B	619	BCR	C27-C26-C25	2.54	126.42	122.73
27	A	412	SQD	O8-S-C6	2.54	109.79	105.74
27	a	412	SQD	O8-S-C6	2.54	109.79	105.74
28	C	517	DGD	O5D-C6D-C5D	-2.53	104.36	109.05
35	V	201	HEC	C1D-C2D-C3D	-2.53	105.23	107.00
22	C	504	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	c	504	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	a	406	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
22	C	501	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	c	501	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	b	618	BCR	C2-C1-C6	2.53	114.38	110.48
22	B	615	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	c	513	CLA	CHD-C1D-ND	-2.53	122.13	124.45
22	d	405	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
22	C	506	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	c	506	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	B	603	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	b	604	CLA	CHB-C4A-NA	2.52	127.99	124.51
32	B	623	LMT	C3'-C4'-C5'	-2.51	105.17	110.93
32	b	624	LMT	C3'-C4'-C5'	-2.51	105.17	110.93
24	D	407	PL9	C20-C19-C21	2.51	119.49	115.27
32	M	102	LMT	C1'-O5'-C5'	-2.51	108.76	113.69
32	m	101	LMT	C1'-O5'-C5'	-2.51	108.76	113.69
23	B	617	BCR	C2-C1-C6	2.51	114.34	110.48
22	C	503	CLA	CHD-C1D-ND	-2.51	122.15	124.45
22	c	503	CLA	CHD-C1D-ND	-2.51	122.15	124.45
22	D	405	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
27	b	621	SQD	O48-C23-C24	2.50	119.77	111.91
26	D	402	LMG	O1-C7-C8	-2.50	105.15	111.78
22	C	510	CLA	CHD-C1D-ND	-2.50	122.16	124.45
22	c	510	CLA	CHD-C1D-ND	-2.50	122.16	124.45
22	b	616	CLA	CHB-C4A-NA	2.50	127.97	124.51
31	d	411	LHG	O8-C23-C24	2.50	119.75	111.91
22	C	513	CLA	CHD-C1D-ND	-2.50	122.16	124.45
22	a	406	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
31	L	101	LHG	O8-C23-C24	2.50	119.74	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	602	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
23	C	515	BCR	C15-C16-C17	-2.50	118.36	123.47
22	A	406	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
31	D	411	LHG	O8-C23-C24	2.49	119.73	111.91
23	c	514	BCR	C15-C16-C17	-2.49	118.37	123.47
26	d	402	LMG	O1-C7-C8	-2.49	105.18	111.78
23	c	515	BCR	C15-C16-C17	-2.49	118.38	123.47
22	B	613	CLA	CMB-C2B-C3B	2.49	129.33	124.68
22	c	502	CLA	CMB-C2B-C3B	2.49	129.33	124.68
31	l	101	LHG	O8-C23-C24	2.49	119.71	111.91
28	c	518	DGD	C1D-C2D-C3D	-2.48	104.83	110.00
22	C	509	CLA	CHB-C4A-NA	2.48	127.94	124.51
27	X	101	SQD	O48-C23-C24	2.47	119.67	111.91
22	a	406	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	c	508	CLA	O2D-CGD-CBD	2.47	115.66	111.27
22	b	617	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
22	b	614	CLA	CMB-C2B-C3B	2.47	129.30	124.68
24	d	407	PL9	C22-C23-C24	-2.47	121.72	127.66
28	C	518	DGD	C1D-C2D-C3D	-2.47	104.86	110.00
23	H	102	BCR	C15-C16-C17	-2.47	118.42	123.47
24	D	407	PL9	C22-C23-C24	-2.47	121.72	127.66
22	c	509	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	C	506	CLA	CHD-C1D-ND	-2.46	122.19	124.45
22	c	506	CLA	CHD-C1D-ND	-2.46	122.19	124.45
22	B	602	CLA	O2D-CGD-CBD	2.46	115.65	111.27
22	B	608	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	b	609	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	C	502	CLA	CMB-C2B-C3B	2.46	129.29	124.68
23	C	514	BCR	C15-C16-C17	-2.46	118.43	123.47
23	k	101	BCR	C33-C5-C6	-2.46	121.76	124.53
22	B	601	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
26	D	408	LMG	C40-C39-C38	-2.46	101.92	114.42
23	K	101	BCR	C33-C5-C6	-2.46	121.76	124.53
22	A	406	CLA	CHB-C4A-NA	2.46	127.91	124.51
26	d	408	LMG	C40-C39-C38	-2.46	101.94	114.42
22	B	616	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
22	A	406	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
27	x	101	SQD	O48-C23-C24	2.46	119.61	111.91
22	C	508	CLA	O2D-CGD-CBD	2.45	115.63	111.27
23	h	102	BCR	C15-C16-C17	-2.45	118.45	123.47
26	H	101	LMG	O1-C7-C8	-2.45	105.28	111.78
26	h	101	LMG	O1-C7-C8	-2.45	105.29	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D	411	LHG	C11-C10-C9	-2.45	102.00	114.42
31	d	411	LHG	C11-C10-C9	-2.45	102.00	114.42
22	B	608	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
22	b	609	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
22	B	609	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
23	a	407	BCR	C33-C5-C6	-2.44	121.79	124.53
23	H	102	BCR	C33-C5-C6	-2.44	121.79	124.53
22	B	604	CLA	C1-C2-C3	-2.43	121.83	126.04
22	b	605	CLA	C1-C2-C3	-2.43	121.83	126.04
23	B	618	BCR	C33-C5-C6	-2.43	121.80	124.53
27	A	411	SQD	O48-C23-C24	2.43	119.54	111.91
22	B	605	CLA	CMB-C2B-C3B	2.43	129.23	124.68
22	b	606	CLA	CMB-C2B-C3B	2.43	129.23	124.68
22	b	603	CLA	O2D-CGD-CBD	2.43	115.59	111.27
22	b	610	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
23	K	103	BCR	C27-C26-C25	2.43	126.26	122.73
27	a	411	SQD	O48-C23-C24	2.43	119.53	111.91
22	C	512	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	h	102	BCR	C33-C5-C6	-2.42	121.81	124.53
32	C	523	LMT	C4'-C3'-C2'	2.42	115.06	110.82
23	C	515	BCR	C33-C5-C6	-2.42	121.81	124.53
23	c	515	BCR	C33-C5-C6	-2.42	121.81	124.53
22	B	611	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	b	612	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	B	603	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	b	604	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	b	618	BCR	C29-C30-C25	2.42	114.20	110.48
22	C	503	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	C	502	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
27	a	412	SQD	O48-C23-C24	2.42	119.49	111.91
22	B	601	CLA	CHD-C1D-ND	-2.42	122.23	124.45
28	C	519	DGD	CDB-CCB-CBB	-2.42	102.16	114.42
22	c	503	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
28	c	519	DGD	CDB-CCB-CBB	-2.41	102.17	114.42
26	C	524	LMG	O2-C2-C1	-2.41	104.19	110.05
27	A	412	SQD	O48-C23-C24	2.41	119.47	111.91
23	B	617	BCR	C29-C30-C25	2.41	114.19	110.48
26	c	524	LMG	O2-C2-C1	-2.40	104.20	110.05
22	c	502	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	C	509	CLA	CMB-C2B-C3B	2.40	129.17	124.68
22	c	509	CLA	CMB-C2B-C3B	2.40	129.17	124.68
22	b	617	CLA	CHB-C4A-NA	2.40	127.83	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	k	103	BCR	C27-C26-C25	2.40	126.22	122.73
31	D	410	LHG	C11-C10-C9	-2.40	102.26	114.42
28	H	103	DGD	C3D-C4D-C5D	-2.40	105.97	110.24
28	h	103	DGD	C3D-C4D-C5D	-2.40	105.97	110.24
23	A	407	BCR	C33-C5-C6	-2.39	121.84	124.53
23	T	101	BCR	C27-C26-C25	2.39	126.20	122.73
22	c	512	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	b	619	BCR	C33-C5-C6	-2.39	121.84	124.53
22	B	616	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	b	625	LMG	O6-C1-O1	-2.39	104.32	109.97
23	D	406	BCR	C33-C5-C6	-2.39	121.85	124.53
22	c	508	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
26	c	524	LMG	C38-C37-C36	-2.39	102.32	114.42
26	A	410	LMG	O6-C1-O1	-2.38	104.33	109.97
22	B	614	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
23	t	102	BCR	C27-C26-C25	2.38	126.19	122.73
26	C	524	LMG	C38-C37-C36	-2.38	102.33	114.42
22	B	609	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
22	b	610	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
31	d	411	LHG	C20-C19-C18	-2.37	102.37	114.42
22	b	610	CLA	O1D-CGD-CBD	2.37	129.34	124.48
22	b	615	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
31	D	411	LHG	C20-C19-C18	-2.37	102.40	114.42
26	a	410	LMG	O6-C1-O1	-2.37	104.37	109.97
22	B	607	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
22	b	608	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
22	b	612	CLA	O2D-CGD-CBD	2.36	115.47	111.27
26	B	624	LMG	O6-C1-O1	-2.36	104.38	109.97
23	c	514	BCR	C27-C26-C25	2.36	126.16	122.73
22	C	501	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
22	c	501	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
31	D	410	LHG	O8-C23-C24	2.36	119.31	111.91
26	b	625	LMG	C38-C37-C36	-2.36	102.46	114.42
22	D	404	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
22	d	404	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
22	B	609	CLA	O1D-CGD-CBD	2.36	129.30	124.48
25	B	622	STE	C3-C2-C1	-2.35	108.54	114.47
22	b	602	CLA	C1-C2-C3	-2.35	121.97	126.04
22	B	611	CLA	O2D-CGD-CBD	2.35	115.45	111.27
22	C	508	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
23	a	407	BCR	C2-C1-C6	2.35	114.10	110.48
25	b	623	STE	C3-C2-C1	-2.35	108.55	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	413	DGD	CDB-CCB-CBB	-2.35	102.50	114.42
31	d	410	LHG	O8-C23-C24	2.35	119.27	111.91
26	B	624	LMG	C38-C37-C36	-2.35	102.51	114.42
22	b	612	CLA	C1-C2-C3	-2.35	121.99	126.04
23	A	407	BCR	C2-C1-C6	2.35	114.09	110.48
26	h	101	LMG	C40-C39-C38	-2.34	102.53	114.42
23	d	406	BCR	C33-C5-C6	-2.34	121.90	124.53
22	b	602	CLA	CHD-C1D-ND	-2.34	122.31	124.45
23	c	514	BCR	C2-C1-C6	2.34	114.08	110.48
26	B	624	LMG	C40-C39-C38	-2.34	102.56	114.42
23	C	514	BCR	C27-C26-C25	2.34	126.12	122.73
26	H	101	LMG	C40-C39-C38	-2.34	102.57	114.42
23	C	514	BCR	C2-C1-C6	2.33	114.08	110.48
22	B	601	CLA	C1-C2-C3	-2.33	122.01	126.04
26	c	520	LMG	O1-C7-C8	-2.33	105.27	110.90
26	b	625	LMG	C40-C39-C38	-2.33	102.59	114.42
26	C	520	LMG	O1-C7-C8	-2.32	105.29	110.90
31	d	410	LHG	C11-C10-C9	-2.32	102.63	114.42
28	a	413	DGD	CDB-CCB-CBB	-2.32	102.66	114.42
22	C	511	CLA	CHD-C1D-ND	-2.32	122.32	124.45
22	c	511	CLA	CHD-C1D-ND	-2.32	122.33	124.45
35	v	201	HEC	CMC-C2C-C1C	-2.31	124.91	128.46
30	d	401	PHO	CMC-C2C-C3C	2.31	129.30	124.94
22	A	406	CLA	O2D-CGD-CBD	2.31	115.37	111.27
28	C	518	DGD	CDB-CCB-CBB	-2.30	102.73	114.42
28	c	518	DGD	CDB-CCB-CBB	-2.30	102.73	114.42
22	B	611	CLA	C1-C2-C3	-2.30	122.06	126.04
22	B	609	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	a	406	CLA	O2D-CGD-CBD	2.30	115.36	111.27
22	b	614	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
22	B	605	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	b	606	CLA	CHD-C1D-ND	-2.30	122.34	124.45
30	D	401	PHO	CMC-C2C-C3C	2.30	129.27	124.94
22	C	503	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
31	D	411	LHG	C18-C17-C16	-2.30	102.77	114.42
31	d	411	LHG	C18-C17-C16	-2.30	102.77	114.42
30	a	418	PHO	O2D-CGD-O1D	-2.29	119.35	123.84
22	c	508	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
22	b	610	CLA	CHB-C4A-NA	2.29	127.68	124.51
35	V	201	HEC	CMC-C2C-C1C	-2.28	124.95	128.46
22	C	508	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
28	c	517	DGD	C3G-C2G-C1G	-2.28	106.39	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	515	BCR	C27-C26-C25	2.28	126.04	122.73
23	c	515	BCR	C27-C26-C25	2.28	126.04	122.73
32	J	102	LMT	C1'-O5'-C5'	-2.28	109.22	113.69
22	c	503	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
24	d	407	PL9	C27-C28-C29	-2.28	122.18	127.66
22	C	509	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
22	c	509	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
28	C	517	DGD	C3G-C2G-C1G	-2.27	106.41	111.79
32	j	102	LMT	C1'-O5'-C5'	-2.27	109.23	113.69
22	C	505	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
22	c	505	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
26	C	520	LMG	O3-C3-C2	-2.27	105.11	110.35
24	D	407	PL9	C27-C28-C29	-2.26	122.21	127.66
30	A	418	PHO	O2D-CGD-O1D	-2.26	119.41	123.84
22	B	604	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	b	605	CLA	CHB-C4A-NA	2.26	127.64	124.51
26	c	520	LMG	O3-C3-C2	-2.26	105.12	110.35
31	l	101	LHG	C11-C10-C9	-2.26	102.94	114.42
31	A	420	LHG	C20-C19-C18	-2.26	102.95	114.42
22	B	613	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
22	B	611	CLA	CHB-C4A-NA	2.26	127.63	124.51
22	b	612	CLA	CHB-C4A-NA	2.26	127.63	124.51
22	C	506	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
31	L	101	LHG	C11-C10-C9	-2.25	102.98	114.42
24	D	407	PL9	C7-C8-C9	-2.25	123.04	126.79
31	a	420	LHG	C20-C19-C18	-2.25	102.99	114.42
24	d	407	PL9	C7-C8-C9	-2.25	123.05	126.79
28	A	413	DGD	C1D-C2D-C3D	-2.24	105.33	110.00
22	C	511	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	c	506	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
22	A	419	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
32	e	104	LMT	C1'-O5'-C5'	-2.24	109.30	113.69
22	C	506	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
22	c	506	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
31	A	420	LHG	C18-C17-C16	-2.23	103.09	114.42
26	a	410	LMG	O3-C3-C2	-2.23	105.19	110.35
28	a	413	DGD	C1D-C2D-C3D	-2.23	105.35	110.00
22	C	504	CLA	CHD-C1D-ND	-2.23	122.41	124.45
22	c	504	CLA	CHD-C1D-ND	-2.23	122.41	124.45
31	a	420	LHG	C18-C17-C16	-2.23	103.12	114.42
34	e	105	HEM	CBD-CAD-C3D	-2.22	106.45	112.63
26	A	410	LMG	O3-C3-C2	-2.22	105.21	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	E	105	HEM	CBD-CAD-C3D	-2.22	106.45	112.63
22	d	404	CLA	CHD-C1D-ND	-2.22	122.41	124.45
24	a	408	PL9	C12-C13-C14	-2.22	122.31	127.66
23	K	101	BCR	C24-C23-C22	-2.22	122.88	126.23
23	k	101	BCR	C24-C23-C22	-2.22	122.88	126.23
32	E	104	LMT	C1'-O5'-C5'	-2.22	109.34	113.69
23	b	619	BCR	C38-C26-C25	-2.21	122.05	124.53
26	C	524	LMG	O6-C1-O1	-2.21	104.74	109.97
27	A	411	SQD	C3-C4-C5	2.21	114.18	110.24
28	c	517	DGD	C4E-C3E-C2E	-2.21	106.97	110.82
22	A	404	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
31	L	101	LHG	C20-C19-C18	-2.20	103.25	114.42
31	l	101	LHG	C20-C19-C18	-2.20	103.25	114.42
22	C	508	CLA	CHD-C1D-ND	-2.20	122.43	124.45
22	c	508	CLA	CHD-C1D-ND	-2.20	122.43	124.45
22	A	405	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
22	a	419	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
31	D	409	LHG	C20-C19-C18	-2.20	103.26	114.42
22	D	404	CLA	CHD-C1D-ND	-2.20	122.43	124.45
28	a	413	DGD	CBB-CAB-C9B	-2.19	103.28	114.42
22	a	405	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
26	b	625	LMG	O3-C3-C2	-2.19	105.28	110.35
22	a	404	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
26	c	524	LMG	O3-C3-C2	-2.19	105.28	110.35
31	d	409	LHG	C20-C19-C18	-2.19	103.30	114.42
22	A	405	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
26	C	524	LMG	O3-C3-C2	-2.19	105.29	110.35
22	B	608	CLA	C2D-C1D-ND	-2.19	108.49	110.10
22	b	609	CLA	C2D-C1D-ND	-2.19	108.49	110.10
28	A	413	DGD	O6E-C1E-O5D	-2.19	104.80	109.97
22	C	510	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
28	C	517	DGD	C4E-C3E-C2E	-2.18	107.01	110.82
22	C	509	CLA	C1-C2-C3	-2.18	122.27	126.04
22	c	509	CLA	C1-C2-C3	-2.18	122.27	126.04
23	B	619	BCR	C38-C26-C25	-2.18	122.08	124.53
27	a	411	SQD	C3-C4-C5	2.18	114.13	110.24
22	a	405	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
22	c	510	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
22	B	602	CLA	CHB-C4A-NA	2.18	127.52	124.51
22	B	612	CLA	C2D-C1D-ND	-2.17	108.50	110.10
22	b	613	CLA	C2D-C1D-ND	-2.17	108.50	110.10
26	B	624	LMG	O3-C3-C2	-2.17	105.33	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	413	DGD	O6E-C1E-O5D	-2.17	104.83	109.97
23	K	101	BCR	C2-C1-C6	2.17	113.82	110.48
22	b	603	CLA	CHB-C4A-NA	2.17	127.51	124.51
26	c	520	LMG	O2-C2-C1	-2.17	104.77	110.05
22	c	511	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	b	618	BCR	C7-C8-C9	-2.17	122.96	126.23
26	C	524	LMG	O7-C10-O9	-2.16	118.47	123.70
24	A	408	PL9	C12-C13-C14	-2.16	122.45	127.66
22	C	504	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
22	c	504	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
26	c	520	LMG	O1-C1-C2	-2.16	104.93	108.30
22	B	615	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
22	a	405	CLA	CHD-C1D-ND	-2.16	122.47	124.45
23	B	617	BCR	C7-C8-C9	-2.16	122.97	126.23
24	A	408	PL9	O2-C1-C2	-2.16	116.84	121.78
22	A	406	CLA	CHD-C1D-ND	-2.16	122.47	124.45
26	d	408	LMG	C38-C37-C36	-2.16	103.48	114.42
23	B	617	BCR	C28-C27-C26	-2.15	110.23	114.08
24	d	407	PL9	C12-C13-C14	-2.15	122.48	127.66
26	C	520	LMG	O2-C2-C1	-2.15	104.82	110.05
23	k	101	BCR	C2-C1-C6	2.15	113.79	110.48
22	A	419	CLA	O2D-CGD-CBD	2.15	115.08	111.27
28	A	413	DGD	CBB-CAB-C9B	-2.15	103.53	114.42
26	a	410	LMG	C40-C39-C38	-2.15	103.53	114.42
26	b	625	LMG	C1-C2-C3	-2.14	105.53	110.00
22	B	614	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
24	a	408	PL9	O2-C1-C2	-2.14	116.87	121.78
26	c	524	LMG	O6-C1-O1	-2.14	104.91	109.97
22	b	614	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
22	b	616	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
22	c	501	CLA	O2D-CGD-CBD	2.14	115.07	111.27
22	B	612	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
22	c	512	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
24	D	407	PL9	C12-C13-C14	-2.14	122.52	127.66
22	C	512	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
23	b	620	BCR	C3-C4-C5	-2.13	110.27	114.08
26	B	624	LMG	C1-C2-C3	-2.13	105.55	110.00
26	d	408	LMG	O1-C7-C8	-2.13	105.75	110.90
26	c	524	LMG	O7-C10-O9	-2.13	118.55	123.70
22	D	404	CLA	CHB-C4A-NA	2.13	127.46	124.51
22	d	404	CLA	CHB-C4A-NA	2.13	127.46	124.51
23	B	619	BCR	C33-C5-C6	-2.13	122.14	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	410	LMG	C40-C39-C38	-2.13	103.61	114.42
22	D	404	CLA	O2D-CGD-CBD	2.13	115.05	111.27
22	a	419	CLA	O2D-CGD-CBD	2.13	115.05	111.27
24	a	408	PL9	C37-C38-C39	-2.13	122.54	127.66
26	D	408	LMG	C38-C37-C36	-2.13	103.63	114.42
23	H	102	BCR	C7-C8-C9	-2.12	123.03	126.23
22	B	613	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
23	b	620	BCR	C38-C26-C25	-2.12	122.14	124.53
28	C	517	DGD	CBB-CAB-C9B	-2.12	103.65	114.42
26	C	520	LMG	O1-C1-C2	-2.12	104.99	108.30
23	B	617	BCR	C15-C16-C17	-2.12	119.13	123.47
26	a	410	LMG	C38-C37-C36	-2.12	103.66	114.42
23	B	619	BCR	C3-C4-C5	-2.12	110.29	114.08
22	C	513	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
22	b	613	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	d	404	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
28	c	517	DGD	CBB-CAB-C9B	-2.12	103.68	114.42
28	h	103	DGD	CAB-C9B-C8B	-2.12	103.68	114.42
24	a	408	PL9	C20-C19-C21	2.12	118.83	115.27
26	A	410	LMG	C38-C37-C36	-2.12	103.69	114.42
31	l	101	LHG	C27-C26-C25	-2.12	103.69	114.42
22	D	404	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
22	a	406	CLA	CHD-C1D-ND	-2.11	122.51	124.45
22	b	615	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
28	a	413	DGD	CFB-CEB-CDB	-2.11	103.70	114.42
26	D	408	LMG	O1-C7-C8	-2.11	105.80	110.90
24	A	408	PL9	C37-C38-C39	-2.11	122.58	127.66
23	h	102	BCR	C7-C8-C9	-2.11	123.04	126.23
23	b	618	BCR	C15-C16-C17	-2.11	119.15	123.47
22	B	610	CLA	C2D-C1D-ND	-2.11	108.55	110.10
23	b	618	BCR	C28-C27-C26	-2.11	110.31	114.08
23	b	620	BCR	C33-C5-C6	-2.11	122.16	124.53
30	A	418	PHO	CMC-C2C-C3C	2.11	128.92	124.94
28	H	103	DGD	CAB-C9B-C8B	-2.11	103.72	114.42
26	d	408	LMG	O2-C2-C1	-2.11	104.93	110.05
31	L	101	LHG	C27-C26-C25	-2.11	103.74	114.42
22	c	513	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
22	d	404	CLA	O2D-CGD-CBD	2.10	115.00	111.27
22	B	609	CLA	CED-O2D-CGD	2.10	120.69	115.94
22	C	501	CLA	O2D-CGD-CBD	2.10	115.00	111.27
22	C	503	CLA	CHB-C4A-NA	2.10	127.42	124.51
24	A	408	PL9	C20-C19-C21	2.10	118.80	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	413	DGD	CAB-C9B-C8B	-2.10	103.77	114.42
28	C	519	DGD	O3E-C3E-C2E	-2.10	105.50	110.35
31	d	410	LHG	C18-C17-C16	-2.10	103.78	114.42
22	b	611	CLA	C2D-C1D-ND	-2.10	108.56	110.10
22	c	507	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
26	c	520	LMG	C38-C37-C36	-2.09	103.79	114.42
24	a	408	PL9	C41-C39-C38	-2.09	116.88	121.12
26	C	520	LMG	C38-C37-C36	-2.09	103.80	114.42
22	b	610	CLA	CED-O2D-CGD	2.09	120.67	115.94
22	B	605	CLA	O1D-CGD-CBD	2.09	128.76	124.48
26	D	408	LMG	O2-C2-C1	-2.09	104.97	110.05
31	d	411	LHG	C27-C26-C25	-2.09	103.81	114.42
22	c	503	CLA	CHB-C4A-NA	2.09	127.40	124.51
23	h	102	BCR	C15-C14-C13	-2.09	124.33	127.31
31	D	411	LHG	C27-C26-C25	-2.09	103.82	114.42
28	c	519	DGD	O3E-C3E-C2E	-2.09	105.52	110.35
23	H	102	BCR	C15-C14-C13	-2.08	124.33	127.31
30	a	418	PHO	CMC-C2C-C3C	2.08	128.87	124.94
22	C	507	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	C	515	BCR	C38-C26-C25	-2.08	122.19	124.53
23	c	515	BCR	C38-C26-C25	-2.08	122.19	124.53
23	C	514	BCR	C15-C14-C13	-2.08	124.34	127.31
31	D	409	LHG	C27-C26-C25	-2.08	103.86	114.42
31	d	409	LHG	C27-C26-C25	-2.08	103.86	114.42
23	K	103	BCR	C15-C16-C17	-2.08	119.21	123.47
31	d	409	LHG	C11-C10-C9	-2.08	103.87	114.42
31	D	409	LHG	C11-C10-C9	-2.08	103.88	114.42
24	A	408	PL9	O2-C1-C6	2.08	124.19	120.59
24	a	408	PL9	O2-C1-C6	2.08	124.19	120.59
23	k	103	BCR	C15-C16-C17	-2.08	119.22	123.47
22	A	404	CLA	C2D-C1D-ND	-2.07	108.58	110.10
23	T	101	BCR	C15-C16-C17	-2.07	119.23	123.47
22	b	610	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
23	D	406	BCR	C15-C16-C17	-2.07	119.23	123.47
23	c	514	BCR	C15-C14-C13	-2.07	124.36	127.31
24	d	407	PL9	C37-C38-C39	-2.07	122.67	127.66
22	B	606	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
22	b	607	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
24	D	407	PL9	C37-C38-C39	-2.07	122.68	127.66
28	A	413	DGD	CAB-C9B-C8B	-2.07	103.94	114.42
22	a	419	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	H	102	BCR	C28-C27-C26	-2.06	110.39	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	602	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	b	603	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	b	606	CLA	O1D-CGD-CBD	2.06	128.70	124.48
22	B	609	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	c	511	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
30	D	401	PHO	C1-C2-C3	-2.06	122.48	126.04
28	C	519	DGD	CBB-CAB-C9B	-2.06	103.98	114.42
31	A	420	LHG	C27-C26-C25	-2.06	103.98	114.42
23	K	101	BCR	C15-C16-C17	-2.06	119.26	123.47
23	k	101	BCR	C15-C16-C17	-2.06	119.26	123.47
23	B	618	BCR	C38-C26-C25	-2.06	122.22	124.53
23	d	406	BCR	C15-C16-C17	-2.06	119.26	123.47
23	t	102	BCR	C15-C16-C17	-2.05	119.27	123.47
30	a	418	PHO	O1D-CGD-CBD	2.05	128.16	124.74
22	A	419	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
22	C	511	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
22	c	512	CLA	O2D-CGD-CBD	2.05	114.92	111.27
28	c	518	DGD	CAB-C9B-C8B	-2.05	104.01	114.42
28	c	519	DGD	CBB-CAB-C9B	-2.05	104.01	114.42
25	t	101	STE	C3-C2-C1	-2.05	109.30	114.47
22	B	603	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
24	A	408	PL9	C41-C39-C38	-2.05	116.97	121.12
28	a	413	DGD	C5B-C4B-C3B	-2.05	104.02	114.42
31	a	420	LHG	C27-C26-C25	-2.05	104.04	114.42
28	A	413	DGD	CFB-CEB-CDB	-2.04	104.04	114.42
22	C	512	CLA	O2D-CGD-CBD	2.04	114.90	111.27
22	C	505	CLA	C1-C2-C3	-2.04	122.51	126.04
28	C	518	DGD	CAB-C9B-C8B	-2.04	104.06	114.42
22	A	405	CLA	CHD-C1D-ND	-2.04	122.58	124.45
28	A	413	DGD	C5B-C4B-C3B	-2.04	104.06	114.42
31	A	420	LHG	C5-O7-C7	-2.04	112.77	117.79
22	B	613	CLA	C2D-C1D-ND	-2.04	108.60	110.10
22	b	614	CLA	C2D-C1D-ND	-2.04	108.60	110.10
23	h	102	BCR	C28-C27-C26	-2.04	110.44	114.08
22	C	507	CLA	O2D-CGD-CBD	2.04	114.89	111.27
22	B	604	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	D	405	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	D	406	BCR	C2-C1-C6	2.04	113.61	110.48
26	b	625	LMG	O1-C7-C8	-2.04	105.99	110.90
26	c	524	LMG	C40-C39-C38	-2.04	104.09	114.42
22	a	404	CLA	C2D-C1D-ND	-2.04	108.60	110.10
28	H	103	DGD	C1D-C2D-C3D	-2.03	105.76	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	h	103	DGD	C1D-C2D-C3D	-2.03	105.76	110.00
22	b	614	CLA	O1D-CGD-CBD	2.03	128.65	124.48
22	b	604	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
23	B	618	BCR	C15-C16-C17	-2.03	119.31	123.47
22	B	610	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
22	b	611	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
23	d	406	BCR	C2-C1-C6	2.03	113.61	110.48
26	C	524	LMG	C40-C39-C38	-2.03	104.12	114.42
22	d	405	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	b	605	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
31	D	410	LHG	C18-C17-C16	-2.03	104.13	114.42
26	a	410	LMG	O2-C2-C1	-2.03	105.12	110.05
30	d	401	PHO	C1-C2-C3	-2.03	122.54	126.04
22	B	612	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
22	B	605	CLA	CHB-C4A-NA	2.02	127.31	124.51
22	b	606	CLA	CHB-C4A-NA	2.02	127.31	124.51
22	C	502	CLA	CHD-C1D-ND	-2.02	122.59	124.45
22	c	505	CLA	C1-C2-C3	-2.02	122.54	126.04
22	c	507	CLA	O2D-CGD-CBD	2.02	114.86	111.27
25	c	516	STE	C3-C2-C1	-2.02	109.38	114.47
22	c	513	CLA	O2D-CGD-CBD	2.02	114.86	111.27
26	B	624	LMG	O1-C7-C8	-2.02	106.03	110.90
22	C	509	CLA	C2D-C1D-ND	-2.02	108.62	110.10
22	b	613	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
28	a	413	DGD	O2D-C2D-C1D	-2.02	105.14	110.05
30	A	418	PHO	O1D-CGD-CBD	2.02	128.10	124.74
26	A	410	LMG	O2-C2-C1	-2.02	105.15	110.05
22	C	513	CLA	O2D-CGD-CBD	2.02	114.85	111.27
22	B	602	CLA	C2D-C1D-ND	-2.02	108.62	110.10
22	b	603	CLA	C2D-C1D-ND	-2.02	108.62	110.10
22	C	505	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	c	505	CLA	CHD-C1D-ND	-2.02	122.60	124.45
26	D	402	LMG	O7-C10-O9	-2.02	118.83	123.70
22	B	608	CLA	O2D-CGD-CBD	2.02	114.85	111.27
22	B	602	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
22	b	603	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
23	C	515	BCR	C2-C1-C6	2.02	113.58	110.48
23	c	515	BCR	C2-C1-C6	2.02	113.58	110.48
25	C	516	STE	C3-C2-C1	-2.01	109.40	114.47
26	d	402	LMG	O7-C10-O9	-2.01	118.83	123.70
22	B	605	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
22	b	606	CLA	O2A-CGA-O1A	-2.01	118.51	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	413	DGD	O3G-C1D-C2D	-2.01	105.16	108.30
23	t	102	BCR	C38-C26-C25	-2.01	122.27	124.53
30	a	418	PHO	OBD-CAD-CBD	-2.01	122.88	125.82
28	A	413	DGD	O3E-C3E-C2E	-2.01	105.71	110.35
22	B	616	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
22	C	513	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
22	c	513	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
23	T	101	BCR	C38-C26-C25	-2.00	122.28	124.53
22	c	502	CLA	C2D-C1D-ND	-2.00	108.63	110.10
22	B	613	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	b	614	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (56) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	404	CLA	ND
22	A	405	CLA	ND
22	A	406	CLA	ND
22	A	419	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	608	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	C	501	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND

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Mol	Chain	Res	Type	Atom
22	C	513	CLA	ND
22	a	404	CLA	ND
22	a	405	CLA	ND
22	a	406	CLA	ND
22	a	419	CLA	ND
22	b	602	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND
22	b	605	CLA	ND
22	b	607	CLA	ND
22	b	608	CLA	ND
22	b	609	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	b	617	CLA	ND
22	c	501	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND

All (1586) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	406	CLA	C2-C3-C5-C6
22	A	406	CLA	C4-C3-C5-C6
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	C3A-C2A-CAA-CBA
22	B	605	CLA	C4-C3-C5-C6
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
22	B	614	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	a	406	CLA	C2-C3-C5-C6
22	a	406	CLA	C4-C3-C5-C6
22	b	602	CLA	C1A-C2A-CAA-CBA
22	b	602	CLA	C3A-C2A-CAA-CBA
22	b	606	CLA	C4-C3-C5-C6
22	b	607	CLA	CHA-CBD-CGD-O1D
22	b	607	CLA	CHA-CBD-CGD-O2D
22	b	615	CLA	CHA-CBD-CGD-O1D
22	b	615	CLA	CHA-CBD-CGD-O2D
22	b	615	CLA	CAD-CBD-CGD-O1D
22	b	615	CLA	CAD-CBD-CGD-O2D
22	b	615	CLA	C11-C12-C13-C15
22	c	508	CLA	CHA-CBD-CGD-O1D
23	H	102	BCR	C16-C17-C18-C36
23	h	102	BCR	C16-C17-C18-C36
24	A	408	PL9	C22-C23-C24-C25
24	A	408	PL9	C24-C26-C27-C28
24	A	408	PL9	C27-C28-C29-C30
24	A	408	PL9	C27-C28-C29-C31
24	A	408	PL9	C32-C33-C34-C36
24	A	408	PL9	C37-C38-C39-C40
24	A	408	PL9	C38-C39-C41-C42
24	D	407	PL9	C37-C38-C39-C41
24	a	408	PL9	C22-C23-C24-C25
24	a	408	PL9	C24-C26-C27-C28
24	a	408	PL9	C27-C28-C29-C30
24	a	408	PL9	C27-C28-C29-C31
24	a	408	PL9	C32-C33-C34-C36
24	a	408	PL9	C37-C38-C39-C40
24	a	408	PL9	C38-C39-C41-C42
24	d	407	PL9	C37-C38-C39-C41
26	A	410	LMG	O6-C1-O1-C7
26	A	410	LMG	O1-C7-C8-O7
26	A	410	LMG	O9-C10-O7-C8
26	C	524	LMG	O9-C10-O7-C8
26	C	524	LMG	C11-C10-O7-C8
26	a	410	LMG	O6-C1-O1-C7
26	a	410	LMG	O1-C7-C8-O7
26	a	410	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
26	c	524	LMG	O9-C10-O7-C8
26	c	524	LMG	C11-C10-O7-C8
27	B	620	SQD	C2-C1-O6-C44
27	B	620	SQD	O5-C1-O6-C44
27	B	620	SQD	O49-C7-O47-C45
27	B	620	SQD	C8-C7-O47-C45
27	B	620	SQD	O5-C5-C6-S
27	X	101	SQD	C45-C44-O6-C1
27	b	621	SQD	O5-C1-O6-C44
27	b	621	SQD	C8-C7-O47-C45
27	b	621	SQD	O5-C5-C6-S
27	x	101	SQD	C45-C44-O6-C1
28	A	413	DGD	O1A-C1A-O1G-C1G
28	A	413	DGD	C2B-C1B-O2G-C2G
28	a	413	DGD	O1A-C1A-O1G-C1G
28	a	413	DGD	C2B-C1B-O2G-C2G
31	A	420	LHG	O1-C1-C2-C3
31	A	420	LHG	C3-O3-P-O5
31	A	420	LHG	C3-O3-P-O6
31	D	409	LHG	O1-C1-C2-C3
31	D	409	LHG	O2-C2-C3-O3
31	D	409	LHG	C3-O3-P-O5
31	D	409	LHG	C4-O6-P-O4
31	a	420	LHG	O1-C1-C2-C3
31	a	420	LHG	C3-O3-P-O5
31	a	420	LHG	C3-O3-P-O6
31	d	409	LHG	O1-C1-C2-C3
31	d	409	LHG	O2-C2-C3-O3
31	d	409	LHG	C3-O3-P-O5
31	d	409	LHG	C4-O6-P-O4
22	b	602	CLA	CBD-CGD-O2D-CED
22	B	601	CLA	O1A-CGA-O2A-C1
22	B	616	CLA	O1A-CGA-O2A-C1
22	b	602	CLA	O1A-CGA-O2A-C1
22	b	617	CLA	O1A-CGA-O2A-C1
22	B	601	CLA	CBA-CGA-O2A-C1
22	b	602	CLA	CBA-CGA-O2A-C1
28	A	413	DGD	C2A-C1A-O1G-C1G
28	a	413	DGD	C2A-C1A-O1G-C1G
22	B	601	CLA	CBD-CGD-O2D-CED
22	C	506	CLA	CBD-CGD-O2D-CED
22	c	506	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	C	524	LMG	O10-C28-O8-C9
26	c	524	LMG	O10-C28-O8-C9
27	X	101	SQD	O10-C23-O48-C46
27	x	101	SQD	O10-C23-O48-C46
27	b	621	SQD	O49-C7-O47-C45
27	X	101	SQD	C44-C45-C46-O48
27	x	101	SQD	C44-C45-C46-O48
22	C	512	CLA	C3-C5-C6-C7
22	c	512	CLA	C3-C5-C6-C7
22	B	616	CLA	CBA-CGA-O2A-C1
22	b	617	CLA	CBA-CGA-O2A-C1
26	C	524	LMG	C29-C28-O8-C9
26	c	524	LMG	C29-C28-O8-C9
26	A	410	LMG	C11-C10-O7-C8
26	a	410	LMG	C11-C10-O7-C8
32	Z	101	LMT	O5'-C5'-C6'-O6'
32	z	101	LMT	O5'-C5'-C6'-O6'
26	c	524	LMG	O6-C5-C6-O5
22	B	605	CLA	C2-C3-C5-C6
22	b	606	CLA	C2-C3-C5-C6
22	B	606	CLA	C2A-CAA-CBA-CGA
22	b	607	CLA	C2A-CAA-CBA-CGA
26	C	520	LMG	C29-C28-O8-C9
26	c	520	LMG	C29-C28-O8-C9
27	X	101	SQD	C24-C23-O48-C46
27	x	101	SQD	C24-C23-O48-C46
26	C	524	LMG	O6-C5-C6-O5
24	A	408	PL9	C32-C33-C34-C35
24	a	408	PL9	C32-C33-C34-C35
24	A	408	PL9	C22-C23-C24-C26
24	A	408	PL9	C37-C38-C39-C41
24	a	408	PL9	C22-C23-C24-C26
24	a	408	PL9	C37-C38-C39-C41
32	Z	101	LMT	C4B-C5B-C6B-O6B
32	z	101	LMT	C4B-C5B-C6B-O6B
22	B	603	CLA	CBD-CGD-O2D-CED
22	b	604	CLA	CBD-CGD-O2D-CED
26	H	101	LMG	C11-C10-O7-C8
26	h	101	LMG	C11-C10-O7-C8
32	Z	101	LMT	C4'-C5'-C6'-O6'
32	z	101	LMT	C4'-C5'-C6'-O6'
31	D	409	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	a	420	LHG	C30-C31-C32-C33
31	d	409	LHG	C32-C33-C34-C35
32	Z	101	LMT	O5B-C5B-C6B-O6B
32	z	101	LMT	O5B-C5B-C6B-O6B
25	a	415	STE	C13-C14-C15-C16
26	C	524	LMG	C4-C5-C6-O5
26	c	524	LMG	C4-C5-C6-O5
25	A	415	STE	C13-C14-C15-C16
32	J	102	LMT	O5'-C5'-C6'-O6'
32	j	102	LMT	O5'-C5'-C6'-O6'
32	Z	101	LMT	O5'-C1'-O1'-C1
32	z	101	LMT	O5'-C1'-O1'-C1
24	A	408	PL9	C34-C36-C37-C38
24	D	407	PL9	C39-C41-C42-C43
24	a	408	PL9	C34-C36-C37-C38
24	d	407	PL9	C39-C41-C42-C43
27	B	620	SQD	C24-C23-O48-C46
27	b	621	SQD	C24-C23-O48-C46
22	b	602	CLA	O1D-CGD-O2D-CED
22	B	601	CLA	O1D-CGD-O2D-CED
27	b	621	SQD	O10-C23-O48-C46
24	a	408	PL9	C31-C32-C33-C34
27	B	620	SQD	O10-C23-O48-C46
22	C	506	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
22	c	504	CLA	CBD-CGD-O2D-CED
28	C	518	DGD	C1A-C2A-C3A-C4A
22	B	608	CLA	C15-C16-C17-C18
22	b	609	CLA	C15-C16-C17-C18
32	J	102	LMT	C4'-C5'-C6'-O6'
32	j	102	LMT	C4'-C5'-C6'-O6'
22	b	615	CLA	C5-C6-C7-C8
28	c	518	DGD	C1A-C2A-C3A-C4A
22	A	405	CLA	C11-C10-C8-C9
22	B	601	CLA	C11-C12-C13-C14
22	B	604	CLA	C6-C7-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	C	509	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	D	405	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C12-C13-C14
22	b	605	CLA	C6-C7-C8-C9
22	b	615	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C10-C8-C9
22	c	509	CLA	C6-C7-C8-C9
22	c	512	CLA	C11-C10-C8-C9
22	d	405	CLA	C14-C13-C15-C16
23	H	102	BCR	C37-C22-C23-C24
23	b	619	BCR	C36-C18-C19-C20
23	h	102	BCR	C37-C22-C23-C24
32	E	104	LMT	O5'-C5'-C6'-O6'
32	e	104	LMT	O5'-C5'-C6'-O6'
32	C	525	LMT	C4B-C5B-C6B-O6B
32	c	525	LMT	C4B-C5B-C6B-O6B
31	A	420	LHG	C7-C8-C9-C10
31	a	420	LHG	C7-C8-C9-C10
22	B	604	CLA	CBD-CGD-O2D-CED
22	b	605	CLA	CBD-CGD-O2D-CED
26	B	624	LMG	C28-C29-C30-C31
22	B	614	CLA	C5-C6-C7-C8
22	B	616	CLA	C8-C10-C11-C12
22	C	512	CLA	C13-C15-C16-C17
22	b	617	CLA	C8-C10-C11-C12
22	c	512	CLA	C13-C15-C16-C17
31	a	420	LHG	O1-C1-C2-O2
26	A	410	LMG	C10-C11-C12-C13
26	a	410	LMG	C10-C11-C12-C13
26	b	625	LMG	C28-C29-C30-C31
28	a	413	DGD	O1B-C1B-O2G-C2G
25	a	416	STE	C12-C13-C14-C15
25	a	421	STE	C1-C2-C3-C4
25	A	416	STE	C12-C13-C14-C15
22	B	614	CLA	C11-C12-C13-C15
22	B	615	CLA	C6-C7-C8-C10
22	D	404	CLA	C12-C13-C15-C16
22	b	615	CLA	C12-C13-C15-C16
22	b	616	CLA	C6-C7-C8-C10
22	d	404	CLA	C12-C13-C15-C16
22	B	604	CLA	C5-C6-C7-C8
22	C	505	CLA	C15-C16-C17-C18
22	C	513	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C5-C6-C7-C8
22	c	505	CLA	C15-C16-C17-C18
22	c	513	CLA	C5-C6-C7-C8
22	d	404	CLA	C15-C16-C17-C18
26	C	520	LMG	O10-C28-O8-C9
26	c	520	LMG	O10-C28-O8-C9
32	Z	101	LMT	O1'-C1-C2-C3
32	z	101	LMT	O1'-C1-C2-C3
26	H	101	LMG	C28-C29-C30-C31
26	h	101	LMG	C28-C29-C30-C31
31	A	420	LHG	O2-C2-C3-O3
31	a	420	LHG	O2-C2-C3-O3
28	A	413	DGD	O1B-C1B-O2G-C2G
32	B	623	LMT	C4'-C5'-C6'-O6'
32	b	624	LMT	C4'-C5'-C6'-O6'
22	B	605	CLA	C15-C16-C17-C18
22	b	606	CLA	C15-C16-C17-C18
31	l	101	LHG	C32-C33-C34-C35
24	A	408	PL9	C31-C32-C33-C34
22	C	503	CLA	C5-C6-C7-C8
22	D	404	CLA	C15-C16-C17-C18
22	c	503	CLA	C5-C6-C7-C8
31	D	409	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O3
31	d	409	LHG	C4-O6-P-O3
31	l	101	LHG	C4-O6-P-O3
25	A	421	STE	C1-C2-C3-C4
27	B	620	SQD	C23-C24-C25-C26
31	L	101	LHG	C32-C33-C34-C35
31	A	420	LHG	C1-C2-C3-O3
31	D	409	LHG	C1-C2-C3-O3
31	a	420	LHG	C1-C2-C3-O3
31	d	409	LHG	C1-C2-C3-O3
22	B	601	CLA	C10-C11-C12-C13
22	b	602	CLA	C10-C11-C12-C13
22	b	607	CLA	C16-C17-C18-C19
25	D	412	STE	C5-C6-C7-C8
26	C	520	LMG	C33-C34-C35-C36
26	h	101	LMG	C33-C34-C35-C36
31	L	101	LHG	C30-C31-C32-C33
31	l	101	LHG	C30-C31-C32-C33
32	z	101	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
23	H	102	BCR	C20-C21-C22-C37
23	T	101	BCR	C20-C21-C22-C37
23	h	102	BCR	C20-C21-C22-C37
23	t	102	BCR	C20-C21-C22-C37
32	B	623	LMT	O5'-C5'-C6'-O6'
32	b	624	LMT	O5'-C5'-C6'-O6'
25	B	625	STE	C6-C7-C8-C9
25	J	101	STE	C10-C11-C12-C13
25	b	601	STE	C6-C7-C8-C9
25	d	412	STE	C5-C6-C7-C8
25	j	101	STE	C10-C11-C12-C13
26	C	520	LMG	C35-C36-C37-C38
26	H	101	LMG	C33-C34-C35-C36
26	c	520	LMG	C33-C34-C35-C36
26	c	520	LMG	C35-C36-C37-C38
27	A	411	SQD	C14-C15-C16-C17
27	a	411	SQD	C14-C15-C16-C17
28	C	518	DGD	C6A-C7A-C8A-C9A
28	C	518	DGD	C4B-C5B-C6B-C7B
28	C	519	DGD	C9A-CAA-CBA-CCA
28	H	103	DGD	CBA-CCA-CDA-CEA
28	a	413	DGD	CEA-CFA-CGA-CHA
28	c	518	DGD	C6A-C7A-C8A-C9A
28	c	518	DGD	C4B-C5B-C6B-C7B
28	c	519	DGD	C5A-C6A-C7A-C8A
28	c	519	DGD	C9A-CAA-CBA-CCA
28	h	103	DGD	CBA-CCA-CDA-CEA
22	C	513	CLA	C16-C17-C18-C20
27	A	412	SQD	C24-C23-O48-C46
27	a	412	SQD	C24-C23-O48-C46
25	A	416	STE	C14-C15-C16-C17
25	C	516	STE	C5-C6-C7-C8
25	a	416	STE	C14-C15-C16-C17
25	c	516	STE	C5-C6-C7-C8
26	A	410	LMG	C16-C17-C18-C19
26	A	410	LMG	C29-C30-C31-C32
26	a	410	LMG	C16-C17-C18-C19
26	a	410	LMG	C29-C30-C31-C32
28	C	518	DGD	C5B-C6B-C7B-C8B
28	C	519	DGD	C5A-C6A-C7A-C8A
28	c	518	DGD	C5B-C6B-C7B-C8B
31	l	101	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	J	102	LMT	C4-C5-C6-C7
32	Z	101	LMT	C3-C4-C5-C6
32	j	102	LMT	C4-C5-C6-C7
26	C	524	LMG	C9-C8-O7-C10
26	c	524	LMG	C9-C8-O7-C10
27	B	620	SQD	C46-C45-O47-C7
27	b	621	SQD	C46-C45-O47-C7
25	B	621	STE	C11-C12-C13-C14
25	E	102	STE	C14-C15-C16-C17
25	T	102	STE	C6-C7-C8-C9
25	b	622	STE	C11-C12-C13-C14
25	e	102	STE	C14-C15-C16-C17
26	d	408	LMG	C18-C19-C20-C21
27	B	620	SQD	C11-C12-C13-C14
28	A	413	DGD	CDB-CEB-CFB-CGB
28	H	103	DGD	C6B-C7B-C8B-C9B
28	h	103	DGD	C6B-C7B-C8B-C9B
31	L	101	LHG	C14-C15-C16-C17
31	a	420	LHG	C33-C34-C35-C36
26	D	408	LMG	C18-C19-C20-C21
27	A	411	SQD	C29-C30-C31-C32
27	B	620	SQD	C31-C32-C33-C34
27	b	621	SQD	C17-C18-C19-C20
28	C	519	DGD	C8A-C9A-CAA-CBA
28	c	519	DGD	C8A-C9A-CAA-CBA
25	i	101	STE	C4-C5-C6-C7
26	D	408	LMG	C16-C17-C18-C19
26	d	408	LMG	C16-C17-C18-C19
27	b	621	SQD	C13-C14-C15-C16
27	b	621	SQD	C15-C16-C17-C18
28	C	518	DGD	C6B-C7B-C8B-C9B
28	H	103	DGD	C4B-C5B-C6B-C7B
28	h	103	DGD	C4B-C5B-C6B-C7B
23	H	102	BCR	C16-C17-C18-C19
23	h	102	BCR	C16-C17-C18-C19
32	Z	101	LMT	C2'-C1'-O1'-C1
32	z	101	LMT	C2'-C1'-O1'-C1
25	C	521	STE	C4-C5-C6-C7
25	I	101	STE	C4-C5-C6-C7
25	c	521	STE	C4-C5-C6-C7
26	d	408	LMG	C30-C31-C32-C33
28	H	103	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
28	a	413	DGD	CDA-CEA-CFA-CGA
28	c	518	DGD	C6B-C7B-C8B-C9B
28	h	103	DGD	C9B-CAB-CBB-CCB
31	L	101	LHG	C29-C30-C31-C32
26	D	402	LMG	O10-C28-O8-C9
26	d	402	LMG	O10-C28-O8-C9
22	c	513	CLA	C16-C17-C18-C20
25	t	101	STE	C12-C13-C14-C15
26	D	408	LMG	C30-C31-C32-C33
26	h	101	LMG	C37-C38-C39-C40
31	l	101	LHG	C29-C30-C31-C32
32	E	104	LMT	C4-C5-C6-C7
32	e	104	LMT	C4-C5-C6-C7
22	B	611	CLA	C14-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C9
22	b	612	CLA	C14-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C9
26	D	402	LMG	C28-C29-C30-C31
25	C	516	STE	C2-C3-C4-C5
25	c	516	STE	C2-C3-C4-C5
26	D	408	LMG	C32-C33-C34-C35
26	H	101	LMG	C11-C12-C13-C14
26	H	101	LMG	C35-C36-C37-C38
26	H	101	LMG	C37-C38-C39-C40
26	d	408	LMG	C32-C33-C34-C35
26	h	101	LMG	C35-C36-C37-C38
27	a	412	SQD	C11-C12-C13-C14
28	C	517	DGD	C4B-C5B-C6B-C7B
28	c	517	DGD	C4B-C5B-C6B-C7B
31	A	420	LHG	C26-C27-C28-C29
22	C	512	CLA	C2A-CAA-CBA-CGA
22	c	512	CLA	C2A-CAA-CBA-CGA
25	a	415	STE	C12-C13-C14-C15
26	C	520	LMG	C38-C39-C40-C41
26	D	408	LMG	C35-C36-C37-C38
26	c	520	LMG	C38-C39-C40-C41
26	d	408	LMG	C35-C36-C37-C38
27	A	411	SQD	C31-C32-C33-C34
27	B	620	SQD	C27-C28-C29-C30
27	b	621	SQD	C16-C17-C18-C19
31	D	410	LHG	O1-C1-C2-C3
31	d	410	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	A	410	LMG	C31-C32-C33-C34
26	A	410	LMG	C33-C34-C35-C36
26	a	410	LMG	C31-C32-C33-C34
26	a	410	LMG	C33-C34-C35-C36
26	h	101	LMG	C11-C12-C13-C14
27	A	412	SQD	C9-C10-C11-C12
27	X	101	SQD	C33-C34-C35-C36
27	b	621	SQD	C29-C30-C31-C32
27	x	101	SQD	C33-C34-C35-C36
28	A	413	DGD	CCB-CDB-CEB-CFB
28	C	519	DGD	C2A-C3A-C4A-C5A
28	H	103	DGD	C7A-C8A-C9A-CAA
31	A	420	LHG	C32-C33-C34-C35
31	L	101	LHG	C10-C11-C12-C13
31	l	101	LHG	C10-C11-C12-C13
32	C	525	LMT	C2-C3-C4-C5
32	c	525	LMT	C2-C3-C4-C5
25	C	521	STE	C6-C7-C8-C9
25	a	409	STE	C4-C5-C6-C7
25	c	521	STE	C6-C7-C8-C9
27	A	411	SQD	C16-C17-C18-C19
27	A	411	SQD	C33-C34-C35-C36
27	A	412	SQD	C11-C12-C13-C14
27	A	412	SQD	C32-C33-C34-C35
27	B	620	SQD	C33-C34-C35-C36
27	a	411	SQD	C31-C32-C33-C34
27	a	411	SQD	C33-C34-C35-C36
27	a	412	SQD	C9-C10-C11-C12
28	C	519	DGD	CBB-CCB-CDB-CEB
28	a	413	DGD	C2A-C3A-C4A-C5A
28	c	519	DGD	C2A-C3A-C4A-C5A
28	c	519	DGD	CBB-CCB-CDB-CEB
28	h	103	DGD	C7A-C8A-C9A-CAA
32	B	623	LMT	C3-C4-C5-C6
32	b	624	LMT	C3-C4-C5-C6
28	C	517	DGD	O6E-C5E-C6E-O5E
28	c	517	DGD	O6E-C5E-C6E-O5E
22	C	513	CLA	C16-C17-C18-C19
25	A	409	STE	C4-C5-C6-C7
25	T	102	STE	C3-C4-C5-C6
25	a	415	STE	C9-C10-C11-C12
27	a	411	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	c	519	DGD	C9B-CAB-CBB-CCB
31	A	420	LHG	C33-C34-C35-C36
22	B	603	CLA	O1D-CGD-O2D-CED
22	b	604	CLA	O1D-CGD-O2D-CED
25	a	421	STE	C4-C5-C6-C7
26	C	520	LMG	C37-C38-C39-C40
26	C	524	LMG	C37-C38-C39-C40
26	c	520	LMG	C37-C38-C39-C40
26	c	524	LMG	C37-C38-C39-C40
28	A	413	DGD	C2A-C3A-C4A-C5A
28	C	519	DGD	C9B-CAB-CBB-CCB
31	d	410	LHG	C13-C14-C15-C16
26	d	402	LMG	C28-C29-C30-C31
25	A	421	STE	C4-C5-C6-C7
26	H	101	LMG	C13-C14-C15-C16
27	a	411	SQD	C29-C30-C31-C32
27	a	412	SQD	C33-C34-C35-C36
28	C	517	DGD	C2B-C3B-C4B-C5B
26	A	410	LMG	C32-C33-C34-C35
26	B	624	LMG	C38-C39-C40-C41
26	C	524	LMG	C35-C36-C37-C38
31	L	101	LHG	C27-C28-C29-C30
28	A	413	DGD	O6E-C5E-C6E-O5E
26	a	410	LMG	C30-C31-C32-C33
26	a	410	LMG	C32-C33-C34-C35
26	b	625	LMG	C38-C39-C40-C41
26	c	524	LMG	C35-C36-C37-C38
28	c	517	DGD	C2B-C3B-C4B-C5B
28	h	103	DGD	C9A-CAA-CBA-CCA
31	l	101	LHG	C27-C28-C29-C30
22	B	601	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C20
22	c	513	CLA	C16-C17-C18-C19
26	A	410	LMG	C30-C31-C32-C33
27	X	101	SQD	C25-C26-C27-C28
28	H	103	DGD	C9A-CAA-CBA-CCA
28	a	413	DGD	O6E-C5E-C6E-O5E
27	x	101	SQD	C25-C26-C27-C28
27	X	101	SQD	O6-C44-C45-C46
27	x	101	SQD	O6-C44-C45-C46
26	C	524	LMG	C29-C30-C31-C32
26	H	101	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
24	D	407	PL9	C45-C44-C46-C47
24	d	407	PL9	C45-C44-C46-C47
24	A	408	PL9	C33-C34-C36-C37
24	D	407	PL9	C43-C44-C46-C47
24	a	408	PL9	C33-C34-C36-C37
24	d	407	PL9	C43-C44-C46-C47
26	b	625	LMG	C17-C18-C19-C20
26	d	402	LMG	C33-C34-C35-C36
26	h	101	LMG	C13-C14-C15-C16
26	h	101	LMG	C38-C39-C40-C41
27	A	411	SQD	C30-C31-C32-C33
31	A	420	LHG	O1-C1-C2-O2
25	I	101	STE	C3-C4-C5-C6
25	i	101	STE	C3-C4-C5-C6
25	t	101	STE	C10-C11-C12-C13
26	B	624	LMG	C17-C18-C19-C20
26	C	520	LMG	C14-C15-C16-C17
26	D	402	LMG	C33-C34-C35-C36
27	B	620	SQD	C9-C10-C11-C12
27	X	101	SQD	C31-C32-C33-C34
27	a	412	SQD	C26-C27-C28-C29
28	A	413	DGD	C3B-C4B-C5B-C6B
31	D	410	LHG	C29-C30-C31-C32
31	d	410	LHG	C29-C30-C31-C32
27	A	412	SQD	O10-C23-O48-C46
27	a	412	SQD	O10-C23-O48-C46
26	a	410	LMG	C38-C39-C40-C41
26	c	520	LMG	C14-C15-C16-C17
27	a	411	SQD	C30-C31-C32-C33
28	C	519	DGD	C4A-C5A-C6A-C7A
28	c	519	DGD	C4A-C5A-C6A-C7A
26	A	410	LMG	C38-C39-C40-C41
26	c	524	LMG	C29-C30-C31-C32
27	x	101	SQD	C31-C32-C33-C34
31	D	411	LHG	C29-C30-C31-C32
25	m	102	STE	C4-C5-C6-C7
25	t	101	STE	C6-C7-C8-C9
27	A	411	SQD	C12-C13-C14-C15
27	a	411	SQD	C12-C13-C14-C15
31	d	411	LHG	C29-C30-C31-C32
26	H	101	LMG	O9-C10-O7-C8
26	h	101	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
25	M	101	STE	C4-C5-C6-C7
26	C	524	LMG	C33-C34-C35-C36
26	D	408	LMG	C38-C39-C40-C41
26	c	524	LMG	C33-C34-C35-C36
27	A	411	SQD	C32-C33-C34-C35
27	B	620	SQD	C13-C14-C15-C16
27	a	411	SQD	C32-C33-C34-C35
31	d	410	LHG	C11-C12-C13-C14
25	B	622	STE	C2-C3-C4-C5
26	D	402	LMG	C32-C33-C34-C35
26	d	402	LMG	C32-C33-C34-C35
26	d	408	LMG	C38-C39-C40-C41
28	a	413	DGD	C3B-C4B-C5B-C6B
31	L	101	LHG	C9-C10-C11-C12
31	l	101	LHG	C9-C10-C11-C12
23	B	617	BCR	C1-C6-C7-C8
23	B	617	BCR	C5-C6-C7-C8
23	H	102	BCR	C23-C24-C25-C26
23	H	102	BCR	C23-C24-C25-C30
23	K	103	BCR	C1-C6-C7-C8
23	K	103	BCR	C5-C6-C7-C8
23	b	618	BCR	C1-C6-C7-C8
23	b	618	BCR	C5-C6-C7-C8
23	h	102	BCR	C23-C24-C25-C26
23	h	102	BCR	C23-C24-C25-C30
23	k	103	BCR	C1-C6-C7-C8
23	k	103	BCR	C5-C6-C7-C8
25	e	103	STE	C14-C15-C16-C17
31	a	420	LHG	C28-C29-C30-C31
26	C	520	LMG	C11-C10-O7-C8
26	c	520	LMG	C11-C10-O7-C8
25	A	415	STE	C12-C13-C14-C15
25	E	103	STE	C14-C15-C16-C17
25	d	412	STE	C2-C3-C4-C5
26	H	101	LMG	C39-C40-C41-C42
26	c	520	LMG	C17-C18-C19-C20
32	E	104	LMT	C11-C10-C9-C8
32	e	104	LMT	C11-C10-C9-C8
25	a	421	STE	C3-C4-C5-C6
26	h	101	LMG	C39-C40-C41-C42
27	A	412	SQD	C17-C18-C19-C20
27	b	621	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	A	420	LHG	C24-C25-C26-C27
25	D	412	STE	C2-C3-C4-C5
25	T	102	STE	C5-C6-C7-C8
25	b	623	STE	C4-C5-C6-C7
26	B	624	LMG	C30-C31-C32-C33
26	C	520	LMG	C17-C18-C19-C20
26	C	520	LMG	C18-C19-C20-C21
27	B	620	SQD	C34-C35-C36-C37
28	h	103	DGD	CAA-CBA-CCA-CDA
31	A	420	LHG	C31-C32-C33-C34
22	B	601	CLA	C6-C7-C8-C10
22	B	601	CLA	C11-C12-C13-C15
22	C	503	CLA	C11-C10-C8-C7
22	C	510	CLA	C6-C7-C8-C10
22	C	513	CLA	C11-C12-C13-C15
22	b	602	CLA	C6-C7-C8-C10
22	b	602	CLA	C11-C12-C13-C15
22	c	503	CLA	C11-C10-C8-C7
22	c	510	CLA	C6-C7-C8-C10
22	c	512	CLA	C11-C10-C8-C7
22	c	513	CLA	C11-C12-C13-C15
24	a	408	PL9	C13-C14-C16-C17
26	c	520	LMG	C18-C19-C20-C21
28	H	103	DGD	CAA-CBA-CCA-CDA
28	C	517	DGD	C1A-C2A-C3A-C4A
28	c	517	DGD	C1A-C2A-C3A-C4A
31	D	411	LHG	C7-C8-C9-C10
31	d	411	LHG	C7-C8-C9-C10
22	C	513	CLA	CBA-CGA-O2A-C1
22	c	513	CLA	CBA-CGA-O2A-C1
28	a	413	DGD	C5B-C6B-C7B-C8B
25	b	622	STE	C9-C10-C11-C12
26	A	410	LMG	C18-C19-C20-C21
26	a	410	LMG	C18-C19-C20-C21
26	b	625	LMG	C30-C31-C32-C33
28	a	413	DGD	CAA-CBA-CCA-CDA
31	a	420	LHG	C31-C32-C33-C34
25	B	621	STE	C9-C10-C11-C12
26	H	101	LMG	C14-C15-C16-C17
27	x	101	SQD	C26-C27-C28-C29
28	C	518	DGD	C8A-C9A-CAA-CBA
25	B	622	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	E	103	STE	C9-C10-C11-C12
25	e	103	STE	C9-C10-C11-C12
26	h	101	LMG	C14-C15-C16-C17
27	X	101	SQD	C26-C27-C28-C29
27	a	412	SQD	C17-C18-C19-C20
28	c	518	DGD	C8A-C9A-CAA-CBA
31	D	411	LHG	C24-C25-C26-C27
31	d	411	LHG	C24-C25-C26-C27
25	T	102	STE	C9-C10-C11-C12
27	B	620	SQD	C32-C33-C34-C35
22	B	606	CLA	C16-C17-C18-C19
28	C	518	DGD	O6E-C1E-O5D-C6D
28	c	518	DGD	O6E-C1E-O5D-C6D
22	C	513	CLA	C10-C11-C12-C13
22	c	513	CLA	C10-C11-C12-C13
25	A	421	STE	C3-C4-C5-C6
32	C	525	LMT	O5B-C5B-C6B-O6B
32	c	525	LMT	O5B-C5B-C6B-O6B
25	C	516	STE	C7-C8-C9-C10
25	c	516	STE	C7-C8-C9-C10
31	a	420	LHG	C32-C33-C34-C35
31	d	410	LHG	C15-C16-C17-C18
22	C	506	CLA	C15-C16-C17-C18
22	c	506	CLA	C15-C16-C17-C18
25	E	101	STE	C6-C7-C8-C9
28	A	413	DGD	C5B-C6B-C7B-C8B
28	C	517	DGD	C6A-C7A-C8A-C9A
28	c	517	DGD	C6A-C7A-C8A-C9A
25	B	622	STE	C3-C4-C5-C6
25	e	101	STE	C6-C7-C8-C9
28	A	413	DGD	CEB-CFB-CGB-CHB
31	a	420	LHG	C26-C27-C28-C29
28	C	518	DGD	C2E-C1E-O5D-C6D
28	c	518	DGD	C2E-C1E-O5D-C6D
26	A	410	LMG	O7-C8-C9-O8
27	B	620	SQD	O6-C44-C45-O47
25	K	102	STE	C12-C13-C14-C15
25	i	101	STE	C5-C6-C7-C8
22	B	601	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C19
22	b	607	CLA	C16-C17-C18-C20
25	I	101	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	A	411	SQD	C13-C14-C15-C16
22	C	509	CLA	C13-C15-C16-C17
24	A	408	PL9	C35-C34-C36-C37
27	a	411	SQD	C13-C14-C15-C16
28	A	413	DGD	C9A-CAA-CBA-CCA
32	E	104	LMT	C7-C8-C9-C10
32	e	104	LMT	C7-C8-C9-C10
22	B	601	CLA	C6-C7-C8-C9
22	B	614	CLA	C14-C13-C15-C16
22	C	513	CLA	C11-C12-C13-C14
22	b	602	CLA	C6-C7-C8-C9
22	b	615	CLA	C14-C13-C15-C16
22	c	513	CLA	C11-C12-C13-C14
24	A	408	PL9	C47-C48-C49-C51
24	a	408	PL9	C47-C48-C49-C51
26	B	624	LMG	C36-C37-C38-C39
26	b	625	LMG	C36-C37-C38-C39
26	d	408	LMG	C15-C16-C17-C18
26	D	408	LMG	C15-C16-C17-C18
26	D	408	LMG	C36-C37-C38-C39
26	D	408	LMG	O6-C5-C6-O5
26	d	408	LMG	O6-C5-C6-O5
22	B	609	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED
22	c	509	CLA	C13-C15-C16-C17
28	C	519	DGD	CAB-CBB-CCB-CDB
28	c	519	DGD	CAB-CBB-CCB-CDB
32	z	101	LMT	C4-C5-C6-C7
22	C	503	CLA	C1A-C2A-CAA-CBA
22	c	503	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	C16-C17-C18-C20
26	D	408	LMG	C39-C40-C41-C42
26	d	408	LMG	C14-C15-C16-C17
28	a	413	DGD	C7A-C8A-C9A-CAA
32	Z	101	LMT	C4-C5-C6-C7
25	b	623	STE	C2-C3-C4-C5
26	D	408	LMG	C14-C15-C16-C17
26	d	408	LMG	C36-C37-C38-C39
31	L	101	LHG	O6-C4-C5-C6
31	l	101	LHG	O6-C4-C5-C6
22	A	404	CLA	C2C-C3C-CAC-CBC
22	a	404	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	d	408	LMG	C39-C40-C41-C42
26	D	408	LMG	C28-C29-C30-C31
26	d	408	LMG	C28-C29-C30-C31
25	K	102	STE	C11-C10-C9-C8
27	a	412	SQD	C30-C31-C32-C33
31	D	409	LHG	C34-C35-C36-C37
31	d	409	LHG	C34-C35-C36-C37
22	A	419	CLA	C2C-C3C-CAC-CBC
22	a	419	CLA	C2C-C3C-CAC-CBC
25	t	101	STE	C4-C5-C6-C7
27	A	412	SQD	C30-C31-C32-C33
27	a	411	SQD	C11-C12-C13-C14
28	c	519	DGD	C2B-C3B-C4B-C5B
24	A	408	PL9	C15-C14-C16-C17
22	a	406	CLA	C5-C6-C7-C8
27	A	411	SQD	C9-C10-C11-C12
22	B	609	CLA	C15-C16-C17-C18
22	b	610	CLA	C15-C16-C17-C18
22	A	406	CLA	C5-C6-C7-C8
27	A	411	SQD	C11-C12-C13-C14
27	a	411	SQD	C9-C10-C11-C12
31	d	411	LHG	C27-C28-C29-C30
31	l	101	LHG	C34-C35-C36-C37
22	c	513	CLA	O1A-CGA-O2A-C1
27	b	621	SQD	C12-C13-C14-C15
28	A	413	DGD	C6B-C7B-C8B-C9B
28	C	519	DGD	C2B-C3B-C4B-C5B
31	L	101	LHG	C34-C35-C36-C37
32	E	104	LMT	C6-C7-C8-C9
32	e	104	LMT	C6-C7-C8-C9
25	C	516	STE	C6-C7-C8-C9
25	c	516	STE	C6-C7-C8-C9
26	A	410	LMG	O1-C7-C8-C9
26	C	520	LMG	O1-C7-C8-C9
26	a	410	LMG	O1-C7-C8-C9
26	c	520	LMG	O1-C7-C8-C9
31	D	411	LHG	C27-C28-C29-C30
22	B	614	CLA	C13-C15-C16-C17
28	a	413	DGD	C8B-C9B-CAB-CBB
22	C	513	CLA	O1A-CGA-O2A-C1
26	c	524	LMG	C8-C7-O1-C1
28	C	518	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
28	C	518	DGD	C5D-C6D-O5D-C1E
28	c	518	DGD	C2G-C3G-O3G-C1D
28	c	518	DGD	C5D-C6D-O5D-C1E
27	A	412	SQD	C33-C34-C35-C36
25	A	415	STE	C9-C10-C11-C12
26	D	402	LMG	C36-C37-C38-C39
32	j	102	LMT	C3-C4-C5-C6
22	c	504	CLA	C11-C12-C13-C14
25	c	521	STE	C5-C6-C7-C8
26	B	624	LMG	C15-C16-C17-C18
27	A	412	SQD	C31-C32-C33-C34
32	J	102	LMT	C3-C4-C5-C6
31	D	409	LHG	O1-C1-C2-O2
31	d	409	LHG	O1-C1-C2-O2
22	C	504	CLA	C11-C12-C13-C14
26	B	624	LMG	C14-C15-C16-C17
26	d	402	LMG	C36-C37-C38-C39
28	A	413	DGD	C6A-C7A-C8A-C9A
24	D	407	PL9	C37-C38-C39-C40
24	d	407	PL9	C37-C38-C39-C40
26	A	410	LMG	C34-C35-C36-C37
26	b	625	LMG	C14-C15-C16-C17
27	b	621	SQD	C11-C10-C9-C8
28	H	103	DGD	CDB-CEB-CFB-CGB
28	h	103	DGD	CDB-CEB-CFB-CGB
25	t	101	STE	C13-C14-C15-C16
26	b	625	LMG	C15-C16-C17-C18
26	b	625	LMG	C29-C30-C31-C32
26	d	408	LMG	C40-C41-C42-C43
22	C	504	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	O1D-CGD-O2D-CED
22	d	405	CLA	C10-C11-C12-C13
23	D	406	BCR	C20-C21-C22-C37
24	a	408	PL9	C35-C34-C36-C37
26	D	408	LMG	C40-C41-C42-C43
26	a	410	LMG	C34-C35-C36-C37
27	A	412	SQD	C26-C27-C28-C29
26	C	524	LMG	C28-C29-C30-C31
26	c	524	LMG	C28-C29-C30-C31
22	C	507	CLA	C16-C17-C18-C20
22	c	507	CLA	C16-C17-C18-C20
26	B	624	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
26	b	625	LMG	C18-C19-C20-C21
31	D	409	LHG	C11-C10-C9-C8
31	d	409	LHG	C11-C10-C9-C8
25	C	521	STE	C5-C6-C7-C8
25	a	416	STE	C11-C10-C9-C8
26	B	624	LMG	C29-C30-C31-C32
25	A	416	STE	C11-C10-C9-C8
25	E	103	STE	C13-C14-C15-C16
25	e	103	STE	C13-C14-C15-C16
28	a	413	DGD	CEB-CFB-CGB-CHB
25	T	102	STE	C2-C3-C4-C5
27	a	412	SQD	C31-C32-C33-C34
31	D	410	LHG	C35-C36-C37-C38
22	D	405	CLA	C10-C11-C12-C13
25	J	101	STE	C5-C6-C7-C8
28	A	413	DGD	C8A-C9A-CAA-CBA
26	a	410	LMG	O7-C8-C9-O8
25	D	412	STE	C11-C10-C9-C8
26	C	520	LMG	C36-C37-C38-C39
26	c	520	LMG	C36-C37-C38-C39
31	A	420	LHG	C11-C10-C9-C8
31	A	420	LHG	C34-C35-C36-C37
25	j	101	STE	C5-C6-C7-C8
28	C	519	DGD	CAA-CBA-CCA-CDA
31	d	410	LHG	C35-C36-C37-C38
32	B	623	LMT	C11-C10-C9-C8
32	b	624	LMT	C11-C10-C9-C8
22	B	601	CLA	C11-C10-C8-C7
22	B	614	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	b	602	CLA	C11-C10-C8-C7
22	c	507	CLA	C11-C10-C8-C7
24	A	408	PL9	C13-C14-C16-C17
28	c	519	DGD	CAA-CBA-CCA-CDA
22	B	601	CLA	C11-C10-C8-C9
22	B	614	CLA	C11-C10-C8-C9
22	B	615	CLA	C6-C7-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	D	404	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	616	CLA	C6-C7-C8-C9
22	c	506	CLA	C6-C7-C8-C9
22	c	506	CLA	C14-C13-C15-C16
22	c	512	CLA	C14-C13-C15-C16
25	d	412	STE	C11-C10-C9-C8
31	A	420	LHG	C17-C18-C19-C20
32	Z	101	LMT	C2-C3-C4-C5
32	z	101	LMT	C2-C3-C4-C5
25	A	421	STE	C6-C7-C8-C9
28	H	103	DGD	C7B-C8B-C9B-CAB
28	h	103	DGD	C7B-C8B-C9B-CAB
25	E	102	STE	C7-C8-C9-C10
28	a	413	DGD	C6B-C7B-C8B-C9B
31	a	420	LHG	C11-C10-C9-C8
31	a	420	LHG	C17-C18-C19-C20
22	b	608	CLA	C15-C16-C17-C18
25	c	521	STE	C2-C3-C4-C5
25	e	102	STE	C7-C8-C9-C10
22	B	607	CLA	C15-C16-C17-C18
22	c	512	CLA	C8-C10-C11-C12
28	a	413	DGD	CFA-CGA-CHA-CIA
22	c	507	CLA	C16-C17-C18-C19
25	a	421	STE	C6-C7-C8-C9
22	C	509	CLA	C10-C11-C12-C13
22	C	512	CLA	C8-C10-C11-C12
22	c	509	CLA	C10-C11-C12-C13
31	a	420	LHG	C24-C25-C26-C27
22	C	507	CLA	C16-C17-C18-C19
25	D	413	STE	C10-C11-C12-C13
25	d	413	STE	C10-C11-C12-C13
26	D	402	LMG	C29-C28-O8-C9
26	d	402	LMG	C29-C28-O8-C9
26	C	520	LMG	C28-C29-C30-C31
26	c	520	LMG	C28-C29-C30-C31
28	C	518	DGD	C2B-C3B-C4B-C5B
28	c	518	DGD	C2B-C3B-C4B-C5B
22	C	509	CLA	C8-C10-C11-C12
22	c	509	CLA	C8-C10-C11-C12
26	B	624	LMG	C19-C20-C21-C22
22	B	616	CLA	C11-C12-C13-C15
22	b	617	CLA	C11-C12-C13-C15
26	b	625	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
27	B	620	SQD	C10-C11-C12-C13
22	B	601	CLA	C15-C16-C17-C18
22	b	602	CLA	C15-C16-C17-C18
26	A	410	LMG	C7-C8-C9-O8
26	C	520	LMG	C7-C8-C9-O8
26	a	410	LMG	C7-C8-C9-O8
26	c	520	LMG	C7-C8-C9-O8
27	B	620	SQD	O6-C44-C45-C46
25	t	101	STE	C3-C4-C5-C6
31	L	101	LHG	C12-C13-C14-C15
31	l	101	LHG	C12-C13-C14-C15
32	B	623	LMT	C7-C8-C9-C10
32	b	624	LMT	C7-C8-C9-C10
22	C	512	CLA	O2A-C1-C2-C3
22	c	512	CLA	O2A-C1-C2-C3
25	C	521	STE	C2-C3-C4-C5
25	b	622	STE	C2-C3-C4-C5
32	e	104	LMT	C4'-C5'-C6'-O6'
22	B	604	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
25	t	101	STE	C11-C10-C9-C8
32	E	104	LMT	C4'-C5'-C6'-O6'
25	B	621	STE	C2-C3-C4-C5
32	j	102	LMT	C1-C2-C3-C4
26	C	524	LMG	C38-C39-C40-C41
28	c	519	DGD	C3B-C4B-C5B-C6B
25	M	101	STE	C7-C8-C9-C10
25	m	102	STE	C7-C8-C9-C10
26	c	524	LMG	C38-C39-C40-C41
26	D	402	LMG	C16-C17-C18-C19
26	d	402	LMG	C16-C17-C18-C19
28	C	519	DGD	C3B-C4B-C5B-C6B
32	J	102	LMT	C1-C2-C3-C4
32	J	102	LMT	O1'-C1-C2-C3
32	j	102	LMT	O1'-C1-C2-C3
22	B	616	CLA	C11-C12-C13-C14
22	d	405	CLA	C16-C17-C18-C20
25	C	521	STE	C3-C4-C5-C6
25	c	521	STE	C3-C4-C5-C6
22	b	617	CLA	C11-C12-C13-C14
25	m	102	STE	C5-C6-C7-C8
27	X	101	SQD	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
25	A	409	STE	C5-C6-C7-C8
25	a	409	STE	C5-C6-C7-C8
22	B	603	CLA	C11-C10-C8-C9
22	B	614	CLA	C11-C12-C13-C14
22	b	604	CLA	C11-C10-C8-C9
22	d	404	CLA	C14-C13-C15-C16
25	E	103	STE	C2-C3-C4-C5
25	e	103	STE	C2-C3-C4-C5
26	C	520	LMG	C39-C40-C41-C42
26	c	520	LMG	C39-C40-C41-C42
27	B	620	SQD	C28-C29-C30-C31
25	E	102	STE	C15-C16-C17-C18
25	M	101	STE	C5-C6-C7-C8
25	c	516	STE	C11-C10-C9-C8
27	x	101	SQD	C30-C31-C32-C33
22	D	405	CLA	C16-C17-C18-C20
23	D	406	BCR	C23-C24-C25-C26
23	D	406	BCR	C23-C24-C25-C30
23	d	406	BCR	C23-C24-C25-C26
23	d	406	BCR	C23-C24-C25-C30
25	k	102	STE	C11-C12-C13-C14
27	b	621	SQD	C30-C31-C32-C33
28	A	413	DGD	C4A-C5A-C6A-C7A
25	C	516	STE	C11-C10-C9-C8
25	I	101	STE	C6-C7-C8-C9
25	e	102	STE	C15-C16-C17-C18
26	b	625	LMG	C33-C34-C35-C36
22	B	611	CLA	C13-C15-C16-C17
22	b	612	CLA	C13-C15-C16-C17
25	i	101	STE	C6-C7-C8-C9
26	B	624	LMG	C33-C34-C35-C36
32	j	102	LMT	C7-C8-C9-C10
32	J	102	LMT	C7-C8-C9-C10
25	b	623	STE	C5-C6-C7-C8
27	b	621	SQD	C27-C28-C29-C30
28	C	517	DGD	CAA-CBA-CCA-CDA
22	B	603	CLA	C11-C10-C8-C7
22	B	611	CLA	C12-C13-C15-C16
22	B	613	CLA	C12-C13-C15-C16
22	B	615	CLA	C11-C12-C13-C15
22	B	616	CLA	C6-C7-C8-C10
22	C	506	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C12-C13-C15
22	C	509	CLA	C6-C7-C8-C10
22	C	512	CLA	C12-C13-C15-C16
22	D	405	CLA	C12-C13-C15-C16
22	b	604	CLA	C11-C10-C8-C7
22	b	612	CLA	C12-C13-C15-C16
22	b	616	CLA	C11-C12-C13-C15
22	b	617	CLA	C6-C7-C8-C10
22	c	506	CLA	C6-C7-C8-C10
22	c	506	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C12-C13-C15
22	c	509	CLA	C6-C7-C8-C10
22	c	512	CLA	C12-C13-C15-C16
22	d	405	CLA	C12-C13-C15-C16
32	c	523	LMT	C1-C2-C3-C4
26	B	624	LMG	C31-C32-C33-C34
28	c	517	DGD	CAA-CBA-CCA-CDA
32	E	104	LMT	C5-C6-C7-C8
22	D	405	CLA	C16-C17-C18-C19
22	d	405	CLA	C16-C17-C18-C19
32	C	523	LMT	C1-C2-C3-C4
32	e	104	LMT	C5-C6-C7-C8
28	C	519	DGD	C1B-C2B-C3B-C4B
25	K	102	STE	C10-C11-C12-C13
25	a	409	STE	C6-C7-C8-C9
32	C	525	LMT	C6-C7-C8-C9
26	b	625	LMG	C31-C32-C33-C34
28	C	517	DGD	CBA-CCA-CDA-CEA
28	c	517	DGD	CBA-CCA-CDA-CEA
22	b	615	CLA	C13-C15-C16-C17
23	B	619	BCR	C20-C21-C22-C37
23	b	619	BCR	C20-C21-C22-C37
23	b	620	BCR	C20-C21-C22-C37
23	d	406	BCR	C20-C21-C22-C37
25	A	409	STE	C6-C7-C8-C9
32	c	525	LMT	C6-C7-C8-C9
28	c	519	DGD	C1B-C2B-C3B-C4B
22	B	609	CLA	C13-C15-C16-C17
22	b	610	CLA	C13-C15-C16-C17
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	616	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	CAD-CBD-CGD-O2D
22	C	510	CLA	CAD-CBD-CGD-O2D
22	b	605	CLA	CAD-CBD-CGD-O2D
22	b	617	CLA	CAD-CBD-CGD-O2D
22	c	509	CLA	CAD-CBD-CGD-O2D
22	c	510	CLA	CAD-CBD-CGD-O2D
28	C	517	DGD	C5A-C6A-C7A-C8A
31	D	411	LHG	C33-C34-C35-C36
31	d	411	LHG	C33-C34-C35-C36
25	A	421	STE	C2-C3-C4-C5
25	k	102	STE	C10-C11-C12-C13
28	c	517	DGD	C5A-C6A-C7A-C8A
32	c	523	LMT	C5-C6-C7-C8
25	I	101	STE	C12-C13-C14-C15
31	D	410	LHG	C15-C16-C17-C18
31	D	410	LHG	C2-C3-O3-P
31	d	410	LHG	C2-C3-O3-P
27	A	412	SQD	C8-C7-O47-C45
28	a	413	DGD	CCA-CDA-CEA-CFA
31	L	101	LHG	O6-C4-C5-O7
31	l	101	LHG	O6-C4-C5-O7
25	a	421	STE	C2-C3-C4-C5
27	X	101	SQD	C29-C30-C31-C32
32	C	523	LMT	C5-C6-C7-C8
22	c	505	CLA	C13-C15-C16-C17
25	b	623	STE	C3-C4-C5-C6
27	b	621	SQD	C9-C10-C11-C12
28	C	517	DGD	CCA-CDA-CEA-CFA
28	c	517	DGD	CCA-CDA-CEA-CFA
26	d	408	LMG	C22-C23-C24-C25
22	B	605	CLA	CHA-CBD-CGD-O1D
22	C	502	CLA	CHA-CBD-CGD-O1D
22	C	502	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	512	CLA	CHA-CBD-CGD-O1D
22	b	606	CLA	CHA-CBD-CGD-O1D
22	c	502	CLA	CHA-CBD-CGD-O1D
22	c	502	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	512	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	C13-C15-C16-C17
26	H	101	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	x	101	SQD	C29-C30-C31-C32
26	A	410	LMG	C2-C1-O1-C7
26	a	410	LMG	C2-C1-O1-C7
26	C	520	LMG	O7-C8-C9-O8
26	c	520	LMG	O7-C8-C9-O8
22	A	404	CLA	C4C-C3C-CAC-CBC
22	a	404	CLA	C4C-C3C-CAC-CBC
25	B	621	STE	C6-C7-C8-C9
25	b	622	STE	C6-C7-C8-C9
25	a	415	STE	C11-C10-C9-C8
26	h	101	LMG	C15-C16-C17-C18
27	B	620	SQD	C29-C30-C31-C32
27	a	412	SQD	C8-C7-O47-C45
24	a	408	PL9	C15-C14-C16-C17
30	A	418	PHO	C4-C3-C5-C6
30	a	418	PHO	C4-C3-C5-C6
27	A	412	SQD	C7-C8-C9-C10
24	A	408	PL9	C4-C3-C7-C8
24	a	408	PL9	C4-C3-C7-C8
27	A	412	SQD	O49-C7-O47-C45
27	a	412	SQD	O49-C7-O47-C45
22	C	507	CLA	C11-C12-C13-C14
22	C	512	CLA	C14-C13-C15-C16
22	c	507	CLA	C11-C12-C13-C14
25	t	101	STE	C11-C12-C13-C14
24	a	408	PL9	C47-C48-C49-C50
27	b	621	SQD	C24-C25-C26-C27
25	i	101	STE	C12-C13-C14-C15
28	A	413	DGD	CDA-CEA-CFA-CGA
22	C	510	CLA	C16-C17-C18-C20
22	c	510	CLA	C16-C17-C18-C20
26	A	410	LMG	C15-C16-C17-C18
22	A	406	CLA	CBA-CGA-O2A-C1
22	a	406	CLA	CBA-CGA-O2A-C1
26	a	410	LMG	C15-C16-C17-C18
25	E	102	STE	C9-C10-C11-C12
22	C	506	CLA	C4-C3-C5-C6
22	c	506	CLA	C4-C3-C5-C6
28	C	517	DGD	C5B-C6B-C7B-C8B
31	A	420	LHG	C3-O3-P-O4
31	D	409	LHG	C4-O6-P-O5
31	D	411	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
31	L	101	LHG	C4-O6-P-O5
31	a	420	LHG	C3-O3-P-O4
31	d	409	LHG	C4-O6-P-O5
31	d	411	LHG	C3-O3-P-O4
31	l	101	LHG	C4-O6-P-O5
27	a	412	SQD	C7-C8-C9-C10
28	A	413	DGD	C4B-C5B-C6B-C7B
28	c	517	DGD	C5B-C6B-C7B-C8B
26	B	624	LMG	C20-C21-C22-C23
26	b	625	LMG	C20-C21-C22-C23
27	B	620	SQD	C35-C36-C37-C38
22	A	419	CLA	C4C-C3C-CAC-CBC
22	a	419	CLA	C4C-C3C-CAC-CBC
25	e	102	STE	C11-C10-C9-C8
22	B	605	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	b	606	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
27	A	411	SQD	C5-C6-S-O7
27	a	411	SQD	C5-C6-S-O7
26	C	520	LMG	C10-C11-C12-C13
26	D	408	LMG	C22-C23-C24-C25
24	A	408	PL9	C47-C48-C49-C50
26	c	520	LMG	C10-C11-C12-C13
25	B	625	STE	C7-C8-C9-C10
27	B	620	SQD	C18-C19-C20-C21
28	a	413	DGD	CCB-CDB-CEB-CFB
32	M	102	LMT	C11-C10-C9-C8
28	C	517	DGD	C4D-C5D-C6D-O5D
28	c	517	DGD	C4D-C5D-C6D-O5D
28	C	517	DGD	O6D-C5D-C6D-O5D
25	E	102	STE	C11-C10-C9-C8
25	e	102	STE	C9-C10-C11-C12
28	a	413	DGD	C4B-C5B-C6B-C7B
22	B	601	CLA	C12-C13-C15-C16
22	B	603	CLA	C6-C7-C8-C10
22	B	604	CLA	C6-C7-C8-C10
22	B	606	CLA	C11-C10-C8-C7
22	C	504	CLA	C6-C7-C8-C10
22	b	602	CLA	C12-C13-C15-C16
22	b	604	CLA	C6-C7-C8-C10
22	b	605	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C12-C13-C15-C16
22	c	504	CLA	C6-C7-C8-C10
28	c	517	DGD	O6D-C5D-C6D-O5D
32	E	104	LMT	C2-C1-O1'-C1'
32	e	104	LMT	C2-C1-O1'-C1'
32	m	101	LMT	C11-C10-C9-C8
27	A	411	SQD	C23-C24-C25-C26
27	B	620	SQD	C24-C25-C26-C27
22	A	406	CLA	O1A-CGA-O2A-C1
22	a	406	CLA	O1A-CGA-O2A-C1
25	b	601	STE	C7-C8-C9-C10
27	a	412	SQD	C32-C33-C34-C35
28	A	413	DGD	O6D-C5D-C6D-O5D
26	C	524	LMG	C7-C8-C9-O8
26	c	524	LMG	C7-C8-C9-O8
26	c	520	LMG	O1-C7-C8-O7
28	a	413	DGD	C4A-C5A-C6A-C7A
26	C	524	LMG	C8-C7-O1-C1
27	a	412	SQD	C27-C28-C29-C30
28	a	413	DGD	O6D-C5D-C6D-O5D
22	b	615	CLA	C11-C12-C13-C14
28	A	413	DGD	C4D-C5D-C6D-O5D
28	a	413	DGD	C4D-C5D-C6D-O5D
22	B	608	CLA	C13-C15-C16-C17
22	b	609	CLA	C13-C15-C16-C17
26	H	101	LMG	C19-C20-C21-C22
26	d	408	LMG	C20-C21-C22-C23
22	C	502	CLA	C16-C17-C18-C19
22	c	502	CLA	C16-C17-C18-C19
26	h	101	LMG	C19-C20-C21-C22
31	d	411	LHG	C11-C12-C13-C14
25	K	102	STE	C11-C12-C13-C14
22	D	404	CLA	C2C-C3C-CAC-CBC
22	d	404	CLA	C2C-C3C-CAC-CBC
25	k	102	STE	C9-C10-C11-C12
31	D	411	LHG	C11-C12-C13-C14
30	a	418	PHO	C2-C3-C5-C6
22	C	510	CLA	C8-C10-C11-C12
22	c	510	CLA	C8-C10-C11-C12
25	D	412	STE	C1-C2-C3-C4
25	A	409	STE	C3-C4-C5-C6
31	d	410	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
31	d	410	LHG	C34-C35-C36-C37
31	A	420	LHG	O8-C23-C24-C25
25	a	409	STE	C3-C4-C5-C6
26	A	410	LMG	C13-C14-C15-C16
26	a	410	LMG	C13-C14-C15-C16
26	H	101	LMG	C9-C8-O7-C10
26	h	101	LMG	C9-C8-O7-C10
22	C	501	CLA	C2A-CAA-CBA-CGA
22	c	501	CLA	C2A-CAA-CBA-CGA
32	C	525	LMT	C4-C5-C6-C7
32	c	525	LMT	C4-C5-C6-C7
28	C	517	DGD	O1B-C1B-O2G-C2G
28	c	517	DGD	O1B-C1B-O2G-C2G
28	A	413	DGD	O2G-C1B-C2B-C3B
25	k	102	STE	C14-C15-C16-C17
28	A	413	DGD	C8B-C9B-CAB-CBB
26	D	408	LMG	C20-C21-C22-C23
22	c	508	CLA	C15-C16-C17-C18
28	c	518	DGD	C3A-C4A-C5A-C6A
22	B	601	CLA	C8-C10-C11-C12
22	b	602	CLA	C8-C10-C11-C12
26	a	410	LMG	C14-C15-C16-C17
23	b	619	BCR	C23-C24-C25-C30
30	A	418	PHO	C2-C3-C5-C6
26	A	410	LMG	C14-C15-C16-C17
25	d	412	STE	C1-C2-C3-C4
28	a	413	DGD	O2G-C1B-C2B-C3B
22	B	606	CLA	C10-C11-C12-C13
28	C	518	DGD	C3A-C4A-C5A-C6A
31	a	420	LHG	O8-C23-C24-C25
26	C	520	LMG	O1-C7-C8-O7
25	k	102	STE	C15-C16-C17-C18
26	H	101	LMG	C40-C41-C42-C43
26	h	101	LMG	C40-C41-C42-C43
27	A	412	SQD	C27-C28-C29-C30
28	A	413	DGD	CEA-CFA-CGA-CHA
22	C	508	CLA	C15-C16-C17-C18
28	H	103	DGD	CCA-CDA-CEA-CFA
26	H	101	LMG	C30-C31-C32-C33
22	B	604	CLA	C11-C12-C13-C15
22	B	606	CLA	C11-C12-C13-C15
22	C	503	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C11-C12-C13-C15
22	c	503	CLA	C6-C7-C8-C10
28	A	413	DGD	CCA-CDA-CEA-CFA
28	c	518	DGD	C7B-C8B-C9B-CAB
31	D	410	LHG	C34-C35-C36-C37
22	B	603	CLA	C6-C7-C8-C9
22	B	606	CLA	C11-C10-C8-C9
22	B	616	CLA	C6-C7-C8-C9
22	C	504	CLA	C6-C7-C8-C9
22	C	507	CLA	C11-C10-C8-C9
22	b	604	CLA	C6-C7-C8-C9
22	b	617	CLA	C6-C7-C8-C9
22	c	504	CLA	C6-C7-C8-C9
22	c	507	CLA	C11-C10-C8-C9
22	b	615	CLA	C16-C17-C18-C19
28	C	518	DGD	C7B-C8B-C9B-CAB
31	D	411	LHG	C11-C10-C9-C8
31	d	411	LHG	C11-C10-C9-C8
25	A	416	STE	C9-C10-C11-C12
25	a	416	STE	C9-C10-C11-C12
28	h	103	DGD	CCA-CDA-CEA-CFA
25	A	409	STE	C2-C3-C4-C5
25	C	516	STE	C4-C5-C6-C7
27	A	411	SQD	O49-C7-O47-C45
22	C	505	CLA	C8-C10-C11-C12
26	C	524	LMG	C34-C35-C36-C37
24	D	407	PL9	C13-C14-C16-C17
24	d	407	PL9	C13-C14-C16-C17
26	c	524	LMG	C34-C35-C36-C37
22	c	505	CLA	C8-C10-C11-C12
25	K	102	STE	C14-C15-C16-C17
25	a	409	STE	C2-C3-C4-C5
27	b	621	SQD	C14-C15-C16-C17
31	a	420	LHG	C24-C23-O8-C6
22	B	603	CLA	C2A-CAA-CBA-CGA
22	b	604	CLA	C2A-CAA-CBA-CGA
22	C	502	CLA	C16-C17-C18-C20
22	c	502	CLA	C16-C17-C18-C20
28	C	518	DGD	O6D-C1D-O3G-C3G
28	c	518	DGD	O6D-C1D-O3G-C3G
25	c	516	STE	C4-C5-C6-C7
31	A	420	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	A	410	LMG	C11-C12-C13-C14
26	a	410	LMG	C11-C12-C13-C14
22	C	512	CLA	C4-C3-C5-C6
22	A	405	CLA	C10-C11-C12-C13
32	J	102	LMT	C6-C7-C8-C9
32	j	102	LMT	C6-C7-C8-C9
28	h	103	DGD	C5B-C6B-C7B-C8B
27	a	411	SQD	O49-C7-O47-C45
28	H	103	DGD	C5B-C6B-C7B-C8B
35	v	201	HEC	CAD-CBD-CGD-O1D
25	b	601	STE	C9-C10-C11-C12
32	M	102	LMT	C3-C4-C5-C6
31	A	420	LHG	C24-C23-O8-C6
22	B	613	CLA	C15-C16-C17-C18
25	c	522	STE	C12-C13-C14-C15
26	h	101	LMG	C30-C31-C32-C33
22	c	512	CLA	C4-C3-C5-C6
22	C	506	CLA	C2-C3-C5-C6
22	c	506	CLA	C2-C3-C5-C6
31	D	410	LHG	C33-C34-C35-C36
22	B	601	CLA	C14-C13-C15-C16
22	B	611	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C12-C13-C14
22	b	602	CLA	C14-C13-C15-C16
22	b	612	CLA	C11-C12-C13-C14
22	c	505	CLA	C11-C12-C13-C14
25	C	522	STE	C12-C13-C14-C15
35	V	201	HEC	CAD-CBD-CGD-O1D
27	b	621	SQD	C11-C12-C13-C14
28	C	519	DGD	C6A-C7A-C8A-C9A
23	B	618	BCR	C20-C21-C22-C37
28	c	519	DGD	C6A-C7A-C8A-C9A
32	m	101	LMT	C3-C4-C5-C6
25	B	625	STE	C9-C10-C11-C12
26	C	524	LMG	O6-C1-O1-C7
26	c	524	LMG	O6-C1-O1-C7
28	A	413	DGD	CAB-CBB-CCB-CDB
26	A	410	LMG	C9-C8-O7-C10
26	a	410	LMG	C9-C8-O7-C10
24	D	407	PL9	C40-C39-C41-C42
24	d	407	PL9	C40-C39-C41-C42
22	b	607	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C15-C16-C17-C18
32	M	102	LMT	O5'-C5'-C6'-O6'
32	m	101	LMT	O5'-C5'-C6'-O6'
27	A	412	SQD	C15-C16-C17-C18
31	D	409	LHG	O6-C4-C5-C6
31	d	409	LHG	O6-C4-C5-C6
27	A	411	SQD	C27-C28-C29-C30
26	D	402	LMG	C35-C36-C37-C38
22	b	616	CLA	C5-C6-C7-C8
25	B	621	STE	C1-C2-C3-C4
22	B	615	CLA	C5-C6-C7-C8
25	D	412	STE	O2-C1-C2-C3
26	C	524	LMG	O7-C8-C9-O8
27	A	412	SQD	O6-C44-C45-O47
27	a	412	SQD	O6-C44-C45-O47
25	b	622	STE	C1-C2-C3-C4
22	B	612	CLA	C3-C5-C6-C7
22	b	613	CLA	C3-C5-C6-C7
25	E	103	STE	O1-C1-C2-C3
25	e	103	STE	O1-C1-C2-C3
28	C	517	DGD	C8A-C9A-CAA-CBA
28	c	517	DGD	C8A-C9A-CAA-CBA
24	A	408	PL9	C29-C31-C32-C33
24	a	408	PL9	C29-C31-C32-C33
31	D	411	LHG	C1-C2-C3-O3
31	d	411	LHG	C1-C2-C3-O3
25	d	412	STE	O2-C1-C2-C3
22	b	607	CLA	C10-C11-C12-C13
28	h	103	DGD	O1A-C1A-O1G-C1G
31	a	420	LHG	C23-C24-C25-C26
28	H	103	DGD	O1A-C1A-O1G-C1G
25	E	103	STE	O2-C1-C2-C3
25	e	103	STE	O2-C1-C2-C3
27	a	411	SQD	C27-C28-C29-C30
25	d	412	STE	O1-C1-C2-C3
25	e	102	STE	C10-C11-C12-C13
26	c	520	LMG	C30-C31-C32-C33
23	B	618	BCR	C23-C24-C25-C30
23	b	619	BCR	C23-C24-C25-C26
25	E	101	STE	C7-C8-C9-C10
28	a	413	DGD	C1G-C2G-C3G-O3G
25	e	101	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C4-C3-C5-C6
22	b	616	CLA	C4-C3-C5-C6
32	B	623	LMT	C9-C10-C11-C12
32	b	624	LMT	C9-C10-C11-C12
25	D	412	STE	O1-C1-C2-C3
28	C	519	DGD	O6D-C5D-C6D-O5D
28	c	519	DGD	O6D-C5D-C6D-O5D
28	C	517	DGD	C5D-C6D-O5D-C1E
28	c	517	DGD	C5D-C6D-O5D-C1E
26	C	520	LMG	C30-C31-C32-C33
26	A	410	LMG	C12-C13-C14-C15
26	a	410	LMG	C12-C13-C14-C15
26	d	402	LMG	C35-C36-C37-C38
31	a	420	LHG	C14-C15-C16-C17
22	A	405	CLA	C11-C12-C13-C14
22	B	614	CLA	C16-C17-C18-C19
22	b	607	CLA	C13-C15-C16-C17
28	H	103	DGD	O2G-C1B-C2B-C3B
22	B	601	CLA	C4-C3-C5-C6
22	b	602	CLA	C4-C3-C5-C6
31	A	420	LHG	C35-C36-C37-C38
22	c	506	CLA	C16-C17-C18-C20
25	C	516	STE	C9-C10-C11-C12
25	c	516	STE	C9-C10-C11-C12
27	A	412	SQD	C24-C25-C26-C27
26	c	524	LMG	O7-C8-C9-O8
28	a	413	DGD	O2G-C2G-C3G-O3G
27	a	411	SQD	C23-C24-C25-C26
28	h	103	DGD	O2G-C1B-C2B-C3B
22	C	506	CLA	C16-C17-C18-C20
35	v	201	HEC	CAD-CBD-CGD-O2D
22	C	510	CLA	CAA-CBA-CGA-O2A
27	A	411	SQD	O47-C7-C8-C9
27	a	411	SQD	O47-C7-C8-C9
28	C	519	DGD	O1G-C1A-C2A-C3A
28	c	519	DGD	O1G-C1A-C2A-C3A
27	a	412	SQD	C24-C25-C26-C27
25	E	101	STE	O2-C1-C2-C3
25	e	101	STE	O2-C1-C2-C3
22	c	510	CLA	CAA-CBA-CGA-O2A
25	I	101	STE	C2-C3-C4-C5
25	i	101	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	C14-C13-C15-C16
22	B	615	CLA	C11-C12-C13-C14
22	b	606	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C9
22	b	616	CLA	C11-C12-C13-C14
25	B	622	STE	O1-C1-C2-C3
27	B	620	SQD	C16-C17-C18-C19
22	B	608	CLA	O1A-CGA-O2A-C1
22	b	609	CLA	O1A-CGA-O2A-C1
25	t	101	STE	O2-C1-C2-C3
35	V	201	HEC	CAD-CBD-CGD-O2D
22	B	613	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	CAD-CBD-CGD-O2D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	c	503	CLA	CAD-CBD-CGD-O2D
22	c	512	CLA	CAD-CBD-CGD-O2D
27	B	620	SQD	C14-C15-C16-C17
22	b	602	CLA	CAA-CBA-CGA-O2A
31	A	420	LHG	C14-C15-C16-C17
22	B	602	CLA	C16-C17-C18-C20
22	b	603	CLA	C16-C17-C18-C20
25	E	101	STE	O1-C1-C2-C3
25	e	101	STE	O1-C1-C2-C3
32	J	102	LMT	O5'-C1'-O1'-C1
32	j	102	LMT	O5'-C1'-O1'-C1
22	B	615	CLA	C2-C3-C5-C6
22	b	616	CLA	C2-C3-C5-C6
22	B	601	CLA	CAA-CBA-CGA-O2A
32	c	525	LMT	C3-C4-C5-C6
26	D	408	LMG	C10-C11-C12-C13
25	c	521	STE	O2-C1-C2-C3
28	C	518	DGD	C4A-C5A-C6A-C7A
28	c	518	DGD	C4A-C5A-C6A-C7A
32	C	525	LMT	C11-C10-C9-C8
32	Z	101	LMT	C7-C8-C9-C10
22	b	614	CLA	C16-C17-C18-C20
25	C	521	STE	O2-C1-C2-C3
22	a	405	CLA	C2C-C3C-CAC-CBC
26	A	410	LMG	C19-C20-C21-C22
26	a	410	LMG	C19-C20-C21-C22
32	z	101	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	B	602	CLA	O2A-C1-C2-C3
22	C	509	CLA	O2A-C1-C2-C3
22	b	603	CLA	O2A-C1-C2-C3
22	c	509	CLA	O2A-C1-C2-C3
30	A	418	PHO	O2A-C1-C2-C3
30	a	418	PHO	O2A-C1-C2-C3
26	b	625	LMG	C16-C17-C18-C19
31	a	420	LHG	C27-C28-C29-C30
22	B	614	CLA	C2A-CAA-CBA-CGA
25	B	622	STE	O2-C1-C2-C3
25	t	101	STE	O1-C1-C2-C3
22	A	405	CLA	C2C-C3C-CAC-CBC
25	a	416	STE	C15-C16-C17-C18
22	B	613	CLA	C16-C17-C18-C20
26	d	408	LMG	C10-C11-C12-C13
32	c	525	LMT	C11-C10-C9-C8
22	A	405	CLA	CHA-CBD-CGD-O1D
22	A	405	CLA	CHA-CBD-CGD-O2D
22	A	419	CLA	CHA-CBD-CGD-O1D
22	A	419	CLA	CHA-CBD-CGD-O2D
22	B	601	CLA	CHA-CBD-CGD-O1D
22	B	602	CLA	CHA-CBD-CGD-O1D
22	B	602	CLA	CHA-CBD-CGD-O2D
22	B	604	CLA	CHA-CBD-CGD-O2D
22	B	605	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	a	405	CLA	CHA-CBD-CGD-O1D
22	a	405	CLA	CHA-CBD-CGD-O2D
22	a	419	CLA	CHA-CBD-CGD-O1D
22	a	419	CLA	CHA-CBD-CGD-O2D
22	b	602	CLA	CHA-CBD-CGD-O1D
22	b	603	CLA	CHA-CBD-CGD-O1D
22	b	603	CLA	CHA-CBD-CGD-O2D
22	b	605	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CHA-CBD-CGD-O2D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	CHA-CBD-CGD-O2D
22	C	506	CLA	C13-C15-C16-C17
25	c	521	STE	O1-C1-C2-C3
27	a	412	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	c	517	DGD	C2A-C3A-C4A-C5A
32	E	104	LMT	C1-C2-C3-C4
32	e	104	LMT	C1-C2-C3-C4
25	C	521	STE	O1-C1-C2-C3
26	B	624	LMG	C16-C17-C18-C19
31	l	101	LHG	C17-C18-C19-C20
32	C	525	LMT	C3-C4-C5-C6
22	c	506	CLA	C13-C15-C16-C17
28	C	517	DGD	C2A-C3A-C4A-C5A
31	A	420	LHG	C15-C16-C17-C18
31	L	101	LHG	C17-C18-C19-C20
28	A	413	DGD	O2G-C2G-C3G-O3G
26	B	624	LMG	C10-C11-C12-C13
25	A	416	STE	C15-C16-C17-C18
26	b	625	LMG	C10-C11-C12-C13
27	A	412	SQD	O47-C7-C8-C9
31	L	101	LHG	O7-C7-C8-C9
31	l	101	LHG	O7-C7-C8-C9
25	E	103	STE	C11-C10-C9-C8
25	e	103	STE	C11-C10-C9-C8
26	H	101	LMG	C32-C33-C34-C35
22	b	615	CLA	C2A-CAA-CBA-CGA
31	D	410	LHG	O1-C1-C2-O2
31	d	410	LHG	O1-C1-C2-O2
22	B	608	CLA	CBA-CGA-O2A-C1
22	b	609	CLA	CBA-CGA-O2A-C1
25	a	415	STE	C10-C11-C12-C13
22	C	505	CLA	C12-C13-C15-C16
22	c	505	CLA	C12-C13-C15-C16
28	H	103	DGD	C3B-C4B-C5B-C6B
28	h	103	DGD	C3B-C4B-C5B-C6B
31	D	410	LHG	C32-C33-C34-C35
31	a	420	LHG	C15-C16-C17-C18
22	B	606	CLA	C11-C12-C13-C14
22	B	613	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	a	405	CLA	C6-C7-C8-C9
22	b	614	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
22	c	508	CLA	C11-C10-C8-C9
27	B	620	SQD	C4-C5-C6-S

