Full wwPDB EM Validation Report ⓘ

Jun 20, 2024 – 06:22 PM JST

PDB ID	:	8ZEE
EMDB ID	:	EMD-60026
Title	:	Cryo-EM structure of an intermediate-state PSII-PRF2' complex during the process of photosystem II repair
Authors	:	Li, A.; Liu, Z.
Deposited on	:	2024-05-06
Resolution	:	2.90 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:

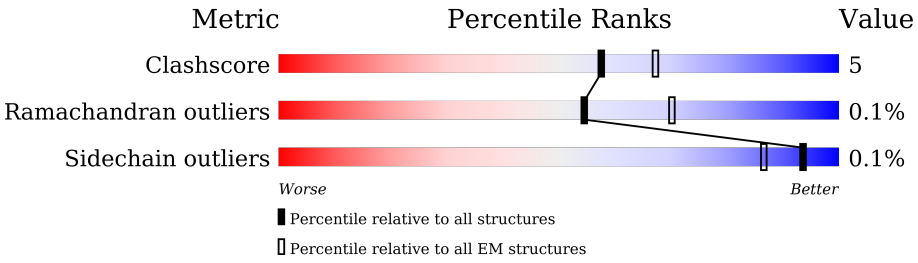
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	B	508	86% 9% 5%
2	D	352	5% 91% 9%
3	E	82	7% 83% 12% 5%
4	F	44	5% 59% 18% 23%
5	H	88	7% 74% 9% 17%
6	I	37	8% 84% 11% 5%
7	K	46	65% 15% 20%
8	L	38	5% 97%

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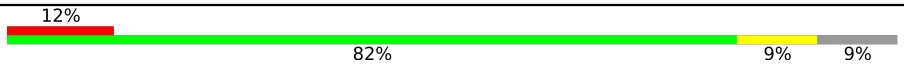
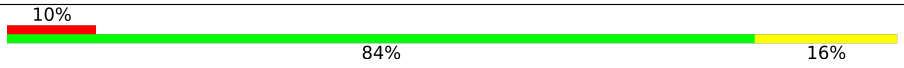
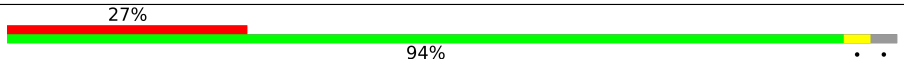
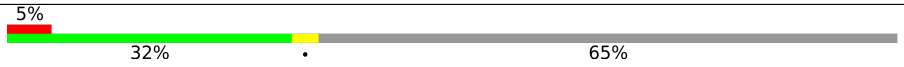
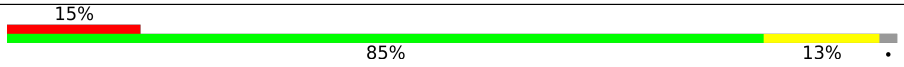
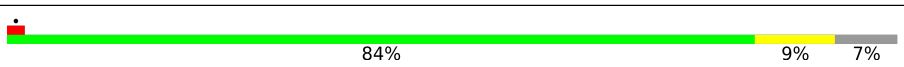
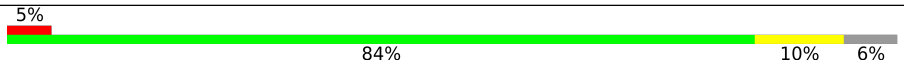
Mol	Chain	Length	Quality of chain
9	M	34	
10	T	31	
11	V	33	
12	X	101	
13	Z	62	
14	C	461	
15	A	329	
16	1	99	

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
17	CLA	A	402	X	-	-	-
17	CLA	A	403	X	-	-	-
17	CLA	A	404	X	-	-	-
17	CLA	B	601	X	-	-	-
17	CLA	B	602	X	-	-	-
17	CLA	B	603	X	-	-	-
17	CLA	B	604	X	-	-	-
17	CLA	B	605	X	-	-	-
17	CLA	B	606	X	-	-	-
17	CLA	B	607	X	-	-	-
17	CLA	B	608	X	-	-	-
17	CLA	B	609	X	-	-	-
17	CLA	B	610	X	-	-	-
17	CLA	B	611	X	-	-	-
17	CLA	B	612	X	-	-	-
17	CLA	B	613	X	-	-	-
17	CLA	B	614	X	-	-	-
17	CLA	B	615	X	-	-	-
17	CLA	B	616	X	-	-	-
17	CLA	C	602	X	-	-	-
17	CLA	C	603	X	-	-	-
17	CLA	C	604	X	-	-	-
17	CLA	C	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	C	606	X	-	-	-
17	CLA	C	607	X	-	-	-
17	CLA	C	608	X	-	-	-
17	CLA	C	609	X	-	-	-
17	CLA	C	610	X	-	-	-
17	CLA	C	611	X	-	-	-
17	CLA	C	612	X	-	-	-
17	CLA	C	613	X	-	-	-
17	CLA	C	614	X	-	-	-
17	CLA	D	402	X	-	-	-
17	CLA	D	403	X	-	-	-
17	CLA	D	410	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 20218 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 CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	482	3766	2469	629	656	12	0	0

- Molecule 2 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	351	2791	1841	459	479	12	0	0

- Molecule 3 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	78	633	414	104	115	0	0

- Molecule 4 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	34	277	190	45	41	1	0	0

- Molecule 5 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	73	561	372	84	103	2	0	0

- Molecule 6 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	35	283	193	43	45	2	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	38	Total	C	N	O	S	0	0
			314	210	51	52	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	M	31	Total	C	N	O	0	0
			239	163	33	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	31	Total	C	N	O	S	0	0
			256	177	38	39	2		

- Molecule 11 is a protein called Photosystem II reaction center protein Psb30.

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

- Molecule 12 is a protein called 4.1 kDa photosystem II subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	35	Total	C	N	O	0	0
			242	159	39	44		

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

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

- Molecule 14 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	430	Total	C	N	O	S	0	0
			3368	2209	561	581	17		

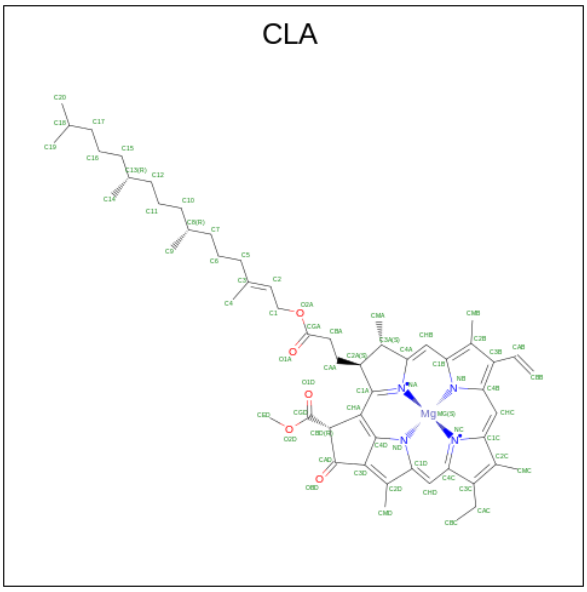
- Molecule 15 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A	309	Total	C	N	O	S	0	0
			2418	1587	401	415	15		

- Molecule 16 is a protein called Chains: 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	1	44	Total	C	N	O	0	0
			313	204	51	58		

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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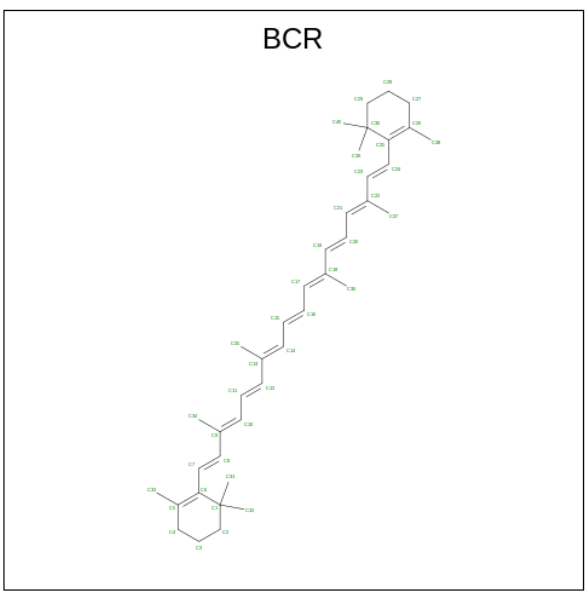
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
17	C	1	65	55	1	4	5	0
17	C	1	65	55	1	4	5	0
17	C	1	65	55	1	4	5	0
17	C	1	65	55	1	4	5	0
17	C	1	65	55	1	4	5	0
17	C	1	65	55	1	4	5	0
17	C	1	65	55	1	4	5	0
17	A	1	65	55	1	4	5	0
17	A	1	49	39	1	4	5	0
17	A	1	60	50	1	4	5	0

- Molecule 18 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
18	B	1	40	40	0

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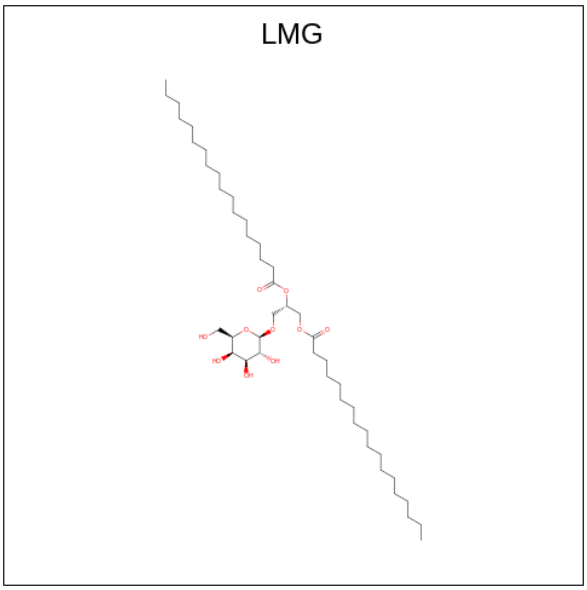
Mol	Chain	Residues	Atoms	AltConf
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	D	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	K	1	Total C 40 40	0
18	Z	1	Total C 40 40	0
18	C	1	Total C 40 40	0
18	C	1	Total C 40 40	0
18	A	1	Total C 40 40	0

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total C O 46 36 10	0
19	D	1	Total C O 46 36 10	0

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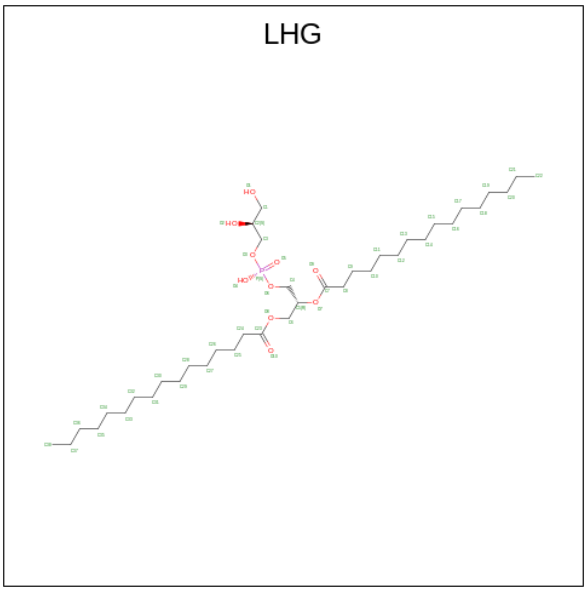
Mol	Chain	Residues	Atoms	AltConf
19	H	1	Total C O 48 38 10	0
19	K	1	Total C O 51 41 10	0
19	C	1	Total C O 49 39 10	0
19	C	1	Total C O 48 38 10	0

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C O P 44 33 10 1	0
20	B	1	Total C O P 47 36 10 1	0
20	B	1	Total C O P 49 38 10 1	0
20	D	1	Total C O P 49 38 10 1	0
20	D	1	Total C O P 43 32 10 1	0
20	D	1	Total C O P 49 38 10 1	0
20	K	1	Total C O P 41 30 10 1	0

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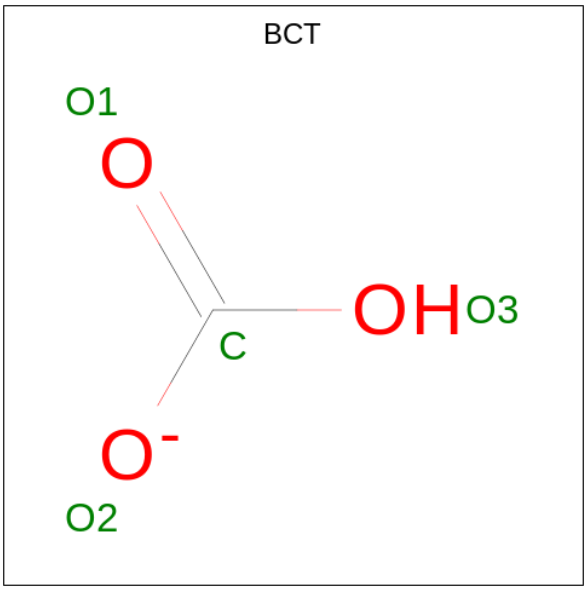
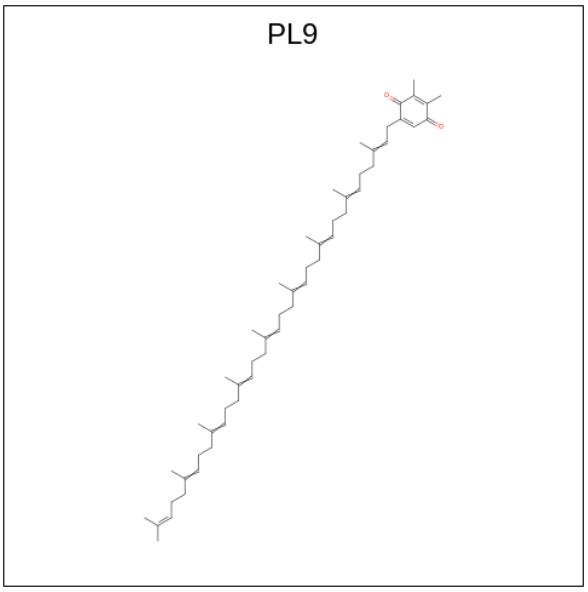
Mol	Chain	Residues	Atoms				AltConf
20	L	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



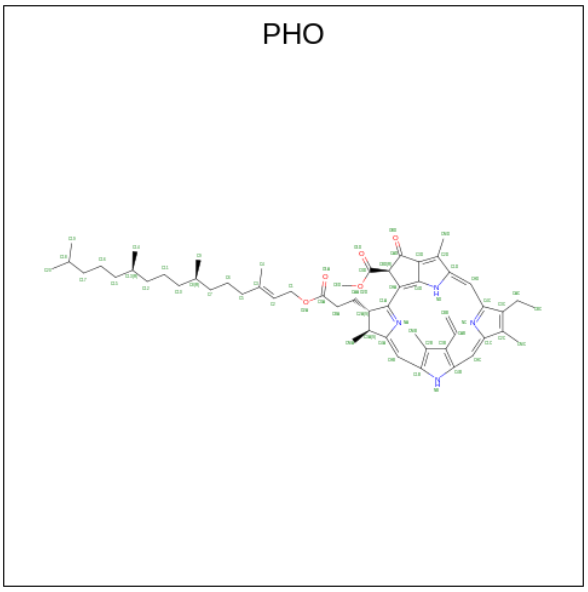
Mol	Chain	Residues	Atoms			AltConf
21	D	1	Total	C	O	0
			4	1	3	

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



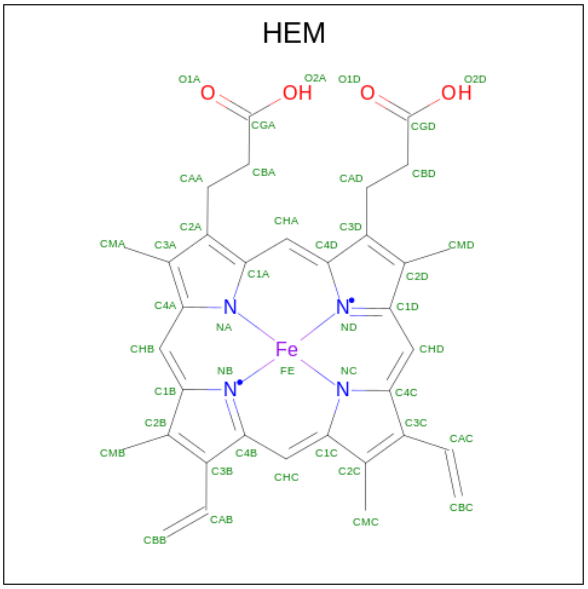
Mol	Chain	Residues	Atoms			AltConf
22	D	1	Total	C	O	0
			55	53	2	

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



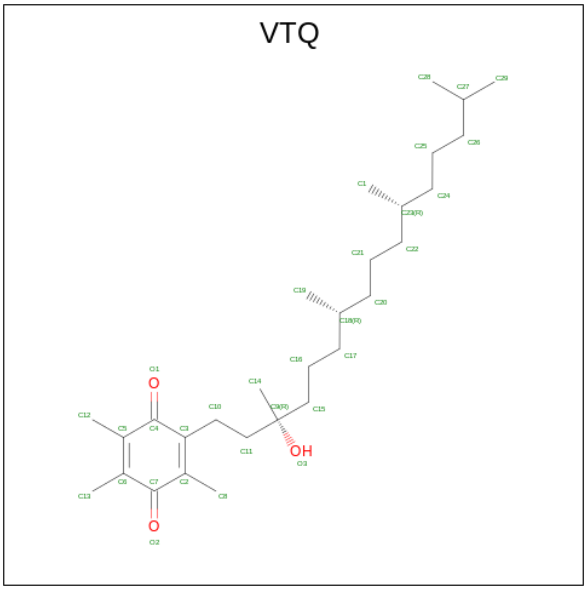
Mol	Chain	Residues	Atoms				AltConf
23	D	1	Total	C	N	O	0
			64	55	4	5	
23	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



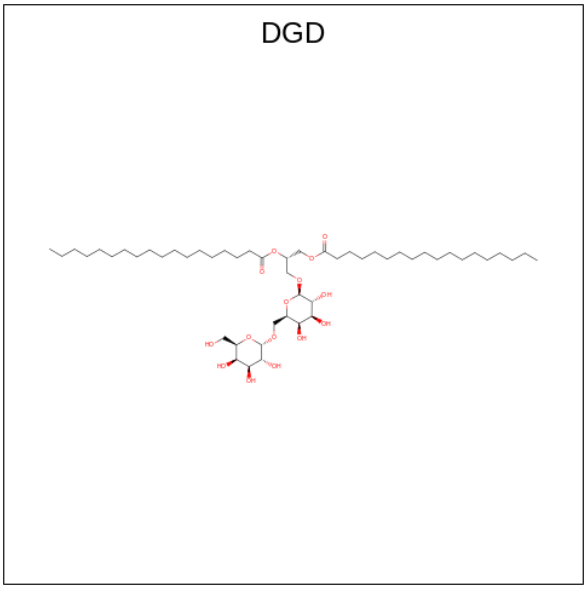
Mol	Chain	Residues	Atoms					AltConf
24	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 25 is RRR-ALPHA-TOCOPHERYLQUINONE (three-letter code: VTQ) (formula: $C_{29}H_{50}O_3$) (labeled as "Ligand of Interest" by depositor).



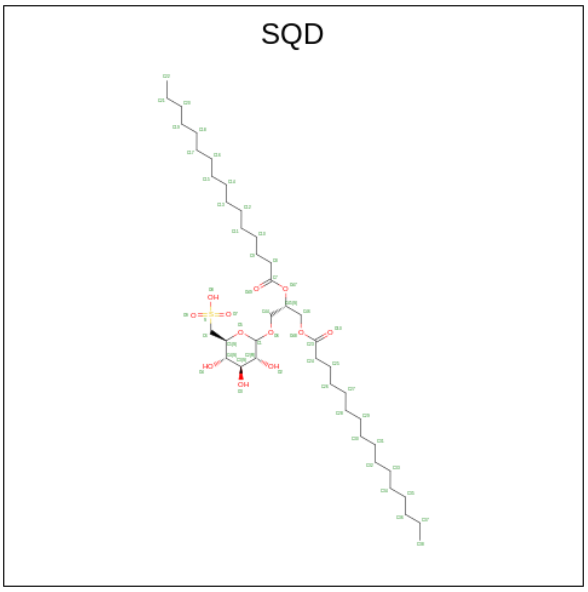
Mol	Chain	Residues	Atoms				AltConf
25	X	1	Total	C	O		0
			32	29	3		

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
26	C	1	Total C O 55 40 15	0
26	C	1	Total C O 57 42 15	0
26	C	1	Total C O 59 44 15	0

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



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

- Molecule 28 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

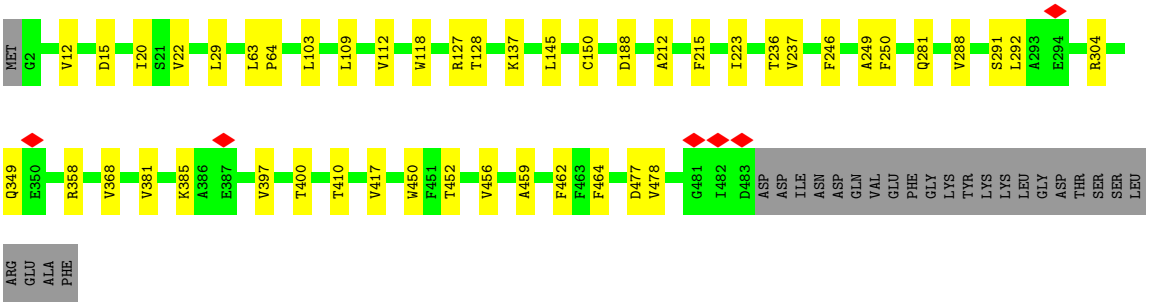
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	Fe	0
			1	1	

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.

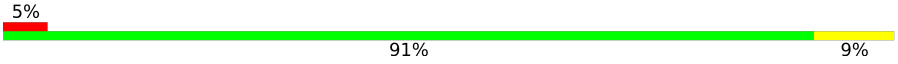
• Molecule 1: Photosystem II CP47 reaction center protein

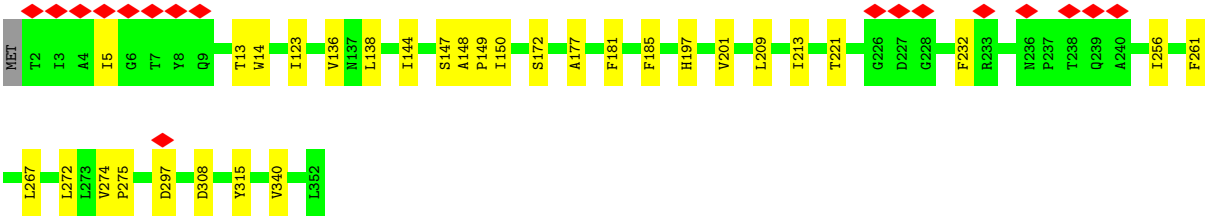
Chain B:



• Molecule 2: Photosystem II D2 protein

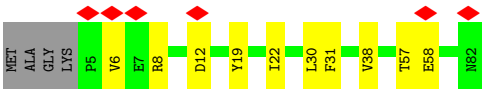
Chain D:





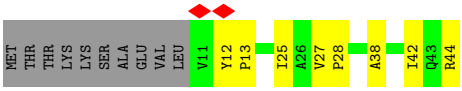
• Molecule 3: Cytochrome b559 subunit alpha

Chain E:

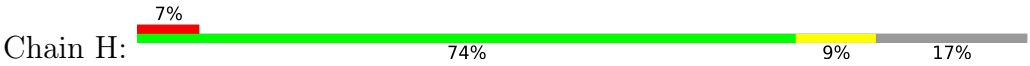


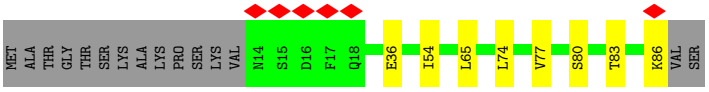
• Molecule 4: Cytochrome b559 subunit beta

Chain F:

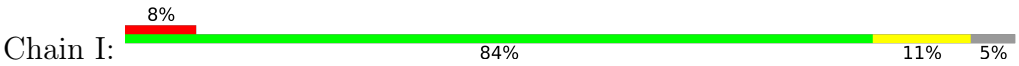


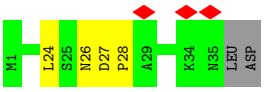
• Molecule 5: Photosystem II reaction center protein H



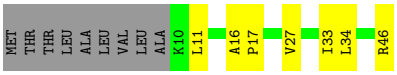


• Molecule 6: Photosystem II reaction center protein I

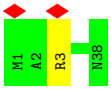




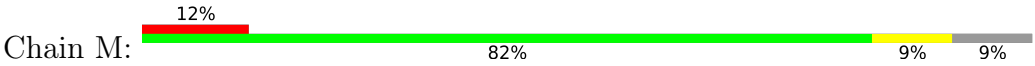
• Molecule 7: Photosystem II reaction center protein K

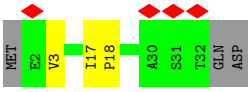


• Molecule 8: Photosystem II reaction center protein L

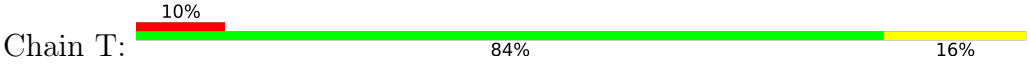


• Molecule 9: Photosystem II reaction center protein M



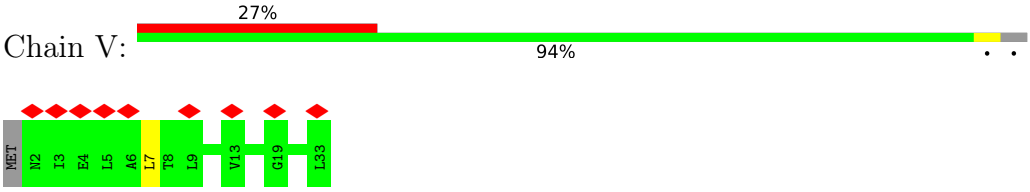


• Molecule 10: Photosystem II reaction center protein T



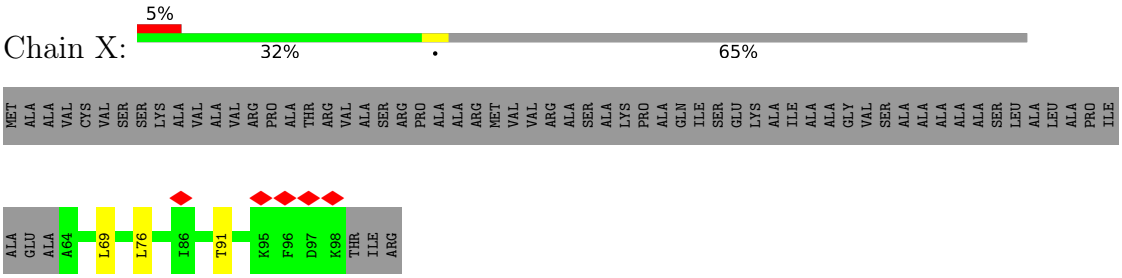
• Molecule 11: Photosystem II reaction center protein Psb30

Chain V:



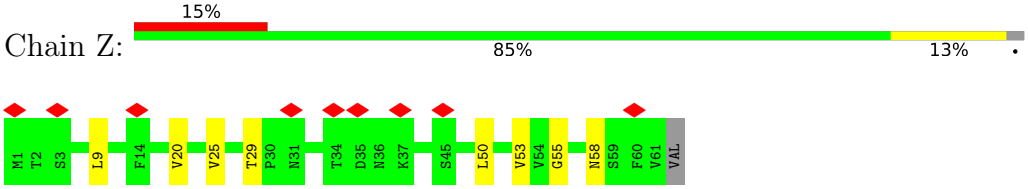
• Molecule 12: 4.1 kDa photosystem II subunit

Chain X:



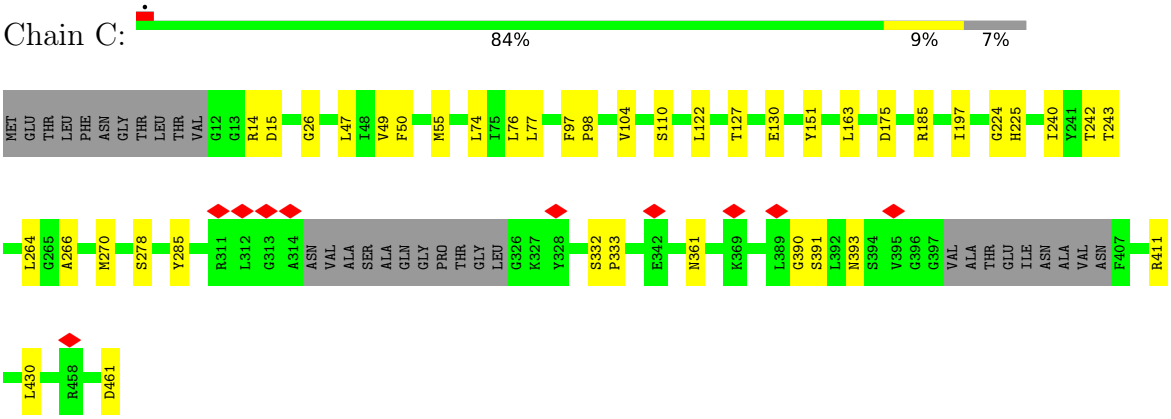
• Molecule 13: Photosystem II reaction center protein Z

Chain Z:



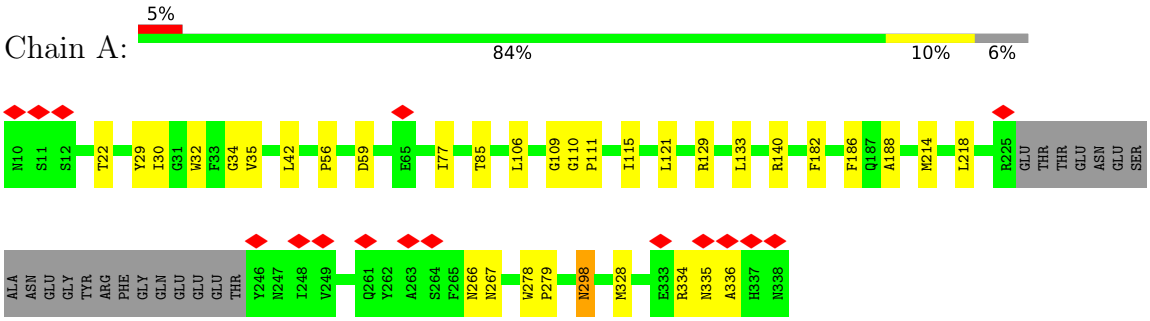
• Molecule 14: Photosystem II CP43 reaction center protein

Chain C:



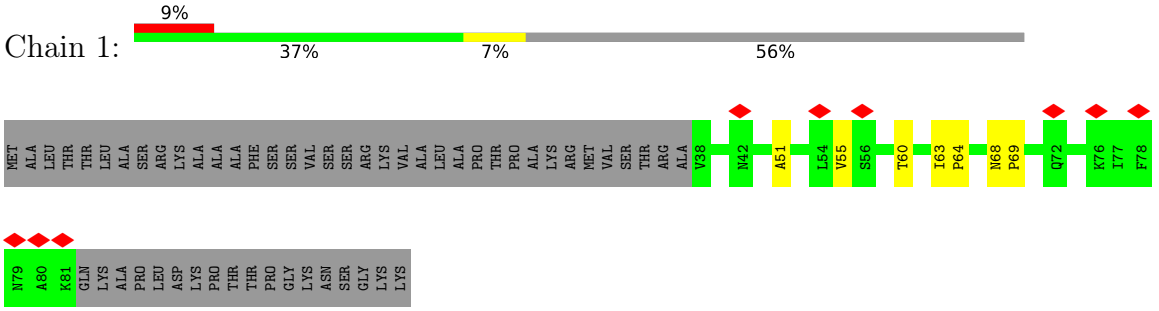
• Molecule 15: Photosystem II protein D1

Chain A:



• Molecule 16: Chains: 1

Chain 1:


9%
37%
7%
56%
MET ALA LEU THR THR LEU ALA SER ARG LYS ALA ALA ALA PHE SER SER VAL SER SER ARG LYS VAL ALA LEU ALA PRO THR PRO ALA LYS ARG MET VAL SER THR ARG ALA V38 N42 A51 L54 V55 S56 T60 I63 P64 N68 P69 Q72 K76 I77 F78
N79 A80 K81 GLN LYS ALA PRO LEU ASP LYS PRO THR THR PRO GLY LYS ASN SER GLY LYS LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	159928	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.215	Depositor
Minimum map value	-0.004	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	280.80002, 280.80002, 280.80002	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3500001, 1.3500001, 1.3500001	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.26	0/3894	0.48	0/5302
2	D	0.26	0/2886	0.46	0/3937
3	E	0.24	0/652	0.45	0/890
4	F	0.25	0/286	0.45	0/389
5	H	0.24	0/573	0.43	0/783
6	I	0.29	0/291	0.49	0/394
7	K	0.26	0/309	0.41	0/425
8	L	0.26	0/322	0.44	0/437
9	M	0.24	0/243	0.37	0/333
10	T	0.28	0/263	0.43	0/354
11	V	0.23	0/224	0.41	0/307
12	X	0.25	0/244	0.37	0/330
13	Z	0.25	0/469	0.37	0/644
14	C	0.25	0/3486	0.45	0/4743
15	A	0.26	0/2495	0.47	0/3402
16	1	0.26	0/317	0.42	0/435
All	All	0.26	0/16954	0.46	0/23105

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	B	3766	0	3649	38	0
2	D	2791	0	2678	27	0
3	E	633	0	622	10	0
4	F	277	0	288	6	0
5	H	561	0	581	5	0
6	I	283	0	293	3	0
7	K	297	0	308	4	0
8	L	314	0	327	1	0
9	M	239	0	258	2	0
10	T	256	0	273	4	0
11	V	224	0	256	1	0
12	X	242	0	266	3	0
13	Z	458	0	490	6	0
14	C	3368	0	3240	34	0
15	A	2418	0	2349	23	0
16	1	313	0	331	8	0
17	A	174	0	170	2	0
17	B	1020	0	1113	23	0
17	C	845	0	936	22	0
17	D	195	0	216	4	0
18	A	40	0	56	2	0
18	B	120	0	168	3	0
18	C	80	0	112	11	0
18	D	40	0	56	0	0
18	H	40	0	56	5	0
18	K	40	0	56	1	0
18	Z	40	0	56	7	0
19	B	46	0	62	0	0
19	C	97	0	134	0	0
19	D	46	0	62	0	0
19	H	48	0	66	2	0
19	K	51	0	72	0	0
20	B	140	0	202	0	0
20	D	141	0	204	2	0
20	K	41	0	52	0	0
20	L	49	0	74	1	0
21	D	4	0	0	0	0
22	D	55	0	80	1	0
23	D	128	0	148	1	0
24	E	43	0	30	5	0
25	X	32	0	50	0	0
26	C	171	0	216	2	0
27	C	51	0	69	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	A	1	0	0	0	0
All	All	20218	0	20725	204	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 (204) 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)
24:E:101:HEM:HHC	24:E:101:HEM:HBB2	1.67	0.77
14:C:390:GLY:O	15:A:298:ASN:ND2	2.19	0.76
14:C:74:LEU:HD13	14:C:77:LEU:HD12	1.70	0.74
1:B:145:LEU:HD11	17:B:615:CLA:HMB2	1.71	0.73
20:D:407:LHG:O5	15:A:140:ARG:NH2	2.22	0.73
18:C:616:BCR:H383	18:C:616:BCR:H23C	1.72	0.72
18:Z:101:BCR:H333	14:C:104:VAL:HG11	1.73	0.71
2:D:297:ASP:O	2:D:315:TYR:OH	2.08	0.69
14:C:47:LEU:HD21	17:C:611:CLA:HMD2	1.74	0.68
7:K:46:ARG:NH1	14:C:14:ARG:O	2.27	0.67
15:A:32:TRP:O	15:A:35:VAL:HG22	1.95	0.66
18:B:618:BCR:H383	18:B:618:BCR:H23C	1.78	0.65
18:K:101:BCR:H343	13:Z:20:VAL:HG11	1.78	0.65
24:E:101:HEM:HBC2	24:E:101:HEM:HMC2	1.80	0.63
1:B:103:LEU:HD21	17:B:605:CLA:HMC3	1.79	0.63
17:C:603:CLA:HED2	17:C:604:CLA:H43	1.81	0.62
1:B:477:ASP:OD1	1:B:478:VAL:N	2.34	0.60
17:B:602:CLA:H43	5:H:65:LEU:HA	1.83	0.60
3:E:19:TYR:OH	16:1:60:THR:O	2.18	0.60
14:C:285:TYR:OH	17:C:603:CLA:HED3	2.01	0.59
15:A:334:ARG:O	15:A:336:ALA:N	2.35	0.59
17:B:613:CLA:HBB1	17:B:613:CLA:HMB1	1.85	0.59
1:B:212:ALA:HB2	17:B:609:CLA:HMC3	1.86	0.58
1:B:291:SER:OG	1:B:304:ARG:NH2	2.36	0.58
15:A:56:PRO:HG3	15:A:106:LEU:HD13	1.85	0.58
5:H:54:ILE:HG13	18:H:101:BCR:H333	1.85	0.58
17:B:612:CLA:HBB1	17:B:612:CLA:HMB1	1.86	0.56
10:T:6:TYR:HB3	15:A:77:ILE:HD11	1.86	0.56
14:C:224:GLY:HA3	18:C:615:BCR:H402	1.86	0.56
14:C:393:ASN:ND2	26:C:619:DGD:O1B	2.38	0.56
3:E:8:ARG:NH2	3:E:12:ASP:OD2	2.39	0.55
26:C:619:DGD:O5D	26:C:619:DGD:O4D	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ARG:O	1:B:128:THR:OG1	2.22	0.55
1:B:368:VAL:HG22	1:B:381:VAL:HG22	1.88	0.55
17:B:602:CLA:H42	19:H:102:LMG:H112	1.88	0.55
18:Z:101:BCR:H382	18:Z:101:BCR:H23C	1.88	0.55
17:C:610:CLA:HBB1	17:C:610:CLA:HMB1	1.89	0.54
3:E:6:VAL:O	3:E:6:VAL:HG22	2.08	0.54
17:C:606:CLA:H11	18:C:615:BCR:H333	1.89	0.54
2:D:261:PHE:HB2	22:D:405:PL9:H522	1.89	0.54
18:B:617:BCR:H382	18:B:617:BCR:H23C	1.88	0.53
2:D:221:THR:O	2:D:221:THR:HG22	2.09	0.53
14:C:49:VAL:HG23	14:C:110:SER:HB2	1.91	0.53
2:D:13:THR:HG22	2:D:14:TRP:N	2.24	0.53
2:D:136:VAL:HG13	2:D:138:LEU:HD13	1.91	0.53
15:A:85:THR:HG22	15:A:109:GLY:O	2.09	0.53
18:H:101:BCR:H383	18:H:101:BCR:H23C	1.91	0.52
14:C:47:LEU:CD2	17:C:611:CLA:HMD2	2.40	0.52
17:D:403:CLA:H43	12:X:76:LEU:HD23	1.90	0.52
10:T:30:ILE:HG23	10:T:30:ILE:O	2.08	0.52
17:C:602:CLA:H171	17:C:608:CLA:HMB3	1.91	0.52
2:D:340:VAL:HG13	2:D:340:VAL:O	2.08	0.52
3:E:38:VAL:CG1	4:F:38:ALA:HB3	2.39	0.52
1:B:462:PHE:CZ	17:B:613:CLA:HMB3	2.45	0.52
4:F:27:VAL:HB	4:F:28:PRO:HD3	1.91	0.52
2:D:232:PHE:O	15:A:267:ASN:ND2	2.42	0.52
2:D:201:VAL:HG22	17:D:402:CLA:C1B	2.41	0.51
7:K:27:VAL:HG12	7:K:27:VAL:O	2.11	0.51
13:Z:55:GLY:HA2	18:Z:101:BCR:H323	1.93	0.51
16:1:51:ALA:O	16:1:55:VAL:HG12	2.11	0.50
1:B:450:TRP:HB3	17:B:607:CLA:HMB2	1.92	0.50
6:I:24:LEU:O	6:I:24:LEU:HD23	2.11	0.50
18:Z:101:BCR:H23C	18:Z:101:BCR:C38	2.40	0.50
14:C:26:GLY:HA3	17:C:612:CLA:HMD3	1.93	0.50
1:B:22:VAL:HG13	17:B:614:CLA:HMB3	1.94	0.50
20:D:407:LHG:O3	20:D:407:LHG:O1	2.24	0.50
14:C:163:LEU:HD23	14:C:225:HIS:CD2	2.48	0.49
3:E:38:VAL:HG11	4:F:38:ALA:HB3	1.94	0.49
3:E:57:THR:HG22	3:E:58:GLU:N	2.28	0.49
1:B:12:VAL:O	1:B:12:VAL:HG12	2.12	0.49
24:E:101:HEM:HBC2	24:E:101:HEM:CMC	2.41	0.49
2:D:197:HIS:O	2:D:201:VAL:HG23	2.13	0.49
1:B:250:PHE:CE2	1:B:459:ALA:HB1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:175:ASP:OD1	14:C:185:ARG:NH2	2.46	0.48
14:C:242:THR:HG22	14:C:243:THR:N	2.28	0.48
1:B:281:GLN:OE1	1:B:358:ARG:NH1	2.46	0.48
17:C:611:CLA:HBB1	17:C:611:CLA:HMB1	1.94	0.48
13:Z:50:LEU:HA	13:Z:53:VAL:HG12	1.96	0.48
14:C:391:SER:HA	15:A:298:ASN:HB2	1.94	0.48
1:B:215:PHE:CZ	17:B:609:CLA:HMD3	2.49	0.48
2:D:148:ALA:HB3	2:D:149:PRO:CD	2.44	0.48
18:Z:101:BCR:C33	14:C:104:VAL:HG11	2.42	0.48
18:C:615:BCR:HC8	18:C:615:BCR:H311	1.95	0.47
17:C:605:CLA:HBB1	17:C:605:CLA:HMB1	1.96	0.47
3:E:30:LEU:HD11	24:E:101:HEM:HBB1	1.96	0.47
1:B:349:GLN:HA	1:B:349:GLN:OE1	2.14	0.47
11:V:7:LEU:HD23	11:V:7:LEU:O	2.14	0.47
14:C:264:LEU:HD21	17:C:609:CLA:HAB	1.96	0.47
2:D:261:PHE:CD2	2:D:267:LEU:HD13	2.49	0.47
14:C:197:ILE:HG23	18:C:615:BCR:H403	1.97	0.47
18:H:101:BCR:H393	12:X:69:LEU:HD21	1.97	0.47
18:Z:101:BCR:H333	14:C:104:VAL:CG1	2.41	0.47
18:C:615:BCR:H382	18:C:615:BCR:H23C	1.97	0.47
17:C:606:CLA:C1	18:C:615:BCR:H333	2.46	0.46
17:C:612:CLA:HBB1	17:C:612:CLA:HMB1	1.98	0.46
18:A:405:BCR:H382	18:A:405:BCR:H23C	1.98	0.46
9:M:3:VAL:HG11	10:T:2:GLU:OE2	2.16	0.46
15:A:278:TRP:HB3	15:A:279:PRO:HD3	1.97	0.46
17:C:609:CLA:HMB1	17:C:609:CLA:HBB1	1.97	0.46
1:B:223:ILE:HD12	2:D:5:ILE:HG21	1.98	0.46
14:C:127:THR:OG1	14:C:130:GLU:OE2	2.28	0.46
16:1:63:ILE:N	16:1:64:PRO:CD	2.78	0.46
18:H:101:BCR:HC8	18:H:101:BCR:H331	1.98	0.46
14:C:430:LEU:HD21	17:C:606:CLA:HMB3	1.96	0.46
15:A:111:PRO:O	15:A:115:ILE:HG12	2.15	0.46
17:B:602:CLA:H41	17:B:602:CLA:H71	1.97	0.46
13:Z:9:LEU:HD11	18:C:616:BCR:H312	1.97	0.45
14:C:15:ASP:N	14:C:15:ASP:OD1	2.48	0.45
17:B:604:CLA:HBB1	17:B:604:CLA:HMB1	1.98	0.45
17:D:410:CLA:H142	17:D:410:CLA:HMA1	1.97	0.45
2:D:14:TRP:NE1	12:X:91:THR:OG1	2.40	0.45
2:D:209:LEU:HD21	2:D:213:ILE:HD12	1.97	0.45
14:C:266:ALA:O	14:C:270:MET:HG3	2.16	0.45
1:B:462:PHE:CE2	17:B:613:CLA:HMB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:172:SER:HB2	2:D:177:ALA:HB1	1.98	0.45
15:A:110:GLY:N	15:A:111:PRO:HD2	2.32	0.45
17:B:602:CLA:H41	17:B:602:CLA:C7	2.46	0.45
14:C:55:MET:HG3	14:C:76:LEU:HD12	1.98	0.45
15:A:59:ASP:O	15:A:59:ASP:OD2	2.35	0.45
1:B:400:THR:HG23	1:B:410:THR:HG22	1.98	0.45
1:B:452:THR:O	1:B:456:VAL:HG23	2.17	0.44
15:A:30:ILE:O	15:A:34:GLY:HA3	2.17	0.44
17:A:402:CLA:HBB1	17:A:402:CLA:HMB1	1.99	0.44
15:A:182:PHE:CE1	15:A:186:PHE:HE2	2.35	0.44
17:B:604:CLA:HAA2	17:B:612:CLA:H141	1.99	0.44
14:C:50:PHE:HB2	14:C:110:SER:OG	2.17	0.44
17:C:606:CLA:HBB1	17:C:606:CLA:HMB1	1.99	0.44
15:A:266:ASN:OD1	15:A:266:ASN:O	2.36	0.44
1:B:109:LEU:O	1:B:112:VAL:HG12	2.18	0.44
1:B:464:PHE:HE1	2:D:144:ILE:HG23	1.83	0.44
3:E:22:ILE:HD13	24:E:101:HEM:HMA3	1.99	0.43
15:A:214:MET:O	15:A:218:LEU:HD13	2.18	0.43
2:D:181:PHE:CZ	2:D:185:PHE:CZ	3.05	0.43
4:F:42:ILE:HG22	4:F:44:ARG:H	1.83	0.43
13:Z:25:VAL:O	13:Z:29:THR:HG23	2.18	0.43
1:B:20:ILE:HG23	17:B:615:CLA:HED1	2.01	0.43
18:C:616:BCR:H383	18:C:616:BCR:C23	2.47	0.43
2:D:123:ILE:HD11	19:H:102:LMG:H401	1.99	0.43
2:D:308:ASP:OD1	2:D:308:ASP:O	2.37	0.43
4:F:25:ILE:O	4:F:25:ILE:HG22	2.18	0.43
17:C:606:CLA:C2	18:C:615:BCR:H333	2.48	0.43
14:C:14:ARG:HG3	14:C:14:ARG:HH11	1.84	0.43
14:C:122:LEU:HD11	17:C:612:CLA:H92	2.01	0.43
14:C:278:SER:O	14:C:411:ARG:NH1	2.52	0.43
15:A:188:ALA:HB2	15:A:328:MET:HB3	2.00	0.43
16:1:63:ILE:N	16:1:64:PRO:HD2	2.33	0.42
2:D:136:VAL:HG22	2:D:136:VAL:O	2.18	0.42
1:B:249:ALA:HB2	17:B:604:CLA:HBC3	2.02	0.42
17:B:615:CLA:H91	17:B:616:CLA:C11	2.49	0.42
2:D:147:SER:HA	2:D:150:ILE:HG22	2.01	0.42
2:D:209:LEU:CD2	2:D:213:ILE:HD12	2.49	0.42
17:B:615:CLA:HBB1	17:B:615:CLA:HMB1	2.00	0.42
1:B:477:ASP:OD1	1:B:478:VAL:HG23	2.19	0.42
14:C:97:PHE:N	14:C:98:PRO:CD	2.83	0.42
14:C:151:TYR:CE1	14:C:240:ILE:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:68:ASN:HB3	16:1:69:PRO:CD	2.49	0.42
1:B:29:LEU:HD13	17:B:613:CLA:HMD2	2.00	0.42
2:D:274:VAL:HB	2:D:275:PRO:HD3	2.01	0.42
1:B:397:VAL:HG23	1:B:417:VAL:HG11	2.01	0.42
5:H:74:LEU:HB2	5:H:77:VAL:HG22	2.01	0.42
10:T:12:GLY:O	10:T:16:ILE:HG12	2.20	0.42
1:B:288:VAL:O	1:B:292:LEU:HD13	2.20	0.42
2:D:148:ALA:HB3	2:D:149:PRO:HD3	2.01	0.42
9:M:17:ILE:HB	9:M:18:PRO:HD3	2.02	0.42
1:B:150:CYS:HB2	17:B:603:CLA:HMC3	2.02	0.42
2:D:272:LEU:C	2:D:272:LEU:HD23	2.40	0.42
3:E:38:VAL:O	3:E:38:VAL:HG22	2.19	0.42
1:B:246:PHE:HE1	1:B:250:PHE:CE2	2.38	0.41
18:H:101:BCR:H321	18:H:101:BCR:HC7	1.87	0.41
1:B:188:ASP:OD1	1:B:188:ASP:N	2.53	0.41
4:F:12:TYR:N	4:F:13:PRO:HD2	2.35	0.41
6:I:26:ASN:OD1	6:I:26:ASN:O	2.38	0.41
14:C:361:ASN:OD1	14:C:361:ASN:N	2.54	0.41
1:B:137:LYS:NZ	5:H:36:GLU:OE2	2.41	0.41
23:D:412:PHO:HBB1	23:D:412:PHO:HMB1	2.02	0.41
1:B:15:ASP:N	1:B:15:ASP:OD1	2.53	0.41
6:I:27:ASP:N	6:I:28:PRO:HD2	2.36	0.41
1:B:118:TRP:NE1	8:L:3:ARG:O	2.46	0.41
5:H:80:SER:O	5:H:83:THR:HG22	2.19	0.41
7:K:33:ILE:HG23	7:K:34:LEU:N	2.35	0.41
13:Z:55:GLY:CA	18:Z:101:BCR:H323	2.51	0.41
15:A:29:TYR:O	15:A:129:ARG:NH1	2.54	0.41
15:A:42:LEU:HB3	18:A:405:BCR:H353	2.02	0.41
2:D:256:ILE:HG12	15:A:133:LEU:HD23	2.03	0.41
17:C:604:CLA:HBB1	17:C:604:CLA:HMB1	2.02	0.41
15:A:22:THR:HG22	15:A:22:THR:O	2.21	0.41
15:A:121:LEU:HD13	17:A:404:CLA:HMB3	2.03	0.41
16:1:63:ILE:CG2	16:1:64:PRO:HD3	2.51	0.41
1:B:246:PHE:CE1	1:B:250:PHE:HE2	2.39	0.41
1:B:385:LYS:HG2	1:B:385:LYS:O	2.21	0.41
2:D:144:ILE:HD12	2:D:144:ILE:H	1.86	0.41
1:B:236:THR:HG23	1:B:237:VAL:N	2.36	0.41
17:C:602:CLA:H141	17:C:602:CLA:H162	1.91	0.41
17:C:607:CLA:H43	18:C:615:BCR:H313	2.02	0.41
16:1:55:VAL:O	16:1:55:VAL:HG22	2.20	0.40
18:B:619:BCR:H23C	18:B:619:BCR:H383	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:410:CLA:H92	20:L:101:LHG:H222	2.03	0.40
3:E:31:PHE:CE2	16:1:55:VAL:HG11	2.57	0.40
14:C:163:LEU:HD22	17:C:602:CLA:C2D	2.51	0.40
14:C:461:ASP:OD1	14:C:461:ASP:N	2.53	0.40
7:K:16:ALA:N	7:K:17:PRO:HD2	2.37	0.40
14:C:332:SER:OG	14:C:333:PRO:HD2	2.21	0.40
1:B:63:LEU:N	1:B:64:PRO:HD2	2.36	0.40
1:B:145:LEU:CD1	17:B:615:CLA:HMB2	2.46	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	B	480/508 (94%)	470 (98%)	10 (2%)	0	100	100
2	D	349/352 (99%)	337 (97%)	12 (3%)	0	100	100
3	E	76/82 (93%)	72 (95%)	4 (5%)	0	100	100
4	F	32/44 (73%)	31 (97%)	1 (3%)	0	100	100
5	H	71/88 (81%)	68 (96%)	3 (4%)	0	100	100
6	I	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
7	K	35/46 (76%)	34 (97%)	0	1 (3%)	4	18
8	L	36/38 (95%)	36 (100%)	0	0	100	100
9	M	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
10	T	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	V	30/33 (91%)	30 (100%)	0	0	100	100
12	X	33/101 (33%)	33 (100%)	0	0	100	100
13	Z	59/62 (95%)	59 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	C	424/461 (92%)	415 (98%)	9 (2%)	0	100 100
15	A	305/329 (93%)	290 (95%)	13 (4%)	2 (1%)	22 54
16	1	42/99 (42%)	42 (100%)	0	0	100 100
All	All	2063/2345 (88%)	2005 (97%)	55 (3%)	3 (0%)	54 82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	A	298	ASN
15	A	335	ASN
7	K	11	LEU

