Full wwPDB EM Validation Report ⓘ

Nov 2, 2026 – 07:09 PM JST

PDB ID	:	9XKK / pdb_00009xkk
EMDB ID	:	EMD-66967
Title	:	Cryo-EM structure of a PSI supercomplex in the leaves of Hevea brasiliensis
Authors	:	Wang, M.; Yang, Y.; Li, Z.H.; Wang, W.D.; Wang, X.C.
Deposited on	:	2025-11-05
Resolution	:	2.50 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:

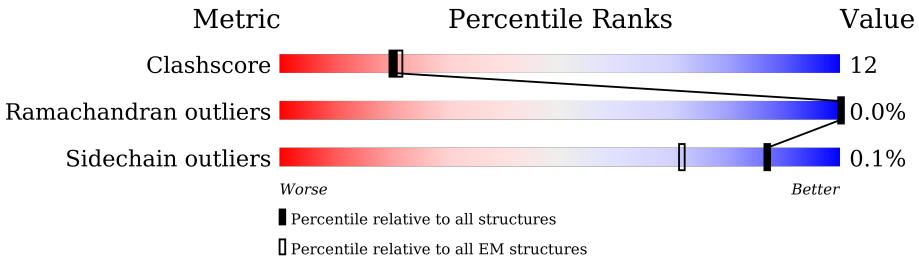
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

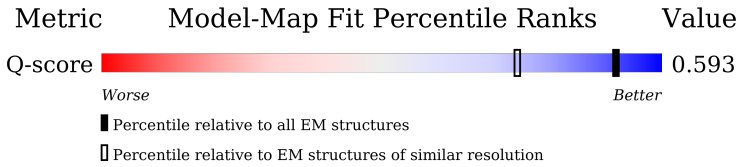
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	A	708	75% 25%
2	B	733	79% 21%
3	C	80	84% 16%
4	E	65	91% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	H	95	80% 20%
6	I	35	74% 26%
7	L	159	74% 26%
8	D	142	89% 10%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 21338 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 I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	708	Total	C	N	O	S	0	0
			5564	3650	944	952	18		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5851	3841	998	999	13		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			617	381	107	118	11		

- Molecule 4 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	65	Total	C	N	O	0	0
			525	335	92	98		

- Molecule 5 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	95	Total	C	N	O	0	0
			727	477	116	134		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	35	Total	C	N	O	S	0	0
			267	181	41	44	1		

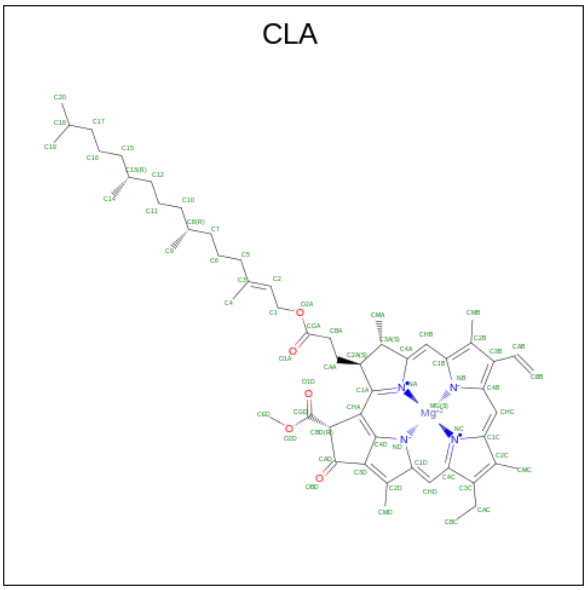
- Molecule 7 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	159	Total	C	N	O	S	0	0
			1185	782	187	214	2		

- Molecule 8 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	142	Total	C	N	O	S	0	0
			1129	726	196	204	3		

- Molecule 9 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

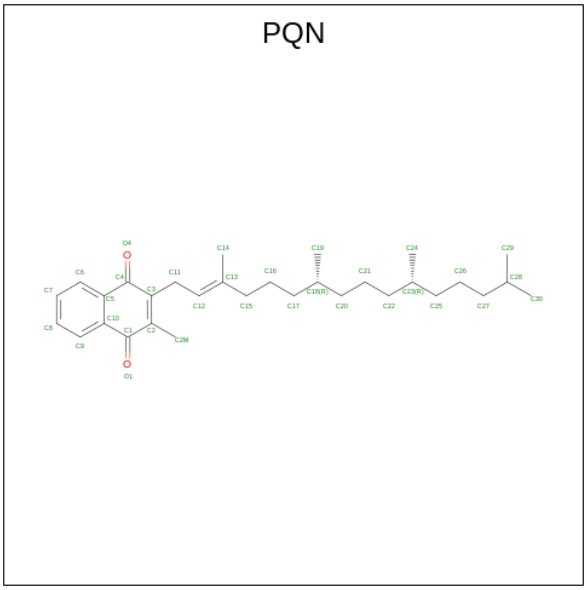
Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

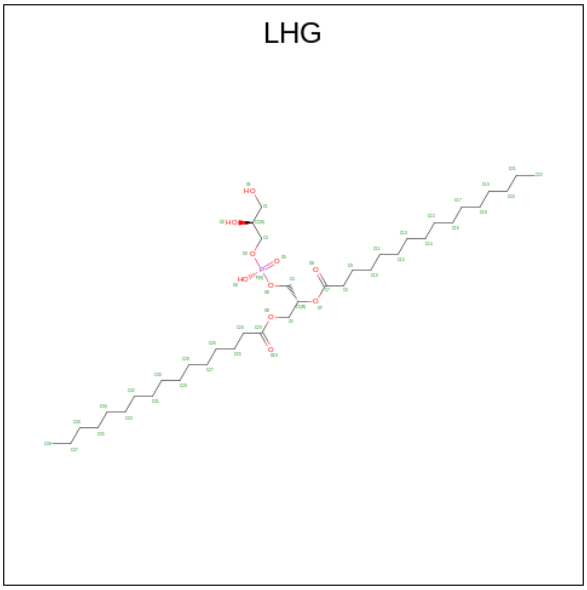
Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	L	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
9	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 10 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



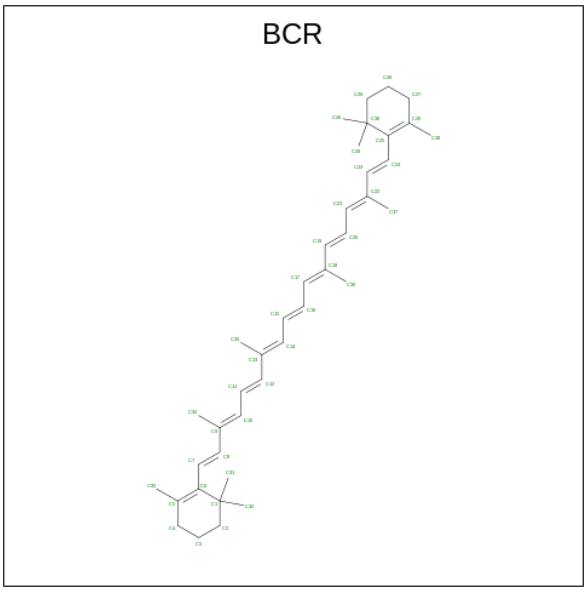
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total 33	C 31	O 2	0
10	B	1	Total 33	C 31	O 2	0

- Molecule 11 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



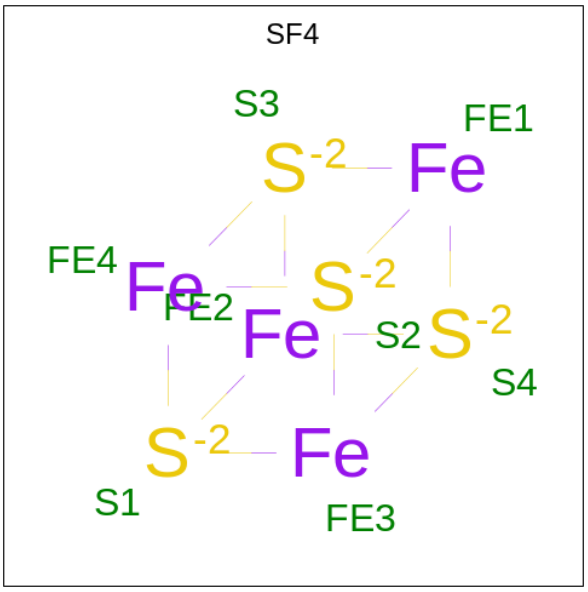
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total 49	C 38	O 10	P 1	0
11	A	1	Total 27	C 16	O 10	P 1	0
11	L	1	Total 49	C 38	O 10	P 1	0

- Molecule 12 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



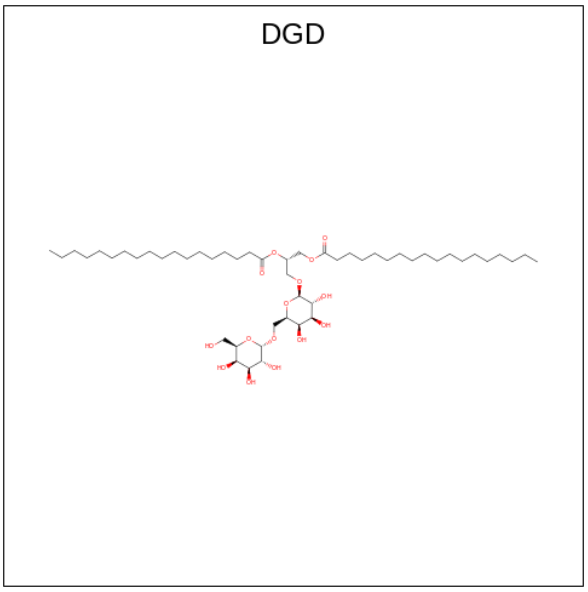
Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total C 40 40	0
12	A	1	Total C 40 40	0
12	A	1	Total C 40 40	0
12	A	1	Total C 40 40	0
12	B	1	Total C 40 40	0
12	B	1	Total C 40 40	0
12	B	1	Total C 40 40	0
12	I	1	Total C 40 40	0
12	L	1	Total C 40 40	0
12	L	1	Total C 40 40	0
12	L	1	Total C 40 40	0
12	L	1	Total C 40 40	0

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



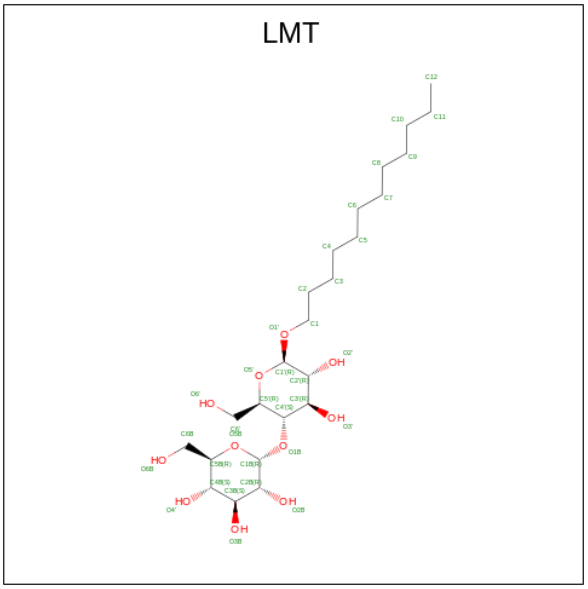
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total Fe S 8 4 4	0
13	C	1	Total Fe S 8 4 4	0
13	C	1	Total Fe S 8 4 4	0

- Molecule 14 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



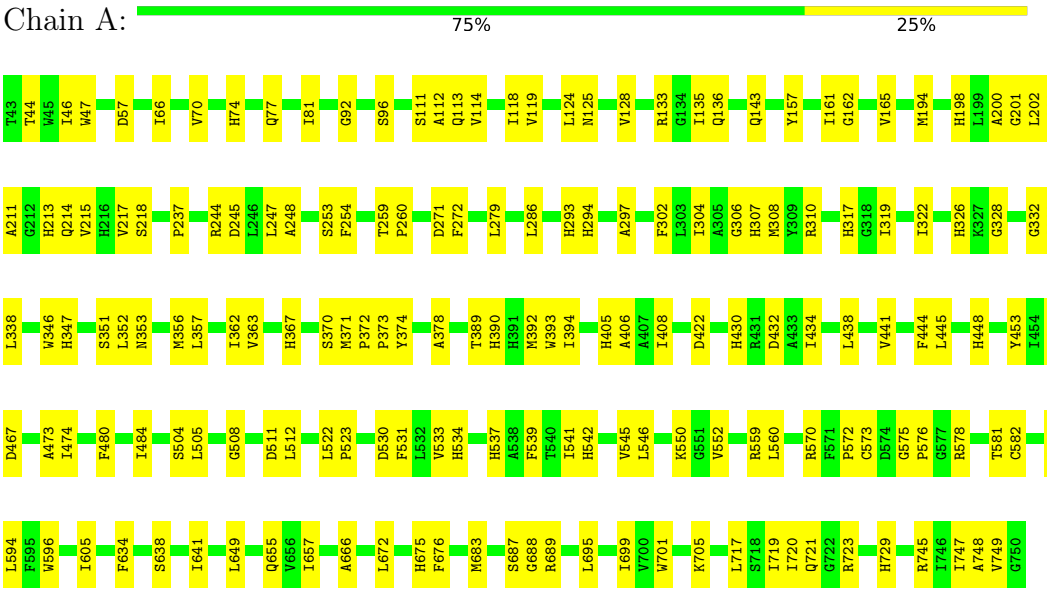
Mol	Chain	Residues	Atoms			AltConf
15	B	1	Total	C	O	0
			35	24	11	

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.

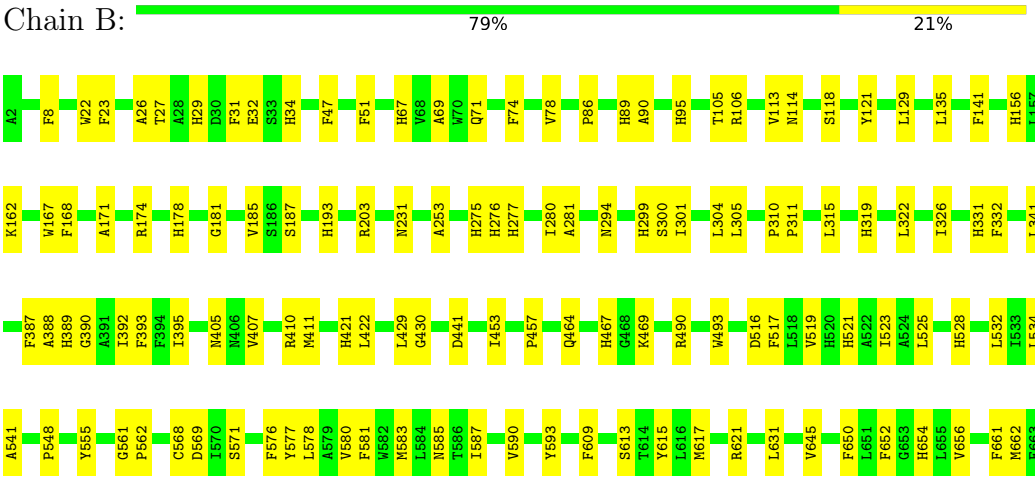
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

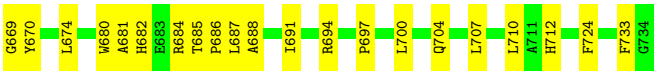
Chain A:



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:





• Molecule 3: Photosystem I iron-sulfur center

Chain C:

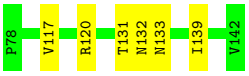




• Molecule 4: PsaE

Chain E:

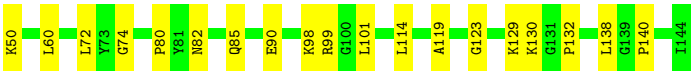




• Molecule 5: PsaH

Chain H:

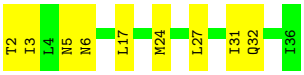




• Molecule 6: Photosystem I reaction center subunit VIII

Chain I:



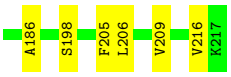


• Molecule 7: PsaL

Chain L:



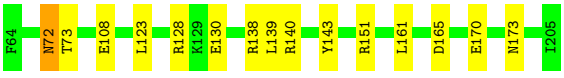




• Molecule 8: PsaD

Chain D:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3309024	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.681	Depositor
Minimum map value	-0.385	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.0233	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, BCR, SF4, LHG, DGD, LMT, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.14	0/5754	0.30	0/7852
2	B	0.14	0/6063	0.29	0/8280
3	C	0.15	0/630	0.31	0/853
4	E	0.11	0/537	0.24	0/728
5	H	0.13	0/748	0.28	0/1014
6	I	0.19	0/272	0.35	0/371
7	L	0.17	0/1218	0.35	0/1664
8	D	0.12	0/1159	0.29	0/1565
All	All	0.14	0/16381	0.30	0/22327

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	A	5564	0	5418	160	0
2	B	5851	0	5636	149	0
3	C	617	0	592	13	0
4	E	525	0	526	4	0
5	H	727	0	734	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	267	0	296	7	0
7	L	1185	0	1199	40	0
8	D	1129	0	1134	11	0
9	A	2482	0	2502	124	0
9	B	1966	0	1928	129	0
9	H	65	0	72	2	0
9	L	164	0	150	11	0
10	A	33	0	46	5	0
10	B	33	0	46	4	0
11	A	76	0	98	2	0
11	L	49	0	74	9	0
12	A	160	0	224	10	0
12	B	120	0	168	7	0
12	I	40	0	56	2	0
12	L	160	0	224	15	0
13	A	8	0	0	0	0
13	C	16	0	0	2	0
14	B	66	0	96	8	0
15	B	35	0	45	3	0
All	All	21338	0	21264	523	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 12.