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Mol	Chain	Res	Type	Atoms
27	a	412	SQD	C15-C16-C17-C18
25	E	103	STE	C5-C6-C7-C8
25	e	103	STE	C5-C6-C7-C8
27	A	411	SQD	C8-C7-O47-C45
27	a	411	SQD	C8-C7-O47-C45
31	A	420	LHG	C8-C7-O7-C5
26	h	101	LMG	O9-C10-C11-C12
27	A	411	SQD	O49-C7-C8-C9
27	a	411	SQD	O49-C7-C8-C9
26	C	524	LMG	O8-C28-C29-C30
22	b	603	CLA	C16-C17-C18-C19
25	A	414	STE	C11-C12-C13-C14
31	L	101	LHG	C16-C17-C18-C19
32	J	102	LMT	C5-C6-C7-C8
22	b	602	CLA	CAA-CBA-CGA-O1A
31	l	101	LHG	C16-C17-C18-C19
22	B	612	CLA	C13-C15-C16-C17
22	b	613	CLA	C13-C15-C16-C17
27	B	620	SQD	C25-C26-C27-C28
32	j	102	LMT	C5-C6-C7-C8
28	A	413	DGD	CAA-CBA-CCA-CDA
22	B	602	CLA	C16-C17-C18-C19
22	B	607	CLA	C16-C17-C18-C20
22	B	609	CLA	C16-C17-C18-C19
22	b	608	CLA	C16-C17-C18-C20
22	b	610	CLA	C16-C17-C18-C19
22	B	601	CLA	CAA-CBA-CGA-O1A
26	H	101	LMG	O9-C10-C11-C12
22	B	604	CLA	C13-C15-C16-C17
22	C	510	CLA	CAA-CBA-CGA-O1A
28	C	517	DGD	O1B-C1B-C2B-C3B
28	c	517	DGD	O1B-C1B-C2B-C3B
22	B	608	CLA	C2A-CAA-CBA-CGA
22	b	609	CLA	C2A-CAA-CBA-CGA
26	c	524	LMG	O10-C28-C29-C30
27	a	412	SQD	O49-C7-C8-C9
25	a	414	STE	C11-C12-C13-C14
22	b	605	CLA	C13-C15-C16-C17
26	C	524	LMG	O10-C28-C29-C30
27	A	412	SQD	O49-C7-C8-C9
22	c	510	CLA	CAA-CBA-CGA-O1A
26	c	524	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
23	T	101	BCR	C1-C6-C7-C8
23	T	101	BCR	C5-C6-C7-C8
23	t	102	BCR	C1-C6-C7-C8
23	t	102	BCR	C5-C6-C7-C8
32	Z	101	LMT	C5-C6-C7-C8
31	a	420	LHG	C8-C7-O7-C5
22	A	405	CLA	C11-C12-C13-C15
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	607	CLA	CAD-CBD-CGD-O1D
22	b	602	CLA	CAD-CBD-CGD-O1D
22	b	608	CLA	CAD-CBD-CGD-O1D
22	b	613	CLA	CAA-CBA-CGA-O2A
22	A	405	CLA	C6-C7-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	D	405	CLA	C6-C7-C8-C9
22	c	511	CLA	C6-C7-C8-C9
22	d	405	CLA	C6-C7-C8-C9
25	B	625	STE	C12-C13-C14-C15
26	B	624	LMG	C35-C36-C37-C38
22	B	603	CLA	C5-C6-C7-C8
28	C	517	DGD	C7A-C8A-C9A-CAA
22	B	612	CLA	CAA-CBA-CGA-O2A
22	b	604	CLA	C5-C6-C7-C8
25	b	623	STE	O1-C1-C2-C3
28	c	517	DGD	C7A-C8A-C9A-CAA
22	b	613	CLA	O1A-CGA-O2A-C1
22	a	405	CLA	C4C-C3C-CAC-CBC
22	C	501	CLA	CAA-CBA-CGA-O2A
31	D	410	LHG	O8-C23-C24-C25
31	d	410	LHG	O8-C23-C24-C25
32	z	101	LMT	C5-C6-C7-C8
26	b	625	LMG	C35-C36-C37-C38
22	B	612	CLA	O1A-CGA-O2A-C1
22	C	506	CLA	C11-C10-C8-C7
22	C	508	CLA	C11-C10-C8-C7
22	C	512	CLA	C2-C3-C5-C6
22	a	405	CLA	C6-C7-C8-C10
22	b	607	CLA	C11-C12-C13-C15
22	b	615	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	c	508	CLA	C11-C10-C8-C7
22	c	512	CLA	C2-C3-C5-C6

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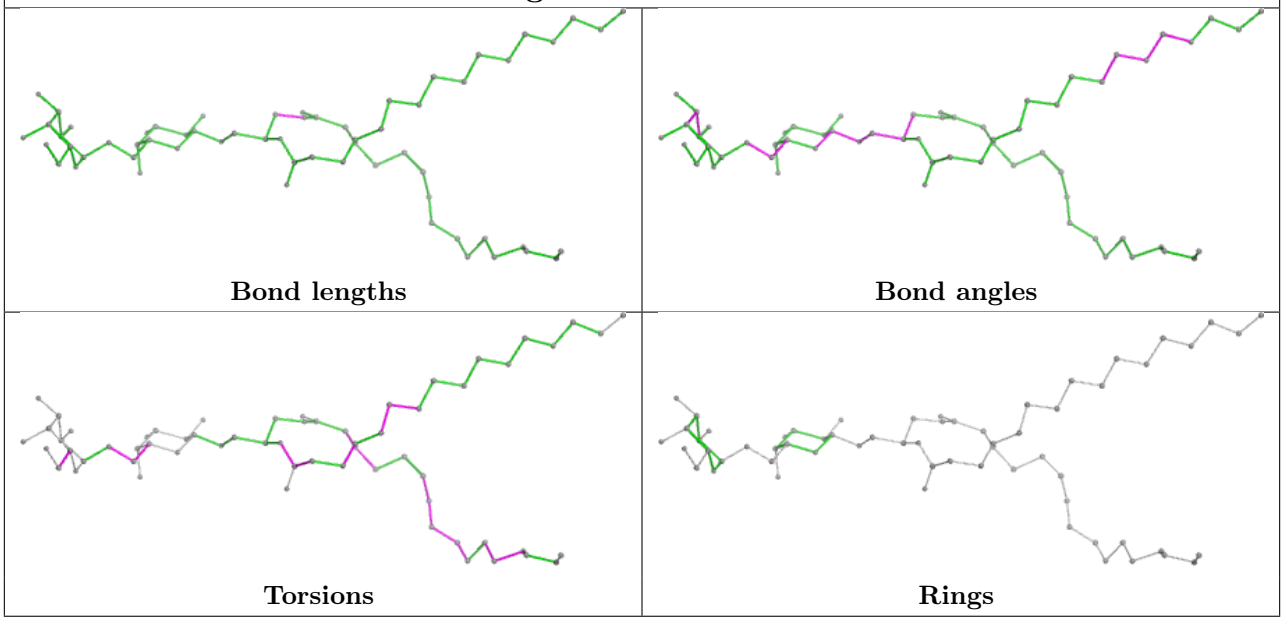
Mol	Chain	Res	Type	Atoms
31	L	101	LHG	O9-C7-C8-C9
31	l	101	LHG	O9-C7-C8-C9
22	c	501	CLA	CAA-CBA-CGA-O2A
22	A	405	CLA	C4C-C3C-CAC-CBC
31	a	420	LHG	O9-C7-C8-C9
25	C	516	STE	O1-C1-C2-C3
25	c	516	STE	O1-C1-C2-C3
23	H	102	BCR	C15-C16-C17-C18
22	B	613	CLA	CAA-CBA-CGA-O2A
22	b	614	CLA	CAA-CBA-CGA-O2A
26	C	520	LMG	O6-C1-O1-C7
28	C	517	DGD	O6E-C1E-O5D-C6D
22	C	512	CLA	C15-C16-C17-C18
32	c	525	LMT	C5'-C4'-O1B-C1B
31	A	420	LHG	O9-C7-C8-C9
31	d	410	LHG	C27-C28-C29-C30
22	C	505	CLA	CAA-CBA-CGA-O2A
22	c	505	CLA	CAA-CBA-CGA-O2A
22	B	612	CLA	C8-C10-C11-C12
22	b	613	CLA	C8-C10-C11-C12
26	C	520	LMG	O10-C28-C29-C30
26	c	520	LMG	O10-C28-C29-C30
32	C	525	LMT	C5'-C4'-O1B-C1B

There are no ring outliers.

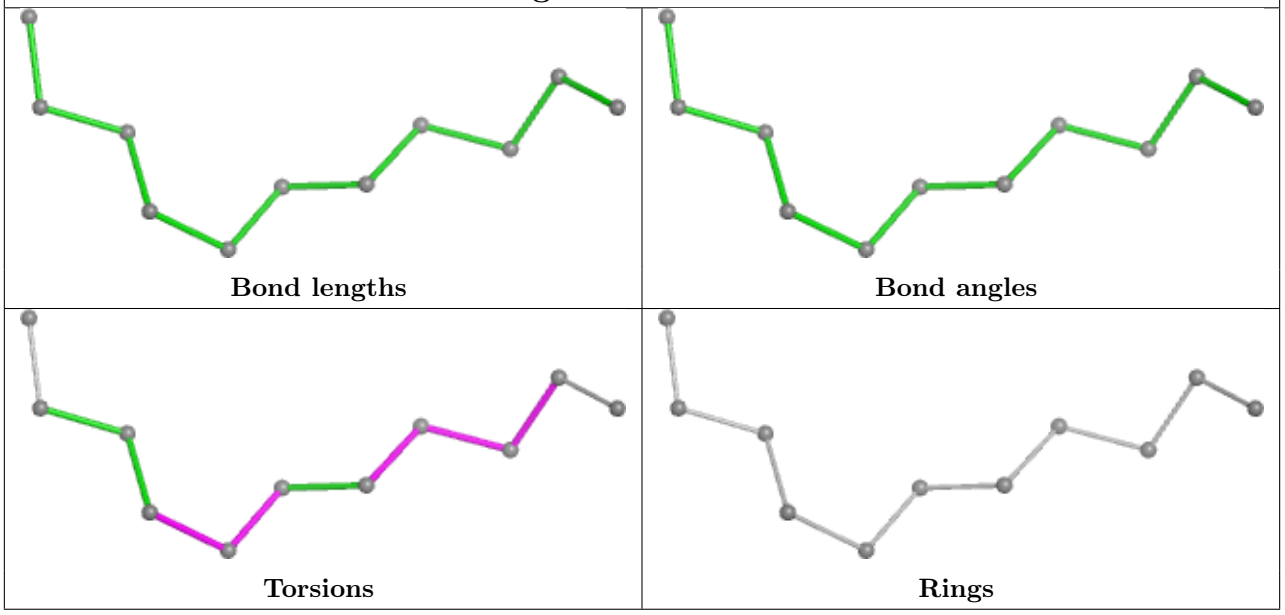
No monomer is involved in short contacts.

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.