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	B	384/407 (94%)	384 (100%)	0	100 100
2	D	280/281 (100%)	280 (100%)	0	100 100
3	E	69/71 (97%)	69 (100%)	0	100 100
4	F	28/37 (76%)	28 (100%)	0	100 100
5	H	63/75 (84%)	62 (98%)	1 (2%)	62 86
6	I	32/34 (94%)	32 (100%)	0	100 100
7	K	31/38 (82%)	31 (100%)	0	100 100
8	L	35/35 (100%)	35 (100%)	0	100 100
9	M	27/30 (90%)	27 (100%)	0	100 100
10	T	28/28 (100%)	28 (100%)	0	100 100
11	V	26/27 (96%)	26 (100%)	0	100 100
12	X	25/67 (37%)	25 (100%)	0	100 100
13	Z	51/52 (98%)	50 (98%)	1 (2%)	55 82
14	C	338/362 (93%)	338 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	A	251/268 (94%)	251 (100%)	0	100 100
16	1	32/75 (43%)	32 (100%)	0	100 100
All	All	1700/1887 (90%)	1698 (100%)	2 (0%)	93 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	H	86	LYS
13	Z	58	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	201	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 70 ligands modelled in this entry, 1 is monoatomic - leaving 69 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	$\#\|Z\|>2$
17	CLA	D	402	-	65,73,73	1.53	7 (10%)	76,113,113	1.38	7 (9%)
19	LMG	C	621	-	48,48,55	0.99	3 (6%)	56,56,63	1.06	3 (5%)
17	CLA	C	608	-	65,73,73	1.51	6 (9%)	76,113,113	1.22	7 (9%)
22	PL9	D	405	-	55,55,55	1.04	4 (7%)	68,69,69	1.53	13 (19%)
17	CLA	A	404	-	60,68,73	1.58	7 (11%)	70,107,113	1.21	8 (11%)
17	CLA	C	610	-	65,73,73	1.51	6 (9%)	76,113,113	1.21	7 (9%)
17	CLA	B	611	-	65,73,73	1.50	5 (7%)	76,113,113	1.21	8 (10%)
17	CLA	B	605	-	65,73,73	1.50	6 (9%)	76,113,113	1.15	8 (10%)
26	DGD	C	617	-	56,56,67	0.93	2 (3%)	70,70,81	0.92	3 (4%)
20	LHG	B	621	-	43,43,48	0.99	2 (4%)	46,49,54	1.00	2 (4%)
18	BCR	Z	101	-	41,41,41	0.82	1 (2%)	56,56,56	1.91	21 (37%)
18	BCR	D	404	-	41,41,41	0.75	0	56,56,56	2.08	22 (39%)
21	BCT	D	401	28	2,3,3	1.25	0	2,3,3	4.13	2 (100%)
19	LMG	C	601	-	49,49,55	0.96	2 (4%)	57,57,63	0.90	2 (3%)
26	DGD	C	619	-	60,60,67	0.90	2 (3%)	74,74,81	0.80	2 (2%)
17	CLA	B	612	-	65,73,73	1.51	6 (9%)	76,113,113	1.23	7 (9%)
17	CLA	C	604	-	65,73,73	1.52	6 (9%)	76,113,113	1.23	9 (11%)
17	CLA	C	611	-	65,73,73	1.53	7 (10%)	76,113,113	1.23	8 (10%)
19	LMG	K	102	-	51,51,55	0.95	2 (3%)	59,59,63	0.88	2 (3%)
17	CLA	B	604	-	65,73,73	1.53	7 (10%)	76,113,113	1.19	8 (10%)
20	LHG	B	623	-	48,48,48	0.94	2 (4%)	51,54,54	0.93	2 (3%)
23	PHO	D	412	-	51,69,69	1.01	3 (5%)	47,99,99	1.04	4 (8%)
25	VTQ	X	201	-	30,32,32	1.48	5 (16%)	39,44,44	1.03	2 (5%)
18	BCR	K	101	-	41,41,41	0.75	0	56,56,56	2.15	20 (35%)
17	CLA	C	603	-	65,73,73	1.51	6 (9%)	76,113,113	1.28	7 (9%)
17	CLA	C	609	-	65,73,73	1.53	5 (7%)	76,113,113	1.17	8 (10%)
20	LHG	D	407	-	42,42,48	1.01	2 (4%)	45,48,54	1.11	3 (6%)
17	CLA	B	610	-	65,73,73	1.49	5 (7%)	76,113,113	1.25	8 (10%)
19	LMG	H	102	-	48,48,55	0.96	2 (4%)	56,56,63	0.95	2 (3%)
18	BCR	C	616	-	41,41,41	0.75	1 (2%)	56,56,56	1.94	16 (28%)
17	CLA	C	605	-	65,73,73	1.53	7 (10%)	76,113,113	1.21	8 (10%)
24	HEM	E	101	4,3	41,50,50	1.48	3 (7%)	45,82,82	1.41	5 (11%)
18	BCR	H	101	-	41,41,41	0.68	0	56,56,56	2.11	20 (35%)
19	LMG	B	620	-	46,46,55	0.98	2 (4%)	54,54,63	0.87	2 (3%)
17	CLA	B	601	-	65,73,73	1.52	6 (9%)	76,113,113	1.17	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	B	608	-	65,73,73	1.51	6 (9%)	76,113,113	1.18	8 (10%)
20	LHG	K	103	-	40,40,48	1.03	2 (5%)	43,46,54	1.01	2 (4%)
27	SQD	C	620	-	50,51,54	1.22	4 (8%)	59,62,65	1.07	6 (10%)
18	BCR	B	618	-	41,41,41	0.75	0	56,56,56	1.92	20 (35%)
20	LHG	B	622	-	46,46,48	0.97	2 (4%)	49,52,54	0.95	2 (4%)
17	CLA	B	615	-	65,73,73	1.52	5 (7%)	76,113,113	1.18	8 (10%)
23	PHO	D	411	-	51,69,69	1.02	4 (7%)	47,99,99	1.15	5 (10%)
17	CLA	A	403	-	49,57,73	1.74	6 (12%)	55,93,113	1.40	8 (14%)
17	CLA	B	607	-	65,73,73	1.52	5 (7%)	76,113,113	1.21	7 (9%)
17	CLA	B	616	-	65,73,73	1.51	5 (7%)	76,113,113	1.21	8 (10%)
17	CLA	D	410	-	65,73,73	1.52	5 (7%)	76,113,113	1.23	9 (11%)
17	CLA	A	402	-	65,73,73	1.52	6 (9%)	76,113,113	1.23	7 (9%)
17	CLA	B	613	-	65,73,73	1.51	6 (9%)	76,113,113	1.23	8 (10%)
20	LHG	L	101	-	48,48,48	0.93	2 (4%)	51,54,54	0.91	2 (3%)
26	DGD	C	618	-	58,58,67	0.92	2 (3%)	72,72,81	0.87	2 (2%)
18	BCR	B	617	-	41,41,41	0.78	1 (2%)	56,56,56	1.96	21 (37%)
17	CLA	B	606	-	65,73,73	1.52	7 (10%)	76,113,113	1.21	7 (9%)
19	LMG	D	408	-	46,46,55	0.99	2 (4%)	54,54,63	0.86	2 (3%)
17	CLA	C	606	-	65,73,73	1.53	5 (7%)	76,113,113	1.15	8 (10%)
17	CLA	B	609	-	65,73,73	1.53	6 (9%)	76,113,113	1.18	8 (10%)
17	CLA	B	614	-	45,53,73	1.79	6 (13%)	52,89,113	1.38	7 (13%)
17	CLA	C	612	14	65,73,73	1.53	6 (9%)	76,113,113	1.20	8 (10%)
17	CLA	C	614	-	65,73,73	1.50	6 (9%)	76,113,113	1.29	8 (10%)
17	CLA	B	603	-	65,73,73	1.52	7 (10%)	76,113,113	1.20	8 (10%)
17	CLA	C	602	-	65,73,73	1.52	6 (9%)	76,113,113	1.20	7 (9%)
17	CLA	C	613	-	65,73,73	1.52	5 (7%)	76,113,113	1.23	7 (9%)
18	BCR	B	619	-	41,41,41	0.76	0	56,56,56	2.02	20 (35%)
18	BCR	C	615	-	41,41,41	0.78	1 (2%)	56,56,56	2.28	22 (39%)
18	BCR	A	405	-	41,41,41	0.76	1 (2%)	56,56,56	2.01	21 (37%)
17	CLA	D	403	-	65,73,73	1.52	5 (7%)	76,113,113	1.22	8 (10%)
17	CLA	B	602	-	65,73,73	1.53	6 (9%)	76,113,113	1.21	8 (10%)
20	LHG	D	406	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	2 (3%)
20	LHG	D	409	-	48,48,48	0.94	2 (4%)	51,54,54	1.01	3 (5%)
17	CLA	C	607	-	65,73,73	1.51	5 (7%)	76,113,113	1.22	8 (10%)

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
17	CLA	D	402	-	1/1/15/20	19/37/115/115	-
19	LMG	C	621	-	-	8/43/63/70	0/1/1/1
17	CLA	C	608	-	1/1/15/20	7/37/115/115	-
22	PL9	D	405	-	-	8/53/73/73	0/1/1/1
17	CLA	A	404	-	1/1/14/20	6/31/109/115	-
17	CLA	C	610	-	1/1/15/20	16/37/115/115	-
17	CLA	B	611	-	1/1/15/20	15/37/115/115	-
17	CLA	B	605	-	1/1/15/20	16/37/115/115	-
26	DGD	C	617	-	-	5/44/84/95	0/2/2/2
20	LHG	B	621	-	-	10/48/48/53	-
18	BCR	Z	101	-	-	4/29/63/63	0/2/2/2
18	BCR	D	404	-	-	4/29/63/63	0/2/2/2
19	LMG	C	601	-	-	5/44/64/70	0/1/1/1
26	DGD	C	619	-	-	5/48/88/95	0/2/2/2
17	CLA	B	612	-	1/1/15/20	13/37/115/115	-
17	CLA	C	604	-	1/1/15/20	17/37/115/115	-
17	CLA	C	611	-	1/1/15/20	10/37/115/115	-
19	LMG	K	102	-	-	7/46/66/70	0/1/1/1
17	CLA	B	604	-	1/1/15/20	18/37/115/115	-
20	LHG	B	623	-	-	11/53/53/53	-
23	PHO	D	412	-	-	10/37/103/103	0/5/6/6
25	VTQ	X	201	-	-	7/25/49/49	0/1/1/1
18	BCR	K	101	-	-	4/29/63/63	0/2/2/2
17	CLA	C	603	-	1/1/15/20	15/37/115/115	-
17	CLA	C	609	-	1/1/15/20	16/37/115/115	-
20	LHG	D	407	-	-	16/47/47/53	-
17	CLA	B	610	-	1/1/15/20	13/37/115/115	-
19	LMG	H	102	-	-	10/43/63/70	0/1/1/1
18	BCR	C	616	-	-	4/29/63/63	0/2/2/2
17	CLA	C	605	-	1/1/15/20	8/37/115/115	-
24	HEM	E	101	4,3	-	3/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	H	101	-	-	5/29/63/63	0/2/2/2
19	LMG	B	620	-	-	3/41/61/70	0/1/1/1
17	CLA	B	601	-	1/1/15/20	14/37/115/115	-
17	CLA	B	608	-	1/1/15/20	10/37/115/115	-
20	LHG	K	103	-	-	8/45/45/53	-
27	SQD	C	620	-	-	12/46/66/69	0/1/1/1
18	BCR	B	618	-	-	4/29/63/63	0/2/2/2
20	LHG	B	622	-	-	8/51/51/53	-
17	CLA	B	615	-	1/1/15/20	6/37/115/115	-
23	PHO	D	411	-	-	12/37/103/103	0/5/6/6
17	CLA	A	403	-	1/1/11/20	6/18/96/115	-
17	CLA	B	607	-	1/1/15/20	19/37/115/115	-
17	CLA	B	616	-	1/1/15/20	11/37/115/115	-
17	CLA	D	410	-	1/1/15/20	6/37/115/115	-
17	CLA	A	402	-	1/1/15/20	11/37/115/115	-
17	CLA	B	613	-	1/1/15/20	13/37/115/115	-
20	LHG	L	101	-	-	14/53/53/53	-
26	DGD	C	618	-	-	7/46/86/95	0/2/2/2
18	BCR	B	617	-	-	4/29/63/63	0/2/2/2
17	CLA	B	606	-	1/1/15/20	13/37/115/115	-
19	LMG	D	408	-	-	6/41/61/70	0/1/1/1
17	CLA	C	606	-	1/1/15/20	16/37/115/115	-
17	CLA	B	609	-	1/1/15/20	15/37/115/115	-
17	CLA	B	614	-	1/1/11/20	5/13/91/115	-
17	CLA	C	612	14	1/1/15/20	15/37/115/115	-
17	CLA	C	614	-	1/1/15/20	15/37/115/115	-
17	CLA	B	603	-	1/1/15/20	12/37/115/115	-
17	CLA	C	602	-	1/1/15/20	16/37/115/115	-
17	CLA	C	613	-	1/1/15/20	15/37/115/115	-
18	BCR	B	619	-	-	4/29/63/63	0/2/2/2
18	BCR	C	615	-	-	2/29/63/63	0/2/2/2
18	BCR	A	405	-	-	4/29/63/63	0/2/2/2
17	CLA	D	403	-	1/1/15/20	20/37/115/115	-
17	CLA	B	602	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LHG	D	406	-	-	8/53/53/53	-
20	LHG	D	409	-	-	11/53/53/53	-
17	CLA	C	607	-	1/1/15/20	24/37/115/115	-

All (269) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	613	CLA	C4B-NB	7.88	1.42	1.35
17	C	606	CLA	C4B-NB	7.83	1.42	1.35
17	C	609	CLA	C4B-NB	7.83	1.42	1.35
17	C	605	CLA	C4B-NB	7.82	1.42	1.35
17	C	611	CLA	C4B-NB	7.80	1.42	1.35
17	B	602	CLA	C4B-NB	7.79	1.42	1.35
17	B	604	CLA	C4B-NB	7.79	1.42	1.35
17	B	615	CLA	C4B-NB	7.79	1.42	1.35
17	D	402	CLA	C4B-NB	7.76	1.42	1.35
17	A	403	CLA	C4B-NB	7.76	1.42	1.35
17	C	610	CLA	C4B-NB	7.75	1.42	1.35
17	B	603	CLA	C4B-NB	7.75	1.42	1.35
17	B	609	CLA	C4B-NB	7.74	1.42	1.35
17	C	612	CLA	C4B-NB	7.74	1.42	1.35
17	C	604	CLA	C4B-NB	7.73	1.42	1.35
17	B	606	CLA	C4B-NB	7.72	1.42	1.35
17	D	403	CLA	C4B-NB	7.72	1.42	1.35
17	D	410	CLA	C4B-NB	7.72	1.42	1.35
17	C	614	CLA	C4B-NB	7.69	1.42	1.35
17	C	602	CLA	C4B-NB	7.69	1.42	1.35
17	B	607	CLA	C4B-NB	7.68	1.42	1.35
17	B	613	CLA	C4B-NB	7.66	1.42	1.35
17	B	608	CLA	C4B-NB	7.64	1.42	1.35
17	B	612	CLA	C4B-NB	7.64	1.42	1.35
17	B	611	CLA	C4B-NB	7.63	1.42	1.35
17	C	607	CLA	C4B-NB	7.63	1.42	1.35
17	B	601	CLA	C4B-NB	7.62	1.42	1.35
17	A	404	CLA	C4B-NB	7.62	1.42	1.35
17	B	616	CLA	C4B-NB	7.62	1.42	1.35
17	A	402	CLA	C4B-NB	7.60	1.42	1.35
17	C	603	CLA	C4B-NB	7.57	1.42	1.35
17	B	614	CLA	C4B-NB	7.52	1.41	1.35
17	C	608	CLA	C4B-NB	7.52	1.41	1.35
17	B	605	CLA	C4B-NB	7.49	1.41	1.35
17	B	610	CLA	C4B-NB	7.43	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	620	SQD	O8-S	4.62	1.63	1.47
20	D	407	LHG	O8-C23	4.29	1.45	1.33
19	C	621	LMG	O8-C28	4.29	1.45	1.33
19	C	601	LMG	O8-C28	4.29	1.45	1.33
26	C	618	DGD	O1G-C1A	4.27	1.45	1.33
19	K	102	LMG	O7-C10	4.27	1.46	1.34
20	B	622	LHG	O8-C23	4.26	1.45	1.33
19	K	102	LMG	O8-C28	4.25	1.45	1.33
19	D	408	LMG	O7-C10	4.25	1.46	1.34
27	C	620	SQD	O48-C23	4.25	1.45	1.33
20	B	623	LHG	O8-C23	4.24	1.45	1.33
20	D	409	LHG	O8-C23	4.24	1.45	1.33
19	D	408	LMG	O8-C28	4.23	1.45	1.33
26	C	617	DGD	O1G-C1A	4.23	1.45	1.33
20	L	101	LHG	O8-C23	4.23	1.45	1.33
19	H	102	LMG	O8-C28	4.23	1.45	1.33
20	K	103	LHG	O8-C23	4.23	1.45	1.33
26	C	619	DGD	O1G-C1A	4.22	1.45	1.33
26	C	618	DGD	O2G-C1B	4.22	1.46	1.34
20	B	621	LHG	O8-C23	4.22	1.45	1.33
19	B	620	LMG	O8-C28	4.21	1.45	1.33
20	B	622	LHG	O7-C7	4.20	1.46	1.34
19	B	620	LMG	O7-C10	4.19	1.46	1.34
20	B	621	LHG	O7-C7	4.18	1.46	1.34
20	D	407	LHG	O7-C7	4.18	1.46	1.34
26	C	619	DGD	O2G-C1B	4.18	1.46	1.34
20	K	103	LHG	O7-C7	4.16	1.46	1.34
19	H	102	LMG	O7-C10	4.15	1.46	1.34
20	D	406	LHG	O8-C23	4.15	1.45	1.33
26	C	617	DGD	O2G-C1B	4.14	1.46	1.34
20	D	409	LHG	O7-C7	4.14	1.46	1.34
20	D	406	LHG	O7-C7	4.14	1.46	1.34
20	B	623	LHG	O7-C7	4.13	1.46	1.34
19	C	621	LMG	O7-C10	4.13	1.45	1.34
24	E	101	HEM	C3C-C2C	-4.11	1.34	1.40
19	C	601	LMG	O7-C10	4.09	1.45	1.34
27	C	620	SQD	O47-C7	4.08	1.45	1.34
20	L	101	LHG	O7-C7	4.07	1.45	1.34
17	D	402	CLA	C1D-ND	3.94	1.42	1.37
17	C	611	CLA	C1D-ND	3.92	1.42	1.37
17	C	610	CLA	C1D-ND	3.90	1.42	1.37
17	B	614	CLA	C1D-ND	3.89	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	606	CLA	C1D-ND	3.89	1.42	1.37
17	B	616	CLA	C1D-ND	3.87	1.42	1.37
17	D	403	CLA	C1D-ND	3.87	1.42	1.37
17	D	410	CLA	C1D-ND	3.86	1.42	1.37
17	C	613	CLA	C1D-ND	3.86	1.42	1.37
17	B	612	CLA	C1D-ND	3.86	1.42	1.37
17	A	402	CLA	C1D-ND	3.86	1.42	1.37
17	B	601	CLA	C1D-ND	3.85	1.42	1.37
17	B	615	CLA	C1D-ND	3.85	1.42	1.37
17	B	607	CLA	C1D-ND	3.85	1.42	1.37
17	C	612	CLA	C1D-ND	3.84	1.42	1.37
17	B	609	CLA	C1D-ND	3.84	1.42	1.37
17	C	604	CLA	C1D-ND	3.84	1.42	1.37
17	A	404	CLA	C1D-ND	3.84	1.42	1.37
17	B	608	CLA	C1D-ND	3.83	1.42	1.37
17	B	613	CLA	C1D-ND	3.82	1.42	1.37
17	C	603	CLA	C1D-ND	3.82	1.42	1.37
17	C	614	CLA	C1D-ND	3.81	1.42	1.37
17	B	610	CLA	C1D-ND	3.81	1.42	1.37
17	B	602	CLA	C1D-ND	3.81	1.42	1.37
17	C	605	CLA	C1D-ND	3.81	1.42	1.37
17	B	611	CLA	C1D-ND	3.80	1.42	1.37
17	C	609	CLA	C1D-ND	3.80	1.42	1.37
17	B	606	CLA	C1D-ND	3.80	1.42	1.37
17	B	605	CLA	C1D-ND	3.79	1.42	1.37
17	C	607	CLA	C1D-ND	3.78	1.42	1.37
17	C	608	CLA	C1D-ND	3.78	1.42	1.37
17	B	604	CLA	C1D-ND	3.78	1.42	1.37
17	A	403	CLA	C1D-ND	3.77	1.42	1.37
17	C	602	CLA	C1D-ND	3.74	1.42	1.37
17	B	603	CLA	C1D-ND	3.70	1.42	1.37
24	E	101	HEM	C3C-CAC	3.67	1.55	1.47
22	D	405	PL9	C7-C3	-3.46	1.47	1.51
25	X	201	VTQ	O3-C9	-3.08	1.40	1.44
17	C	608	CLA	CHC-C1C	3.07	1.42	1.35
22	D	405	PL9	C3-C4	-3.06	1.44	1.49
17	B	613	CLA	CHC-C1C	3.06	1.42	1.35
17	D	402	CLA	CHC-C1C	3.05	1.42	1.35
17	C	602	CLA	CHC-C1C	3.05	1.42	1.35
17	B	602	CLA	CHC-C1C	3.04	1.42	1.35
17	B	611	CLA	C4D-ND	-3.03	1.33	1.37
17	C	611	CLA	CHC-C1C	3.03	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	605	CLA	CHC-C1C	3.03	1.42	1.35
17	A	403	CLA	C4D-ND	-3.02	1.33	1.37
17	C	604	CLA	C4D-ND	-3.01	1.33	1.37
17	C	605	CLA	C4D-ND	-3.01	1.33	1.37
17	A	402	CLA	CHC-C1C	3.00	1.42	1.35
17	B	610	CLA	C4D-ND	-3.00	1.33	1.37
17	B	608	CLA	C4D-ND	-3.00	1.33	1.37
17	C	609	CLA	CHC-C1C	3.00	1.42	1.35
17	B	605	CLA	C4D-ND	-3.00	1.33	1.37
17	B	616	CLA	CHC-C1C	2.99	1.42	1.35
17	C	603	CLA	C4D-ND	-2.99	1.33	1.37
17	B	602	CLA	C4D-ND	-2.99	1.33	1.37
17	C	606	CLA	CHC-C1C	2.99	1.42	1.35
17	C	609	CLA	C4D-ND	-2.98	1.33	1.37
17	B	607	CLA	CHC-C1C	2.98	1.42	1.35
17	B	601	CLA	CHC-C1C	2.98	1.42	1.35
17	C	612	CLA	CHC-C1C	2.98	1.42	1.35
17	B	607	CLA	C4D-ND	-2.98	1.33	1.37
17	C	614	CLA	C4D-ND	-2.98	1.33	1.37
17	D	410	CLA	C4D-ND	-2.98	1.33	1.37
17	D	410	CLA	CHC-C1C	2.97	1.42	1.35
17	C	612	CLA	C4D-ND	-2.97	1.33	1.37
17	A	403	CLA	CHC-C1C	2.97	1.42	1.35
17	C	608	CLA	C4D-ND	-2.97	1.33	1.37
17	B	612	CLA	CHC-C1C	2.97	1.42	1.35
17	C	614	CLA	CHC-C1C	2.97	1.42	1.35
17	B	609	CLA	C4D-ND	-2.97	1.33	1.37
17	B	614	CLA	CHC-C1C	2.96	1.42	1.35
17	B	604	CLA	C4D-ND	-2.96	1.33	1.37
17	C	613	CLA	CHC-C1C	2.96	1.42	1.35
17	B	603	CLA	CHC-C1C	2.95	1.42	1.35
17	B	601	CLA	C4D-ND	-2.94	1.33	1.37
17	B	608	CLA	CHC-C1C	2.94	1.42	1.35
17	B	604	CLA	CHC-C1C	2.94	1.42	1.35
17	B	610	CLA	CHC-C1C	2.94	1.42	1.35
17	D	403	CLA	CHC-C1C	2.94	1.42	1.35
17	B	606	CLA	CHC-C1C	2.93	1.42	1.35
17	C	607	CLA	CHC-C1C	2.93	1.42	1.35
17	B	609	CLA	CHC-C1C	2.93	1.42	1.35
17	A	402	CLA	C4D-ND	-2.92	1.33	1.37
17	A	404	CLA	CHC-C1C	2.92	1.42	1.35
27	C	620	SQD	C6-S	-2.92	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	603	CLA	C4D-ND	-2.91	1.33	1.37
17	C	607	CLA	C4D-ND	-2.91	1.33	1.37
17	B	605	CLA	CHC-C1C	2.91	1.42	1.35
17	B	611	CLA	CHC-C1C	2.91	1.42	1.35
17	C	610	CLA	CHC-C1C	2.91	1.42	1.35
17	C	604	CLA	CHC-C1C	2.90	1.42	1.35
17	C	602	CLA	C4D-ND	-2.90	1.33	1.37
17	C	603	CLA	CHC-C1C	2.89	1.42	1.35
17	B	615	CLA	CHC-C1C	2.89	1.42	1.35
17	C	611	CLA	C4D-ND	-2.88	1.33	1.37
17	D	403	CLA	C4D-ND	-2.88	1.33	1.37
17	A	404	CLA	C4D-ND	-2.88	1.33	1.37
17	C	606	CLA	C4D-ND	-2.88	1.33	1.37
17	B	606	CLA	C4D-ND	-2.86	1.33	1.37
17	C	610	CLA	C4D-ND	-2.86	1.33	1.37
17	B	613	CLA	C4D-ND	-2.85	1.33	1.37
24	E	101	HEM	CAB-C3B	2.83	1.55	1.47
17	B	614	CLA	C4D-ND	-2.83	1.33	1.37
17	B	612	CLA	C4D-ND	-2.81	1.33	1.37
17	B	616	CLA	C4D-ND	-2.78	1.33	1.37
17	B	615	CLA	C4D-ND	-2.77	1.33	1.37
17	C	613	CLA	C4D-ND	-2.73	1.33	1.37
23	D	411	PHO	CAC-C3C	-2.72	1.47	1.52
23	D	412	PHO	CAC-C3C	-2.68	1.47	1.52
17	D	402	CLA	C4D-ND	-2.59	1.34	1.37
17	C	607	CLA	CMB-C2B	-2.58	1.46	1.51
17	B	603	CLA	CMB-C2B	-2.56	1.46	1.51
25	X	201	VTQ	C10-C3	2.54	1.57	1.51
25	X	201	VTQ	C3-C4	2.51	1.53	1.46
17	C	603	CLA	CMB-C2B	-2.50	1.46	1.51
17	C	612	CLA	CMB-C2B	-2.48	1.46	1.51
17	B	612	CLA	CMB-C2B	-2.48	1.46	1.51
17	D	410	CLA	CMB-C2B	-2.48	1.46	1.51
17	A	403	CLA	CMB-C2B	-2.45	1.46	1.51
17	B	601	CLA	CMB-C2B	-2.45	1.46	1.51
17	B	606	CLA	CMB-C2B	-2.43	1.46	1.51
17	C	602	CLA	CMB-C2B	-2.43	1.46	1.51
17	B	615	CLA	CMB-C2B	-2.43	1.46	1.51
17	B	604	CLA	CMB-C2B	-2.42	1.46	1.51
17	A	402	CLA	CMB-C2B	-2.41	1.46	1.51
17	C	609	CLA	CMB-C2B	-2.41	1.46	1.51
17	C	605	CLA	CMB-C2B	-2.40	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	607	CLA	CMB-C2B	-2.40	1.46	1.51
17	D	403	CLA	CMB-C2B	-2.39	1.46	1.51
17	B	610	CLA	CMB-C2B	-2.39	1.46	1.51
17	B	616	CLA	CMB-C2B	-2.38	1.46	1.51
17	C	608	CLA	CMB-C2B	-2.38	1.46	1.51
17	B	611	CLA	CMB-C2B	-2.38	1.46	1.51
17	B	602	CLA	CMB-C2B	-2.38	1.46	1.51
17	C	614	CLA	CMB-C2B	-2.38	1.46	1.51
17	C	610	CLA	CMB-C2B	-2.38	1.46	1.51
17	A	404	CLA	CMB-C2B	-2.38	1.46	1.51
17	C	604	CLA	CMB-C2B	-2.38	1.46	1.51
17	D	402	CLA	CMB-C2B	-2.37	1.46	1.51
17	B	609	CLA	CMB-C2B	-2.36	1.46	1.51
17	B	614	CLA	CMB-C2B	-2.36	1.46	1.51
17	B	608	CLA	CMB-C2B	-2.35	1.46	1.51
17	C	606	CLA	CMB-C2B	-2.34	1.46	1.51
17	C	611	CLA	CMB-C2B	-2.34	1.46	1.51
17	B	613	CLA	CMB-C2B	-2.33	1.46	1.51
17	B	605	CLA	CMB-C2B	-2.29	1.46	1.51
22	D	405	PL9	C6-C1	-2.28	1.44	1.48
22	D	405	PL9	C53-C6	-2.25	1.46	1.50
19	C	621	LMG	O1-C1	2.21	1.44	1.40
23	D	412	PHO	CMD-C2D	-2.18	1.46	1.51
17	C	612	CLA	C3B-C2B	-2.15	1.37	1.40
17	C	613	CLA	CMB-C2B	-2.15	1.47	1.51
25	X	201	VTQ	O1-C4	-2.11	1.18	1.23
18	Z	101	BCR	C1-C6	-2.10	1.50	1.53
25	X	201	VTQ	C5-C4	2.10	1.54	1.47
18	C	615	BCR	C30-C25	-2.09	1.50	1.53
17	B	603	CLA	C3B-C2B	-2.08	1.37	1.40
17	B	612	CLA	CMD-C2D	-2.08	1.46	1.50
23	D	411	PHO	CMB-C2B	-2.08	1.46	1.51
23	D	412	PHO	CMC-C2C	-2.08	1.46	1.51
18	A	405	BCR	C30-C25	-2.07	1.50	1.53
23	D	411	PHO	CMD-C2D	-2.07	1.46	1.51
17	A	402	CLA	CMD-C2D	-2.06	1.46	1.50
18	C	616	BCR	C1-C6	-2.05	1.50	1.53
23	D	411	PHO	CMC-C2C	-2.05	1.46	1.51
17	B	606	CLA	CMD-C2D	-2.05	1.46	1.50
17	C	602	CLA	CMD-C2D	-2.05	1.46	1.50
17	D	402	CLA	CMD-C2D	-2.04	1.46	1.50
17	B	601	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	602	CLA	CMD-C2D	-2.04	1.46	1.50
17	C	611	CLA	CMD-C2D	-2.04	1.46	1.50
17	A	404	CLA	CMD-C2D	-2.04	1.46	1.50
18	B	617	BCR	C30-C25	-2.04	1.51	1.53
17	B	603	CLA	CMD-C2D	-2.03	1.46	1.50
17	B	608	CLA	CMD-C2D	-2.03	1.46	1.50
17	B	606	CLA	C3B-C2B	-2.03	1.37	1.40
17	A	403	CLA	CMD-C2D	-2.02	1.46	1.50
17	C	605	CLA	C3B-C2B	-2.02	1.37	1.40
17	A	404	CLA	C3B-C2B	-2.02	1.37	1.40
17	C	608	CLA	CMD-C2D	-2.02	1.46	1.50
17	C	614	CLA	CMD-C2D	-2.02	1.46	1.50
17	B	605	CLA	CMD-C2D	-2.02	1.46	1.50
17	C	610	CLA	CMD-C2D	-2.02	1.46	1.50
17	B	609	CLA	CMD-C2D	-2.01	1.46	1.50
17	B	614	CLA	CMD-C2D	-2.01	1.46	1.50
17	C	604	CLA	C3B-C2B	-2.01	1.37	1.40
17	C	603	CLA	CMD-C2D	-2.01	1.46	1.50
17	B	613	CLA	CMD-C2D	-2.01	1.46	1.50
17	C	605	CLA	CMD-C2D	-2.01	1.46	1.50
17	B	604	CLA	C3B-C2B	-2.00	1.37	1.40
17	D	402	CLA	C3B-CAB	-2.00	1.43	1.47
17	B	604	CLA	CMD-C2D	-2.00	1.46	1.50
17	C	611	CLA	C3B-C2B	-2.00	1.37	1.40