All (523) 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)
1:A:405:HIS:HE1	9:A:828:CLA:NA	1.70	0.89
1:A:390:HIS:HE1	9:A:826:CLA:ND	1.74	0.86
1:A:96:SER:HA	1:A:112:ALA:HB3	1.63	0.80
1:A:550:LYS:NZ	2:B:670:TYR:O	2.14	0.80
9:A:849:CLA:HBB1	9:B:802:CLA:C4B	2.11	0.78
1:A:111:SER:HB3	1:A:136:GLN:HA	1.66	0.77
2:B:389:HIS:HE1	9:B:825:CLA:NA	1.82	0.77
2:B:294:ASN:HB3	2:B:299:HIS:HA	1.67	0.76
9:H:201:CLA:HBB2	12:L:307:BCR:H311	1.66	0.76
2:B:662:MET:HB2	9:B:804:CLA:C1C	2.16	0.76
5:H:50:LYS:N	8:D:72:ASN:HD21	1.85	0.74
9:B:807:CLA:H151	9:B:824:CLA:HBB2	1.72	0.72
1:A:531:PHE:HA	9:A:835:CLA:HED1	1.71	0.72
7:L:88:ASN:HB3	9:L:303:CLA:HAC1	1.70	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:MET:HB2	9:A:820:CLA:HBC3	1.73	0.70
1:A:689:ARG:H	2:B:568:CYS:HB2	1.55	0.70
2:B:95:HIS:HE1	9:B:811:CLA:NB	1.86	0.68
1:A:455:HIS:HE1	9:A:831:CLA:NA	1.90	0.67
9:A:802:CLA:C4B	9:B:804:CLA:HBB1	2.22	0.67
2:B:168:PHE:O	2:B:174:ARG:NH2	2.28	0.67
7:L:216:VAL:HG11	11:L:301:LHG:H311	1.76	0.67
2:B:712:HIS:HE1	9:B:832:CLA:ND	1.92	0.67
7:L:63:ILE:HA	7:L:73:GLU:HB2	1.77	0.67
1:A:550:LYS:HZ2	2:B:674:LEU:HB2	1.60	0.67
1:A:200:ALA:HB2	1:A:306:GLY:HA3	1.77	0.67
1:A:508:GLY:HA2	1:A:523:PRO:HB3	1.75	0.67
1:A:125:ASN:HB3	1:A:133:ARG:HB3	1.78	0.66
1:A:356:MET:HG3	9:A:823:CLA:HHB	1.77	0.66
2:B:464:GLN:NE2	9:B:828:CLA:OBD	2.29	0.66
2:B:305:LEU:HD13	2:B:322:LEU:HB3	1.78	0.65
2:B:395:ILE:HD13	2:B:555:TYR:HA	1.79	0.65
7:L:205:PHE:HA	7:L:209:VAL:HG22	1.78	0.65
1:A:596:TRP:HH2	9:A:802:CLA:HAB	1.62	0.65
1:A:390:HIS:HE1	9:A:826:CLA:C1D	2.10	0.65
9:A:831:CLA:HED3	7:L:122:PRO:HA	1.79	0.64
2:B:181:GLY:HA2	2:B:185:VAL:HB	1.78	0.64
2:B:193:HIS:HE1	9:B:815:CLA:NA	1.88	0.64
1:A:649:LEU:HD11	9:A:801:CLA:H71	1.78	0.64
10:B:833:PQN:H162	12:B:836:BCR:H382	1.79	0.64
7:L:206:LEU:HD11	12:L:308:BCR:H393	1.80	0.64
2:B:694:ARG:HG3	9:B:831:CLA:HED2	1.80	0.64
8:D:128:ARG:NH2	8:D:130:GLU:OE1	2.31	0.64
9:B:822:CLA:HED2	12:B:835:BCR:H332	1.80	0.63
1:A:335:HIS:CD2	9:A:822:CLA:ND	2.67	0.63
9:A:807:CLA:H2A	9:A:807:CLA:HED2	1.79	0.63
2:B:521:HIS:HE1	9:B:829:CLA:ND	1.96	0.63
4:E:120:ARG:NH1	4:E:131:THR:OG1	2.32	0.62
9:A:829:CLA:HMA2	7:L:74:THR:HG21	1.82	0.62
1:A:319:ILE:HG21	9:A:823:CLA:HAC1	1.81	0.62
9:A:838:CLA:H172	9:A:838:CLA:H91	1.82	0.62
1:A:585:SER:OG	1:A:588:ASP:OD2	2.18	0.61
1:A:596:TRP:CH2	9:A:802:CLA:HAB	2.35	0.61
9:A:817:CLA:H203	9:A:825:CLA:H3A	1.82	0.61
1:A:111:SER:HB2	1:A:128:VAL:HG11	1.81	0.61
1:A:480:PHE:HB3	9:A:834:CLA:H11	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:HIS:HE1	9:A:830:CLA:NA	1.94	0.61
2:B:171:ALA:HB1	9:B:820:CLA:HAB	1.82	0.61
2:B:305:LEU:HB3	2:B:319:HIS:HB2	1.81	0.61
1:A:44:THR:HA	1:A:47:TRP:HD1	1.65	0.60
9:B:806:CLA:HBA1	9:B:814:CLA:HBA1	1.82	0.60
1:A:215:VAL:HG13	1:A:272:PHE:CZ	2.36	0.60
1:A:683:MET:HB3	9:A:849:CLA:C1C	2.32	0.60
2:B:517:PHE:HA	9:B:829:CLA:HED1	1.82	0.60
2:B:523:ILE:HG12	2:B:590:VAL:HG12	1.84	0.59
5:H:123:GLY:HA3	5:H:130:LYS:HB3	1.84	0.59
9:A:816:CLA:H151	9:A:833:CLA:HBA1	1.82	0.59
1:A:537:HIS:HB3	9:A:834:CLA:HAB	1.84	0.59
2:B:684:ARG:HE	7:L:71:SER:HB3	1.68	0.59
7:L:109:HIS:HE1	9:L:304:CLA:C4D	2.14	0.59
2:B:587:ILE:HA	2:B:590:VAL:HG22	1.85	0.59
2:B:422:LEU:HD13	2:B:532:LEU:HA	1.85	0.58
9:A:817:CLA:HAB	9:A:817:CLA:H8	1.85	0.58
9:B:829:CLA:HBC2	15:B:838:LMT:H81	1.84	0.58
6:I:5:ASN:OD1	6:I:6:ASN:N	2.36	0.58
9:B:811:CLA:H41	7:L:136:ALA:HB2	1.86	0.58
6:I:27:LEU:O	6:I:31:ILE:HG12	2.04	0.58
1:A:202:LEU:HD22	1:A:203:LEU:HD12	1.85	0.58
2:B:174:ARG:HB3	9:B:814:CLA:HBC2	1.85	0.58
9:A:831:CLA:HAC1	9:B:810:CLA:HBB2	1.85	0.57
2:B:26:ALA:HB2	14:B:837:DGD:HA32	1.86	0.57
2:B:464:GLN:HB3	2:B:469:LYS:HD3	1.85	0.57
9:B:802:CLA:HHB	9:B:803:CLA:H202	1.86	0.57
7:L:85:TYR:OH	9:L:304:CLA:O1A	2.16	0.57
2:B:277:HIS:HE1	9:B:819:CLA:NA	2.01	0.56
3:C:18:VAL:HG21	3:C:28:MET:HG2	1.87	0.56
1:A:214:GLN:HA	1:A:218:SER:HB2	1.87	0.56
1:A:455:HIS:HE1	9:A:831:CLA:C1A	2.18	0.56
5:H:74:GLY:HA2	7:L:92:TYR:HB3	1.87	0.56
1:A:448:HIS:HE1	9:A:830:CLA:C1A	2.18	0.56
2:B:322:LEU:O	2:B:326:ILE:HG12	2.06	0.56
2:B:631:LEU:HD22	2:B:724:PHE:HA	1.88	0.56
9:B:801:CLA:H192	9:L:304:CLA:C1C	2.35	0.56
9:H:201:CLA:H101	12:L:307:BCR:H19C	1.87	0.56
2:B:681:ALA:O	2:B:685:THR:OG1	2.22	0.56
9:B:806:CLA:H2	9:B:814:CLA:H43	1.88	0.55
1:A:201:GLY:O	1:A:205:LEU:HB2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:ASP:HB2	4:E:132:ASN:ND2	2.21	0.55
7:L:75:PRO:HA	7:L:78:SER:OG	2.05	0.55
1:A:405:HIS:HA	1:A:408:ILE:HD12	1.87	0.55
2:B:106:ARG:NH2	2:B:113:VAL:O	2.35	0.55
1:A:729:HIS:HE1	9:A:839:CLA:C4D	2.19	0.55
9:B:801:CLA:HBC3	9:B:801:CLA:HHD	1.89	0.55
9:B:801:CLA:HBC2	9:B:831:CLA:C1C	2.36	0.55
1:A:92:GLY:O	1:A:96:SER:OG	2.14	0.55
2:B:389:HIS:HA	2:B:392:ILE:HD12	1.89	0.55
1:A:512:LEU:HD12	1:A:522:LEU:HD21	1.89	0.55
1:A:634:PHE:O	1:A:638:SER:OG	2.23	0.54
2:B:654:HIS:CD2	9:B:803:CLA:NB	2.76	0.54
7:L:198:SER:HB3	12:L:307:BCR:HC7	1.90	0.54
1:A:74:HIS:CE1	9:A:804:CLA:ND	2.75	0.54
1:A:113:GLN:HB2	1:A:135:ILE:HG12	1.89	0.54
2:B:661:PHE:HA	2:B:664:LEU:HD12	1.89	0.54
8:D:108:GLU:O	8:D:138:ARG:NH1	2.40	0.54
2:B:519:VAL:HG21	2:B:593:TYR:HB2	1.89	0.54
5:H:72:LEU:HA	7:L:169:LEU:HD13	1.88	0.54
5:H:114:LEU:HD21	6:I:17:LEU:HD12	1.90	0.54
9:B:819:CLA:HAB	9:B:819:CLA:H102	1.88	0.54
9:A:831:CLA:O1D	9:A:831:CLA:H2A	2.08	0.54
2:B:277:HIS:HA	2:B:280:ILE:HG12	1.89	0.54
2:B:178:HIS:CD2	9:B:814:CLA:NB	2.75	0.54
8:D:151:ARG:HB2	8:D:161:LEU:HD11	1.89	0.54
7:L:120:ALA:HB2	11:L:301:LHG:HC81	1.90	0.54
8:D:140:ARG:NH2	8:D:170:GLU:OE2	2.41	0.54
2:B:193:HIS:HE1	9:B:815:CLA:C1A	2.21	0.53
2:B:490:ARG:H	2:B:493:TRP:HE1	1.57	0.53
1:A:542:HIS:HA	1:A:545:VAL:HG22	1.90	0.53
9:B:804:CLA:HED2	9:B:804:CLA:HBA2	1.90	0.53
1:A:371:MET:HG2	1:A:504:SER:HB2	1.90	0.53
1:A:297:ALA:HA	9:A:815:CLA:HMC2	1.90	0.53
1:A:333:GLN:HB2	1:A:422:ASP:HB2	1.91	0.53
1:A:745:ARG:O	1:A:749:VAL:HG22	2.09	0.53
1:A:576:PRO:HB2	3:C:69:LEU:HD11	1.91	0.53
2:B:691:ILE:HG21	9:B:801:CLA:HAB	1.91	0.53
1:A:394:ILE:HD12	9:A:805:CLA:H143	1.91	0.52
9:A:816:CLA:H92	9:A:816:CLA:H41	1.91	0.52
1:A:729:HIS:HE1	9:A:839:CLA:ND	2.07	0.52
4:E:117:VAL:HG11	4:E:139:ILE:HD13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:LEU:HD23	2:B:135:LEU:HD23	1.89	0.52
2:B:89:HIS:CD2	9:B:809:CLA:NA	2.77	0.52
9:B:825:CLA:H203	9:B:832:CLA:H3A	1.92	0.52
1:A:253:SER:OG	1:A:271:ASP:OD1	2.28	0.52
9:B:809:CLA:O1A	9:B:823:CLA:HBD	2.10	0.52
2:B:315:LEU:HA	2:B:410:ARG:HG3	1.90	0.51
2:B:276:HIS:HB2	9:B:818:CLA:C1B	2.40	0.51
2:B:429:LEU:HD11	9:B:829:CLA:HMB2	1.91	0.51
2:B:31:PHE:HA	2:B:34:HIS:CD2	2.45	0.51
2:B:707:LEU:HD23	14:B:837:DGD:HA21	1.91	0.51
10:B:833:PQN:H28	14:B:837:DGD:HA82	1.91	0.51
1:A:676:PHE:HB2	9:B:802:CLA:O1A	2.10	0.51
1:A:118:ILE:HG23	1:A:119:VAL:HG22	1.92	0.51
1:A:655:GLN:HG2	1:A:748:ALA:HB3	1.93	0.51
2:B:90:ALA:HA	2:B:113:VAL:HG12	1.93	0.51
7:L:144:LEU:HD13	12:L:306:BCR:H401	1.93	0.51
1:A:346:TRP:HB3	9:A:804:CLA:HAC1	1.93	0.51
2:B:26:ALA:HA	9:B:825:CLA:H42	1.93	0.51
1:A:372:PRO:HG2	1:A:378:ALA:HB2	1.94	0.50
1:A:198:HIS:CD2	9:A:811:CLA:NB	2.80	0.50
1:A:466:GLN:HB2	11:L:301:LHG:HC11	1.92	0.50
1:A:474:ILE:HG12	11:L:301:LHG:HC41	1.94	0.50
1:A:683:MET:HB3	9:A:849:CLA:C2C	2.41	0.50
1:A:541:ILE:O	1:A:545:VAL:HG13	2.11	0.50
2:B:694:ARG:NH1	6:I:32:GLN:O	2.45	0.50
1:A:588:ASP:OD1	1:A:723:ARG:NH1	2.45	0.50
1:A:596:TRP:HE1	9:B:804:CLA:C1D	2.24	0.50
7:L:61:GLU:HG2	7:L:62:PRO:HD2	1.93	0.50
1:A:111:SER:CB	1:A:136:GLN:HA	2.39	0.49
1:A:552:VAL:HG21	12:A:847:BCR:HC31	1.94	0.49
2:B:733:PHE:CD2	5:H:140:PRO:HG2	2.46	0.49
1:A:194:MET:HB2	9:A:811:CLA:HBC2	1.93	0.49
1:A:717:LEU:HD22	1:A:721:GLN:HB3	1.93	0.49
1:A:304:ILE:O	9:A:820:CLA:HBC1	2.13	0.49
6:I:24:MET:HE3	12:L:306:BCR:H352	1.94	0.49
6:I:27:LEU:HD13	12:L:306:BCR:HC8	1.93	0.49
1:A:245:ASP:O	1:A:248:ALA:N	2.45	0.49
1:A:286:LEU:HD21	1:A:371:MET:HB3	1.94	0.49
2:B:23:PHE:O	2:B:27:THR:OG1	2.26	0.49
5:H:119:ALA:O	5:H:129:LYS:NZ	2.46	0.49
1:A:390:HIS:HB2	9:A:826:CLA:CHB	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:109:HIS:HE1	9:L:304:CLA:ND	2.10	0.49
9:A:814:CLA:HHC	9:A:814:CLA:HBB1	1.93	0.49
2:B:305:LEU:HB3	2:B:319:HIS:CB	2.43	0.49
2:B:697:PRO:O	3:C:81:TYR:OH	2.19	0.49
12:L:306:BCR:H23C	12:L:306:BCR:H392	1.94	0.49
9:A:807:CLA:H2	9:A:826:CLA:H12	1.95	0.49
9:A:816:CLA:H2	9:A:825:CLA:HBB2	1.95	0.49
2:B:141:PHE:HZ	9:B:815:CLA:H102	1.77	0.49
9:A:831:CLA:H52	7:L:116:PRO:HB2	1.94	0.49
9:A:850:CLA:H52	9:L:304:CLA:H43	1.94	0.49
2:B:467:HIS:CD2	9:B:827:CLA:NA	2.80	0.49
2:B:332:PHE:CE1	12:B:835:BCR:H291	2.47	0.49
2:B:332:PHE:HB2	2:B:393:PHE:CD1	2.48	0.48
2:B:680:TRP:NE1	7:L:70:GLY:O	2.42	0.48
1:A:405:HIS:HE1	9:A:828:CLA:C4A	2.25	0.48
2:B:156:HIS:HE1	9:B:812:CLA:NA	2.08	0.48
2:B:203:ARG:NH2	2:B:253:ALA:O	2.38	0.48
1:A:353:ASN:ND2	9:A:804:CLA:OBD	2.26	0.48
1:A:511:ASP:OD1	1:A:512:LEU:N	2.46	0.48
9:B:810:CLA:H3A	9:B:811:CLA:HBB1	1.94	0.48
1:A:559:ARG:O	8:D:128:ARG:NH1	2.44	0.48
1:A:328:GLY:H	11:A:843:LHG:HC2	1.78	0.48
1:A:695:LEU:O	1:A:699:ILE:HD12	2.14	0.48
9:A:826:CLA:HBA2	9:A:826:CLA:H3A	1.35	0.48
9:B:825:CLA:H143	14:B:837:DGD:HAF1	1.96	0.48
5:H:99:ARG:HG2	7:L:186:ALA:HB2	1.94	0.48
9:A:802:CLA:HBB1	9:A:802:CLA:HMB3	1.96	0.48
2:B:358:TYR:OH	9:B:824:CLA:OBD	2.21	0.48
2:B:528:HIS:CD2	9:B:830:CLA:NB	2.81	0.48
1:A:136:GLN:OE1	1:A:747:ILE:HG12	2.13	0.48
1:A:455:HIS:HE1	9:A:831:CLA:C4D	2.27	0.48
2:B:687:LEU:HD21	7:L:89:LEU:HD23	1.96	0.48
1:A:317:HIS:HB3	1:A:322:ILE:HD11	1.96	0.48
1:A:445:LEU:HD23	1:A:539:PHE:HA	1.96	0.48
9:B:824:CLA:H143	9:B:824:CLA:H112	1.67	0.48
9:A:830:CLA:H102	9:B:831:CLA:H52	1.95	0.47
9:A:817:CLA:HBA2	9:A:817:CLA:H3A	1.58	0.47
7:L:118:VAL:HG23	7:L:130:GLY:H	1.79	0.47
8:D:73:THR:HG23	8:D:123:LEU:HB2	1.95	0.47
1:A:326:HIS:CD2	9:A:821:CLA:NB	2.81	0.47
1:A:573:CYS:SG	1:A:582:CYS:HA	2.55	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:HIS:CD2	9:A:825:CLA:NC	2.82	0.47
1:A:688:GLY:HA3	2:B:569:ASP:HB2	1.97	0.47
11:L:301:LHG:H361	9:L:305:CLA:ND	2.28	0.47
8:D:139:LEU:HA	8:D:143:TYR:HD2	1.79	0.47
1:A:201:GLY:HA3	9:A:811:CLA:HBB1	1.97	0.47
1:A:307:HIS:CD2	9:A:818:CLA:NA	2.81	0.47
9:A:804:CLA:H72	12:A:845:BCR:HC8	1.97	0.47
9:A:804:CLA:HBA1	9:A:804:CLA:H3A	1.64	0.47
1:A:582:CYS:O	2:B:669:GLY:N	2.48	0.47
2:B:700:LEU:HD22	2:B:704:GLN:NE2	2.30	0.47
4:E:132:ASN:OD1	4:E:133:ASN:N	2.48	0.47
1:A:572:PRO:HB3	1:A:719:ILE:HB	1.96	0.47
9:A:826:CLA:HMB3	9:A:826:CLA:HBB1	1.97	0.47
2:B:29:HIS:HE1	9:B:805:CLA:C1C	2.28	0.47
2:B:71:GLN:NE2	9:B:808:CLA:O1D	2.46	0.47
2:B:577:TYR:CE1	2:B:710:LEU:HB2	2.49	0.47
9:B:801:CLA:H141	7:L:140:LEU:HD11	1.97	0.47
1:A:66:ILE:O	1:A:70:VAL:HG13	2.15	0.46
1:A:576:PRO:HD3	2:B:561:GLY:HA2	1.97	0.46
12:A:846:BCR:H351	12:A:846:BCR:H15C	1.80	0.46
2:B:645:VAL:HG21	9:B:809:CLA:HAC1	1.96	0.46
7:L:124:ARG:NH2	11:L:301:LHG:O2	2.47	0.46
1:A:362:ILE:HG23	1:A:392:MET:HE1	1.97	0.46
2:B:555:TYR:O	2:B:571:SER:OG	2.32	0.46
9:B:831:CLA:HBB2	10:B:833:PQN:H141	1.97	0.46
9:B:831:CLA:H193	12:I:101:BCR:H362	1.98	0.46
1:A:356:MET:HA	1:A:356:MET:HE2	1.97	0.46
9:A:850:CLA:HBA1	2:B:686:PRO:HD3	1.96	0.46
2:B:32:GLU:OE1	2:B:331:HIS:NE2	2.41	0.46
9:B:818:CLA:H92	9:B:818:CLA:H41	1.98	0.46
9:B:824:CLA:H62	9:B:824:CLA:H41	1.56	0.46
6:I:2:THR:OG1	6:I:3:ILE:N	2.48	0.46
1:A:213:HIS:HB2	9:A:812:CLA:CHC	2.46	0.46
9:B:809:CLA:H8	9:B:809:CLA:H51	1.71	0.46
7:L:59:VAL:HG23	7:L:60:VAL:HG23	1.97	0.46
7:L:79:SER:O	7:L:81:LEU:N	2.48	0.46
1:A:444:PHE:HE2	9:A:835:CLA:HAB	1.81	0.46
9:B:806:CLA:H11	9:B:806:CLA:HBA2	1.59	0.46
7:L:61:GLU:O	7:L:73:GLU:HB3	2.14	0.46
1:A:445:LEU:HD21	9:A:835:CLA:HMB2	1.97	0.46
9:A:801:CLA:HBC3	9:B:803:CLA:HAC2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:803:CLA:HBA1	9:A:803:CLA:H3A	1.74	0.46
2:B:421:HIS:HE1	9:B:826:CLA:NA	2.12	0.46
2:B:661:PHE:HB3	9:B:804:CLA:HMC2	1.97	0.46
12:A:844:BCR:H20C	12:A:844:BCR:H361	1.82	0.46
2:B:326:ILE:HD12	2:B:332:PHE:CE2	2.51	0.46
2:B:341:LEU:HD21	9:B:807:CLA:CBB	2.46	0.46
2:B:581:PHE:HZ	2:B:664:LEU:HD21	1.81	0.46
9:B:801:CLA:H121	12:L:302:BCR:H351	1.98	0.46
1:A:560:LEU:HD21	1:A:581:THR:HG22	1.97	0.46
9:B:802:CLA:H61	9:B:802:CLA:H41	1.49	0.46
9:B:829:CLA:H93	9:B:830:CLA:HBC1	1.98	0.46
1:A:211:ALA:O	1:A:215:VAL:HG23	2.15	0.45
1:A:363:VAL:HG11	9:A:817:CLA:H201	1.96	0.45
7:L:64:ASN:ND2	7:L:169:LEU:O	2.49	0.45
1:A:657:ILE:HD12	2:B:621:ARG:HG3	1.97	0.45
12:A:846:BCR:H20C	12:A:846:BCR:H361	1.82	0.45
2:B:583:MET:HG2	9:B:821:CLA:HBC1	1.99	0.45
9:B:807:CLA:H192	9:B:807:CLA:H161	1.76	0.45
1:A:717:LEU:HB2	10:A:840:PQN:H6	1.97	0.45
9:A:838:CLA:HBA1	9:A:838:CLA:H3A	1.48	0.45
2:B:193:HIS:HB2	9:B:815:CLA:C1C	2.47	0.45
2:B:441:ASP:OD1	2:B:615:TYR:HB2	2.17	0.45
1:A:351:SER:OG	1:A:406:ALA:HB2	2.17	0.45
9:A:801:CLA:HED3	9:A:801:CLA:HBD	1.74	0.45
9:B:805:CLA:HHC	9:B:807:CLA:OBD	2.17	0.45
1:A:203:LEU:HD23	1:A:302:PHE:CE2	2.52	0.45
9:A:832:CLA:H3A	9:A:832:CLA:HBA2	1.41	0.45
9:B:831:CLA:H152	9:B:832:CLA:H13	1.98	0.45
1:A:370:SER:OG	9:A:825:CLA:HAC2	2.17	0.45
10:A:840:PQN:H141	10:A:840:PQN:H161	1.62	0.45
2:B:389:HIS:HE1	9:B:825:CLA:C4A	2.29	0.45
2:B:22:TRP:CG	2:B:704:GLN:HE22	2.34	0.45
2:B:95:HIS:HE1	9:B:811:CLA:C4B	2.30	0.45
2:B:47:PHE:CE2	2:B:51:PHE:HE2	2.35	0.45
9:B:806:CLA:H61	9:B:806:CLA:H41	1.42	0.45
1:A:473:ALA:HA	11:L:301:LHG:HC2	1.98	0.44
1:A:530:ASP:HA	1:A:533:VAL:HG22	1.99	0.44
2:B:193:HIS:HB2	9:B:815:CLA:CHC	2.47	0.44
2:B:453:ILE:HG23	15:B:838:LMT:H1B	1.98	0.44
5:H:82:ASN:HB3	5:H:85:GLN:HG3	1.99	0.44
1:A:124:LEU:HD22	1:A:666:ALA:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:HIS:CE1	9:A:831:CLA:C4D	3.01	0.44
9:A:807:CLA:H101	9:A:807:CLA:H61	1.47	0.44
9:A:831:CLA:H41	9:A:831:CLA:H61	1.48	0.44
9:A:849:CLA:H41	9:A:849:CLA:H62	1.67	0.44
9:A:850:CLA:HBA2	9:A:850:CLA:H3A	1.61	0.44
2:B:585:ASN:HB2	9:B:802:CLA:HBC2	1.98	0.44
2:B:712:HIS:HE1	9:B:832:CLA:C4D	2.29	0.44
9:B:829:CLA:HBB1	9:B:829:CLA:HMB3	1.99	0.44
1:A:438:LEU:HG	1:A:546:LEU:HB2	1.98	0.44
2:B:159:PRO:HA	2:B:162:LYS:HE2	1.98	0.44
10:B:833:PQN:H211	10:B:833:PQN:H252	1.84	0.44
1:A:467:ASP:CG	9:A:831:CLA:HED1	2.42	0.44
1:A:534:HIS:CD2	9:A:834:CLA:NB	2.84	0.44
1:A:259:THR:OG1	1:A:260:PRO:HD3	2.17	0.44
2:B:407:VAL:HG12	2:B:411:MET:HE2	2.00	0.44
9:B:804:CLA:H111	12:B:836:BCR:H362	1.99	0.44
1:A:453:TYR:OH	9:A:801:CLA:H152	2.18	0.44
1:A:672:LEU:HD11	2:B:617:MET:HB2	2.00	0.44
2:B:378:ILE:HD13	9:B:824:CLA:HBB1	2.00	0.44
9:A:804:CLA:H61	9:A:804:CLA:H2	1.68	0.44
2:B:74:PHE:O	2:B:78:VAL:HG13	2.18	0.44
2:B:167:TRP:CZ2	9:B:812:CLA:HHB	2.52	0.44
9:B:801:CLA:H142	9:B:801:CLA:H111	1.66	0.44
11:L:301:LHG:H371	11:L:301:LHG:H341	1.71	0.44
1:A:57:ASP:OD2	1:A:347:HIS:NE2	2.50	0.44
1:A:143:GLN:HB3	1:A:374:TYR:HB3	2.00	0.44
9:A:802:CLA:H111	9:A:802:CLA:H142	1.69	0.44
9:A:827:CLA:H91	9:A:827:CLA:H111	1.68	0.44
10:A:840:PQN:H18	10:A:840:PQN:H221	1.83	0.44
2:B:187:SER:HB3	2:B:281:ALA:HB2	2.00	0.44
9:B:823:CLA:H61	9:B:823:CLA:H102	1.79	0.44
8:D:165:ASP:OD2	8:D:173:ASN:ND2	2.36	0.44
9:A:850:CLA:HMB1	9:B:801:CLA:HAA2	1.99	0.44
9:B:825:CLA:H71	9:B:832:CLA:HED1	2.00	0.44
1:A:279:LEU:HD13	1:A:505:LEU:HD23	2.00	0.43
1:A:338:LEU:HD21	9:A:822:CLA:HBC3	1.99	0.43
9:A:815:CLA:H162	9:A:815:CLA:H193	1.73	0.43
9:A:835:CLA:HBB1	9:A:836:CLA:CHD	2.48	0.43
2:B:609:PHE:O	2:B:613:SER:OG	2.24	0.43
9:B:824:CLA:H61	9:B:824:CLA:H101	1.79	0.43
1:A:247:LEU:HD13	1:A:254:PHE:CE2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:827:CLA:H161	9:A:827:CLA:H122	1.92	0.43
9:A:837:CLA:HBA2	9:A:837:CLA:H3A	1.65	0.43
2:B:86:PRO:HB3	2:B:121:TYR:CG	2.53	0.43
2:B:388:ALA:HB2	2:B:576:PHE:CD1	2.53	0.43
7:L:147:CYS:HA	7:L:150:MET:HE2	1.99	0.43
9:A:826:CLA:H111	9:A:826:CLA:H72	1.63	0.43
10:A:840:PQN:H242	10:A:840:PQN:H212	1.85	0.43
2:B:276:HIS:HB2	9:B:818:CLA:CHB	2.48	0.43
2:B:310:PRO:HA	2:B:311:PRO:HD3	1.89	0.43
1:A:453:TYR:HA	1:A:456:ASN:HB2	2.01	0.43
1:A:596:TRP:HE1	9:B:804:CLA:CHD	2.30	0.43
12:A:846:BCR:H17C	12:A:846:BCR:H14C	1.80	0.43
2:B:27:THR:HG23	14:B:837:DGD:HG31	2.00	0.43
2:B:105:THR:HG21	5:H:132:PRO:HG3	2.00	0.43
2:B:583:MET:O	2:B:587:ILE:HG12	2.17	0.43
12:I:101:BCR:H20C	12:I:101:BCR:H361	1.81	0.43
1:A:484:ILE:CD1	9:A:834:CLA:H12	2.48	0.43
9:A:810:CLA:HBA2	9:A:810:CLA:H3A	1.27	0.43
9:A:826:CLA:H13	9:A:826:CLA:H102	1.85	0.43
9:B:821:CLA:H62	9:B:821:CLA:H102	1.57	0.43
12:B:836:BCR:H361	12:B:836:BCR:H20C	1.78	0.43
8:D:72:ASN:HD22	8:D:72:ASN:HA	1.70	0.43
1:A:202:LEU:HD12	9:A:811:CLA:CHB	2.49	0.43
1:A:372:PRO:HA	1:A:373:PRO:HD3	1.84	0.43
1:A:594:LEU:HD21	9:A:828:CLA:HBC1	1.99	0.43
1:A:687:SER:HA	2:B:578:LEU:HD21	2.00	0.43
9:A:828:CLA:H93	9:A:839:CLA:HED3	2.00	0.43
2:B:650:PHE:HZ	9:B:803:CLA:C1D	2.32	0.43
1:A:357:LEU:HD21	9:A:805:CLA:HBB1	2.01	0.43
9:A:806:CLA:H112	9:A:806:CLA:H72	1.59	0.43
9:A:808:CLA:H142	9:A:808:CLA:H112	1.82	0.43
9:A:817:CLA:H122	9:A:817:CLA:H162	1.65	0.43
12:A:844:BCR:H24C	12:A:844:BCR:H371	1.80	0.43
2:B:457:PRO:HG3	2:B:517:PHE:HB2	2.01	0.43
2:B:577:TYR:HE1	2:B:710:LEU:HB2	1.84	0.43
1:A:293:HIS:CD2	9:A:816:CLA:HAB	2.54	0.43
1:A:328:GLY:HA3	11:A:843:LHG:P	2.59	0.43
2:B:576:PHE:O	2:B:580:VAL:HG23	2.19	0.43
3:C:47:ASP:OD1	8:D:151:ARG:NH2	2.52	0.43
1:A:570:ARG:HD2	1:A:720:ILE:HG21	1.99	0.43
12:A:847:BCR:H15C	12:A:847:BCR:H351	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:814:CLA:H101	9:B:819:CLA:HBC2	2.01	0.42
9:A:816:CLA:CGA	9:A:816:CLA:H3A	2.48	0.42
9:A:838:CLA:H2	9:A:838:CLA:H102	2.01	0.42
3:C:17:CYS:HB3	13:C:102:SF4:S4	2.58	0.42
9:A:806:CLA:HMB3	9:A:807:CLA:H3A	2.01	0.42
9:A:824:CLA:HBA2	9:A:824:CLA:H3A	1.85	0.42
2:B:300:SER:O	2:B:304:LEU:HG	2.19	0.42
2:B:387:PHE:HB3	2:B:534:LEU:HB3	2.02	0.42
2:B:390:GLY:O	2:B:393:PHE:HB3	2.19	0.42
2:B:405:ASN:HA	2:B:410:ARG:NH1	2.34	0.42
9:B:801:CLA:H201	7:L:109:HIS:HB3	2.01	0.42
9:B:821:CLA:H162	9:B:821:CLA:H141	1.81	0.42
9:B:832:CLA:H111	9:B:832:CLA:H152	1.79	0.42
2:B:712:HIS:CE1	9:B:832:CLA:C4D	3.01	0.42
9:B:807:CLA:H8	14:B:837:DGD:HBH1	2.01	0.42
9:B:831:CLA:H2	9:B:832:CLA:H122	2.02	0.42
2:B:652:PHE:O	2:B:656:VAL:HG23	2.19	0.42
9:B:806:CLA:H102	9:B:806:CLA:H62	1.57	0.42
12:B:834:BCR:H392	12:B:834:BCR:H371	2.02	0.42
5:H:80:PRO:HG3	7:L:93:ARG:CZ	2.49	0.42
5:H:99:ARG:NH1	7:L:152:GLY:O	2.52	0.42
1:A:352:LEU:HD21	9:A:823:CLA:C4B	2.50	0.42
2:B:8:PHE:HB2	2:B:34:HIS:CG	2.53	0.42
2:B:67:HIS:HE1	9:B:808:CLA:C4D	2.33	0.42
2:B:118:SER:HA	9:B:823:CLA:HMA2	2.01	0.42
1:A:332:GLY:N	1:A:422:ASP:OD2	2.52	0.42
1:A:641:ILE:HD13	1:A:641:ILE:HA	1.88	0.42
1:A:672:LEU:HD23	1:A:672:LEU:HA	1.91	0.42
9:A:823:CLA:H141	9:A:823:CLA:H161	1.79	0.42
2:B:301:ILE:HD12	2:B:304:LEU:HD12	2.02	0.42
9:B:802:CLA:H142	9:B:802:CLA:H111	1.86	0.42
9:B:822:CLA:CAB	9:B:827:CLA:H3A	2.48	0.42
1:A:430:HIS:CE1	1:A:434:ILE:HD11	2.55	0.42
1:A:434:ILE:HG23	9:A:836:CLA:HBB2	2.00	0.42
2:B:536:LYS:O	2:B:540:ASP:HB2	2.19	0.42
12:L:307:BCR:H11C	12:L:307:BCR:H341	1.90	0.42
1:A:213:HIS:HE1	9:A:812:CLA:C1A	2.27	0.42
1:A:215:VAL:HG13	1:A:272:PHE:HZ	1.80	0.42
2:B:516:ASP:HA	2:B:519:VAL:HG12	2.02	0.42
9:B:810:CLA:H161	9:B:810:CLA:H192	1.76	0.42
12:A:845:BCR:H24C	12:A:845:BCR:H371	1.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:829:CLA:H112	9:B:829:CLA:H152	1.75	0.42
3:C:70:TRP:CE3	3:C:70:TRP:HA	2.55	0.42
9:A:835:CLA:H111	9:A:835:CLA:H142	1.70	0.41
2:B:275:HIS:HE1	9:B:817:CLA:ND	2.11	0.41
2:B:395:ILE:HD11	2:B:541:ALA:HB1	2.01	0.41
9:B:810:CLA:CMA	9:B:811:CLA:HBB1	2.49	0.41
3:C:70:TRP:CG	3:C:71:HIS:H	2.38	0.41
5:H:90:GLU:HG2	7:L:99:LEU:HD23	2.01	0.41
1:A:157:TYR:O	1:A:161:ILE:HG12	2.20	0.41
1:A:455:HIS:HE1	9:A:831:CLA:CHA	2.32	0.41
9:A:817:CLA:H92	9:A:827:CLA:H91	2.01	0.41
2:B:301:ILE:HA	2:B:304:LEU:HD12	2.02	0.41
9:B:809:CLA:CGA	9:B:809:CLA:C1A	2.97	0.41
9:B:825:CLA:H2	14:B:837:DGD:HB51	2.02	0.41
12:L:306:BCR:H361	12:L:306:BCR:H20C	1.80	0.41
12:L:307:BCR:H15C	12:L:307:BCR:H351	1.82	0.41
1:A:77:GLN:HE21	1:A:81:ILE:HG13	1.84	0.41
1:A:432:ASP:OD2	1:A:559:ARG:NH1	2.50	0.41
2:B:684:ARG:NE	7:L:71:SER:HB3	2.32	0.41
2:B:704:GLN:HG3	14:B:837:DGD:HA22	2.02	0.41
9:B:814:CLA:H2	9:B:814:CLA:H61	1.80	0.41
9:B:821:CLA:CHB	9:B:830:CLA:HAA2	2.51	0.41
9:B:824:CLA:H91	9:B:824:CLA:H111	1.72	0.41
1:A:701:TRP:CH2	1:A:705:LYS:HD2	2.55	0.41
2:B:583:MET:HE3	2:B:583:MET:HB3	1.84	0.41
9:L:304:CLA:H112	9:L:304:CLA:H142	1.72	0.41
1:A:699:ILE:HG21	9:A:838:CLA:HBC1	2.01	0.41
2:B:662:MET:O	2:B:666:SER:OG	2.29	0.41
2:B:682:HIS:HE1	2:B:691:ILE:O	2.04	0.41
2:B:687:LEU:HD11	7:L:89:LEU:HD21	2.03	0.41
9:L:304:CLA:H162	9:L:304:CLA:H141	1.76	0.41
12:L:306:BCR:H11C	12:L:306:BCR:H341	1.92	0.41
1:A:92:GLY:HA2	1:A:96:SER:HB3	2.02	0.41
1:A:389:THR:HG23	1:A:605:ILE:HG21	2.02	0.41
2:B:89:HIS:CE1	2:B:114:ASN:HD22	2.39	0.41
3:C:15:THR:HG22	3:C:28:MET:HG3	2.03	0.41
5:H:138:LEU:HD23	5:H:138:LEU:HA	1.88	0.41
7:L:109:HIS:CE1	9:L:304:CLA:C4D	3.00	0.41
1:A:294:HIS:HB2	9:A:816:CLA:C1B	2.50	0.41
1:A:675:HIS:CD2	9:A:801:CLA:NB	2.89	0.41
2:B:528:HIS:HE1	9:B:830:CLA:C4D	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:656:VAL:HG12	2:B:712:HIS:O	2.21	0.41
12:L:302:BCR:H351	12:L:302:BCR:H15C	1.84	0.41
1:A:217:VAL:HG13	1:A:237:PRO:HB3	2.02	0.41
1:A:319:ILE:HD12	1:A:319:ILE:H	1.86	0.41
9:A:807:CLA:H3A	9:A:807:CLA:HBA2	1.51	0.41
9:A:831:CLA:H162	9:A:831:CLA:H202	1.75	0.41
2:B:548:PRO:HD2	3:C:62:PHE:CE1	2.56	0.41
2:B:670:TYR:OH	9:B:804:CLA:OBD	2.32	0.41
1:A:111:SER:OG	1:A:136:GLN:HG3	2.21	0.41
1:A:203:LEU:HB3	1:A:302:PHE:CD2	2.56	0.41
1:A:244:ARG:HD2	1:A:254:PHE:O	2.21	0.41
1:A:438:LEU:HA	1:A:441:VAL:HG12	2.02	0.41
10:A:840:PQN:H293	10:A:840:PQN:H261	1.91	0.41
2:B:156:HIS:HE1	9:B:812:CLA:C1A	2.32	0.41
2:B:158:GLN:HB2	2:B:161:TRP:HE3	1.85	0.41
2:B:521:HIS:HE1	9:B:829:CLA:C4D	2.33	0.41
9:B:817:CLA:H62	9:B:817:CLA:H41	1.63	0.41
9:B:819:CLA:H91	9:B:819:CLA:H112	1.74	0.41
5:H:98:LYS:HB2	5:H:101:LEU:HB2	2.03	0.41
7:L:109:HIS:HA	7:L:112:LEU:CD2	2.51	0.41
1:A:162:GLY:O	1:A:165:VAL:HG22	2.21	0.41
1:A:393:TRP:CD1	9:A:826:CLA:HAB	2.55	0.41
1:A:393:TRP:HB3	9:A:826:CLA:HMC3	2.03	0.41
9:A:802:CLA:HBB2	9:B:804:CLA:HAA1	2.03	0.41
9:A:850:CLA:H61	9:A:850:CLA:H92	1.83	0.41
2:B:231:ASN:HA	9:B:817:CLA:HAA2	2.03	0.41
2:B:548:PRO:HD2	3:C:62:PHE:CZ	2.56	0.41
3:C:13:GLY:HA2	3:C:28:MET:HE1	2.03	0.41
1:A:46:ILE:HG13	1:A:47:TRP:N	2.36	0.40
1:A:390:HIS:HB2	9:A:826:CLA:C1B	2.51	0.40
2:B:686:PRO:C	2:B:688:ALA:H	2.29	0.40
9:B:809:CLA:H192	9:B:809:CLA:H162	1.77	0.40
9:B:818:CLA:H92	9:B:818:CLA:H61	1.80	0.40
9:B:818:CLA:O1A	9:B:822:CLA:HBB1	2.21	0.40
3:C:21:CYS:HA	13:C:101:SF4:S4	2.61	0.40
1:A:560:LEU:HD11	1:A:578:ARG:HB3	2.02	0.40
9:A:808:CLA:H3A	9:A:808:CLA:HBA2	1.93	0.40
9:A:825:CLA:H152	9:A:825:CLA:H112	1.96	0.40
12:A:847:BCR:H361	12:A:847:BCR:H20C	1.79	0.40
2:B:694:ARG:HD2	7:L:155:SER:HA	2.03	0.40
9:B:809:CLA:H162	9:B:809:CLA:H141	1.80	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:838:LMT:H1B	15:B:838:LMT:H5'	1.69	0.40
5:H:60:LEU:HD23	5:H:60:LEU:HA	1.82	0.40
1:A:310:ARG:N	1:A:317:HIS:O	2.50	0.40
2:B:430:GLY:HA2	2:B:525:LEU:HD22	2.03	0.40
9:B:802:CLA:HMB2	9:B:803:CLA:H193	2.02	0.40
9:B:815:CLA:H112	9:B:815:CLA:H142	1.79	0.40
9:B:819:CLA:H3A	9:B:819:CLA:HBA2	1.40	0.40
9:L:303:CLA:HBB2	12:L:307:BCR:H392	2.04	0.40
9:A:841:CLA:H12	9:A:841:CLA:H52	1.91	0.40
2:B:69:ALA:HB2	2:B:135:LEU:HB2	2.03	0.40
9:B:801:CLA:HBC2	9:B:831:CLA:CHC	2.51	0.40
11:L:301:LHG:H212	11:L:301:LHG:H182	1.97	0.40
1:A:575:GLY:HA2	2:B:562:PRO:HD3	2.04	0.40
2:B:332:PHE:CD1	12:B:835:BCR:H391	2.56	0.40
9:B:804:CLA:H111	9:B:804:CLA:H143	1.73	0.40
9:B:831:CLA:H192	9:B:831:CLA:H161	1.88	0.40
9:B:832:CLA:H92	9:B:832:CLA:H62	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	706/708 (100%)	681 (96%)	24 (3%)	1 (0%)	48 68
2	B	731/733 (100%)	713 (98%)	18 (2%)	0	100 100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100 100
4	E	63/65 (97%)	62 (98%)	1 (2%)	0	100 100
5	H	93/95 (98%)	92 (99%)	1 (1%)	0	100 100
6	I	33/35 (94%)	32 (97%)	1 (3%)	0	100 100
7	L	157/159 (99%)	148 (94%)	9 (6%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	D	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
All	All	2001/2017 (99%)	1941 (97%)	59 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	571/571 (100%)	571 (100%)	0	100	100
2	B	596/596 (100%)	596 (100%)	0	100	100
3	C	71/71 (100%)	71 (100%)	0	100	100
4	E	58/58 (100%)	58 (100%)	0	100	100
5	H	77/77 (100%)	77 (100%)	0	100	100
6	I	31/31 (100%)	31 (100%)	0	100	100
7	L	123/123 (100%)	123 (100%)	0	100	100
8	D	121/121 (100%)	120 (99%)	1 (1%)	73	88
All	All	1648/1648 (100%)	1647 (100%)	1 (0%)	87	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	D	72	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	312	ASN
1	A	347	HIS
1	A	439	ASN
2	B	10	GLN
2	B	114	ASN
2	B	170	ASN
2	B	248	GLN
2	B	294	ASN
2	B	328	ASN
2	B	502	ASN
8	D	181	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