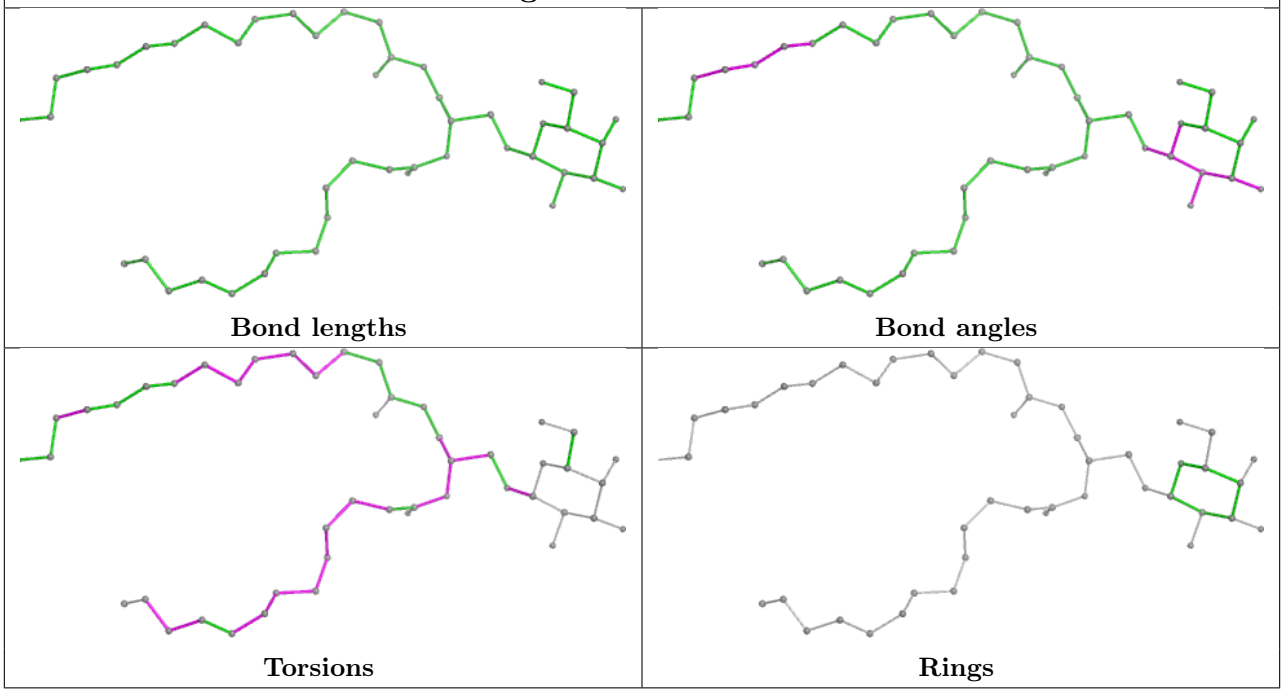
Ligand DGD c 517



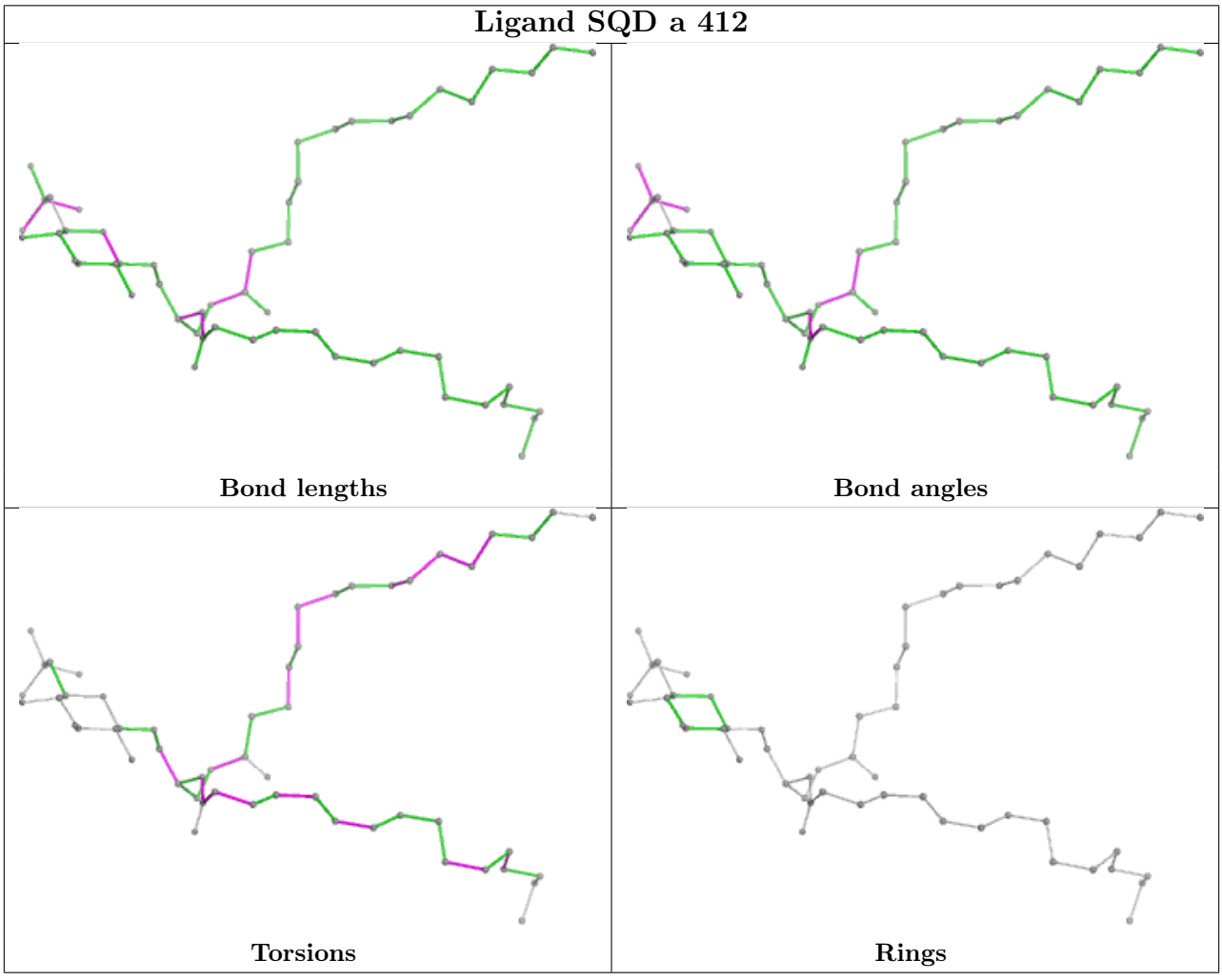
Ligand STE a 415



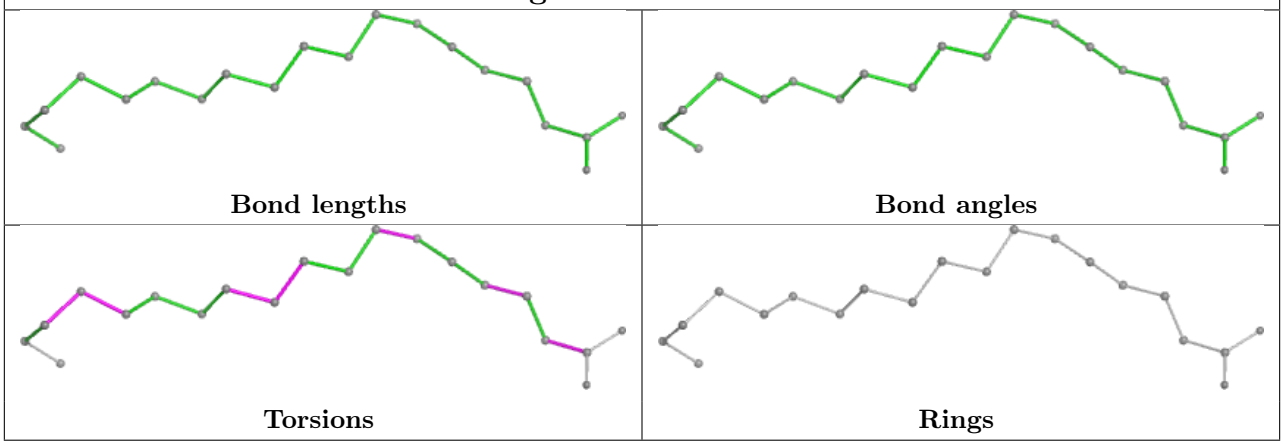
Ligand LMG A 410



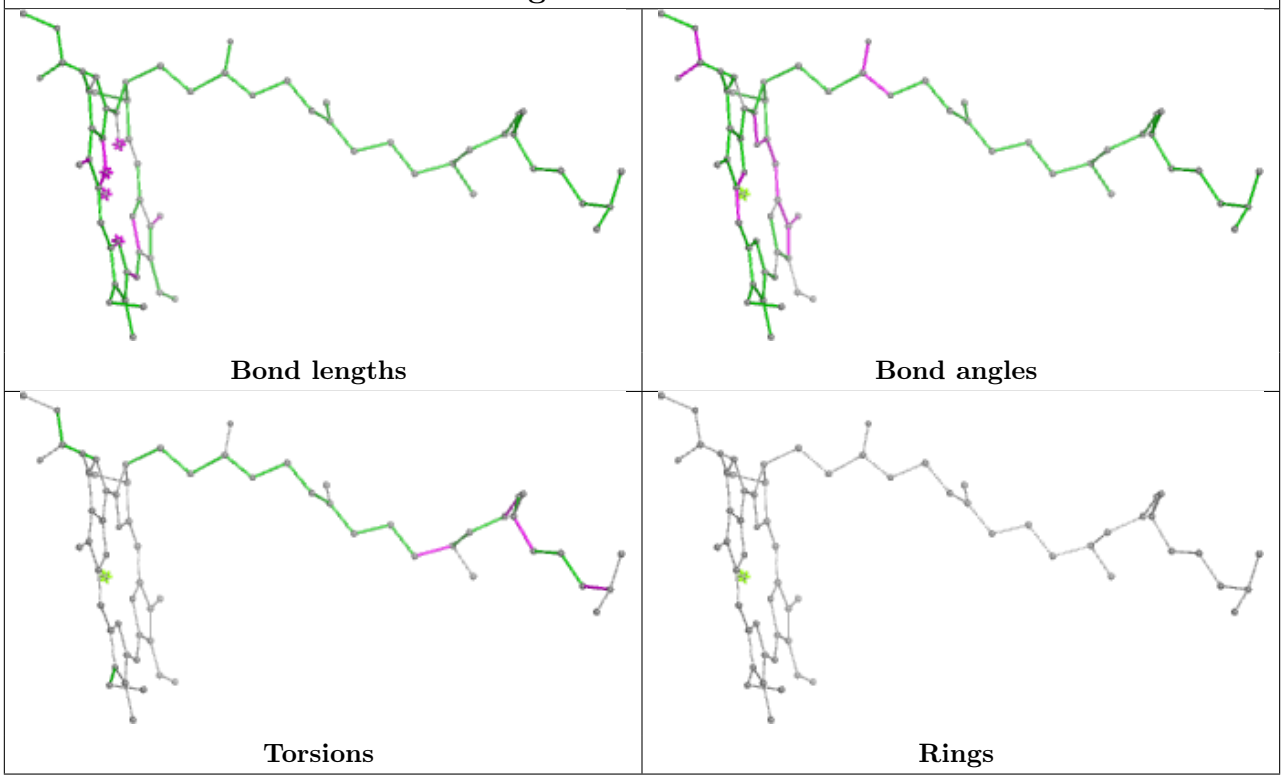
Ligand SQD a 412



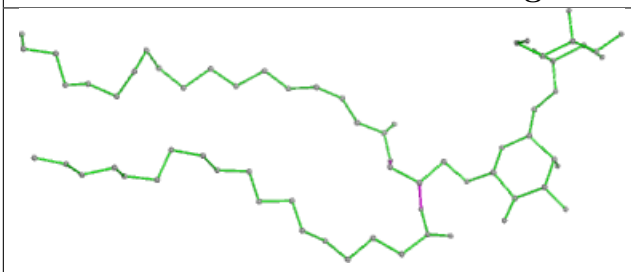
Ligand STE E 103



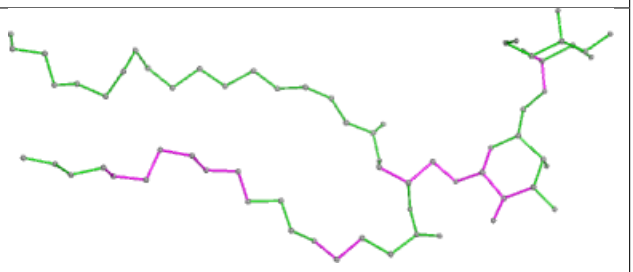
Ligand CLA d 405



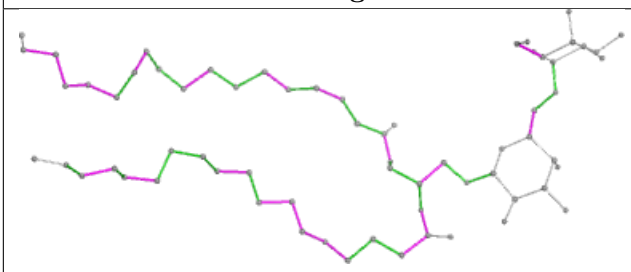
Ligand DGD a 413



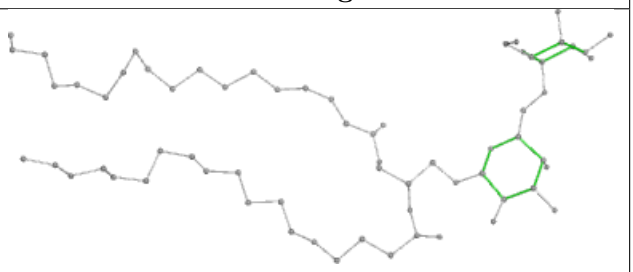
Bond lengths



Bond angles

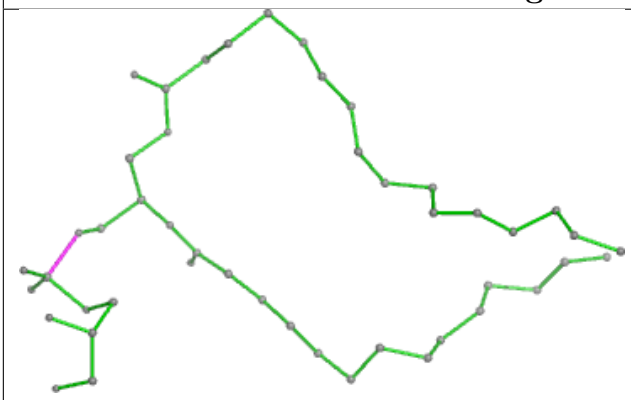


Torsions

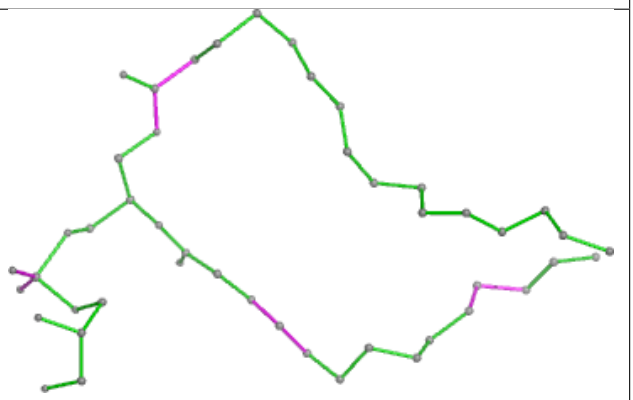


Rings

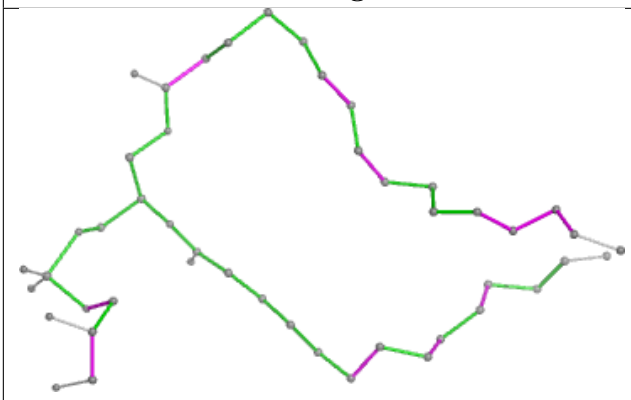
Ligand LHG d 410



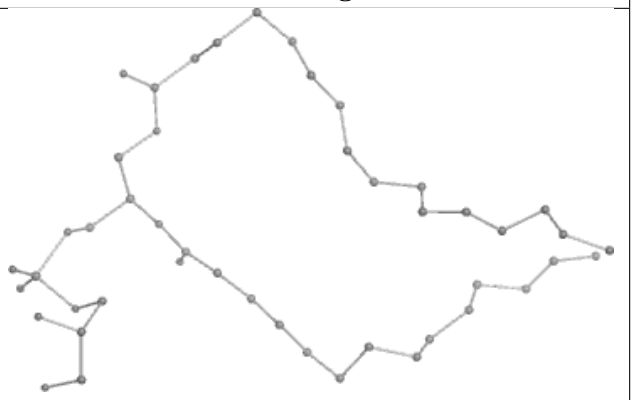
Bond lengths



Bond angles

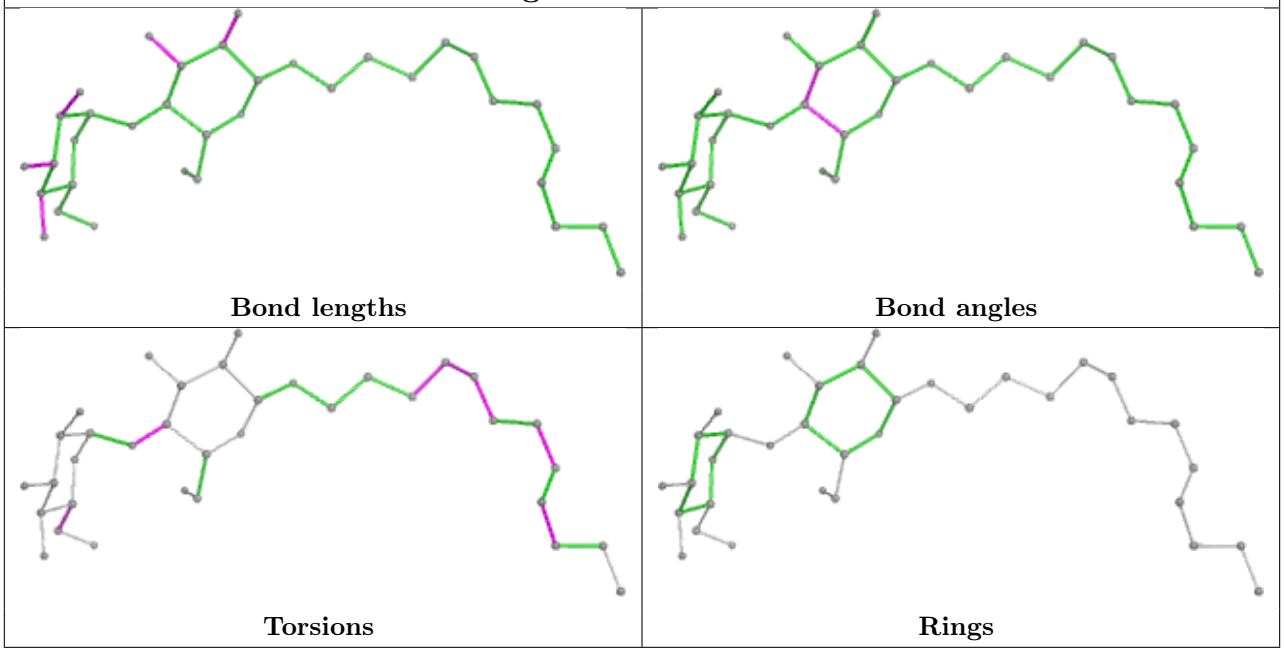


Torsions

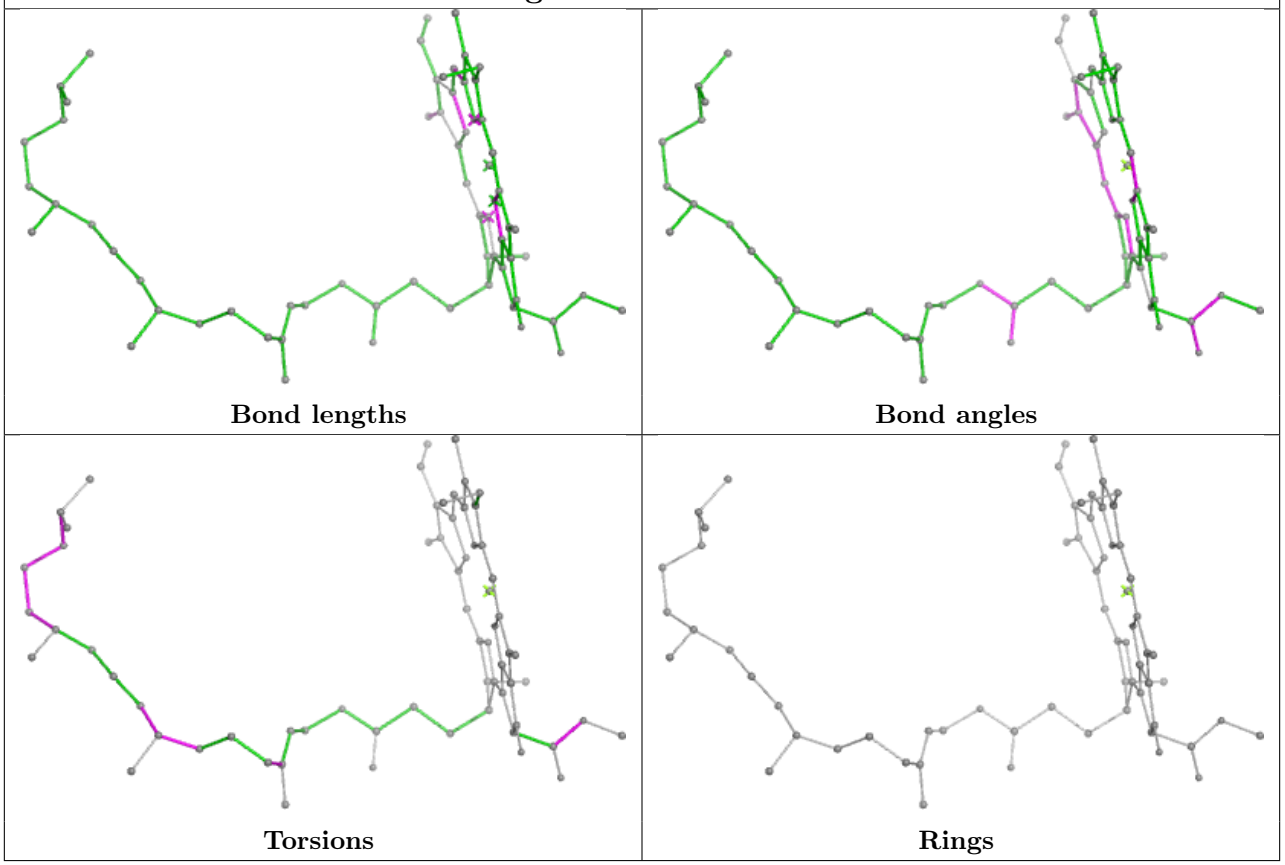


Rings

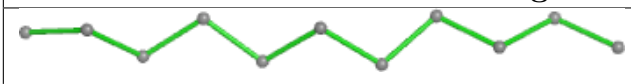
Ligand LMT C 525



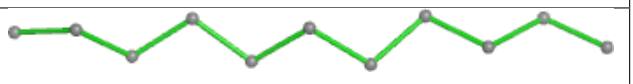
Ligand CLA C 506



Ligand STE k 102

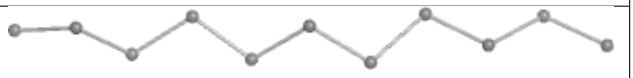


Bond lengths



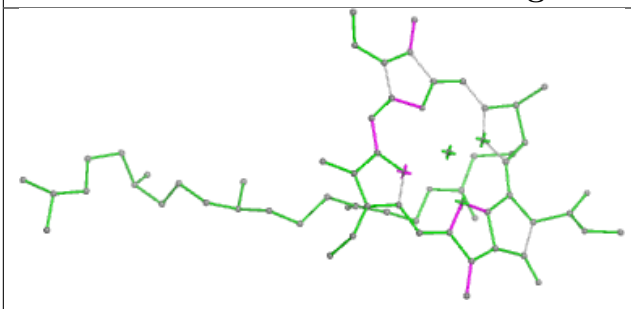
Bond angles

Torsions

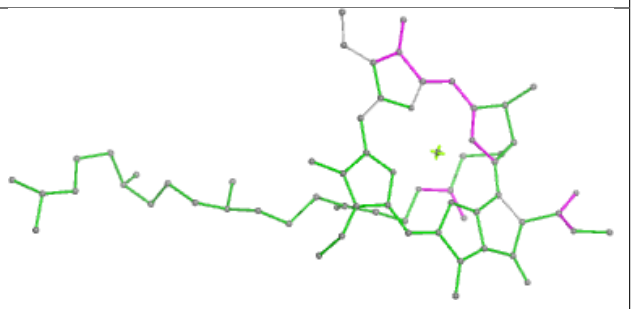


Rings

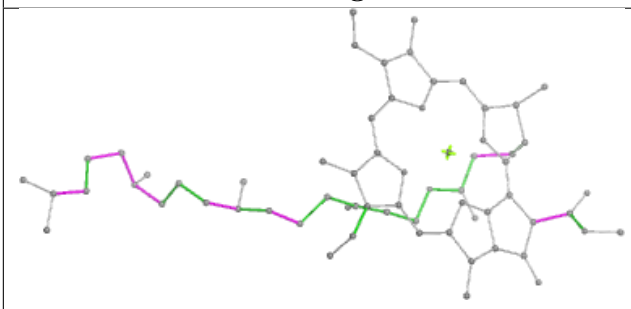
Ligand CLA b 615



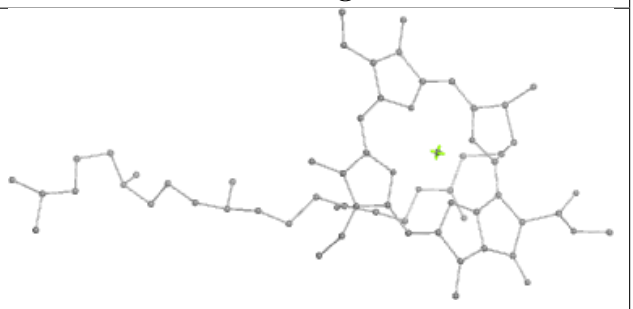
Bond lengths



Bond angles

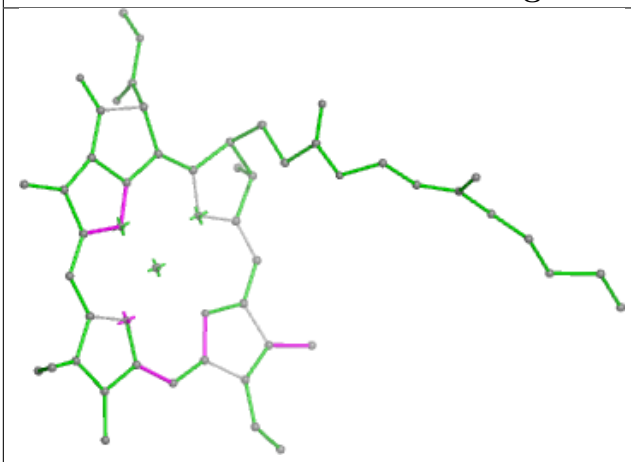


Torsions

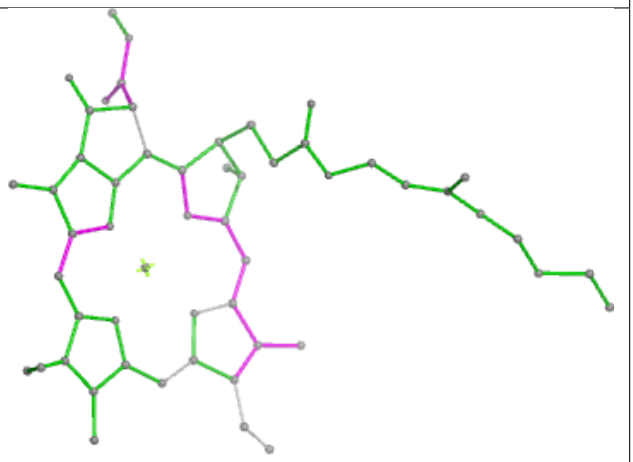


Rings

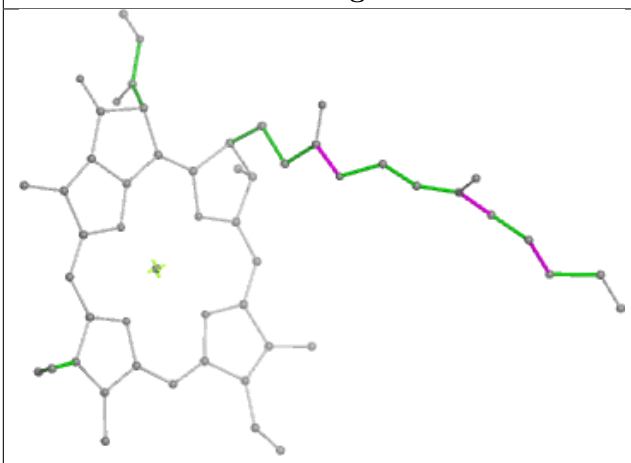
Ligand CLA A 406



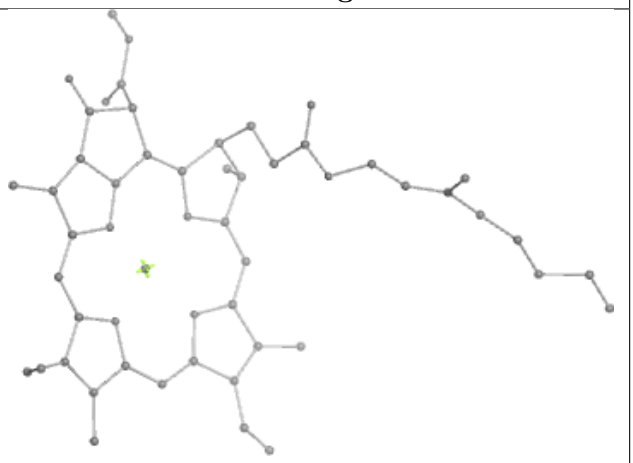
Bond lengths



Bond angles

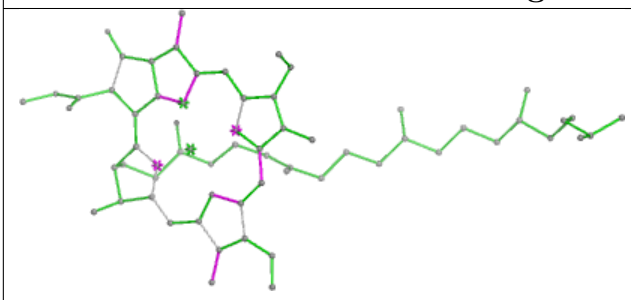


Torsions

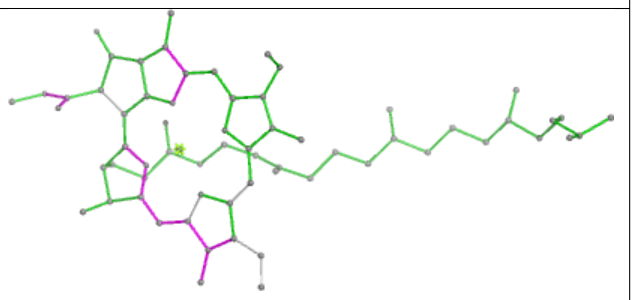


Rings

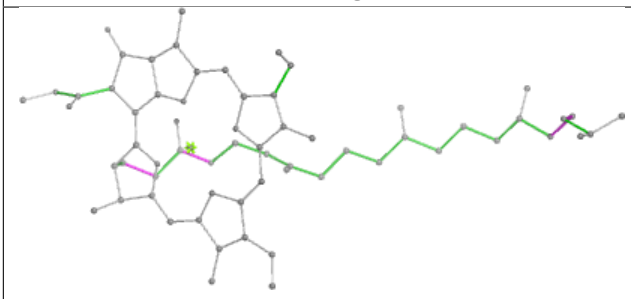
Ligand CLA b 609



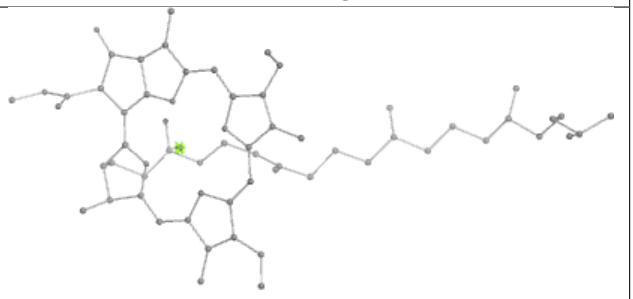
Bond lengths



Bond angles

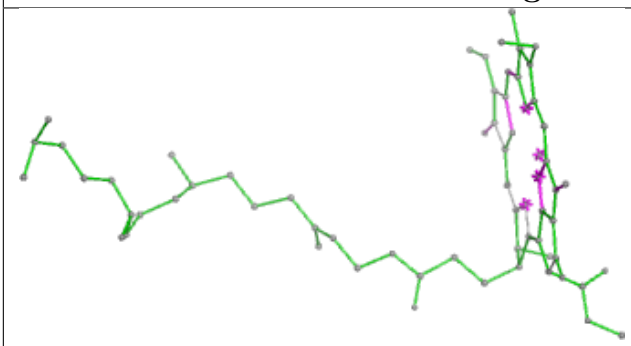


Torsions

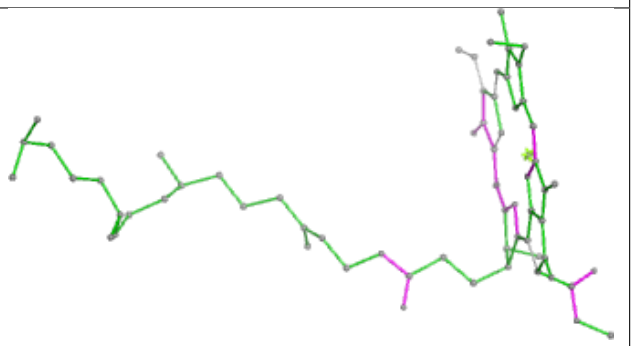


Rings

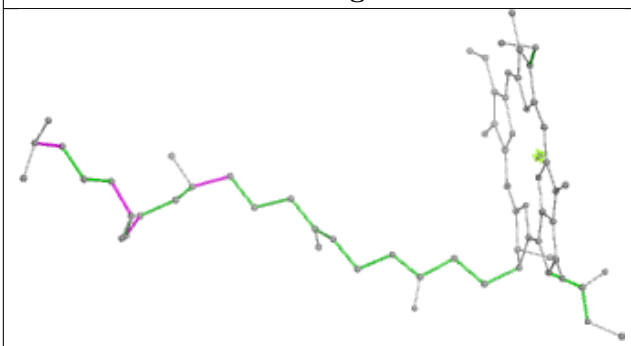
Ligand CLA D 405



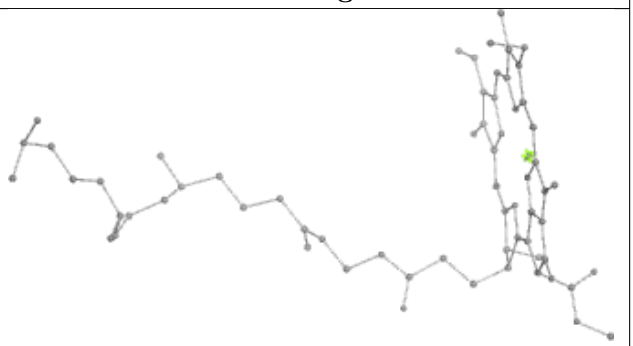
Bond lengths



Bond angles

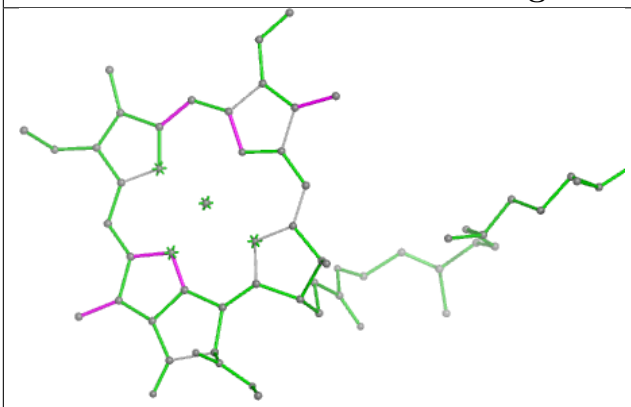


Torsions

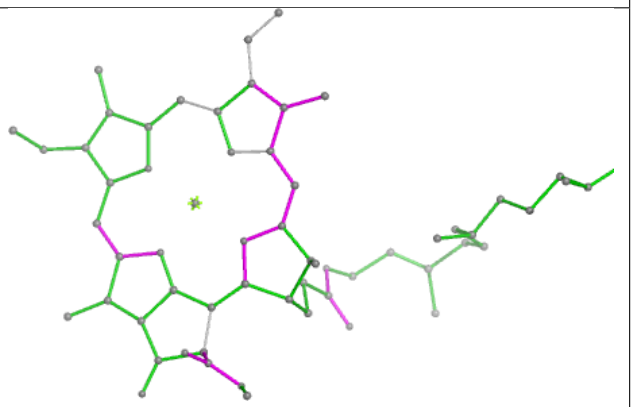


Rings

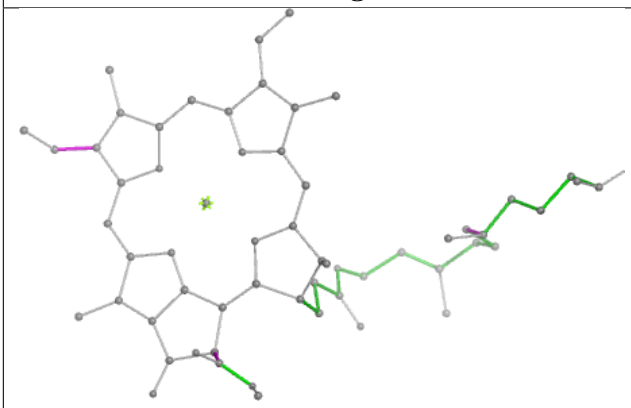
Ligand CLA a 405



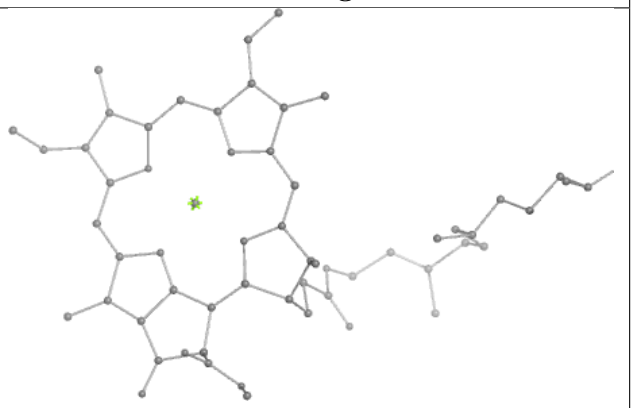
Bond lengths



Bond angles

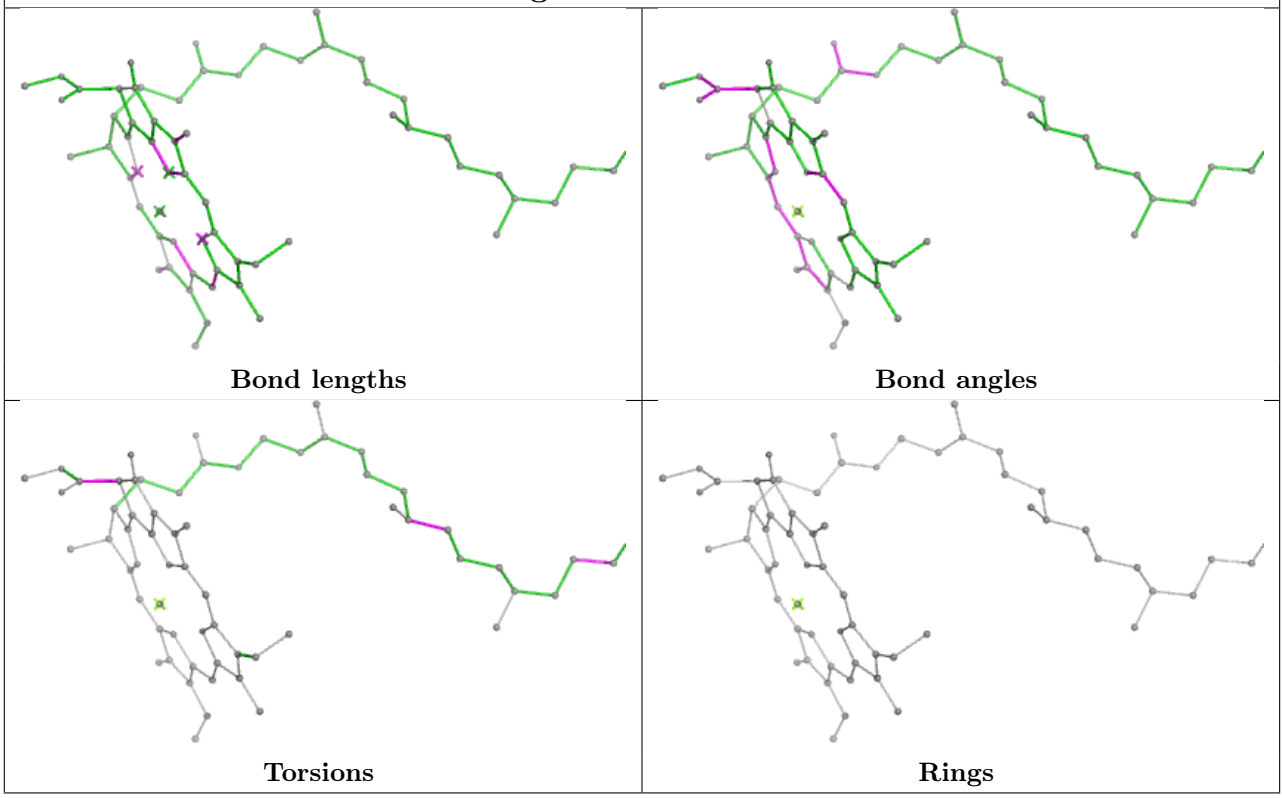


Torsions

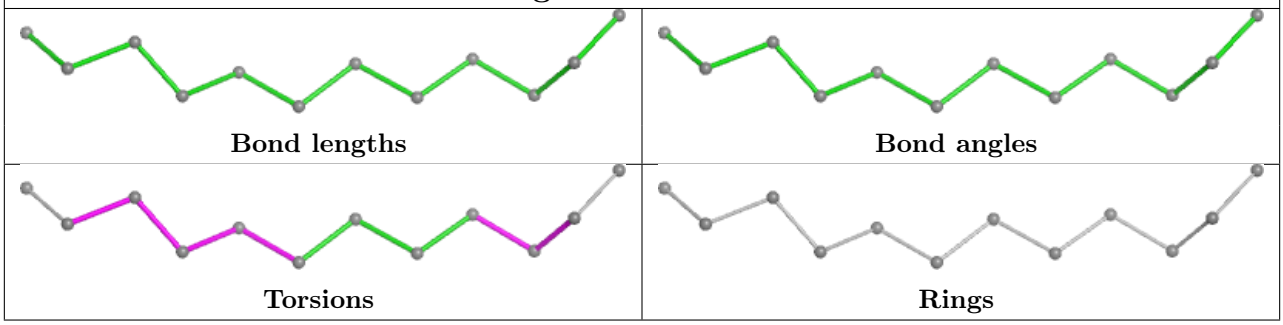


Rings

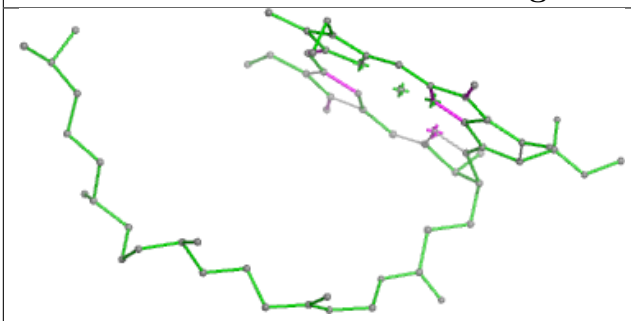
Ligand CLA c 508



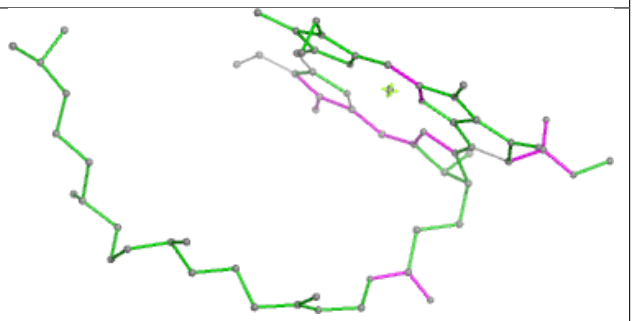
Ligand STE e 102



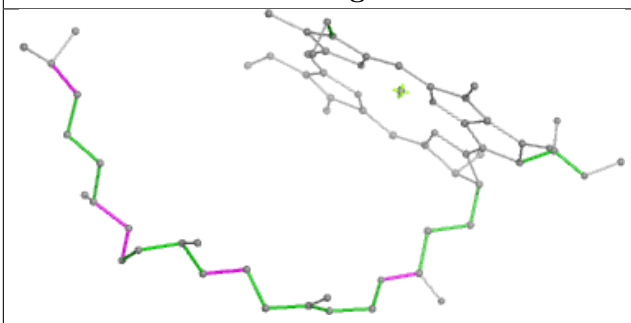
Ligand CLA c 513



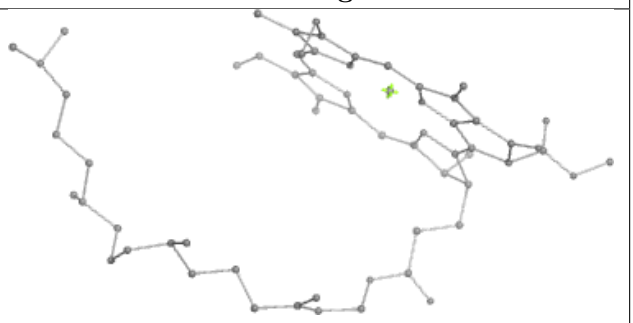
Bond lengths



Bond angles

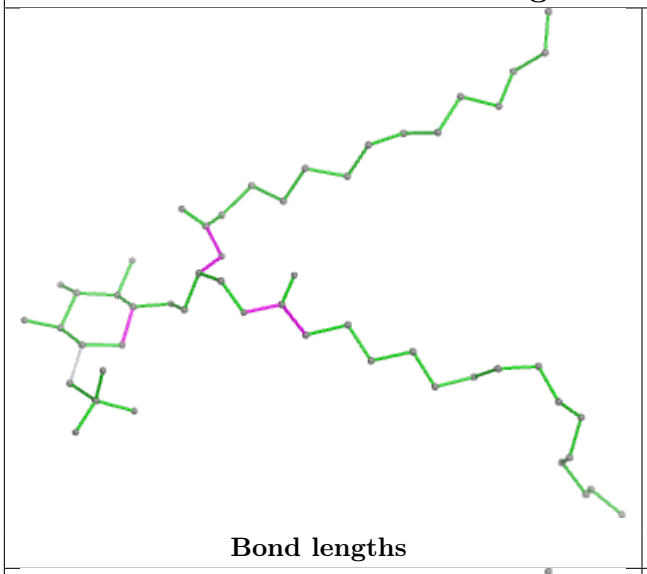


Torsions

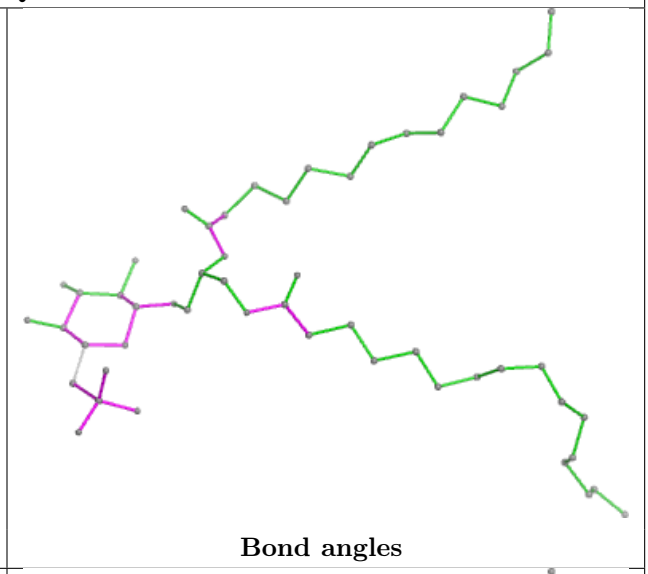


Rings

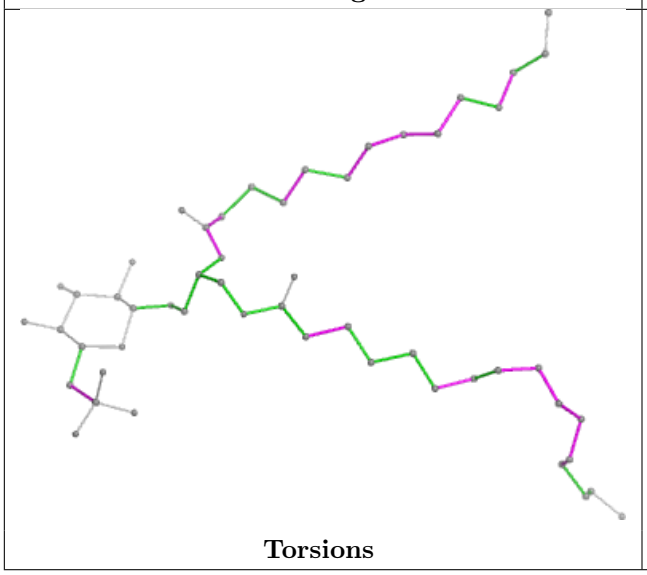
Ligand SQD a 411



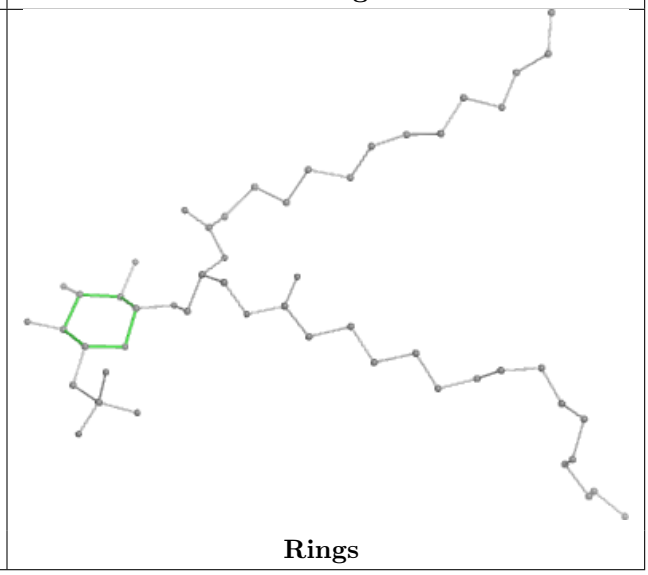
Bond lengths



Bond angles

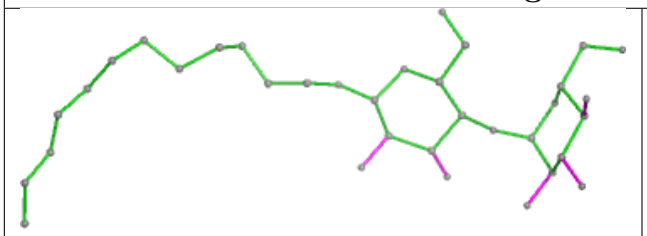


Torsions

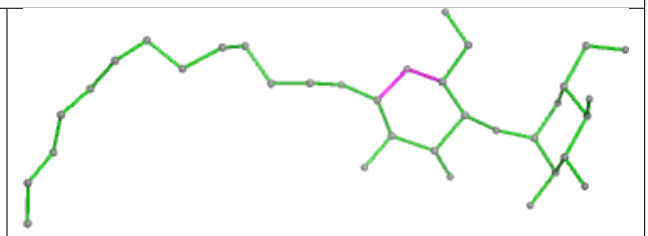


Rings

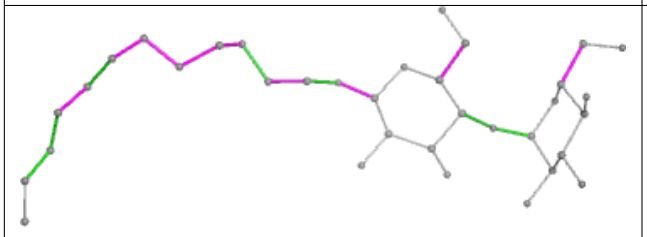
Ligand LMT Z 101



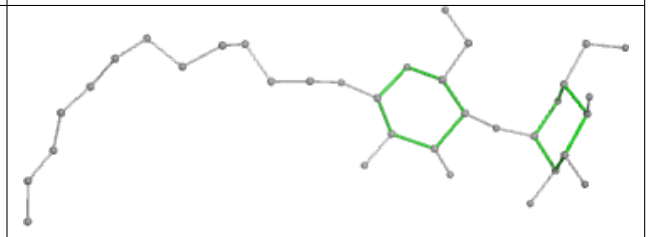
Bond lengths



Bond angles

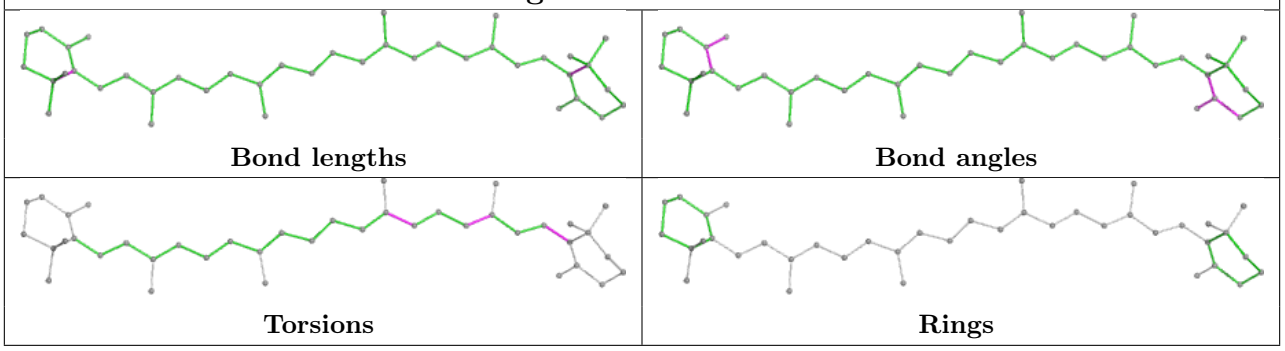


Torsions

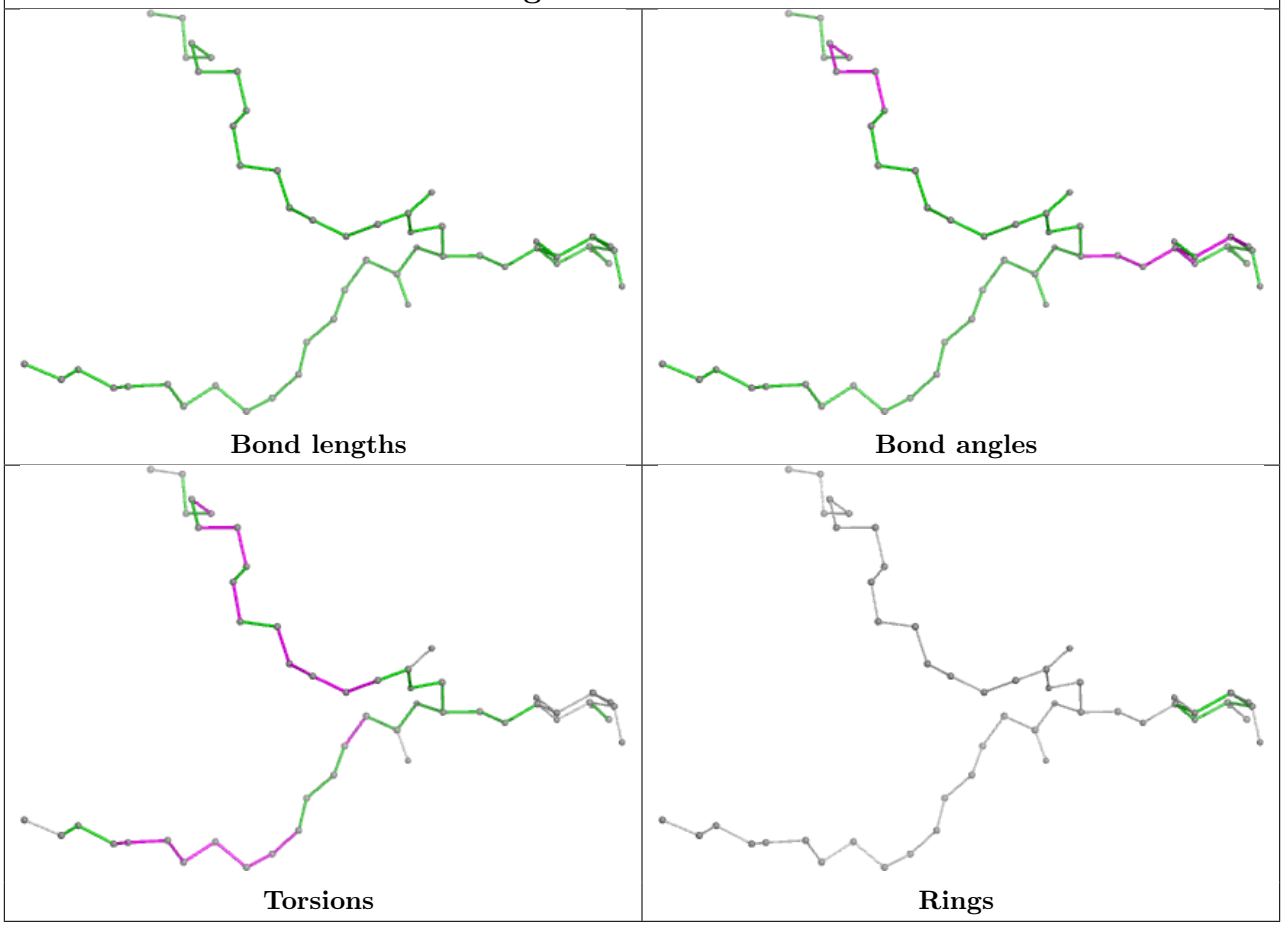


Rings

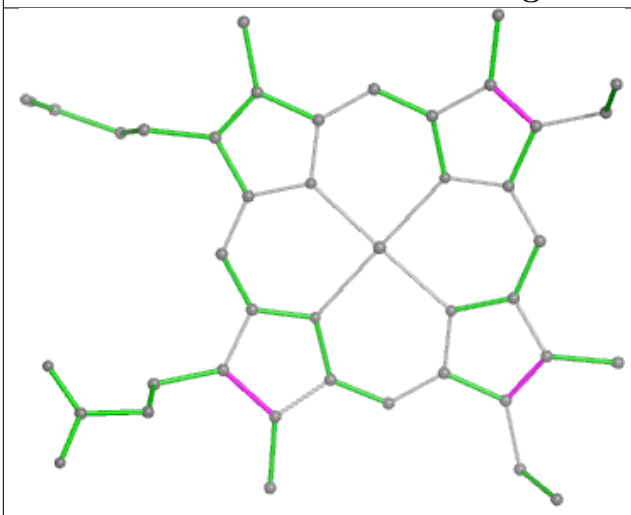
Ligand BCR b 619



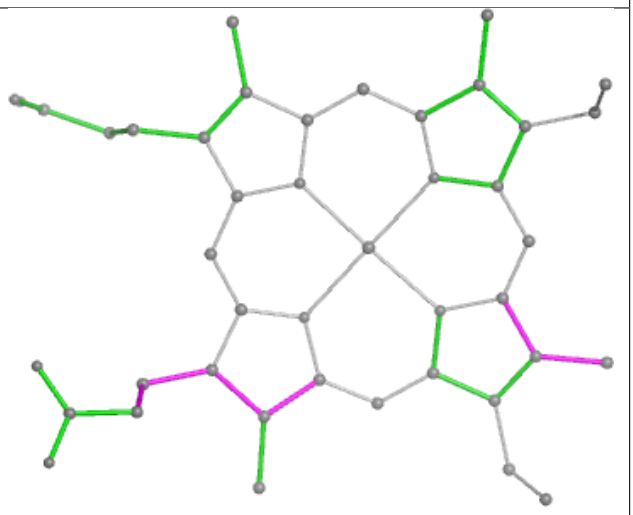
Ligand LMG b 625



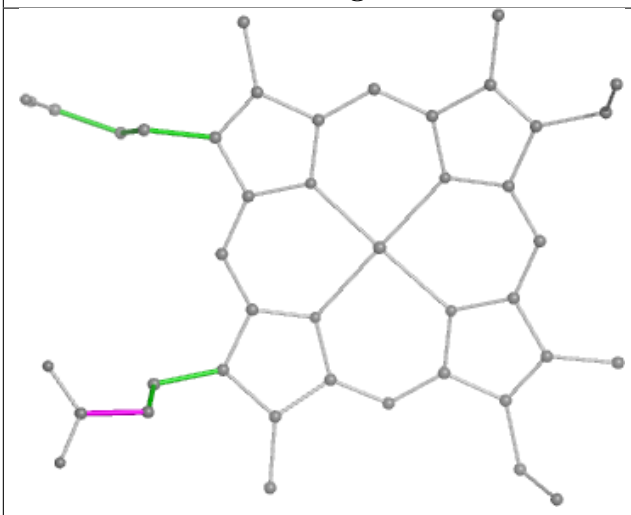
Ligand HEC V 201



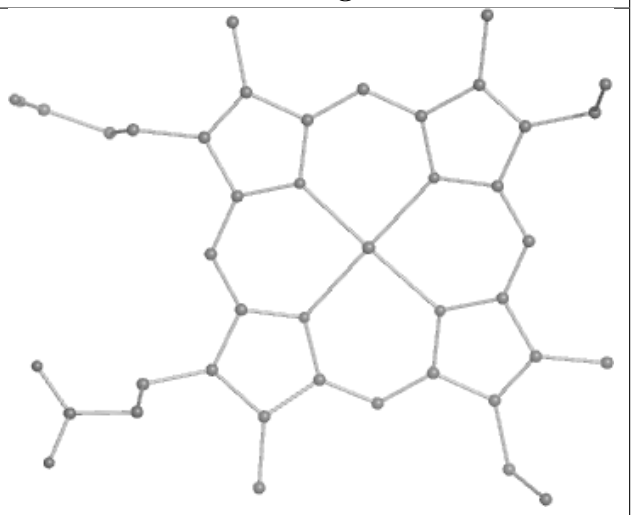
Bond lengths



Bond angles

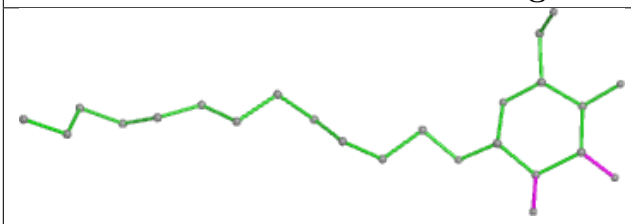


Torsions

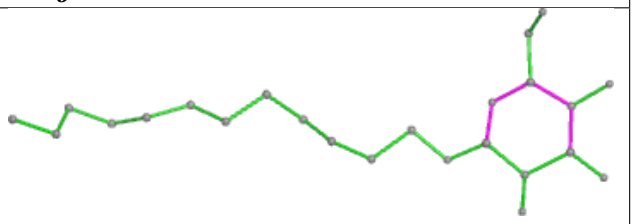


Rings

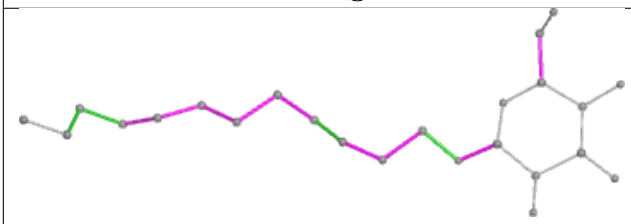
Ligand LMT j 102



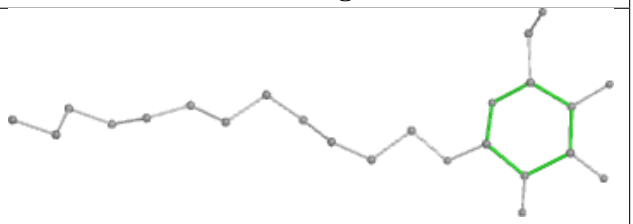
Bond lengths



Bond angles

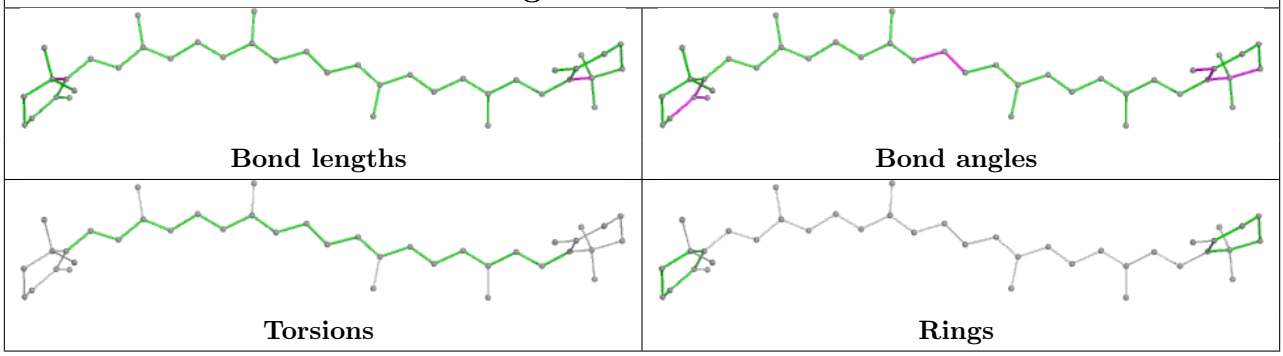


Torsions

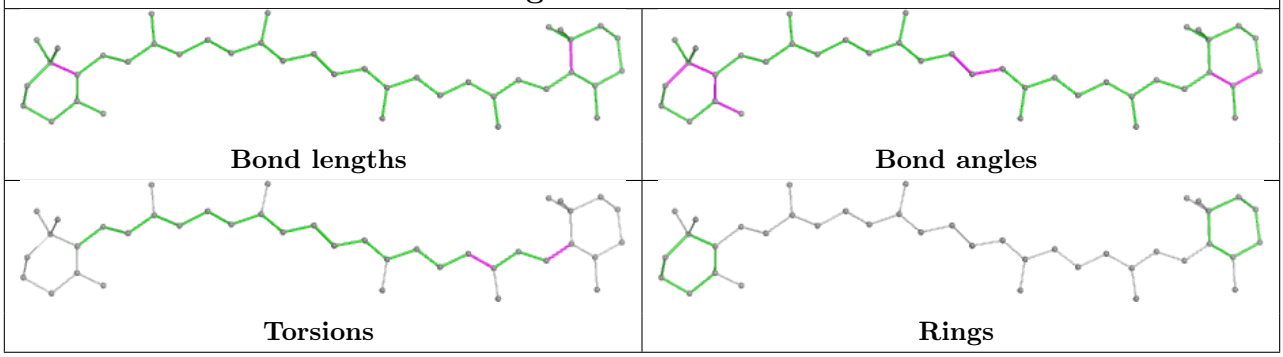


Rings

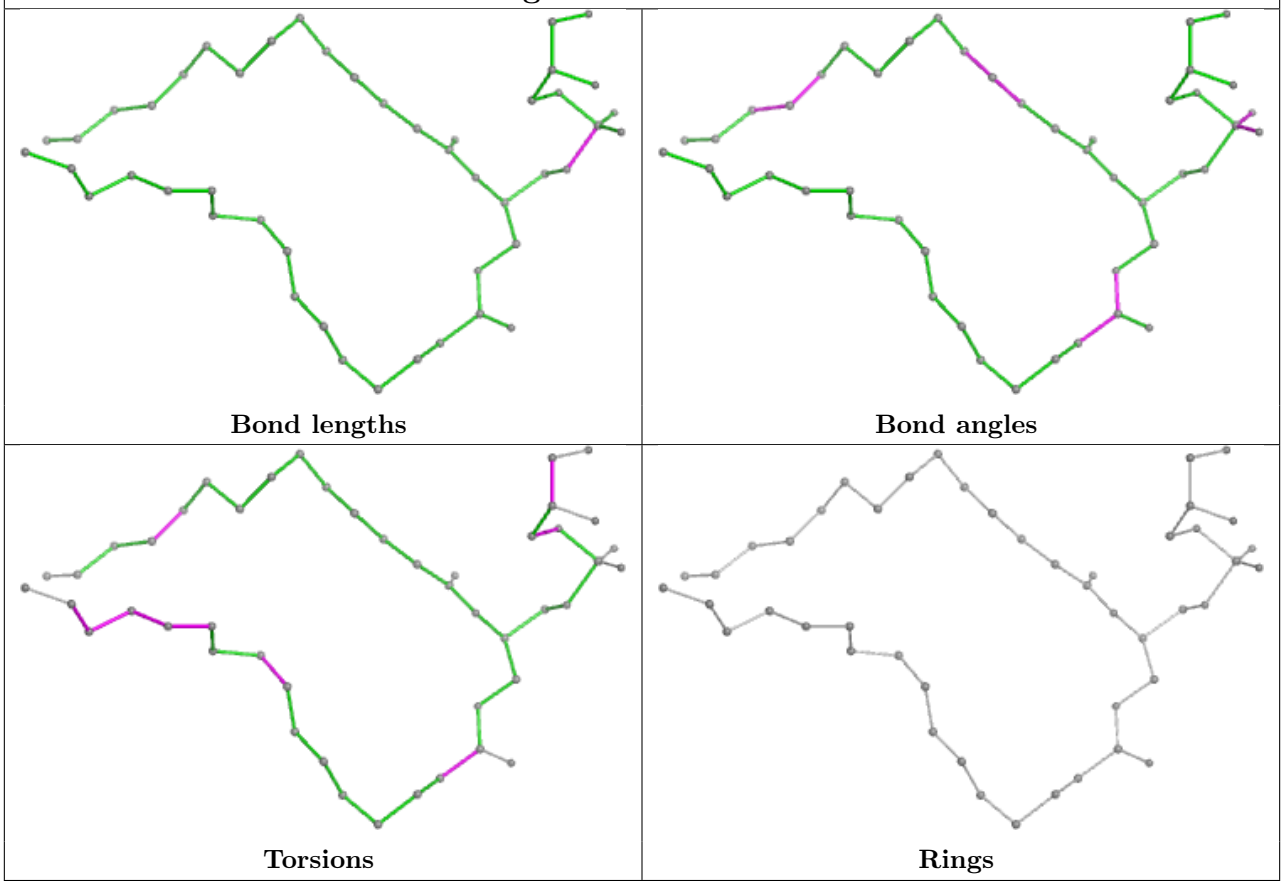
Ligand BCR C 515



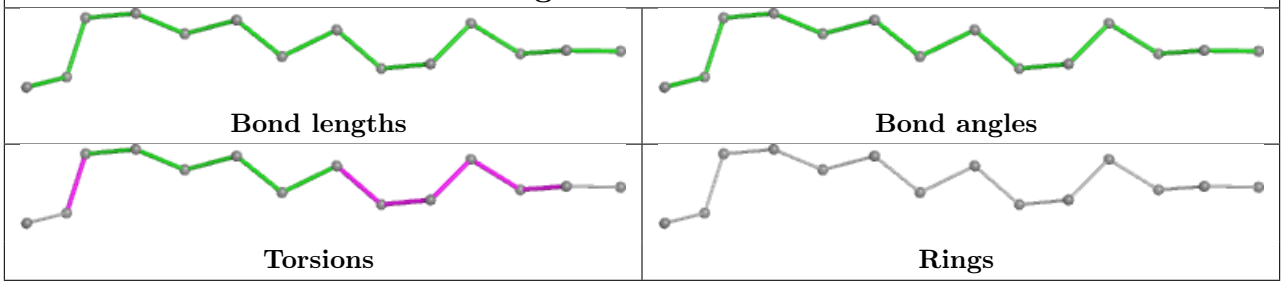
Ligand BCR d 406



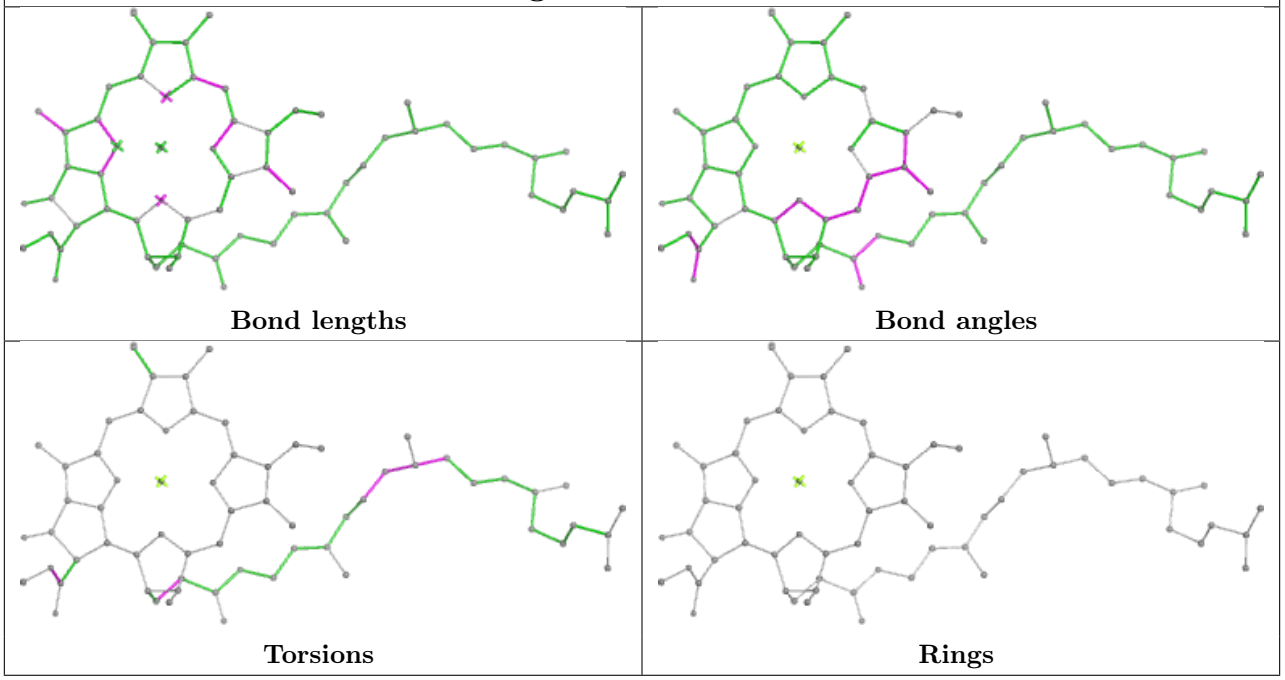
Ligand LHG D 410



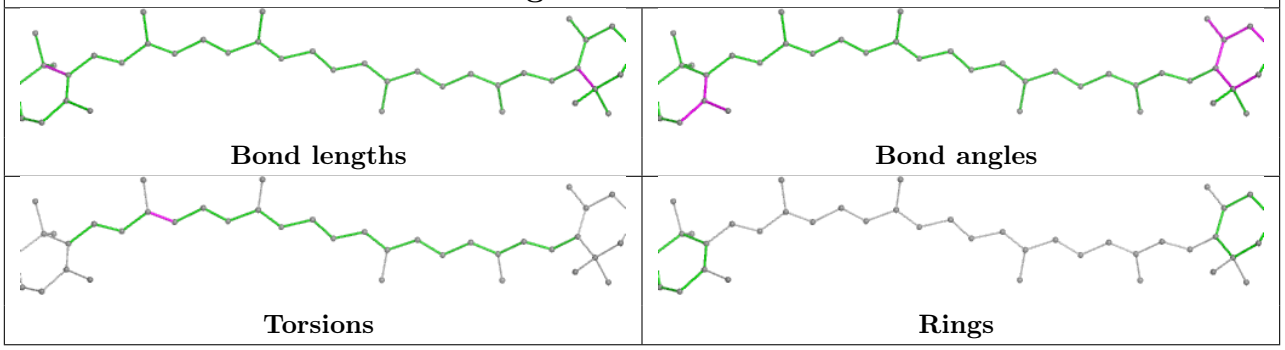
Ligand STE I 101



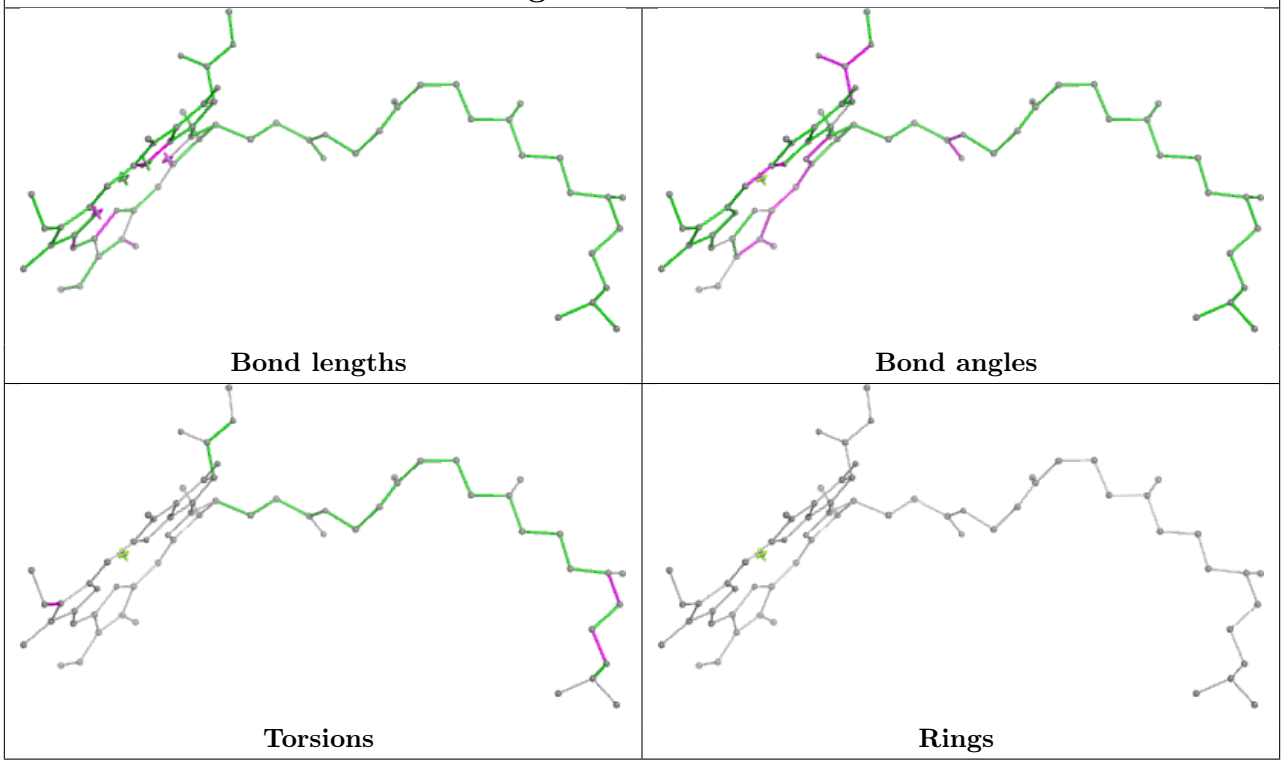
Ligand CLA b 604



Ligand BCR b 620



Ligand CLA d 404



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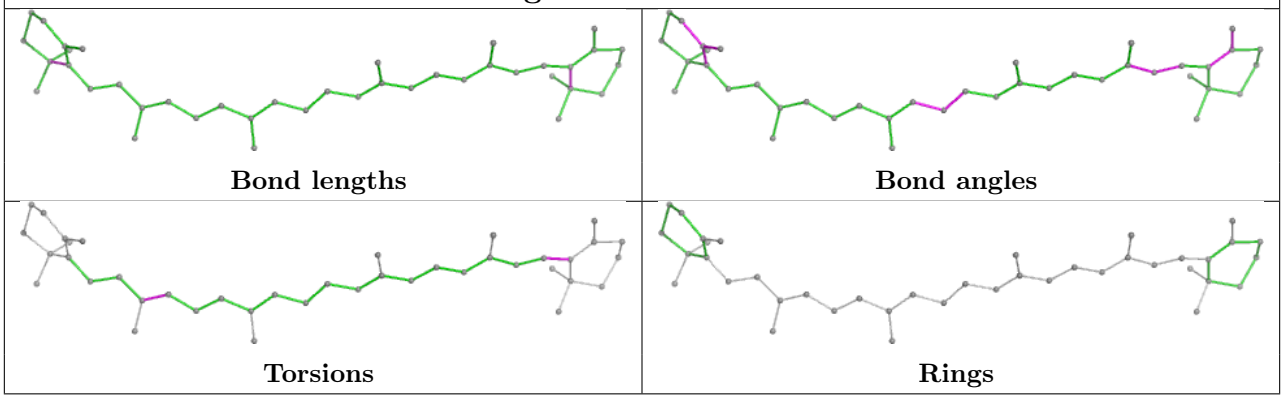
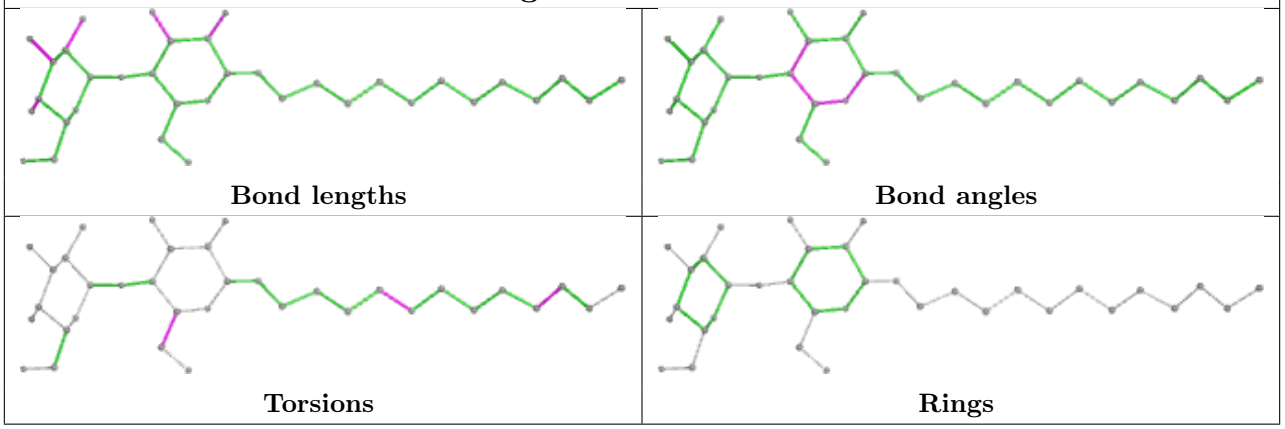
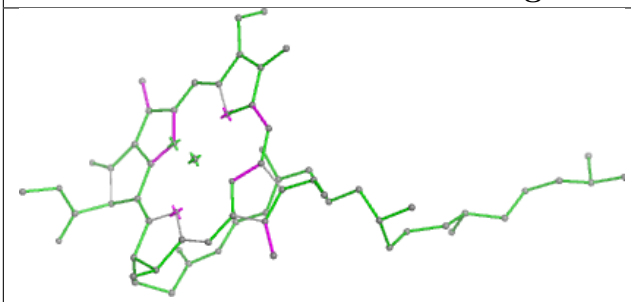