All (549) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	C	615	BCR	C3-C4-C5	-5.93	103.49	114.08
17	D	402	CLA	C4A-NA-C1A	5.52	109.19	106.71
18	C	615	BCR	C30-C25-C26	-5.52	114.84	122.61
21	D	401	BCT	O2-C-O1	5.47	133.74	119.55
17	C	603	CLA	C4A-NA-C1A	5.47	109.16	106.71
22	D	405	PL9	C7-C3-C4	5.31	121.19	116.88
17	C	608	CLA	C4A-NA-C1A	5.23	109.06	106.71
17	B	612	CLA	C4A-NA-C1A	5.22	109.05	106.71
18	K	101	BCR	C30-C25-C26	-4.97	115.62	122.61
18	B	619	BCR	C30-C25-C26	-4.96	115.62	122.61
18	Z	101	BCR	C33-C5-C6	-4.94	118.98	124.53
17	B	610	CLA	C4A-NA-C1A	4.92	108.92	106.71
17	B	613	CLA	C4A-NA-C1A	4.92	108.92	106.71
18	H	101	BCR	C7-C8-C9	-4.82	118.95	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	405	BCR	C30-C25-C26	-4.79	115.87	122.61
17	C	611	CLA	C4A-NA-C1A	4.78	108.86	106.71
18	H	101	BCR	C28-C27-C26	-4.75	105.59	114.08
18	H	101	BCR	C3-C4-C5	-4.66	105.75	114.08
17	C	610	CLA	C4A-NA-C1A	4.63	108.79	106.71
17	C	602	CLA	C4A-NA-C1A	4.59	108.77	106.71
17	C	614	CLA	C4A-NA-C1A	4.57	108.76	106.71
17	B	602	CLA	C4A-NA-C1A	4.55	108.75	106.71
17	B	607	CLA	C4A-NA-C1A	4.55	108.75	106.71
17	C	605	CLA	C4A-NA-C1A	4.52	108.74	106.71
17	C	613	CLA	C4A-NA-C1A	4.52	108.74	106.71
18	Z	101	BCR	C1-C6-C5	-4.50	116.27	122.61
17	D	403	CLA	C4A-NA-C1A	4.47	108.72	106.71
17	B	616	CLA	C4A-NA-C1A	4.44	108.70	106.71
17	C	614	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
18	C	616	BCR	C28-C27-C26	-4.42	106.19	114.08
17	C	612	CLA	C4A-NA-C1A	4.40	108.68	106.71
17	B	611	CLA	C4A-NA-C1A	4.40	108.68	106.71
18	D	404	BCR	C30-C25-C26	-4.39	116.43	122.61
18	D	404	BCR	C1-C6-C5	-4.35	116.48	122.61
17	B	606	CLA	C4A-NA-C1A	4.34	108.66	106.71
17	B	615	CLA	C4A-NA-C1A	4.33	108.65	106.71
18	K	101	BCR	C3-C4-C5	-4.31	106.39	114.08
17	B	605	CLA	C4A-NA-C1A	4.26	108.62	106.71
17	A	403	CLA	C4A-NA-C1A	4.26	108.62	106.71
17	C	609	CLA	C4A-NA-C1A	4.26	108.62	106.71
18	K	101	BCR	C1-C6-C5	-4.25	116.63	122.61
17	B	601	CLA	C4A-NA-C1A	4.24	108.61	106.71
17	A	404	CLA	C4A-NA-C1A	4.23	108.61	106.71
18	C	615	BCR	C33-C5-C4	4.22	121.72	113.62
20	D	407	LHG	O7-C7-C8	4.20	120.56	111.50
17	C	607	CLA	C4A-NA-C1A	4.20	108.59	106.71
17	D	410	CLA	C4A-NA-C1A	4.13	108.56	106.71
18	B	618	BCR	C28-C27-C26	-4.07	106.80	114.08
18	B	617	BCR	C1-C6-C5	-4.06	116.89	122.61
20	K	103	LHG	O7-C7-C8	4.05	120.22	111.50
18	C	615	BCR	C33-C5-C6	-4.04	120.00	124.53
18	A	405	BCR	C3-C4-C5	-4.02	106.90	114.08
18	D	404	BCR	C3-C4-C5	-4.02	106.91	114.08
20	D	406	LHG	O7-C7-C8	4.01	120.15	111.50
20	D	409	LHG	O7-C7-C8	4.00	120.12	111.50
18	Z	101	BCR	C33-C5-C4	3.98	121.27	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	614	CLA	C4A-NA-C1A	3.97	108.49	106.71
19	C	621	LMG	O7-C10-C11	3.96	120.03	111.50
17	A	403	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
26	C	618	DGD	O2G-C1B-C2B	3.88	119.87	111.50
18	C	616	BCR	C20-C21-C22	-3.88	121.78	127.31
17	A	402	CLA	C4A-NA-C1A	3.84	108.43	106.71
20	B	621	LHG	O7-C7-C8	3.84	119.78	111.50
26	C	617	DGD	O2G-C1B-C2B	3.81	119.72	111.50
18	K	101	BCR	C37-C22-C23	3.81	124.08	118.08
18	K	101	BCR	C28-C27-C26	-3.81	107.28	114.08
18	H	101	BCR	C20-C21-C22	-3.80	121.88	127.31
17	D	402	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
19	H	102	LMG	O7-C10-C11	3.80	119.69	111.50
18	C	616	BCR	C16-C17-C18	-3.78	121.91	127.31
18	H	101	BCR	C16-C17-C18	-3.74	121.97	127.31
18	C	615	BCR	C28-C27-C26	-3.74	107.40	114.08
19	K	102	LMG	O7-C10-C11	3.73	119.53	111.50
18	B	619	BCR	C28-C27-C26	-3.72	107.43	114.08
18	B	619	BCR	C1-C6-C5	-3.68	117.43	122.61
18	D	404	BCR	C16-C17-C18	-3.68	122.06	127.31
17	C	614	CLA	CMB-C2B-C3B	3.67	131.55	124.68
18	C	615	BCR	C1-C6-C7	3.67	126.16	115.78
27	C	620	SQD	O47-C7-C8	3.65	119.37	111.50
17	B	603	CLA	C4A-NA-C1A	3.65	108.35	106.71
26	C	619	DGD	O2G-C1B-C2B	3.65	119.36	111.50
17	B	604	CLA	C4A-NA-C1A	3.63	108.34	106.71
18	K	101	BCR	C16-C17-C18	-3.62	122.14	127.31
18	C	616	BCR	C1-C6-C5	-3.62	117.52	122.61
19	B	620	LMG	O7-C10-C11	3.61	119.29	111.50
20	B	622	LHG	O7-C7-C8	3.60	119.27	111.50
18	B	618	BCR	C20-C21-C22	-3.60	122.17	127.31
18	B	617	BCR	C20-C21-C22	-3.59	122.19	127.31
17	B	608	CLA	C4A-NA-C1A	3.58	108.32	106.71
18	B	617	BCR	C30-C25-C26	-3.57	117.59	122.61
19	C	601	LMG	O7-C10-C11	3.57	119.19	111.50
18	B	618	BCR	C37-C22-C23	3.56	123.69	118.08
18	B	617	BCR	C36-C18-C19	3.55	123.68	118.08
25	X	201	VTQ	C10-C11-C9	-3.55	109.23	118.08
18	A	405	BCR	C20-C21-C22	-3.54	122.25	127.31
18	B	619	BCR	C16-C17-C18	-3.54	122.26	127.31
22	D	405	PL9	C7-C3-C2	-3.52	118.67	123.30
18	B	619	BCR	C20-C21-C22	-3.52	122.29	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	C	604	CLA	C4A-NA-C1A	3.52	108.29	106.71
18	A	405	BCR	C38-C26-C27	3.52	120.37	113.62
17	C	607	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
19	D	408	LMG	O7-C10-C11	3.50	119.04	111.50
17	B	611	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
17	D	402	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
20	B	623	LHG	O7-C7-C8	3.49	119.02	111.50
18	B	619	BCR	C37-C22-C23	3.49	123.57	118.08
18	A	405	BCR	C7-C8-C9	-3.48	120.98	126.23
18	B	617	BCR	C37-C22-C23	3.48	123.55	118.08
17	B	610	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
18	D	404	BCR	C20-C21-C22	-3.45	122.39	127.31
17	D	410	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
18	D	404	BCR	C37-C22-C23	3.41	123.45	118.08
18	H	101	BCR	C36-C18-C19	3.39	123.42	118.08
18	K	101	BCR	C36-C18-C19	3.38	123.41	118.08
18	K	101	BCR	C27-C26-C25	-3.38	117.83	122.73
17	B	614	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
17	A	402	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
18	A	405	BCR	C16-C17-C18	-3.36	122.51	127.31
20	L	101	LHG	O7-C7-C8	3.36	118.74	111.50
18	B	619	BCR	C36-C18-C19	3.36	123.37	118.08
18	B	618	BCR	C36-C18-C19	3.35	123.36	118.08
18	C	616	BCR	C7-C8-C9	-3.35	121.17	126.23
18	C	615	BCR	C1-C6-C5	-3.35	117.90	122.61
17	B	606	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
18	B	618	BCR	C7-C8-C9	-3.34	121.19	126.23
18	D	404	BCR	C38-C26-C27	3.33	120.00	113.62
17	D	402	CLA	CMB-C2B-C3B	3.32	130.89	124.68
18	Z	101	BCR	C37-C22-C23	3.31	123.29	118.08
17	A	403	CLA	CMB-C2B-C3B	3.31	130.86	124.68
17	B	602	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
18	B	618	BCR	C33-C5-C6	-3.30	120.83	124.53
17	B	608	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
18	K	101	BCR	C38-C26-C27	3.28	119.92	113.62
17	C	613	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
17	C	603	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
18	B	618	BCR	C1-C6-C5	-3.27	118.01	122.61
18	H	101	BCR	C4-C5-C6	-3.26	118.00	122.73
18	B	617	BCR	C33-C5-C4	3.26	119.87	113.62
18	K	101	BCR	C20-C21-C22	-3.25	122.67	127.31
17	B	609	CLA	C4A-NA-C1A	3.24	108.16	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	617	BCR	C3-C4-C5	-3.24	108.30	114.08
18	D	404	BCR	C28-C27-C26	-3.23	108.30	114.08
17	B	609	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
18	A	405	BCR	C36-C18-C19	3.22	123.15	118.08
18	D	404	BCR	C27-C26-C25	-3.22	118.06	122.73
17	B	612	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
18	H	101	BCR	C30-C25-C26	-3.20	118.11	122.61
18	D	404	BCR	C36-C18-C19	3.19	123.10	118.08
18	Z	101	BCR	C3-C4-C5	-3.19	108.38	114.08
18	H	101	BCR	C37-C22-C23	3.17	123.08	118.08
17	B	606	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
18	B	619	BCR	C38-C26-C27	3.16	119.69	113.62
17	C	609	CLA	CMB-C2B-C1B	-3.15	123.61	128.46
17	B	603	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
17	B	604	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
17	C	605	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
17	B	609	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
18	B	619	BCR	C33-C5-C4	3.14	119.64	113.62
18	C	615	BCR	C38-C26-C27	3.13	119.64	113.62
18	C	615	BCR	C4-C5-C6	-3.13	118.18	122.73
18	B	618	BCR	C30-C25-C26	-3.12	118.22	122.61
18	B	619	BCR	C33-C5-C6	-3.11	121.04	124.53
18	H	101	BCR	C11-C10-C9	-3.10	122.88	127.31
18	D	404	BCR	C4-C5-C6	-3.09	118.24	122.73
18	C	615	BCR	C37-C22-C23	3.09	122.94	118.08
17	C	606	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
17	B	616	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
18	B	618	BCR	C33-C5-C4	3.08	119.53	113.62
17	C	604	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
18	B	618	BCR	C16-C17-C18	-3.07	122.92	127.31
18	D	404	BCR	C33-C5-C4	3.07	119.52	113.62
17	C	602	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
18	B	618	BCR	C37-C22-C21	-3.07	118.62	122.92
18	C	615	BCR	C7-C8-C9	-3.07	121.60	126.23
18	A	405	BCR	C27-C26-C25	-3.06	118.28	122.73
17	B	611	CLA	CMB-C2B-C3B	3.06	130.40	124.68
17	B	610	CLA	CMB-C2B-C3B	3.05	130.38	124.68
17	C	606	CLA	C4A-NA-C1A	3.04	108.07	106.71
18	Z	101	BCR	C16-C17-C18	-3.03	122.98	127.31
18	A	405	BCR	C38-C26-C25	-3.03	121.12	124.53
18	B	617	BCR	C37-C22-C21	-3.03	118.68	122.92
17	B	615	CLA	O2D-CGD-O1D	-3.02	117.93	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	C	615	BCR	C36-C18-C19	3.02	122.84	118.08
17	C	606	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
17	B	608	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
17	C	613	CLA	CMB-C2B-C3B	3.00	130.29	124.68
18	C	616	BCR	C33-C5-C6	-3.00	121.16	124.53
18	C	615	BCR	C38-C26-C25	-2.99	121.17	124.53
17	C	604	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
17	A	402	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
17	B	614	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
17	C	613	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
17	D	403	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
18	A	405	BCR	C1-C6-C5	-2.98	118.41	122.61
17	C	603	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
17	B	611	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
17	C	610	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
17	A	404	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
18	B	617	BCR	C33-C5-C6	-2.97	121.19	124.53
17	B	608	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
17	A	403	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
18	B	617	BCR	C38-C26-C25	-2.96	121.20	124.53
17	B	603	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
18	Z	101	BCR	C36-C18-C19	2.96	122.74	118.08
18	A	405	BCR	C37-C22-C23	2.96	122.74	118.08
18	B	617	BCR	C16-C17-C18	-2.96	123.09	127.31
17	C	611	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
17	D	403	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
18	B	619	BCR	C7-C8-C9	-2.95	121.78	126.23
17	B	604	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
17	D	410	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
17	C	606	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
17	B	614	CLA	CMB-C2B-C3B	2.93	130.17	124.68
17	B	604	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
18	C	616	BCR	C24-C23-C22	-2.93	121.80	126.23
17	B	601	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
24	E	101	HEM	C1B-NB-C4B	2.93	108.09	105.07
17	D	410	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
17	C	613	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
17	B	612	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
17	B	606	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
18	Z	101	BCR	C20-C21-C22	-2.91	123.16	127.31
17	C	612	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
18	C	616	BCR	C33-C5-C4	2.90	119.19	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	C	616	BCR	C37-C22-C23	2.90	122.65	118.08
17	A	403	CLA	C1B-CHB-C4A	-2.89	124.38	130.12
17	A	402	CLA	CMB-C2B-C3B	2.89	130.08	124.68
17	B	608	CLA	CMB-C2B-C3B	2.89	130.08	124.68
18	C	616	BCR	C29-C30-C25	2.89	114.92	110.48
17	B	606	CLA	CMB-C2B-C3B	2.89	130.08	124.68
17	D	402	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
18	H	101	BCR	C38-C26-C27	2.88	119.15	113.62
18	B	619	BCR	C27-C26-C25	-2.88	118.55	122.73
27	C	620	SQD	O48-C23-C24	2.87	120.92	111.91
17	C	612	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
17	B	607	CLA	CMB-C2B-C1B	-2.86	124.06	128.46
17	C	608	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
18	A	405	BCR	C11-C10-C9	-2.86	123.23	127.31
22	D	405	PL9	C40-C39-C41	2.85	120.06	115.27
17	C	605	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
17	C	607	CLA	CMB-C2B-C3B	2.84	129.99	124.68
17	C	610	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
17	B	613	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
17	B	609	CLA	CMB-C2B-C3B	2.84	129.99	124.68
18	K	101	BCR	C33-C5-C6	-2.84	121.34	124.53
24	E	101	HEM	C4D-ND-C1D	2.83	108.00	105.07
23	D	411	PHO	O2D-CGD-O1D	-2.83	118.30	123.84
18	K	101	BCR	C33-C5-C4	2.83	119.05	113.62
18	B	617	BCR	C7-C8-C9	-2.83	121.96	126.23
23	D	411	PHO	O1D-CGD-CBD	2.82	129.44	124.74
17	B	603	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
17	B	616	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
18	B	617	BCR	C38-C26-C27	2.81	119.02	113.62
17	B	602	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
17	B	610	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
17	C	609	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
17	C	607	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
18	H	101	BCR	C2-C1-C6	2.80	114.80	110.48
17	D	403	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
18	A	405	BCR	C28-C27-C26	-2.80	109.08	114.08
17	C	608	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
17	D	410	CLA	CMB-C2B-C3B	2.80	129.91	124.68
17	B	607	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
18	C	616	BCR	C36-C18-C19	2.80	122.48	118.08
17	B	605	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
17	C	609	CLA	C1B-CHB-C4A	-2.80	124.58	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	602	CLA	CMB-C2B-C3B	2.79	129.90	124.68
17	C	604	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	C	615	BCR	C20-C21-C22	-2.79	123.33	127.31
17	C	605	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
17	B	607	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
17	B	614	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
17	C	611	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
17	B	615	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
22	D	405	PL9	C22-C23-C24	-2.77	120.99	127.66
17	D	402	CLA	O2D-CGD-CBD	2.77	116.19	111.27
17	B	604	CLA	CMB-C2B-C3B	2.77	129.86	124.68
17	B	601	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
17	B	616	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
17	B	609	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	D	412	PHO	O2D-CGD-O1D	-2.75	118.45	123.84
17	C	607	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	D	412	PHO	O1D-CGD-CBD	2.75	129.31	124.74
17	B	610	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
17	C	614	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
19	C	621	LMG	O8-C28-C29	2.74	120.51	111.91
20	D	407	LHG	O8-C23-C24	2.74	120.50	111.91
17	C	605	CLA	CMB-C2B-C3B	2.74	129.80	124.68
18	B	619	BCR	C37-C22-C21	-2.73	119.09	122.92
17	B	601	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	C	601	LMG	O8-C28-C29	2.73	120.48	111.91
17	B	616	CLA	CMB-C2B-C3B	2.73	129.78	124.68
18	B	617	BCR	C15-C16-C17	-2.73	117.89	123.47
17	A	402	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
18	H	101	BCR	C1-C6-C5	-2.72	118.79	122.61
18	C	615	BCR	C27-C26-C25	-2.71	118.80	122.73
17	C	609	CLA	CMB-C2B-C3B	2.70	129.74	124.68
18	B	619	BCR	C36-C18-C17	-2.70	119.14	122.92
17	C	602	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
17	C	610	CLA	CMB-C2B-C3B	2.70	129.73	124.68
18	H	101	BCR	C36-C18-C17	-2.70	119.14	122.92
18	D	404	BCR	C16-C15-C14	-2.70	117.95	123.47
17	B	605	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
18	C	615	BCR	C16-C17-C18	-2.70	123.46	127.31
17	C	602	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
17	A	404	CLA	CMB-C2B-C1B	-2.69	124.32	128.46
17	A	404	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
20	B	622	LHG	O8-C23-C24	2.69	120.36	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	405	BCR	C33-C5-C4	2.69	118.79	113.62
17	B	611	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
20	D	409	LHG	C5-O7-C7	-2.69	111.17	117.79
17	C	610	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
17	C	602	CLA	CMB-C2B-C3B	2.68	129.69	124.68
17	B	602	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
17	B	615	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
17	C	606	CLA	CMB-C2B-C3B	2.67	129.68	124.68
18	B	618	BCR	C3-C4-C5	-2.67	109.30	114.08
17	B	603	CLA	CMB-C2B-C3B	2.67	129.68	124.68
18	H	101	BCR	C27-C26-C25	-2.67	118.85	122.73
17	C	612	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
18	C	615	BCR	C15-C16-C17	-2.67	118.00	123.47
17	C	603	CLA	CMB-C2B-C3B	2.67	129.67	124.68
24	E	101	HEM	C4B-CHC-C1C	2.67	126.08	122.56
17	C	614	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
17	B	605	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
18	B	617	BCR	C4-C5-C6	-2.64	118.90	122.73
18	C	616	BCR	C16-C15-C14	-2.64	118.07	123.47
17	C	604	CLA	CMB-C2B-C3B	2.64	129.61	124.68
17	C	611	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
17	B	616	CLA	CHB-C4A-NA	2.63	128.14	124.51
17	C	603	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
18	A	405	BCR	C24-C23-C22	-2.62	122.28	126.23
26	C	617	DGD	O1G-C1A-C2A	2.61	120.11	111.91
17	C	611	CLA	CMB-C2B-C3B	2.61	129.56	124.68
26	C	618	DGD	O1G-C1A-C2A	2.61	120.10	111.91
18	B	618	BCR	C36-C18-C17	-2.61	119.27	122.92
18	C	616	BCR	C11-C10-C9	-2.61	123.59	127.31
17	B	601	CLA	CMB-C2B-C3B	2.60	129.55	124.68
18	B	619	BCR	C38-C26-C25	-2.60	121.61	124.53
17	D	403	CLA	CMB-C2B-C3B	2.59	129.53	124.68
20	B	623	LHG	O8-C23-C24	2.59	120.04	111.91
17	B	615	CLA	CHB-C4A-NA	2.58	128.07	124.51
17	C	610	CLA	CHB-C4A-NA	2.57	128.07	124.51
17	B	612	CLA	CMB-C2B-C3B	2.56	129.47	124.68
23	D	411	PHO	CMB-C2B-C3B	2.56	129.47	124.68
20	B	621	LHG	O8-C23-C24	2.56	119.94	111.91
23	D	411	PHO	C1-C2-C3	-2.55	121.63	126.04
17	C	613	CLA	CHB-C4A-NA	2.55	128.03	124.51
18	B	618	BCR	C11-C10-C9	-2.54	123.68	127.31
20	L	101	LHG	O8-C23-C24	2.54	119.88	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	E	101	HEM	C3B-C2B-C1B	2.51	108.35	106.49
17	B	607	CLA	CMB-C2B-C3B	2.51	129.37	124.68
17	B	613	CLA	CMB-C2B-C3B	2.50	129.35	124.68
17	C	612	CLA	CMB-C2B-C3B	2.50	129.35	124.68
17	C	608	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
17	C	604	CLA	CHB-C4A-NA	2.50	127.97	124.51
17	D	402	CLA	CHD-C1D-ND	-2.50	122.16	124.45
22	D	405	PL9	C7-C8-C9	-2.49	122.64	126.79
17	B	613	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
18	H	101	BCR	C37-C22-C21	-2.48	119.44	122.92
18	A	405	BCR	C33-C5-C6	-2.48	121.74	124.53
17	B	606	CLA	CHB-C4A-NA	2.47	127.93	124.51
17	C	612	CLA	CHD-C1D-ND	-2.47	122.19	124.45
18	K	101	BCR	C16-C15-C14	-2.46	118.43	123.47
17	B	612	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
26	C	617	DGD	O6D-C5D-C6D	2.45	111.60	106.67
19	B	620	LMG	O8-C28-C29	2.45	119.58	111.91
17	B	613	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
18	B	619	BCR	C3-C4-C5	-2.43	109.74	114.08
17	C	608	CLA	CMB-C2B-C3B	2.43	129.22	124.68
17	C	611	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	H	101	BCR	C38-C26-C25	-2.42	121.81	124.53
18	Z	101	BCR	C7-C8-C9	-2.42	122.58	126.23
18	D	404	BCR	C38-C26-C25	-2.41	121.82	124.53
18	Z	101	BCR	C29-C30-C25	2.41	114.19	110.48
18	D	404	BCR	C36-C18-C17	-2.41	119.55	122.92
18	B	618	BCR	C15-C16-C17	-2.41	118.55	123.47
18	K	101	BCR	C37-C22-C21	-2.41	119.55	122.92
18	D	404	BCR	C7-C8-C9	-2.40	122.61	126.23
18	Z	101	BCR	C8-C7-C6	-2.40	120.46	127.20
18	B	619	BCR	C4-C5-C6	-2.39	119.26	122.73
17	B	612	CLA	CHB-C4A-NA	2.39	127.81	124.51
17	D	403	CLA	C1-C2-C3	-2.38	121.93	126.04
17	A	402	CLA	CHD-C1D-ND	-2.38	122.27	124.45
17	A	404	CLA	CMB-C2B-C3B	2.38	129.12	124.68
20	D	406	LHG	O8-C23-C24	2.38	119.36	111.91
17	B	613	CLA	CHB-C4A-NA	2.37	127.79	124.51
17	B	605	CLA	CMB-C2B-C3B	2.37	129.11	124.68
17	B	604	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	D	405	PL9	C20-C19-C21	2.36	119.25	115.27
17	B	609	CLA	CHB-C4A-NA	2.36	127.78	124.51
17	B	602	CLA	CHD-C1D-ND	-2.36	122.28	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	615	CLA	CMB-C2B-C3B	2.36	129.09	124.68
27	C	620	SQD	O9-S-C6	2.36	109.74	106.94
17	B	607	CLA	CHB-C4A-NA	2.35	127.76	124.51
18	K	101	BCR	C7-C8-C9	-2.35	122.68	126.23
17	B	610	CLA	CHB-C4A-NA	2.35	127.76	124.51
18	B	618	BCR	C15-C14-C13	-2.35	123.95	127.31
19	D	408	LMG	O8-C28-C29	2.35	119.28	111.91
18	B	617	BCR	C15-C14-C13	-2.35	123.96	127.31
17	B	607	CLA	CHD-C1D-ND	-2.34	122.30	124.45
17	B	610	CLA	CHD-C1D-ND	-2.34	122.30	124.45
17	C	609	CLA	CHD-C1D-ND	-2.34	122.30	124.45
18	K	101	BCR	C34-C9-C8	2.34	121.77	118.08
20	D	409	LHG	O8-C23-C24	2.34	119.25	111.91
17	C	605	CLA	CHD-C1D-ND	-2.34	122.30	124.45
18	K	101	BCR	C30-C25-C24	2.34	122.40	115.78
19	K	102	LMG	O8-C28-C29	2.34	119.24	111.91
18	H	101	BCR	C16-C15-C14	-2.33	118.69	123.47
17	B	605	CLA	CHD-C1D-ND	-2.33	122.31	124.45
17	C	611	CLA	C1-C2-C3	-2.33	122.01	126.04
18	A	405	BCR	C15-C16-C17	-2.32	118.71	123.47
18	A	405	BCR	C36-C18-C17	-2.32	119.67	122.92
24	E	101	HEM	C4C-CHD-C1D	2.32	125.62	122.56
18	D	404	BCR	C37-C22-C21	-2.32	119.67	122.92
17	A	402	CLA	CHB-C4A-NA	2.32	127.72	124.51
18	A	405	BCR	C4-C5-C6	-2.32	119.36	122.73
17	C	608	CLA	CHB-C4A-NA	2.32	127.72	124.51
18	C	615	BCR	C7-C6-C5	-2.32	115.85	121.46
17	C	602	CLA	CHD-C1D-ND	-2.31	122.33	124.45
17	B	611	CLA	CHD-C1D-ND	-2.31	122.33	124.45
17	C	608	CLA	CHD-C1D-ND	-2.31	122.33	124.45
17	C	614	CLA	CHD-C1D-ND	-2.31	122.33	124.45
18	H	101	BCR	C24-C23-C22	-2.31	122.74	126.23
18	Z	101	BCR	C15-C14-C13	-2.31	124.01	127.31
17	D	403	CLA	CHB-C4A-NA	2.31	127.71	124.51
17	B	603	CLA	CHB-C4A-NA	2.30	127.69	124.51
17	B	614	CLA	CHB-C4A-NA	2.30	127.69	124.51
17	C	612	CLA	CHB-C4A-NA	2.30	127.69	124.51
17	C	606	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
17	B	601	CLA	CHD-C1D-ND	-2.29	122.34	124.45
18	K	101	BCR	C36-C18-C17	-2.29	119.71	122.92
18	A	405	BCR	C15-C14-C13	-2.29	124.04	127.31
18	C	615	BCR	C15-C14-C13	-2.29	124.05	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	C	603	CLA	CHB-C4A-NA	2.28	127.67	124.51
17	C	603	CLA	CHD-C1D-ND	-2.27	122.36	124.45
18	H	101	BCR	C31-C1-C6	-2.27	106.61	110.30
17	B	605	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
18	Z	101	BCR	C37-C22-C21	-2.27	119.74	122.92
17	C	602	CLA	CHB-C4A-NA	2.27	127.65	124.51
17	B	609	CLA	CHD-C1D-ND	-2.26	122.37	124.45
17	C	609	CLA	CHB-C4A-NA	2.26	127.64	124.51
17	C	611	CLA	CHD-C1D-ND	-2.25	122.38	124.45
17	D	410	CLA	CHD-C1D-ND	-2.25	122.39	124.45
17	B	605	CLA	CHB-C4A-NA	2.25	127.62	124.51
17	C	613	CLA	CHD-C1D-ND	-2.24	122.39	124.45
18	K	101	BCR	C4-C5-C6	-2.24	119.47	122.73
18	B	619	BCR	C30-C25-C24	2.24	122.13	115.78
17	B	604	CLA	CHD-C1D-ND	-2.24	122.39	124.45
17	B	611	CLA	CHB-C4A-NA	2.24	127.61	124.51
17	A	403	CLA	CHD-C1D-ND	-2.23	122.40	124.45
17	C	604	CLA	CHD-C1D-ND	-2.22	122.41	124.45
17	C	607	CLA	CHB-C4A-NA	2.21	127.57	124.51
17	A	404	CLA	CHB-C4A-NA	2.21	127.57	124.51
27	C	620	SQD	O8-S-C6	2.21	109.26	105.74
17	B	616	CLA	CHD-C1D-ND	-2.21	122.42	124.45
18	Z	101	BCR	C1-C6-C7	2.21	122.03	115.78
20	K	103	LHG	O8-C23-C24	2.20	118.82	111.91
26	C	619	DGD	O1G-C1A-C2A	2.20	118.80	111.91
17	C	609	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
20	D	407	LHG	C5-O7-C7	-2.19	112.39	117.79
17	B	601	CLA	CHB-C4A-NA	2.19	127.54	124.51
17	C	614	CLA	CHB-C4A-NA	2.18	127.53	124.51
18	B	617	BCR	C28-C27-C26	-2.18	110.18	114.08
22	D	405	PL9	O2-C1-C6	2.18	124.37	120.59
27	C	620	SQD	O7-S-C6	2.18	109.53	106.94
17	B	615	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
18	C	616	BCR	C4-C5-C6	-2.18	119.57	122.73
23	D	412	PHO	CMB-C2B-C3B	2.17	128.75	124.68
17	B	613	CLA	CHD-C1D-ND	-2.17	122.46	124.45
17	B	602	CLA	CHB-C4A-NA	2.17	127.52	124.51
17	C	606	CLA	CHB-C4A-NA	2.17	127.52	124.51
22	D	405	PL9	O1-C4-C3	-2.17	118.33	120.72
17	C	604	CLA	C4-C3-C5	2.17	118.92	115.27
17	C	605	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	D	412	PHO	CMC-C2C-C3C	2.17	129.03	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	C	616	BCR	C27-C26-C25	-2.17	119.58	122.73
17	B	611	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
19	H	102	LMG	O8-C28-C29	2.16	118.70	111.91
17	B	608	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	D	410	CLA	CHB-C4A-NA	2.16	127.50	124.51
18	B	618	BCR	C4-C5-C6	-2.16	119.59	122.73
17	C	606	CLA	CHD-C1D-ND	-2.16	122.47	124.45
17	A	403	CLA	CHB-C4A-NA	2.16	127.49	124.51
17	C	604	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
17	B	608	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
17	D	403	CLA	CHD-C1D-ND	-2.15	122.48	124.45
23	D	411	PHO	O2A-CGA-O1A	-2.15	118.16	123.59
17	B	606	CLA	CHD-C1D-ND	-2.15	122.48	124.45
17	C	607	CLA	CHD-C1D-ND	-2.15	122.48	124.45
17	A	404	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	A	405	BCR	C37-C22-C21	-2.15	119.92	122.92
18	D	404	BCR	C12-C13-C14	-2.14	115.66	118.94
18	Z	101	BCR	C4-C5-C6	-2.14	119.62	122.73
22	D	405	PL9	C32-C33-C34	-2.14	122.51	127.66
17	B	603	CLA	CHD-C1D-ND	-2.14	122.49	124.45
18	D	404	BCR	C8-C9-C10	-2.13	115.67	118.94
18	B	619	BCR	C11-C10-C9	-2.13	124.27	127.31
18	C	615	BCR	C23-C24-C25	-2.13	121.21	127.20
18	B	617	BCR	C27-C26-C25	-2.13	119.64	122.73
17	C	610	CLA	CHD-C1D-ND	-2.13	122.50	124.45
22	D	405	PL9	O2-C1-C2	-2.12	116.91	121.78
18	D	404	BCR	C33-C5-C6	-2.12	122.15	124.53
18	Z	101	BCR	C36-C18-C17	-2.12	119.96	122.92
17	C	612	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
27	C	620	SQD	C45-O47-C7	-2.11	112.58	117.79
22	D	405	PL9	C12-C13-C14	-2.11	122.57	127.66
18	Z	101	BCR	C24-C25-C26	2.11	126.58	121.46
18	B	617	BCR	C24-C23-C22	-2.11	123.05	126.23
18	B	617	BCR	C36-C18-C17	-2.10	119.98	122.92
18	C	616	BCR	C37-C22-C21	-2.10	119.98	122.92
18	K	101	BCR	C38-C26-C25	-2.09	122.18	124.53
18	Z	101	BCR	C15-C16-C17	-2.09	119.19	123.47
17	C	614	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
17	C	607	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
19	C	621	LMG	C8-O7-C10	-2.08	112.68	117.79
18	B	618	BCR	C38-C26-C27	2.08	117.60	113.62
18	Z	101	BCR	C11-C10-C9	-2.07	124.35	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	X	201	VTQ	C8-C2-C3	-2.07	121.02	124.40
17	B	608	CLA	CHD-C1D-ND	-2.07	122.55	124.45
17	B	601	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
17	B	616	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
17	B	612	CLA	CHD-C1D-ND	-2.07	122.56	124.45
17	D	410	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
17	B	604	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
18	B	618	BCR	C27-C26-C25	-2.05	119.75	122.73
21	D	401	BCT	O3-C-O1	-2.05	114.22	119.55
18	B	619	BCR	C15-C14-C13	-2.05	124.38	127.31
17	C	605	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
18	C	615	BCR	C11-C10-C9	-2.05	124.39	127.31
18	B	618	BCR	C24-C23-C22	-2.05	123.14	126.23
17	D	410	CLA	O2D-CGD-CBD	2.04	114.90	111.27
18	Z	101	BCR	C29-C28-C27	-2.04	106.81	111.38
17	B	603	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
17	A	404	CLA	C1-C2-C3	-2.04	122.52	126.04
18	Z	101	BCR	C24-C23-C22	-2.04	123.16	126.23
18	D	404	BCR	C10-C11-C12	-2.04	116.86	123.22
18	D	404	BCR	C1-C6-C7	2.03	121.53	115.78
17	B	615	CLA	CHD-C1D-ND	-2.03	122.59	124.45
17	B	613	CLA	C1-C2-C3	-2.03	122.54	126.04
22	D	405	PL9	C27-C28-C29	-2.02	122.79	127.66
18	C	615	BCR	C2-C1-C6	2.02	113.59	110.48
17	B	614	CLA	CHD-C1D-ND	-2.02	122.60	124.45
17	B	602	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
17	B	609	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
17	A	403	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
17	B	610	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
18	B	617	BCR	C11-C10-C9	-2.01	124.45	127.31
22	D	405	PL9	C31-C32-C33	-2.01	105.29	111.88

All (35) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	B	601	CLA	ND
17	B	602	CLA	ND
17	B	603	CLA	ND
17	B	604	CLA	ND
17	B	605	CLA	ND
17	B	606	CLA	ND
17	B	607	CLA	ND

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Mol	Chain	Res	Type	Atom
17	B	608	CLA	ND
17	B	609	CLA	ND
17	B	610	CLA	ND
17	B	611	CLA	ND
17	B	612	CLA	ND
17	B	613	CLA	ND
17	B	614	CLA	ND
17	B	615	CLA	ND
17	B	616	CLA	ND
17	D	402	CLA	ND
17	D	403	CLA	ND
17	D	410	CLA	ND
17	C	602	CLA	ND
17	C	603	CLA	ND
17	C	604	CLA	ND
17	C	605	CLA	ND
17	C	606	CLA	ND
17	C	607	CLA	ND
17	C	608	CLA	ND
17	C	609	CLA	ND
17	C	610	CLA	ND
17	C	611	CLA	ND
17	C	612	CLA	ND
17	C	613	CLA	ND
17	C	614	CLA	ND
17	A	402	CLA	ND
17	A	403	CLA	ND
17	A	404	CLA	ND