102 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	BCR	A	846	-	41,41,41	1.10	2 (4%)	56,56,56	1.34	10 (17%)
9	CLA	B	829	2	69,73,73	1.24	8 (11%)	83,113,113	1.30	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	A	819	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	8 (9%)
9	CLA	A	825	1	69,73,73	1.25	10 (14%)	83,113,113	1.30	6 (7%)
9	CLA	B	839	2	52,56,73	1.44	9 (17%)	62,92,113	1.36	7 (11%)
9	CLA	A	828	1	69,73,73	1.26	9 (13%)	83,113,113	1.28	7 (8%)
9	CLA	A	814	-	49,53,73	1.49	9 (18%)	59,89,113	1.44	5 (8%)
9	CLA	B	826	2	52,56,73	1.44	7 (13%)	62,92,113	1.41	7 (11%)
9	CLA	A	824	-	69,73,73	1.24	8 (11%)	83,113,113	1.30	8 (9%)
12	BCR	B	835	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
9	CLA	A	801	1	69,73,73	1.24	9 (13%)	83,113,113	1.23	6 (7%)
9	CLA	L	305	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	6 (9%)
9	CLA	B	828	2	55,59,73	1.40	8 (14%)	66,96,113	1.39	8 (12%)
9	CLA	B	816	-	50,54,73	1.44	9 (18%)	60,90,113	1.42	4 (6%)
9	CLA	A	816	1	69,73,73	1.25	8 (11%)	83,113,113	1.27	6 (7%)
9	CLA	B	822	2	51,55,73	1.44	10 (19%)	61,91,113	1.44	5 (8%)
9	CLA	A	831	1	69,73,73	1.25	8 (11%)	83,113,113	1.33	7 (8%)
9	CLA	B	824	-	64,68,73	1.30	9 (14%)	77,107,113	1.23	6 (7%)
9	CLA	A	830	1	69,73,73	1.26	9 (13%)	83,113,113	1.29	9 (10%)
9	CLA	A	834	1	55,59,73	1.41	9 (16%)	66,96,113	1.37	8 (12%)
9	CLA	B	803	2	69,73,73	1.23	9 (13%)	83,113,113	1.22	6 (7%)
9	CLA	A	808	1	69,73,73	1.26	9 (13%)	83,113,113	1.28	6 (7%)
9	CLA	L	303	7	53,57,73	1.41	9 (16%)	62,93,113	1.46	6 (9%)
9	CLA	B	840	-	52,56,73	1.44	7 (13%)	62,92,113	1.41	4 (6%)
9	CLA	A	812	1	49,53,73	1.48	8 (16%)	59,89,113	1.44	7 (11%)
9	CLA	A	820	1	53,57,73	1.43	8 (15%)	62,93,113	1.43	5 (8%)
9	CLA	B	819	2	64,68,73	1.29	9 (14%)	77,107,113	1.27	8 (10%)
9	CLA	A	822	1	59,63,73	1.35	9 (15%)	71,101,113	1.35	5 (7%)
9	CLA	A	833	1	49,53,73	1.49	9 (18%)	59,89,113	1.44	7 (11%)
9	CLA	A	839	1	52,56,73	1.44	8 (15%)	62,92,113	1.41	5 (8%)
9	CLA	A	817	1	69,73,73	1.25	9 (13%)	83,113,113	1.26	6 (7%)
9	CLA	B	813	2	47,52,73	1.58	7 (14%)	55,87,113	1.45	5 (9%)
9	CLA	L	304	7	69,73,73	1.24	9 (13%)	83,113,113	1.31	6 (7%)
12	BCR	L	302	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	5 (8%)
11	LHG	A	843	9	26,26,48	0.80	0	29,32,54	1.36	4 (13%)
9	CLA	B	831	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
9	CLA	B	802	-	69,73,73	1.24	9 (13%)	83,113,113	1.25	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	B	825	2	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
9	CLA	B	809	2	69,73,73	1.23	10 (14%)	83,113,113	1.32	6 (7%)
9	CLA	A	827	1	69,73,73	1.24	10 (14%)	83,113,113	1.26	6 (7%)
9	CLA	H	201	5	69,73,73	1.25	8 (11%)	83,113,113	1.32	6 (7%)
15	LMT	B	838	-	36,36,36	1.17	6 (16%)	47,47,47	0.95	1 (2%)
9	CLA	A	811	1	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
12	BCR	I	101	-	41,41,41	1.16	2 (4%)	56,56,56	1.16	4 (7%)
9	CLA	B	810	2	69,73,73	1.24	8 (11%)	83,113,113	1.31	6 (7%)
9	CLA	A	813	-	54,58,73	1.41	9 (16%)	65,95,113	1.39	8 (12%)
9	CLA	B	820	-	54,58,73	1.41	7 (12%)	65,95,113	1.40	5 (7%)
9	CLA	B	821	-	68,72,73	1.31	10 (14%)	85,112,113	1.33	9 (10%)
9	CLA	B	801	-	69,73,73	1.25	10 (14%)	83,113,113	1.37	9 (10%)
9	CLA	B	817	2	59,63,73	1.35	9 (15%)	71,101,113	1.33	6 (8%)
9	CLA	A	818	1	49,53,73	1.48	8 (16%)	59,89,113	1.42	4 (6%)
9	CLA	A	807	-	69,73,73	1.26	7 (10%)	83,113,113	1.26	5 (6%)
11	LHG	L	301	-	48,48,48	0.60	1 (2%)	51,54,54	1.26	6 (11%)
9	CLA	A	805	1	69,73,73	1.25	8 (11%)	83,113,113	1.31	8 (9%)
12	BCR	A	845	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	6 (10%)
9	CLA	A	823	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
9	CLA	B	811	2	69,73,73	1.25	9 (13%)	83,113,113	1.29	4 (4%)
9	CLA	A	835	-	69,73,73	1.24	9 (13%)	83,113,113	1.32	7 (8%)
9	CLA	A	803	-	59,63,73	1.36	7 (11%)	71,101,113	1.35	7 (9%)
9	CLA	B	818	2	63,67,73	1.31	10 (15%)	75,105,113	1.37	6 (8%)
9	CLA	B	830	2	51,55,73	1.44	8 (15%)	61,91,113	1.38	6 (9%)
9	CLA	A	806	-	69,73,73	1.27	8 (11%)	83,113,113	1.27	6 (7%)
12	BCR	L	306	-	41,41,41	1.14	2 (4%)	56,56,56	1.30	8 (14%)
12	BCR	A	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.28	8 (14%)
12	BCR	L	308	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	8 (14%)
9	CLA	B	823	2	69,73,73	1.24	8 (11%)	83,113,113	1.26	7 (8%)
9	CLA	B	827	2	49,53,73	1.49	9 (18%)	59,89,113	1.47	7 (11%)
13	SF4	C	101	3	0,12,12	-	-	-		
9	CLA	A	836	1	69,73,73	1.23	7 (10%)	83,113,113	1.36	7 (8%)
12	BCR	B	834	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	5 (8%)
9	CLA	A	810	1	58,62,73	1.38	9 (15%)	69,99,113	1.34	7 (10%)
11	LHG	A	842	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	B	808	2	59,63,73	1.34	9 (15%)	71,101,113	1.35	6 (8%)
10	PQN	B	833	-	34,34,34	0.36	0	42,45,45	0.58	1 (2%)
9	CLA	B	807	2	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
9	CLA	B	805	2	49,53,73	1.48	10 (20%)	59,89,113	1.44	5 (8%)
9	CLA	A	802	-	69,73,73	1.26	8 (11%)	83,113,113	1.24	7 (8%)
9	CLA	A	804	1	69,73,73	1.25	8 (11%)	83,113,113	1.32	6 (7%)
9	CLA	B	806	2	69,73,73	1.24	7 (10%)	83,113,113	1.33	7 (8%)
9	CLA	B	812	2	58,62,73	1.41	9 (15%)	73,100,113	1.34	7 (9%)
9	CLA	A	841	11	56,60,73	1.41	6 (10%)	67,97,113	1.38	5 (7%)
12	BCR	B	836	-	41,41,41	1.17	3 (7%)	56,56,56	1.24	5 (8%)
14	DGD	B	837	-	67,67,67	0.87	2 (2%)	81,81,81	1.45	12 (14%)
9	CLA	A	849	-	69,73,73	1.25	9 (13%)	83,113,113	1.27	6 (7%)
10	PQN	A	840	-	34,34,34	0.36	0	42,45,45	0.54	0
12	BCR	L	307	-	41,41,41	1.16	2 (4%)	56,56,56	1.26	7 (12%)
9	CLA	B	832	2	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
9	CLA	B	814	2	69,73,73	1.25	9 (13%)	83,113,113	1.27	5 (6%)
9	CLA	A	838	-	69,73,73	1.27	9 (13%)	83,113,113	1.27	5 (6%)
9	CLA	A	837	1	51,55,73	1.44	7 (13%)	61,91,113	1.43	6 (9%)
9	CLA	A	832	1	54,58,73	1.42	6 (11%)	65,95,113	1.44	7 (10%)
9	CLA	B	815	2	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
9	CLA	B	804	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	4 (4%)
9	CLA	A	815	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
12	BCR	A	844	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
9	CLA	A	809	-	69,73,73	1.27	8 (11%)	83,113,113	1.28	7 (8%)
9	CLA	A	826	1	69,73,73	1.24	7 (10%)	83,113,113	1.28	8 (9%)
9	CLA	A	829	1	54,58,73	1.40	9 (16%)	65,95,113	1.40	6 (9%)
13	SF4	C	102	3	0,12,12	-	-	-		
9	CLA	A	821	1	55,59,73	1.40	8 (14%)	66,96,113	1.36	6 (9%)
13	SF4	A	848	2,1	0,12,12	-	-	-		
9	CLA	A	850	1	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)

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
12	BCR	A	846	-	-	7/29/63/63	0/2/2/2
9	CLA	B	829	2	-	10/39/115/115	-
9	CLA	A	819	-	-	4/39/115/115	-
9	CLA	A	825	1	-	10/39/115/115	-
9	CLA	B	839	2	-	6/19/95/115	-
9	CLA	A	828	1	-	9/39/115/115	-
9	CLA	A	814	-	-	1/15/91/115	-
9	CLA	B	826	2	-	9/19/95/115	-
9	CLA	A	824	-	-	7/39/115/115	-
12	BCR	B	835	-	-	21/29/63/63	0/2/2/2
9	CLA	A	801	1	-	12/39/115/115	-
9	CLA	L	305	-	-	2/21/97/115	-
9	CLA	B	828	2	-	6/23/99/115	-
9	CLA	B	816	-	-	7/17/93/115	-
9	CLA	A	816	1	-	18/39/115/115	-
9	CLA	B	822	2	-	10/18/94/115	-
9	CLA	A	831	1	-	24/39/115/115	-
9	CLA	B	824	-	-	16/33/109/115	-
9	CLA	A	830	1	-	9/39/115/115	-
9	CLA	A	834	1	-	11/23/99/115	-
9	CLA	B	803	2	-	9/39/115/115	-
9	CLA	A	808	1	-	14/39/115/115	-
9	CLA	L	303	7	-	8/20/96/115	-
9	CLA	B	840	-	-	10/19/95/115	-
9	CLA	A	812	1	-	4/15/91/115	-
9	CLA	A	820	1	-	9/20/96/115	-
9	CLA	B	819	2	-	15/33/109/115	-
9	CLA	A	822	1	-	9/27/103/115	-
9	CLA	A	833	1	-	5/15/91/115	-
9	CLA	A	839	1	-	5/19/95/115	-
9	CLA	A	817	1	-	15/39/115/115	-
9	CLA	B	813	2	-	4/14/91/115	-
9	CLA	L	304	7	-	8/39/115/115	-
12	BCR	L	302	-	-	7/29/63/63	0/2/2/2
11	LHG	A	843	9	-	13/31/31/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	B	831	-	-	8/39/115/115	-
9	CLA	B	802	-	-	15/39/115/115	-
9	CLA	B	825	2	-	8/39/115/115	-
9	CLA	B	809	2	-	10/39/115/115	-
9	CLA	A	827	1	-	13/39/115/115	-
9	CLA	H	201	5	-	10/39/115/115	-
15	LMT	B	838	-	-	13/21/61/61	0/2/2/2
9	CLA	A	811	1	-	13/39/115/115	-
12	BCR	I	101	-	-	7/29/63/63	0/2/2/2
9	CLA	B	810	2	-	9/39/115/115	-
9	CLA	A	813	-	-	7/21/97/115	-
9	CLA	B	820	-	-	8/21/97/115	-
9	CLA	B	821	-	-	12/37/113/115	-
9	CLA	B	801	-	-	20/39/115/115	-
9	CLA	B	817	2	-	8/27/103/115	-
9	CLA	A	818	1	-	6/15/91/115	-
9	CLA	A	807	-	-	21/39/115/115	-
11	LHG	L	301	-	-	24/53/53/53	-
9	CLA	A	805	1	-	10/39/115/115	-
12	BCR	A	845	-	-	10/29/63/63	0/2/2/2
9	CLA	A	823	-	-	8/39/115/115	-
9	CLA	B	811	2	-	21/39/115/115	-
9	CLA	A	835	-	-	11/39/115/115	-
9	CLA	A	803	-	-	7/27/103/115	-
9	CLA	B	818	2	-	9/32/108/115	-
9	CLA	B	830	2	-	1/18/94/115	-
9	CLA	A	806	-	-	15/39/115/115	-
12	BCR	L	306	-	-	8/29/63/63	0/2/2/2
12	BCR	A	847	-	-	9/29/63/63	0/2/2/2
12	BCR	L	308	-	-	10/29/63/63	0/2/2/2
9	CLA	B	823	2	-	12/39/115/115	-
9	CLA	B	827	2	-	4/15/91/115	-
13	SF4	C	101	3	-	-	0/6/5/5
9	CLA	A	836	1	-	12/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BCR	B	834	-	-	9/29/63/63	0/2/2/2
9	CLA	A	810	1	-	8/26/102/115	-
11	LHG	A	842	-	-	24/53/53/53	-
9	CLA	B	808	2	-	5/27/103/115	-
10	PQN	B	833	-	-	2/23/43/43	0/2/2/2
9	CLA	B	807	2	-	13/39/115/115	-
9	CLA	B	805	2	-	3/15/91/115	-
9	CLA	A	802	-	-	8/39/115/115	-
9	CLA	A	804	1	-	7/39/115/115	-
9	CLA	B	806	2	-	14/39/115/115	-
9	CLA	B	812	2	-	8/25/101/115	-
9	CLA	A	841	11	-	9/24/100/115	-
12	BCR	B	836	-	-	8/29/63/63	0/2/2/2
14	DGD	B	837	-	-	24/55/95/95	0/2/2/2
9	CLA	A	849	-	-	19/39/115/115	-
10	PQN	A	840	-	-	12/23/43/43	0/2/2/2
12	BCR	L	307	-	-	8/29/63/63	0/2/2/2
9	CLA	B	832	2	-	12/39/115/115	-
9	CLA	B	814	2	-	16/39/115/115	-
9	CLA	A	838	-	-	16/39/115/115	-
9	CLA	A	837	1	-	11/18/94/115	-
9	CLA	A	832	1	-	7/21/97/115	-
9	CLA	B	815	2	-	10/39/115/115	-
9	CLA	B	804	-	-	13/39/115/115	-
9	CLA	A	815	-	-	16/39/115/115	-
12	BCR	A	844	-	-	7/29/63/63	0/2/2/2
9	CLA	A	809	-	-	16/39/115/115	-
9	CLA	A	826	1	-	18/39/115/115	-
9	CLA	A	829	1	-	6/21/97/115	-
13	SF4	C	102	3	-	-	0/6/5/5
9	CLA	A	821	1	-	9/23/99/115	-
13	SF4	A	848	2,1	-	-	0/6/5/5
9	CLA	A	850	1	-	13/39/115/115	-