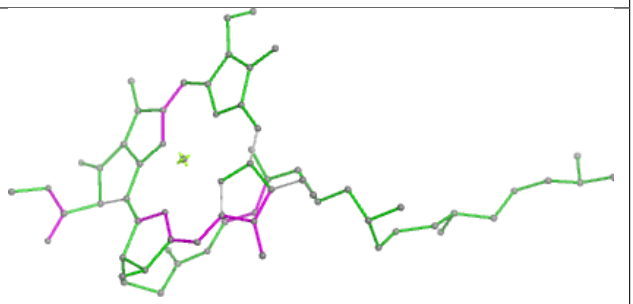
Ligand LMT m 101



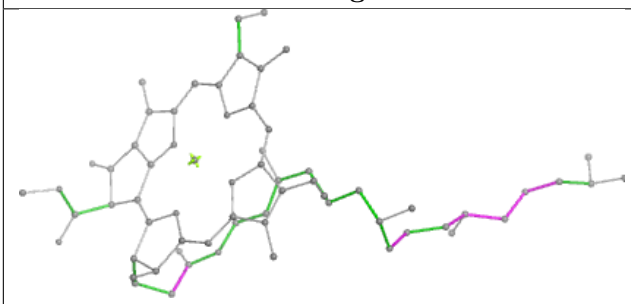
Ligand CLA C 505



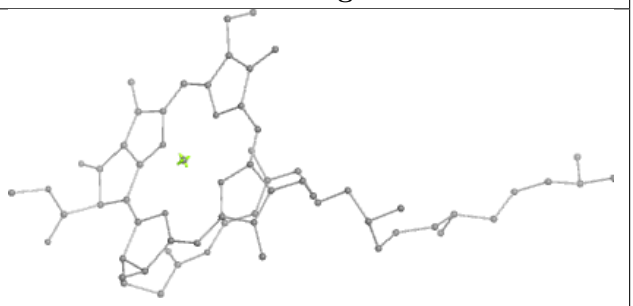
Bond lengths



Bond angles

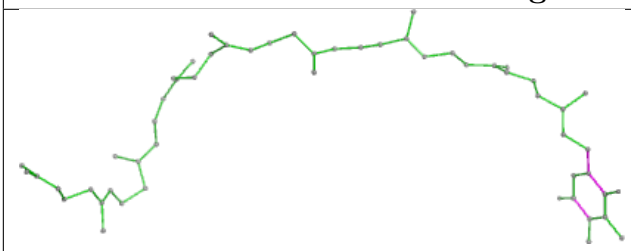


Torsions

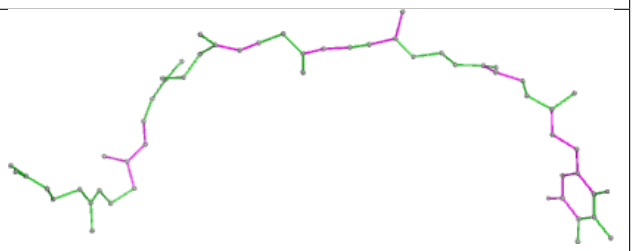


Rings

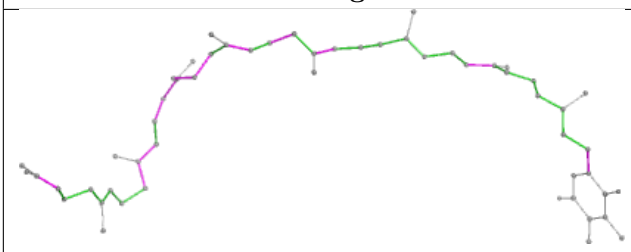
Ligand PL9 A 408



Bond lengths



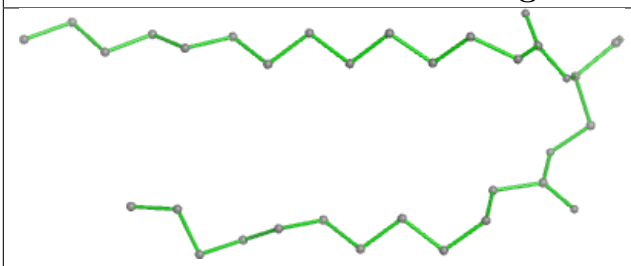
Bond angles



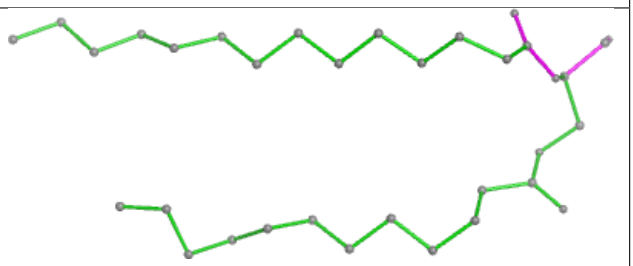
Torsions

Rings

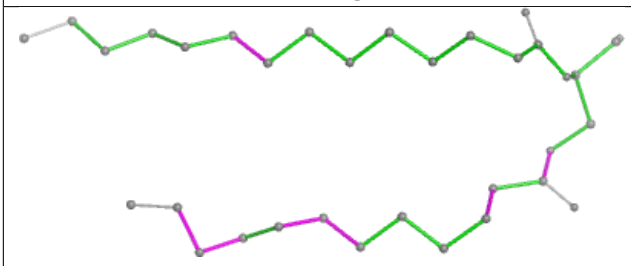
Ligand LMG D 402



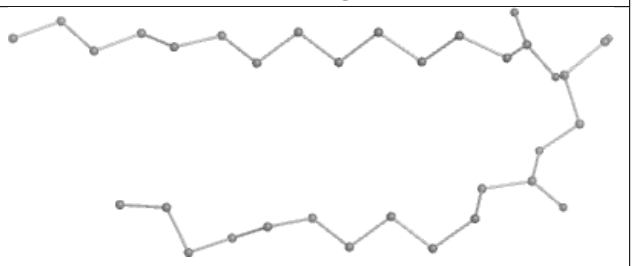
Bond lengths



Bond angles

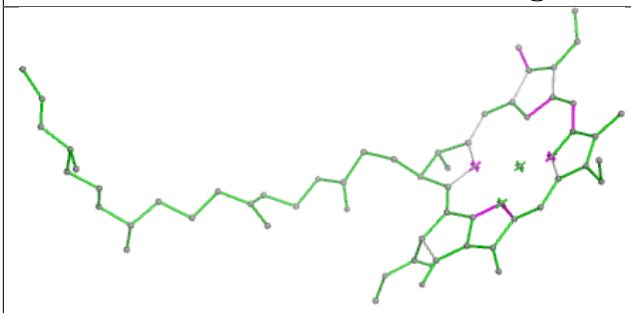


Torsions

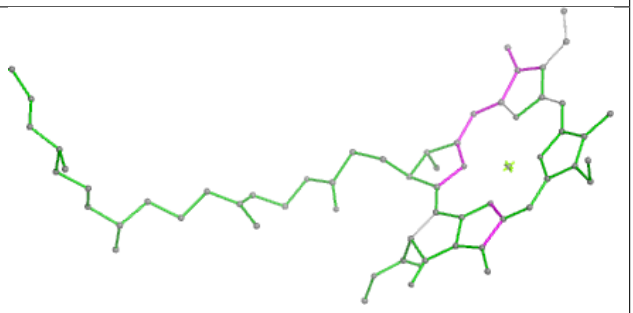


Rings

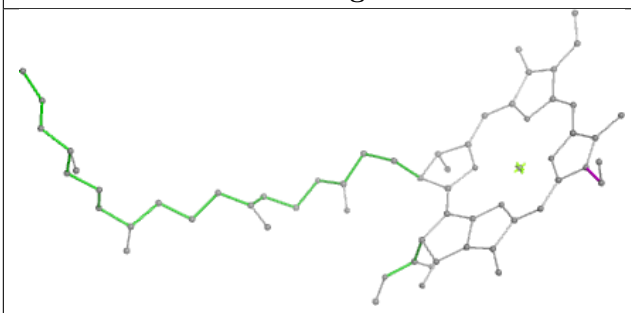
Ligand CLA a 404



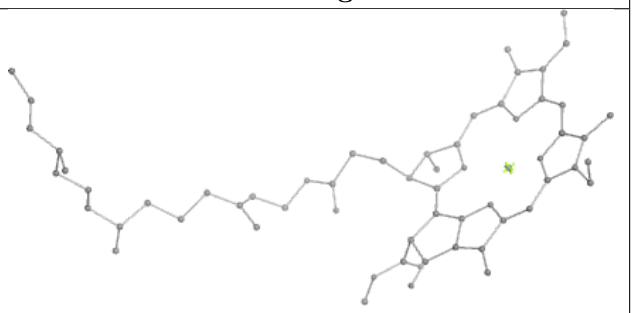
Bond lengths



Bond angles

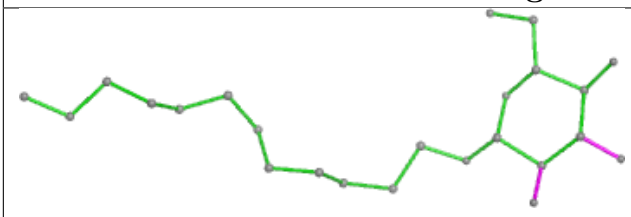


Torsions

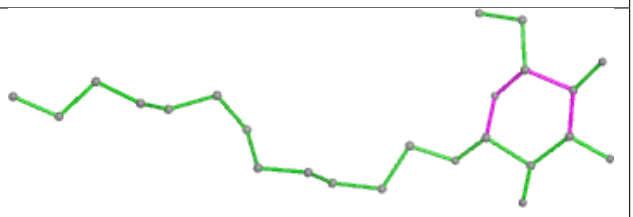


Rings

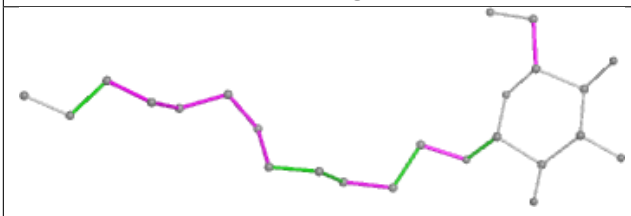
Ligand LMT e 104



Bond lengths



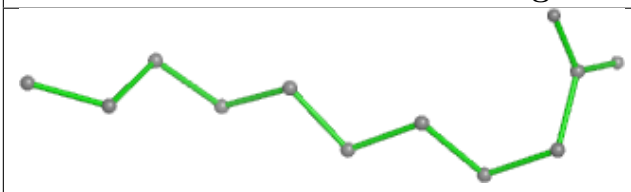
Bond angles



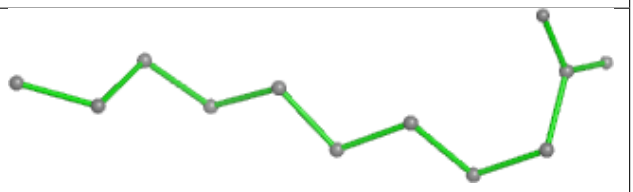
Torsions

Rings

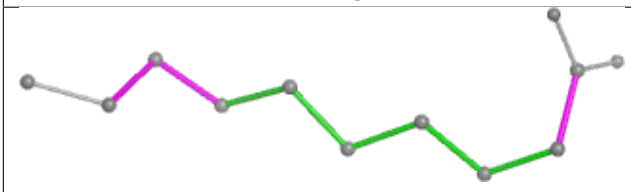
Ligand STE e 101



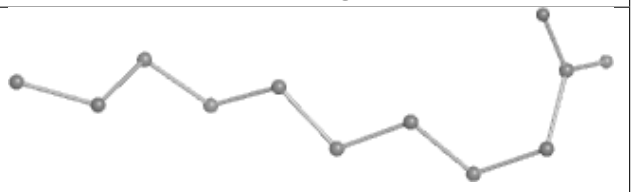
Bond lengths



Bond angles

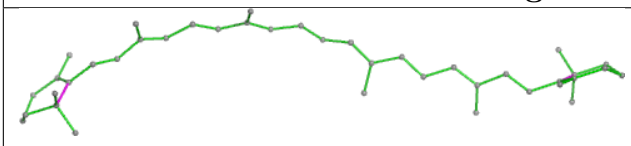


Torsions

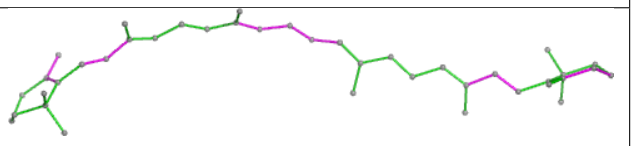


Rings

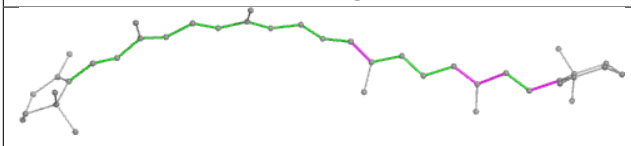
Ligand BCR h 102



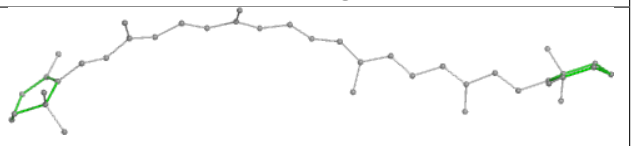
Bond lengths



Bond angles

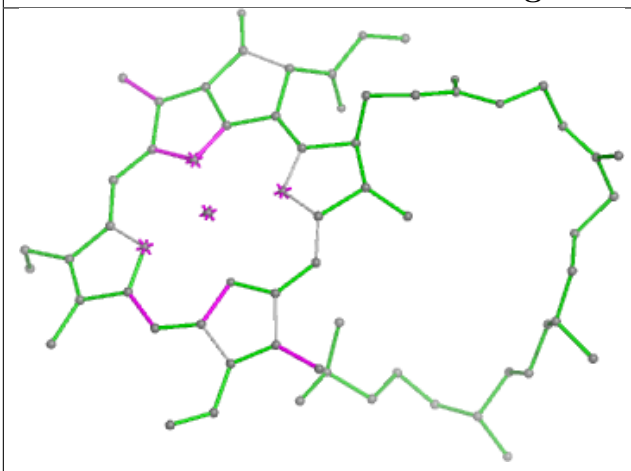


Torsions

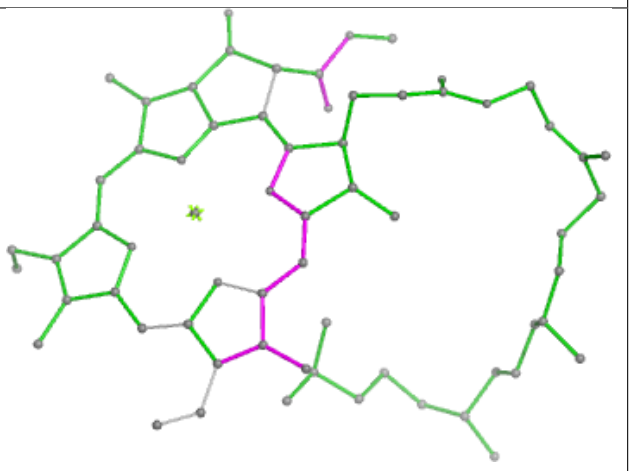


Rings

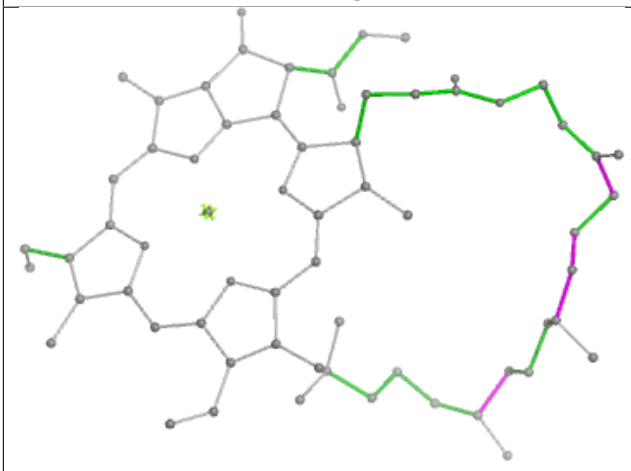
Ligand CLA B 615



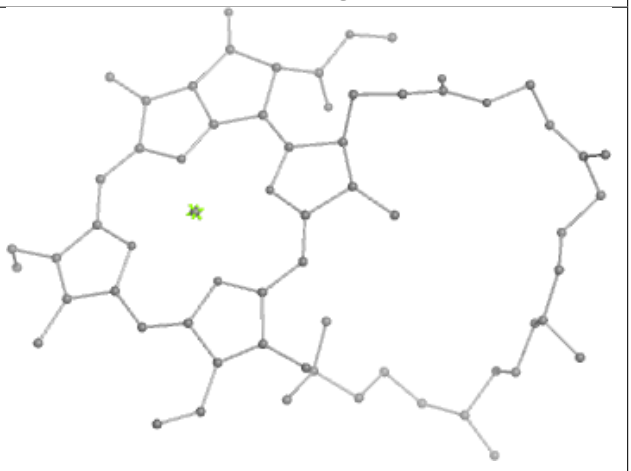
Bond lengths



Bond angles

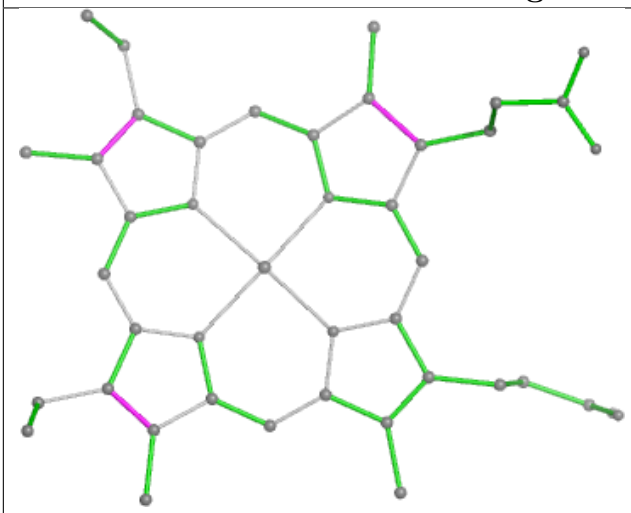


Torsions

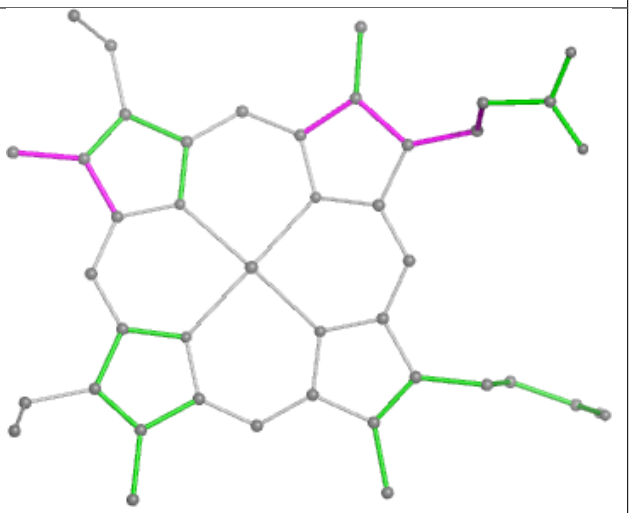


Rings

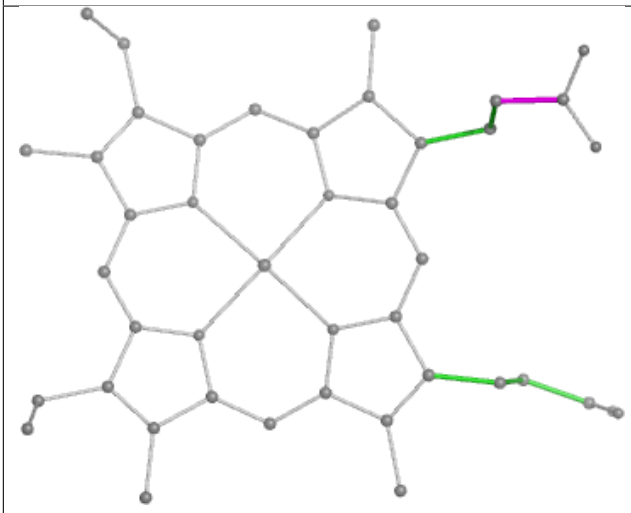
Ligand HEC v 201



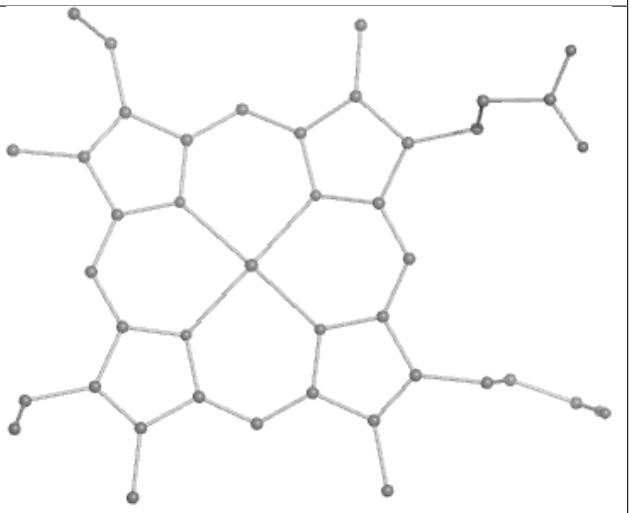
Bond lengths



Bond angles

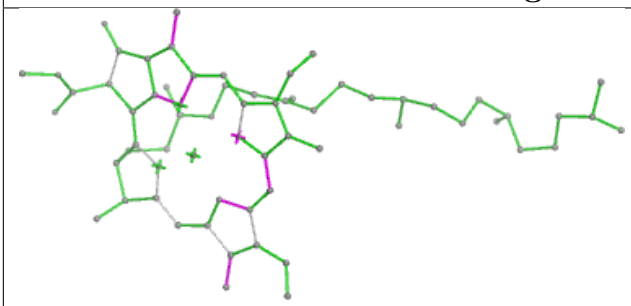


Torsions

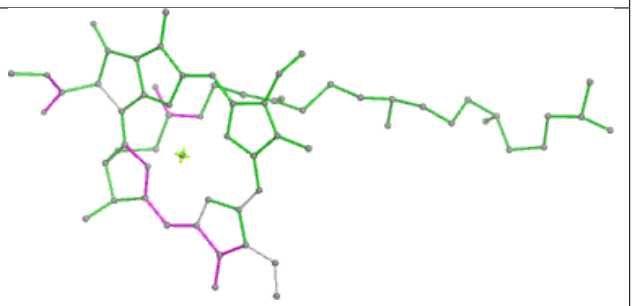


Rings

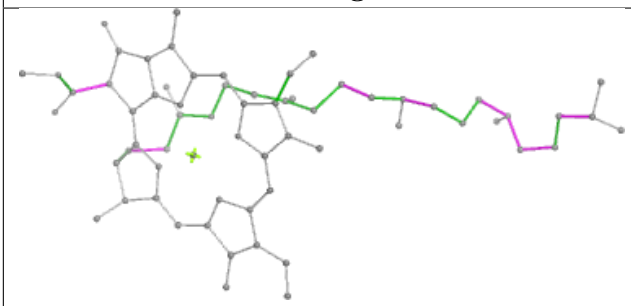
Ligand CLA B 614



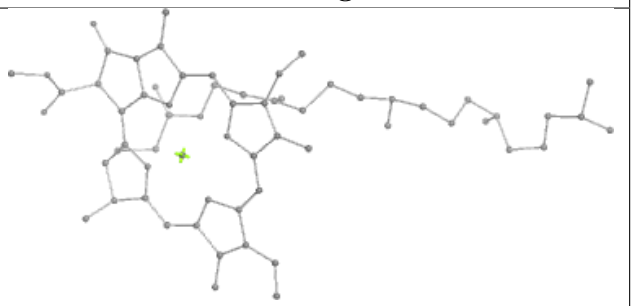
Bond lengths



Bond angles

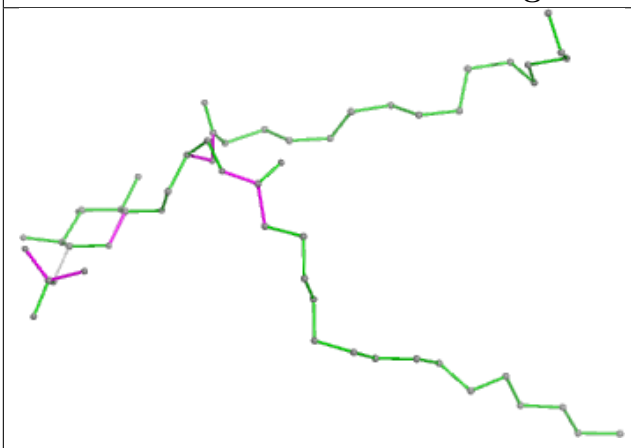


Torsions

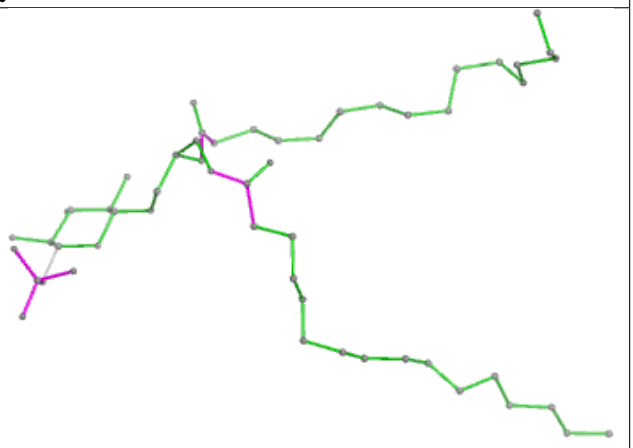


Rings

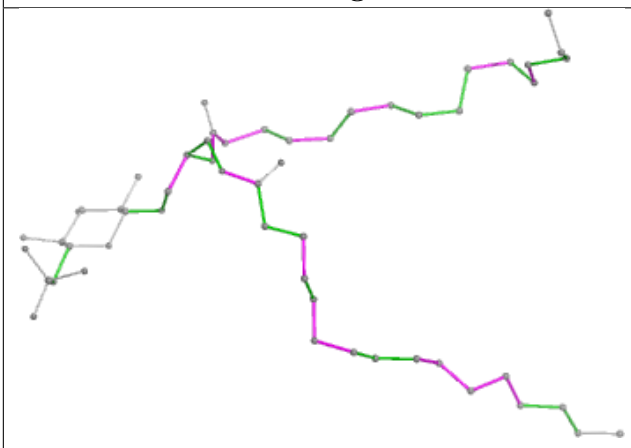
Ligand SQD A 412



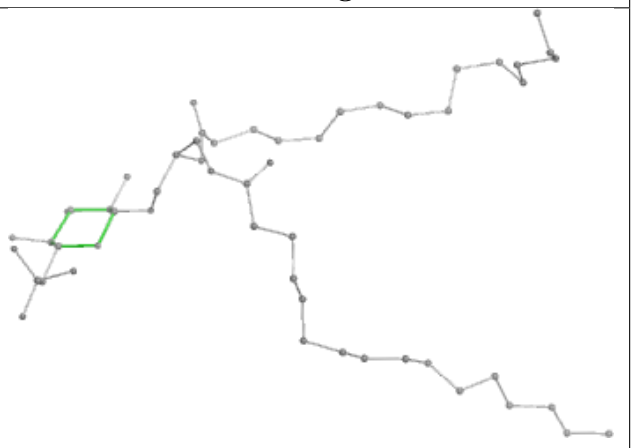
Bond lengths



Bond angles

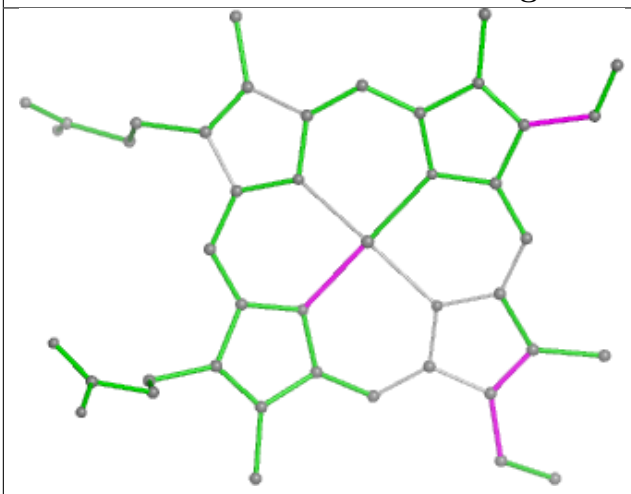


Torsions

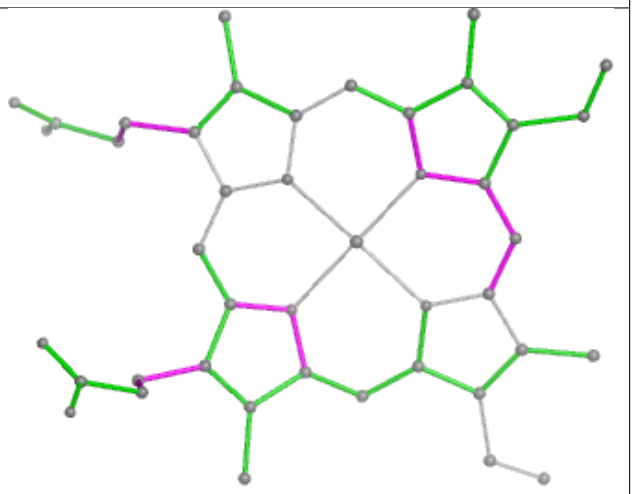


Rings

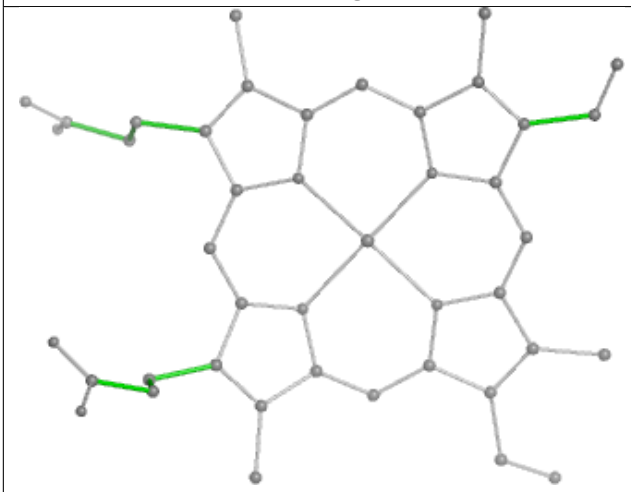
Ligand HEM E 105



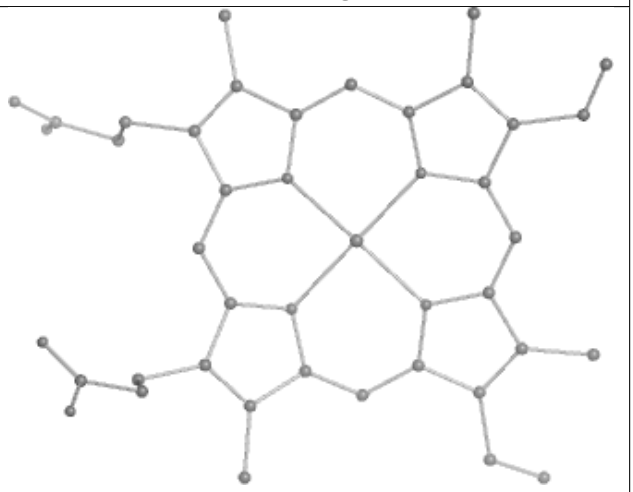
Bond lengths



Bond angles

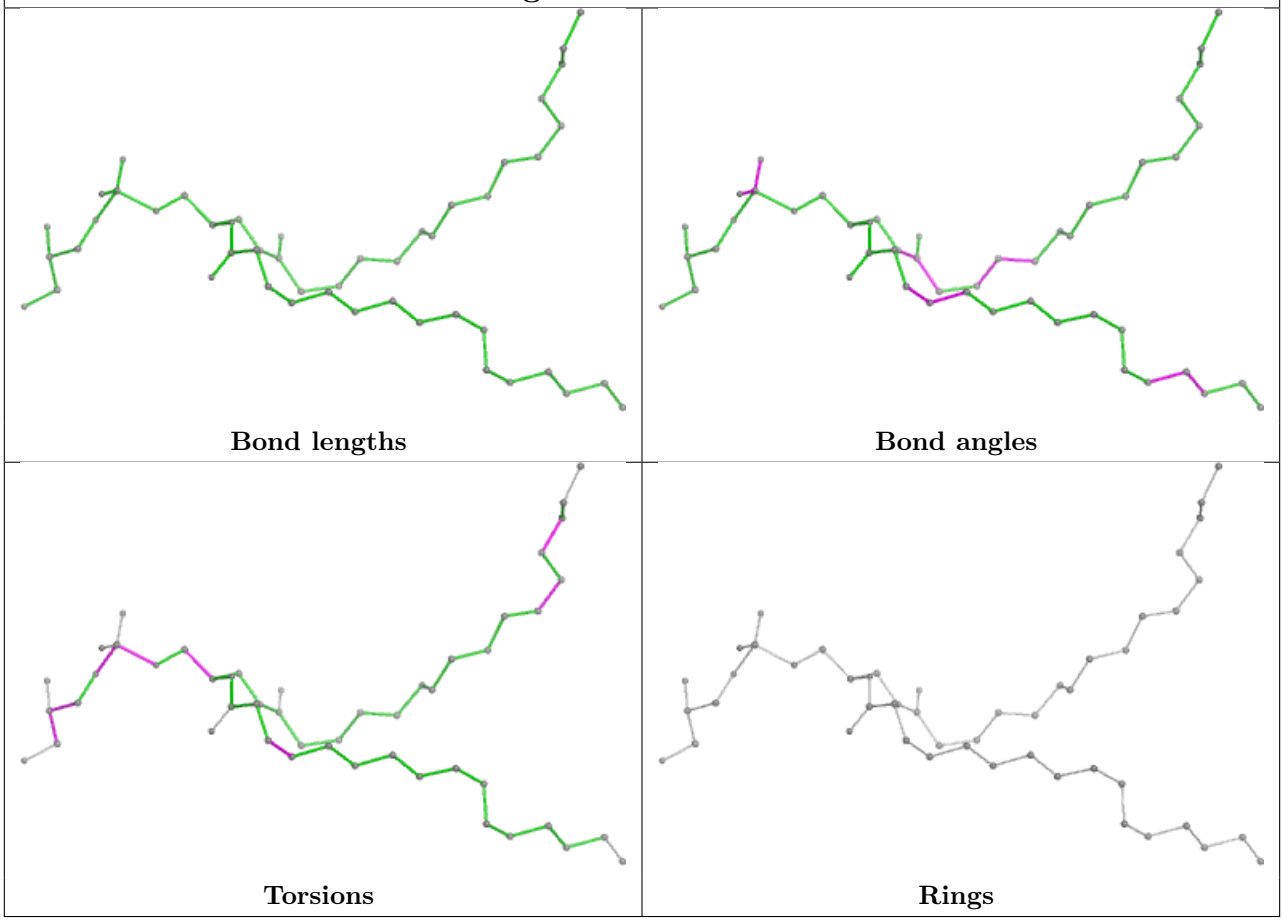


Torsions

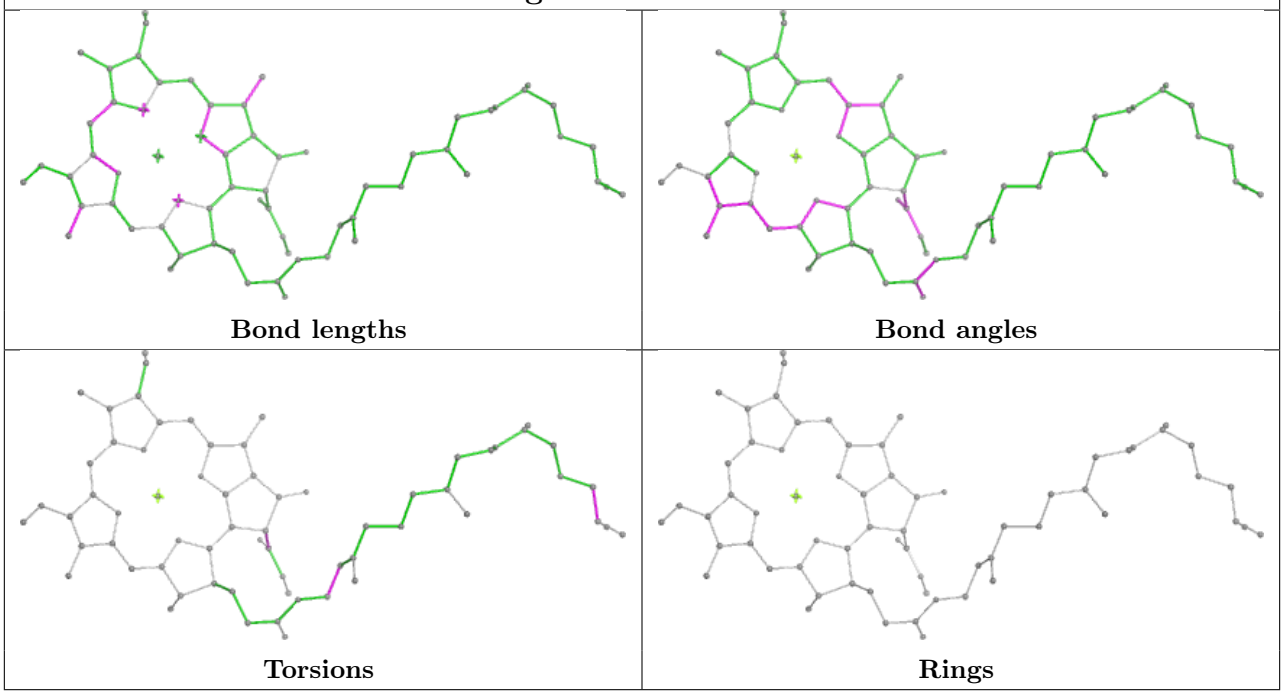


Rings

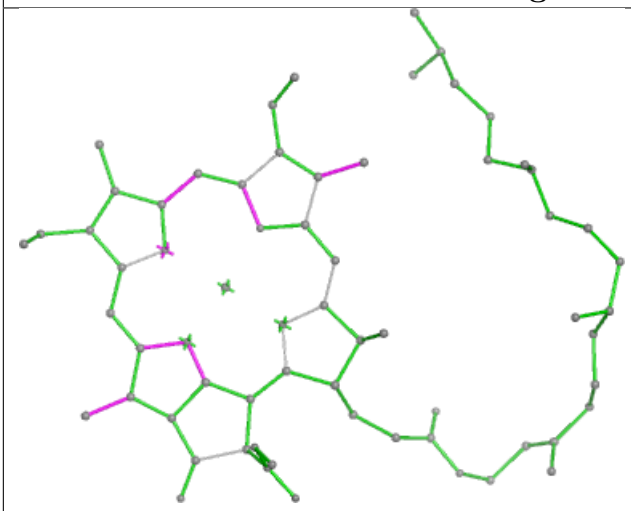
Ligand LHG D 409



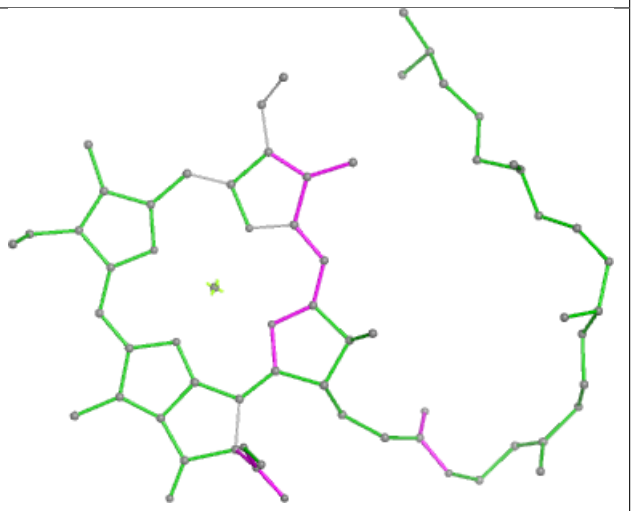
Ligand CLA B 602



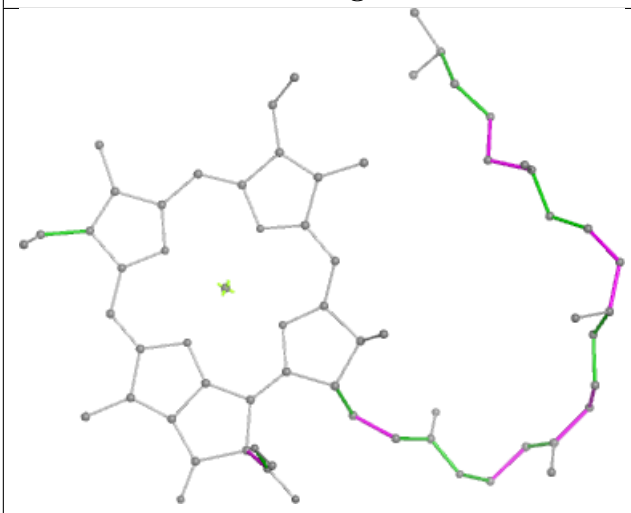
Ligand CLA c 512



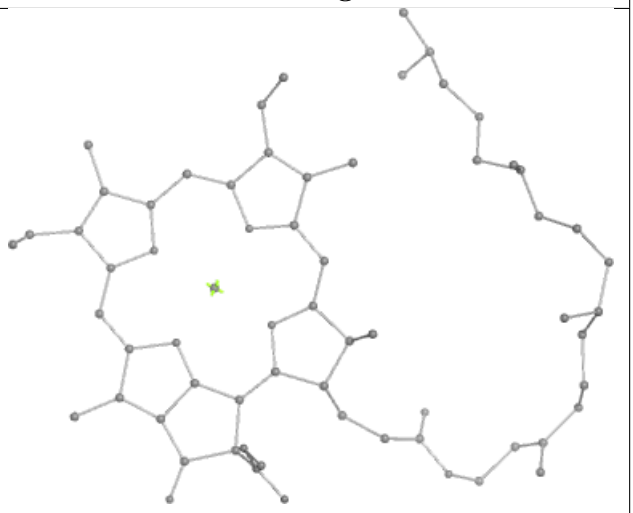
Bond lengths



Bond angles

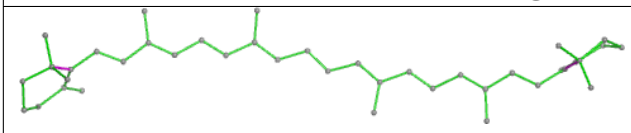


Torsions

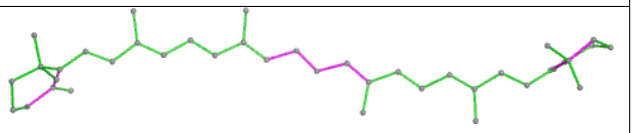


Rings

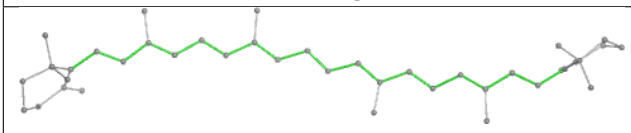
Ligand BCR c 514



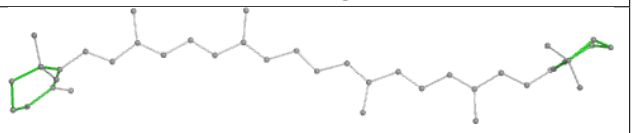
Bond lengths



Bond angles

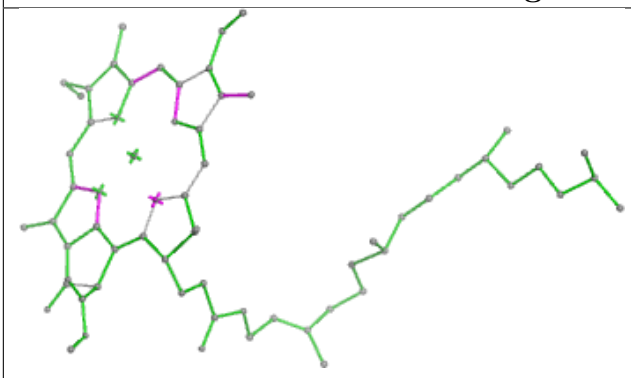


Torsions

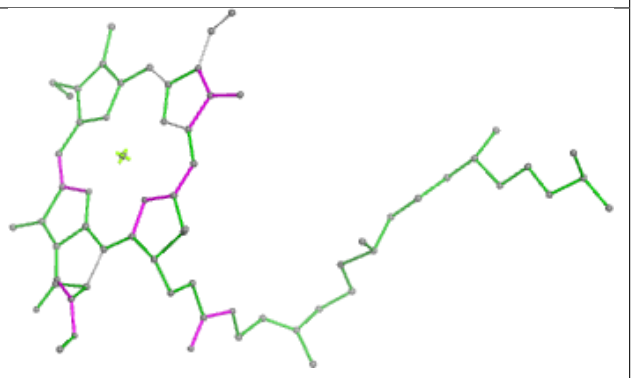


Rings

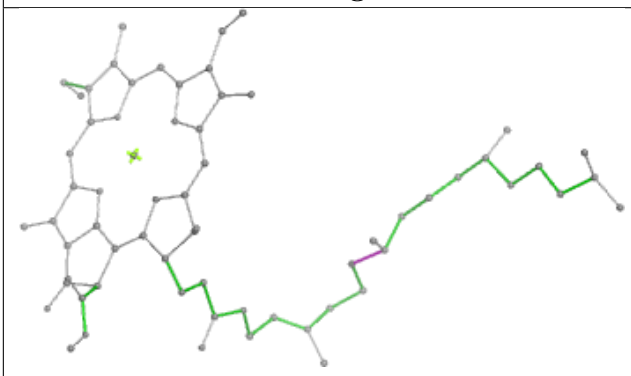
Ligand CLA C 511



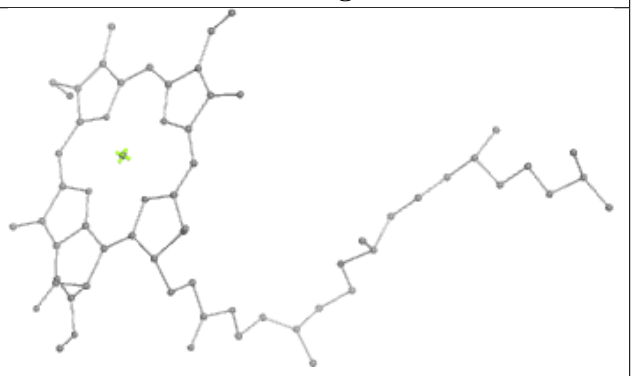
Bond lengths



Bond angles

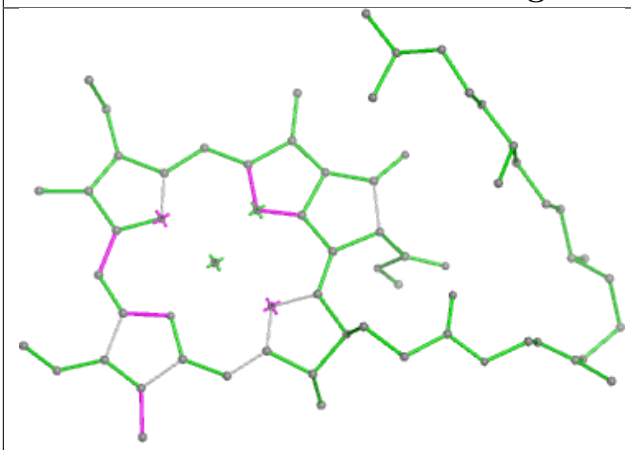


Torsions

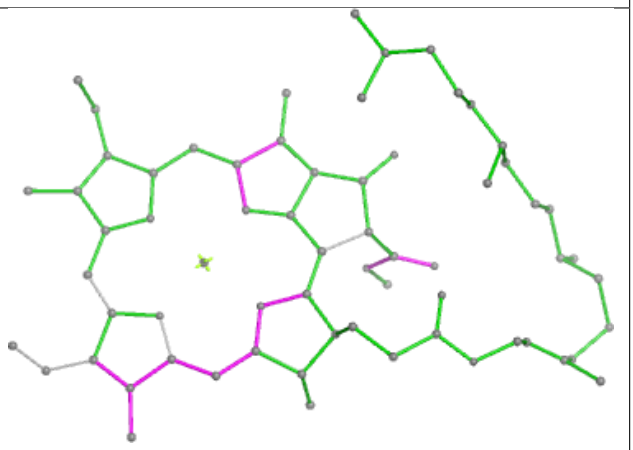


Rings

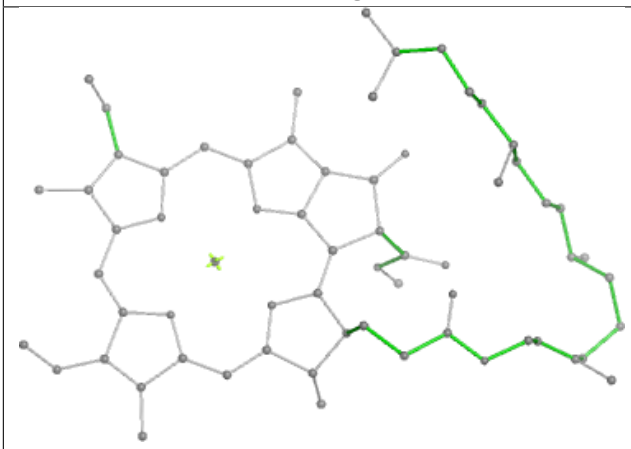
Ligand CLA b 611



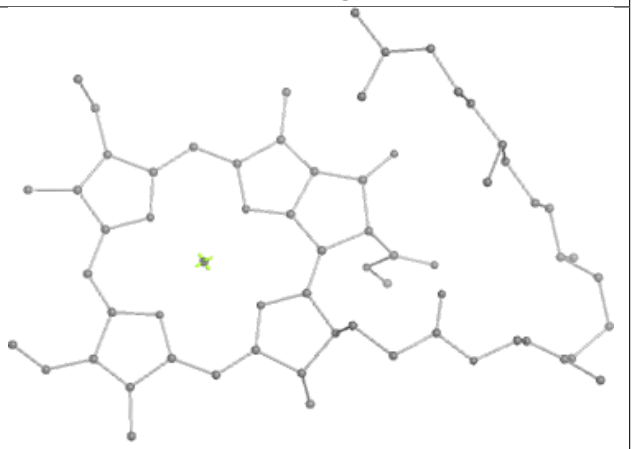
Bond lengths



Bond angles

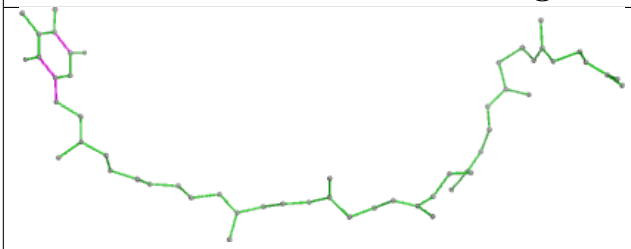


Torsions

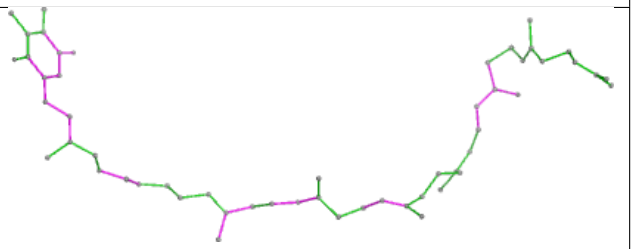


Rings

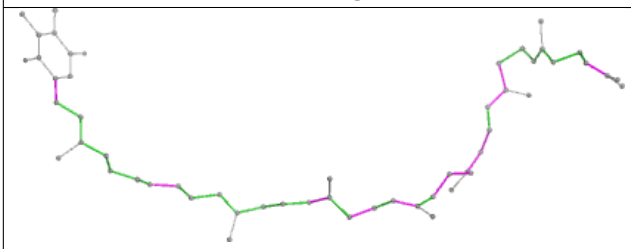
Ligand PL9 a 408



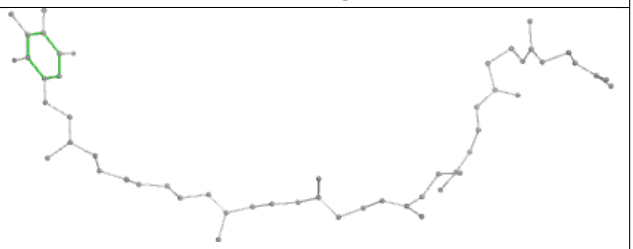
Bond lengths



Bond angles

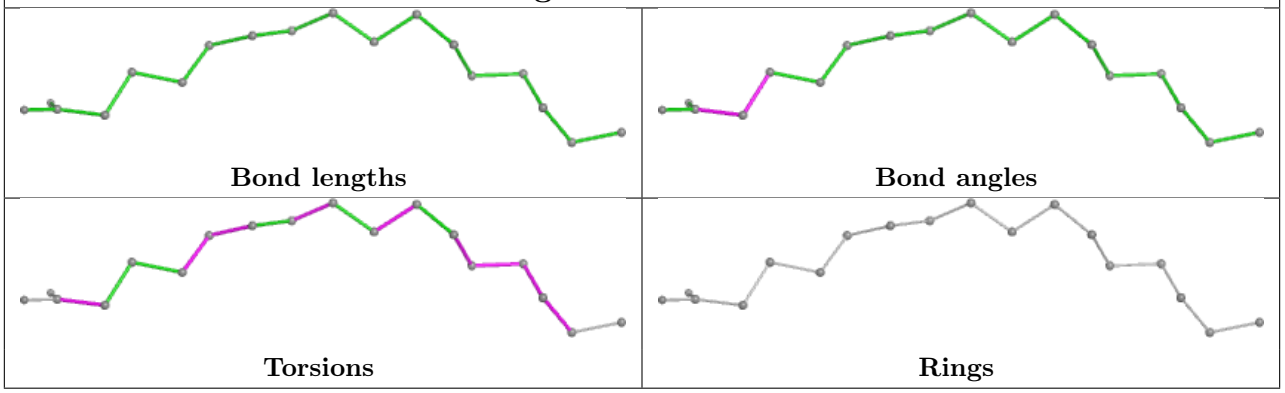


Torsions

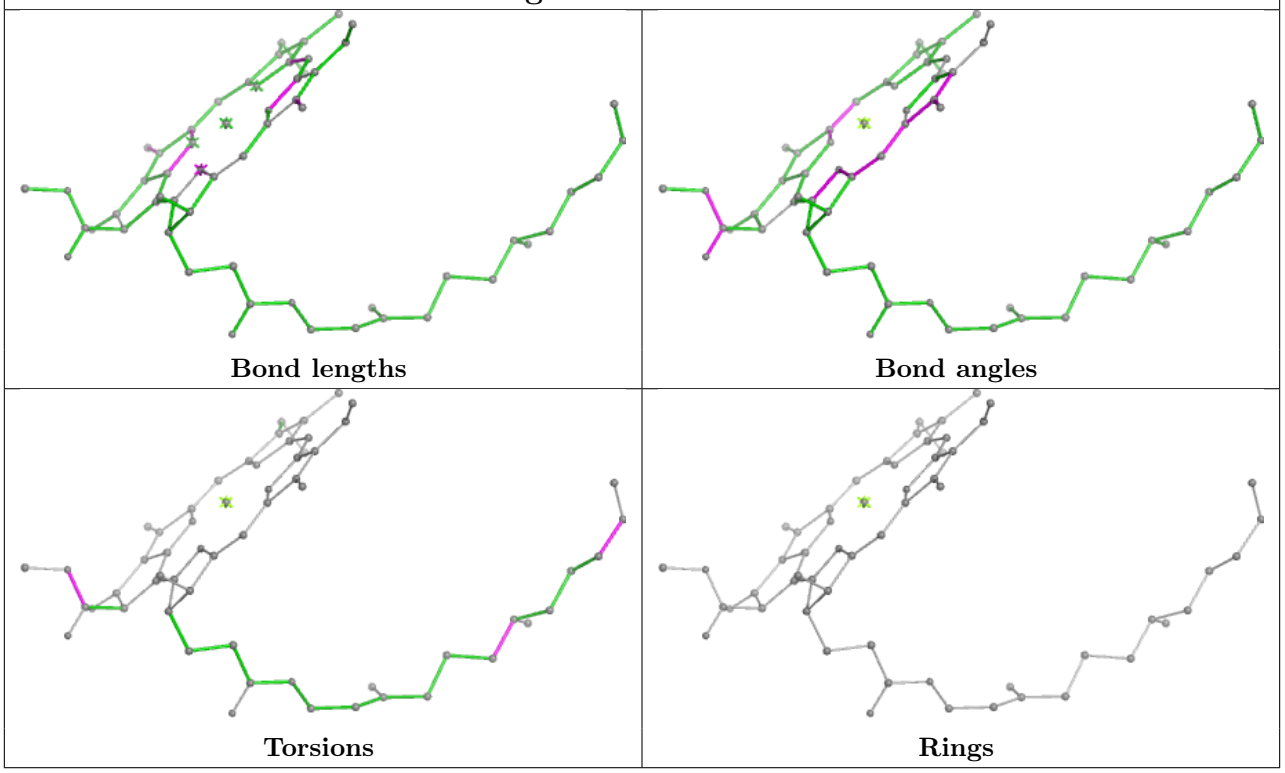


Rings

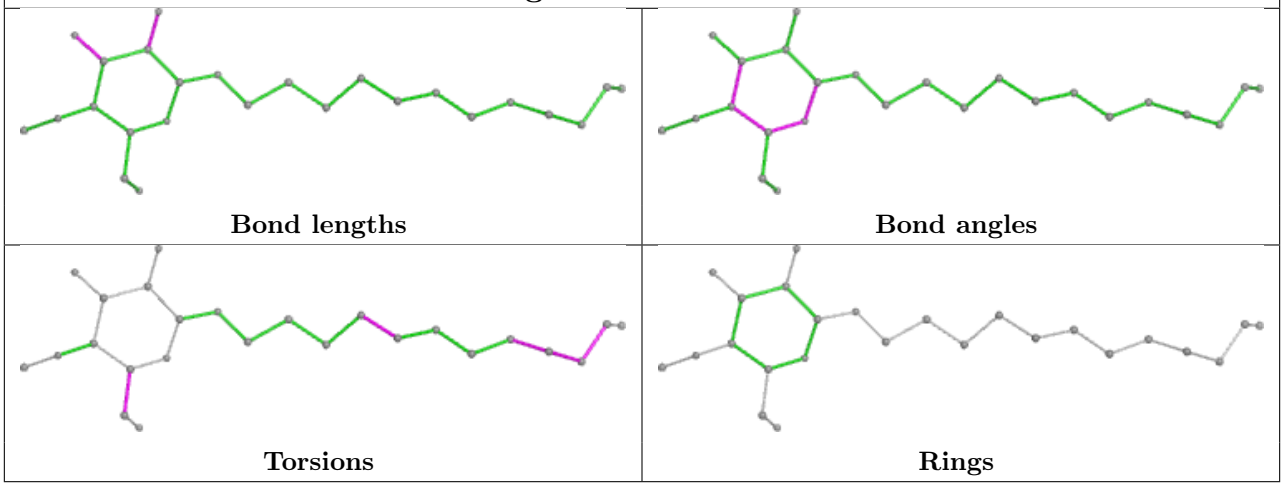
Ligand STE t 101



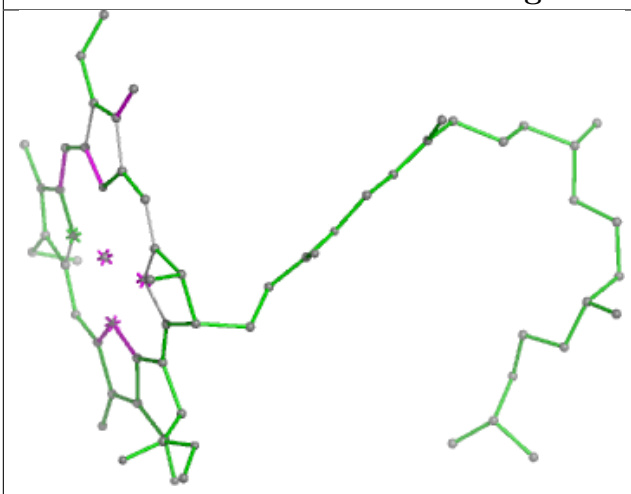
Ligand CLA C 504



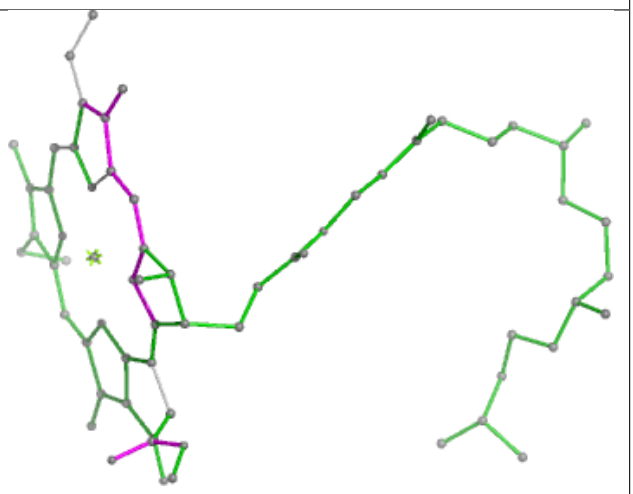
Ligand LMT b 624



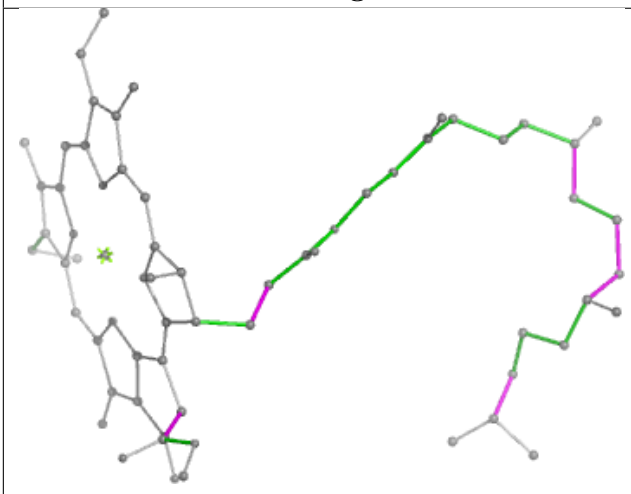
Ligand CLA B 606



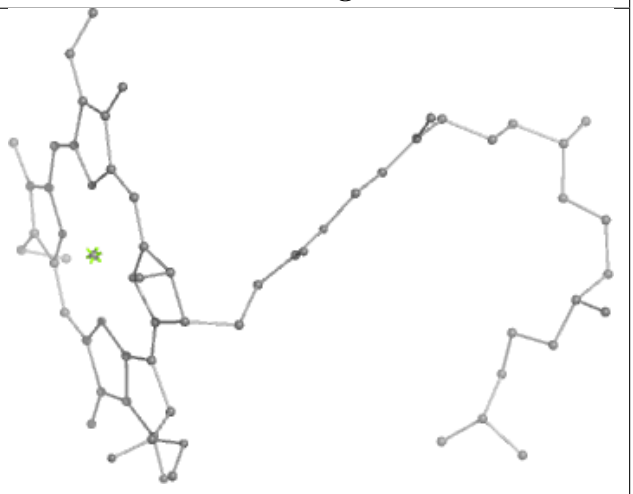
Bond lengths



Bond angles

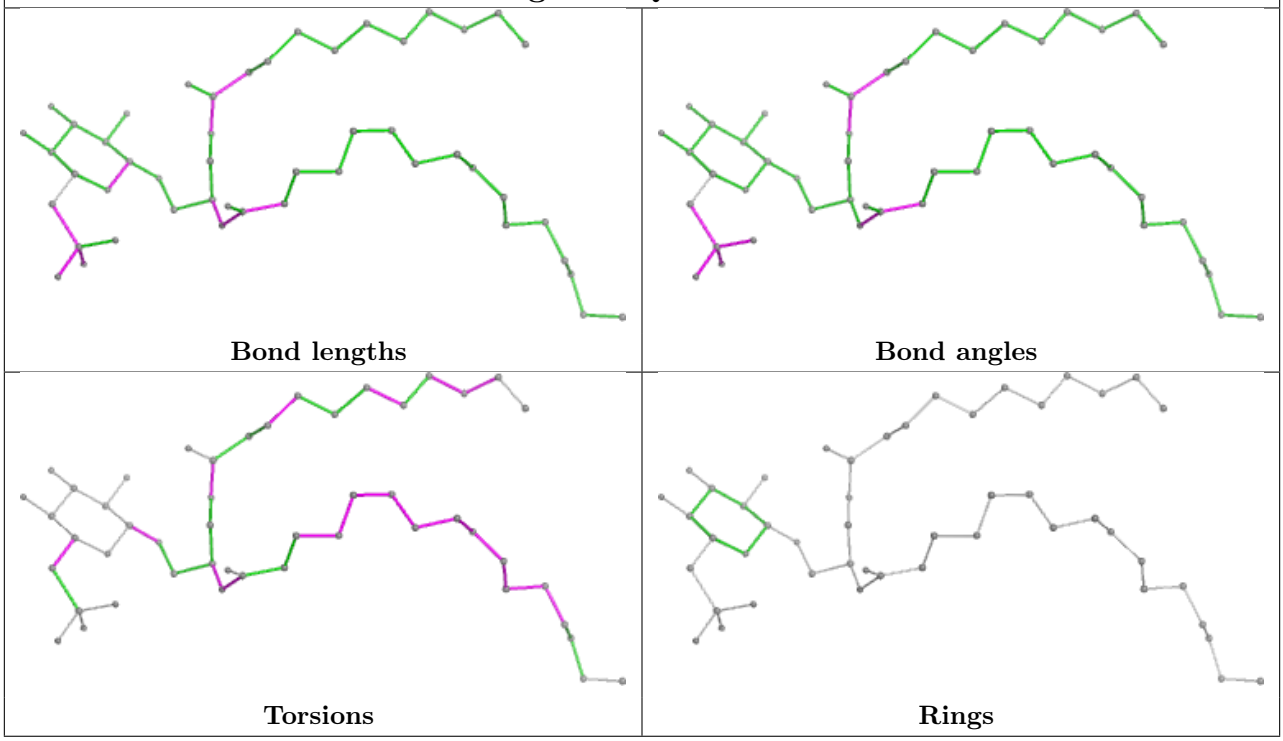


Torsions

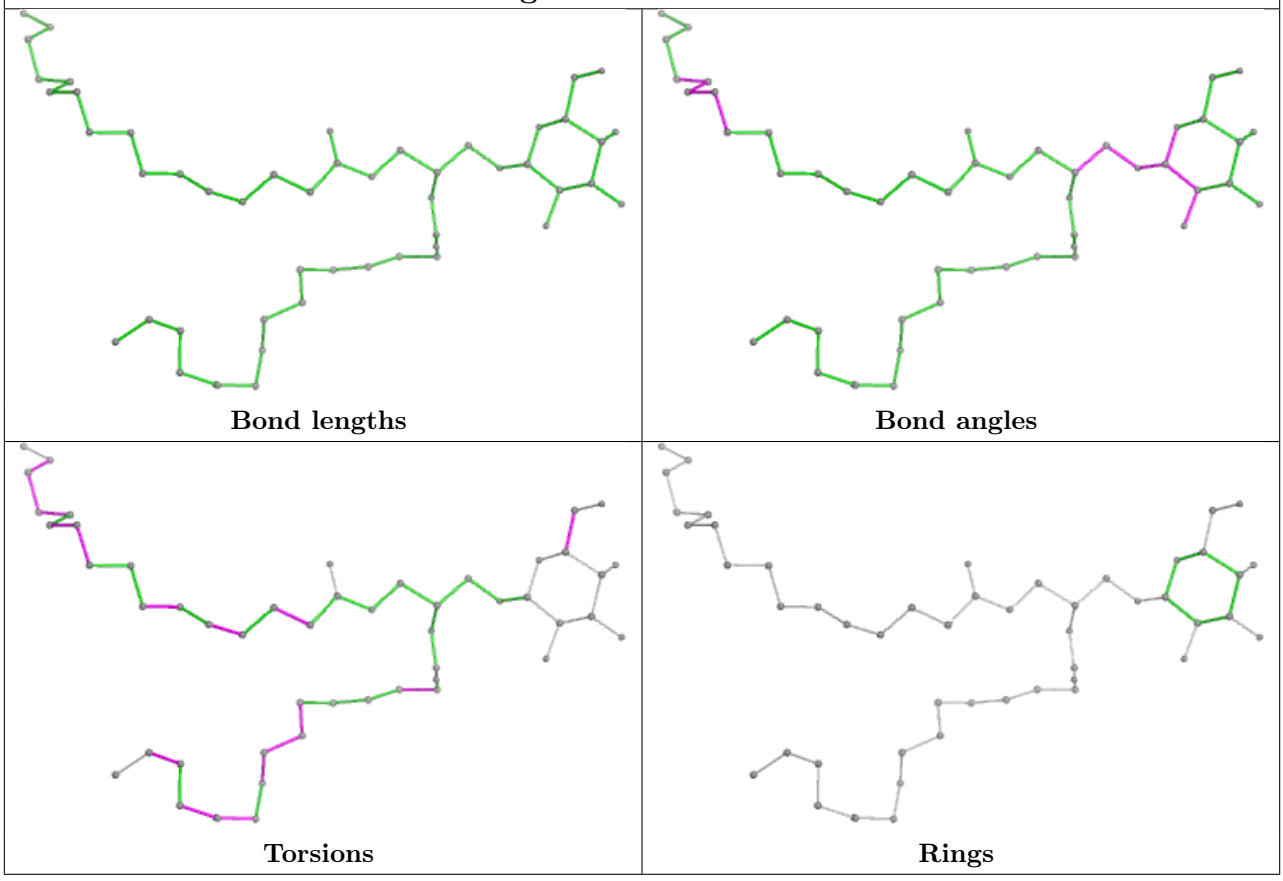


Rings

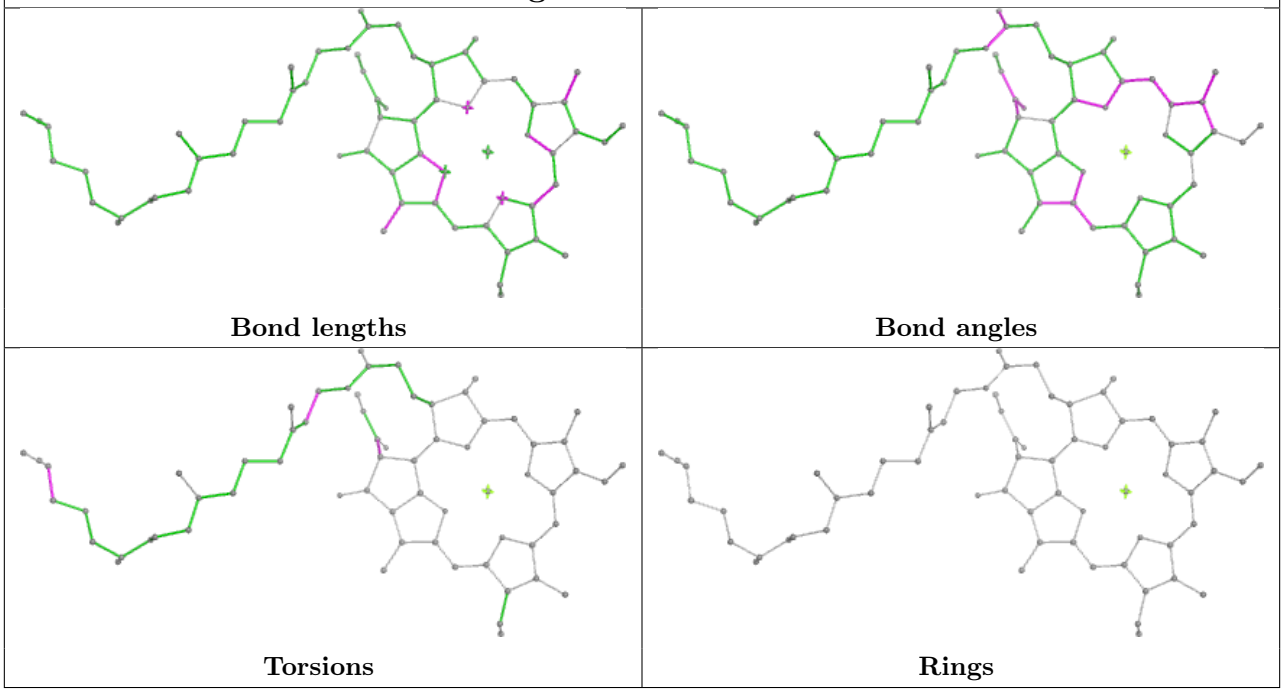
Ligand SQD b 621



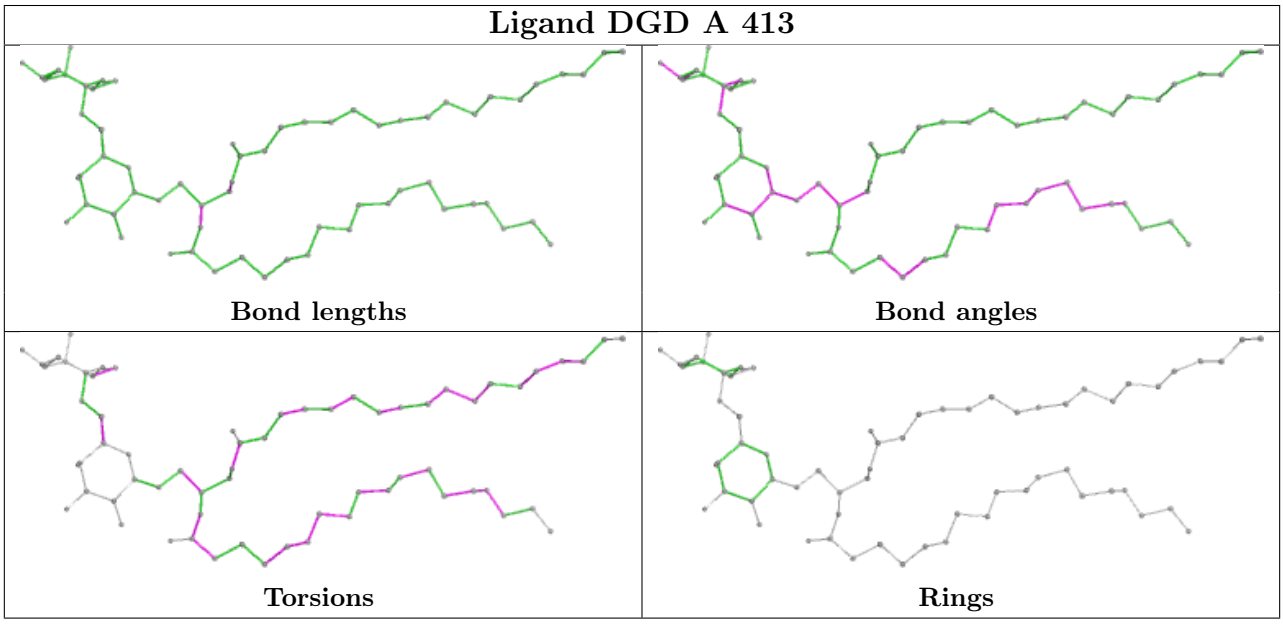
Ligand LMG D 408



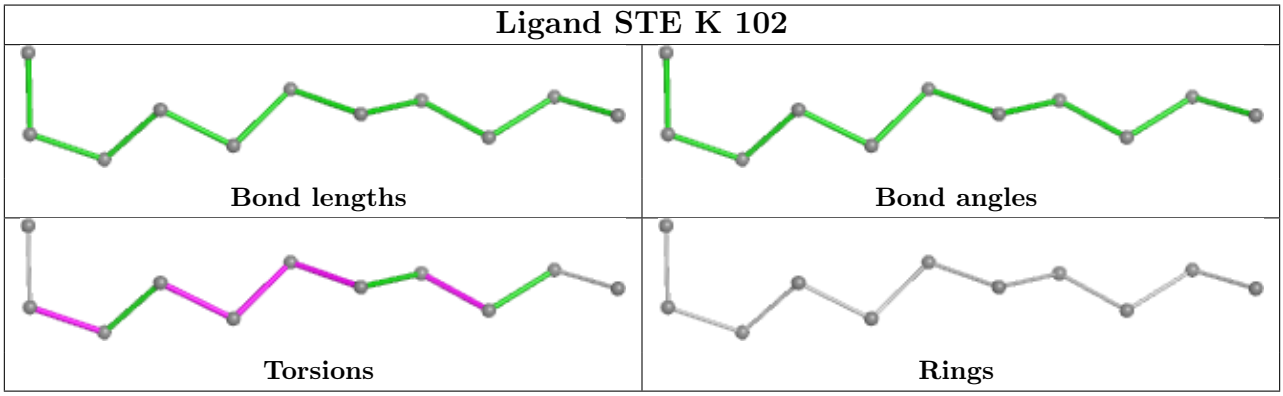
Ligand CLA b 603



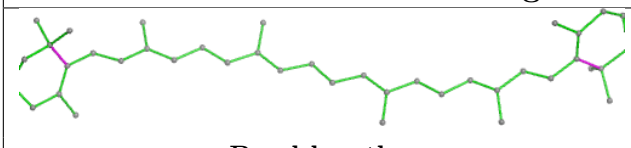
Ligand DGD A 413



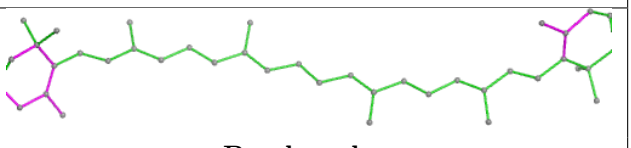
Ligand STE K 102



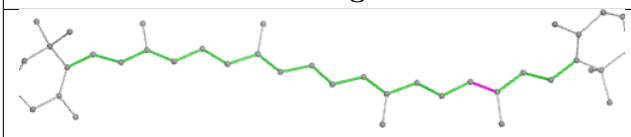
Ligand BCR B 619



Bond lengths



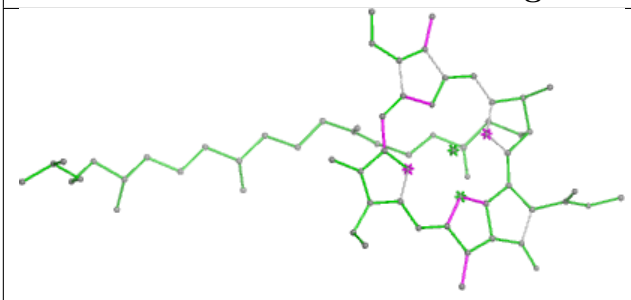
Bond angles



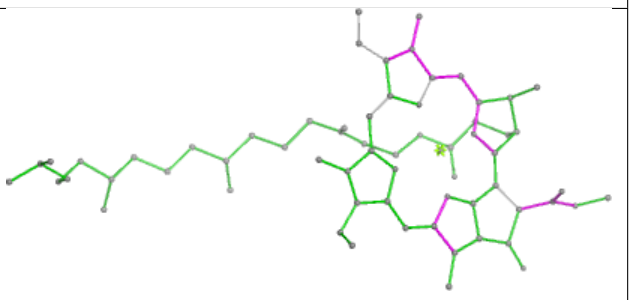
Torsions

Rings

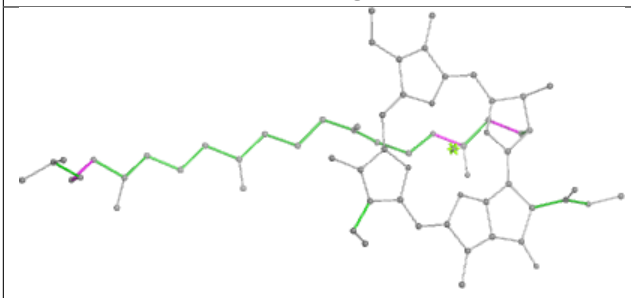
Ligand CLA B 608



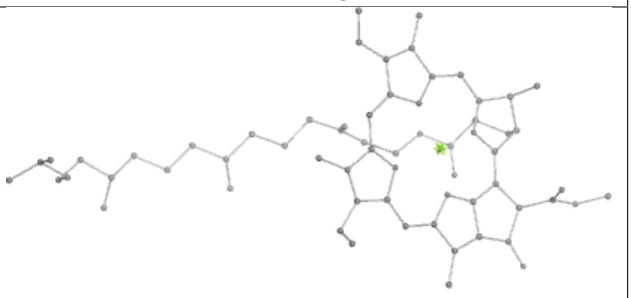
Bond lengths



Bond angles

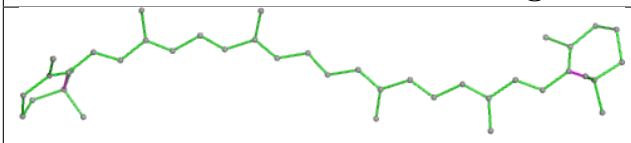


Torsions

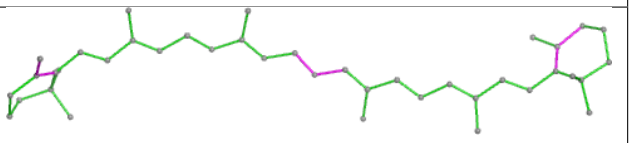


Rings

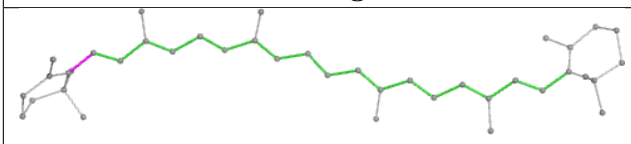
Ligand BCR k 103



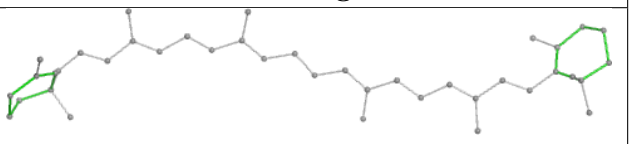
Bond lengths



Bond angles

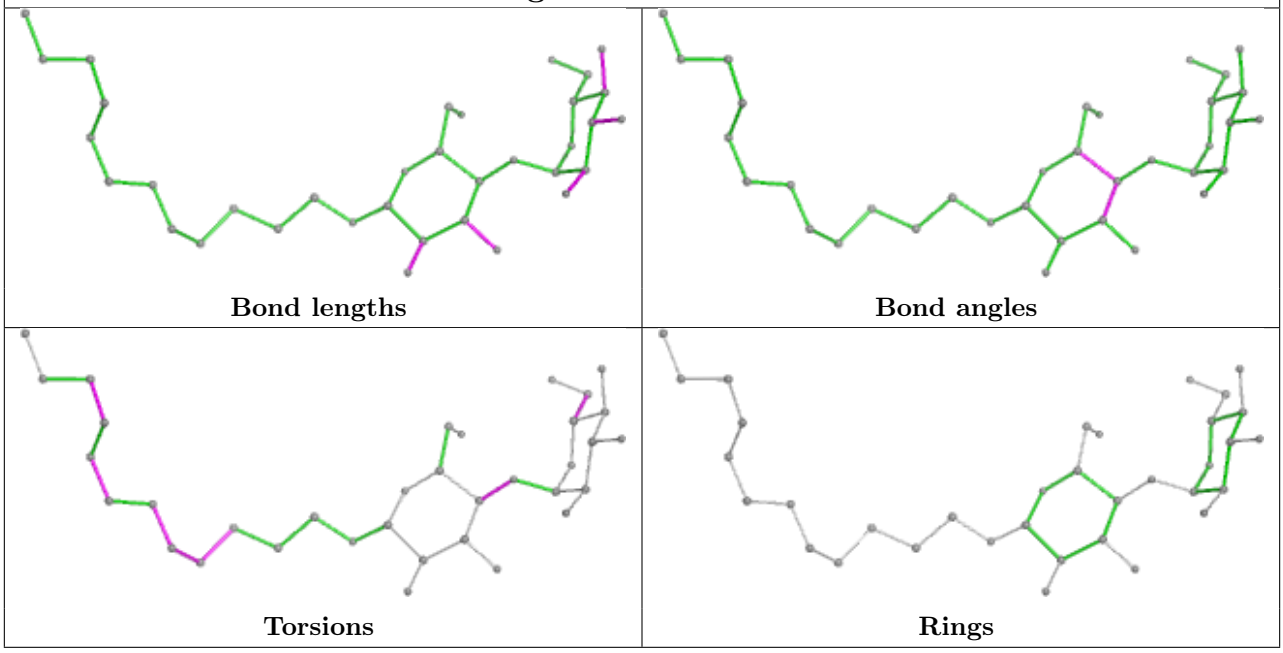


Torsions

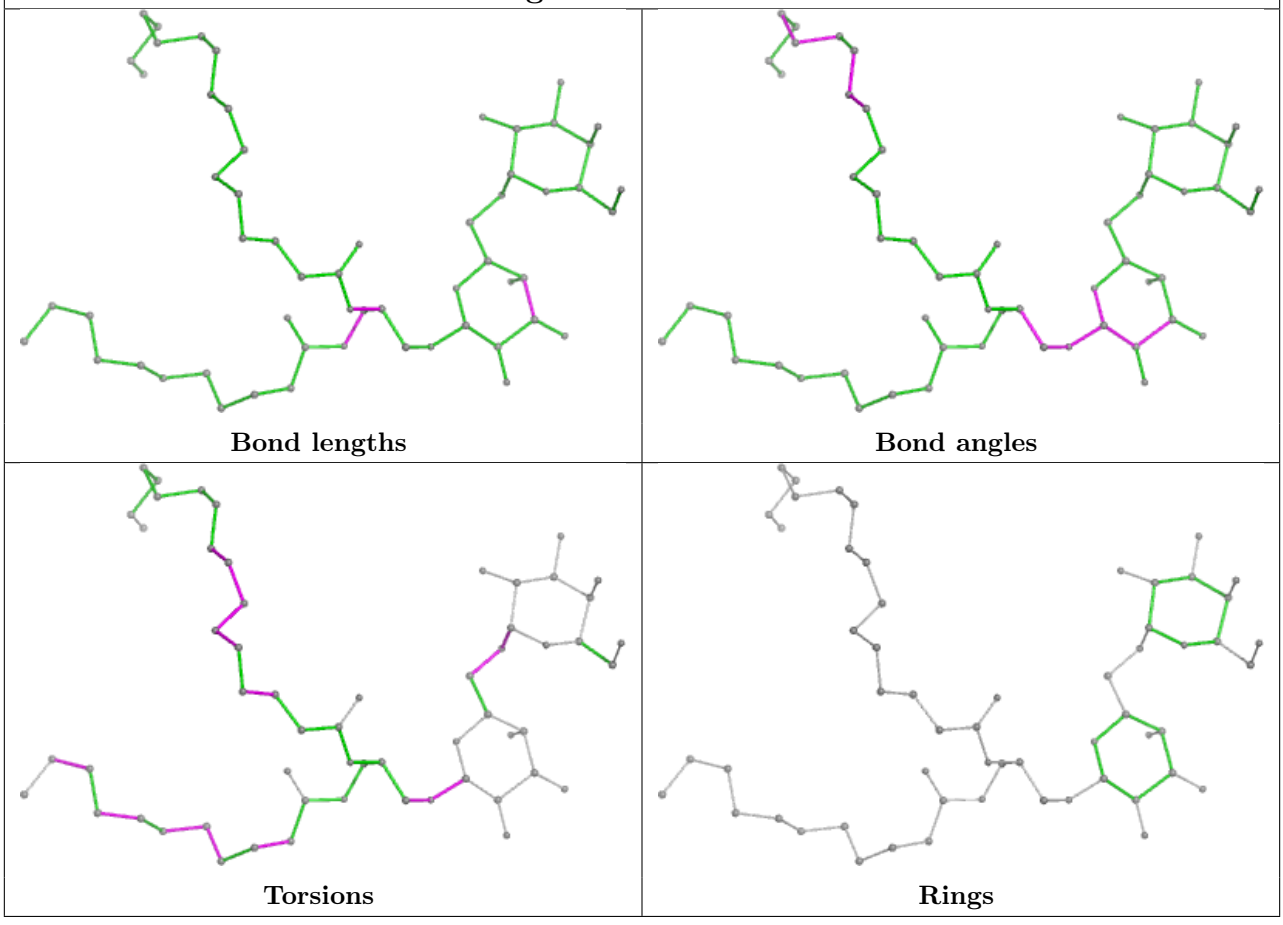


Rings

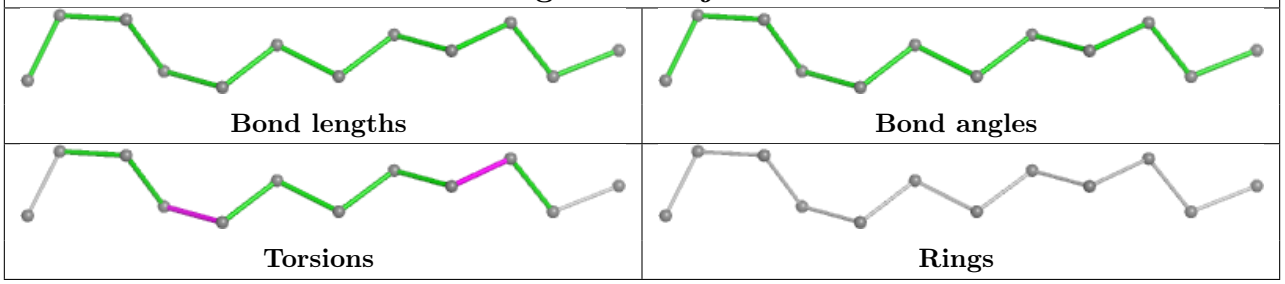
Ligand LMT c 525



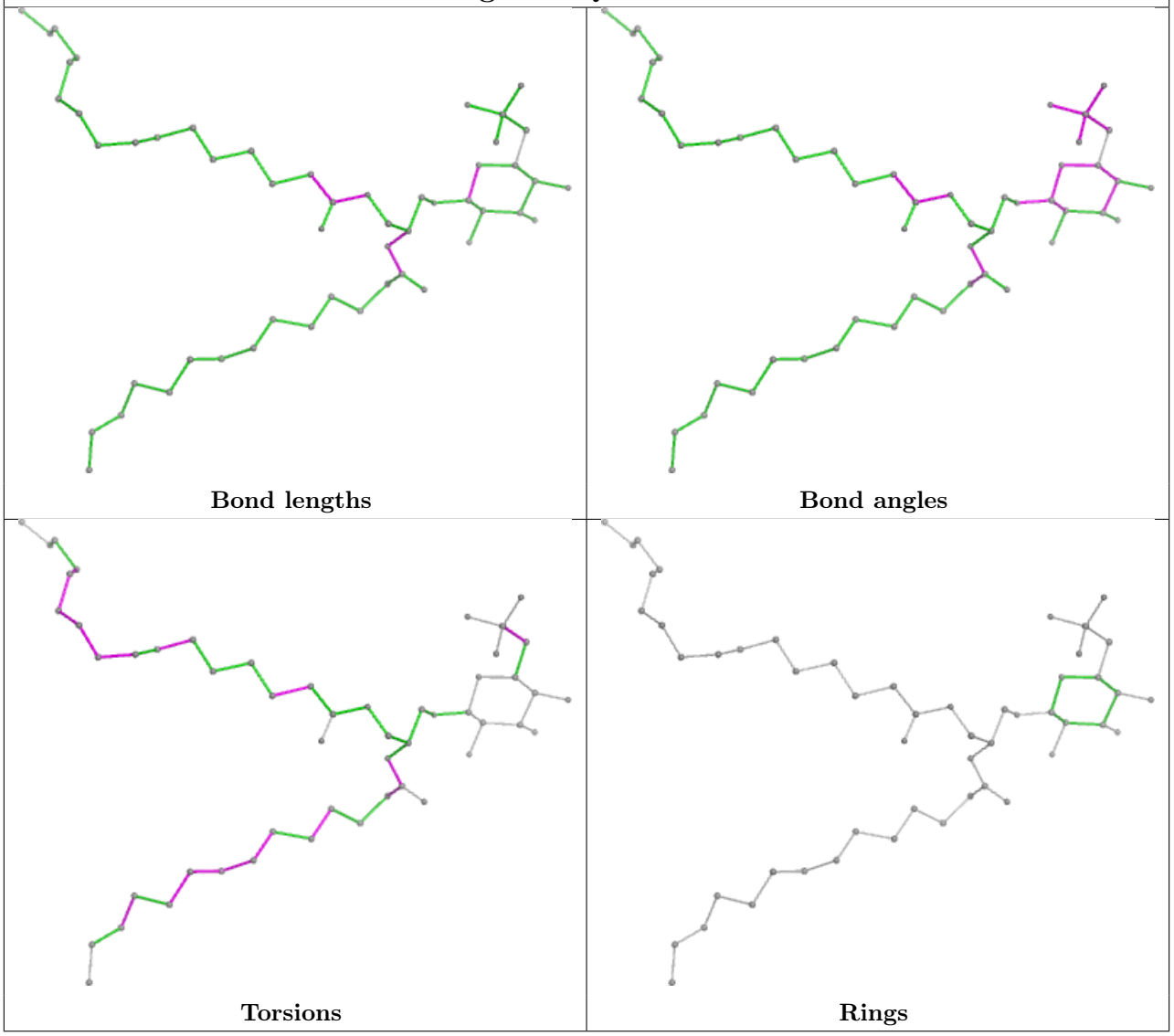
Ligand DGD c 518



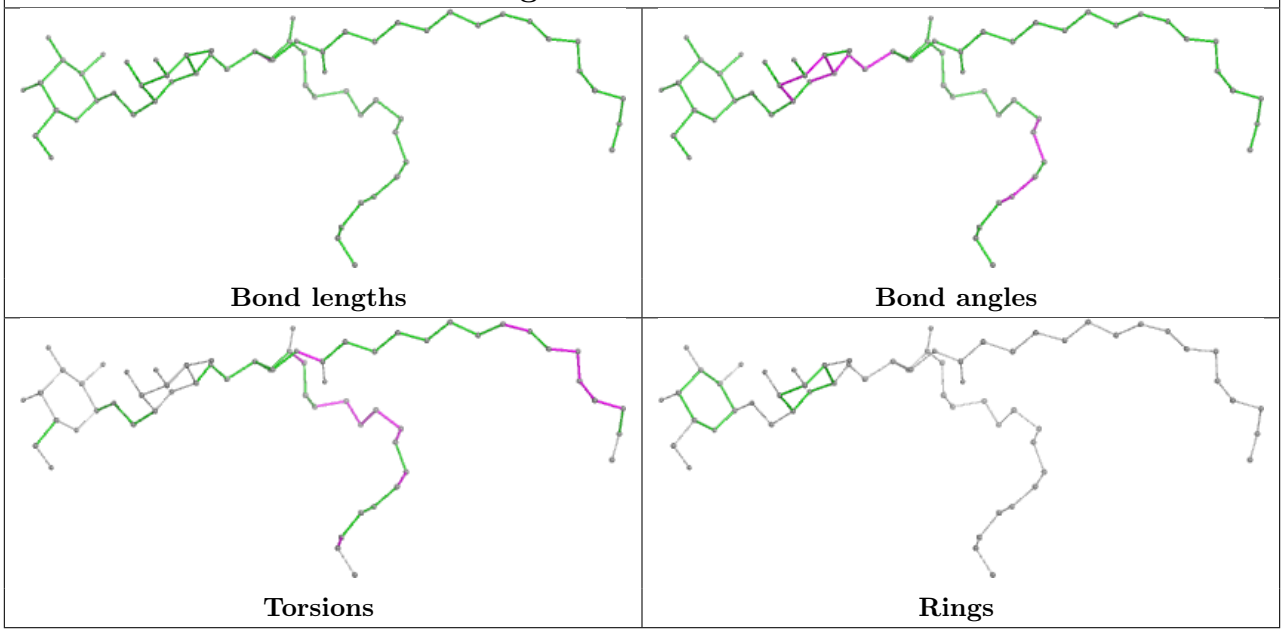
Ligand STE j 101



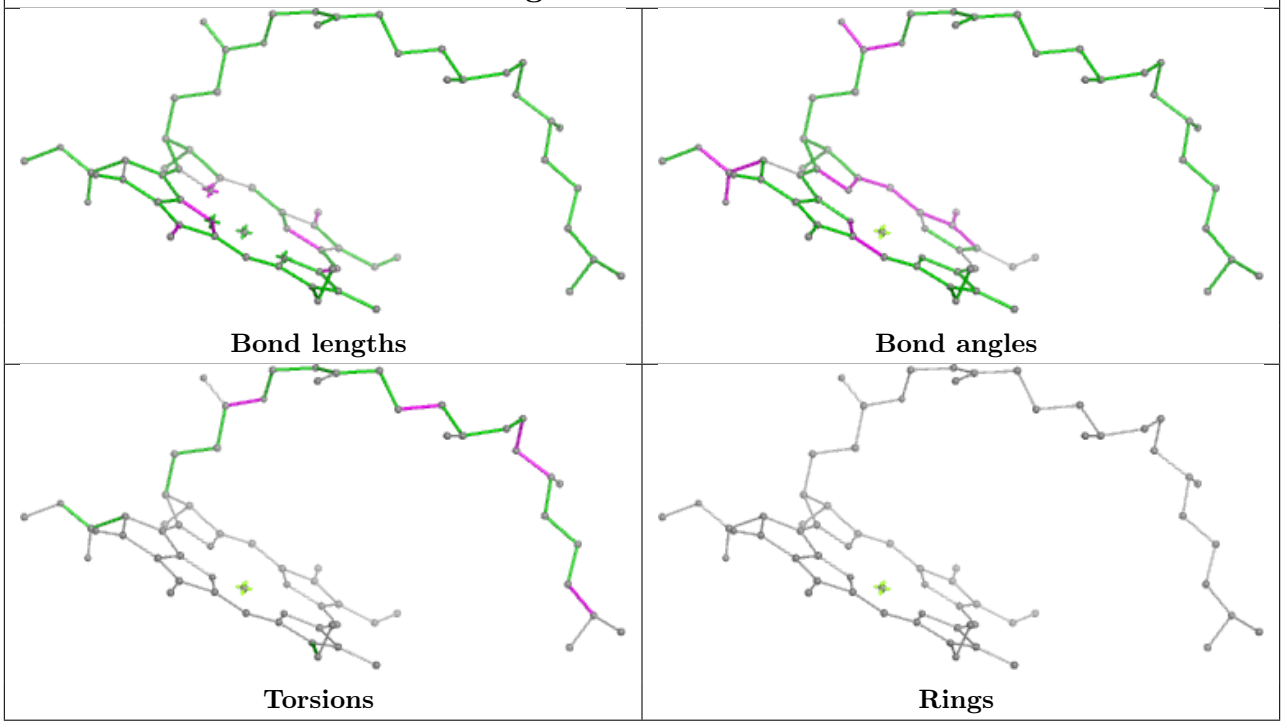
Ligand SQD A 411



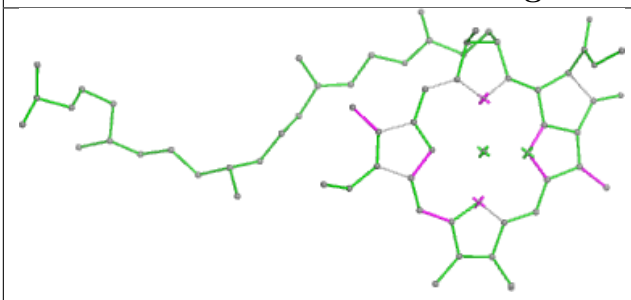
Ligand DGD H 103



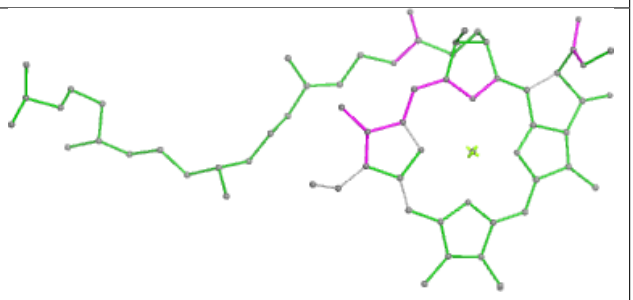
Ligand CLA C 513



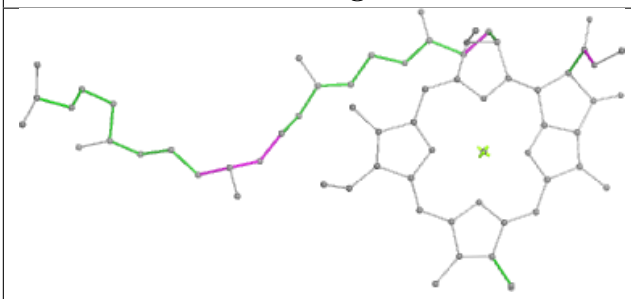
Ligand CLA B 603



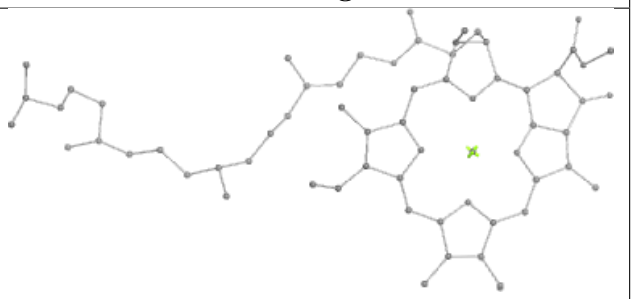
Bond lengths



Bond angles

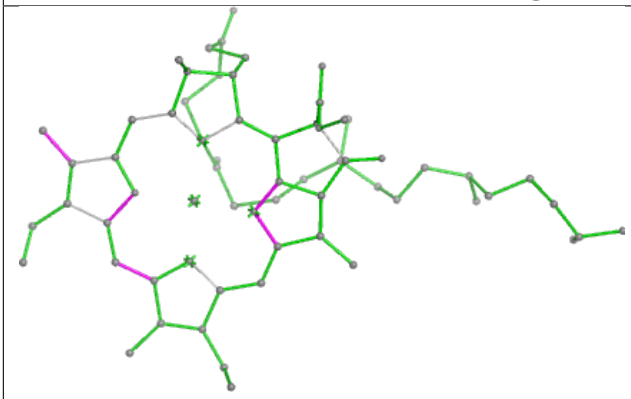


Torsions

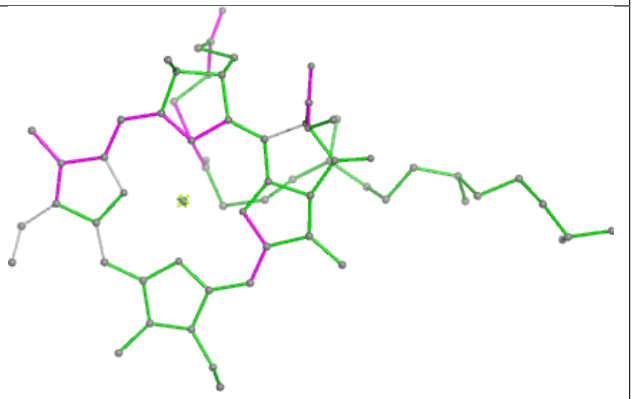


Rings

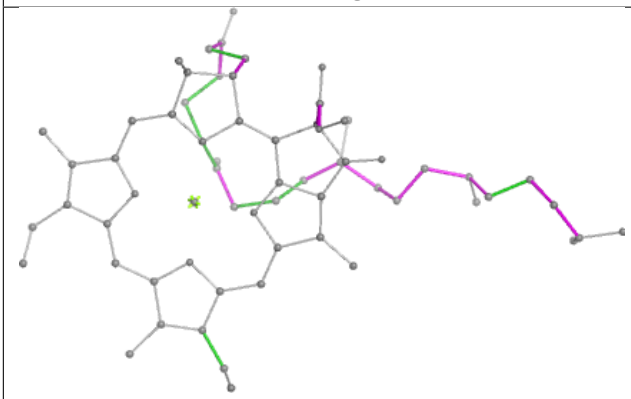
Ligand CLA b 602



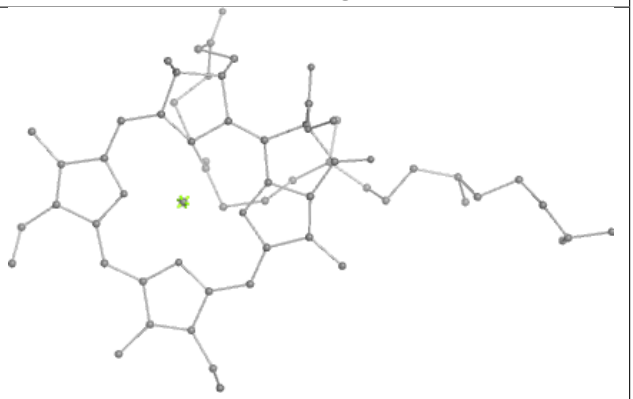
Bond lengths



Bond angles

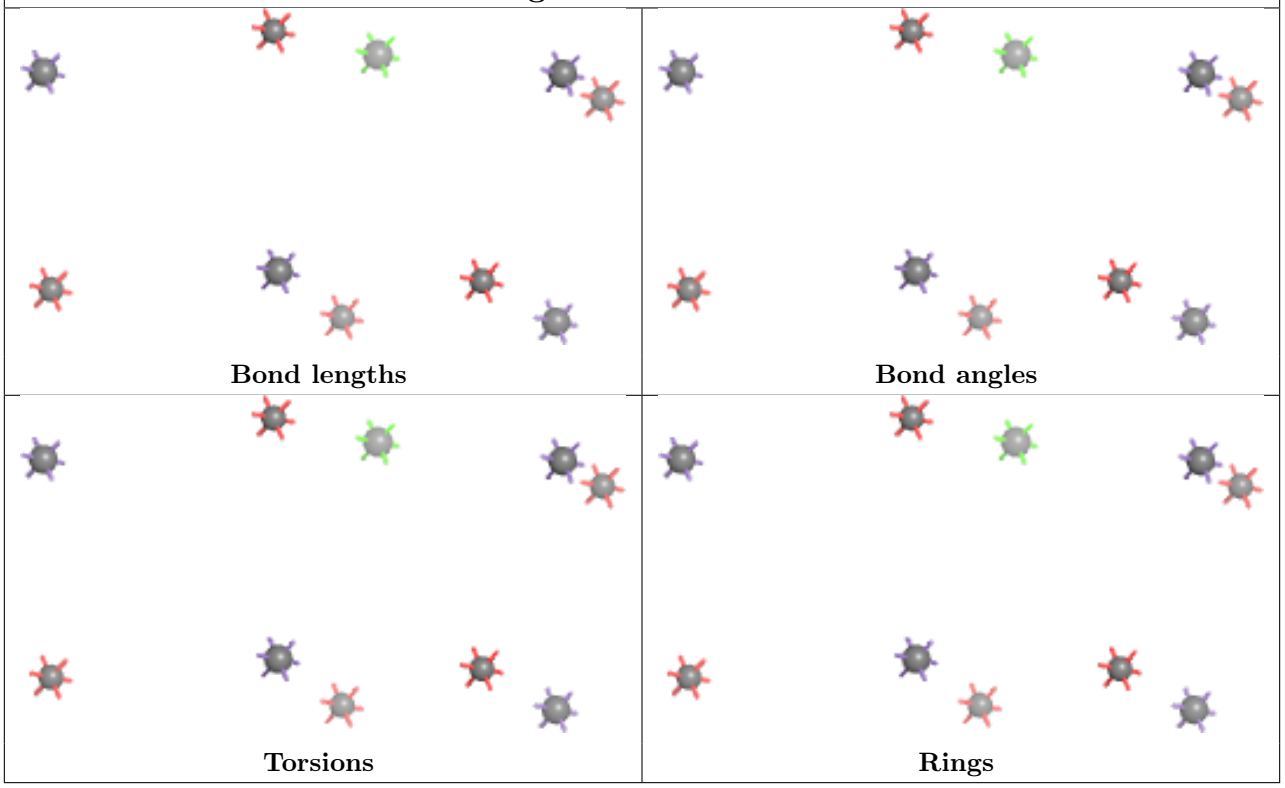


Torsions

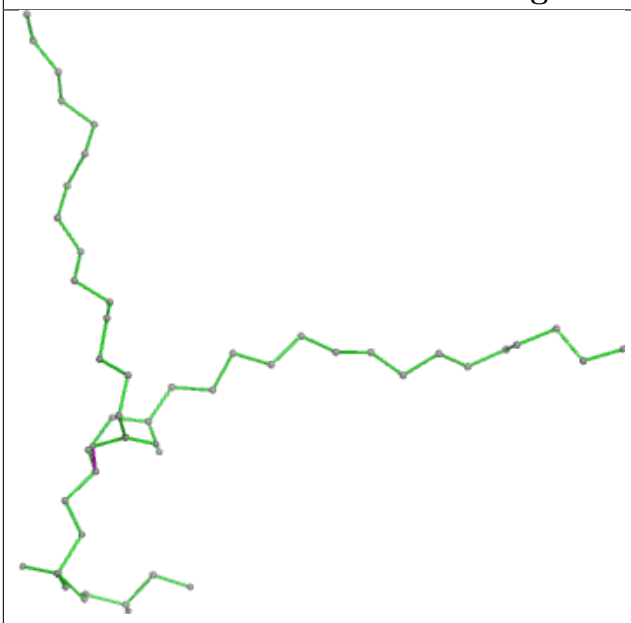