All (694) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	B	601	CLA	CHA-CBD-CGD-O1D
17	B	601	CLA	CHA-CBD-CGD-O2D
17	B	603	CLA	C1A-C2A-CAA-CBA
17	B	603	CLA	C3A-C2A-CAA-CBA
17	B	603	CLA	CHA-CBD-CGD-O1D
17	B	603	CLA	CHA-CBD-CGD-O2D
17	B	603	CLA	CAD-CBD-CGD-O1D
17	B	604	CLA	C1A-C2A-CAA-CBA
17	B	604	CLA	CHA-CBD-CGD-O1D
17	B	604	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	B	605	CLA	C1A-C2A-CAA-CBA
17	B	606	CLA	CAD-CBD-CGD-O1D
17	B	606	CLA	CAD-CBD-CGD-O2D
17	B	606	CLA	CBD-CGD-O2D-CED
17	B	607	CLA	C1A-C2A-CAA-CBA
17	B	607	CLA	C3A-C2A-CAA-CBA
17	B	608	CLA	C1A-C2A-CAA-CBA
17	B	608	CLA	CHA-CBD-CGD-O1D
17	B	608	CLA	CHA-CBD-CGD-O2D
17	B	608	CLA	CAD-CBD-CGD-O1D
17	B	609	CLA	CHA-CBD-CGD-O1D
17	B	609	CLA	CHA-CBD-CGD-O2D
17	B	609	CLA	CAD-CBD-CGD-O1D
17	B	609	CLA	CAD-CBD-CGD-O2D
17	B	611	CLA	CHA-CBD-CGD-O1D
17	B	611	CLA	CHA-CBD-CGD-O2D
17	B	611	CLA	CBD-CGD-O2D-CED
17	B	614	CLA	CHA-CBD-CGD-O1D
17	B	614	CLA	CHA-CBD-CGD-O2D
17	B	614	CLA	CAD-CBD-CGD-O1D
17	B	614	CLA	CAD-CBD-CGD-O2D
17	B	615	CLA	O2A-C1-C2-C3
17	D	402	CLA	CAD-CBD-CGD-O1D
17	D	402	CLA	CAD-CBD-CGD-O2D
17	D	403	CLA	C1A-C2A-CAA-CBA
17	D	403	CLA	C3A-C2A-CAA-CBA
17	D	403	CLA	CHA-CBD-CGD-O1D
17	D	403	CLA	CHA-CBD-CGD-O2D
17	D	403	CLA	CAD-CBD-CGD-O1D
17	D	403	CLA	CAD-CBD-CGD-O2D
17	C	602	CLA	CHA-CBD-CGD-O1D
17	C	602	CLA	CHA-CBD-CGD-O2D
17	C	602	CLA	CAD-CBD-CGD-O1D
17	C	603	CLA	CBD-CGD-O2D-CED
17	C	604	CLA	C1A-C2A-CAA-CBA
17	C	604	CLA	CHA-CBD-CGD-O1D
17	C	604	CLA	CHA-CBD-CGD-O2D
17	C	604	CLA	CAD-CBD-CGD-O1D
17	C	604	CLA	C2-C3-C5-C6
17	C	604	CLA	C4-C3-C5-C6
17	C	606	CLA	C1A-C2A-CAA-CBA
17	C	607	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	C	607	CLA	CHA-CBD-CGD-O2D
17	C	607	CLA	CAD-CBD-CGD-O1D
17	C	607	CLA	CBD-CGD-O2D-CED
17	C	608	CLA	C1A-C2A-CAA-CBA
17	C	608	CLA	C3A-C2A-CAA-CBA
17	C	612	CLA	CHA-CBD-CGD-O1D
17	C	612	CLA	CHA-CBD-CGD-O2D
17	C	612	CLA	CAD-CBD-CGD-O1D
17	C	612	CLA	CAD-CBD-CGD-O2D
17	C	613	CLA	CHA-CBD-CGD-O1D
17	C	613	CLA	CHA-CBD-CGD-O2D
17	C	614	CLA	CBD-CGD-O2D-CED
17	A	404	CLA	CHA-CBD-CGD-O2D
18	B	617	BCR	C1-C6-C7-C8
18	B	617	BCR	C5-C6-C7-C8
18	B	617	BCR	C23-C24-C25-C26
18	B	617	BCR	C23-C24-C25-C30
18	B	618	BCR	C1-C6-C7-C8
18	B	618	BCR	C5-C6-C7-C8
18	B	618	BCR	C23-C24-C25-C26
18	B	619	BCR	C1-C6-C7-C8
18	B	619	BCR	C5-C6-C7-C8
18	B	619	BCR	C23-C24-C25-C26
18	D	404	BCR	C1-C6-C7-C8
18	D	404	BCR	C5-C6-C7-C8
18	D	404	BCR	C23-C24-C25-C26
18	D	404	BCR	C23-C24-C25-C30
18	H	101	BCR	C1-C6-C7-C8
18	H	101	BCR	C5-C6-C7-C8
18	H	101	BCR	C23-C24-C25-C26
18	K	101	BCR	C5-C6-C7-C8
18	K	101	BCR	C23-C24-C25-C26
18	Z	101	BCR	C5-C6-C7-C8
18	Z	101	BCR	C23-C24-C25-C26
18	C	616	BCR	C5-C6-C7-C8
18	A	405	BCR	C5-C6-C7-C8
18	A	405	BCR	C23-C24-C25-C26
18	A	405	BCR	C23-C24-C25-C30
19	C	621	LMG	C2-C1-O1-C7
19	C	621	LMG	O6-C1-O1-C7
20	B	621	LHG	C3-O3-P-O6
20	B	621	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
20	B	622	LHG	C4-O6-P-O3
20	B	623	LHG	C4-O6-P-O3
20	D	406	LHG	C3-O3-P-O6
20	D	406	LHG	C4-O6-P-O4
20	K	103	LHG	C3-O3-P-O5
20	K	103	LHG	C3-O3-P-O6
20	L	101	LHG	C3-O3-P-O5
25	X	201	VTQ	C16-C15-C9-C11
26	C	618	DGD	C4D-C5D-C6D-O5D
17	C	603	CLA	O1D-CGD-O2D-CED
17	B	609	CLA	O1D-CGD-O2D-CED
17	B	601	CLA	CBD-CGD-O2D-CED
17	B	604	CLA	CBD-CGD-O2D-CED
17	B	609	CLA	CBD-CGD-O2D-CED
17	C	604	CLA	CBD-CGD-O2D-CED
17	C	605	CLA	CBD-CGD-O2D-CED
17	A	402	CLA	CBD-CGD-O2D-CED
17	B	607	CLA	O1A-CGA-O2A-C1
17	B	616	CLA	O1A-CGA-O2A-C1
17	B	611	CLA	O1D-CGD-O2D-CED
17	C	604	CLA	O1D-CGD-O2D-CED
17	C	607	CLA	O1D-CGD-O2D-CED
17	B	606	CLA	O1D-CGD-O2D-CED
17	B	616	CLA	CBA-CGA-O2A-C1
23	D	411	PHO	CBA-CGA-O2A-C1
17	C	611	CLA	CBD-CGD-O2D-CED
17	D	410	CLA	O1A-CGA-O2A-C1
17	C	607	CLA	O1A-CGA-O2A-C1
23	D	411	PHO	O1A-CGA-O2A-C1
17	C	614	CLA	O1D-CGD-O2D-CED
17	B	603	CLA	CBD-CGD-O2D-CED
17	A	404	CLA	C3-C5-C6-C7
17	B	605	CLA	CBA-CGA-O2A-C1
17	B	607	CLA	CBA-CGA-O2A-C1
17	D	410	CLA	CBA-CGA-O2A-C1
17	C	606	CLA	CBA-CGA-O2A-C1
17	C	607	CLA	CBA-CGA-O2A-C1
22	D	405	PL9	C47-C48-C49-C51
17	B	606	CLA	O1A-CGA-O2A-C1
17	B	615	CLA	C4-C3-C5-C6
17	C	612	CLA	CBD-CGD-O2D-CED
17	B	611	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
17	B	616	CLA	C2A-CAA-CBA-CGA
17	D	410	CLA	C2A-CAA-CBA-CGA
17	C	603	CLA	C2A-CAA-CBA-CGA
17	C	609	CLA	C2A-CAA-CBA-CGA
17	C	612	CLA	C2A-CAA-CBA-CGA
17	A	402	CLA	O1D-CGD-O2D-CED
17	D	402	CLA	C3-C5-C6-C7
17	C	605	CLA	C3-C5-C6-C7
17	B	606	CLA	CBA-CGA-O2A-C1
17	C	609	CLA	CBA-CGA-O2A-C1
17	C	605	CLA	O1D-CGD-O2D-CED
17	B	605	CLA	O1A-CGA-O2A-C1
17	B	611	CLA	O1A-CGA-O2A-C1
17	C	609	CLA	O1A-CGA-O2A-C1
17	C	612	CLA	O1A-CGA-O2A-C1
17	B	615	CLA	CBD-CGD-O2D-CED
17	D	403	CLA	CBD-CGD-O2D-CED
17	B	604	CLA	O1D-CGD-O2D-CED
17	B	603	CLA	C3-C5-C6-C7
23	D	412	PHO	C3-C5-C6-C7
17	B	601	CLA	CBA-CGA-O2A-C1
17	B	602	CLA	CBA-CGA-O2A-C1
17	C	614	CLA	CBA-CGA-O2A-C1
17	C	606	CLA	O1A-CGA-O2A-C1
20	D	409	LHG	C8-C7-O7-C5
17	C	614	CLA	O1A-CGA-O2A-C1
17	B	611	CLA	CBA-CGA-O2A-C1
17	C	612	CLA	CBA-CGA-O2A-C1
17	B	602	CLA	O1A-CGA-O2A-C1
17	B	605	CLA	C2A-CAA-CBA-CGA
17	B	601	CLA	O1A-CGA-O2A-C1
17	B	601	CLA	O1D-CGD-O2D-CED
26	C	618	DGD	O6D-C5D-C6D-O5D
20	L	101	LHG	C1-C2-C3-O3
20	D	409	LHG	O9-C7-O7-C5
17	C	613	CLA	CBA-CGA-O2A-C1
17	C	612	CLA	C15-C16-C17-C18
20	L	101	LHG	O2-C2-C3-O3
22	D	405	PL9	C47-C48-C49-C50
17	C	613	CLA	O1A-CGA-O2A-C1
17	C	614	CLA	C10-C11-C12-C13
17	C	605	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	B	605	CLA	C13-C15-C16-C17
17	D	402	CLA	C13-C15-C16-C17
17	C	602	CLA	C13-C15-C16-C17
17	B	611	CLA	C5-C6-C7-C8
17	B	612	CLA	C13-C15-C16-C17
17	C	606	CLA	C8-C10-C11-C12
17	C	611	CLA	C10-C11-C12-C13
17	C	611	CLA	O1D-CGD-O2D-CED
17	B	602	CLA	C10-C11-C12-C13
23	D	412	PHO	CBA-CGA-O2A-C1
17	C	613	CLA	C2-C1-O2A-CGA
22	D	405	PL9	C42-C43-C44-C46
17	B	601	CLA	C10-C11-C12-C13
25	X	201	VTQ	C15-C16-C17-C18
17	C	614	CLA	C6-C7-C8-C10
17	C	607	CLA	C2A-CAA-CBA-CGA
17	B	603	CLA	O1D-CGD-O2D-CED
25	X	201	VTQ	C16-C15-C9-C14
17	D	403	CLA	C3-C5-C6-C7
17	C	605	CLA	O1A-CGA-O2A-C1
17	B	604	CLA	C15-C16-C17-C18
17	C	602	CLA	C10-C11-C12-C13
17	C	609	CLA	C8-C10-C11-C12
17	B	601	CLA	C5-C6-C7-C8
17	B	616	CLA	C10-C11-C12-C13
17	D	403	CLA	C15-C16-C17-C18
20	B	621	LHG	C4-O6-P-O3
20	D	406	LHG	C4-O6-P-O3
20	D	407	LHG	C4-O6-P-O3
20	D	409	LHG	C4-O6-P-O3
17	A	403	CLA	CBA-CGA-O2A-C1
23	D	412	PHO	O1A-CGA-O2A-C1
17	B	613	CLA	CBA-CGA-O2A-C1
17	C	602	CLA	CBA-CGA-O2A-C1
17	C	610	CLA	CBA-CGA-O2A-C1
17	A	402	CLA	CBA-CGA-O2A-C1
17	B	607	CLA	CBD-CGD-O2D-CED
19	C	601	LMG	C11-C12-C13-C14
17	C	612	CLA	O1D-CGD-O2D-CED
17	D	402	CLA	C10-C11-C12-C13
20	B	621	LHG	C30-C31-C32-C33
26	C	619	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
17	B	615	CLA	C2-C3-C5-C6
17	B	604	CLA	C11-C12-C13-C14
17	B	607	CLA	C6-C7-C8-C9
17	B	610	CLA	C11-C10-C8-C9
17	C	604	CLA	C6-C7-C8-C9
17	C	606	CLA	C6-C7-C8-C9
17	C	608	CLA	C14-C13-C15-C16
26	C	619	DGD	C3B-C4B-C5B-C6B
26	C	618	DGD	C6B-C7B-C8B-C9B
17	C	609	CLA	C16-C17-C18-C19
17	B	607	CLA	C5-C6-C7-C8
17	D	403	CLA	O1D-CGD-O2D-CED
27	C	620	SQD	C27-C28-C29-C30
17	C	602	CLA	O1A-CGA-O2A-C1
17	B	604	CLA	C3A-C2A-CAA-CBA
17	B	608	CLA	C3A-C2A-CAA-CBA
17	B	609	CLA	C3A-C2A-CAA-CBA
17	D	402	CLA	C3A-C2A-CAA-CBA
17	C	606	CLA	C3A-C2A-CAA-CBA
17	C	609	CLA	C16-C17-C18-C20
17	B	615	CLA	O1D-CGD-O2D-CED
17	B	612	CLA	O2A-C1-C2-C3
17	C	607	CLA	O2A-C1-C2-C3
17	C	611	CLA	C4-C3-C5-C6
17	C	611	CLA	C2-C3-C5-C6
27	C	620	SQD	C8-C7-O47-C45
17	B	613	CLA	O1A-CGA-O2A-C1
17	C	610	CLA	O1A-CGA-O2A-C1
17	A	403	CLA	O1A-CGA-O2A-C1
17	A	402	CLA	O1A-CGA-O2A-C1
17	C	612	CLA	C2-C1-O2A-CGA
18	B	618	BCR	C23-C24-C25-C30
18	B	619	BCR	C23-C24-C25-C30
18	H	101	BCR	C23-C24-C25-C30
18	K	101	BCR	C1-C6-C7-C8
18	K	101	BCR	C23-C24-C25-C30
18	Z	101	BCR	C1-C6-C7-C8
18	Z	101	BCR	C23-C24-C25-C30
18	C	615	BCR	C23-C24-C25-C26
18	C	615	BCR	C23-C24-C25-C30
18	C	616	BCR	C1-C6-C7-C8
18	C	616	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	C	616	BCR	C23-C24-C25-C30
18	A	405	BCR	C1-C6-C7-C8
17	D	403	CLA	CBA-CGA-O2A-C1
20	L	101	LHG	C8-C7-O7-C5
17	C	607	CLA	C4-C3-C5-C6
23	D	411	PHO	C4-C3-C5-C6
17	B	603	CLA	C11-C12-C13-C15
17	B	604	CLA	C11-C12-C13-C15
17	B	607	CLA	C6-C7-C8-C10
17	B	610	CLA	C11-C10-C8-C7
17	C	604	CLA	C6-C7-C8-C10
17	C	606	CLA	C6-C7-C8-C10
17	C	607	CLA	C2-C3-C5-C6
17	C	610	CLA	C12-C13-C15-C16
17	A	402	CLA	C12-C13-C15-C16
22	D	405	PL9	C28-C29-C31-C32
22	D	405	PL9	C43-C44-C46-C47
17	B	608	CLA	C3-C5-C6-C7
17	B	616	CLA	C13-C15-C16-C17
17	D	403	CLA	C10-C11-C12-C13
17	B	610	CLA	C15-C16-C17-C18
26	C	617	DGD	C4B-C5B-C6B-C7B
19	K	102	LMG	C15-C16-C17-C18
17	D	403	CLA	O1A-CGA-O2A-C1
17	B	604	CLA	CBA-CGA-O2A-C1
17	C	614	CLA	C16-C17-C18-C20
20	B	623	LHG	C11-C12-C13-C14
20	D	407	LHG	O6-C4-C5-O7
17	D	402	CLA	CBD-CGD-O2D-CED
17	C	606	CLA	CBD-CGD-O2D-CED
27	C	620	SQD	O49-C7-O47-C45
17	B	602	CLA	C3-C5-C6-C7
27	C	620	SQD	O6-C44-C45-O47
19	B	620	LMG	O6-C5-C6-O5
23	D	411	PHO	C2-C3-C5-C6
17	B	603	CLA	C11-C12-C13-C14
17	C	610	CLA	C14-C13-C15-C16
17	C	611	CLA	C6-C7-C8-C9
17	C	614	CLA	C6-C7-C8-C9
20	D	409	LHG	C26-C27-C28-C29
17	B	609	CLA	C1A-C2A-CAA-CBA
17	B	614	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
17	C	602	CLA	C1A-C2A-CAA-CBA
17	C	607	CLA	C1A-C2A-CAA-CBA
17	C	614	CLA	C16-C17-C18-C19
20	L	101	LHG	O9-C7-O7-C5
19	C	621	LMG	C11-C10-O7-C8
20	B	623	LHG	C8-C7-O7-C5
20	D	407	LHG	C3-O3-P-O6
17	C	614	CLA	C3-C5-C6-C7
20	B	621	LHG	C11-C12-C13-C14
17	C	610	CLA	C5-C6-C7-C8
20	D	407	LHG	O6-C4-C5-C6
17	B	604	CLA	C8-C10-C11-C12
17	C	604	CLA	C8-C10-C11-C12
19	K	102	LMG	O6-C5-C6-O5
17	B	602	CLA	C5-C6-C7-C8
17	B	609	CLA	C16-C17-C18-C20
19	H	102	LMG	C38-C39-C40-C41
17	B	609	CLA	C8-C10-C11-C12
17	C	608	CLA	C8-C10-C11-C12
20	B	621	LHG	C11-C10-C9-C8
23	D	411	PHO	C3-C5-C6-C7
19	H	102	LMG	C11-C10-O7-C8
19	D	408	LMG	O6-C5-C6-O5
22	D	405	PL9	C45-C44-C46-C47
19	D	408	LMG	C14-C15-C16-C17
17	B	613	CLA	C2-C1-O2A-CGA
17	C	609	CLA	C2-C1-O2A-CGA
26	C	617	DGD	O6E-C5E-C6E-O5E
19	C	621	LMG	O9-C10-O7-C8
17	B	604	CLA	O1A-CGA-O2A-C1
23	D	412	PHO	CHA-CBD-CGD-O1D
23	D	412	PHO	CHA-CBD-CGD-O2D
17	B	601	CLA	C11-C10-C8-C7
17	B	605	CLA	C11-C12-C13-C15
17	B	608	CLA	C11-C12-C13-C15
17	B	610	CLA	C12-C13-C15-C16
17	B	612	CLA	C11-C10-C8-C7
17	D	402	CLA	C6-C7-C8-C10
17	C	602	CLA	C11-C12-C13-C15
17	C	603	CLA	C12-C13-C15-C16
17	C	611	CLA	C6-C7-C8-C10
17	C	614	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	X	201	VTQ	C16-C17-C18-C20
19	H	102	LMG	C35-C36-C37-C38
17	B	601	CLA	C11-C10-C8-C9
17	B	605	CLA	C11-C12-C13-C14
17	B	608	CLA	C11-C12-C13-C14
17	B	612	CLA	C11-C10-C8-C9
17	B	616	CLA	C11-C10-C8-C9
17	C	603	CLA	C14-C13-C15-C16
17	A	402	CLA	C14-C13-C15-C16
25	X	201	VTQ	C21-C22-C23-C1
20	D	409	LHG	C23-C24-C25-C26
17	B	606	CLA	C5-C6-C7-C8
20	D	406	LHG	C9-C10-C11-C12
20	B	623	LHG	O9-C7-O7-C5
17	C	607	CLA	C5-C6-C7-C8
26	C	618	DGD	C2A-C1A-O1G-C1G
17	B	607	CLA	O1D-CGD-O2D-CED
17	C	606	CLA	C4-C3-C5-C6
17	B	605	CLA	C3A-C2A-CAA-CBA
17	B	610	CLA	C3A-C2A-CAA-CBA
17	C	610	CLA	C3A-C2A-CAA-CBA
20	L	101	LHG	C14-C15-C16-C17
17	B	613	CLA	C10-C11-C12-C13
17	C	611	CLA	C8-C10-C11-C12
27	C	620	SQD	O6-C44-C45-C46
19	D	408	LMG	C10-C11-C12-C13
17	B	609	CLA	C16-C17-C18-C19
20	B	623	LHG	C25-C26-C27-C28
17	B	604	CLA	C2A-CAA-CBA-CGA
17	C	604	CLA	CBA-CGA-O2A-C1
20	D	409	LHG	C11-C12-C13-C14
19	C	621	LMG	C34-C35-C36-C37
19	H	102	LMG	O7-C8-C9-O8
19	H	102	LMG	O9-C10-O7-C8
17	C	606	CLA	C2-C3-C5-C6
17	B	610	CLA	C14-C13-C15-C16
17	D	403	CLA	C11-C10-C8-C9
23	D	411	PHO	C15-C16-C17-C18
20	D	406	LHG	C11-C10-C9-C8
17	C	614	CLA	C5-C6-C7-C8
17	B	616	CLA	C11-C10-C8-C7
17	D	403	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
17	C	605	CLA	C11-C10-C8-C7
17	C	608	CLA	C11-C12-C13-C15
17	C	609	CLA	C12-C13-C15-C16
17	C	614	CLA	C12-C13-C15-C16
23	D	411	PHO	C11-C12-C13-C15
17	C	609	CLA	C5-C6-C7-C8
20	B	622	LHG	C31-C32-C33-C34
17	C	605	CLA	C15-C16-C17-C18
17	B	610	CLA	CBA-CGA-O2A-C1
17	C	603	CLA	CBA-CGA-O2A-C1
19	B	620	LMG	C11-C12-C13-C14
17	B	602	CLA	CAD-CBD-CGD-O2D
17	B	612	CLA	CAD-CBD-CGD-O2D
17	B	615	CLA	CAD-CBD-CGD-O2D
17	D	410	CLA	CAD-CBD-CGD-O2D
17	C	607	CLA	CAD-CBD-CGD-O2D
17	C	607	CLA	C15-C16-C17-C18
19	H	102	LMG	C7-C8-C9-O8
20	B	623	LHG	O6-C4-C5-O7
24	E	101	HEM	C4B-C3B-CAB-CBB
17	B	613	CLA	C16-C17-C18-C20
17	B	605	CLA	CHA-CBD-CGD-O1D
17	B	605	CLA	CHA-CBD-CGD-O2D
17	B	607	CLA	CHA-CBD-CGD-O1D
17	B	607	CLA	CHA-CBD-CGD-O2D
17	D	402	CLA	CHA-CBD-CGD-O1D
17	C	610	CLA	CHA-CBD-CGD-O1D
17	C	610	CLA	CHA-CBD-CGD-O2D
17	A	404	CLA	CHA-CBD-CGD-O1D
17	C	612	CLA	C3-C5-C6-C7
17	B	605	CLA	CBD-CGD-O2D-CED
17	C	602	CLA	CBD-CGD-O2D-CED
26	C	618	DGD	O1A-C1A-O1G-C1G
17	C	606	CLA	O1D-CGD-O2D-CED
17	C	604	CLA	O1A-CGA-O2A-C1
17	C	605	CLA	C11-C10-C8-C9
23	D	412	PHO	C11-C10-C8-C9
23	D	412	PHO	C14-C13-C15-C16
17	B	613	CLA	C3-C5-C6-C7
17	B	610	CLA	O1A-CGA-O2A-C1
17	C	603	CLA	O1A-CGA-O2A-C1
20	D	406	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
17	B	610	CLA	C1A-C2A-CAA-CBA
17	D	402	CLA	C1A-C2A-CAA-CBA
20	D	409	LHG	C3-O3-P-O6
20	K	103	LHG	C4-O6-P-O3
20	B	621	LHG	C3-O3-P-O4
20	B	622	LHG	C4-O6-P-O4
20	B	623	LHG	C4-O6-P-O4
20	D	406	LHG	C3-O3-P-O4
20	D	407	LHG	C4-O6-P-O4
20	D	409	LHG	C4-O6-P-O5
20	B	622	LHG	O6-C4-C5-C6
20	B	623	LHG	O6-C4-C5-C6
22	D	405	PL9	C34-C36-C37-C38
17	D	402	CLA	O1D-CGD-O2D-CED
20	B	623	LHG	C31-C32-C33-C34
27	C	620	SQD	C33-C34-C35-C36
20	L	101	LHG	C11-C12-C13-C14
19	D	408	LMG	C33-C34-C35-C36
17	B	601	CLA	CAD-CBD-CGD-O1D
17	B	604	CLA	CAD-CBD-CGD-O1D
17	B	605	CLA	CAD-CBD-CGD-O1D
17	B	607	CLA	CAD-CBD-CGD-O1D
17	B	611	CLA	CAD-CBD-CGD-O1D
19	K	102	LMG	C17-C18-C19-C20
19	C	601	LMG	C28-C29-C30-C31
17	B	609	CLA	CBA-CGA-O2A-C1
22	D	405	PL9	C30-C29-C31-C32
17	B	606	CLA	C3A-C2A-CAA-CBA
17	B	607	CLA	C11-C12-C13-C15
17	B	611	CLA	C6-C7-C8-C10
17	B	612	CLA	C6-C7-C8-C10
17	B	616	CLA	C11-C12-C13-C15
17	D	402	CLA	C11-C12-C13-C15
17	C	604	CLA	C3A-C2A-CAA-CBA
17	C	604	CLA	C11-C10-C8-C7
17	C	606	CLA	C12-C13-C15-C16
17	C	607	CLA	C3A-C2A-CAA-CBA
17	C	609	CLA	C6-C7-C8-C10
17	C	610	CLA	C6-C7-C8-C10
17	A	404	CLA	C11-C10-C8-C7
20	B	622	LHG	O6-C4-C5-O7
23	D	412	PHO	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
17	B	609	CLA	O1A-CGA-O2A-C1
17	A	404	CLA	C11-C12-C13-C15
19	C	601	LMG	O7-C8-C9-O8
26	C	618	DGD	O1G-C1G-C2G-O2G
27	C	620	SQD	C25-C26-C27-C28
17	C	613	CLA	C4-C3-C5-C6
17	B	612	CLA	C14-C13-C15-C16
17	D	402	CLA	C6-C7-C8-C9
17	C	602	CLA	C14-C13-C15-C16
17	C	609	CLA	C14-C13-C15-C16
17	C	613	CLA	C14-C13-C15-C16
17	C	614	CLA	C14-C13-C15-C16
23	D	411	PHO	C11-C12-C13-C14
25	X	201	VTQ	C16-C17-C18-C19
17	B	613	CLA	C16-C17-C18-C19
20	D	409	LHG	C10-C11-C12-C13
17	C	602	CLA	O1D-CGD-O2D-CED
17	C	607	CLA	C13-C15-C16-C17
20	D	407	LHG	C33-C34-C35-C36
20	B	622	LHG	C30-C31-C32-C33
27	C	620	SQD	C9-C10-C11-C12
17	B	605	CLA	O1D-CGD-O2D-CED
17	C	603	CLA	C3-C5-C6-C7
20	D	407	LHG	O9-C7-O7-C5
17	B	611	CLA	C16-C17-C18-C19
17	D	410	CLA	C13-C15-C16-C17
20	B	622	LHG	C3-O3-P-O6
20	B	623	LHG	C3-O3-P-O6
20	L	101	LHG	C3-O3-P-O6
20	L	101	LHG	C4-O6-P-O3
20	B	621	LHG	C23-C24-C25-C26
23	D	412	PHO	C11-C12-C13-C15
25	X	201	VTQ	C21-C22-C23-C24
17	B	607	CLA	C11-C12-C13-C14
17	B	611	CLA	C6-C7-C8-C9
17	C	602	CLA	C11-C12-C13-C14
17	C	604	CLA	C11-C10-C8-C9
17	C	606	CLA	C14-C13-C15-C16
17	C	609	CLA	C6-C7-C8-C9
17	C	610	CLA	C6-C7-C8-C9
17	C	614	CLA	C11-C10-C8-C9
17	A	404	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
17	D	402	CLA	C16-C17-C18-C19
17	C	606	CLA	C16-C17-C18-C20
19	C	601	LMG	C12-C13-C14-C15
17	A	403	CLA	O2A-C1-C2-C3
17	B	613	CLA	CBD-CGD-O2D-CED
17	A	402	CLA	C4C-C3C-CAC-CBC
26	C	619	DGD	O6D-C5D-C6D-O5D
20	D	407	LHG	C24-C25-C26-C27
23	D	411	PHO	C5-C6-C7-C8
19	C	621	LMG	C33-C34-C35-C36
17	B	613	CLA	O1D-CGD-O2D-CED
17	B	607	CLA	C3-C5-C6-C7
17	C	613	CLA	C16-C17-C18-C19
17	B	605	CLA	C6-C7-C8-C9
17	C	603	CLA	C11-C10-C8-C9
17	B	611	CLA	C16-C17-C18-C20
19	C	621	LMG	C16-C17-C18-C19
20	D	409	LHG	C30-C31-C32-C33
19	C	601	LMG	C7-C8-C9-O8
20	K	103	LHG	C24-C25-C26-C27
17	D	402	CLA	C16-C17-C18-C20
17	C	606	CLA	C16-C17-C18-C19
17	A	402	CLA	O2A-C1-C2-C3
17	B	606	CLA	C1A-C2A-CAA-CBA
17	C	610	CLA	C1A-C2A-CAA-CBA
17	B	613	CLA	C6-C7-C8-C10
17	D	403	CLA	C5-C6-C7-C8
20	D	407	LHG	C11-C10-C9-C8
17	B	602	CLA	C2A-CAA-CBA-CGA
17	C	603	CLA	C13-C15-C16-C17
19	H	102	LMG	C33-C34-C35-C36
20	D	407	LHG	C8-C7-O7-C5
17	C	613	CLA	C2-C3-C5-C6
17	B	603	CLA	C13-C15-C16-C17
17	C	607	CLA	C3-C5-C6-C7
17	C	607	CLA	C16-C17-C18-C20
19	B	620	LMG	C10-C11-C12-C13
17	D	403	CLA	C2-C1-O2A-CGA
20	D	407	LHG	C32-C33-C34-C35
17	B	608	CLA	C14-C13-C15-C16
17	C	607	CLA	C8-C10-C11-C12
17	B	601	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
19	C	621	LMG	C15-C16-C17-C18
17	D	403	CLA	C4-C3-C5-C6
19	K	102	LMG	O9-C10-O7-C8
19	K	102	LMG	C14-C15-C16-C17
17	C	613	CLA	C12-C13-C15-C16
23	D	411	PHO	C6-C7-C8-C10
17	B	607	CLA	C16-C17-C18-C19
26	C	617	DGD	O6D-C5D-C6D-O5D
20	L	101	LHG	O7-C5-C6-O8
27	C	620	SQD	O47-C45-C46-O48
19	D	408	LMG	C29-C30-C31-C32
20	D	407	LHG	O8-C23-C24-C25
20	K	103	LHG	C10-C11-C12-C13
17	C	613	CLA	C16-C17-C18-C20
17	B	611	CLA	CAA-CBA-CGA-O2A
17	C	603	CLA	C4-C3-C5-C6
17	B	612	CLA	C6-C7-C8-C9
17	B	616	CLA	C11-C12-C13-C14
17	D	402	CLA	C11-C12-C13-C14
17	D	403	CLA	C14-C13-C15-C16
19	D	408	LMG	C19-C20-C21-C22
17	B	612	CLA	C3A-C2A-CAA-CBA
17	C	613	CLA	C3A-C2A-CAA-CBA
17	B	606	CLA	CAA-CBA-CGA-O2A
17	B	610	CLA	CAA-CBA-CGA-O2A
17	B	612	CLA	CAA-CBA-CGA-O2A
17	C	610	CLA	CAA-CBA-CGA-O2A
17	B	603	CLA	CAD-CBD-CGD-O2D
17	C	608	CLA	CAD-CBD-CGD-O2D
19	K	102	LMG	C28-C29-C30-C31
17	D	402	CLA	CAA-CBA-CGA-O2A
17	C	609	CLA	CAA-CBA-CGA-O2A
19	K	102	LMG	C32-C33-C34-C35
17	C	613	CLA	CAA-CBA-CGA-O2A
26	C	617	DGD	C4A-C5A-C6A-C7A
26	C	618	DGD	O1G-C1G-C2G-C3G
20	D	407	LHG	C25-C26-C27-C28
17	C	606	CLA	O2A-C1-C2-C3
17	C	609	CLA	C10-C11-C12-C13
17	C	604	CLA	C15-C16-C17-C18
17	D	410	CLA	C16-C17-C18-C19
17	B	606	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	B	610	CLA	CHA-CBD-CGD-O1D
17	B	610	CLA	CHA-CBD-CGD-O2D
17	B	613	CLA	CHA-CBD-CGD-O1D
17	B	613	CLA	CHA-CBD-CGD-O2D
17	B	616	CLA	CHA-CBD-CGD-O1D
17	B	616	CLA	CHA-CBD-CGD-O2D
17	D	402	CLA	CHA-CBD-CGD-O2D
17	C	603	CLA	CHA-CBD-CGD-O1D
17	C	603	CLA	CHA-CBD-CGD-O2D
17	C	609	CLA	CHA-CBD-CGD-O2D
17	C	611	CLA	CHA-CBD-CGD-O1D
23	D	411	PHO	C10-C11-C12-C13
17	B	604	CLA	C10-C11-C12-C13
17	C	610	CLA	C8-C10-C11-C12
26	C	619	DGD	O1B-C1B-O2G-C2G
17	B	607	CLA	CAA-CBA-CGA-O2A
17	B	609	CLA	CAA-CBA-CGA-O2A
20	K	103	LHG	O7-C7-C8-C9
20	K	103	LHG	C24-C23-O8-C6
17	B	604	CLA	C13-C15-C16-C17
17	B	612	CLA	C12-C13-C15-C16
17	C	602	CLA	C6-C7-C8-C10
17	B	601	CLA	C13-C15-C16-C17
17	B	605	CLA	CAA-CBA-CGA-O2A
17	C	607	CLA	CAA-CBA-CGA-O2A
26	C	617	DGD	C3A-C4A-C5A-C6A
17	C	608	CLA	C11-C12-C13-C14
24	E	101	HEM	CAA-CBA-CGA-O2A
17	C	607	CLA	C16-C17-C18-C19
26	C	619	DGD	C2B-C1B-O2G-C2G
19	H	102	LMG	C12-C13-C14-C15
19	H	102	LMG	C15-C16-C17-C18
17	B	610	CLA	CAA-CBA-CGA-O1A
17	B	612	CLA	CAA-CBA-CGA-O1A
17	B	607	CLA	C16-C17-C18-C20
17	B	602	CLA	C1A-C2A-CAA-CBA
17	B	612	CLA	C1A-C2A-CAA-CBA
17	C	612	CLA	C1A-C2A-CAA-CBA
17	C	613	CLA	C1A-C2A-CAA-CBA
17	A	403	CLA	C1A-C2A-CAA-CBA
17	D	402	CLA	CAA-CBA-CGA-O1A
17	C	610	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	C	607	CLA	C2-C1-O2A-CGA
17	A	402	CLA	C5-C6-C7-C8
17	B	611	CLA	CAA-CBA-CGA-O1A
17	C	613	CLA	CAA-CBA-CGA-O1A
17	B	613	CLA	C2A-CAA-CBA-CGA
17	C	610	CLA	C16-C17-C18-C20
17	C	603	CLA	CAA-CBA-CGA-O2A
20	D	407	LHG	C3-O3-P-O4
20	L	101	LHG	C4-O6-P-O5
20	D	407	LHG	O10-C23-C24-C25
20	K	103	LHG	O9-C7-C8-C9
20	D	409	LHG	C12-C13-C14-C15
17	B	606	CLA	CAA-CBA-CGA-O1A
17	C	609	CLA	CAA-CBA-CGA-O1A
17	B	604	CLA	CAA-CBA-CGA-O2A
20	B	622	LHG	O8-C23-C24-C25
27	C	620	SQD	C32-C33-C34-C35
20	L	101	LHG	O8-C23-C24-C25
27	C	620	SQD	O47-C7-C8-C9
17	B	606	CLA	C8-C10-C11-C12
17	C	611	CLA	CAD-CBD-CGD-O1D
23	D	412	PHO	CAA-CBA-CGA-O2A
17	C	602	CLA	C6-C7-C8-C9
17	C	612	CLA	C14-C13-C15-C16
23	D	411	PHO	C6-C7-C8-C9
19	H	102	LMG	C11-C12-C13-C14
17	B	609	CLA	CAA-CBA-CGA-O1A
17	B	602	CLA	CAA-CBA-CGA-O2A
17	A	403	CLA	CAA-CBA-CGA-O2A
24	E	101	HEM	CAA-CBA-CGA-O1A
17	C	607	CLA	CAA-CBA-CGA-O1A
17	C	610	CLA	C13-C15-C16-C17
17	A	402	CLA	CAA-CBA-CGA-O2A
20	B	621	LHG	C35-C36-C37-C38
20	L	101	LHG	C12-C13-C14-C15
17	C	612	CLA	C12-C13-C15-C16
17	B	607	CLA	CAA-CBA-CGA-O1A
27	C	620	SQD	O49-C7-C8-C9
20	D	407	LHG	C29-C30-C31-C32
18	H	101	BCR	C7-C8-C9-C10
17	B	604	CLA	CAA-CBA-CGA-O1A
17	B	605	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	C	603	CLA	CAA-CBA-CGA-O1A
17	B	601	CLA	CAA-CBA-CGA-O2A
17	D	403	CLA	CAA-CBA-CGA-O2A
20	B	621	LHG	O7-C7-C8-C9
17	B	602	CLA	CAA-CBA-CGA-O1A
17	A	402	CLA	CAA-CBA-CGA-O1A
17	C	602	CLA	C15-C16-C17-C18
20	L	101	LHG	O10-C23-C24-C25
20	D	406	LHG	C25-C26-C27-C28
17	A	403	CLA	CAA-CBA-CGA-O1A
17	B	608	CLA	CAA-CBA-CGA-O2A
20	B	623	LHG	O8-C23-C24-C25

There are no ring outliers.

43 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	402	CLA	1	0
17	C	608	CLA	1	0
22	D	405	PL9	1	0
17	A	404	CLA	1	0
17	C	610	CLA	1	0
17	B	605	CLA	1	0
18	Z	101	BCR	7	0
26	C	619	DGD	2	0
17	B	612	CLA	2	0
17	C	604	CLA	2	0
17	C	611	CLA	3	0
17	B	604	CLA	3	0
23	D	412	PHO	1	0
18	K	101	BCR	1	0
17	C	603	CLA	2	0
17	C	609	CLA	2	0
20	D	407	LHG	2	0
19	H	102	LMG	2	0
18	C	616	BCR	3	0
17	C	605	CLA	1	0
24	E	101	HEM	5	0
18	H	101	BCR	5	0
18	B	618	BCR	1	0
17	B	615	CLA	5	0
17	B	607	CLA	1	0

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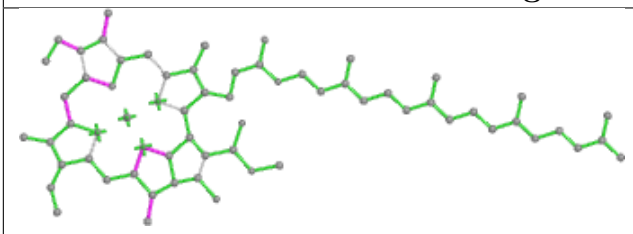
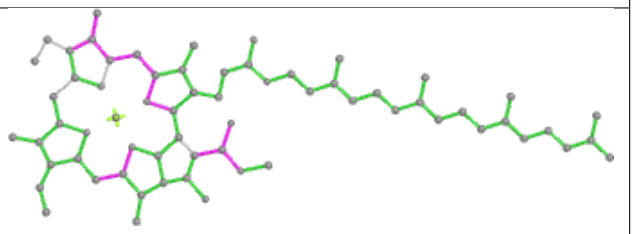
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	616	CLA	1	0
17	D	410	CLA	2	0
17	A	402	CLA	1	0
17	B	613	CLA	4	0
20	L	101	LHG	1	0
18	B	617	BCR	1	0
17	C	606	CLA	5	0
17	B	609	CLA	2	0
17	B	614	CLA	1	0
17	C	612	CLA	3	0
17	B	603	CLA	1	0
17	C	602	CLA	3	0
18	B	619	BCR	1	0
18	C	615	BCR	8	0
18	A	405	BCR	2	0
17	D	403	CLA	1	0
17	B	602	CLA	4	0
17	C	607	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.

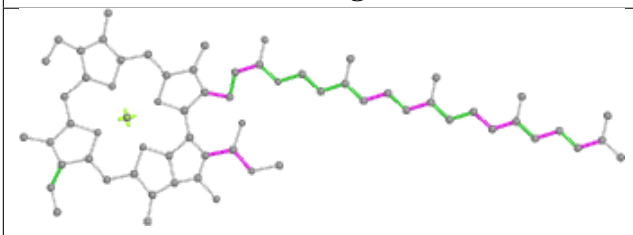
Ligand CLA D 402



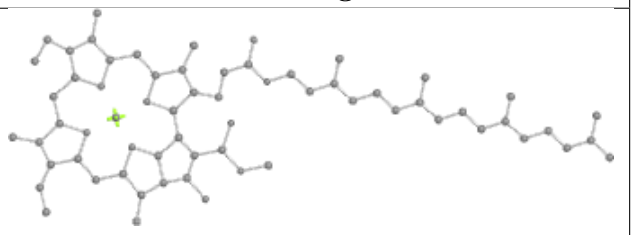
Bond lengths



Bond angles

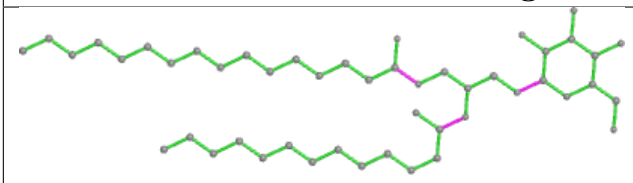


Torsions

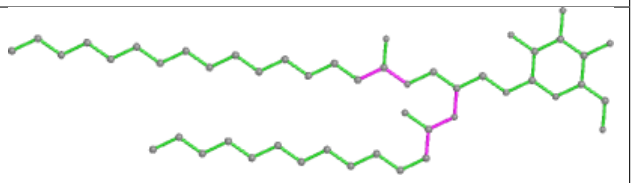


Rings

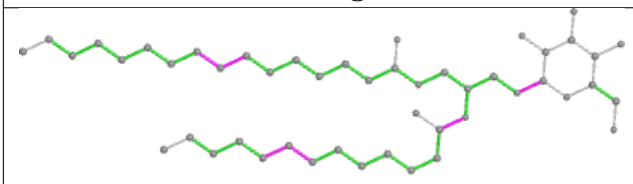
Ligand LMG C 621



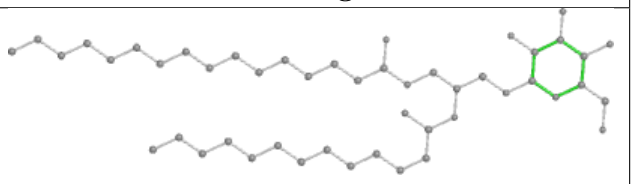
Bond lengths



Bond angles

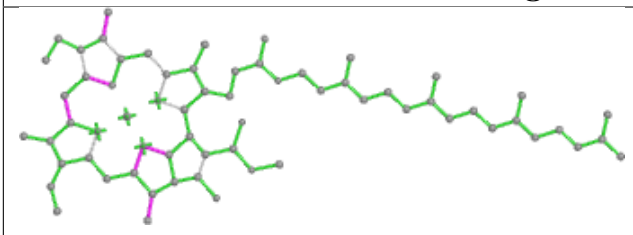


Torsions

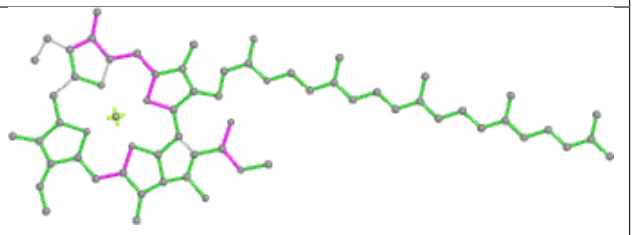


Rings

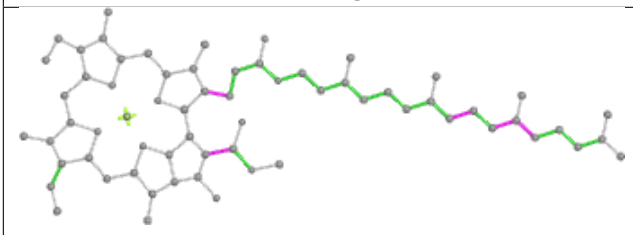
Ligand CLA C 608



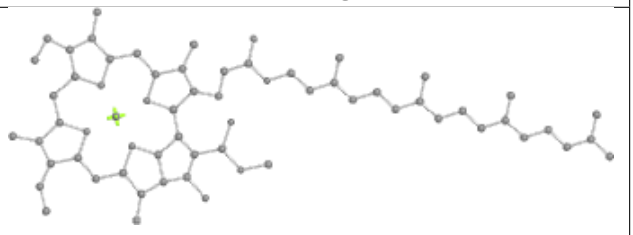
Bond lengths



Bond angles

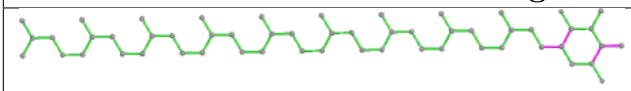


Torsions

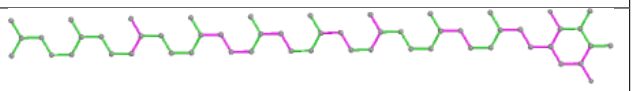


Rings

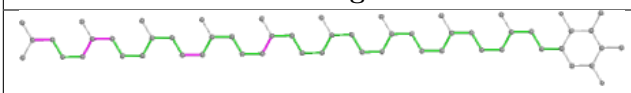
Ligand PL9 D 405



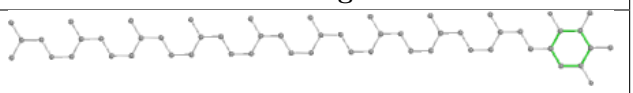
Bond lengths



Bond angles

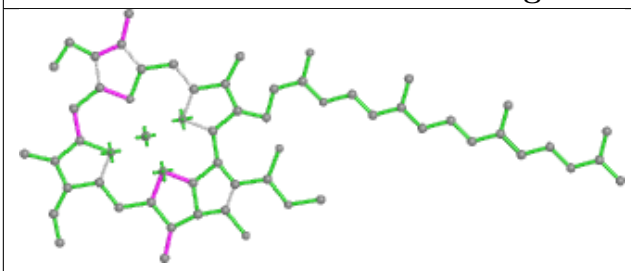


Torsions

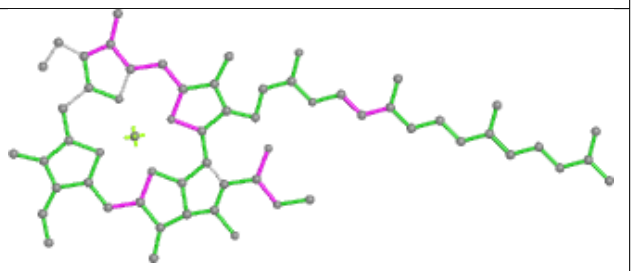


Rings

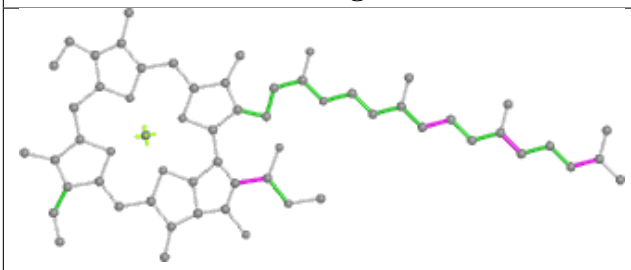
Ligand CLA A 404



Bond lengths



Bond angles



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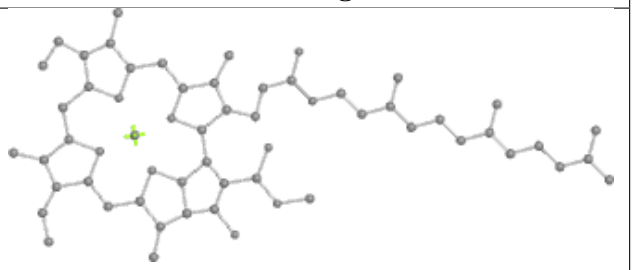
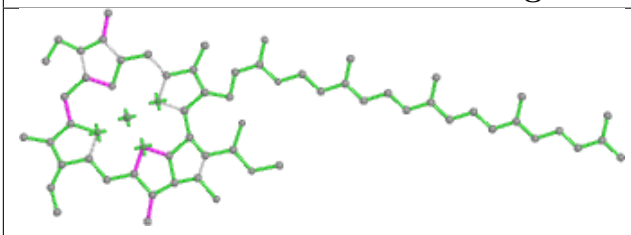


Rings

Ligand CLA C 610



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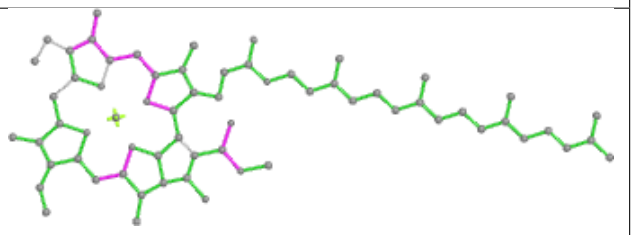
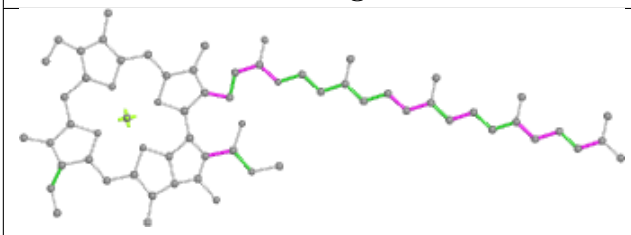
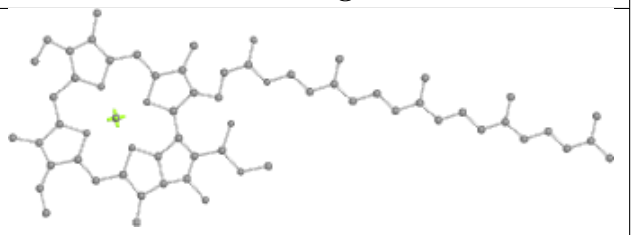