All (714) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	813	CLA	C2B-C1B	4.83	1.49	1.39
9	A	826	CLA	C1D-ND	4.01	1.42	1.37
9	A	838	CLA	C1D-ND	3.97	1.42	1.37
9	A	841	CLA	C1D-ND	3.95	1.42	1.37
9	B	818	CLA	C1D-ND	3.90	1.42	1.37
9	A	836	CLA	C1D-ND	3.89	1.42	1.37
9	A	832	CLA	C1D-ND	3.88	1.42	1.37
9	A	809	CLA	C1D-ND	3.87	1.42	1.37
9	A	801	CLA	C1D-ND	3.87	1.42	1.37
9	A	839	CLA	C1D-ND	3.87	1.42	1.37
9	B	840	CLA	C1D-ND	3.86	1.42	1.37
9	A	820	CLA	C1D-ND	3.86	1.42	1.37
9	A	822	CLA	C1D-ND	3.85	1.42	1.37
9	A	806	CLA	C1D-ND	3.85	1.42	1.37
9	A	807	CLA	C1D-ND	3.84	1.42	1.37
9	A	821	CLA	C1D-ND	3.83	1.42	1.37
9	A	803	CLA	C1D-ND	3.82	1.42	1.37
9	A	816	CLA	C1D-ND	3.82	1.42	1.37
9	B	826	CLA	C1D-ND	3.81	1.42	1.37
9	H	201	CLA	C1D-ND	3.81	1.42	1.37
9	A	815	CLA	C1D-ND	3.80	1.42	1.37
9	A	833	CLA	C1D-ND	3.80	1.42	1.37
9	A	808	CLA	C1D-ND	3.80	1.42	1.37
9	A	810	CLA	C1D-ND	3.80	1.42	1.37
9	B	832	CLA	C1D-ND	3.80	1.42	1.37
9	B	823	CLA	C1D-ND	3.80	1.42	1.37
9	B	827	CLA	C1D-ND	3.80	1.42	1.37
9	A	823	CLA	C1D-ND	3.79	1.42	1.37
9	B	813	CLA	C1D-ND	3.79	1.42	1.37
9	B	820	CLA	C1D-ND	3.78	1.42	1.37
9	A	805	CLA	C1D-ND	3.77	1.42	1.37
9	B	814	CLA	C1D-ND	3.77	1.42	1.37
9	B	803	CLA	C1D-ND	3.76	1.42	1.37
9	A	818	CLA	C1D-ND	3.76	1.42	1.37
9	A	819	CLA	C1D-ND	3.76	1.42	1.37
9	A	831	CLA	C1D-ND	3.76	1.42	1.37
9	A	814	CLA	C1D-ND	3.75	1.42	1.37
9	L	305	CLA	C1D-ND	3.75	1.42	1.37
9	B	806	CLA	C1D-ND	3.75	1.42	1.37
9	A	811	CLA	C1D-ND	3.75	1.42	1.37
9	B	830	CLA	C1D-ND	3.75	1.42	1.37
9	A	834	CLA	C1D-ND	3.74	1.42	1.37
9	B	839	CLA	C1D-ND	3.74	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	804	CLA	C1D-ND	3.73	1.42	1.37
9	A	817	CLA	C1D-ND	3.73	1.42	1.37
9	A	825	CLA	C1D-ND	3.73	1.42	1.37
9	B	829	CLA	C1D-ND	3.73	1.42	1.37
9	A	813	CLA	C1D-ND	3.73	1.42	1.37
9	B	825	CLA	C1D-ND	3.73	1.42	1.37
9	A	828	CLA	C1D-ND	3.72	1.42	1.37
9	B	821	CLA	C1D-ND	3.72	1.42	1.37
9	B	822	CLA	C1D-ND	3.72	1.42	1.37
9	B	808	CLA	C1D-ND	3.71	1.42	1.37
9	B	812	CLA	C1D-ND	3.70	1.42	1.37
9	L	303	CLA	C1D-ND	3.69	1.42	1.37
9	A	830	CLA	C1D-ND	3.69	1.42	1.37
9	A	837	CLA	C1D-ND	3.68	1.42	1.37
9	B	807	CLA	C1D-ND	3.68	1.42	1.37
9	A	802	CLA	C1D-ND	3.67	1.42	1.37
9	B	815	CLA	C1D-ND	3.67	1.42	1.37
9	B	828	CLA	C1D-ND	3.67	1.42	1.37
9	A	812	CLA	C1D-ND	3.67	1.42	1.37
9	B	802	CLA	C1D-ND	3.67	1.42	1.37
9	B	811	CLA	C1D-ND	3.66	1.42	1.37
9	A	835	CLA	C1D-ND	3.66	1.42	1.37
9	A	850	CLA	C1D-ND	3.65	1.42	1.37
9	B	809	CLA	C1D-ND	3.65	1.42	1.37
9	B	805	CLA	C1D-ND	3.65	1.42	1.37
9	B	824	CLA	C1D-ND	3.65	1.42	1.37
9	B	819	CLA	C1D-ND	3.64	1.42	1.37
9	A	824	CLA	C1D-ND	3.63	1.42	1.37
9	B	817	CLA	C1D-ND	3.62	1.42	1.37
9	A	829	CLA	C1D-ND	3.62	1.42	1.37
9	B	816	CLA	C1D-ND	3.62	1.42	1.37
9	B	831	CLA	C1D-ND	3.57	1.42	1.37
9	L	304	CLA	C1D-ND	3.57	1.42	1.37
12	L	302	BCR	C1-C6	-3.57	1.48	1.53
12	I	101	BCR	C1-C6	-3.56	1.48	1.53
9	A	849	CLA	C1D-ND	3.56	1.42	1.37
9	B	810	CLA	C1D-ND	3.55	1.42	1.37
12	L	307	BCR	C1-C6	-3.53	1.48	1.53
9	A	827	CLA	C1D-ND	3.52	1.42	1.37
12	A	847	BCR	C1-C6	-3.50	1.49	1.53
9	A	839	CLA	C4B-NB	3.49	1.42	1.37
9	B	801	CLA	C1D-ND	3.46	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	849	CLA	C4B-NB	3.45	1.42	1.37
9	B	804	CLA	C1D-ND	3.45	1.42	1.37
9	A	814	CLA	C4B-NB	3.44	1.42	1.37
12	A	844	BCR	C1-C6	-3.43	1.49	1.53
9	A	809	CLA	C4B-NB	3.42	1.42	1.37
9	B	832	CLA	C4B-NB	3.42	1.42	1.37
9	B	839	CLA	C4B-NB	3.40	1.42	1.37
9	A	838	CLA	C4B-NB	3.38	1.41	1.37
12	L	306	BCR	C1-C6	-3.38	1.49	1.53
9	A	806	CLA	C4B-NB	3.37	1.41	1.37
9	B	830	CLA	C4B-NB	3.37	1.41	1.37
12	A	847	BCR	C30-C25	-3.36	1.49	1.53
9	B	827	CLA	C4B-NB	3.36	1.41	1.37
9	B	817	CLA	C4B-NB	3.36	1.41	1.37
12	B	836	BCR	C30-C25	-3.36	1.49	1.53
12	B	836	BCR	C1-C6	-3.35	1.49	1.53
12	L	308	BCR	C1-C6	-3.35	1.49	1.53
9	A	810	CLA	C4B-NB	3.35	1.41	1.37
9	A	833	CLA	C4B-NB	3.35	1.41	1.37
9	A	837	CLA	C4B-NB	3.35	1.41	1.37
9	B	824	CLA	C4B-NB	3.35	1.41	1.37
9	A	828	CLA	C4B-NB	3.34	1.41	1.37
9	A	841	CLA	C4B-NB	3.33	1.41	1.37
9	A	803	CLA	C4B-NB	3.33	1.41	1.37
9	B	804	CLA	C4B-NB	3.33	1.41	1.37
9	A	821	CLA	C4B-NB	3.33	1.41	1.37
9	A	830	CLA	C4B-NB	3.33	1.41	1.37
9	B	826	CLA	C4B-NB	3.32	1.41	1.37
9	B	805	CLA	C4B-NB	3.31	1.41	1.37
9	A	820	CLA	C4B-NB	3.31	1.41	1.37
9	A	832	CLA	C4B-NB	3.31	1.41	1.37
9	A	817	CLA	C4B-NB	3.30	1.41	1.37
9	A	826	CLA	C4B-NB	3.28	1.41	1.37
9	L	303	CLA	C4B-NB	3.28	1.41	1.37
9	A	829	CLA	C4B-NB	3.26	1.41	1.37
9	B	840	CLA	C4B-NB	3.26	1.41	1.37
9	B	809	CLA	C4B-NB	3.26	1.41	1.37
9	A	834	CLA	C4B-NB	3.26	1.41	1.37
9	B	812	CLA	C4B-NB	3.26	1.41	1.37
9	A	808	CLA	C4B-NB	3.26	1.41	1.37
9	A	802	CLA	C4B-NB	3.25	1.41	1.37
9	A	813	CLA	C4B-NB	3.25	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	807	CLA	C4B-NB	3.25	1.41	1.37
9	A	818	CLA	C4B-NB	3.24	1.41	1.37
9	B	820	CLA	C4B-NB	3.23	1.41	1.37
9	A	815	CLA	C4B-NB	3.23	1.41	1.37
9	B	823	CLA	C4B-NB	3.23	1.41	1.37
9	L	304	CLA	C4B-NB	3.23	1.41	1.37
9	B	802	CLA	C4B-NB	3.23	1.41	1.37
9	A	836	CLA	C4B-NB	3.23	1.41	1.37
9	B	815	CLA	C4B-NB	3.23	1.41	1.37
9	B	813	CLA	C4B-NB	3.22	1.41	1.37
9	A	804	CLA	C4B-NB	3.22	1.41	1.37
9	B	811	CLA	C4B-NB	3.22	1.41	1.37
9	B	825	CLA	C4B-NB	3.21	1.41	1.37
9	B	819	CLA	C4B-NB	3.21	1.41	1.37
9	A	823	CLA	C4B-NB	3.21	1.41	1.37
9	A	816	CLA	C4B-NB	3.20	1.41	1.37
12	L	307	BCR	C30-C25	-3.20	1.49	1.53
9	L	305	CLA	C4B-NB	3.20	1.41	1.37
9	A	831	CLA	C4B-NB	3.19	1.41	1.37
9	B	801	CLA	C4B-NB	3.18	1.41	1.37
9	A	827	CLA	C4B-NB	3.18	1.41	1.37
9	A	819	CLA	C4B-NB	3.18	1.41	1.37
12	A	845	BCR	C1-C6	-3.17	1.49	1.53
9	A	822	CLA	C4B-NB	3.17	1.41	1.37
9	B	821	CLA	C4B-NB	3.17	1.41	1.37
9	B	806	CLA	C4B-NB	3.17	1.41	1.37
9	B	831	CLA	C4B-NB	3.17	1.41	1.37
9	A	802	CLA	C4D-ND	-3.17	1.33	1.37
9	B	829	CLA	C4B-NB	3.16	1.41	1.37
9	B	803	CLA	C4B-NB	3.16	1.41	1.37
9	B	808	CLA	C4B-NB	3.15	1.41	1.37
9	A	812	CLA	C4B-NB	3.15	1.41	1.37
9	B	816	CLA	C4B-NB	3.14	1.41	1.37
9	A	814	CLA	C3B-C4B	3.13	1.50	1.42
9	A	825	CLA	C4B-NB	3.13	1.41	1.37
9	B	818	CLA	C4B-NB	3.13	1.41	1.37
9	B	821	CLA	CAB-C3B	-3.12	1.44	1.50
9	A	850	CLA	C4B-NB	3.12	1.41	1.37
12	B	834	BCR	C30-C25	-3.12	1.49	1.53
9	B	821	CLA	C4D-ND	-3.12	1.33	1.37
9	B	814	CLA	C4B-NB	3.11	1.41	1.37
9	B	830	CLA	C4D-ND	-3.11	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	845	BCR	C30-C25	-3.11	1.49	1.53
9	A	811	CLA	C4B-NB	3.10	1.41	1.37
9	H	201	CLA	C4B-NB	3.10	1.41	1.37
9	B	807	CLA	C4D-ND	-3.10	1.33	1.37
9	B	819	CLA	C4D-ND	-3.10	1.33	1.37
12	I	101	BCR	C30-C25	-3.10	1.49	1.53
9	B	811	CLA	C4D-ND	-3.10	1.33	1.37
9	B	810	CLA	C4D-ND	-3.09	1.33	1.37
9	B	810	CLA	C4B-NB	3.09	1.41	1.37
9	A	824	CLA	C4B-NB	3.09	1.41	1.37
9	A	805	CLA	C4B-NB	3.08	1.41	1.37
12	B	834	BCR	C1-C6	-3.08	1.49	1.53
9	B	828	CLA	C4B-NB	3.08	1.41	1.37
9	A	835	CLA	C4B-NB	3.08	1.41	1.37
9	B	817	CLA	C4D-ND	-3.07	1.33	1.37
9	A	849	CLA	C3B-C4B	3.07	1.49	1.42
9	B	812	CLA	CAB-C3B	-3.07	1.44	1.50
9	A	824	CLA	C4D-ND	-3.06	1.33	1.37
9	B	822	CLA	C4B-NB	3.06	1.41	1.37
9	B	806	CLA	C4D-ND	-3.05	1.33	1.37
9	A	817	CLA	C4D-ND	-3.05	1.33	1.37
9	B	801	CLA	C4D-ND	-3.05	1.33	1.37
9	B	808	CLA	C4D-ND	-3.04	1.33	1.37
12	A	846	BCR	C30-C25	-3.04	1.49	1.53
9	A	828	CLA	C4D-ND	-3.04	1.33	1.37
9	A	827	CLA	C4D-ND	-3.04	1.33	1.37
9	A	830	CLA	C4D-ND	-3.03	1.33	1.37
9	A	805	CLA	C4D-ND	-3.03	1.33	1.37
9	A	801	CLA	C4B-NB	3.03	1.41	1.37
9	A	825	CLA	C4D-ND	-3.02	1.33	1.37
9	A	804	CLA	C4D-ND	-3.02	1.33	1.37
9	A	812	CLA	C4D-ND	-3.02	1.33	1.37
9	B	825	CLA	C4D-ND	-3.02	1.33	1.37
9	B	828	CLA	C4D-ND	-3.02	1.33	1.37
9	L	304	CLA	C4D-ND	-3.02	1.33	1.37
9	B	831	CLA	C4D-ND	-3.02	1.33	1.37
9	B	807	CLA	C4B-NB	3.02	1.41	1.37
9	B	818	CLA	C4D-ND	-3.01	1.33	1.37
9	B	839	CLA	C3B-C4B	3.01	1.49	1.42
9	A	835	CLA	C4D-ND	-3.01	1.33	1.37
9	B	829	CLA	C4D-ND	-3.01	1.33	1.37
9	B	822	CLA	C4D-ND	-3.00	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	839	CLA	C4D-ND	-3.00	1.33	1.37
9	L	303	CLA	C4D-ND	-3.00	1.33	1.37
9	B	824	CLA	C3B-C4B	3.00	1.49	1.42
12	L	302	BCR	C30-C25	-3.00	1.49	1.53
9	B	824	CLA	C4D-ND	-2.99	1.33	1.37
12	A	846	BCR	C1-C6	-2.98	1.49	1.53
9	A	850	CLA	C4D-ND	-2.98	1.33	1.37
9	B	804	CLA	C4D-ND	-2.98	1.33	1.37
9	A	809	CLA	C3B-C4B	2.98	1.49	1.42
9	A	830	CLA	C3B-C4B	2.98	1.49	1.42
9	A	810	CLA	C3B-C4B	2.98	1.49	1.42
9	B	814	CLA	C4D-ND	-2.98	1.33	1.37
9	A	816	CLA	C4D-ND	-2.97	1.33	1.37
9	B	802	CLA	C4D-ND	-2.97	1.33	1.37
9	A	831	CLA	C4D-ND	-2.97	1.33	1.37
9	A	803	CLA	C3B-C4B	2.97	1.49	1.42
9	B	823	CLA	C4D-ND	-2.97	1.33	1.37
9	A	810	CLA	C4D-ND	-2.97	1.33	1.37
9	A	819	CLA	C4D-ND	-2.96	1.33	1.37
9	A	815	CLA	C4D-ND	-2.96	1.33	1.37
9	B	816	CLA	C4D-ND	-2.96	1.33	1.37
9	B	805	CLA	C4D-ND	-2.95	1.33	1.37
9	A	839	CLA	C3B-C4B	2.95	1.49	1.42
9	A	818	CLA	C4D-ND	-2.95	1.33	1.37
9	A	822	CLA	C4D-ND	-2.95	1.33	1.37
9	A	829	CLA	C4D-ND	-2.95	1.33	1.37
9	A	832	CLA	C4D-ND	-2.95	1.33	1.37
9	A	823	CLA	C4D-ND	-2.94	1.33	1.37
9	B	809	CLA	C4D-ND	-2.94	1.33	1.37
9	B	813	CLA	C4D-ND	-2.94	1.33	1.37
9	A	808	CLA	C4D-ND	-2.94	1.33	1.37
9	B	827	CLA	C4D-ND	-2.94	1.33	1.37
9	A	834	CLA	C3B-C4B	2.93	1.49	1.42
9	A	814	CLA	C4D-ND	-2.93	1.33	1.37
9	L	305	CLA	C4D-ND	-2.93	1.33	1.37
9	A	813	CLA	C4D-ND	-2.93	1.33	1.37
9	A	833	CLA	C3B-C4B	2.93	1.49	1.42
9	A	811	CLA	C4D-ND	-2.93	1.33	1.37
9	A	826	CLA	C3B-C4B	2.93	1.49	1.42
9	A	813	CLA	C3B-C4B	2.93	1.49	1.42
9	A	803	CLA	C4D-ND	-2.92	1.33	1.37
9	B	815	CLA	C4D-ND	-2.92	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	802	CLA	C3B-C4B	2.92	1.49	1.42
9	B	831	CLA	C3B-C4B	2.92	1.49	1.42
9	A	834	CLA	C4D-ND	-2.92	1.33	1.37
9	A	806	CLA	C3B-C4B	2.92	1.49	1.42
9	B	805	CLA	C3B-C4B	2.92	1.49	1.42
9	A	837	CLA	C3B-C4B	2.91	1.49	1.42
9	A	820	CLA	C4D-ND	-2.91	1.33	1.37
9	A	833	CLA	C4D-ND	-2.91	1.33	1.37
9	A	841	CLA	C4D-ND	-2.91	1.33	1.37
9	B	802	CLA	C3B-C4B	2.91	1.49	1.42
9	A	832	CLA	C3B-C4B	2.91	1.49	1.42
9	B	826	CLA	C4D-ND	-2.90	1.33	1.37
9	A	811	CLA	C3B-C4B	2.90	1.49	1.42
12	B	835	BCR	C1-C6	-2.90	1.49	1.53
9	A	824	CLA	C3B-C4B	2.90	1.49	1.42
9	H	201	CLA	C4D-ND	-2.90	1.33	1.37
9	A	816	CLA	C3B-C4B	2.90	1.49	1.42
9	A	838	CLA	C4D-ND	-2.89	1.33	1.37
9	A	818	CLA	C3B-C4B	2.89	1.49	1.42
9	B	832	CLA	C4D-ND	-2.89	1.33	1.37
9	A	839	CLA	C4D-ND	-2.89	1.33	1.37
9	A	819	CLA	C3B-C4B	2.88	1.49	1.42
9	A	807	CLA	C4D-ND	-2.88	1.33	1.37
9	B	826	CLA	C3B-C4B	2.88	1.49	1.42
9	B	840	CLA	C3B-C4B	2.88	1.49	1.42
9	B	820	CLA	C4D-ND	-2.87	1.33	1.37
9	B	827	CLA	C3B-C4B	2.87	1.49	1.42
9	B	812	CLA	C4D-ND	-2.87	1.33	1.37
9	A	815	CLA	C3B-C4B	2.87	1.49	1.42
9	A	804	CLA	C3B-C4B	2.87	1.49	1.42
9	B	820	CLA	C3B-C4B	2.87	1.49	1.42
9	L	303	CLA	C3B-C4B	2.87	1.49	1.42
9	B	814	CLA	C3B-C4B	2.87	1.49	1.42
12	L	306	BCR	C30-C25	-2.87	1.49	1.53
9	A	808	CLA	C3B-C4B	2.87	1.49	1.42
9	A	826	CLA	C4D-ND	-2.86	1.33	1.37
9	B	829	CLA	C3B-C4B	2.86	1.49	1.42
12	B	835	BCR	C30-C25	-2.86	1.49	1.53
9	B	804	CLA	C3B-C4B	2.86	1.49	1.42
9	A	836	CLA	C3B-C4B	2.86	1.49	1.42
9	A	838	CLA	C3B-C4B	2.86	1.49	1.42
9	A	821	CLA	C3B-C4B	2.85	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	806	CLA	C3B-C4B	2.85	1.49	1.42
9	B	828	CLA	C3B-C4B	2.84	1.49	1.42
9	A	837	CLA	C4D-ND	-2.84	1.33	1.37
9	A	807	CLA	C3B-C4B	2.84	1.49	1.42
9	A	841	CLA	C3B-C4B	2.84	1.49	1.42
9	B	817	CLA	C3B-C4B	2.84	1.49	1.42
9	A	849	CLA	C4D-ND	-2.84	1.33	1.37
9	A	825	CLA	C3B-C4B	2.84	1.49	1.42
9	A	806	CLA	C4D-ND	-2.83	1.33	1.37
9	B	816	CLA	C3B-C4B	2.83	1.49	1.42
9	A	809	CLA	C4D-ND	-2.83	1.33	1.37
9	A	812	CLA	C3B-C4B	2.82	1.49	1.42
9	B	815	CLA	C3B-C4B	2.82	1.49	1.42
9	A	850	CLA	C3B-C4B	2.82	1.49	1.42
9	B	840	CLA	C4D-ND	-2.82	1.33	1.37
12	A	844	BCR	C30-C25	-2.82	1.49	1.53
9	B	803	CLA	C4D-ND	-2.82	1.33	1.37
9	H	201	CLA	C3B-C4B	2.81	1.49	1.42
9	B	809	CLA	C3B-C4B	2.81	1.49	1.42
9	A	821	CLA	C4D-ND	-2.81	1.33	1.37
9	A	817	CLA	C3B-C4B	2.81	1.49	1.42
9	A	820	CLA	C3B-C4B	2.81	1.49	1.42
9	A	801	CLA	C4D-ND	-2.81	1.33	1.37
9	B	801	CLA	C3B-C4B	2.81	1.49	1.42
9	B	823	CLA	C3B-C4B	2.80	1.49	1.42
9	B	818	CLA	C3B-C4B	2.80	1.49	1.42
9	L	305	CLA	C3B-C4B	2.79	1.49	1.42
9	B	822	CLA	C3B-C4B	2.79	1.49	1.42
9	B	819	CLA	C3B-C4B	2.78	1.49	1.42
9	A	805	CLA	C3B-C4B	2.78	1.49	1.42
9	A	823	CLA	C3B-C4B	2.77	1.49	1.42
9	A	829	CLA	C3B-C4B	2.77	1.49	1.42
9	A	822	CLA	C3B-C4B	2.77	1.49	1.42
9	B	803	CLA	C1B-C2B	2.76	1.49	1.43
9	A	827	CLA	C3B-C4B	2.76	1.49	1.42
9	A	831	CLA	C3B-C4B	2.76	1.49	1.42
9	B	808	CLA	C3B-C4B	2.76	1.49	1.42
9	A	841	CLA	C1B-C2B	2.75	1.49	1.43
9	L	304	CLA	C3B-C4B	2.75	1.49	1.42
9	A	835	CLA	C3B-C4B	2.75	1.49	1.42
9	A	801	CLA	C3B-C4B	2.75	1.49	1.42
9	B	830	CLA	C3B-C4B	2.73	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	828	CLA	C3B-C4B	2.73	1.49	1.42
9	A	806	CLA	C1B-C2B	2.73	1.49	1.43
9	A	836	CLA	C4D-ND	-2.72	1.33	1.37
9	B	807	CLA	C3B-C4B	2.72	1.49	1.42
9	B	832	CLA	C3B-C4B	2.72	1.49	1.42
9	B	811	CLA	C3B-C4B	2.72	1.49	1.42
9	A	836	CLA	C1B-C2B	2.71	1.49	1.43
9	A	807	CLA	C1B-C2B	2.71	1.49	1.43
9	A	808	CLA	C1B-C2B	2.70	1.49	1.43
9	B	825	CLA	C3B-C4B	2.70	1.49	1.42
9	B	810	CLA	C3B-C4B	2.69	1.49	1.42
9	A	820	CLA	C1B-C2B	2.68	1.49	1.43
9	A	822	CLA	C1B-C2B	2.68	1.49	1.43
9	B	803	CLA	C3B-C4B	2.68	1.49	1.42
9	A	805	CLA	C1B-C2B	2.67	1.49	1.43
9	A	823	CLA	C1B-C2B	2.67	1.49	1.43
9	A	839	CLA	C1B-C2B	2.67	1.49	1.43
9	A	832	CLA	C1B-C2B	2.66	1.49	1.43
9	B	821	CLA	C4B-C3B	2.66	1.49	1.43
9	B	822	CLA	C1B-C2B	2.66	1.49	1.43
9	L	304	CLA	C1B-C2B	2.66	1.49	1.43
9	A	821	CLA	C1B-C2B	2.66	1.49	1.43
9	B	812	CLA	C1B-C2B	2.65	1.49	1.43
9	A	801	CLA	C1B-C2B	2.65	1.49	1.43
9	B	840	CLA	C1B-C2B	2.65	1.49	1.43
9	A	837	CLA	C1B-C2B	2.65	1.49	1.43
9	L	305	CLA	C1B-C2B	2.65	1.49	1.43
12	L	308	BCR	C30-C25	-2.65	1.50	1.53
9	B	820	CLA	C1B-C2B	2.65	1.49	1.43
9	A	809	CLA	C1B-C2B	2.64	1.49	1.43
9	B	809	CLA	C1B-C2B	2.63	1.49	1.43
9	B	827	CLA	C1B-C2B	2.63	1.49	1.43
9	B	806	CLA	C1B-C2B	2.63	1.49	1.43
9	B	811	CLA	C1B-C2B	2.63	1.49	1.43
9	H	201	CLA	C1B-C2B	2.63	1.49	1.43
15	B	838	LMT	O3'-C3'	-2.63	1.36	1.43
9	B	816	CLA	C1B-C2B	2.62	1.49	1.43
9	B	804	CLA	C1B-C2B	2.62	1.49	1.43
9	B	815	CLA	C1B-C2B	2.62	1.49	1.43
9	A	818	CLA	C1B-C2B	2.62	1.49	1.43
9	B	812	CLA	C4B-C3B	2.62	1.49	1.43
9	B	832	CLA	C1B-C2B	2.62	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	808	CLA	C1B-C2B	2.62	1.49	1.43
9	B	817	CLA	C1B-C2B	2.62	1.49	1.43
9	A	838	CLA	C1B-C2B	2.61	1.49	1.43
9	B	818	CLA	C1B-C2B	2.61	1.49	1.43
9	A	815	CLA	C1B-C2B	2.61	1.49	1.43
9	B	826	CLA	C1B-C2B	2.60	1.49	1.43
9	A	811	CLA	C1B-C2B	2.60	1.49	1.43
9	A	804	CLA	C1B-C2B	2.59	1.49	1.43
9	A	813	CLA	C1B-C2B	2.59	1.49	1.43
9	A	825	CLA	C1B-C2B	2.59	1.49	1.43
9	A	810	CLA	C1B-C2B	2.58	1.49	1.43
9	B	814	CLA	C1B-C2B	2.58	1.49	1.43
9	B	823	CLA	C1B-C2B	2.58	1.49	1.43
9	B	807	CLA	C1B-C2B	2.58	1.49	1.43
9	B	830	CLA	C1B-C2B	2.58	1.49	1.43
9	A	812	CLA	C1B-C2B	2.57	1.49	1.43
9	B	821	CLA	C1B-C2B	2.57	1.49	1.43
9	A	850	CLA	C1B-C2B	2.57	1.49	1.43
9	A	829	CLA	C1B-C2B	2.57	1.49	1.43
9	A	831	CLA	C1B-C2B	2.57	1.49	1.43
9	A	833	CLA	C1B-C2B	2.56	1.49	1.43
9	A	816	CLA	C1B-C2B	2.56	1.49	1.43
9	B	839	CLA	C1B-C2B	2.56	1.49	1.43
9	L	303	CLA	C1B-C2B	2.56	1.49	1.43
9	A	849	CLA	C1B-C2B	2.55	1.49	1.43
9	A	803	CLA	C1B-C2B	2.55	1.49	1.43
9	A	834	CLA	C1B-C2B	2.55	1.49	1.43
9	B	810	CLA	C1B-C2B	2.55	1.49	1.43
9	B	829	CLA	C1B-C2B	2.55	1.49	1.43
9	A	824	CLA	C1B-C2B	2.54	1.49	1.43
9	B	828	CLA	C1B-C2B	2.54	1.49	1.43
9	A	835	CLA	C1B-C2B	2.53	1.49	1.43
9	A	827	CLA	C1B-C2B	2.53	1.49	1.43
9	B	831	CLA	C1B-C2B	2.52	1.49	1.43
9	B	801	CLA	C1B-C2B	2.52	1.49	1.43
9	B	819	CLA	C1B-C2B	2.51	1.49	1.43
9	A	819	CLA	C1B-C2B	2.51	1.49	1.43
9	A	828	CLA	C1B-C2B	2.51	1.49	1.43
9	A	826	CLA	C1B-C2B	2.51	1.49	1.43
9	A	814	CLA	C1B-C2B	2.50	1.49	1.43
9	B	805	CLA	C1B-C2B	2.50	1.49	1.43
9	B	813	CLA	C3B-C4B	2.48	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	817	CLA	C1B-C2B	2.46	1.49	1.43
9	B	825	CLA	C1B-C2B	2.46	1.49	1.43
9	B	824	CLA	C1B-C2B	2.46	1.49	1.43
9	B	802	CLA	C1B-C2B	2.43	1.49	1.43
15	B	838	LMT	O2B-C2B	-2.40	1.37	1.43
9	A	830	CLA	C1B-C2B	2.39	1.48	1.43
9	A	802	CLA	C1B-C2B	2.39	1.48	1.43
9	B	818	CLA	CMC-C2C	-2.36	1.45	1.50
14	B	837	DGD	O1G-C1G	-2.36	1.39	1.45
15	B	838	LMT	O3B-C3B	-2.34	1.37	1.43
9	B	805	CLA	CHC-C1C	2.34	1.43	1.38
9	B	802	CLA	CHC-C1C	2.31	1.43	1.38
9	B	810	CLA	CMB-C2B	-2.31	1.45	1.50
14	B	837	DGD	O2G-C2G	-2.30	1.40	1.46
15	B	838	LMT	O2'-C2'	-2.28	1.37	1.43
9	A	802	CLA	CHC-C1C	2.28	1.43	1.38
9	A	809	CLA	CHC-C1C	2.28	1.43	1.38
9	A	803	CLA	CHC-C1C	2.27	1.43	1.38
9	A	833	CLA	CHC-C1C	2.27	1.43	1.38
9	A	828	CLA	CMB-C2B	-2.27	1.46	1.50
9	B	821	CLA	CHC-C1C	2.27	1.43	1.38
9	B	825	CLA	CMB-C2B	-2.26	1.46	1.50
9	B	831	CLA	CHC-C1C	2.26	1.43	1.38
9	B	840	CLA	CHC-C1C	2.26	1.43	1.38
9	B	807	CLA	MG-NB	-2.26	2.01	2.05
9	A	804	CLA	CHC-C1C	2.26	1.43	1.38
9	A	807	CLA	CHC-C1C	2.26	1.43	1.38
9	A	849	CLA	CHC-C1C	2.25	1.43	1.38
9	A	832	CLA	CHC-C1C	2.25	1.43	1.38
9	A	806	CLA	CHC-C1C	2.24	1.43	1.38
9	B	806	CLA	CHC-C1C	2.24	1.43	1.38
9	A	810	CLA	CHC-C1C	2.24	1.43	1.38
9	A	835	CLA	MG-NB	-2.24	2.01	2.05
9	B	813	CLA	CHC-C1C	2.23	1.43	1.38
9	A	815	CLA	CHC-C1C	2.23	1.43	1.38
9	A	830	CLA	CHC-C1C	2.23	1.43	1.38
9	B	804	CLA	CHC-C1C	2.23	1.43	1.38
9	B	829	CLA	CHC-C1C	2.23	1.43	1.38
9	A	821	CLA	CHC-C1C	2.22	1.43	1.38
9	B	832	CLA	CMB-C2B	-2.22	1.46	1.50
9	B	815	CLA	CHC-C1C	2.22	1.43	1.38
9	B	804	CLA	CMC-C2C	-2.22	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	827	CLA	CHC-C1C	2.22	1.43	1.38
9	A	841	CLA	CHC-C1C	2.22	1.43	1.38
9	A	826	CLA	CHC-C1C	2.21	1.43	1.38
9	A	825	CLA	CHC-C1C	2.21	1.43	1.38
9	B	839	CLA	CHC-C1C	2.21	1.43	1.38
9	B	831	CLA	CMD-C2D	-2.21	1.46	1.50
9	A	824	CLA	CHC-C1C	2.21	1.43	1.38
9	A	819	CLA	CHC-C1C	2.21	1.43	1.38
9	B	828	CLA	CHC-C1C	2.21	1.43	1.38
9	A	808	CLA	CHC-C1C	2.20	1.43	1.38
9	B	817	CLA	CHC-C1C	2.20	1.43	1.38
9	B	810	CLA	MG-NB	-2.20	2.01	2.05
9	B	801	CLA	CMB-C2B	-2.19	1.46	1.50
11	A	842	LHG	O7-C5	-2.19	1.41	1.46
9	B	814	CLA	CHC-C1C	2.19	1.43	1.38
9	A	812	CLA	MG-NB	-2.19	2.01	2.05
9	A	834	CLA	CHC-C1C	2.19	1.43	1.38
9	B	819	CLA	MG-NB	-2.19	2.01	2.05
9	A	812	CLA	CHC-C1C	2.19	1.43	1.38
9	B	826	CLA	CHC-C1C	2.19	1.43	1.38
9	A	811	CLA	CHC-C1C	2.18	1.42	1.38
9	A	816	CLA	CHC-C1C	2.18	1.42	1.38
9	B	828	CLA	MG-NB	-2.18	2.01	2.05
9	A	850	CLA	MG-NB	-2.17	2.01	2.05
9	B	830	CLA	MG-NB	-2.17	2.01	2.05
9	A	837	CLA	CHC-C1C	2.17	1.42	1.38
9	A	813	CLA	CHC-C1C	2.17	1.42	1.38
9	B	818	CLA	CHC-C1C	2.17	1.42	1.38
9	B	816	CLA	CHC-C1C	2.17	1.42	1.38
9	A	850	CLA	CHC-C1C	2.16	1.42	1.38
9	A	827	CLA	CMD-C2D	-2.16	1.46	1.50
9	A	802	CLA	MG-NB	-2.16	2.01	2.05
9	A	824	CLA	MG-NB	-2.16	2.01	2.05
9	A	818	CLA	CHC-C1C	2.16	1.42	1.38
9	B	820	CLA	CHC-C1C	2.16	1.42	1.38
9	A	801	CLA	CHC-C1C	2.16	1.42	1.38
9	B	823	CLA	CHC-C1C	2.16	1.42	1.38
9	A	817	CLA	CHC-C1C	2.15	1.42	1.38
9	A	827	CLA	MG-NB	-2.15	2.01	2.05
9	B	825	CLA	MG-NB	-2.15	2.01	2.05
9	A	823	CLA	MG-NB	-2.15	2.01	2.05
9	L	303	CLA	CHC-C1C	2.15	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	808	CLA	MG-NB	-2.15	2.01	2.05
9	B	831	CLA	MG-NB	-2.14	2.01	2.05
9	B	825	CLA	CMD-C2D	-2.14	1.46	1.50
9	L	304	CLA	CHC-C1C	2.14	1.42	1.38
9	B	815	CLA	MG-NB	-2.14	2.01	2.05
9	A	817	CLA	MG-NB	-2.13	2.01	2.05
9	B	822	CLA	MG-NB	-2.13	2.01	2.05
9	B	824	CLA	CMB-C2B	-2.13	1.46	1.50
9	A	838	CLA	CMB-C2B	-2.13	1.46	1.50
9	B	803	CLA	CMD-C2D	-2.13	1.46	1.50
9	A	819	CLA	MG-NB	-2.13	2.01	2.05
9	A	831	CLA	CHC-C1C	2.13	1.42	1.38
9	A	838	CLA	CHC-C1C	2.13	1.42	1.38
9	B	824	CLA	CHC-C1C	2.13	1.42	1.38
9	B	809	CLA	CMD-C2D	-2.13	1.46	1.50
9	A	830	CLA	MG-NB	-2.12	2.01	2.05
9	A	829	CLA	CMD-C2D	-2.12	1.46	1.50
9	B	823	CLA	MG-NB	-2.12	2.01	2.05
9	A	828	CLA	MG-NB	-2.12	2.01	2.05
9	B	805	CLA	MG-NB	-2.12	2.01	2.05
9	B	821	CLA	MG-NB	-2.12	2.01	2.05
9	B	819	CLA	CMB-C2B	-2.12	1.46	1.50
9	A	829	CLA	CHC-C1C	2.12	1.42	1.38
9	B	828	CLA	CMD-C2D	-2.12	1.46	1.50
9	B	824	CLA	CMD-C2D	-2.12	1.46	1.50
9	B	801	CLA	MG-NB	-2.12	2.01	2.05
9	B	811	CLA	CHC-C1C	2.12	1.42	1.38
9	B	830	CLA	CHC-C1C	2.12	1.42	1.38
9	A	805	CLA	CHC-C1C	2.12	1.42	1.38
9	L	305	CLA	CHC-C1C	2.12	1.42	1.38
9	L	304	CLA	MG-NB	-2.12	2.01	2.05
9	A	825	CLA	MG-NB	-2.11	2.01	2.05
9	A	833	CLA	MG-NB	-2.11	2.01	2.05
9	A	820	CLA	CHC-C1C	2.11	1.42	1.38
9	A	834	CLA	MG-NB	-2.11	2.01	2.05
9	B	829	CLA	MG-NB	-2.11	2.01	2.05
9	A	835	CLA	CHC-C1C	2.11	1.42	1.38
9	A	817	CLA	CMB-C2B	-2.11	1.46	1.50
9	A	813	CLA	MG-NB	-2.11	2.01	2.05
9	B	811	CLA	CMD-C2D	-2.10	1.46	1.50
9	A	816	CLA	MG-NB	-2.10	2.01	2.05
9	B	817	CLA	MG-NB	-2.10	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	807	CLA	CHC-C1C	2.10	1.42	1.38
9	A	829	CLA	MG-NB	-2.10	2.01	2.05
9	B	803	CLA	CHC-C1C	2.10	1.42	1.38
9	A	811	CLA	MG-NB	-2.10	2.01	2.05
9	A	815	CLA	MG-NB	-2.10	2.01	2.05
9	B	812	CLA	CHC-C1C	2.10	1.42	1.38
9	B	809	CLA	CMC-C2C	-2.10	1.46	1.50
9	B	832	CLA	MG-NB	-2.10	2.01	2.05
9	B	812	CLA	MG-NB	-2.10	2.01	2.05
9	B	816	CLA	MG-NB	-2.09	2.01	2.05
9	B	811	CLA	MG-NB	-2.09	2.01	2.05
9	L	305	CLA	MG-NB	-2.09	2.01	2.05
9	A	814	CLA	CHC-C1C	2.09	1.42	1.38
9	A	849	CLA	CMB-C2B	-2.09	1.46	1.50
9	B	803	CLA	CMC-C2C	-2.09	1.46	1.50
9	B	815	CLA	CMD-C2D	-2.09	1.46	1.50
9	A	801	CLA	MG-NB	-2.09	2.01	2.05
9	L	303	CLA	MG-NB	-2.09	2.01	2.05
9	A	835	CLA	CMB-C2B	-2.09	1.46	1.50
9	A	831	CLA	MG-NB	-2.09	2.01	2.05
9	A	801	CLA	CMD-C2D	-2.09	1.46	1.50
9	B	814	CLA	MG-NB	-2.09	2.01	2.05
9	H	201	CLA	CMB-C2B	-2.09	1.46	1.50
12	B	836	BCR	C38-C26	-2.09	1.47	1.50
15	B	838	LMT	O4'-C4B	-2.08	1.38	1.43
9	B	819	CLA	CHC-C1C	2.08	1.42	1.38
9	H	201	CLA	CHC-C1C	2.08	1.42	1.38
9	B	839	CLA	MG-NB	-2.08	2.01	2.05
9	B	822	CLA	CHC-C1C	2.08	1.42	1.38
9	B	818	CLA	CMB-C2B	-2.08	1.46	1.50
9	A	822	CLA	CHC-C1C	2.07	1.42	1.38
9	A	827	CLA	CHC-C1C	2.07	1.42	1.38
9	B	801	CLA	CMD-C2D	-2.07	1.46	1.50
9	A	803	CLA	MG-NB	-2.07	2.01	2.05
9	A	819	CLA	CMB-C2B	-2.07	1.46	1.50
9	A	823	CLA	CHC-C1C	2.07	1.42	1.38
9	A	808	CLA	MG-NB	-2.07	2.01	2.05
9	B	803	CLA	MG-NB	-2.07	2.01	2.05
9	B	814	CLA	CMC-C2C	-2.07	1.46	1.50
9	A	824	CLA	CMD-C2D	-2.07	1.46	1.50
9	B	805	CLA	CMD-C2D	-2.07	1.46	1.50
9	L	304	CLA	CMB-C2B	-2.07	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	818	CLA	MG-NB	-2.07	2.01	2.05
9	A	804	CLA	CMD-C2D	-2.07	1.46	1.50
9	B	822	CLA	CMC-C2C	-2.07	1.46	1.50
9	A	805	CLA	MG-NB	-2.07	2.01	2.05
9	A	823	CLA	CMB-C2B	-2.07	1.46	1.50
9	B	824	CLA	MG-NB	-2.06	2.01	2.05
9	B	809	CLA	CHC-C1C	2.06	1.42	1.38
9	A	839	CLA	CHC-C1C	2.06	1.42	1.38
9	B	816	CLA	CMD-C2D	-2.06	1.46	1.50
9	A	821	CLA	MG-NB	-2.06	2.01	2.05
9	B	813	CLA	MG-NB	-2.06	2.01	2.05
9	A	850	CLA	CMD-C2D	-2.06	1.46	1.50
9	B	818	CLA	MG-NB	-2.06	2.01	2.05
9	B	827	CLA	CMB-C2B	-2.06	1.46	1.50
9	B	822	CLA	CMD-C2D	-2.06	1.46	1.50
9	A	820	CLA	MG-NB	-2.06	2.01	2.05
9	A	849	CLA	CMD-C2D	-2.06	1.46	1.50
9	B	802	CLA	MG-NB	-2.06	2.01	2.05
9	A	802	CLA	CMD-C2D	-2.06	1.46	1.50
9	B	807	CLA	CMD-C2D	-2.06	1.46	1.50
9	A	818	CLA	CMD-C2D	-2.06	1.46	1.50
9	B	825	CLA	CHC-C1C	2.06	1.42	1.38
9	A	836	CLA	CHC-C1C	2.06	1.42	1.38
9	B	820	CLA	MG-NB	-2.05	2.01	2.05
9	A	814	CLA	CMD-C2D	-2.05	1.46	1.50
9	B	829	CLA	CMD-C2D	-2.05	1.46	1.50
9	A	821	CLA	CMD-C2D	-2.05	1.46	1.50
9	B	808	CLA	CHC-C1C	2.05	1.42	1.38
9	B	839	CLA	CMB-C2B	-2.05	1.46	1.50
9	A	834	CLA	CMD-C2D	-2.05	1.46	1.50
9	L	303	CLA	CMB-C2B	-2.05	1.46	1.50
9	H	201	CLA	MG-NB	-2.05	2.01	2.05
9	A	836	CLA	MG-NB	-2.05	2.01	2.05
9	A	817	CLA	CMD-C2D	-2.05	1.46	1.50
9	A	828	CLA	CMD-C2D	-2.05	1.46	1.50
9	A	807	CLA	MG-NB	-2.05	2.01	2.05
9	B	814	CLA	CMD-C2D	-2.05	1.46	1.50
9	B	821	CLA	CMD-C2D	-2.04	1.46	1.50
9	B	804	CLA	CMB-C2B	-2.04	1.46	1.50
9	A	825	CLA	CMC-C2C	-2.04	1.46	1.50
9	B	801	CLA	CHC-C1C	2.04	1.42	1.38
11	L	301	LHG	O7-C5	-2.04	1.41	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	816	CLA	CMD-C2D	-2.04	1.46	1.50
9	A	828	CLA	CHC-C1C	2.04	1.42	1.38
9	L	305	CLA	CMD-C2D	-2.04	1.46	1.50
9	B	821	CLA	CMB-C2B	-2.04	1.46	1.50
9	A	835	CLA	CMD-C2D	-2.04	1.46	1.50
9	B	831	CLA	CMB-C2B	-2.04	1.46	1.50
9	B	807	CLA	CMB-C2B	-2.04	1.46	1.50
9	A	810	CLA	MG-NB	-2.04	2.01	2.05
9	B	804	CLA	CMD-C2D	-2.03	1.46	1.50
9	A	809	CLA	CMD-C2D	-2.03	1.46	1.50
9	A	822	CLA	MG-NB	-2.03	2.01	2.05
9	B	823	CLA	CMD-C2D	-2.03	1.46	1.50
9	A	805	CLA	CMD-C2D	-2.03	1.46	1.50
9	A	830	CLA	CMB-C2B	-2.03	1.46	1.50
9	A	839	CLA	MG-NB	-2.03	2.01	2.05
9	B	802	CLA	CMD-C2D	-2.03	1.46	1.50
9	B	811	CLA	CMB-C2B	-2.03	1.46	1.50
9	B	827	CLA	MG-NB	-2.03	2.01	2.05
9	A	850	CLA	CMB-C2B	-2.03	1.46	1.50
9	A	823	CLA	CMD-C2D	-2.02	1.46	1.50
9	B	801	CLA	CMC-C2C	-2.02	1.46	1.50
9	A	827	CLA	CMB-C2B	-2.02	1.46	1.50
9	B	819	CLA	CMD-C2D	-2.02	1.46	1.50
9	B	808	CLA	CMD-C2D	-2.02	1.46	1.50
9	B	809	CLA	MG-NB	-2.02	2.01	2.05
9	B	840	CLA	MG-NB	-2.02	2.01	2.05
9	A	825	CLA	CMD-C2D	-2.02	1.46	1.50
9	B	817	CLA	CMD-C2D	-2.02	1.46	1.50
9	B	830	CLA	CMD-C2D	-2.02	1.46	1.50
9	B	839	CLA	CMD-C2D	-2.02	1.46	1.50
9	A	820	CLA	CMB-C2B	-2.02	1.46	1.50
9	B	827	CLA	CMD-C2D	-2.02	1.46	1.50
9	B	806	CLA	CMD-C2D	-2.02	1.46	1.50
9	L	304	CLA	CMD-C2D	-2.02	1.46	1.50
9	A	801	CLA	CMB-C2B	-2.02	1.46	1.50
9	A	813	CLA	CMD-C2D	-2.02	1.46	1.50
9	A	829	CLA	CMB-C2B	-2.02	1.46	1.50
9	A	815	CLA	CMD-C2D	-2.02	1.46	1.50
9	A	822	CLA	CMD-C2D	-2.02	1.46	1.50
9	B	809	CLA	CMB-C2B	-2.02	1.46	1.50
9	A	837	CLA	MG-NB	-2.02	2.01	2.05
9	B	817	CLA	CMB-C2B	-2.02	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	832	CLA	CMD-C2D	-2.02	1.46	1.50
9	A	810	CLA	CMD-C2D	-2.02	1.46	1.50
9	A	815	CLA	CMC-C2C	-2.02	1.46	1.50
9	A	814	CLA	CMB-C2B	-2.02	1.46	1.50
9	B	810	CLA	CMD-C2D	-2.02	1.46	1.50
9	B	805	CLA	CMC-C2C	-2.02	1.46	1.50
9	B	808	CLA	CMB-C2B	-2.02	1.46	1.50
9	A	830	CLA	CMD-C2D	-2.02	1.46	1.50
9	A	849	CLA	CMC-C2C	-2.01	1.46	1.50
9	L	303	CLA	CMD-C2D	-2.01	1.46	1.50
9	A	833	CLA	CMD-C2D	-2.01	1.46	1.50
9	A	809	CLA	MG-NB	-2.01	2.01	2.05
9	A	839	CLA	CMB-C2B	-2.01	1.46	1.50
9	B	812	CLA	CMD-C2D	-2.01	1.46	1.50
9	A	806	CLA	MG-NB	-2.01	2.01	2.05
9	A	814	CLA	MG-NB	-2.01	2.01	2.05
9	A	808	CLA	CMD-C2D	-2.01	1.46	1.50
9	A	838	CLA	CMD-C2D	-2.01	1.46	1.50
9	A	822	CLA	CMB-C2B	-2.01	1.46	1.50
9	A	834	CLA	CMB-C2B	-2.01	1.46	1.50
9	A	838	CLA	CMC-C2C	-2.01	1.46	1.50
15	B	838	LMT	O1'-C1'	-2.01	1.36	1.40
9	A	831	CLA	CMD-C2D	-2.01	1.46	1.50
9	B	818	CLA	CMD-C2D	-2.01	1.46	1.50
9	L	305	CLA	CMB-C2B	-2.01	1.46	1.50
9	A	819	CLA	CMD-C2D	-2.01	1.46	1.50
9	B	802	CLA	CMC-C2C	-2.01	1.46	1.50
9	A	810	CLA	CMB-C2B	-2.01	1.46	1.50
9	B	816	CLA	CMB-C2B	-2.01	1.46	1.50
9	A	804	CLA	MG-NB	-2.00	2.01	2.05
9	A	806	CLA	CMD-C2D	-2.00	1.46	1.50
9	A	813	CLA	CMB-C2B	-2.00	1.46	1.50
9	B	822	CLA	CMB-C2B	-2.00	1.46	1.50
9	A	826	CLA	CMD-C2D	-2.00	1.46	1.50
9	A	827	CLA	CMC-C2C	-2.00	1.46	1.50
9	A	808	CLA	CMC-C2C	-2.00	1.46	1.50
9	B	805	CLA	CMB-C2B	-2.00	1.46	1.50
9	B	826	CLA	CMD-C2D	-2.00	1.46	1.50
9	A	812	CLA	CMD-C2D	-2.00	1.46	1.50
9	A	833	CLA	CMB-C2B	-2.00	1.46	1.50
9	A	825	CLA	CMB-C2B	-2.00	1.46	1.50

