Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 12:18 PM JST

PDB ID	:	9IIU / pdb_00009iiu
EMDB ID	:	EMD-60605
Title	:	Cryo-EM structure of an TEF30-associated intermediate PSII core complex from Chlamydomonas reinhardtii
Authors	:	Wang, Y.; Wang, C.; Li, A.; Liu, Z.
Deposited on	:	2024-06-21
Resolution	:	2.98 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:

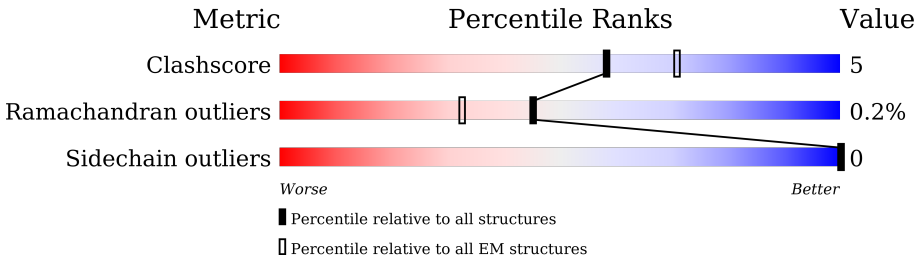
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.98 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	326	82% 10% 8%
2	B	480	91% 9%
3	C	450	85% 12%
4	D	349	83% 13%
5	E	75	92% 8%
6	F	31	6% 90% 10%
7	G	258	24% 91% 9%
8	H	70	90% 9%

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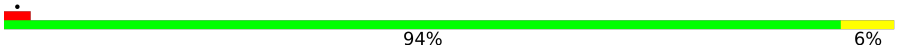
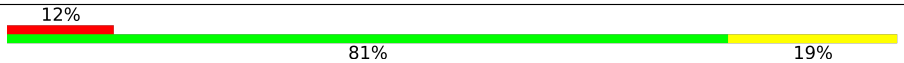
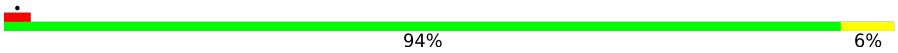
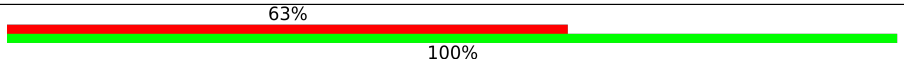
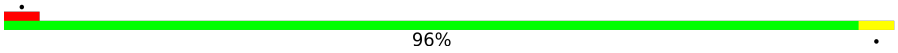
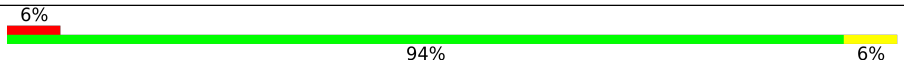
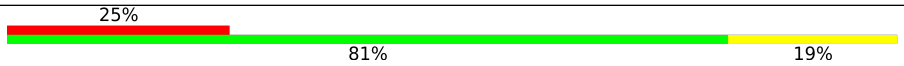
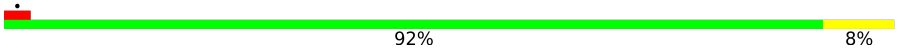
Mol	Chain	Length	Quality of chain
9	I	34	
10	J	32	
11	K	37	
12	L	35	
13	M	27	
14	T	24	
15	V	32	
16	X	32	
17	Z	61	

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
19	CLA	A	402	X	-	-	-
19	CLA	A	403	X	-	-	-
19	CLA	B	501	X	-	-	-
19	CLA	B	502	X	-	-	-
19	CLA	B	503	X	-	-	-
19	CLA	B	504	X	-	-	-
19	CLA	B	505	X	-	-	-
19	CLA	B	506	X	-	-	-
19	CLA	B	507	X	-	-	-
19	CLA	B	508	X	-	-	-
19	CLA	B	509	X	-	-	-
19	CLA	B	510	X	-	-	-
19	CLA	B	511	X	-	-	-
19	CLA	B	512	X	-	-	-
19	CLA	B	513	X	-	-	-
19	CLA	B	514	X	-	-	-
19	CLA	B	515	X	-	-	-
19	CLA	B	516	X	-	-	-
19	CLA	C	501	X	-	-	-
19	CLA	C	502	X	-	-	-
19	CLA	C	503	X	-	-	-
19	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	C	505	X	-	-	-
19	CLA	C	506	X	-	-	-
19	CLA	C	507	X	-	-	-
19	CLA	C	508	X	-	-	-
19	CLA	C	509	X	-	-	-
19	CLA	C	510	X	-	-	-
19	CLA	C	511	X	-	-	-
19	CLA	C	512	X	-	-	-
19	CLA	C	513	X	-	-	-
19	CLA	D	401	X	-	-	-
19	CLA	D	405	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 21452 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	301	2355	1547	389	404	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	480	3755	2462	630	651	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	438	3431	2249	571	594	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	335	2671	1767	437	455	12	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	75	610	399	101	110	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	31	251	171	42	37	1	0	0

- Molecule 7 is a protein called PDZ domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	258	Total	C	N	O	S	0	0
			1806	1116	334	349	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	69	Total	C	N	O	S	0	0
			532	356	79	95	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			275	189	41	43	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	32	Total	C	N	O	0	0
			232	160	33	39		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	209	43	45		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	35	Total	C	N	O	0	0
			290	196	45	49		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	27	Total	C	N	O	0	0
			210	146	29	35		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	24	Total	C	N	O	S	0	0
			198	140	27	30	1		

- Molecule 15 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	V	32	Total	C	N	O	0	0
			224	147	37	40		

- Molecule 16 is a protein called Chloroplast photosystem II subunit X.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	X	32	Total	C	N	O	0	0
			214	140	35	39		

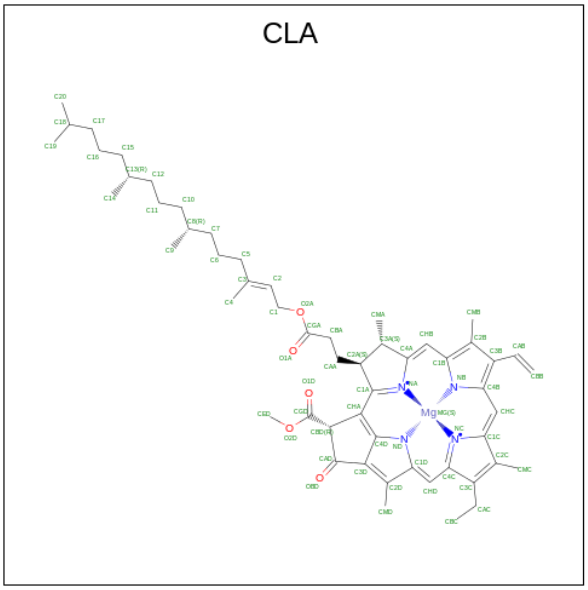
- Molecule 17 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

- Molecule 18 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C Mg N O 65 55 1 4 5	0
19	A	1	Total C Mg N O 49 39 1 4 5	0
19	A	1	Total C Mg N O 60 50 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0

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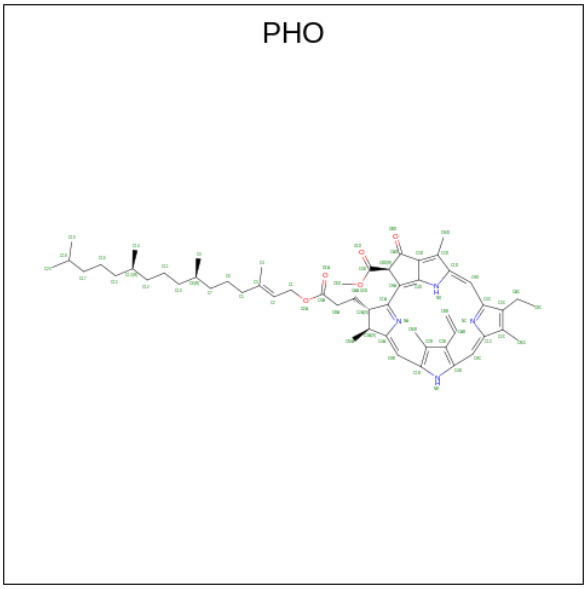
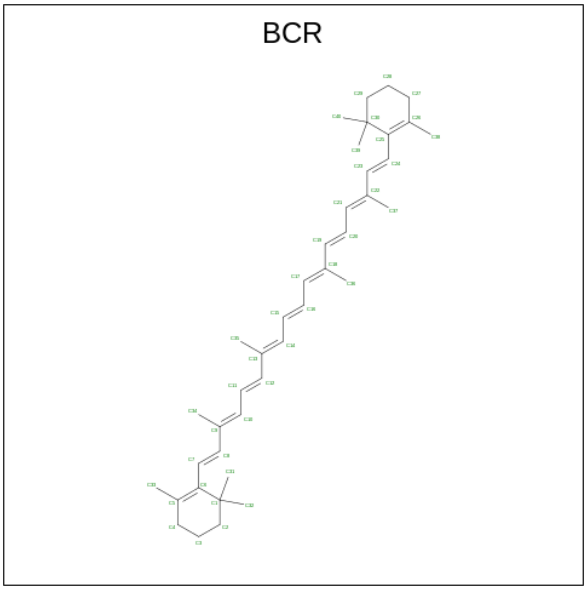
Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 45 35 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	D	1	Total C Mg N O 65 55 1 4 5	0
19	D	1	Total C Mg N O 65 55 1 4 5	0
19	D	1	Total C Mg N O 65 55 1 4 5	0

- Molecule 20 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



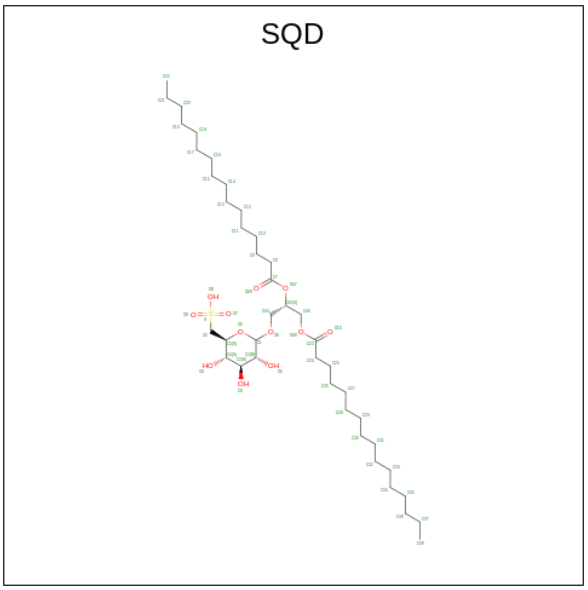
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	N	O	0
			64	55	4	5	
20	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



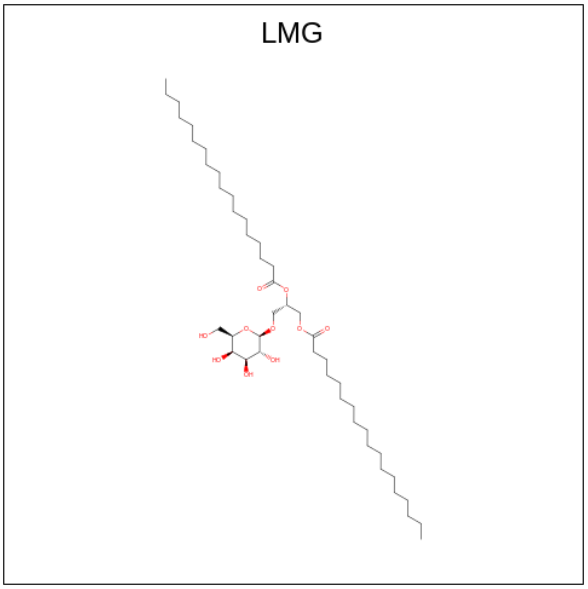
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	D	1	Total C 40 40	0
21	H	1	Total C 40 40	0
21	K	1	Total C 40 40	0

- Molecule 22 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



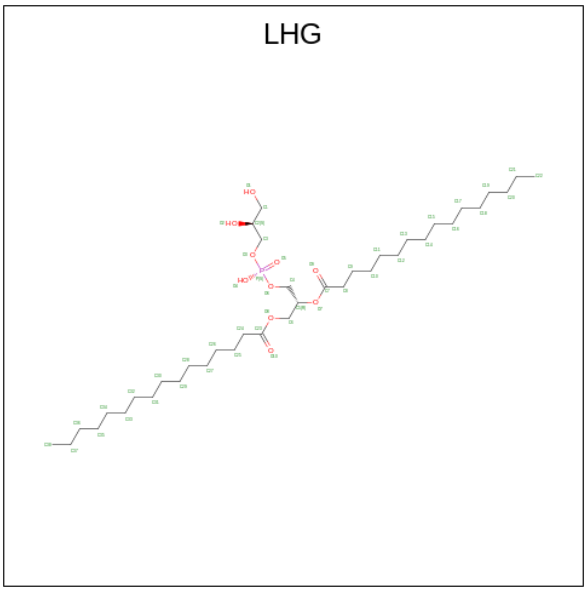
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C O S 51 38 12 1	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



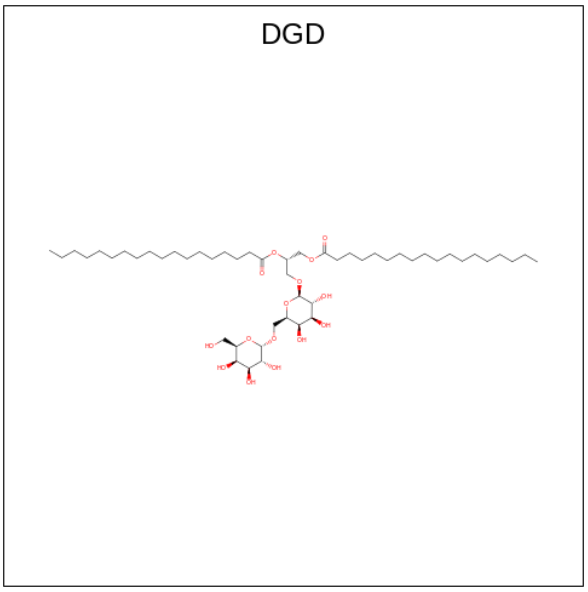
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C O 46 36 10	0
23	B	1	Total C O 42 32 10	0
23	B	1	Total C O 48 38 10	0
23	C	1	Total C O 51 41 10	0
23	D	1	Total C O 46 36 10	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



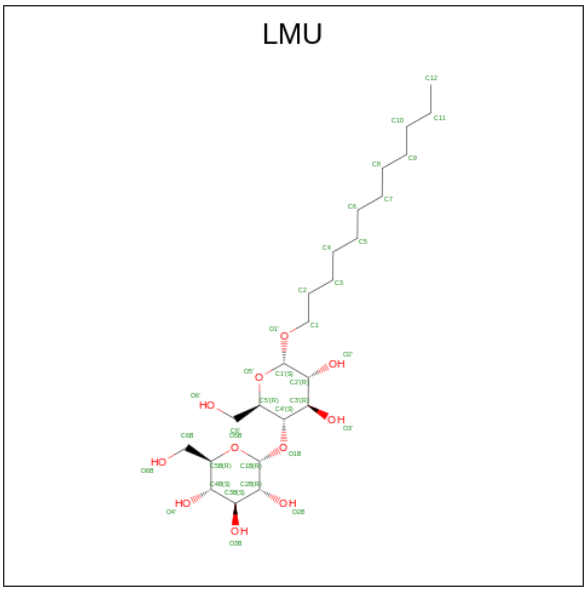
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			43	32	10	1	
24	B	1	Total	C	O	P	0
			44	33	10	1	
24	D	1	Total	C	O	P	0
			49	38	10	1	
24	D	1	Total	C	O	P	0
			49	38	10	1	
24	D	1	Total	C	O	P	0
			49	38	10	1	
24	L	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



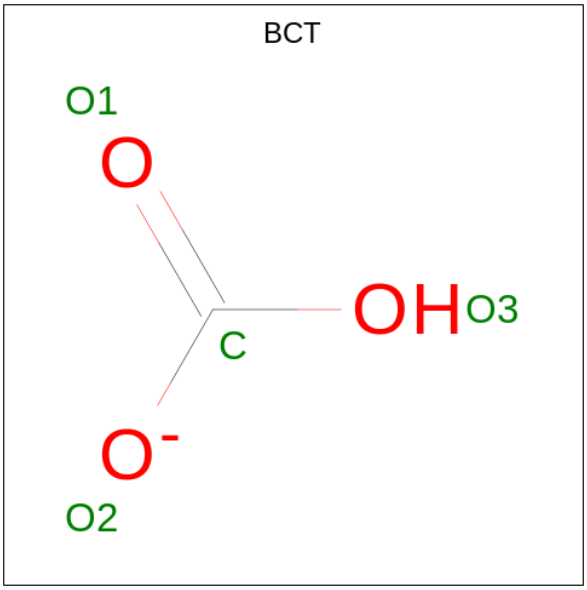
Mol	Chain	Residues	Atoms			AltConf
25	C	1	Total 53	C 38	O 15	0
25	C	1	Total 62	C 47	O 15	0
25	J	1	Total 59	C 44	O 15	0

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



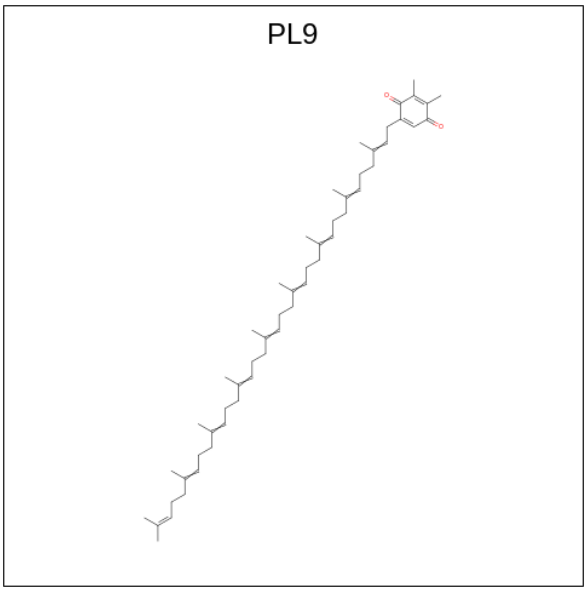
Mol	Chain	Residues	Atoms			AltConf
26	C	1	Total	C	O	0
			35	24	11	

- Molecule 27 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



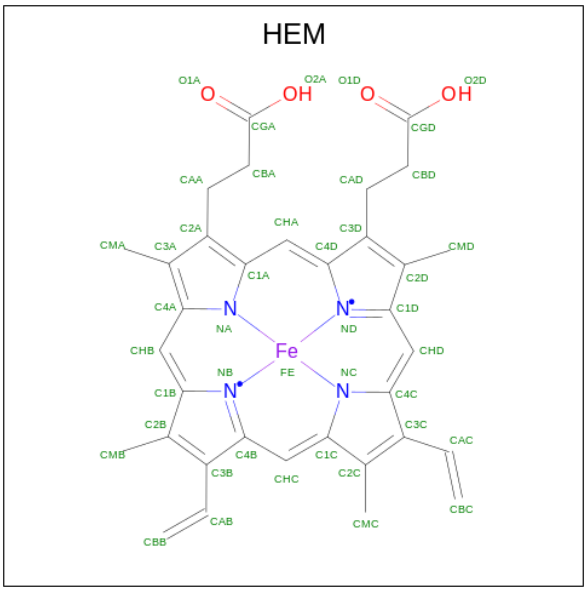
Mol	Chain	Residues	Atoms			AltConf
27	D	1	Total	C	O	0
			4	1	3	

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

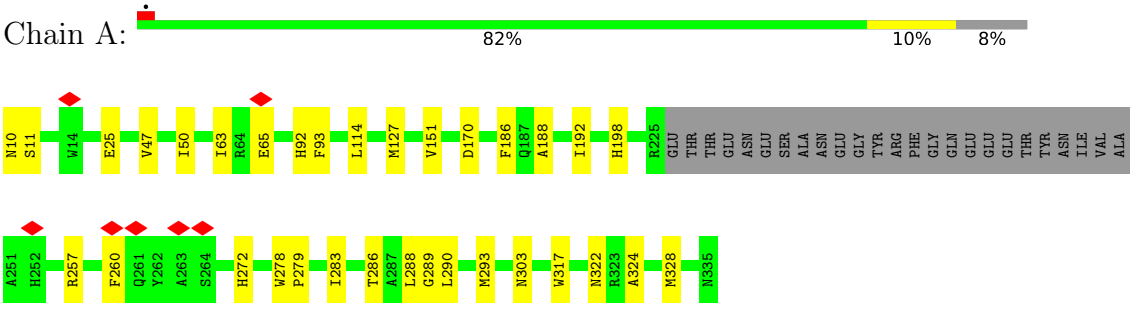
- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	A	2	Total	O	0
			2	2	

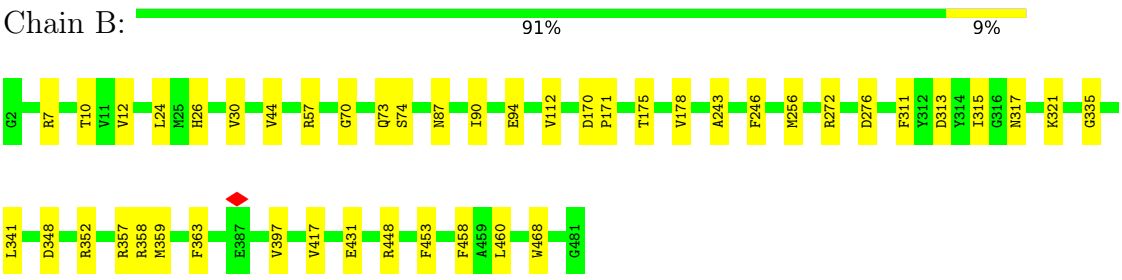
3 Residue-property plots (i)

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.

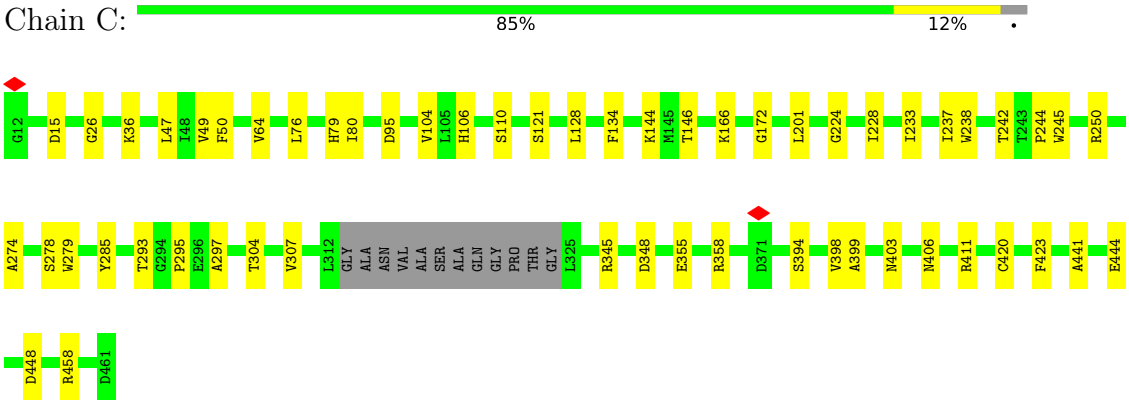
• Molecule 1: Photosystem II protein D1



• Molecule 2: Photosystem II CP47 reaction center protein

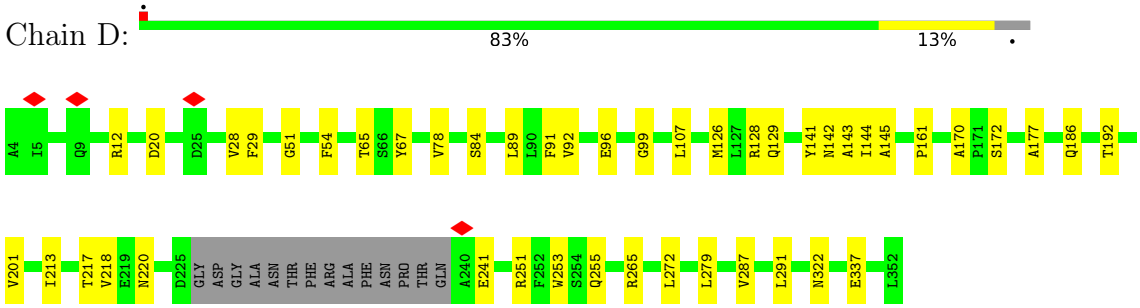


• Molecule 3: Photosystem II CP43 reaction center protein



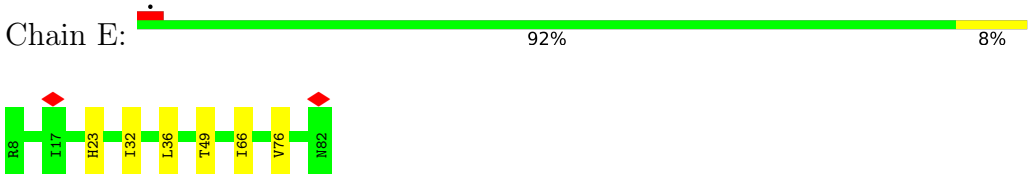
• Molecule 4: Photosystem II D2 protein

Chain D:



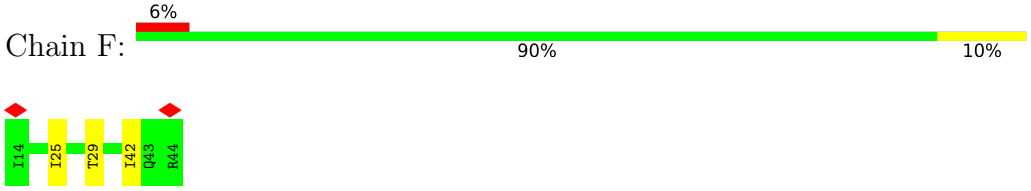
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



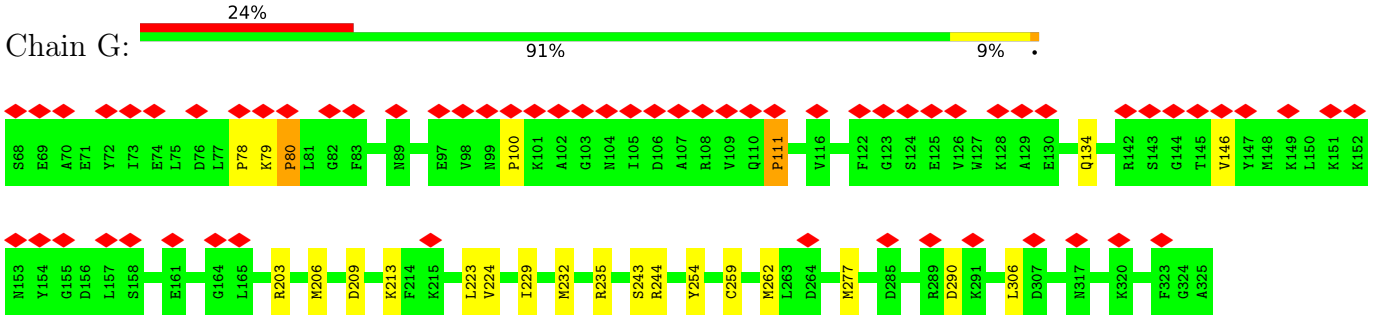
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



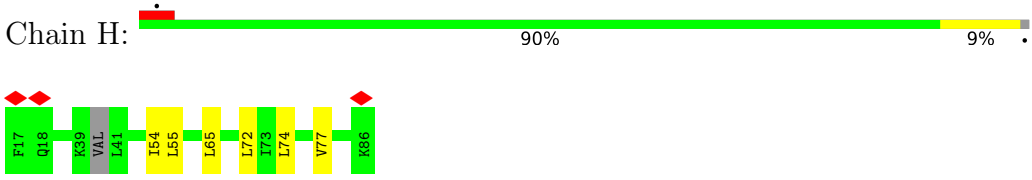
• Molecule 7: PDZ domain-containing protein

Chain G:



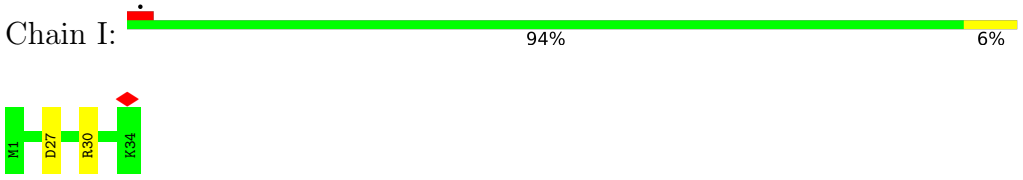
• Molecule 8: Photosystem II reaction center protein H

Chain H:



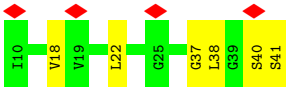
• Molecule 9: Photosystem II reaction center protein I

Chain I:



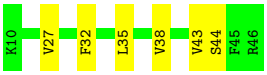
• Molecule 10: Photosystem II reaction center protein J

Chain J:



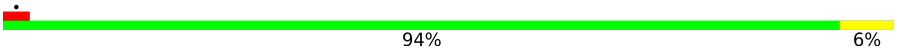
• Molecule 11: Photosystem II reaction center protein K

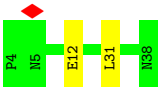
Chain K:



• Molecule 12: Photosystem II reaction center protein L

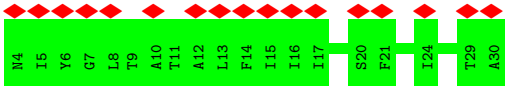
Chain L:





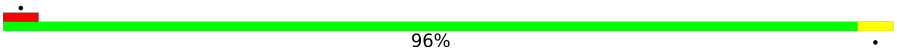
• Molecule 13: Photosystem II reaction center protein M

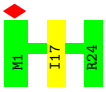
Chain M:



• Molecule 14: Photosystem II reaction center protein T

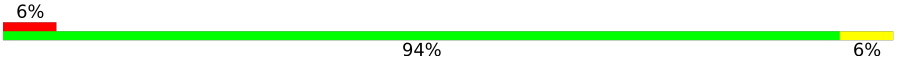
Chain T:

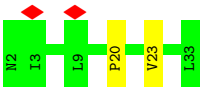




• Molecule 15: Photosystem II reaction center protein Psb30

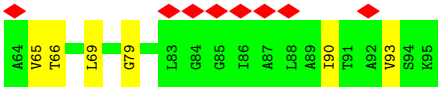
Chain V:





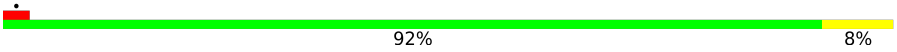
• Molecule 16: Chloroplast photosystem II subunit X

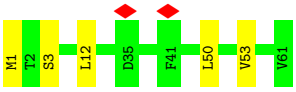
Chain X:



• Molecule 17: Photosystem II reaction center protein Z

Chain Z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45968	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.397	Depositor
Minimum map value	-0.883	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.174	Depositor
Map size (Å)	280.0, 280.0, 280.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, LHG, LMG, HEM, BCT, BCR, FE2, LMU, PHO, CLA, PL9, DGD

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	0.16	0/2430	0.31	0/3312
2	B	0.13	0/3883	0.26	0/5286
3	C	0.13	0/3550	0.27	0/4834
4	D	0.14	0/2762	0.27	0/3766
5	E	0.11	0/628	0.27	0/857
6	F	0.12	0/258	0.27	0/349
7	G	0.16	0/1830	0.43	4/2476 (0.2%)
8	H	0.11	0/543	0.27	0/740
9	I	0.16	0/283	0.24	0/383
10	J	0.10	0/238	0.23	0/326
11	K	0.16	0/309	0.37	0/425
12	L	0.11	0/298	0.22	0/405
13	M	0.10	0/214	0.28	0/293
14	T	0.15	0/203	0.25	0/273
15	V	0.10	0/224	0.25	0/307
16	X	0.11	0/215	0.27	0/292
17	Z	0.15	0/469	0.29	0/644
All	All	0.14	0/18337	0.29	4/24968 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	78	PRO	N-CA-CB	7.86	110.28	103.36
7	G	80	PRO	N-CA-CB	7.31	110.92	103.25
7	G	100	PRO	N-CA-CB	7.13	109.97	103.20
7	G	111	PRO	N-CA-CB	6.93	110.53	103.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2355	0	2291	30	0
2	B	3755	0	3642	30	0
3	C	3431	0	3308	45	0
4	D	2671	0	2567	40	0
5	E	610	0	599	5	0
6	F	251	0	263	2	0
7	G	1806	0	1549	13	0
8	H	532	0	556	6	0
9	I	275	0	287	2	0
10	J	232	0	242	5	0
11	K	297	0	308	5	0
12	L	290	0	298	2	0
13	M	210	0	231	0	0
14	T	198	0	209	2	0
15	V	224	0	256	1	0
16	X	214	0	240	4	0
17	Z	458	0	490	4	0
18	A	1	0	0	0	0
19	A	174	0	170	2	0
19	B	1020	0	1113	9	0
19	C	845	0	936	5	0
19	D	195	0	216	7	0
20	A	64	0	74	1	0
20	D	64	0	74	3	0
21	A	40	0	56	3	0
21	B	120	0	168	3	0
21	C	120	0	168	12	0
21	D	40	0	56	2	0
21	H	40	0	56	3	0
21	K	40	0	56	1	0
22	A	51	0	69	0	0
23	A	46	0	62	0	0
23	B	90	0	120	1	0
23	C	51	0	72	0	0
23	D	46	0	62	2	0
24	A	43	0	56	1	0
24	B	44	0	61	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	147	0	222	2	0
24	L	49	0	74	2	0
25	C	115	0	146	0	0
25	J	59	0	76	0	0
26	C	35	0	46	1	0
27	D	4	0	0	0	0
28	D	55	0	80	1	0
29	F	43	0	30	5	0
30	A	2	0	0	0	0
All	All	21452	0	21655	195	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:ARG:NH1	2:B:276:ASP:OD2	2.10	0.85
1:A:286:THR:OG1	19:A:402:CLA:O1D	2.01	0.77
3:C:285:TYR:O	3:C:411:ARG:NH2	2.20	0.74
3:C:104:VAL:HG11	21:C:514:BCR:H333	1.69	0.74
4:D:217:THR:HG21	4:D:253:TRP:HE1	1.54	0.72
3:C:274:ALA:HB2	19:C:502:CLA:HMD1	1.71	0.72
4:D:241:GLU:N	4:D:241:GLU:OE2	2.25	0.70
11:K:43:VAL:O	11:K:44:SER:OG	2.11	0.69
3:C:444:GLU:N	3:C:444:GLU:OE2	2.27	0.67
2:B:311:PHE:O	2:B:317:ASN:ND2	2.28	0.66
3:C:36:LYS:NZ	3:C:121:SER:O	2.28	0.66
17:Z:1:MET:SD	17:Z:3:SER:N	2.68	0.66
16:X:65:VAL:HG13	16:X:66:THR:HG23	1.78	0.65
3:C:394:SER:O	3:C:406:ASN:ND2	2.30	0.65
4:D:12:ARG:NH2	4:D:20:ASP:OD2	2.30	0.64
1:A:303:ASN:OD1	1:A:322:ASN:ND2	2.30	0.64
24:B:521:LHG:O2	4:D:265:ARG:NH1	2.30	0.64
3:C:441:ALA:O	7:G:244:ARG:NH2	2.31	0.64
7:G:209:ASP:OD2	7:G:213:LYS:NZ	2.31	0.64
3:C:134:PHE:O	3:C:144:LYS:NZ	2.31	0.63
5:E:23:HIS:CE1	29:F:101:HEM:ND	2.66	0.62
7:G:134:GLN:NE2	7:G:224:VAL:HG21	2.15	0.62
21:H:101:BCR:H23C	21:H:101:BCR:H383	1.81	0.62
3:C:224:GLY:HA3	21:C:515:BCR:H402	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:409:LHG:O10	4:D:220:ASN:ND2	2.34	0.60
3:C:79:HIS:NE2	19:C:502:CLA:O1D	2.34	0.60
4:D:186:GLN:NE2	4:D:322:ASN:OD1	2.34	0.60
3:C:278:SER:O	3:C:411:ARG:NH1	2.35	0.59
3:C:355:GLU:OE2	3:C:358:ARG:NH1	2.35	0.59
21:D:406:BCR:H23C	21:D:406:BCR:H403	1.83	0.59
4:D:186:GLN:HB2	19:D:404:CLA:HBC1	1.86	0.58
4:D:192:THR:HG23	19:D:404:CLA:HBC2	1.85	0.58
21:A:406:BCR:H23C	21:A:406:BCR:H383	1.86	0.57
4:D:54:PHE:O	5:E:49:THR:OG1	2.22	0.57
2:B:73:GLN:NE2	2:B:87:ASN:O	2.38	0.57
19:D:404:CLA:HHD	19:D:404:CLA:HBC3	1.86	0.56
21:C:516:BCR:H383	21:C:516:BCR:H23C	1.87	0.56
2:B:7:ARG:O	2:B:10:THR:OG1	2.11	0.56
3:C:233:ILE:O	3:C:237:ILE:HD12	2.05	0.55
24:B:521:LHG:O4	4:D:141:TYR:OH	2.25	0.55
1:A:303:ASN:O	3:C:403:ASN:ND2	2.39	0.55
6:F:25:ILE:O	6:F:29:THR:OG1	2.17	0.55
1:A:288:LEU:HD21	3:C:423:PHE:CD2	2.40	0.55
29:F:101:HEM:HMC2	29:F:101:HEM:HBC2	1.89	0.55
21:B:519:BCR:H23C	21:B:519:BCR:H383	1.90	0.54
4:D:96:GLU:OE1	4:D:96:GLU:N	2.38	0.54
2:B:357:ARG:NH2	4:D:337:GLU:OE1	2.41	0.54
7:G:223:LEU:HD21	7:G:259:CYS:HB2	1.87	0.54
3:C:201:LEU:HD11	21:C:515:BCR:H20C	1.90	0.54
21:C:514:BCR:H23C	21:C:514:BCR:H383	1.89	0.53
3:C:104:VAL:CG1	21:C:514:BCR:H333	2.37	0.53
1:A:10:ASN:OD1	1:A:11:SER:N	2.42	0.53
15:V:20:PRO:HA	15:V:23:VAL:HG22	1.91	0.53
1:A:25:GLU:OE1	3:C:458:ARG:NH2	2.43	0.52
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.92	0.52
19:B:502:CLA:H42	23:B:522:LMG:H111	1.92	0.52
3:C:26:GLY:HA3	19:C:511:CLA:HMD2	1.91	0.52
3:C:76:LEU:O	3:C:80:ILE:HD12	2.10	0.52
3:C:95:ASP:OD2	26:C:520:LMU:O6B	2.13	0.52
7:G:254:TYR:OH	7:G:290:ASP:OD2	2.26	0.52
1:A:288:LEU:HD22	3:C:420:CYS:HA	1.92	0.52
3:C:279:TRP:O	3:C:293:THR:HG23	2.10	0.51
4:D:217:THR:HG21	4:D:253:TRP:NE1	2.23	0.51
1:A:170:ASP:OD2	3:C:345:ARG:NH1	2.44	0.51
1:A:283:ILE:HA	1:A:286:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:HIS:O	2:B:30:VAL:HG23	2.11	0.51
7:G:203:ARG:NH1	7:G:229:ILE:O	2.45	0.50
1:A:92:HIS:NE2	3:C:348:ASP:OD2	2.45	0.50
21:C:514:BCR:H311	21:C:514:BCR:HC8	1.93	0.50
19:D:405:CLA:H92	8:H:55:LEU:HD22	1.94	0.50
1:A:63:ILE:HG22	1:A:63:ILE:O	2.12	0.49
1:A:192:ILE:HD12	1:A:293:MET:HE1	1.95	0.49
2:B:397:VAL:HG23	2:B:417:VAL:HG11	1.93	0.49
19:B:502:CLA:H43	8:H:65:LEU:HA	1.95	0.49
3:C:448:ASP:OD2	7:G:235:ARG:NH2	2.46	0.49
4:D:279:LEU:HD22	20:D:402:PHO:HBC3	1.94	0.49
4:D:201:VAL:HG23	19:D:404:CLA:C2B	2.43	0.49
29:F:101:HEM:HMB2	29:F:101:HEM:HBB2	1.94	0.49
3:C:166:LYS:NZ	3:C:172:GLY:O	2.46	0.49
1:A:260:PHE:HD1	4:D:28:VAL:HG23	1.78	0.48
19:B:502:CLA:C7	19:B:502:CLA:H41	2.44	0.48
24:L:101:LHG:O3	24:L:101:LHG:O1	2.16	0.48
4:D:279:LEU:HD11	20:D:402:PHO:HMC3	1.95	0.48
2:B:321:LYS:NZ	2:B:363:PHE:O	2.46	0.48
1:A:290:LEU:O	1:A:290:LEU:HD23	2.13	0.48
3:C:285:TYR:OH	19:C:502:CLA:O2D	2.32	0.48
4:D:213:ILE:O	4:D:217:THR:HG23	2.13	0.48
4:D:29:PHE:O	4:D:128:ARG:NH1	2.46	0.48
2:B:243:ALA:HA	2:B:246:PHE:CE1	2.49	0.47
2:B:70:GLY:HA2	2:B:178:VAL:HG11	1.96	0.47
1:A:186:PHE:HE2	1:A:192:ILE:HD13	1.80	0.47
19:B:513:CLA:H141	21:B:518:BCR:H322	1.96	0.47
11:K:27:VAL:O	11:K:27:VAL:HG12	2.13	0.47
4:D:129:GLN:NE2	20:D:402:PHO:OBD	2.48	0.47
1:A:317:TRP:CD1	4:D:65:THR:HG21	2.50	0.47
7:G:259:CYS:HA	7:G:262:MET:HE2	1.96	0.47
2:B:74:SER:OG	2:B:94:GLU:OE2	2.33	0.47
1:A:257:ARG:O	4:D:128:ARG:NH2	2.48	0.47
3:C:15:ASP:N	3:C:15:ASP:OD1	2.47	0.47
3:C:293:THR:O	3:C:297:ALA:N	2.43	0.47
3:C:201:LEU:HD11	21:C:515:BCR:H373	1.97	0.47
1:A:127:MET:HE2	1:A:151:VAL:HG11	1.97	0.46
2:B:12:VAL:HG22	2:B:12:VAL:O	2.15	0.46
7:G:277:MET:HE1	7:G:306:LEU:HD12	1.97	0.46
3:C:228:ILE:HD11	21:C:515:BCR:C21	2.45	0.46
7:G:206:MET:HE1	7:G:232:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:MET:O	2:B:448:ARG:NH1	2.42	0.46
4:D:161:PRO:CG	4:D:170:ALA:HB2	2.45	0.46
4:D:67:TYR:OH	23:D:409:LMG:O10	2.32	0.46
6:F:42:ILE:HG21	10:J:38:LEU:HD12	1.97	0.46
4:D:201:VAL:HG23	19:D:404:CLA:CMB	2.45	0.46
10:J:37:GLY:O	10:J:40:SER:OG	2.27	0.46
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.98	0.46
7:G:243:SER:O	9:I:30:ARG:NH1	2.49	0.46
1:A:283:ILE:HG13	20:A:404:PHO:HBC3	1.99	0.45
2:B:170:ASP:HB2	2:B:171:PRO:HD2	1.98	0.45
3:C:49:VAL:HG12	3:C:106:HIS:O	2.16	0.45
23:D:409:LMG:O3	10:J:38:LEU:O	2.25	0.45
2:B:24:LEU:HD21	19:B:516:CLA:CAB	2.46	0.45
21:C:516:BCR:H383	21:C:516:BCR:C23	2.46	0.45
3:C:146:THR:HG21	3:C:244:PRO:HD3	1.99	0.45
17:Z:50:LEU:HA	17:Z:53:VAL:HG22	1.99	0.45
2:B:44:VAL:O	2:B:44:VAL:HG22	2.17	0.45
28:D:407:PL9:H352	12:L:31:LEU:HD22	1.98	0.45
29:F:101:HEM:HBB2	29:F:101:HEM:CMB	2.47	0.44
2:B:468:TRP:CZ3	4:D:144:ILE:HD13	2.53	0.44
1:A:188:ALA:HB2	1:A:328:MET:CB	2.48	0.44
2:B:313:ASP:OD1	2:B:358:ARG:NH1	2.45	0.44
4:D:84:SER:OG	5:E:66:ILE:O	2.12	0.44
8:H:54:ILE:CD1	21:H:101:BCR:H333	2.48	0.44
12:L:12:GLU:OE2	24:L:101:LHG:O2	2.12	0.43
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.00	0.43
10:J:40:SER:O	10:J:41:SER:OG	2.26	0.43
3:C:238:TRP:O	3:C:242:THR:OG1	2.27	0.43
1:A:289:GLY:O	1:A:293:MET:HG3	2.19	0.43
2:B:112:VAL:HG11	21:B:519:BCR:H381	2.00	0.43
11:K:35:LEU:HA	11:K:38:VAL:HG12	2.00	0.43
19:B:505:CLA:H142	19:B:510:CLA:H2	2.00	0.43
10:J:18:VAL:O	10:J:22:LEU:HD23	2.17	0.43
3:C:304:THR:HA	3:C:307:VAL:HG22	2.01	0.43
7:G:223:LEU:HD21	7:G:259:CYS:CB	2.48	0.43
17:Z:12:LEU:HA	17:Z:50:LEU:HD23	2.01	0.43
2:B:348:ASP:OD1	2:B:352:ARG:N	2.51	0.43
1:A:93:PHE:CE1	19:A:405:CLA:HED1	2.54	0.43
3:C:245:TRP:NE1	19:C:506:CLA:OBD	2.49	0.43
2:B:453:PHE:HB2	4:D:291:LEU:HD12	2.01	0.42
11:K:32:PHE:CZ	21:K:101:BCR:H341	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:X:90:ILE:HA	16:X:93:VAL:HG12	2.01	0.42
1:A:65:GLU:OE2	1:A:65:GLU:HA	2.19	0.42
3:C:201:LEU:HD11	21:C:515:BCR:C20	2.49	0.42
2:B:458:PHE:HB3	19:B:504:CLA:HBC2	2.01	0.42
3:C:293:THR:HG22	3:C:295:PRO:HD2	1.99	0.42
8:H:74:LEU:HB2	8:H:77:VAL:HG22	2.01	0.42
3:C:47:LEU:HD21	11:K:32:PHE:CD2	2.54	0.42
3:C:250:ARG:NH2	9:I:27:ASP:OD1	2.53	0.42
1:A:272:HIS:CG	4:D:218:VAL:HG11	2.54	0.42
3:C:50:PHE:HB2	3:C:110:SER:OG	2.19	0.42
1:A:192:ILE:HD11	1:A:198:HIS:HB2	2.02	0.42
4:D:251:ARG:NE	4:D:255:GLN:OE1	2.48	0.42
29:F:101:HEM:HBC2	29:F:101:HEM:CMC	2.49	0.42
7:G:277:MET:HE1	7:G:306:LEU:CD1	2.49	0.42
8:H:72:LEU:HD11	16:X:69:LEU:HA	2.02	0.42
4:D:89:LEU:HD12	4:D:91:PHE:CZ	2.55	0.42
19:D:405:CLA:H42	16:X:79:GLY:HA3	2.02	0.42
3:C:398:VAL:HG12	3:C:399:ALA:N	2.35	0.42
1:A:47:VAL:HG21	1:A:114:LEU:HD22	2.02	0.41
2:B:57:ARG:NH2	2:B:335:GLY:O	2.53	0.41
3:C:64:VAL:O	3:C:64:VAL:HG23	2.20	0.41
4:D:145:ALA:HB2	4:D:272:LEU:CD1	2.50	0.41
2:B:175:THR:HG23	2:B:175:THR:O	2.20	0.41
21:D:406:BCR:H311	21:D:406:BCR:HC8	2.02	0.41
1:A:50:ILE:CG2	21:A:406:BCR:H393	2.51	0.41
4:D:142:ASN:C	4:D:142:ASN:HD22	2.25	0.41
5:E:32:ILE:O	5:E:36:LEU:HD23	2.21	0.41
19:B:504:CLA:HBB1	19:B:513:CLA:HBC2	2.01	0.41
8:H:54:ILE:HD13	21:H:101:BCR:H333	2.03	0.41
17:Z:1:MET:SD	17:Z:3:SER:OG	2.76	0.41
1:A:324:ALA:O	1:A:328:MET:HG3	2.20	0.41
2:B:7:ARG:NH1	24:B:521:LHG:O5	2.54	0.41
2:B:90:ILE:HD12	2:B:90:ILE:H	1.85	0.41
2:B:341:LEU:HD21	2:B:431:GLU:HB2	2.03	0.41
2:B:460:LEU:HD12	4:D:287:VAL:HG21	2.02	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.03	0.41
24:D:408:LHG:H302	14:T:17:ILE:HG23	2.03	0.41
2:B:357:ARG:NH1	2:B:358:ARG:O	2.54	0.41
24:D:408:LHG:C30	14:T:17:ILE:HG23	2.51	0.41
19:B:502:CLA:H41	19:B:502:CLA:H71	2.04	0.40
4:D:126:MET:HE3	4:D:143:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:406:BCR:H383	21:A:406:BCR:C23	2.49	0.40
4:D:107:LEU:HD23	5:E:76:VAL:HG21	2.04	0.40
3:C:128:LEU:O	3:C:128:LEU:HD12	2.21	0.40
4:D:92:VAL:O	4:D:99:GLY:N	2.48	0.40
2:B:315:ILE:HD13	2:B:359:MET:HE2	2.02	0.40
21:C:515:BCR:H11C	21:C:515:BCR:H341	1.96	0.40
4:D:142:ASN:O	4:D:142:ASN:ND2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/326 (91%)	289 (97%)	8 (3%)	0	100	100
2	B	478/480 (100%)	466 (98%)	12 (2%)	0	100	100
3	C	434/450 (96%)	418 (96%)	16 (4%)	0	100	100
4	D	331/349 (95%)	324 (98%)	7 (2%)	0	100	100
5	E	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
6	F	29/31 (94%)	29 (100%)	0	0	100	100
7	G	256/258 (99%)	236 (92%)	16 (6%)	4 (2%)	8	32
8	H	65/70 (93%)	64 (98%)	1 (2%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
10	J	30/32 (94%)	30 (100%)	0	0	100	100
11	K	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
12	L	33/35 (94%)	33 (100%)	0	0	100	100
13	M	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
14	T	22/24 (92%)	22 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
16	X	30/32 (94%)	30 (100%)	0	0	100	100
17	Z	59/61 (97%)	59 (100%)	0	0	100	100
All	All	2259/2353 (96%)	2189 (97%)	66 (3%)	4 (0%)	45	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	79	LYS
7	G	80	PRO
7	G	111	PRO
7	G	146	VAL