Bond angles

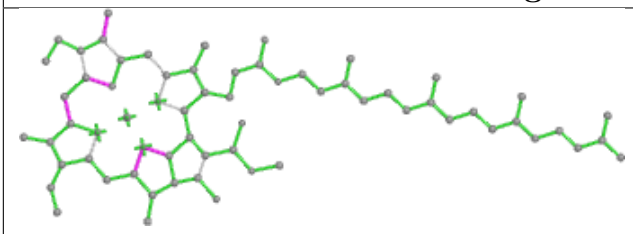


Torsions

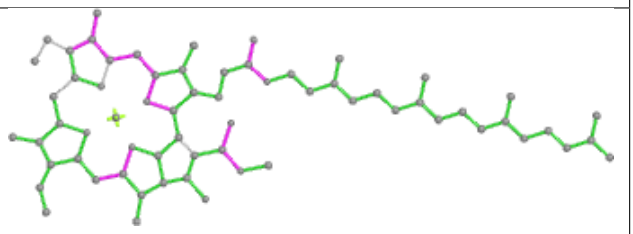


Rings

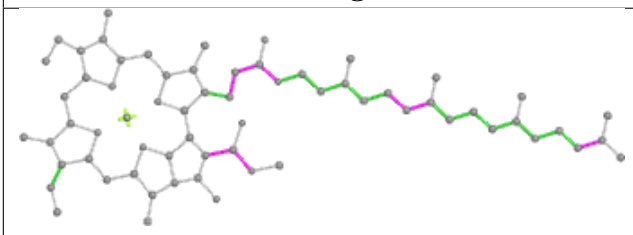
Ligand CLA B 611



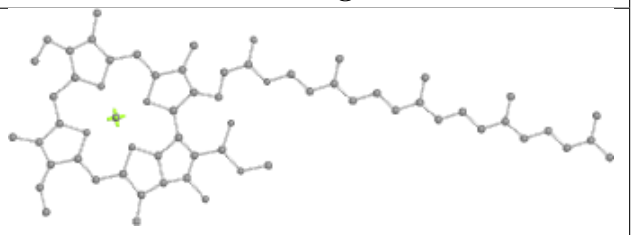
Bond lengths



Bond angles

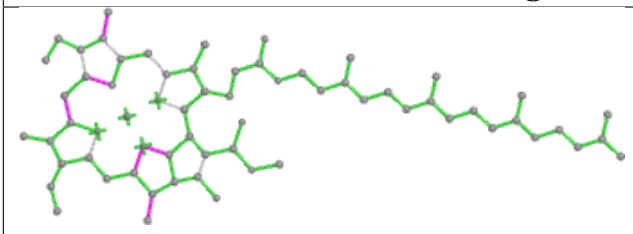


Torsions

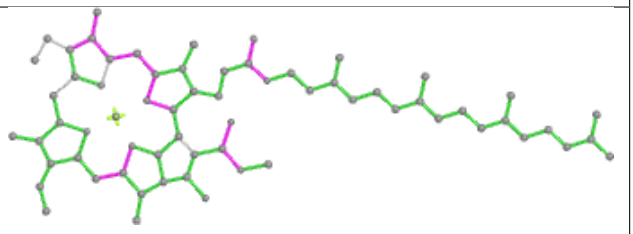


Rings

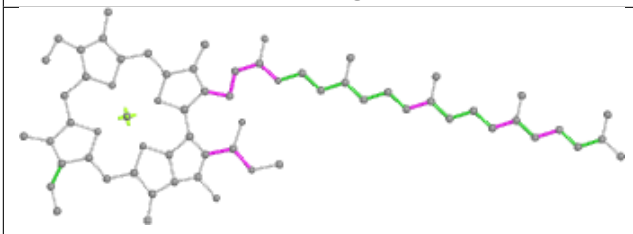
Ligand CLA B 605



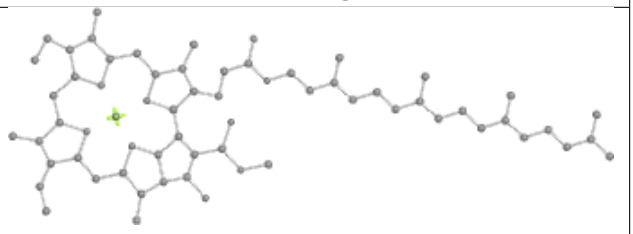
Bond lengths



Bond angles

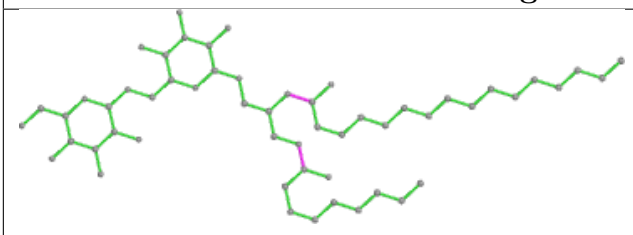


Torsions

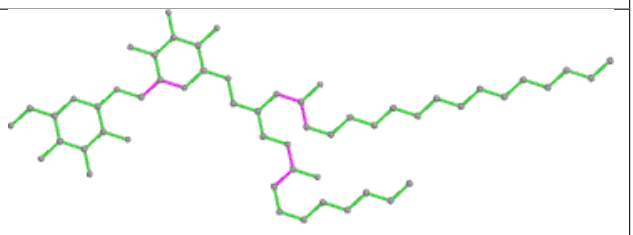


Rings

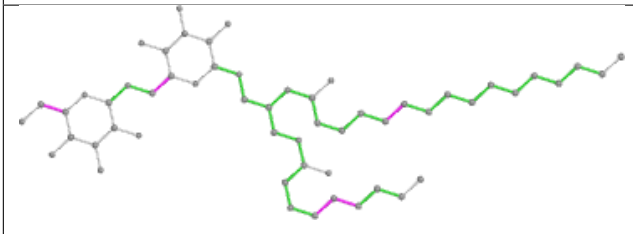
Ligand DGD C 617



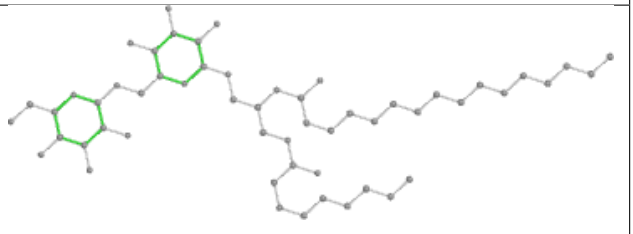
Bond lengths



Bond angles

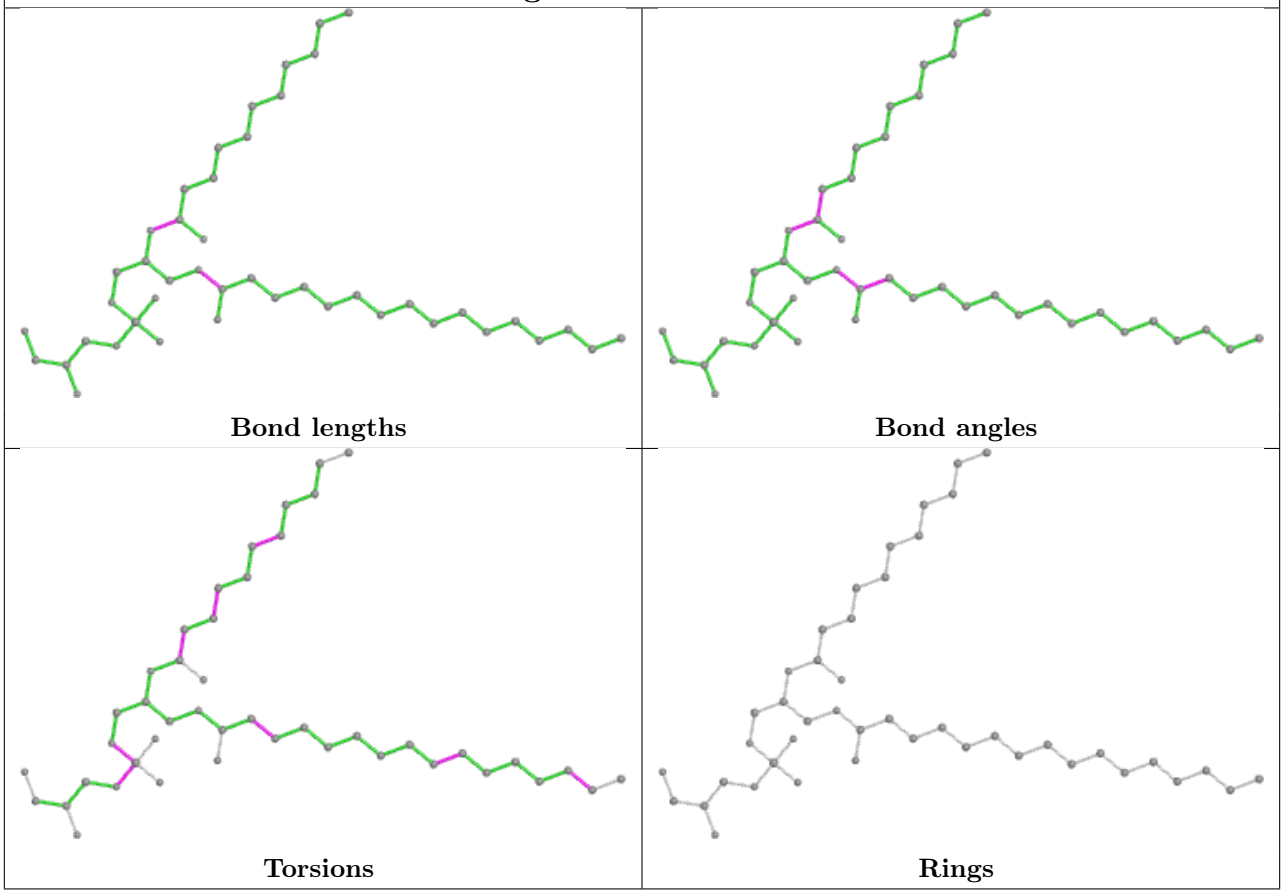


Torsions

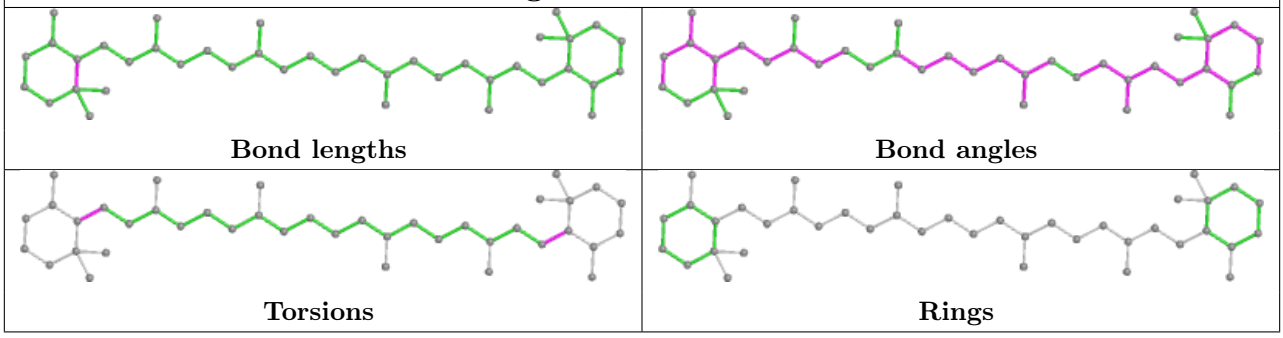


Rings

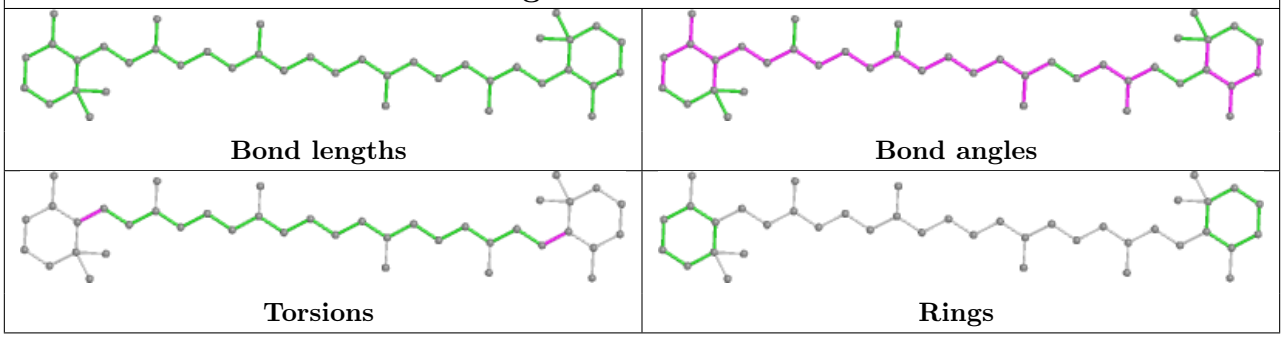
Ligand LHG B 621



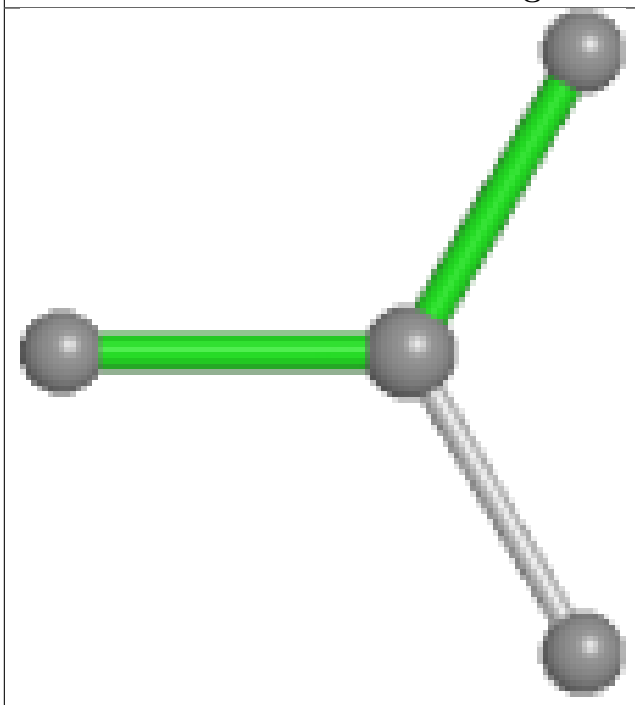
Ligand BCR Z 101



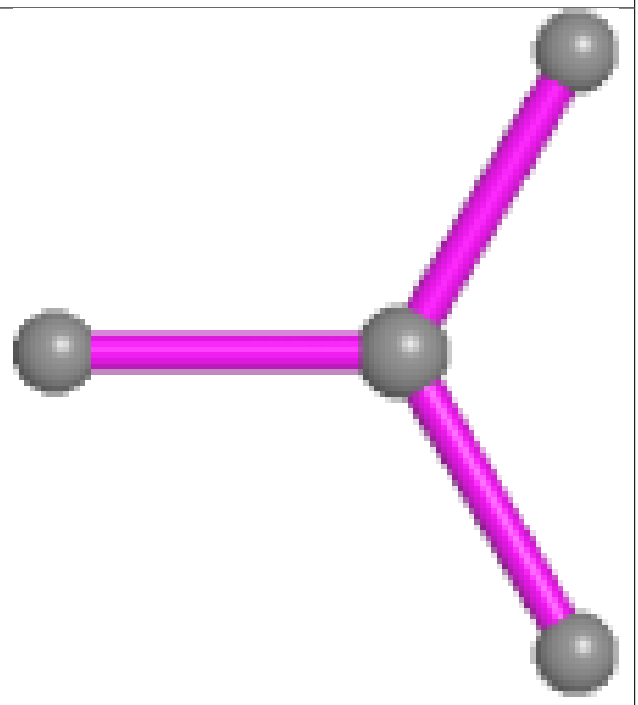
Ligand BCR D 404



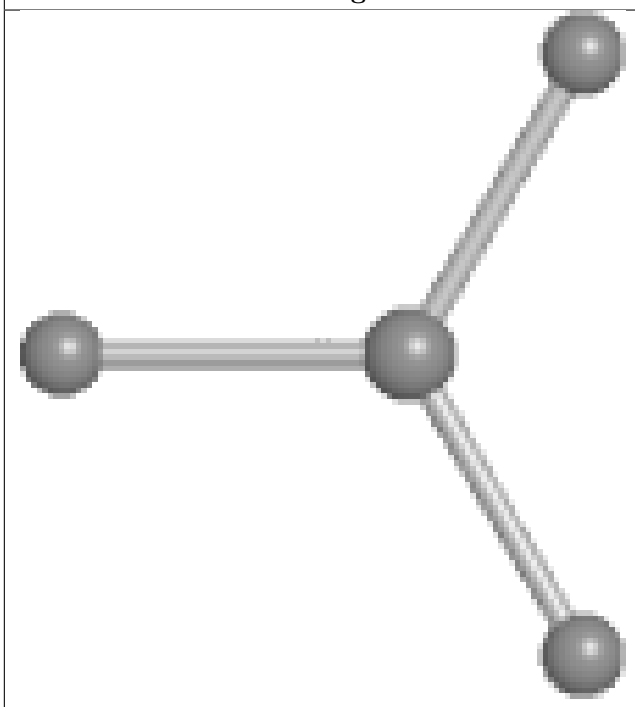
Ligand BCT D 401



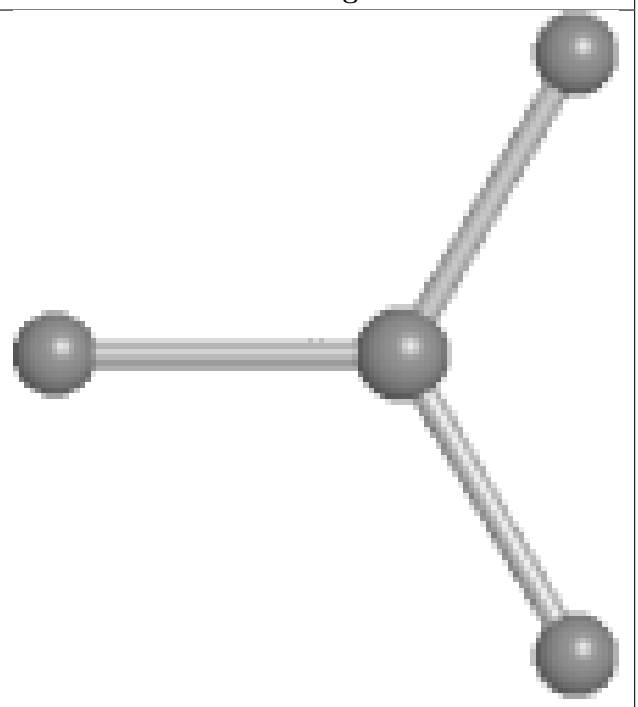
Bond lengths



Bond angles

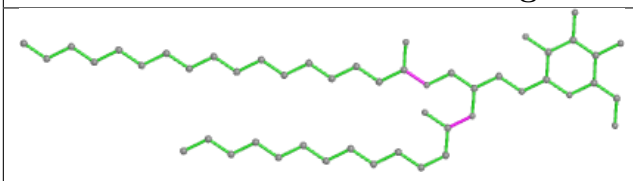


Torsions

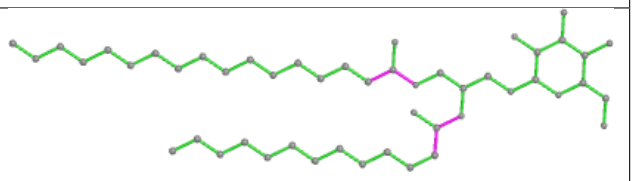


Rings

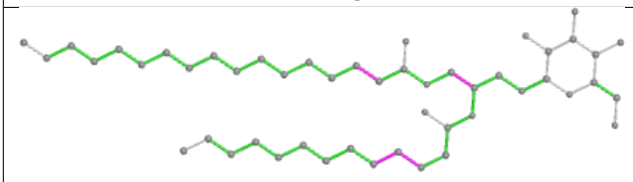
Ligand LMG C 601



Bond lengths



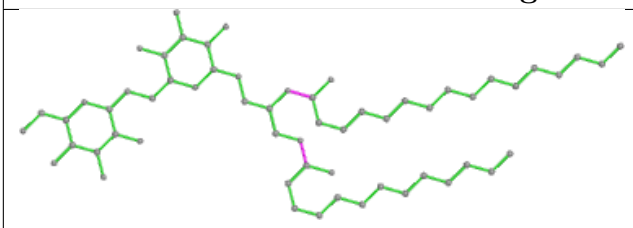
Bond angles



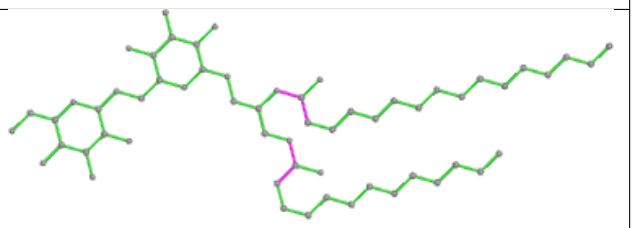
Torsions

Rings

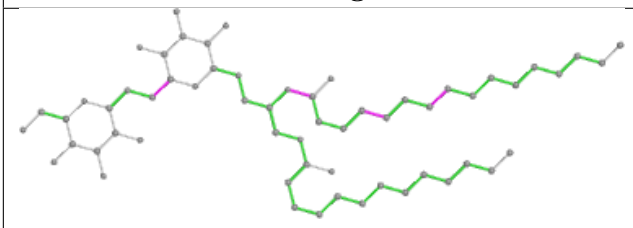
Ligand DGD C 619



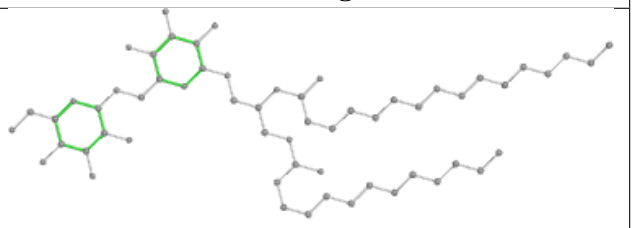
Bond lengths



Bond angles

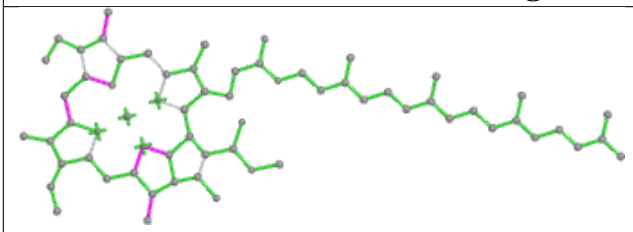


Torsions

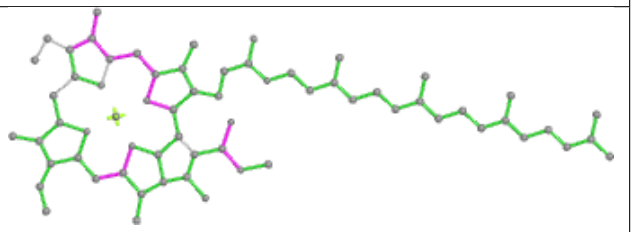


Rings

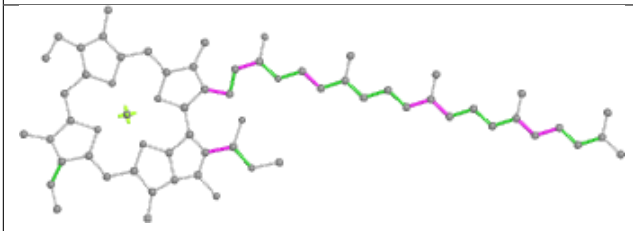
Ligand CLA B 612



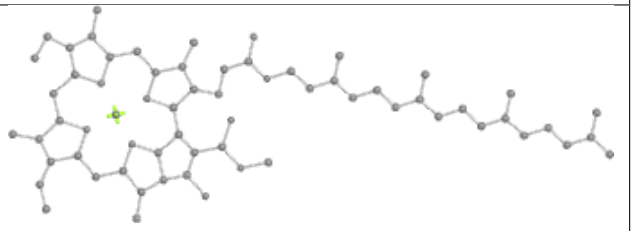
Bond lengths



Bond angles

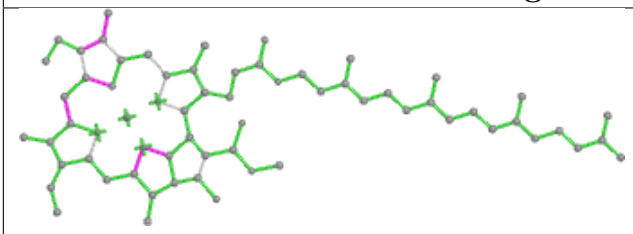


Torsions

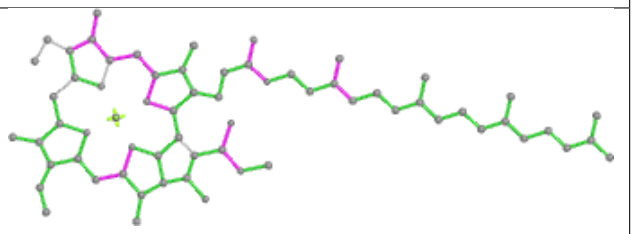


Rings

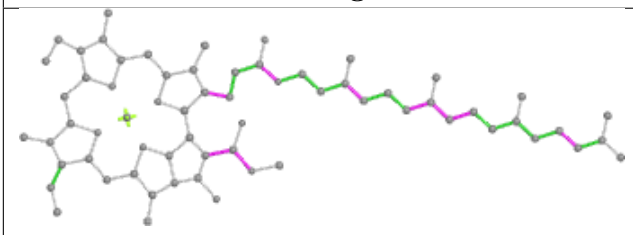
Ligand CLA C 604



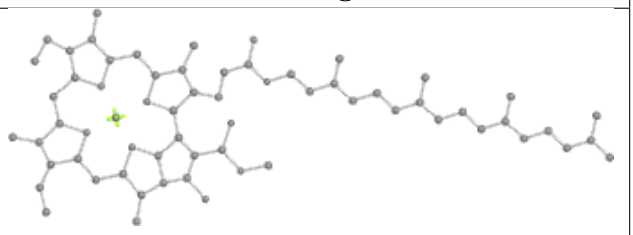
Bond lengths



Bond angles

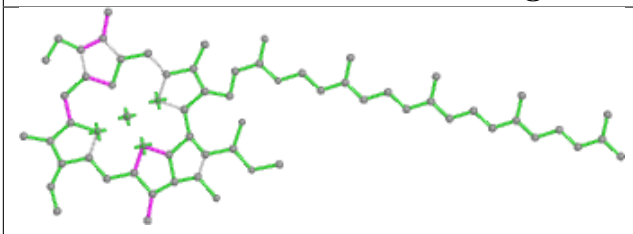


Torsions

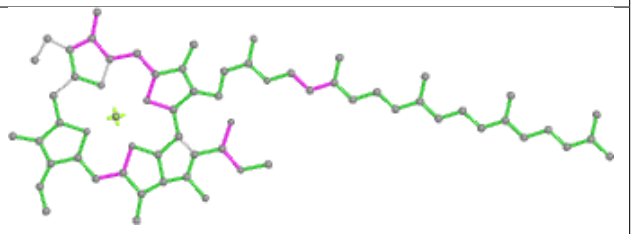


Rings

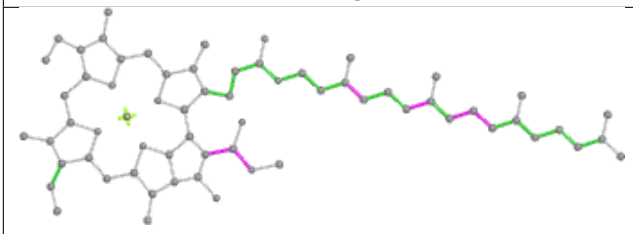
Ligand CLA C 611



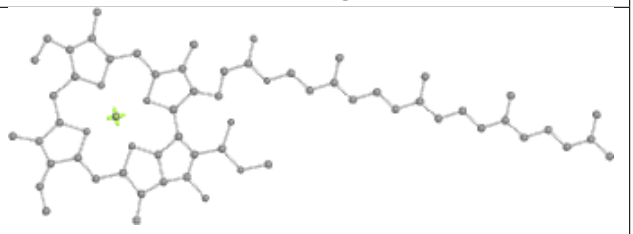
Bond lengths



Bond angles

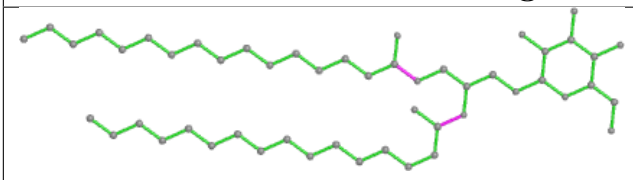


Torsions

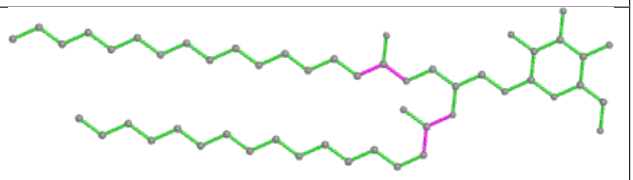


Rings

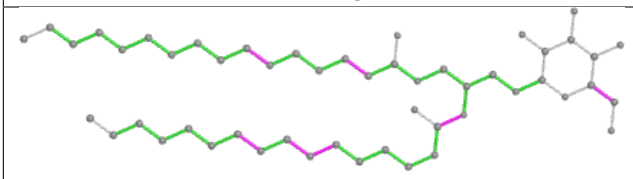
Ligand LMG K 102



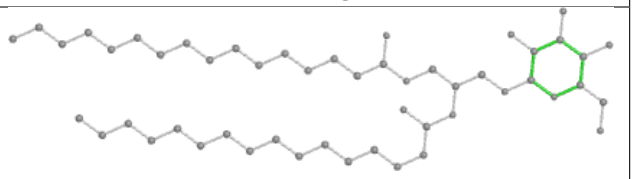
Bond lengths



Bond angles

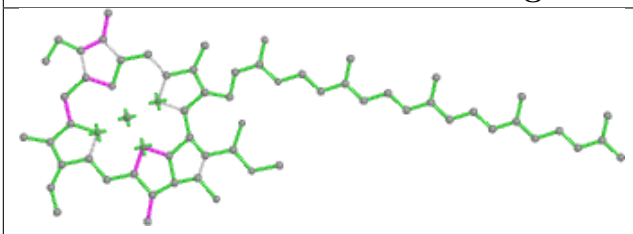


Torsions

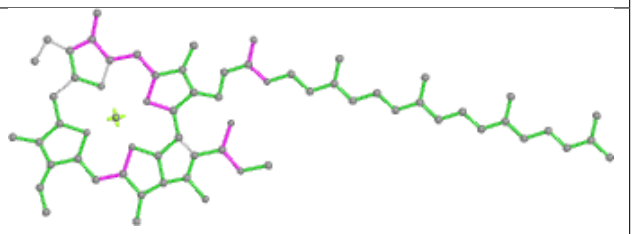


Rings

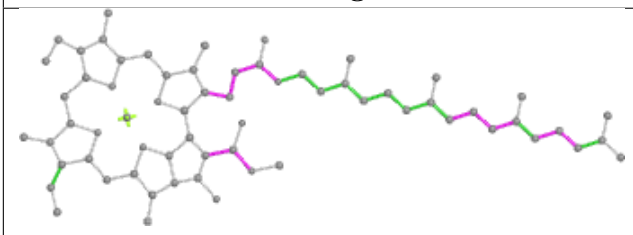
Ligand CLA B 604



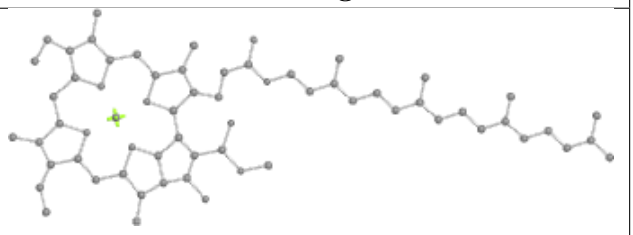
Bond lengths



Bond angles

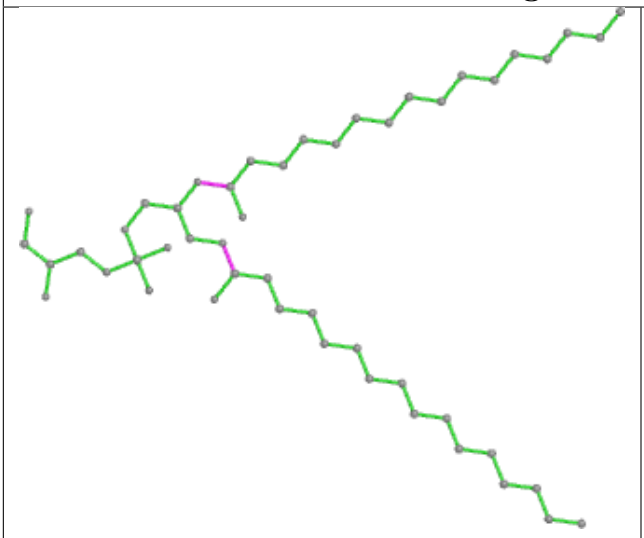


Torsions

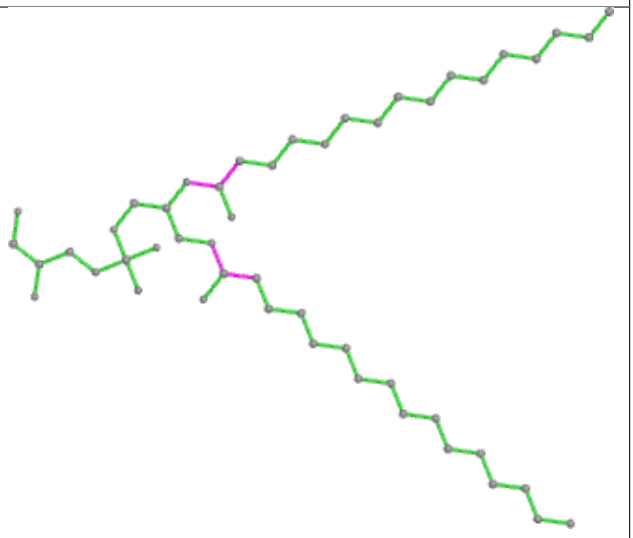


Rings

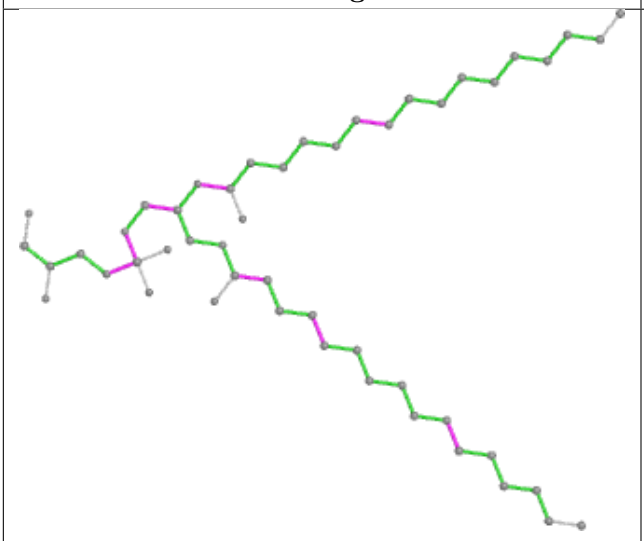
Ligand LHG B 623



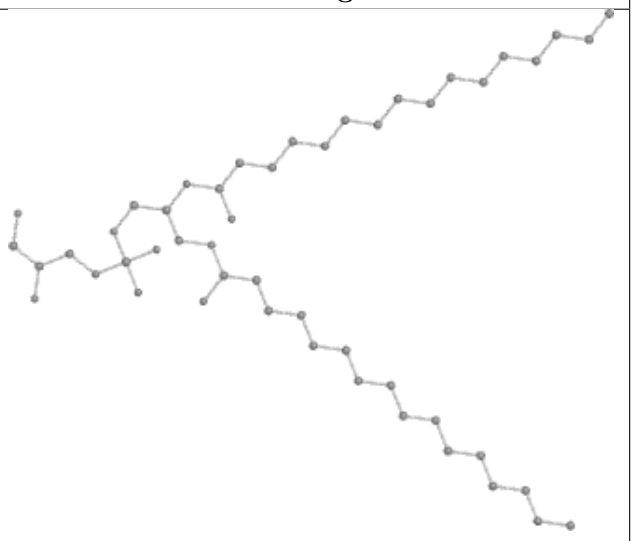
Bond lengths



Bond angles

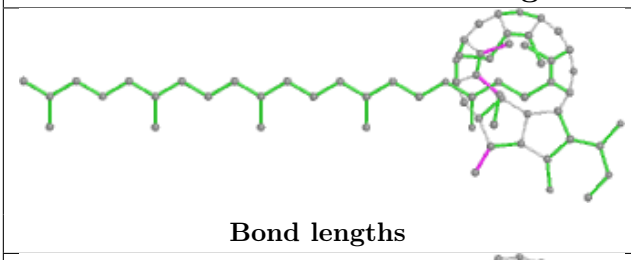


Torsions

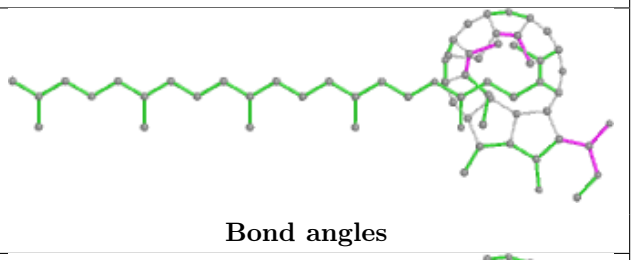


Rings

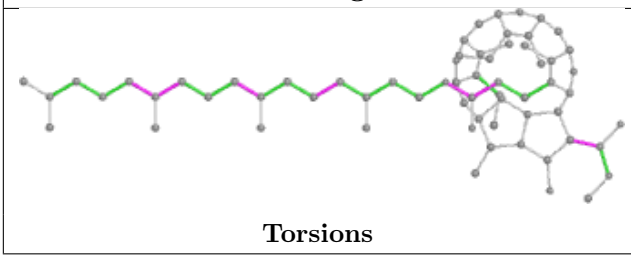
Ligand PHO D 412



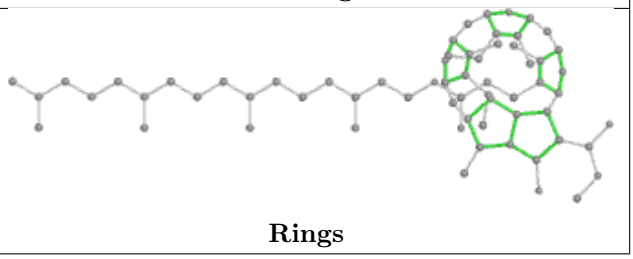
Bond lengths



Bond angles

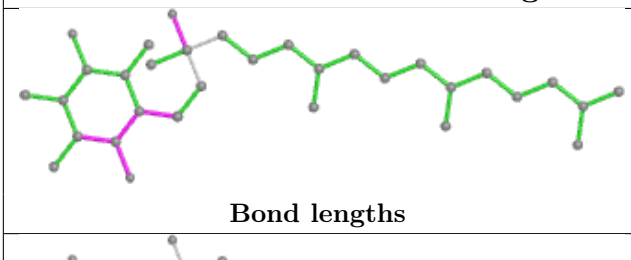


Torsions

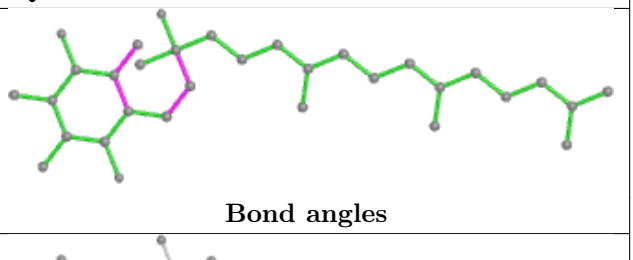


Rings

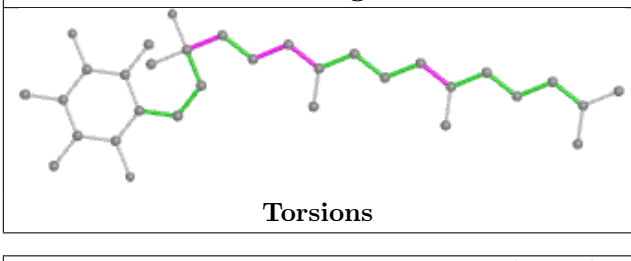
Ligand VTQ X 201



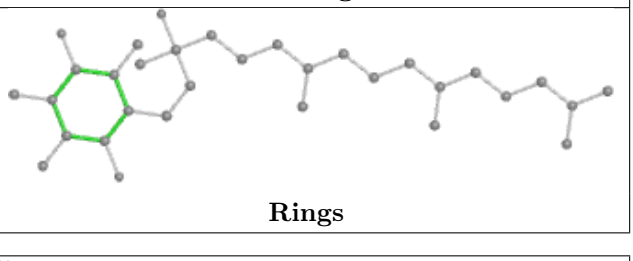
Bond lengths



Bond angles



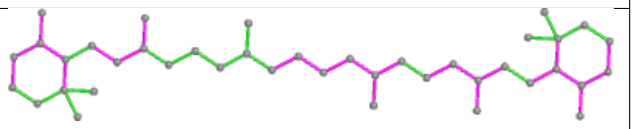
Torsions



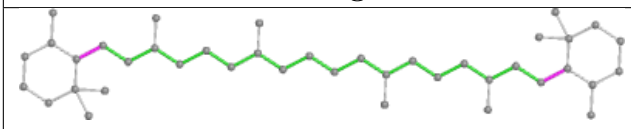
Rings

Ligand BCR K 101

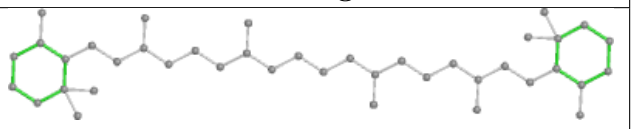
Bond lengths



Bond angles

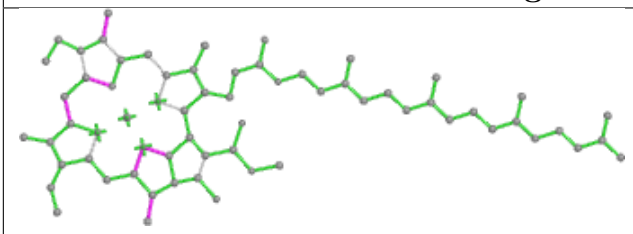


Torsions

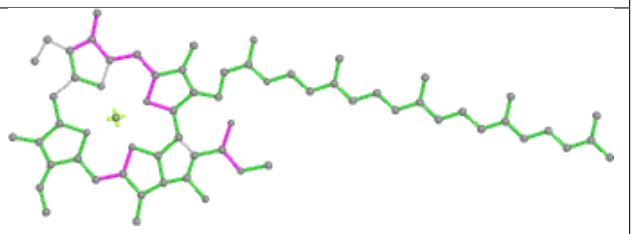


Rings

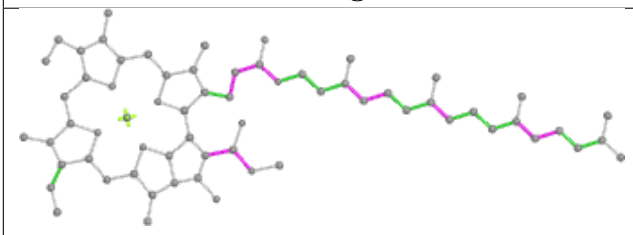
Ligand CLA C 603



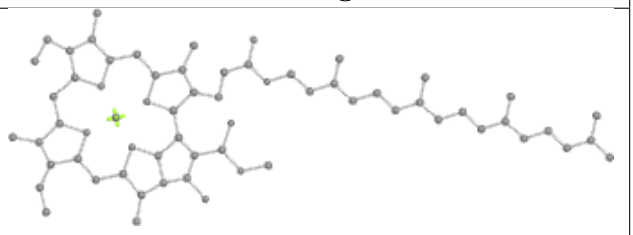
Bond lengths



Bond angles

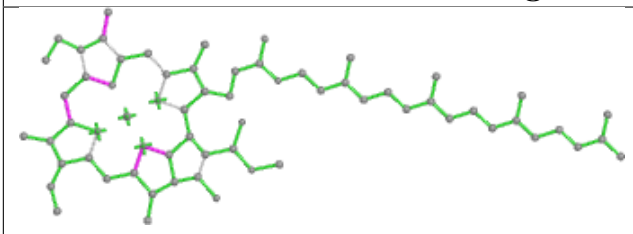


Torsions

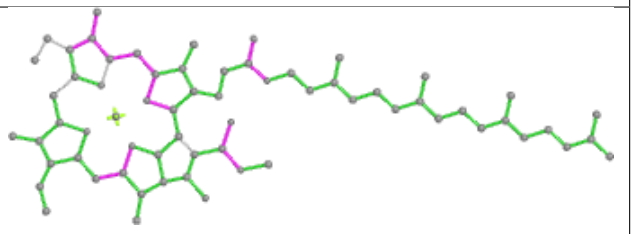


Rings

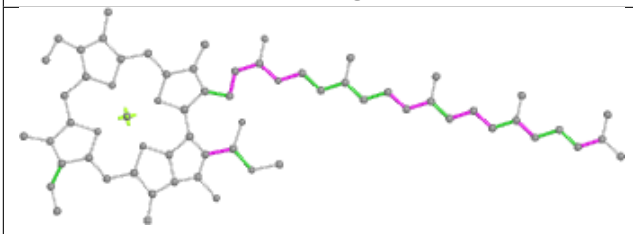
Ligand CLA C 609



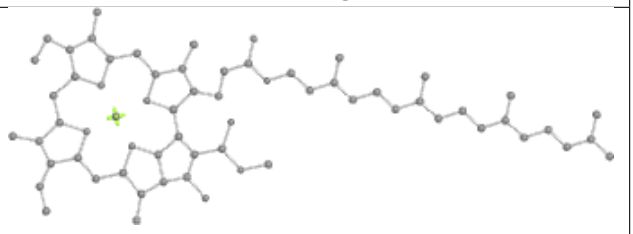
Bond lengths



Bond angles

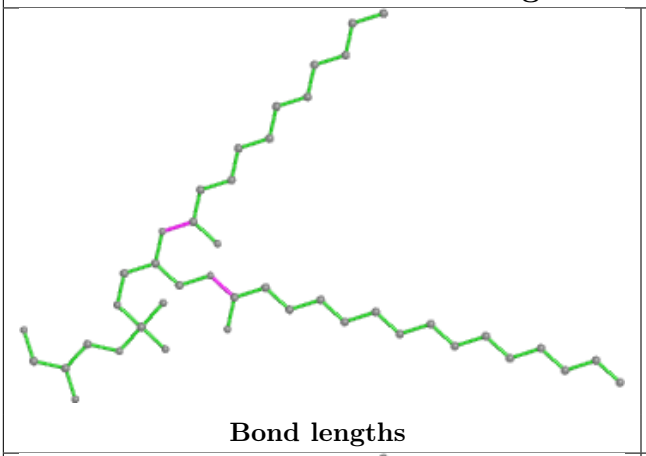


Torsions

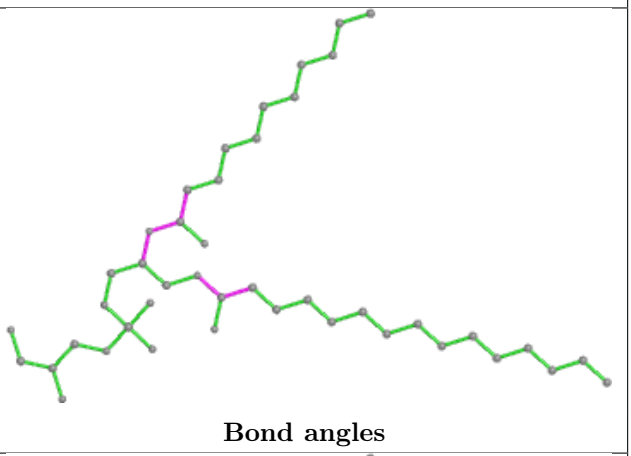


Rings

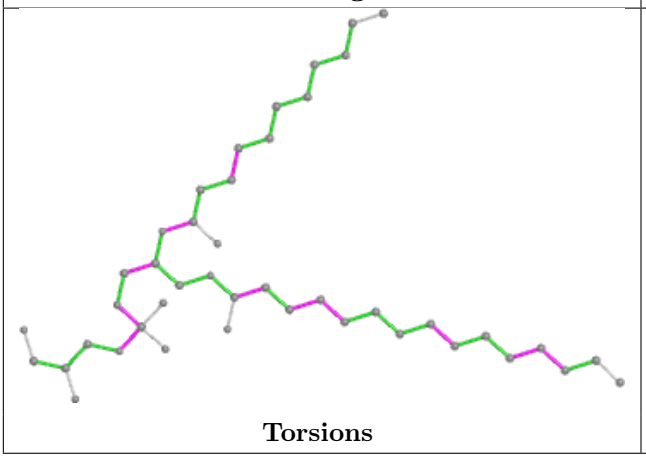
Ligand LHG D 407



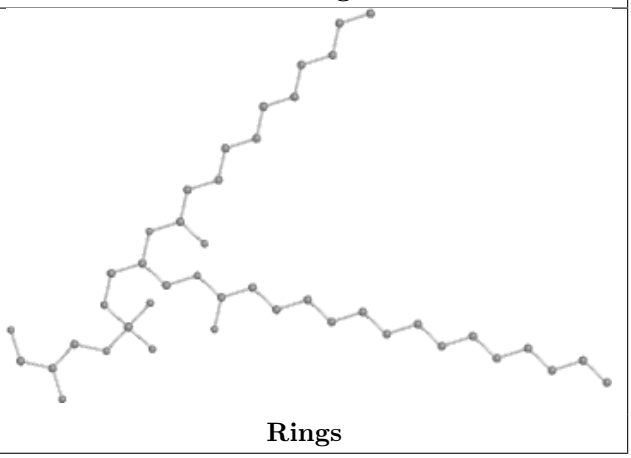
Bond lengths



Bond angles

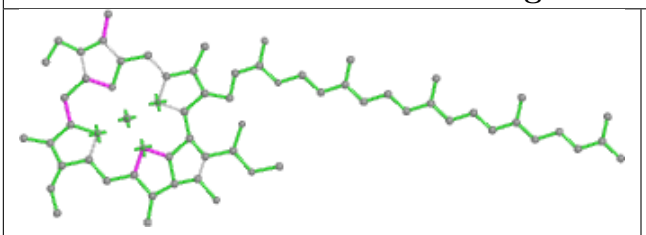


Torsions

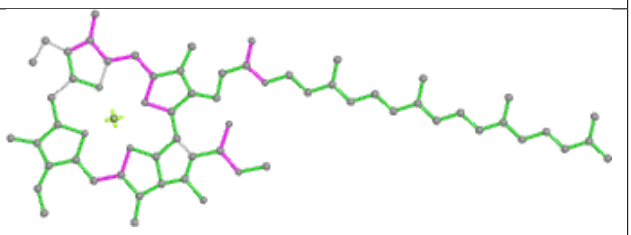


Rings

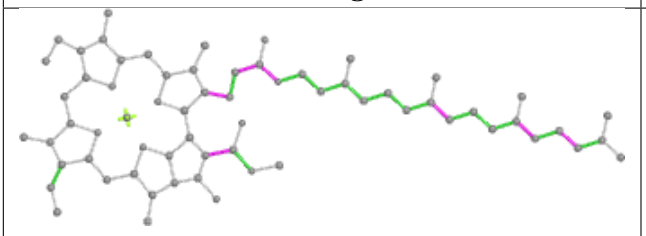
Ligand CLA B 610



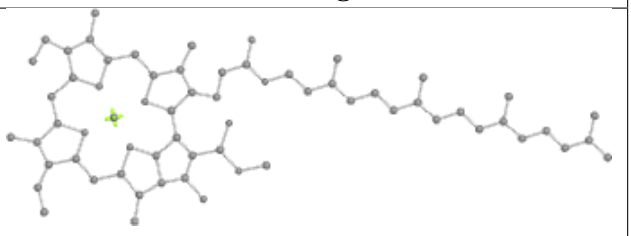
Bond lengths



Bond angles

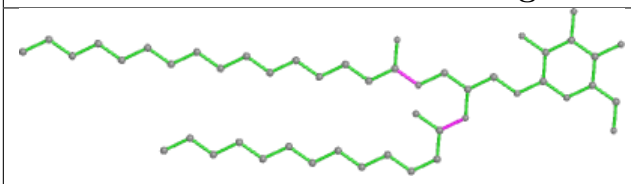


Torsions

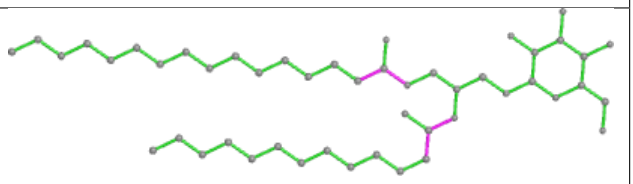


Rings