All (613) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	818	CLA	C4A-NA-C1A	7.21	109.95	106.71
9	B	809	CLA	C4A-NA-C1A	7.12	109.91	106.71
9	B	806	CLA	C4A-NA-C1A	7.05	109.88	106.71
9	B	832	CLA	C4A-NA-C1A	7.03	109.86	106.71
9	A	832	CLA	C4A-NA-C1A	7.01	109.86	106.71
9	A	839	CLA	C4A-NA-C1A	7.01	109.86	106.71
9	B	804	CLA	C4A-NA-C1A	6.96	109.84	106.71
9	L	304	CLA	C4A-NA-C1A	6.87	109.79	106.71
9	B	811	CLA	C4A-NA-C1A	6.81	109.77	106.71
9	L	303	CLA	C4A-NA-C1A	6.81	109.77	106.71
9	A	836	CLA	C4A-NA-C1A	6.76	109.75	106.71
9	B	822	CLA	C4A-NA-C1A	6.74	109.74	106.71
9	A	820	CLA	C4A-NA-C1A	6.72	109.73	106.71
9	A	823	CLA	C4A-NA-C1A	6.72	109.73	106.71
9	B	810	CLA	C4A-NA-C1A	6.70	109.72	106.71
9	B	827	CLA	C4A-NA-C1A	6.70	109.72	106.71
9	H	201	CLA	C4A-NA-C1A	6.70	109.72	106.71
9	B	808	CLA	C4A-NA-C1A	6.69	109.72	106.71
9	A	804	CLA	C4A-NA-C1A	6.69	109.71	106.71
9	A	825	CLA	C4A-NA-C1A	6.67	109.70	106.71
9	A	837	CLA	C4A-NA-C1A	6.66	109.70	106.71
9	A	838	CLA	C4A-NA-C1A	6.61	109.68	106.71
9	A	814	CLA	C4A-NA-C1A	6.61	109.68	106.71
9	B	815	CLA	C4A-NA-C1A	6.59	109.67	106.71
9	B	817	CLA	C4A-NA-C1A	6.59	109.67	106.71
9	A	805	CLA	C4A-NA-C1A	6.58	109.67	106.71
9	A	815	CLA	C4A-NA-C1A	6.58	109.67	106.71
9	L	305	CLA	C4A-NA-C1A	6.58	109.66	106.71
9	B	823	CLA	C4A-NA-C1A	6.57	109.66	106.71
9	A	822	CLA	C4A-NA-C1A	6.57	109.66	106.71
9	B	840	CLA	C4A-NA-C1A	6.56	109.65	106.71
9	A	809	CLA	C4A-NA-C1A	6.55	109.65	106.71
9	B	807	CLA	C4A-NA-C1A	6.55	109.65	106.71
9	A	808	CLA	C4A-NA-C1A	6.53	109.64	106.71
9	A	841	CLA	C4A-NA-C1A	6.53	109.64	106.71
9	B	816	CLA	C4A-NA-C1A	6.53	109.64	106.71
9	A	835	CLA	C4A-NA-C1A	6.51	109.63	106.71
9	A	803	CLA	C4A-NA-C1A	6.51	109.63	106.71
9	A	850	CLA	C4A-NA-C1A	6.50	109.63	106.71
9	B	829	CLA	C4A-NA-C1A	6.50	109.63	106.71
9	A	828	CLA	C4A-NA-C1A	6.49	109.62	106.71
9	B	814	CLA	C4A-NA-C1A	6.49	109.62	106.71
9	A	833	CLA	C4A-NA-C1A	6.47	109.62	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	826	CLA	C4A-NA-C1A	6.47	109.62	106.71
9	A	821	CLA	C4A-NA-C1A	6.47	109.61	106.71
9	A	829	CLA	C4A-NA-C1A	6.47	109.61	106.71
9	B	820	CLA	C4A-NA-C1A	6.47	109.61	106.71
9	A	811	CLA	C4A-NA-C1A	6.45	109.61	106.71
9	A	816	CLA	C4A-NA-C1A	6.44	109.60	106.71
9	B	830	CLA	C4A-NA-C1A	6.43	109.60	106.71
9	B	803	CLA	C4A-NA-C1A	6.43	109.59	106.71
9	B	831	CLA	C4A-NA-C1A	6.41	109.59	106.71
9	A	819	CLA	C4A-NA-C1A	6.38	109.58	106.71
9	A	813	CLA	C4A-NA-C1A	6.38	109.57	106.71
9	A	806	CLA	C4A-NA-C1A	6.36	109.57	106.71
9	A	807	CLA	C4A-NA-C1A	6.36	109.56	106.71
9	A	818	CLA	C4A-NA-C1A	6.35	109.56	106.71
9	B	813	CLA	C4A-NA-C1A	6.35	109.56	106.71
9	B	805	CLA	C4A-NA-C1A	6.32	109.55	106.71
9	A	826	CLA	C4A-NA-C1A	6.30	109.54	106.71
9	B	821	CLA	C4A-NA-C1A	6.29	109.53	106.71
9	A	812	CLA	C4A-NA-C1A	6.28	109.53	106.71
9	A	810	CLA	C4A-NA-C1A	6.27	109.52	106.71
9	A	824	CLA	C4A-NA-C1A	6.23	109.51	106.71
9	B	801	CLA	C4A-NA-C1A	6.20	109.50	106.71
9	B	812	CLA	C4A-NA-C1A	6.17	109.48	106.71
9	A	849	CLA	C4A-NA-C1A	6.16	109.48	106.71
9	A	801	CLA	C4A-NA-C1A	6.15	109.47	106.71
9	A	817	CLA	C4A-NA-C1A	6.15	109.47	106.71
9	A	831	CLA	C4A-NA-C1A	6.13	109.46	106.71
9	A	827	CLA	C4A-NA-C1A	6.11	109.45	106.71
9	B	824	CLA	C4A-NA-C1A	6.09	109.44	106.71
9	B	819	CLA	C4A-NA-C1A	6.05	109.42	106.71
9	B	839	CLA	C4A-NA-C1A	6.04	109.42	106.71
9	A	834	CLA	C4A-NA-C1A	6.04	109.42	106.71
9	B	828	CLA	C4A-NA-C1A	6.01	109.41	106.71
9	B	825	CLA	C4A-NA-C1A	5.99	109.40	106.71
9	A	830	CLA	C4A-NA-C1A	5.94	109.38	106.71
9	B	802	CLA	C4A-NA-C1A	5.62	109.23	106.71
9	A	802	CLA	C4A-NA-C1A	5.44	109.15	106.71
11	L	301	LHG	O4-P-O5	4.22	133.08	112.24
11	A	842	LHG	O4-P-O5	4.18	132.90	112.24
11	A	843	LHG	O4-P-O5	4.14	132.70	112.24
14	B	837	DGD	O3G-C3G-C2G	-4.01	101.21	110.90
9	B	801	CLA	CAC-C3C-C4C	3.74	129.66	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	831	CLA	O2D-CGD-O1D	-3.60	116.81	123.84
9	B	821	CLA	C3B-C4B-NB	-3.57	107.84	110.23
12	L	307	BCR	C11-C10-C9	-3.46	122.38	127.31
9	A	835	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
9	A	836	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
14	B	837	DGD	O6D-C1D-O3G	-3.38	101.97	109.97
11	A	843	LHG	O8-C23-C24	3.29	120.00	111.38
12	A	846	BCR	C2-C1-C6	3.26	115.50	110.48
12	B	834	BCR	C2-C1-C6	3.24	115.47	110.48
9	B	829	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
12	L	306	BCR	C24-C23-C22	-3.19	121.42	126.23
9	L	304	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
9	B	809	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
9	B	808	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
14	B	837	DGD	O5D-C6D-C5D	-3.10	103.31	109.05
9	L	303	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
12	A	846	BCR	C15-C14-C13	-3.09	122.91	127.31
9	B	812	CLA	C3B-C4B-NB	-3.08	108.16	110.23
9	B	819	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
9	B	805	CLA	C3B-C4B-NB	-3.07	107.67	110.52
9	B	839	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
9	A	834	CLA	C3B-C4B-NB	-3.05	107.69	110.52
9	A	815	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
12	A	846	BCR	C24-C23-C22	-3.03	121.65	126.23
9	A	828	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
9	B	830	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
9	B	803	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
9	B	805	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
9	A	812	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
9	B	816	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
9	B	825	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
9	B	804	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
9	A	834	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
9	A	823	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
9	A	829	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
9	B	811	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
9	A	810	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
9	A	824	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
9	A	804	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
9	A	802	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
9	A	830	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
9	A	849	CLA	O2D-CGD-O1D	-2.94	118.09	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	305	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
9	A	837	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
9	B	827	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
9	A	827	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
9	B	840	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
12	B	835	BCR	C15-C14-C13	-2.93	123.14	127.31
9	A	825	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
9	B	802	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
9	B	831	CLA	C3B-C4B-NB	-2.92	107.81	110.52
9	A	850	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
9	A	811	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
9	B	806	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
9	B	810	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
9	A	807	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
9	B	815	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
9	A	814	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
9	A	809	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
9	B	818	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
9	B	822	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
9	A	833	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
9	A	817	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
9	A	805	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
9	A	816	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
9	B	811	CLA	C3B-C4B-NB	-2.89	107.83	110.52
9	B	817	CLA	C3B-C4B-NB	-2.89	107.83	110.52
12	A	847	BCR	C24-C23-C22	-2.89	121.87	126.23
12	L	302	BCR	C15-C16-C17	-2.89	117.56	123.47
9	B	820	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
9	H	201	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
12	L	308	BCR	C28-C27-C26	-2.89	108.92	114.08
9	B	814	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
9	A	839	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
9	B	813	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
9	B	823	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
9	A	813	CLA	C3B-C4B-NB	-2.88	107.84	110.52
9	B	826	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
9	B	801	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
9	A	822	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
9	A	826	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
9	A	816	CLA	C3B-C4B-NB	-2.87	107.86	110.52
9	A	841	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
9	A	810	CLA	C3B-C4B-NB	-2.87	107.86	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	817	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
12	L	307	BCR	C15-C14-C13	-2.86	123.23	127.31
9	A	818	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
9	B	821	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
12	A	844	BCR	C33-C5-C6	-2.85	121.33	124.53
9	A	812	CLA	C3B-C4B-NB	-2.85	107.87	110.52
9	A	820	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
9	A	821	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
9	B	812	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
9	A	832	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
9	A	808	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
14	B	837	DGD	CDB-CCB-CBB	-2.84	100.02	114.42
9	A	803	CLA	C3B-C4B-NB	-2.84	107.88	110.52
9	A	806	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
9	A	835	CLA	C3B-C4B-NB	-2.83	107.89	110.52
9	B	828	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
9	B	807	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
9	A	838	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
9	A	803	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
9	A	830	CLA	C3B-C4B-NB	-2.81	107.91	110.52
9	A	819	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
9	B	813	CLA	C4B-NB-C1B	2.81	108.33	106.33
9	A	801	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
9	A	813	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
9	B	820	CLA	C3B-C4B-NB	-2.80	107.92	110.52
9	B	831	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
9	B	832	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
9	B	824	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
9	A	832	CLA	CHB-C4A-NA	2.77	128.34	124.51
9	A	814	CLA	C3B-C4B-NB	-2.76	107.95	110.52
9	A	811	CLA	C3B-C4B-NB	-2.76	107.96	110.52
9	A	836	CLA	CHC-C4B-NB	2.76	127.17	124.26
12	L	302	BCR	C33-C5-C6	-2.75	121.44	124.53
9	A	818	CLA	C3B-C4B-NB	-2.74	107.97	110.52
11	A	842	LHG	O8-C23-C24	2.74	120.51	111.91
12	A	845	BCR	C24-C23-C22	-2.74	122.10	126.23
9	A	836	CLA	CHB-C4A-NA	2.73	128.29	124.51
12	A	845	BCR	C11-C10-C9	-2.73	123.41	127.31
9	B	839	CLA	C3B-C4B-NB	-2.73	107.99	110.52
9	B	814	CLA	C3B-C4B-NB	-2.72	107.99	110.52
9	A	809	CLA	C3B-C4B-NB	-2.72	107.99	110.52
9	A	806	CLA	C3B-C4B-NB	-2.72	107.99	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	815	CLA	C3B-C4B-NB	-2.71	108.00	110.52
9	B	807	CLA	C3B-C4B-NB	-2.71	108.00	110.52
12	B	835	BCR	C15-C16-C17	-2.70	117.94	123.47
9	A	832	CLA	C3B-C4B-NB	-2.70	108.01	110.52
12	A	846	BCR	C11-C10-C9	-2.70	123.46	127.31
9	A	825	CLA	C3B-C4B-NB	-2.70	108.01	110.52
9	A	837	CLA	C3B-C4B-NB	-2.69	108.02	110.52
9	B	801	CLA	C3B-C4B-NB	-2.69	108.02	110.52
9	B	816	CLA	C3B-C4B-NB	-2.69	108.02	110.52
9	L	303	CLA	C3B-C4B-NB	-2.69	108.02	110.52
9	A	801	CLA	C3B-C4B-NB	-2.69	108.02	110.52
12	I	101	BCR	C33-C5-C6	-2.68	121.52	124.53
9	A	815	CLA	C3B-C4B-NB	-2.68	108.03	110.52
9	B	818	CLA	CHB-C4A-NA	2.67	128.21	124.51
9	B	824	CLA	C3B-C4B-NB	-2.67	108.03	110.52
9	A	808	CLA	C3B-C4B-NB	-2.67	108.04	110.52
9	B	822	CLA	C3B-C4B-NB	-2.67	108.04	110.52
9	B	827	CLA	C3B-C4B-NB	-2.66	108.05	110.52
11	L	301	LHG	O8-C23-C24	2.65	120.22	111.91
9	A	819	CLA	C3B-C4B-NB	-2.64	108.06	110.52
12	L	306	BCR	C27-C26-C25	2.64	126.56	122.73
9	A	824	CLA	C3B-C4B-NB	-2.63	108.07	110.52
12	L	308	BCR	C33-C5-C6	-2.63	121.58	124.53
9	L	304	CLA	C3B-C4B-NB	-2.63	108.08	110.52
9	B	809	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
9	L	305	CLA	C3B-C4B-NB	-2.62	108.08	110.52
12	A	847	BCR	C33-C5-C6	-2.62	121.59	124.53
9	L	303	CLA	CHB-C4A-NA	2.61	128.13	124.51
9	A	837	CLA	CHB-C4A-NA	2.61	128.12	124.51
9	A	803	CLA	CHB-C4A-NA	2.61	128.12	124.51
9	A	804	CLA	C3B-C4B-NB	-2.60	108.10	110.52
9	A	850	CLA	C3B-C4B-NB	-2.60	108.10	110.52
9	B	840	CLA	C3B-C4B-NB	-2.60	108.10	110.52
9	A	807	CLA	C3B-C4B-NB	-2.60	108.11	110.52
9	B	829	CLA	C3B-C4B-NB	-2.59	108.11	110.52
14	B	837	DGD	C3G-C2G-C1G	-2.59	105.66	111.79
12	A	847	BCR	C15-C16-C17	-2.59	118.17	123.47
9	H	201	CLA	CHB-C4A-NA	2.59	128.09	124.51
12	L	306	BCR	C15-C14-C13	-2.59	123.62	127.31
12	L	302	BCR	C15-C14-C13	-2.58	123.62	127.31
9	B	806	CLA	CHB-C4A-NA	2.58	128.08	124.51
9	A	839	CLA	C3B-C4B-NB	-2.57	108.13	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	809	CLA	CHB-C4A-NA	2.57	128.07	124.51
9	A	816	CLA	CHB-C4A-NA	2.57	128.06	124.51
12	A	847	BCR	C15-C14-C13	-2.57	123.65	127.31
9	B	818	CLA	C3B-C4B-NB	-2.56	108.14	110.52
9	B	822	CLA	CHB-C4A-NA	2.55	128.04	124.51
9	A	805	CLA	CHB-C4A-NA	2.55	128.04	124.51
15	B	838	LMT	C1'-O5'-C5'	-2.55	108.69	113.69
9	A	849	CLA	C3B-C4B-NB	-2.54	108.16	110.52
12	A	847	BCR	C27-C26-C25	2.54	126.42	122.73
12	B	834	BCR	C15-C16-C17	-2.54	118.27	123.47
9	B	816	CLA	CHB-C4A-NA	2.54	128.02	124.51
9	A	839	CLA	CHB-C4A-NA	2.53	128.00	124.51
9	B	826	CLA	CHB-C4A-NA	2.52	128.00	124.51
9	B	806	CLA	C3B-C4B-NB	-2.52	108.17	110.52
9	A	820	CLA	CHB-C4A-NA	2.52	128.00	124.51
9	A	834	CLA	CHB-C4A-NA	2.52	128.00	124.51
9	A	813	CLA	CHB-C4A-NA	2.52	128.00	124.51
9	B	809	CLA	C3B-C4B-NB	-2.52	108.18	110.52
9	B	815	CLA	CHB-C4A-NA	2.52	128.00	124.51
11	A	842	LHG	C11-C10-C9	-2.52	101.64	114.42
9	B	814	CLA	CHB-C4A-NA	2.51	127.99	124.51
9	B	840	CLA	CHB-C4A-NA	2.51	127.98	124.51
9	A	833	CLA	C3B-C4B-NB	-2.50	108.19	110.52
9	B	820	CLA	CHB-C4A-NA	2.50	127.97	124.51
9	B	828	CLA	CHB-C4A-NA	2.50	127.97	124.51
9	B	807	CLA	CHB-C4A-NA	2.50	127.97	124.51
12	L	307	BCR	C15-C16-C17	-2.50	118.35	123.47
9	B	817	CLA	CHB-C4A-NA	2.50	127.97	124.51
9	B	812	CLA	CAB-C3B-C2B	2.50	130.06	123.59
9	A	825	CLA	CHB-C4A-NA	2.50	127.97	124.51
9	A	818	CLA	CHB-C4A-NA	2.49	127.96	124.51
9	A	808	CLA	CHB-C4A-NA	2.49	127.96	124.51
9	A	841	CLA	C3B-C4B-NB	-2.49	108.20	110.52
12	L	306	BCR	C15-C16-C17	-2.49	118.37	123.47
9	A	820	CLA	C3B-C4B-NB	-2.49	108.20	110.52
9	B	811	CLA	CHB-C4A-NA	2.49	127.95	124.51
9	A	815	CLA	CHB-C4A-NA	2.49	127.95	124.51
9	L	304	CLA	CHB-C4A-NA	2.48	127.95	124.51
12	L	307	BCR	C33-C5-C6	-2.48	121.74	124.53
9	B	808	CLA	CHB-C4A-NA	2.48	127.95	124.51
9	A	831	CLA	CHB-C4A-NA	2.48	127.95	124.51
12	L	307	BCR	C24-C23-C22	-2.48	122.49	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	836	BCR	C27-C26-C25	2.48	126.33	122.73
9	A	822	CLA	CHB-C4A-NA	2.48	127.94	124.51
9	B	829	CLA	CHB-C4A-NA	2.48	127.94	124.51
9	A	835	CLA	CHB-C4A-NA	2.48	127.94	124.51
9	B	804	CLA	C3B-C4B-NB	-2.47	108.22	110.52
9	B	803	CLA	C3B-C4B-NB	-2.47	108.22	110.52
9	A	811	CLA	CHB-C4A-NA	2.47	127.93	124.51
12	A	844	BCR	C15-C16-C17	-2.47	118.42	123.47
9	A	829	CLA	C3B-C4B-NB	-2.47	108.23	110.52
9	A	809	CLA	CHB-C4A-NA	2.46	127.92	124.51
9	B	826	CLA	C3B-C4B-NB	-2.46	108.23	110.52
9	B	827	CLA	CHB-C4A-NA	2.46	127.92	124.51
12	B	836	BCR	C24-C23-C22	-2.46	122.52	126.23
9	A	814	CLA	CHB-C4A-NA	2.46	127.92	124.51
9	A	830	CLA	CHB-C4A-NA	2.46	127.92	124.51
9	A	826	CLA	CHD-C1D-ND	-2.46	122.19	124.45
12	L	307	BCR	C27-C26-C25	2.46	126.30	122.73
9	H	201	CLA	C3B-C4B-NB	-2.46	108.24	110.52
9	A	819	CLA	CHB-C4A-NA	2.46	127.91	124.51
9	B	802	CLA	C3B-C4B-NB	-2.45	108.24	110.52
9	A	804	CLA	CHB-C4A-NA	2.45	127.90	124.51
9	L	305	CLA	CHB-C4A-NA	2.45	127.90	124.51
9	A	807	CLA	CHB-C4A-NA	2.45	127.90	124.51
9	B	821	CLA	CMB-C2B-C3B	2.45	129.93	123.59
9	A	828	CLA	C3B-C4B-NB	-2.45	108.24	110.52
12	A	845	BCR	C27-C26-C25	2.45	126.28	122.73
9	A	836	CLA	C3B-C4B-NB	-2.45	108.25	110.52
9	A	823	CLA	C3B-C4B-NB	-2.44	108.25	110.52
9	A	838	CLA	CHB-C4A-NA	2.44	127.89	124.51
9	A	841	CLA	CHB-C4A-NA	2.44	127.89	124.51
9	A	805	CLA	C3B-C4B-NB	-2.43	108.26	110.52
9	A	826	CLA	CHB-C4A-NA	2.43	127.88	124.51
9	B	813	CLA	CHB-C4A-NA	2.43	127.88	124.51
12	L	308	BCR	C11-C10-C9	-2.43	123.84	127.31
9	B	831	CLA	CHB-C4A-NA	2.43	127.87	124.51
11	L	301	LHG	C11-C10-C9	-2.43	102.09	114.42
9	A	810	CLA	CHB-C4A-NA	2.43	127.87	124.51
12	B	835	BCR	C11-C10-C9	-2.43	123.85	127.31
9	B	801	CLA	CHB-C4A-NA	2.42	127.86	124.51
11	A	843	LHG	C11-C10-C9	-2.42	102.12	114.42
9	B	812	CLA	CMB-C2B-C3B	2.42	129.86	123.59
9	B	802	CLA	C1-C2-C3	-2.42	121.86	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	833	CLA	CHB-C4A-NA	2.41	127.85	124.51
9	A	829	CLA	CHB-C4A-NA	2.41	127.85	124.51
9	A	823	CLA	CHB-C4A-NA	2.41	127.85	124.51
9	B	804	CLA	CHB-C4A-NA	2.41	127.85	124.51
9	B	828	CLA	C3B-C4B-NB	-2.41	108.28	110.52
9	B	805	CLA	CHB-C4A-NA	2.40	127.83	124.51
9	A	821	CLA	CHB-C4A-NA	2.39	127.82	124.51
9	B	828	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
9	B	802	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
12	L	306	BCR	C33-C5-C6	-2.39	121.84	124.53
9	B	819	CLA	C3B-C4B-NB	-2.39	108.30	110.52
9	A	850	CLA	CHB-C4A-NA	2.39	127.81	124.51
9	B	825	CLA	C3B-C4B-NB	-2.38	108.31	110.52
9	A	835	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
11	L	301	LHG	C20-C19-C18	-2.38	102.36	114.42
12	L	302	BCR	C27-C26-C25	2.37	126.18	122.73
9	B	825	CLA	CHB-C1B-NB	2.37	126.77	124.26
11	A	842	LHG	C20-C19-C18	-2.37	102.38	114.42
12	B	836	BCR	C33-C5-C6	-2.37	121.87	124.53
9	B	803	CLA	CHC-C4B-NB	2.37	126.76	124.26
12	A	845	BCR	C15-C14-C13	-2.37	123.93	127.31
9	A	806	CLA	CHB-C4A-NA	2.37	127.78	124.51
9	A	838	CLA	C3B-C4B-NB	-2.36	108.32	110.52
9	B	821	CLA	CHB-C4A-NA	2.36	127.78	124.51
14	B	837	DGD	CFB-CEB-CDB	-2.36	102.44	114.42
9	B	820	CLA	C1-C2-C3	-2.36	122.93	126.75
9	A	802	CLA	CHD-C1D-ND	-2.36	122.29	124.45
9	B	810	CLA	CHB-C4A-NA	2.36	127.77	124.51
9	A	828	CLA	CHB-C1B-NB	2.36	126.75	124.26
9	A	849	CLA	CHB-C4A-NA	2.35	127.77	124.51
12	A	845	BCR	C2-C1-C6	2.35	114.10	110.48
12	A	846	BCR	C27-C26-C25	2.34	126.13	122.73
9	B	832	CLA	CHB-C4A-NA	2.34	127.75	124.51
9	B	821	CLA	CAB-C3B-C2B	2.34	129.66	123.59
9	A	824	CLA	CHB-C4A-NA	2.34	127.75	124.51
12	B	834	BCR	C27-C26-C25	2.34	126.12	122.73
9	B	839	CLA	CHB-C4A-NA	2.34	127.74	124.51
9	A	802	CLA	C3B-C4B-NB	-2.33	108.35	110.52
9	A	849	CLA	CHD-C1D-ND	-2.33	122.31	124.45
9	A	813	CLA	C1-C2-C3	-2.31	123.01	126.75
12	L	306	BCR	C11-C10-C9	-2.31	124.01	127.31
12	B	835	BCR	C33-C5-C6	-2.31	121.93	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	812	CLA	CHB-C4A-NA	2.31	127.71	124.51
12	A	844	BCR	C15-C14-C13	-2.31	124.01	127.31
9	A	822	CLA	C3B-C4B-NB	-2.30	108.38	110.52
9	A	850	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
12	B	835	BCR	C27-C26-C25	2.30	126.06	122.73
9	A	827	CLA	CHB-C4A-NA	2.29	127.68	124.51
9	A	802	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
9	B	808	CLA	C3B-C4B-NB	-2.29	108.39	110.52
9	B	823	CLA	CHB-C4A-NA	2.28	127.67	124.51
9	A	817	CLA	C3B-C4B-NB	-2.28	108.40	110.52
9	A	814	CLA	CHB-C1B-NB	2.28	126.67	124.26
9	B	829	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
12	L	302	BCR	C24-C23-C22	-2.27	122.80	126.23
9	B	812	CLA	CHB-C4A-NA	2.27	127.66	124.51
9	A	830	CLA	CHB-C1B-NB	2.27	126.66	124.26
9	A	831	CLA	C3B-C4B-NB	-2.26	108.41	110.52
9	B	805	CLA	CHB-C1B-NB	2.26	126.65	124.26
9	B	825	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
9	L	304	CLA	CHD-C1D-ND	-2.26	122.38	124.45
9	A	817	CLA	CHB-C4A-NA	2.26	127.63	124.51
9	B	831	CLA	CHB-C1B-NB	2.25	126.64	124.26
12	B	836	BCR	C16-C15-C14	-2.25	118.87	123.47
9	A	829	CLA	C1-C2-C3	-2.25	123.12	126.75
9	A	821	CLA	C3B-C4B-NB	-2.25	108.43	110.52
12	A	844	BCR	C24-C23-C22	-2.24	122.85	126.23
12	A	846	BCR	C15-C16-C17	-2.24	118.88	123.47
9	B	819	CLA	CHB-C4A-NA	2.23	127.59	124.51
9	A	849	CLA	C1-C2-C3	-2.23	122.19	126.04
11	A	842	LHG	C18-C17-C16	-2.23	103.13	114.42
9	B	824	CLA	CHB-C4A-NA	2.22	127.59	124.51
9	A	801	CLA	CHB-C4A-NA	2.22	127.59	124.51
12	A	846	BCR	C7-C8-C9	-2.22	122.88	126.23
12	A	844	BCR	C27-C26-C25	2.22	125.96	122.73
9	A	828	CLA	CHB-C4A-NA	2.22	127.58	124.51
9	L	305	CLA	C1-C2-C3	-2.22	123.16	126.75
11	L	301	LHG	C18-C17-C16	-2.22	103.17	114.42
9	B	821	CLA	CHD-C1D-ND	-2.22	122.42	124.45
12	B	834	BCR	C15-C14-C13	-2.22	124.15	127.31
12	L	308	BCR	C15-C16-C17	-2.21	118.94	123.47
9	L	304	CLA	O2D-CGD-CBD	2.21	115.19	111.27
12	I	101	BCR	C15-C16-C17	-2.21	118.95	123.47
12	L	306	BCR	C2-C1-C6	2.21	113.88	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	817	CLA	CHD-C1D-ND	-2.21	122.43	124.45
9	B	802	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
9	B	821	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
9	B	803	CLA	CHB-C4A-NA	2.20	127.56	124.51
9	B	801	CLA	CHB-C1B-NB	2.20	126.58	124.26
9	A	830	CLA	CHD-C1D-ND	-2.20	122.43	124.45
11	A	842	LHG	C27-C26-C25	-2.20	103.27	114.42
9	B	810	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
9	B	823	CLA	C3B-C4B-NB	-2.19	108.48	110.52
9	B	829	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
9	B	801	CLA	CAC-C3C-C2C	-2.19	123.78	127.53
12	L	306	BCR	C38-C26-C25	-2.19	122.07	124.53
14	B	837	DGD	CBB-CAB-C9B	-2.19	103.32	114.42
9	B	825	CLA	CHB-C4A-NA	2.19	127.53	124.51
9	B	828	CLA	CHB-C1B-NB	2.19	126.57	124.26
9	A	827	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
9	A	805	CLA	C1-C2-C3	-2.18	122.28	126.04
9	A	816	CLA	CHD-C1D-ND	-2.17	122.46	124.45
9	A	825	CLA	C1-C2-C3	-2.17	122.30	126.04
14	B	837	DGD	O2D-C2D-C1D	-2.17	104.78	110.05
9	A	827	CLA	C3B-C4B-NB	-2.17	108.51	110.52
9	A	824	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
9	A	824	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
9	A	830	CLA	C1-C2-C3	-2.16	122.31	126.04
11	L	301	LHG	C27-C26-C25	-2.16	103.46	114.42
10	B	833	PQN	C11-C3-C4	-2.16	116.19	118.50
9	A	824	CLA	CHB-C1B-NB	2.16	126.54	124.26
9	B	818	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
14	B	837	DGD	C3D-C4D-C5D	-2.15	106.41	110.24
9	A	802	CLA	CMB-C2B-C3B	2.15	131.79	126.59
12	L	308	BCR	C29-C30-C25	2.15	113.79	110.48
9	A	815	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
9	A	839	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
9	A	826	CLA	CMB-C2B-C1B	-2.15	122.10	125.37
9	A	827	CLA	C1-C2-C3	-2.14	122.34	126.04
9	B	810	CLA	C3B-C4B-NB	-2.14	108.53	110.52
9	B	819	CLA	CHB-C1B-NB	2.14	126.52	124.26
12	A	846	BCR	C20-C21-C22	-2.13	124.27	127.31
12	L	308	BCR	C15-C14-C13	-2.13	124.27	127.31
9	A	838	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
9	L	303	CLA	CHB-C1B-NB	2.13	126.51	124.26
9	B	810	CLA	C1-C2-C3	-2.13	122.36	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	101	BCR	C27-C26-C25	2.13	125.82	122.73
9	A	835	CLA	CHB-C1B-NB	2.13	126.51	124.26
9	A	826	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
9	A	831	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
9	B	830	CLA	CHC-C4B-NB	2.12	126.50	124.26
14	B	837	DGD	CAB-C9B-C8B	-2.12	103.65	114.42
9	B	825	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
9	B	830	CLA	CHB-C4A-NA	2.12	127.44	124.51
9	A	815	CLA	C1-C2-C3	-2.12	122.38	126.04
12	A	847	BCR	C38-C26-C25	-2.12	122.15	124.53
9	A	813	CLA	CHD-C1D-ND	-2.11	122.51	124.45
9	A	836	CLA	C1-C2-C3	-2.11	122.39	126.04
9	A	804	CLA	CHD-C1D-ND	-2.11	122.51	124.45
9	B	801	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
9	B	817	CLA	CHD-C1D-ND	-2.11	122.52	124.45
9	B	829	CLA	CHD-C1D-ND	-2.11	122.52	124.45
9	B	832	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
9	A	809	CLA	C1-C2-C3	-2.11	122.40	126.04
9	A	830	CLA	CMB-C2B-C1B	-2.10	122.16	125.37
9	A	828	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
9	B	819	CLA	CHD-C1D-ND	-2.10	122.52	124.45
9	B	823	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
9	A	803	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
9	B	802	CLA	CHD-C1D-ND	-2.10	122.52	124.45
9	B	801	CLA	CHD-C1D-ND	-2.10	122.52	124.45
9	A	832	CLA	C1-C2-C3	-2.10	123.36	126.75
9	B	809	CLA	O2D-CGD-CBD	2.10	115.00	111.27
9	B	803	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
9	H	201	CLA	CHD-C1D-ND	-2.10	122.53	124.45
9	B	806	CLA	CMB-C2B-C1B	-2.10	122.18	125.37
9	A	805	CLA	CHD-C1D-ND	-2.09	122.53	124.45
9	B	827	CLA	CHD-C1D-ND	-2.09	122.53	124.45
12	B	835	BCR	C24-C23-C22	-2.09	123.07	126.23
9	B	839	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
9	A	841	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
9	A	816	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
9	A	819	CLA	CHB-C1B-NB	2.09	126.47	124.26
9	A	819	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
9	A	825	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
9	A	834	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
9	A	807	CLA	CHD-C1D-ND	-2.08	122.54	124.45
9	B	823	CLA	CHD-C1D-ND	-2.08	122.54	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	805	CLA	CMB-C2B-C1B	-2.08	122.19	125.37
9	B	830	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
12	A	845	BCR	C33-C5-C6	-2.08	122.19	124.53
9	B	819	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
9	A	806	CLA	CHD-C1D-ND	-2.08	122.54	124.45
9	B	824	CLA	CHB-C1B-NB	2.08	126.46	124.26
9	A	804	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
12	A	846	BCR	C33-C5-C6	-2.08	122.19	124.53
9	A	801	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
9	A	850	CLA	C1-C2-C3	-2.08	122.45	126.04
9	A	837	CLA	CHB-C1B-NB	2.07	126.45	124.26
9	A	815	CLA	O2D-CGD-CBD	2.07	114.95	111.27
9	A	824	CLA	CHD-C1D-ND	-2.07	122.55	124.45
9	A	819	CLA	CHD-C1D-ND	-2.07	122.55	124.45
9	A	834	CLA	CHD-C1D-ND	-2.07	122.55	124.45
9	A	809	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
9	B	828	CLA	CMB-C2B-C3B	2.07	131.60	126.59
9	B	818	CLA	CHD-C1D-ND	-2.07	122.55	124.45
9	A	822	CLA	CHD-C1D-ND	-2.07	122.55	124.45
9	A	810	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
9	B	826	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
9	A	810	CLA	CHB-C1B-NB	2.07	126.45	124.26
9	B	827	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
9	A	810	CLA	CHD-C1D-ND	-2.07	122.56	124.45
9	B	826	CLA	CHD-C1D-ND	-2.07	122.56	124.45
12	B	834	BCR	C7-C8-C9	-2.06	123.11	126.23
12	L	308	BCR	C8-C7-C6	-2.06	121.41	127.20
9	A	819	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
9	A	834	CLA	C1-C2-C3	-2.06	122.47	126.04
9	A	808	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
9	B	806	CLA	CHD-C1D-ND	-2.06	122.56	124.45
14	B	837	DGD	C5B-C4B-C3B	-2.06	103.97	114.42
9	A	833	CLA	CHB-C1B-NB	2.06	126.44	124.26
9	B	814	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
9	A	812	CLA	O2A-CGA-O1A	-2.06	118.17	123.30
12	L	308	BCR	C2-C1-C6	2.06	113.65	110.48
9	A	812	CLA	CHD-C1D-ND	-2.06	122.56	124.45
9	A	837	CLA	CHD-C1D-ND	-2.06	122.56	124.45
9	A	811	CLA	CHD-C1D-ND	-2.06	122.56	124.45
9	A	834	CLA	CHB-C1B-NB	2.06	126.43	124.26
9	A	833	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
9	A	808	CLA	CHD-C1D-ND	-2.05	122.57	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	808	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
9	A	813	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
9	B	812	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
12	B	835	BCR	C28-C27-C26	-2.05	110.42	114.08
9	A	850	CLA	CHB-C1B-NB	2.05	126.43	124.26
9	A	832	CLA	CHD-C1D-ND	-2.05	122.57	124.45
9	H	201	CLA	C1-C2-C3	-2.05	122.50	126.04
12	L	307	BCR	C8-C7-C6	-2.05	121.45	127.20
9	A	820	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
9	A	811	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
9	A	812	CLA	CHB-C1B-NB	2.04	126.42	124.26
12	A	847	BCR	C37-C22-C21	-2.04	120.06	122.92
12	B	836	BCR	C8-C7-C6	-2.04	121.46	127.20
9	L	305	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
9	A	809	CLA	CHB-C1B-NB	2.04	126.42	124.26
9	B	819	CLA	O2D-CGD-CBD	2.04	114.89	111.27
9	A	823	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
9	A	817	CLA	CHB-C1B-NB	2.04	126.42	124.26
9	B	807	CLA	CHB-C1B-NB	2.04	126.42	124.26
9	A	828	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
9	A	802	CLA	C1-C2-C3	-2.04	122.52	126.04
9	B	839	CLA	CHD-C1D-ND	-2.04	122.58	124.45
9	A	826	CLA	CMB-C2B-C3B	2.04	131.52	126.59
9	A	833	CLA	CHD-C1D-ND	-2.03	122.58	124.45
9	A	806	CLA	C1-C2-C3	-2.03	122.53	126.04
9	B	828	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
9	B	826	CLA	CHB-C1B-NB	2.03	126.41	124.26
9	B	831	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
9	A	803	CLA	CHB-C1B-NB	2.03	126.41	124.26
9	A	803	CLA	CHD-C1D-ND	-2.03	122.59	124.45
9	B	807	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
9	A	811	CLA	C1-C2-C3	-2.03	122.53	126.04
9	A	805	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
12	A	847	BCR	C8-C7-C6	-2.03	121.51	127.20
12	I	101	BCR	C8-C7-C6	-2.03	121.51	127.20
9	A	829	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
9	B	829	CLA	CHB-C1B-NB	2.03	126.40	124.26
9	B	815	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
9	B	807	CLA	C1-C2-C3	-2.02	122.54	126.04
9	B	824	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
11	A	843	LHG	C5-O7-C7	-2.02	112.81	117.79
9	B	808	CLA	O2D-CGD-CBD	2.02	114.86	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	822	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
9	B	821	CLA	CHB-C1B-NB	2.01	126.39	124.26
9	B	806	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
9	B	827	CLA	CHB-C1B-NB	2.01	126.39	124.26
9	L	303	CLA	CHD-C1D-ND	-2.01	122.61	124.45
9	A	821	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
9	B	813	CLA	CHB-C1B-NB	2.01	126.31	124.27
9	A	836	CLA	CHB-C1B-NB	2.01	126.39	124.26
9	B	830	CLA	CHD-C1D-ND	-2.01	122.61	124.45
9	B	832	CLA	C3B-C4B-NB	-2.01	108.65	110.52
9	A	830	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
9	A	831	CLA	CHB-C1B-NB	2.01	126.38	124.26
14	B	837	DGD	O6E-C1E-O5D	-2.01	105.22	109.97
12	A	846	BCR	C3-C4-C5	-2.01	110.50	114.08
9	A	831	CLA	CHD-C1D-ND	-2.01	122.61	124.45
9	A	826	CLA	C1-C2-C3	-2.00	122.58	126.04
9	B	839	CLA	CHB-C1B-NB	2.00	126.38	124.26
9	B	823	CLA	C1-C2-C3	-2.00	122.58	126.04
9	B	817	CLA	CHB-C1B-NB	2.00	126.38	124.26
9	A	835	CLA	C1-C2-C3	-2.00	122.58	126.04
9	A	821	CLA	C1-C2-C3	-2.00	122.58	126.04
9	A	832	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
9	A	801	CLA	O1D-CGD-CBD	2.00	128.58	124.48
9	A	813	CLA	CHB-C1B-NB	2.00	126.38	124.26