Rings

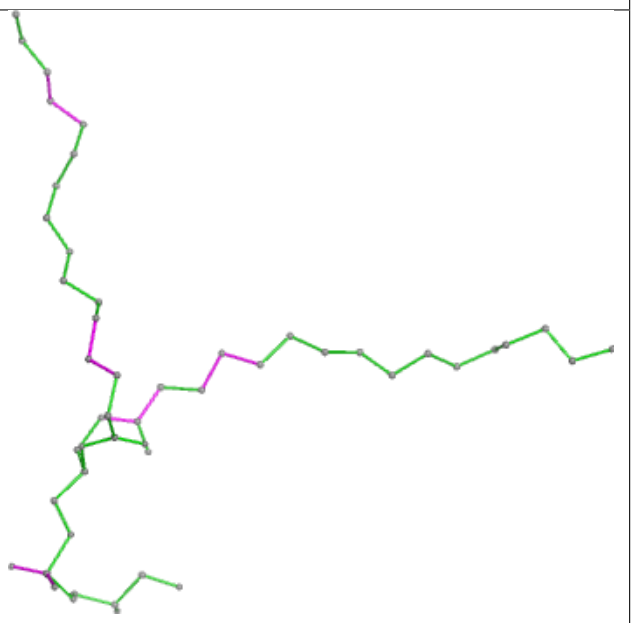
Ligand OEX a 417



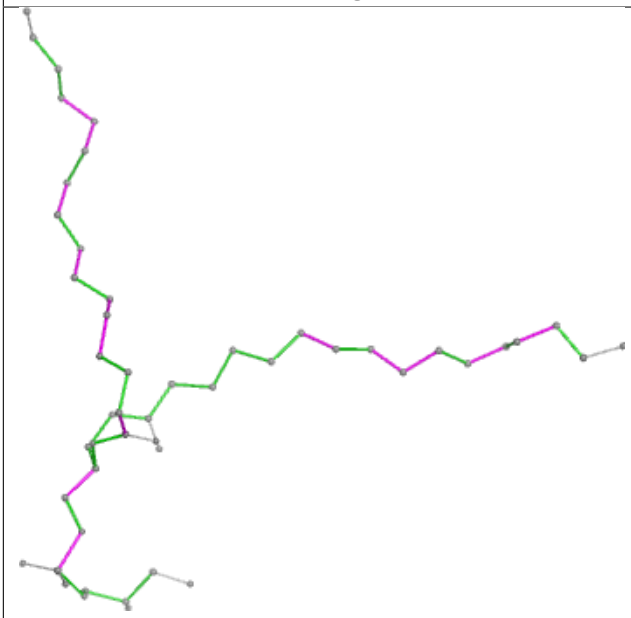
Ligand LHG l 101



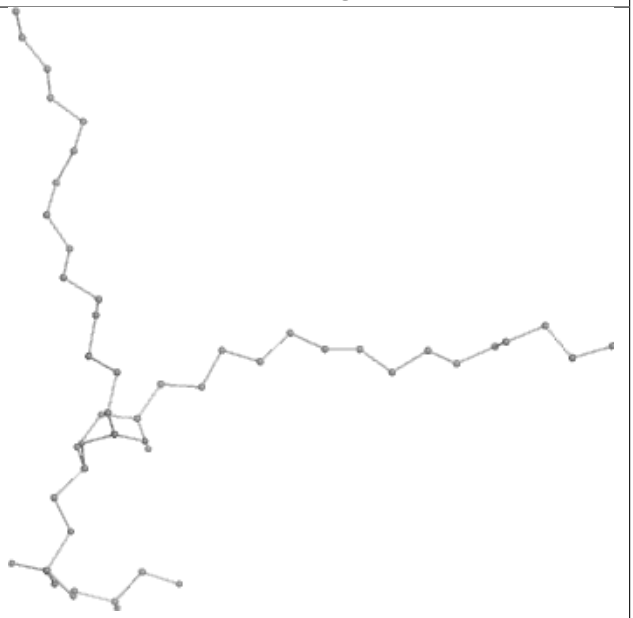
Bond lengths



Bond angles

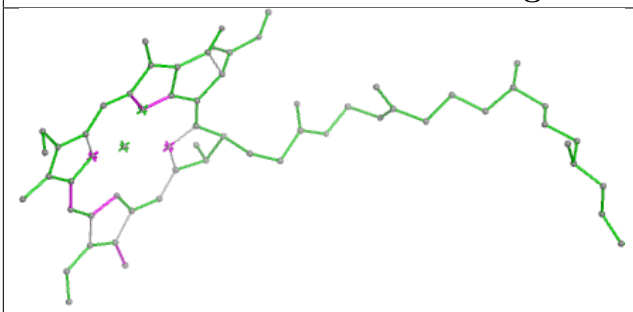


Torsions

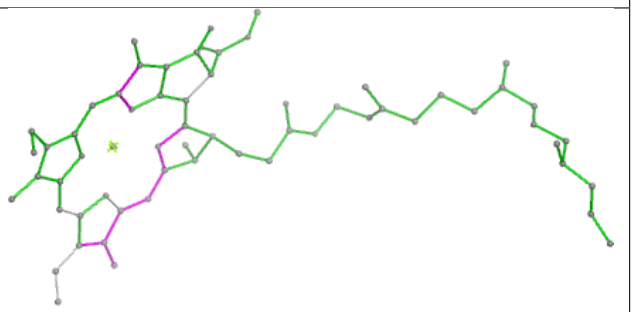


Rings

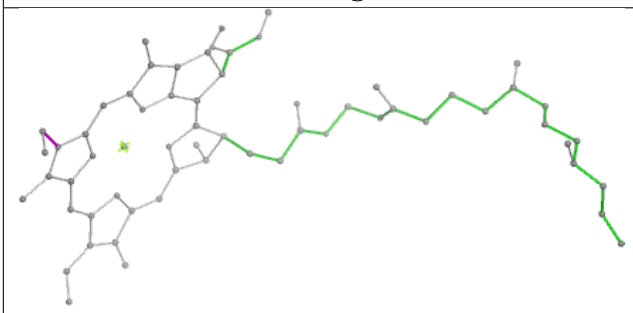
Ligand CLA A 404



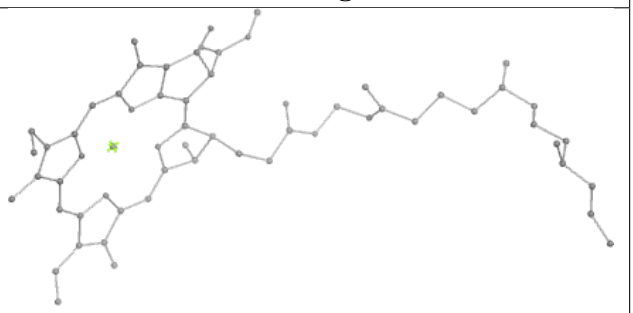
Bond lengths



Bond angles

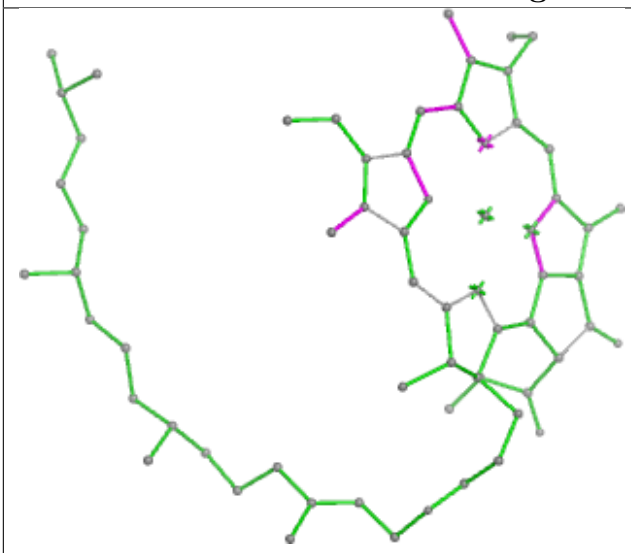


Torsions

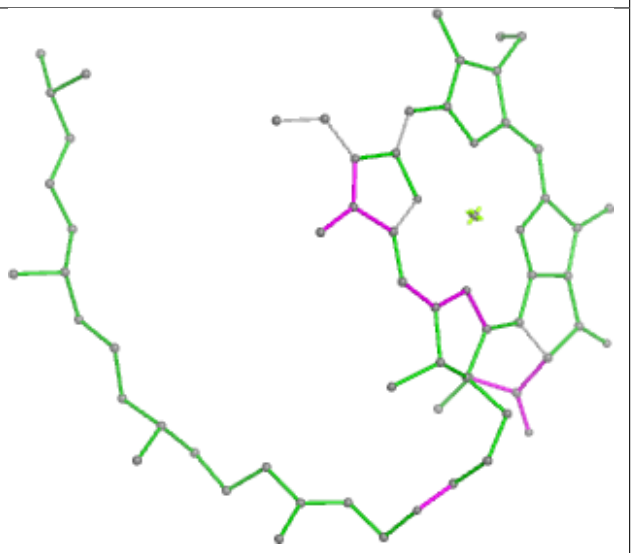


Rings

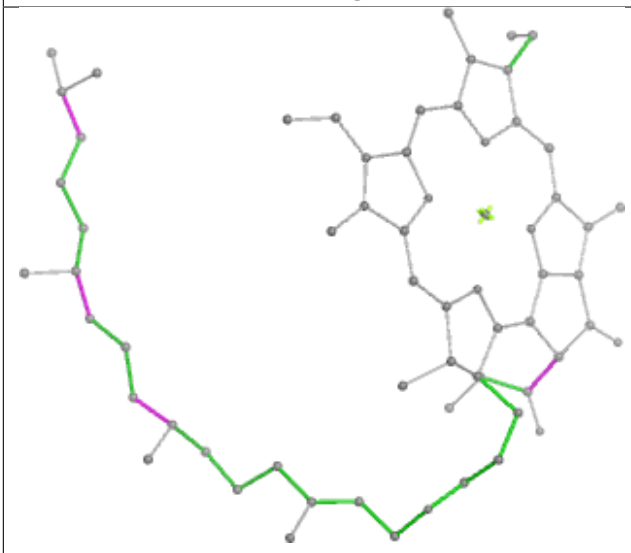
Ligand CLA c 507



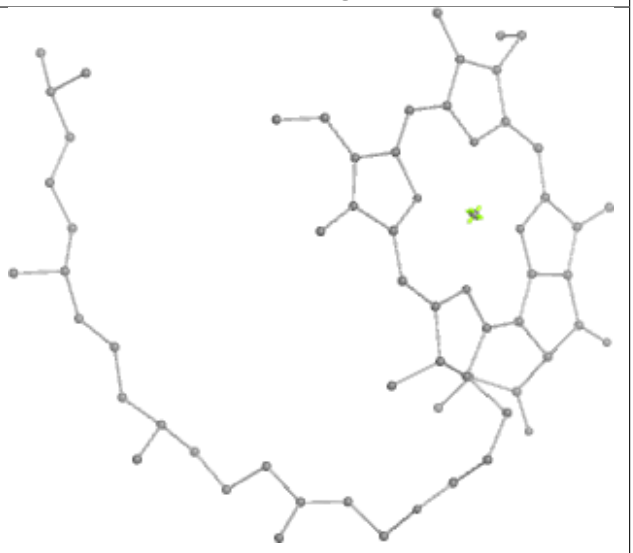
Bond lengths



Bond angles

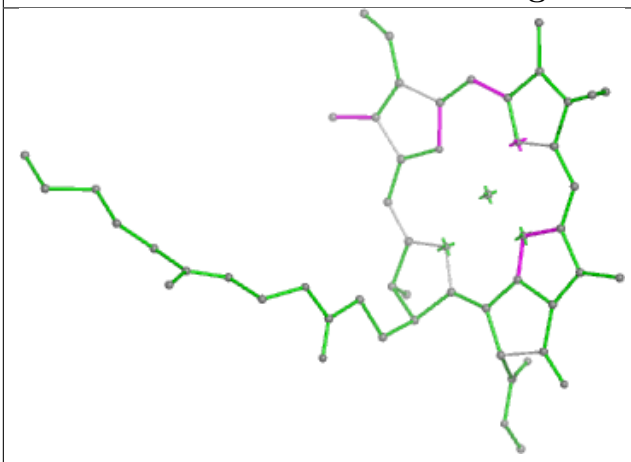


Torsions

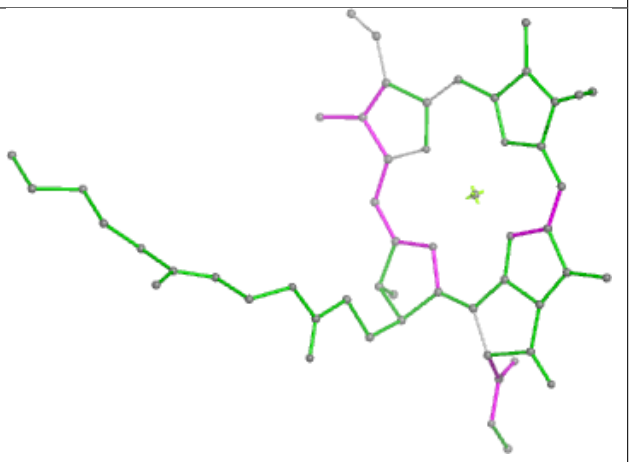


Rings

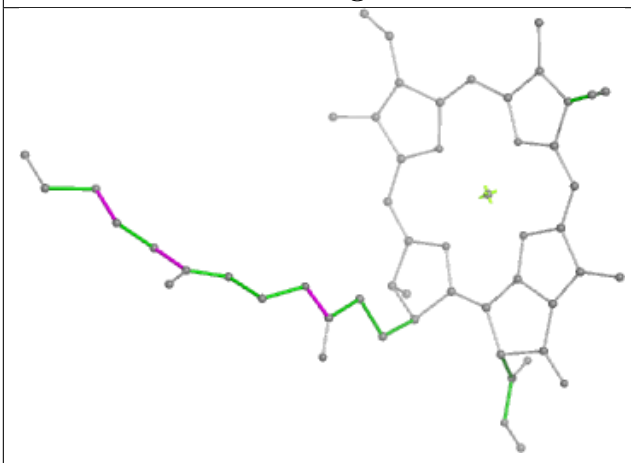
Ligand CLA a 406



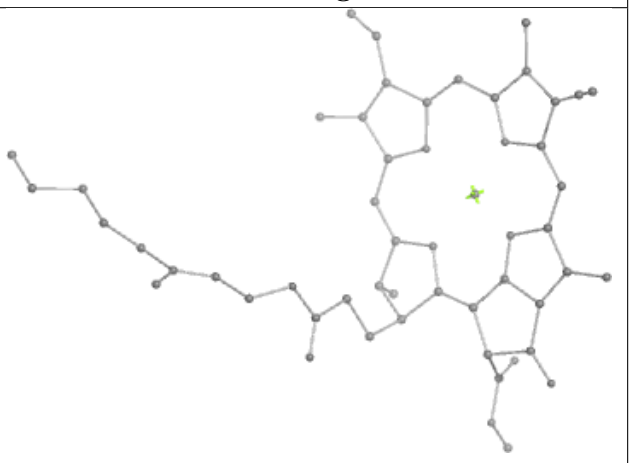
Bond lengths



Bond angles

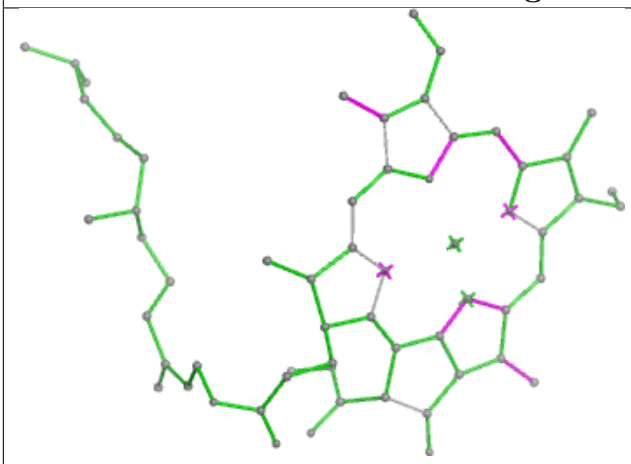


Torsions

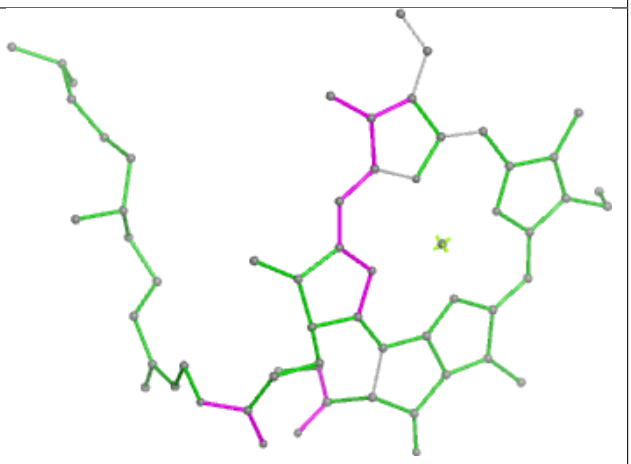


Rings

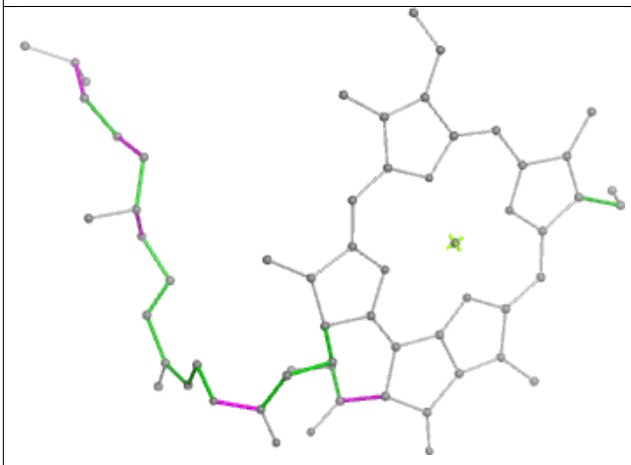
Ligand CLA B 616



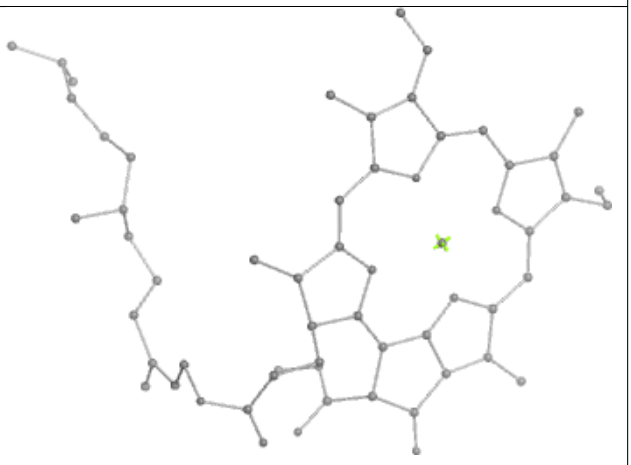
Bond lengths



Bond angles

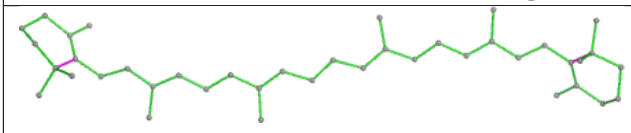


Torsions

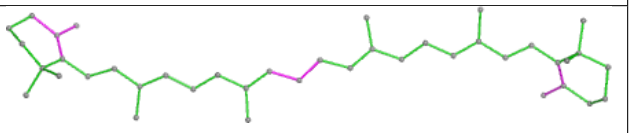


Rings

Ligand BCR B 618

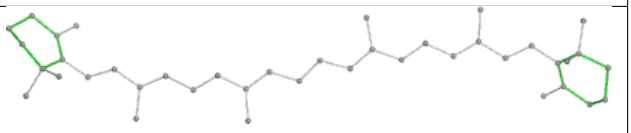


Bond lengths



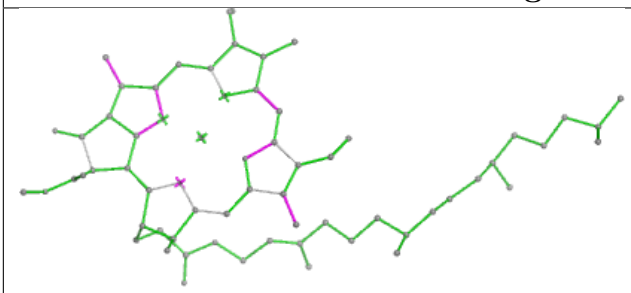
Bond angles

Torsions

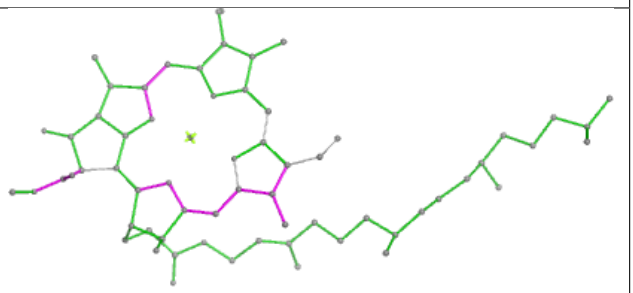


Rings

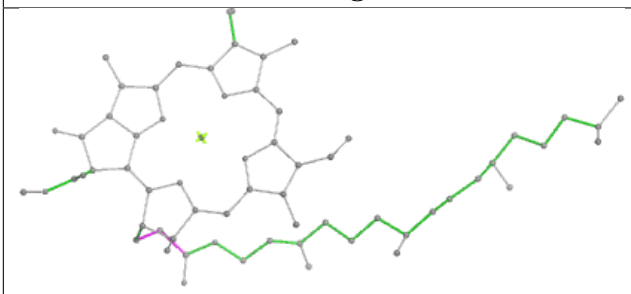
Ligand CLA C 501



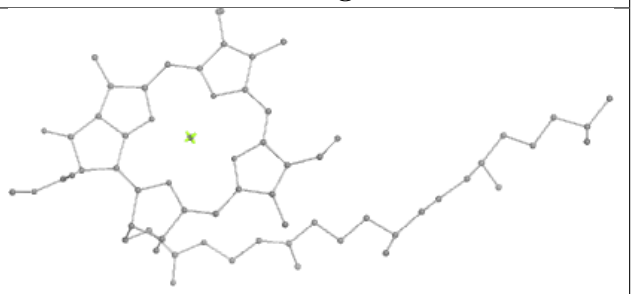
Bond lengths



Bond angles

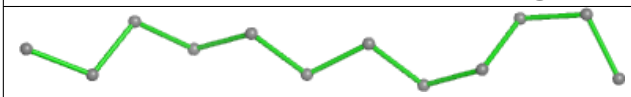


Torsions

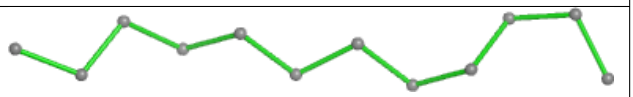


Rings

Ligand STE J 101

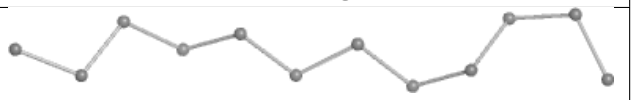


Bond lengths



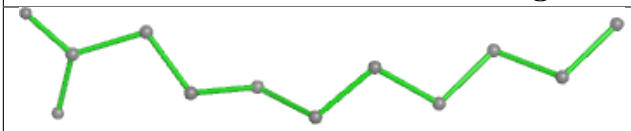
Bond angles

Torsions

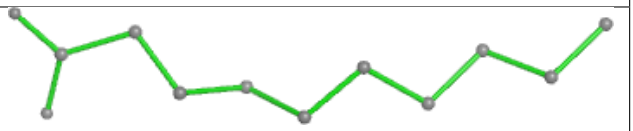


Rings

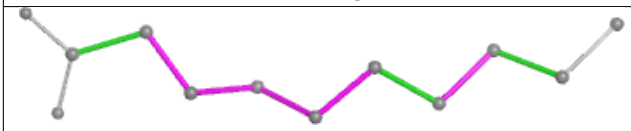
Ligand STE a 421



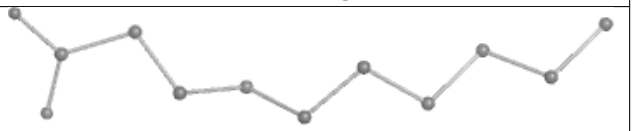
Bond lengths



Bond angles

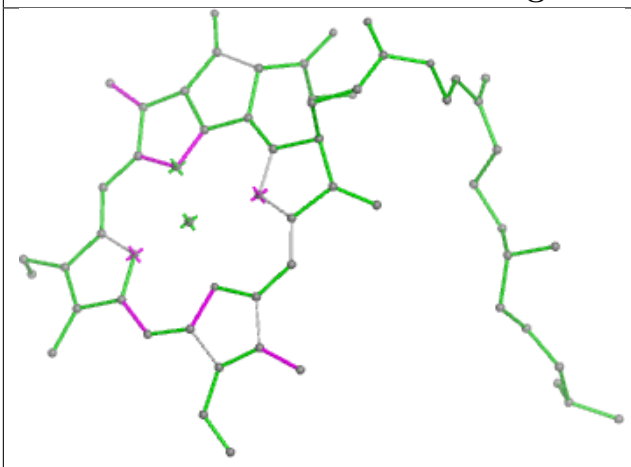


Torsions

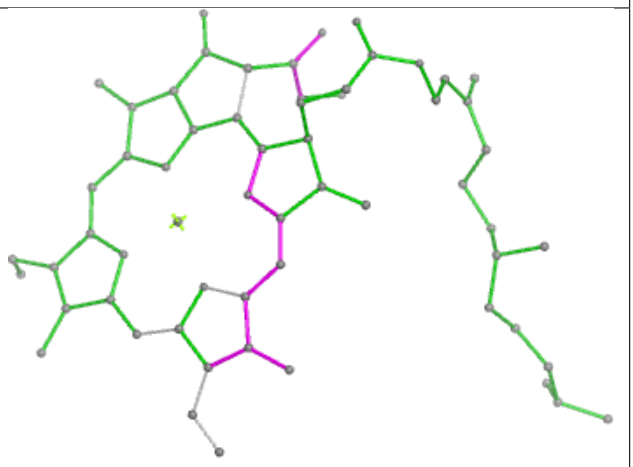


Rings

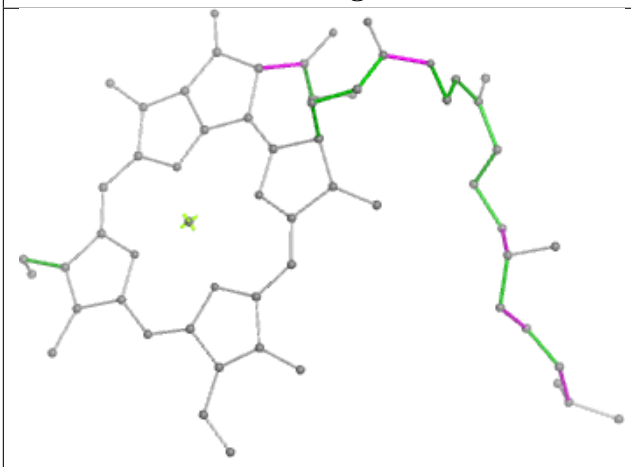
Ligand CLA b 617



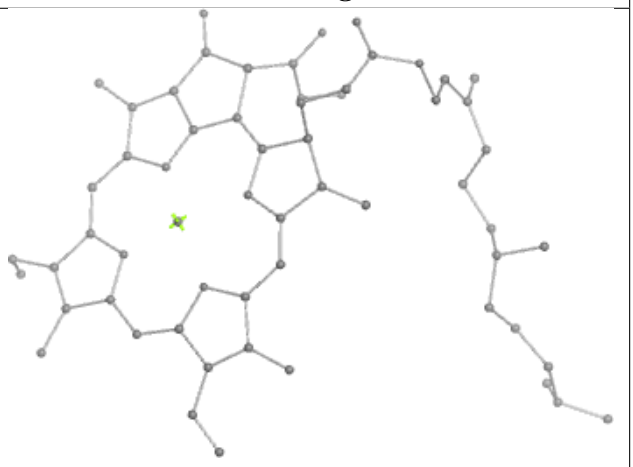
Bond lengths



Bond angles

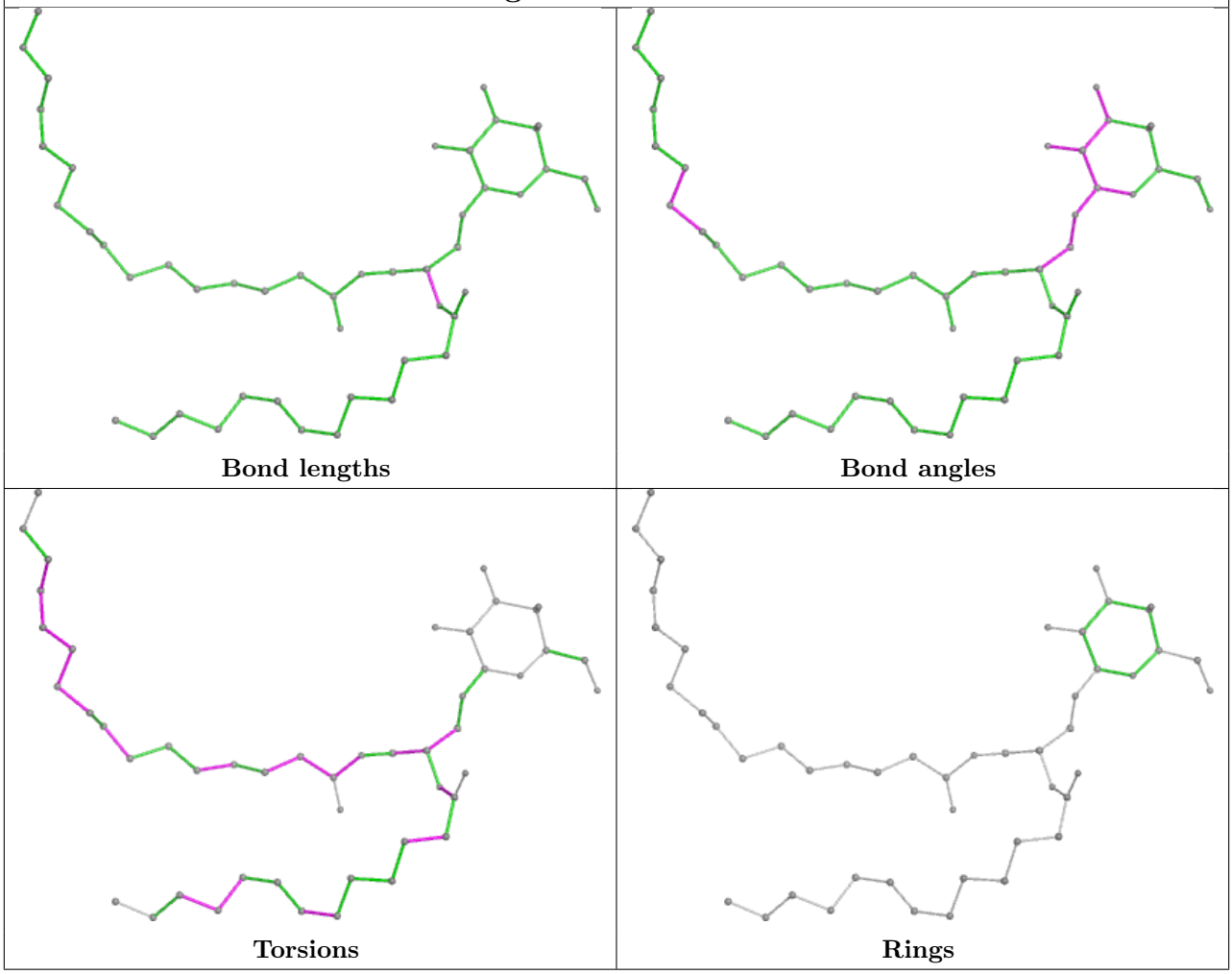


Torsions

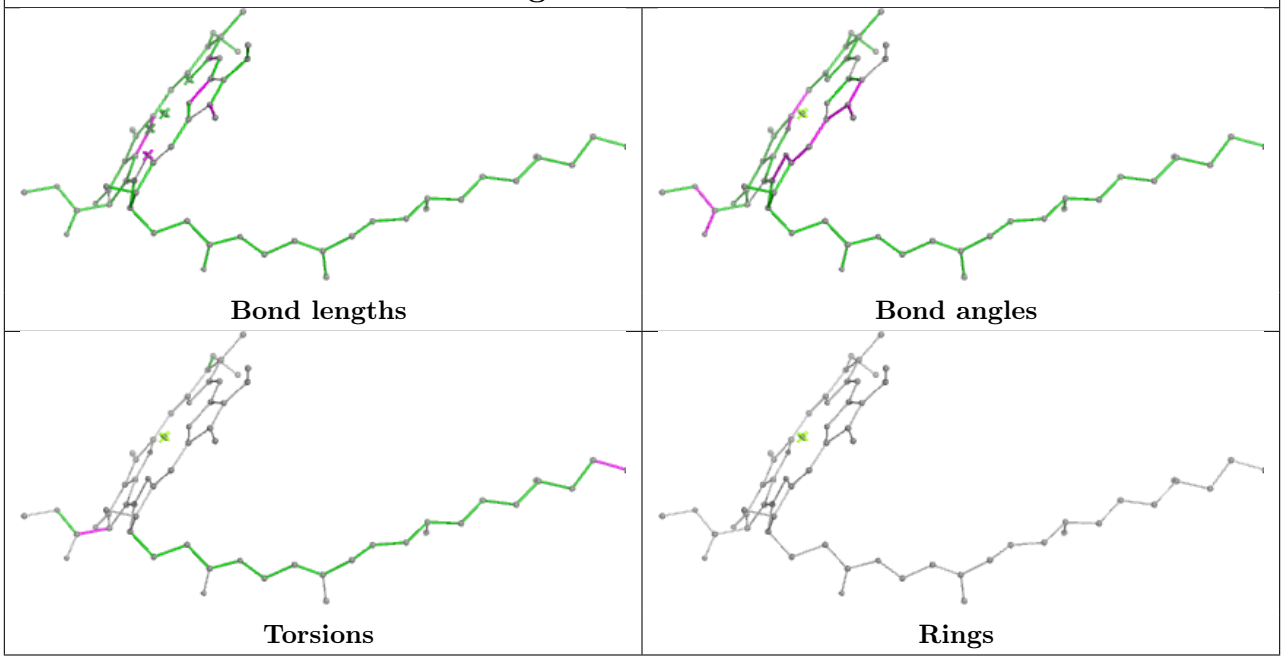


Rings

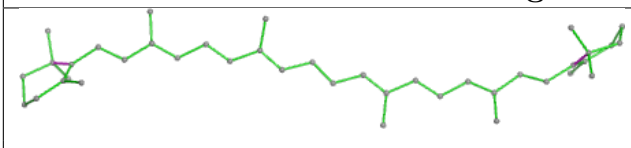
Ligand LMG c 520



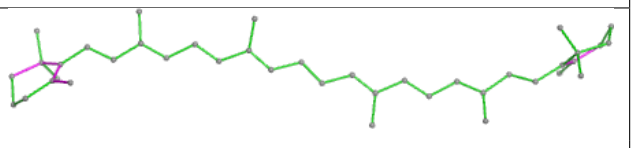
Ligand CLA b 608



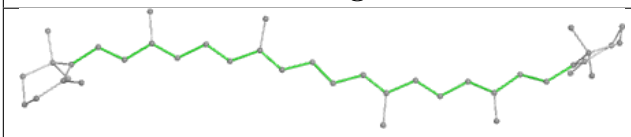
Ligand BCR a 407



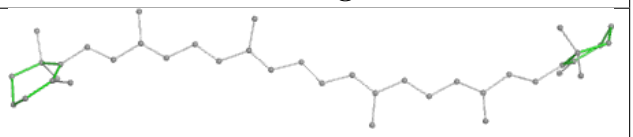
Bond lengths



Bond angles

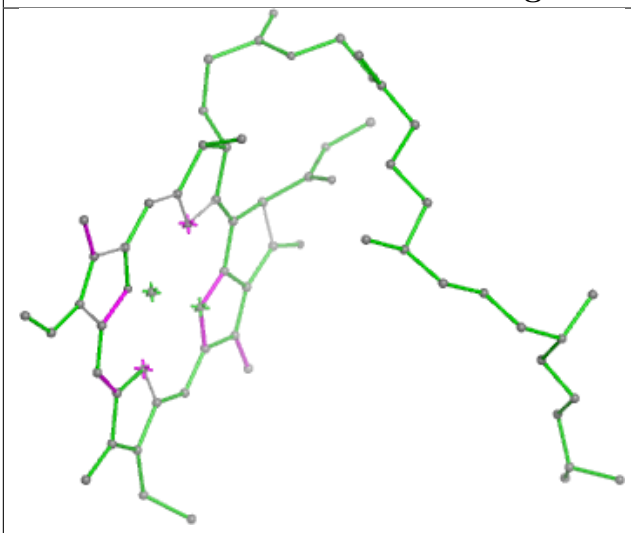


Torsions

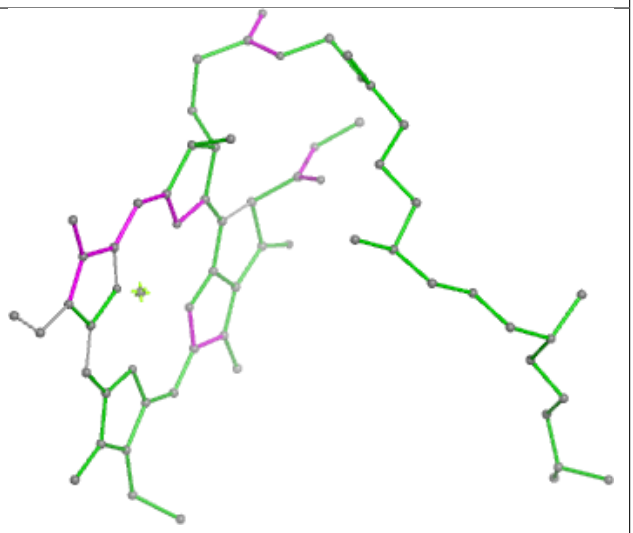


Rings

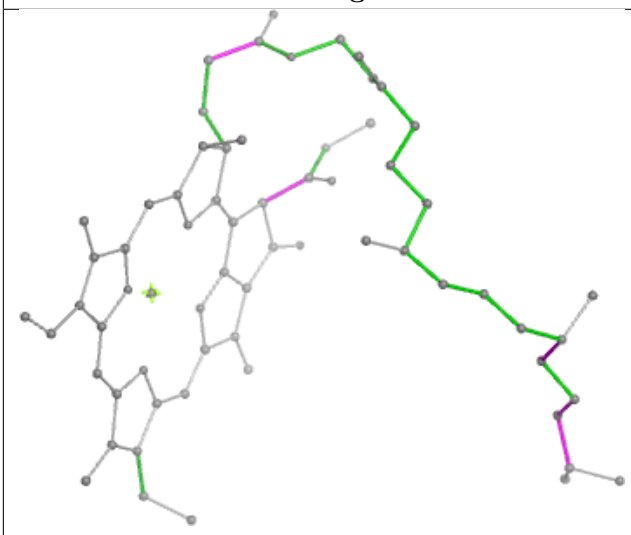
Ligand CLA B 613



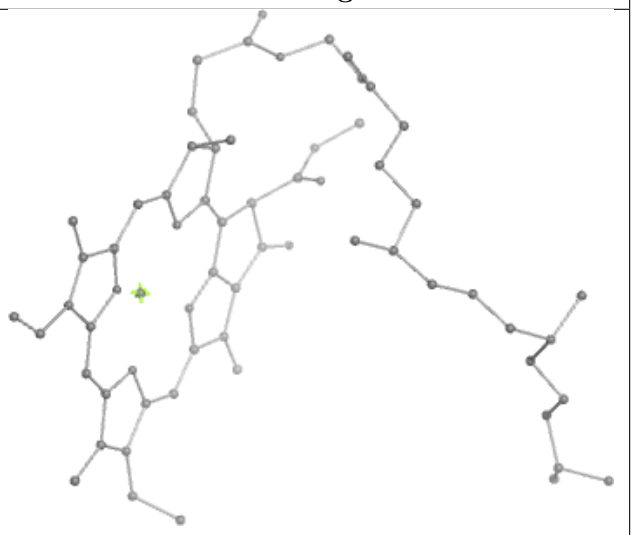
Bond lengths



Bond angles

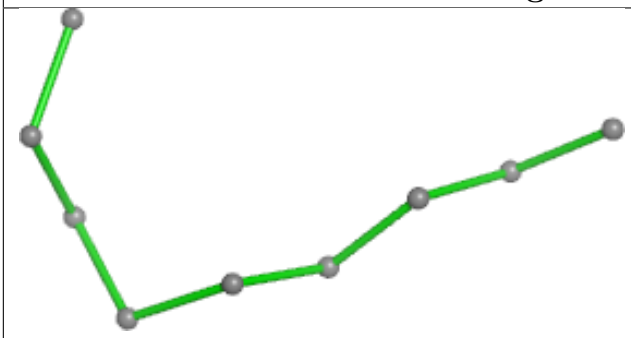


Torsions

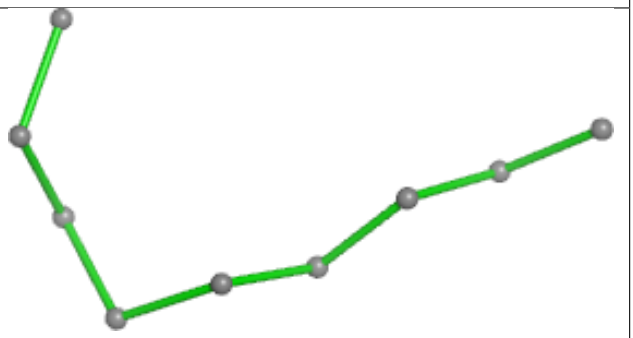


Rings

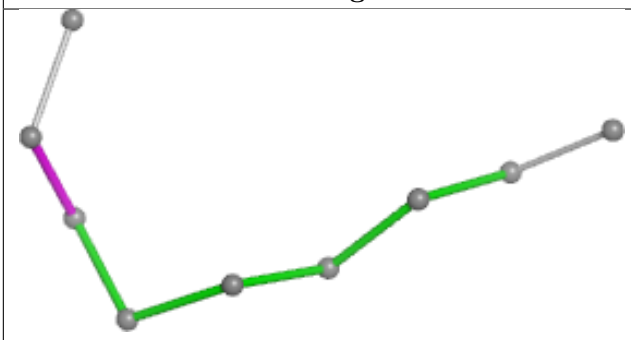
Ligand STE D 413



Bond lengths



Bond angles

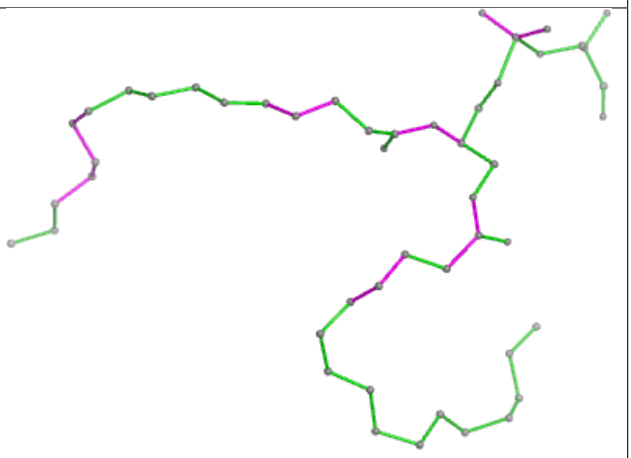


Torsions

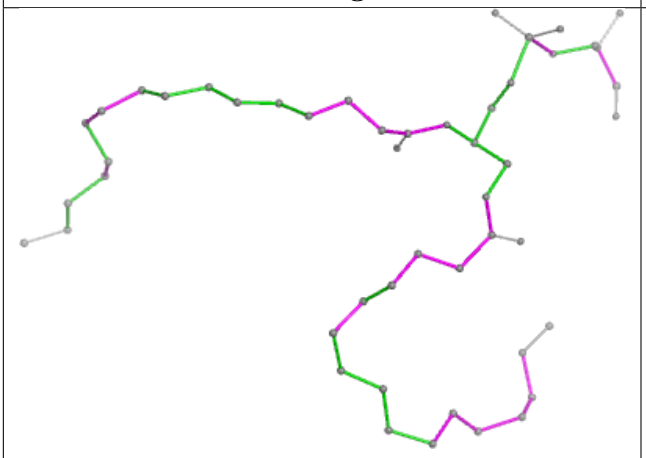
Rings

Ligand LHG A 420

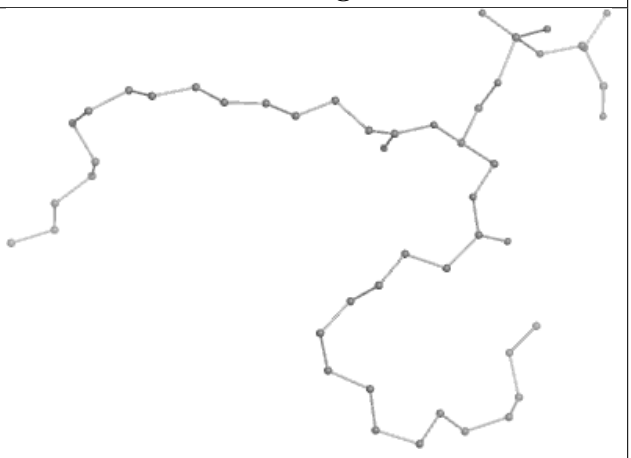
Bond lengths



Bond angles

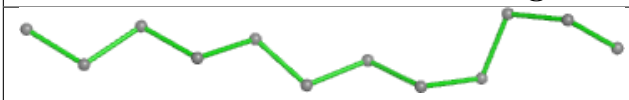


Torsions

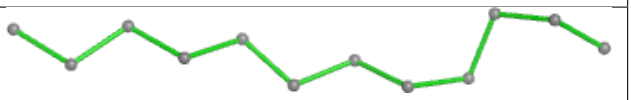


Rings

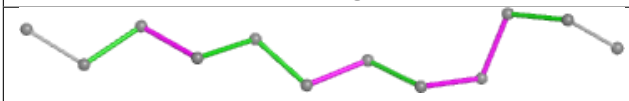
Ligand STE B 625



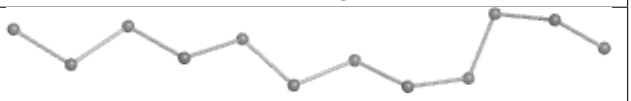
Bond lengths



Bond angles

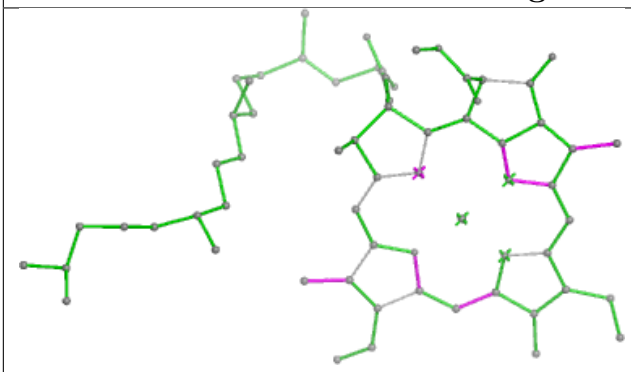


Torsions

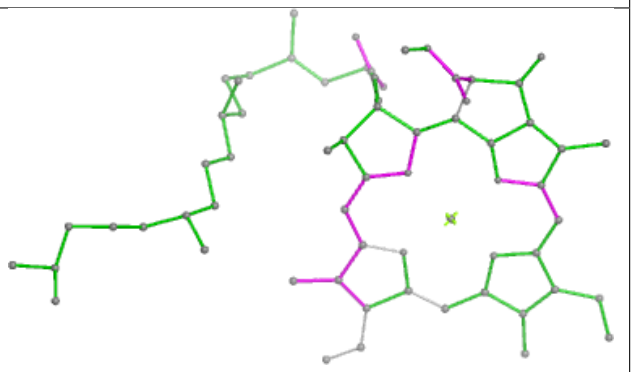


Rings

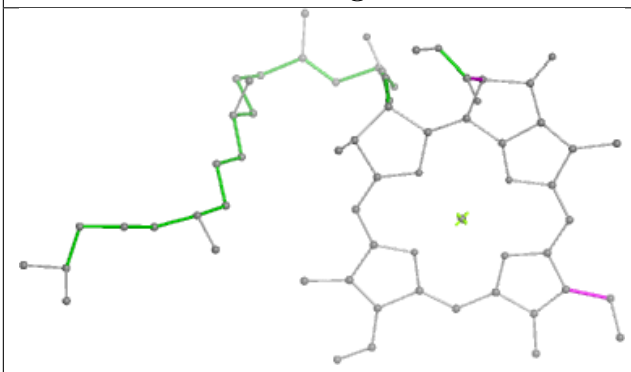
Ligand CLA a 419



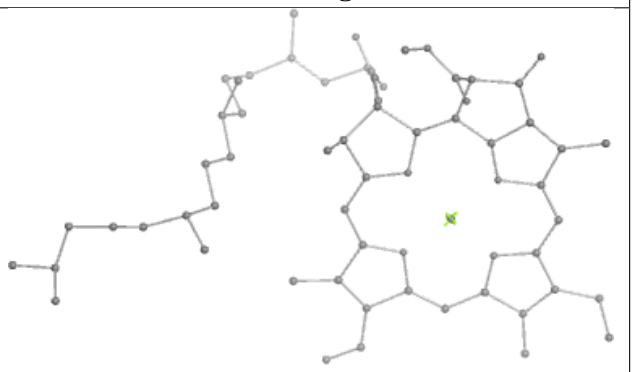
Bond lengths



Bond angles

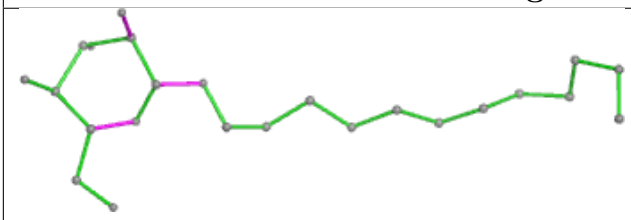


Torsions

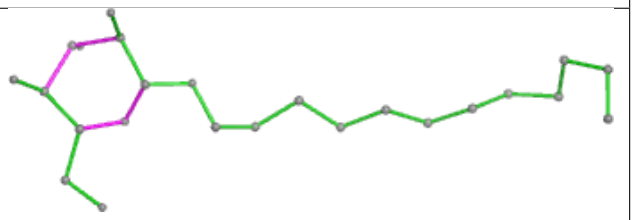


Rings

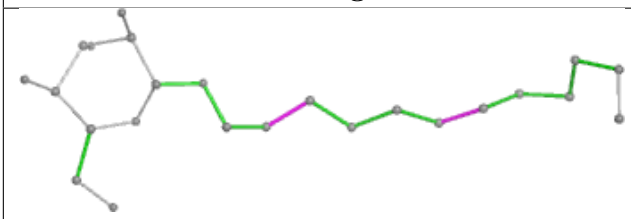
Ligand LMT c 523



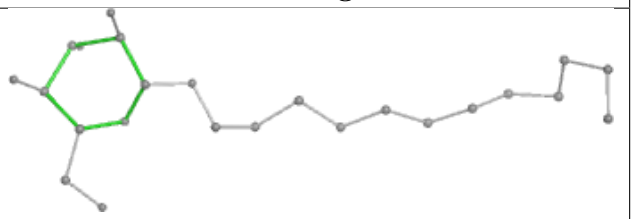
Bond lengths



Bond angles

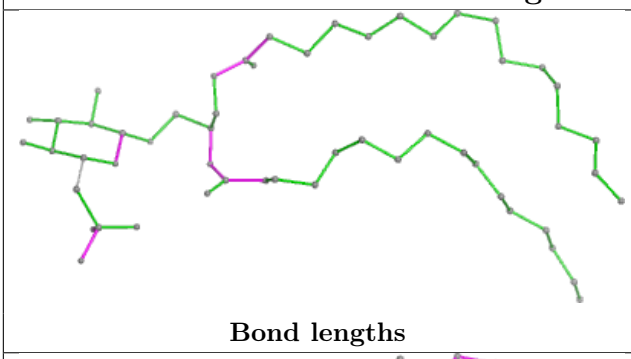


Torsions

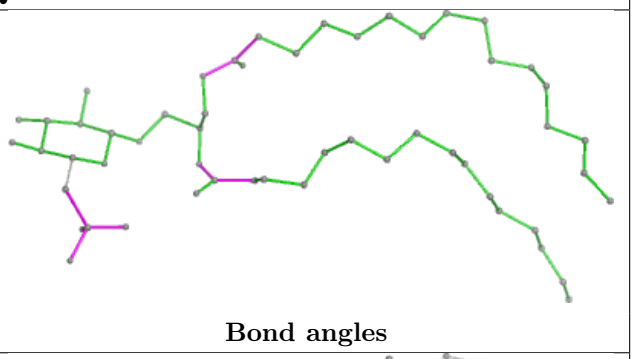


Rings

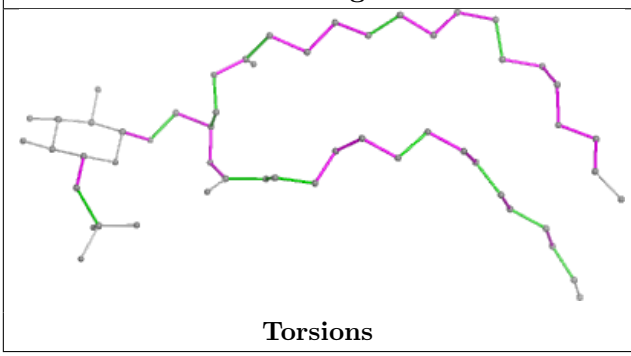
Ligand SQD B 620



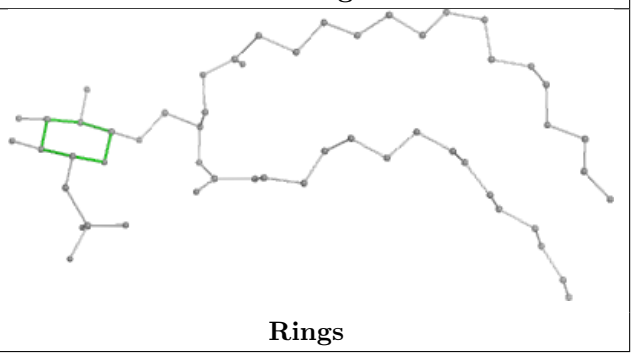
Bond lengths



Bond angles

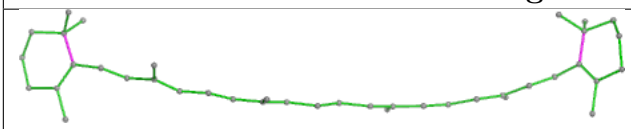


Torsions

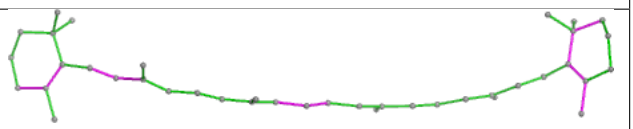


Rings

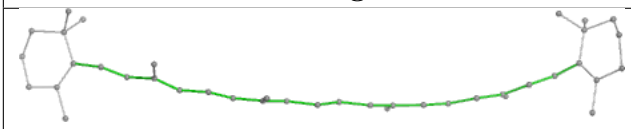
Ligand BCR k 101



Bond lengths



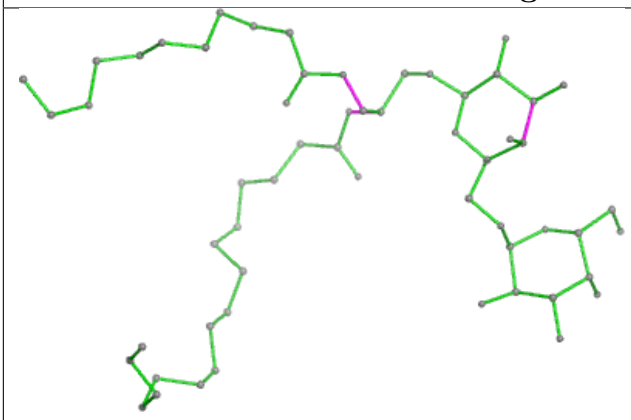
Bond angles



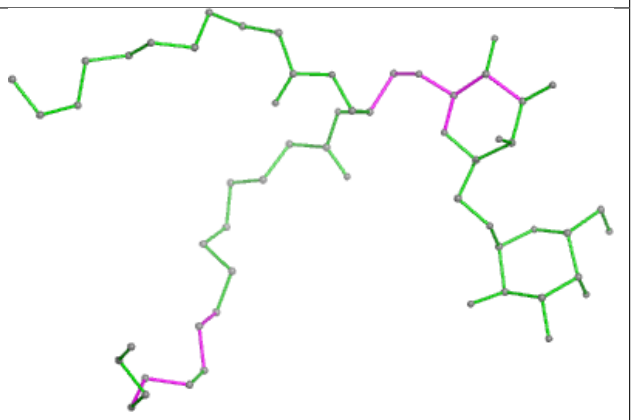
Torsions

Rings

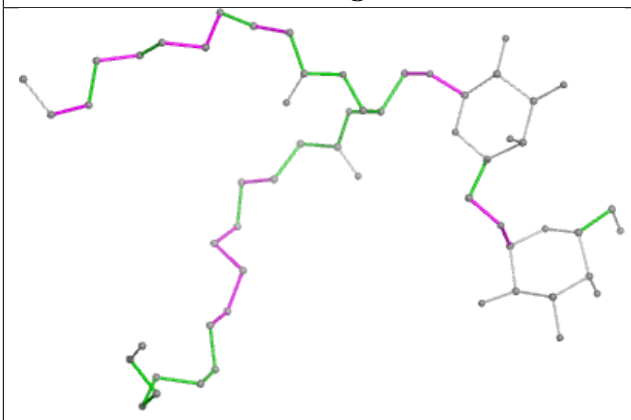
Ligand DGD C 518



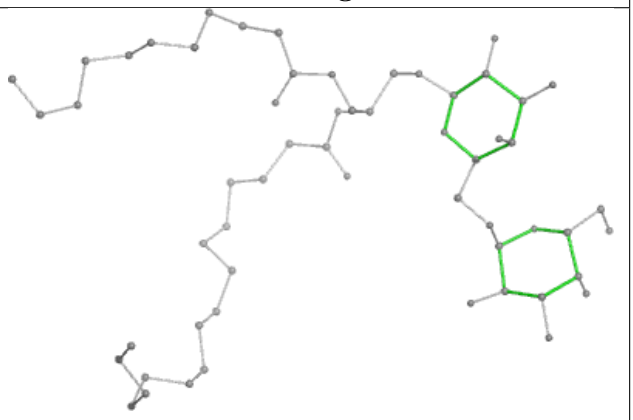
Bond lengths



Bond angles

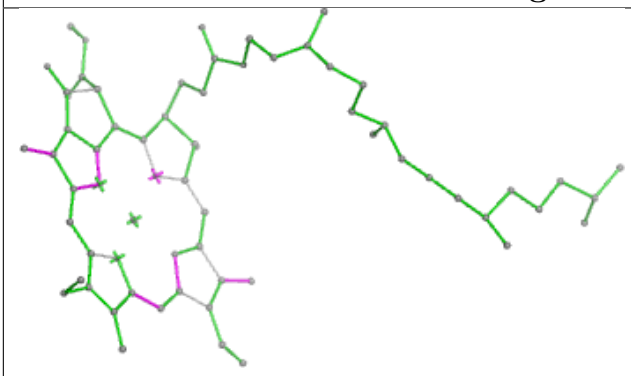


Torsions

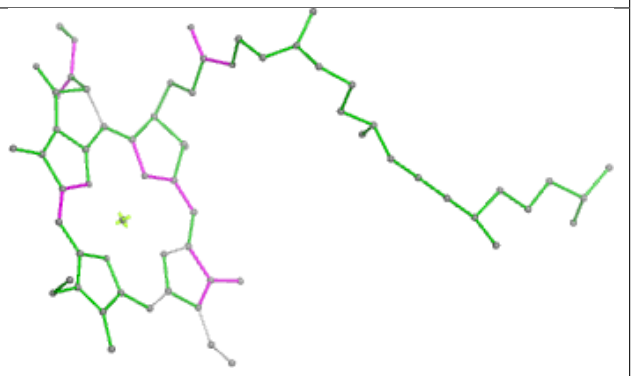


Rings

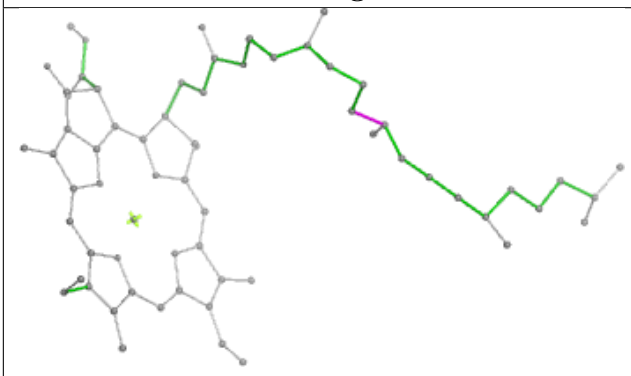
Ligand CLA c 511



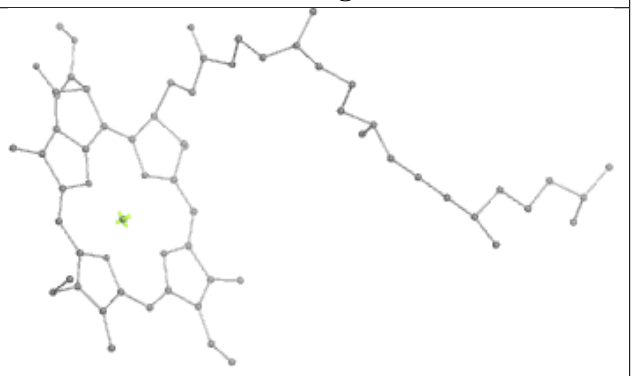
Bond lengths



Bond angles

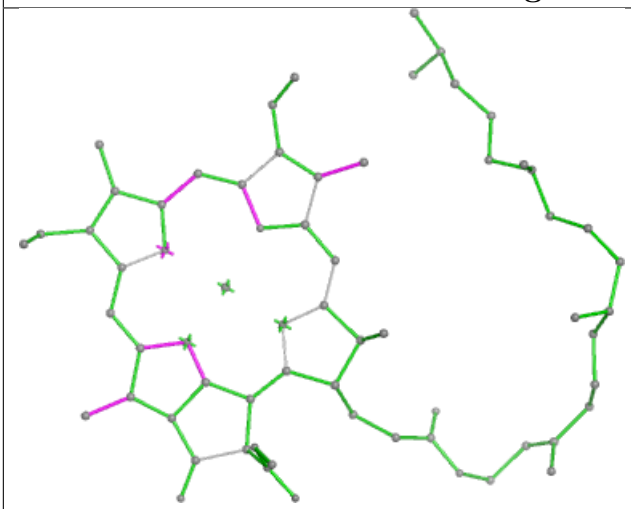


Torsions

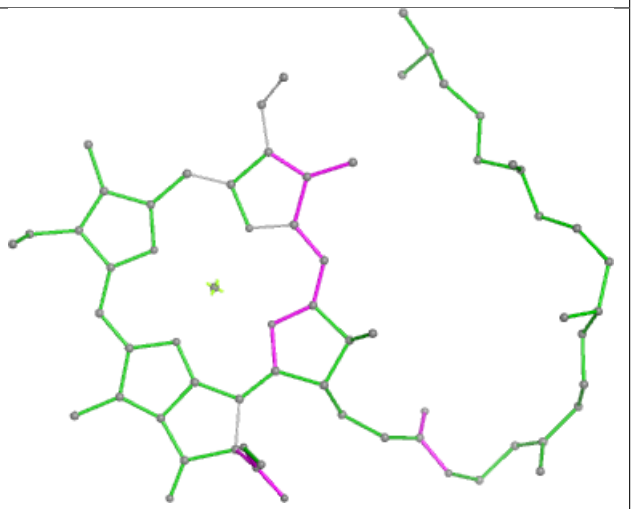


Rings

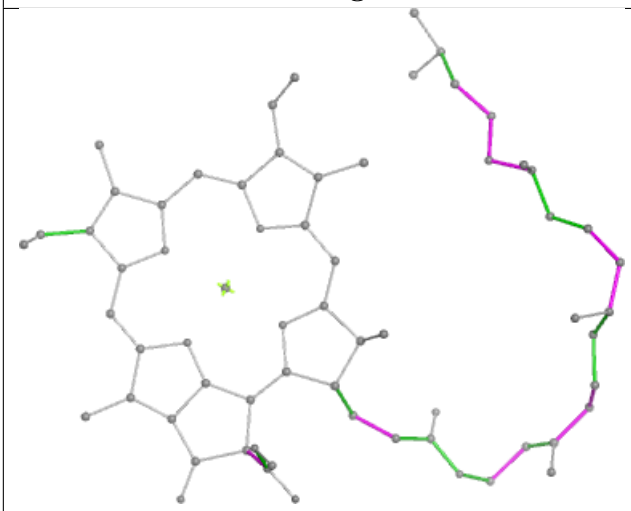
Ligand CLA C 512



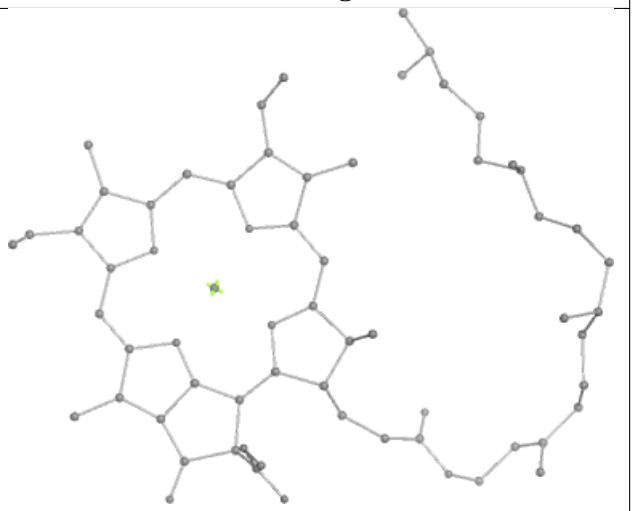
Bond lengths



Bond angles

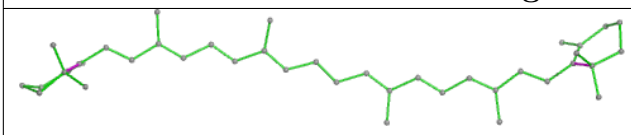


Torsions

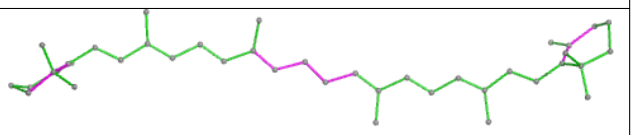


Rings

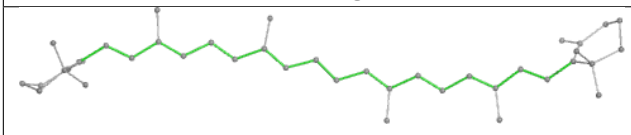
Ligand BCR C 514



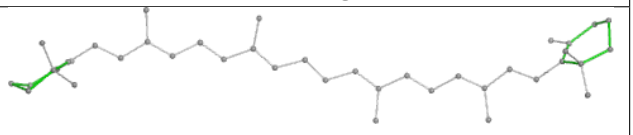
Bond lengths



Bond angles

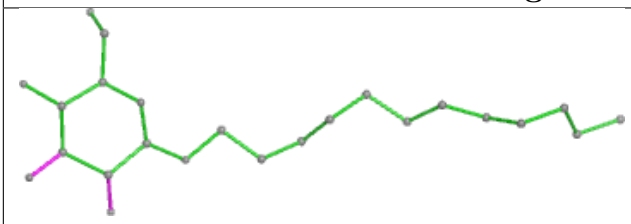


Torsions

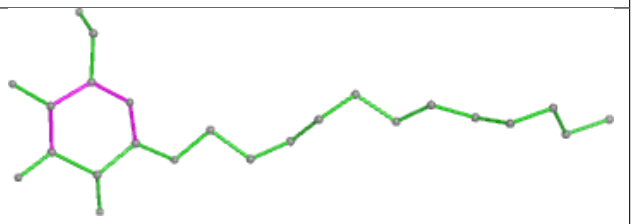


Rings

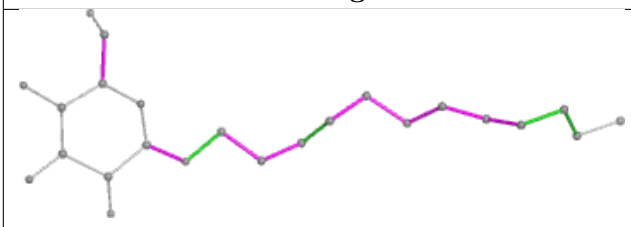
Ligand LMT J 102



Bond lengths



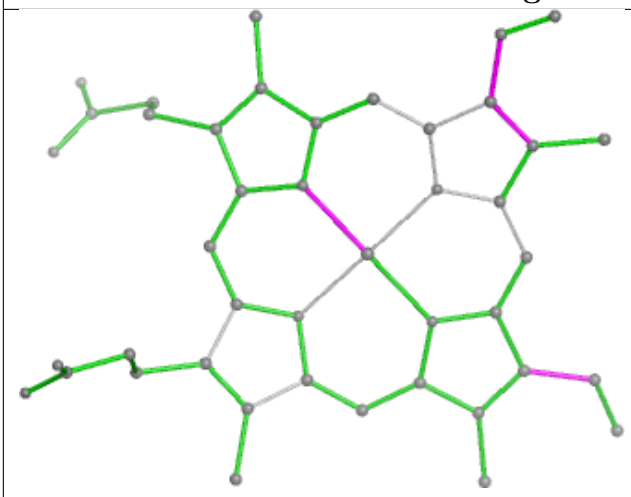
Bond angles



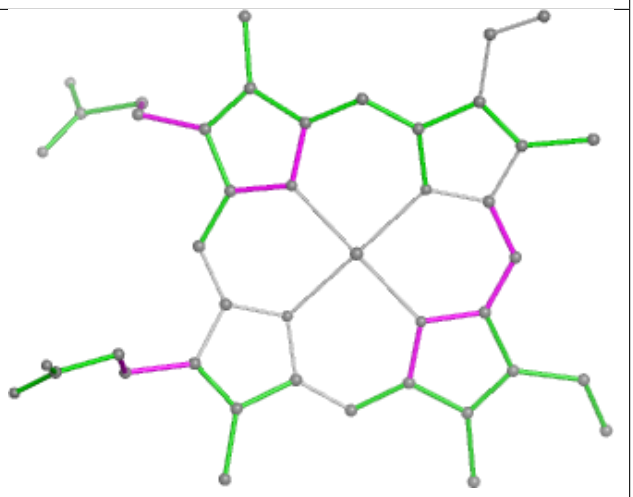
Torsions

Rings

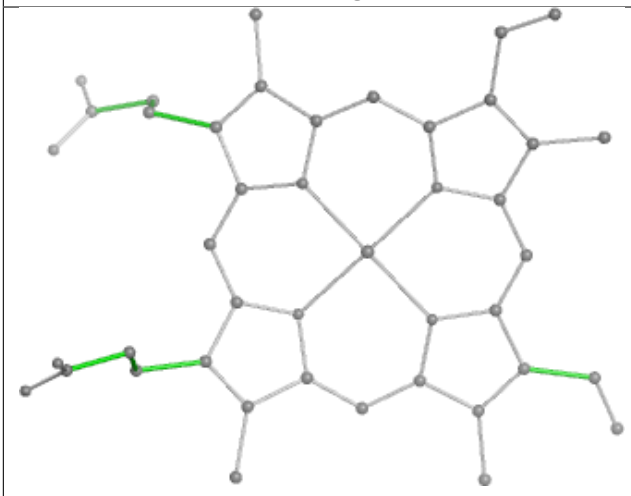
Ligand HEM e 105



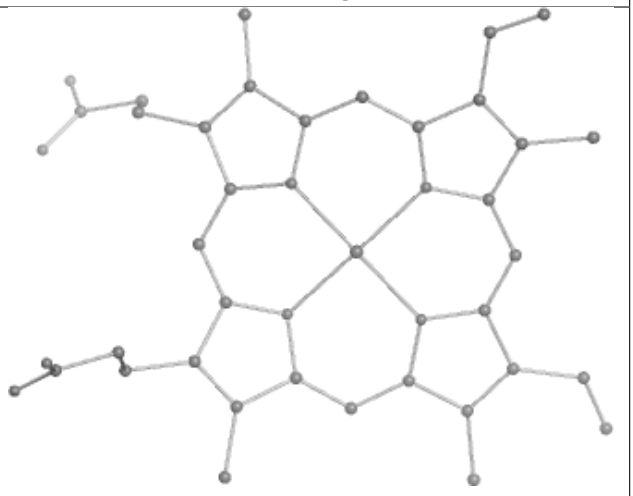
Bond lengths



Bond angles

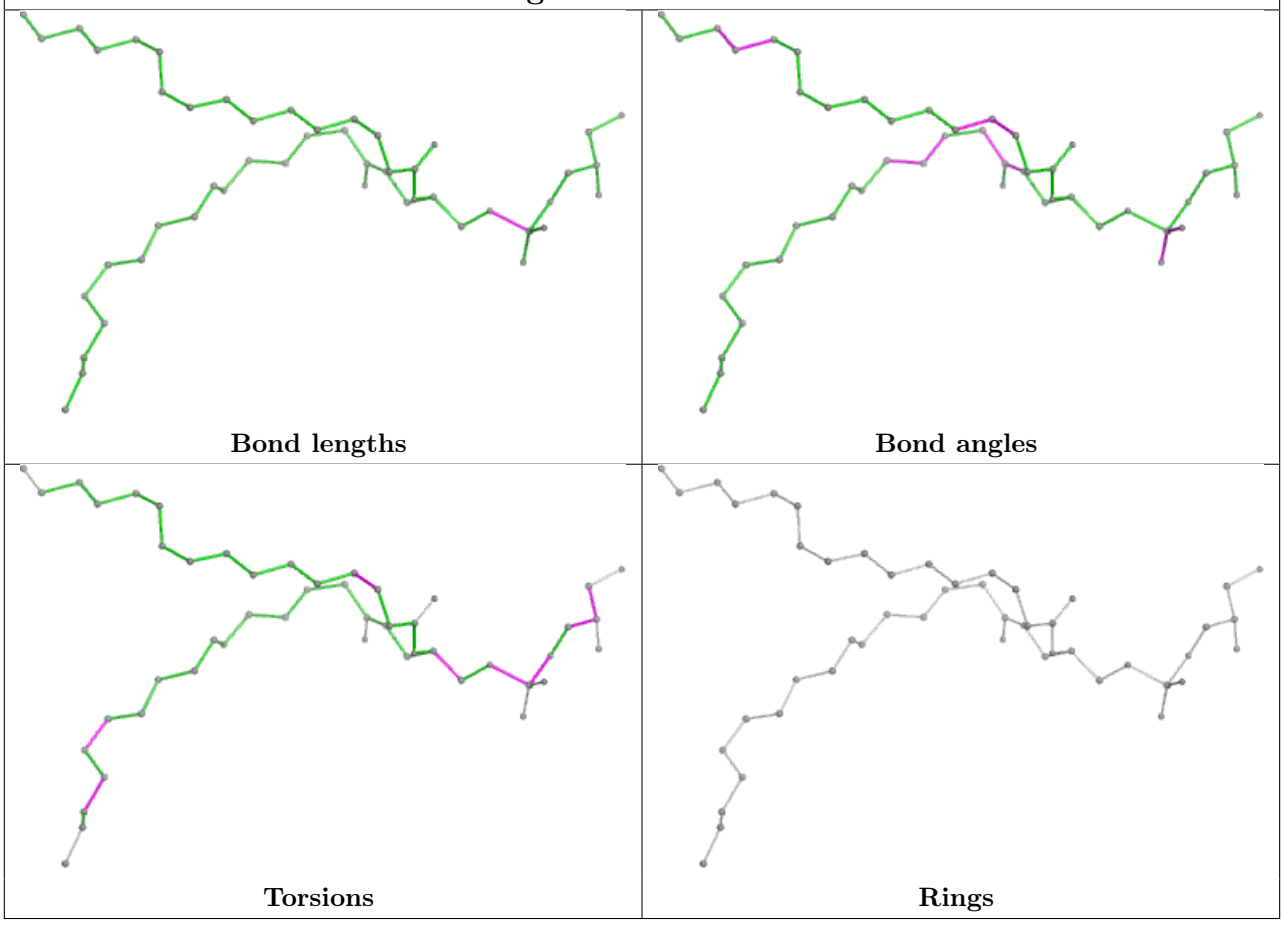


Torsions

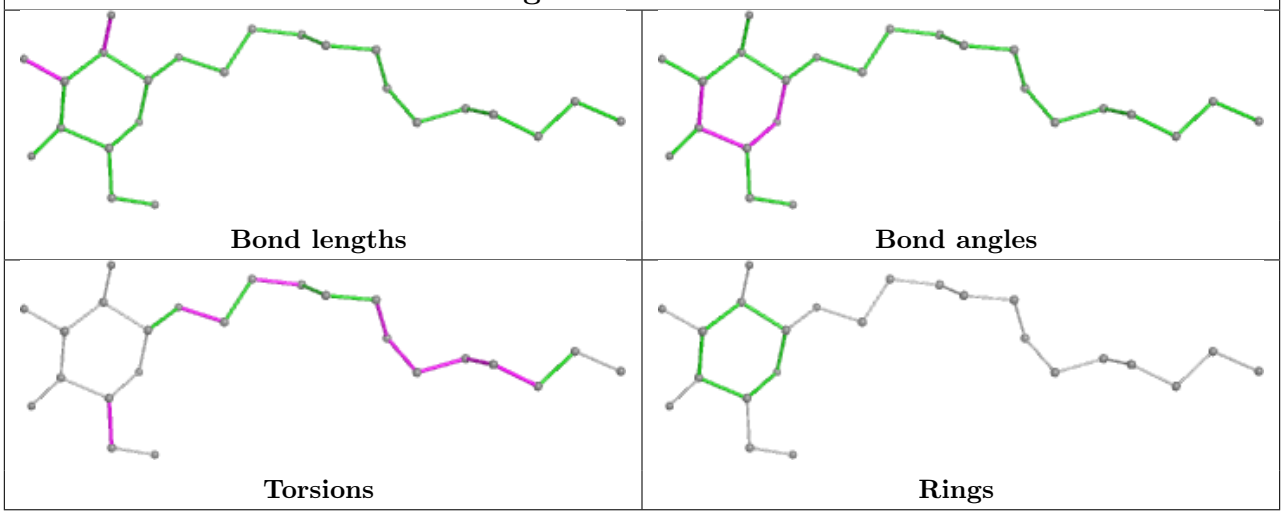


Rings

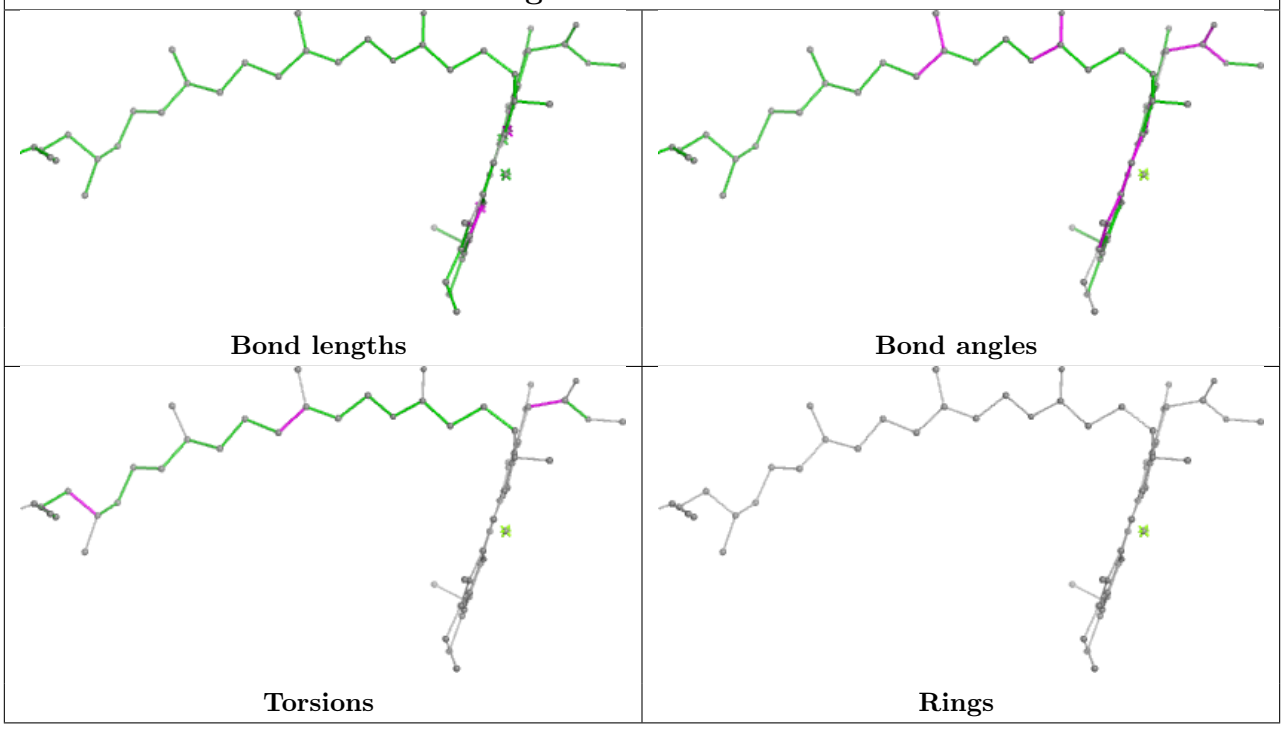
Ligand LHG d 409



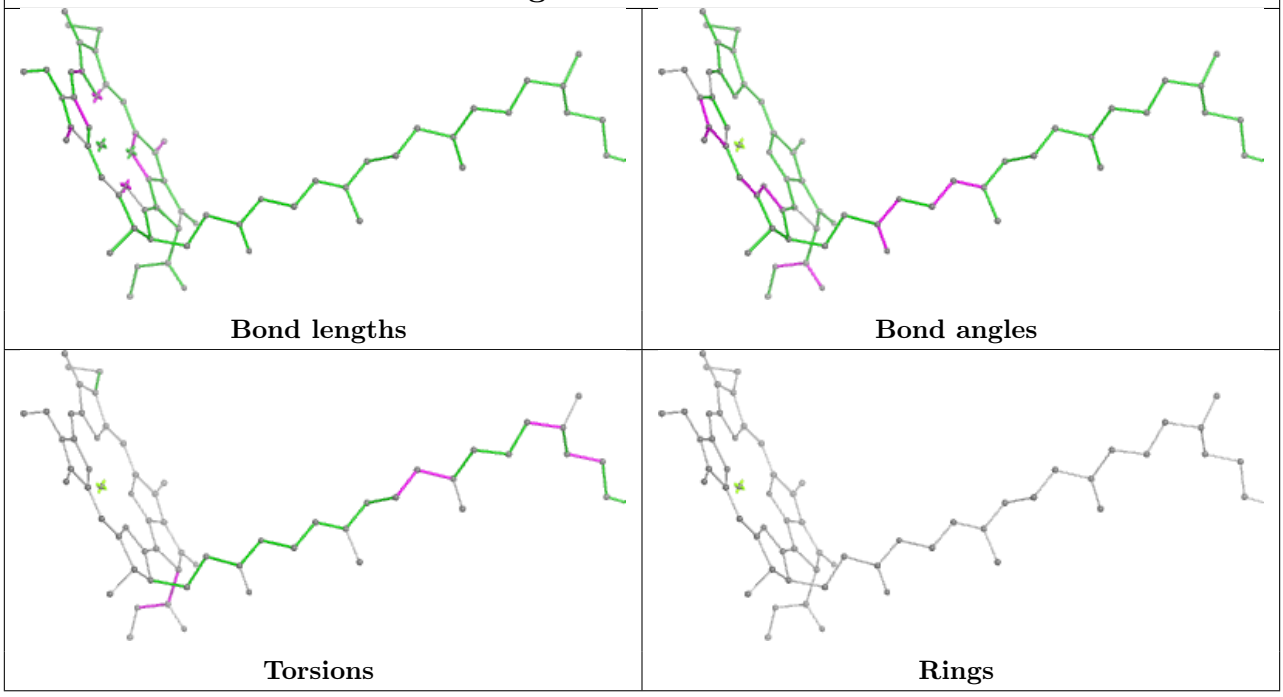
Ligand LMT E 104



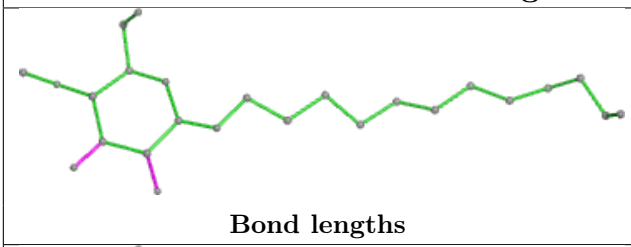
Ligand CLA B 605



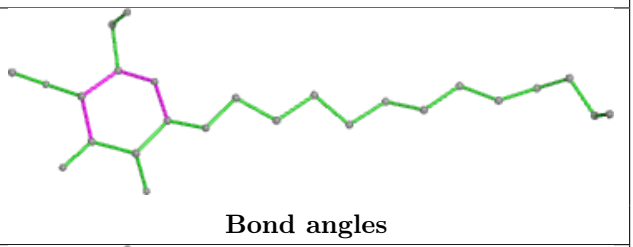
Ligand CLA b 605



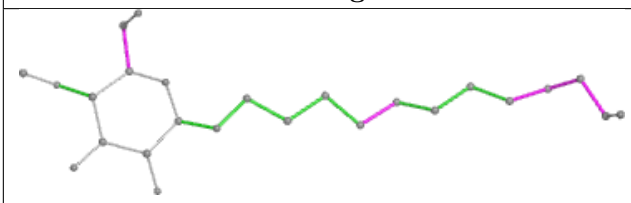
Ligand LMT B 623



Bond lengths



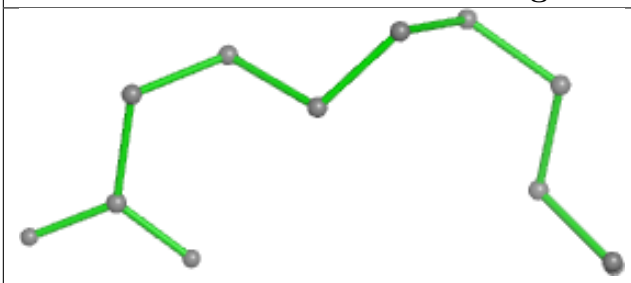
Bond angles



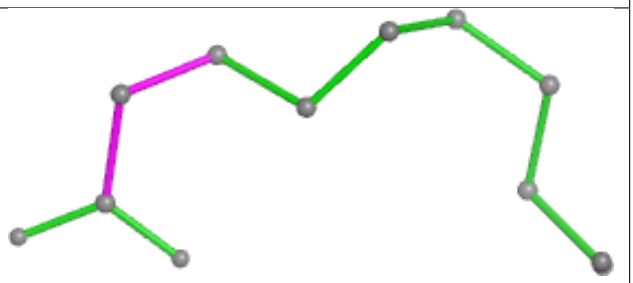
Torsions

Rings

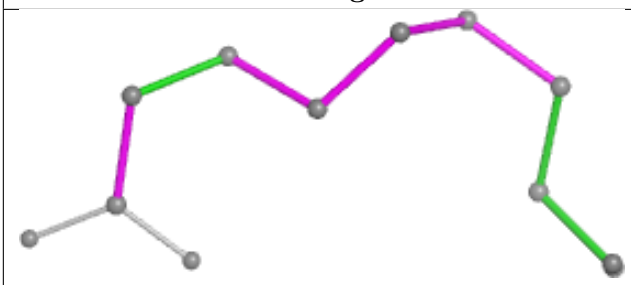
Ligand STE b 623