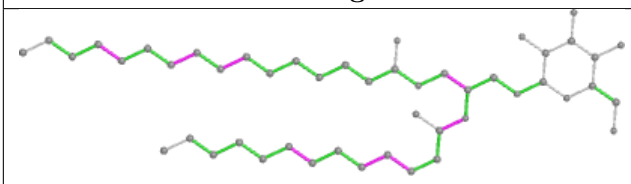
Ligand LMG H 102



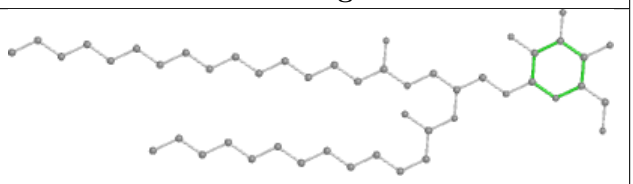
Bond lengths



Bond angles

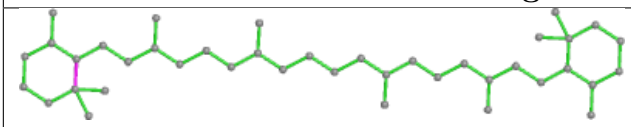


Torsions

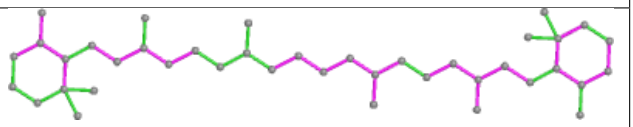


Rings

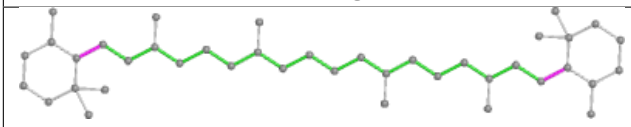
Ligand BCR C 616



Bond lengths



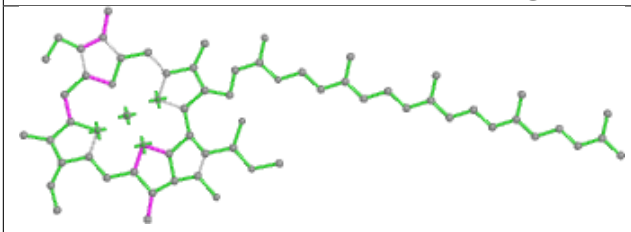
Bond angles



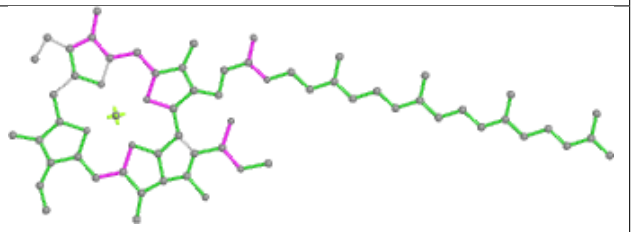
Torsions

Rings

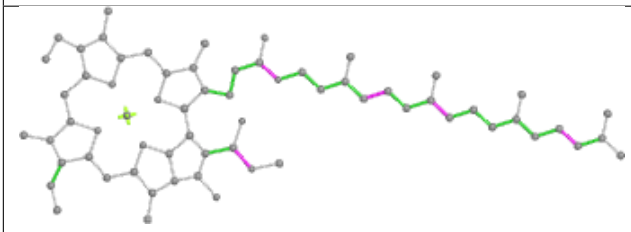
Ligand CLA C 605



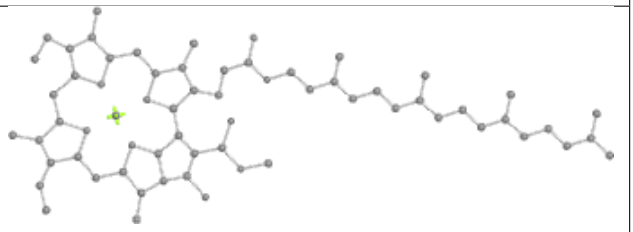
Bond lengths



Bond angles

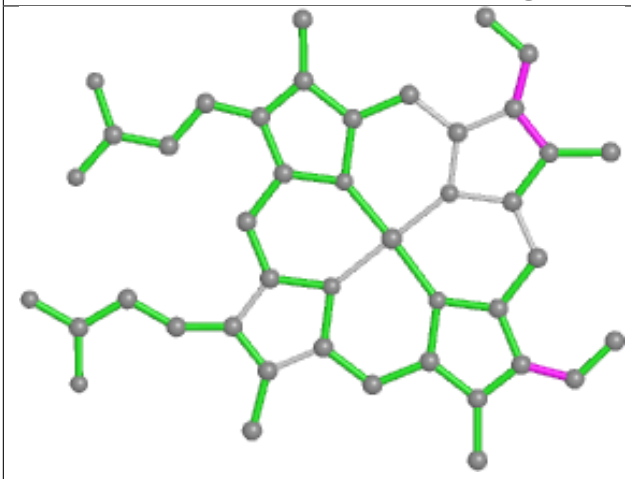


Torsions

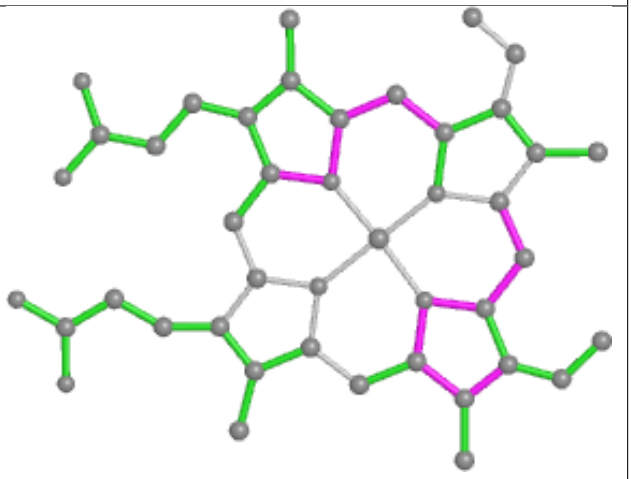


Rings

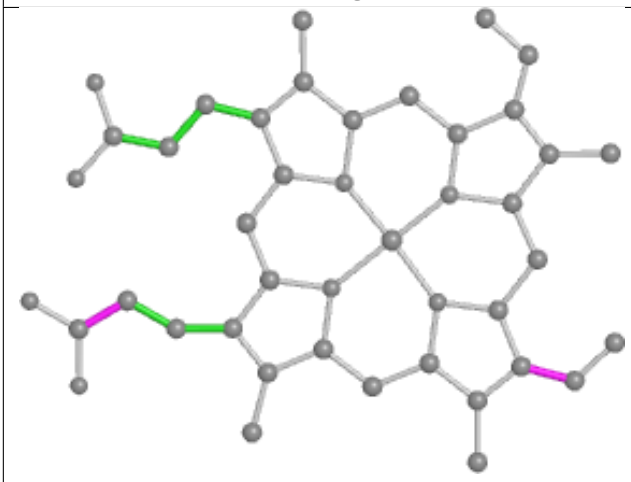
Ligand HEM E 101



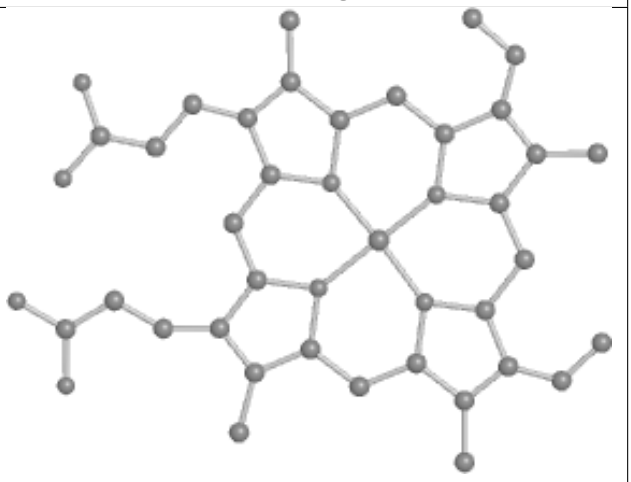
Bond lengths



Bond angles

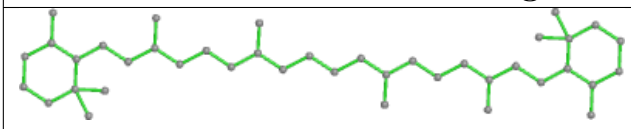


Torsions

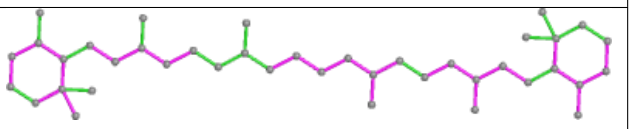


Rings

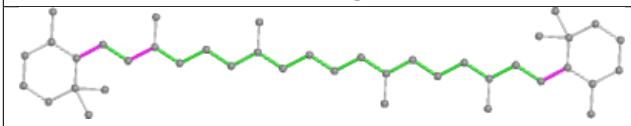
Ligand BCR H 101



Bond lengths



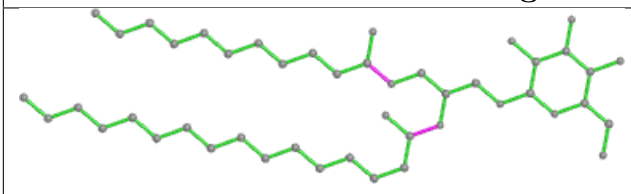
Bond angles



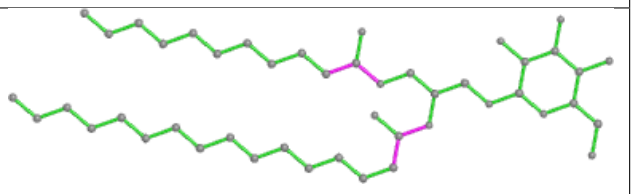
Torsions

Rings

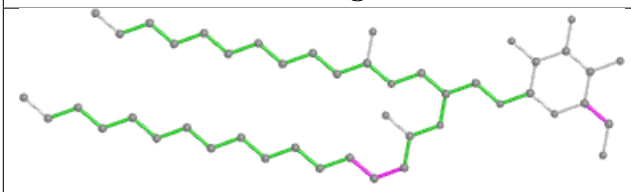
Ligand LMG B 620



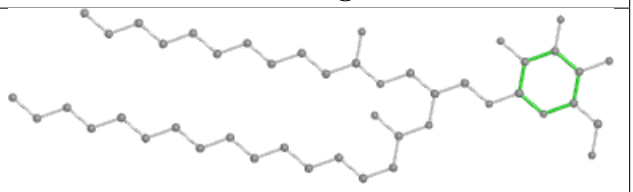
Bond lengths



Bond angles

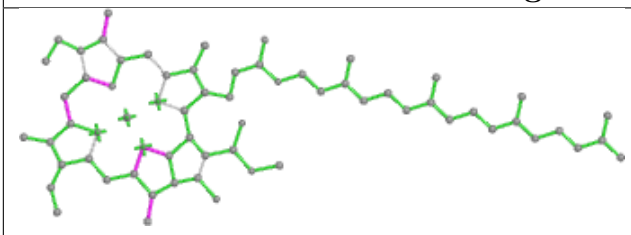


Torsions

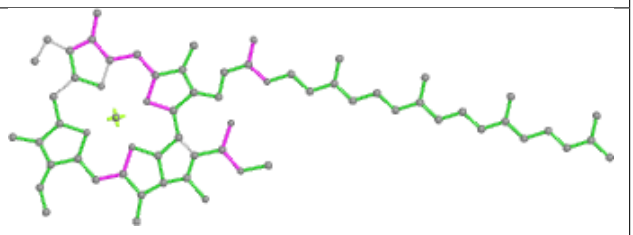


Rings

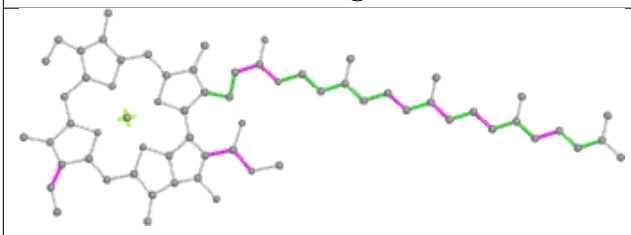
Ligand CLA B 601



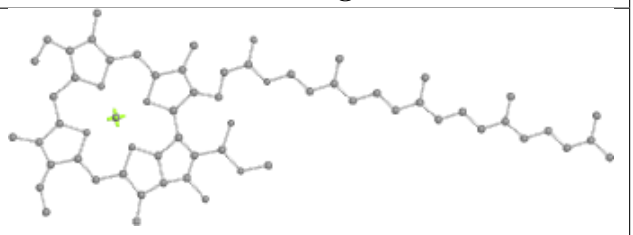
Bond lengths



Bond angles

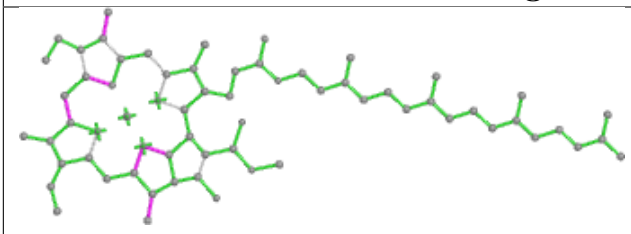


Torsions

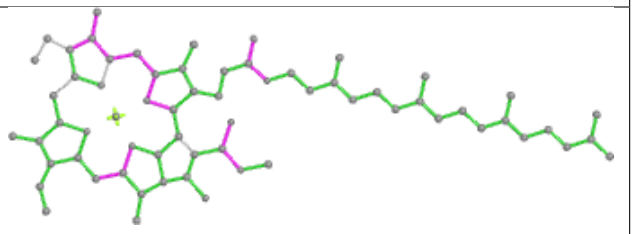


Rings

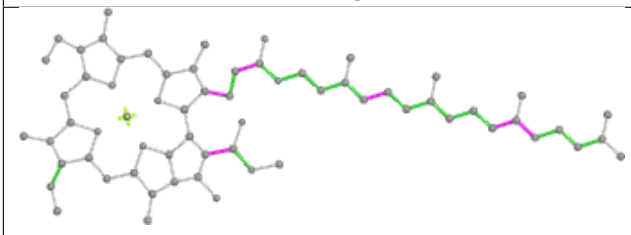
Ligand CLA B 608



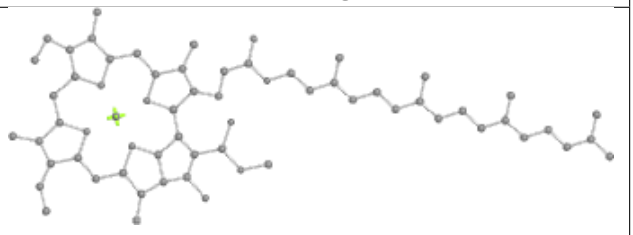
Bond lengths



Bond angles

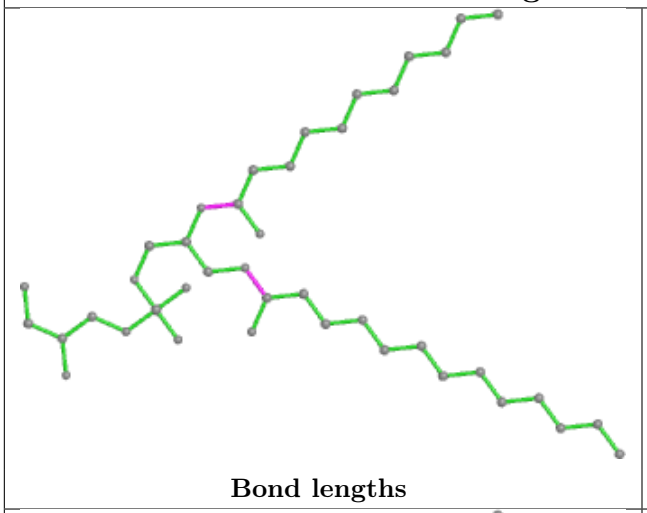


Torsions

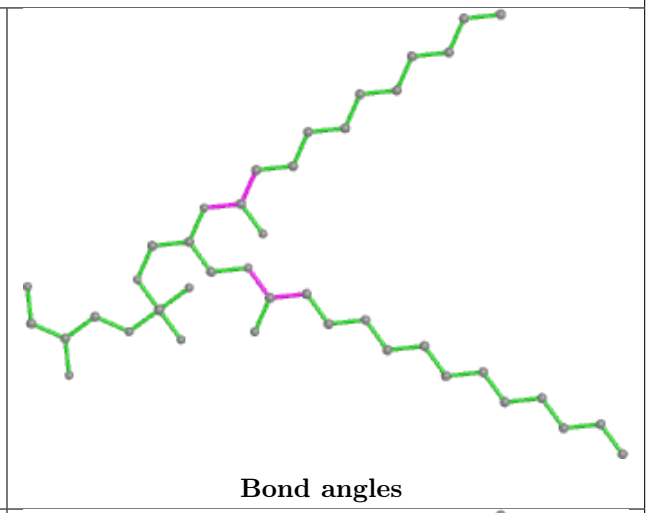


Rings

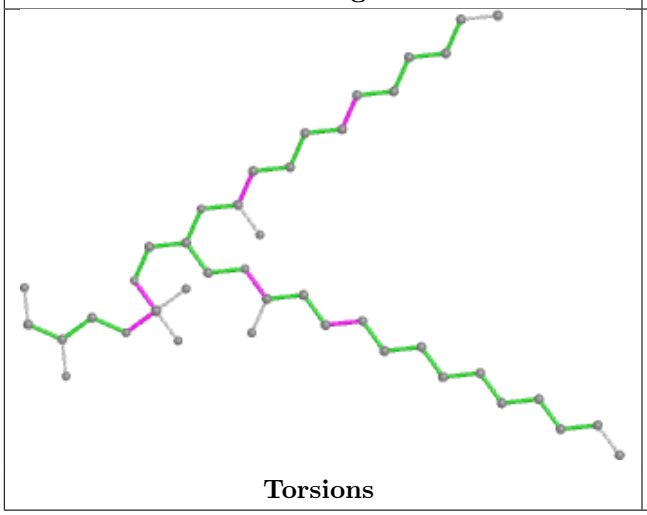
Ligand LHG K 103



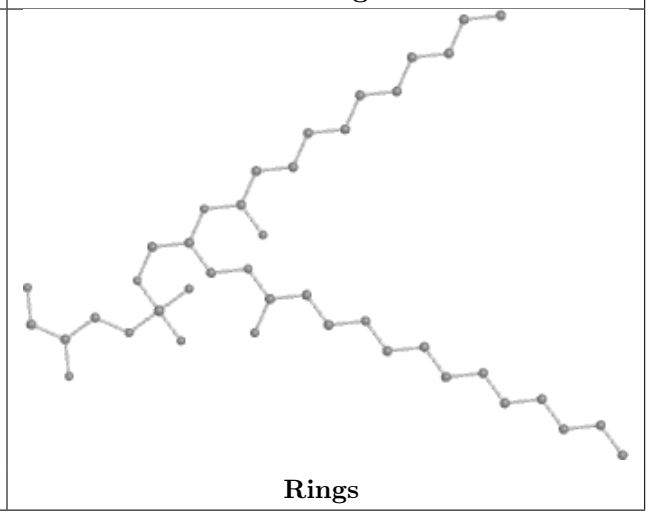
Bond lengths



Bond angles

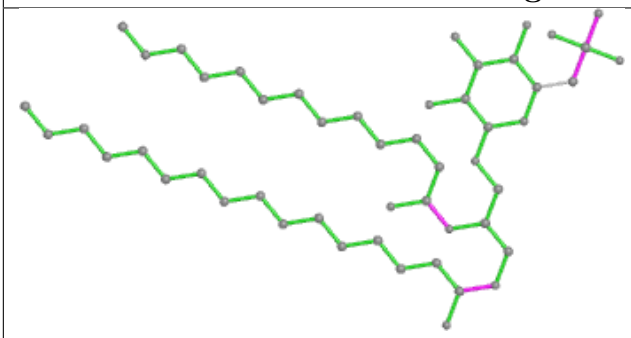


Torsions

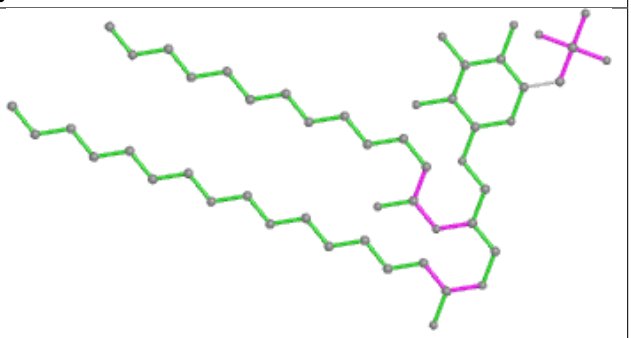


Rings

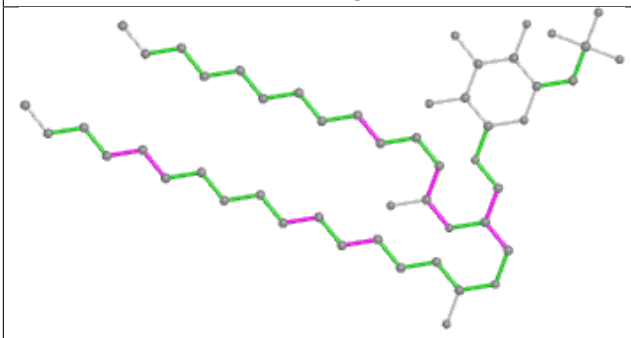
Ligand SQD C 620



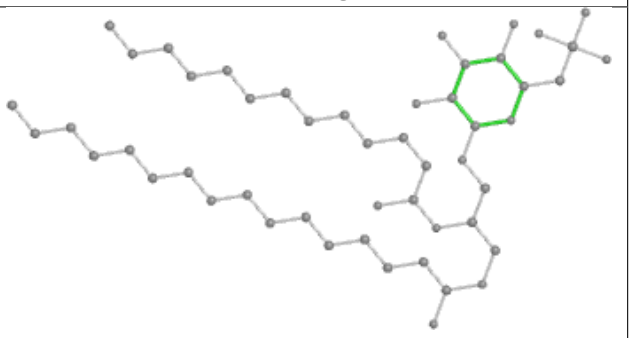
Bond lengths



Bond angles



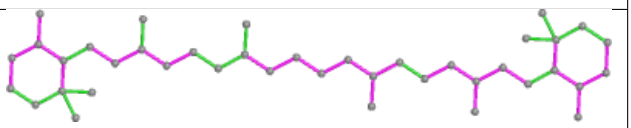
Torsions



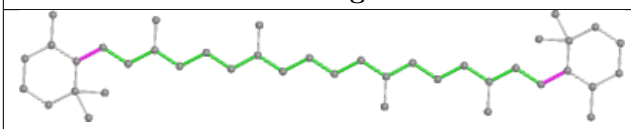
Rings

Ligand BCR B 618

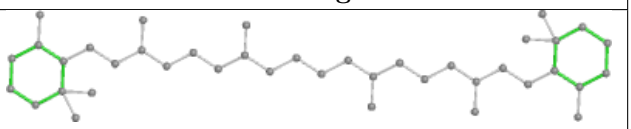
Bond lengths



Bond angles

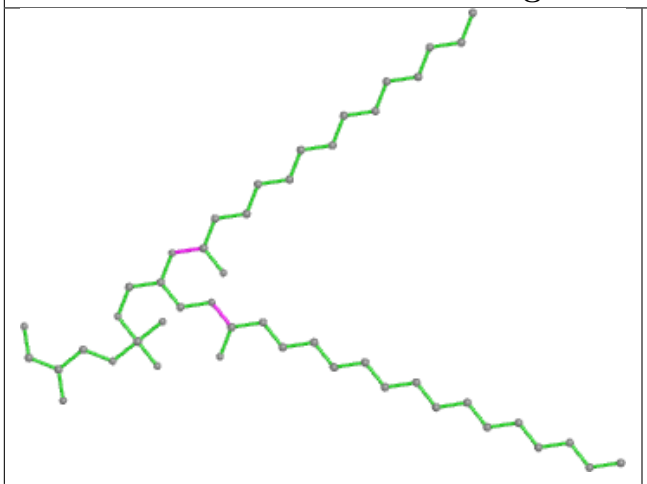


Torsions

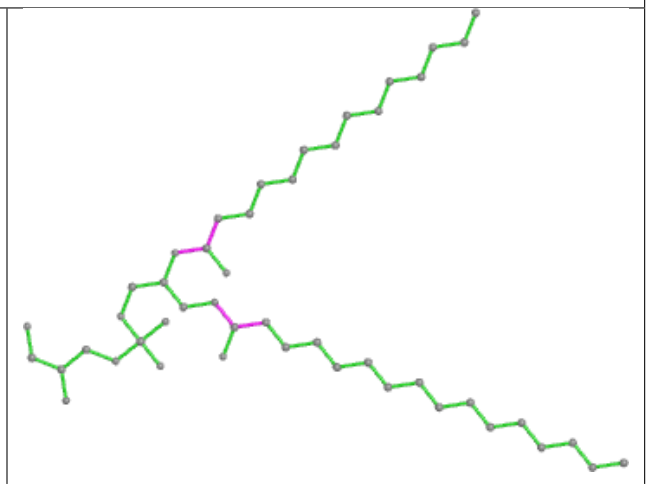


Rings

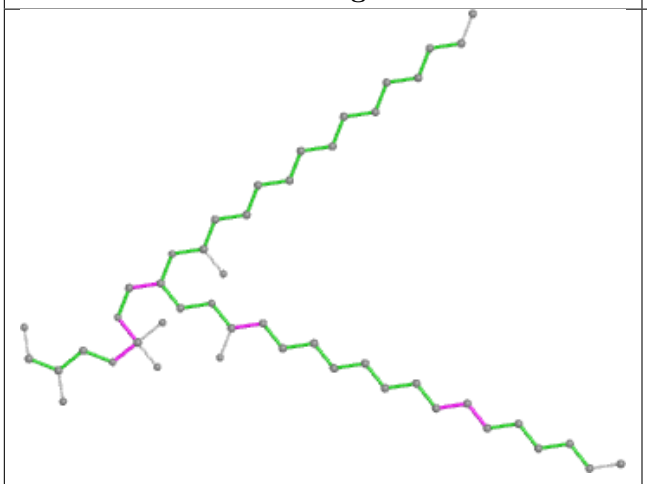
Ligand LHG B 622



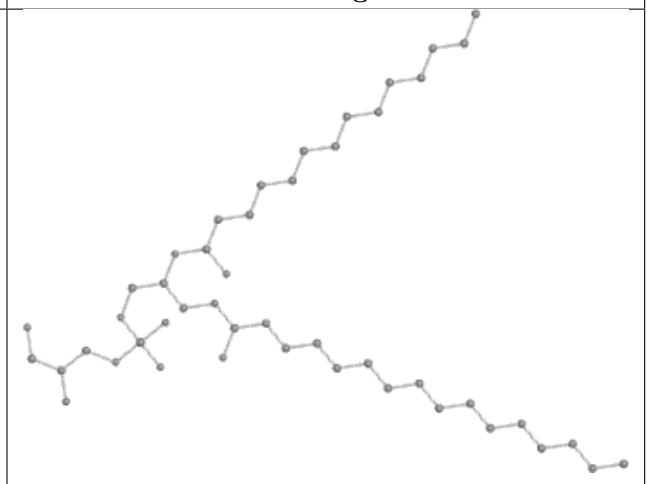
Bond lengths



Bond angles

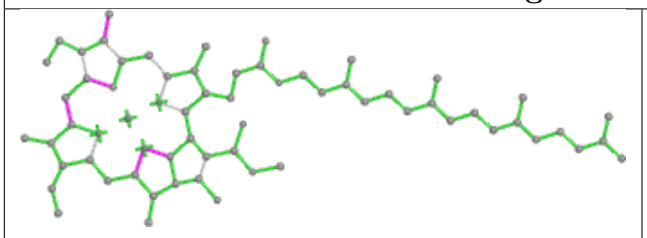


Torsions

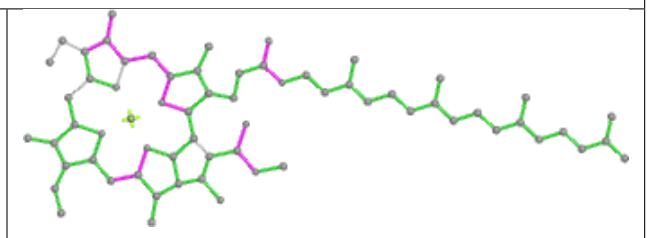


Rings

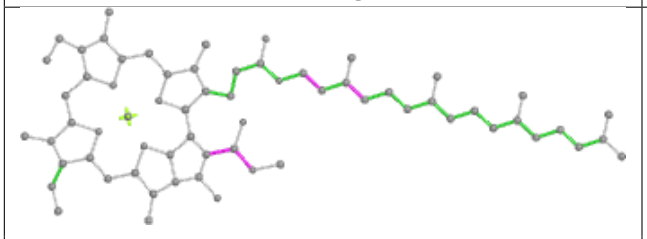
Ligand CLA B 615



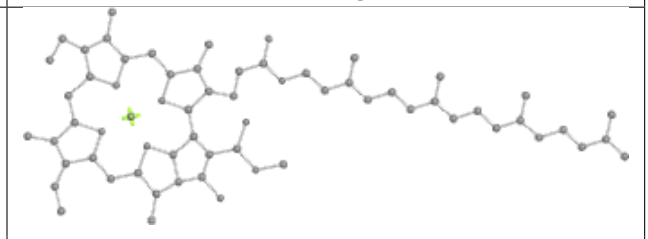
Bond lengths



Bond angles

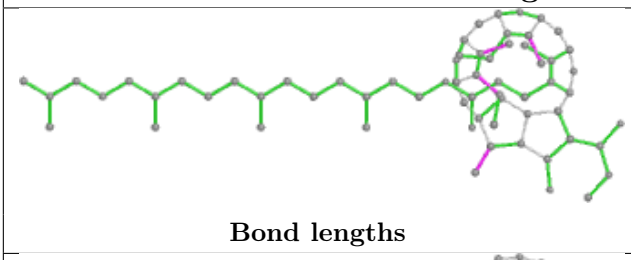


Torsions

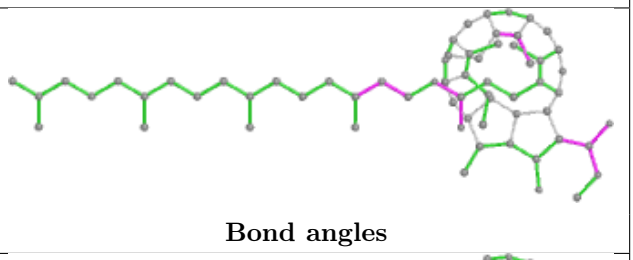


Rings

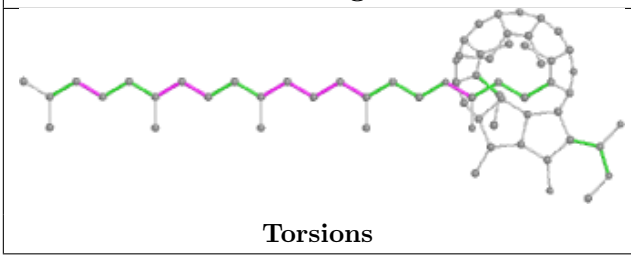
Ligand PHO D 411



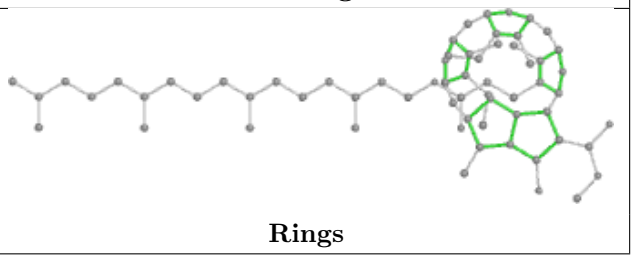
Bond lengths



Bond angles

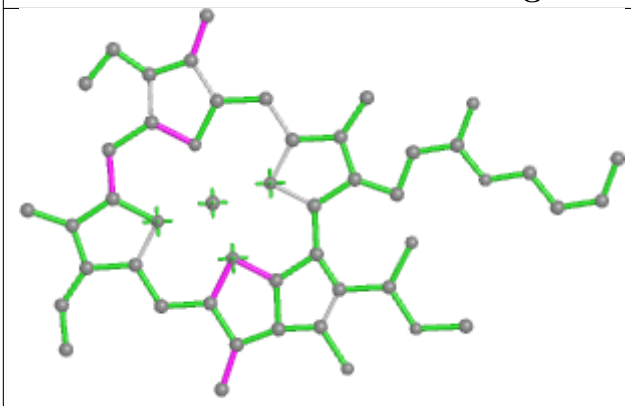


Torsions

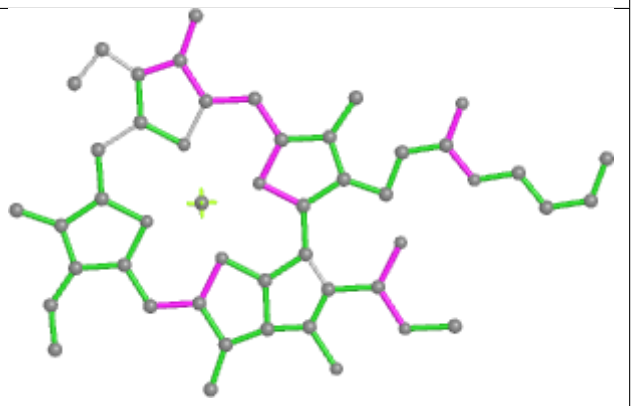


Rings

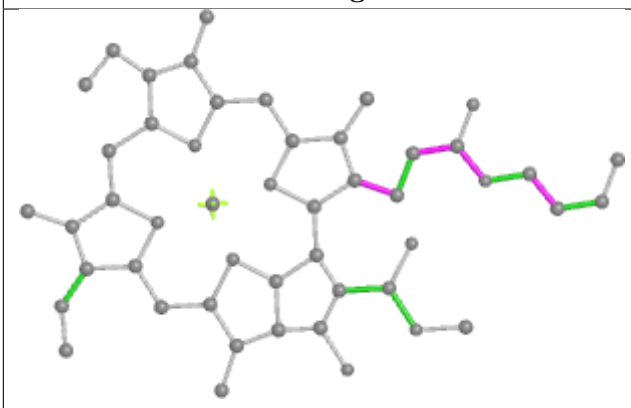
Ligand CLA A 403



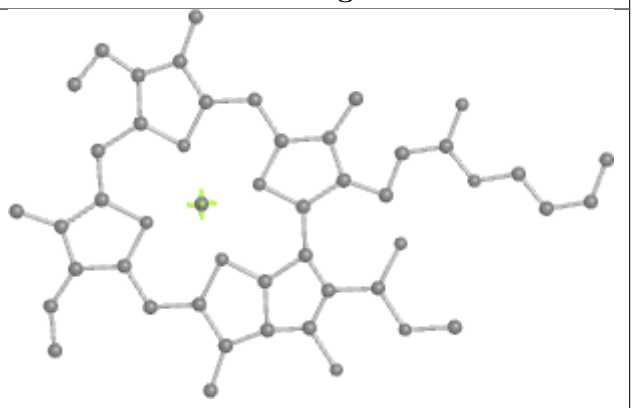
Bond lengths



Bond angles

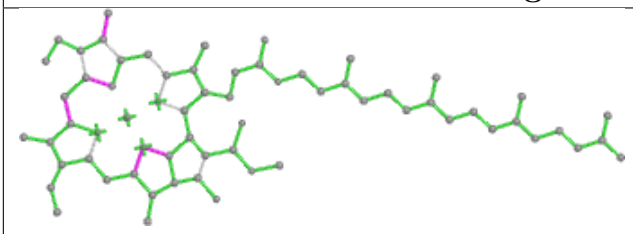


Torsions

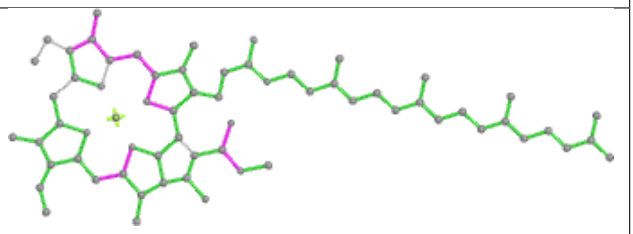


Rings

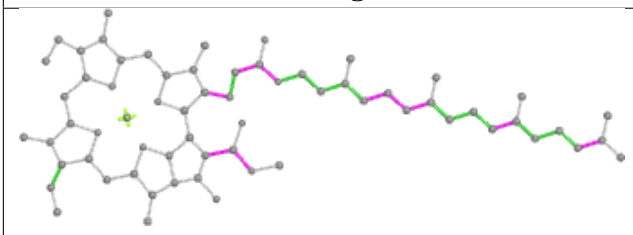
Ligand CLA B 607



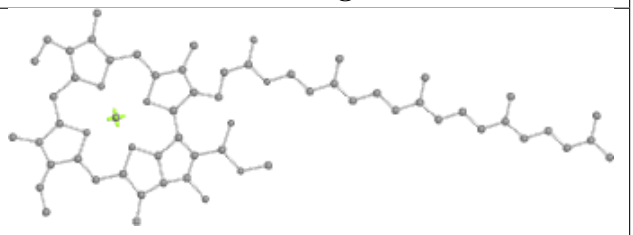
Bond lengths



Bond angles

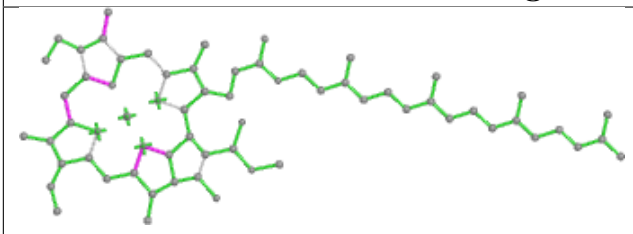


Torsions

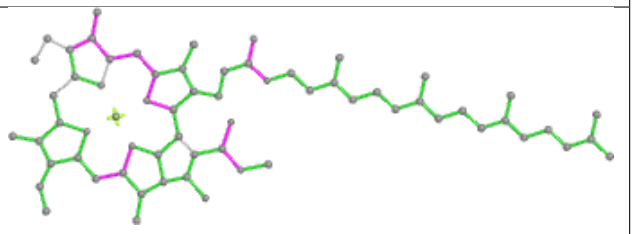


Rings

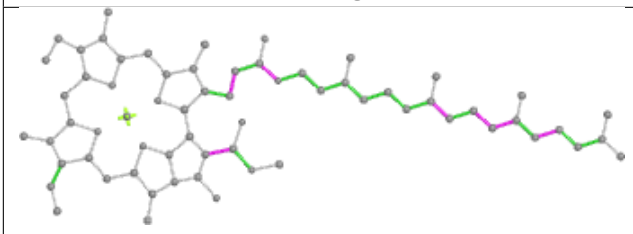
Ligand CLA B 616



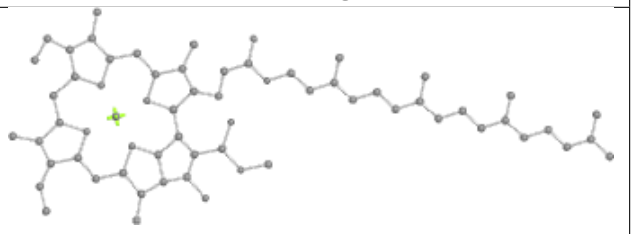
Bond lengths



Bond angles

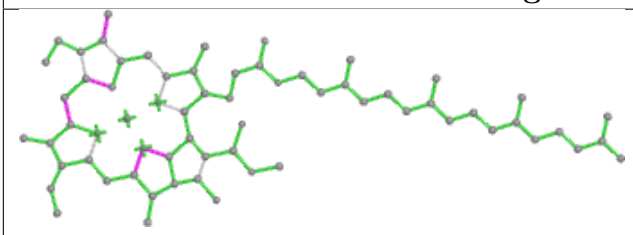


Torsions

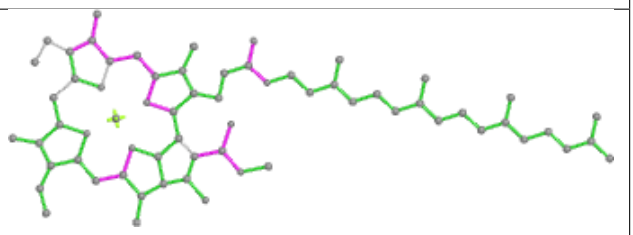


Rings

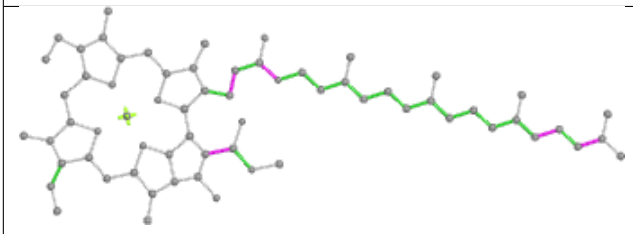
Ligand CLA D 410



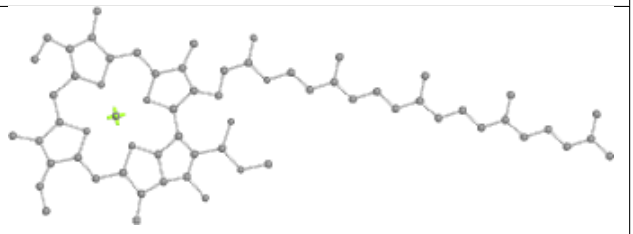
Bond lengths



Bond angles

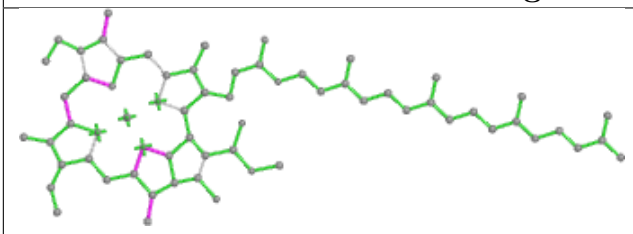


Torsions

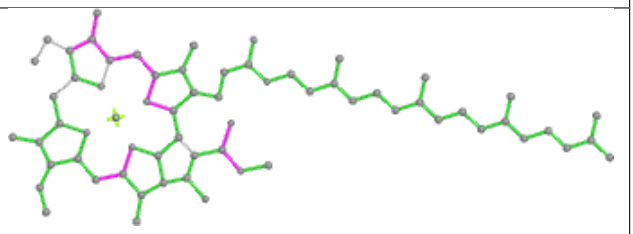


Rings

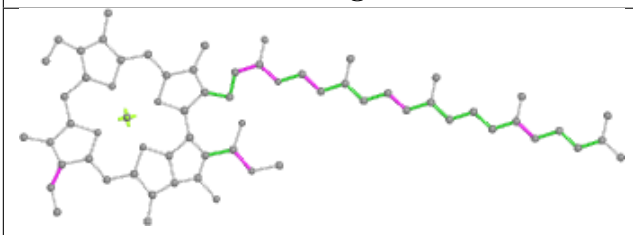
Ligand CLA A 402



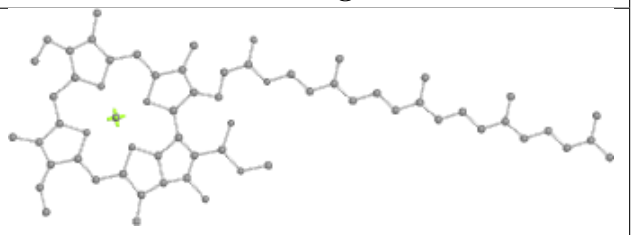
Bond lengths



Bond angles

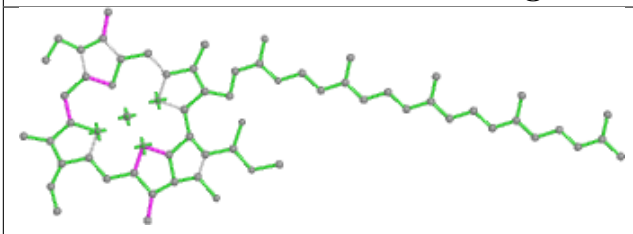


Torsions

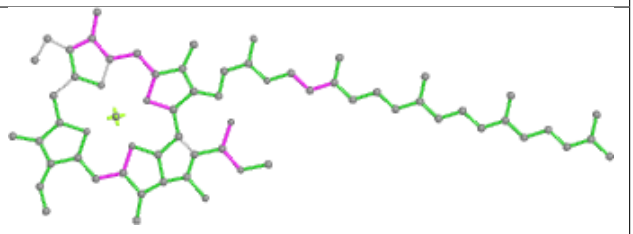


Rings

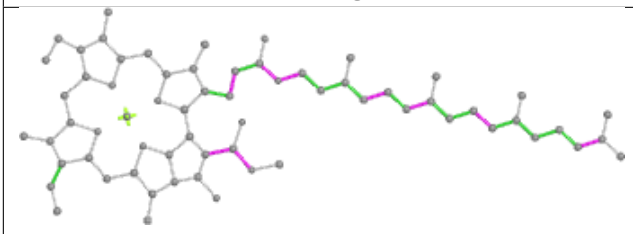
Ligand CLA B 613



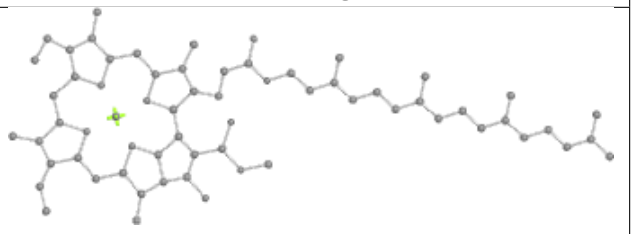
Bond lengths



Bond angles

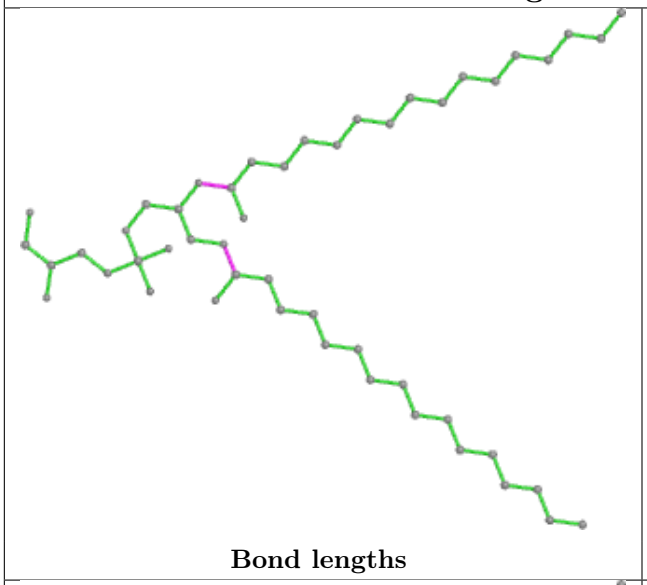


Torsions

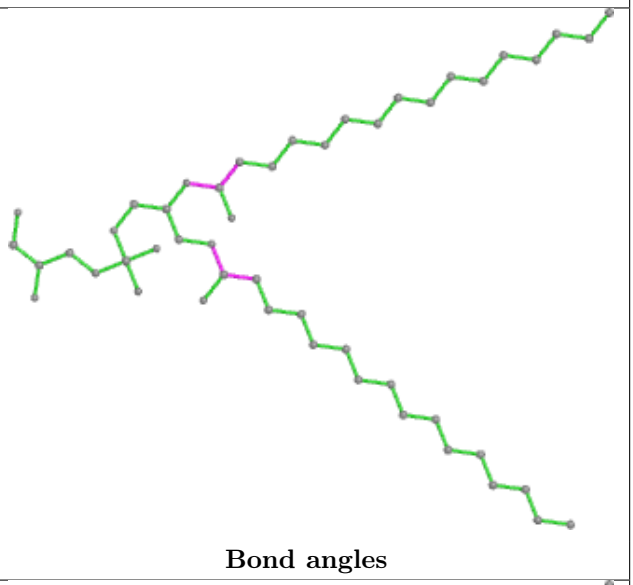


Rings

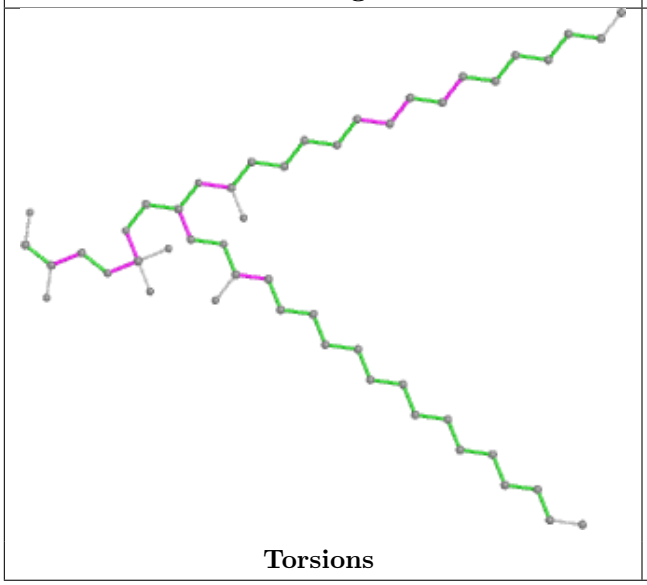
Ligand LHG L 101



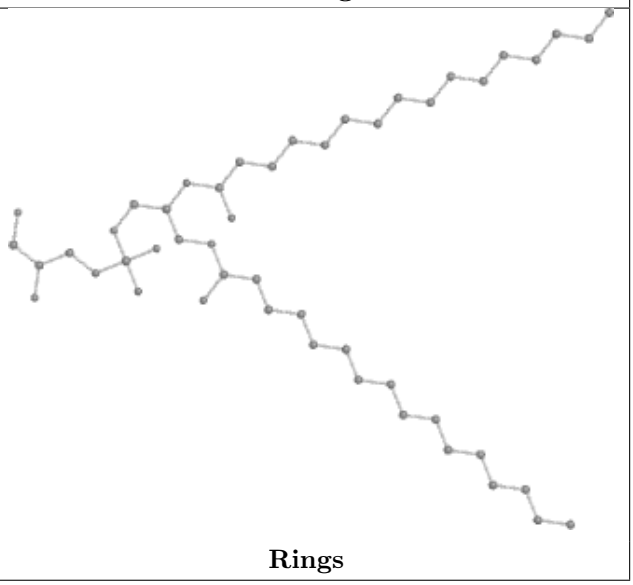
Bond lengths



Bond angles