There are no chirality outliers.

All (1044) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	801	CLA	CBD-CGD-O2D-CED
9	A	803	CLA	C1A-C2A-CAA-CBA
9	A	803	CLA	CHA-CBD-CGD-O1D
9	A	803	CLA	CHA-CBD-CGD-O2D
9	A	804	CLA	CHA-CBD-CGD-O1D
9	A	804	CLA	CHA-CBD-CGD-O2D
9	A	804	CLA	CAD-CBD-CGD-O1D
9	A	805	CLA	C1A-C2A-CAA-CBA
9	A	805	CLA	C3A-C2A-CAA-CBA
9	A	807	CLA	C1A-C2A-CAA-CBA
9	A	807	CLA	C3A-C2A-CAA-CBA
9	A	807	CLA	CBD-CGD-O2D-CED
9	A	808	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	808	CLA	O1D-CGD-O2D-CED
9	A	808	CLA	C11-C12-C13-C14
9	A	809	CLA	CBD-CGD-O2D-CED
9	A	810	CLA	C3A-C2A-CAA-CBA
9	A	812	CLA	C1A-C2A-CAA-CBA
9	A	812	CLA	C3A-C2A-CAA-CBA
9	A	815	CLA	C1A-C2A-CAA-CBA
9	A	815	CLA	CHA-CBD-CGD-O1D
9	A	815	CLA	CHA-CBD-CGD-O2D
9	A	816	CLA	C1A-C2A-CAA-CBA
9	A	816	CLA	C3A-C2A-CAA-CBA
9	A	817	CLA	C1A-C2A-CAA-CBA
9	A	817	CLA	C3A-C2A-CAA-CBA
9	A	817	CLA	CHA-CBD-CGD-O1D
9	A	817	CLA	CHA-CBD-CGD-O2D
9	A	820	CLA	CBD-CGD-O2D-CED
9	A	822	CLA	CHA-CBD-CGD-O1D
9	A	822	CLA	CHA-CBD-CGD-O2D
9	A	825	CLA	C1A-C2A-CAA-CBA
9	A	826	CLA	C1A-C2A-CAA-CBA
9	A	826	CLA	C3A-C2A-CAA-CBA
9	A	826	CLA	CHA-CBD-CGD-O1D
9	A	826	CLA	CHA-CBD-CGD-O2D
9	A	826	CLA	C4-C3-C5-C6
9	A	831	CLA	C1A-C2A-CAA-CBA
9	A	831	CLA	CAD-CBD-CGD-O1D
9	A	831	CLA	CAD-CBD-CGD-O2D
9	A	832	CLA	C1A-C2A-CAA-CBA
9	A	832	CLA	C3A-C2A-CAA-CBA
9	A	832	CLA	C2A-CAA-CBA-CGA
9	A	833	CLA	C1A-C2A-CAA-CBA
9	A	833	CLA	C3A-C2A-CAA-CBA
9	A	833	CLA	CHA-CBD-CGD-O1D
9	A	833	CLA	CHA-CBD-CGD-O2D
9	A	834	CLA	C1A-C2A-CAA-CBA
9	A	834	CLA	C3A-C2A-CAA-CBA
9	A	836	CLA	CHA-CBD-CGD-O1D
9	A	836	CLA	CHA-CBD-CGD-O2D
9	A	837	CLA	CHA-CBD-CGD-O1D
9	A	837	CLA	CHA-CBD-CGD-O2D
9	A	838	CLA	C1A-C2A-CAA-CBA
9	A	838	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	838	CLA	CBD-CGD-O2D-CED
9	A	849	CLA	C2B-C3B-CAB-CBB
9	A	849	CLA	C4B-C3B-CAB-CBB
9	A	849	CLA	CBD-CGD-O2D-CED
9	A	849	CLA	C4-C3-C5-C6
9	A	850	CLA	C1A-C2A-CAA-CBA
9	A	850	CLA	C3A-C2A-CAA-CBA
9	A	850	CLA	C2A-CAA-CBA-CGA
9	B	802	CLA	C2A-CAA-CBA-CGA
9	B	802	CLA	CHA-CBD-CGD-O1D
9	B	802	CLA	CHA-CBD-CGD-O2D
9	B	802	CLA	CAD-CBD-CGD-O1D
9	B	802	CLA	CAD-CBD-CGD-O2D
9	B	802	CLA	C4-C3-C5-C6
9	B	803	CLA	CHA-CBD-CGD-O1D
9	B	803	CLA	CHA-CBD-CGD-O2D
9	B	803	CLA	CBD-CGD-O2D-CED
9	B	804	CLA	C2B-C3B-CAB-CBB
9	B	804	CLA	C4B-C3B-CAB-CBB
9	B	804	CLA	CBD-CGD-O2D-CED
9	B	808	CLA	CHA-CBD-CGD-O1D
9	B	808	CLA	CHA-CBD-CGD-O2D
9	B	809	CLA	CHA-CBD-CGD-O2D
9	B	811	CLA	C2B-C3B-CAB-CBB
9	B	811	CLA	C4B-C3B-CAB-CBB
9	B	812	CLA	CHA-CBD-CGD-O1D
9	B	812	CLA	CHA-CBD-CGD-O2D
9	B	812	CLA	CAD-CBD-CGD-O1D
9	B	814	CLA	C1A-C2A-CAA-CBA
9	B	818	CLA	C1A-C2A-CAA-CBA
9	B	818	CLA	C3A-C2A-CAA-CBA
9	B	819	CLA	C3A-C2A-CAA-CBA
9	B	819	CLA	C11-C10-C8-C9
9	B	824	CLA	C1A-C2A-CAA-CBA
9	B	824	CLA	C3A-C2A-CAA-CBA
9	B	824	CLA	C2-C3-C5-C6
9	B	824	CLA	C4-C3-C5-C6
9	B	825	CLA	CHA-CBD-CGD-O1D
9	B	825	CLA	CHA-CBD-CGD-O2D
9	B	827	CLA	C2A-CAA-CBA-CGA
9	B	840	CLA	CHA-CBD-CGD-O1D
9	B	840	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	L	301	LHG	C3-O3-P-O5
11	L	301	LHG	C4-O6-P-O5
12	A	844	BCR	C6-C7-C8-C9
12	A	844	BCR	C7-C8-C9-C34
12	A	844	BCR	C23-C24-C25-C30
12	A	845	BCR	C14-C15-C16-C17
12	A	847	BCR	C1-C6-C7-C8
12	A	847	BCR	C7-C8-C9-C34
12	A	847	BCR	C22-C23-C24-C25
12	B	834	BCR	C21-C22-C23-C24
12	B	834	BCR	C22-C23-C24-C25
12	B	835	BCR	C6-C7-C8-C9
12	B	835	BCR	C7-C8-C9-C10
12	B	835	BCR	C7-C8-C9-C34
12	B	835	BCR	C14-C15-C16-C17
12	B	835	BCR	C16-C17-C18-C19
12	B	835	BCR	C16-C17-C18-C36
12	B	835	BCR	C17-C18-C19-C20
12	B	835	BCR	C36-C18-C19-C20
12	B	835	BCR	C18-C19-C20-C21
12	B	835	BCR	C20-C21-C22-C37
12	B	835	BCR	C37-C22-C23-C24
12	B	835	BCR	C22-C23-C24-C25
12	B	836	BCR	C21-C22-C23-C24
12	B	836	BCR	C37-C22-C23-C24
12	B	836	BCR	C22-C23-C24-C25
12	I	101	BCR	C21-C22-C23-C24
12	I	101	BCR	C37-C22-C23-C24
12	I	101	BCR	C22-C23-C24-C25
12	L	306	BCR	C7-C8-C9-C34
12	L	306	BCR	C21-C22-C23-C24
12	L	306	BCR	C37-C22-C23-C24
12	L	306	BCR	C23-C24-C25-C26
12	L	306	BCR	C23-C24-C25-C30
12	L	308	BCR	C1-C6-C7-C8
12	L	308	BCR	C7-C8-C9-C10
12	L	308	BCR	C7-C8-C9-C34
12	L	308	BCR	C20-C21-C22-C37
12	L	308	BCR	C21-C22-C23-C24
12	L	308	BCR	C37-C22-C23-C24
12	L	308	BCR	C23-C24-C25-C26
12	L	308	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	801	CLA	O1D-CGD-O2D-CED
9	A	809	CLA	O1D-CGD-O2D-CED
9	A	821	CLA	O1D-CGD-O2D-CED
9	A	838	CLA	O1D-CGD-O2D-CED
9	B	804	CLA	O1D-CGD-O2D-CED
9	A	826	CLA	O1D-CGD-O2D-CED
9	A	821	CLA	CBD-CGD-O2D-CED
9	A	826	CLA	CBD-CGD-O2D-CED
9	A	841	CLA	CBD-CGD-O2D-CED
9	B	820	CLA	CBD-CGD-O2D-CED
9	B	823	CLA	CBD-CGD-O2D-CED
9	B	806	CLA	O1A-CGA-O2A-C1
11	L	301	LHG	O10-C23-O8-C6
9	A	841	CLA	O1D-CGD-O2D-CED
9	B	803	CLA	O1D-CGD-O2D-CED
9	A	849	CLA	O1D-CGD-O2D-CED
9	B	820	CLA	O1D-CGD-O2D-CED
9	B	806	CLA	CBA-CGA-O2A-C1
9	A	811	CLA	CBD-CGD-O2D-CED
9	A	829	CLA	CBD-CGD-O2D-CED
9	A	832	CLA	CBD-CGD-O2D-CED
9	A	837	CLA	CBD-CGD-O2D-CED
9	B	810	CLA	CBD-CGD-O2D-CED
9	B	811	CLA	CBD-CGD-O2D-CED
9	B	813	CLA	CBD-CGD-O2D-CED
9	B	822	CLA	CBD-CGD-O2D-CED
9	A	821	CLA	O1A-CGA-O2A-C1
9	A	837	CLA	O1A-CGA-O2A-C1
9	B	814	CLA	O1A-CGA-O2A-C1
9	A	807	CLA	O1D-CGD-O2D-CED
9	A	820	CLA	O1D-CGD-O2D-CED
9	A	813	CLA	CBD-CGD-O2D-CED
14	B	837	DGD	O1B-C1B-O2G-C2G
9	A	806	CLA	C3-C5-C6-C7
9	A	830	CLA	C3-C5-C6-C7
9	A	838	CLA	C3-C5-C6-C7
9	B	802	CLA	C3-C5-C6-C7
9	A	805	CLA	CBA-CGA-O2A-C1
9	A	819	CLA	CBA-CGA-O2A-C1
9	A	834	CLA	CBA-CGA-O2A-C1
9	B	814	CLA	CBA-CGA-O2A-C1
9	H	201	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	L	301	LHG	C24-C23-O8-C6
9	B	802	CLA	CBD-CGD-O2D-CED
9	B	801	CLA	C2C-C3C-CAC-CBC
9	B	817	CLA	C4-C3-C5-C6
10	A	840	PQN	C14-C13-C15-C16
9	A	826	CLA	C2-C3-C5-C6
9	B	802	CLA	C2-C3-C5-C6
9	A	812	CLA	CBD-CGD-O2D-CED
9	A	810	CLA	C2A-CAA-CBA-CGA
9	A	826	CLA	C2A-CAA-CBA-CGA
9	A	839	CLA	C2A-CAA-CBA-CGA
9	A	841	CLA	C2A-CAA-CBA-CGA
9	B	820	CLA	C2A-CAA-CBA-CGA
9	B	831	CLA	C2A-CAA-CBA-CGA
9	A	850	CLA	C3-C5-C6-C7
9	B	801	CLA	C3-C5-C6-C7
9	A	821	CLA	CBA-CGA-O2A-C1
9	A	837	CLA	CBA-CGA-O2A-C1
9	B	818	CLA	CBA-CGA-O2A-C1
9	B	823	CLA	O1D-CGD-O2D-CED
9	A	805	CLA	O1A-CGA-O2A-C1
9	A	834	CLA	O1A-CGA-O2A-C1
9	B	801	CLA	O1A-CGA-O2A-C1
9	A	804	CLA	CBD-CGD-O2D-CED
9	A	823	CLA	CBD-CGD-O2D-CED
9	B	828	CLA	CBD-CGD-O2D-CED
9	B	806	CLA	C3-C5-C6-C7
9	B	807	CLA	C3-C5-C6-C7
9	A	817	CLA	CBA-CGA-O2A-C1
9	A	831	CLA	CBA-CGA-O2A-C1
9	B	801	CLA	CBA-CGA-O2A-C1
9	A	819	CLA	O1A-CGA-O2A-C1
9	H	201	CLA	O1A-CGA-O2A-C1
9	B	807	CLA	CBD-CGD-O2D-CED
9	B	816	CLA	CBD-CGD-O2D-CED
9	B	840	CLA	CBD-CGD-O2D-CED
9	L	303	CLA	CBD-CGD-O2D-CED
9	A	817	CLA	O1A-CGA-O2A-C1
15	B	838	LMT	C5'-C4'-O1B-C1B
9	A	831	CLA	C3-C5-C6-C7
9	A	831	CLA	O1A-CGA-O2A-C1
9	B	818	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	837	DGD	O6E-C5E-C6E-O5E
9	A	831	CLA	C4-C3-C5-C6
9	B	806	CLA	C4-C3-C5-C6
9	A	831	CLA	C2-C3-C5-C6
9	A	849	CLA	C2-C3-C5-C6
9	B	806	CLA	C2-C3-C5-C6
9	B	817	CLA	C2-C3-C5-C6
9	A	822	CLA	CBD-CGD-O2D-CED
9	A	837	CLA	O1D-CGD-O2D-CED
9	B	810	CLA	O1D-CGD-O2D-CED
9	B	822	CLA	O1D-CGD-O2D-CED
9	A	809	CLA	CBA-CGA-O2A-C1
9	A	813	CLA	CBA-CGA-O2A-C1
9	A	822	CLA	CBA-CGA-O2A-C1
9	B	817	CLA	CBA-CGA-O2A-C1
14	B	837	DGD	C4E-C5E-C6E-O5E
9	B	801	CLA	C4C-C3C-CAC-CBC
12	B	835	BCR	C19-C20-C21-C22
9	B	811	CLA	O1D-CGD-O2D-CED
9	A	835	CLA	C8-C10-C11-C12
9	B	821	CLA	C10-C11-C12-C13
9	A	849	CLA	C3-C5-C6-C7
10	A	840	PQN	C12-C13-C15-C16
9	A	807	CLA	C11-C10-C8-C9
9	A	809	CLA	C11-C12-C13-C14
9	A	824	CLA	C6-C7-C8-C9
9	A	830	CLA	C6-C7-C8-C9
9	A	831	CLA	C6-C7-C8-C9
9	A	849	CLA	C11-C10-C8-C9
9	A	850	CLA	C11-C12-C13-C14
9	B	801	CLA	C11-C10-C8-C9
9	B	801	CLA	C11-C12-C13-C14
9	B	804	CLA	C11-C12-C13-C14
9	B	807	CLA	C6-C7-C8-C9
9	B	810	CLA	C14-C13-C15-C16
9	B	814	CLA	C6-C7-C8-C9
9	B	814	CLA	C11-C12-C13-C14
9	B	824	CLA	C11-C10-C8-C9
9	L	304	CLA	C6-C7-C8-C9
10	A	840	PQN	C21-C22-C23-C24
10	A	840	PQN	C24-C23-C25-C26
9	A	811	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	813	CLA	O1D-CGD-O2D-CED
9	A	836	CLA	CBD-CGD-O2D-CED
9	A	827	CLA	C8-C10-C11-C12
9	A	831	CLA	C10-C11-C12-C13
9	B	840	CLA	C2A-CAA-CBA-CGA
12	A	847	BCR	C37-C22-C23-C24
12	B	834	BCR	C37-C22-C23-C24
12	L	307	BCR	C7-C8-C9-C34
12	A	844	BCR	C7-C8-C9-C10
12	A	847	BCR	C21-C22-C23-C24
12	B	835	BCR	C21-C22-C23-C24
12	L	306	BCR	C7-C8-C9-C10
9	A	809	CLA	O1A-CGA-O2A-C1
9	A	822	CLA	O1A-CGA-O2A-C1
9	A	849	CLA	C15-C16-C17-C18
9	B	801	CLA	C5-C6-C7-C8
9	B	804	CLA	C10-C11-C12-C13
9	A	832	CLA	O1D-CGD-O2D-CED
9	B	826	CLA	CBD-CGD-O2D-CED
9	A	807	CLA	C3-C5-C6-C7
9	A	808	CLA	C8-C10-C11-C12
9	A	817	CLA	C15-C16-C17-C18
9	A	849	CLA	C13-C15-C16-C17
9	B	801	CLA	C10-C11-C12-C13
9	B	819	CLA	C8-C10-C11-C12
9	A	829	CLA	O1D-CGD-O2D-CED
9	A	801	CLA	C15-C16-C17-C18
9	A	817	CLA	C5-C6-C7-C8
9	A	824	CLA	C15-C16-C17-C18
9	B	814	CLA	C8-C10-C11-C12
9	B	821	CLA	C8-C10-C11-C12
9	B	824	CLA	C8-C10-C11-C12
9	A	813	CLA	O1A-CGA-O2A-C1
11	L	301	LHG	C23-C24-C25-C26
9	A	801	CLA	C13-C15-C16-C17
9	B	809	CLA	C15-C16-C17-C18
9	B	831	CLA	C15-C16-C17-C18
9	A	832	CLA	CBA-CGA-O2A-C1
9	A	811	CLA	C10-C11-C12-C13
9	B	821	CLA	C13-C15-C16-C17
9	A	831	CLA	CBD-CGD-O2D-CED
9	B	816	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	826	CLA	O2A-C1-C2-C3
10	A	840	PQN	C20-C21-C22-C23
9	A	807	CLA	C6-C7-C8-C10
9	A	830	CLA	C6-C7-C8-C10
9	B	811	CLA	C11-C12-C13-C15
9	B	823	CLA	C12-C13-C15-C16
9	A	806	CLA	CBD-CGD-O2D-CED
9	A	820	CLA	C2A-CAA-CBA-CGA
9	A	813	CLA	O1D-CGD-O2D-CED
9	A	850	CLA	C13-C15-C16-C17
15	B	838	LMT	O1'-C1-C2-C3
9	B	827	CLA	CBD-CGD-O2D-CED
9	A	807	CLA	C15-C16-C17-C18
12	A	845	BCR	C10-C11-C12-C13
12	A	845	BCR	C18-C19-C20-C21
12	A	846	BCR	C10-C11-C12-C13
12	L	307	BCR	C10-C11-C12-C13
9	A	808	CLA	C10-C11-C12-C13
9	A	809	CLA	C13-C15-C16-C17
9	B	817	CLA	O1A-CGA-O2A-C1
9	A	809	CLA	C5-C6-C7-C8
9	A	830	CLA	C5-C6-C7-C8
9	A	835	CLA	C10-C11-C12-C13
9	B	829	CLA	C5-C6-C7-C8
9	A	802	CLA	C10-C11-C12-C13
9	A	802	CLA	C15-C16-C17-C18
9	A	815	CLA	C15-C16-C17-C18
9	A	831	CLA	C8-C10-C11-C12
9	B	811	CLA	C5-C6-C7-C8
9	B	824	CLA	C10-C11-C12-C13
11	A	843	LHG	C4-O6-P-O3
11	L	301	LHG	C4-O6-P-O3
9	A	810	CLA	CBA-CGA-O2A-C1
9	A	850	CLA	CBA-CGA-O2A-C1
9	B	823	CLA	CBA-CGA-O2A-C1
9	B	824	CLA	CBA-CGA-O2A-C1
9	A	839	CLA	O2A-C1-C2-C3
11	A	842	LHG	C28-C29-C30-C31
9	B	816	CLA	C2A-CAA-CBA-CGA
9	L	303	CLA	C2A-CAA-CBA-CGA
12	A	845	BCR	C35-C13-C14-C15
12	A	845	BCR	C20-C21-C22-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	A	846	BCR	C16-C17-C18-C36
12	B	834	BCR	C20-C21-C22-C37
12	L	302	BCR	C16-C17-C18-C36
14	B	837	DGD	C2B-C3B-C4B-C5B
9	B	802	CLA	O1D-CGD-O2D-CED
14	B	837	DGD	C2A-C3A-C4A-C5A
9	A	834	CLA	CBD-CGD-O2D-CED
9	B	814	CLA	CBD-CGD-O2D-CED
11	L	301	LHG	C32-C33-C34-C35
9	A	832	CLA	O1A-CGA-O2A-C1
11	A	842	LHG	C32-C33-C34-C35
9	A	812	CLA	O1D-CGD-O2D-CED
11	L	301	LHG	O2-C2-C3-O3
15	B	838	LMT	C4-C5-C6-C7
9	B	817	CLA	C3-C5-C6-C7
12	A	845	BCR	C12-C13-C14-C15
12	A	845	BCR	C20-C21-C22-C23
12	A	847	BCR	C20-C21-C22-C23
12	B	835	BCR	C20-C21-C22-C23
12	L	308	BCR	C20-C21-C22-C23
9	B	840	CLA	CBA-CGA-O2A-C1
11	A	842	LHG	C9-C10-C11-C12
9	A	810	CLA	O1A-CGA-O2A-C1
9	B	823	CLA	O1A-CGA-O2A-C1
9	A	822	CLA	C6-C7-C8-C10
9	B	815	CLA	C16-C17-C18-C20
9	A	801	CLA	C4-C3-C5-C6
9	A	838	CLA	C4-C3-C5-C6
14	B	837	DGD	C7A-C8A-C9A-CAA
9	A	801	CLA	C2-C3-C5-C6
9	A	816	CLA	C11-C12-C13-C14
9	A	849	CLA	C11-C12-C13-C14
9	B	804	CLA	C11-C10-C8-C9
9	A	824	CLA	C13-C15-C16-C17
9	A	826	CLA	C5-C6-C7-C8
9	A	809	CLA	C2A-CAA-CBA-CGA
9	B	819	CLA	C2A-CAA-CBA-CGA
9	B	824	CLA	O1A-CGA-O2A-C1
11	A	843	LHG	O1-C1-C2-C3
11	L	301	LHG	O1-C1-C2-C3
12	L	307	BCR	C7-C8-C9-C10
9	B	814	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	842	LHG	C24-C25-C26-C27
9	A	804	CLA	O1D-CGD-O2D-CED
11	A	842	LHG	C11-C10-C9-C8
14	B	837	DGD	C4A-C5A-C6A-C7A
9	B	817	CLA	C4B-C3B-CAB-CBB
9	A	826	CLA	C16-C17-C18-C20
9	A	827	CLA	C16-C17-C18-C19
9	A	827	CLA	C16-C17-C18-C20
9	B	819	CLA	C11-C12-C13-C14
9	B	819	CLA	C11-C12-C13-C15
15	B	838	LMT	O5'-C1'-O1'-C1
9	A	807	CLA	C5-C6-C7-C8
9	A	823	CLA	O1D-CGD-O2D-CED
15	B	838	LMT	C3-C4-C5-C6
14	B	837	DGD	C3B-C4B-C5B-C6B
9	A	850	CLA	O1A-CGA-O2A-C1
11	A	842	LHG	C16-C17-C18-C19
9	A	839	CLA	CBA-CGA-O2A-C1
9	B	815	CLA	CBA-CGA-O2A-C1
11	A	842	LHG	C12-C13-C14-C15
9	B	828	CLA	O1D-CGD-O2D-CED
9	A	815	CLA	C3A-C2A-CAA-CBA
9	A	825	CLA	C3A-C2A-CAA-CBA
9	A	830	CLA	C3A-C2A-CAA-CBA
9	A	831	CLA	C3A-C2A-CAA-CBA
9	B	814	CLA	C3A-C2A-CAA-CBA
9	B	828	CLA	C3A-C2A-CAA-CBA
9	B	839	CLA	C3A-C2A-CAA-CBA
11	A	842	LHG	C30-C31-C32-C33
14	B	837	DGD	C4B-C5B-C6B-C7B
9	A	822	CLA	C6-C7-C8-C9
9	A	826	CLA	C16-C17-C18-C19
11	L	301	LHG	C24-C25-C26-C27
9	L	305	CLA	CBD-CGD-O2D-CED
9	A	808	CLA	C4-C3-C5-C6
9	A	808	CLA	C2-C3-C5-C6
9	A	827	CLA	C2-C3-C5-C6
9	A	838	CLA	C2-C3-C5-C6
11	A	843	LHG	C8-C7-O7-C5
11	L	301	LHG	C28-C29-C30-C31
11	A	843	LHG	O1-C1-C2-O2
11	A	842	LHG	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	815	CLA	C16-C17-C18-C19
9	B	817	CLA	C2B-C3B-CAB-CBB
11	L	301	LHG	C10-C11-C12-C13
15	B	838	LMT	C5-C6-C7-C8
9	B	802	CLA	C15-C16-C17-C18
11	A	842	LHG	C7-C8-C9-C10
12	A	844	BCR	C1-C6-C7-C8
12	A	844	BCR	C5-C6-C7-C8
12	A	844	BCR	C23-C24-C25-C26
12	A	847	BCR	C5-C6-C7-C8
12	A	847	BCR	C23-C24-C25-C26
12	A	847	BCR	C23-C24-C25-C30
12	B	835	BCR	C23-C24-C25-C26
12	B	835	BCR	C23-C24-C25-C30
12	I	101	BCR	C1-C6-C7-C8
12	I	101	BCR	C5-C6-C7-C8
12	L	302	BCR	C1-C6-C7-C8
12	L	302	BCR	C5-C6-C7-C8
12	L	307	BCR	C1-C6-C7-C8
12	L	308	BCR	C5-C6-C7-C8
9	B	819	CLA	CBA-CGA-O2A-C1
9	B	823	CLA	C10-C11-C12-C13
9	A	820	CLA	C2C-C3C-CAC-CBC
9	B	840	CLA	O1A-CGA-O2A-C1
15	B	838	LMT	C3'-C4'-O1B-C1B
9	A	827	CLA	C4-C3-C5-C6
9	B	807	CLA	O1D-CGD-O2D-CED
9	L	303	CLA	O1D-CGD-O2D-CED
9	A	802	CLA	C11-C10-C8-C7
9	A	824	CLA	C6-C7-C8-C10
9	A	849	CLA	C11-C12-C13-C15
9	B	804	CLA	C11-C10-C8-C7
9	B	810	CLA	C12-C13-C15-C16
10	A	840	PQN	C16-C17-C18-C20
10	B	833	PQN	C16-C17-C18-C20
9	A	839	CLA	O1A-CGA-O2A-C1
9	B	815	CLA	O1A-CGA-O2A-C1
9	B	832	CLA	CBD-CGD-O2D-CED
9	B	840	CLA	O1D-CGD-O2D-CED
9	A	807	CLA	CBA-CGA-O2A-C1
9	L	304	CLA	CBA-CGA-O2A-C1
9	A	813	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	816	CLA	C2A-CAA-CBA-CGA
9	B	824	CLA	C2A-CAA-CBA-CGA
9	A	850	CLA	C8-C10-C11-C12
9	A	806	CLA	C8-C10-C11-C12
9	B	801	CLA	C8-C10-C11-C12
9	B	816	CLA	O1D-CGD-O2D-CED
11	A	842	LHG	C8-C7-O7-C5
14	B	837	DGD	C2B-C1B-O2G-C2G
9	A	803	CLA	C5-C6-C7-C8
14	B	837	DGD	C6A-C7A-C8A-C9A
9	A	817	CLA	C11-C12-C13-C14
9	A	828	CLA	C14-C13-C15-C16
9	A	836	CLA	C11-C12-C13-C14
9	A	849	CLA	C6-C7-C8-C9
9	B	806	CLA	C11-C10-C8-C9
9	B	823	CLA	C14-C13-C15-C16
10	B	833	PQN	C16-C17-C18-C19
9	B	806	CLA	CBD-CGD-O2D-CED
10	A	840	PQN	C13-C15-C16-C17
9	A	849	CLA	C2A-CAA-CBA-CGA
9	B	811	CLA	C2A-CAA-CBA-CGA
15	B	838	LMT	O5B-C5B-C6B-O6B
9	B	825	CLA	CBA-CGA-O2A-C1
9	A	822	CLA	O1D-CGD-O2D-CED
9	B	819	CLA	O1A-CGA-O2A-C1
9	A	810	CLA	C1A-C2A-CAA-CBA
9	A	830	CLA	C1A-C2A-CAA-CBA
9	A	837	CLA	C1A-C2A-CAA-CBA
9	B	817	CLA	C1A-C2A-CAA-CBA
9	B	819	CLA	C1A-C2A-CAA-CBA
9	B	826	CLA	C1A-C2A-CAA-CBA
9	B	828	CLA	C1A-C2A-CAA-CBA
9	B	839	CLA	C1A-C2A-CAA-CBA
9	A	836	CLA	O1D-CGD-O2D-CED
9	A	838	CLA	C8-C10-C11-C12
9	A	820	CLA	CBA-CGA-O2A-C1
9	B	811	CLA	C4-C3-C5-C6
9	B	831	CLA	C13-C15-C16-C17
9	A	807	CLA	O1A-CGA-O2A-C1
9	B	801	CLA	C2A-CAA-CBA-CGA
11	A	843	LHG	C4-C5-C6-O8
14	B	837	DGD	O1G-C1G-C2G-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	806	CLA	CBA-CGA-O2A-C1