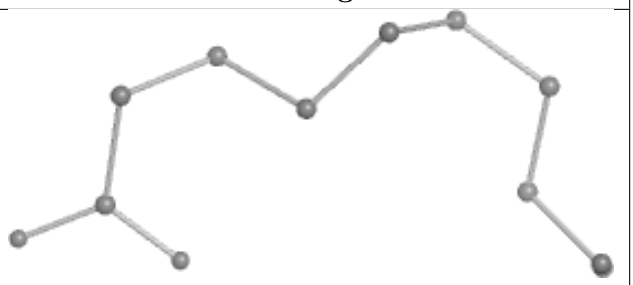
Bond lengths



Bond angles

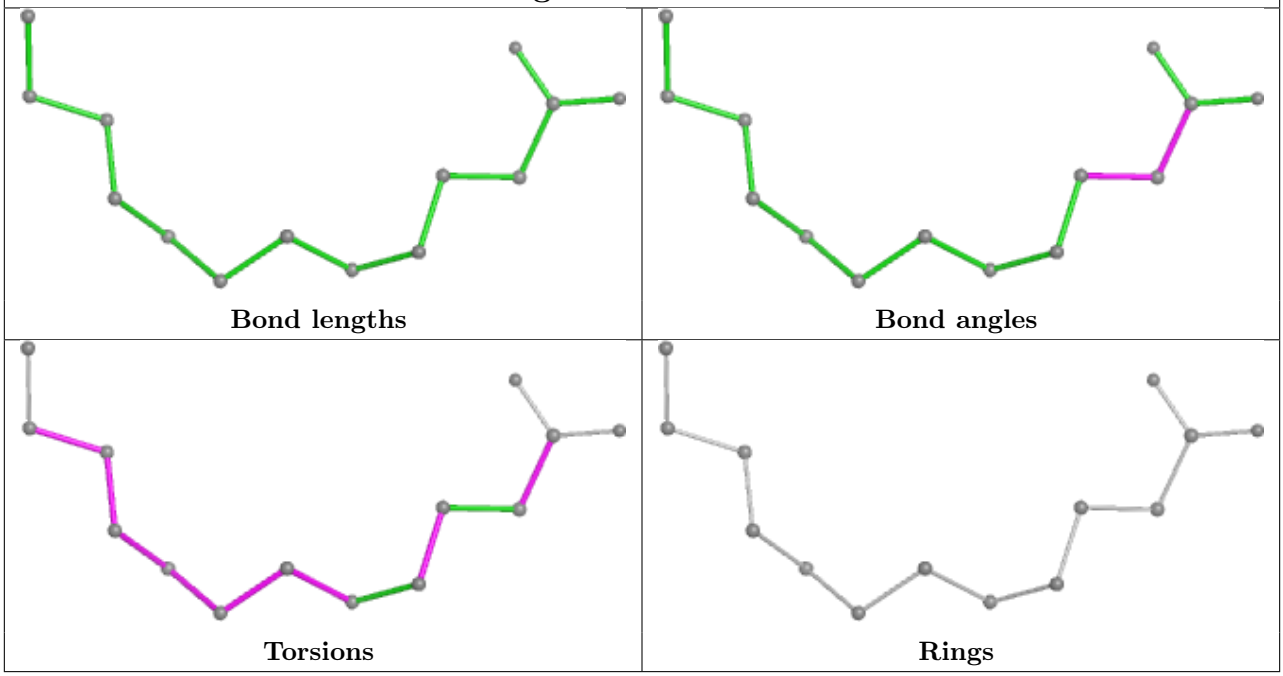


Torsions

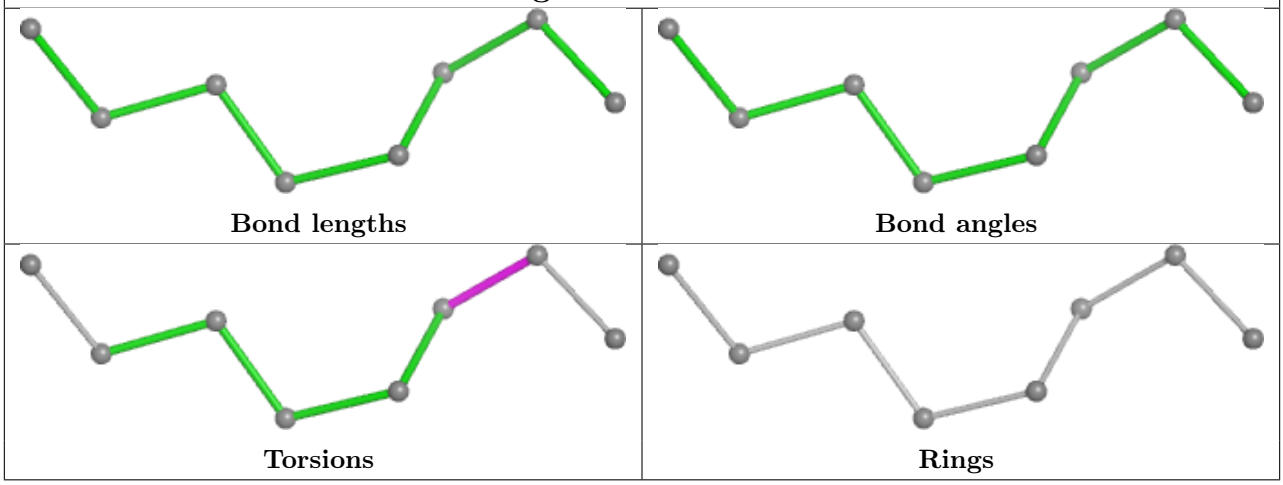


Rings

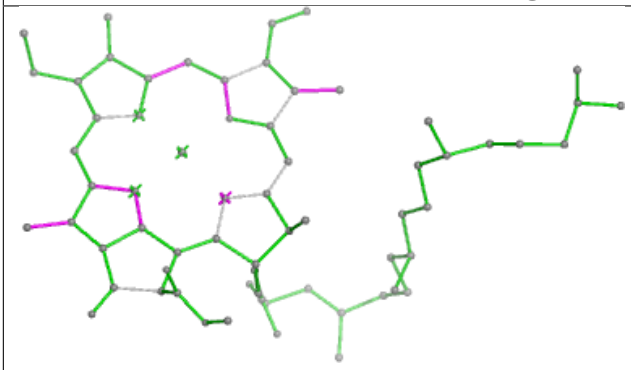
Ligand STE c 516



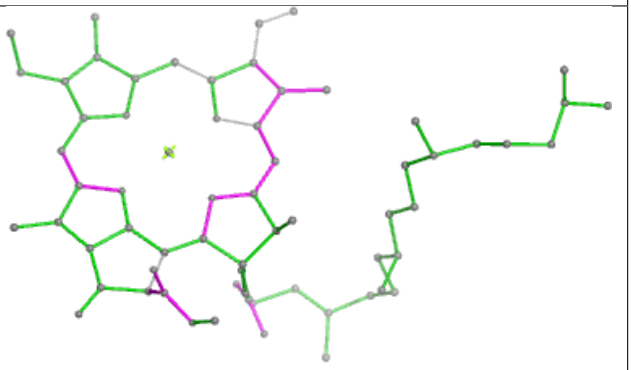
Ligand STE a 414



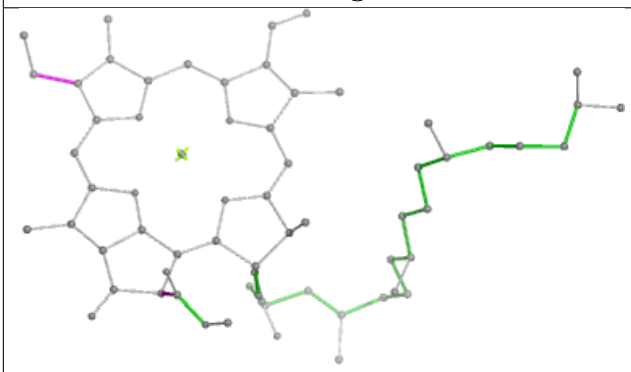
Ligand CLA A 419



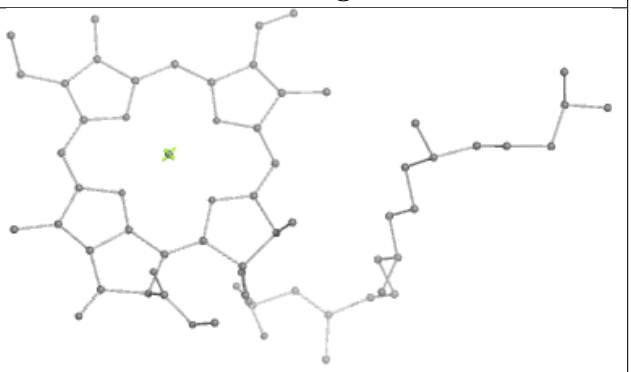
Bond lengths



Bond angles

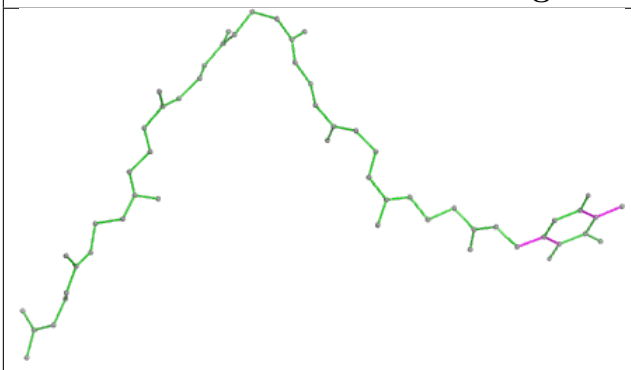


Torsions

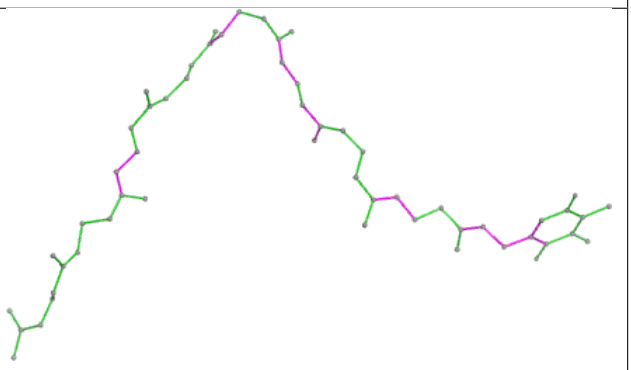


Rings

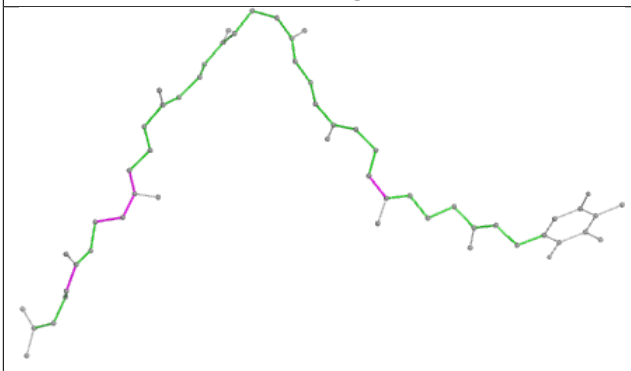
Ligand PL9 d 407



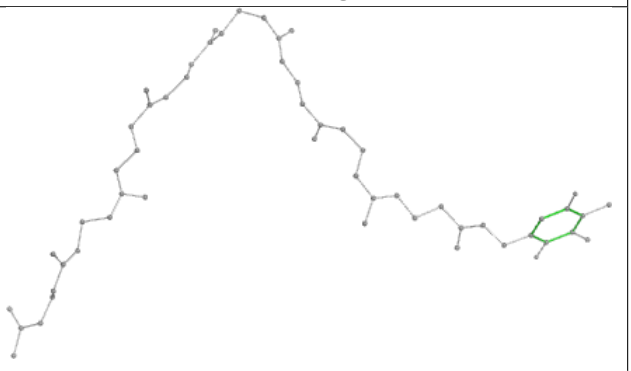
Bond lengths



Bond angles

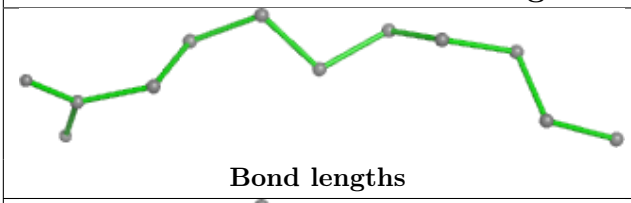


Torsions

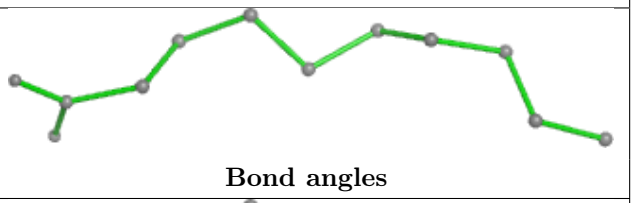


Rings

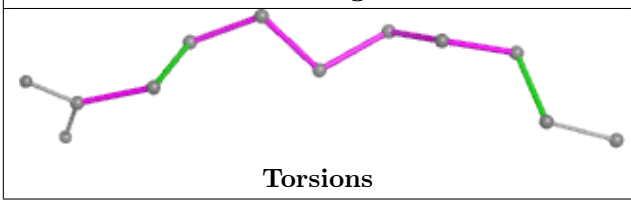
Ligand STE C 521



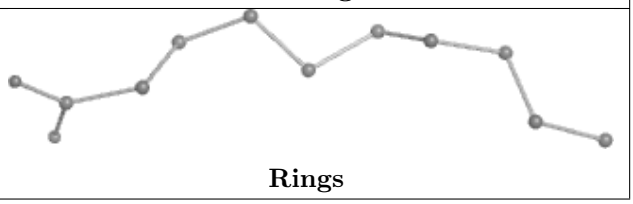
Bond lengths



Bond angles

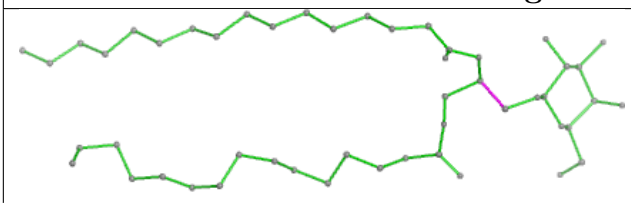


Torsions

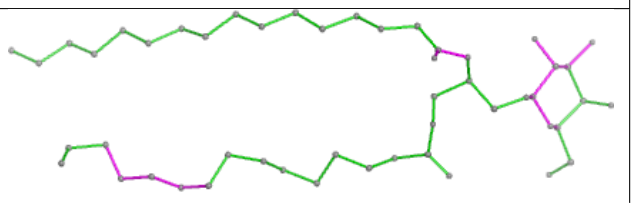


Rings

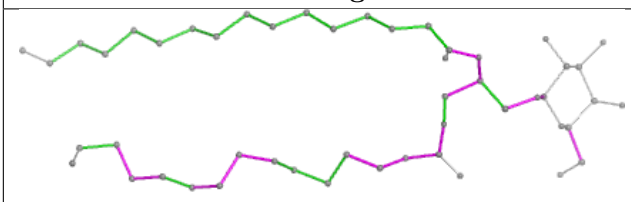
Ligand LMG c 524



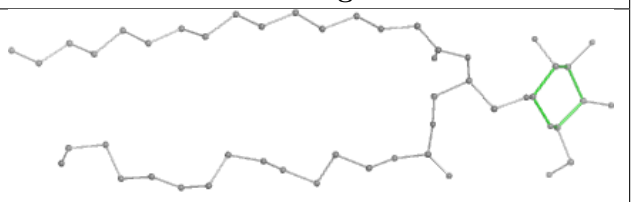
Bond lengths



Bond angles

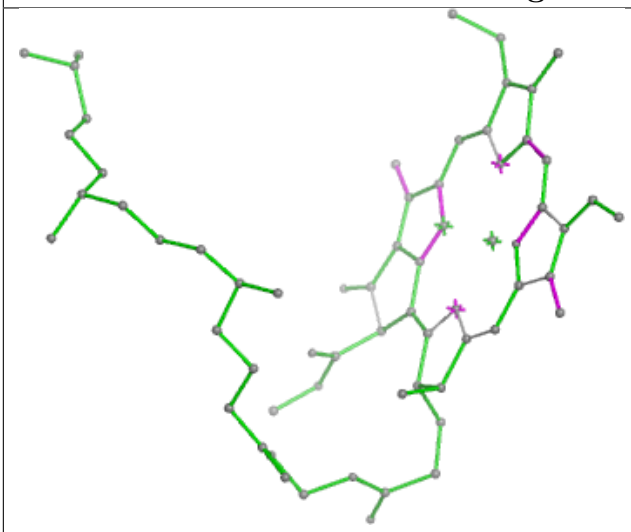


Torsions

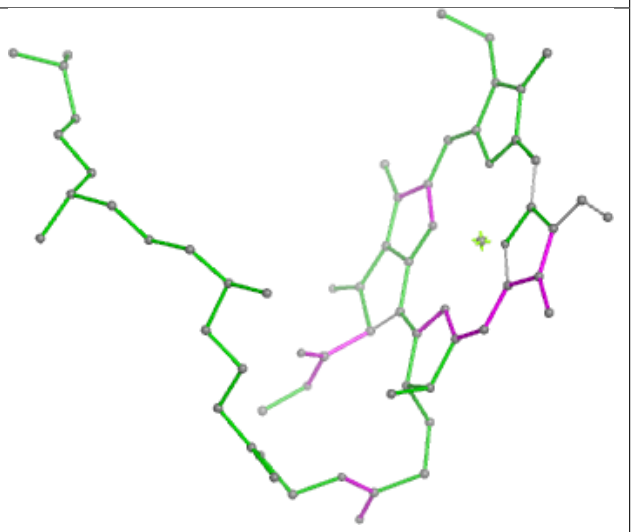


Rings

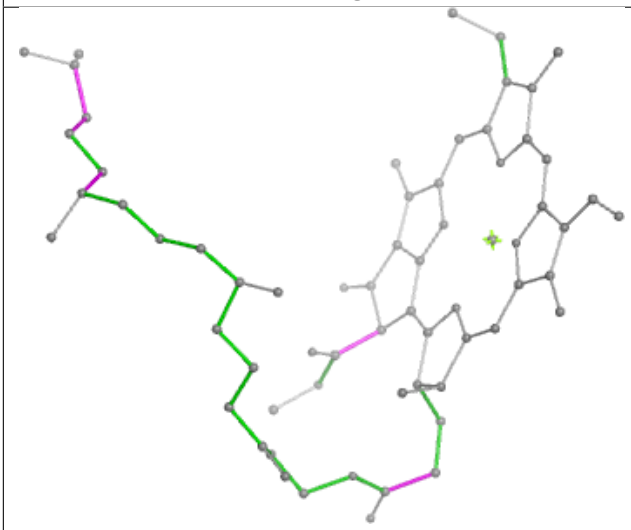
Ligand CLA b 614



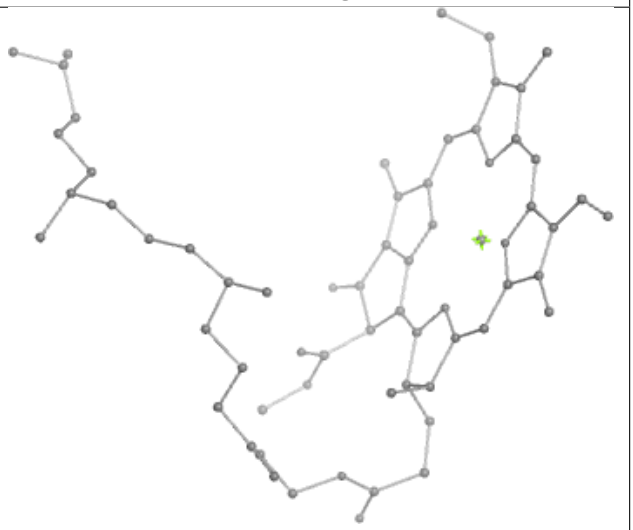
Bond lengths



Bond angles

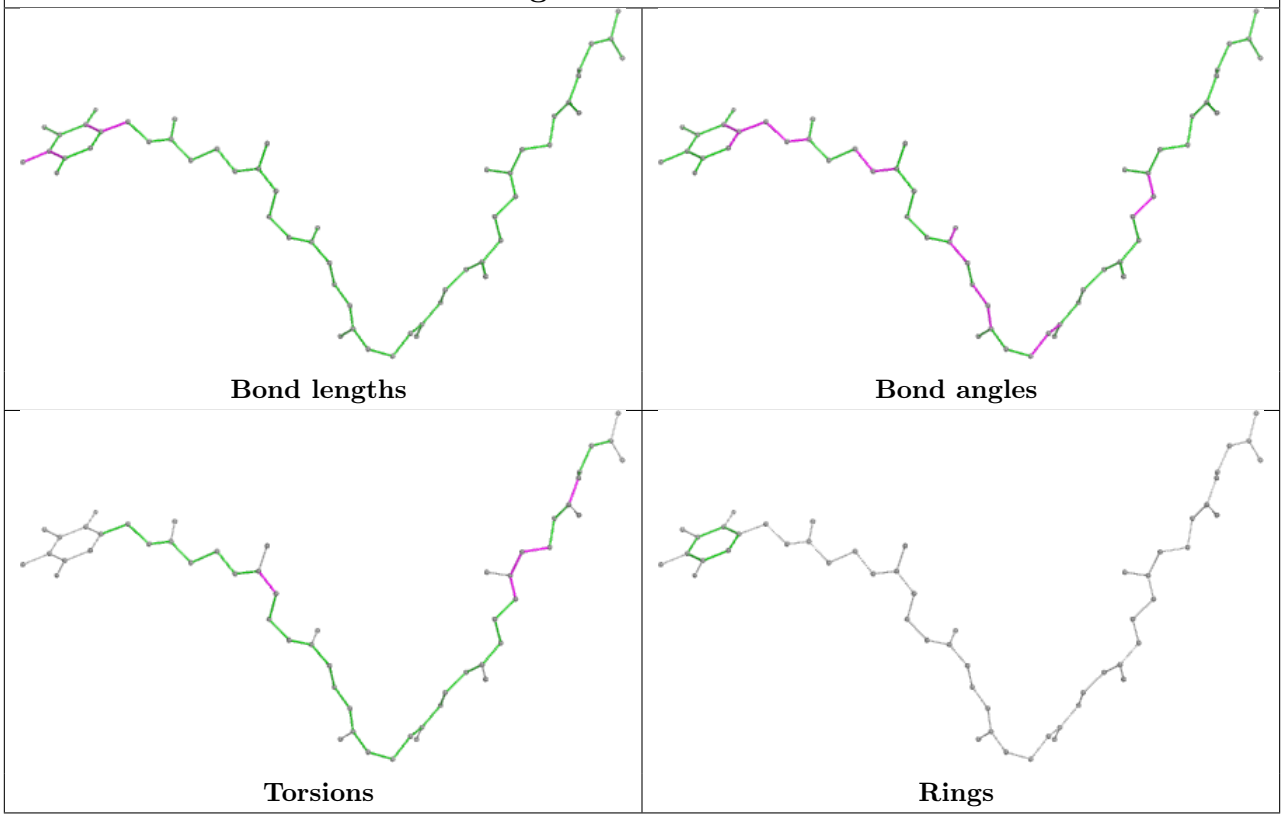


Torsions

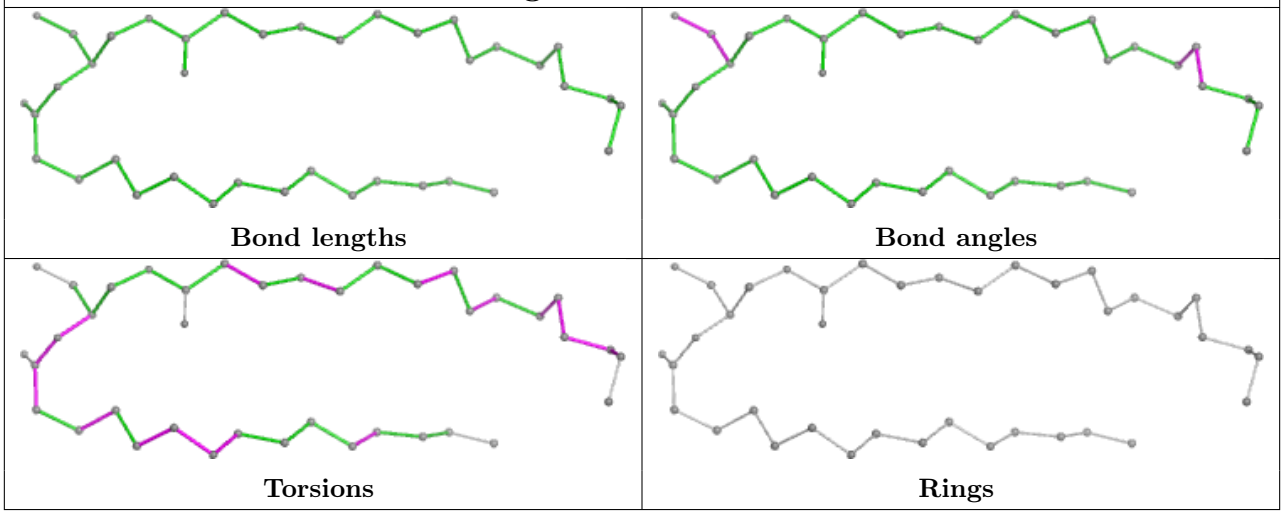


Rings

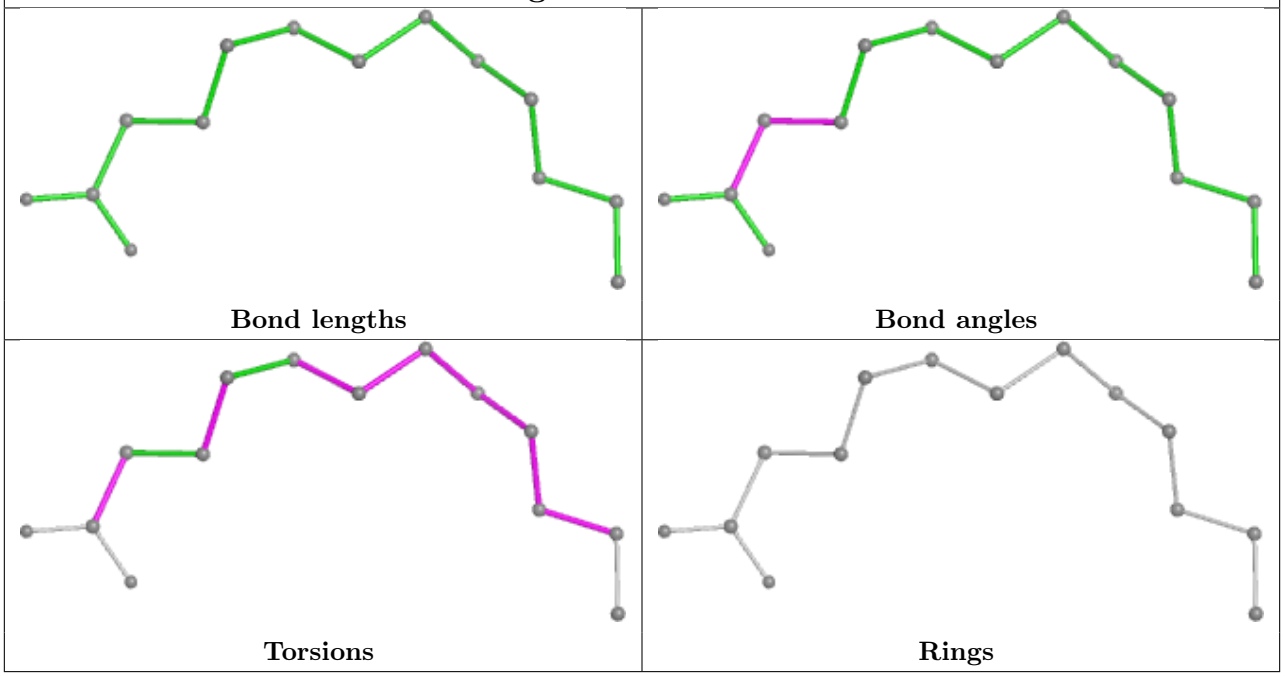
Ligand PL9 D 407



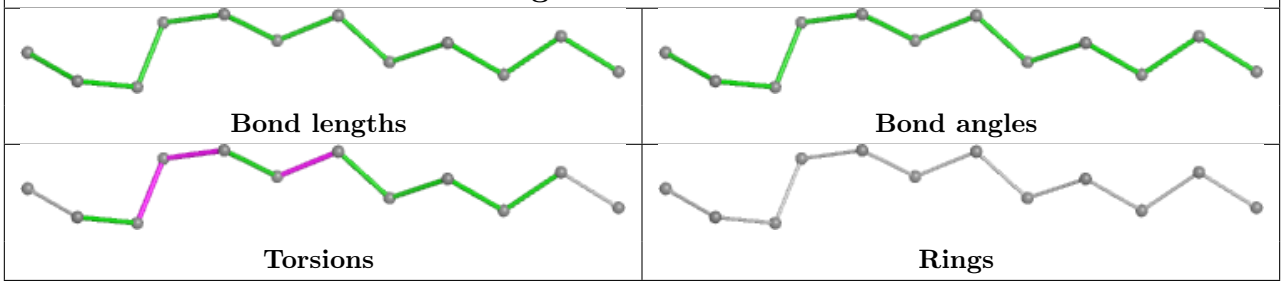
Ligand LMG h 101



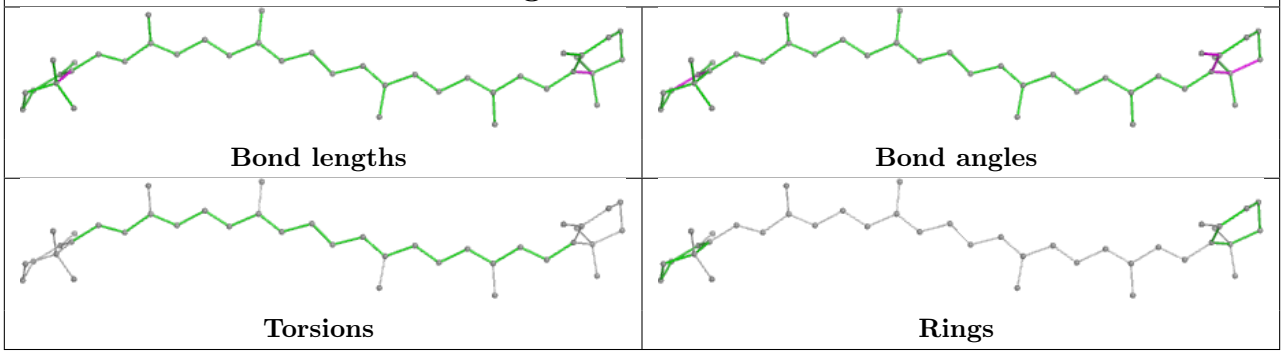
Ligand STE C 516



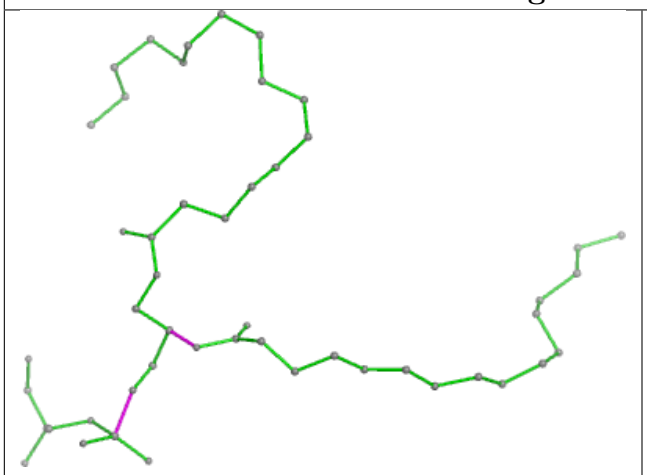
Ligand STE b 601



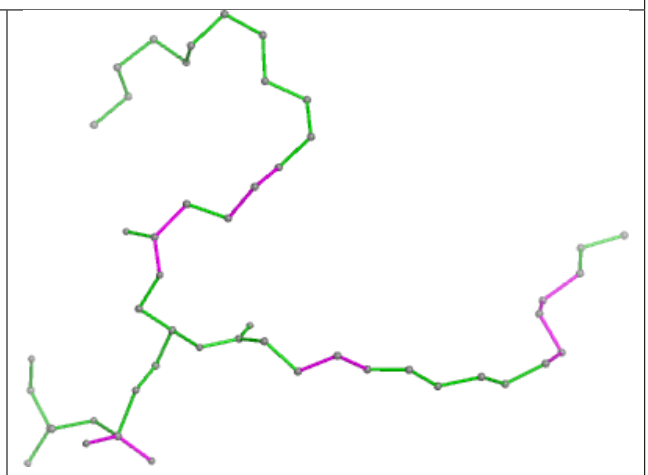
Ligand BCR A 407



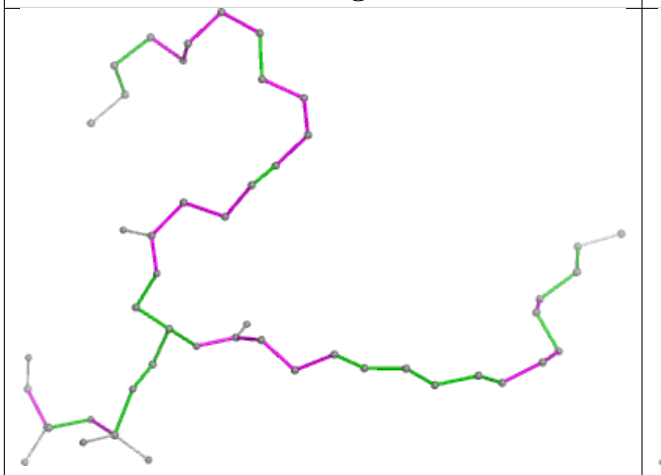
Ligand LHG a 420



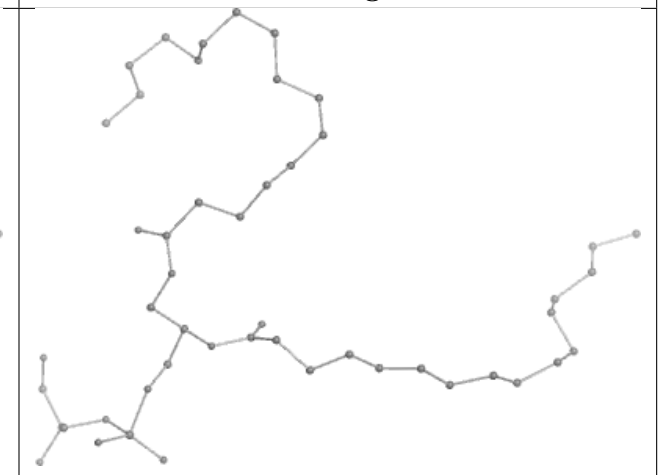
Bond lengths



Bond angles

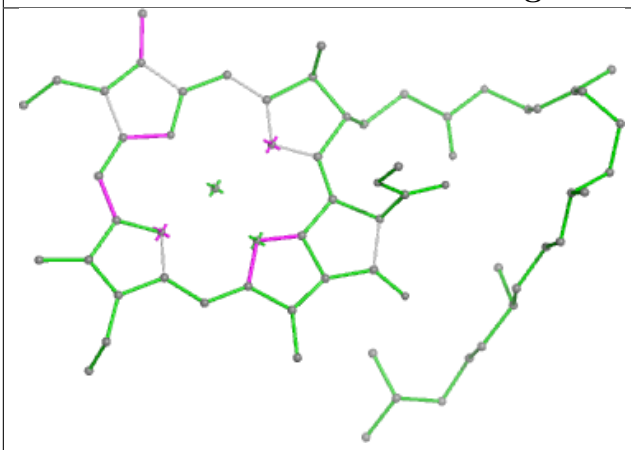


Torsions

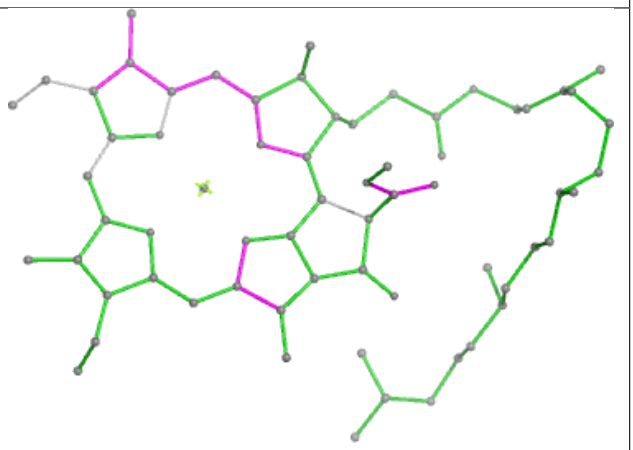


Rings

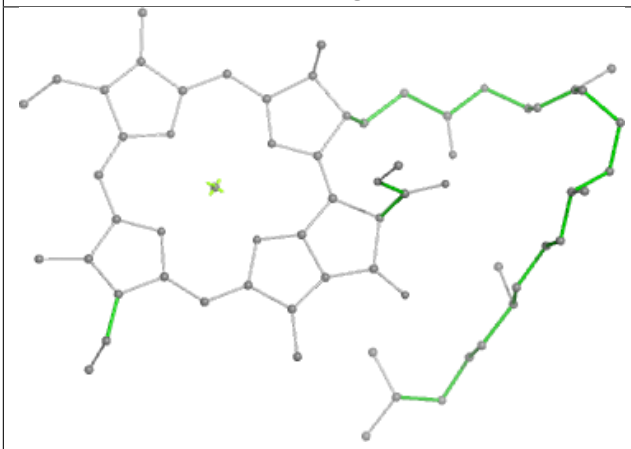
Ligand CLA B 610



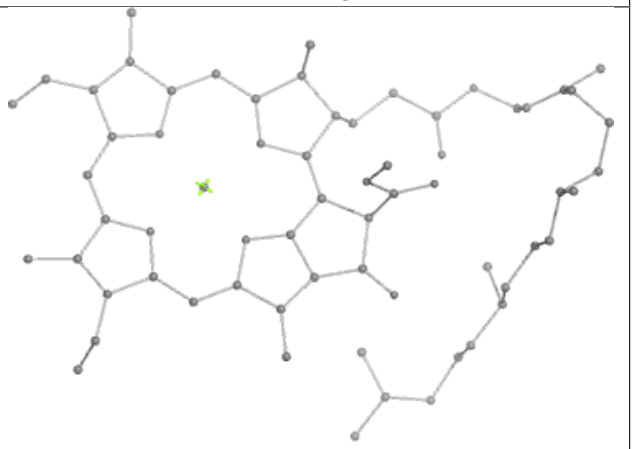
Bond lengths



Bond angles

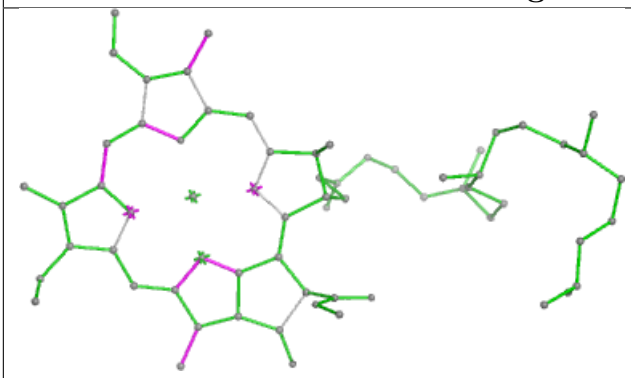


Torsions

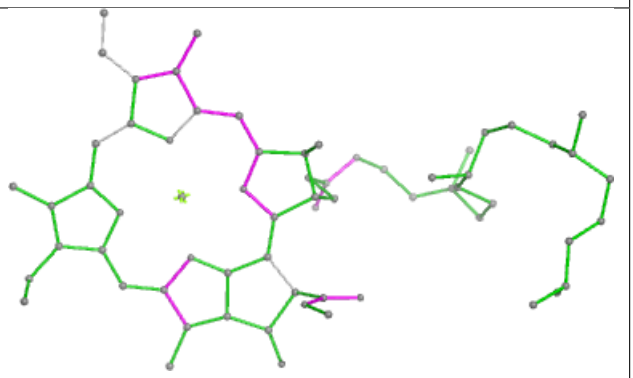


Rings

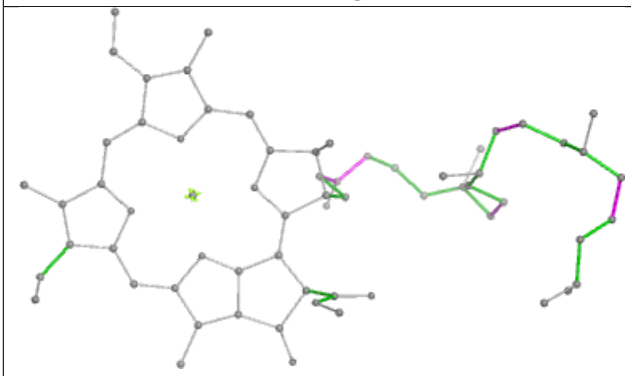
Ligand CLA b 613



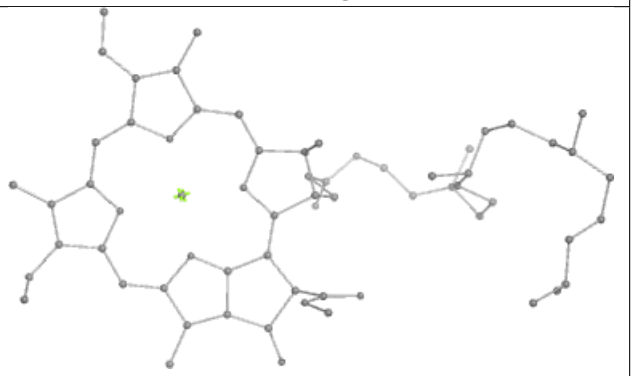
Bond lengths



Bond angles

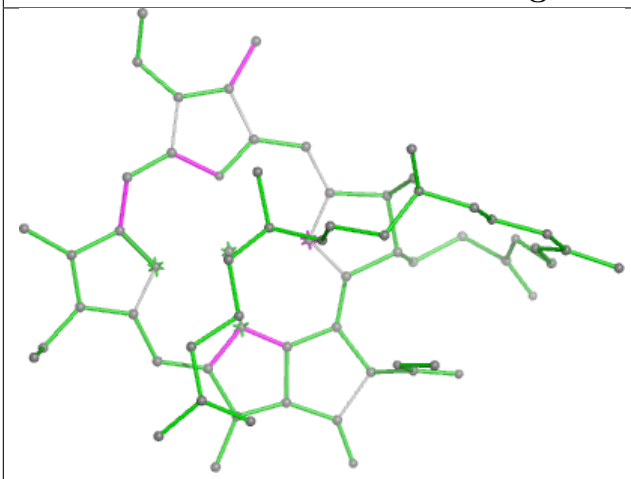


Torsions

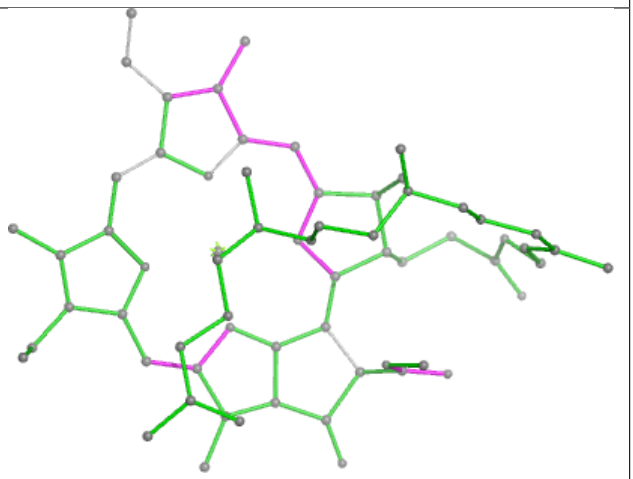


Rings

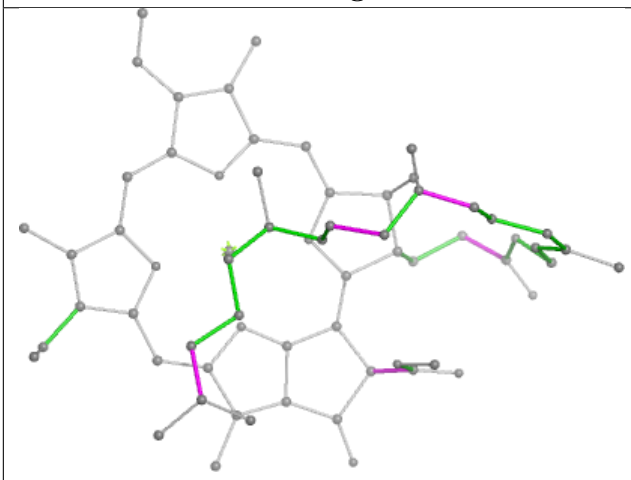
Ligand CLA c 510



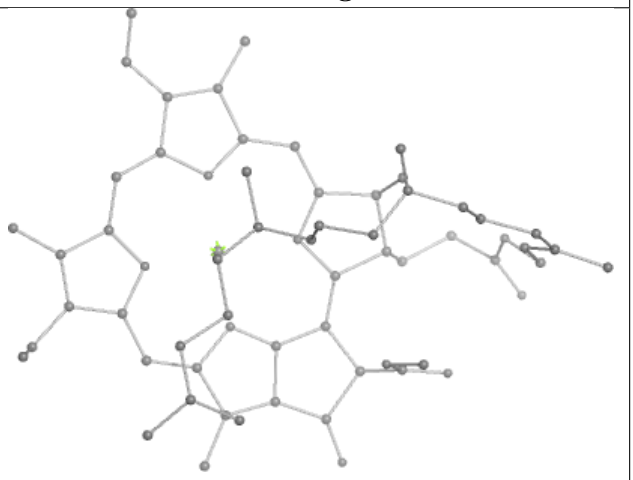
Bond lengths



Bond angles

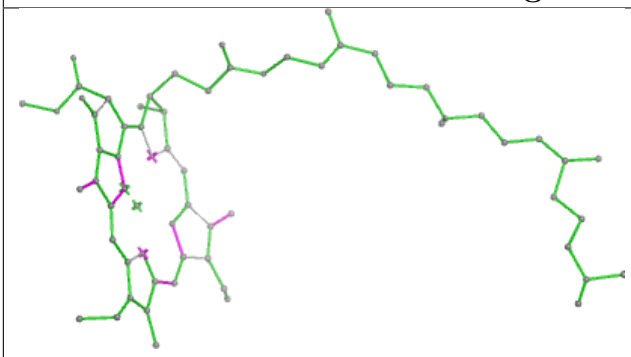


Torsions

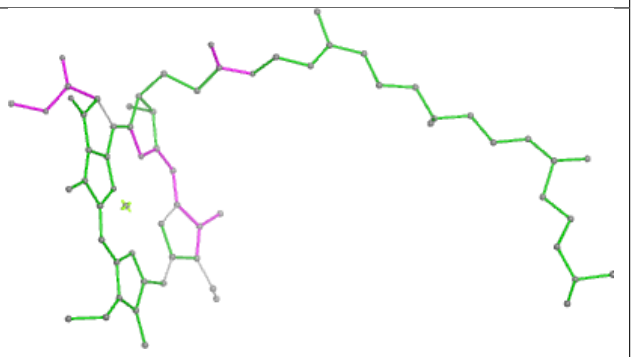


Rings

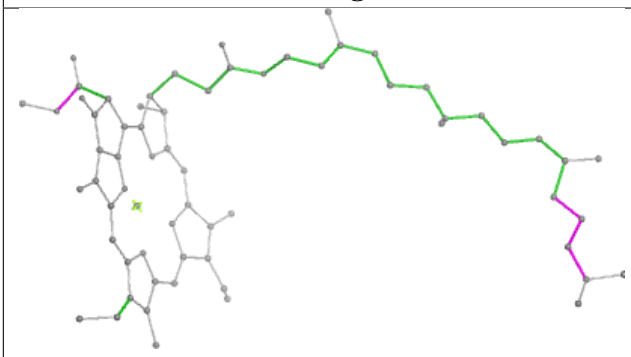
Ligand CLA B 609



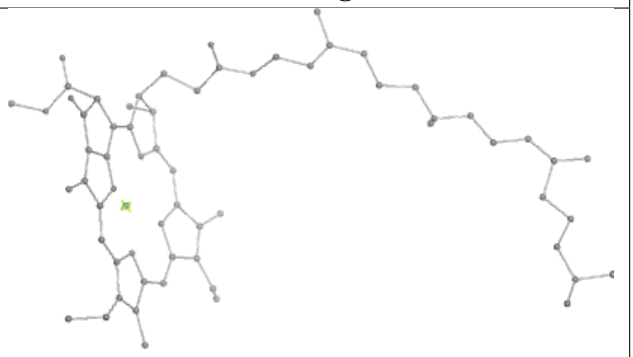
Bond lengths



Bond angles

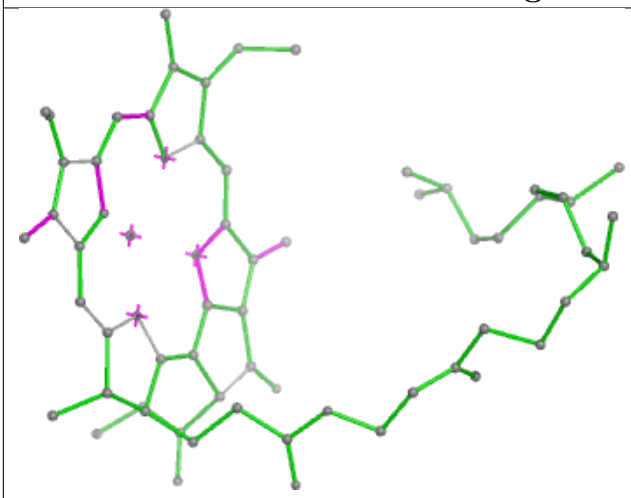


Torsions

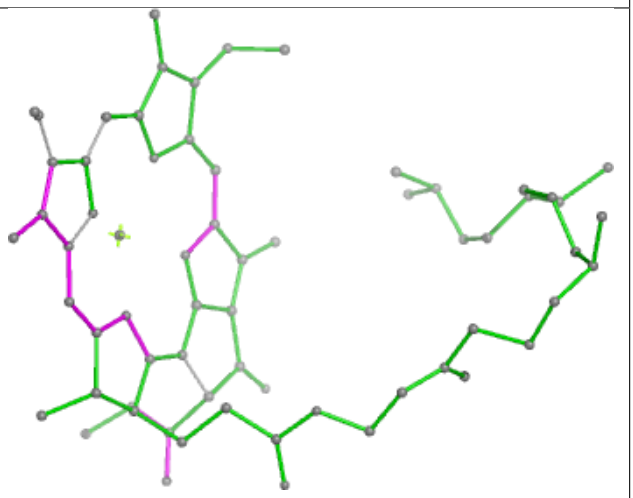


Rings

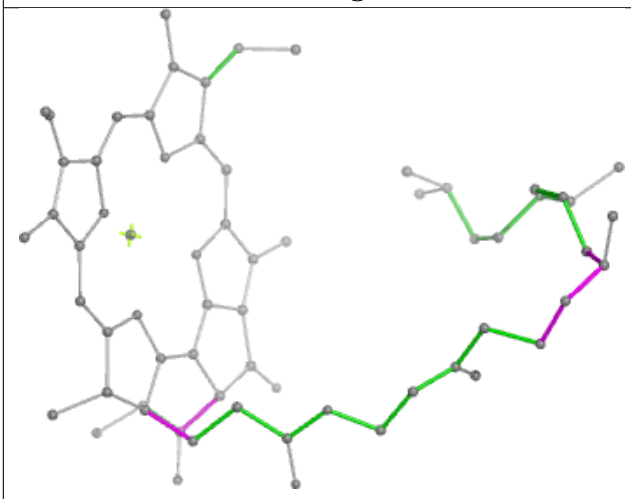
Ligand CLA C 503



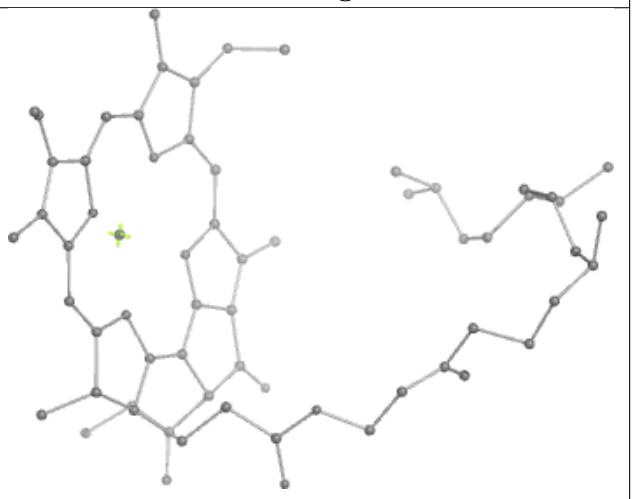
Bond lengths



Bond angles

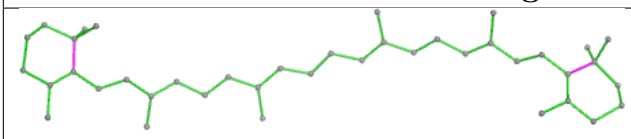


Torsions

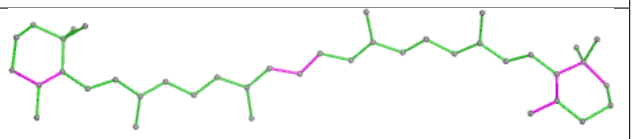


Rings

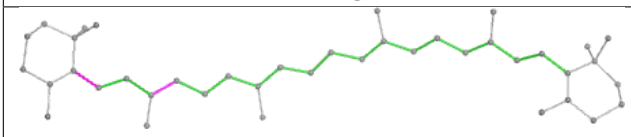
Ligand BCR D 406



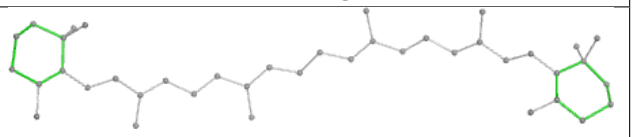
Bond lengths



Bond angles

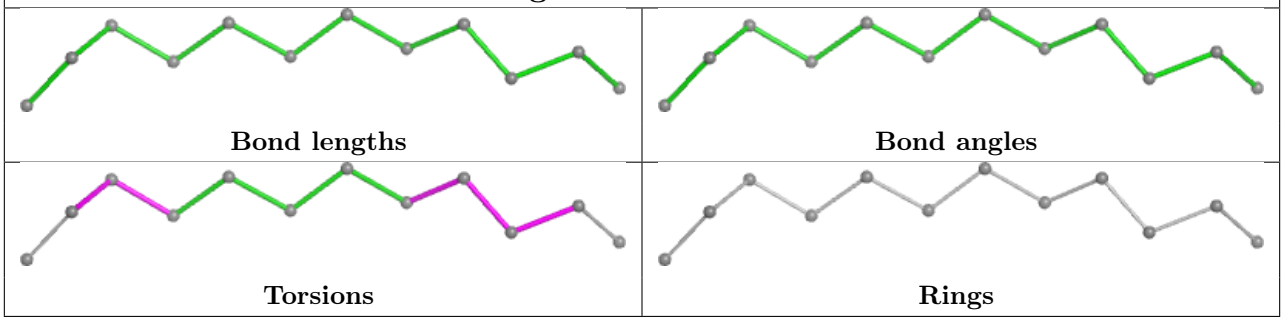


Torsions

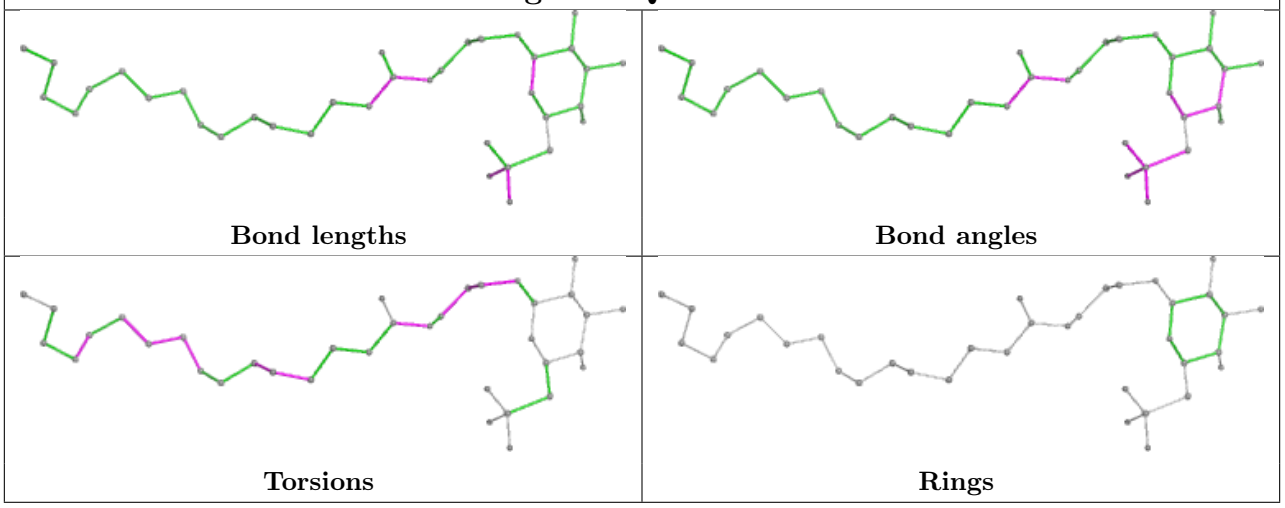


Rings

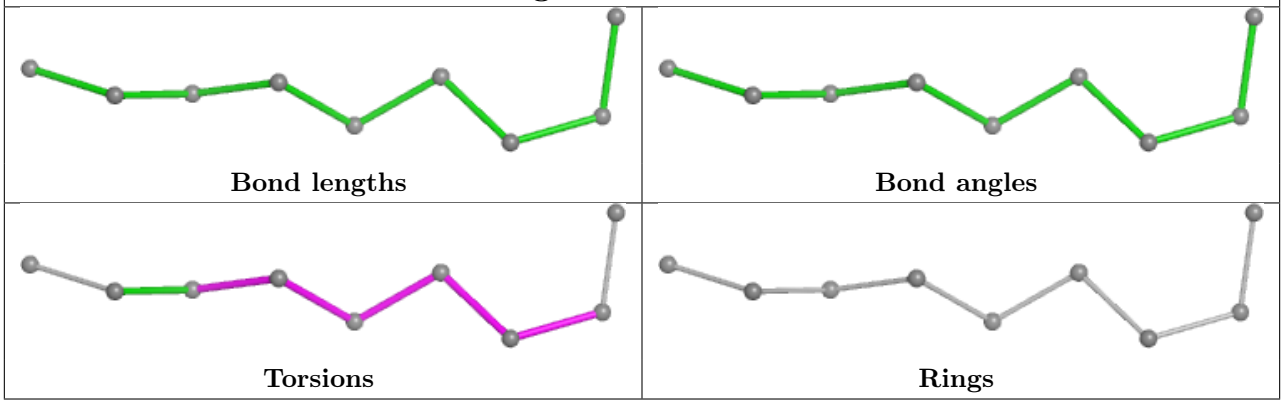
Ligand STE E 102



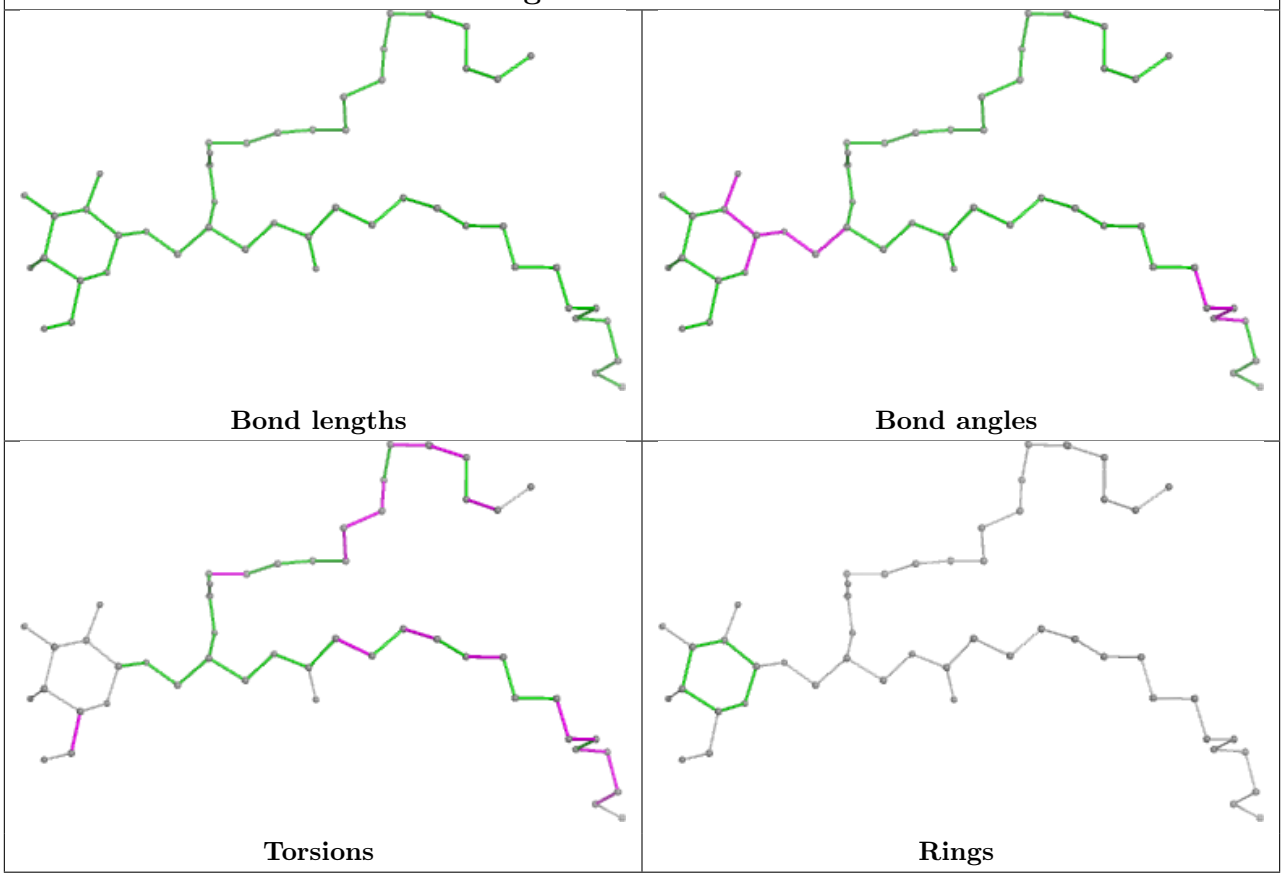
Ligand SQD X 101



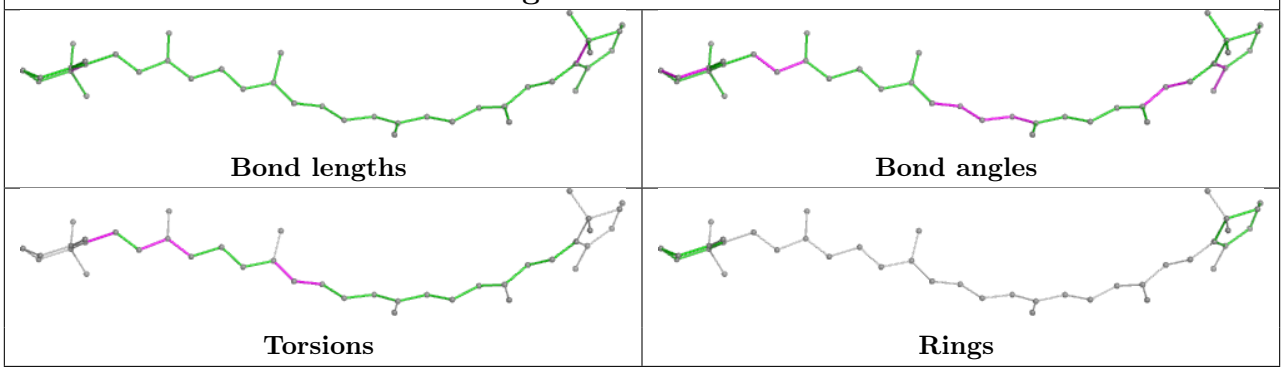
Ligand STE a 409



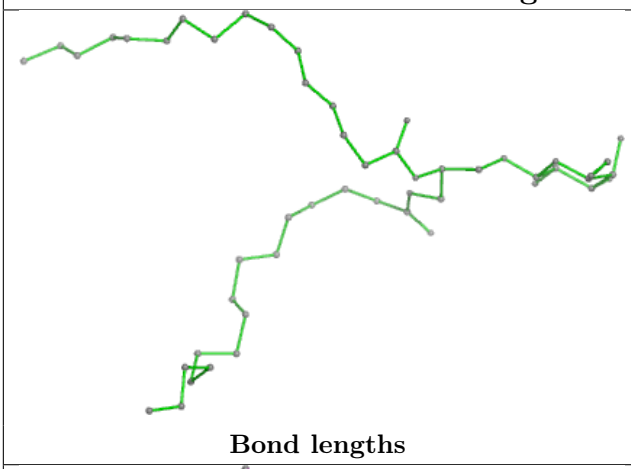
Ligand LMG d 408



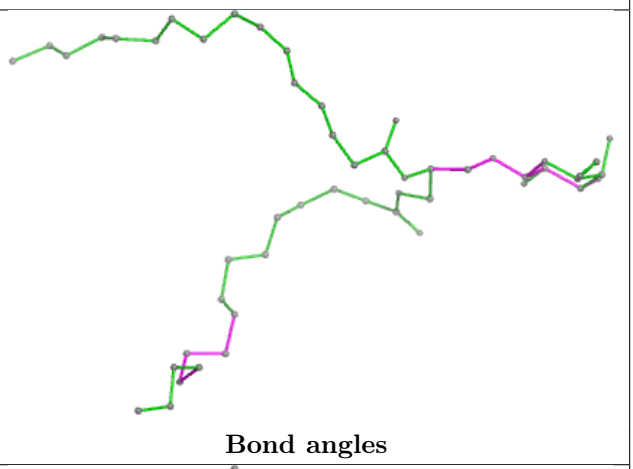
Ligand BCR H 102



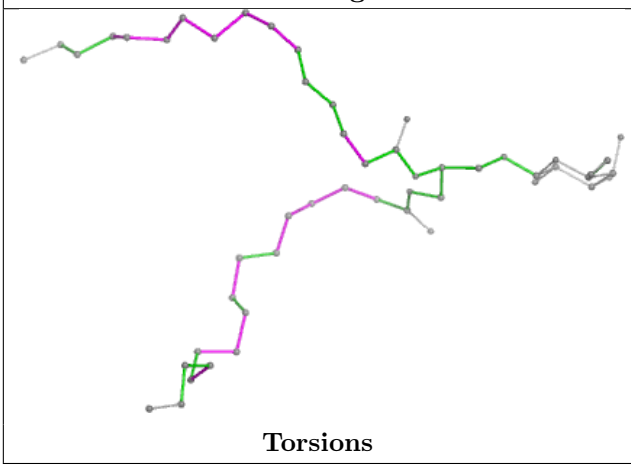
Ligand LMG B 624



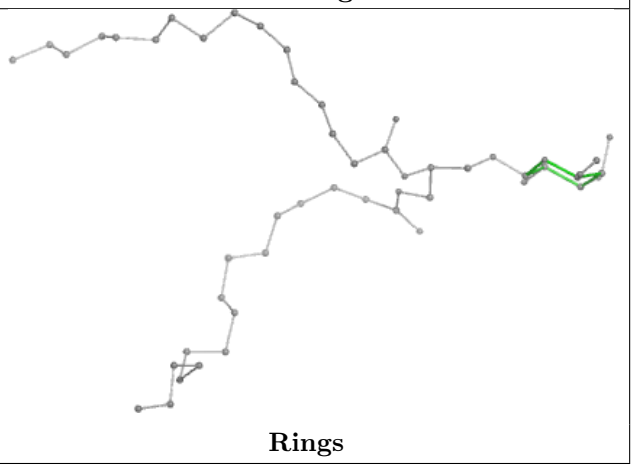
Bond lengths



Bond angles

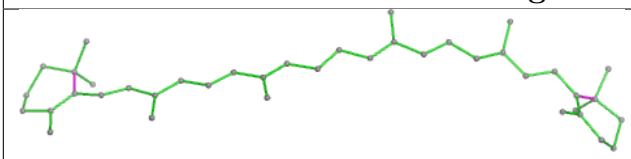


Torsions

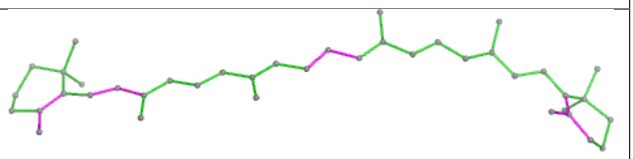


Rings

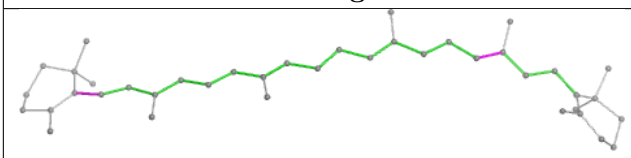
Ligand BCR t 102



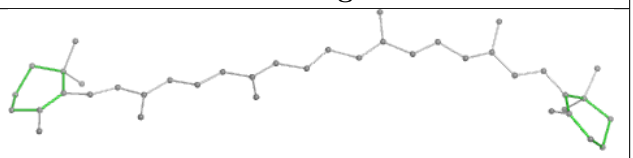
Bond lengths



Bond angles

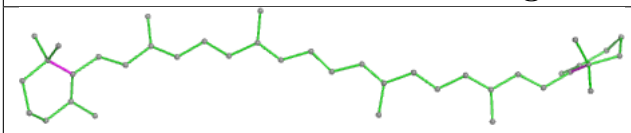


Torsions

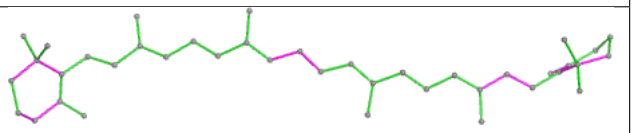


Rings

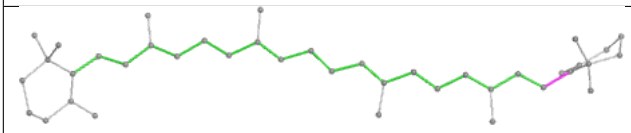
Ligand BCR B 617



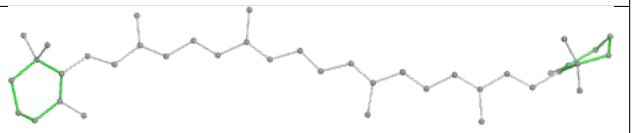
Bond lengths



Bond angles

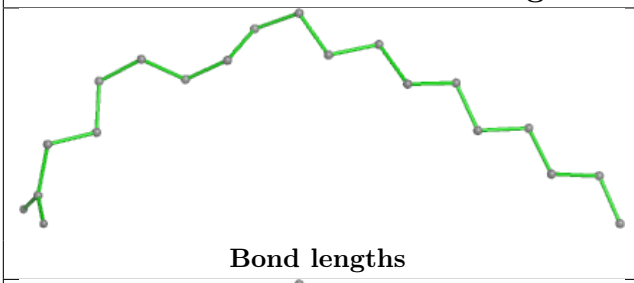


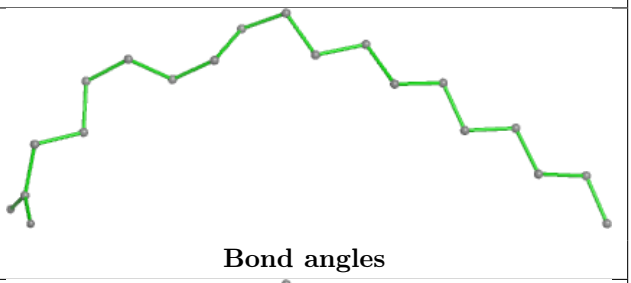
Torsions

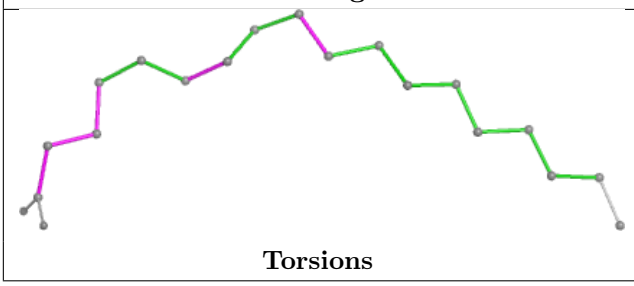


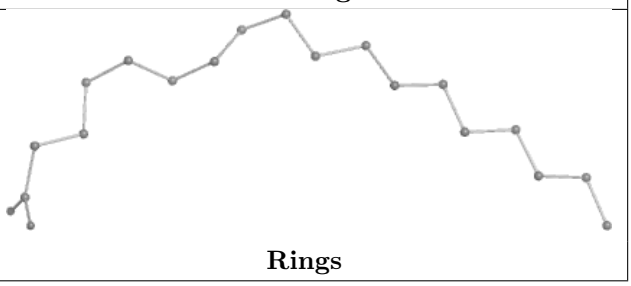
Rings

Ligand STE D 412

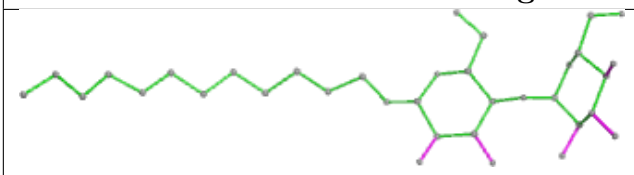

Bond lengths

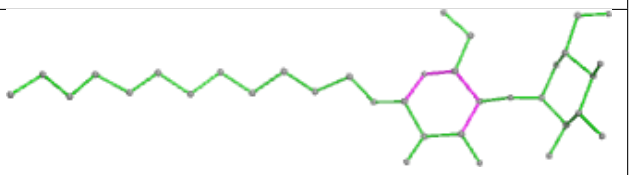

Bond angles

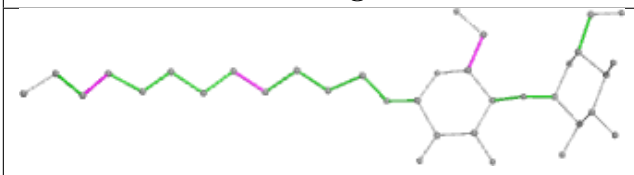

Torsions

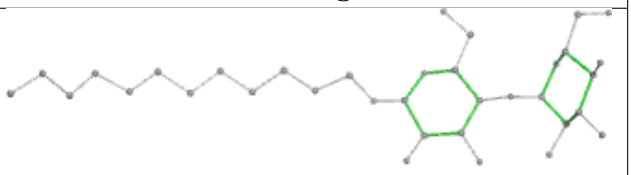

Rings

Ligand LMT M 102

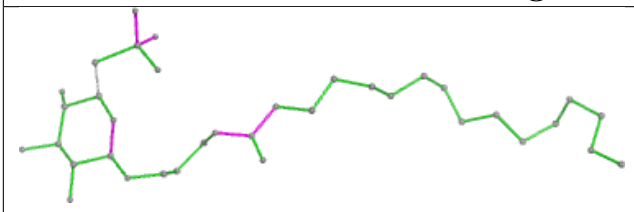

Bond lengths

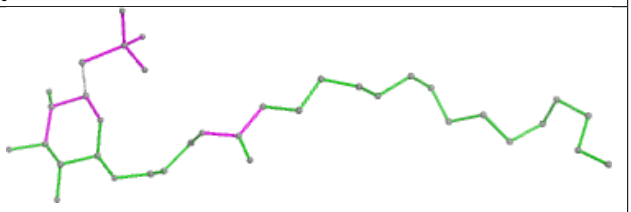

Bond angles

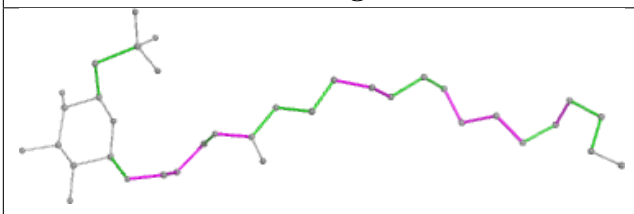

Torsions

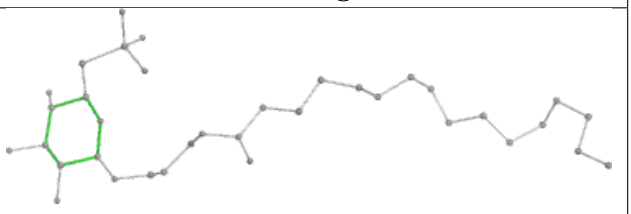

Rings

Ligand SQD x 101

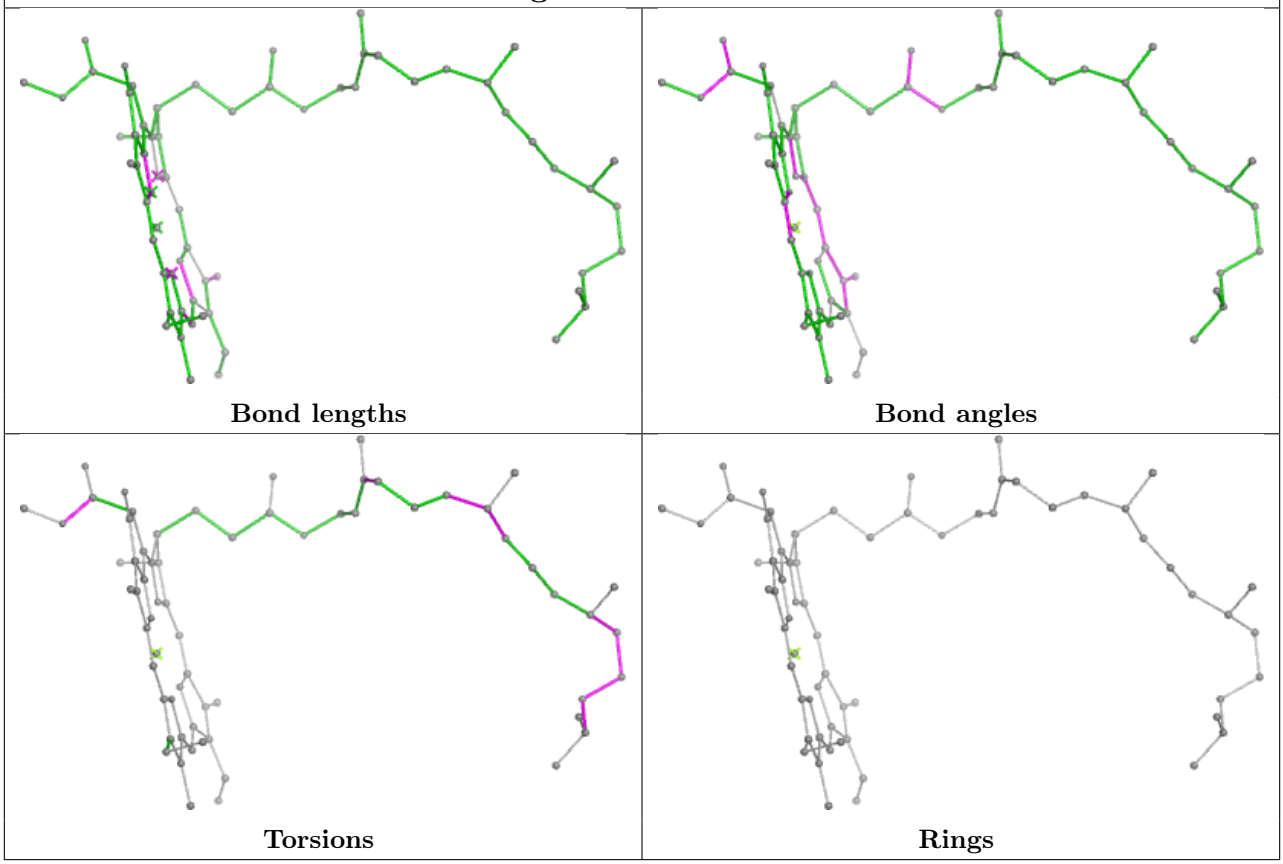

Bond lengths


Bond angles

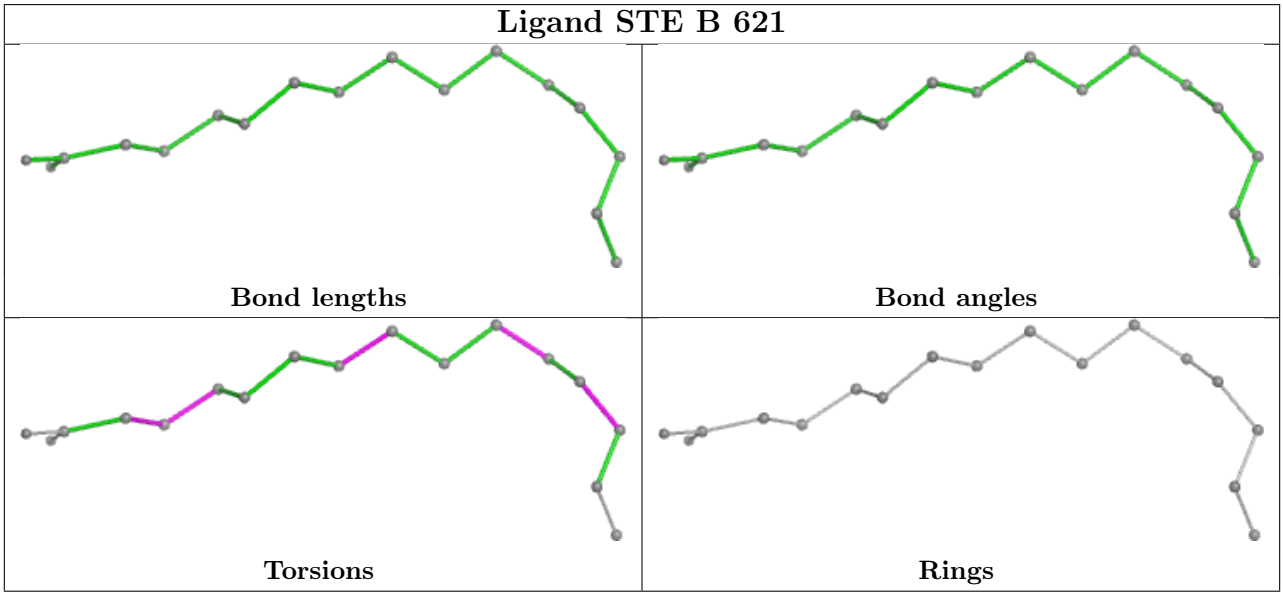

Torsions


Rings

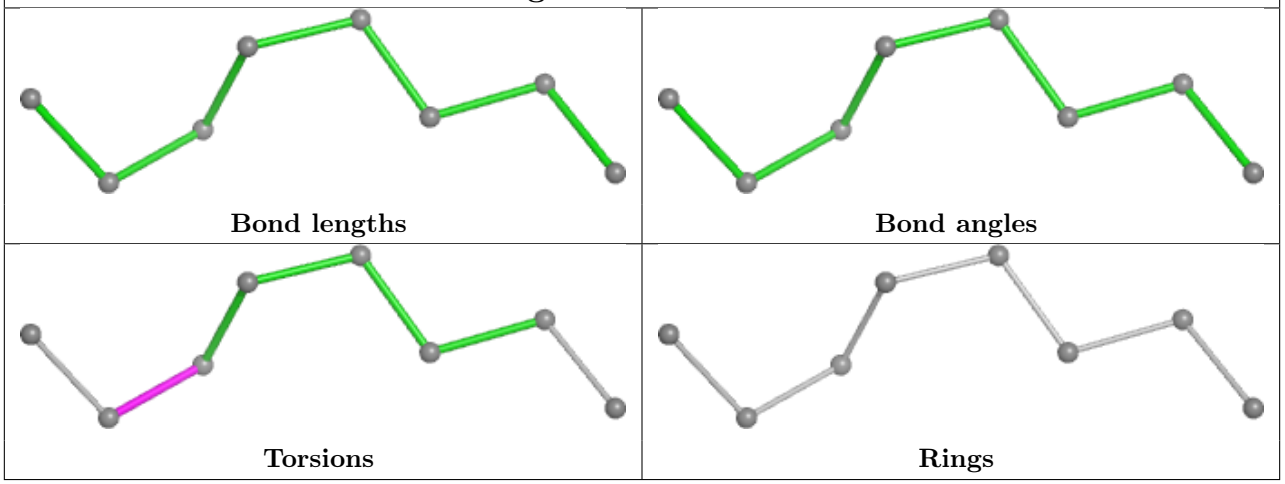
Ligand CLA c 506



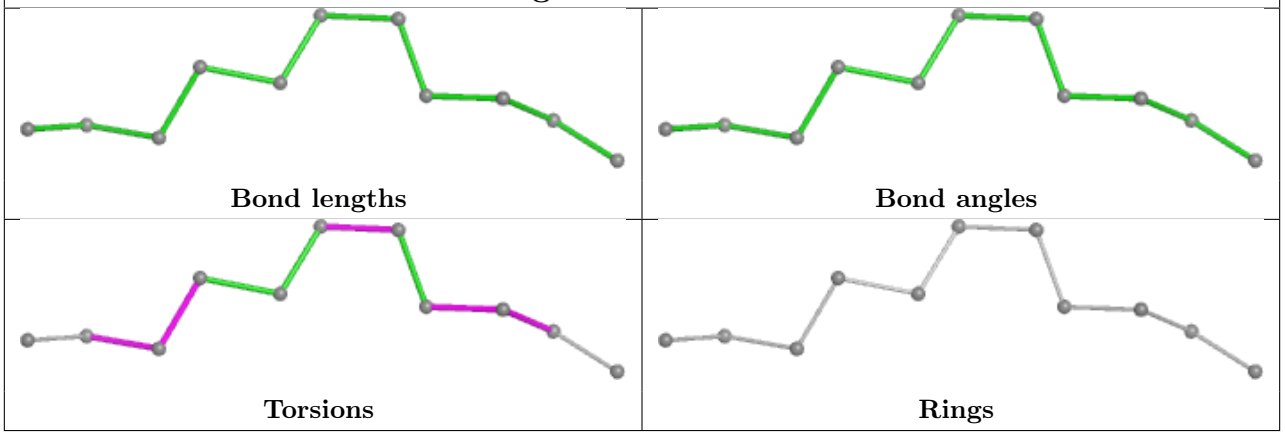
Ligand STE B 621



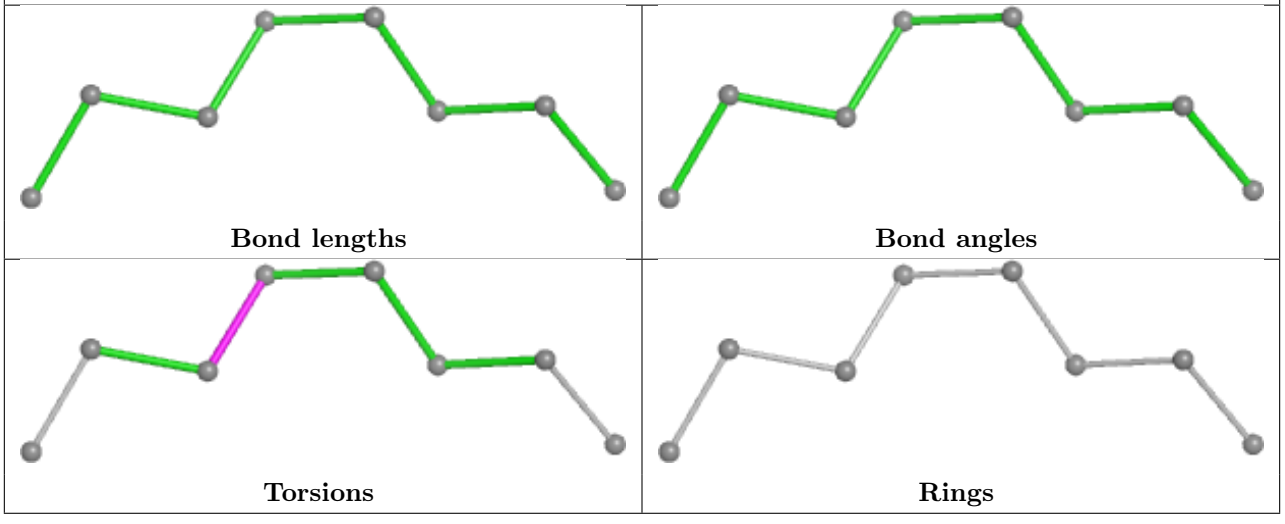
Ligand STE A 414



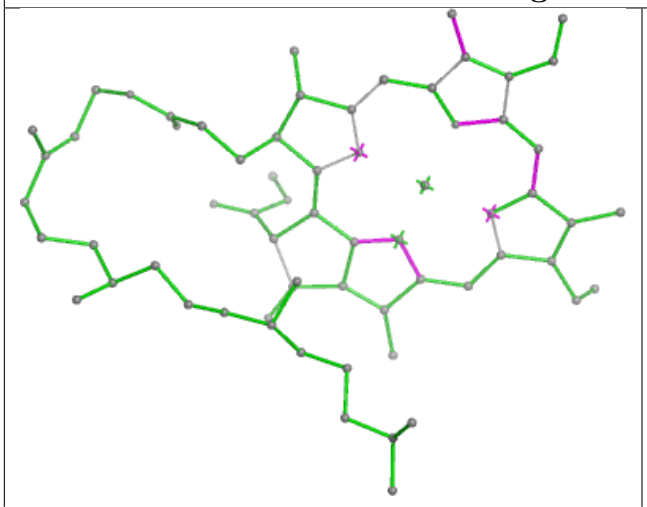
Ligand STE a 416



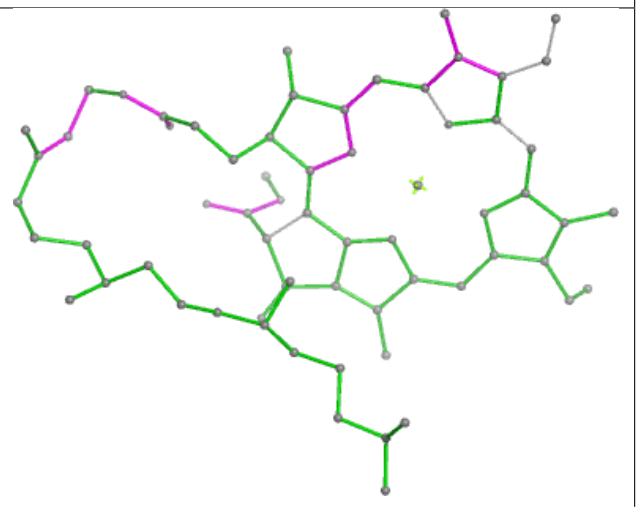
Ligand STE c 522



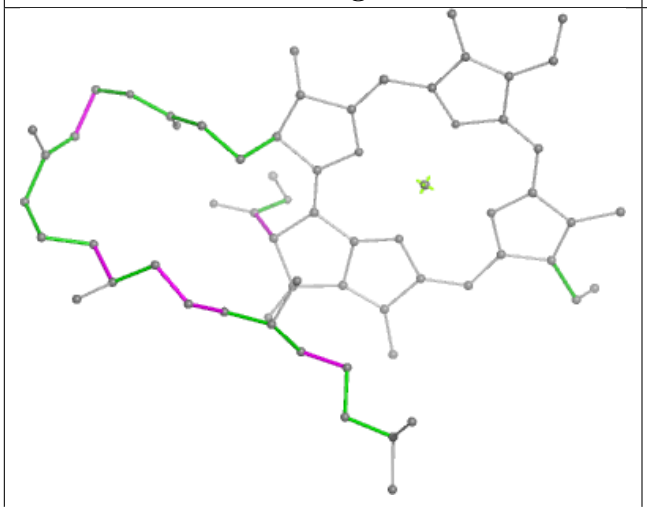
Ligand CLA c 509



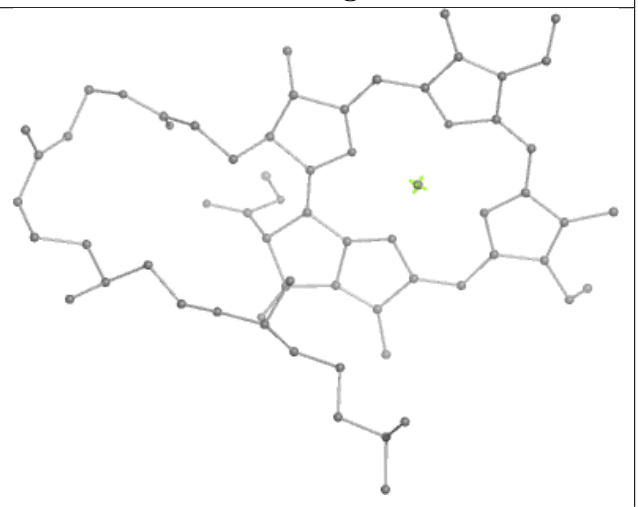
Bond lengths



Bond angles

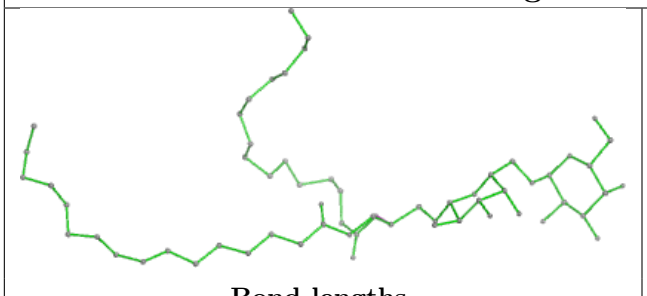


Torsions

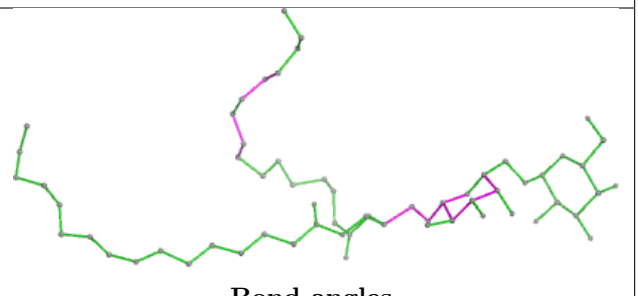


Rings

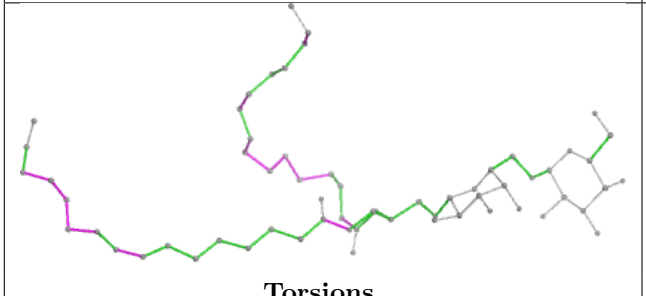
Ligand DGD h 103



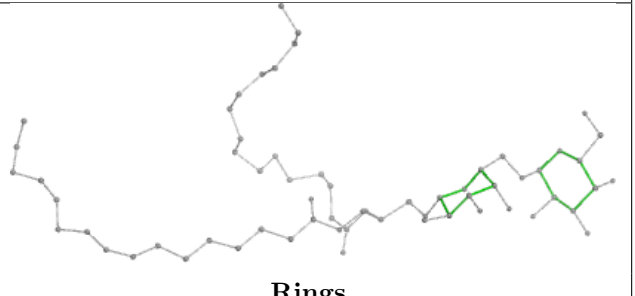
Bond lengths



Bond angles

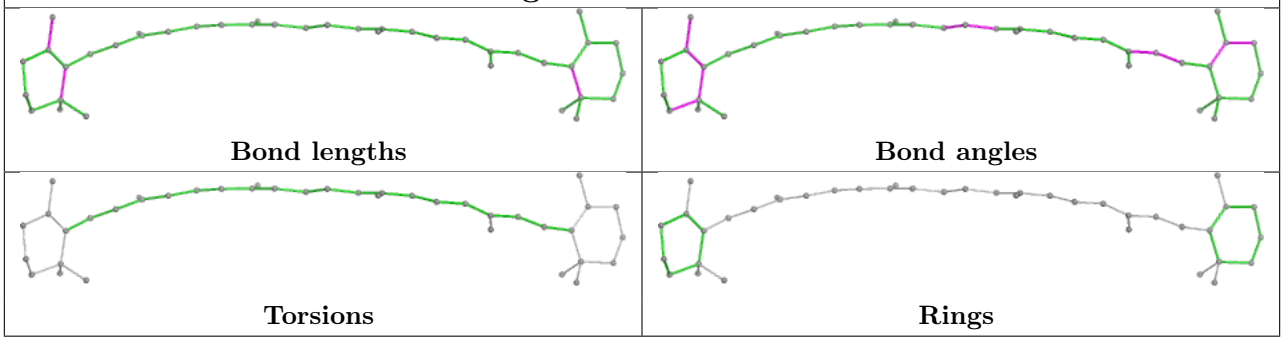


Torsions

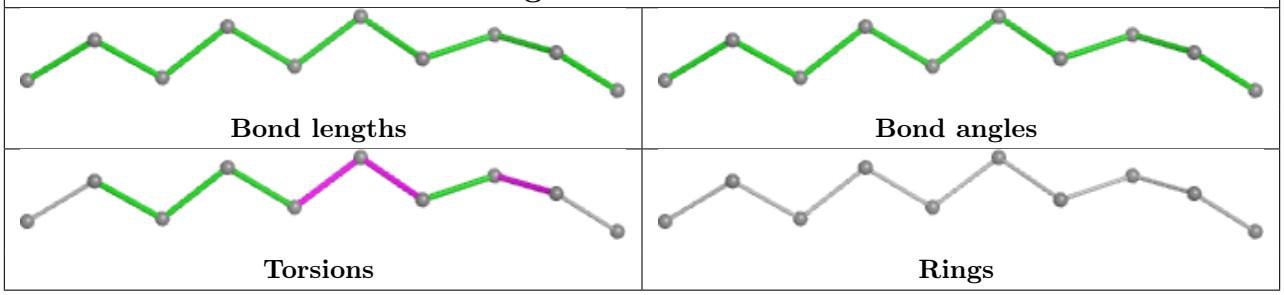


Rings

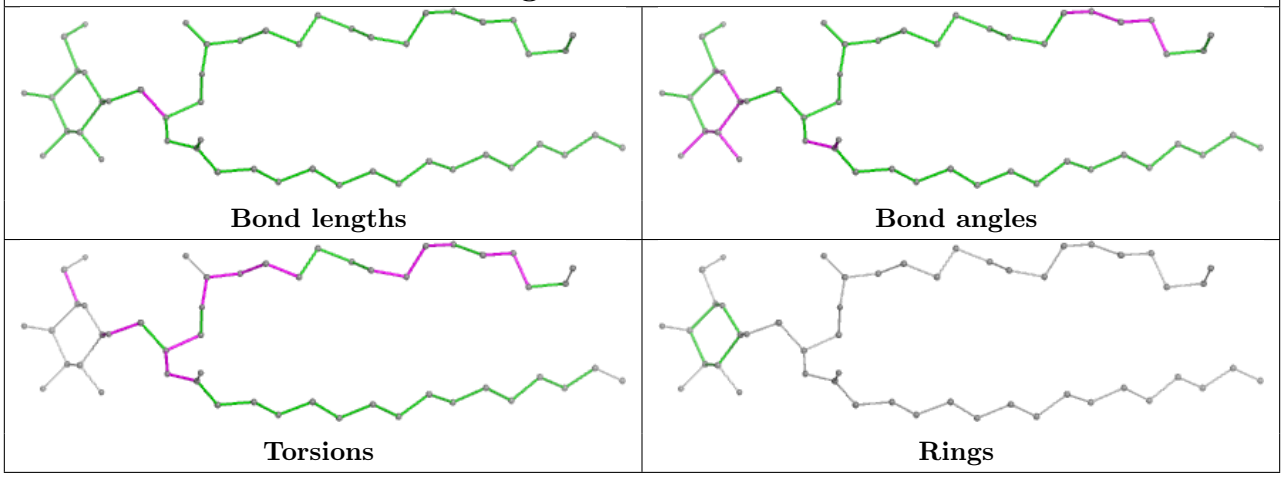
Ligand BCR K 101



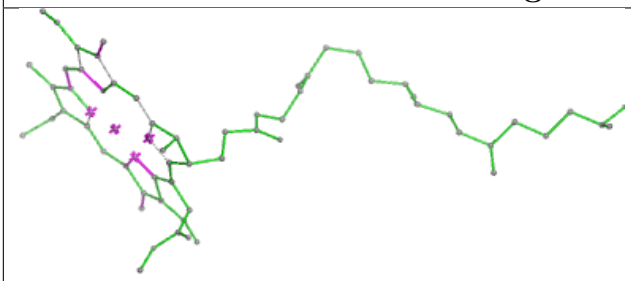
Ligand STE M 101



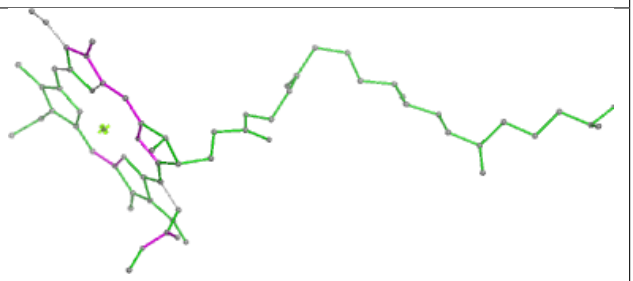
Ligand LMG C 524



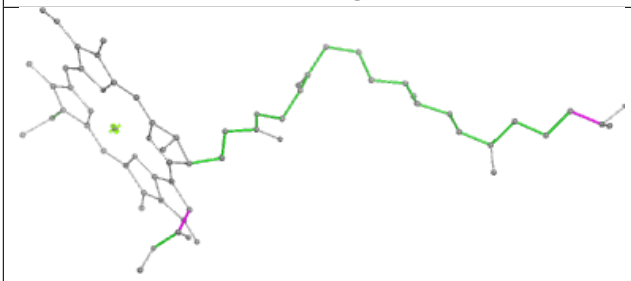
Ligand CLA C 502



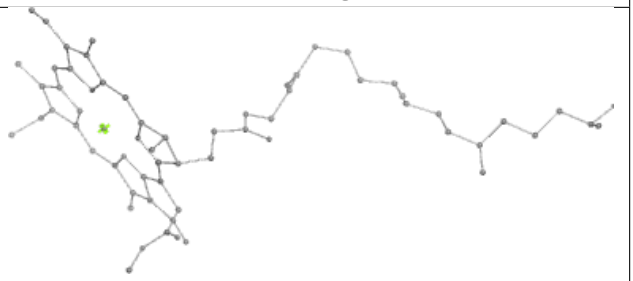
Bond lengths



Bond angles

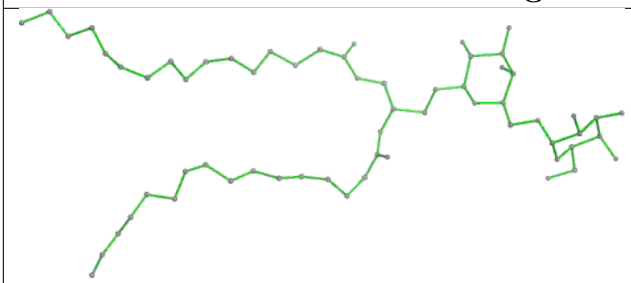


Torsions

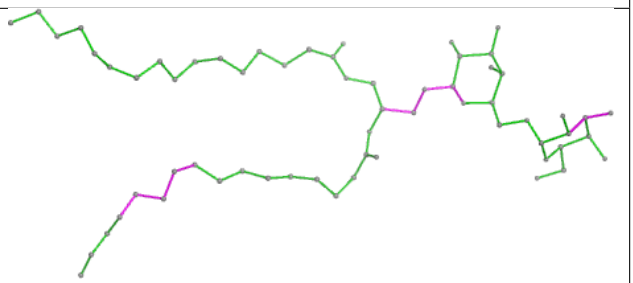