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	245/266 (92%)	245 (100%)	0	100	100
2	B	382/382 (100%)	382 (100%)	0	100	100
3	C	346/352 (98%)	346 (100%)	0	100	100
4	D	268/278 (96%)	268 (100%)	0	100	100
5	E	66/66 (100%)	66 (100%)	0	100	100
6	F	25/25 (100%)	25 (100%)	0	100	100
7	G	141/211 (67%)	141 (100%)	0	100	100
8	H	59/60 (98%)	59 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
10	J	24/24 (100%)	24 (100%)	0	100	100
11	K	31/31 (100%)	31 (100%)	0	100	100
12	L	33/33 (100%)	33 (100%)	0	100	100
13	M	23/23 (100%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	21/21 (100%)	21 (100%)	0	100	100
15	V	26/26 (100%)	26 (100%)	0	100	100
16	X	22/22 (100%)	22 (100%)	0	100	100
17	Z	51/51 (100%)	51 (100%)	0	100	100
All	All	1794/1902 (94%)	1794 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	ASN
4	D	142	ASN
7	G	134	GLN
7	G	220	GLN
12	L	38	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 67 ligands modelled in this entry, 1 is monoatomic - leaving 66 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	$\#\|Z\| > 2$
19	CLA	A	402	-	65,73,73	1.51	7 (10%)	76,113,113	1.25	8 (10%)
19	CLA	B	502	-	65,73,73	1.51	5 (7%)	76,113,113	1.22	8 (10%)
23	LMG	A	408	-	46,46,55	0.99	2 (4%)	54,54,63	1.00	3 (5%)
19	CLA	B	503	-	65,73,73	1.53	7 (10%)	76,113,113	1.31	8 (10%)
19	CLA	B	515	-	65,73,73	1.50	6 (9%)	76,113,113	1.20	7 (9%)
19	CLA	C	501	-	65,73,73	1.50	6 (9%)	76,113,113	1.27	10 (13%)
19	CLA	B	507	-	65,73,73	1.52	6 (9%)	76,113,113	1.20	8 (10%)
21	BCR	C	514	-	41,41,41	0.74	0	56,56,56	2.26	22 (39%)
19	CLA	A	405	-	60,68,73	1.56	8 (13%)	70,107,113	1.25	9 (12%)
23	LMG	D	409	-	46,46,55	1.01	2 (4%)	54,54,63	1.04	3 (5%)
24	LHG	A	409	-	42,42,48	1.01	2 (4%)	45,48,54	1.02	2 (4%)
19	CLA	C	512	-	65,73,73	1.52	7 (10%)	76,113,113	1.31	9 (11%)
21	BCR	B	518	-	41,41,41	0.77	0	56,56,56	2.06	19 (33%)
21	BCR	B	517	-	41,41,41	0.78	0	56,56,56	2.08	20 (35%)
23	LMG	B	520	-	42,42,55	1.01	2 (4%)	50,50,63	1.00	2 (4%)
20	PHO	D	402	-	51,69,69	1.02	5 (9%)	47,99,99	1.12	4 (8%)
19	CLA	B	510	-	65,73,73	1.48	6 (9%)	76,113,113	1.23	7 (9%)
23	LMG	C	519	-	51,51,55	0.93	2 (3%)	59,59,63	0.93	2 (3%)
19	CLA	B	508	-	65,73,73	1.50	7 (10%)	76,113,113	1.23	8 (10%)
19	CLA	B	509	-	65,73,73	1.54	7 (10%)	76,113,113	1.26	9 (11%)
19	CLA	B	516	-	65,73,73	1.52	5 (7%)	76,113,113	1.18	7 (9%)
19	CLA	D	405	-	65,73,73	1.53	5 (7%)	76,113,113	1.25	8 (10%)
21	BCR	H	101	-	41,41,41	0.71	0	56,56,56	2.11	21 (37%)
19	CLA	C	507	-	65,73,73	1.50	6 (9%)	76,113,113	1.24	7 (9%)
25	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	1.02	3 (3%)
21	BCR	B	519	-	41,41,41	0.78	0	56,56,56	1.92	18 (32%)
21	BCR	K	101	-	41,41,41	0.77	1 (2%)	56,56,56	2.21	20 (35%)
21	BCR	D	406	-	41,41,41	0.70	0	56,56,56	2.19	23 (41%)
21	BCR	A	406	-	41,41,41	0.70	0	56,56,56	2.03	18 (32%)
19	CLA	C	509	-	65,73,73	1.47	6 (9%)	76,113,113	1.26	7 (9%)
19	CLA	B	513	-	65,73,73	1.48	6 (9%)	76,113,113	1.24	8 (10%)
19	CLA	C	508	-	65,73,73	1.49	7 (10%)	76,113,113	1.29	8 (10%)
24	LHG	L	101	-	48,48,48	0.93	2 (4%)	51,54,54	0.95	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PL9	D	407	-	55,55,55	1.09	4 (7%)	68,69,69	1.58	12 (17%)
19	CLA	D	401	-	65,73,73	1.49	6 (9%)	76,113,113	1.30	8 (10%)
27	BCT	D	403	18	2,3,3	1.25	0	2,3,3	4.17	2 (100%)
19	CLA	C	504	-	65,73,73	1.52	8 (12%)	76,113,113	1.16	8 (10%)
25	DGD	C	517	-	54,54,67	0.95	2 (3%)	68,68,81	1.03	3 (4%)
24	LHG	D	408	-	48,48,48	0.94	2 (4%)	51,54,54	0.91	2 (3%)
19	CLA	C	505	-	65,73,73	1.50	6 (9%)	76,113,113	1.16	7 (9%)
19	CLA	B	504	-	65,73,73	1.52	7 (10%)	76,113,113	1.26	6 (7%)
19	CLA	A	403	-	49,57,73	1.74	7 (14%)	55,93,113	1.39	8 (14%)
19	CLA	C	510	-	65,73,73	1.52	6 (9%)	76,113,113	1.25	8 (10%)
19	CLA	C	511	3	65,73,73	1.55	6 (9%)	76,113,113	1.20	9 (11%)
21	BCR	C	516	-	41,41,41	0.70	0	56,56,56	1.88	17 (30%)
22	SQD	A	407	-	50,51,54	1.22	4 (8%)	59,62,65	1.16	8 (13%)
19	CLA	B	506	-	65,73,73	1.52	6 (9%)	76,113,113	1.22	7 (9%)
23	LMG	B	522	-	48,48,55	0.96	2 (4%)	56,56,63	0.94	2 (3%)
19	CLA	D	404	-	65,73,73	1.50	7 (10%)	76,113,113	1.21	8 (10%)
29	HEM	F	101	6,5	41,50,50	1.49	5 (12%)	45,82,82	1.32	6 (13%)
19	CLA	B	512	-	65,73,73	1.48	6 (9%)	76,113,113	1.30	8 (10%)
24	LHG	D	410	-	48,48,48	0.95	2 (4%)	51,54,54	0.95	2 (3%)
26	LMU	C	520	-	36,36,36	1.17	2 (5%)	47,47,47	0.87	1 (2%)
24	LHG	B	521	-	43,43,48	1.00	2 (4%)	46,49,54	1.08	3 (6%)
20	PHO	A	404	-	51,69,69	1.03	4 (7%)	47,99,99	1.15	6 (12%)
19	CLA	B	514	-	45,53,73	1.80	6 (13%)	52,89,113	1.35	7 (13%)
19	CLA	C	503	-	65,73,73	1.52	6 (9%)	76,113,113	1.20	9 (11%)
24	LHG	D	411	-	48,48,48	0.94	2 (4%)	51,54,54	0.97	3 (5%)
19	CLA	C	513	-	65,73,73	1.51	5 (7%)	76,113,113	1.21	8 (10%)
19	CLA	B	501	-	65,73,73	1.53	7 (10%)	76,113,113	1.22	7 (9%)
21	BCR	C	515	-	41,41,41	0.77	1 (2%)	56,56,56	1.99	16 (28%)
25	DGD	J	101	-	60,60,67	0.92	2 (3%)	74,74,81	0.96	3 (4%)
19	CLA	B	511	-	65,73,73	1.51	8 (12%)	76,113,113	1.24	9 (11%)
19	CLA	C	502	-	65,73,73	1.52	8 (12%)	76,113,113	1.29	8 (10%)
19	CLA	B	505	-	65,73,73	1.50	5 (7%)	76,113,113	1.17	6 (7%)
19	CLA	C	506	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	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
19	CLA	A	402	-	1/1/15/20	11/37/115/115	-
19	CLA	B	502	-	1/1/15/20	11/37/115/115	-
23	LMG	A	408	-	-	11/41/61/70	0/1/1/1
19	CLA	B	503	-	1/1/15/20	8/37/115/115	-
19	CLA	B	515	-	1/1/15/20	12/37/115/115	-
19	CLA	C	501	-	1/1/15/20	12/37/115/115	-
19	CLA	B	507	-	1/1/15/20	15/37/115/115	-
21	BCR	C	514	-	-	5/29/63/63	0/2/2/2
19	CLA	A	405	-	-	10/31/109/115	-
23	LMG	D	409	-	-	6/41/61/70	0/1/1/1
24	LHG	A	409	-	-	7/47/47/53	-
19	CLA	C	512	-	1/1/15/20	14/37/115/115	-
21	BCR	B	518	-	-	4/29/63/63	0/2/2/2
21	BCR	B	517	-	-	6/29/63/63	0/2/2/2
23	LMG	B	520	-	-	9/37/57/70	0/1/1/1
20	PHO	D	402	-	-	13/37/103/103	0/5/6/6
19	CLA	B	510	-	1/1/15/20	16/37/115/115	-
23	LMG	C	519	-	-	5/46/66/70	0/1/1/1
19	CLA	B	508	-	1/1/15/20	12/37/115/115	-
19	CLA	B	509	-	1/1/15/20	16/37/115/115	-
19	CLA	B	516	-	1/1/15/20	13/37/115/115	-
19	CLA	D	405	-	1/1/15/20	17/37/115/115	-
21	BCR	H	101	-	-	6/29/63/63	0/2/2/2
19	CLA	C	507	-	1/1/15/20	13/37/115/115	-
25	DGD	C	518	-	-	11/51/91/95	0/2/2/2
21	BCR	B	519	-	-	4/29/63/63	0/2/2/2
21	BCR	K	101	-	-	6/29/63/63	0/2/2/2
21	BCR	D	406	-	-	0/29/63/63	0/2/2/2
21	BCR	A	406	-	-	5/29/63/63	0/2/2/2
19	CLA	C	509	-	1/1/15/20	14/37/115/115	-
19	CLA	B	513	-	1/1/15/20	18/37/115/115	-
19	CLA	C	508	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	L	101	-	-	15/53/53/53	-
28	PL9	D	407	-	-	10/53/73/73	0/1/1/1
19	CLA	D	401	-	1/1/15/20	13/37/115/115	-
19	CLA	C	504	-	1/1/15/20	7/37/115/115	-
25	DGD	C	517	-	-	9/42/82/95	0/2/2/2
24	LHG	D	408	-	-	6/53/53/53	-
19	CLA	C	505	-	1/1/15/20	9/37/115/115	-
19	CLA	B	504	-	1/1/15/20	17/37/115/115	-
19	CLA	A	403	-	1/1/11/20	12/18/96/115	-
19	CLA	C	510	-	1/1/15/20	14/37/115/115	-
19	CLA	C	511	3	1/1/15/20	24/37/115/115	-
21	BCR	C	516	-	-	3/29/63/63	0/2/2/2
22	SQD	A	407	-	-	12/46/66/69	0/1/1/1
19	CLA	B	506	-	1/1/15/20	8/37/115/115	-
23	LMG	B	522	-	-	8/43/63/70	0/1/1/1
19	CLA	D	404	-	-	14/37/115/115	-
29	HEM	F	101	6,5	-	0/12/54/54	-
19	CLA	B	512	-	1/1/15/20	14/37/115/115	-
24	LHG	D	410	-	-	10/53/53/53	-
26	LMU	C	520	-	-	12/21/61/61	0/2/2/2
24	LHG	B	521	-	-	12/48/48/53	-
20	PHO	A	404	-	-	13/37/103/103	0/5/6/6
19	CLA	B	514	-	1/1/11/20	4/13/91/115	-
19	CLA	C	503	-	1/1/15/20	17/37/115/115	-
24	LHG	D	411	-	-	19/53/53/53	-
19	CLA	C	513	-	1/1/15/20	14/37/115/115	-
19	CLA	B	501	-	1/1/15/20	14/37/115/115	-
21	BCR	C	515	-	-	4/29/63/63	0/2/2/2
25	DGD	J	101	-	-	6/48/88/95	0/2/2/2
19	CLA	B	511	-	1/1/15/20	11/37/115/115	-
19	CLA	C	502	-	1/1/15/20	19/37/115/115	-
19	CLA	B	505	-	1/1/15/20	17/37/115/115	-
19	CLA	C	506	-	1/1/15/20	17/37/115/115	-

All (277) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	405	CLA	C4B-NB	7.85	1.42	1.35
19	B	509	CLA	C4B-NB	7.77	1.42	1.35
19	B	516	CLA	C4B-NB	7.75	1.42	1.35
19	B	507	CLA	C4B-NB	7.75	1.42	1.35
19	C	511	CLA	C4B-NB	7.73	1.42	1.35
19	B	501	CLA	C4B-NB	7.71	1.42	1.35
19	C	510	CLA	C4B-NB	7.71	1.42	1.35
19	B	503	CLA	C4B-NB	7.70	1.42	1.35
19	C	502	CLA	C4B-NB	7.70	1.42	1.35
19	C	512	CLA	C4B-NB	7.69	1.42	1.35
19	C	504	CLA	C4B-NB	7.68	1.42	1.35
19	B	504	CLA	C4B-NB	7.66	1.42	1.35
19	B	506	CLA	C4B-NB	7.64	1.42	1.35
19	B	511	CLA	C4B-NB	7.63	1.42	1.35
19	C	503	CLA	C4B-NB	7.63	1.42	1.35
19	B	508	CLA	C4B-NB	7.58	1.42	1.35
19	B	502	CLA	C4B-NB	7.58	1.42	1.35
19	C	507	CLA	C4B-NB	7.57	1.42	1.35
19	C	513	CLA	C4B-NB	7.55	1.41	1.35
19	B	515	CLA	C4B-NB	7.54	1.41	1.35
19	D	401	CLA	C4B-NB	7.53	1.41	1.35
19	B	505	CLA	C4B-NB	7.53	1.41	1.35
19	A	403	CLA	C4B-NB	7.52	1.41	1.35
19	D	404	CLA	C4B-NB	7.50	1.41	1.35
19	B	514	CLA	C4B-NB	7.48	1.41	1.35
19	C	505	CLA	C4B-NB	7.47	1.41	1.35
19	C	506	CLA	C4B-NB	7.44	1.41	1.35
19	A	402	CLA	C4B-NB	7.43	1.41	1.35
19	C	509	CLA	C4B-NB	7.41	1.41	1.35
19	C	508	CLA	C4B-NB	7.39	1.41	1.35
19	C	501	CLA	C4B-NB	7.36	1.41	1.35
19	B	512	CLA	C4B-NB	7.28	1.41	1.35
19	A	405	CLA	C4B-NB	7.27	1.41	1.35
19	B	513	CLA	C4B-NB	7.23	1.41	1.35
19	B	510	CLA	C4B-NB	7.14	1.41	1.35
22	A	407	SQD	O8-S	4.65	1.64	1.47
25	C	517	DGD	O2G-C1B	4.35	1.46	1.34
23	D	409	LMG	O7-C10	4.33	1.46	1.34
25	J	101	DGD	O1G-C1A	4.33	1.46	1.33
24	B	521	LHG	O8-C23	4.31	1.45	1.33
24	D	410	LHG	O8-C23	4.31	1.45	1.33
24	A	409	LHG	O8-C23	4.31	1.45	1.33
23	D	409	LMG	O8-C28	4.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	517	DGD	O1G-C1A	4.29	1.45	1.33
23	C	519	LMG	O8-C28	4.25	1.45	1.33
22	A	407	SQD	O48-C23	4.25	1.45	1.33
24	D	411	LHG	O8-C23	4.24	1.45	1.33
24	L	101	LHG	O8-C23	4.22	1.45	1.33
24	D	410	LHG	O7-C7	4.22	1.46	1.34
23	B	522	LMG	O8-C28	4.21	1.45	1.33
25	C	518	DGD	O1G-C1A	4.21	1.45	1.33
24	D	408	LHG	O7-C7	4.20	1.46	1.34
24	D	408	LHG	O8-C23	4.18	1.45	1.33
23	A	408	LMG	O8-C28	4.17	1.45	1.33
23	B	520	LMG	O8-C28	4.17	1.45	1.33
24	B	521	LHG	O7-C7	4.17	1.46	1.34
23	A	408	LMG	O7-C10	4.17	1.46	1.34
24	A	409	LHG	O7-C7	4.13	1.46	1.34
23	C	519	LMG	O7-C10	4.13	1.45	1.34
25	J	101	DGD	O2G-C1B	4.13	1.45	1.34
24	D	411	LHG	O7-C7	4.12	1.45	1.34
23	B	520	LMG	O7-C10	4.09	1.45	1.34
23	B	522	LMG	O7-C10	4.09	1.45	1.34
22	A	407	SQD	O47-C7	4.07	1.45	1.34
25	C	518	DGD	O2G-C1B	4.07	1.45	1.34
24	L	101	LHG	O7-C7	4.04	1.45	1.34
19	C	511	CLA	C1D-ND	4.03	1.42	1.37
29	F	101	HEM	C3C-C2C	-3.92	1.34	1.40
19	B	509	CLA	C1D-ND	3.92	1.42	1.37
19	C	513	CLA	C1D-ND	3.89	1.42	1.37
19	B	513	CLA	C1D-ND	3.88	1.42	1.37
19	D	401	CLA	C1D-ND	3.87	1.42	1.37
19	B	506	CLA	C1D-ND	3.86	1.42	1.37
19	C	503	CLA	C1D-ND	3.86	1.42	1.37
19	B	504	CLA	C1D-ND	3.85	1.42	1.37
19	C	505	CLA	C1D-ND	3.84	1.42	1.37
19	A	405	CLA	C1D-ND	3.82	1.42	1.37
19	C	506	CLA	C1D-ND	3.81	1.42	1.37
19	C	507	CLA	C1D-ND	3.80	1.42	1.37
19	B	501	CLA	C1D-ND	3.79	1.42	1.37
19	B	502	CLA	C1D-ND	3.78	1.42	1.37
19	D	405	CLA	C1D-ND	3.77	1.42	1.37
19	B	507	CLA	C1D-ND	3.76	1.42	1.37
19	B	516	CLA	C1D-ND	3.76	1.42	1.37
19	C	504	CLA	C1D-ND	3.75	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	515	CLA	C1D-ND	3.75	1.42	1.37
19	A	402	CLA	C1D-ND	3.75	1.42	1.37
19	B	512	CLA	C1D-ND	3.75	1.42	1.37
19	C	501	CLA	C1D-ND	3.73	1.42	1.37
19	C	509	CLA	C1D-ND	3.73	1.42	1.37
19	C	512	CLA	C1D-ND	3.72	1.42	1.37
29	F	101	HEM	C3C-CAC	3.71	1.55	1.47
19	B	510	CLA	C1D-ND	3.70	1.42	1.37
28	D	407	PL9	C7-C3	-3.69	1.47	1.51
19	B	511	CLA	C1D-ND	3.68	1.42	1.37
19	C	510	CLA	C1D-ND	3.67	1.42	1.37
19	B	514	CLA	C1D-ND	3.67	1.42	1.37
19	A	403	CLA	C1D-ND	3.66	1.42	1.37
19	B	503	CLA	C1D-ND	3.61	1.42	1.37
19	B	505	CLA	C1D-ND	3.61	1.42	1.37
19	C	508	CLA	C1D-ND	3.58	1.42	1.37
19	B	508	CLA	C1D-ND	3.53	1.42	1.37
19	D	404	CLA	C1D-ND	3.50	1.42	1.37
26	C	520	LMU	O5'-C1'	3.48	1.50	1.41
19	C	502	CLA	C1D-ND	3.48	1.42	1.37
28	D	407	PL9	C3-C4	-3.28	1.44	1.49
26	C	520	LMU	O5B-C1B	3.21	1.50	1.41
19	D	401	CLA	C4D-ND	-3.20	1.33	1.37
19	B	510	CLA	C4D-ND	-3.19	1.33	1.37
19	C	511	CLA	C4D-ND	-3.16	1.33	1.37
19	A	403	CLA	CHC-C1C	3.14	1.43	1.35
19	B	511	CLA	C4D-ND	-3.13	1.33	1.37
19	B	502	CLA	C4D-ND	-3.12	1.33	1.37
19	A	403	CLA	C4D-ND	-3.12	1.33	1.37
19	C	502	CLA	C4D-ND	-3.11	1.33	1.37
19	B	504	CLA	C4D-ND	-3.11	1.33	1.37
19	C	502	CLA	CHC-C1C	3.10	1.42	1.35
19	B	507	CLA	CHC-C1C	3.09	1.42	1.35
19	C	504	CLA	C4D-ND	-3.09	1.33	1.37
19	C	506	CLA	C4D-ND	-3.08	1.33	1.37
19	B	505	CLA	C4D-ND	-3.07	1.33	1.37
19	B	515	CLA	C4D-ND	-3.07	1.33	1.37
19	B	512	CLA	CHC-C1C	3.06	1.42	1.35
19	B	516	CLA	CHC-C1C	3.06	1.42	1.35
19	C	503	CLA	CHC-C1C	3.05	1.42	1.35
19	C	503	CLA	C4D-ND	-3.05	1.33	1.37
19	B	503	CLA	CHC-C1C	3.05	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	511	CLA	CHC-C1C	3.04	1.42	1.35
19	C	508	CLA	C4D-ND	-3.04	1.33	1.37
19	B	503	CLA	C4D-ND	-3.03	1.33	1.37
19	D	404	CLA	CHC-C1C	3.02	1.42	1.35
19	B	505	CLA	CHC-C1C	3.02	1.42	1.35
19	B	501	CLA	CHC-C1C	3.02	1.42	1.35
19	B	508	CLA	C4D-ND	-3.01	1.33	1.37
19	C	507	CLA	CHC-C1C	3.01	1.42	1.35
19	B	507	CLA	C4D-ND	-3.01	1.33	1.37
19	C	506	CLA	CHC-C1C	3.00	1.42	1.35
19	D	405	CLA	CHC-C1C	3.00	1.42	1.35
19	A	405	CLA	C4D-ND	-3.00	1.33	1.37
19	C	510	CLA	CHC-C1C	3.00	1.42	1.35
19	B	509	CLA	C4D-ND	-3.00	1.33	1.37
19	B	506	CLA	CHC-C1C	2.99	1.42	1.35
19	B	514	CLA	CHC-C1C	2.99	1.42	1.35
19	C	507	CLA	C4D-ND	-2.98	1.33	1.37
19	C	504	CLA	CHC-C1C	2.98	1.42	1.35
19	C	513	CLA	C4D-ND	-2.97	1.33	1.37
19	B	513	CLA	CHC-C1C	2.97	1.42	1.35
19	B	514	CLA	C4D-ND	-2.96	1.33	1.37
19	C	510	CLA	C4D-ND	-2.96	1.33	1.37
19	C	509	CLA	C4D-ND	-2.95	1.33	1.37
19	B	501	CLA	C4D-ND	-2.95	1.33	1.37
19	B	516	CLA	C4D-ND	-2.95	1.33	1.37
19	A	405	CLA	CHC-C1C	2.95	1.42	1.35
19	A	402	CLA	C4D-ND	-2.94	1.33	1.37
19	B	513	CLA	C4D-ND	-2.94	1.33	1.37
29	F	101	HEM	CAB-C3B	2.94	1.55	1.47
19	B	506	CLA	C4D-ND	-2.94	1.33	1.37
19	C	501	CLA	C4D-ND	-2.93	1.33	1.37
19	C	508	CLA	CHC-C1C	2.93	1.42	1.35
19	B	509	CLA	CHC-C1C	2.92	1.42	1.35
19	B	502	CLA	CHC-C1C	2.91	1.42	1.35
19	C	505	CLA	CHC-C1C	2.91	1.42	1.35
19	B	511	CLA	CHC-C1C	2.91	1.42	1.35
22	A	407	SQD	C6-S	-2.90	1.66	1.77
19	C	513	CLA	CHC-C1C	2.90	1.42	1.35
19	D	405	CLA	C4D-ND	-2.90	1.33	1.37
19	B	515	CLA	CHC-C1C	2.90	1.42	1.35
19	B	512	CLA	C4D-ND	-2.89	1.33	1.37
19	B	508	CLA	CHC-C1C	2.89	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	501	CLA	CHC-C1C	2.87	1.42	1.35
19	C	512	CLA	C4D-ND	-2.87	1.33	1.37
19	C	512	CLA	CHC-C1C	2.87	1.42	1.35
19	B	504	CLA	CHC-C1C	2.86	1.42	1.35
19	D	404	CLA	C4D-ND	-2.85	1.33	1.37
19	D	401	CLA	CHC-C1C	2.85	1.42	1.35
20	A	404	PHO	CAC-C3C	-2.84	1.47	1.52
19	B	510	CLA	CHC-C1C	2.84	1.42	1.35
19	A	402	CLA	CHC-C1C	2.84	1.42	1.35
19	C	505	CLA	C4D-ND	-2.81	1.33	1.37
28	D	407	PL9	C6-C1	-2.80	1.43	1.48
19	C	509	CLA	CHC-C1C	2.77	1.42	1.35
19	B	503	CLA	CMB-C2B	-2.76	1.45	1.51
20	D	402	PHO	CAC-C3C	-2.69	1.47	1.52
19	B	508	CLA	CMB-C2B	-2.68	1.46	1.51
19	A	403	CLA	CMB-C2B	-2.67	1.46	1.51
19	C	506	CLA	CMB-C2B	-2.63	1.46	1.51
19	C	502	CLA	CMB-C2B	-2.57	1.46	1.51
19	A	402	CLA	CMB-C2B	-2.55	1.46	1.51
19	D	405	CLA	CMB-C2B	-2.53	1.46	1.51
19	B	510	CLA	CMB-C2B	-2.51	1.46	1.51
19	B	506	CLA	CMB-C2B	-2.51	1.46	1.51
19	C	508	CLA	CMB-C2B	-2.51	1.46	1.51
19	B	509	CLA	CMB-C2B	-2.49	1.46	1.51
19	C	511	CLA	CMB-C2B	-2.49	1.46	1.51
19	D	401	CLA	CMB-C2B	-2.48	1.46	1.51
19	B	511	CLA	CMB-C2B	-2.48	1.46	1.51
19	B	501	CLA	CMB-C2B	-2.45	1.46	1.51
19	B	512	CLA	CMB-C2B	-2.44	1.46	1.51
19	B	504	CLA	CMB-C2B	-2.44	1.46	1.51
19	B	507	CLA	CMB-C2B	-2.44	1.46	1.51
19	B	502	CLA	CMB-C2B	-2.42	1.46	1.51
19	C	504	CLA	CMB-C2B	-2.42	1.46	1.51
19	C	512	CLA	CMB-C2B	-2.41	1.46	1.51
19	C	510	CLA	CMB-C2B	-2.41	1.46	1.51
19	A	405	CLA	CMB-C2B	-2.41	1.46	1.51
19	B	513	CLA	CMB-C2B	-2.41	1.46	1.51
19	B	514	CLA	CMB-C2B	-2.40	1.46	1.51
19	C	502	CLA	CMD-C2D	-2.40	1.45	1.50
19	D	404	CLA	CMB-C2B	-2.39	1.46	1.51
19	C	503	CLA	CMB-C2B	-2.38	1.46	1.51
19	B	505	CLA	CMB-C2B	-2.37	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	516	CLA	CMB-C2B	-2.36	1.46	1.51
19	C	507	CLA	CMB-C2B	-2.36	1.46	1.51
19	B	515	CLA	CMB-C2B	-2.36	1.46	1.51
19	C	501	CLA	CMB-C2B	-2.35	1.46	1.51
19	C	513	CLA	CMB-C2B	-2.34	1.46	1.51
19	D	404	CLA	CMD-C2D	-2.32	1.45	1.50
19	C	509	CLA	CMB-C2B	-2.31	1.46	1.51
19	C	501	CLA	CMD-C2D	-2.31	1.45	1.50
19	B	514	CLA	CMD-C2D	-2.31	1.45	1.50
19	C	510	CLA	C3B-C2B	-2.30	1.37	1.40
19	C	505	CLA	CMB-C2B	-2.26	1.46	1.51
29	F	101	HEM	FE-ND	2.25	2.08	1.96
21	K	101	BCR	C1-C6	-2.21	1.50	1.53
19	A	405	CLA	C3B-C2B	-2.20	1.37	1.40
19	C	504	CLA	C3B-C2B	-2.20	1.37	1.40
19	A	403	CLA	C3B-C2B	-2.17	1.37	1.40
19	B	508	CLA	CMD-C2D	-2.17	1.46	1.50
19	B	503	CLA	CMD-C2D	-2.16	1.46	1.50
19	A	402	CLA	CMD-C2D	-2.14	1.46	1.50
19	C	508	CLA	CMC-C2C	-2.13	1.46	1.50
19	C	512	CLA	C3B-C2B	-2.11	1.37	1.40
19	B	504	CLA	CMD-C2D	-2.11	1.46	1.50
20	D	402	PHO	CMD-C2D	-2.11	1.46	1.51
19	A	402	CLA	C3B-C2B	-2.11	1.37	1.40
20	A	404	PHO	CMD-C2D	-2.10	1.46	1.51
20	D	402	PHO	CMB-C2B	-2.10	1.46	1.51
19	C	508	CLA	CMD-C2D	-2.09	1.46	1.50
19	C	505	CLA	CMD-C2D	-2.09	1.46	1.50
19	A	405	CLA	CMD-C2D	-2.08	1.46	1.50
19	B	509	CLA	C3B-C2B	-2.08	1.37	1.40
19	B	507	CLA	CMD-C2D	-2.08	1.46	1.50
19	C	511	CLA	C3B-C2B	-2.08	1.37	1.40
19	C	509	CLA	CMD-C2D	-2.08	1.46	1.50
28	D	407	PL9	C53-C6	-2.07	1.46	1.50
19	A	403	CLA	CMD-C2D	-2.07	1.46	1.50
19	B	512	CLA	CMD-C2D	-2.07	1.46	1.50
20	D	402	PHO	C3B-C2B	-2.07	1.37	1.40
19	B	513	CLA	CMD-C2D	-2.07	1.46	1.50
19	B	503	CLA	C3B-C2B	-2.06	1.37	1.40
19	B	511	CLA	CMD-C2D	-2.06	1.46	1.50
19	A	405	CLA	C3B-CAB	-2.06	1.43	1.47
19	C	502	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	502	CLA	C3B-C2B	-2.06	1.37	1.40
19	B	510	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	404	PHO	CMB-C2B	-2.05	1.46	1.51
20	D	402	PHO	CMC-C2C	-2.05	1.46	1.51
19	C	504	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	404	PHO	CMC-C2C	-2.05	1.46	1.51
19	D	401	CLA	CMD-C2D	-2.05	1.46	1.50
19	B	511	CLA	CMC-C2C	-2.05	1.46	1.50
19	C	503	CLA	CMD-C2D	-2.04	1.46	1.50
19	B	501	CLA	C3B-C2B	-2.03	1.37	1.40
19	B	506	CLA	C3B-C2B	-2.03	1.37	1.40
21	C	515	BCR	C30-C25	-2.03	1.51	1.53
19	B	509	CLA	CMD-C2D	-2.03	1.46	1.50
19	C	507	CLA	CMD-C2D	-2.03	1.46	1.50
19	B	501	CLA	CMD-C2D	-2.02	1.46	1.50
19	B	515	CLA	CMD-C2D	-2.02	1.46	1.50
19	D	404	CLA	CMC-C2C	-2.02	1.46	1.50
29	F	101	HEM	CAA-C2A	2.02	1.55	1.52
19	C	504	CLA	CMC-C2C	-2.02	1.46	1.50
19	C	512	CLA	CMD-C2D	-2.01	1.46	1.50
19	B	508	CLA	C3B-C2B	-2.01	1.37	1.40
19	C	506	CLA	CMD-C2D	-2.01	1.46	1.50
19	B	511	CLA	C3B-C2B	-2.00	1.37	1.40
19	B	504	CLA	CMC-C2C	-2.00	1.46	1.50