9	L	304	CLA	O1A-CGA-O2A-C1
11	A	843	LHG	C9-C10-C11-C12
9	B	826	CLA	O1D-CGD-O2D-CED
9	B	810	CLA	C15-C16-C17-C18
11	L	301	LHG	O1-C1-C2-O2
15	B	838	LMT	C4'-C5'-C6'-O6'
9	A	816	CLA	CBA-CGA-O2A-C1
9	B	826	CLA	CBA-CGA-O2A-C1
9	A	849	CLA	C8-C10-C11-C12
9	B	810	CLA	C10-C11-C12-C13
9	B	810	CLA	C13-C15-C16-C17
9	A	809	CLA	C10-C11-C12-C13
11	L	301	LHG	C33-C34-C35-C36
9	A	806	CLA	O1D-CGD-O2D-CED
9	B	816	CLA	O1A-CGA-O2A-C1
9	A	831	CLA	O1D-CGD-O2D-CED
9	B	825	CLA	O1A-CGA-O2A-C1
15	B	838	LMT	C2'-C1'-O1'-C1
11	L	301	LHG	O7-C5-C6-O8
11	L	301	LHG	C16-C17-C18-C19
9	A	806	CLA	O1A-CGA-O2A-C1
9	A	801	CLA	C6-C7-C8-C10
9	A	805	CLA	C6-C7-C8-C10
9	A	807	CLA	C11-C12-C13-C15
9	A	828	CLA	C12-C13-C15-C16
9	A	831	CLA	C6-C7-C8-C10
9	A	836	CLA	C11-C12-C13-C15
9	A	836	CLA	C12-C13-C15-C16
9	A	849	CLA	C6-C7-C8-C10
9	B	801	CLA	C11-C10-C8-C7
9	B	801	CLA	C12-C13-C15-C16
9	B	804	CLA	C11-C12-C13-C15
9	B	806	CLA	C11-C10-C8-C7
9	B	807	CLA	C6-C7-C8-C10
9	B	810	CLA	C6-C7-C8-C10
9	B	814	CLA	C6-C7-C8-C10
9	B	823	CLA	C11-C10-C8-C7
9	B	824	CLA	C6-C7-C8-C10
9	B	829	CLA	C11-C10-C8-C7
9	B	829	CLA	C11-C12-C13-C15
9	A	826	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	820	CLA	O1A-CGA-O2A-C1
9	A	801	CLA	C6-C7-C8-C9
9	A	802	CLA	C11-C10-C8-C9
9	A	807	CLA	C6-C7-C8-C9
9	A	807	CLA	C11-C12-C13-C14
9	A	815	CLA	C11-C10-C8-C9
9	A	817	CLA	C11-C10-C8-C9
9	A	836	CLA	C14-C13-C15-C16
9	A	838	CLA	C11-C10-C8-C9
9	B	801	CLA	C14-C13-C15-C16
9	B	807	CLA	C14-C13-C15-C16
9	B	810	CLA	C6-C7-C8-C9
9	B	818	CLA	C6-C7-C8-C9
9	B	823	CLA	C11-C10-C8-C9
9	B	825	CLA	C6-C7-C8-C9
9	B	829	CLA	C11-C10-C8-C9
9	H	201	CLA	C11-C12-C13-C14
9	B	812	CLA	CBA-CGA-O2A-C1
9	B	832	CLA	CBA-CGA-O2A-C1
12	I	101	BCR	C11-C12-C13-C35
9	A	820	CLA	C4C-C3C-CAC-CBC
11	A	842	LHG	O1-C1-C2-C3
9	A	827	CLA	C15-C16-C17-C18
9	A	850	CLA	C10-C11-C12-C13
9	B	807	CLA	C15-C16-C17-C18
9	A	801	CLA	C4B-C3B-CAB-CBB
9	A	806	CLA	C4B-C3B-CAB-CBB
9	A	813	CLA	C4B-C3B-CAB-CBB
9	A	818	CLA	C4B-C3B-CAB-CBB
9	A	837	CLA	C4B-C3B-CAB-CBB
9	B	803	CLA	C4B-C3B-CAB-CBB
9	B	807	CLA	C4B-C3B-CAB-CBB
9	A	815	CLA	C10-C11-C12-C13
9	B	815	CLA	C15-C16-C17-C18
9	B	827	CLA	O1D-CGD-O2D-CED
9	A	831	CLA	C2C-C3C-CAC-CBC
9	B	818	CLA	C11-C12-C13-C14
9	A	827	CLA	C2A-CAA-CBA-CGA
11	L	301	LHG	C29-C30-C31-C32
9	A	803	CLA	C3A-C2A-CAA-CBA
9	A	837	CLA	C3A-C2A-CAA-CBA
9	B	822	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	L	303	CLA	C3A-C2A-CAA-CBA
15	B	838	LMT	C2-C1-O1'-C1'
9	B	814	CLA	O1D-CGD-O2D-CED
9	A	826	CLA	CBA-CGA-O2A-C1
9	B	829	CLA	C13-C15-C16-C17
11	L	301	LHG	C4-C5-C6-O8
9	B	826	CLA	O1A-CGA-O2A-C1
9	H	201	CLA	C15-C16-C17-C18
9	A	834	CLA	O1D-CGD-O2D-CED
11	L	301	LHG	C11-C10-C9-C8
14	B	837	DGD	C9B-CAB-CBB-CCB
9	A	816	CLA	O1A-CGA-O2A-C1
11	A	842	LHG	O6-C4-C5-O7
9	A	806	CLA	C2B-C3B-CAB-CBB
9	A	813	CLA	C2B-C3B-CAB-CBB
9	A	818	CLA	C2B-C3B-CAB-CBB
9	B	803	CLA	C2B-C3B-CAB-CBB
9	B	807	CLA	C2B-C3B-CAB-CBB
9	B	832	CLA	O1A-CGA-O2A-C1
9	B	840	CLA	O2A-C1-C2-C3
11	L	301	LHG	C12-C13-C14-C15
11	A	842	LHG	O7-C5-C6-O8
11	A	843	LHG	O7-C5-C6-O8
14	B	837	DGD	O2G-C2G-C3G-O3G
9	A	828	CLA	CBD-CGD-O2D-CED
9	B	812	CLA	CBD-CGD-O2D-CED
10	A	840	PQN	C23-C25-C26-C27
9	B	815	CLA	C2-C1-O2A-CGA
9	B	832	CLA	O1D-CGD-O2D-CED
9	A	827	CLA	C11-C12-C13-C14
9	A	828	CLA	C6-C7-C8-C9
9	A	835	CLA	C11-C10-C8-C9
9	A	827	CLA	CBA-CGA-O2A-C1
14	B	837	DGD	C7B-C8B-C9B-CAB
9	B	812	CLA	O1A-CGA-O2A-C1
9	A	807	CLA	C2A-CAA-CBA-CGA
9	B	808	CLA	C2A-CAA-CBA-CGA
12	A	845	BCR	C23-C24-C25-C26
12	A	845	BCR	C23-C24-C25-C30
12	A	846	BCR	C23-C24-C25-C26
12	B	835	BCR	C1-C6-C7-C8
12	B	835	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	B	836	BCR	C1-C6-C7-C8
12	B	836	BCR	C5-C6-C7-C8
12	B	836	BCR	C23-C24-C25-C26
12	B	836	BCR	C23-C24-C25-C30
12	L	302	BCR	C23-C24-C25-C26
12	L	306	BCR	C1-C6-C7-C8
12	L	307	BCR	C5-C6-C7-C8
9	L	305	CLA	O1D-CGD-O2D-CED
12	B	835	BCR	C11-C12-C13-C14
9	A	827	CLA	C10-C11-C12-C13
9	A	835	CLA	C15-C16-C17-C18
9	A	825	CLA	C10-C11-C12-C13
9	B	802	CLA	C10-C11-C12-C13
11	A	842	LHG	O6-C4-C5-C6
9	A	816	CLA	CAA-CBA-CGA-O2A
9	A	805	CLA	C12-C13-C15-C16
9	A	808	CLA	C11-C12-C13-C15
9	A	811	CLA	C6-C7-C8-C10
9	A	816	CLA	C11-C12-C13-C15
9	A	817	CLA	C11-C10-C8-C7
9	A	817	CLA	C11-C12-C13-C15
9	A	827	CLA	C11-C12-C13-C15
9	A	835	CLA	C11-C10-C8-C7
9	A	838	CLA	C11-C10-C8-C7
9	B	807	CLA	C12-C13-C15-C16
9	B	819	CLA	C6-C7-C8-C10
9	B	819	CLA	C11-C10-C8-C7
9	B	824	CLA	C11-C10-C8-C7
9	B	825	CLA	C6-C7-C8-C10
9	B	831	CLA	C12-C13-C15-C16
9	H	201	CLA	C11-C12-C13-C15
12	B	835	BCR	C15-C16-C17-C18
9	B	801	CLA	C16-C17-C18-C20
9	B	822	CLA	CBA-CGA-O2A-C1
9	B	821	CLA	C15-C16-C17-C18
9	A	804	CLA	CAD-CBD-CGD-O2D
9	A	807	CLA	CAD-CBD-CGD-O2D
9	A	818	CLA	CAD-CBD-CGD-O2D
9	A	824	CLA	CAD-CBD-CGD-O2D
9	A	830	CLA	CAD-CBD-CGD-O2D
9	A	834	CLA	CAD-CBD-CGD-O2D
9	L	304	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	837	DGD	CEB-CFB-CGB-CHB
9	B	814	CLA	C10-C11-C12-C13
9	B	818	CLA	C5-C6-C7-C8
11	A	842	LHG	C2-C3-O3-P
11	A	843	LHG	O6-C4-C5-O7
9	A	841	CLA	CAA-CBA-CGA-O2A
9	L	303	CLA	O2A-C1-C2-C3
9	A	841	CLA	CBA-CGA-O2A-C1
9	A	811	CLA	CHA-CBD-CGD-O1D
9	A	811	CLA	CHA-CBD-CGD-O2D
9	A	821	CLA	CHA-CBD-CGD-O1D
9	A	821	CLA	CHA-CBD-CGD-O2D
9	A	825	CLA	CHA-CBD-CGD-O1D
9	A	825	CLA	CHA-CBD-CGD-O2D
9	A	828	CLA	CHA-CBD-CGD-O1D
9	A	828	CLA	CHA-CBD-CGD-O2D
9	B	806	CLA	CHA-CBD-CGD-O1D
9	B	809	CLA	CHA-CBD-CGD-O1D
9	B	811	CLA	CHA-CBD-CGD-O1D
9	B	811	CLA	CHA-CBD-CGD-O2D
9	B	824	CLA	C3-C5-C6-C7
9	A	815	CLA	CBD-CGD-O2D-CED
9	A	826	CLA	O1A-CGA-O2A-C1
9	A	836	CLA	C10-C11-C12-C13
9	A	825	CLA	C13-C15-C16-C17
9	B	806	CLA	O1D-CGD-O2D-CED
9	A	809	CLA	C15-C16-C17-C18
9	A	810	CLA	C6-C7-C8-C9
9	A	805	CLA	C14-C13-C15-C16
9	B	819	CLA	C6-C7-C8-C9
9	B	821	CLA	C11-C12-C13-C14
9	B	832	CLA	C14-C13-C15-C16
9	H	201	CLA	C11-C10-C8-C9
9	A	827	CLA	O1A-CGA-O2A-C1
9	B	822	CLA	O1A-CGA-O2A-C1
9	A	831	CLA	C2A-CAA-CBA-CGA
12	B	834	BCR	C11-C12-C13-C35
12	L	307	BCR	C11-C12-C13-C14
9	B	822	CLA	C1A-C2A-CAA-CBA
9	B	824	CLA	C11-C12-C13-C14
11	L	301	LHG	C3-O3-P-O6
9	A	828	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	809	CLA	C4B-C3B-CAB-CBB
9	A	810	CLA	C4B-C3B-CAB-CBB
9	A	816	CLA	C4B-C3B-CAB-CBB
9	A	830	CLA	C4B-C3B-CAB-CBB
9	A	838	CLA	C4B-C3B-CAB-CBB
9	B	801	CLA	C4B-C3B-CAB-CBB
9	B	809	CLA	C4B-C3B-CAB-CBB
9	B	820	CLA	C4B-C3B-CAB-CBB
9	B	831	CLA	C4B-C3B-CAB-CBB
9	B	832	CLA	C4B-C3B-CAB-CBB
9	B	839	CLA	C4B-C3B-CAB-CBB
11	A	843	LHG	C4-O6-P-O5
11	L	301	LHG	C4-O6-P-O4
9	L	304	CLA	C10-C11-C12-C13
9	B	839	CLA	CBA-CGA-O2A-C1
9	A	815	CLA	O1D-CGD-O2D-CED
9	A	811	CLA	CAD-CBD-CGD-O1D
9	A	825	CLA	CAD-CBD-CGD-O1D
9	B	806	CLA	CAD-CBD-CGD-O1D
9	B	811	CLA	CAD-CBD-CGD-O1D
9	B	825	CLA	CAD-CBD-CGD-O1D
9	A	841	CLA	O1A-CGA-O2A-C1
11	A	842	LHG	C1-C2-C3-O3
9	B	801	CLA	C16-C17-C18-C19
9	A	806	CLA	C12-C13-C15-C16
9	A	807	CLA	C11-C10-C8-C7
9	A	808	CLA	C6-C7-C8-C10
9	A	815	CLA	C11-C12-C13-C15
9	A	817	CLA	C6-C7-C8-C10
9	A	826	CLA	C6-C7-C8-C10
9	B	801	CLA	C11-C12-C13-C15
9	B	814	CLA	C11-C12-C13-C15
9	B	829	CLA	C12-C13-C15-C16
9	B	832	CLA	C11-C10-C8-C7
9	B	832	CLA	C12-C13-C15-C16
9	H	201	CLA	C11-C10-C8-C7
9	L	304	CLA	C6-C7-C8-C10
9	A	801	CLA	CAA-CBA-CGA-O2A
9	A	806	CLA	C10-C11-C12-C13
14	B	837	DGD	O1G-C1G-C2G-O2G
14	B	837	DGD	CEA-CFA-CGA-CHA
9	A	835	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	811	CLA	C13-C15-C16-C17
9	A	831	CLA	C4C-C3C-CAC-CBC
9	B	839	CLA	O1A-CGA-O2A-C1
9	A	811	CLA	CBA-CGA-O2A-C1
9	H	201	CLA	C8-C10-C11-C12
9	A	811	CLA	C6-C7-C8-C9
9	A	823	CLA	C14-C13-C15-C16
9	A	826	CLA	C6-C7-C8-C9
9	B	811	CLA	C11-C12-C13-C14
9	B	831	CLA	C14-C13-C15-C16
9	B	812	CLA	O1D-CGD-O2D-CED
9	B	808	CLA	CBA-CGA-O2A-C1
9	B	804	CLA	C2C-C3C-CAC-CBC
9	A	801	CLA	C2B-C3B-CAB-CBB
9	A	809	CLA	C2B-C3B-CAB-CBB
9	A	830	CLA	C2B-C3B-CAB-CBB
9	A	834	CLA	C2B-C3B-CAB-CBB
9	A	835	CLA	C2B-C3B-CAB-CBB
9	A	837	CLA	C2B-C3B-CAB-CBB
9	A	838	CLA	C2B-C3B-CAB-CBB
9	B	801	CLA	C2B-C3B-CAB-CBB
9	B	809	CLA	C2B-C3B-CAB-CBB
9	B	839	CLA	C2B-C3B-CAB-CBB
9	B	811	CLA	C2-C3-C5-C6
9	A	816	CLA	C5-C6-C7-C8
9	A	820	CLA	C1-C2-C3-C4
9	L	303	CLA	C1-C2-C3-C4
9	A	802	CLA	C2A-CAA-CBA-CGA
9	A	821	CLA	C2A-CAA-CBA-CGA
9	B	823	CLA	C2A-CAA-CBA-CGA
9	A	811	CLA	O1A-CGA-O2A-C1
9	B	808	CLA	O1A-CGA-O2A-C1
14	B	837	DGD	CBA-CCA-CDA-CEA
9	B	822	CLA	C2-C1-O2A-CGA
12	A	846	BCR	C1-C6-C7-C8
12	A	846	BCR	C5-C6-C7-C8
12	A	846	BCR	C23-C24-C25-C30
12	L	302	BCR	C23-C24-C25-C30
12	L	306	BCR	C5-C6-C7-C8
9	A	836	CLA	C16-C17-C18-C19
9	A	835	CLA	O1A-CGA-O2A-C1
11	A	842	LHG	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	842	LHG	O9-C7-O7-C5
9	A	849	CLA	C5-C6-C7-C8
9	A	835	CLA	C4-C3-C5-C6
9	A	849	CLA	C11-C10-C8-C7
9	A	805	CLA	C6-C7-C8-C9
9	A	806	CLA	C14-C13-C15-C16
9	A	815	CLA	C11-C12-C13-C14
9	A	816	CLA	C6-C7-C8-C9
9	A	817	CLA	C6-C7-C8-C9
9	A	824	CLA	C11-C10-C8-C9
9	B	809	CLA	C14-C13-C15-C16
9	B	829	CLA	C14-C13-C15-C16
9	B	832	CLA	C11-C10-C8-C9
10	A	840	PQN	C16-C17-C18-C19
9	B	824	CLA	C11-C12-C13-C15
12	B	836	BCR	C7-C8-C9-C34
12	I	101	BCR	C7-C8-C9-C34
14	B	837	DGD	C5B-C6B-C7B-C8B
11	A	842	LHG	C5-C4-O6-P
9	B	819	CLA	C5-C6-C7-C8
15	B	838	LMT	O5'-C5'-C6'-O6'
9	B	825	CLA	C5-C6-C7-C8
9	B	828	CLA	CBA-CGA-O2A-C1
9	A	834	CLA	C4B-C3B-CAB-CBB
9	A	835	CLA	C4B-C3B-CAB-CBB
9	B	822	CLA	C4B-C3B-CAB-CBB
9	L	304	CLA	C4B-C3B-CAB-CBB
9	B	828	CLA	O1A-CGA-O2A-C1
9	A	808	CLA	C5-C6-C7-C8
9	A	825	CLA	C2-C1-O2A-CGA
9	B	814	CLA	C2-C1-O2A-CGA
9	B	811	CLA	C16-C17-C18-C19
9	A	811	CLA	C2A-CAA-CBA-CGA
9	B	821	CLA	C3A-C2A-CAA-CBA
9	A	823	CLA	C8-C10-C11-C12
14	B	837	DGD	CAB-CBB-CCB-CDB
10	A	840	PQN	C18-C20-C21-C22
9	A	816	CLA	C11-C10-C8-C9
9	A	827	CLA	C11-C10-C8-C9
9	A	815	CLA	C16-C17-C18-C19
9	A	807	CLA	C13-C15-C16-C17
12	B	834	BCR	C11-C10-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	L	302	BCR	C11-C10-C9-C34
9	A	815	CLA	C2A-CAA-CBA-CGA
9	B	815	CLA	C2A-CAA-CBA-CGA
9	A	836	CLA	C16-C17-C18-C20
9	A	815	CLA	CBA-CGA-O2A-C1
9	A	838	CLA	C5-C6-C7-C8
9	A	802	CLA	C1A-C2A-CAA-CBA
9	A	822	CLA	C1A-C2A-CAA-CBA
9	B	806	CLA	C1A-C2A-CAA-CBA
9	B	812	CLA	C1A-C2A-CAA-CBA
9	B	821	CLA	C1A-C2A-CAA-CBA
9	L	303	CLA	C1A-C2A-CAA-CBA
9	A	809	CLA	C11-C12-C13-C15
9	B	809	CLA	C11-C12-C13-C15
9	B	811	CLA	C6-C7-C8-C10
9	B	821	CLA	C11-C12-C13-C15
9	B	823	CLA	C6-C7-C8-C10
10	A	840	PQN	C22-C23-C25-C26
9	A	806	CLA	C5-C6-C7-C8
9	B	813	CLA	CAA-CBA-CGA-O2A
9	A	819	CLA	C2A-CAA-CBA-CGA
9	A	835	CLA	C2-C3-C5-C6
9	A	810	CLA	C2B-C3B-CAB-CBB
9	A	816	CLA	C2B-C3B-CAB-CBB
9	B	818	CLA	C2B-C3B-CAB-CBB
9	B	820	CLA	C2B-C3B-CAB-CBB
9	B	831	CLA	C2B-C3B-CAB-CBB
9	B	832	CLA	C2B-C3B-CAB-CBB
9	L	304	CLA	C2B-C3B-CAB-CBB
9	A	803	CLA	CBA-CGA-O2A-C1
9	B	813	CLA	CAA-CBA-CGA-O1A
10	A	840	PQN	C15-C16-C17-C18
11	A	843	LHG	O9-C7-O7-C5
9	A	815	CLA	O1A-CGA-O2A-C1
9	B	801	CLA	C4-C3-C5-C6
9	A	817	CLA	C2-C1-O2A-CGA
9	A	808	CLA	CAA-CBA-CGA-O2A
9	A	806	CLA	C6-C7-C8-C9
9	B	815	CLA	C6-C7-C8-C9
9	A	823	CLA	C13-C15-C16-C17
9	A	805	CLA	C2A-CAA-CBA-CGA
9	A	829	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	826	CLA	CAA-CBA-CGA-O1A
9	A	803	CLA	O1A-CGA-O2A-C1
12	B	834	BCR	C1-C6-C7-C8
12	L	307	BCR	C23-C24-C25-C30
15	B	838	LMT	C2-C3-C4-C5
12	L	307	BCR	C21-C22-C23-C24
11	A	842	LHG	C10-C11-C12-C13
9	B	811	CLA	C16-C17-C18-C20
9	A	801	CLA	C3-C5-C6-C7
9	A	816	CLA	C3-C5-C6-C7
9	A	807	CLA	C4B-C3B-CAB-CBB
9	B	818	CLA	C4B-C3B-CAB-CBB
9	A	808	CLA	C12-C13-C15-C16
9	B	815	CLA	C6-C7-C8-C10
9	A	837	CLA	C2C-C3C-CAC-CBC
9	A	820	CLA	O2A-C1-C2-C3
9	A	828	CLA	CBA-CGA-O2A-C1
9	B	820	CLA	CAA-CBA-CGA-O2A
11	L	301	LHG	C7-C8-C9-C10
9	A	808	CLA	C6-C7-C8-C9
9	A	816	CLA	C14-C13-C15-C16
9	B	811	CLA	C6-C7-C8-C9
9	B	809	CLA	O1D-CGD-O2D-CED
9	A	802	CLA	C3A-C2A-CAA-CBA
9	B	804	CLA	C3A-C2A-CAA-CBA
9	B	806	CLA	C3A-C2A-CAA-CBA
9	A	802	CLA	CAD-CBD-CGD-O2D
9	A	806	CLA	CAD-CBD-CGD-O2D
9	A	808	CLA	CAD-CBD-CGD-O2D
9	A	816	CLA	CAD-CBD-CGD-O2D
9	B	805	CLA	CAD-CBD-CGD-O2D
9	B	815	CLA	CAD-CBD-CGD-O2D
9	B	820	CLA	CAD-CBD-CGD-O2D
9	B	821	CLA	CAD-CBD-CGD-O2D
9	B	826	CLA	CAD-CBD-CGD-O2D
9	B	827	CLA	CAD-CBD-CGD-O2D
9	B	829	CLA	CAD-CBD-CGD-O2D
9	B	830	CLA	CAD-CBD-CGD-O2D
9	B	831	CLA	CAD-CBD-CGD-O2D
9	H	201	CLA	CAD-CBD-CGD-O2D
9	L	303	CLA	CAD-CBD-CGD-O2D
9	A	815	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	838	CLA	C2-C1-O2A-CGA
9	A	849	CLA	C2-C1-O2A-CGA
9	A	818	CLA	CAA-CBA-CGA-O2A
9	B	832	CLA	C15-C16-C17-C18
9	A	807	CLA	C4-C3-C5-C6
9	A	825	CLA	C4-C3-C5-C6
9	B	821	CLA	C16-C17-C18-C19
9	B	807	CLA	CAA-CBA-CGA-O2A
9	B	811	CLA	CAA-CBA-CGA-O2A
14	B	837	DGD	C1G-C2G-C3G-O3G
9	A	831	CLA	C15-C16-C17-C18
9	A	807	CLA	O2A-C1-C2-C3
9	A	829	CLA	O2A-C1-C2-C3
9	A	838	CLA	O2A-C1-C2-C3
9	A	850	CLA	O2A-C1-C2-C3
9	B	804	CLA	O2A-C1-C2-C3
9	B	811	CLA	O2A-C1-C2-C3
11	L	301	LHG	C11-C12-C13-C14
9	A	831	CLA	CAA-CBA-CGA-O2A
9	A	809	CLA	CHA-CBD-CGD-O2D
9	A	818	CLA	CHA-CBD-CGD-O2D
9	A	829	CLA	CHA-CBD-CGD-O1D
9	A	829	CLA	CHA-CBD-CGD-O2D
9	A	831	CLA	CHA-CBD-CGD-O1D
9	A	831	CLA	CHA-CBD-CGD-O2D
9	A	841	CLA	CHA-CBD-CGD-O1D
9	A	841	CLA	CHA-CBD-CGD-O2D
9	B	806	CLA	CHA-CBD-CGD-O2D
9	B	814	CLA	CHA-CBD-CGD-O1D
9	B	816	CLA	CHA-CBD-CGD-O1D
9	B	816	CLA	CHA-CBD-CGD-O2D
9	A	834	CLA	CAA-CBA-CGA-O2A
9	B	819	CLA	CAA-CBA-CGA-O2A
12	A	846	BCR	C16-C17-C18-C19
12	B	834	BCR	C11-C10-C9-C8
12	B	834	BCR	C20-C21-C22-C23
12	L	302	BCR	C11-C10-C9-C8
9	B	805	CLA	CAA-CBA-CGA-O2A
9	A	828	CLA	O1A-CGA-O2A-C1
9	A	831	CLA	C13-C15-C16-C17
9	A	805	CLA	C15-C16-C17-C18
9	A	809	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	A	842	LHG	O1-C1-C2-O2
9	A	806	CLA	C6-C7-C8-C10
9	A	823	CLA	C11-C12-C13-C15
9	A	825	CLA	C2-C3-C5-C6
11	A	843	LHG	O7-C7-C8-C9
14	B	837	DGD	O2G-C1B-C2B-C3B
9	A	818	CLA	CAA-CBA-CGA-O1A
9	B	803	CLA	C14-C13-C15-C16
9	B	822	CLA	C2B-C3B-CAB-CBB
9	B	820	CLA	CAA-CBA-CGA-O1A
9	A	850	CLA	C16-C17-C18-C20
9	A	834	CLA	CAA-CBA-CGA-O1A
9	B	807	CLA	CAA-CBA-CGA-O1A
9	A	804	CLA	C1A-C2A-CAA-CBA
9	A	811	CLA	C1A-C2A-CAA-CBA
9	A	814	CLA	C1A-C2A-CAA-CBA
9	A	821	CLA	C1A-C2A-CAA-CBA
9	A	841	CLA	C1A-C2A-CAA-CBA
9	B	802	CLA	C1A-C2A-CAA-CBA
9	B	804	CLA	C1A-C2A-CAA-CBA
9	B	802	CLA	C8-C10-C11-C12
11	A	842	LHG	C15-C16-C17-C18
9	B	832	CLA	C2-C1-O2A-CGA
9	A	831	CLA	CAA-CBA-CGA-O1A
11	A	842	LHG	C4-C5-C6-O8
9	B	809	CLA	CBD-CGD-O2D-CED
11	A	843	LHG	O9-C7-C8-C9
9	A	819	CLA	C13-C15-C16-C17
9	B	811	CLA	CAA-CBA-CGA-O1A
9	A	839	CLA	C4B-C3B-CAB-CBB
9	A	816	CLA	C16-C17-C18-C20
9	B	819	CLA	CAA-CBA-CGA-O1A
11	A	843	LHG	O6-C4-C5-C6
14	B	837	DGD	CFA-CGA-CHA-CIA
9	B	805	CLA	CAA-CBA-CGA-O1A
9	A	816	CLA	CAA-CBA-CGA-O1A
9	A	850	CLA	C5-C6-C7-C8
9	A	838	CLA	C13-C15-C16-C17
9	B	821	CLA	C16-C17-C18-C20
9	A	809	CLA	CAD-CBD-CGD-O1D
9	A	821	CLA	C2-C3-C5-C6
9	B	814	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	836	CLA	C8-C10-C11-C12
9	A	811	CLA	C11-C12-C13-C14
9	A	823	CLA	C11-C12-C13-C14
9	B	809	CLA	C11-C12-C13-C14
9	B	829	CLA	C11-C12-C13-C14
9	B	826	CLA	CAA-CBA-CGA-O2A
9	A	824	CLA	C11-C10-C8-C7
9	B	803	CLA	C12-C13-C15-C16
9	B	821	CLA	C6-C7-C8-C10
9	B	840	CLA	CAA-CBA-CGA-O1A
9	B	803	CLA	CAA-CBA-CGA-O2A
9	B	822	CLA	CAA-CBA-CGA-O2A
9	B	840	CLA	CAA-CBA-CGA-O2A
9	H	201	CLA	CAA-CBA-CGA-O2A
12	A	845	BCR	C19-C20-C21-C22
9	A	823	CLA	CAA-CBA-CGA-O2A
9	B	802	CLA	CAA-CBA-CGA-O2A
9	B	824	CLA	CAA-CBA-CGA-O2A
9	B	807	CLA	C5-C6-C7-C8
9	B	826	CLA	CAA-CBA-CGA-O1A
9	A	833	CLA	CAA-CBA-CGA-O2A
9	B	829	CLA	C8-C10-C11-C12
9	B	823	CLA	C8-C10-C11-C12

There are no ring outliers.