Rings

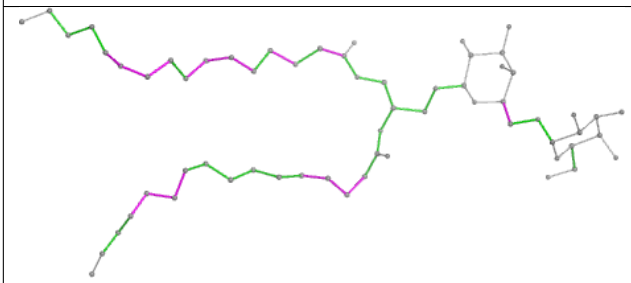
Ligand DGD c 519



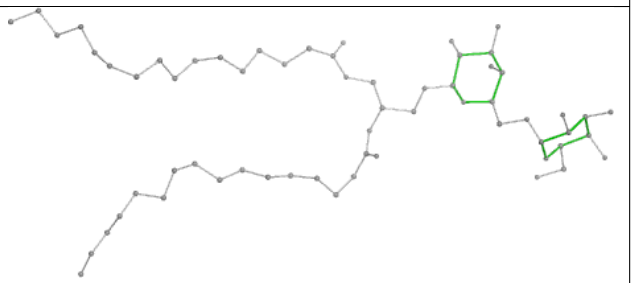
Bond lengths



Bond angles

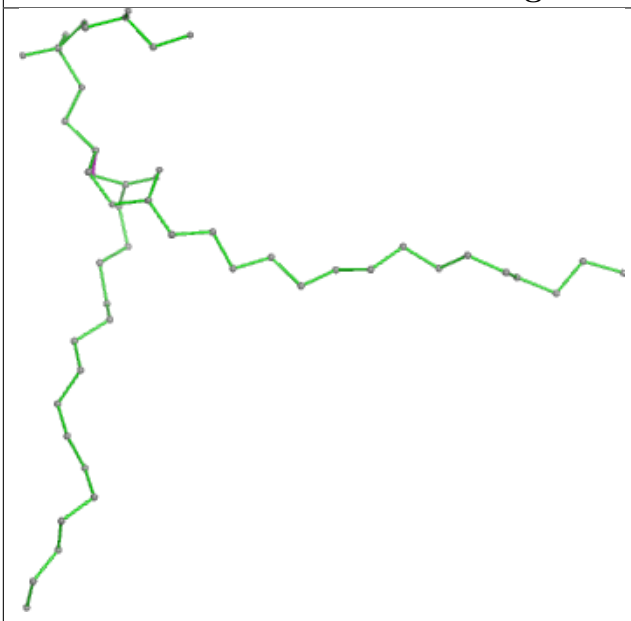


Torsions

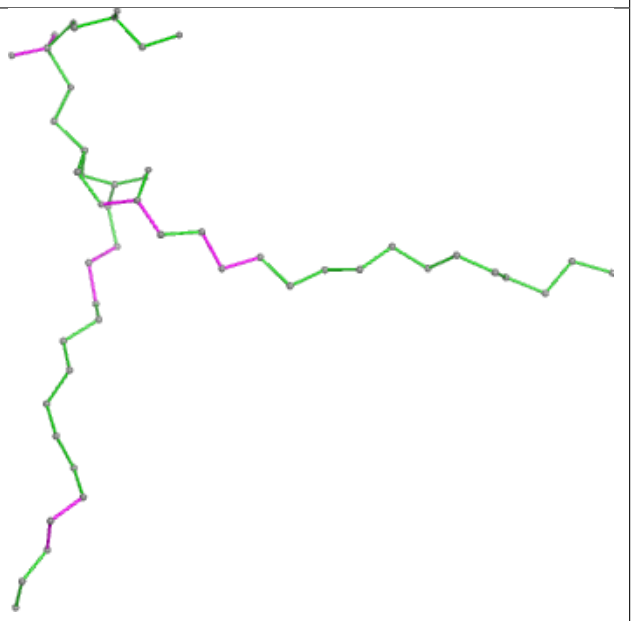


Rings

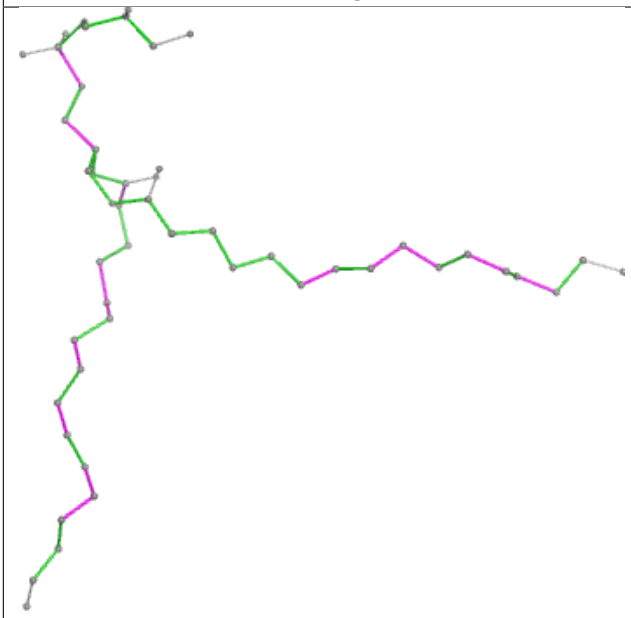
Ligand LHG L 101



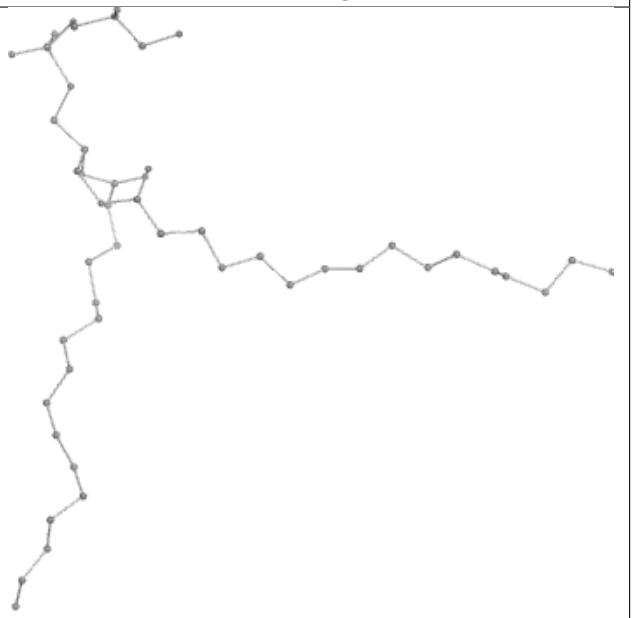
Bond lengths



Bond angles

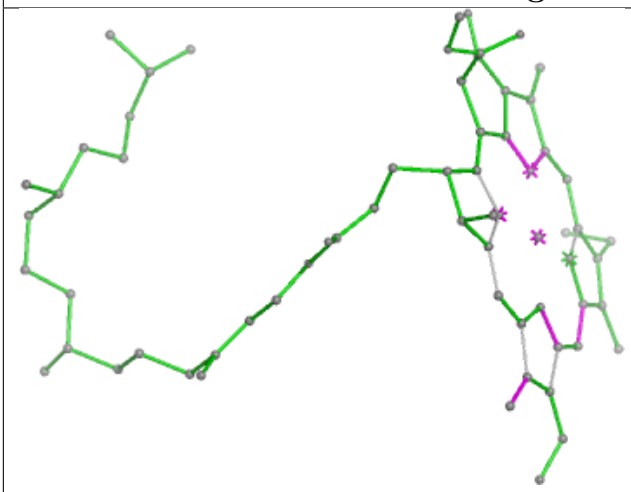


Torsions

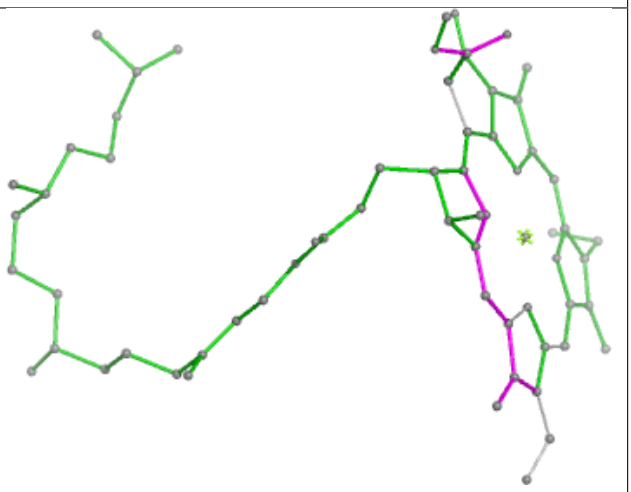


Rings

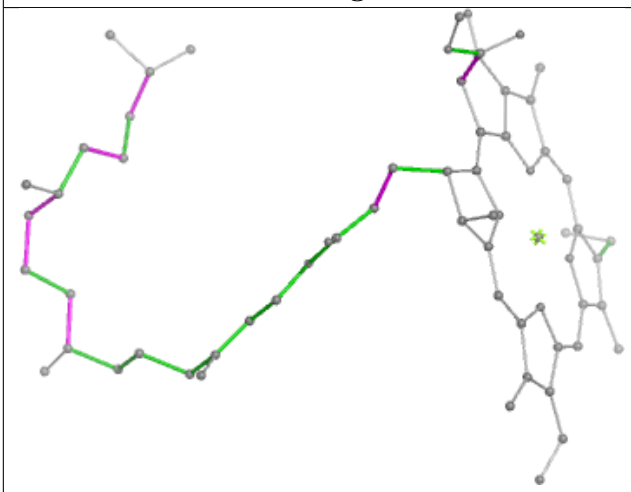
Ligand CLA b 607



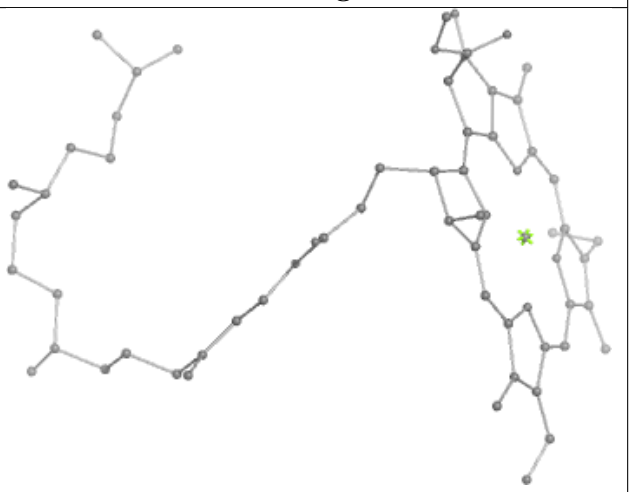
Bond lengths



Bond angles

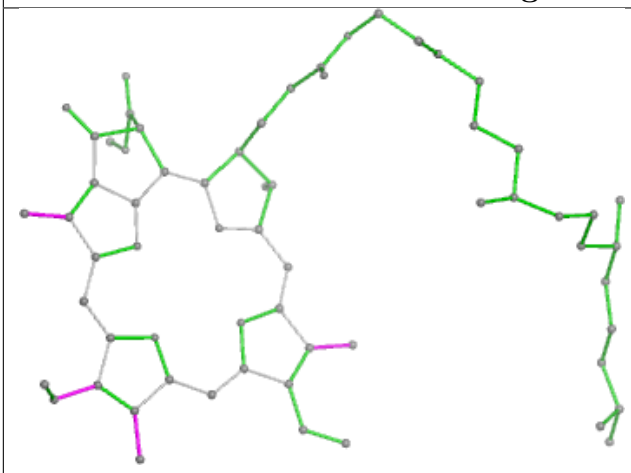


Torsions

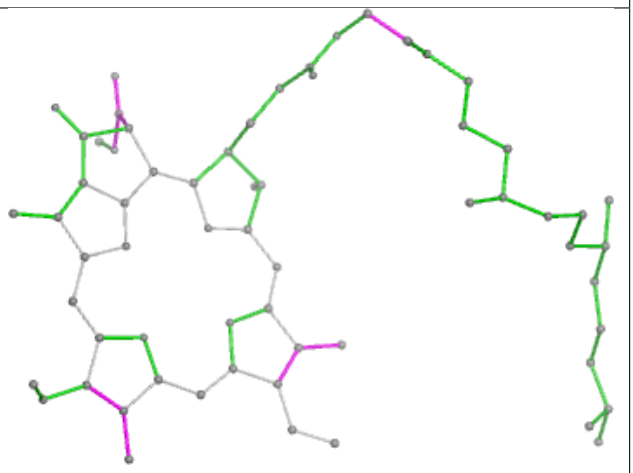


Rings

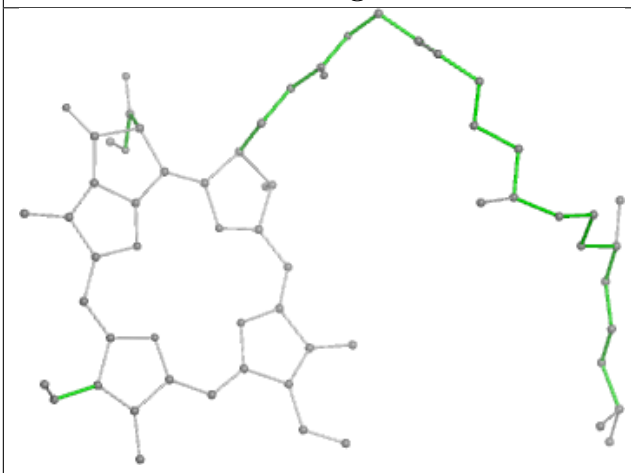
Ligand PHO D 401



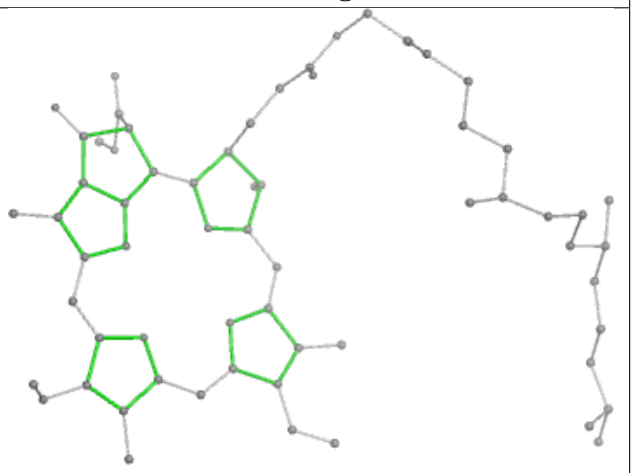
Bond lengths



Bond angles

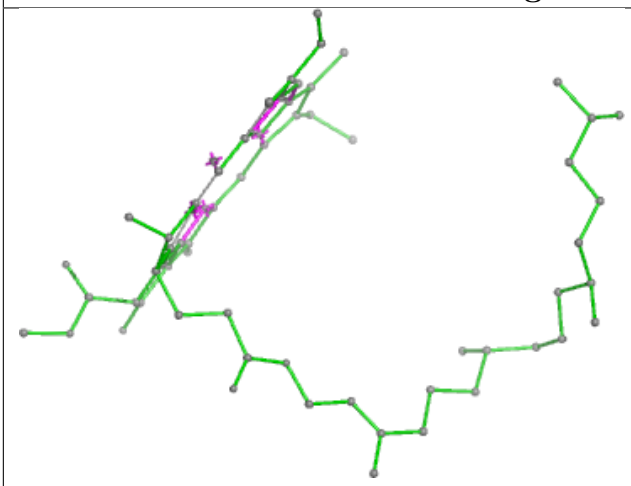


Torsions

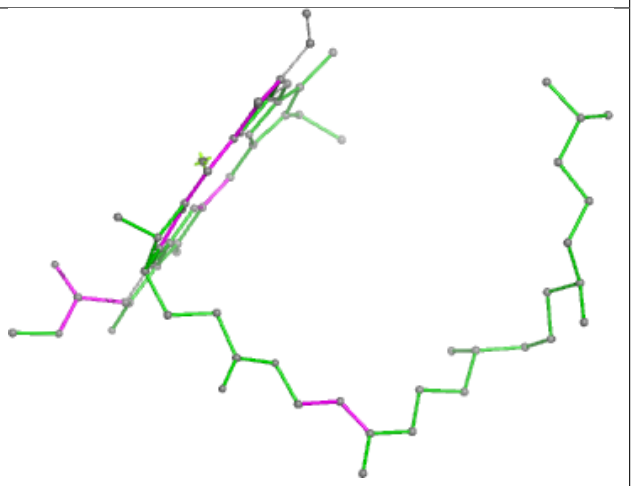


Rings

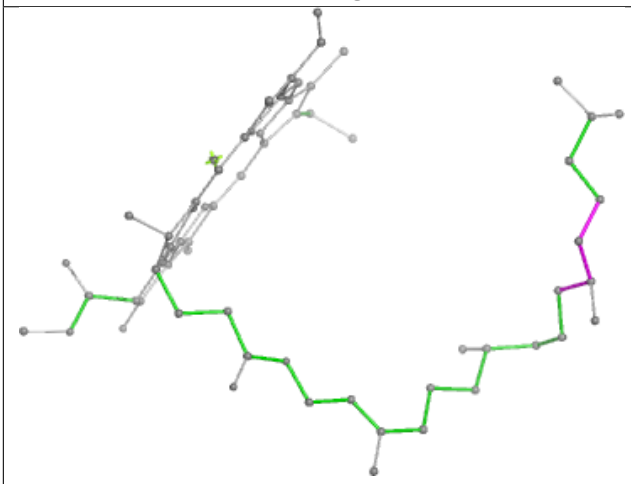
Ligand CLA B 611



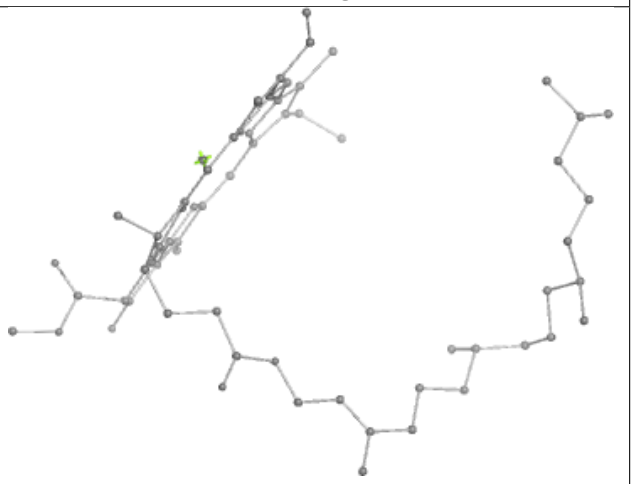
Bond lengths



Bond angles

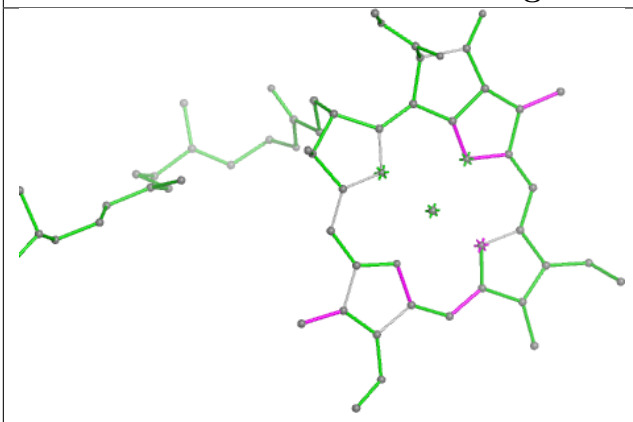


Torsions

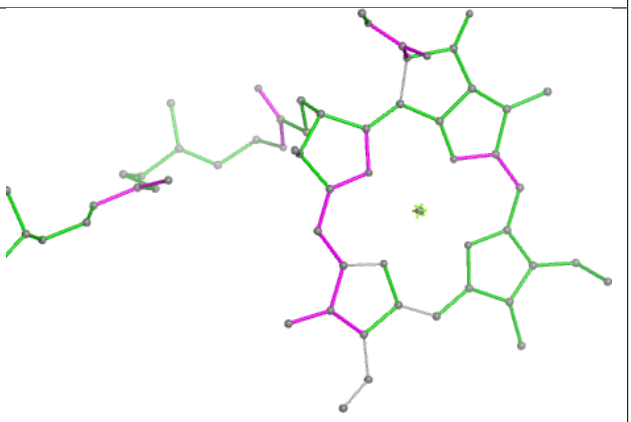


Rings

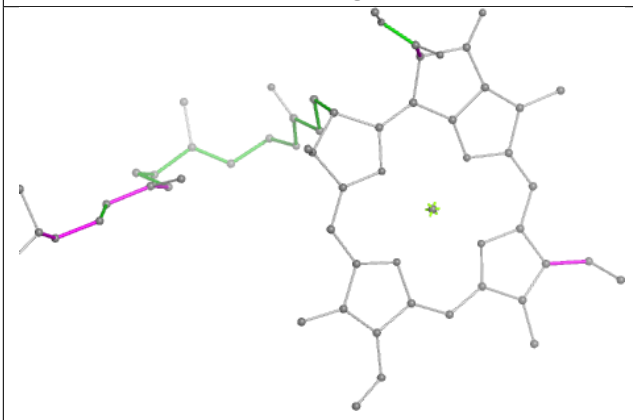
Ligand CLA A 405



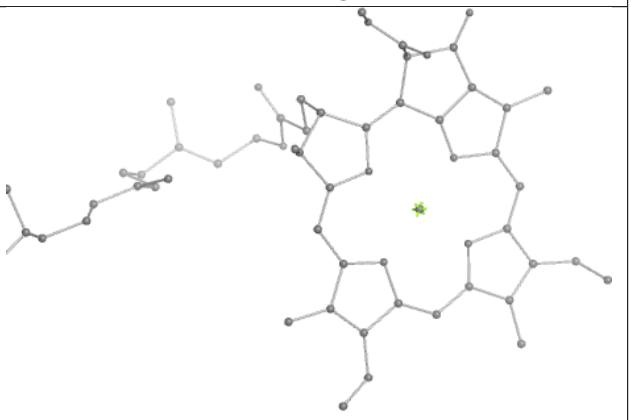
Bond lengths



Bond angles

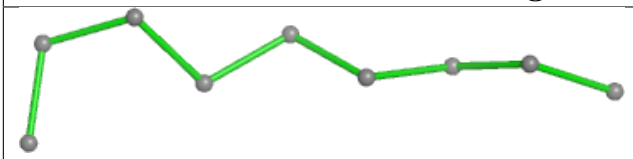


Torsions

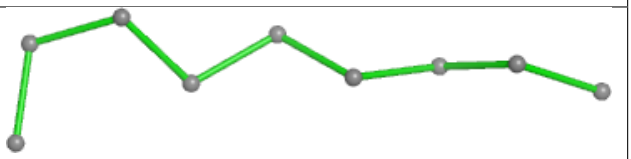


Rings

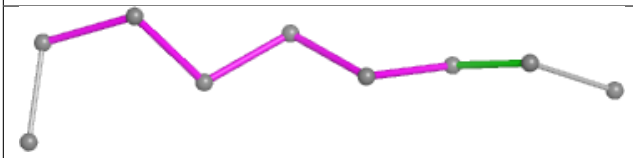
Ligand STE A 409



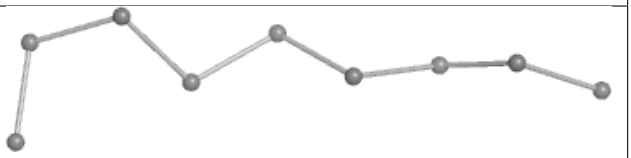
Bond lengths



Bond angles

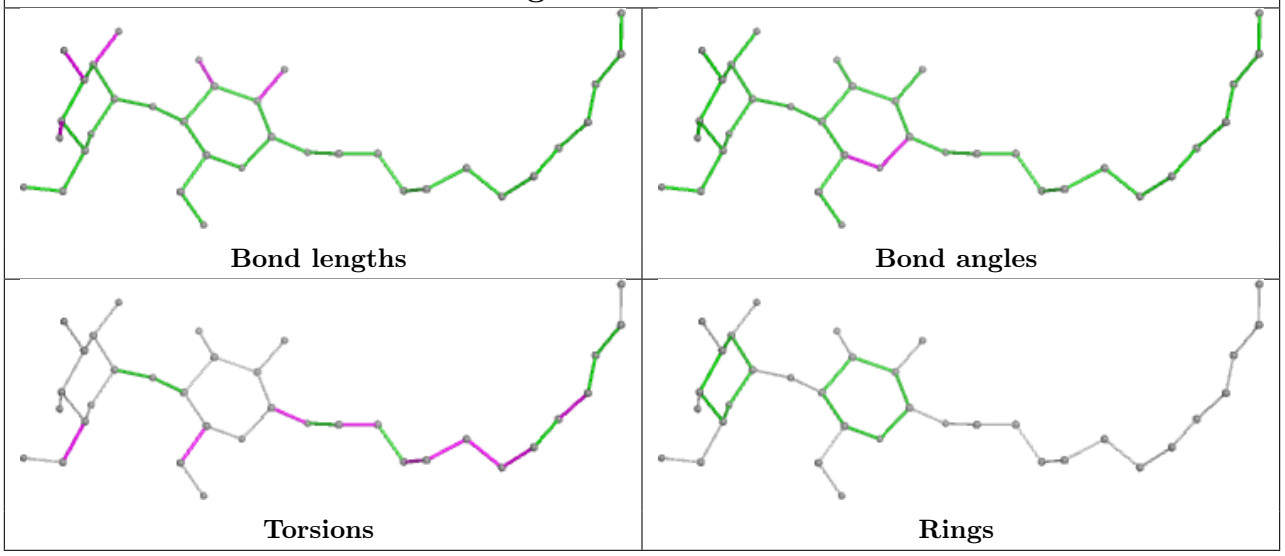


Torsions

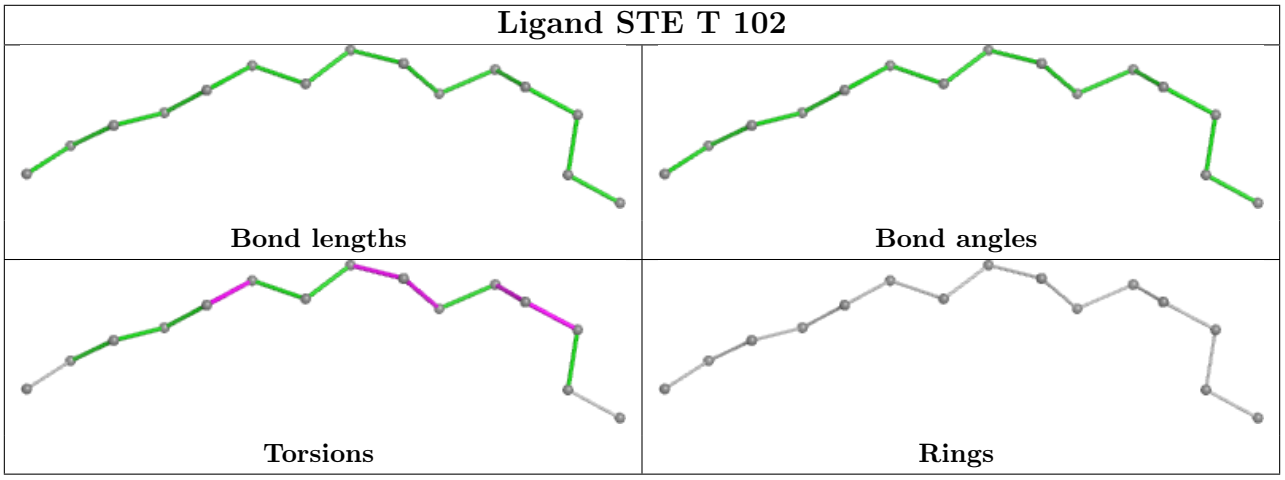


Rings

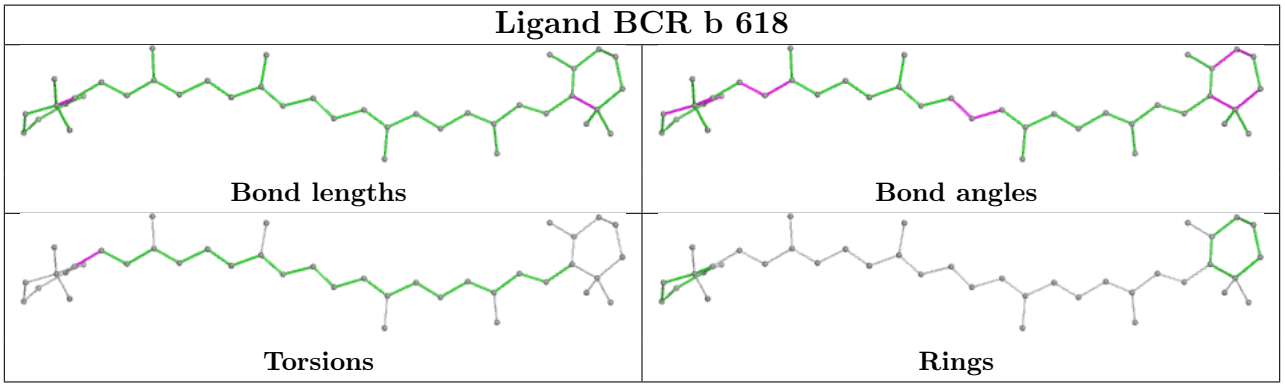
Ligand LMT z 101



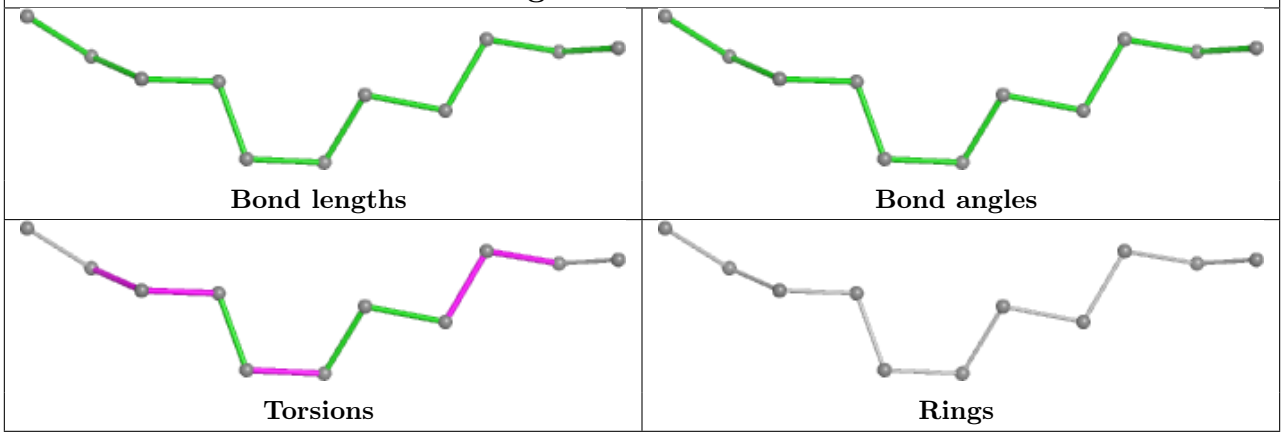
Ligand STE T 102



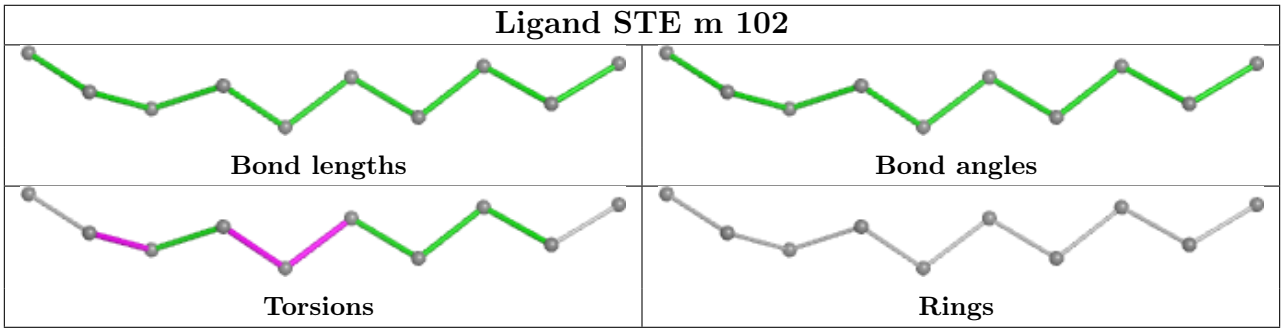
Ligand BCR b 618



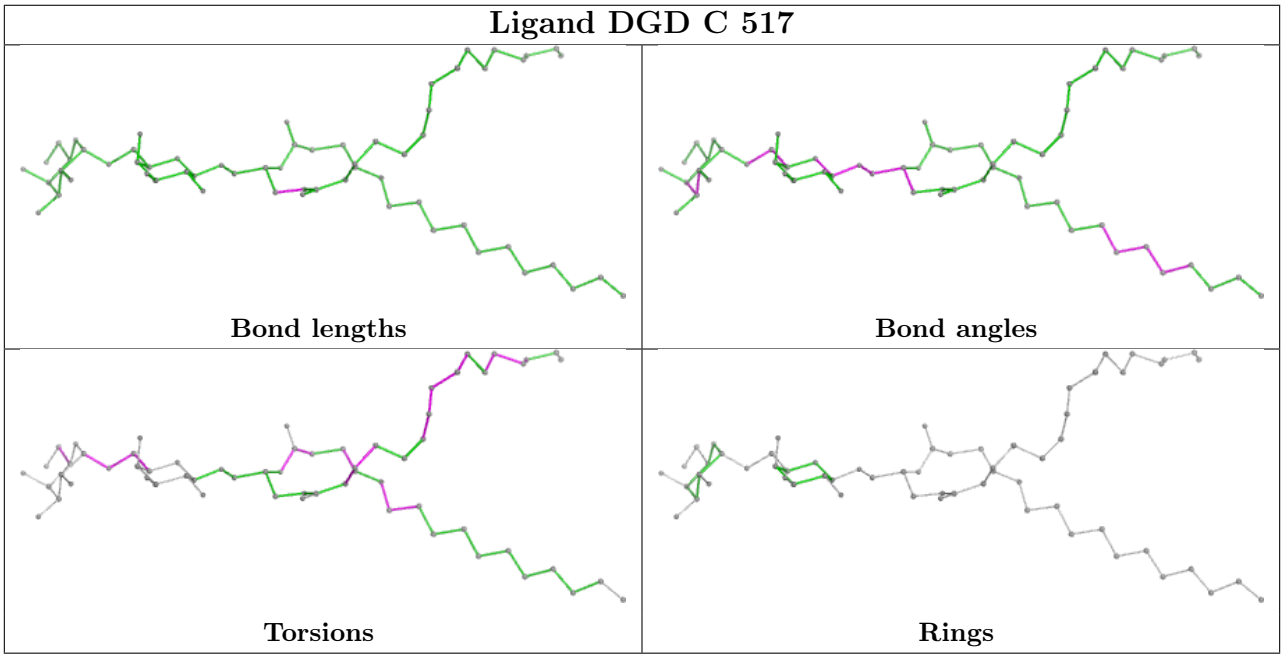
Ligand STE A 416



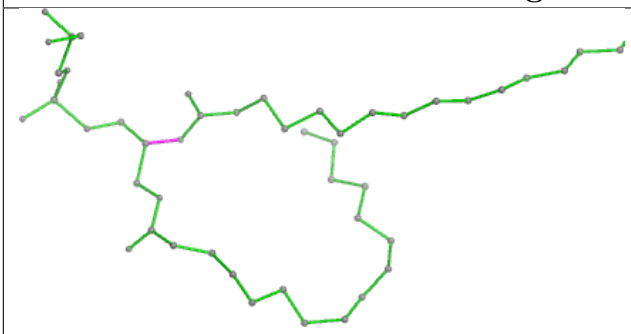
Ligand STE m 102



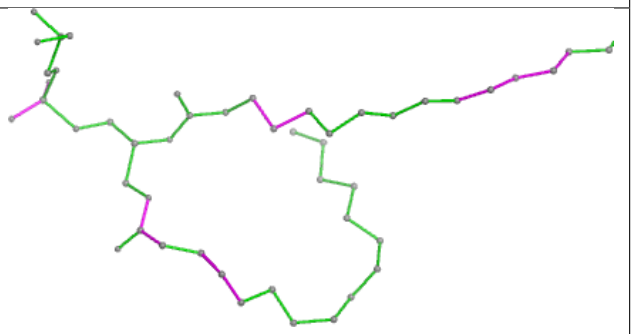
Ligand DGD C 517



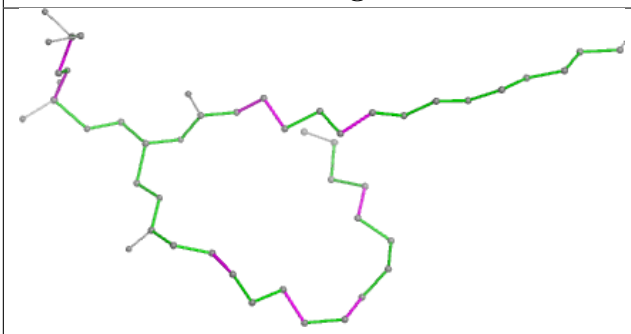
Ligand LHG d 411



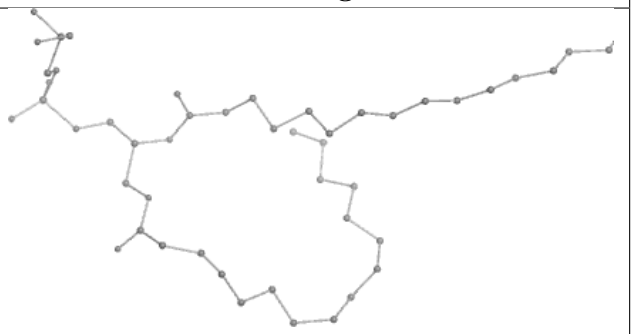
Bond lengths



Bond angles

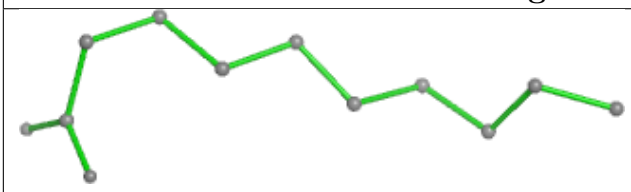


Torsions

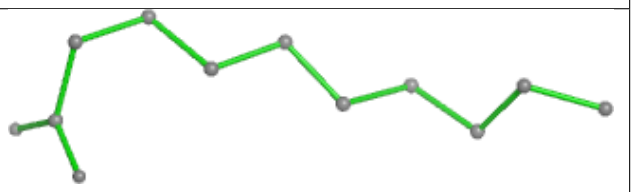


Rings

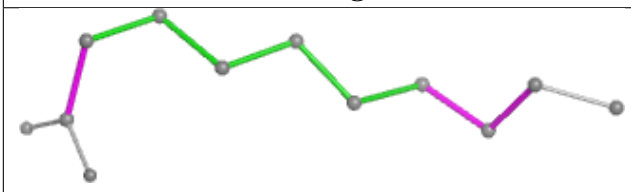
Ligand STE E 101



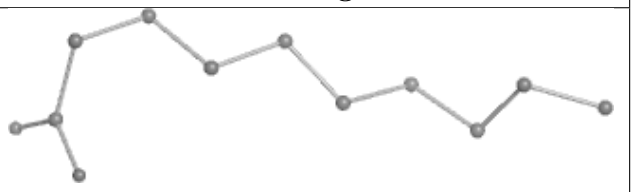
Bond lengths



Bond angles

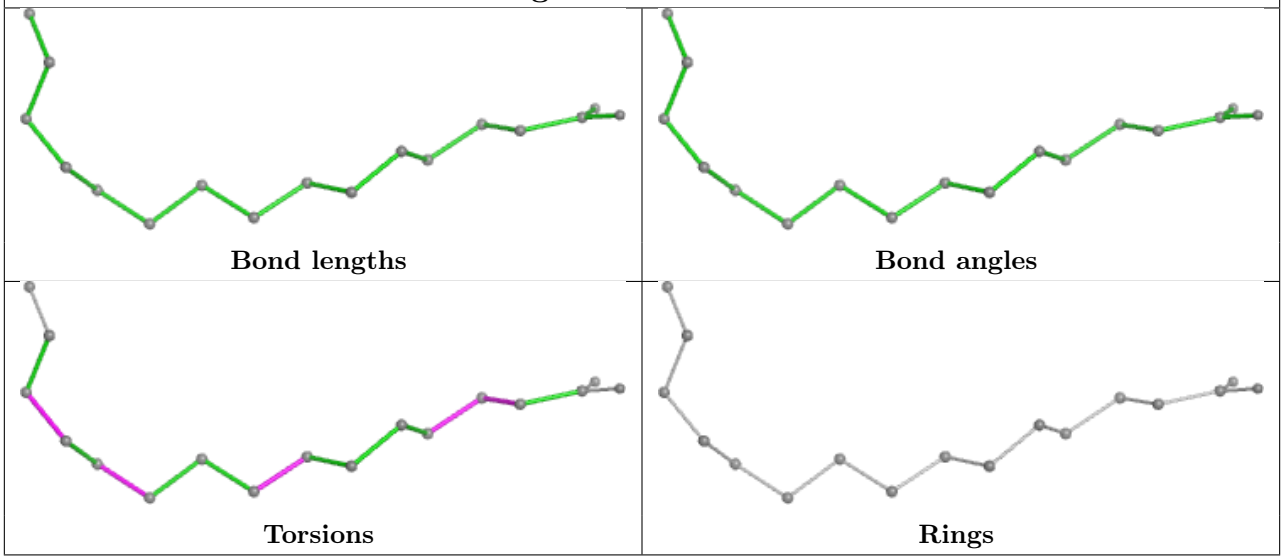


Torsions

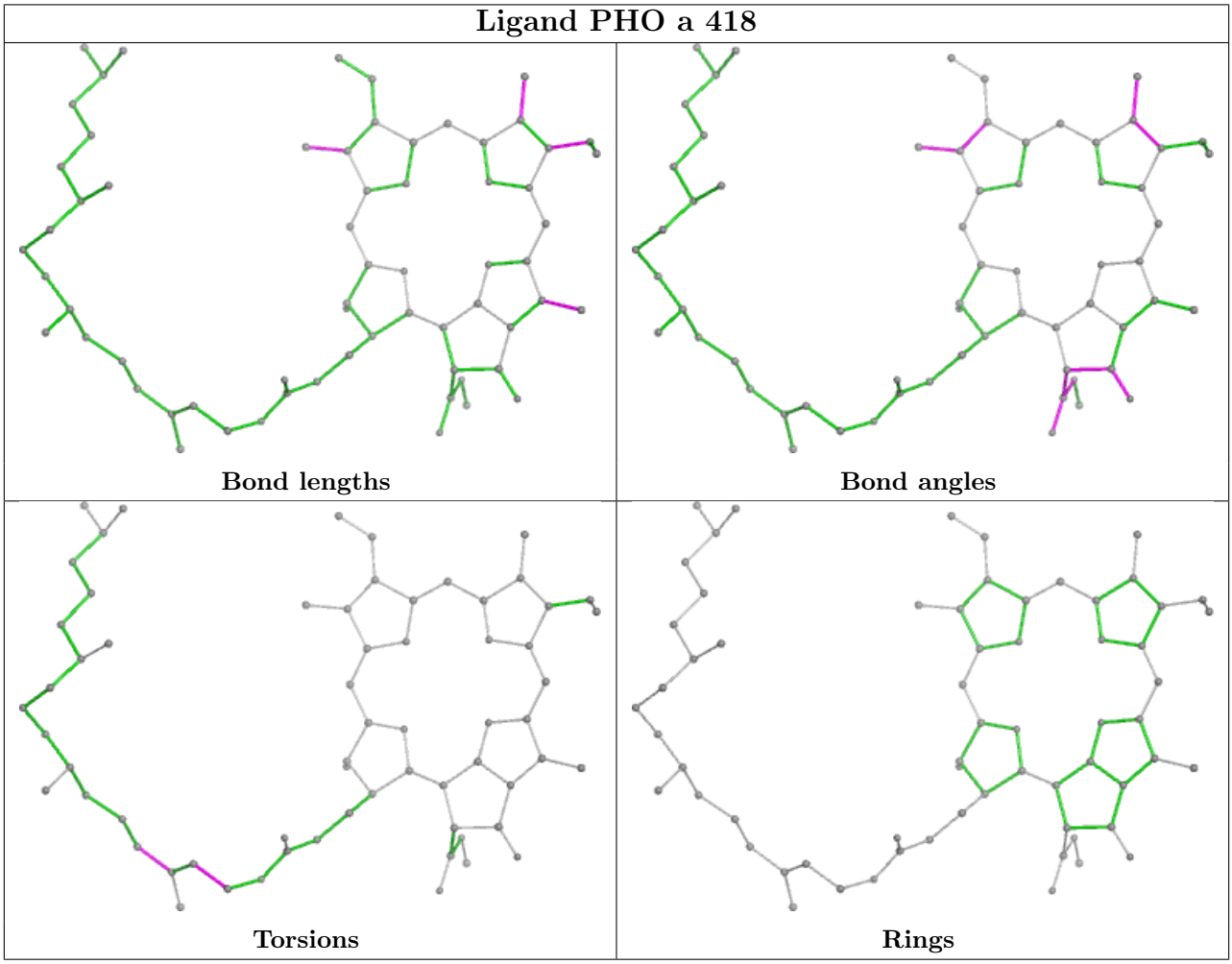


Rings

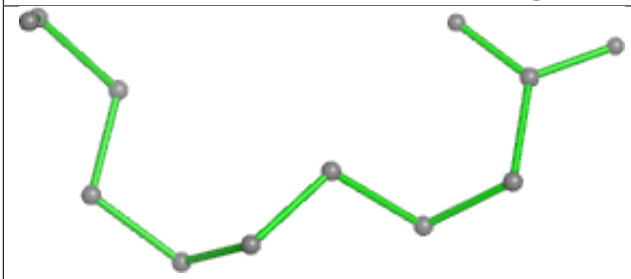
Ligand STE b 622



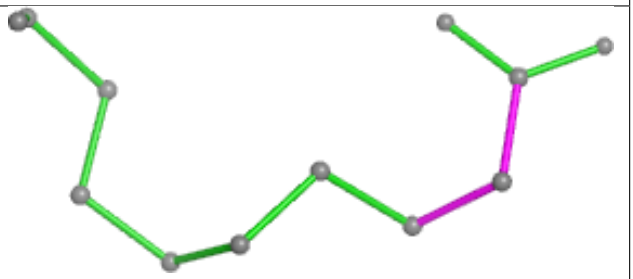
Ligand PHO a 418



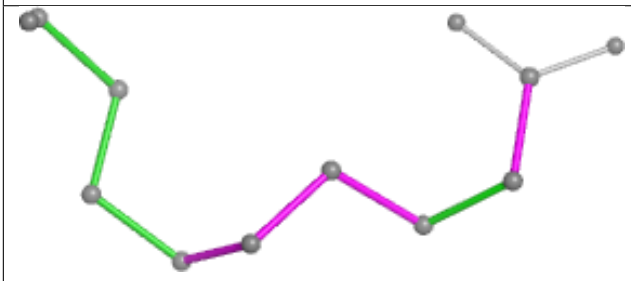
Ligand STE B 622



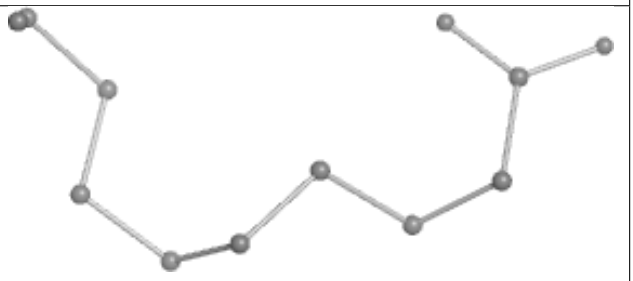
Bond lengths



Bond angles

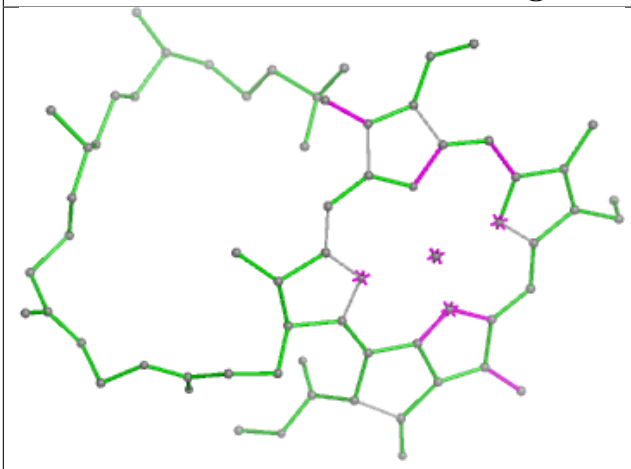


Torsions

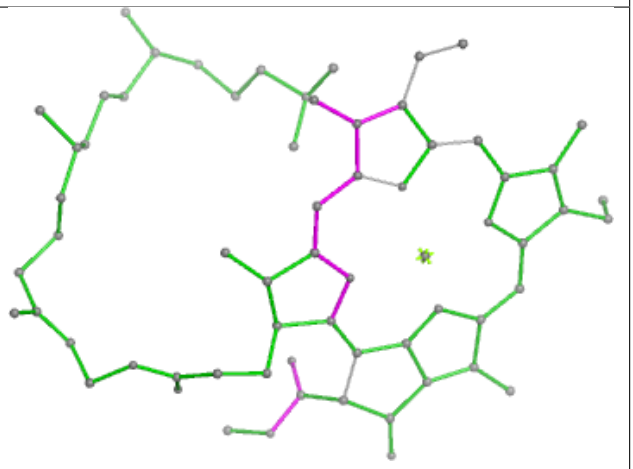


Rings

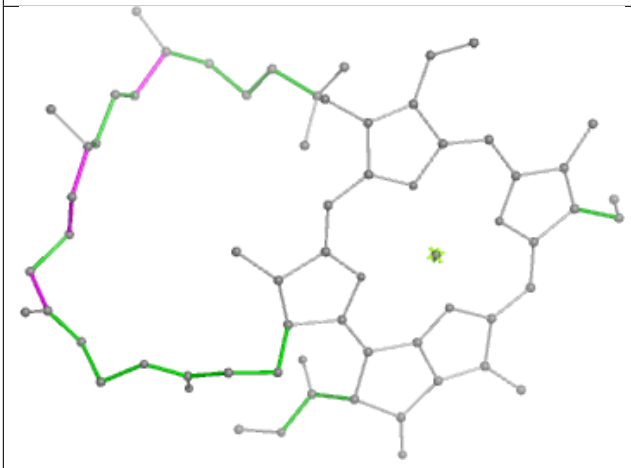
Ligand CLA b 616



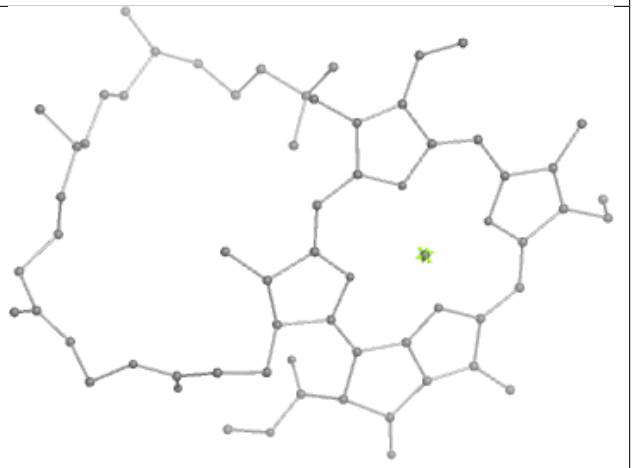
Bond lengths



Bond angles

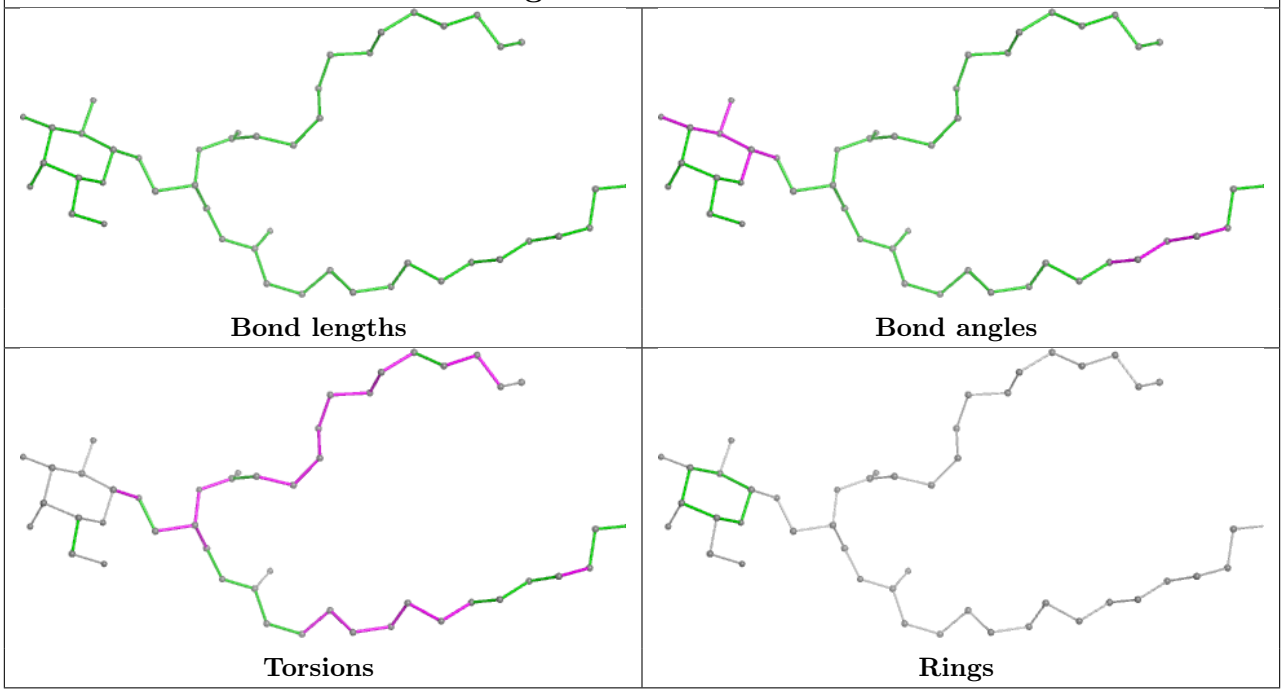


Torsions

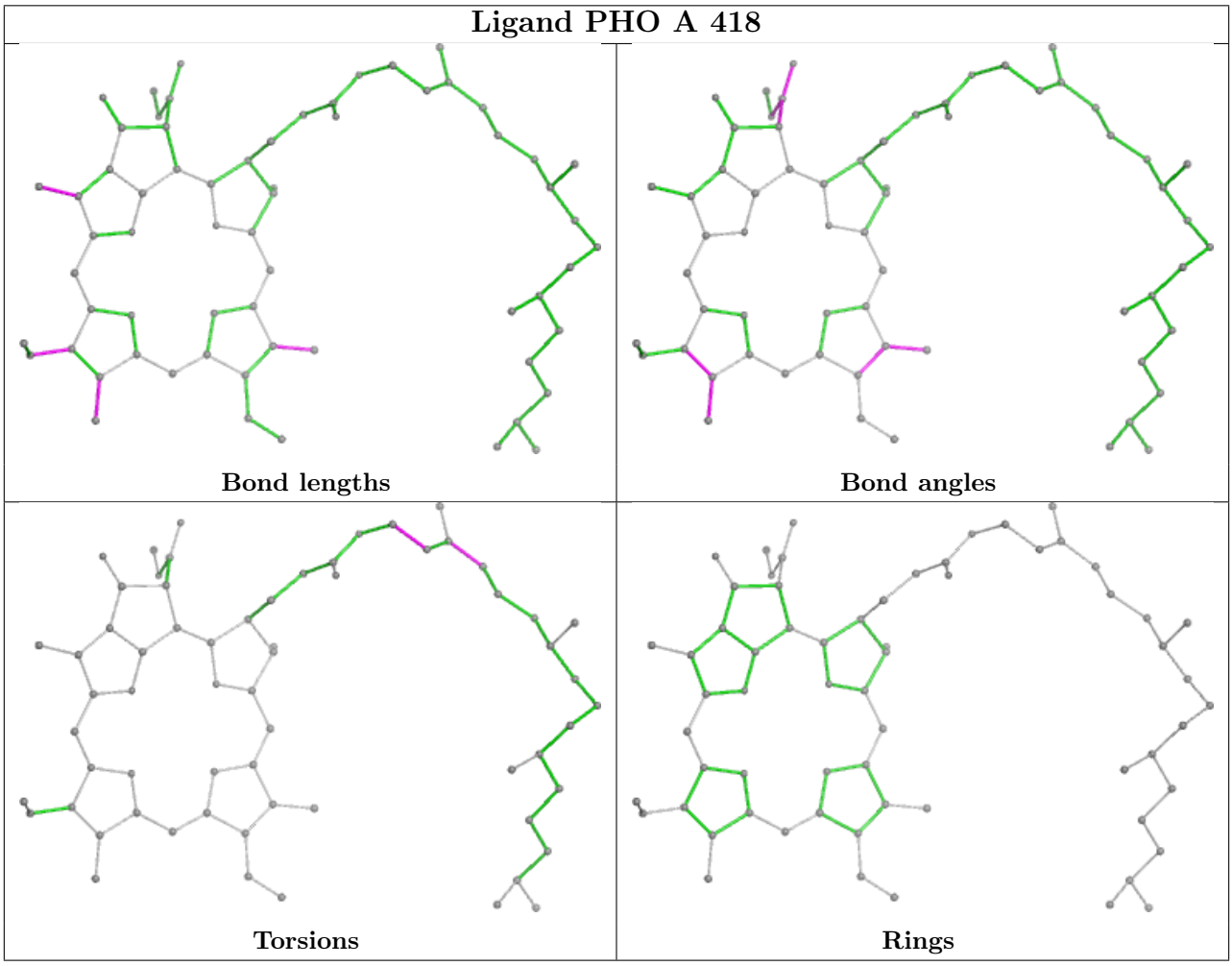


Rings

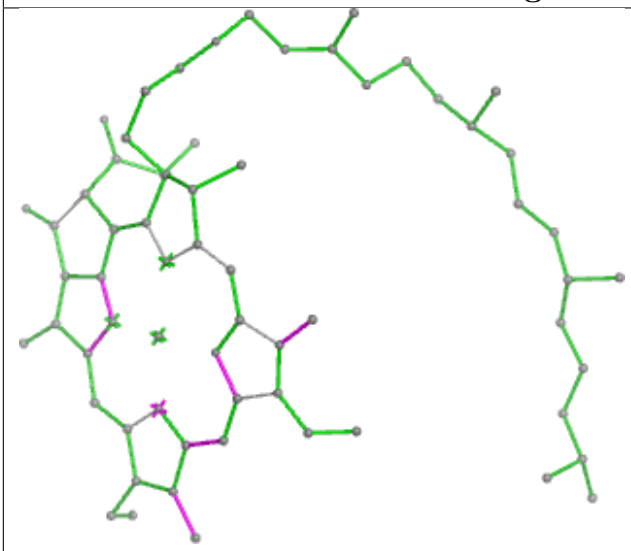
Ligand LMG a 410



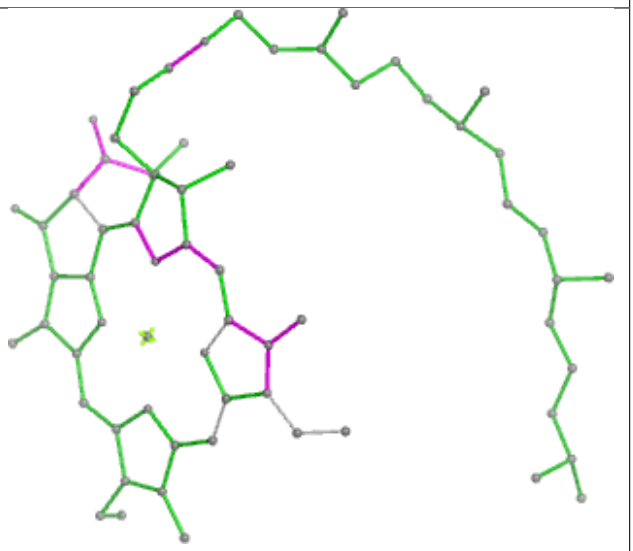
Ligand PHO A 418



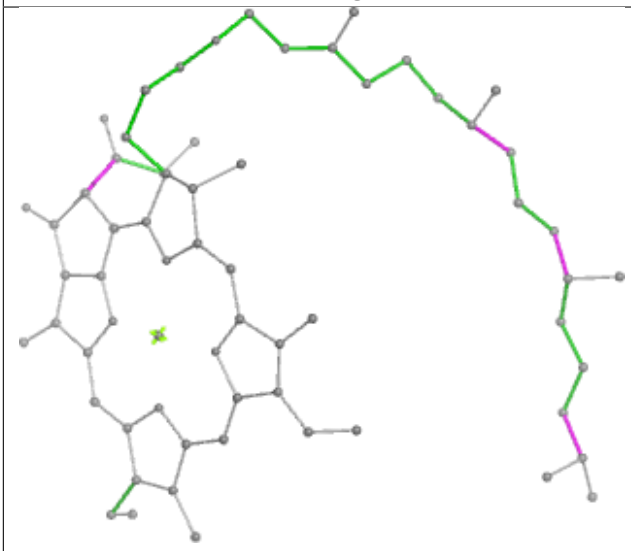
Ligand CLA C 507



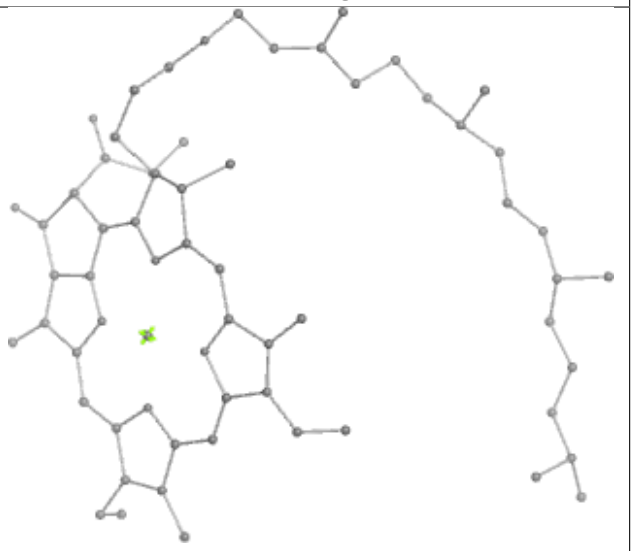
Bond lengths



Bond angles

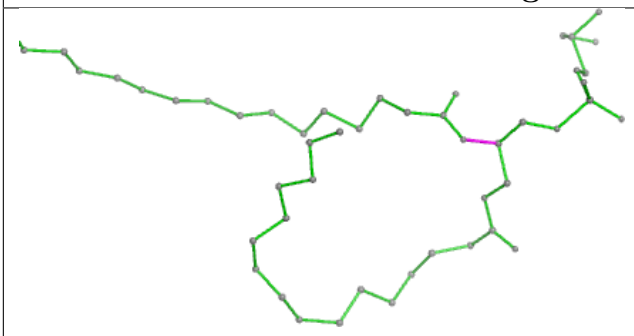


Torsions

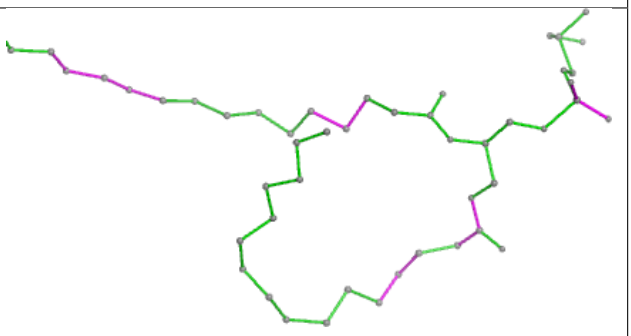


Rings

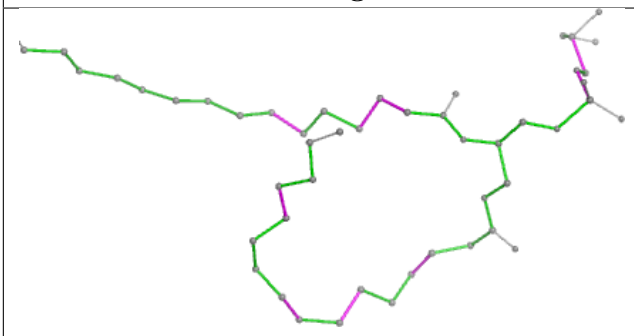
Ligand LHG D 411



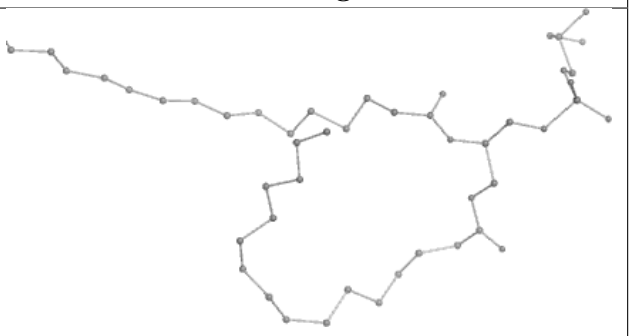
Bond lengths



Bond angles

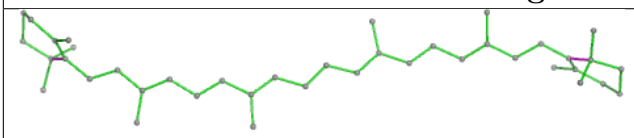


Torsions

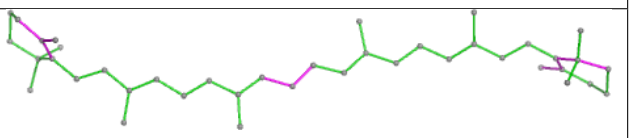


Rings

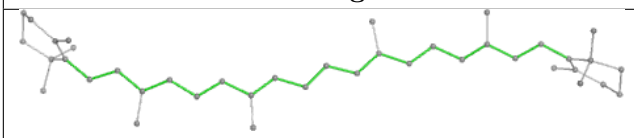
Ligand BCR c 515



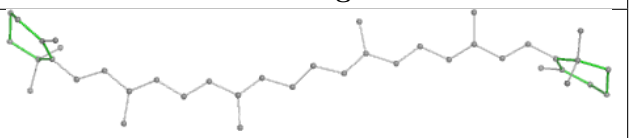
Bond lengths



Bond angles

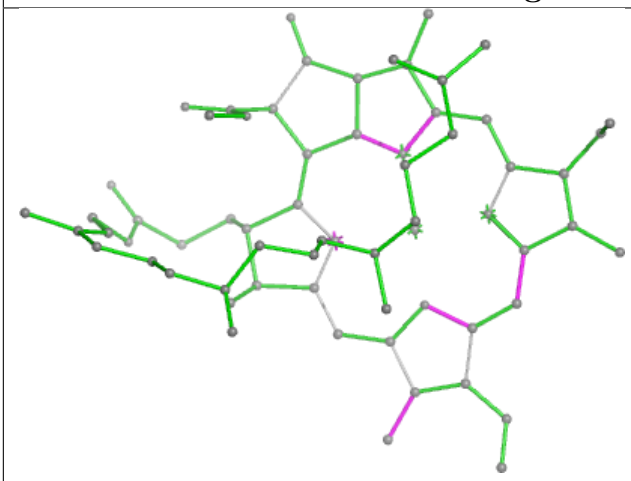


Torsions

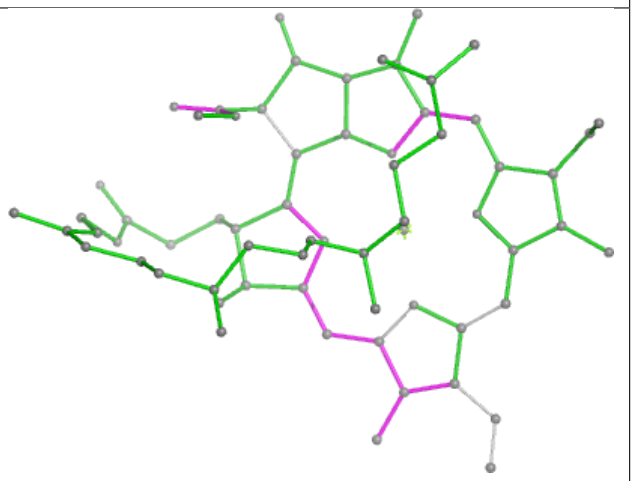


Rings

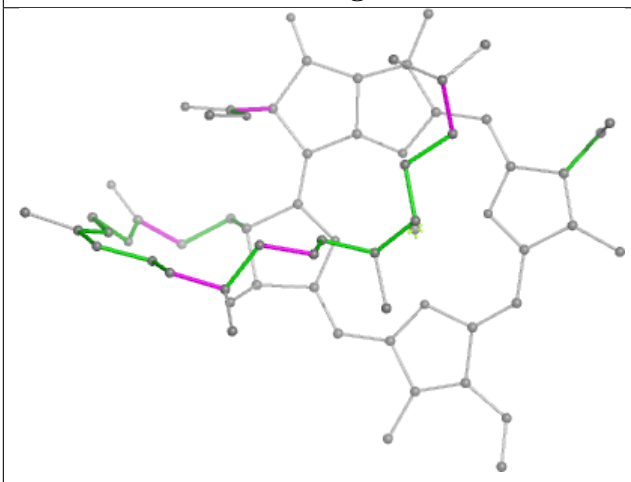
Ligand CLA C 510



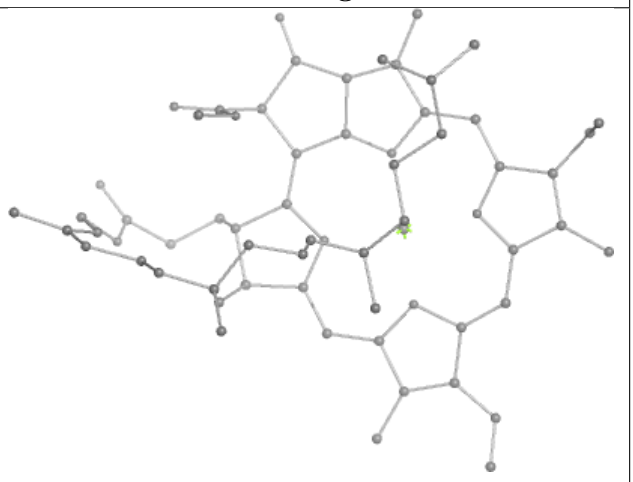
Bond lengths



Bond angles

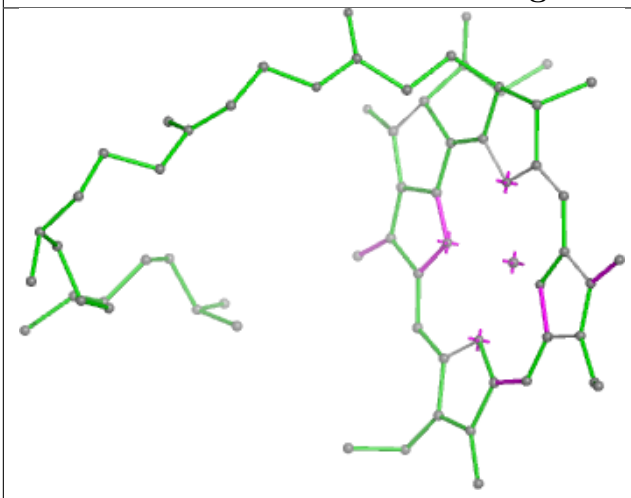


Torsions

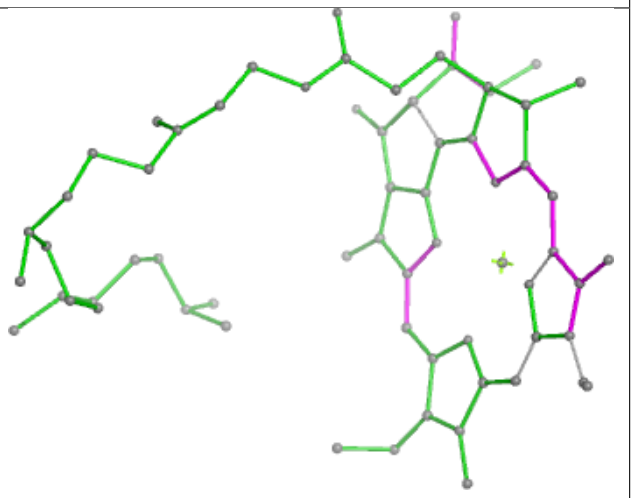


Rings

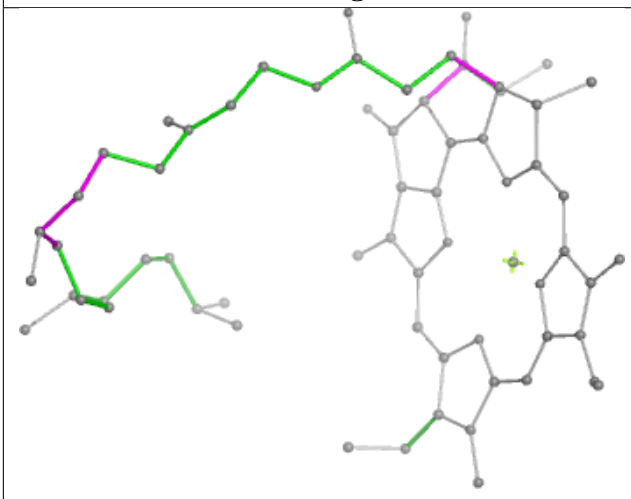
Ligand CLA c 503



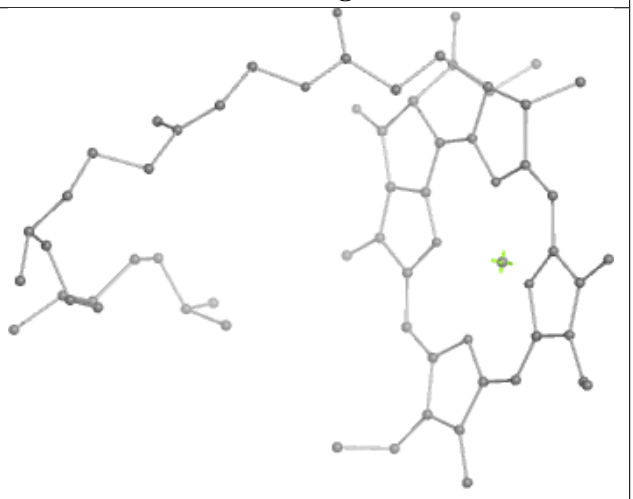
Bond lengths



Bond angles

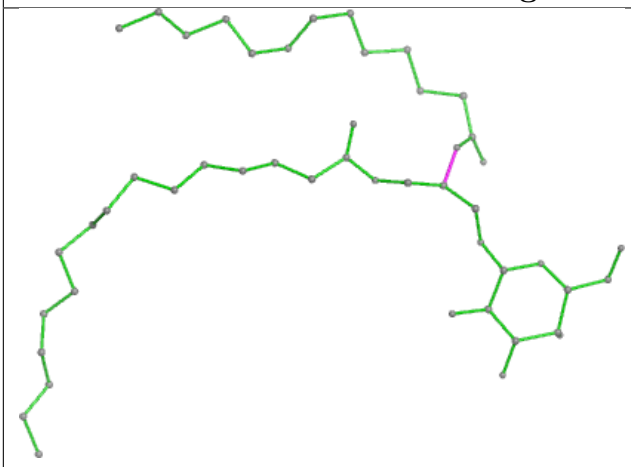


Torsions

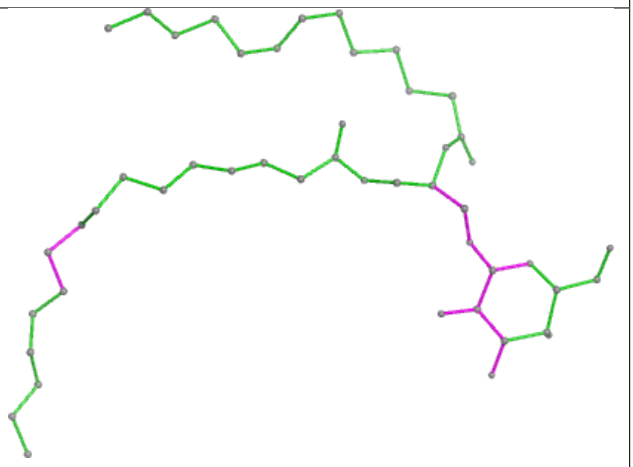


Rings

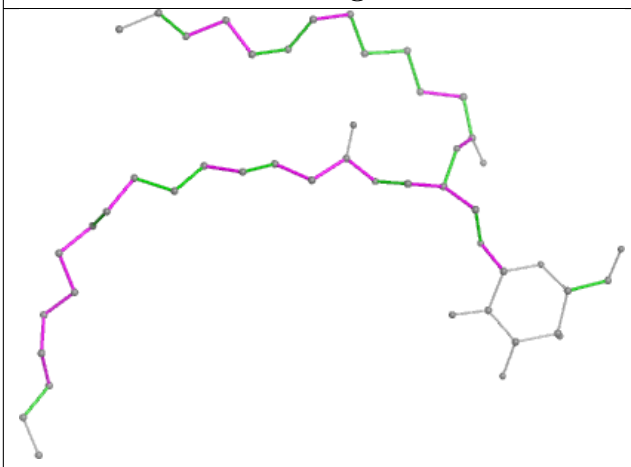
Ligand LMG C 520



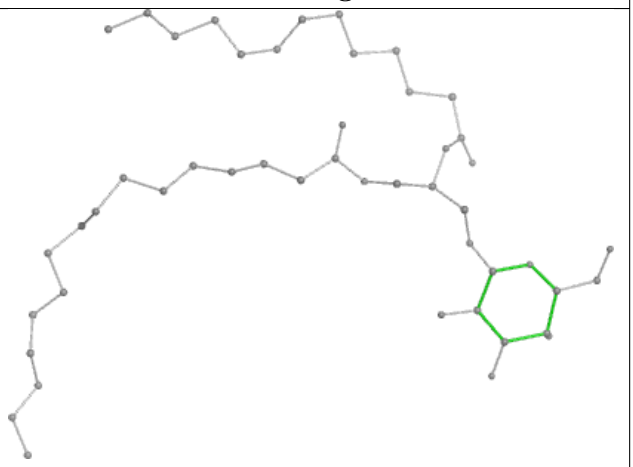
Bond lengths



Bond angles

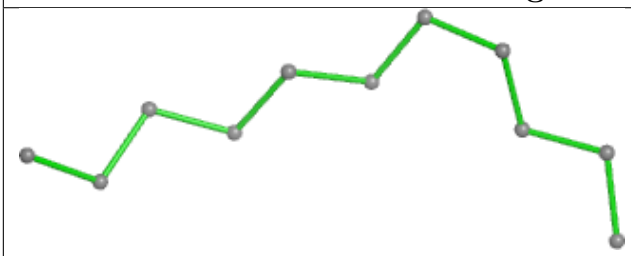


Torsions

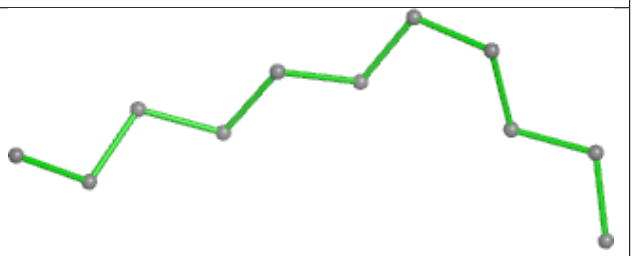


Rings

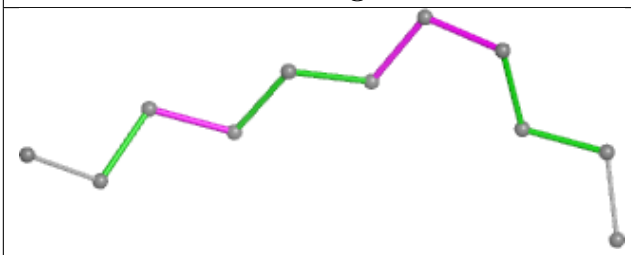
Ligand STE A 415



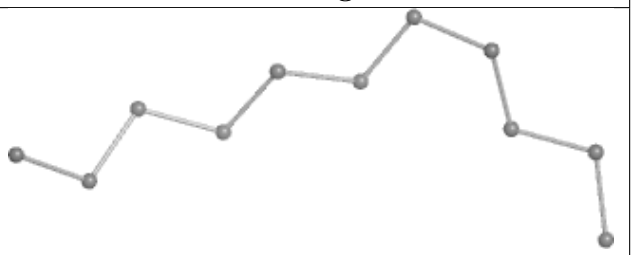
Bond lengths



Bond angles

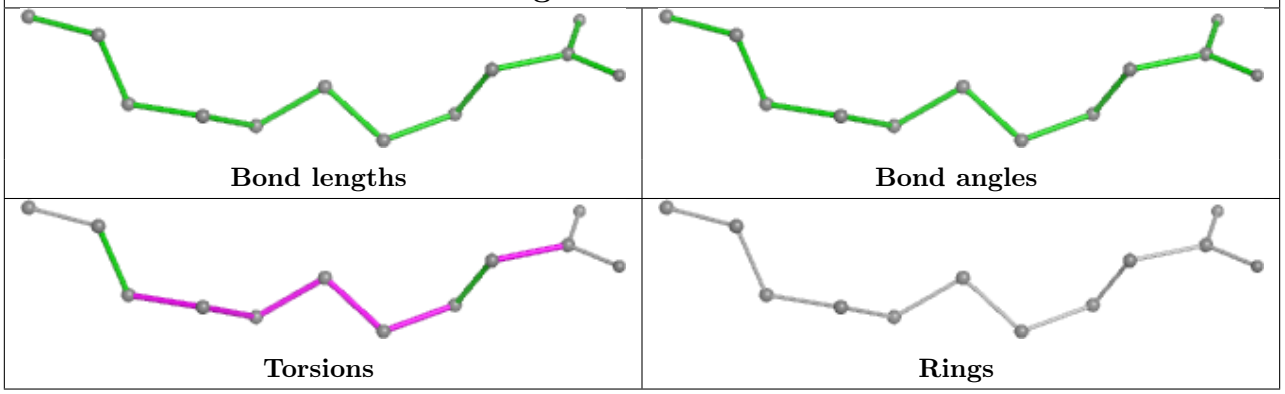


Torsions

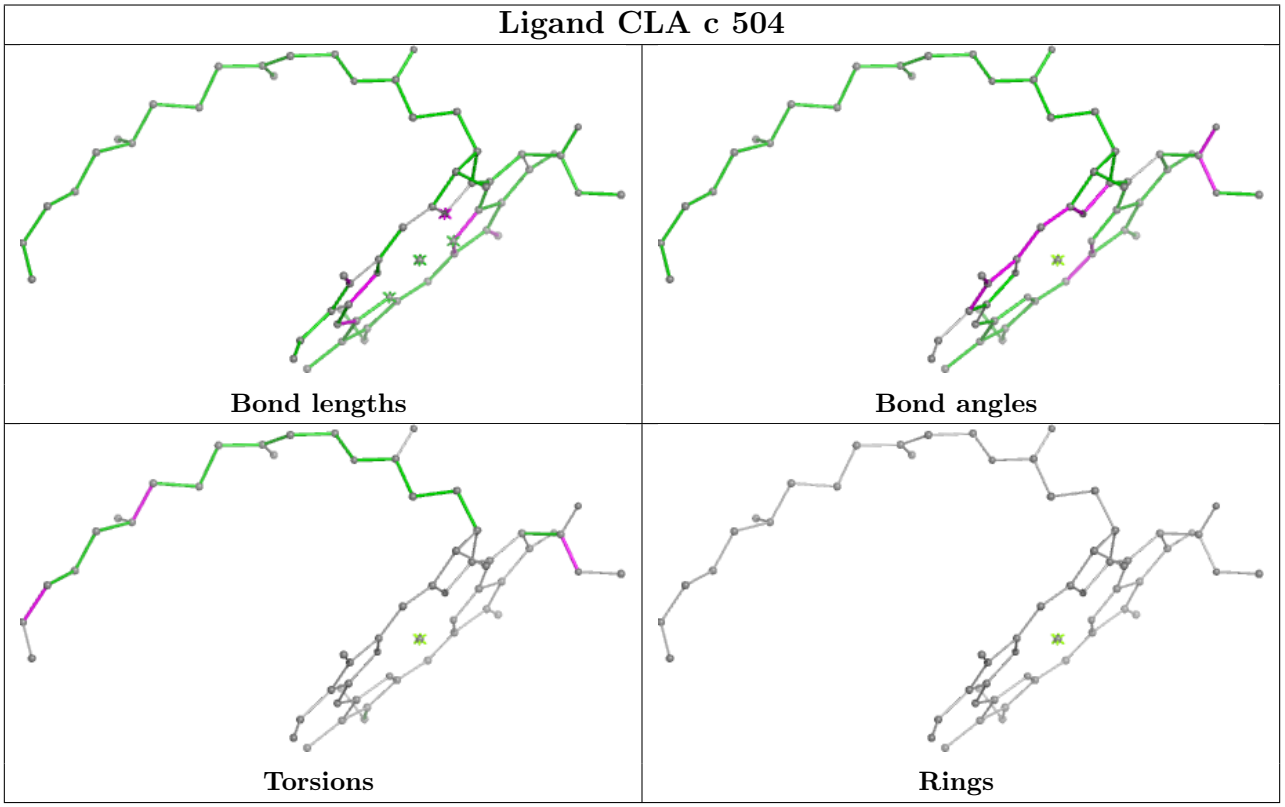


Rings

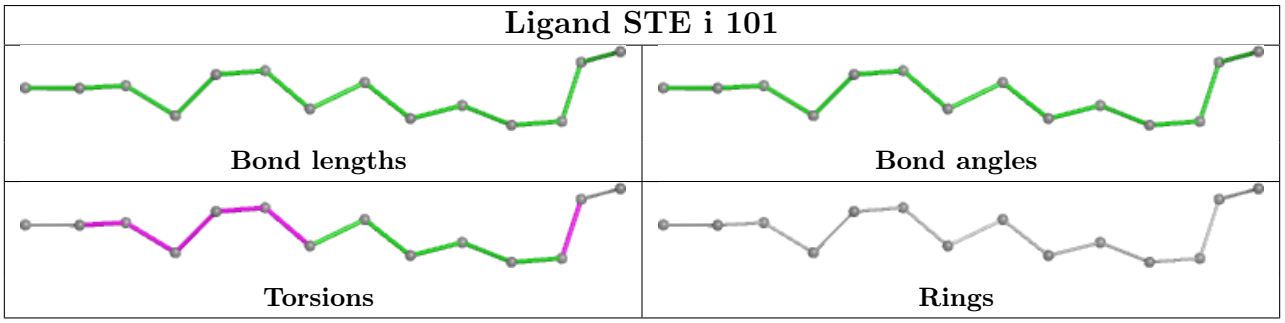
Ligand STE c 521



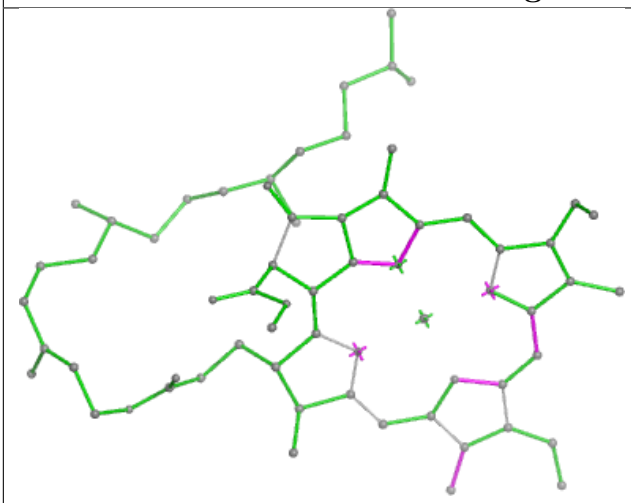
Ligand CLA c 504



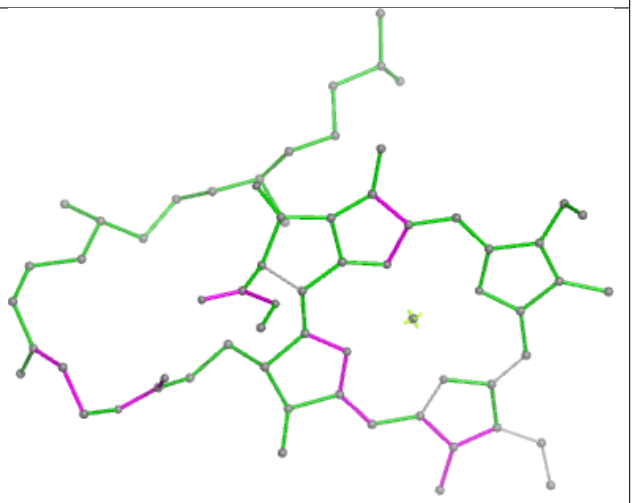
Ligand STE i 101



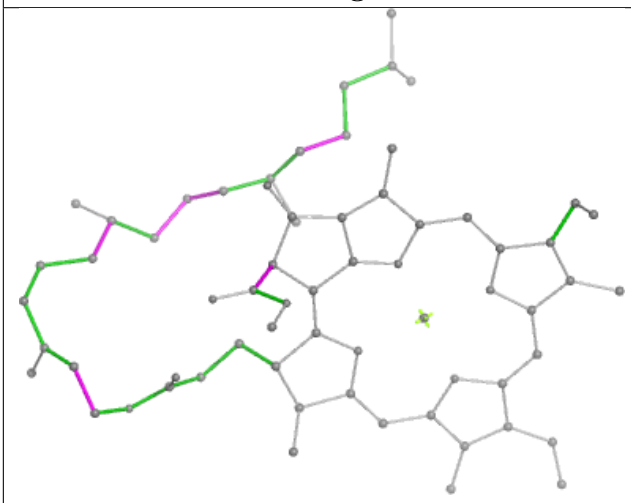
Ligand CLA C 509



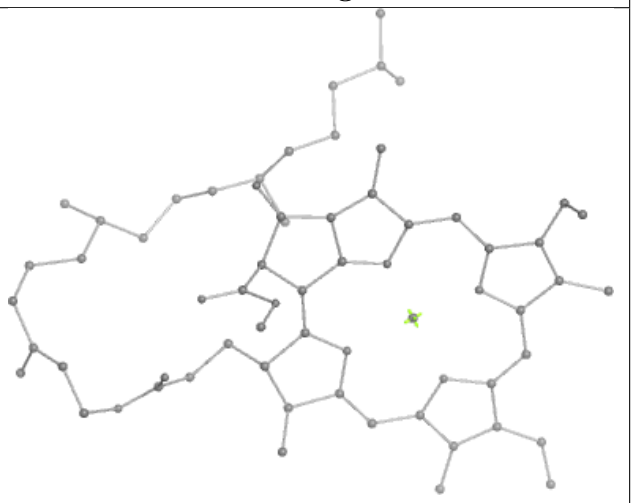
Bond lengths



Bond angles

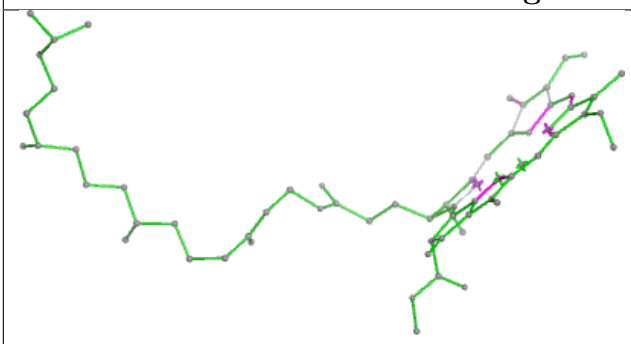


Torsions

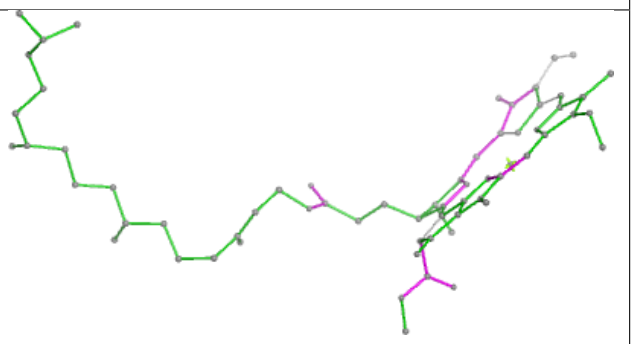


Rings

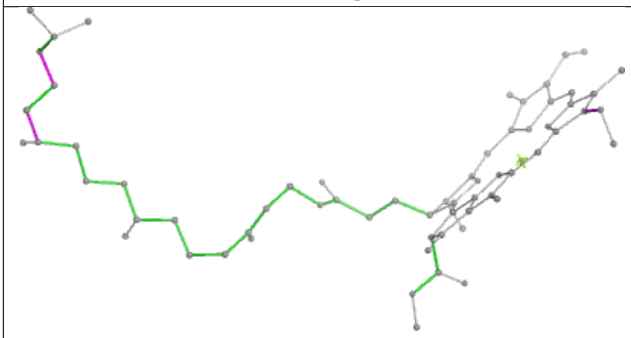
Ligand CLA D 404



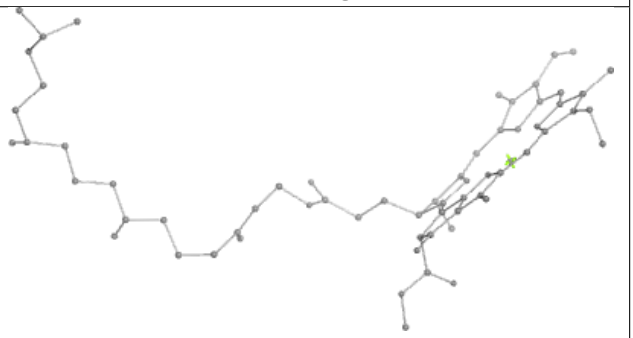
Bond lengths



Bond angles

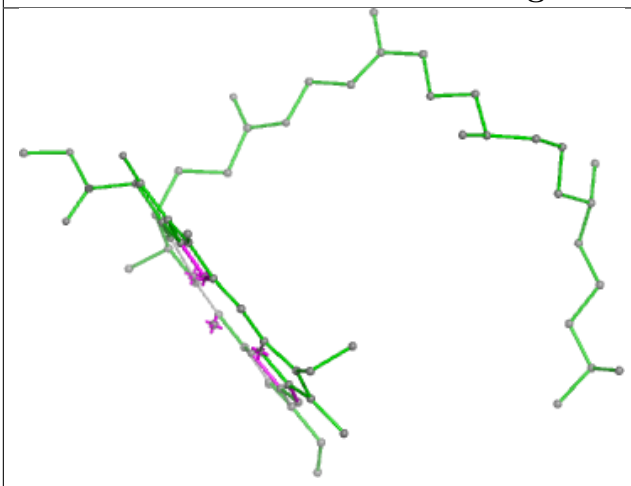


Torsions

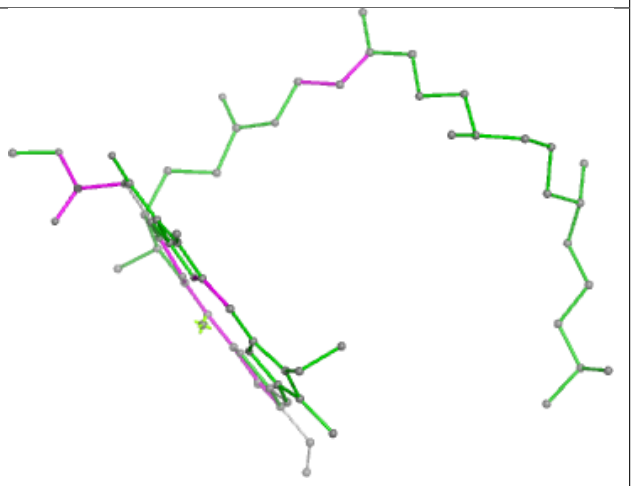


Rings

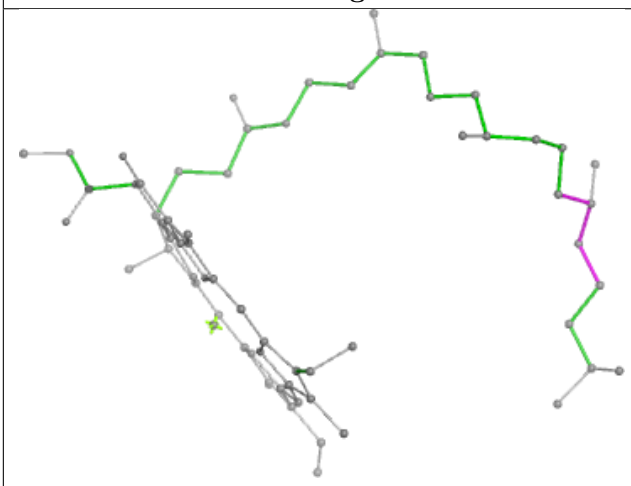
Ligand CLA b 612



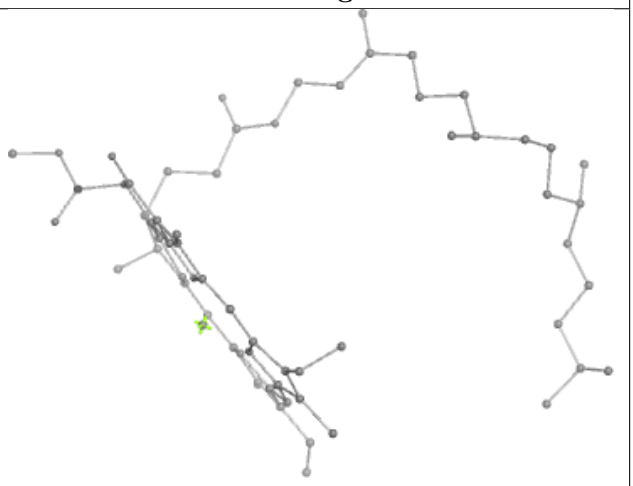
Bond lengths



Bond angles

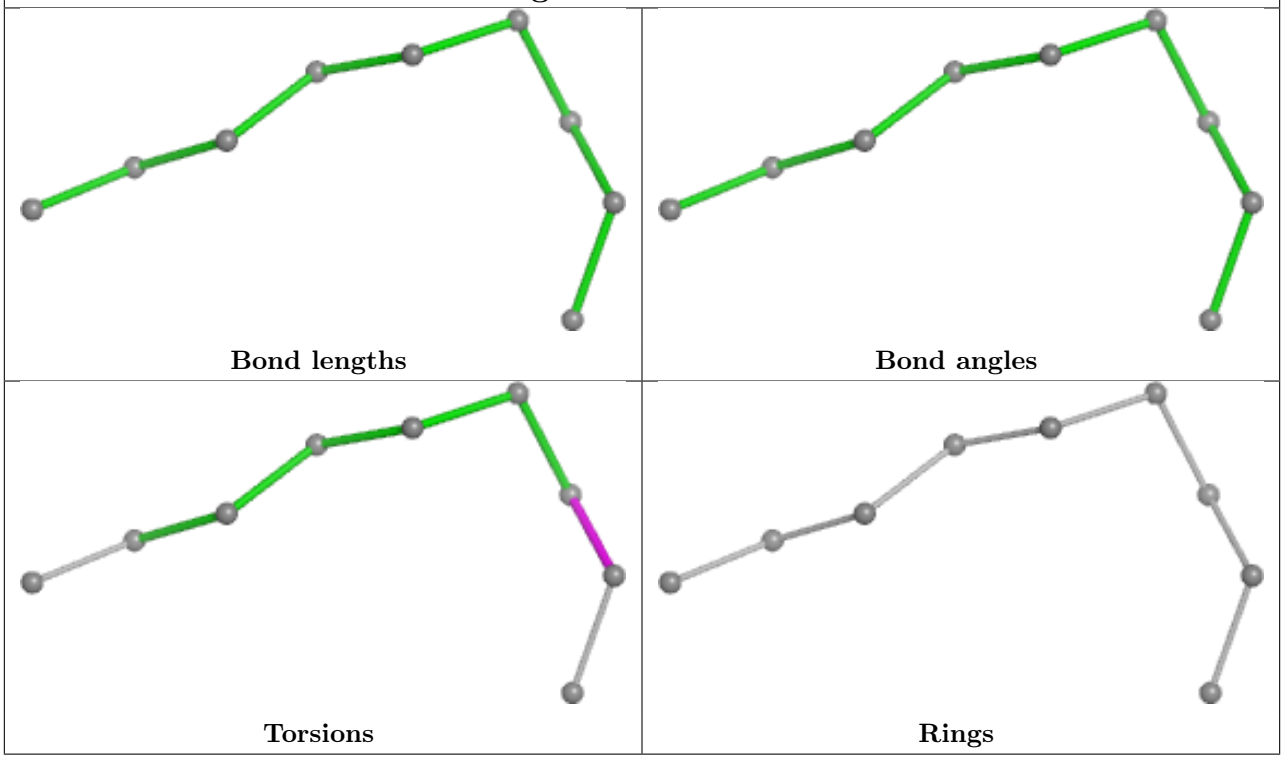


Torsions

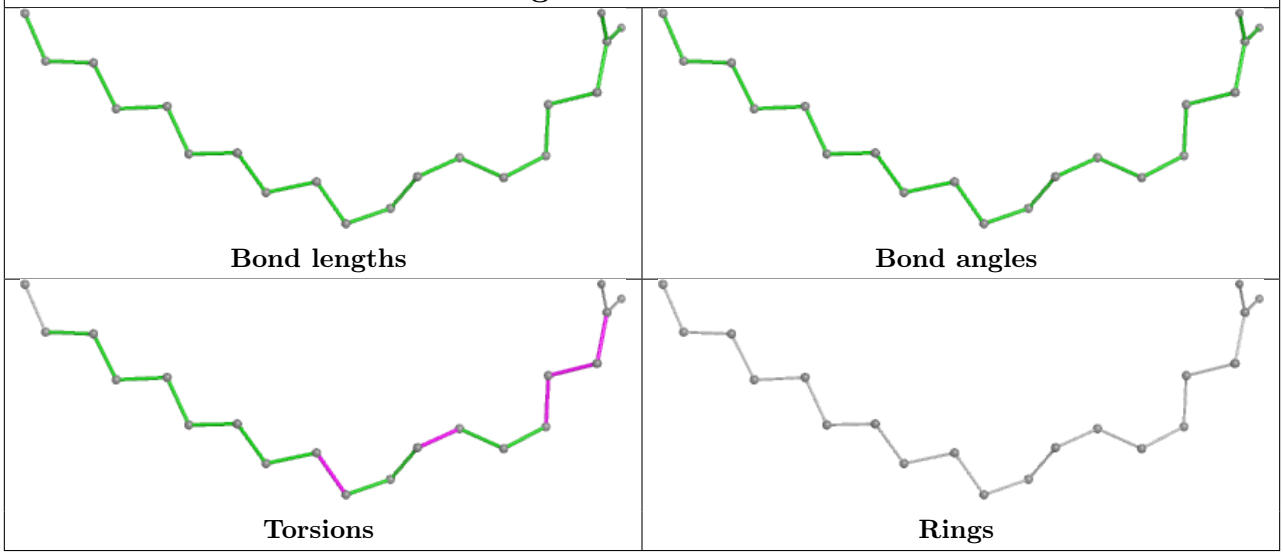


Rings

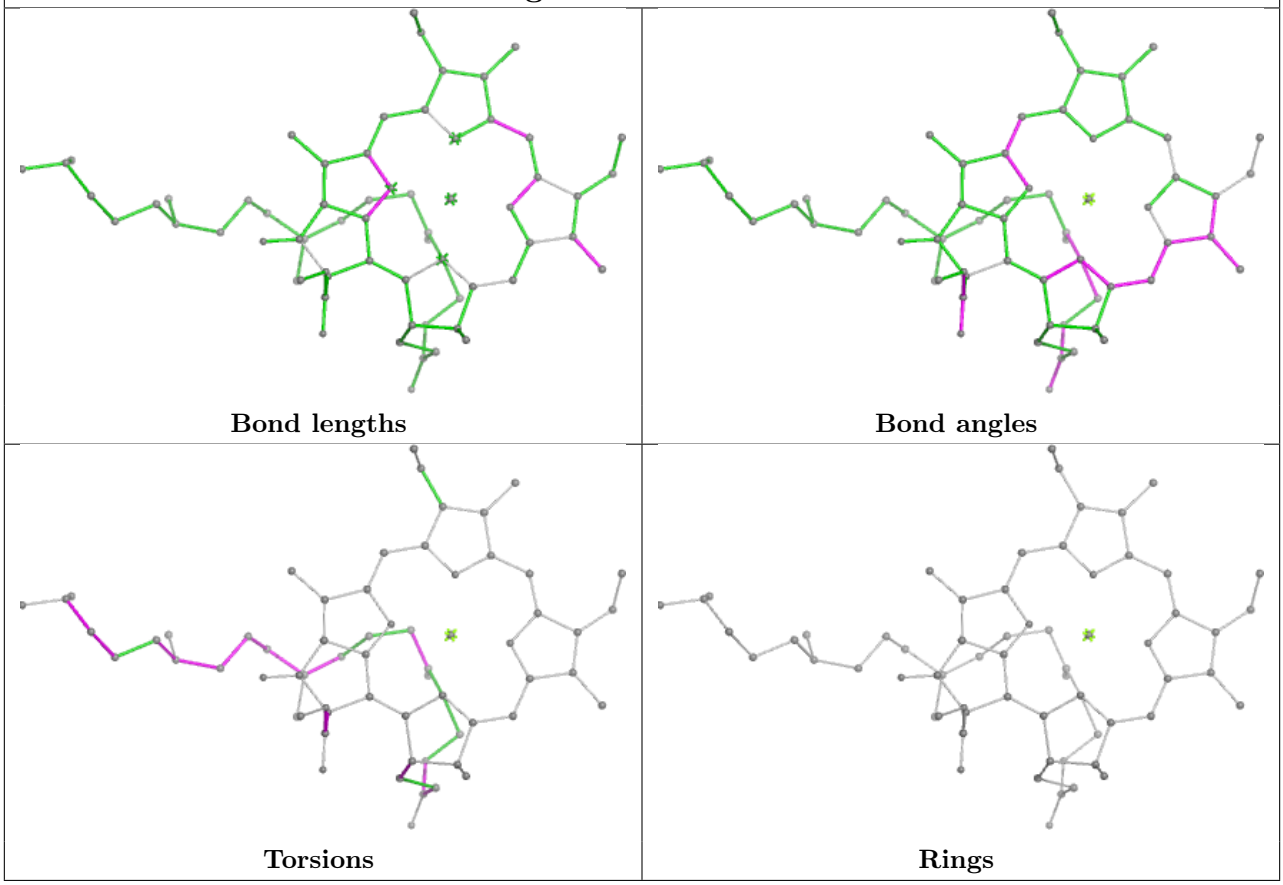
Ligand STE d 413



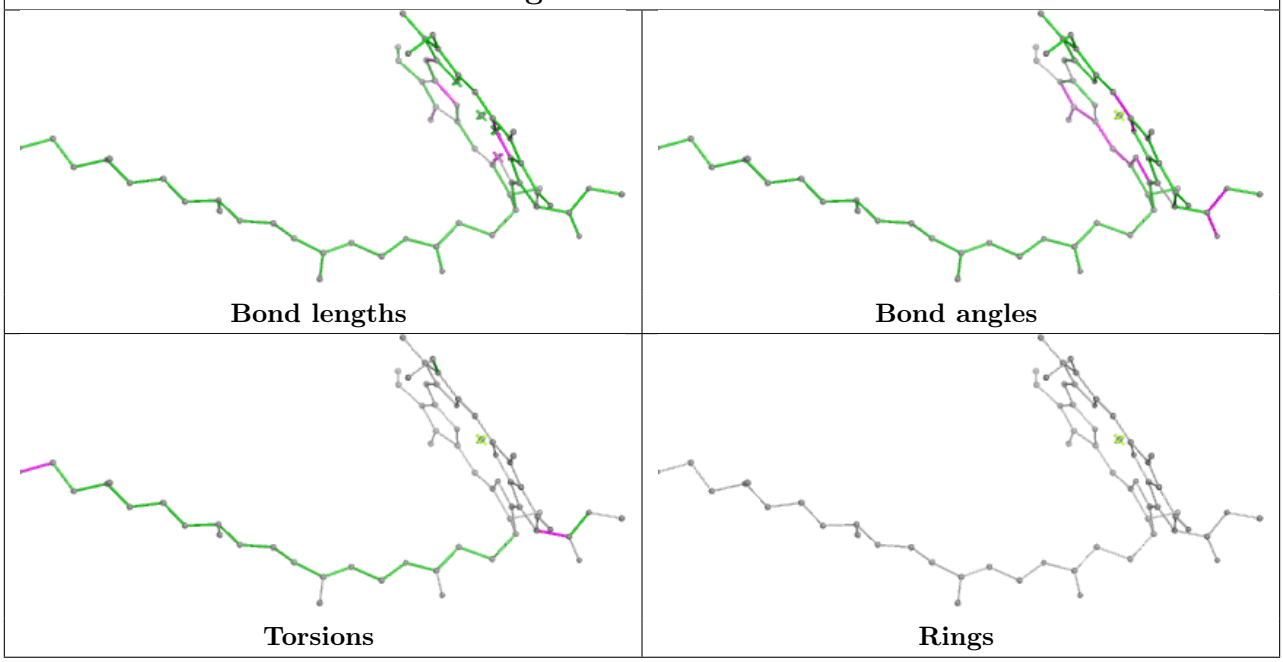
Ligand STE d 412



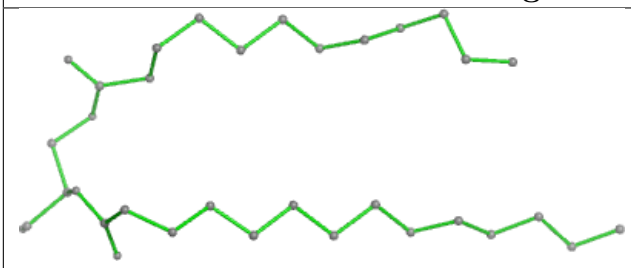
Ligand CLA B 601



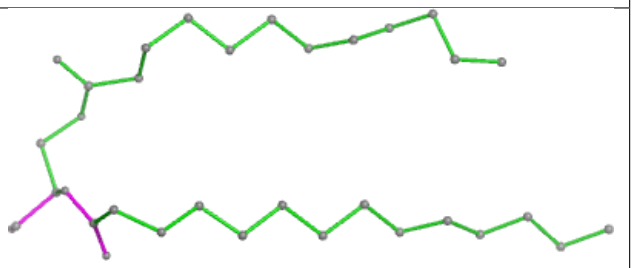
Ligand CLA B 607



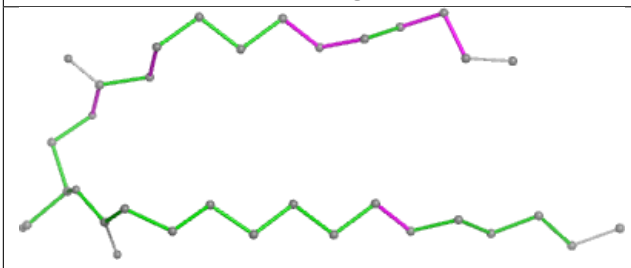
Ligand LMG d 402



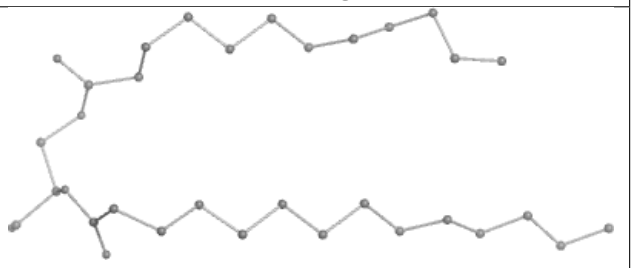
Bond lengths



Bond angles

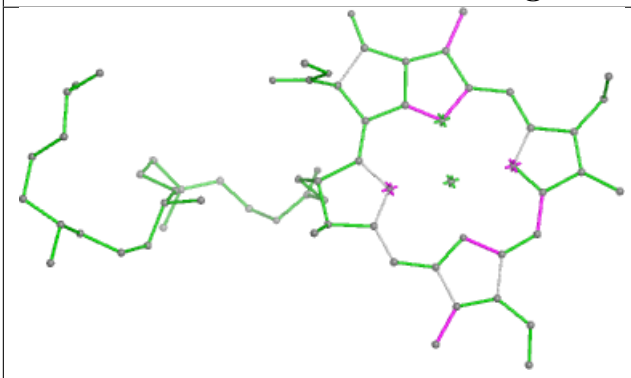


Torsions

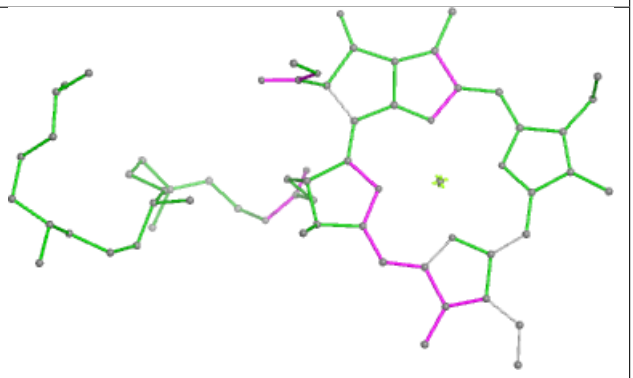


Rings

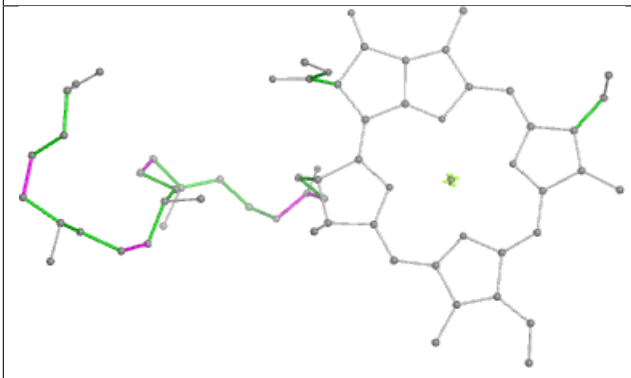
Ligand CLA B 612