All (545) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	D	406	BCR	C28-C27-C26	-6.00	103.36	114.08
21	C	514	BCR	C3-C4-C5	-5.89	103.56	114.08
19	B	513	CLA	C4A-NA-C1A	5.86	109.34	106.71
28	D	407	PL9	C7-C3-C4	5.80	121.59	116.88
21	A	406	BCR	C28-C27-C26	-5.80	103.72	114.08
19	B	512	CLA	C4A-NA-C1A	5.60	109.22	106.71
27	D	403	BCT	O2-C-O1	5.54	133.92	119.55
19	C	510	CLA	C4A-NA-C1A	5.53	109.19	106.71
21	C	515	BCR	C3-C4-C5	-5.34	104.55	114.08
19	C	509	CLA	C4A-NA-C1A	5.33	109.10	106.71
21	C	515	BCR	C30-C25-C26	-5.33	115.11	122.61
19	D	404	CLA	C4A-NA-C1A	5.26	109.07	106.71
21	A	406	BCR	C3-C4-C5	-5.18	104.83	114.08
19	C	507	CLA	C4A-NA-C1A	5.10	109.00	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	K	101	BCR	C28-C27-C26	-5.07	105.02	114.08
19	C	508	CLA	C4A-NA-C1A	5.06	108.98	106.71
19	C	502	CLA	C4A-NA-C1A	5.04	108.97	106.71
21	C	516	BCR	C28-C27-C26	-5.00	105.15	114.08
19	B	505	CLA	C4A-NA-C1A	4.97	108.94	106.71
19	B	510	CLA	C4A-NA-C1A	4.96	108.93	106.71
19	C	506	CLA	CMB-C2B-C1B	-4.94	120.88	128.46
21	B	518	BCR	C30-C25-C26	-4.90	115.71	122.61
21	H	101	BCR	C28-C27-C26	-4.85	105.42	114.08
21	C	514	BCR	C30-C25-C26	-4.84	115.80	122.61
21	C	514	BCR	C33-C5-C6	-4.81	119.13	124.53
19	B	515	CLA	C4A-NA-C1A	4.78	108.85	106.71
21	K	101	BCR	C30-C25-C26	-4.73	115.95	122.61
21	B	518	BCR	C28-C27-C26	-4.67	105.75	114.08
19	B	507	CLA	C4A-NA-C1A	4.62	108.78	106.71
19	B	502	CLA	C4A-NA-C1A	4.61	108.78	106.71
21	B	517	BCR	C3-C4-C5	-4.57	105.91	114.08
19	B	508	CLA	C4A-NA-C1A	4.49	108.72	106.71
19	C	503	CLA	C4A-NA-C1A	4.49	108.72	106.71
21	H	101	BCR	C1-C6-C5	-4.45	116.35	122.61
19	C	512	CLA	C4A-NA-C1A	4.44	108.70	106.71
21	K	101	BCR	C1-C6-C5	-4.43	116.38	122.61
19	A	405	CLA	C4A-NA-C1A	4.42	108.69	106.71
21	B	517	BCR	C1-C6-C5	-4.39	116.43	122.61
19	C	506	CLA	C4A-NA-C1A	4.38	108.68	106.71
19	B	509	CLA	C4A-NA-C1A	4.37	108.67	106.71
19	B	501	CLA	C4A-NA-C1A	4.35	108.66	106.71
21	C	516	BCR	C3-C4-C5	-4.35	106.32	114.08
21	H	101	BCR	C7-C8-C9	-4.31	119.72	126.23
21	B	519	BCR	C28-C27-C26	-4.30	106.39	114.08
19	D	401	CLA	C4A-NA-C1A	4.27	108.62	106.71
21	B	517	BCR	C30-C25-C26	-4.25	116.62	122.61
19	B	504	CLA	C4A-NA-C1A	4.22	108.60	106.71
19	B	503	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
21	K	101	BCR	C37-C22-C23	4.21	124.71	118.08
25	C	517	DGD	O2G-C1B-C2B	4.20	120.56	111.50
19	B	514	CLA	C4A-NA-C1A	4.18	108.58	106.71
19	C	504	CLA	C4A-NA-C1A	4.17	108.58	106.71
19	B	511	CLA	C4A-NA-C1A	4.16	108.58	106.71
23	A	408	LMG	O7-C10-C11	4.14	120.43	111.50
21	C	514	BCR	C28-C27-C26	-4.12	106.72	114.08
24	B	521	LHG	O7-C7-C8	4.12	120.37	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	D	405	CLA	C4A-NA-C1A	4.09	108.55	106.71
24	D	411	LHG	O7-C7-C8	4.01	120.15	111.50
25	J	101	DGD	O2G-C1B-C2B	4.01	120.15	111.50
19	C	506	CLA	CMB-C2B-C3B	3.99	132.15	124.68
19	C	511	CLA	C4A-NA-C1A	3.99	108.50	106.71
21	B	518	BCR	C36-C18-C19	3.95	124.30	118.08
21	B	517	BCR	C37-C22-C23	3.95	124.30	118.08
19	C	505	CLA	C4A-NA-C1A	3.93	108.47	106.71
19	C	513	CLA	C4A-NA-C1A	3.93	108.47	106.71
21	K	101	BCR	C36-C18-C19	3.93	124.26	118.08
19	A	403	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
21	C	514	BCR	C33-C5-C4	3.89	121.08	113.62
19	B	516	CLA	C4A-NA-C1A	3.88	108.45	106.71
23	B	520	LMG	O7-C10-C11	3.88	119.86	111.50
23	C	519	LMG	O7-C10-C11	3.86	119.82	111.50
21	C	515	BCR	C27-C26-C25	-3.85	117.14	122.73
21	B	518	BCR	C37-C22-C23	3.84	124.13	118.08
19	C	502	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
28	D	407	PL9	C7-C3-C2	-3.82	118.28	123.30
24	D	410	LHG	O7-C7-C8	3.81	119.72	111.50
19	B	503	CLA	C4A-NA-C1A	3.79	108.41	106.71
21	D	406	BCR	C36-C18-C19	3.79	124.05	118.08
22	A	407	SQD	O47-C7-C8	3.79	119.66	111.50
21	H	101	BCR	C3-C4-C5	-3.78	107.33	114.08
25	C	518	DGD	O2G-C1B-C2B	3.77	119.64	111.50
21	B	517	BCR	C36-C18-C19	3.76	123.99	118.08
19	C	501	CLA	C4A-NA-C1A	3.74	108.39	106.71
21	B	519	BCR	C1-C6-C5	-3.72	117.38	122.61
24	L	101	LHG	O7-C7-C8	3.71	119.50	111.50
19	D	405	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
21	C	514	BCR	C36-C18-C19	3.70	123.90	118.08
19	B	509	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
24	A	409	LHG	O7-C7-C8	3.67	119.41	111.50
21	C	514	BCR	C1-C6-C7	3.66	126.13	115.78
23	D	409	LMG	O7-C10-C11	3.65	119.37	111.50
19	A	402	CLA	C4A-NA-C1A	3.65	108.35	106.71
19	B	508	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
19	B	506	CLA	C4A-NA-C1A	3.64	108.34	106.71
21	B	519	BCR	C30-C25-C26	-3.64	117.49	122.61
21	D	406	BCR	C30-C25-C24	3.63	126.05	115.78
21	H	101	BCR	C36-C18-C19	3.63	123.80	118.08
24	D	408	LHG	O7-C7-C8	3.62	119.30	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	511	CLA	CMB-C2B-C1B	-3.60	122.92	128.46
19	B	504	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
19	B	506	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
19	D	401	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
19	C	508	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
19	B	510	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
21	D	406	BCR	C1-C6-C5	-3.56	117.60	122.61
21	C	515	BCR	C28-C27-C26	-3.56	107.73	114.08
21	B	519	BCR	C37-C22-C23	3.52	123.62	118.08
21	D	406	BCR	C1-C6-C7	3.52	125.73	115.78
21	D	406	BCR	C33-C5-C6	-3.50	120.59	124.53
21	K	101	BCR	C33-C5-C4	3.50	120.34	113.62
19	A	403	CLA	C4A-NA-C1A	3.50	108.28	106.71
21	B	517	BCR	C34-C9-C8	-3.49	112.58	118.08
21	H	101	BCR	C37-C22-C23	3.48	123.57	118.08
21	D	406	BCR	C37-C22-C23	3.48	123.56	118.08
21	B	519	BCR	C36-C18-C19	3.47	123.54	118.08
21	C	514	BCR	C27-C26-C25	-3.45	117.72	122.73
21	D	406	BCR	C38-C26-C27	3.45	120.24	113.62
21	A	406	BCR	C20-C21-C22	-3.44	122.40	127.31
19	C	501	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
23	B	522	LMG	O7-C10-C11	3.42	118.87	111.50
19	B	503	CLA	CMB-C2B-C3B	3.40	131.04	124.68
21	H	101	BCR	C4-C5-C6	-3.40	117.80	122.73
21	K	101	BCR	C11-C10-C9	-3.39	122.47	127.31
19	C	512	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
21	A	406	BCR	C36-C18-C19	3.39	123.42	118.08
21	B	518	BCR	C1-C6-C5	-3.39	117.84	122.61
21	B	517	BCR	C15-C16-C17	-3.39	116.54	123.47
21	C	515	BCR	C38-C26-C27	3.38	120.10	113.62
21	C	516	BCR	C37-C22-C23	3.38	123.40	118.08
19	D	405	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
21	C	514	BCR	C37-C22-C23	3.34	123.34	118.08
21	D	406	BCR	C30-C25-C26	-3.33	117.92	122.61
19	C	501	CLA	CAA-C2A-C1A	-3.33	101.06	111.97
19	D	401	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
21	K	101	BCR	C38-C26-C27	3.31	119.97	113.62
19	B	504	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
19	C	511	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
21	C	516	BCR	C7-C8-C9	-3.29	121.26	126.23
19	A	405	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
21	H	101	BCR	C11-C10-C9	-3.28	122.63	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	406	BCR	C29-C30-C25	3.28	115.53	110.48
21	C	515	BCR	C36-C18-C19	3.27	123.23	118.08
19	C	512	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
19	B	501	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
21	B	518	BCR	C38-C26-C27	3.23	119.83	113.62
19	B	513	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
21	D	406	BCR	C27-C26-C25	-3.22	118.06	122.73
21	C	514	BCR	C1-C6-C5	-3.21	118.08	122.61
21	C	515	BCR	C24-C23-C22	-3.20	121.39	126.23
21	B	519	BCR	C20-C21-C22	-3.20	122.74	127.31
21	B	519	BCR	C33-C5-C6	-3.18	120.95	124.53
21	H	101	BCR	C20-C21-C22	-3.18	122.77	127.31
21	K	101	BCR	C4-C5-C6	-3.16	118.14	122.73
19	A	403	CLA	CMB-C2B-C3B	3.16	130.59	124.68
21	B	517	BCR	C28-C27-C26	-3.16	108.44	114.08
21	B	519	BCR	C16-C17-C18	-3.16	122.80	127.31
19	B	510	CLA	CMB-C2B-C3B	3.16	130.58	124.68
21	K	101	BCR	C15-C16-C17	-3.15	117.01	123.47
21	B	518	BCR	C33-C5-C6	-3.15	120.99	124.53
19	C	502	CLA	CMB-C2B-C3B	3.15	130.57	124.68
21	B	518	BCR	C27-C26-C25	-3.15	118.16	122.73
21	B	517	BCR	C8-C9-C10	3.14	123.77	118.94
19	B	507	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
21	B	518	BCR	C33-C5-C4	3.13	119.64	113.62
19	D	405	CLA	CMB-C2B-C3B	3.13	130.54	124.68
19	C	511	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
21	A	406	BCR	C16-C17-C18	-3.13	122.84	127.31
19	B	511	CLA	CMB-C2B-C3B	3.11	130.49	124.68
19	B	516	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
19	C	501	CLA	O2D-CGD-O1D	-3.10	117.79	123.84
19	B	504	CLA	CMB-C2B-C3B	3.10	130.47	124.68
21	H	101	BCR	C16-C17-C18	-3.09	122.89	127.31
19	C	501	CLA	CMB-C2B-C3B	3.09	130.46	124.68
19	C	513	CLA	CMB-C2B-C1B	-3.08	123.72	128.46
19	C	507	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
21	A	406	BCR	C7-C8-C9	-3.08	121.58	126.23
19	B	512	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
19	A	403	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
19	B	506	CLA	CMB-C2B-C3B	3.06	130.41	124.68
19	A	405	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
21	C	516	BCR	C20-C21-C22	-3.04	122.97	127.31
21	H	101	BCR	C29-C30-C25	3.03	115.14	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	518	BCR	C20-C21-C22	-3.03	122.99	127.31
19	B	503	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
19	D	401	CLA	CMB-C2B-C3B	3.02	130.33	124.68
28	D	407	PL9	C22-C23-C24	-3.02	120.39	127.66
19	B	506	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
19	C	508	CLA	CMB-C2B-C3B	3.01	130.32	124.68
19	B	503	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
19	B	515	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
19	C	513	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
19	D	405	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
19	C	505	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
19	B	502	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
21	B	519	BCR	C33-C5-C4	2.99	119.37	113.62
21	B	517	BCR	C38-C26-C27	2.98	119.34	113.62
19	B	501	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
19	B	511	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
19	A	403	CLA	CHD-C1D-ND	-2.97	121.72	124.45
19	C	505	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
19	C	509	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
21	B	517	BCR	C38-C26-C25	-2.96	121.21	124.53
19	B	511	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
19	C	505	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
21	D	406	BCR	C3-C4-C5	-2.95	108.81	114.08
19	A	402	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
21	C	516	BCR	C36-C18-C19	2.95	122.72	118.08
19	B	508	CLA	CMB-C2B-C3B	2.95	130.19	124.68
19	B	508	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
19	B	509	CLA	CMB-C2B-C3B	2.94	130.19	124.68
19	B	502	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
19	B	502	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
21	K	101	BCR	C8-C9-C10	2.94	123.45	118.94
19	B	504	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
19	B	514	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
21	K	101	BCR	C38-C26-C25	-2.93	121.24	124.53
19	B	514	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
19	C	512	CLA	CMB-C2B-C3B	2.92	130.15	124.68
19	C	507	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
19	D	404	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
19	D	404	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
19	C	506	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
19	B	506	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	C	510	CLA	O2D-CGD-O1D	-2.88	118.20	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	514	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
19	B	507	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
19	B	512	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	C	512	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
21	B	519	BCR	C36-C18-C17	-2.87	118.90	122.92
19	C	504	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
19	B	508	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
19	C	513	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
19	B	501	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
21	A	406	BCR	C30-C25-C26	-2.85	118.59	122.61
19	C	504	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
21	K	101	BCR	C27-C26-C25	-2.85	118.59	122.73
19	C	509	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
21	K	101	BCR	C3-C4-C5	-2.84	109.00	114.08
21	B	518	BCR	C3-C4-C5	-2.84	109.00	114.08
24	D	410	LHG	O8-C23-C24	2.84	120.81	111.91
20	A	404	PHO	O1D-CGD-CBD	2.83	129.46	124.74
19	A	403	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
21	A	406	BCR	C23-C22-C21	2.83	123.28	118.94
19	C	501	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
19	B	516	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
19	B	507	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
19	B	510	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
19	C	504	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
19	D	401	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
19	A	402	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
19	C	502	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
19	B	509	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	C	519	LMG	O8-C28-C29	2.80	120.71	111.91
19	C	507	CLA	CMB-C2B-C3B	2.80	129.92	124.68
21	D	406	BCR	C16-C17-C18	-2.80	123.31	127.31
19	B	510	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
19	C	508	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
19	B	509	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
24	A	409	LHG	O8-C23-C24	2.79	120.67	111.91
28	D	407	PL9	C40-C39-C41	2.79	119.97	115.27
19	C	513	CLA	CMB-C2B-C3B	2.79	129.89	124.68
25	C	518	DGD	O1G-C1A-C2A	2.79	120.65	111.91
19	C	506	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
21	C	516	BCR	C16-C17-C18	-2.78	123.35	127.31
19	C	511	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
21	C	514	BCR	C16-C17-C18	-2.78	123.35	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	C	508	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	B	501	CLA	CMB-C2B-C3B	2.77	129.87	124.68
19	D	404	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
21	B	518	BCR	C37-C22-C21	-2.77	119.05	122.92
19	B	516	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
21	B	518	BCR	C7-C8-C9	-2.76	122.07	126.23
21	C	515	BCR	C7-C8-C9	-2.76	122.07	126.23
21	B	518	BCR	C16-C17-C18	-2.75	123.38	127.31
21	K	101	BCR	C33-C5-C6	-2.75	121.44	124.53
25	J	101	DGD	O1G-C1A-C2A	2.75	120.53	111.91
23	D	409	LMG	O8-C28-C29	2.75	120.52	111.91
24	B	521	LHG	O8-C23-C24	2.74	120.49	111.91
19	C	509	CLA	CMB-C2B-C3B	2.72	129.78	124.68
25	C	517	DGD	O1G-C1A-C2A	2.72	120.45	111.91
21	D	406	BCR	C33-C5-C4	2.71	118.83	113.62
19	A	402	CLA	CAC-C3C-C4C	2.71	128.33	124.81
19	B	516	CLA	CMB-C2B-C3B	2.71	129.75	124.68
21	D	406	BCR	C29-C30-C25	2.70	114.64	110.48
21	K	101	BCR	C37-C22-C21	-2.70	119.14	122.92
19	A	402	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
21	A	406	BCR	C2-C1-C6	2.69	114.63	110.48
20	D	402	PHO	O1D-CGD-CBD	2.69	129.22	124.74
21	K	101	BCR	C20-C21-C22	-2.69	123.47	127.31
21	B	518	BCR	C15-C16-C17	-2.69	117.97	123.47
21	A	406	BCR	C27-C26-C25	-2.69	118.83	122.73
21	H	101	BCR	C30-C25-C26	-2.68	118.83	122.61
19	B	512	CLA	CMB-C2B-C3B	2.68	129.69	124.68
22	A	407	SQD	O5-C5-C4	2.68	114.55	109.69
22	A	407	SQD	O48-C23-C24	2.68	120.31	111.91
20	D	402	PHO	O2D-CGD-O1D	-2.67	118.61	123.84
19	C	505	CLA	CMB-C2B-C3B	2.67	129.68	124.68
21	C	514	BCR	C8-C9-C10	2.67	123.04	118.94
21	B	519	BCR	C37-C22-C21	-2.67	119.19	122.92
29	F	101	HEM	C1B-NB-C4B	2.66	107.82	105.07
21	B	519	BCR	C3-C4-C5	-2.65	109.34	114.08
21	B	518	BCR	C36-C18-C17	-2.65	119.22	122.92
21	B	519	BCR	C7-C8-C9	-2.65	122.24	126.23
19	B	505	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
19	C	511	CLA	CMB-C2B-C3B	2.65	129.63	124.68
19	B	507	CLA	CMB-C2B-C3B	2.64	129.61	124.68
21	C	515	BCR	C20-C21-C22	-2.63	123.55	127.31
19	B	502	CLA	CMB-C2B-C3B	2.63	129.59	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	515	CLA	CMB-C2B-C1B	-2.63	124.43	128.46
25	C	517	DGD	O6D-C5D-C6D	2.62	111.96	106.67
20	D	402	PHO	CMC-C2C-C3C	2.62	129.88	124.94
21	D	406	BCR	C38-C26-C25	-2.62	121.59	124.53
19	C	503	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
29	F	101	HEM	C4D-ND-C1D	2.61	107.77	105.07
19	C	512	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	D	404	CLA	CMB-C2B-C3B	2.61	129.56	124.68
19	C	504	CLA	CHD-C1D-ND	-2.61	122.06	124.45
21	H	101	BCR	C36-C18-C17	-2.60	119.28	122.92
21	B	517	BCR	C20-C21-C22	-2.60	123.60	127.31
21	H	101	BCR	C27-C26-C25	-2.60	118.96	122.73
19	B	512	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
19	C	510	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
21	C	515	BCR	C16-C17-C18	-2.59	123.61	127.31
19	C	503	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
20	A	404	PHO	O2D-CGD-O1D	-2.58	118.78	123.84
21	B	517	BCR	C37-C22-C21	-2.58	119.31	122.92
19	B	513	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
19	B	515	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
19	C	501	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
24	B	521	LHG	C5-O7-C7	-2.57	111.46	117.79
19	C	511	CLA	CHD-C1D-ND	-2.57	122.09	124.45
21	B	517	BCR	C33-C5-C4	2.57	118.55	113.62
19	C	503	CLA	C1-C2-C3	-2.56	121.61	126.04
19	C	509	CLA	CHB-C4A-NA	2.56	128.05	124.51
19	B	502	CLA	CHD-C1D-ND	-2.56	122.10	124.45
19	D	401	CLA	O2D-CGD-CBD	2.56	115.82	111.27
19	C	507	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
20	A	404	PHO	CMB-C2B-C3B	2.54	129.44	124.68
19	C	503	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
20	A	404	PHO	C1-C2-C3	-2.54	121.65	126.04
19	B	506	CLA	CHD-C1D-ND	-2.54	122.12	124.45
19	A	402	CLA	CHD-C1D-ND	-2.53	122.12	124.45
19	A	405	CLA	CMB-C2B-C1B	-2.53	124.58	128.46
19	B	504	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	C	504	CLA	CMB-C2B-C3B	2.52	129.40	124.68
19	B	505	CLA	CHD-C1D-ND	-2.52	122.14	124.45
21	B	517	BCR	C11-C10-C9	-2.52	123.71	127.31
19	B	512	CLA	CHB-C4A-NA	2.51	127.99	124.51
19	A	405	CLA	CHD-C1D-ND	-2.50	122.15	124.45
20	D	402	PHO	CMB-C2B-C3B	2.50	129.35	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	C	503	CLA	CHD-C1D-ND	-2.50	122.16	124.45
19	A	405	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	C	509	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
21	C	515	BCR	C15-C16-C17	-2.48	118.39	123.47
19	B	514	CLA	CMB-C2B-C3B	2.48	129.32	124.68
21	C	514	BCR	C7-C6-C5	-2.48	115.46	121.46
19	C	505	CLA	CHD-C1D-ND	-2.48	122.18	124.45
20	A	404	PHO	CMC-C2C-C3C	2.48	129.61	124.94
28	D	407	PL9	C36-C34-C33	-2.47	116.12	121.12
19	B	513	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	B	507	CLA	CHD-C1D-ND	-2.47	122.19	124.45
19	B	505	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
28	D	407	PL9	C7-C8-C9	-2.46	122.69	126.79
19	B	513	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
29	F	101	HEM	C4B-CHC-C1C	2.46	125.81	122.56
21	D	406	BCR	C20-C21-C22	-2.46	123.80	127.31
21	K	101	BCR	C16-C17-C18	-2.46	123.80	127.31
19	A	405	CLA	O2D-CGD-CBD	2.46	115.64	111.27
19	C	502	CLA	C1-C2-C3	-2.46	121.80	126.04
25	J	101	DGD	O6D-C5D-C6D	2.46	111.62	106.67
19	C	510	CLA	CHD-C1D-ND	-2.45	122.20	124.45
21	C	514	BCR	C11-C10-C9	-2.45	123.81	127.31
19	D	405	CLA	CHD-C1D-ND	-2.45	122.20	124.45
21	H	101	BCR	C37-C22-C21	-2.45	119.49	122.92
28	D	407	PL9	C20-C19-C21	2.45	119.39	115.27
21	B	517	BCR	C4-C5-C6	-2.45	119.17	122.73
25	C	518	DGD	C1E-C2E-C3E	2.45	115.09	110.00
21	C	515	BCR	C11-C10-C9	-2.44	123.82	127.31
21	B	517	BCR	C19-C18-C17	-2.44	115.19	118.94
21	B	519	BCR	C38-C26-C27	2.44	118.31	113.62
19	B	516	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	C	515	BCR	C4-C5-C6	-2.44	119.19	122.73
21	C	516	BCR	C2-C1-C6	2.43	114.23	110.48
19	B	506	CLA	CHB-C4A-NA	2.43	127.88	124.51
19	C	510	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
19	C	508	CLA	CHB-C4A-NA	2.43	127.87	124.51
21	C	514	BCR	C15-C16-C17	-2.42	118.51	123.47
19	B	511	CLA	CHD-C1D-ND	-2.42	122.23	124.45
23	A	408	LMG	O8-C28-C29	2.42	119.50	111.91
24	D	411	LHG	O8-C23-C24	2.42	119.49	111.91
19	B	507	CLA	CHB-C4A-NA	2.42	127.85	124.51
21	C	514	BCR	C20-C21-C22	-2.41	123.87	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	502	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	B	501	CLA	CHD-C1D-ND	-2.41	122.24	124.45
19	B	503	CLA	C4-C3-C5	2.41	119.32	115.27
21	B	518	BCR	C38-C26-C25	-2.41	121.82	124.53
21	A	406	BCR	C38-C26-C27	2.40	118.23	113.62
19	D	405	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	L	101	LHG	O8-C23-C24	2.40	119.44	111.91
19	A	405	CLA	CMB-C2B-C3B	2.40	129.16	124.68
21	H	101	BCR	C16-C15-C14	-2.39	118.57	123.47
21	C	514	BCR	C34-C9-C8	-2.39	114.31	118.08
21	C	516	BCR	C38-C26-C25	-2.39	121.84	124.53
21	C	515	BCR	C2-C1-C6	2.38	114.14	110.48
21	B	519	BCR	C38-C26-C25	-2.38	121.86	124.53
21	A	406	BCR	C36-C18-C17	-2.36	119.61	122.92
19	B	509	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
19	C	510	CLA	CHB-C4A-NA	2.36	127.78	124.51
19	C	513	CLA	CHB-C4A-NA	2.36	127.77	124.51
21	B	518	BCR	C4-C5-C6	-2.35	119.31	122.73
21	B	517	BCR	C27-C26-C25	-2.35	119.32	122.73
19	B	503	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	C	503	CLA	CMB-C2B-C3B	2.34	129.06	124.68
19	B	515	CLA	CMB-C2B-C3B	2.34	129.06	124.68
24	D	408	LHG	O8-C23-C24	2.34	119.26	111.91
21	B	519	BCR	C16-C15-C14	-2.34	118.68	123.47
21	C	516	BCR	C16-C15-C14	-2.33	118.70	123.47
19	C	502	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
21	D	406	BCR	C15-C16-C17	-2.32	118.72	123.47
19	D	404	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	B	515	CLA	CHB-C4A-NA	2.32	127.72	124.51
23	B	522	LMG	O8-C28-C29	2.32	119.18	111.91
21	A	406	BCR	C16-C15-C14	-2.31	118.73	123.47
19	C	502	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
19	B	511	CLA	CHB-C4A-NA	2.31	127.70	124.51
21	C	516	BCR	C37-C22-C21	-2.31	119.69	122.92
24	D	411	LHG	C5-O7-C7	-2.31	112.11	117.79
19	B	505	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	B	508	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	B	512	CLA	CHD-C1D-ND	-2.29	122.35	124.45
21	B	517	BCR	C15-C14-C13	-2.29	124.04	127.31
21	C	515	BCR	C33-C5-C4	2.29	118.01	113.62
21	D	406	BCR	C36-C18-C17	-2.29	119.72	122.92
19	B	510	CLA	CHB-C4A-NA	2.28	127.67	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	D	405	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
21	K	101	BCR	C19-C18-C17	-2.28	115.45	118.94
19	C	506	CLA	CHD-C1D-ND	-2.28	122.36	124.45
21	D	406	BCR	C7-C8-C9	-2.28	122.80	126.23
19	C	510	CLA	CMB-C2B-C3B	2.28	128.94	124.68
19	B	515	CLA	CHD-C1D-ND	-2.27	122.37	124.45
21	C	516	BCR	C8-C7-C6	-2.27	120.83	127.20
22	A	407	SQD	O7-S-C6	2.26	109.63	106.94
22	A	407	SQD	O8-S-C6	2.26	109.35	105.74
19	A	402	CLA	CMB-C2B-C3B	2.26	128.91	124.68
19	B	501	CLA	CHB-C4A-NA	2.26	127.64	124.51
19	C	509	CLA	CHD-C1D-ND	-2.26	122.38	124.45
19	B	513	CLA	CMB-C2B-C3B	2.25	128.89	124.68
19	A	402	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	D	409	LMG	O1-C1-C2	2.25	111.81	108.30
21	D	406	BCR	C24-C25-C26	-2.24	116.03	121.46
21	A	406	BCR	C24-C23-C22	-2.24	122.85	126.23
19	B	509	CLA	CHD-C1D-ND	-2.24	122.39	124.45
19	B	514	CLA	CHD-C1D-ND	-2.23	122.40	124.45
23	B	520	LMG	O8-C28-C29	2.22	118.88	111.91
28	D	407	PL9	O1-C4-C3	-2.22	118.27	120.72
19	B	514	CLA	CHB-C4A-NA	2.22	127.58	124.51
29	F	101	HEM	C4C-CHD-C1D	2.22	125.49	122.56
19	C	512	CLA	O2D-CGD-CBD	2.22	115.20	111.27
19	C	505	CLA	CHB-C4A-NA	2.21	127.56	124.51
21	C	514	BCR	C15-C14-C13	-2.21	124.16	127.31
19	C	506	CLA	CHB-C4A-NA	2.20	127.56	124.51
19	A	403	CLA	O2D-CGD-CBD	2.20	115.18	111.27
21	C	516	BCR	C29-C30-C25	2.20	113.87	110.48
24	L	101	LHG	C5-O7-C7	-2.20	112.37	117.79
19	B	509	CLA	C1-C2-C3	-2.20	122.24	126.04
19	B	516	CLA	CHD-C1D-ND	-2.20	122.43	124.45
21	C	515	BCR	C1-C6-C5	-2.19	119.53	122.61
19	C	501	CLA	CHB-C4A-NA	2.18	127.53	124.51
21	H	101	BCR	C24-C23-C22	-2.18	122.94	126.23
19	B	503	CLA	CHD-C1D-ND	-2.18	122.45	124.45
21	K	101	BCR	C30-C25-C24	2.17	121.93	115.78
19	C	507	CLA	CHB-C4A-NA	2.17	127.51	124.51
19	B	511	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
22	A	407	SQD	O9-S-C6	2.16	109.50	106.94
21	D	406	BCR	C16-C15-C14	-2.16	119.05	123.47
19	A	403	CLA	CHB-C4A-NA	2.16	127.50	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	D	407	PL9	C31-C32-C33	-2.16	104.79	111.88
21	H	101	BCR	C31-C1-C6	-2.16	106.80	110.30
19	B	512	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
21	B	519	BCR	C4-C5-C6	-2.15	119.61	122.73
21	B	517	BCR	C33-C5-C6	-2.15	122.12	124.53
21	C	514	BCR	C4-C5-C6	-2.14	119.62	122.73
21	B	519	BCR	C27-C26-C25	-2.14	119.62	122.73
28	D	407	PL9	O2-C1-C6	2.14	124.30	120.59
19	B	508	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
19	B	508	CLA	CHD-C1D-ND	-2.14	122.49	124.45
21	C	516	BCR	C32-C1-C6	-2.14	106.83	110.30
19	B	502	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
19	D	404	CLA	O2D-CGD-CBD	2.14	115.06	111.27
19	B	505	CLA	CMB-C2B-C1B	-2.13	125.18	128.46
19	C	512	CLA	CHD-C1D-ND	-2.13	122.50	124.45
28	D	407	PL9	O2-C1-C2	-2.13	116.90	121.78
19	D	401	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
19	C	511	CLA	CHB-C4A-NA	2.13	127.45	124.51
19	C	513	CLA	CHD-C1D-ND	-2.13	122.50	124.45
19	C	513	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
19	C	512	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
21	C	514	BCR	C36-C18-C17	-2.12	119.95	122.92
20	A	404	PHO	O2A-CGA-O1A	-2.12	118.25	123.59
26	C	520	LMU	O1B-C4'-C3'	2.12	112.91	107.28
22	A	407	SQD	C3-C4-C5	2.11	114.01	110.24
19	C	508	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	B	513	CLA	O2D-CGD-CBD	2.10	115.01	111.27
19	B	513	CLA	CHD-C1D-ND	-2.10	122.52	124.45
19	C	511	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
19	C	507	CLA	C1-C2-C3	-2.10	122.41	126.04
21	B	518	BCR	C30-C25-C24	2.10	121.71	115.78
21	A	406	BCR	C33-C5-C4	2.09	117.63	113.62
21	H	101	BCR	C38-C26-C27	2.08	117.62	113.62
19	C	504	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
22	A	407	SQD	C45-O47-C7	-2.08	112.67	117.79
19	B	510	CLA	CHD-C1D-ND	-2.08	122.54	124.45
21	C	514	BCR	C24-C23-C22	-2.08	123.09	126.23
21	A	406	BCR	C4-C5-C6	-2.08	119.72	122.73
19	D	401	CLA	CHB-C4A-NA	2.07	127.38	124.51
21	H	101	BCR	C32-C1-C6	2.07	113.66	110.30
19	C	506	CLA	C1-C2-C3	-2.06	122.49	126.04
19	B	511	CLA	C1-C2-C3	-2.05	122.49	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	C	506	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	B	507	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
21	H	101	BCR	C15-C16-C17	-2.05	119.28	123.47
19	B	509	CLA	CHB-C4A-NA	2.04	127.34	124.51
19	C	501	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	C	516	BCR	C11-C10-C9	-2.04	124.40	127.31
21	A	406	BCR	C23-C24-C25	-2.04	121.48	127.20
19	C	511	CLA	O1D-CGD-CBD	2.03	128.65	124.48
27	D	403	BCT	O3-C-O1	-2.03	114.27	119.55
21	C	516	BCR	C15-C16-C17	-2.03	119.31	123.47
19	C	502	CLA	CHD-C1D-ND	-2.03	122.59	124.45
19	C	508	CLA	C1-C2-C3	-2.03	122.53	126.04
19	C	504	CLA	CHB-C4A-NA	2.03	127.32	124.51
21	C	516	BCR	C23-C24-C25	-2.03	121.51	127.20
21	D	406	BCR	C23-C22-C21	-2.03	115.83	118.94
29	F	101	HEM	CMC-C2C-C3C	2.03	128.47	124.68
19	C	510	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
19	C	503	CLA	CHB-C4A-NA	2.02	127.30	124.51
19	A	405	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
29	F	101	HEM	C3B-C2B-C1B	2.01	107.98	106.49
23	A	408	LMG	C8-O7-C10	-2.01	112.84	117.79
19	D	404	CLA	CHD-C1D-ND	-2.01	122.61	124.45
21	D	406	BCR	C12-C13-C14	-2.01	115.86	118.94
28	D	407	PL9	C27-C28-C29	-2.00	122.83	127.66
21	C	514	BCR	C23-C22-C21	-2.00	115.87	118.94
19	C	503	CLA	C16-C15-C13	-2.00	109.44	115.92
19	C	501	CLA	O2D-CGD-CBD	2.00	114.82	111.27

All (33) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	402	CLA	ND
19	A	403	CLA	ND
19	B	501	CLA	ND
19	B	502	CLA	ND
19	B	503	CLA	ND
19	B	504	CLA	ND
19	B	505	CLA	ND
19	B	506	CLA	ND
19	B	507	CLA	ND
19	B	508	CLA	ND
19	B	509	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	510	CLA	ND
19	B	511	CLA	ND
19	B	512	CLA	ND
19	B	513	CLA	ND
19	B	514	CLA	ND
19	B	515	CLA	ND
19	B	516	CLA	ND
19	C	501	CLA	ND
19	C	502	CLA	ND
19	C	503	CLA	ND
19	C	504	CLA	ND
19	C	505	CLA	ND
19	C	506	CLA	ND
19	C	507	CLA	ND
19	C	508	CLA	ND
19	C	509	CLA	ND
19	C	510	CLA	ND
19	C	511	CLA	ND
19	C	512	CLA	ND
19	C	513	CLA	ND
19	D	401	CLA	ND
19	D	405	CLA	ND