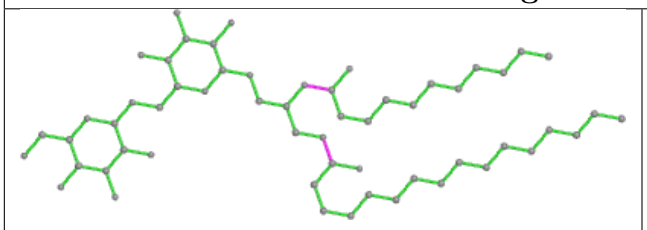


Torsions

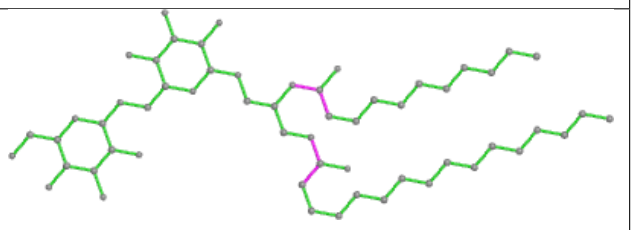


Rings

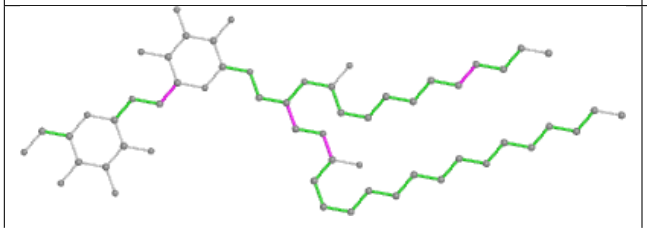
Ligand DGD C 618



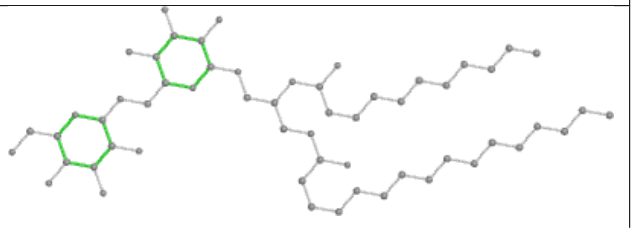
Bond lengths



Bond angles

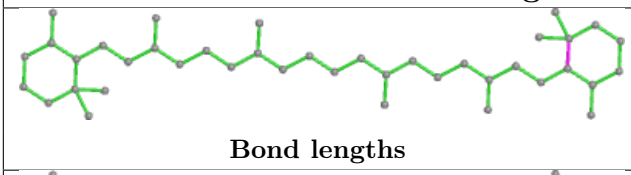


Torsions

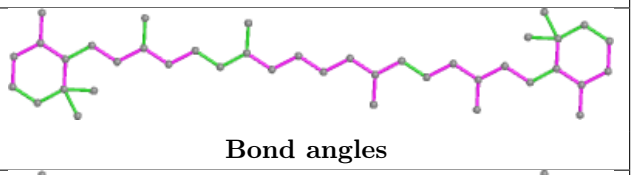


Rings

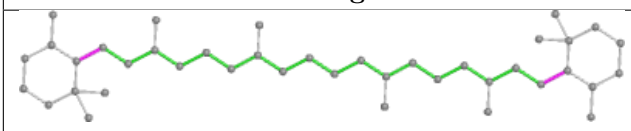
Ligand BCR B 617



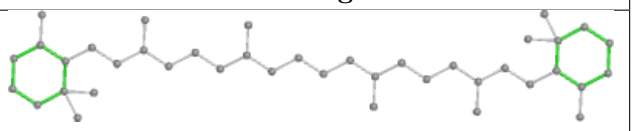
Bond lengths



Bond angles

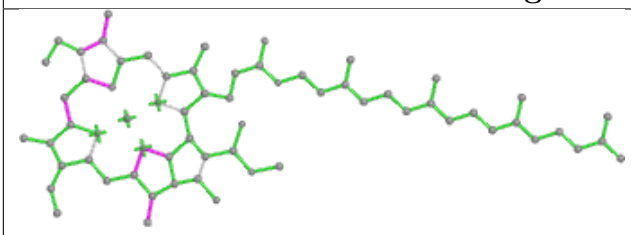


Torsions

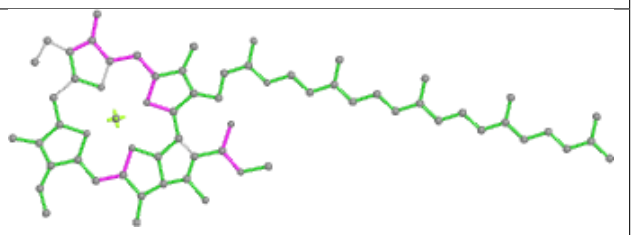


Rings

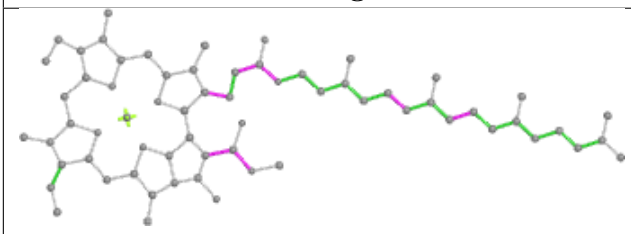
Ligand CLA B 606



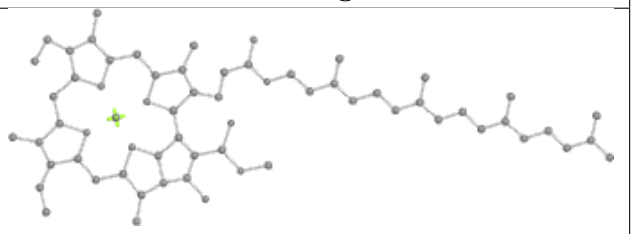
Bond lengths



Bond angles

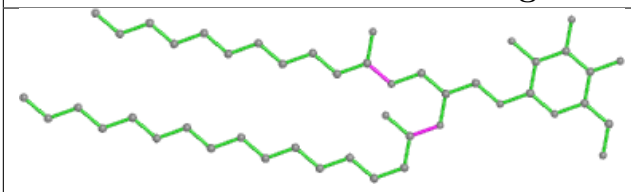


Torsions

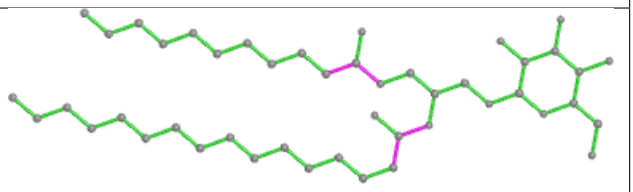


Rings

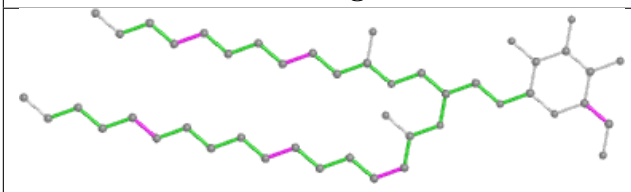
Ligand LMG D 408



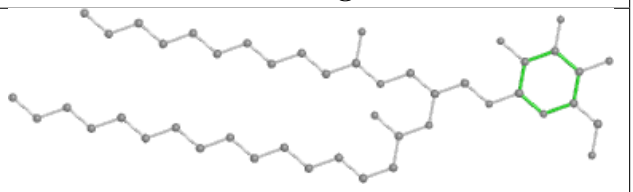
Bond lengths



Bond angles

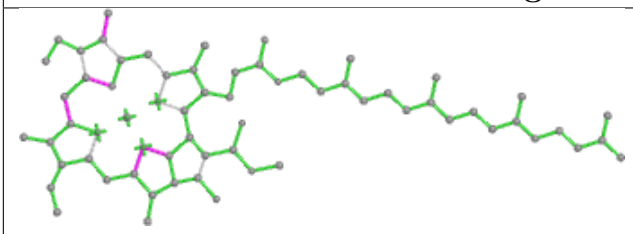


Torsions

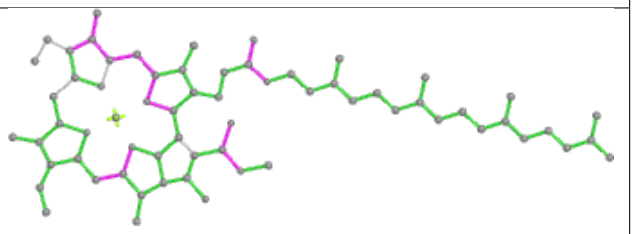


Rings

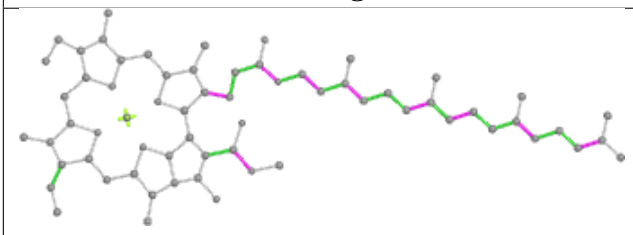
Ligand CLA C 606



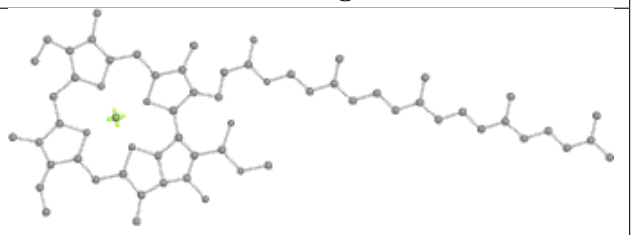
Bond lengths



Bond angles

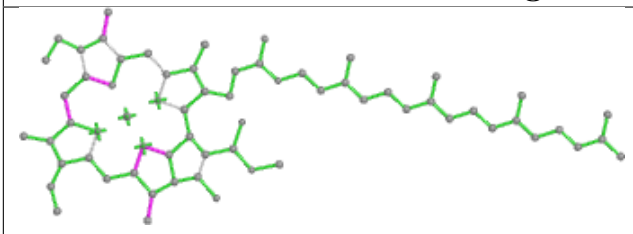


Torsions

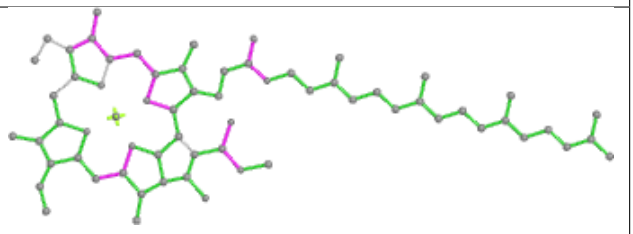


Rings

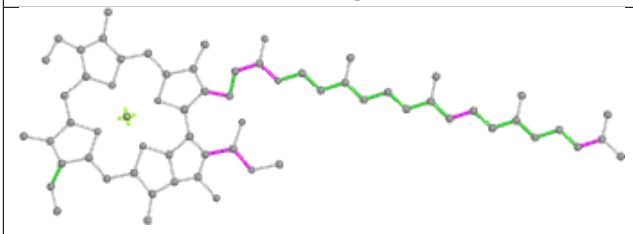
Ligand CLA B 609



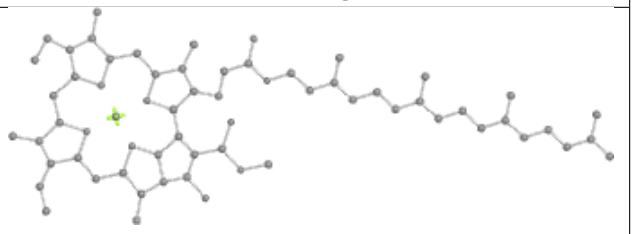
Bond lengths



Bond angles

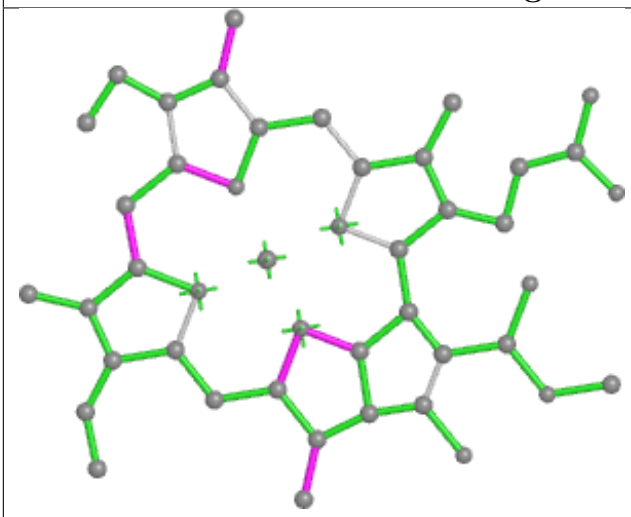


Torsions

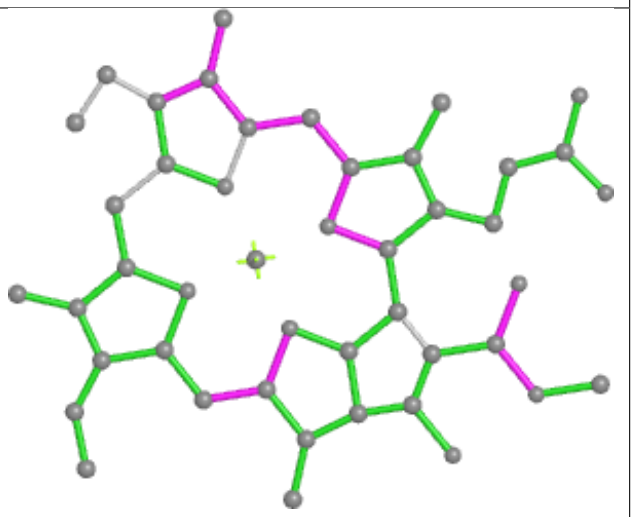


Rings

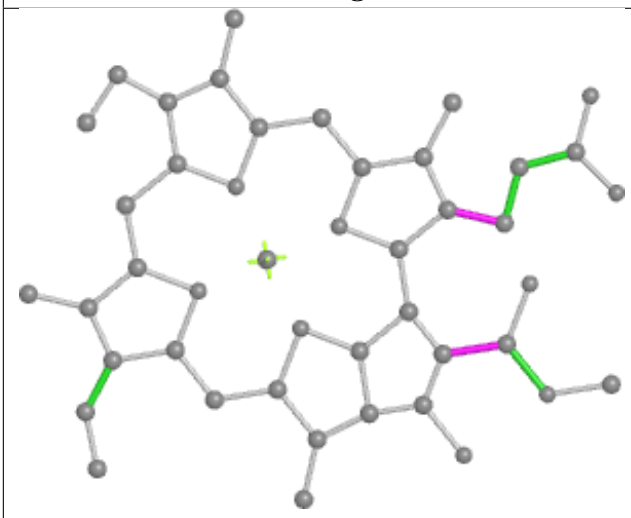
Ligand CLA B 614



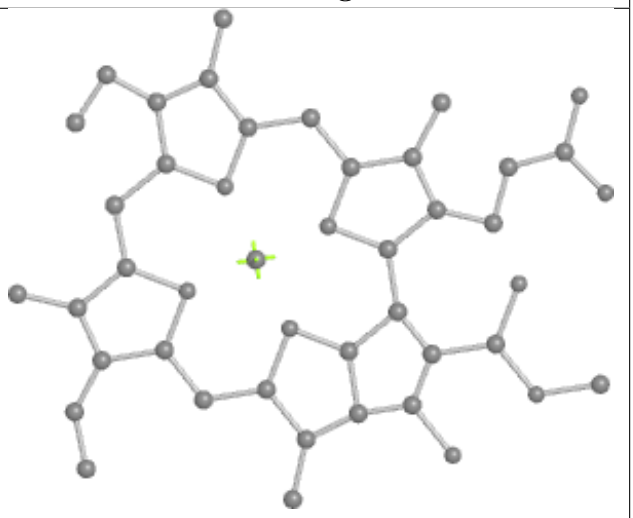
Bond lengths



Bond angles

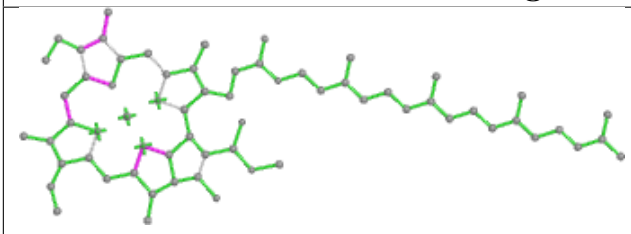


Torsions

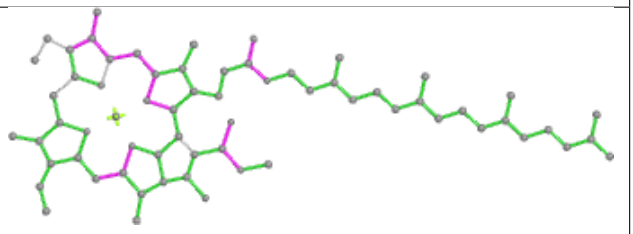


Rings

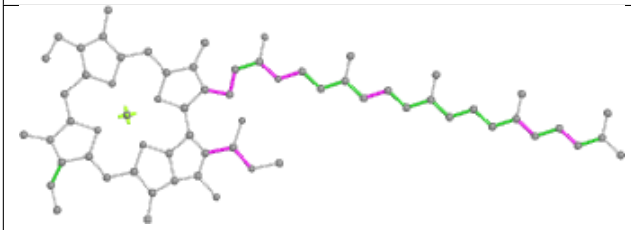
Ligand CLA C 612



Bond lengths



Bond angles



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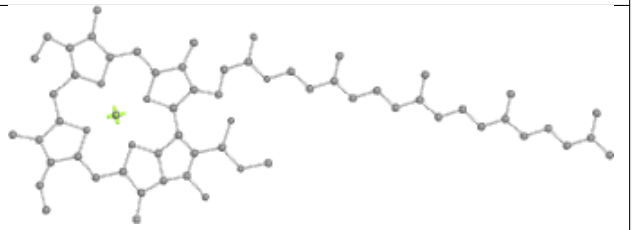
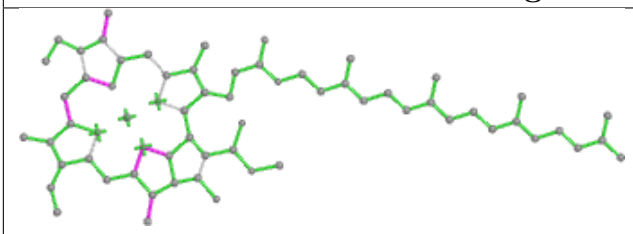
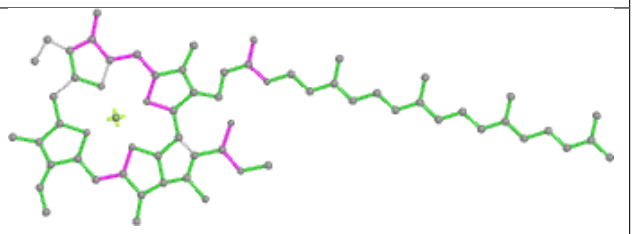


Rings

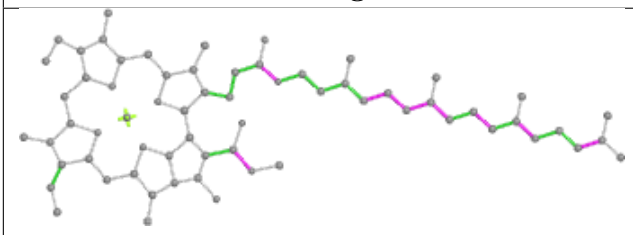
Ligand CLA C 614



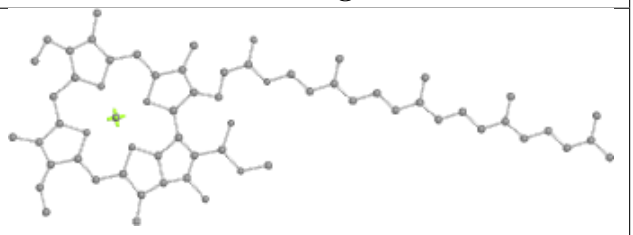
Bond lengths



Bond angles

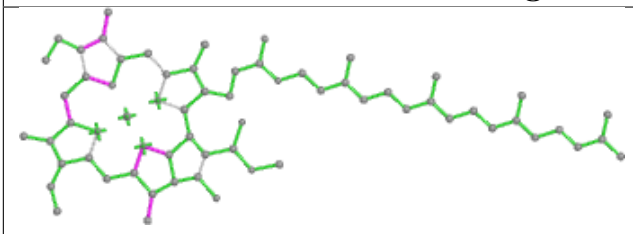


Torsions

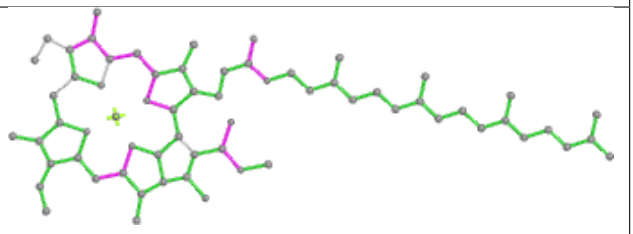


Rings

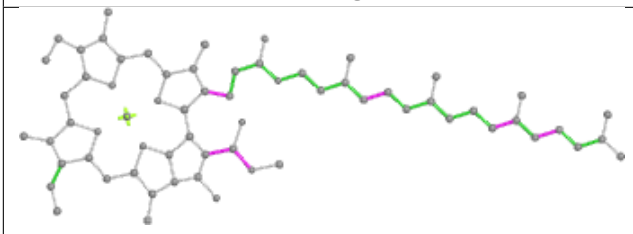
Ligand CLA B 603



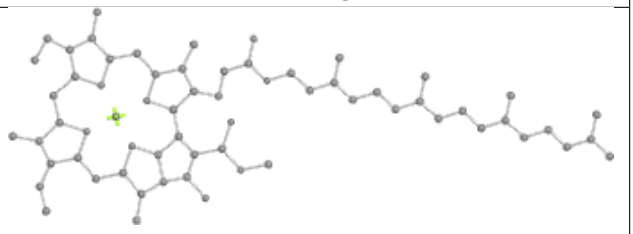
Bond lengths



Bond angles

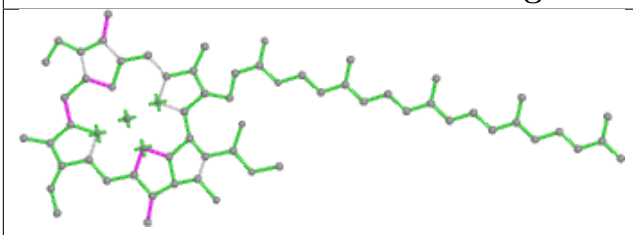


Torsions

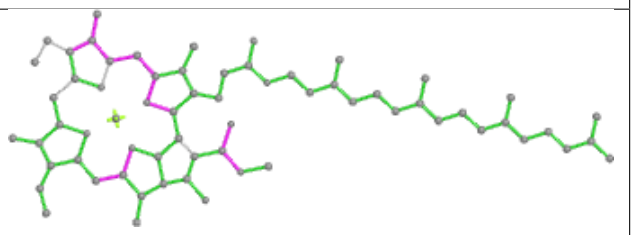


Rings

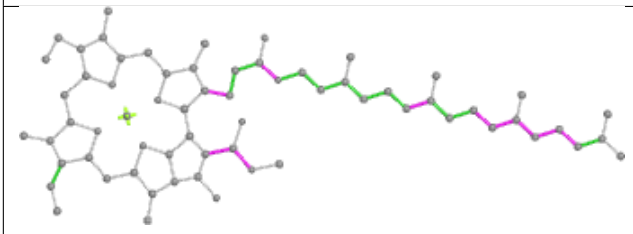
Ligand CLA C 602



Bond lengths



Bond angles



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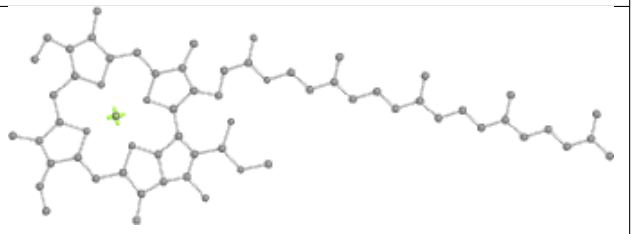
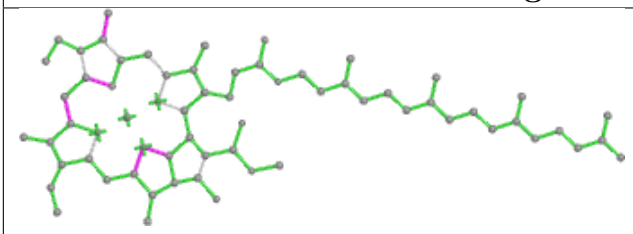
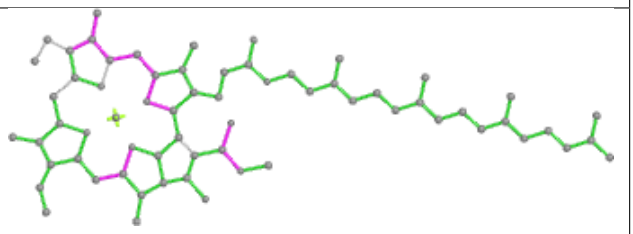
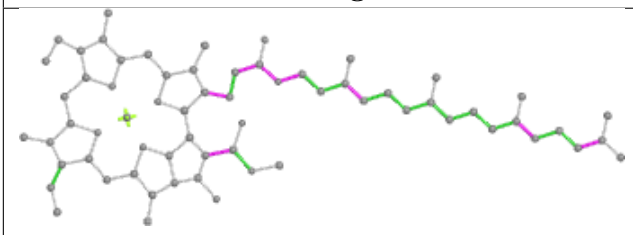


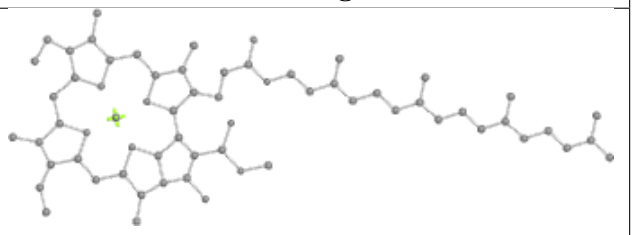
Rings

Ligand CLA C 613

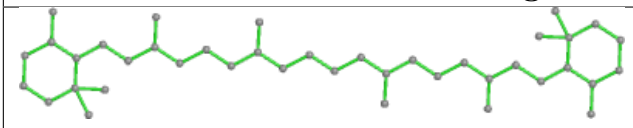

Bond lengths

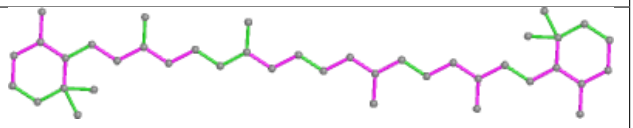

Bond angles

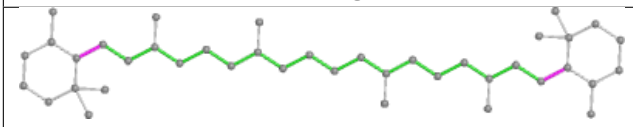

Torsions


Rings

Ligand BCR B 619

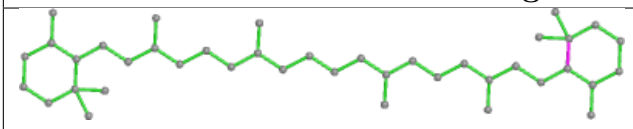

Bond lengths

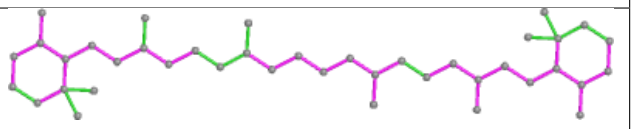

Bond angles

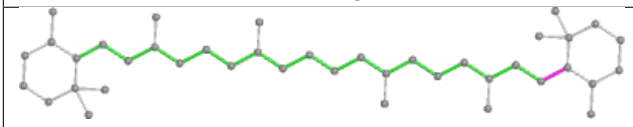

Torsions


Rings

Ligand BCR C 615

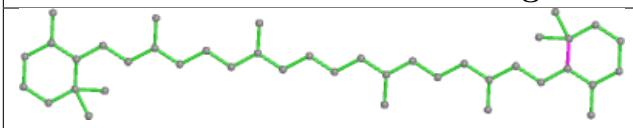

Bond lengths

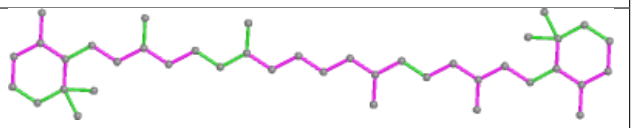

Bond angles

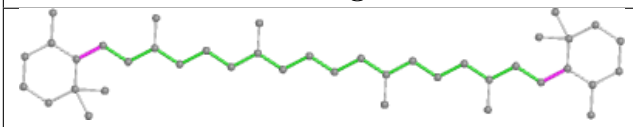

Torsions


Rings

Ligand BCR A 405

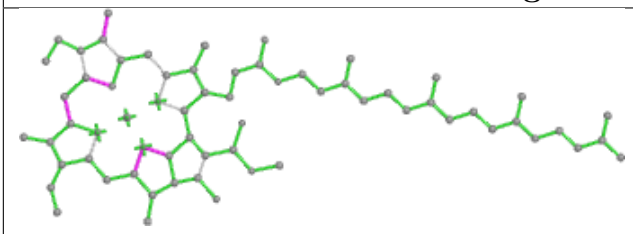

Bond lengths


Bond angles

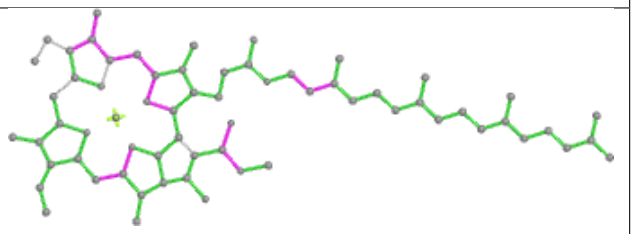

Torsions


Rings

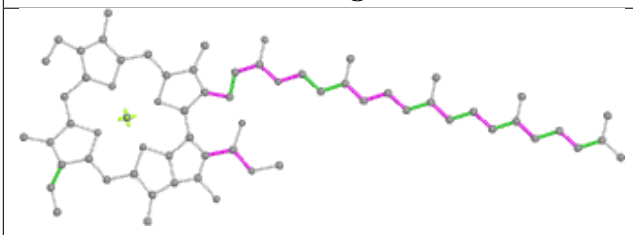
Ligand CLA D 403



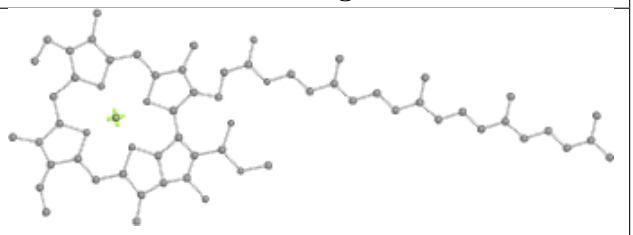
Bond lengths



Bond angles

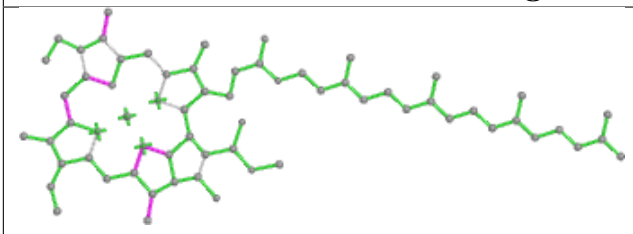


Torsions

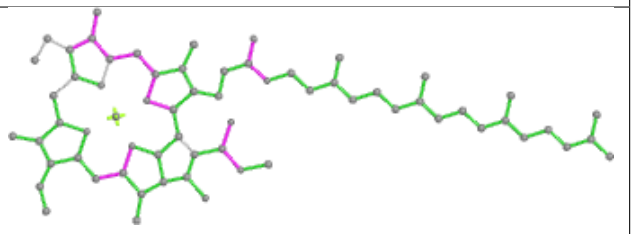


Rings

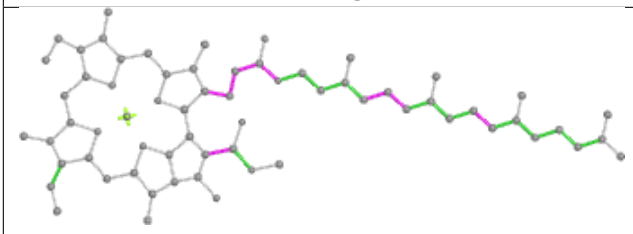
Ligand CLA B 602



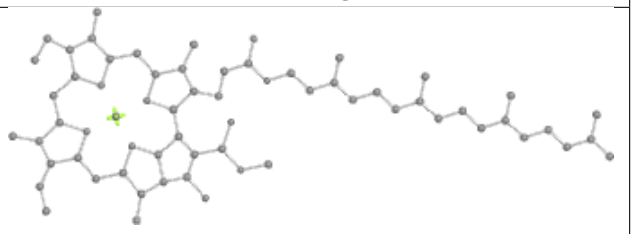
Bond lengths



Bond angles

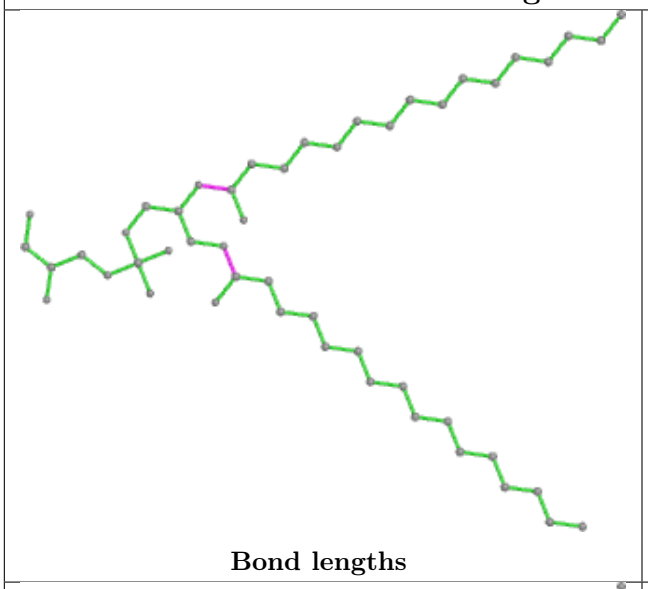


Torsions

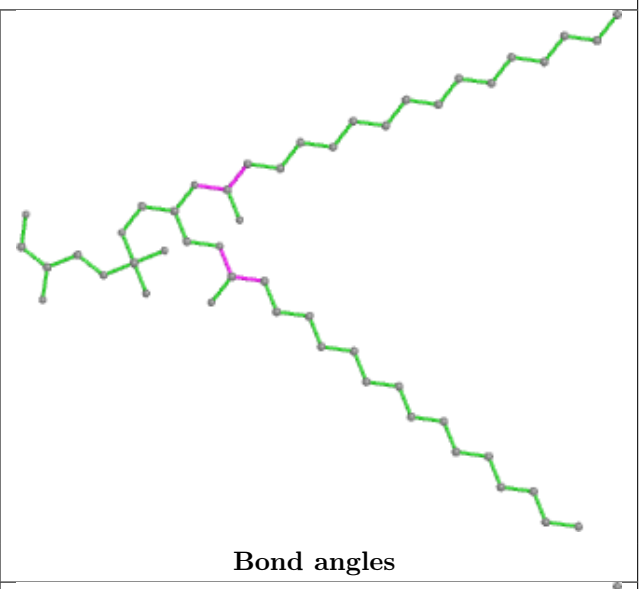


Rings

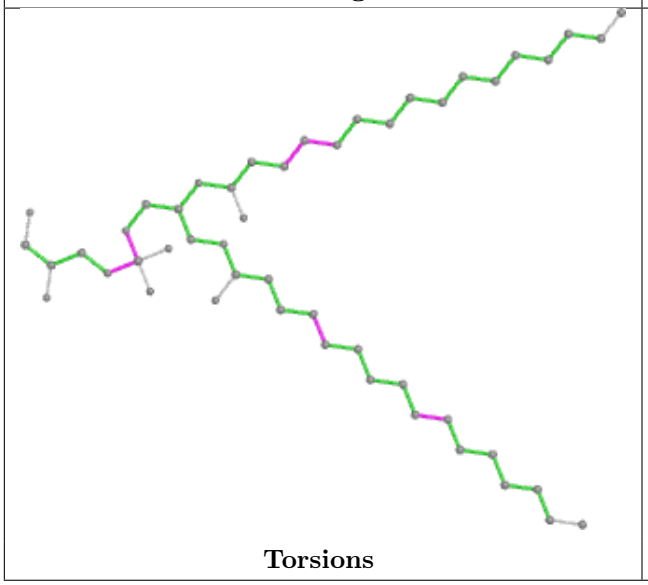
Ligand LHG D 406



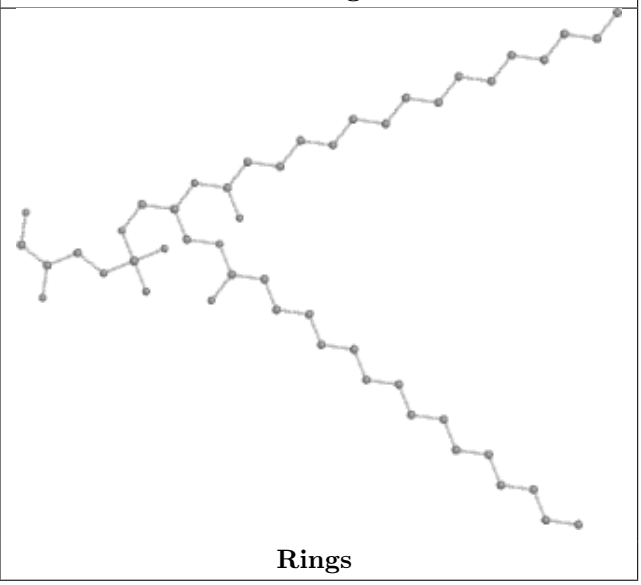
Bond lengths



Bond angles

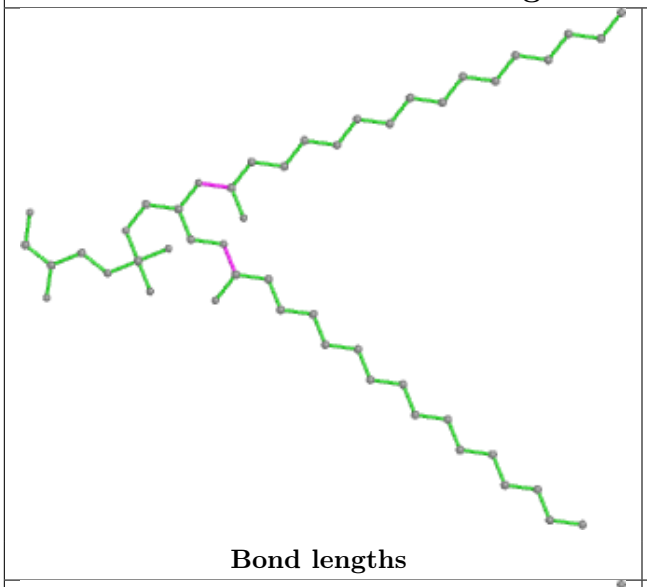


Torsions

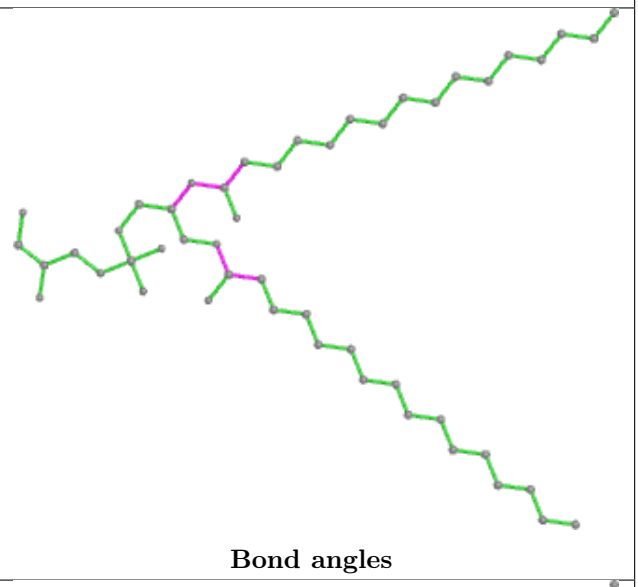


Rings

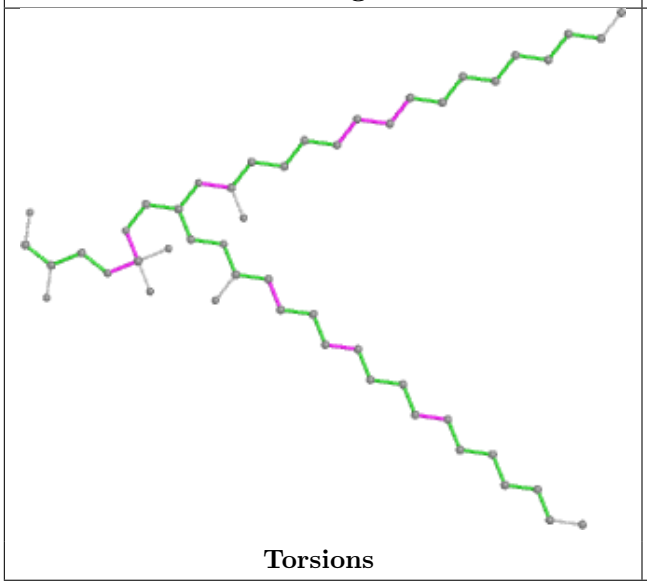
Ligand LHG D 409



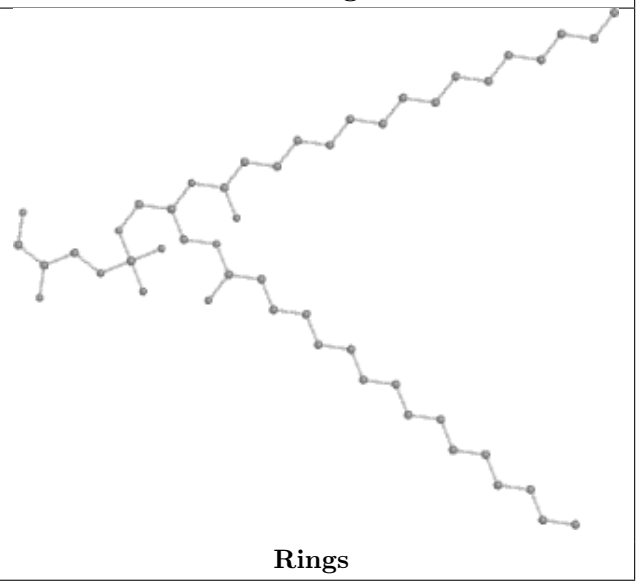
Bond lengths



Bond angles

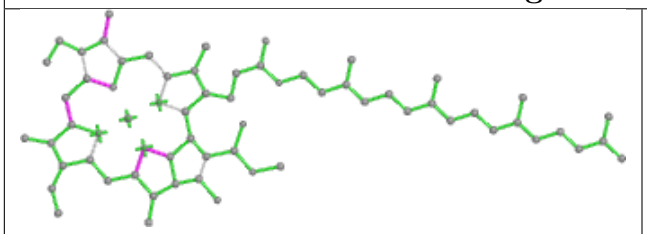


Torsions

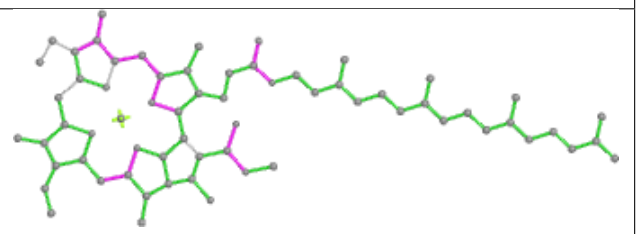


Rings

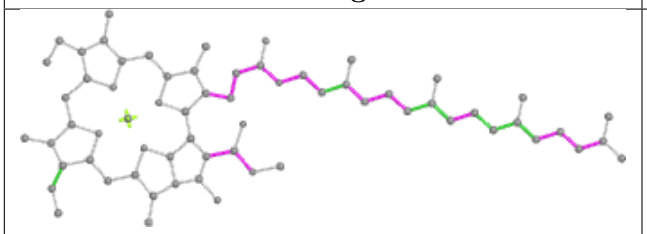
Ligand CLA C 607



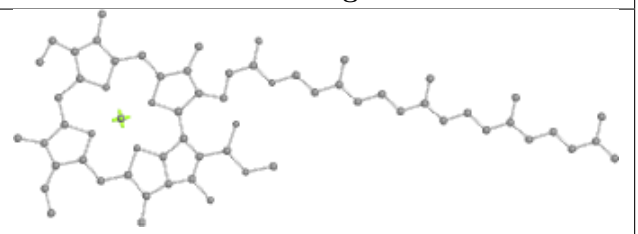
Bond lengths



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.