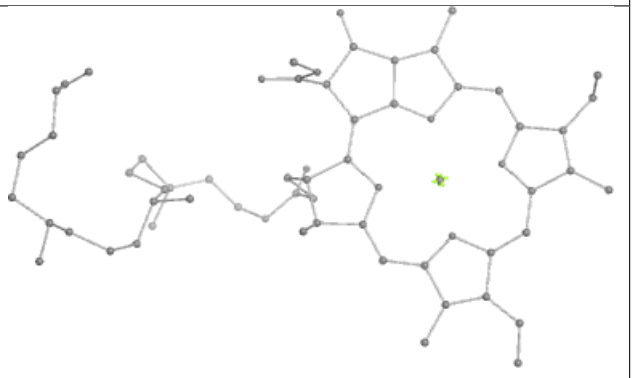
Bond lengths



Bond angles

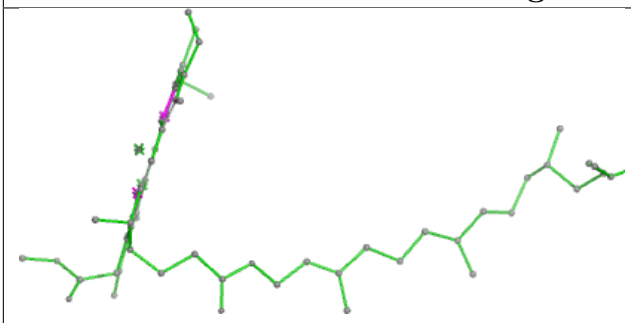


Torsions

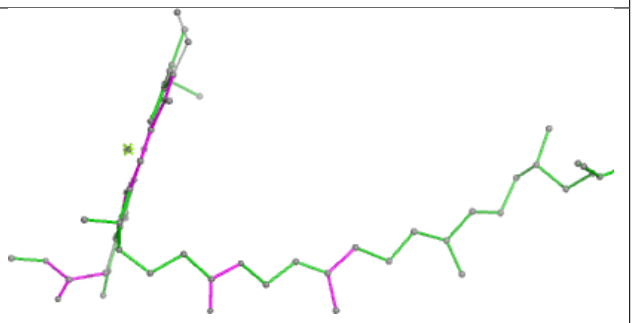


Rings

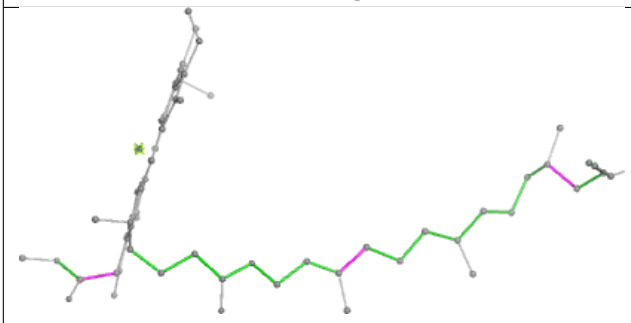
Ligand CLA b 606



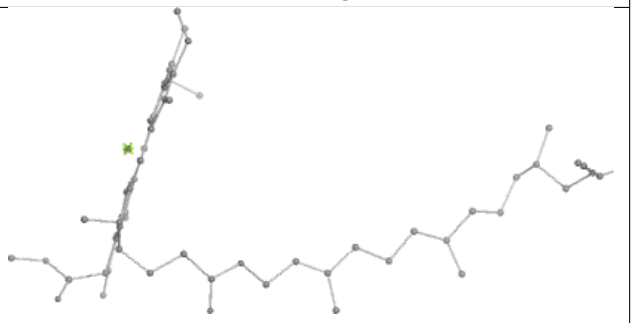
Bond lengths



Bond angles

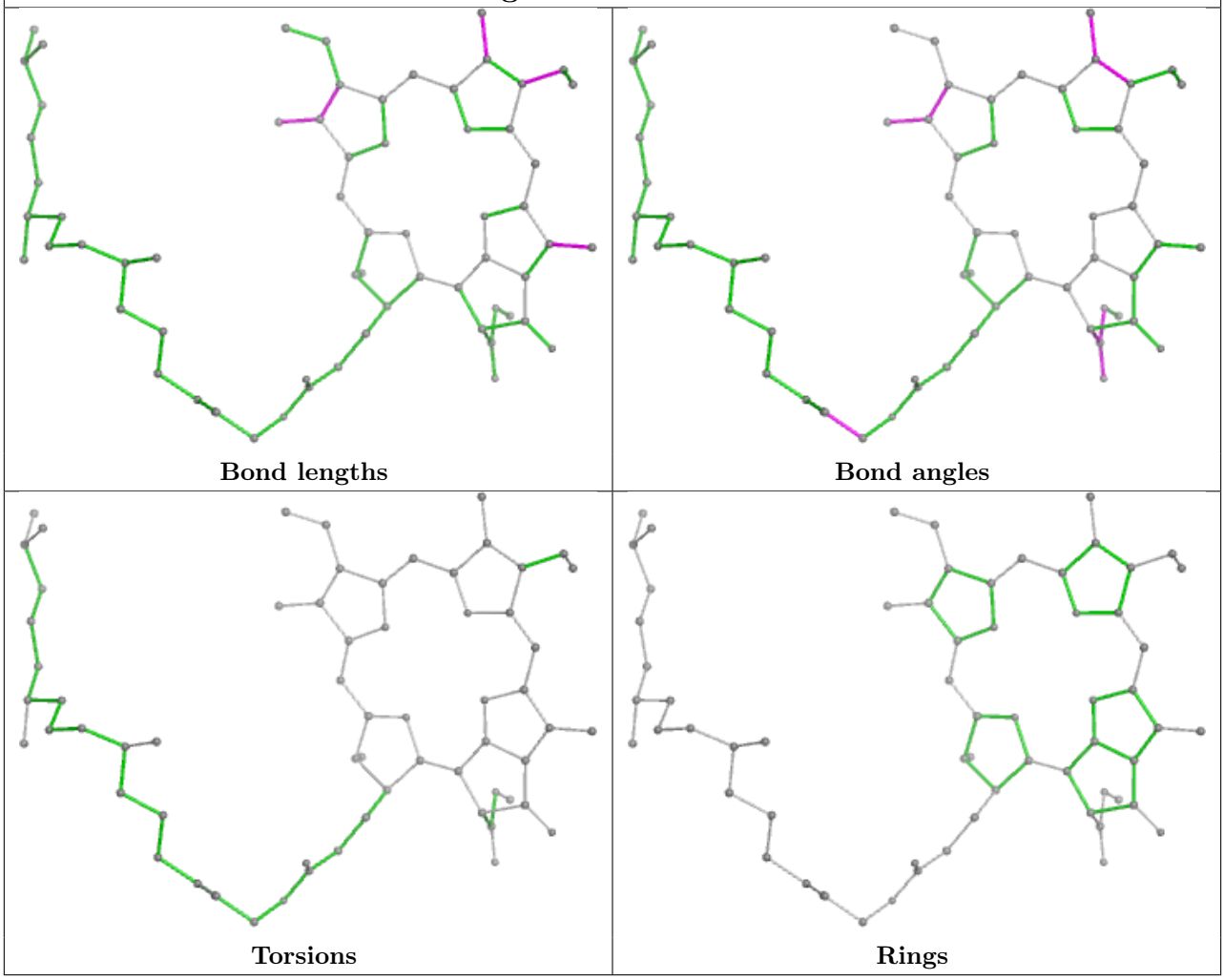


Torsions

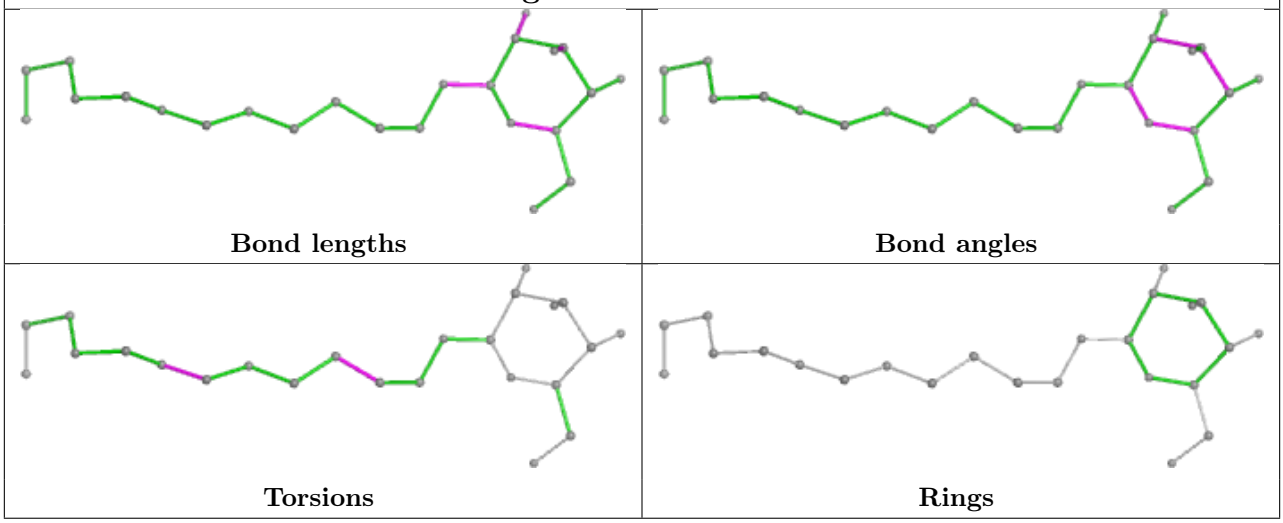


Rings

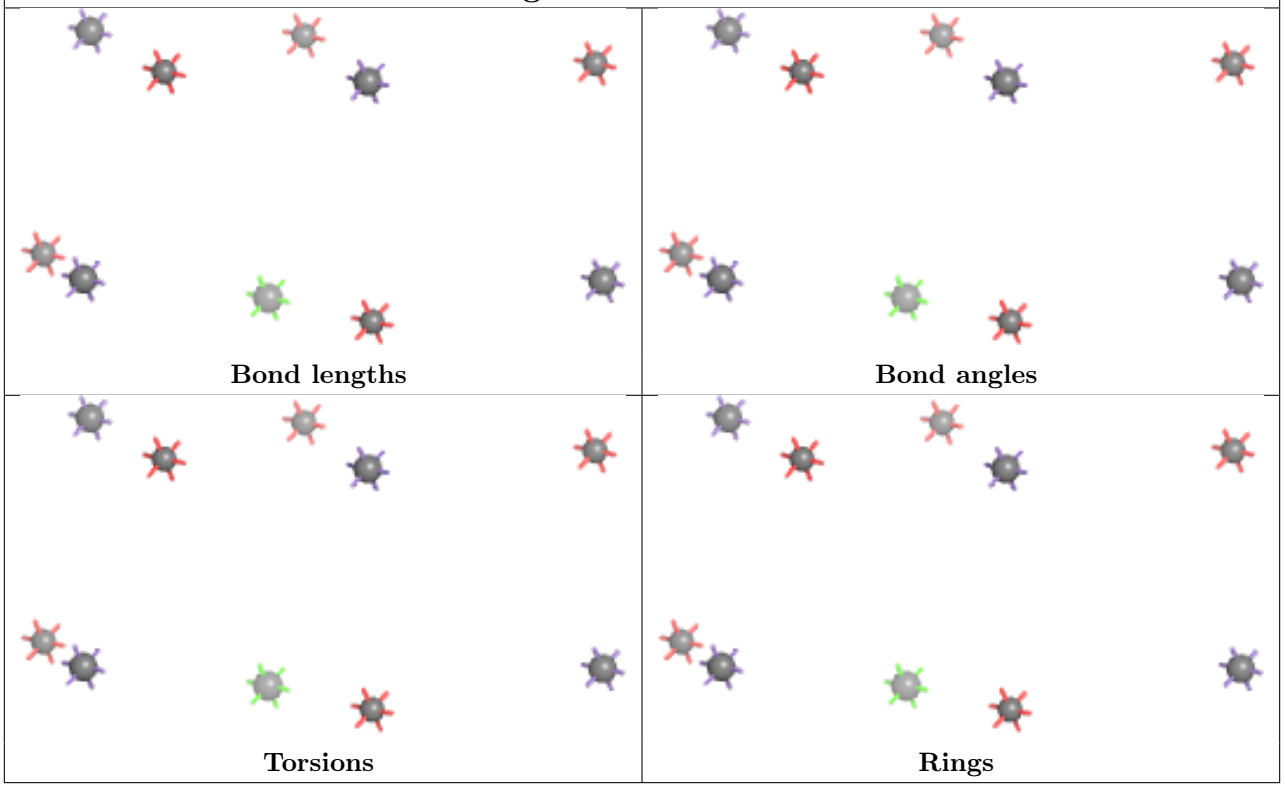
Ligand PHO d 401



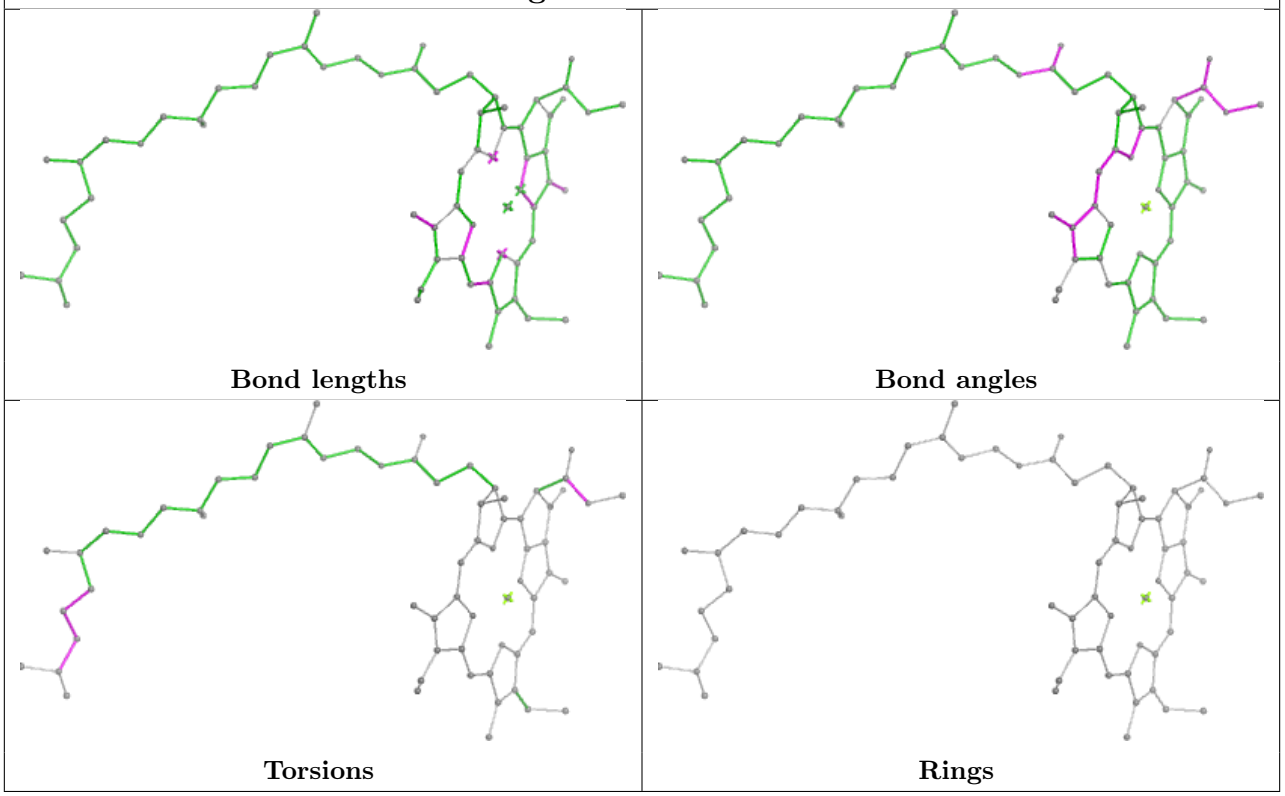
Ligand LMT C 523



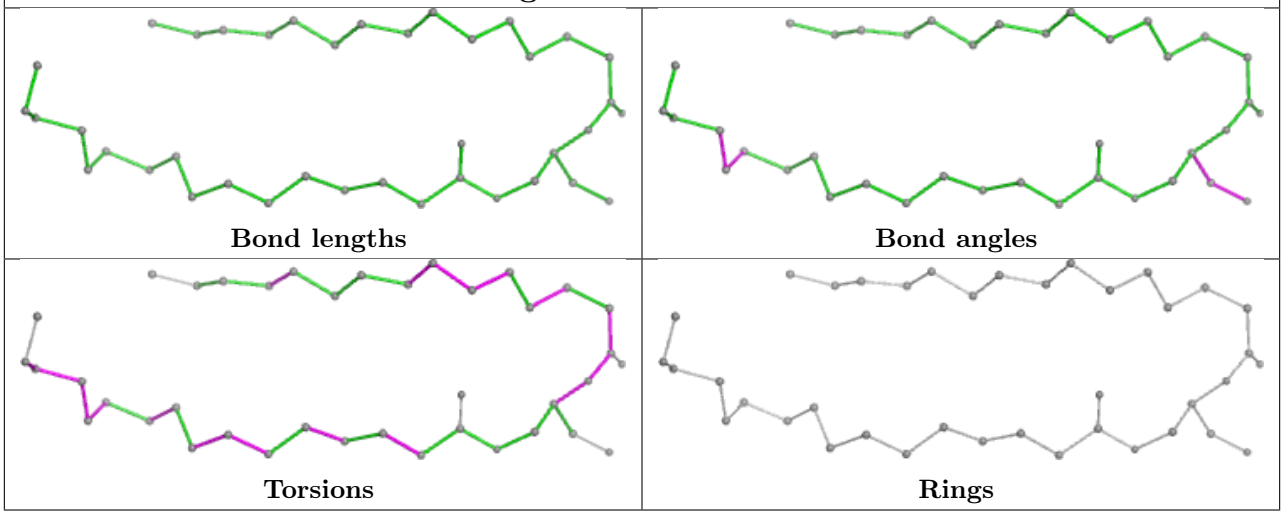
Ligand OEX A 417



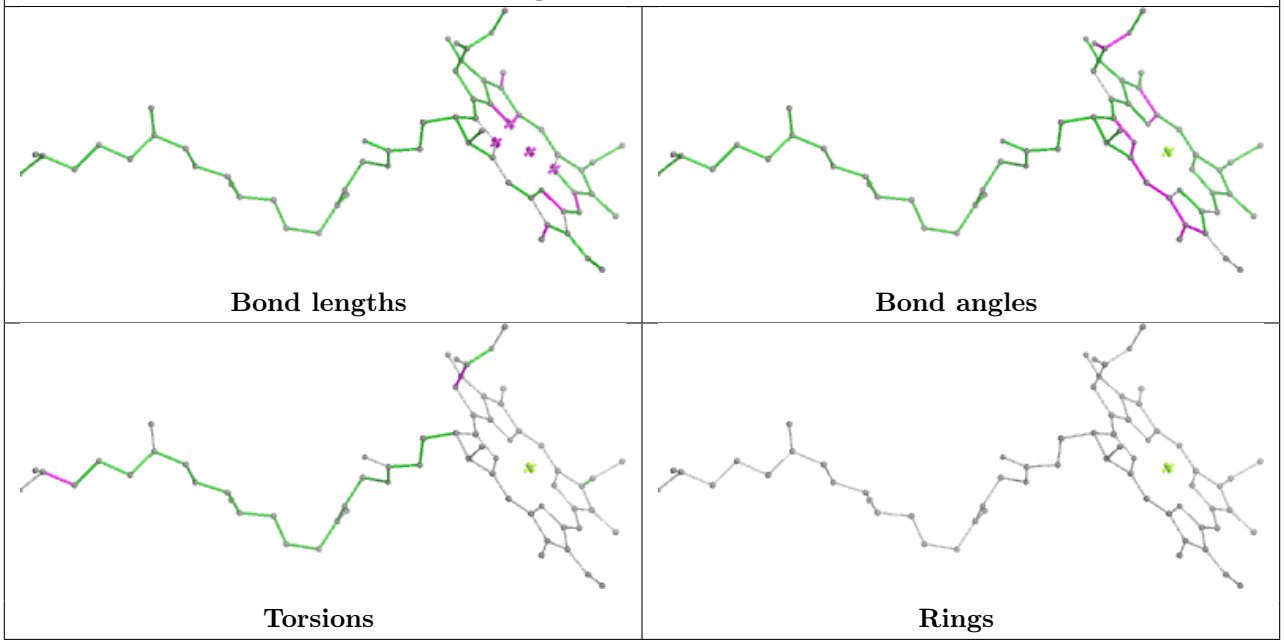
Ligand CLA b 610



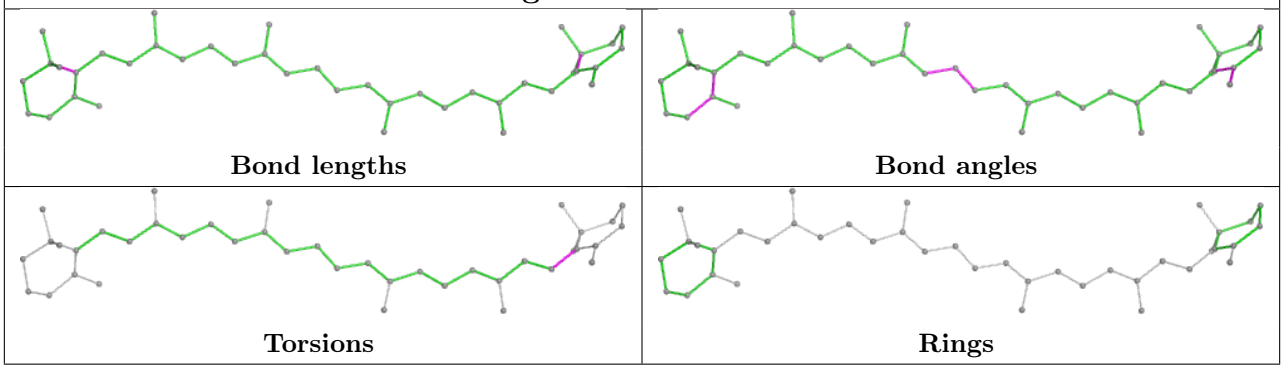
Ligand LMG H 101



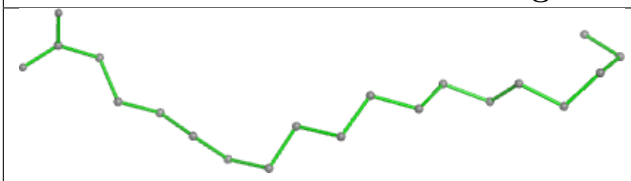
Ligand CLA c 502



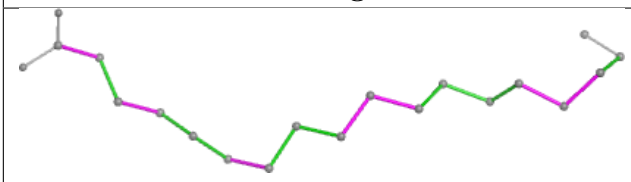
Ligand BCR K 103



Ligand STE e 103

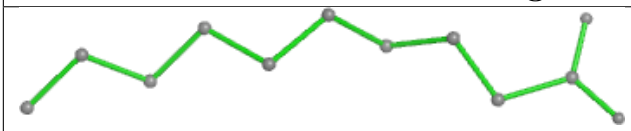

Bond lengths

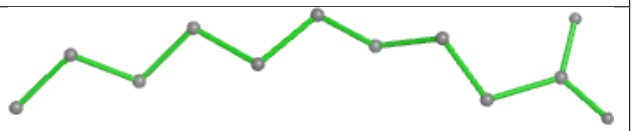

Bond angles

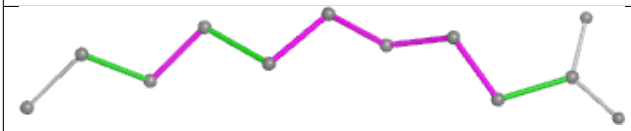

Torsions

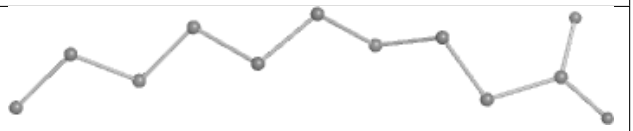

Rings

Ligand STE A 421

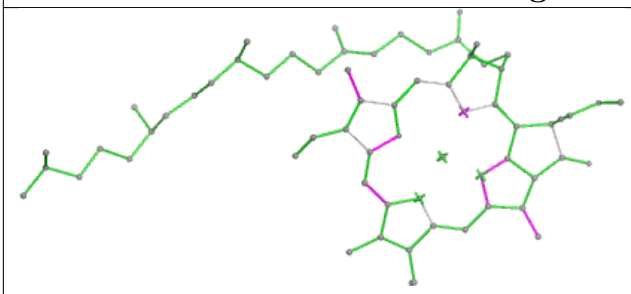

Bond lengths

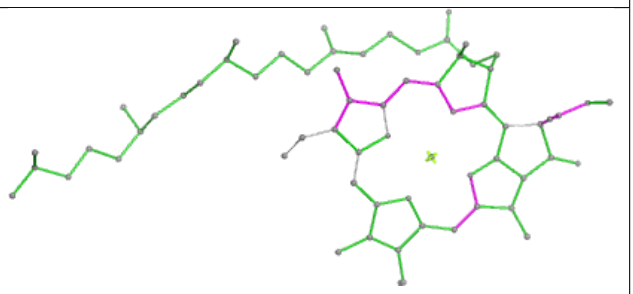

Bond angles

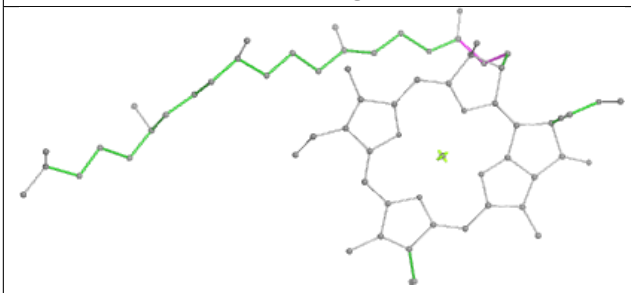

Torsions

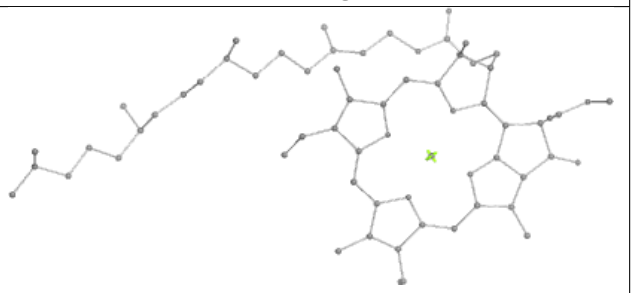

Rings

Ligand CLA c 501

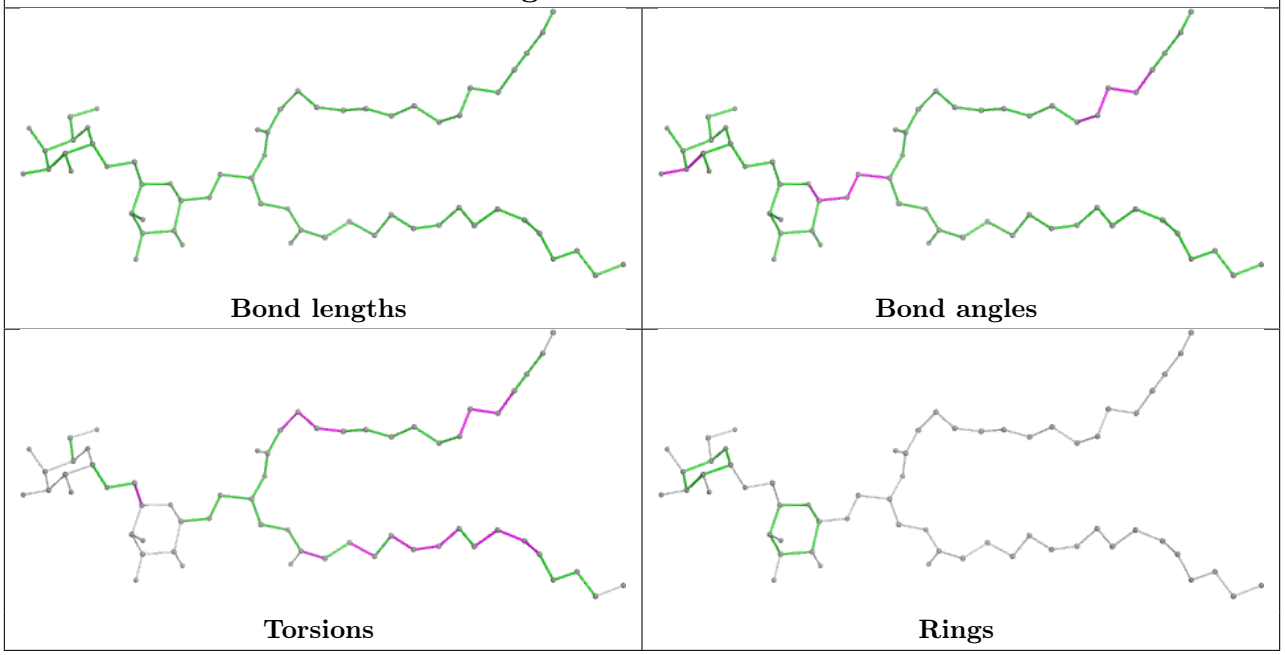

Bond lengths


Bond angles

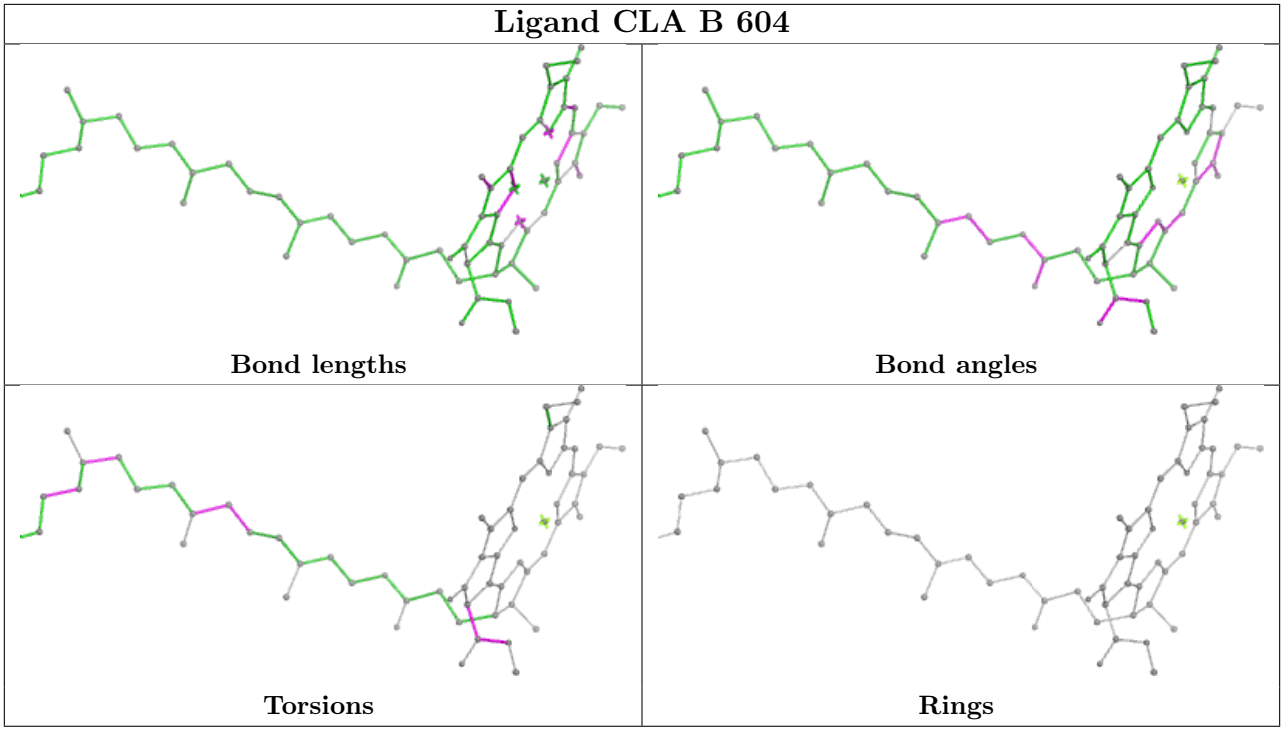

Torsions


Rings

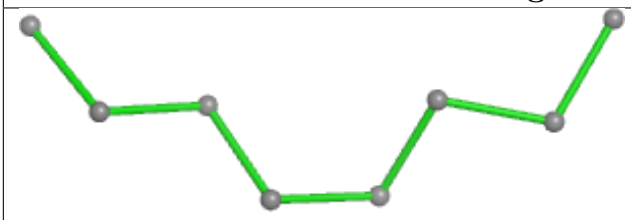
Ligand DGD C 519



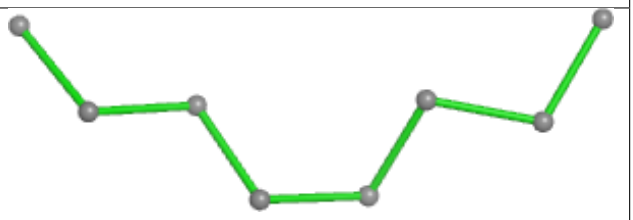
Ligand CLA B 604



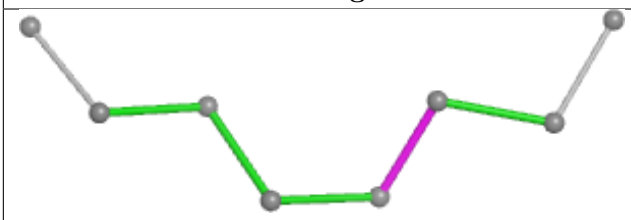
Ligand STE C 522



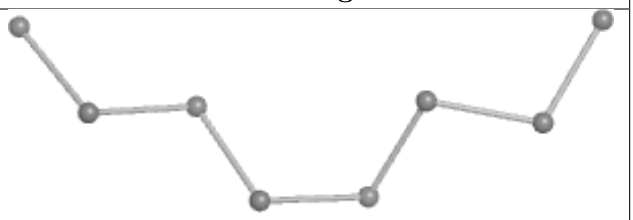
Bond lengths



Bond angles

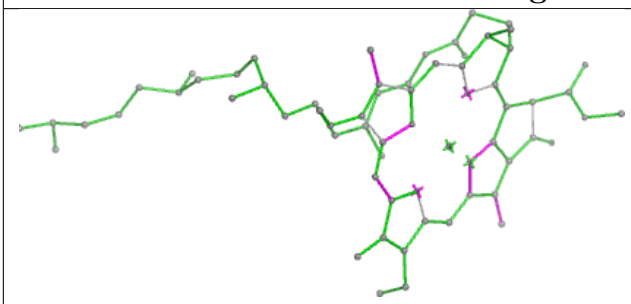


Torsions

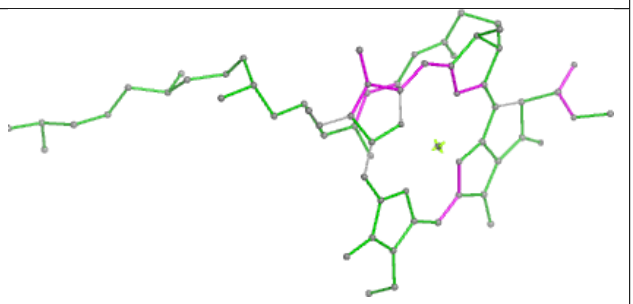


Rings

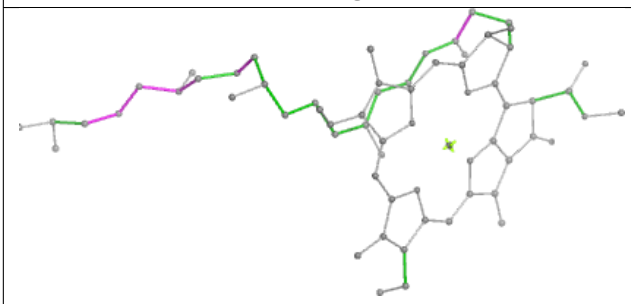
Ligand CLA c 505



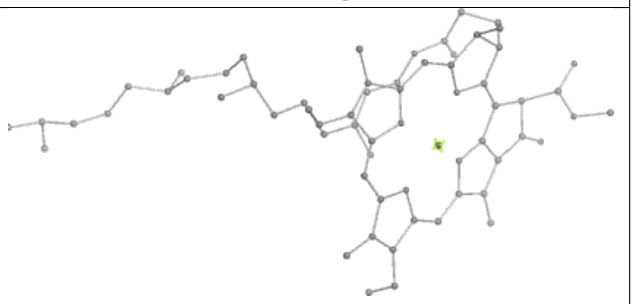
Bond lengths



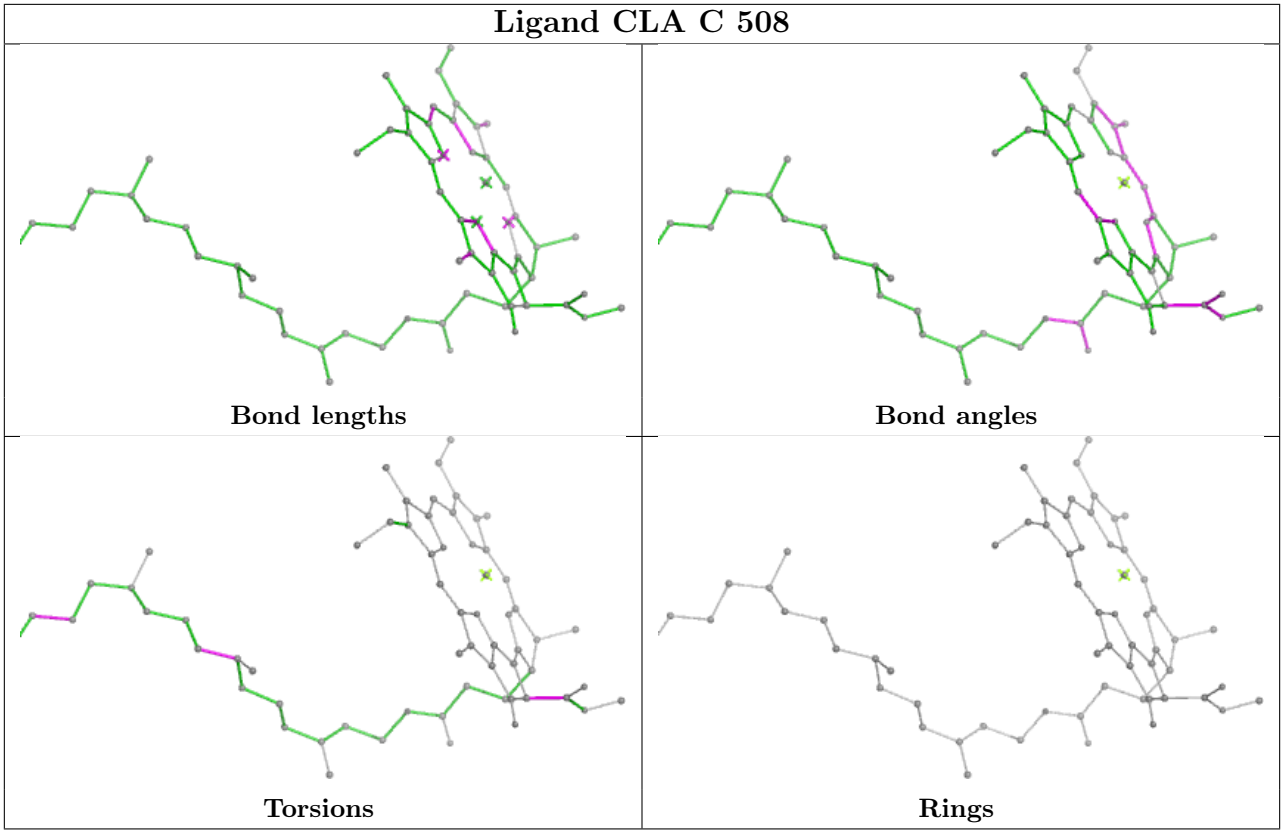
Bond angles



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.

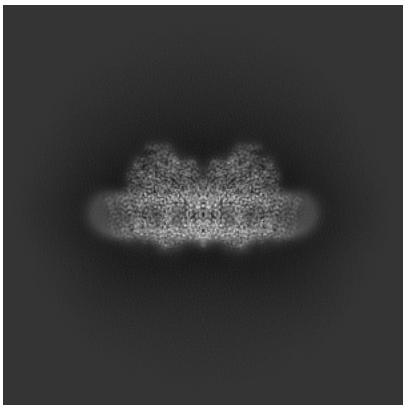
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50019. These allow visual inspection of the internal detail of the map and identification of artifacts.

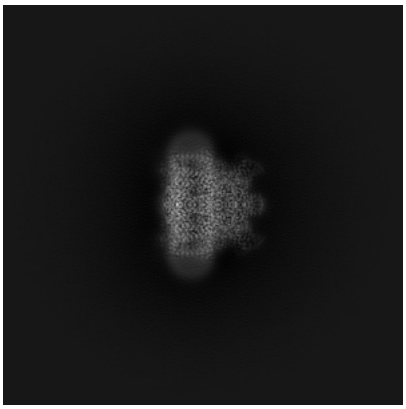
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

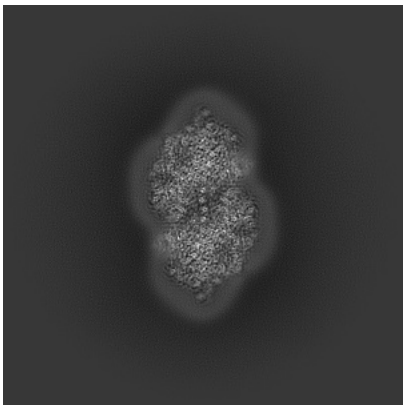
6.1.1 Primary map



X

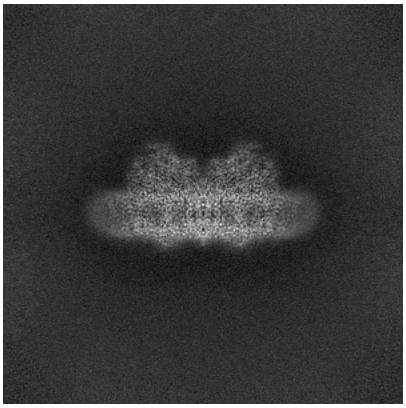


Y

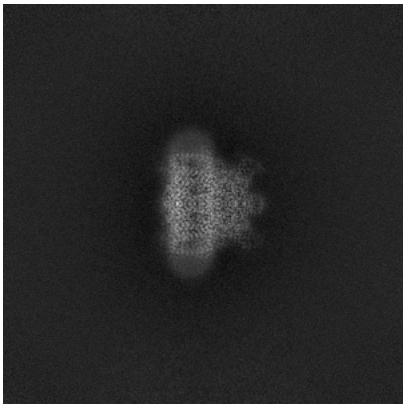


Z

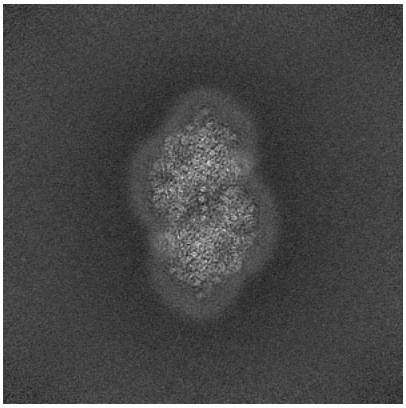
6.1.2 Raw map



X



Y

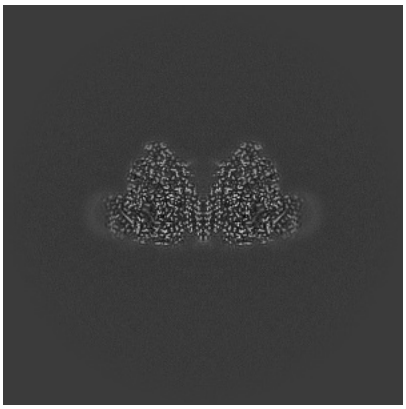


Z

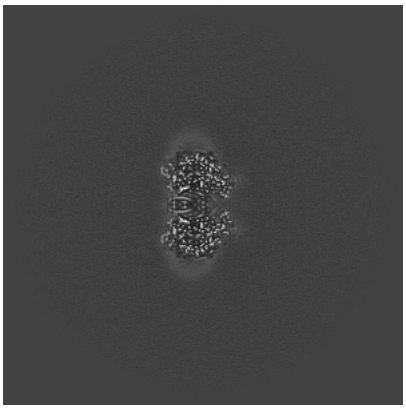
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

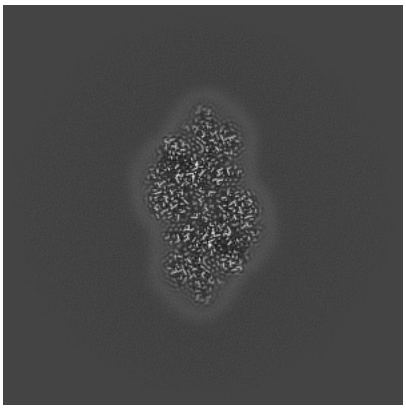
6.2.1 Primary map



X Index: 360

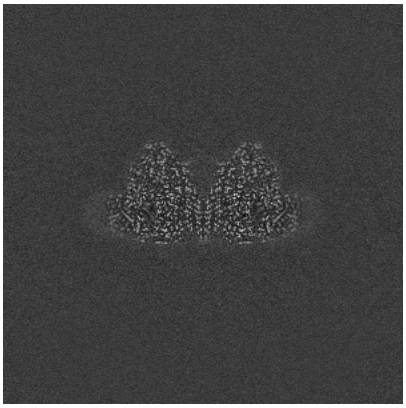


Y Index: 360

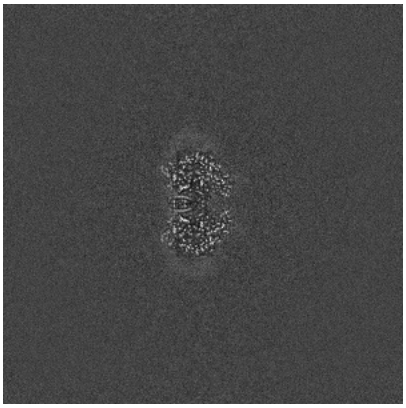


Z Index: 360

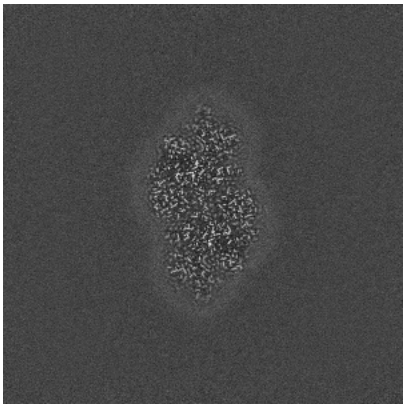
6.2.2 Raw map



X Index: 360



Y Index: 360

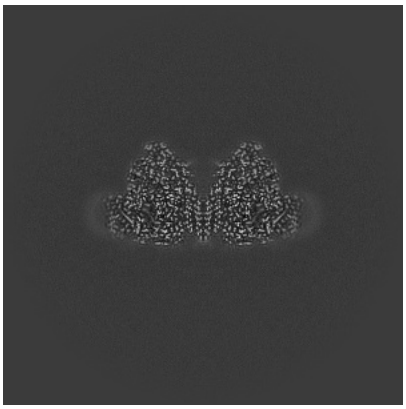


Z Index: 360

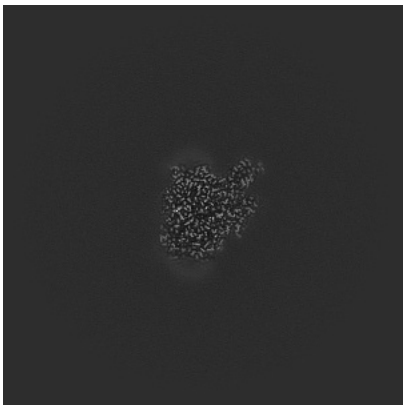
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

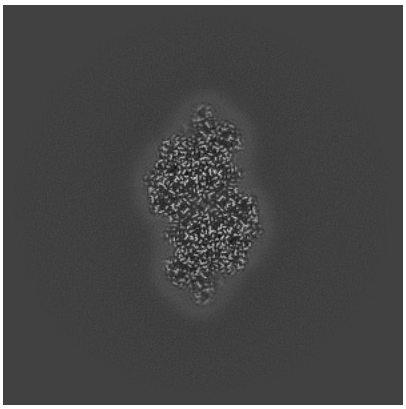
6.3.1 Primary map



X Index: 360

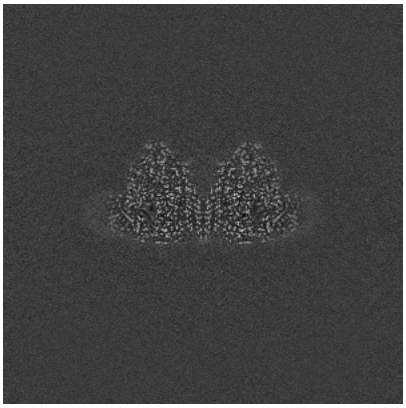


Y Index: 420

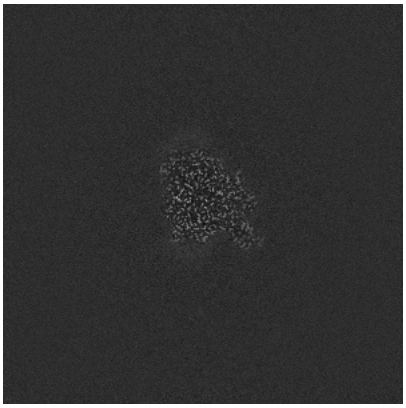


Z Index: 369

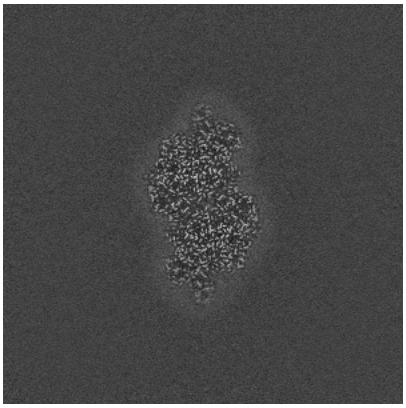
6.3.2 Raw map



X Index: 360



Y Index: 300

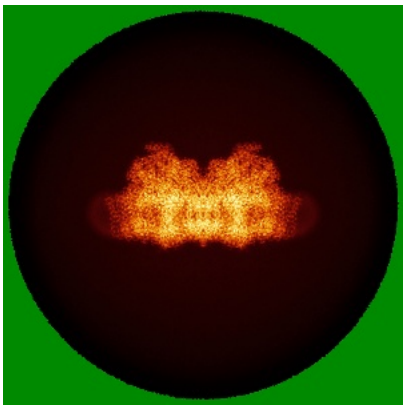


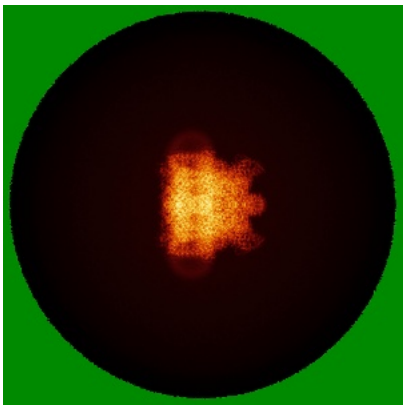
Z Index: 369

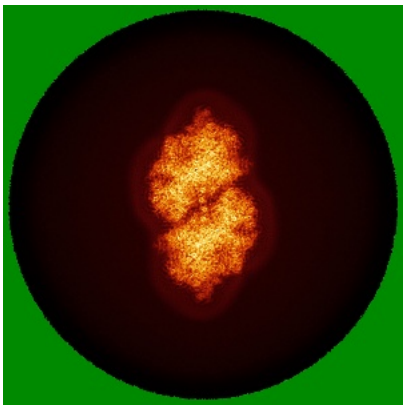
The images above show the largest variance slices of the map in three orthogonal directions.

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

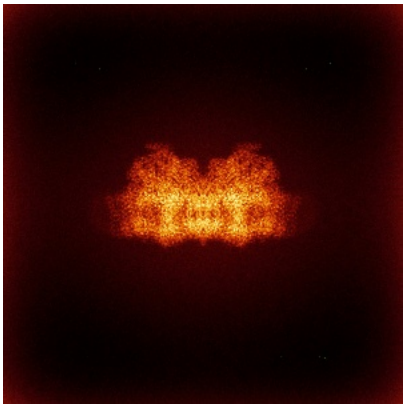
6.4.1 Primary map

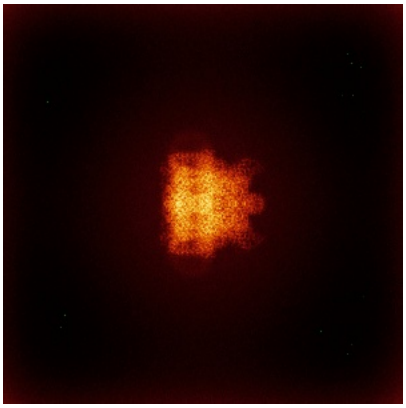

X

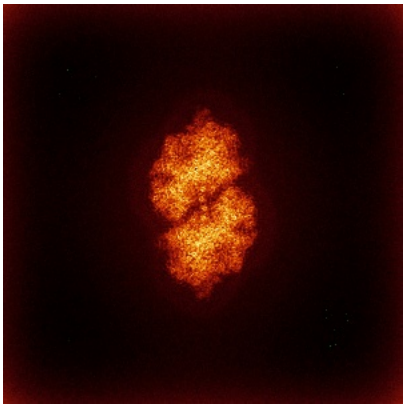

Y


Z

6.4.2 Raw map


X

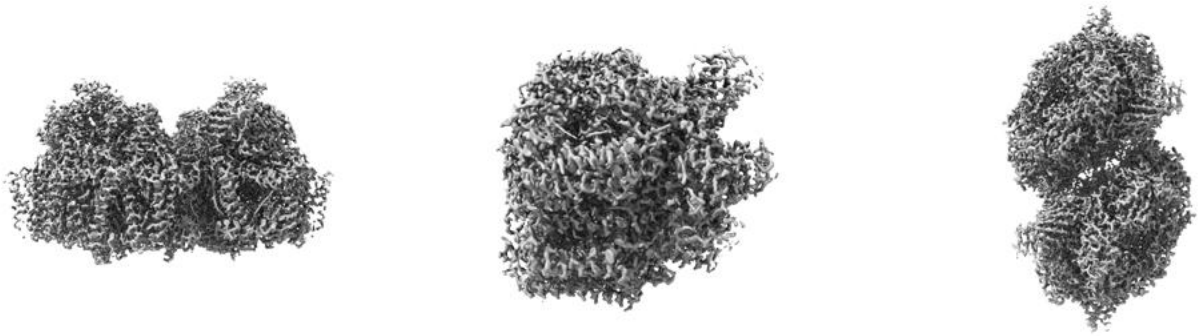

Y


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 0.45. 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.

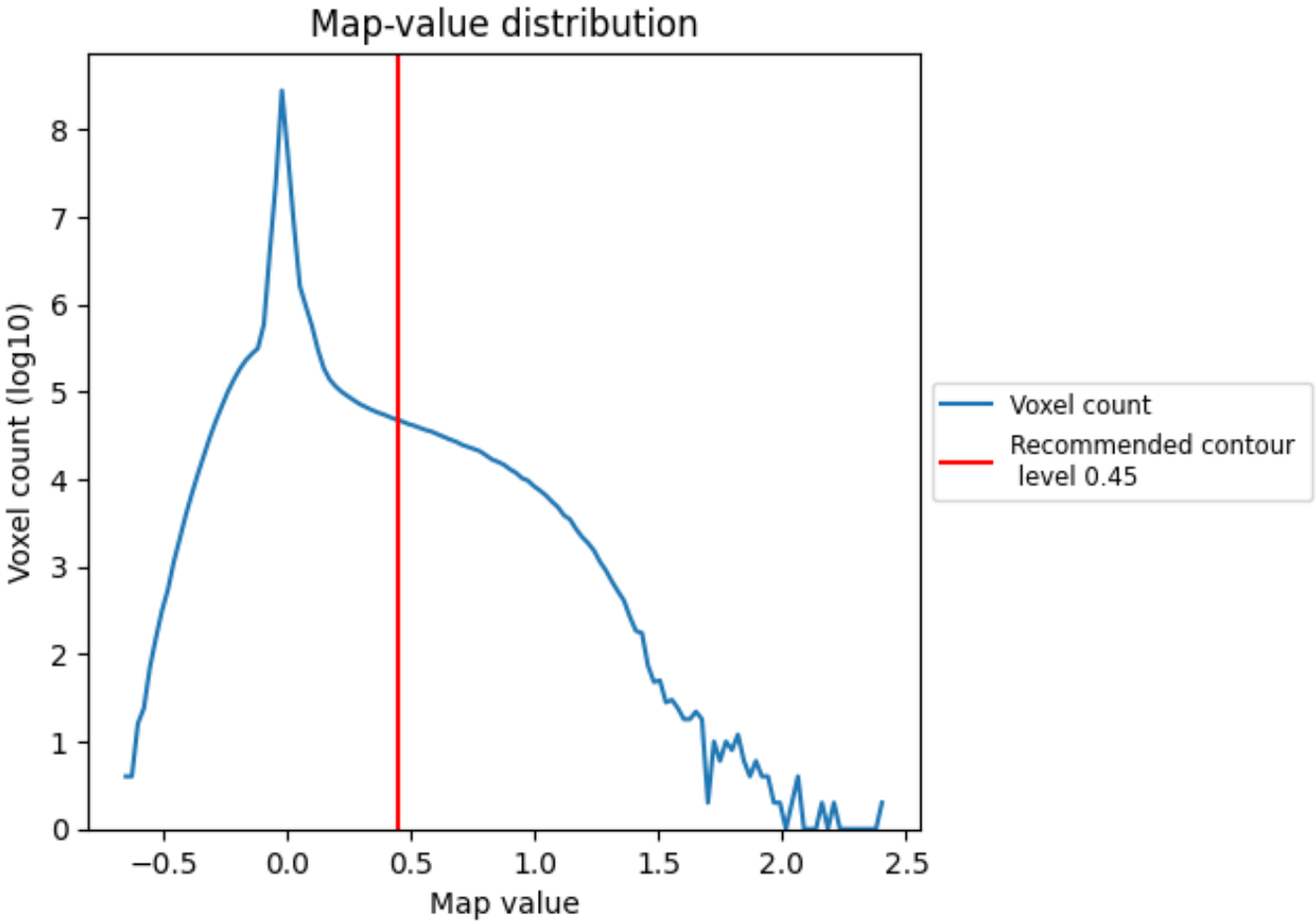
6.6 Mask visualisation (i)

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

7 Map analysis

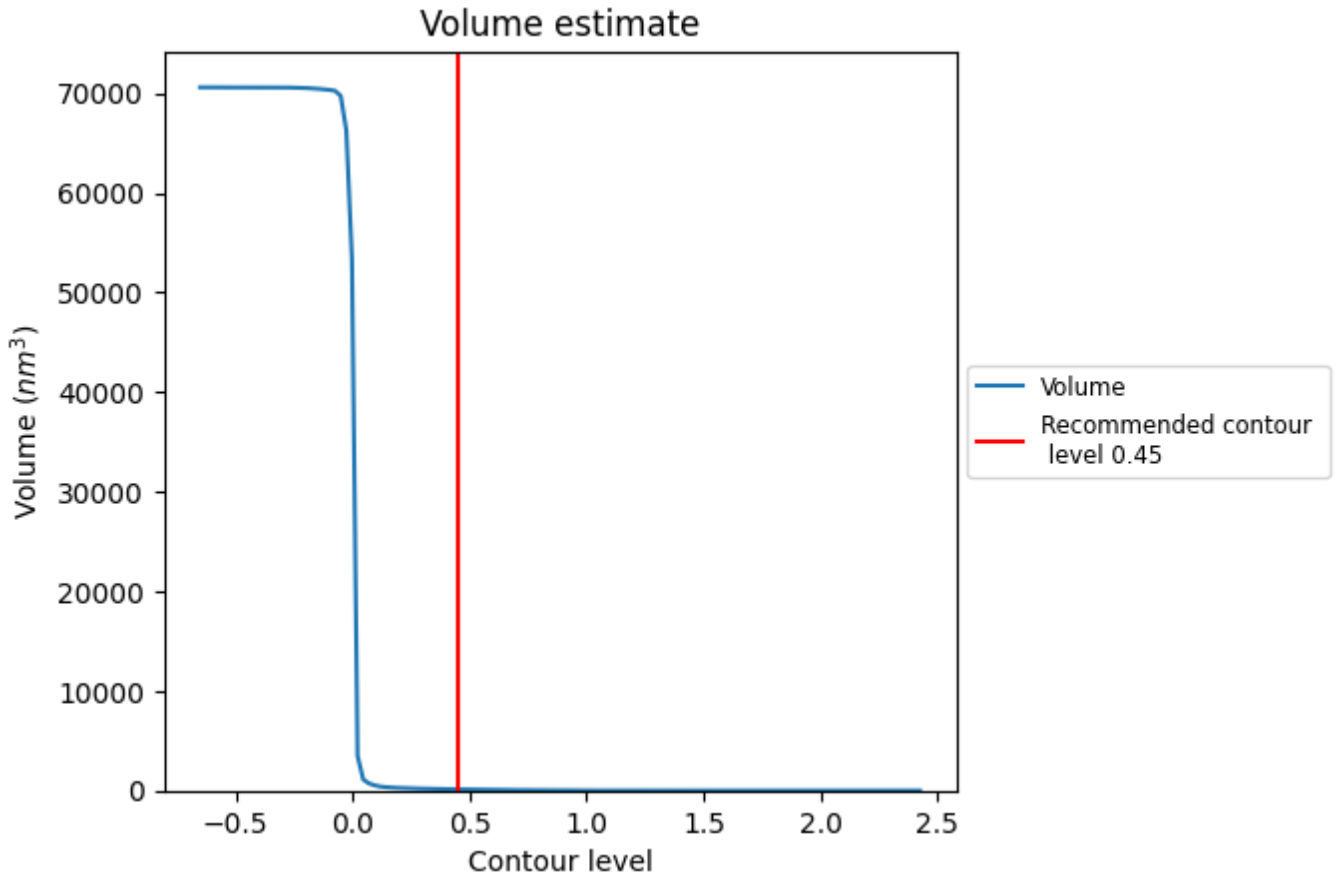
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

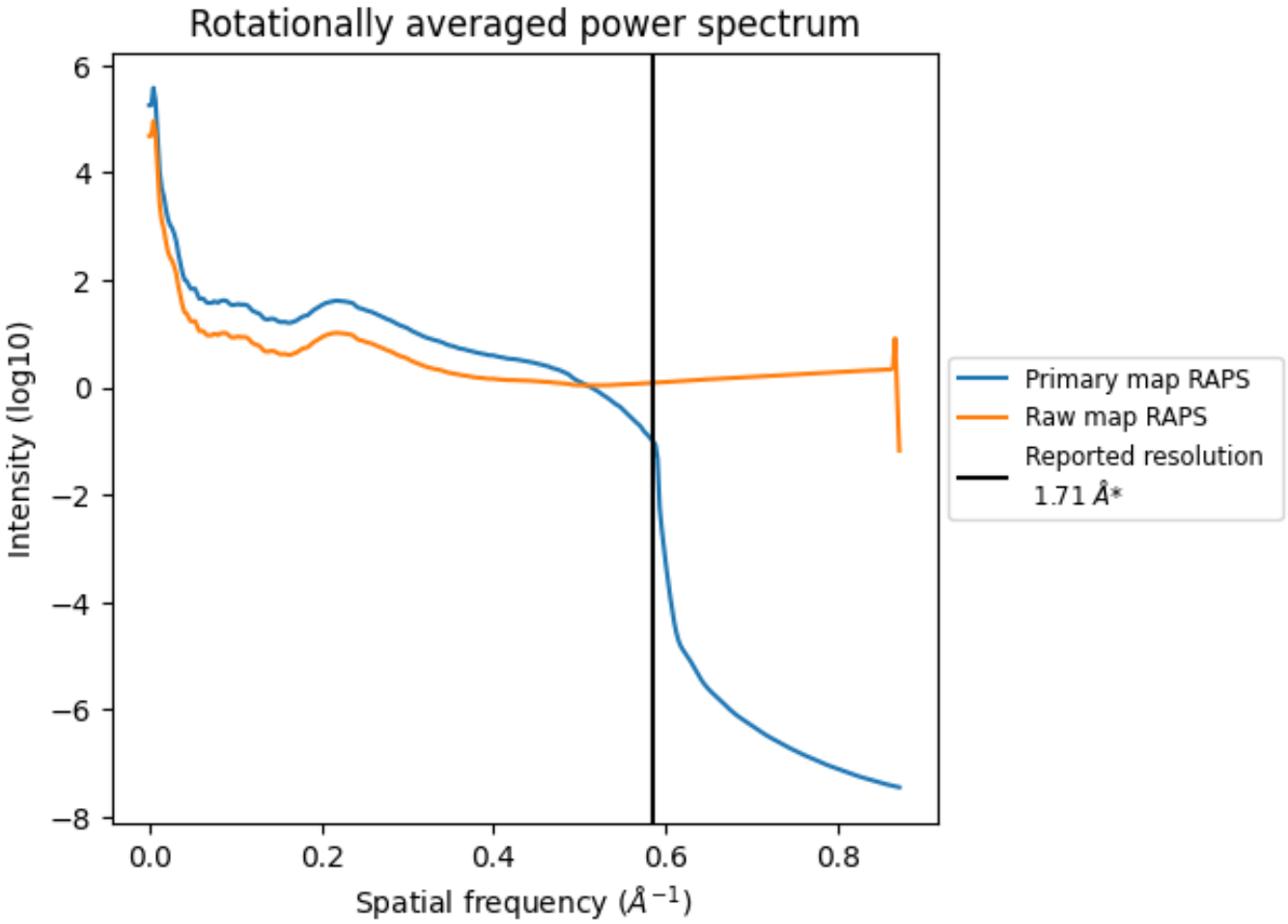
7.2 Volume estimate



The volume at the recommended contour level is 121 nm^3; this corresponds to an approximate mass of 109 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)

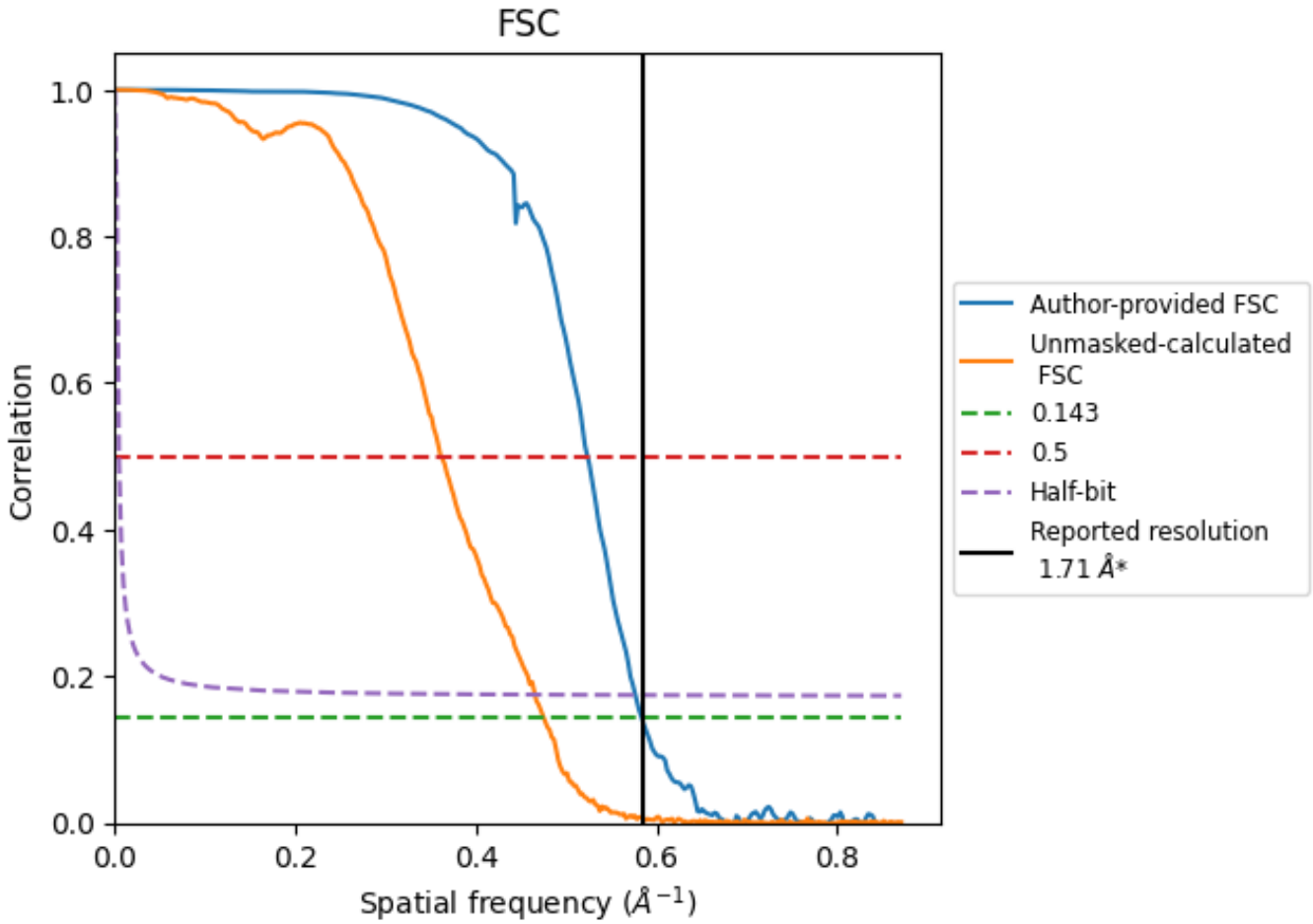


*Reported resolution corresponds to spatial frequency of 0.585 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.585 Å^{-1}

8.2 Resolution estimates (i)

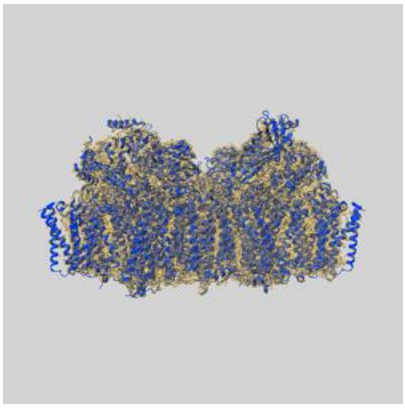
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.71	-	-
Author-provided FSC curve	1.71	1.91	1.73
Unmasked-calculated*	2.10	2.77	2.15

*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 2.10 differs from the reported value 1.71 by more than 10 %

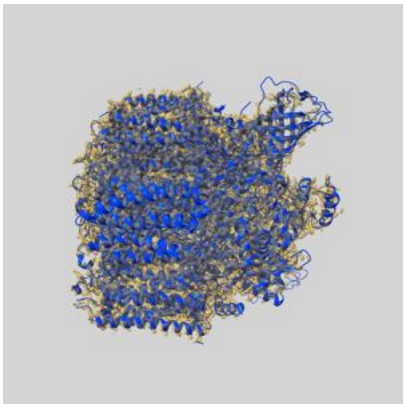
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50019 and PDB model 9EVX. Per-residue inclusion information can be found in section 3 on page 29.

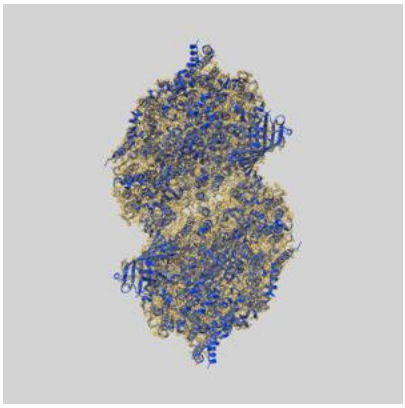
9.1 Map-model overlay



X



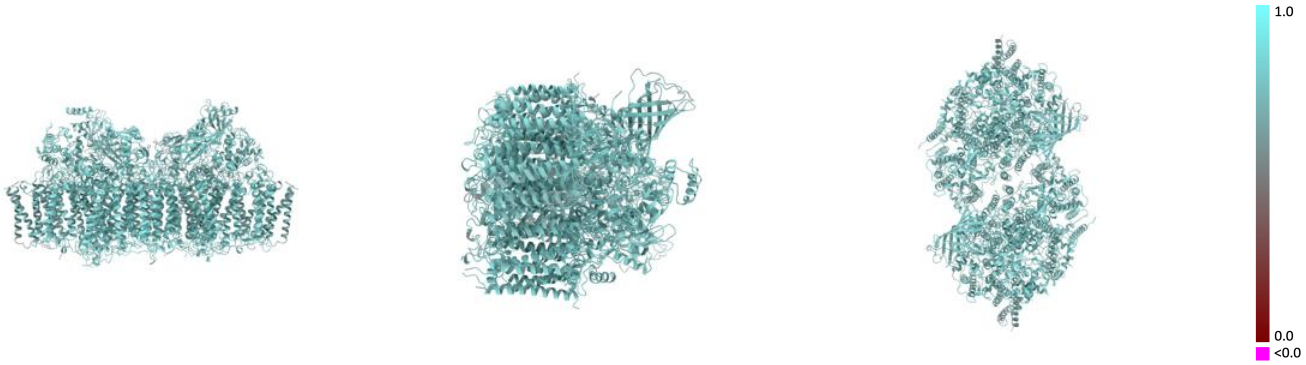
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 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.

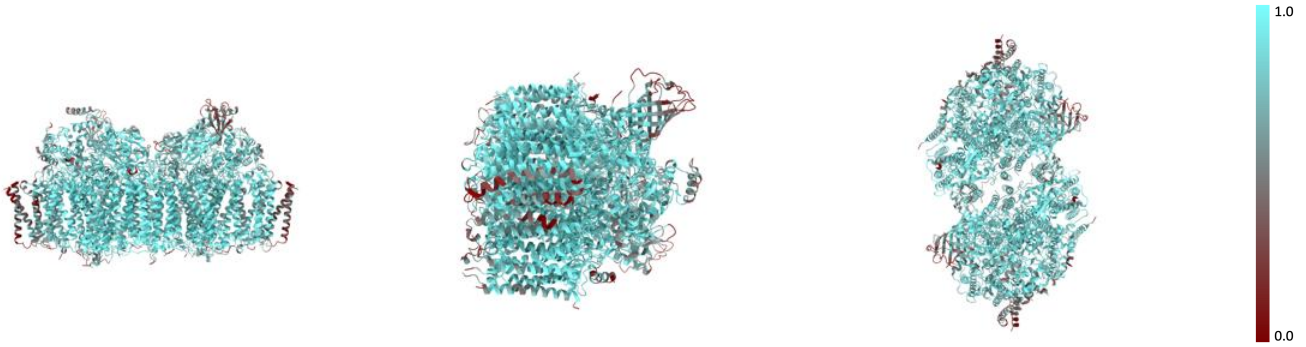
9.2 Q-score mapped to coordinate model (i)



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.

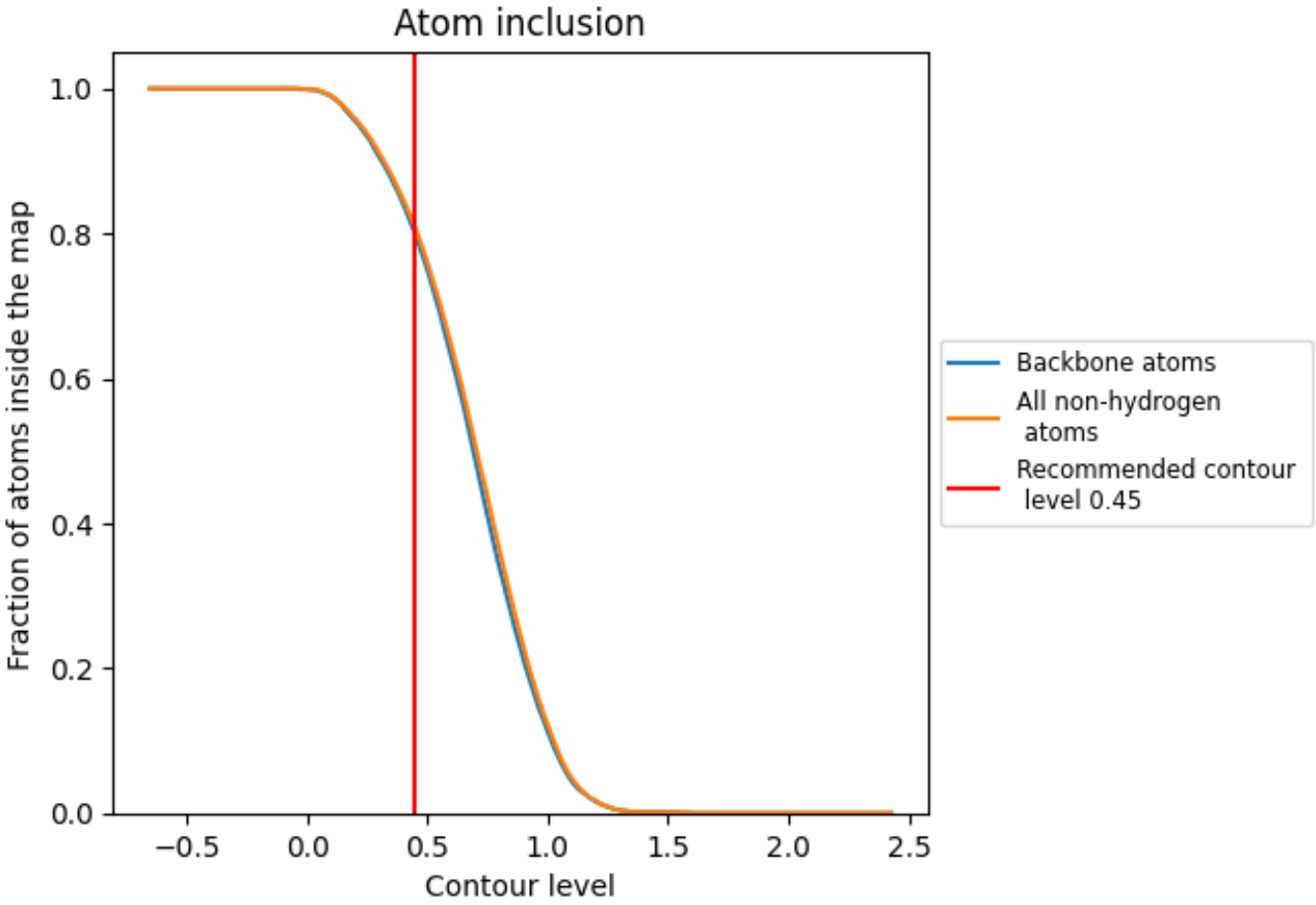
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.7490
A	0.8620	0.7700
B	0.8650	0.7580
C	0.8280	0.7430
D	0.9200	0.7740
E	0.6740	0.7180
F	0.8070	0.7480
H	0.7480	0.7330
I	0.7760	0.7400
J	0.6490	0.7220
K	0.7580	0.7240
L	0.8560	0.7730
M	0.8230	0.7650
O	0.6540	0.7220
T	0.8380	0.7700
U	0.7510	0.7380
V	0.7740	0.7400
X	0.6100	0.7120
Y	0.3950	0.6670
Z	0.3280	0.6400
a	0.8630	0.7680
b	0.8670	0.7610
c	0.8290	0.7420
d	0.9230	0.7760
e	0.6780	0.7250
f	0.8550	0.7490
h	0.7570	0.7350
i	0.7830	0.7380
j	0.6700	0.7280
k	0.7470	0.7310
l	0.8730	0.7740
m	0.8230	0.7690
o	0.6590	0.7240
t	0.8230	0.7690
u	0.7500	0.7460

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
v	0.7880	0.7410
x	0.6160	0.7190
y	0.4200	0.6760
z	0.3520	0.6440