All (703) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	402	CLA	O2A-C1-C2-C3
19	A	405	CLA	C1A-C2A-CAA-CBA
19	A	405	CLA	C3A-C2A-CAA-CBA
19	B	501	CLA	C1A-C2A-CAA-CBA
19	B	501	CLA	CHA-CBD-CGD-O1D
19	B	501	CLA	CHA-CBD-CGD-O2D
19	B	503	CLA	C1A-C2A-CAA-CBA
19	B	503	CLA	C3A-C2A-CAA-CBA
19	B	503	CLA	C2-C3-C5-C6
19	B	503	CLA	C4-C3-C5-C6
19	B	504	CLA	C3A-C2A-CAA-CBA
19	B	504	CLA	CHA-CBD-CGD-O1D
19	B	504	CLA	CHA-CBD-CGD-O2D
19	B	504	CLA	CAD-CBD-CGD-O1D
19	B	504	CLA	CAD-CBD-CGD-O2D
19	B	505	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B	505	CLA	CHA-CBD-CGD-O2D
19	B	506	CLA	C1A-C2A-CAA-CBA
19	B	506	CLA	C3A-C2A-CAA-CBA
19	B	507	CLA	C1A-C2A-CAA-CBA
19	B	507	CLA	C3A-C2A-CAA-CBA
19	B	508	CLA	CHA-CBD-CGD-O1D
19	B	508	CLA	CHA-CBD-CGD-O2D
19	B	509	CLA	C1A-C2A-CAA-CBA
19	B	509	CLA	C3A-C2A-CAA-CBA
19	B	510	CLA	CBD-CGD-O2D-CED
19	B	511	CLA	C11-C12-C13-C14
19	B	512	CLA	C6-C7-C8-C10
19	C	502	CLA	CHA-CBD-CGD-O1D
19	C	502	CLA	CHA-CBD-CGD-O2D
19	C	502	CLA	CAD-CBD-CGD-O1D
19	C	506	CLA	C1A-C2A-CAA-CBA
19	C	506	CLA	C3A-C2A-CAA-CBA
19	C	506	CLA	CHA-CBD-CGD-O1D
19	C	506	CLA	CHA-CBD-CGD-O2D
19	C	507	CLA	CHA-CBD-CGD-O1D
19	C	507	CLA	CHA-CBD-CGD-O2D
19	C	511	CLA	C1A-C2A-CAA-CBA
19	C	511	CLA	C3A-C2A-CAA-CBA
19	C	511	CLA	CAD-CBD-CGD-O1D
19	C	511	CLA	CAD-CBD-CGD-O2D
19	C	511	CLA	CBD-CGD-O2D-CED
19	C	512	CLA	CHA-CBD-CGD-O1D
19	C	512	CLA	CHA-CBD-CGD-O2D
19	C	512	CLA	C4-C3-C5-C6
19	C	513	CLA	CBD-CGD-O2D-CED
19	C	513	CLA	O1D-CGD-O2D-CED
19	C	513	CLA	C11-C10-C8-C9
19	D	404	CLA	C1A-C2A-CAA-CBA
19	D	405	CLA	CHA-CBD-CGD-O1D
19	D	405	CLA	CHA-CBD-CGD-O2D
19	D	405	CLA	CAD-CBD-CGD-O1D
19	D	405	CLA	CAD-CBD-CGD-O2D
21	B	517	BCR	C1-C6-C7-C8
21	B	517	BCR	C5-C6-C7-C8
21	B	517	BCR	C7-C8-C9-C10
21	B	517	BCR	C7-C8-C9-C34
21	B	517	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
21	B	518	BCR	C1-C6-C7-C8
21	B	518	BCR	C5-C6-C7-C8
21	B	518	BCR	C23-C24-C25-C26
21	B	519	BCR	C1-C6-C7-C8
21	B	519	BCR	C5-C6-C7-C8
21	B	519	BCR	C23-C24-C25-C26
21	C	514	BCR	C23-C24-C25-C26
21	C	514	BCR	C23-C24-C25-C30
21	C	515	BCR	C23-C24-C25-C26
21	H	101	BCR	C5-C6-C7-C8
21	H	101	BCR	C23-C24-C25-C26
21	K	101	BCR	C1-C6-C7-C8
21	K	101	BCR	C5-C6-C7-C8
21	K	101	BCR	C7-C8-C9-C10
21	K	101	BCR	C7-C8-C9-C34
21	K	101	BCR	C23-C24-C25-C26
22	A	407	SQD	C8-C7-O47-C45
23	A	408	LMG	O6-C1-O1-C7
24	B	521	LHG	C4-O6-P-O4
24	B	521	LHG	C4-O6-P-O5
24	D	408	LHG	C3-O3-P-O6
24	D	410	LHG	C4-O6-P-O5
24	D	411	LHG	C3-O3-P-O4
24	D	411	LHG	C4-O6-P-O5
28	D	407	PL9	C7-C8-C9-C11
28	D	407	PL9	C42-C43-C44-C46
28	D	407	PL9	C47-C48-C49-C51
19	A	402	CLA	O1D-CGD-O2D-CED
19	B	505	CLA	O1D-CGD-O2D-CED
19	B	514	CLA	O1D-CGD-O2D-CED
19	B	516	CLA	O1D-CGD-O2D-CED
19	C	503	CLA	O1D-CGD-O2D-CED
19	C	506	CLA	O1D-CGD-O2D-CED
19	A	402	CLA	CBD-CGD-O2D-CED
19	B	504	CLA	CBD-CGD-O2D-CED
19	B	505	CLA	CBD-CGD-O2D-CED
19	B	507	CLA	CBD-CGD-O2D-CED
19	B	508	CLA	CBD-CGD-O2D-CED
19	B	509	CLA	CBD-CGD-O2D-CED
19	B	514	CLA	CBD-CGD-O2D-CED
19	B	516	CLA	CBD-CGD-O2D-CED
19	C	502	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	C	503	CLA	CBD-CGD-O2D-CED
19	C	506	CLA	CBD-CGD-O2D-CED
20	D	402	PHO	CBD-CGD-O2D-CED
19	D	405	CLA	O1A-CGA-O2A-C1
20	A	404	PHO	O1A-CGA-O2A-C1
19	C	511	CLA	O1D-CGD-O2D-CED
19	D	405	CLA	CBA-CGA-O2A-C1
19	D	405	CLA	CBD-CGD-O2D-CED
19	B	505	CLA	O1A-CGA-O2A-C1
19	B	507	CLA	O1A-CGA-O2A-C1
19	C	505	CLA	O1A-CGA-O2A-C1
19	C	506	CLA	O1A-CGA-O2A-C1
19	C	510	CLA	O1A-CGA-O2A-C1
19	D	401	CLA	O1A-CGA-O2A-C1
19	B	510	CLA	O1D-CGD-O2D-CED
19	A	405	CLA	CBD-CGD-O2D-CED
22	A	407	SQD	O49-C7-O47-C45
19	B	506	CLA	O1A-CGA-O2A-C1
20	A	404	PHO	CBA-CGA-O2A-C1
23	D	409	LMG	C29-C28-O8-C9
28	D	407	PL9	C47-C48-C49-C50
19	B	508	CLA	O1D-CGD-O2D-CED
19	B	509	CLA	O1D-CGD-O2D-CED
19	A	403	CLA	CBD-CGD-O2D-CED
19	B	516	CLA	O1A-CGA-O2A-C1
19	C	512	CLA	C2-C3-C5-C6
19	B	510	CLA	C2A-CAA-CBA-CGA
19	C	501	CLA	C2A-CAA-CBA-CGA
19	C	502	CLA	C2A-CAA-CBA-CGA
19	D	401	CLA	C2A-CAA-CBA-CGA
26	C	520	LMU	C3'-C4'-O1B-C1B
19	B	506	CLA	C3-C5-C6-C7
19	A	405	CLA	CBA-CGA-O2A-C1
19	B	505	CLA	CBA-CGA-O2A-C1
19	B	506	CLA	CBA-CGA-O2A-C1
19	B	507	CLA	CBA-CGA-O2A-C1
19	B	512	CLA	CBA-CGA-O2A-C1
19	B	516	CLA	CBA-CGA-O2A-C1
19	C	505	CLA	CBA-CGA-O2A-C1
19	C	506	CLA	CBA-CGA-O2A-C1
19	C	510	CLA	CBA-CGA-O2A-C1
19	D	401	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	507	CLA	O1D-CGD-O2D-CED
19	C	502	CLA	O1D-CGD-O2D-CED
28	D	407	PL9	C42-C43-C44-C45
19	C	505	CLA	CBD-CGD-O2D-CED
19	B	504	CLA	O1D-CGD-O2D-CED
23	D	409	LMG	O10-C28-O8-C9
20	D	402	PHO	O1D-CGD-O2D-CED
19	B	507	CLA	C3-C5-C6-C7
19	C	506	CLA	C3-C5-C6-C7
20	D	402	PHO	C3-C5-C6-C7
19	B	502	CLA	CBA-CGA-O2A-C1
19	B	509	CLA	CBA-CGA-O2A-C1
19	C	513	CLA	CBA-CGA-O2A-C1
20	D	402	PHO	CBA-CGA-O2A-C1
19	A	405	CLA	O1A-CGA-O2A-C1
19	B	502	CLA	O1A-CGA-O2A-C1
19	B	508	CLA	O1A-CGA-O2A-C1
19	B	509	CLA	O1A-CGA-O2A-C1
20	D	402	PHO	O1A-CGA-O2A-C1
19	B	508	CLA	CBA-CGA-O2A-C1
19	B	512	CLA	O1A-CGA-O2A-C1
28	D	407	PL9	C39-C41-C42-C43
28	D	407	PL9	C44-C46-C47-C48
19	C	511	CLA	CBA-CGA-O2A-C1
19	C	513	CLA	O1A-CGA-O2A-C1
28	D	407	PL9	C7-C8-C9-C10
26	C	520	LMU	O5'-C5'-C6'-O6'
19	C	511	CLA	O1A-CGA-O2A-C1
19	B	503	CLA	C3-C5-C6-C7
19	A	402	CLA	CBA-CGA-O2A-C1
19	B	501	CLA	CBA-CGA-O2A-C1
19	B	513	CLA	CBA-CGA-O2A-C1
19	B	515	CLA	CBA-CGA-O2A-C1
19	C	508	CLA	CBA-CGA-O2A-C1
19	A	402	CLA	C8-C10-C11-C12
19	B	511	CLA	C8-C10-C11-C12
19	C	503	CLA	C8-C10-C11-C12
23	B	522	LMG	O7-C8-C9-O8
19	C	508	CLA	O1A-CGA-O2A-C1
19	B	505	CLA	C4-C3-C5-C6
19	B	507	CLA	C6-C7-C8-C9
19	B	509	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	C	502	CLA	C11-C10-C8-C9
19	C	511	CLA	C11-C12-C13-C14
20	D	402	PHO	C11-C12-C13-C14
21	A	406	BCR	C37-C22-C23-C24
21	C	514	BCR	C7-C8-C9-C34
21	A	406	BCR	C21-C22-C23-C24
21	C	514	BCR	C7-C8-C9-C10
19	B	515	CLA	O1A-CGA-O2A-C1
19	A	403	CLA	CBA-CGA-O2A-C1
19	C	509	CLA	C5-C6-C7-C8
19	B	501	CLA	CBD-CGD-O2D-CED
19	B	511	CLA	C15-C16-C17-C18
19	D	404	CLA	C10-C11-C12-C13
19	D	405	CLA	C5-C6-C7-C8
24	D	408	LHG	C7-C8-C9-C10
19	D	404	CLA	C8-C10-C11-C12
19	C	501	CLA	CBD-CGD-O2D-CED
19	C	501	CLA	C8-C10-C11-C12
19	A	402	CLA	C11-C10-C8-C7
19	B	502	CLA	C6-C7-C8-C10
19	B	513	CLA	C12-C13-C15-C16
19	C	513	CLA	C6-C7-C8-C10
19	A	402	CLA	O1A-CGA-O2A-C1
19	B	516	CLA	C2A-CAA-CBA-CGA
19	C	505	CLA	C2A-CAA-CBA-CGA
19	D	405	CLA	O1D-CGD-O2D-CED
19	C	512	CLA	C5-C6-C7-C8
19	B	501	CLA	O1A-CGA-O2A-C1
19	B	513	CLA	O1A-CGA-O2A-C1
19	B	502	CLA	C5-C6-C7-C8
19	B	516	CLA	C15-C16-C17-C18
19	C	501	CLA	C13-C15-C16-C17
19	A	405	CLA	O1D-CGD-O2D-CED
23	B	522	LMG	C10-C11-C12-C13
19	B	507	CLA	C13-C15-C16-C17
19	B	511	CLA	C13-C15-C16-C17
19	C	501	CLA	C15-C16-C17-C18
19	C	505	CLA	C15-C16-C17-C18
19	A	403	CLA	O1A-CGA-O2A-C1
19	B	504	CLA	C13-C15-C16-C17
19	B	507	CLA	C10-C11-C12-C13
19	C	511	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	C	512	CLA	C8-C10-C11-C12
24	A	409	LHG	C4-O6-P-O3
24	B	521	LHG	C4-O6-P-O3
24	D	411	LHG	C3-O3-P-O6
24	D	411	LHG	C4-O6-P-O3
24	L	101	LHG	C3-O3-P-O6
19	A	403	CLA	O1D-CGD-O2D-CED
25	J	101	DGD	C1A-C2A-C3A-C4A
19	B	515	CLA	C2A-CAA-CBA-CGA
25	C	518	DGD	C2A-C1A-O1G-C1G
26	C	520	LMU	C4'-C5'-C6'-O6'
23	D	409	LMG	C30-C31-C32-C33
19	C	511	CLA	C3-C5-C6-C7
19	C	505	CLA	O1D-CGD-O2D-CED
23	A	408	LMG	C2-C1-O1-C7
24	D	411	LHG	O7-C5-C6-O8
23	B	520	LMG	C13-C14-C15-C16
19	C	501	CLA	C10-C11-C12-C13
19	C	502	CLA	C5-C6-C7-C8
25	C	518	DGD	O1A-C1A-O1G-C1G
19	C	507	CLA	C16-C17-C18-C19
24	D	410	LHG	C9-C10-C11-C12
19	B	515	CLA	C6-C7-C8-C9
19	C	506	CLA	C6-C7-C8-C9
19	C	507	CLA	C14-C13-C15-C16
19	D	404	CLA	C11-C12-C13-C14
24	D	411	LHG	C7-C8-C9-C10
19	B	509	CLA	C2A-CAA-CBA-CGA
19	C	510	CLA	C2A-CAA-CBA-CGA
20	D	402	PHO	C2A-CAA-CBA-CGA
24	D	411	LHG	O9-C7-O7-C5
24	D	411	LHG	C8-C7-O7-C5
24	L	101	LHG	C17-C18-C19-C20
19	B	510	CLA	C16-C17-C18-C19
19	C	503	CLA	C16-C17-C18-C20
19	C	507	CLA	C16-C17-C18-C20
20	A	404	PHO	C13-C15-C16-C17
23	B	522	LMG	C31-C32-C33-C34
26	C	520	LMU	C4-C5-C6-C7
24	D	410	LHG	C23-C24-C25-C26
19	C	512	CLA	CBA-CGA-O2A-C1
19	B	501	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B	515	CLA	C3A-C2A-CAA-CBA
19	B	516	CLA	C3A-C2A-CAA-CBA
19	C	507	CLA	C3A-C2A-CAA-CBA
19	D	404	CLA	C3A-C2A-CAA-CBA
20	D	402	PHO	C3A-C2A-CAA-CBA
19	B	510	CLA	C16-C17-C18-C20
19	C	503	CLA	C16-C17-C18-C19
19	C	506	CLA	C4-C3-C5-C6
20	A	404	PHO	C4-C3-C5-C6
19	B	510	CLA	CBA-CGA-O2A-C1
19	B	505	CLA	C2-C3-C5-C6
19	C	506	CLA	C2-C3-C5-C6
20	A	404	PHO	C2-C3-C5-C6
19	B	504	CLA	C2A-CAA-CBA-CGA
19	D	405	CLA	C16-C17-C18-C19
19	C	509	CLA	CBA-CGA-O2A-C1
19	B	509	CLA	C2-C1-O2A-CGA
19	C	512	CLA	O1A-CGA-O2A-C1
19	C	512	CLA	C3-C5-C6-C7
21	A	406	BCR	C1-C6-C7-C8
21	A	406	BCR	C5-C6-C7-C8
21	A	406	BCR	C23-C24-C25-C26
21	B	517	BCR	C23-C24-C25-C30
21	B	518	BCR	C23-C24-C25-C30
21	B	519	BCR	C23-C24-C25-C30
21	C	515	BCR	C1-C6-C7-C8
21	C	515	BCR	C5-C6-C7-C8
21	C	515	BCR	C23-C24-C25-C30
21	C	516	BCR	C5-C6-C7-C8
21	C	516	BCR	C23-C24-C25-C26
21	H	101	BCR	C1-C6-C7-C8
21	H	101	BCR	C23-C24-C25-C30
21	K	101	BCR	C23-C24-C25-C30
19	B	502	CLA	C10-C11-C12-C13
24	D	411	LHG	C30-C31-C32-C33
19	B	511	CLA	C12-C13-C15-C16
19	B	513	CLA	C6-C7-C8-C10
19	B	515	CLA	C11-C10-C8-C7
19	C	502	CLA	C11-C10-C8-C7
19	C	506	CLA	C6-C7-C8-C10
19	C	507	CLA	C12-C13-C15-C16
19	D	401	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	D	404	CLA	C11-C12-C13-C15
20	D	402	PHO	C11-C12-C13-C15
19	B	510	CLA	O1A-CGA-O2A-C1
19	B	510	CLA	C10-C11-C12-C13
19	C	504	CLA	CBA-CGA-O2A-C1
19	B	513	CLA	C15-C16-C17-C18
24	D	411	LHG	C32-C33-C34-C35
24	D	411	LHG	C17-C18-C19-C20
19	C	509	CLA	O1A-CGA-O2A-C1
19	C	513	CLA	C16-C17-C18-C19
23	B	520	LMG	C11-C10-O7-C8
24	B	521	LHG	C28-C29-C30-C31
23	B	520	LMG	O9-C10-O7-C8
26	C	520	LMU	C2'-C1'-O1'-C1
25	C	518	DGD	O1G-C1G-C2G-O2G
23	B	522	LMG	O6-C5-C6-O5
19	A	402	CLA	C11-C10-C8-C9
19	B	502	CLA	C6-C7-C8-C9
19	B	511	CLA	C14-C13-C15-C16
19	B	512	CLA	C6-C7-C8-C9
19	B	513	CLA	C14-C13-C15-C16
19	B	515	CLA	C11-C10-C8-C9
19	B	516	CLA	C11-C10-C8-C9
19	C	513	CLA	C6-C7-C8-C9
19	D	401	CLA	C11-C12-C13-C14
25	C	518	DGD	C4B-C5B-C6B-C7B
19	B	504	CLA	C1A-C2A-CAA-CBA
19	B	505	CLA	C1A-C2A-CAA-CBA
19	B	514	CLA	C1A-C2A-CAA-CBA
19	B	515	CLA	C1A-C2A-CAA-CBA
19	B	516	CLA	C1A-C2A-CAA-CBA
19	C	507	CLA	C1A-C2A-CAA-CBA
19	C	508	CLA	C1A-C2A-CAA-CBA
19	D	401	CLA	C1A-C2A-CAA-CBA
19	C	513	CLA	C16-C17-C18-C20
19	D	405	CLA	C16-C17-C18-C20
26	C	520	LMU	C2-C3-C4-C5
19	B	507	CLA	C5-C6-C7-C8
23	A	408	LMG	O6-C5-C6-O5
19	C	504	CLA	O1A-CGA-O2A-C1
23	B	522	LMG	C33-C34-C35-C36
19	B	501	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	D	401	CLA	C2-C3-C5-C6
19	B	513	CLA	CBD-CGD-O2D-CED
19	C	508	CLA	C16-C17-C18-C19
25	C	518	DGD	O6E-C5E-C6E-O5E
24	D	411	LHG	C4-C5-C6-O8
26	C	520	LMU	C1-C2-C3-C4
19	B	501	CLA	O1D-CGD-O2D-CED
19	C	509	CLA	C10-C11-C12-C13
25	J	101	DGD	C7A-C8A-C9A-CAA
26	C	520	LMU	O5B-C5B-C6B-O6B
24	D	410	LHG	C8-C7-O7-C5
19	B	513	CLA	C4-C3-C5-C6
19	D	401	CLA	C4-C3-C5-C6
24	B	521	LHG	C23-C24-C25-C26
19	B	504	CLA	CBA-CGA-O2A-C1
22	A	407	SQD	C24-C23-O48-C46
19	C	512	CLA	CBD-CGD-O2D-CED
23	D	409	LMG	O6-C5-C6-O5
25	C	517	DGD	O6D-C5D-C6D-O5D
19	B	511	CLA	C5-C6-C7-C8
19	B	502	CLA	C3-C5-C6-C7
24	A	409	LHG	O7-C5-C6-O8
23	A	408	LMG	C12-C13-C14-C15
24	B	521	LHG	C30-C31-C32-C33
19	A	405	CLA	C6-C7-C8-C10
19	B	509	CLA	C12-C13-C15-C16
19	B	510	CLA	C6-C7-C8-C10
19	B	515	CLA	C6-C7-C8-C10
19	B	516	CLA	C11-C10-C8-C7
19	C	501	CLA	C12-C13-C15-C16
19	C	502	CLA	C6-C7-C8-C10
19	C	503	CLA	C11-C10-C8-C7
19	C	503	CLA	C12-C13-C15-C16
19	C	505	CLA	C11-C12-C13-C15
19	C	507	CLA	C6-C7-C8-C10
19	C	509	CLA	C6-C7-C8-C10
19	C	511	CLA	C6-C7-C8-C10
19	C	511	CLA	C11-C12-C13-C15
19	A	405	CLA	C6-C7-C8-C9
19	B	503	CLA	C14-C13-C15-C16
19	B	509	CLA	C14-C13-C15-C16
19	B	512	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B	513	CLA	C6-C7-C8-C9
19	C	501	CLA	C14-C13-C15-C16
19	C	503	CLA	C14-C13-C15-C16
19	C	505	CLA	C11-C12-C13-C14
19	C	509	CLA	C6-C7-C8-C9
19	C	511	CLA	C6-C7-C8-C9
19	D	405	CLA	C11-C10-C8-C9
19	D	405	CLA	C14-C13-C15-C16
19	C	501	CLA	O1D-CGD-O2D-CED
24	L	101	LHG	C8-C7-O7-C5
19	C	507	CLA	CBA-CGA-O2A-C1
22	A	407	SQD	C31-C32-C33-C34
19	C	508	CLA	C16-C17-C18-C20
24	D	410	LHG	O9-C7-O7-C5
23	D	409	LMG	C20-C21-C22-C23
19	D	401	CLA	C3A-C2A-CAA-CBA
24	L	101	LHG	C15-C16-C17-C18
26	C	520	LMU	C2-C1-O1'-C1'
19	B	510	CLA	C13-C15-C16-C17
19	B	512	CLA	C5-C6-C7-C8
23	B	522	LMG	C7-C8-C9-O8
24	A	409	LHG	C4-C5-C6-O8
24	L	101	LHG	C4-C5-C6-O8
25	C	518	DGD	O1G-C1G-C2G-C3G
20	D	402	PHO	O2A-C1-C2-C3
23	B	520	LMG	C21-C22-C23-C24
19	C	511	CLA	C4-C3-C5-C6
19	A	402	CLA	C16-C17-C18-C20
19	B	513	CLA	C2-C3-C5-C6
25	C	517	DGD	C4D-C5D-C6D-O5D
19	D	404	CLA	C4C-C3C-CAC-CBC
24	D	408	LHG	C11-C12-C13-C14
19	B	504	CLA	O1A-CGA-O2A-C1
22	A	407	SQD	O10-C23-O48-C46
25	C	517	DGD	C6B-C7B-C8B-C9B
24	L	101	LHG	O7-C5-C6-O8
24	D	410	LHG	C32-C33-C34-C35
19	B	506	CLA	C8-C10-C11-C12
19	C	511	CLA	C15-C16-C17-C18
24	L	101	LHG	O9-C7-O7-C5
19	B	501	CLA	C11-C12-C13-C14
19	C	502	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	C	504	CLA	C11-C12-C13-C14
19	C	508	CLA	C11-C10-C8-C9
24	D	411	LHG	C13-C14-C15-C16
20	D	402	PHO	C1A-C2A-CAA-CBA
19	C	507	CLA	O1A-CGA-O2A-C1
24	L	101	LHG	C11-C10-C9-C8
19	B	505	CLA	C16-C17-C18-C19
19	B	512	CLA	C8-C10-C11-C12
21	H	101	BCR	C7-C8-C9-C10
25	C	517	DGD	CDB-CEB-CFB-CGB
19	B	501	CLA	C11-C12-C13-C15
19	B	503	CLA	C12-C13-C15-C16
19	B	509	CLA	C6-C7-C8-C10
19	B	511	CLA	C11-C12-C13-C15
19	B	512	CLA	C11-C12-C13-C15
19	C	508	CLA	C11-C10-C8-C7
19	C	509	CLA	C11-C12-C13-C15
19	C	511	CLA	C2-C3-C5-C6
19	C	513	CLA	C11-C10-C8-C7
19	D	405	CLA	C11-C10-C8-C7
19	D	405	CLA	C12-C13-C15-C16
19	B	505	CLA	C13-C15-C16-C17
19	B	507	CLA	C15-C16-C17-C18
19	B	508	CLA	C15-C16-C17-C18
19	A	402	CLA	C16-C17-C18-C19
19	B	502	CLA	CAD-CBD-CGD-O2D
19	C	501	CLA	CAD-CBD-CGD-O2D
19	C	502	CLA	CAD-CBD-CGD-O2D
24	D	411	LHG	C12-C13-C14-C15
23	D	409	LMG	O6-C1-O1-C7
19	B	505	CLA	C16-C17-C18-C20
19	A	405	CLA	CHA-CBD-CGD-O1D
19	A	405	CLA	CHA-CBD-CGD-O2D
19	B	510	CLA	CHA-CBD-CGD-O1D
19	C	504	CLA	CHA-CBD-CGD-O1D
19	C	504	CLA	CHA-CBD-CGD-O2D
19	C	508	CLA	CHA-CBD-CGD-O1D
19	C	508	CLA	CHA-CBD-CGD-O2D
19	D	404	CLA	CBD-CGD-O2D-CED
23	A	408	LMG	O7-C8-C9-O8
19	C	510	CLA	C16-C17-C18-C19
25	C	517	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
23	C	519	LMG	C11-C10-O7-C8
23	C	519	LMG	O9-C10-O7-C8
19	B	501	CLA	C6-C7-C8-C9
19	B	513	CLA	O1D-CGD-O2D-CED
26	C	520	LMU	C5'-C4'-O1B-C1B
19	C	513	CLA	C1A-C2A-CAA-CBA
24	B	521	LHG	C3-O3-P-O6
19	C	512	CLA	O1D-CGD-O2D-CED
22	A	407	SQD	O47-C7-C8-C9
24	A	409	LHG	C4-O6-P-O5
24	D	408	LHG	C3-O3-P-O4
24	D	411	LHG	C4-O6-P-O4
24	L	101	LHG	C3-O3-P-O5
19	B	503	CLA	CAD-CBD-CGD-O1D
19	B	505	CLA	CAD-CBD-CGD-O1D
19	B	510	CLA	CAD-CBD-CGD-O1D
19	C	504	CLA	CAD-CBD-CGD-O1D
19	C	506	CLA	CAD-CBD-CGD-O1D
24	D	410	LHG	O8-C23-C24-C25
19	B	501	CLA	C6-C7-C8-C10
19	B	507	CLA	C6-C7-C8-C10
19	C	501	CLA	C6-C7-C8-C10
19	C	502	CLA	C12-C13-C15-C16
19	C	510	CLA	C11-C10-C8-C7
19	C	511	CLA	C12-C13-C15-C16
19	D	404	CLA	C6-C7-C8-C10
20	A	404	PHO	C11-C10-C8-C7
20	A	404	PHO	C12-C13-C15-C16
19	B	512	CLA	C13-C15-C16-C17
24	L	101	LHG	C13-C14-C15-C16
20	A	404	PHO	C3-C5-C6-C7
23	A	408	LMG	C7-C8-C9-O8
19	B	513	CLA	C13-C15-C16-C17
19	B	501	CLA	O2A-C1-C2-C3
22	A	407	SQD	C11-C10-C9-C8
28	D	407	PL9	C30-C29-C31-C32
28	D	407	PL9	C28-C29-C31-C32
19	B	508	CLA	C14-C13-C15-C16
19	B	516	CLA	C11-C12-C13-C14
19	C	501	CLA	C6-C7-C8-C9
19	C	509	CLA	C11-C12-C13-C14
19	C	511	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	C	510	CLA	C16-C17-C18-C20
26	C	520	LMU	O5'-C1'-O1'-C1
23	C	519	LMG	C35-C36-C37-C38
21	H	101	BCR	C7-C8-C9-C34
25	C	518	DGD	C7B-C8B-C9B-CAB
19	B	504	CLA	C15-C16-C17-C18
19	D	405	CLA	C3-C5-C6-C7
23	B	520	LMG	C11-C12-C13-C14
19	B	513	CLA	C2-C1-O2A-CGA
19	C	505	CLA	C2-C1-O2A-CGA
19	C	502	CLA	CBA-CGA-O2A-C1
19	C	511	CLA	CAA-CBA-CGA-O2A
25	C	517	DGD	O1G-C1A-C2A-C3A
24	D	408	LHG	C17-C18-C19-C20
26	C	520	LMU	C6-C7-C8-C9
24	A	409	LHG	C3-O3-P-O6
24	D	408	LHG	C4-O6-P-O3
24	D	410	LHG	C3-O3-P-O6
24	L	101	LHG	C4-O6-P-O3
25	J	101	DGD	O6D-C5D-C6D-O5D
20	D	402	PHO	CHA-CBD-CGD-O1D
20	D	402	PHO	CHA-CBD-CGD-O2D
19	B	509	CLA	C5-C6-C7-C8
25	C	517	DGD	O1G-C1G-C2G-C3G
19	B	510	CLA	C6-C7-C8-C9
19	C	503	CLA	C11-C10-C8-C9
19	C	507	CLA	C6-C7-C8-C9
25	C	517	DGD	C4B-C5B-C6B-C7B
19	C	511	CLA	C16-C17-C18-C20
23	C	519	LMG	C39-C40-C41-C42
24	D	411	LHG	C25-C26-C27-C28
19	A	403	CLA	O2A-C1-C2-C3
19	C	502	CLA	O1A-CGA-O2A-C1
19	C	503	CLA	C3-C5-C6-C7
19	C	513	CLA	C8-C10-C11-C12
19	C	507	CLA	C2-C1-O2A-CGA
19	C	510	CLA	C2-C1-O2A-CGA
23	A	408	LMG	O1-C7-C8-O7
19	A	403	CLA	C3A-C2A-CAA-CBA
19	B	505	CLA	C3A-C2A-CAA-CBA
19	B	512	CLA	C3A-C2A-CAA-CBA
19	A	402	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	L	101	LHG	C14-C15-C16-C17
19	B	513	CLA	C11-C10-C8-C9
19	C	510	CLA	C11-C12-C13-C14
19	D	401	CLA	C14-C13-C15-C16
19	C	511	CLA	C16-C17-C18-C19
19	C	506	CLA	O2A-C1-C2-C3
19	B	513	CLA	C2A-CAA-CBA-CGA
19	B	505	CLA	C8-C10-C11-C12
24	D	411	LHG	C24-C25-C26-C27
23	C	519	LMG	C30-C31-C32-C33
19	B	504	CLA	C16-C17-C18-C19
23	B	522	LMG	C38-C39-C40-C41
19	B	515	CLA	C2-C1-O2A-CGA
19	D	404	CLA	C2C-C3C-CAC-CBC
23	A	408	LMG	C34-C35-C36-C37
19	B	512	CLA	C2A-CAA-CBA-CGA
21	C	514	BCR	C5-C6-C7-C8
21	C	516	BCR	C23-C24-C25-C30
19	C	502	CLA	C13-C15-C16-C17
22	A	407	SQD	C10-C11-C12-C13
19	C	506	CLA	C16-C17-C18-C20
19	B	511	CLA	C2A-CAA-CBA-CGA
25	J	101	DGD	CCB-CDB-CEB-CFB
19	B	516	CLA	C11-C12-C13-C15
23	B	522	LMG	C12-C13-C14-C15
19	C	503	CLA	O1A-CGA-O2A-C1
19	C	503	CLA	CAA-CBA-CGA-O2A
19	C	512	CLA	CAA-CBA-CGA-O2A
23	A	408	LMG	O7-C10-C11-C12
19	C	513	CLA	C13-C15-C16-C17
19	B	510	CLA	CAA-CBA-CGA-O2A
22	A	407	SQD	O48-C23-C24-C25
25	C	518	DGD	O1G-C1A-C2A-C3A
25	C	518	DGD	O6D-C5D-C6D-O5D
19	C	510	CLA	C11-C10-C8-C9
19	D	404	CLA	C6-C7-C8-C9
20	A	404	PHO	C14-C13-C15-C16
19	C	509	CLA	C3A-C2A-CAA-CBA
19	C	510	CLA	CAA-CBA-CGA-O2A
23	B	520	LMG	C19-C20-C21-C22
19	B	506	CLA	CAD-CBD-CGD-O2D
19	B	514	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	C	509	CLA	CAD-CBD-CGD-O2D
19	D	401	CLA	CAD-CBD-CGD-O2D
19	B	504	CLA	C16-C17-C18-C20
19	C	509	CLA	C2A-CAA-CBA-CGA
19	D	404	CLA	CAA-CBA-CGA-O2A
19	D	404	CLA	O1D-CGD-O2D-CED
19	C	504	CLA	C16-C17-C18-C19
19	C	502	CLA	C3-C5-C6-C7
19	C	509	CLA	CAA-CBA-CGA-O2A
19	B	504	CLA	CAA-CBA-CGA-O2A
19	B	505	CLA	CAA-CBA-CGA-O2A
24	L	101	LHG	O7-C7-C8-C9
19	D	401	CLA	O2A-C1-C2-C3
19	C	503	CLA	CBA-CGA-O2A-C1
19	A	403	CLA	CHA-CBD-CGD-O1D
19	A	403	CLA	CHA-CBD-CGD-O2D
19	B	509	CLA	CHA-CBD-CGD-O1D
19	B	510	CLA	CHA-CBD-CGD-O2D
19	B	513	CLA	CHA-CBD-CGD-O2D
19	C	503	CLA	CHA-CBD-CGD-O1D
19	C	510	CLA	CHA-CBD-CGD-O2D
19	C	511	CLA	CHA-CBD-CGD-O1D
19	C	511	CLA	CHA-CBD-CGD-O2D
19	B	507	CLA	CAA-CBA-CGA-O2A
19	B	515	CLA	CAA-CBA-CGA-O2A
25	J	101	DGD	O2G-C1B-C2B-C3B
19	B	502	CLA	CAA-CBA-CGA-O2A
19	B	511	CLA	CAA-CBA-CGA-O2A
24	D	410	LHG	C13-C14-C15-C16
19	B	512	CLA	CAA-CBA-CGA-O2A
19	B	508	CLA	C11-C10-C8-C9
19	C	502	CLA	C14-C13-C15-C16
20	A	404	PHO	C11-C10-C8-C9
24	B	521	LHG	C12-C13-C14-C15
24	B	521	LHG	C24-C25-C26-C27
23	B	520	LMG	C15-C16-C17-C18
19	B	510	CLA	CAA-CBA-CGA-O1A
19	C	509	CLA	CAA-CBA-CGA-O1A
19	C	512	CLA	CAA-CBA-CGA-O1A
24	A	409	LHG	C25-C26-C27-C28
19	A	403	CLA	C1A-C2A-CAA-CBA
19	B	512	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	C	509	CLA	C1A-C2A-CAA-CBA
19	B	515	CLA	CAA-CBA-CGA-O1A
25	C	518	DGD	O1A-C1A-C2A-C3A
23	B	520	LMG	C29-C28-O8-C9
19	B	508	CLA	C2A-CAA-CBA-CGA
19	C	502	CLA	C16-C17-C18-C19
19	C	512	CLA	C16-C17-C18-C20
19	B	507	CLA	CAA-CBA-CGA-O1A
19	B	511	CLA	CAA-CBA-CGA-O1A
19	C	503	CLA	CAA-CBA-CGA-O1A
19	C	510	CLA	CAA-CBA-CGA-O1A
19	A	403	CLA	CAA-CBA-CGA-O2A
22	A	407	SQD	O10-C23-C24-C25
23	A	408	LMG	O9-C10-C11-C12
19	C	513	CLA	C15-C16-C17-C18
24	D	410	LHG	C34-C35-C36-C37
24	A	409	LHG	C3-O3-P-O5
24	B	521	LHG	C3-O3-P-O4
24	L	101	LHG	C4-O6-P-O5
19	B	512	CLA	CAA-CBA-CGA-O1A
19	D	404	CLA	CAA-CBA-CGA-O1A
25	J	101	DGD	O1B-C1B-C2B-C3B
19	B	516	CLA	C8-C10-C11-C12
23	A	408	LMG	C16-C17-C18-C19
19	B	505	CLA	CAA-CBA-CGA-O1A
24	D	411	LHG	C31-C32-C33-C34
25	C	518	DGD	C2B-C3B-C4B-C5B
19	B	504	CLA	CAA-CBA-CGA-O1A
24	L	101	LHG	C12-C13-C14-C15
20	A	404	PHO	O1D-CGD-O2D-CED
19	A	403	CLA	CAD-CBD-CGD-O1D
19	B	509	CLA	CAD-CBD-CGD-O1D
19	C	503	CLA	CAD-CBD-CGD-O1D
22	A	407	SQD	O49-C7-C8-C9
19	C	503	CLA	C11-C12-C13-C14
19	C	510	CLA	C6-C7-C8-C9
19	A	403	CLA	CAA-CBA-CGA-O1A
24	D	411	LHG	C33-C34-C35-C36
19	B	509	CLA	CAA-CBA-CGA-O2A
19	B	502	CLA	CAA-CBA-CGA-O1A
19	B	508	CLA	C11-C10-C8-C7
19	B	508	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	C	510	CLA	C6-C7-C8-C10
19	B	513	CLA	CAA-CBA-CGA-O2A
19	B	502	CLA	C15-C16-C17-C18
20	A	404	PHO	CBD-CGD-O2D-CED
19	B	513	CLA	CAA-CBA-CGA-O1A
23	B	520	LMG	O10-C28-O8-C9
22	A	407	SQD	C27-C28-C29-C30
24	B	521	LHG	C31-C32-C33-C34
19	C	506	CLA	CAA-CBA-CGA-O2A
25	C	517	DGD	O2G-C1B-C2B-C3B
19	D	405	CLA	C8-C10-C11-C12
19	D	401	CLA	C15-C16-C17-C18
20	A	404	PHO	C8-C10-C11-C12
19	B	506	CLA	CAA-CBA-CGA-O2A
24	B	521	LHG	O8-C23-C24-C25

There are no ring outliers.

33 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	402	CLA	1	0
19	B	502	CLA	4	0
21	C	514	BCR	4	0
19	A	405	CLA	1	0
23	D	409	LMG	2	0
24	A	409	LHG	1	0
21	B	518	BCR	1	0
20	D	402	PHO	3	0
19	B	510	CLA	1	0
19	B	516	CLA	1	0
19	D	405	CLA	2	0
21	H	101	BCR	3	0
21	B	519	BCR	2	0
21	K	101	BCR	1	0
21	D	406	BCR	2	0
21	A	406	BCR	3	0
19	B	513	CLA	2	0
24	L	101	LHG	2	0
28	D	407	PL9	1	0
24	D	408	LHG	2	0
19	B	504	CLA	2	0
19	C	511	CLA	1	0

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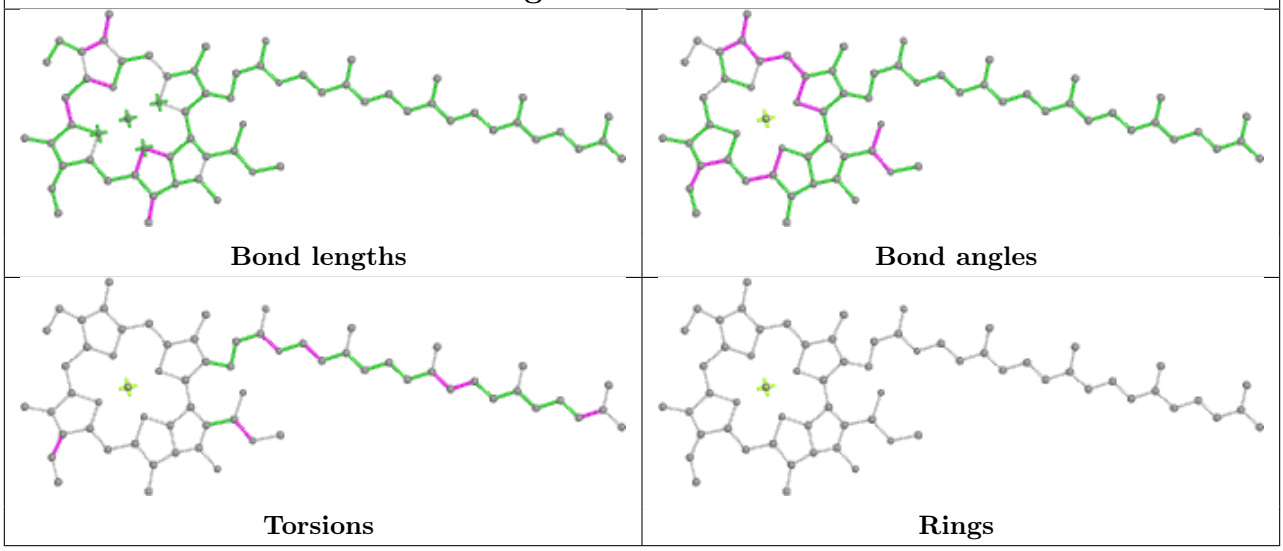
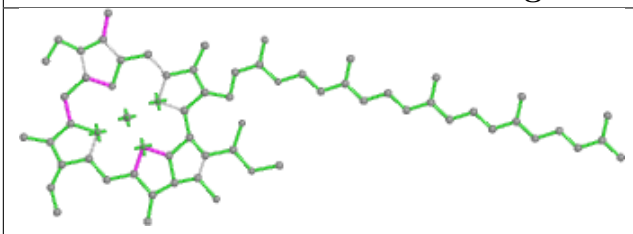
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	C	516	BCR	2	0
23	B	522	LMG	1	0
19	D	404	CLA	5	0
29	F	101	HEM	5	0
26	C	520	LMU	1	0
24	B	521	LHG	3	0
20	A	404	PHO	1	0
21	C	515	BCR	6	0
19	C	502	CLA	3	0
19	B	505	CLA	1	0
19	C	506	CLA	1	0

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

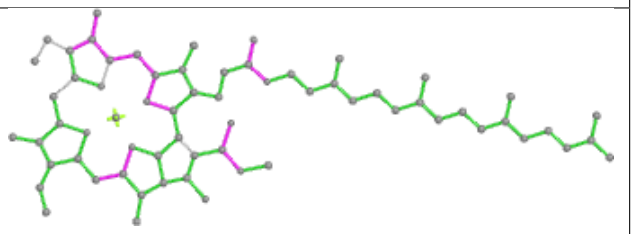
Ligand CLA A 402



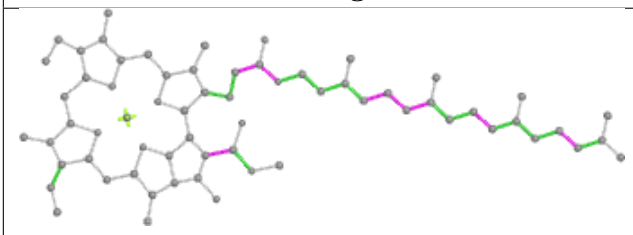
Ligand CLA B 502



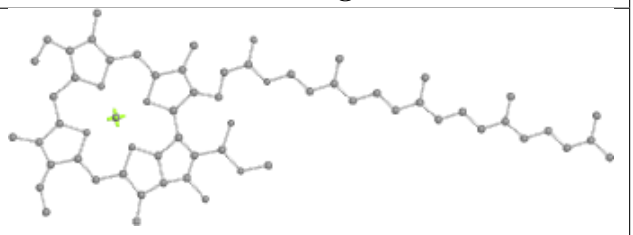
Bond lengths



Bond angles

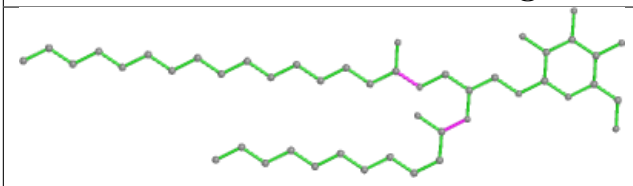


Torsions

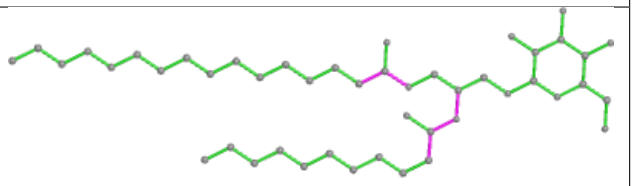


Rings

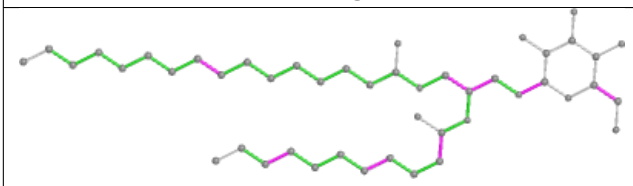
Ligand LMG A 408



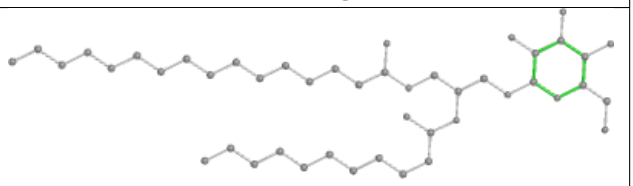
Bond lengths



Bond angles

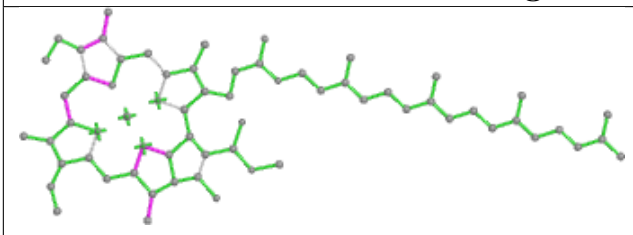


Torsions

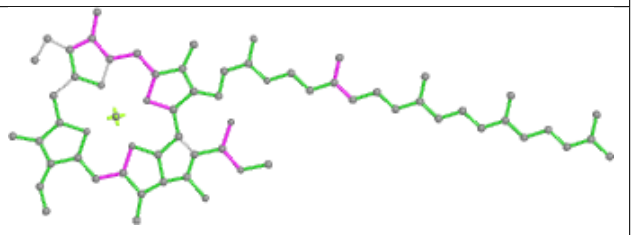


Rings

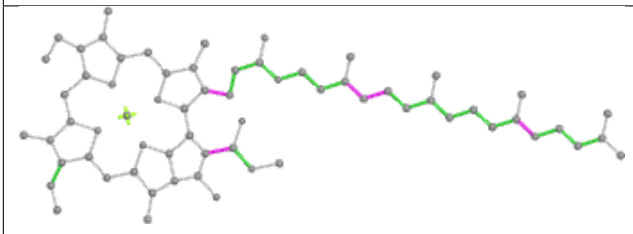
Ligand CLA B 503



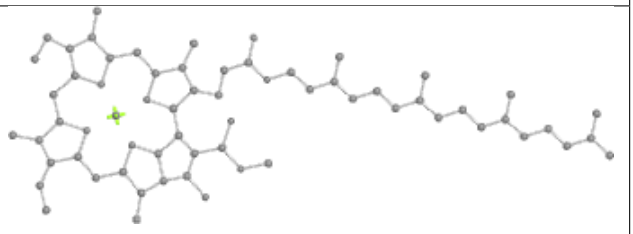
Bond lengths



Bond angles

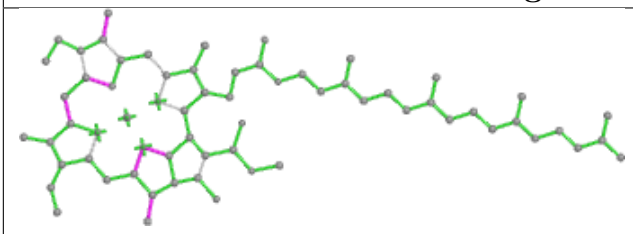


Torsions

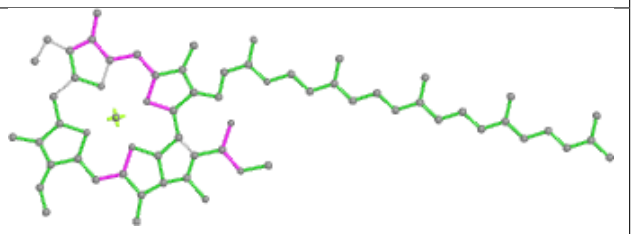


Rings

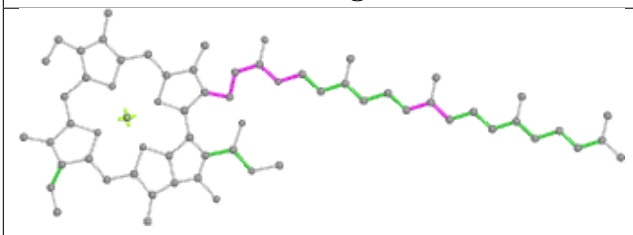
Ligand CLA B 515



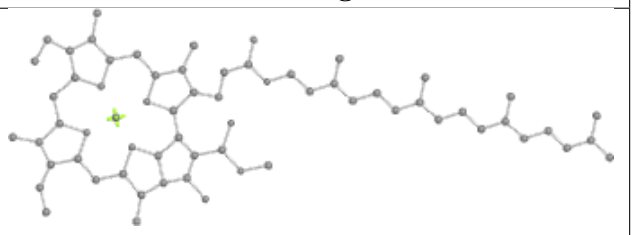
Bond lengths



Bond angles

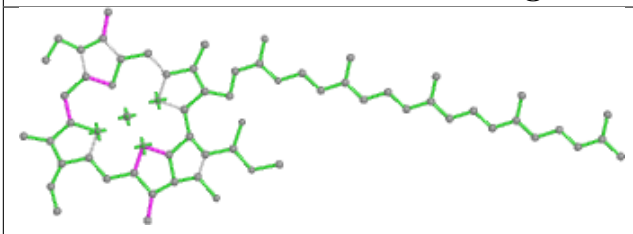


Torsions

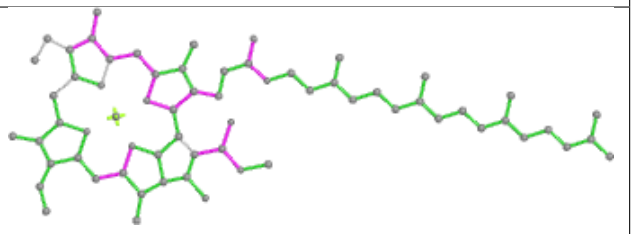


Rings

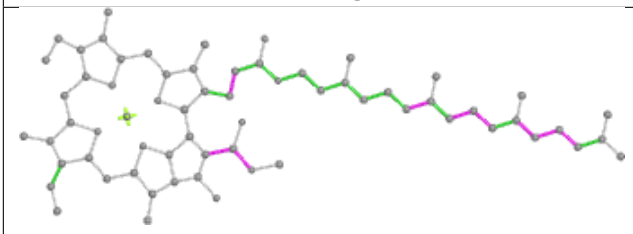
Ligand CLA C 501



Bond lengths



Bond angles



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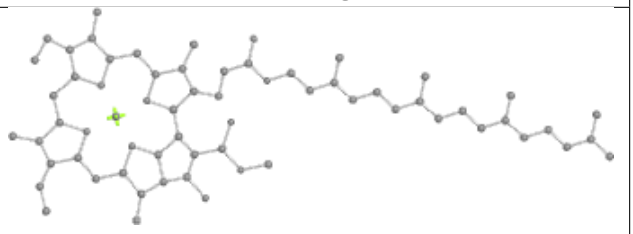
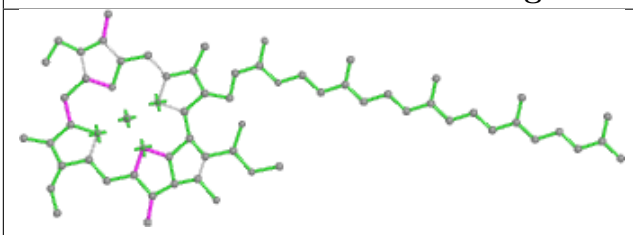
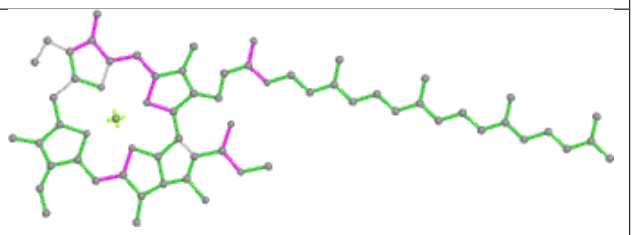