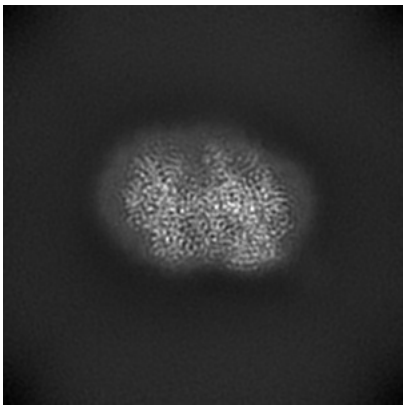
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60026. These allow visual inspection of the internal detail of the map and identification of artifacts.

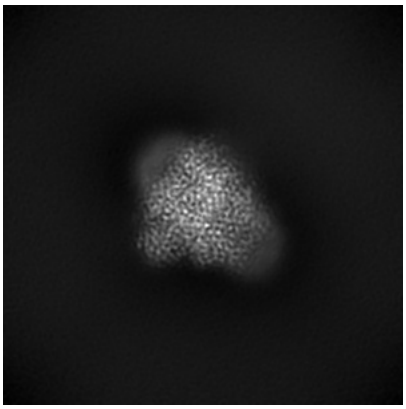
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

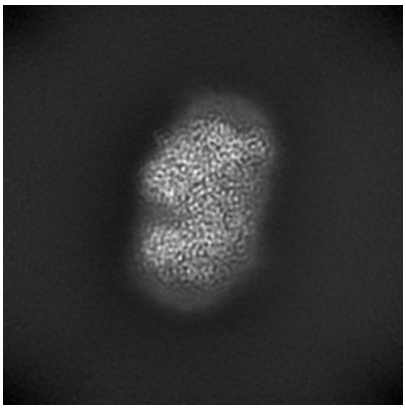
6.1.1 Primary map



X

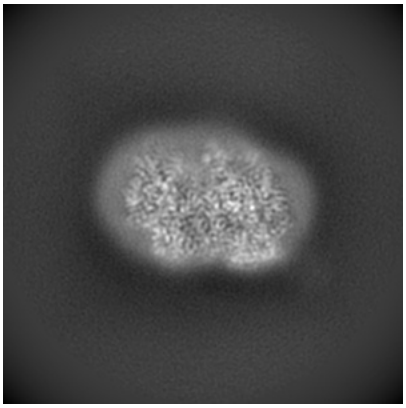


Y

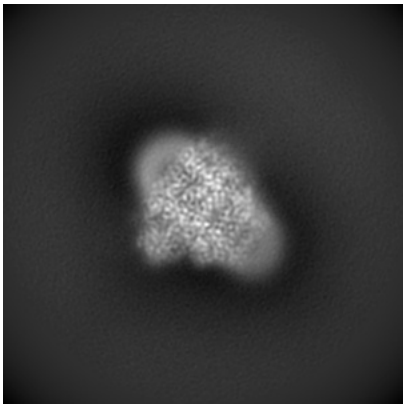


Z

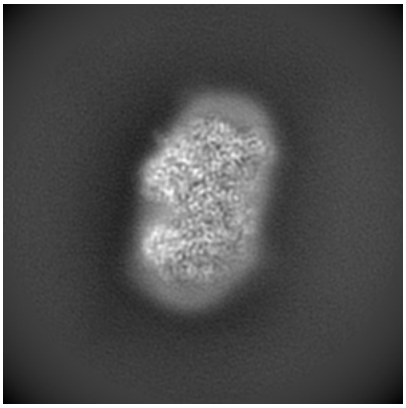
6.1.2 Raw map



X



Y

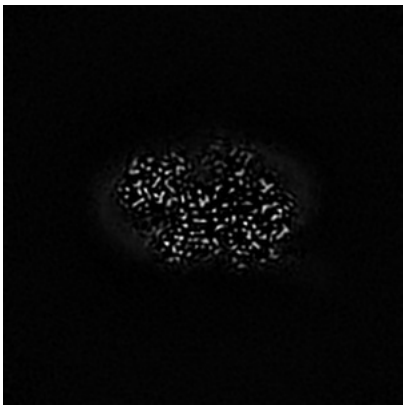


Z

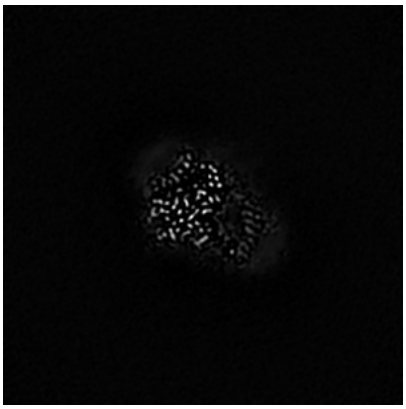
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

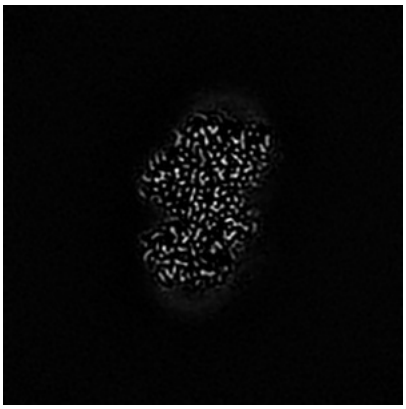
6.2.1 Primary map



X Index: 104

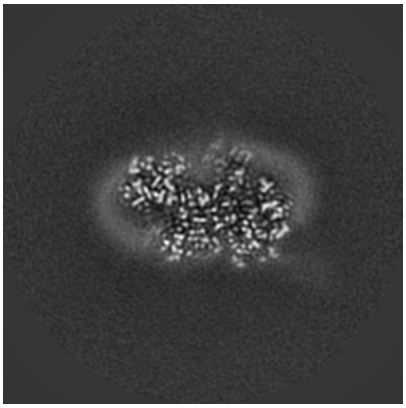


Y Index: 104

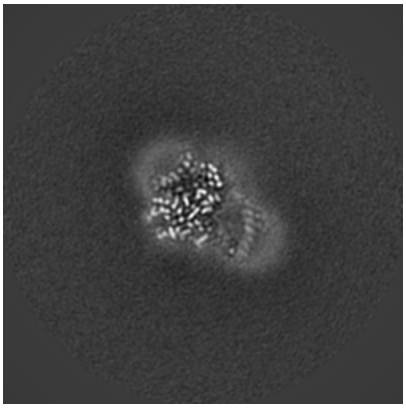


Z Index: 104

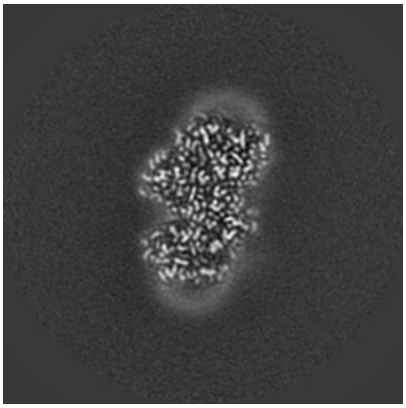
6.2.2 Raw map



X Index: 104



Y Index: 104

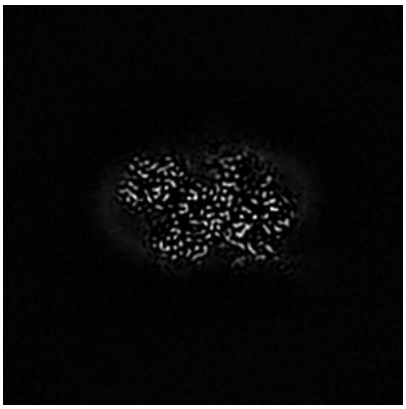


Z Index: 104

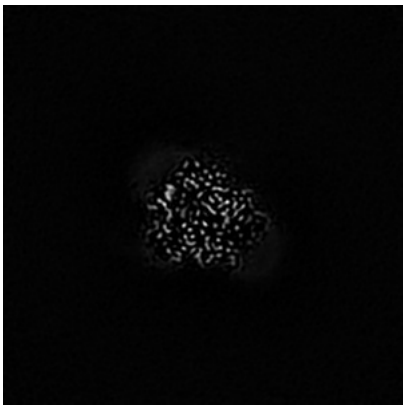
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

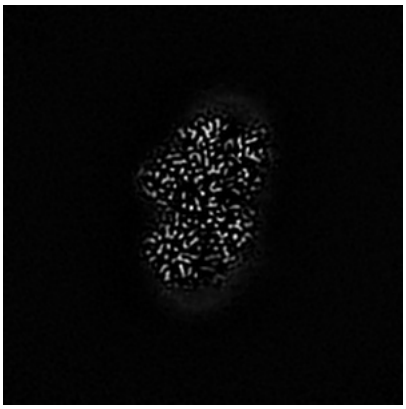
6.3.1 Primary map



X Index: 106

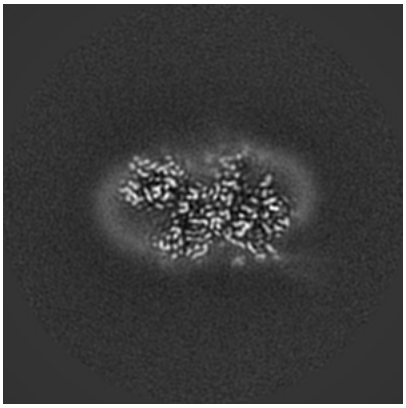


Y Index: 85

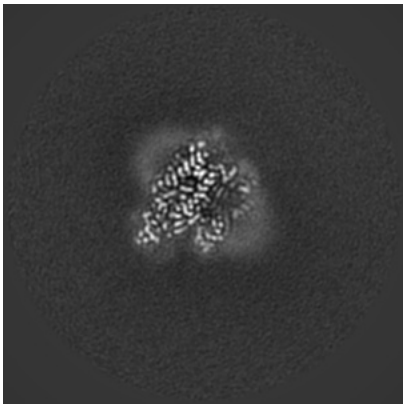


Z Index: 101

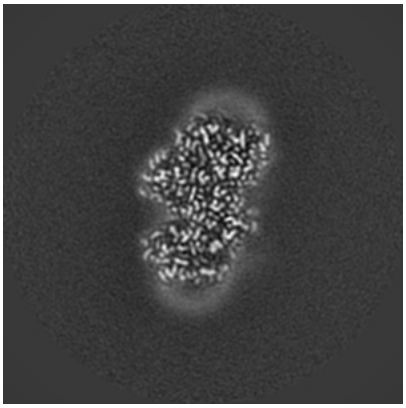
6.3.2 Raw map



X Index: 106



Y Index: 129

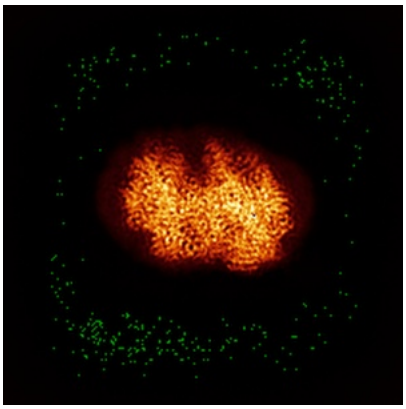


Z Index: 104

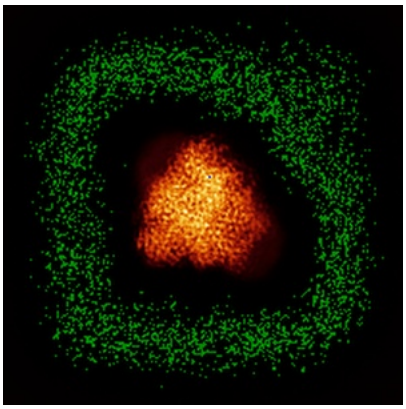
The images above show the largest variance slices of the map in three orthogonal directions.

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

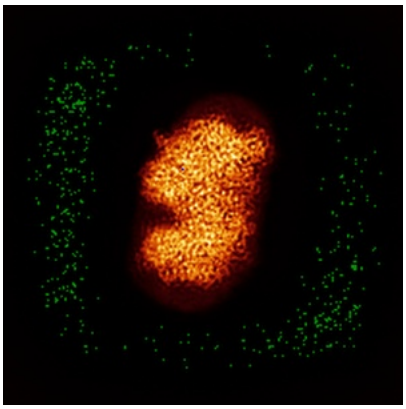
6.4.1 Primary map



X

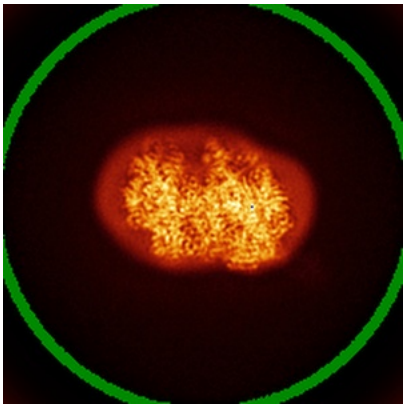


Y

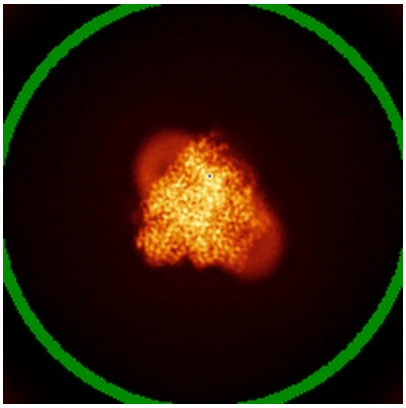


Z

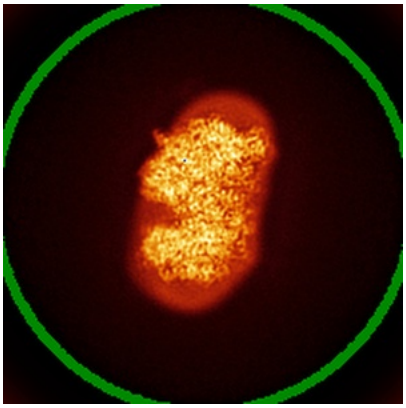
6.4.2 Raw map



X



Y

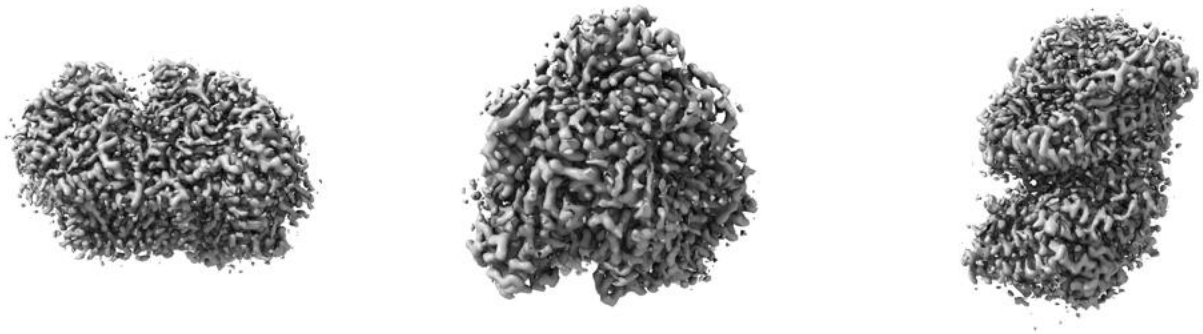


Z

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)

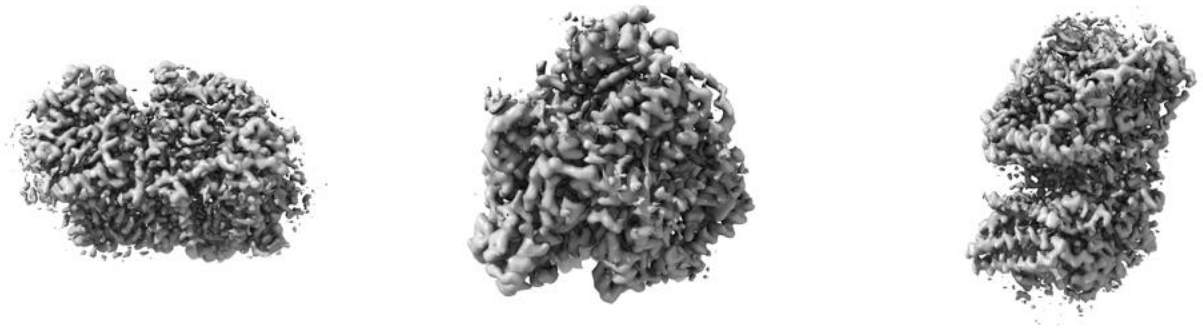
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. 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.

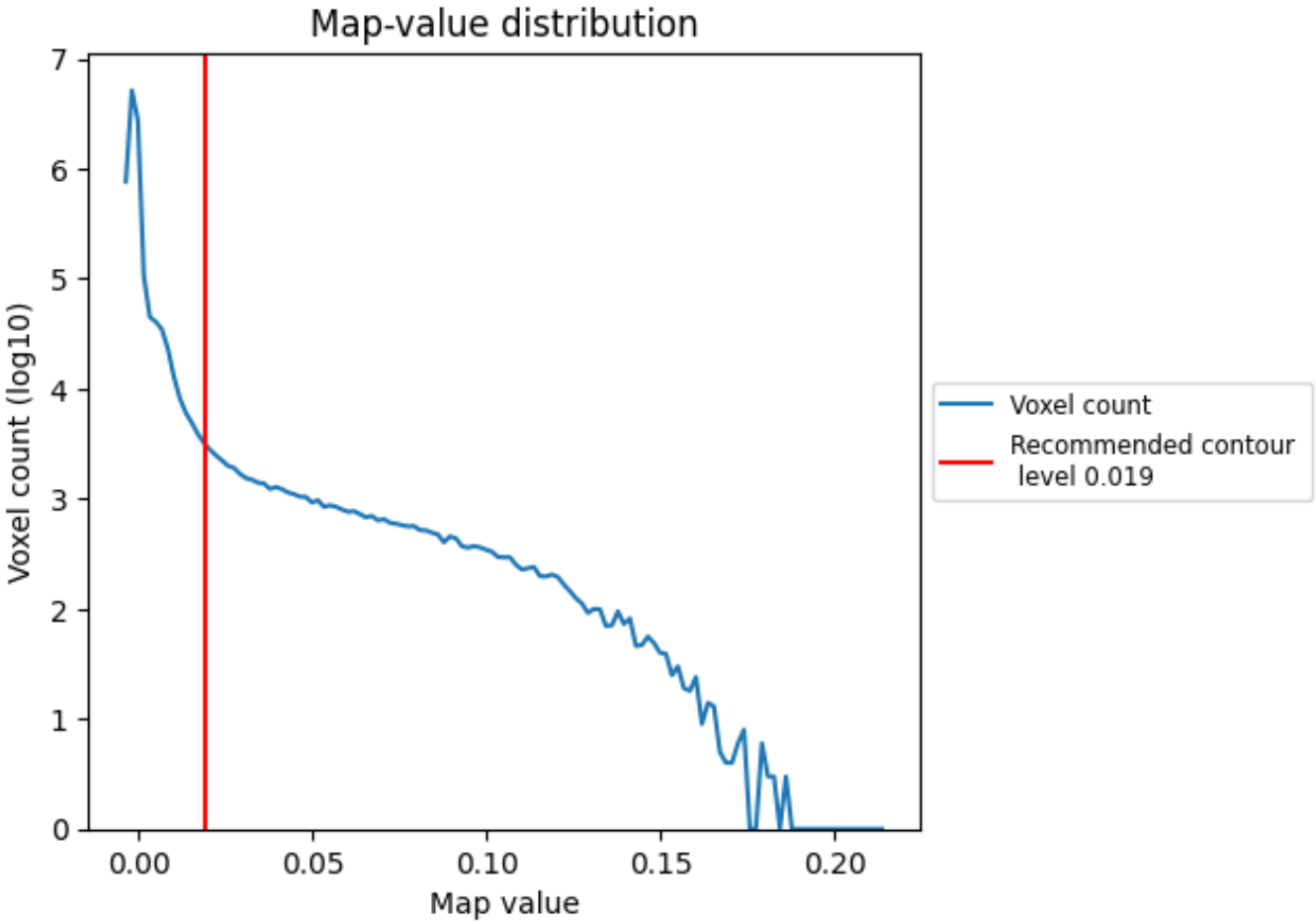
6.6 Mask visualisation (i)

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

7 Map analysis

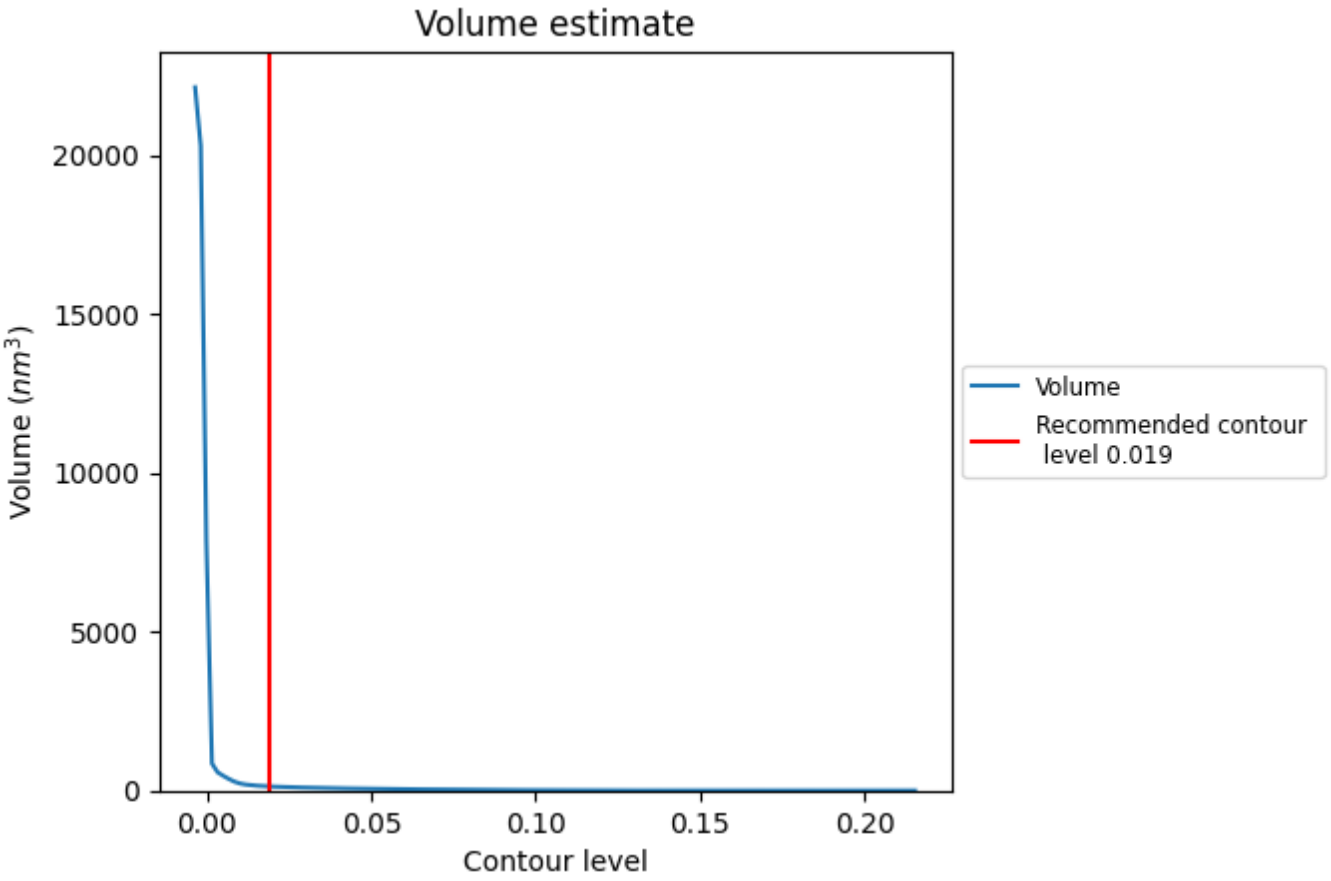
This section contains the results of statistical analysis of the map.

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.

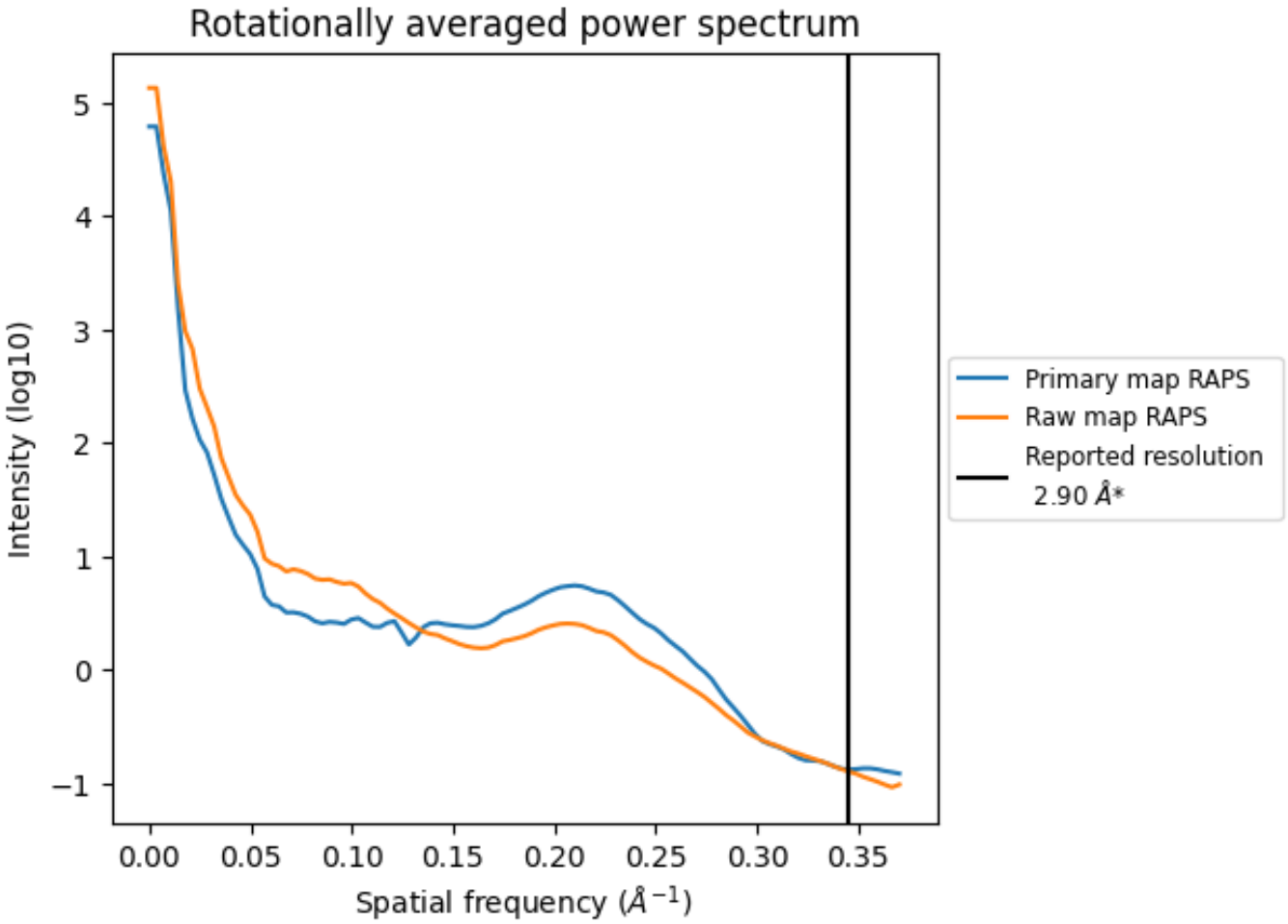
7.2 Volume estimate



The volume at the recommended contour level is 130 nm^3; this corresponds to an approximate mass of 117 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)

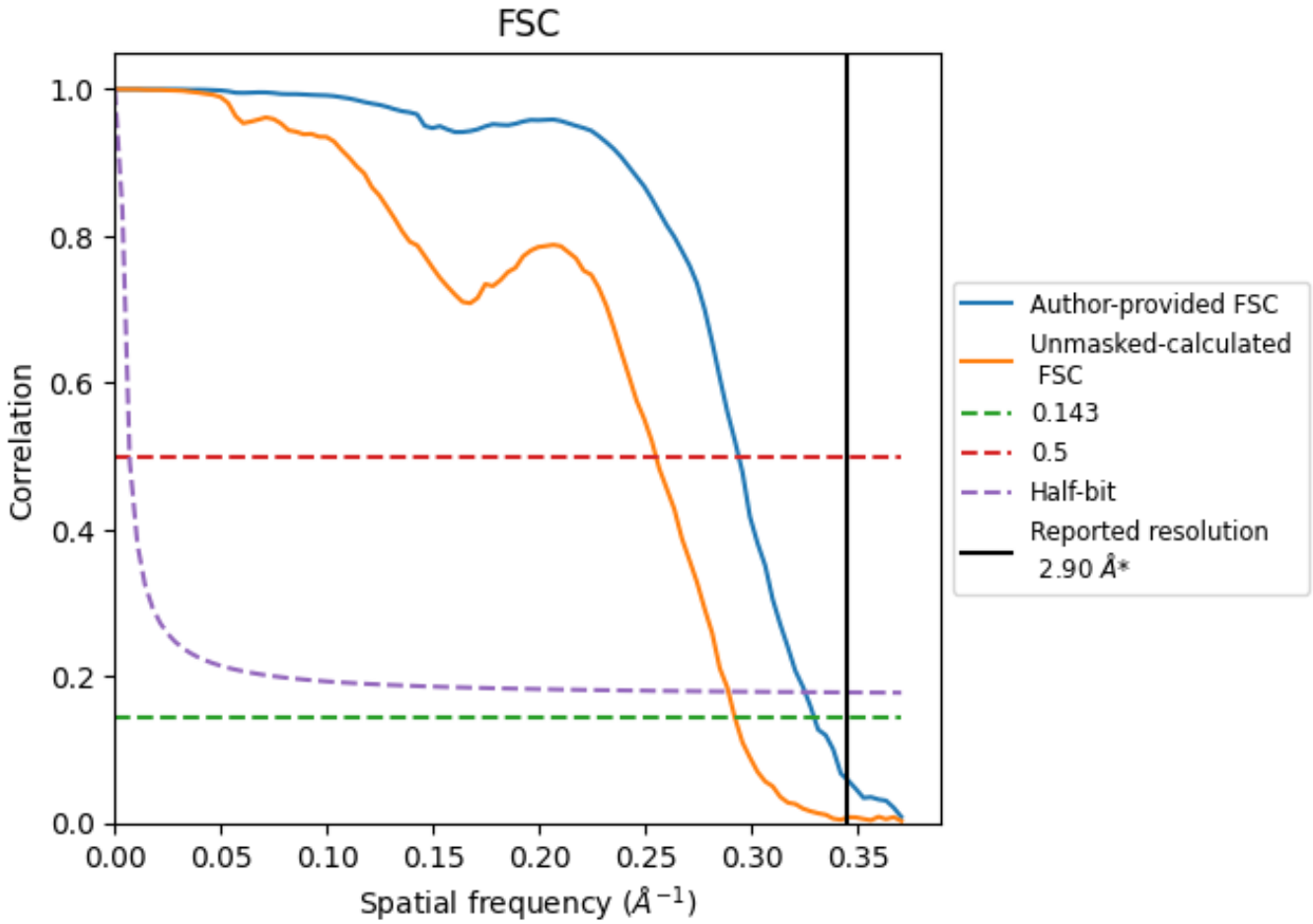


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

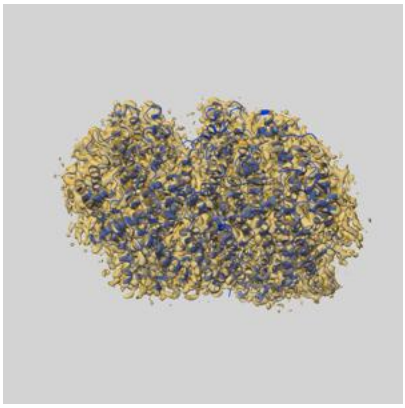
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	3.04	3.40	3.08
Unmasked-calculated*	3.42	3.92	3.46

*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 3.42 differs from the reported value 2.9 by more than 10 %

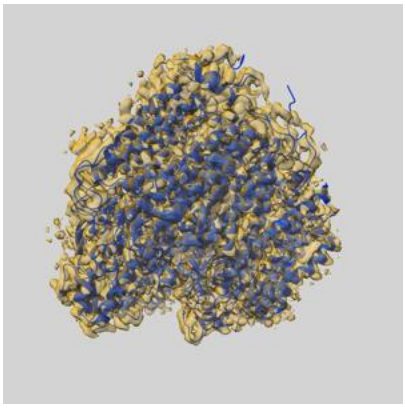
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60026 and PDB model 8ZEE. Per-residue inclusion information can be found in section 3 on page 17.

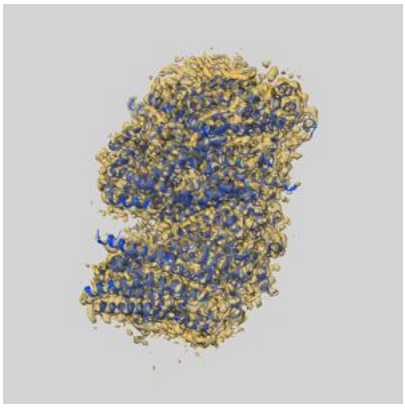
9.1 Map-model overlay



X



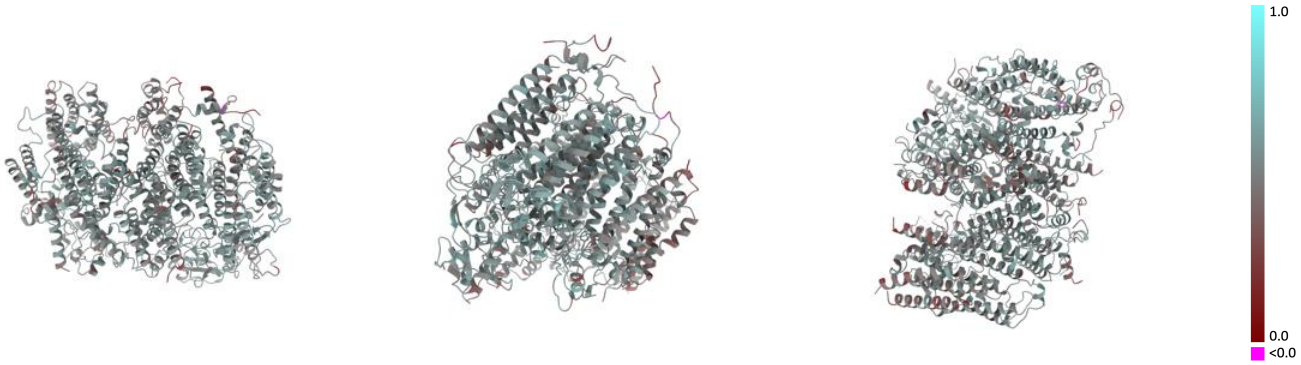
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019 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.

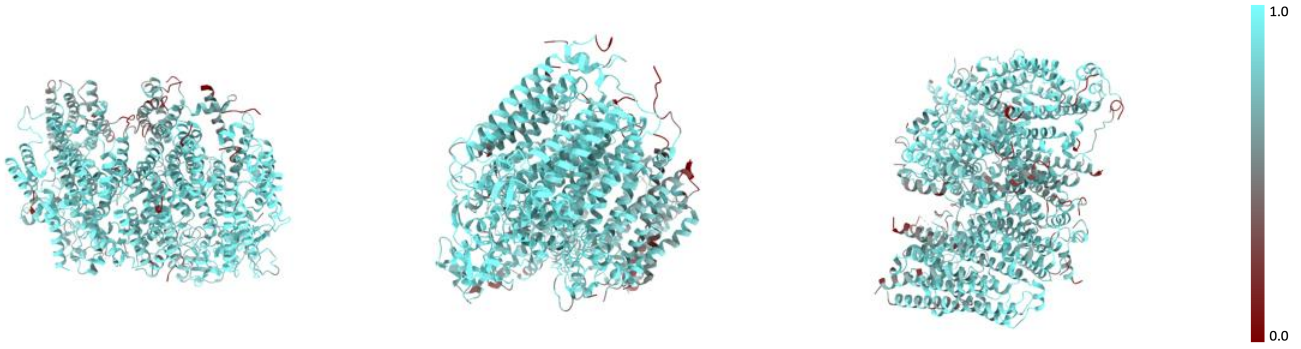
9.2 Q-score mapped to coordinate model (i)



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.

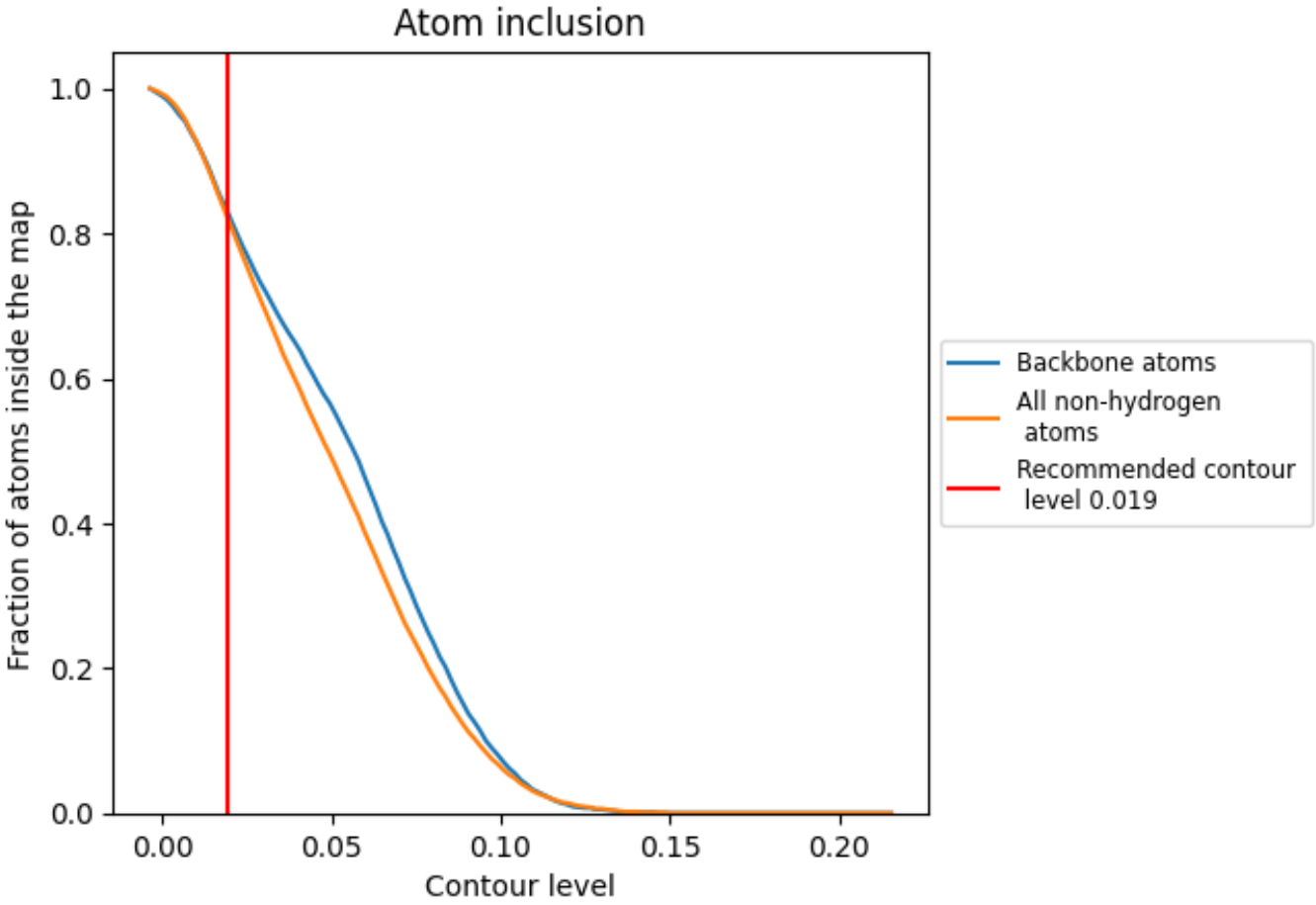
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.5180
1	0.5220	0.4240
A	0.8550	0.5230
B	0.8810	0.5440
C	0.8350	0.5190
D	0.8550	0.5380
E	0.7870	0.4950
F	0.7600	0.4810
H	0.8090	0.5080
I	0.7750	0.4920
K	0.6780	0.4490
L	0.7920	0.5040
M	0.6670	0.4450
T	0.7370	0.4750
V	0.5270	0.4180
X	0.6020	0.4440
Z	0.6390	0.4300