Rings

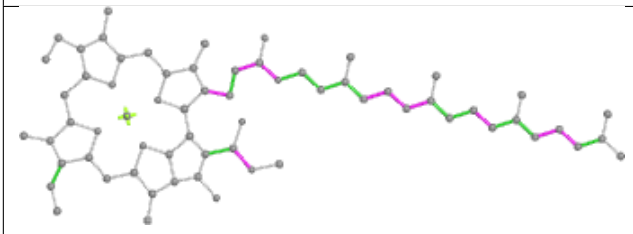
Ligand CLA B 507



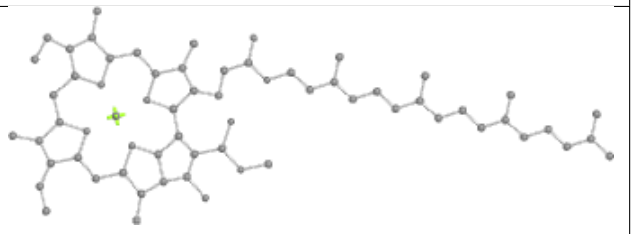
Bond lengths



Bond angles

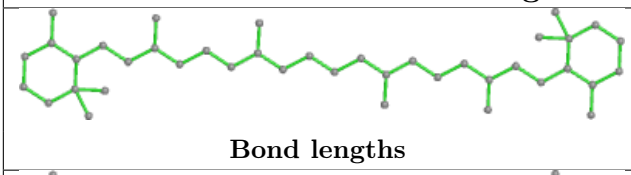


Torsions

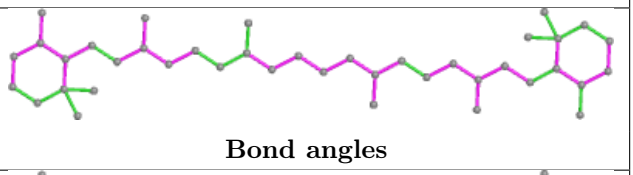


Rings

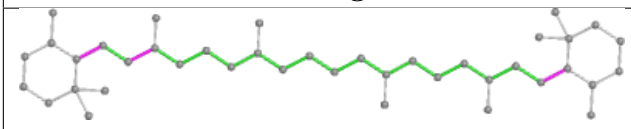
Ligand BCR C 514



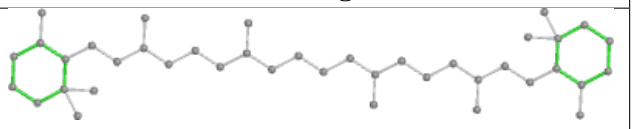
Bond lengths



Bond angles

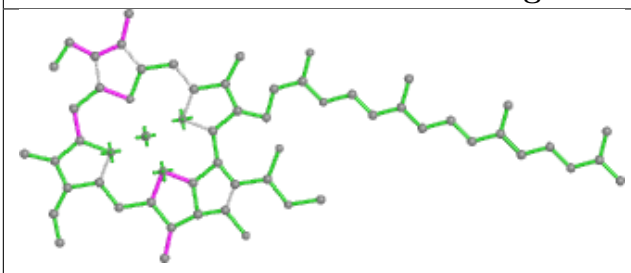


Torsions

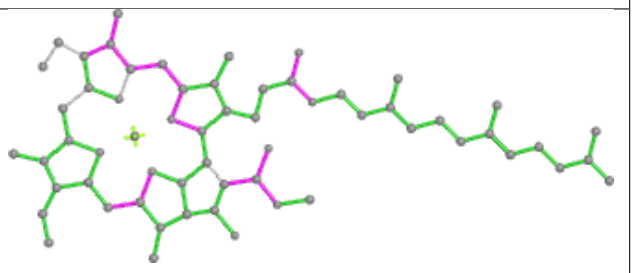


Rings

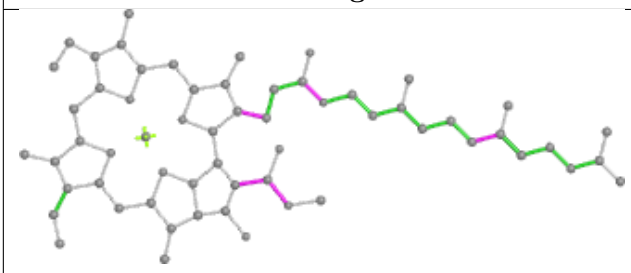
Ligand CLA A 405



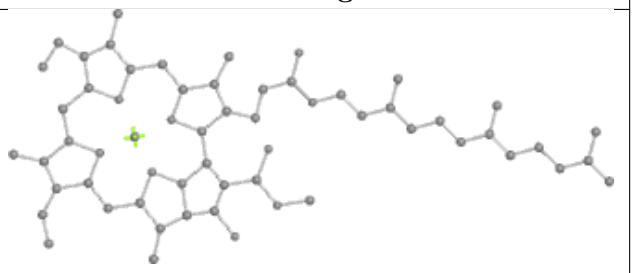
Bond lengths



Bond angles

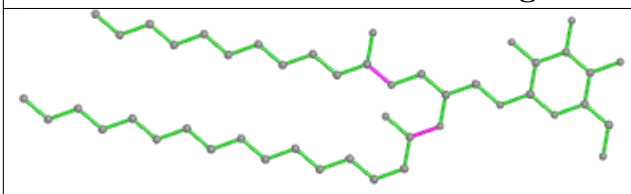


Torsions

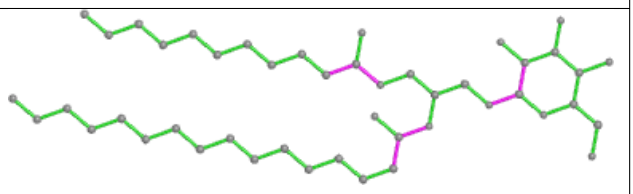


Rings

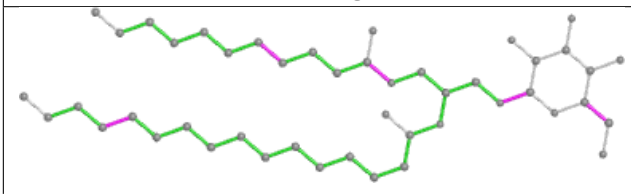
Ligand LMG D 409



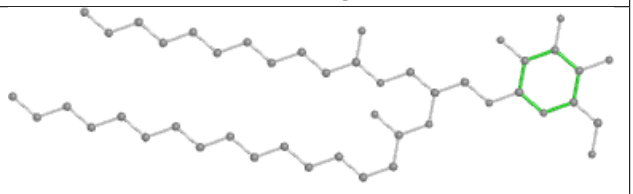
Bond lengths



Bond angles

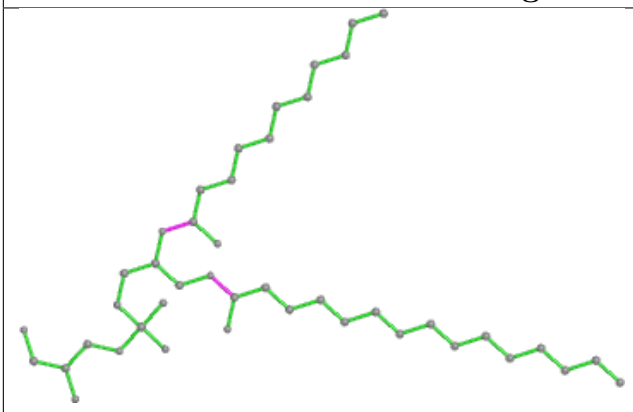


Torsions

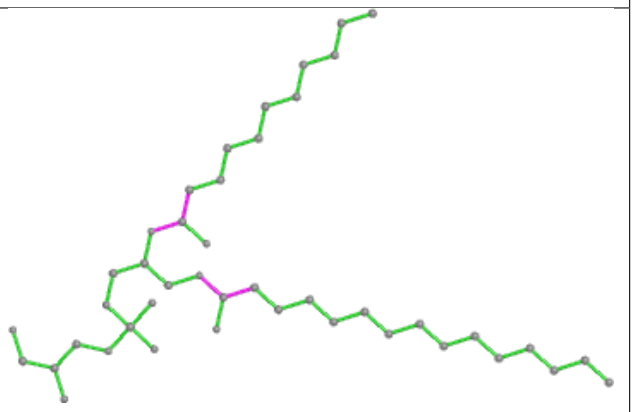


Rings

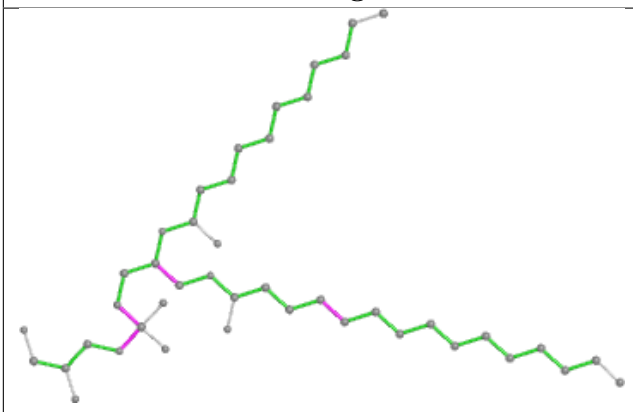
Ligand LHG A 409



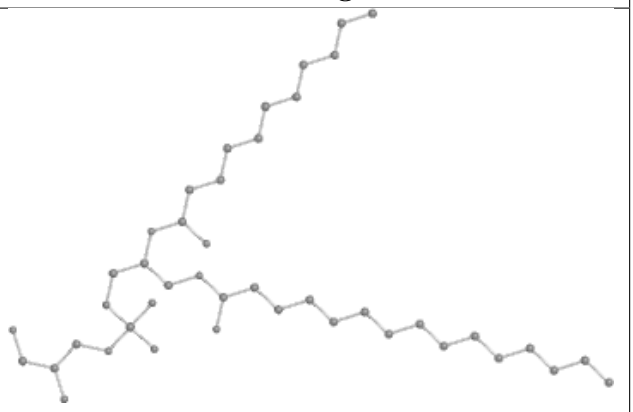
Bond lengths



Bond angles

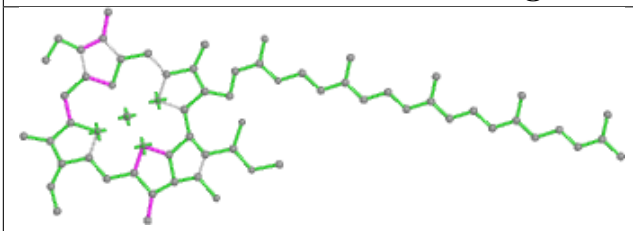


Torsions

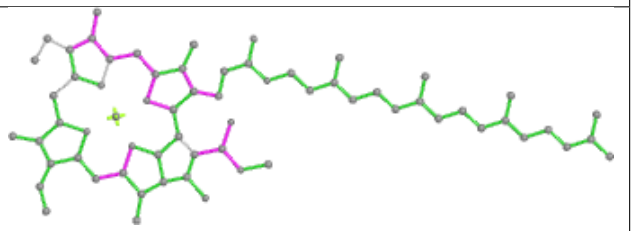


Rings

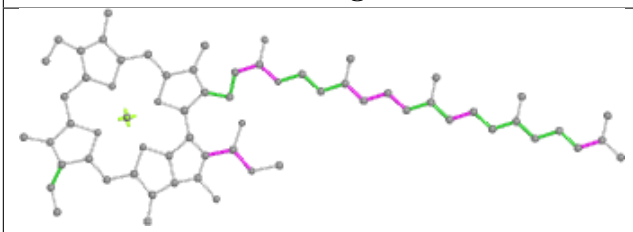
Ligand CLA C 512



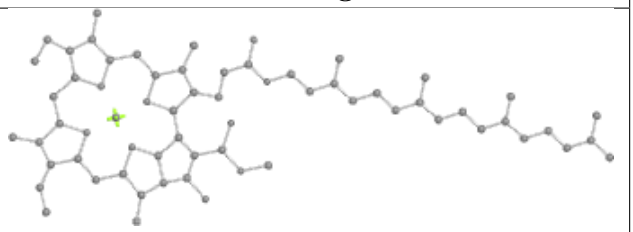
Bond lengths



Bond angles

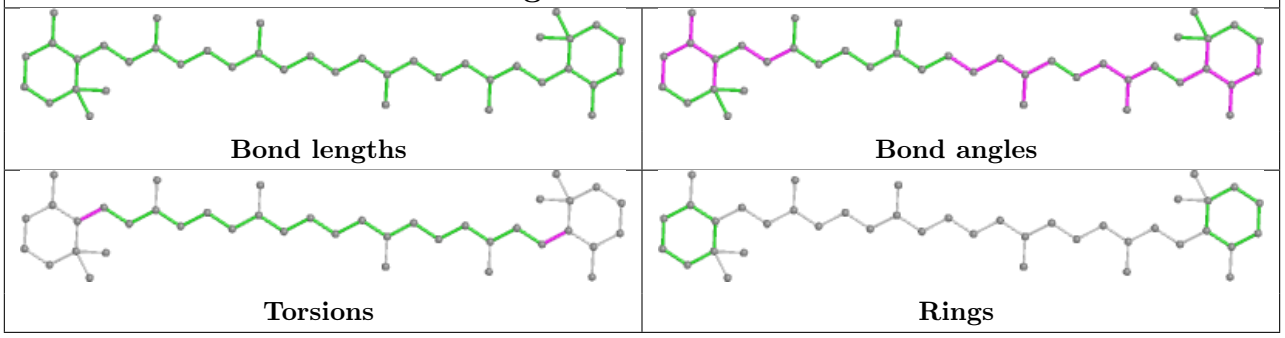


Torsions



Rings

Ligand BCR B 518



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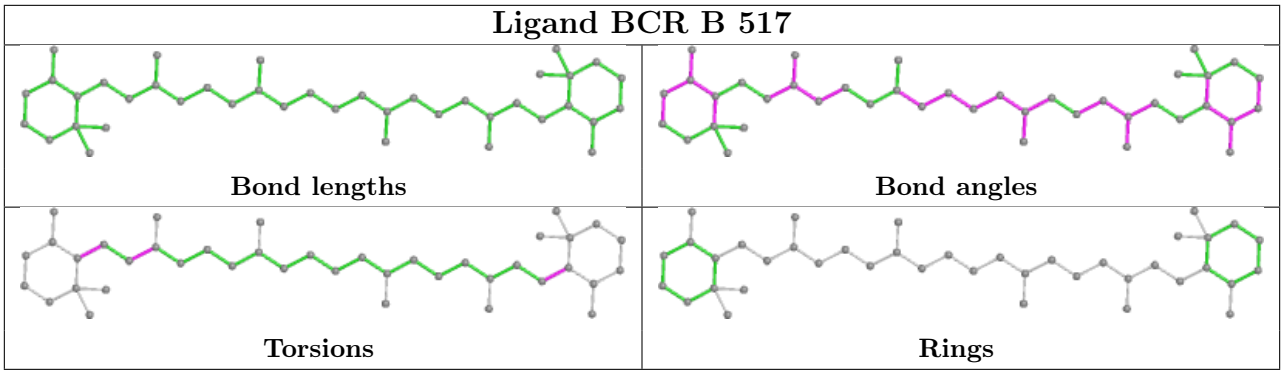
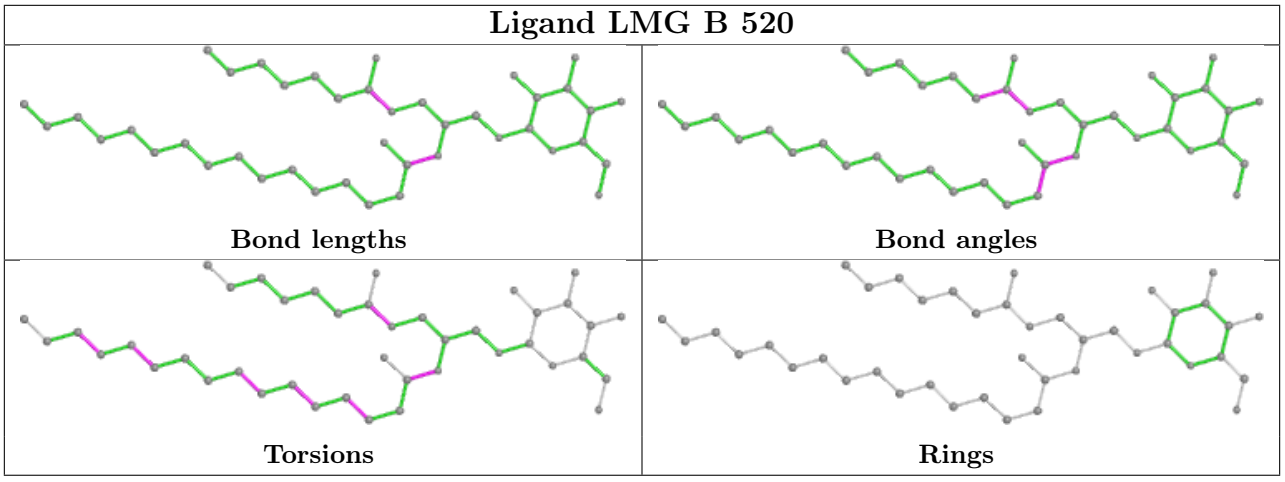
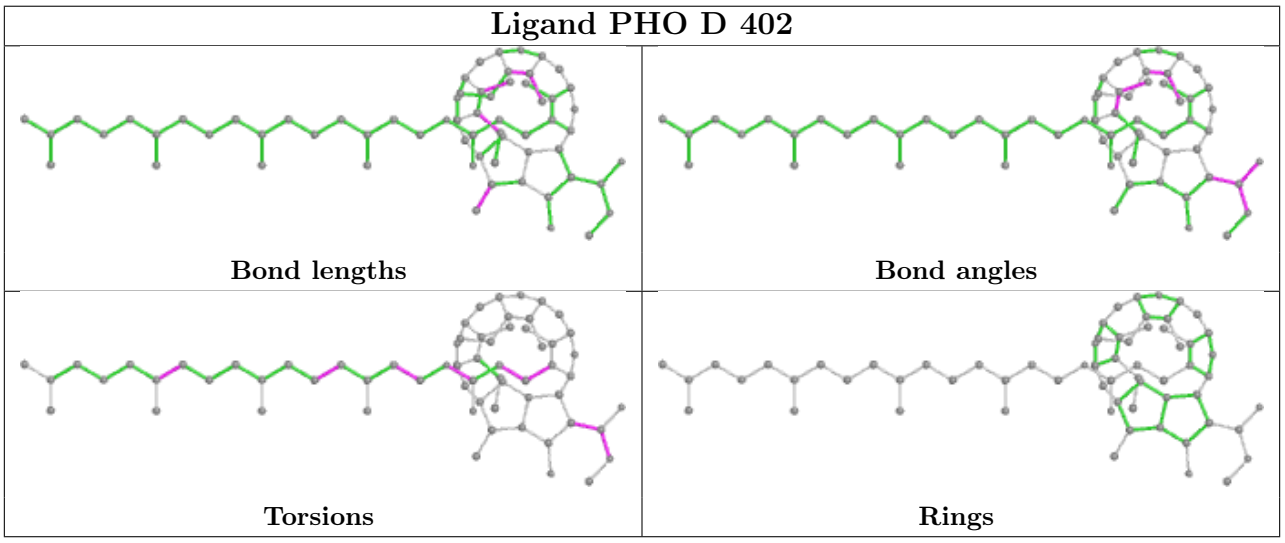


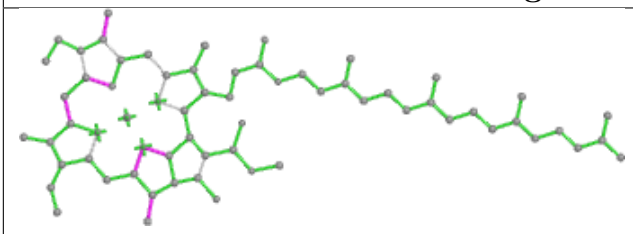
Ligand LMG B 520



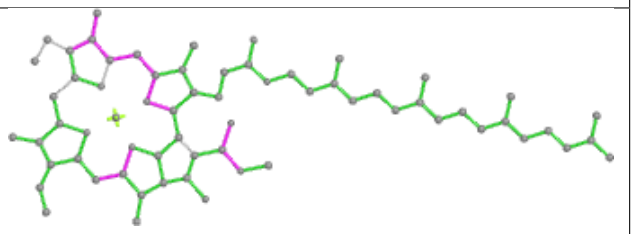
Ligand PHO D 402



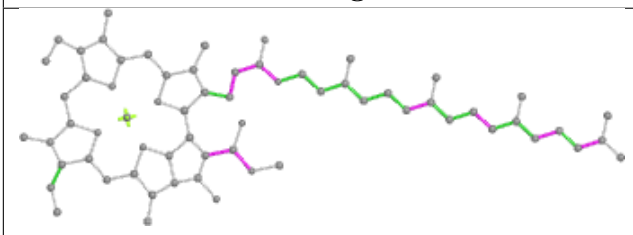
Ligand CLA B 510



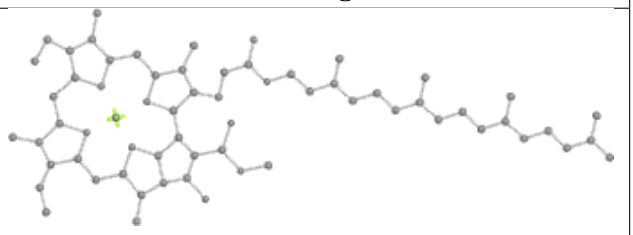
Bond lengths



Bond angles

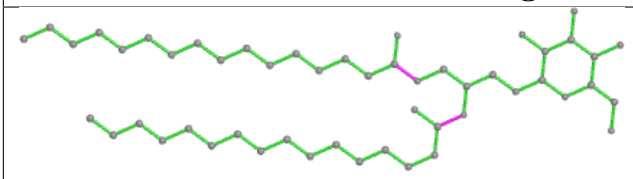


Torsions

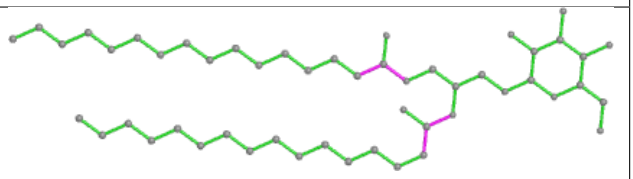


Rings

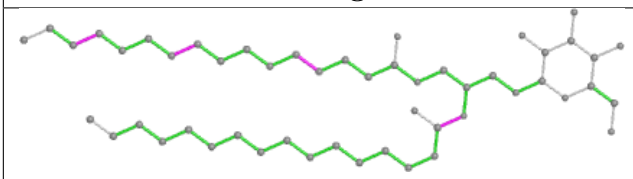
Ligand LMG C 519



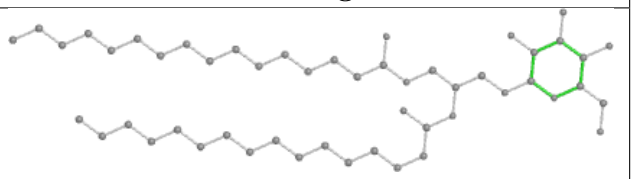
Bond lengths



Bond angles

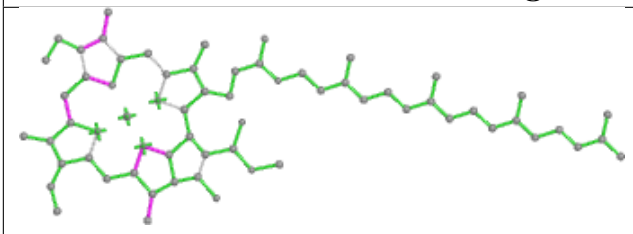


Torsions

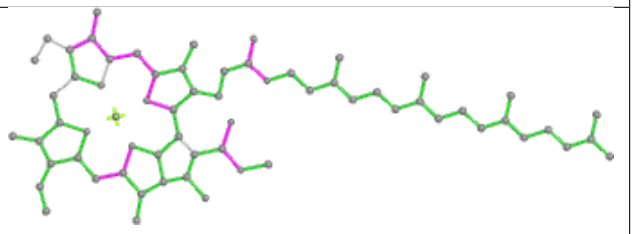


Rings

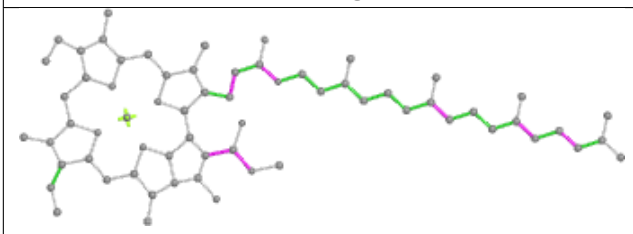
Ligand CLA B 508



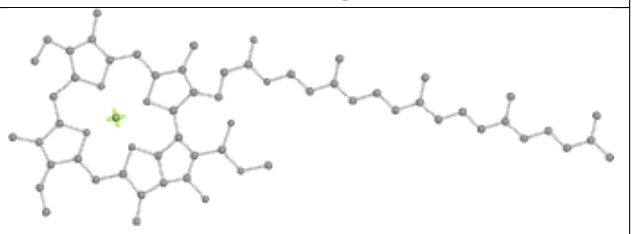
Bond lengths



Bond angles

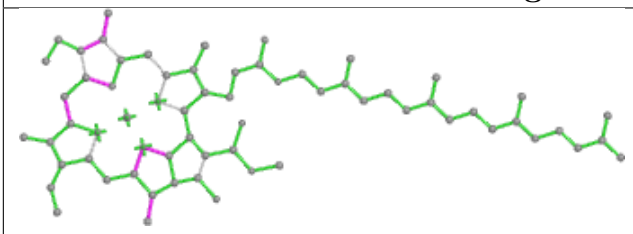


Torsions

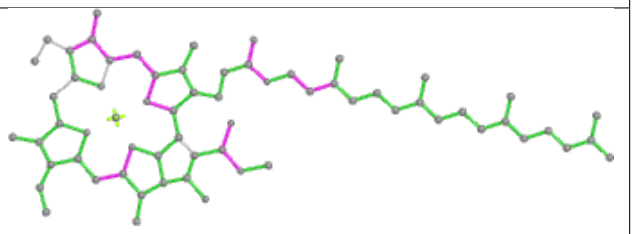


Rings

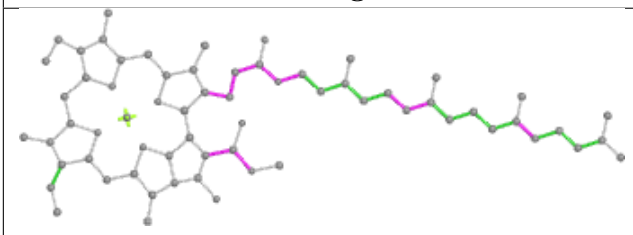
Ligand CLA B 509



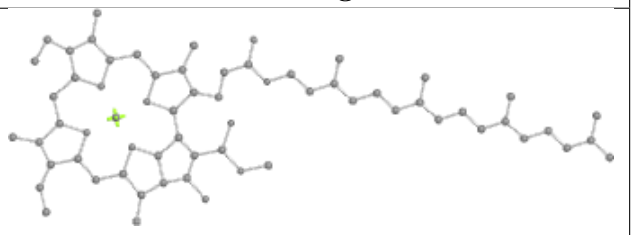
Bond lengths



Bond angles

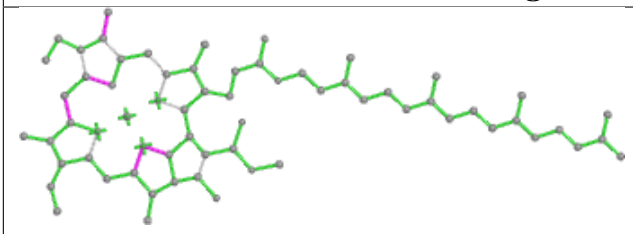


Torsions

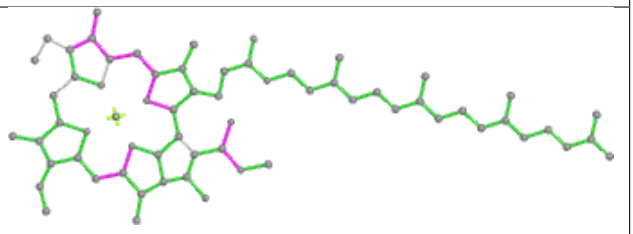


Rings

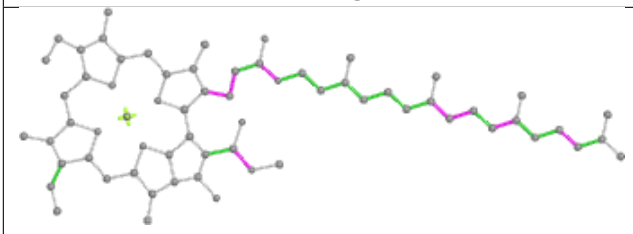
Ligand CLA B 516



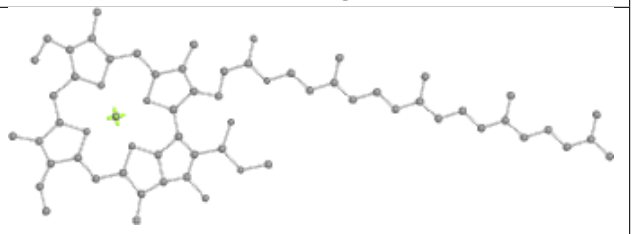
Bond lengths



Bond angles

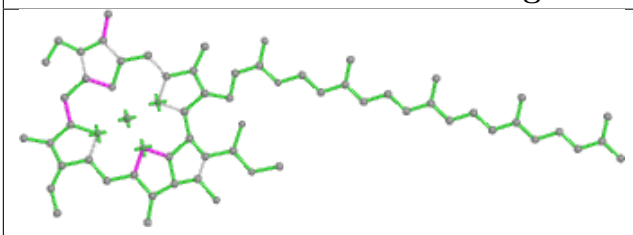


Torsions

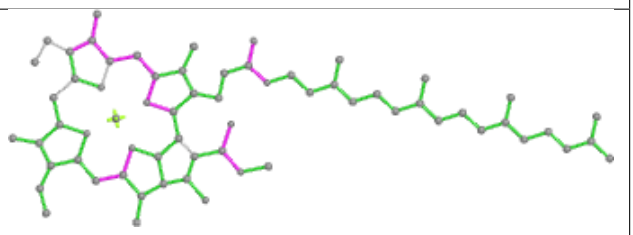


Rings

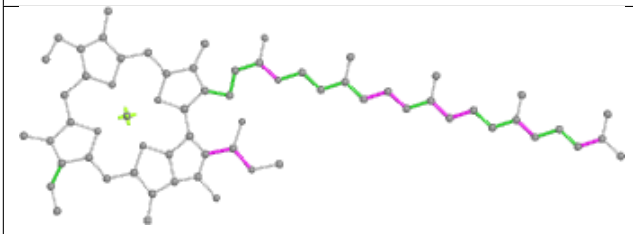
Ligand CLA D 405



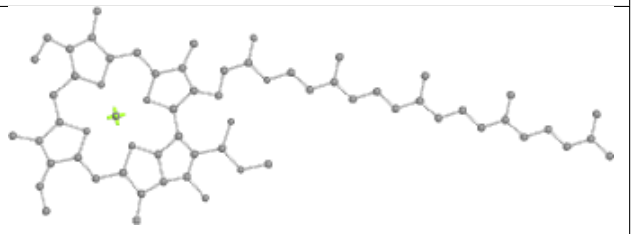
Bond lengths



Bond angles

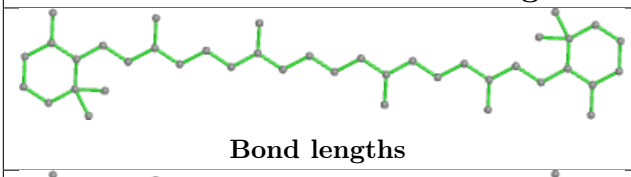


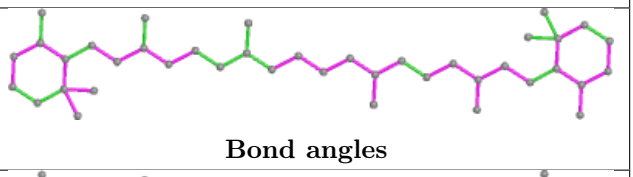
Torsions

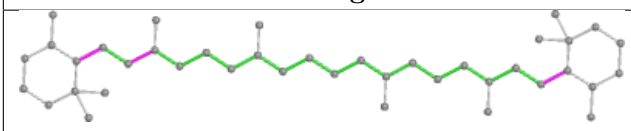


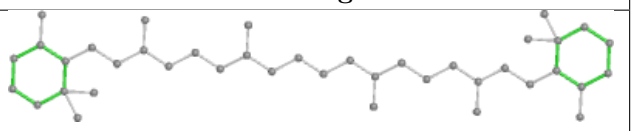
Rings

Ligand BCR H 101

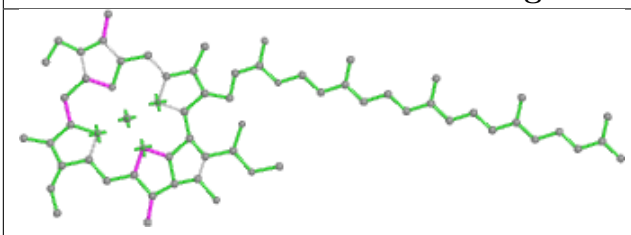

Bond lengths

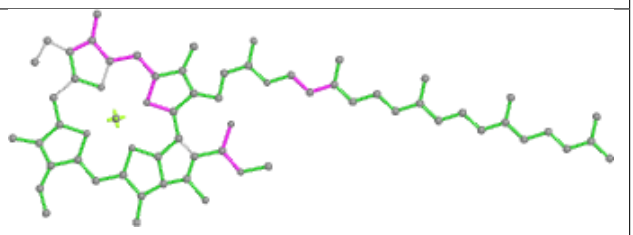

Bond angles

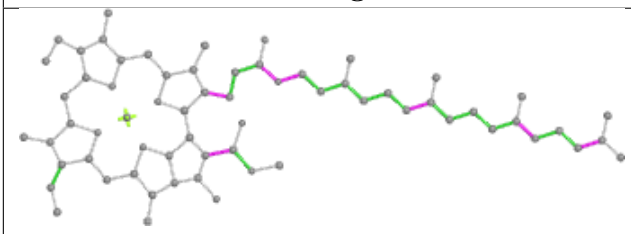

Torsions

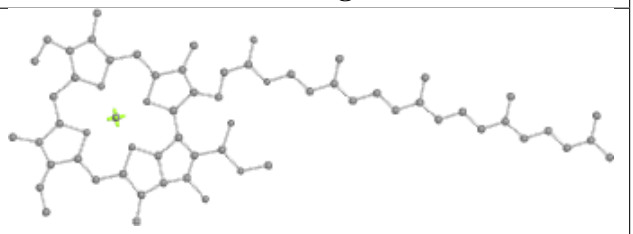

Rings

Ligand CLA C 507

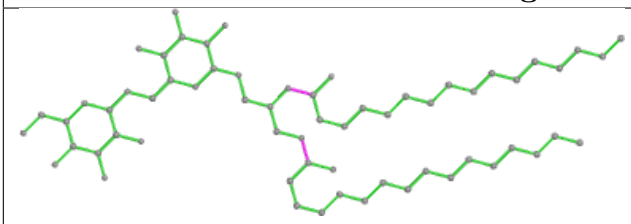

Bond lengths

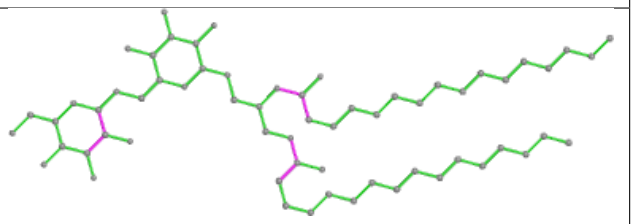

Bond angles

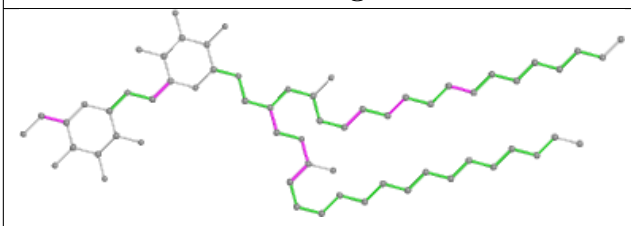

Torsions

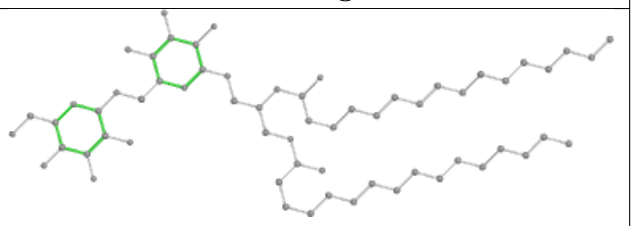

Rings

Ligand DGD C 518

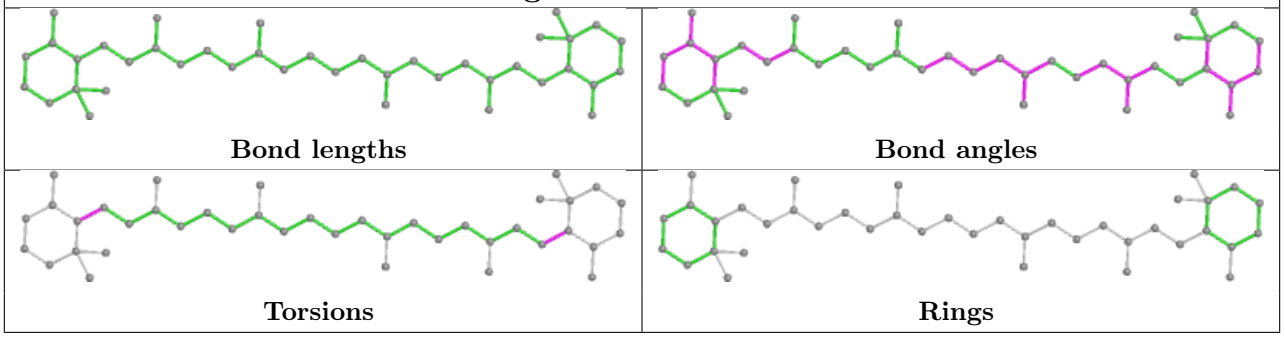

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR B 519



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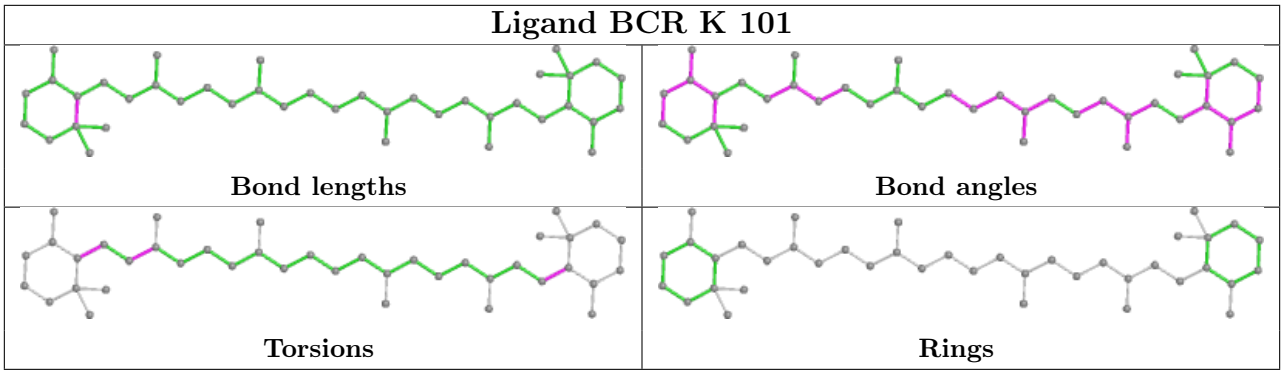

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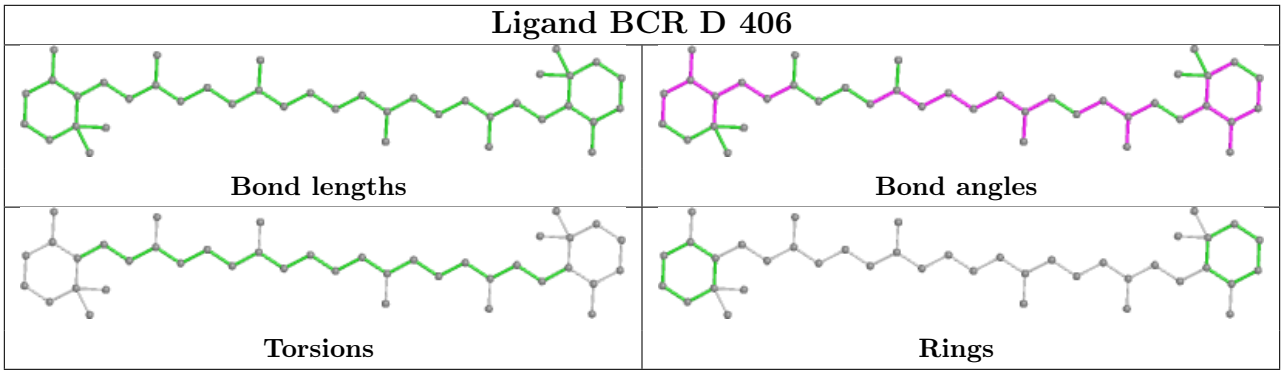

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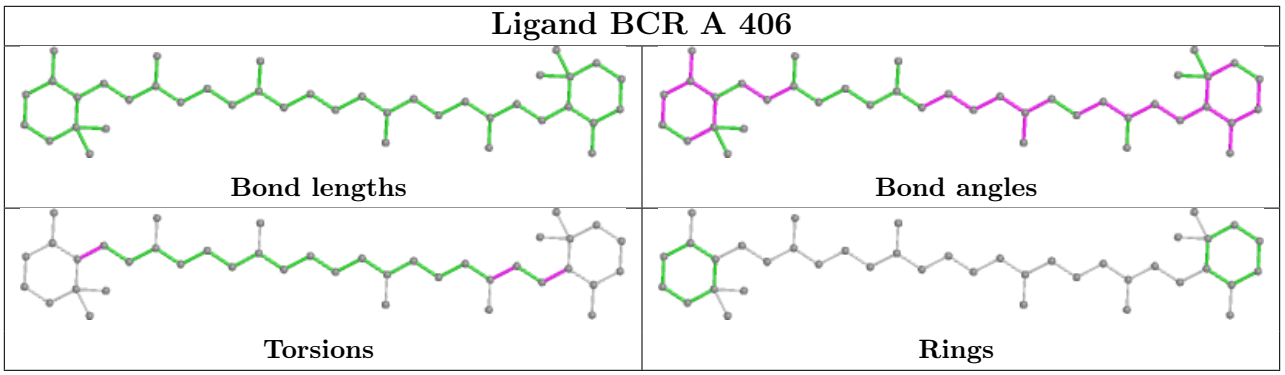
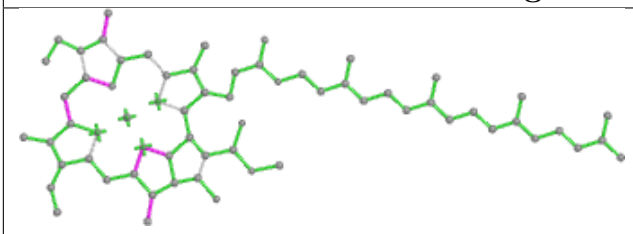
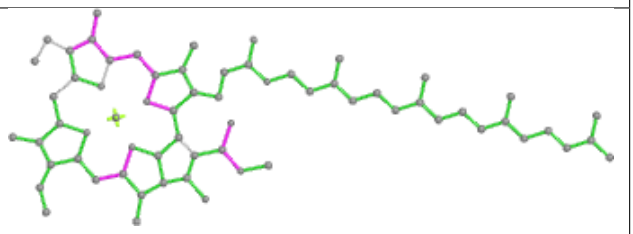


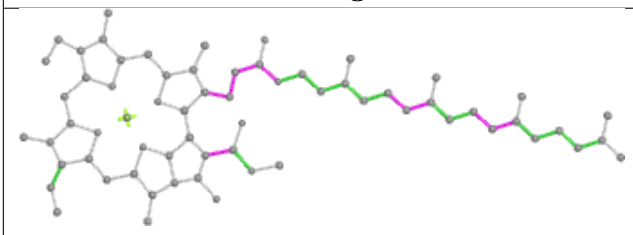
Ligand CLA C 509



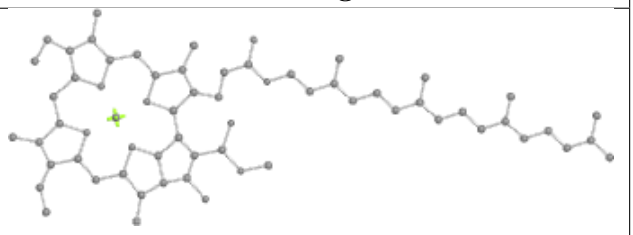
Bond lengths



Bond angles

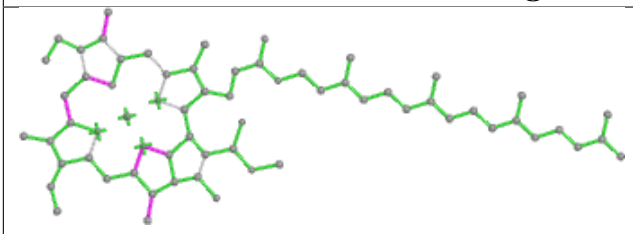


Torsions

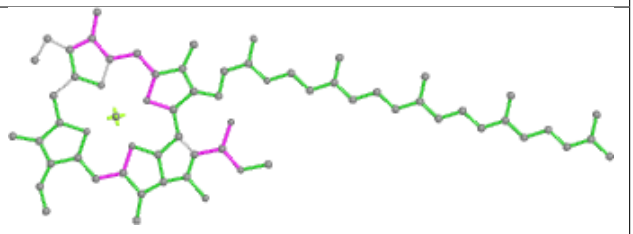


Rings

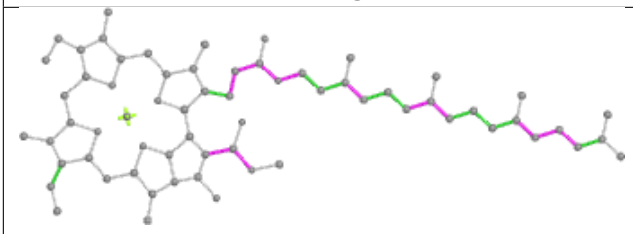
Ligand CLA B 513



Bond lengths



Bond angles



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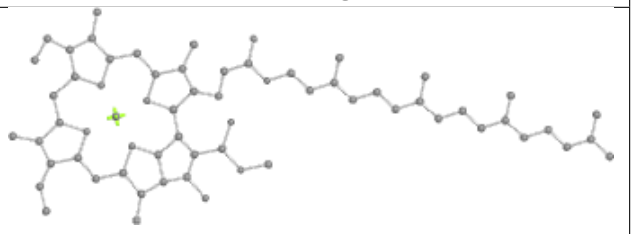
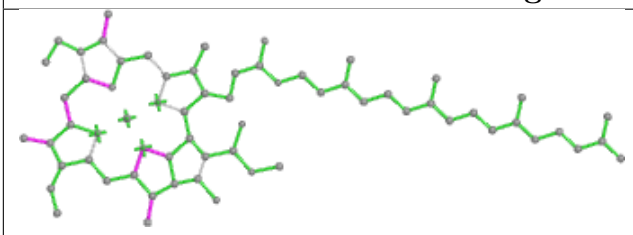


Rings

Ligand CLA C 508



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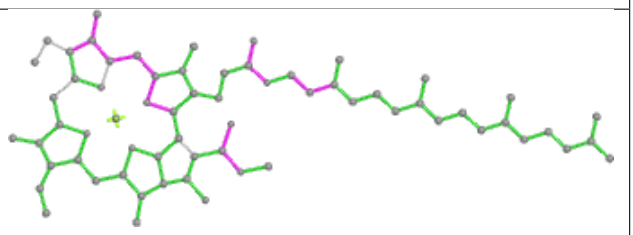
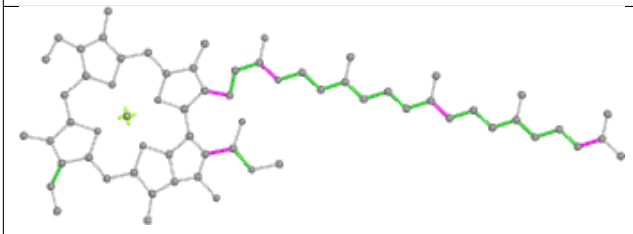


Bond angles



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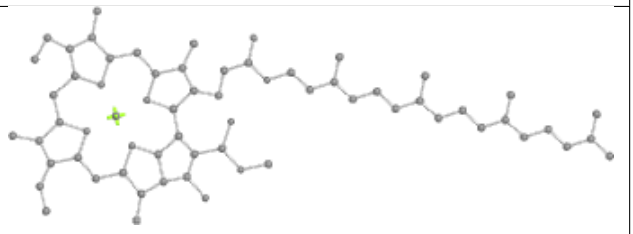
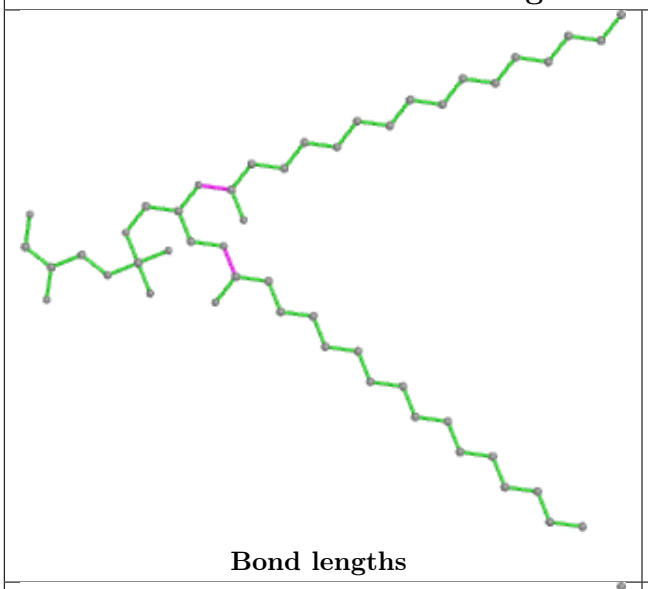


Rings

Ligand LHG L 101



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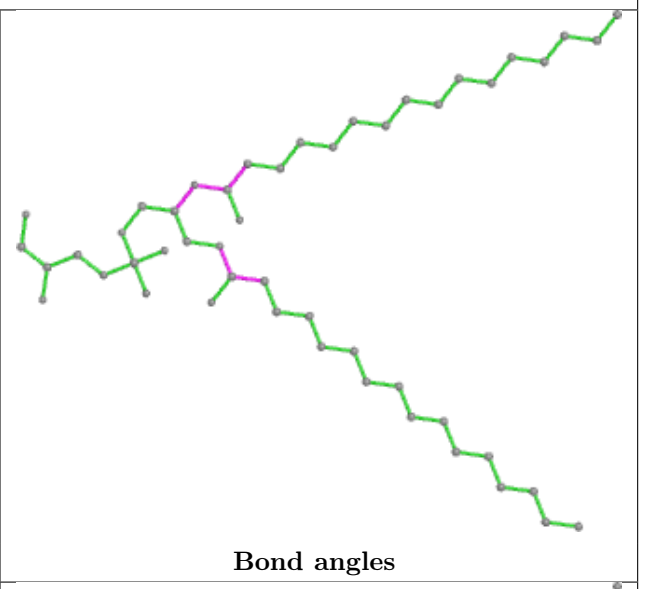
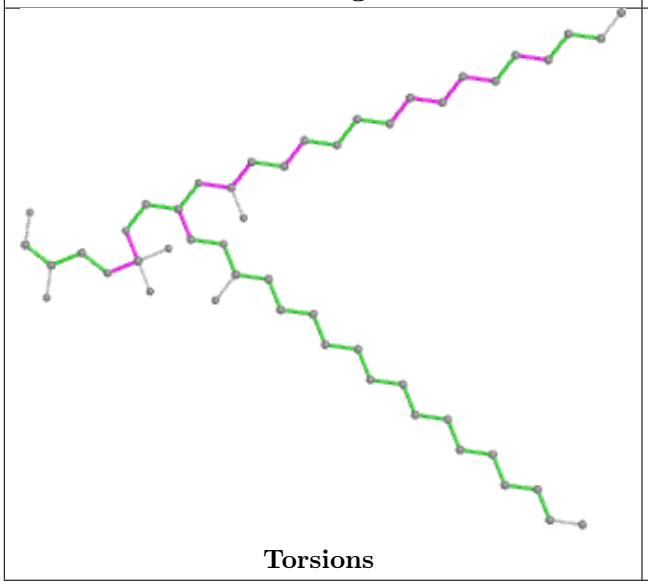


Bond angles



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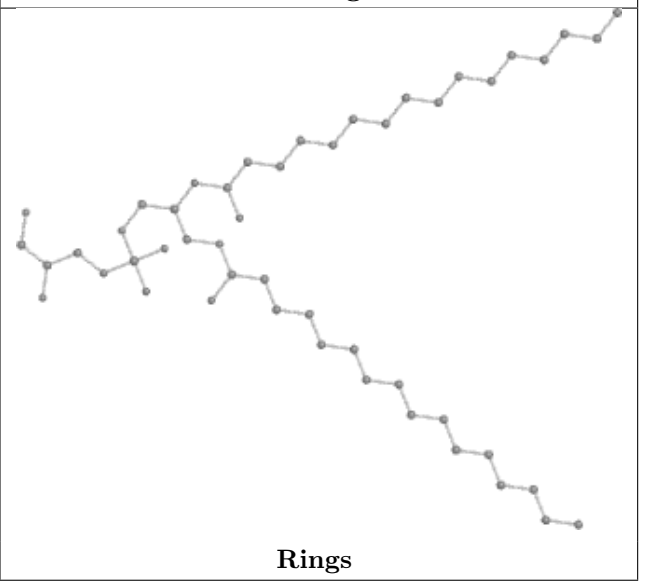
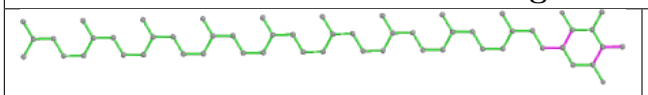


Rings

Ligand PL9 D 407



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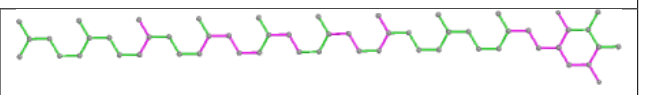
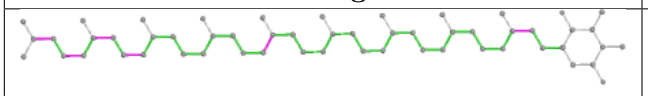


Bond angles



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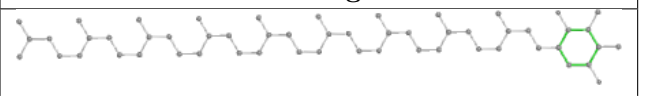
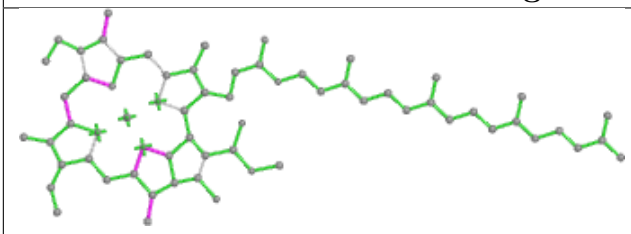


Rings

Ligand CLA D 401



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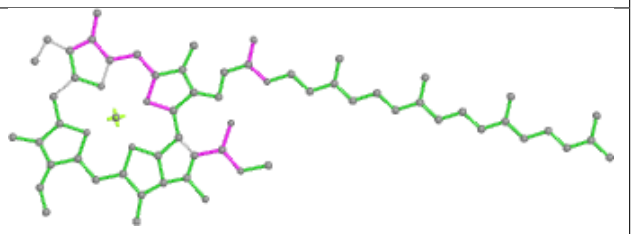
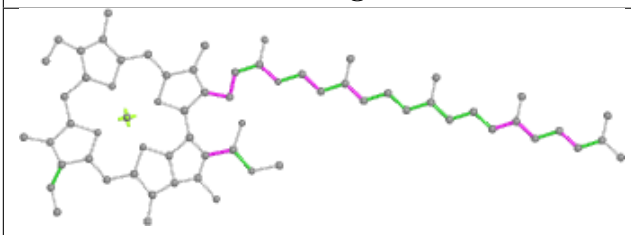


Bond angles



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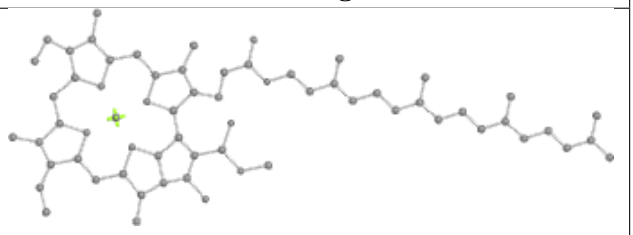
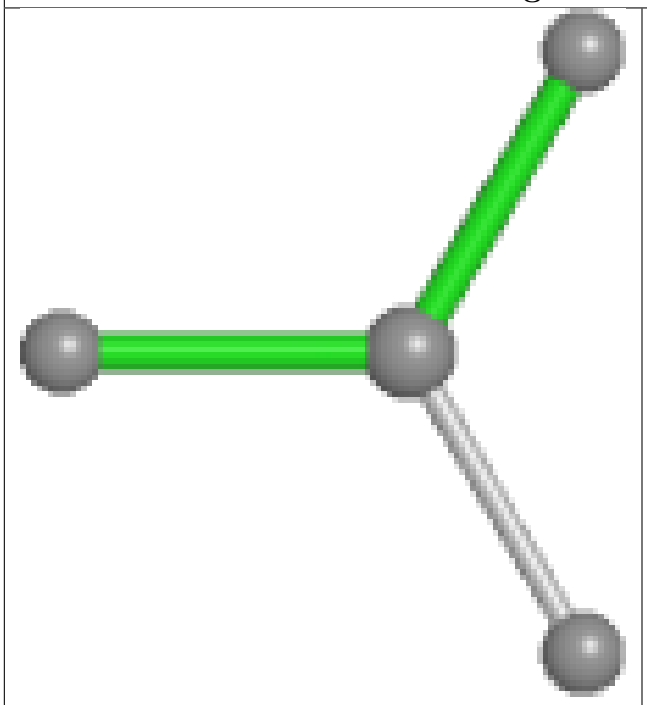


Rings

Ligand BCT D 403



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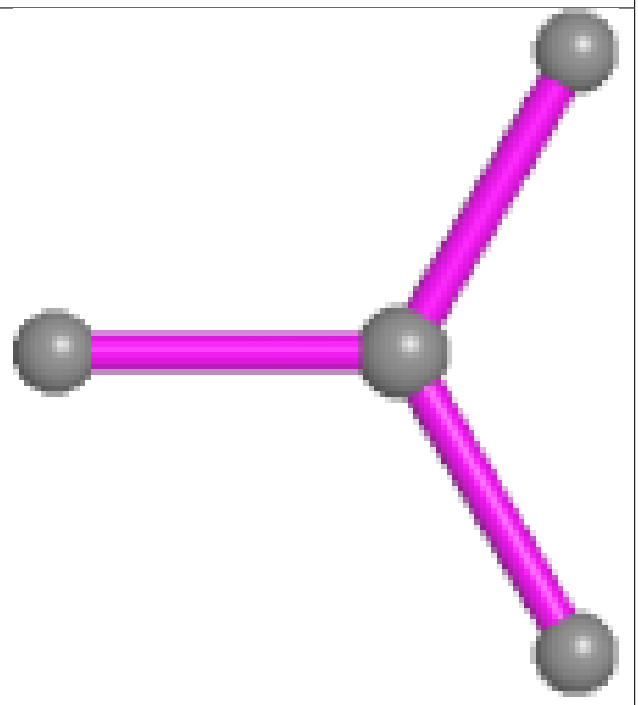
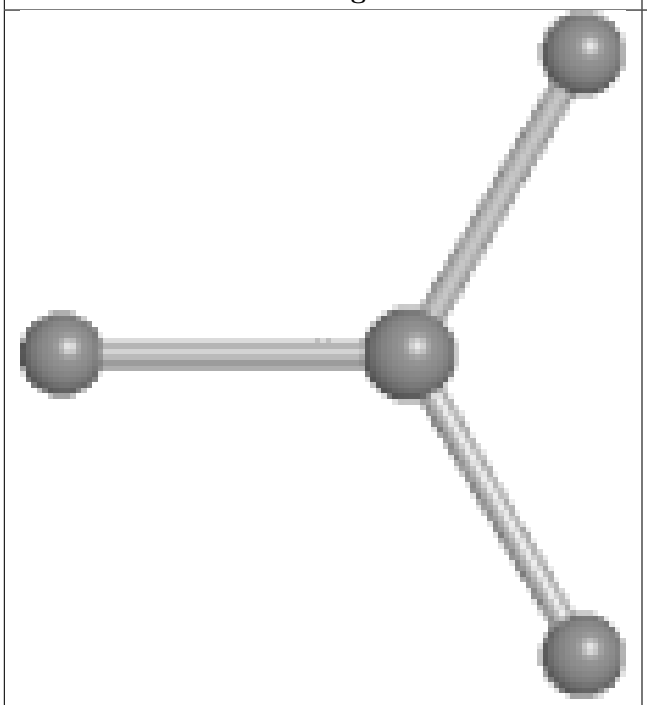


Bond angles



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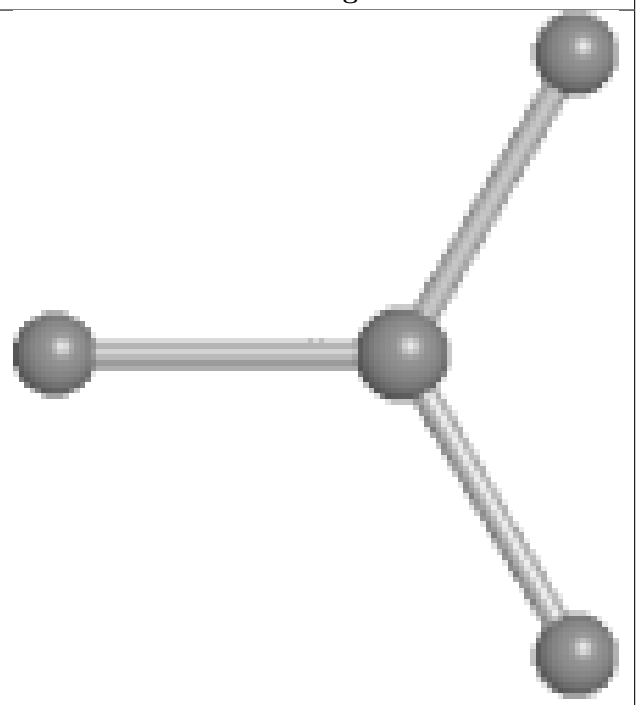
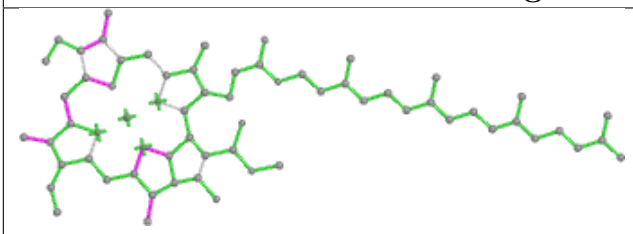


Rings

Ligand CLA C 504



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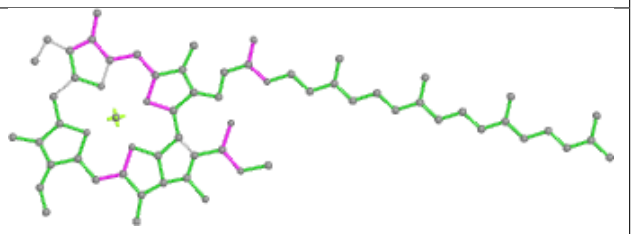
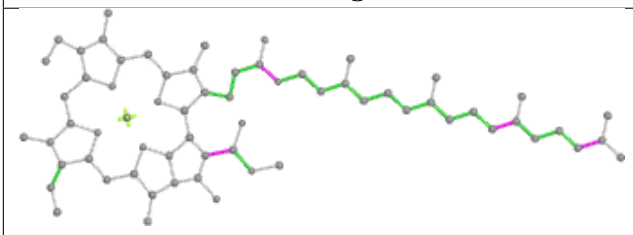


Bond angles



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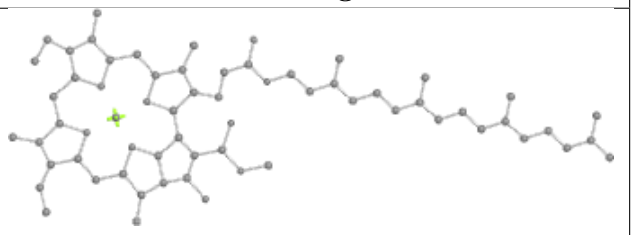
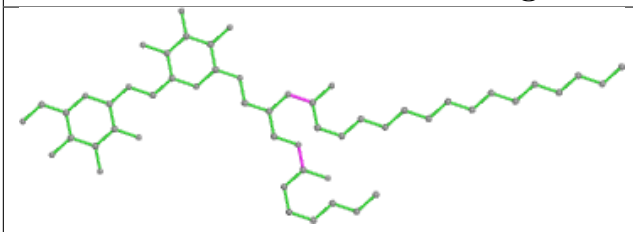


Rings

Ligand DGD C 517



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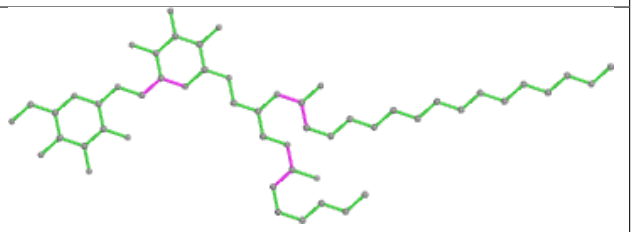
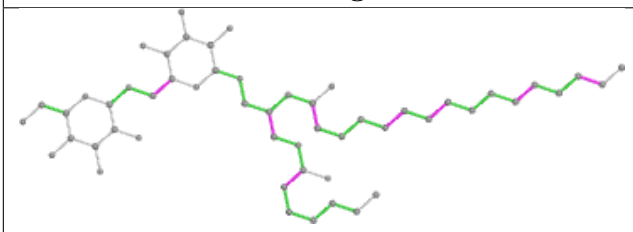
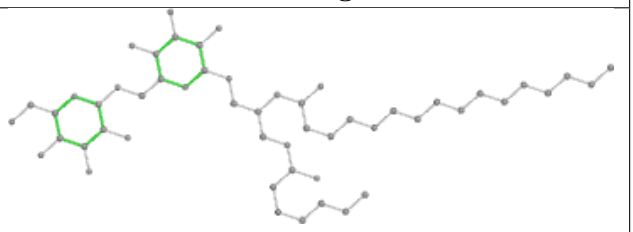


Bond angles

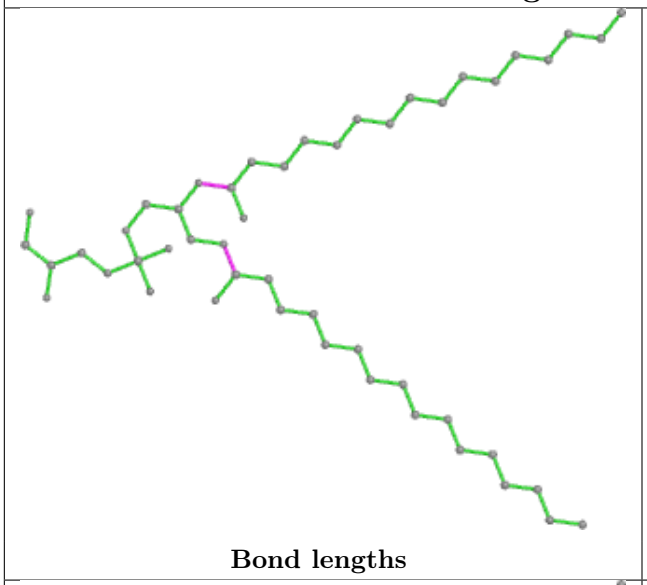


Torsions



Rings

Ligand LHG D 408



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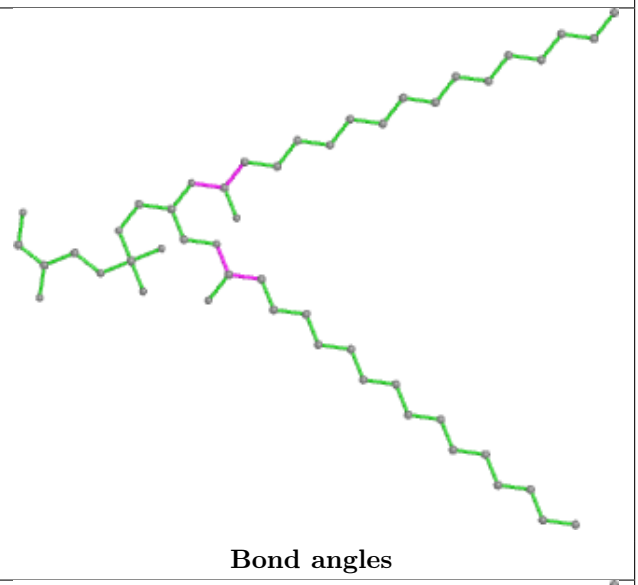
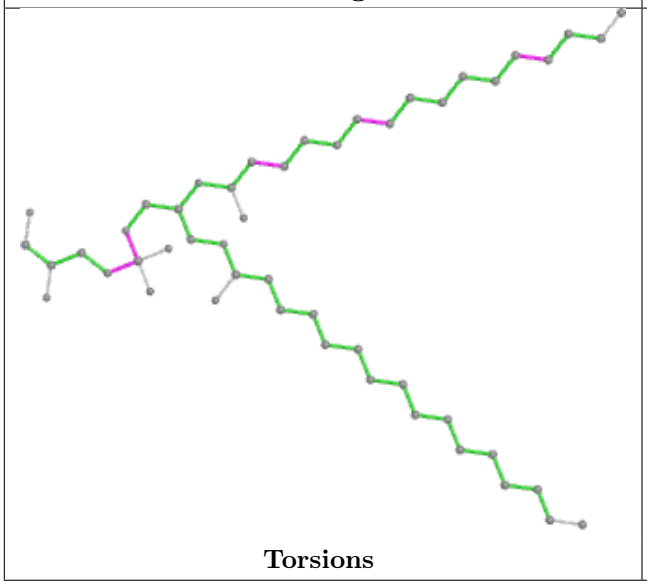


Bond angles



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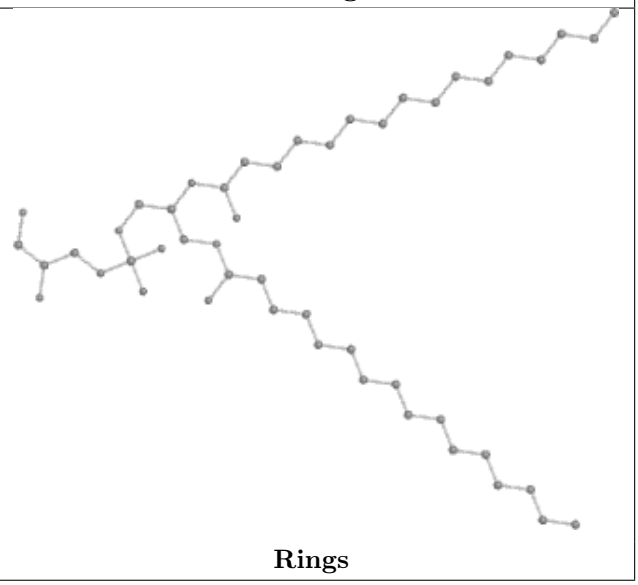
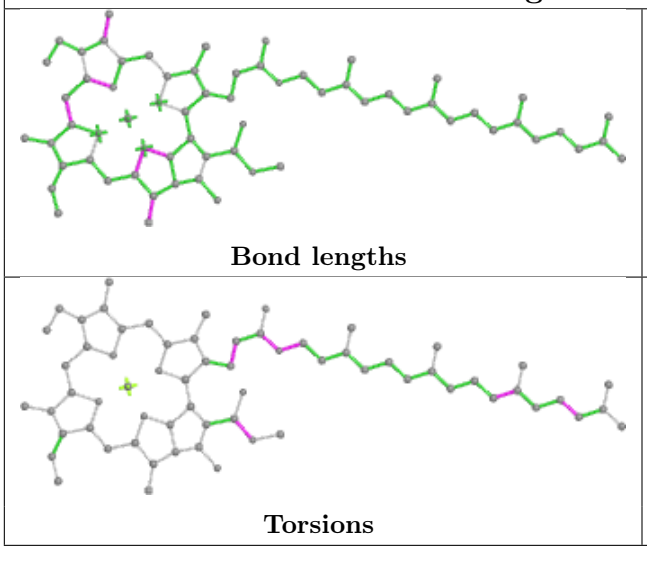


Rings

Ligand CLA C 505



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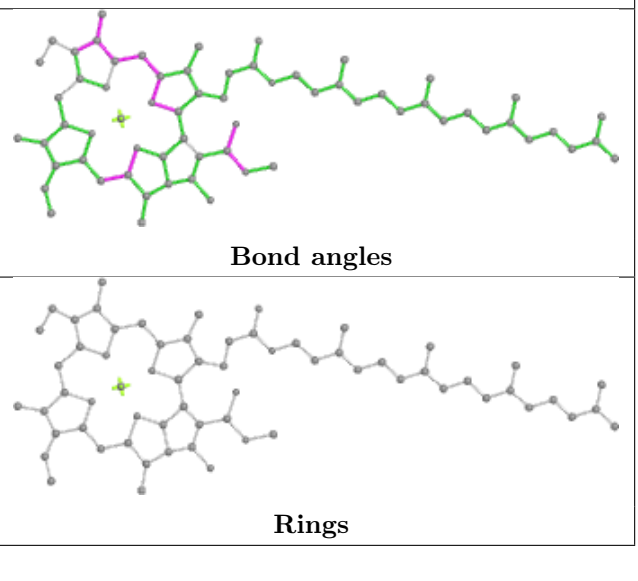
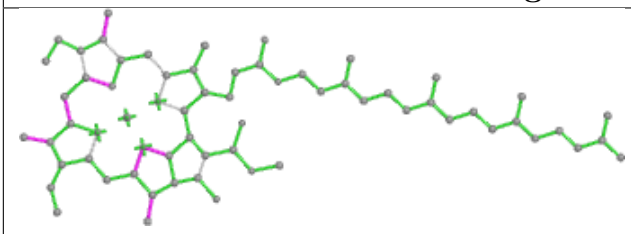


Bond angles

Torsions

Rings

Ligand CLA B 504



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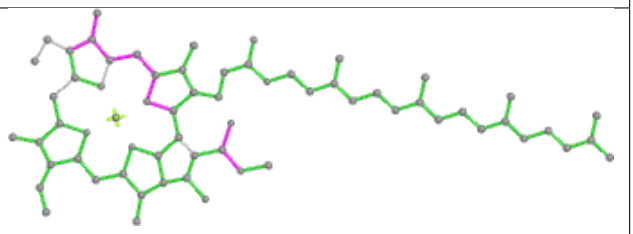
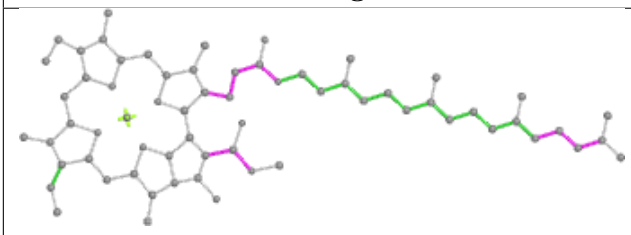
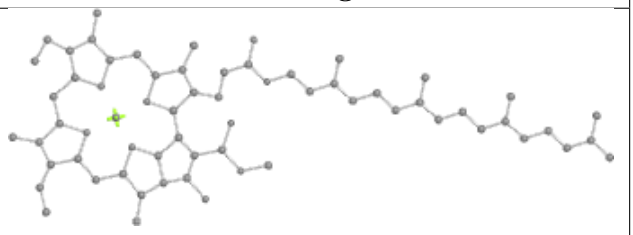


Bond angles

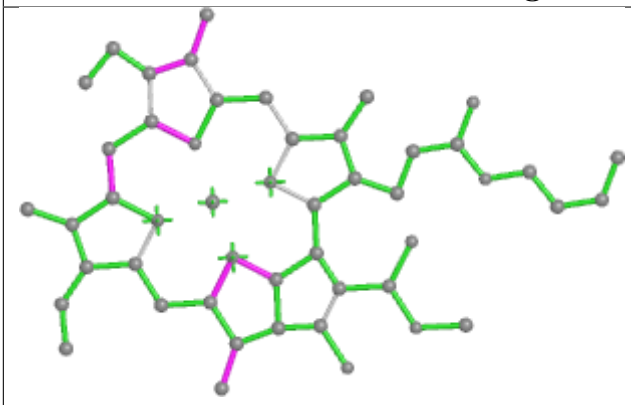


Torsions

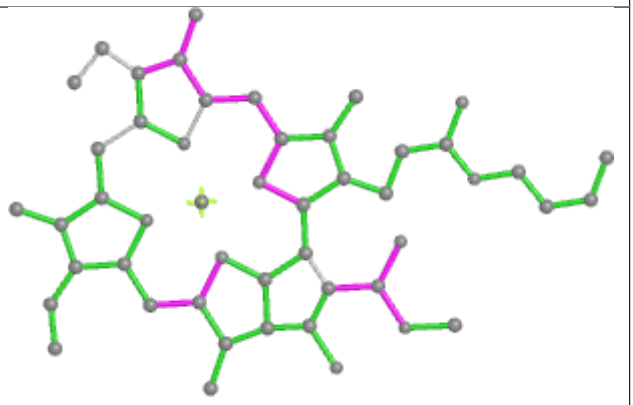


Rings

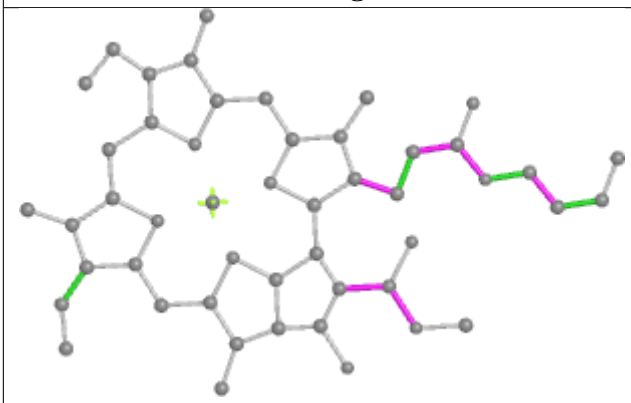
Ligand CLA A 403



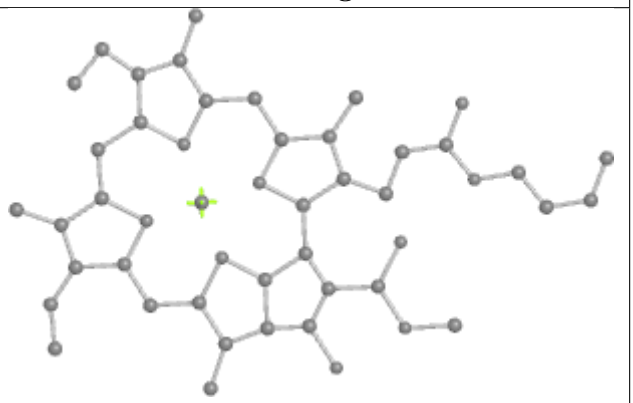
Bond lengths



Bond angles

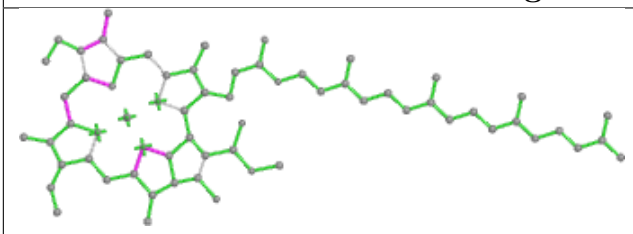


Torsions

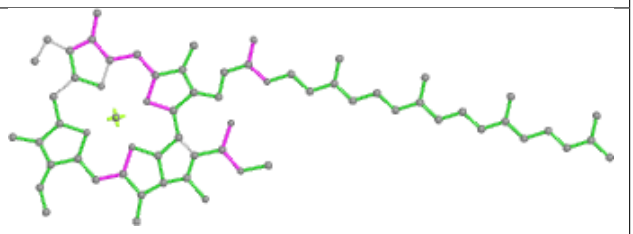


Rings

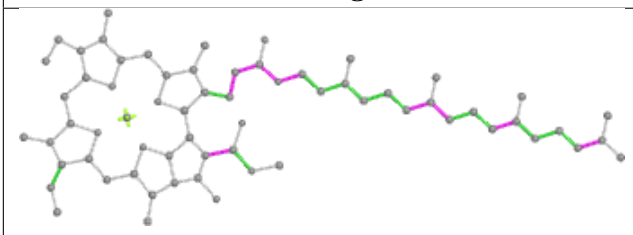
Ligand CLA C 510



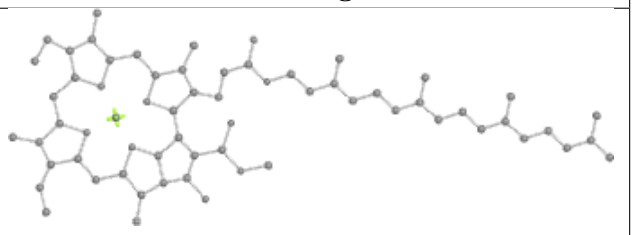
Bond lengths



Bond angles

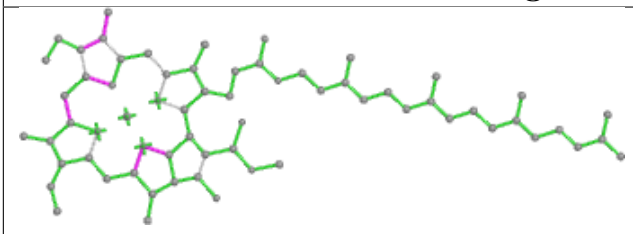


Torsions

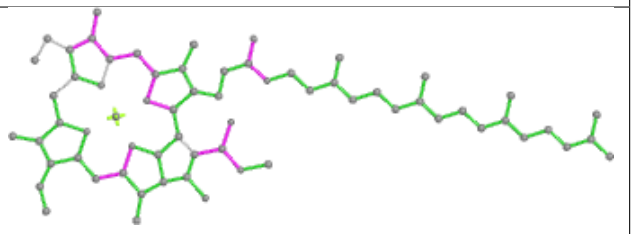


Rings

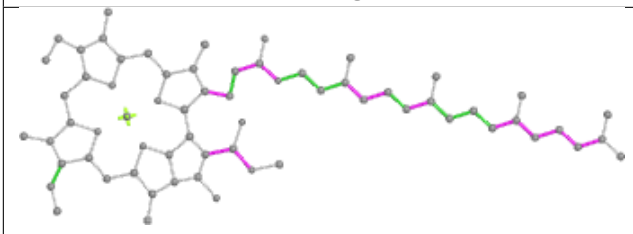
Ligand CLA C 511



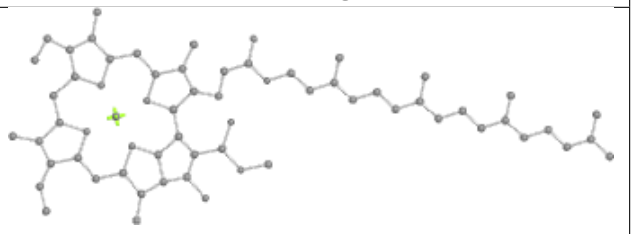
Bond lengths



Bond angles

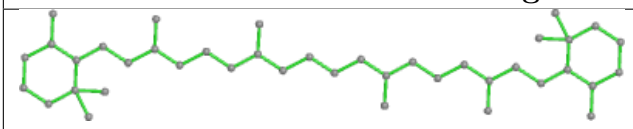


Torsions

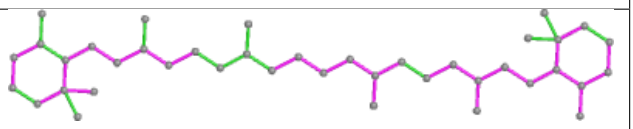


Rings

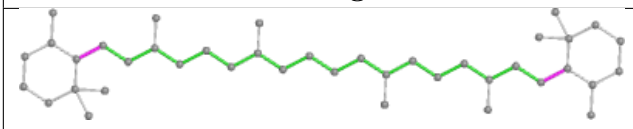
Ligand BCR C 516



Bond lengths



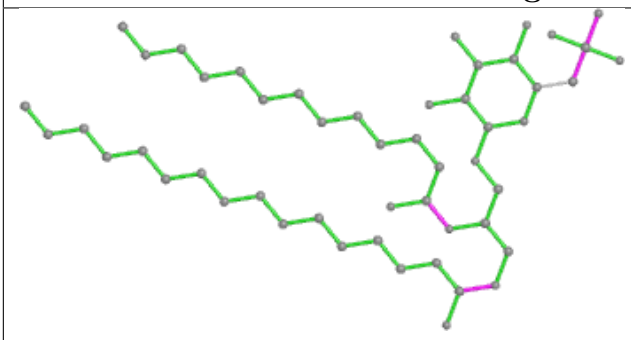
Bond angles



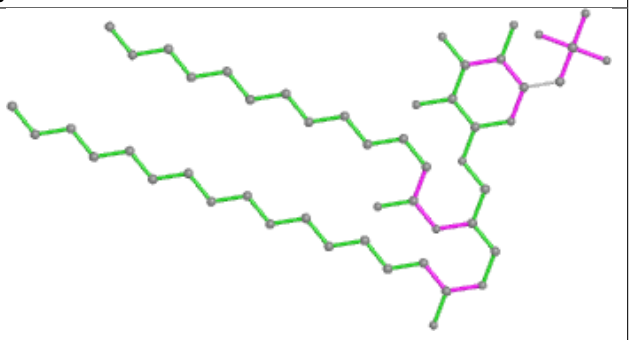
Torsions

Rings

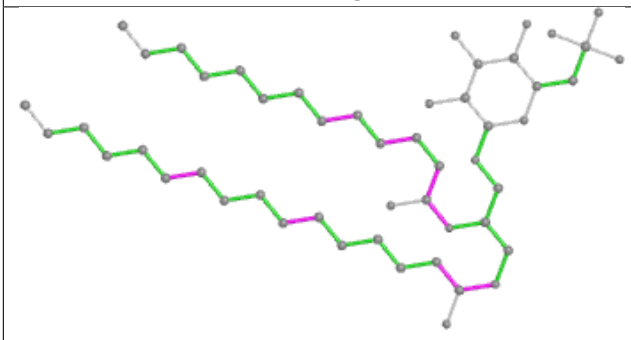
Ligand SQD A 407



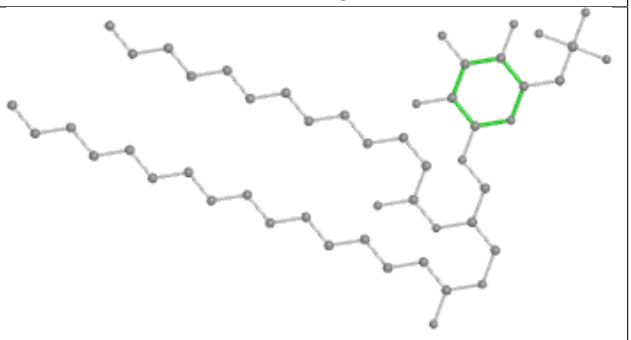
Bond lengths



Bond angles

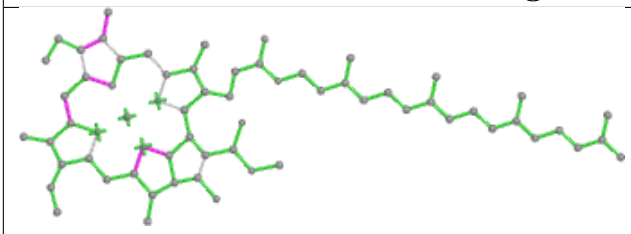


Torsions

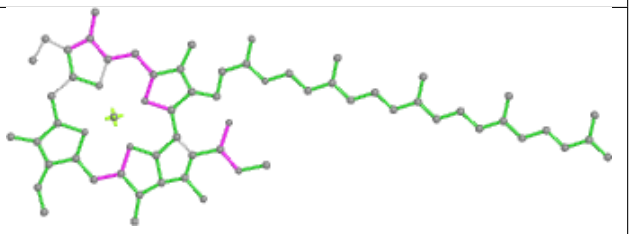


Rings

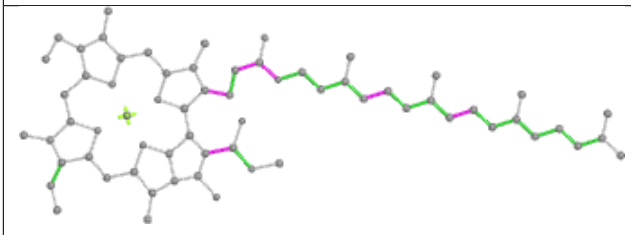
Ligand CLA B 506



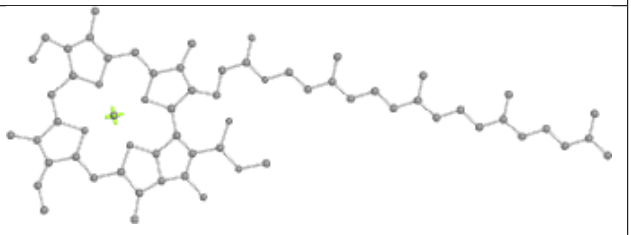
Bond lengths



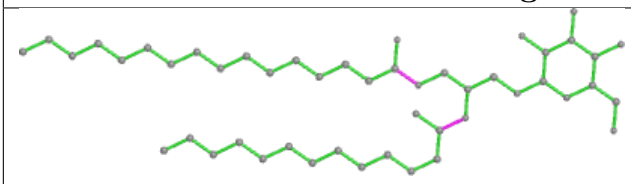
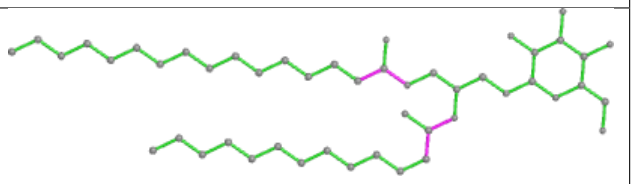
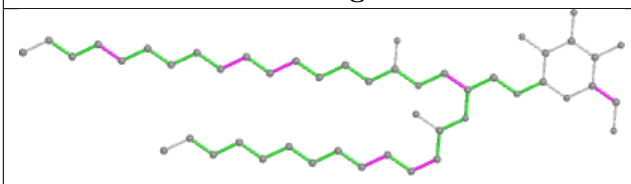
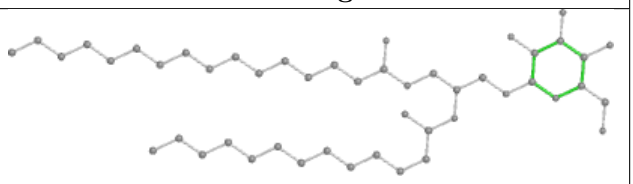
Bond angles

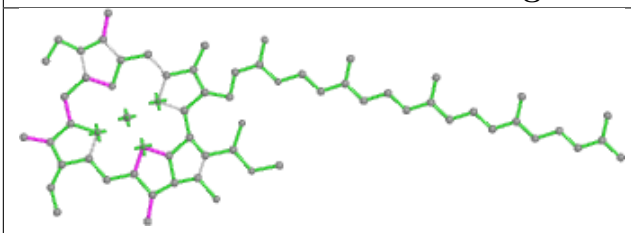
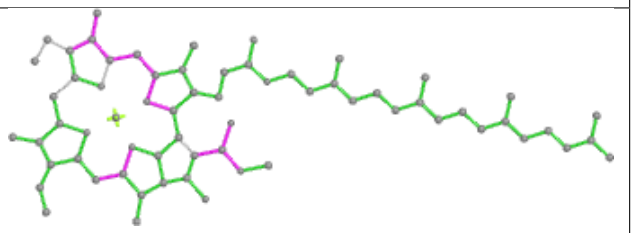
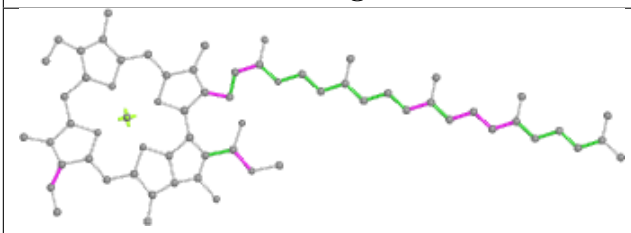
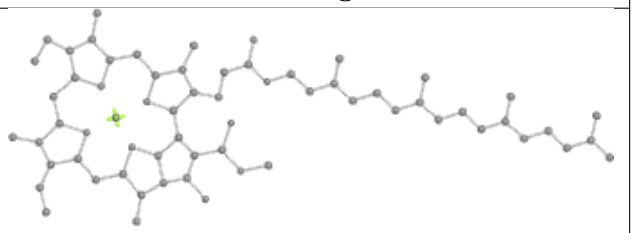


Torsions

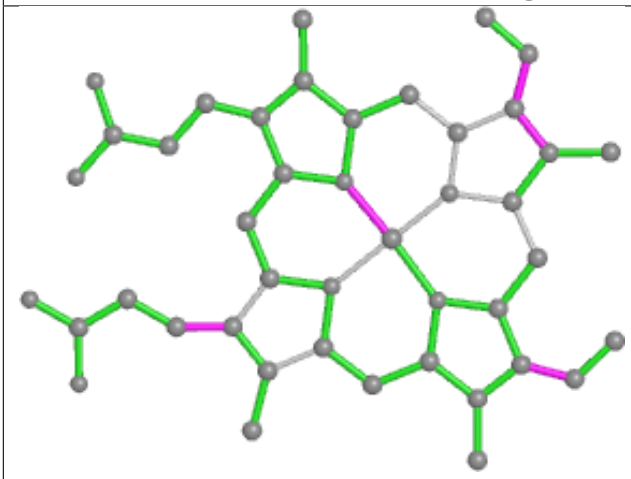


Rings

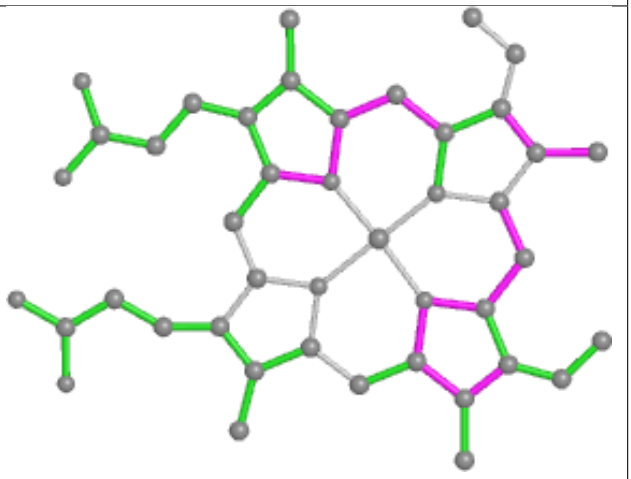
Ligand LMG B 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA D 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

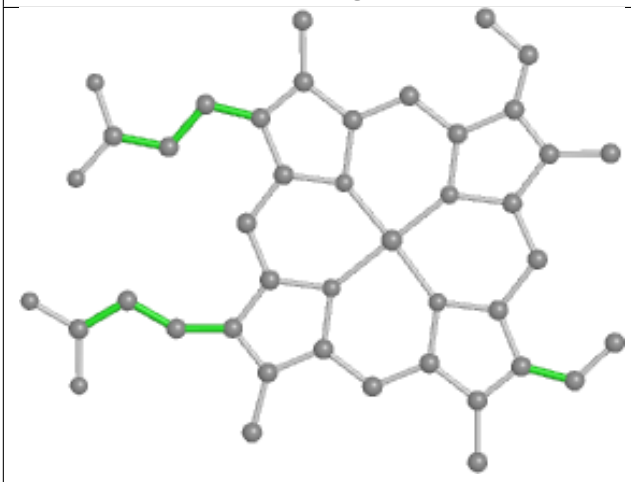
Ligand HEM F 101



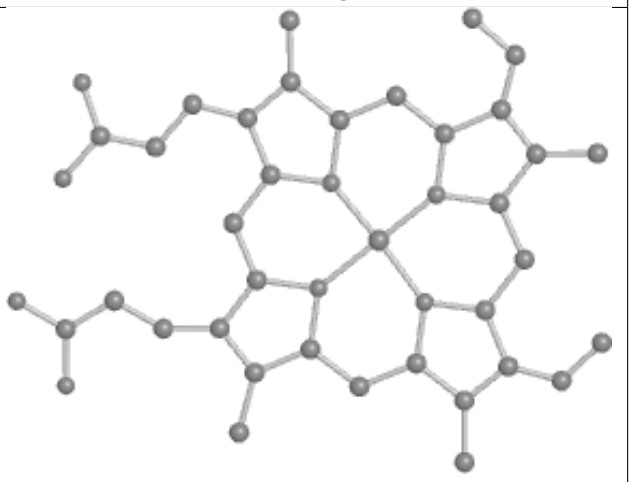
Bond lengths



Bond angles

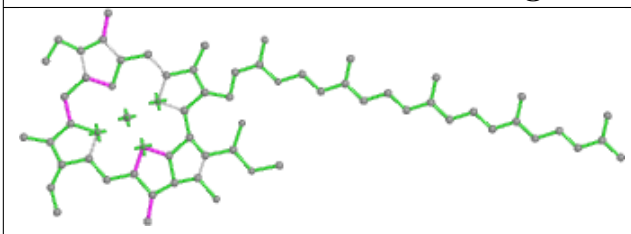


Torsions

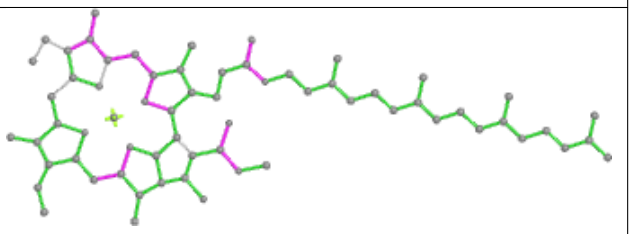


Rings

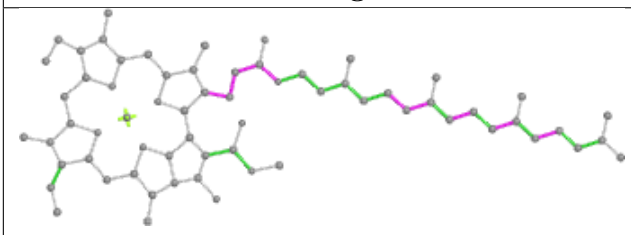
Ligand CLA B 512



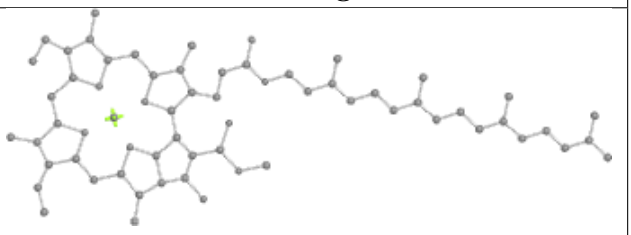
Bond lengths



Bond angles

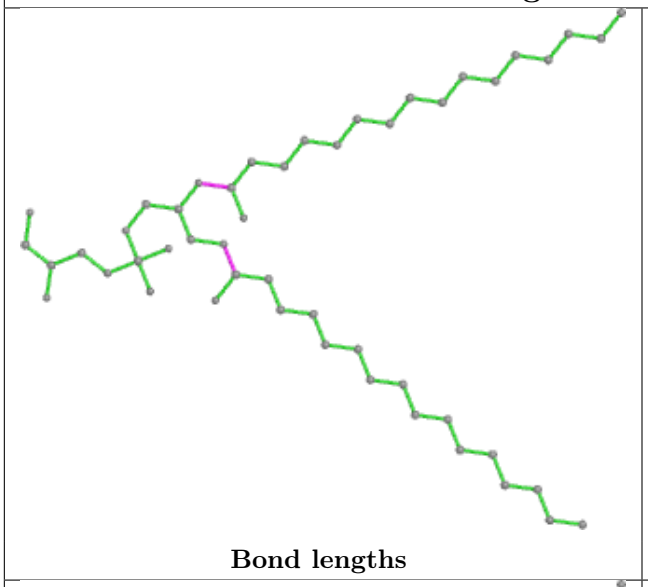


Torsions

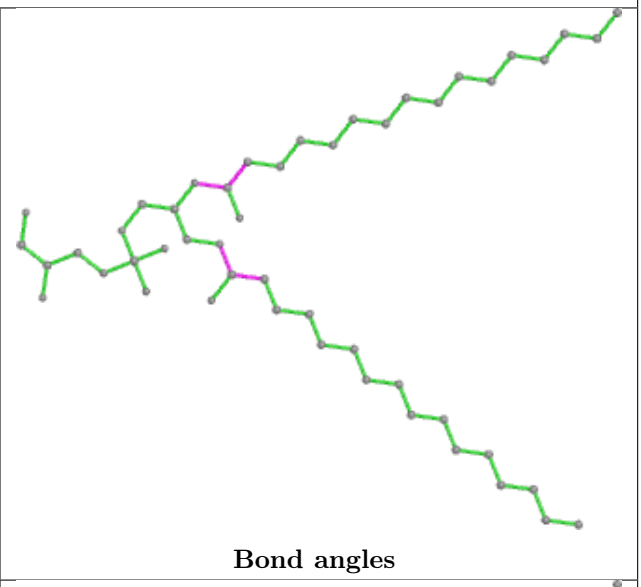


Rings

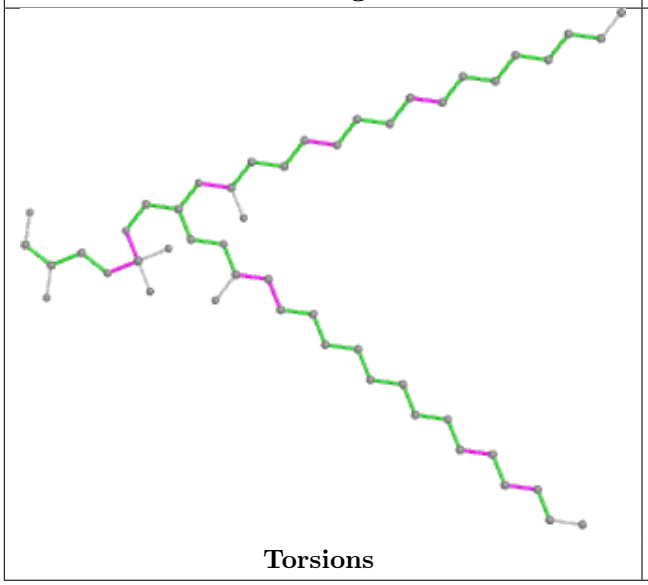
Ligand LHG D 410



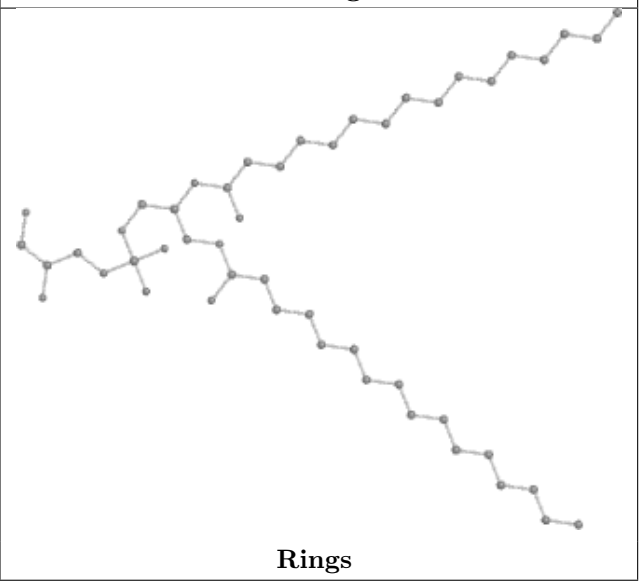
Bond lengths



Bond angles

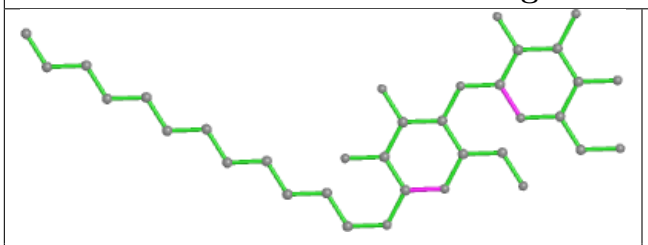


Torsions

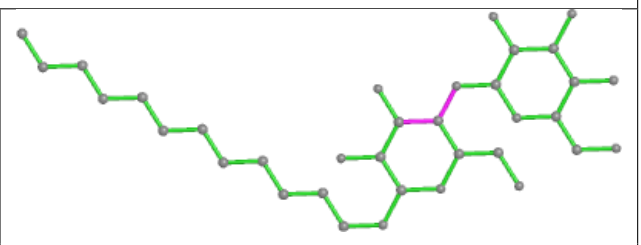


Rings

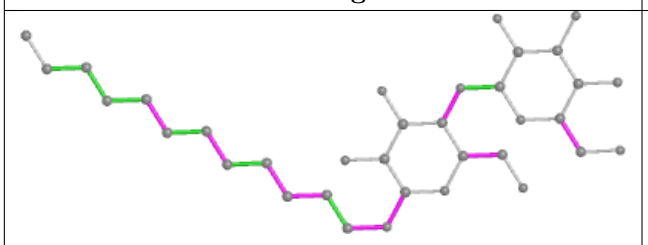
Ligand LMU C 520



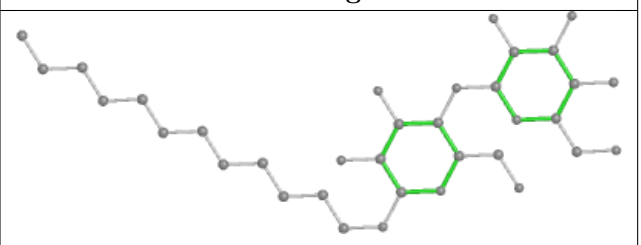
Bond lengths



Bond angles

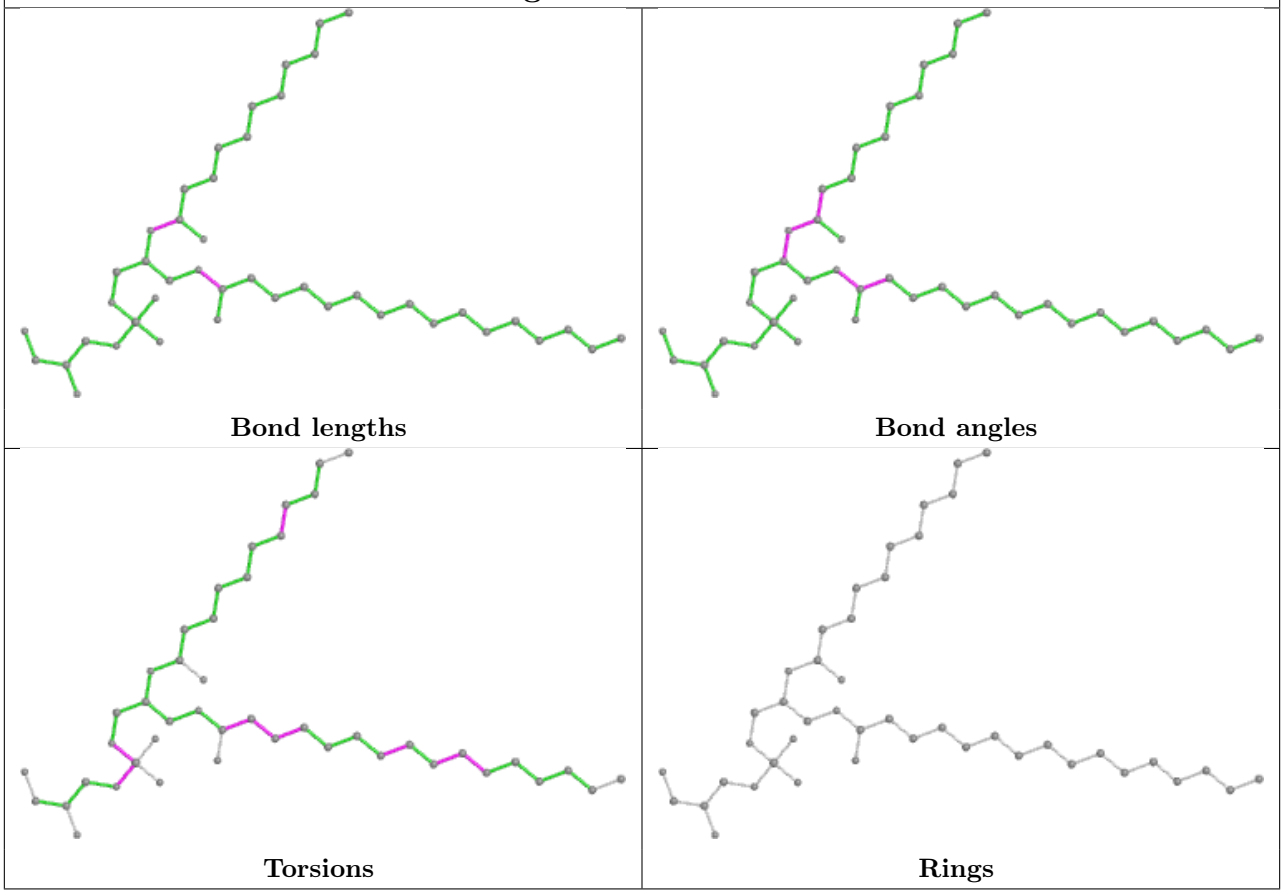


Torsions

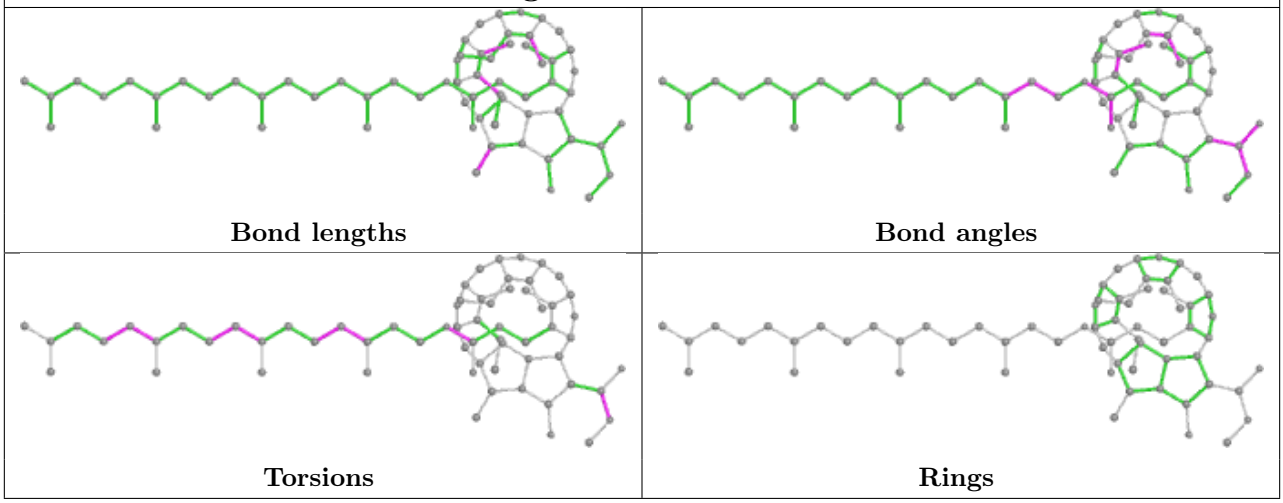


Rings

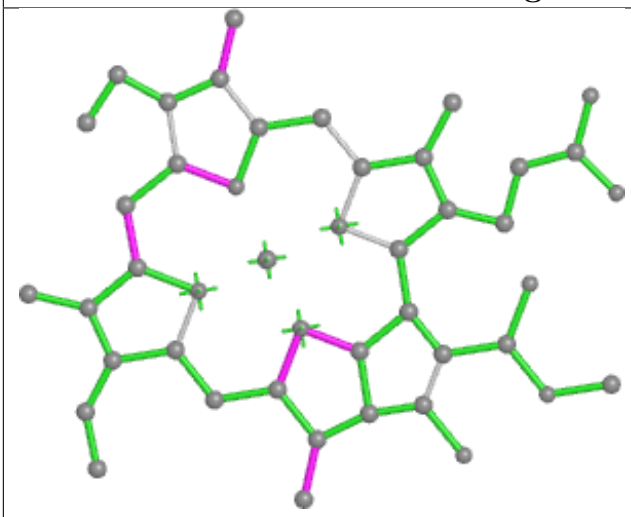
Ligand LHG B 521



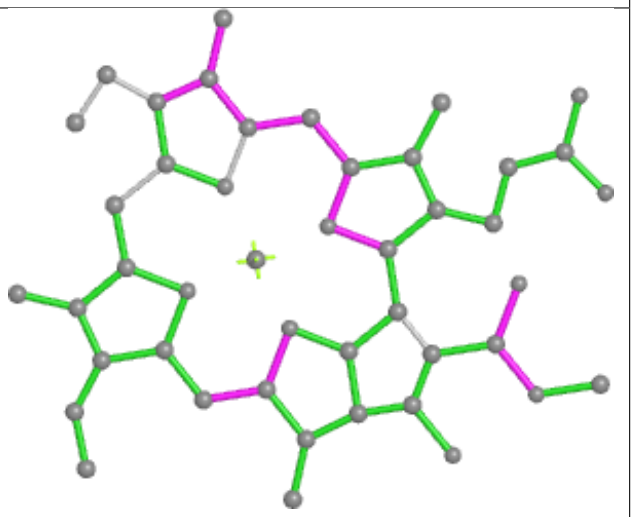
Ligand PHO A 404



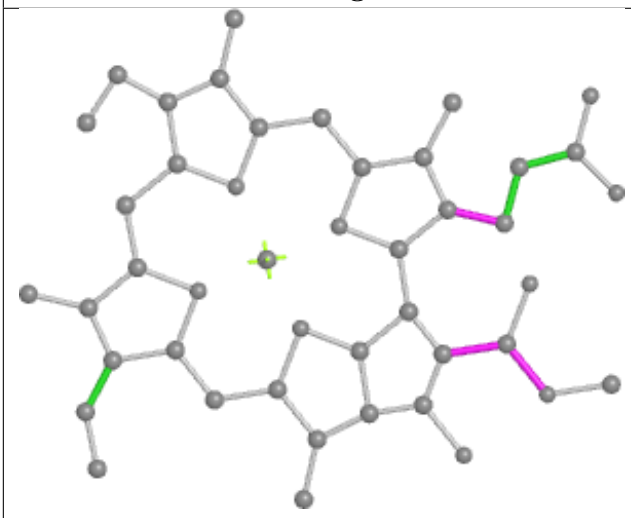
Ligand CLA B 514



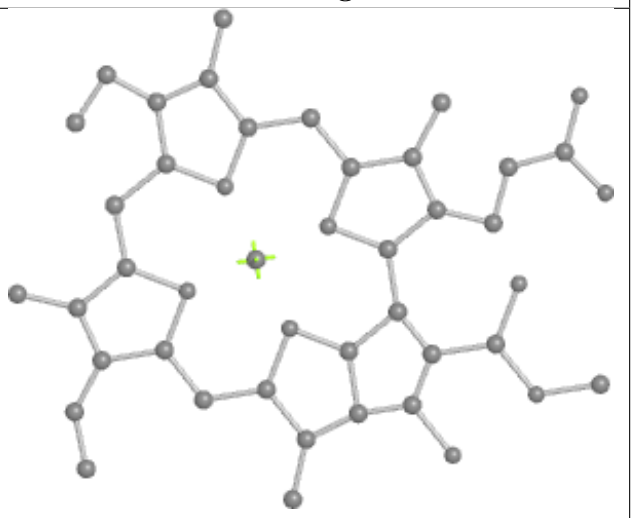
Bond lengths



Bond angles

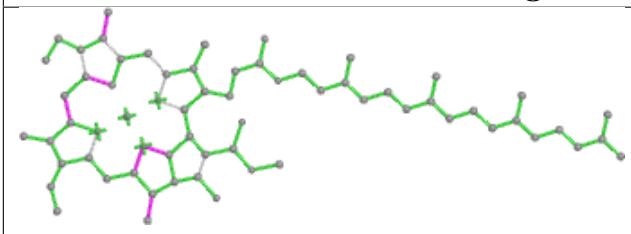


Torsions

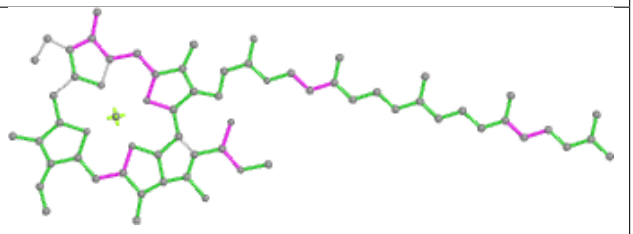


Rings

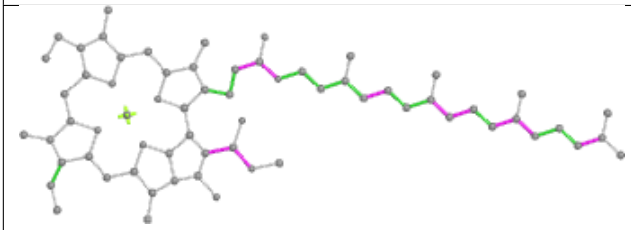
Ligand CLA C 503



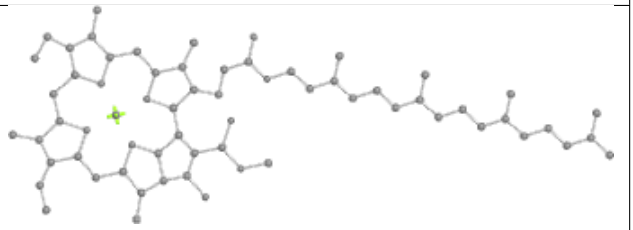
Bond lengths



Bond angles

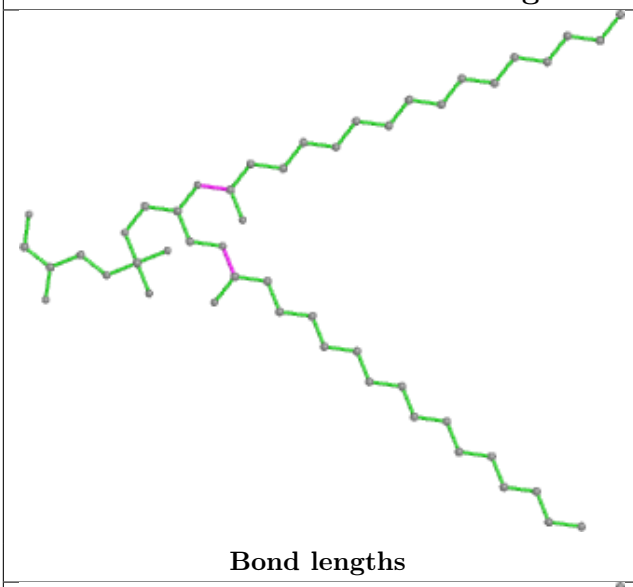


Torsions

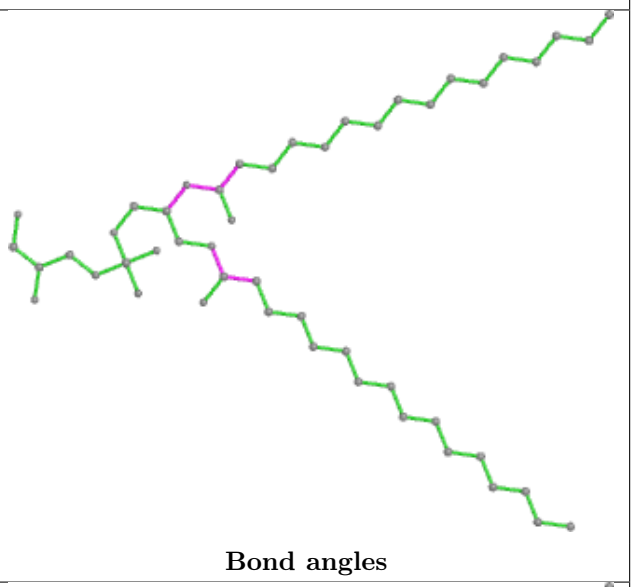


Rings

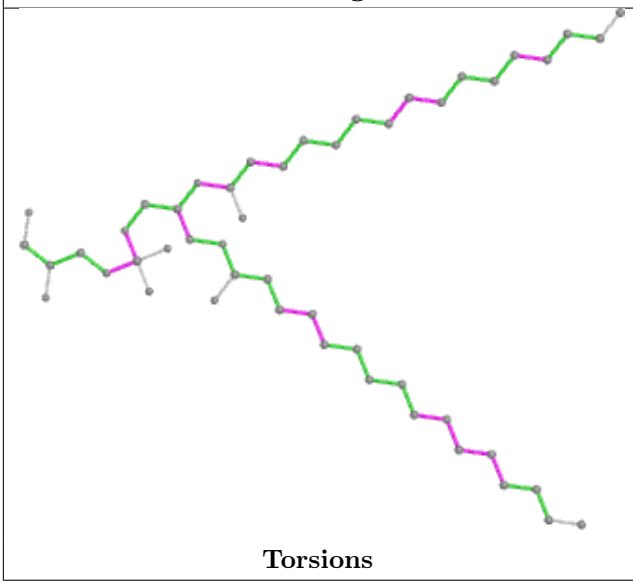
Ligand LHG D 411



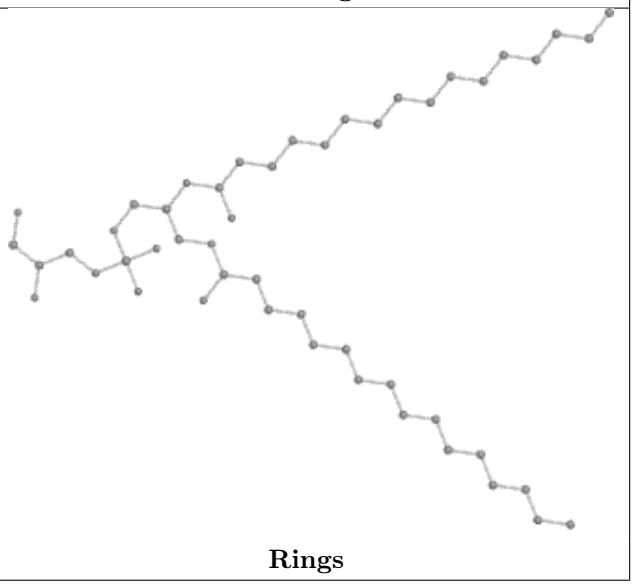
Bond lengths



Bond angles

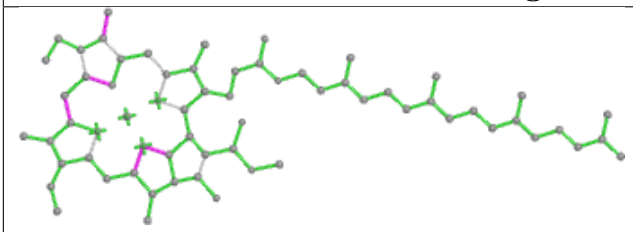


Torsions

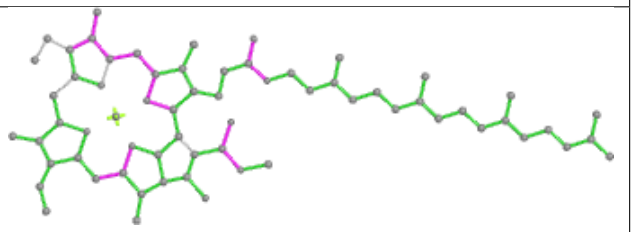


Rings

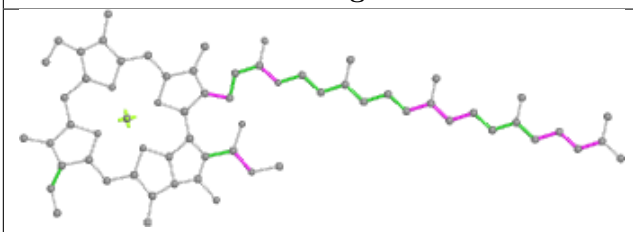
Ligand CLA C 513



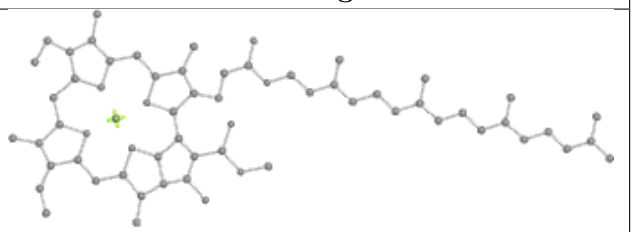
Bond lengths



Bond angles

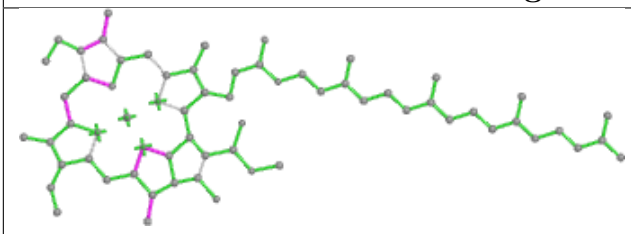


Torsions

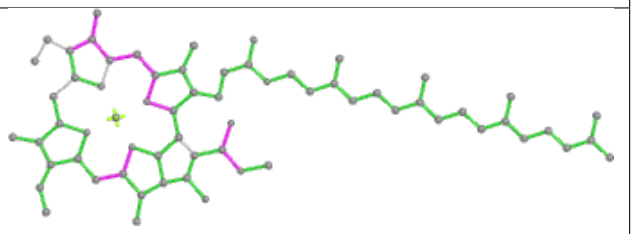


Rings

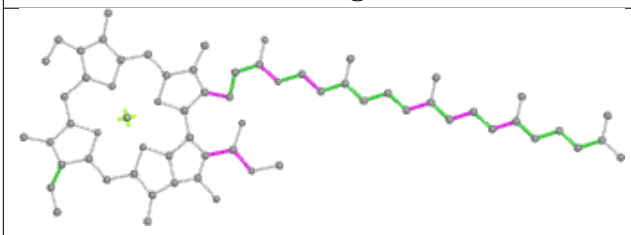
Ligand CLA B 501



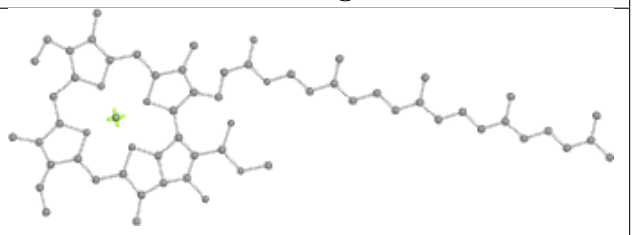
Bond lengths



Bond angles

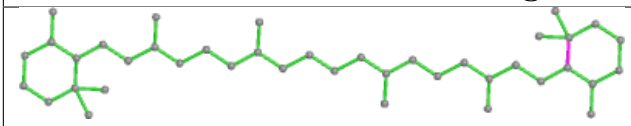


Torsions

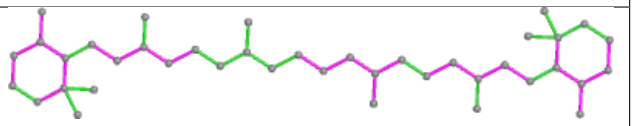


Rings

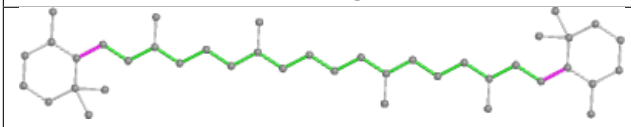
Ligand BCR C 515



Bond lengths



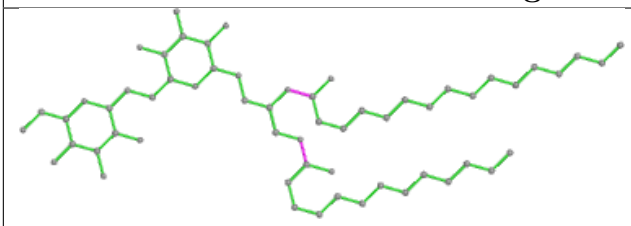
Bond angles



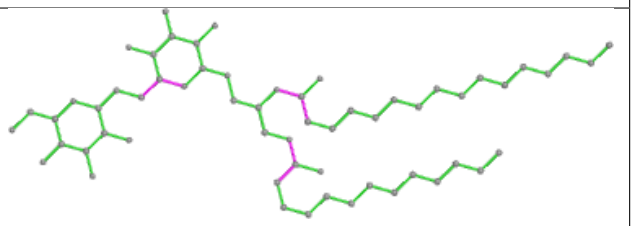
Torsions

Rings

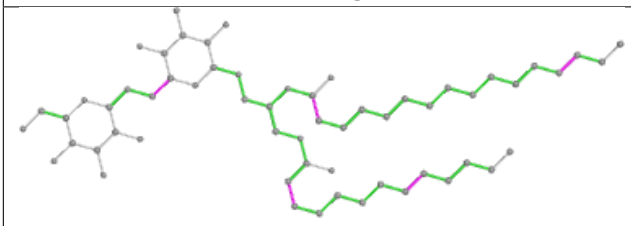
Ligand DGD J 101



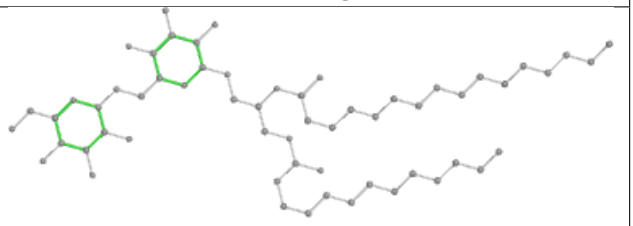
Bond lengths



Bond angles

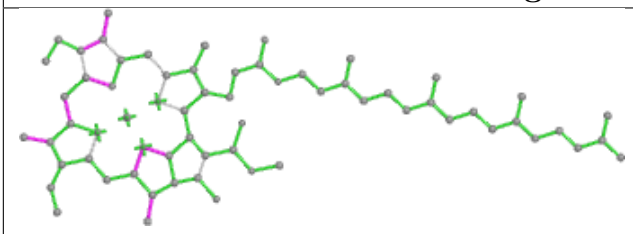


Torsions

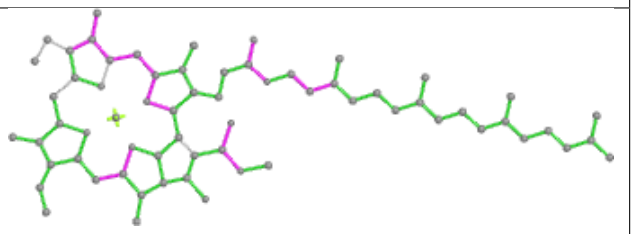


Rings

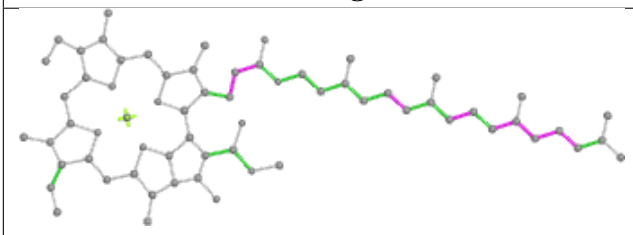
Ligand CLA B 511



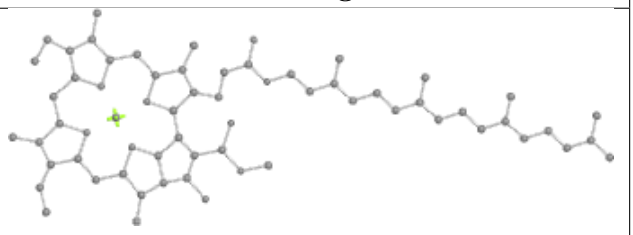
Bond lengths



Bond angles

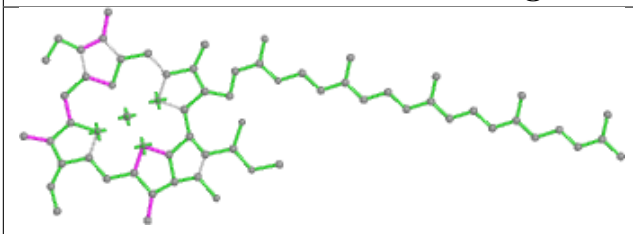


Torsions

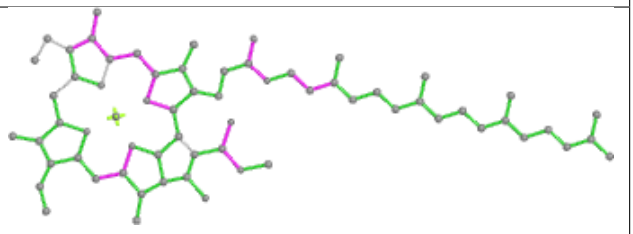


Rings

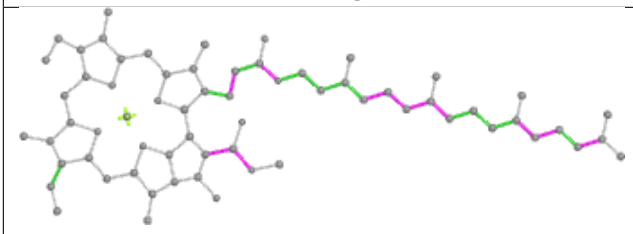
Ligand CLA C 502



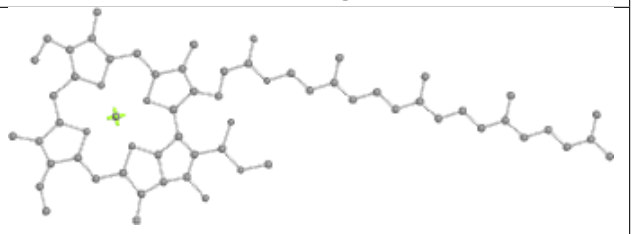
Bond lengths



Bond angles

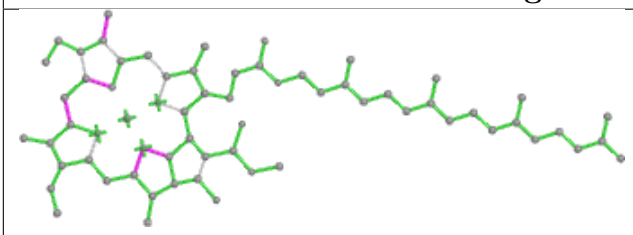


Torsions

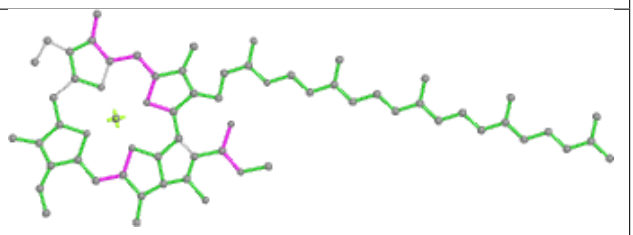


Rings

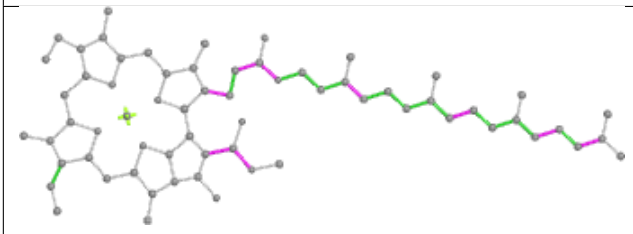
Ligand CLA B 505



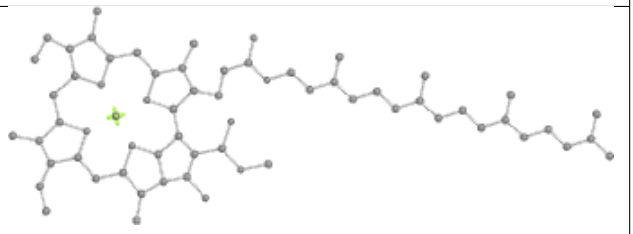
Bond lengths



Bond angles

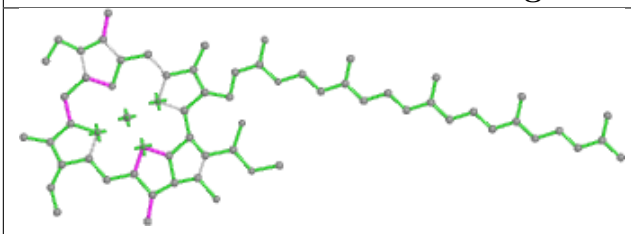


Torsions

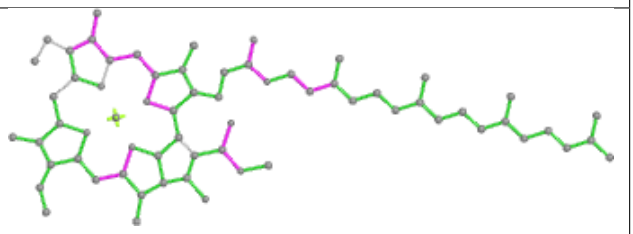


Rings

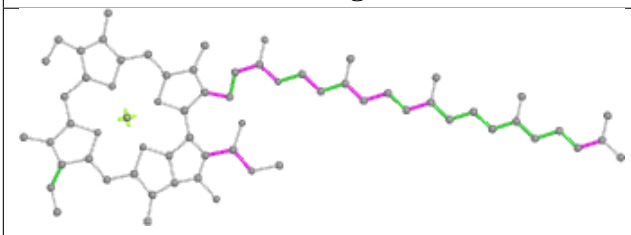
Ligand CLA C 506



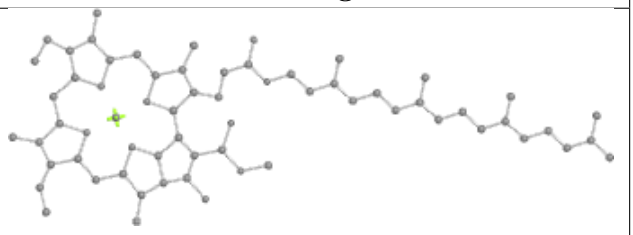
Bond lengths



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.

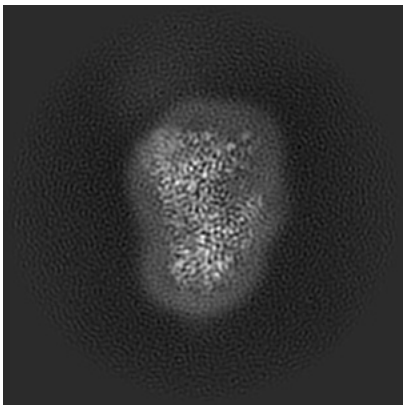
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60605. These allow visual inspection of the internal detail of the map and identification of artifacts.

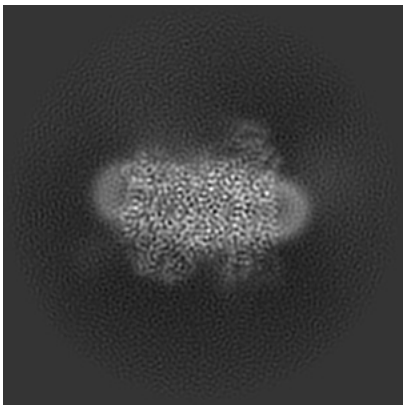
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

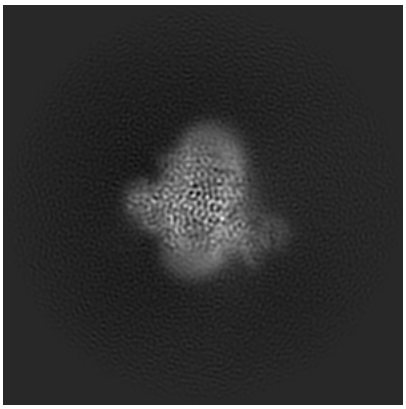
6.1.1 Primary map



X

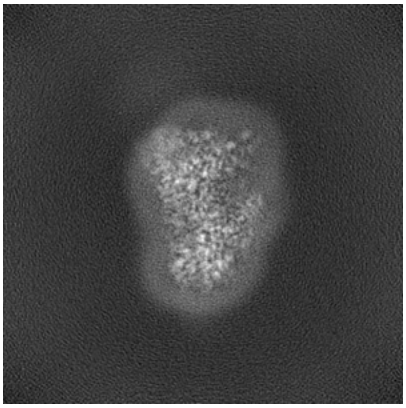


Y

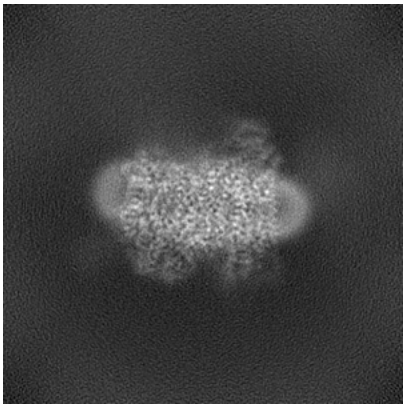


Z

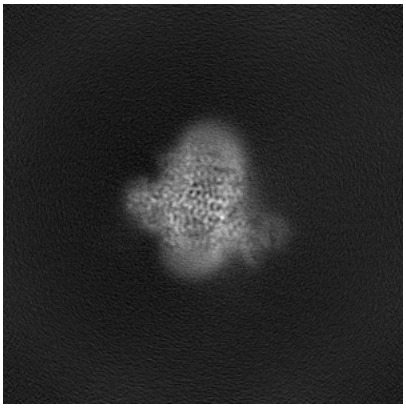
6.1.2 Raw map



X



Y

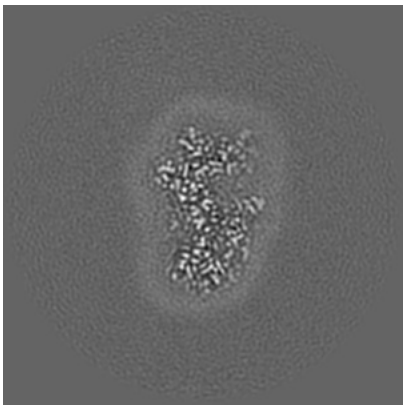


Z

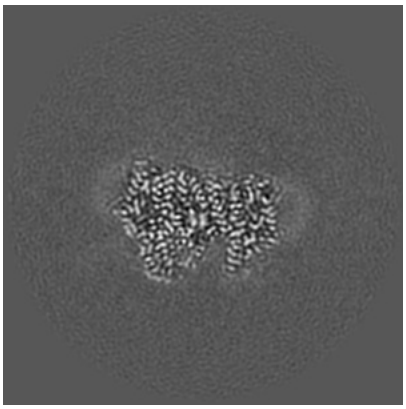
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

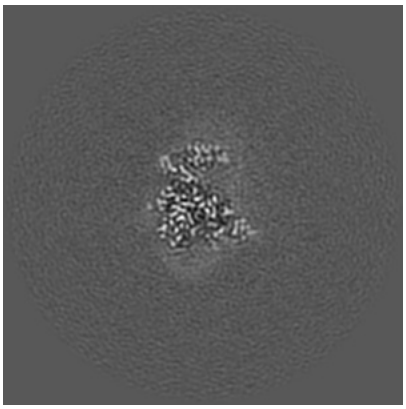
6.2.1 Primary map



X Index: 140

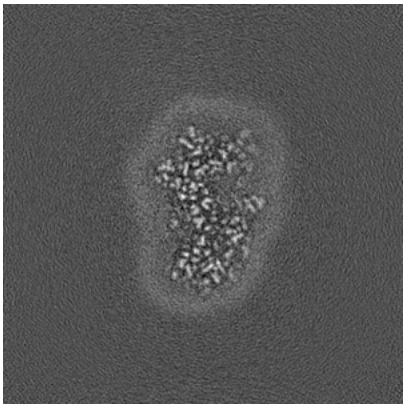


Y Index: 140

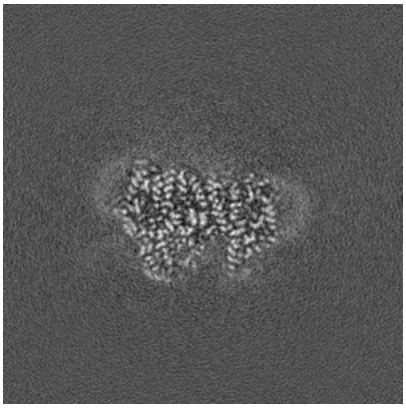


Z Index: 140

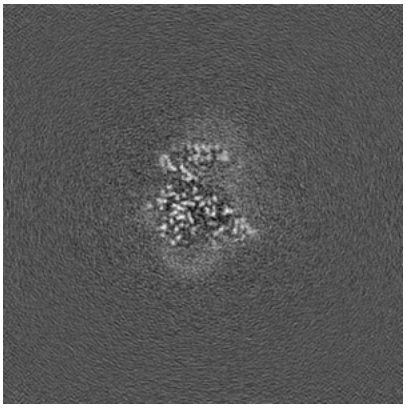
6.2.2 Raw map



X Index: 140



Y Index: 140

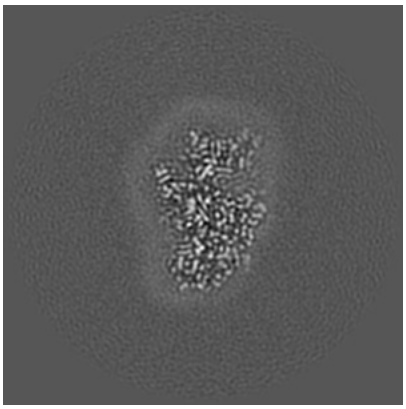


Z Index: 140

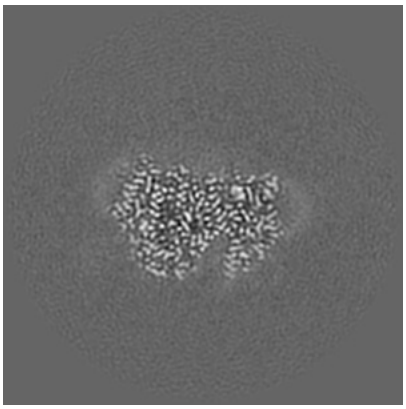
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

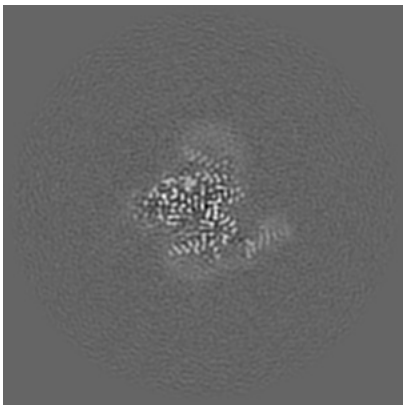
6.3.1 Primary map



X Index: 130

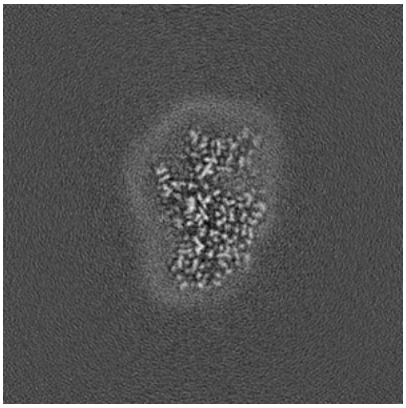


Y Index: 142

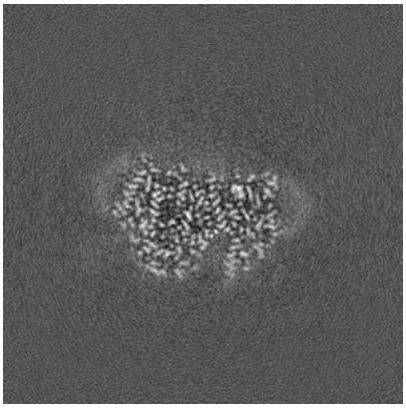


Z Index: 164

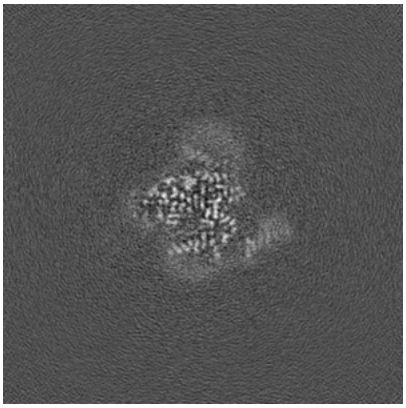
6.3.2 Raw map



X Index: 130



Y Index: 142

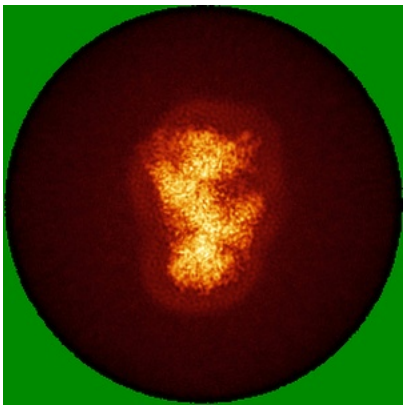


Z Index: 164

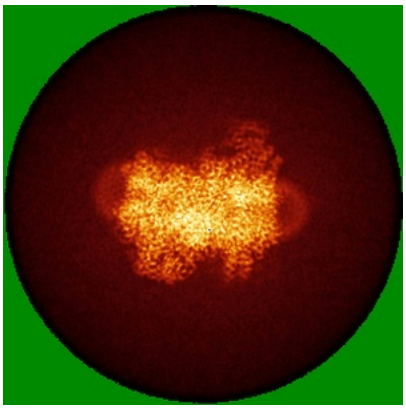
The images above show the largest variance slices of the map in three orthogonal directions.

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

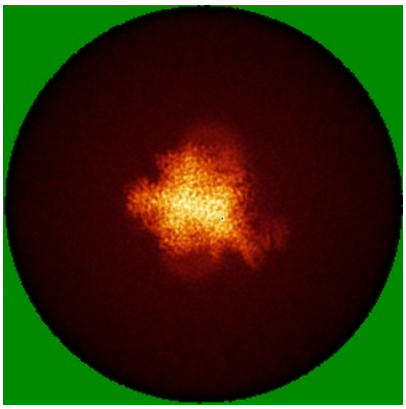
6.4.1 Primary map



X

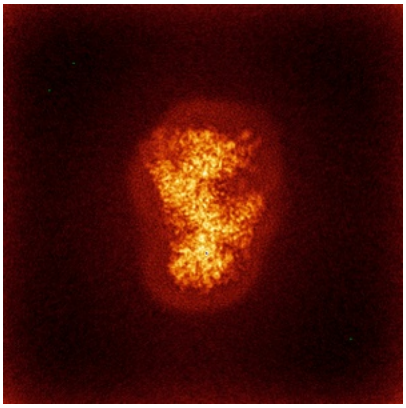


Y

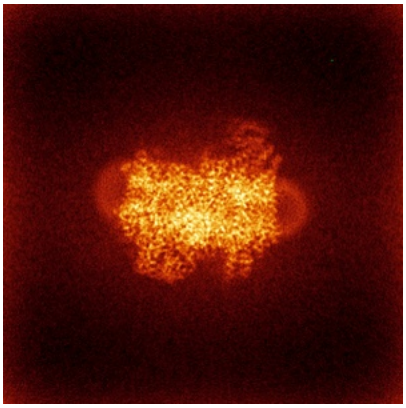


Z

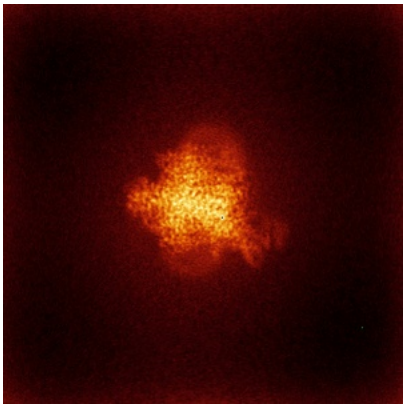
6.4.2 Raw map



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.

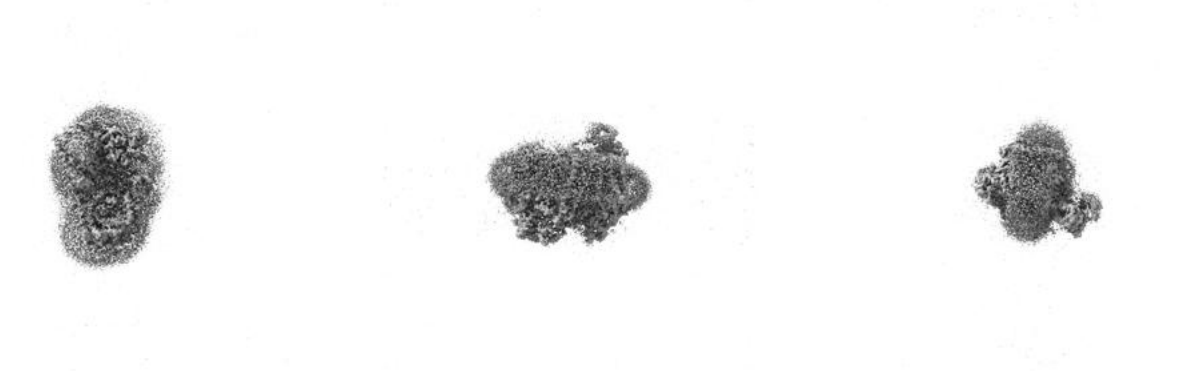
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.174. 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.

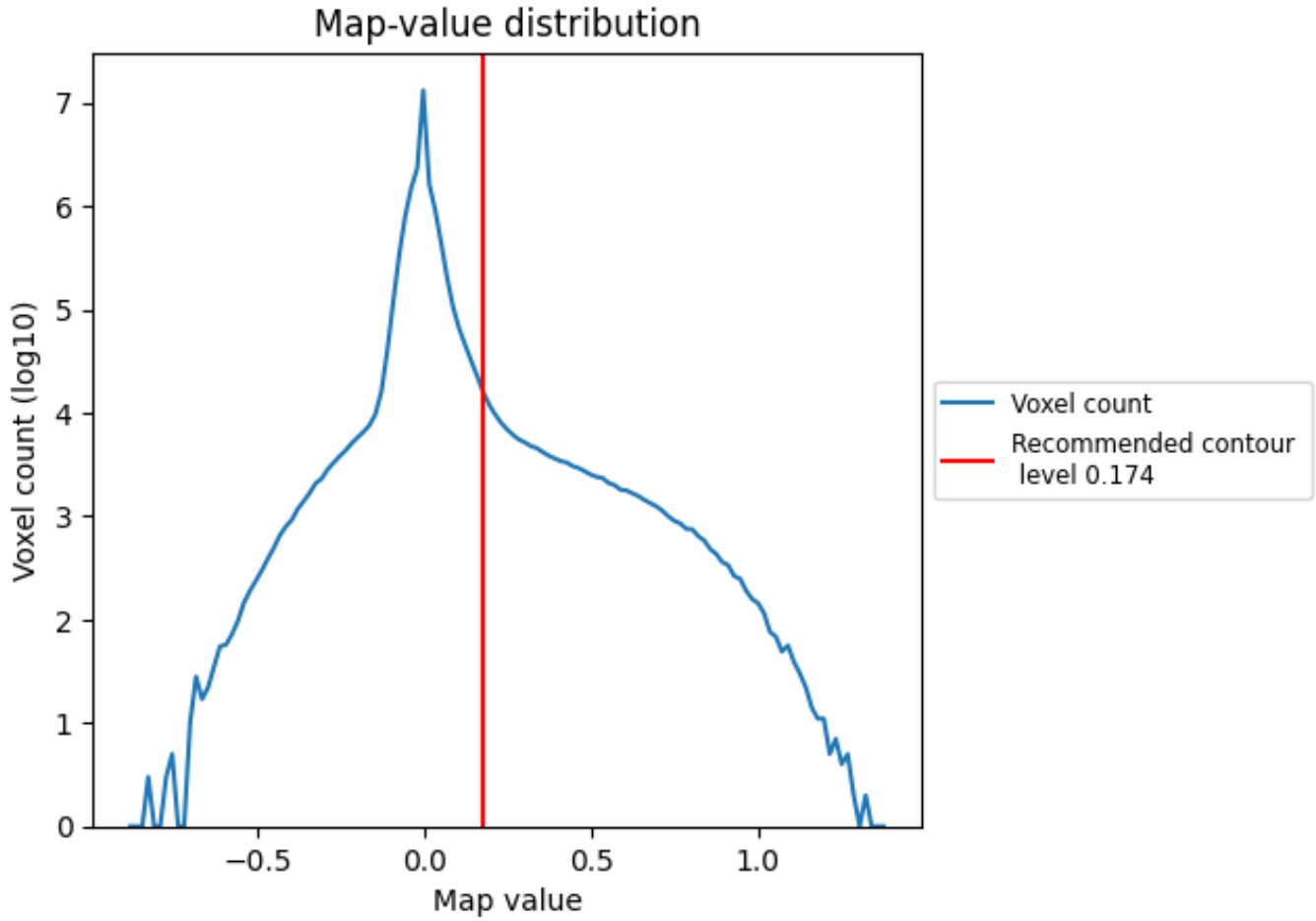
6.6 Mask visualisation (i)

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

7 Map analysis

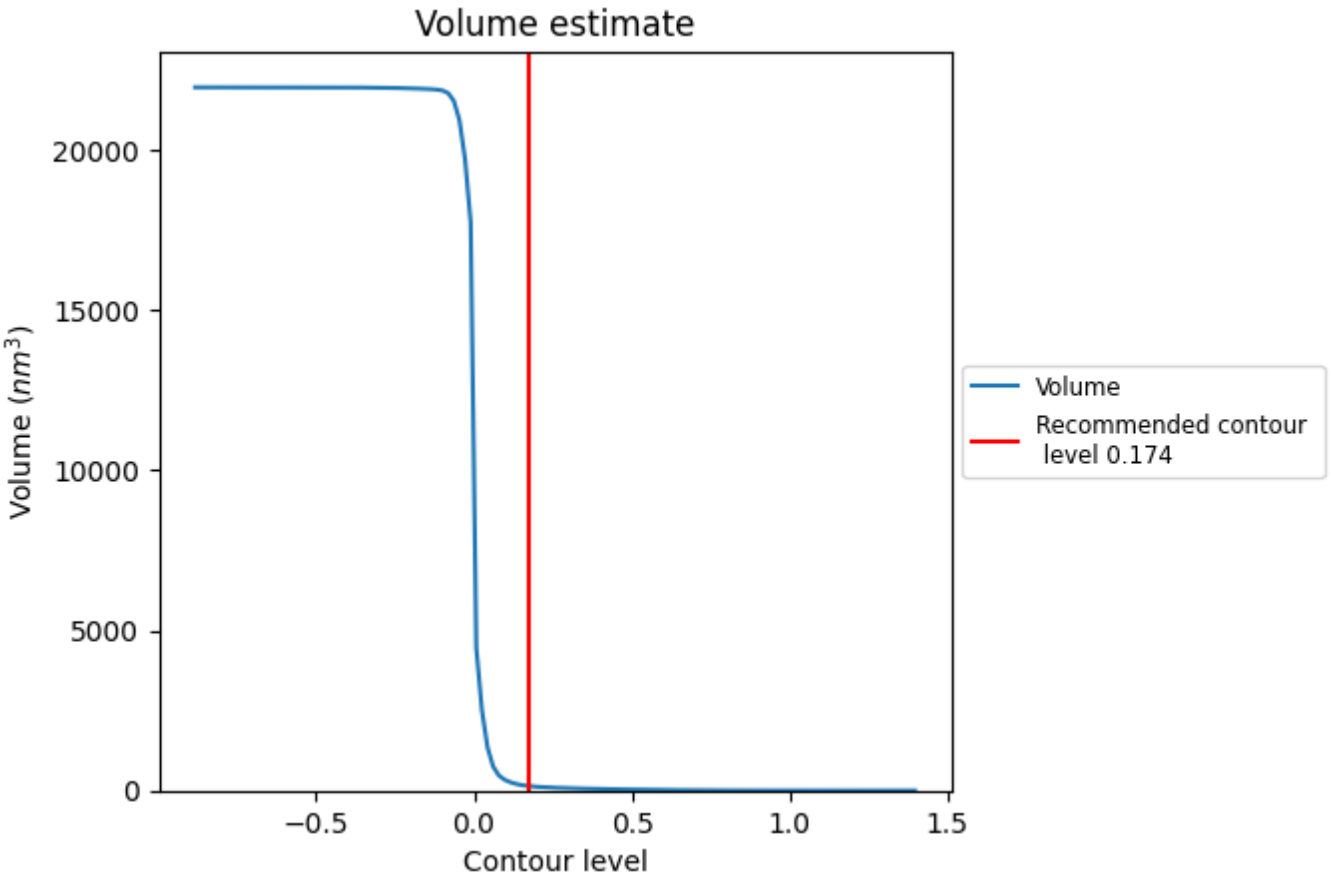
This section contains the results of statistical analysis of the map.

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.

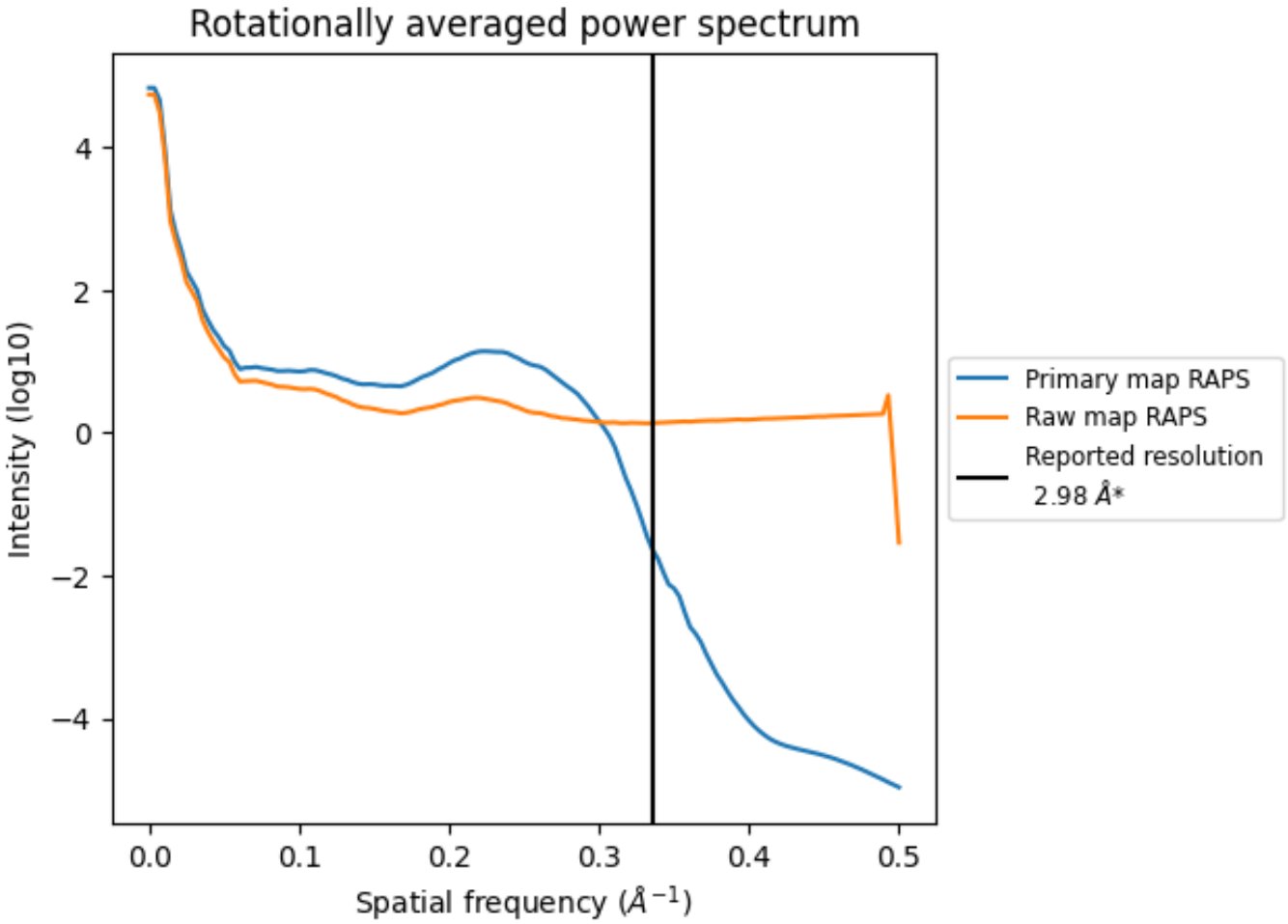
7.2 Volume estimate



The volume at the recommended contour level is 140 nm^3; this corresponds to an approximate mass of 127 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)

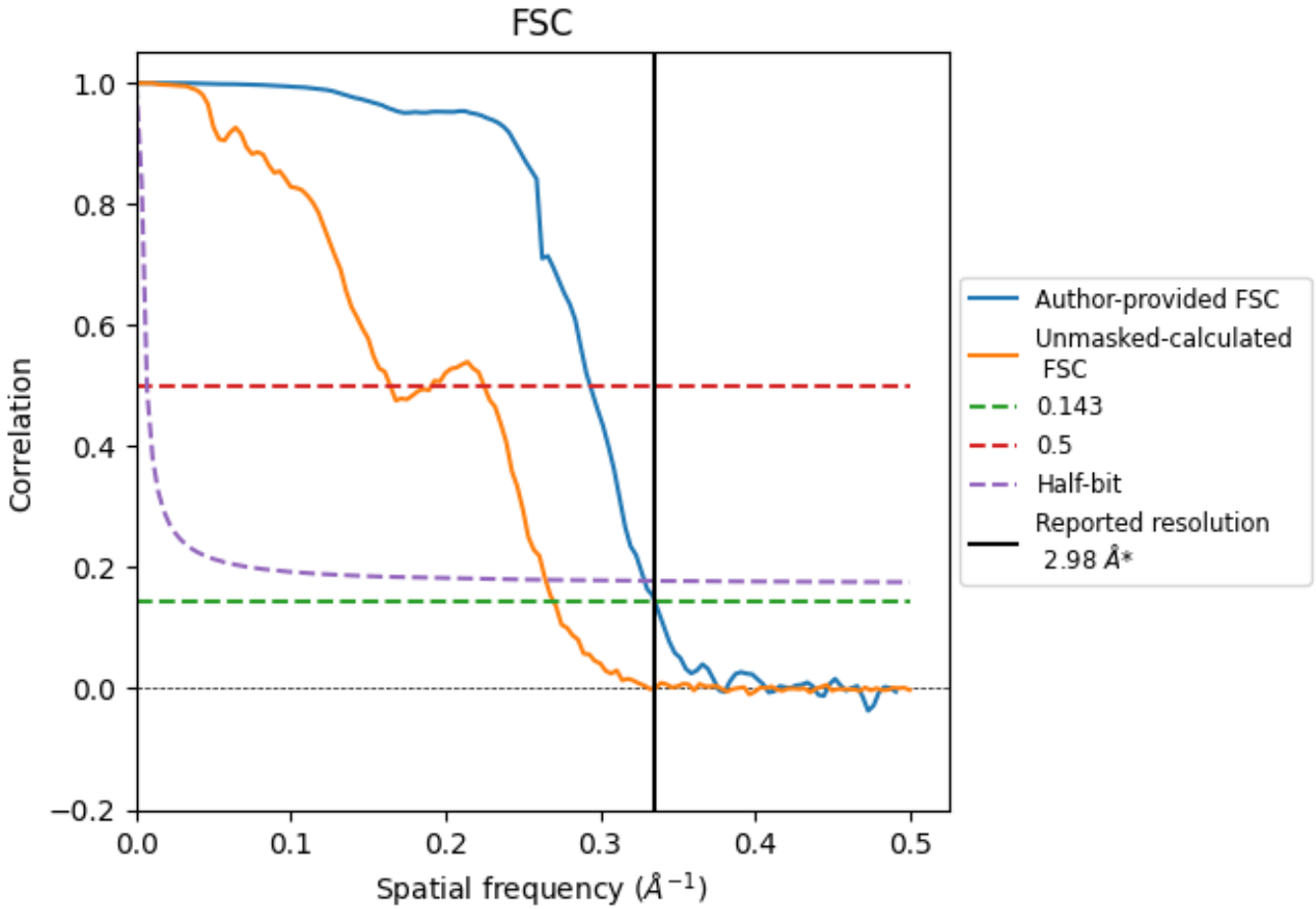


*Reported resolution corresponds to spatial frequency of 0.336 Å^{-1}

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 0.336 Å^{-1}

8.2 Resolution estimates (i)

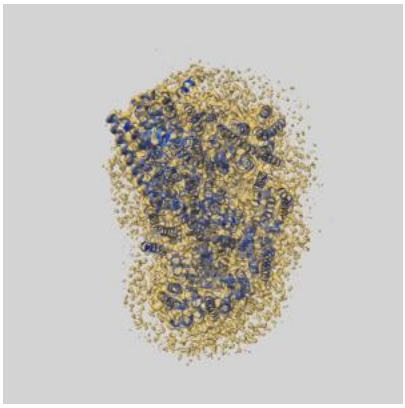
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.41	3.04
Unmasked-calculated*	3.70	6.09	3.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 2.98 by more than 10 %

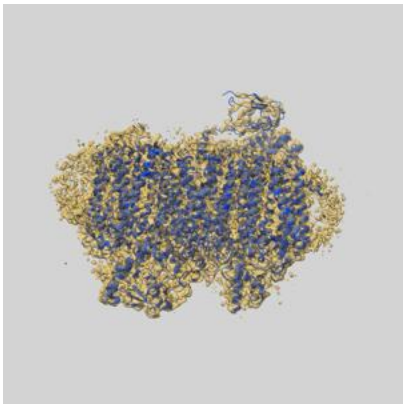
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60605 and PDB model 9IIU. Per-residue inclusion information can be found in section 3 on page 18.

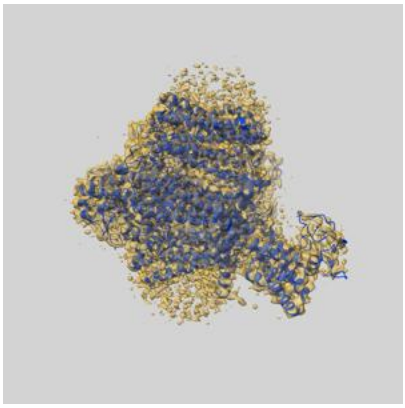
9.1 Map-model overlay



X



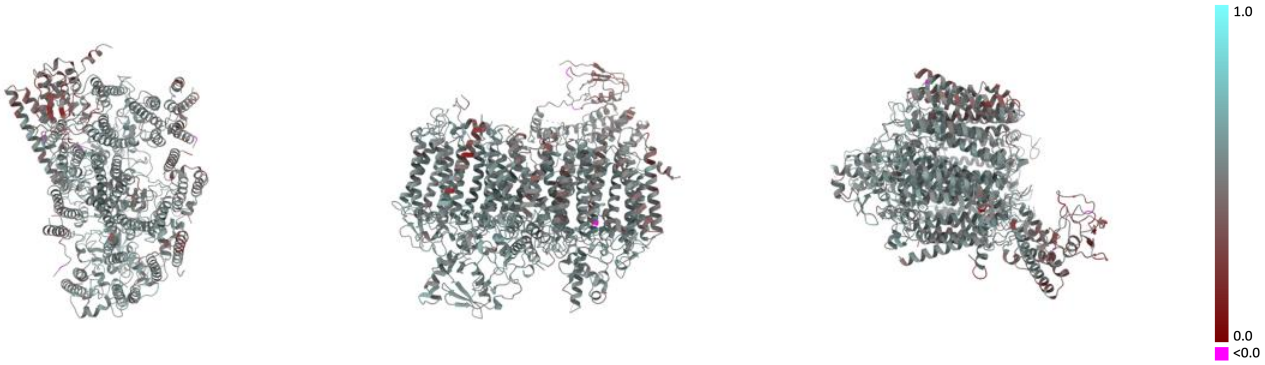
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.174 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.

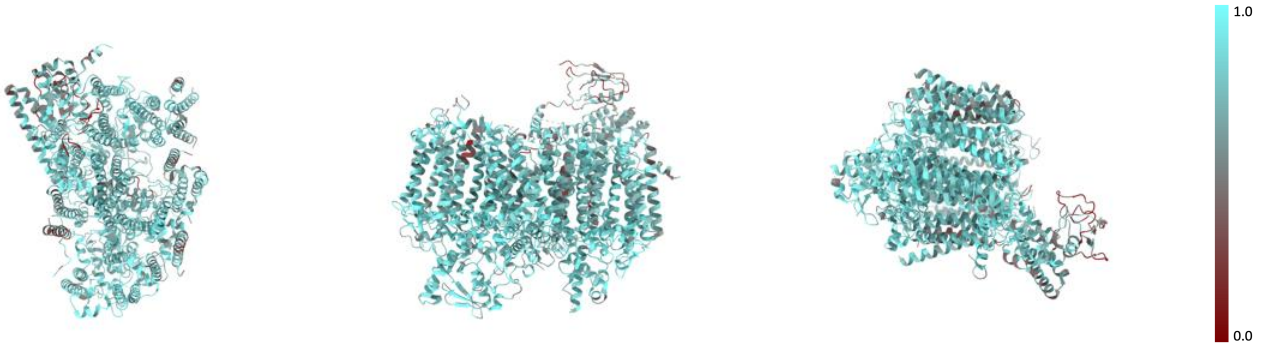
9.2 Q-score mapped to coordinate model (i)



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.

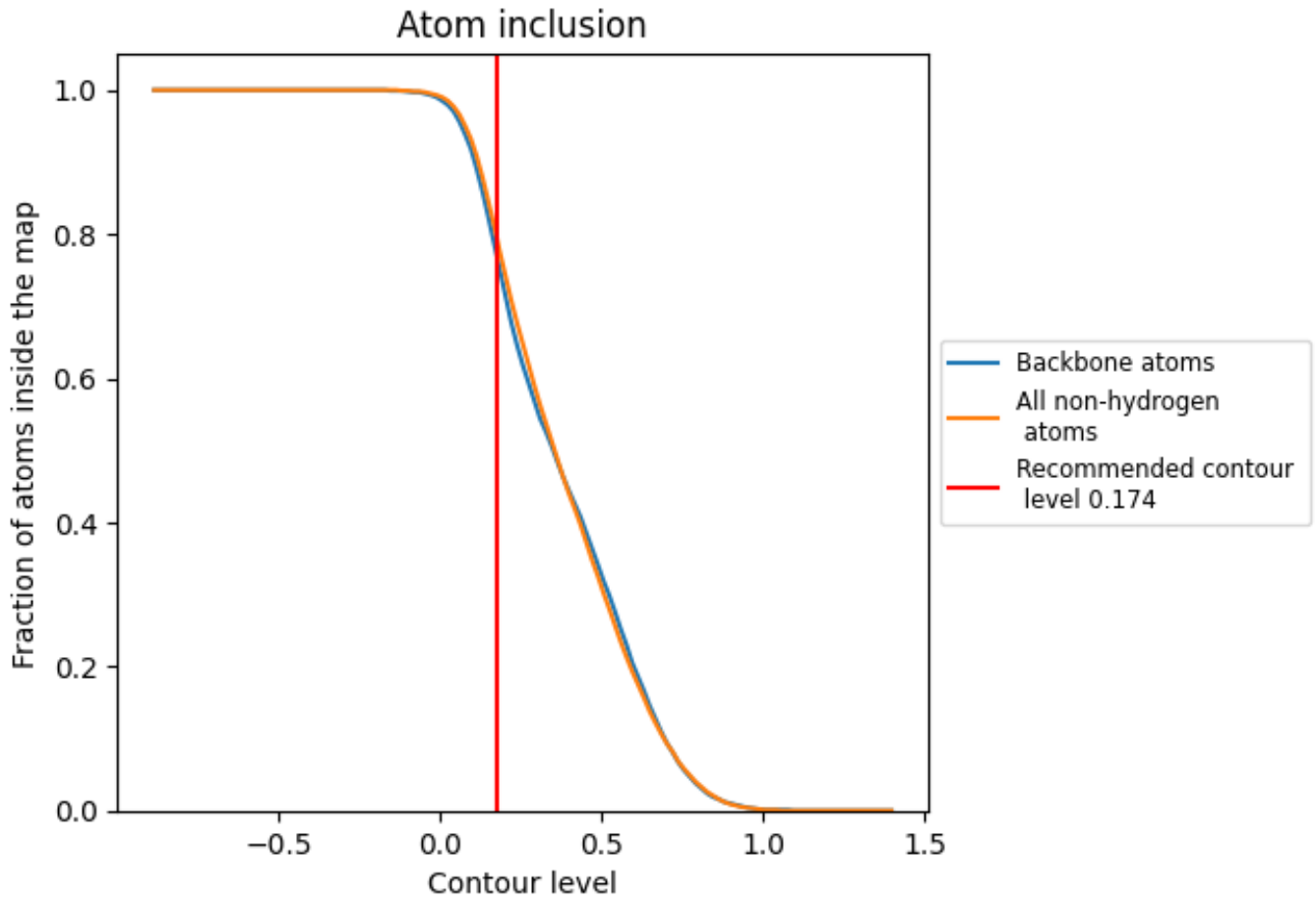
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.174).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 80% 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 (0.174) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.5230
A	0.8410	0.5330
B	0.8480	0.5460
C	0.8420	0.5380
D	0.8560	0.5520
E	0.7710	0.4940
F	0.7820	0.4970
G	0.6600	0.4410
H	0.7690	0.5110
I	0.7940	0.5280
J	0.6770	0.4810
K	0.8050	0.5050
L	0.7430	0.5030
M	0.3560	0.4110
T	0.6260	0.4700
V	0.6260	0.4280
X	0.6400	0.4260
Z	0.6890	0.4500