93 monomers are involved in 308 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	846	BCR	3	0
9	B	829	CLA	8	0
9	A	825	CLA	5	0
9	A	828	CLA	4	0
9	A	814	CLA	1	0
9	B	826	CLA	1	0
9	A	824	CLA	1	0
12	B	835	BCR	3	0
9	A	801	CLA	5	0
9	L	305	CLA	1	0
9	B	828	CLA	1	0
9	A	816	CLA	6	0
9	B	822	CLA	3	0
9	A	831	CLA	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	824	CLA	7	0
9	A	830	CLA	3	0
9	A	834	CLA	4	0
9	B	803	CLA	5	0
9	A	808	CLA	2	0
9	L	303	CLA	2	0
9	A	812	CLA	2	0
9	A	820	CLA	2	0
9	B	819	CLA	5	0
9	A	822	CLA	2	0
9	A	833	CLA	1	0
9	A	839	CLA	3	0
9	A	817	CLA	6	0
9	L	304	CLA	8	0
12	L	302	BCR	2	0
11	A	843	LHG	2	0
9	B	831	CLA	9	0
9	B	802	CLA	7	0
9	B	825	CLA	7	0
9	B	809	CLA	7	0
9	A	827	CLA	3	0
9	H	201	CLA	2	0
15	B	838	LMT	3	0
9	A	811	CLA	4	0
12	I	101	BCR	2	0
9	B	810	CLA	4	0
9	B	820	CLA	1	0
9	B	821	CLA	4	0
9	B	801	CLA	10	0
9	B	817	CLA	3	0
9	A	818	CLA	1	0
9	A	807	CLA	5	0
11	L	301	LHG	9	0
9	A	805	CLA	2	0
12	A	845	BCR	2	0
9	A	823	CLA	4	0
9	B	811	CLA	5	0
9	A	835	CLA	5	0
9	A	803	CLA	1	0
9	B	818	CLA	5	0
9	B	830	CLA	4	0
9	A	806	CLA	2	0

Continued on next page...

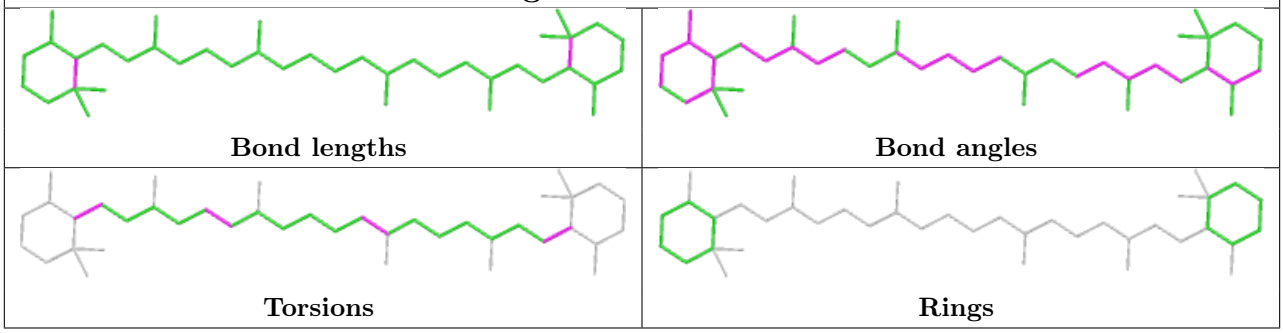
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	306	BCR	6	0
12	A	847	BCR	3	0
12	L	308	BCR	1	0
9	B	823	CLA	3	0
9	B	827	CLA	2	0
13	C	101	SF4	1	0
9	A	836	CLA	2	0
12	B	834	BCR	1	0
9	A	810	CLA	1	0
9	B	808	CLA	2	0
10	B	833	PQN	4	0
9	B	807	CLA	5	0
9	B	805	CLA	2	0
9	A	802	CLA	6	0
9	A	804	CLA	6	0
9	B	806	CLA	5	0
9	B	812	CLA	3	0
9	A	841	CLA	1	0
12	B	836	BCR	3	0
14	B	837	DGD	8	0
9	A	849	CLA	4	0
10	A	840	PQN	5	0
12	L	307	BCR	6	0
9	B	832	CLA	9	0
9	B	814	CLA	6	0
9	A	838	CLA	4	0
9	A	837	CLA	1	0
9	A	832	CLA	1	0
9	B	815	CLA	6	0
9	B	804	CLA	10	0
9	A	815	CLA	2	0
12	A	844	BCR	2	0
9	A	826	CLA	11	0
9	A	829	CLA	1	0
13	C	102	SF4	1	0
9	A	821	CLA	1	0
9	A	850	CLA	5	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.

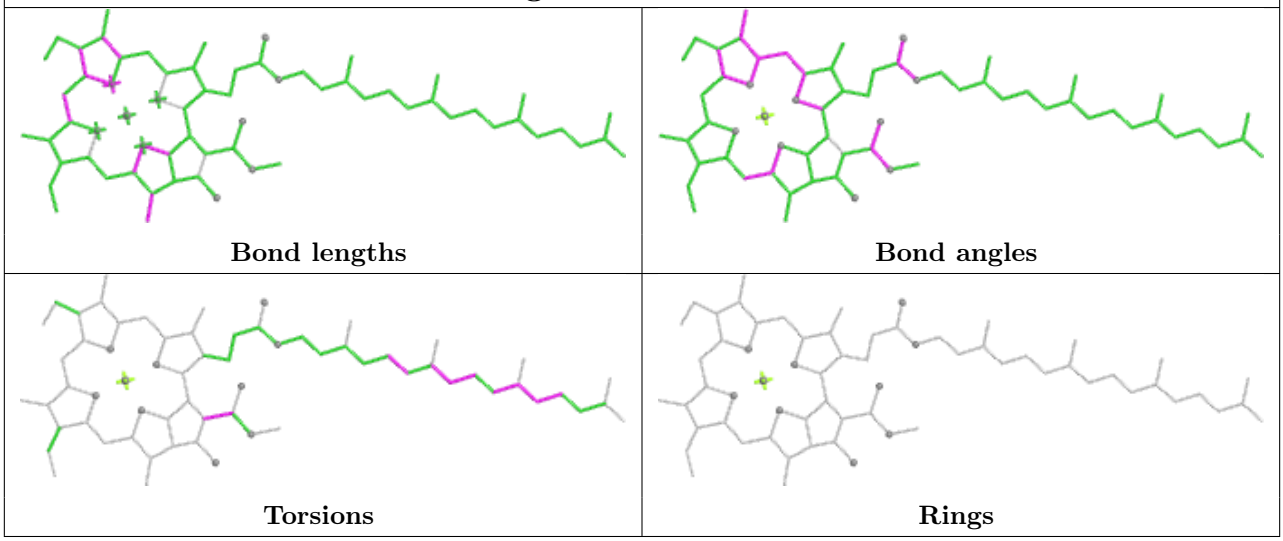
Ligand BCR A 846



Bond lengths | **Bond angles**

Torsions | **Rings**

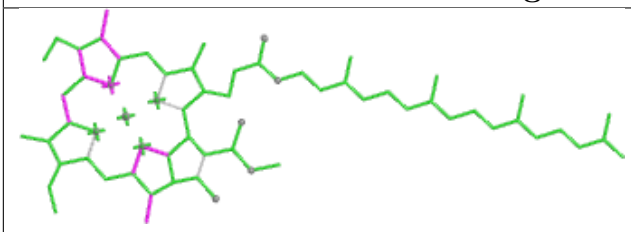
Ligand CLA B 829



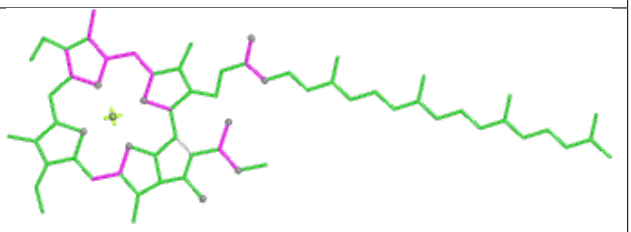
Bond lengths | **Bond angles**

Torsions | **Rings**

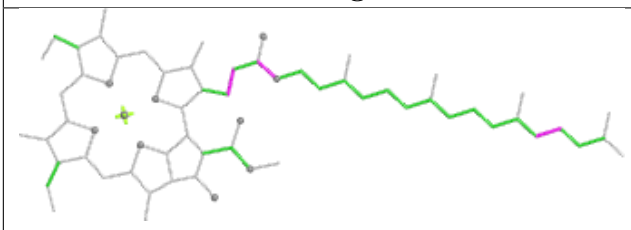
Ligand CLA A 819



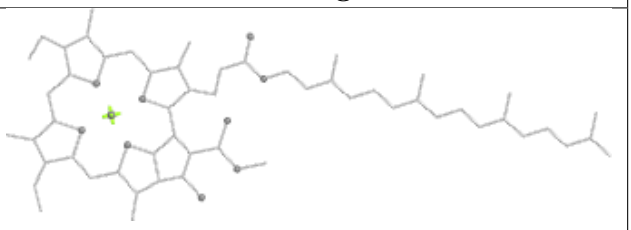
Bond lengths



Bond angles

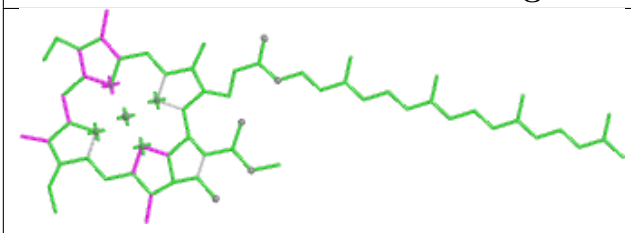


Torsions

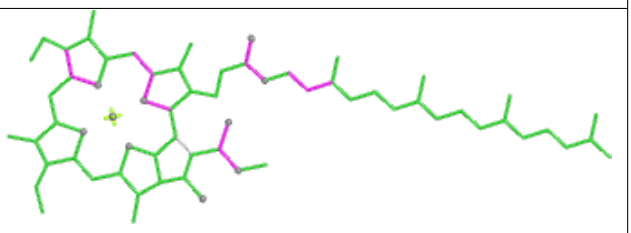


Rings

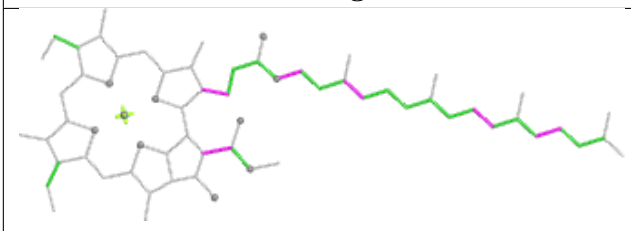
Ligand CLA A 825



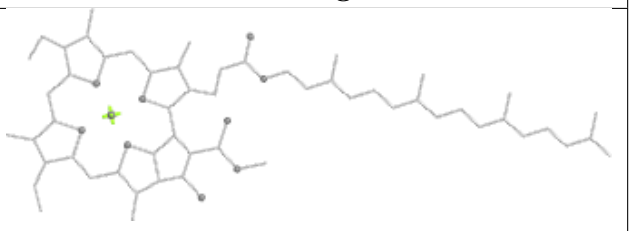
Bond lengths



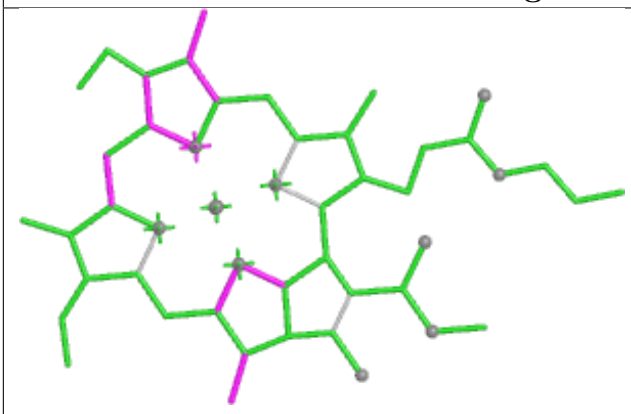
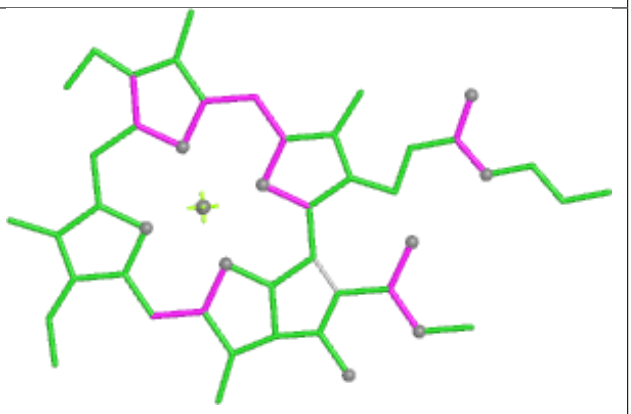
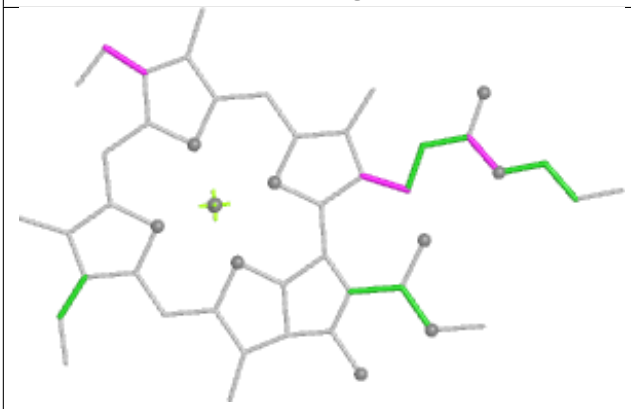
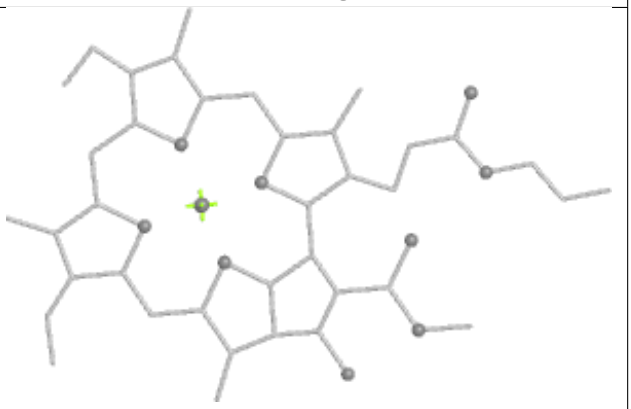
Bond angles

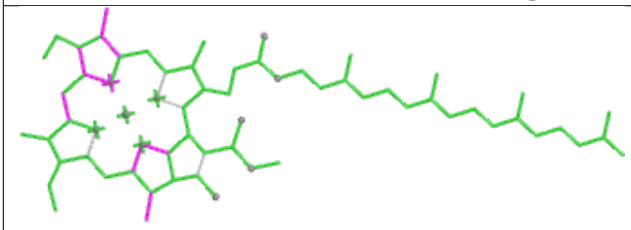
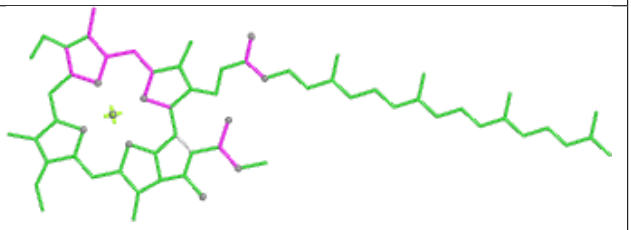
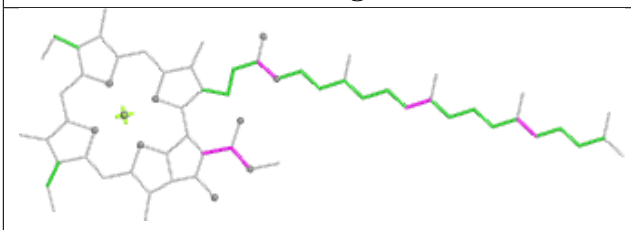
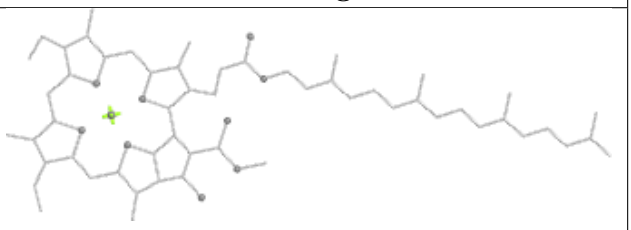


Torsions

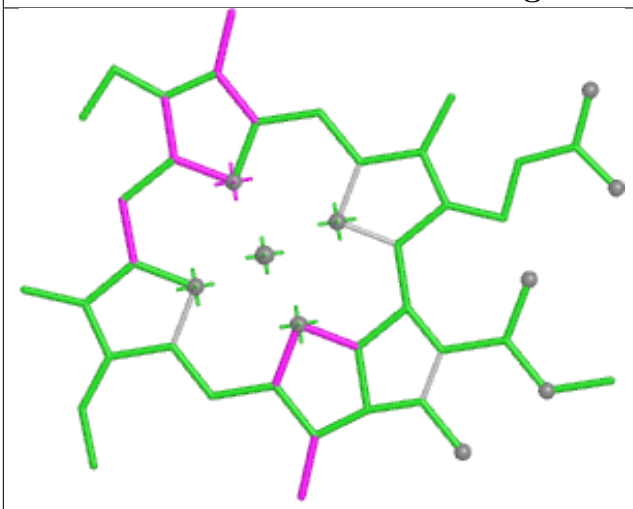


Rings

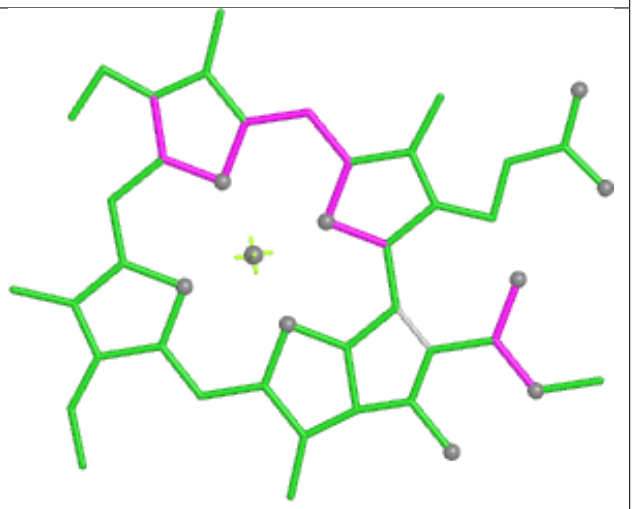
Ligand CLA B 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

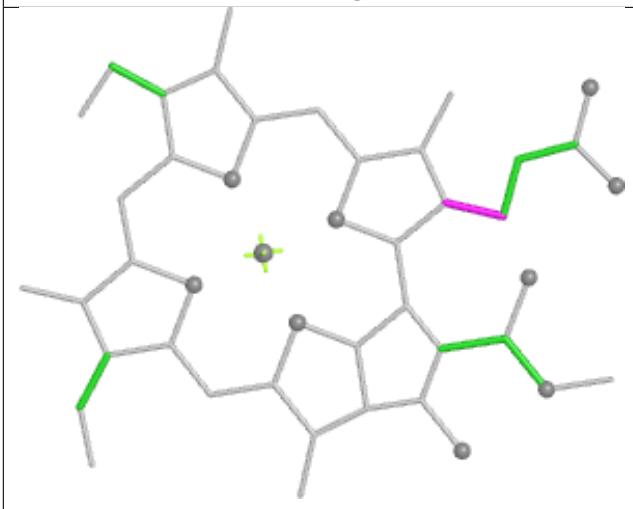
Ligand CLA A 814



Bond lengths



Bond angles

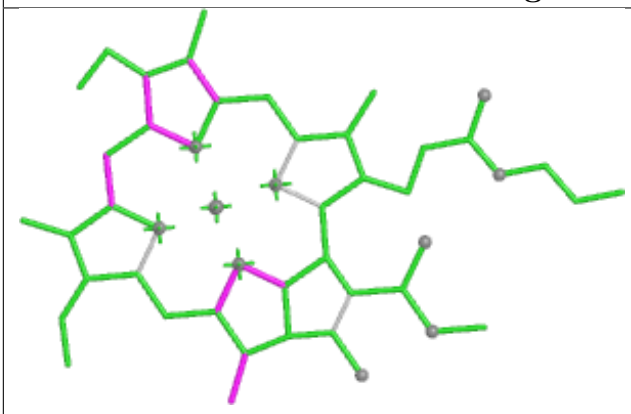


Torsions

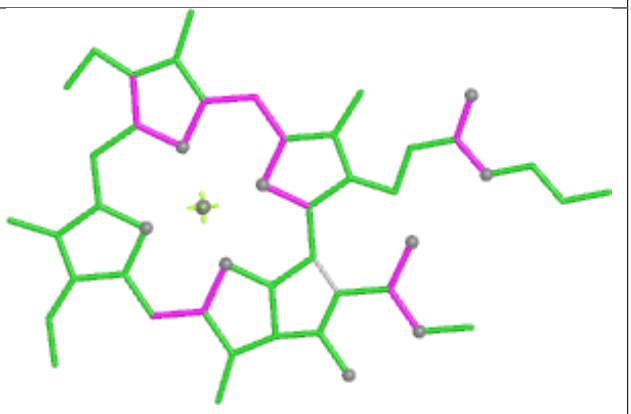


Rings

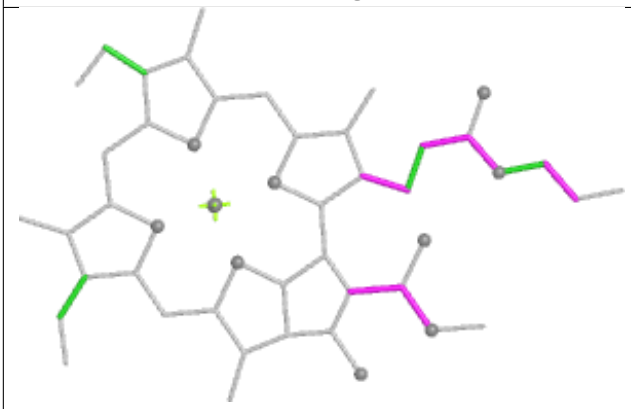
Ligand CLA B 826



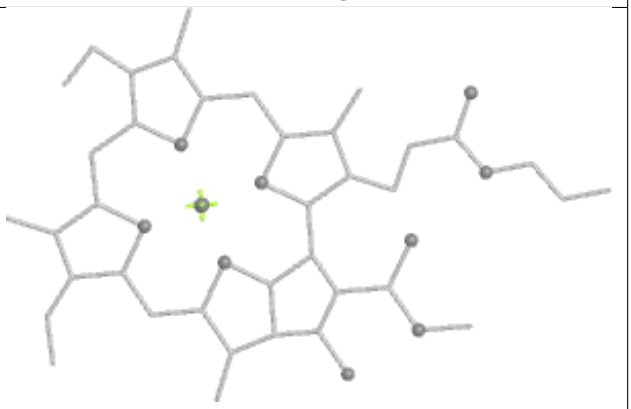
Bond lengths



Bond angles

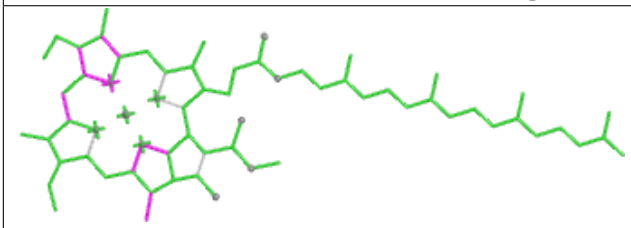


Torsions

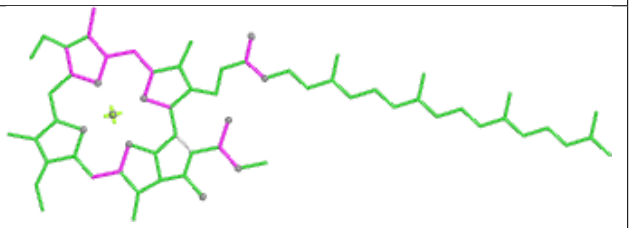


Rings

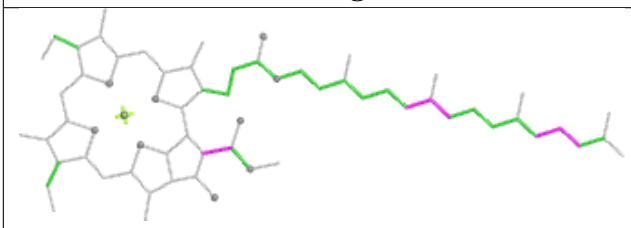
Ligand CLA A 824



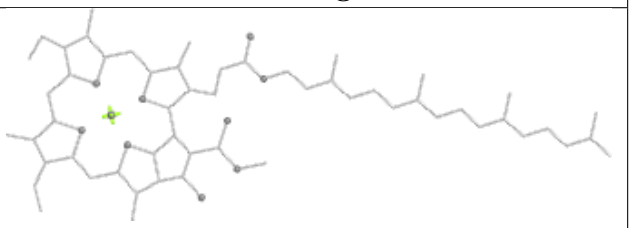
Bond lengths



Bond angles

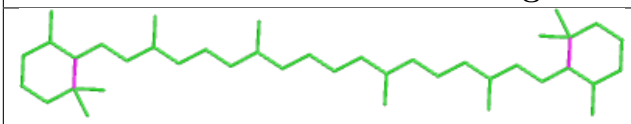


Torsions

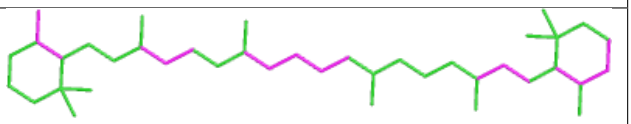


Rings

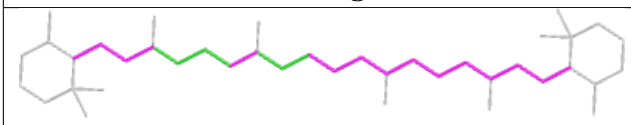
Ligand BCR B 835



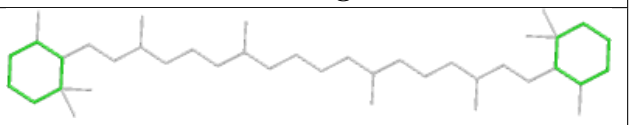
Bond lengths



Bond angles

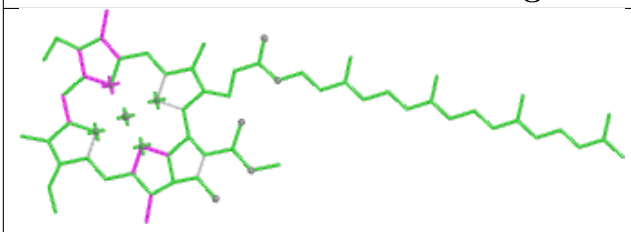


Torsions

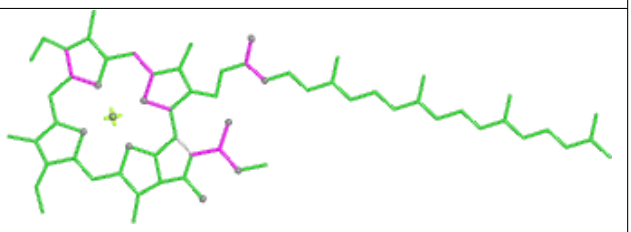


Rings

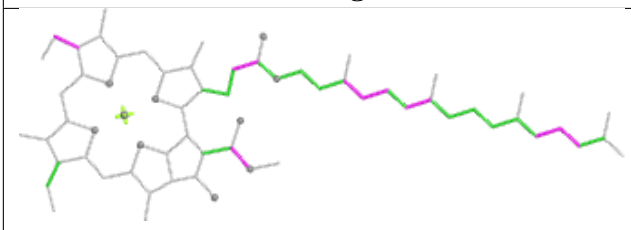
Ligand CLA A 801



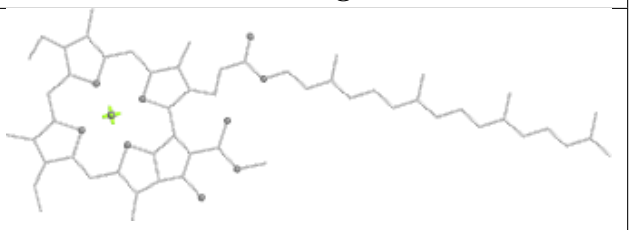
Bond lengths



Bond angles

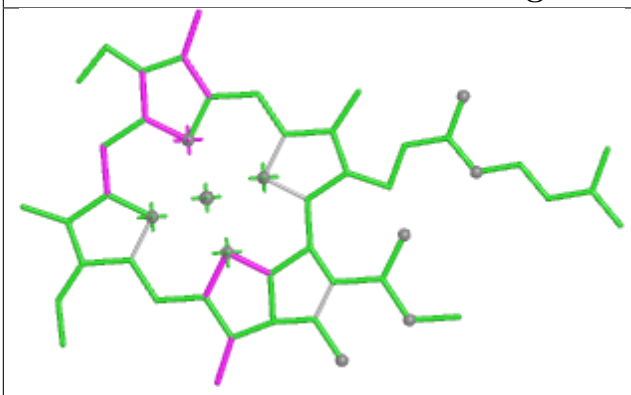


Torsions

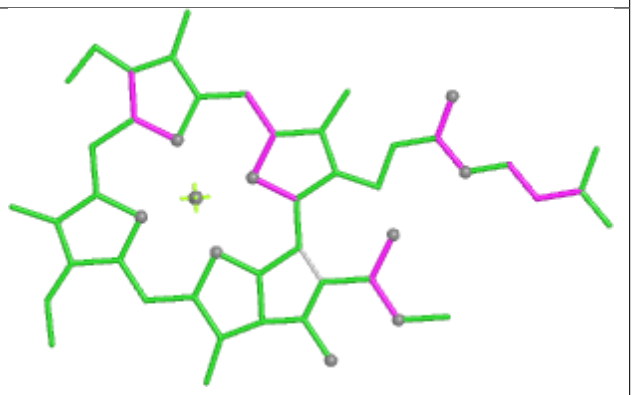


Rings

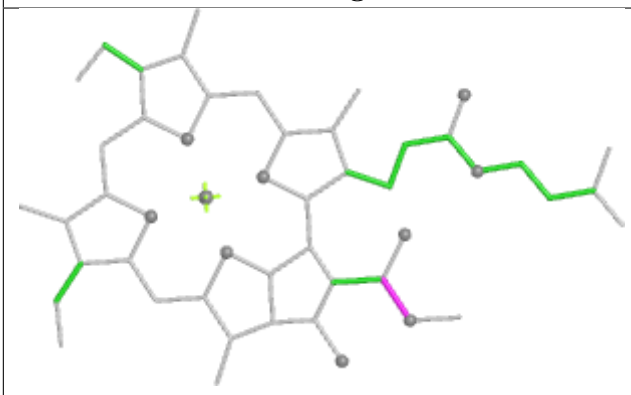
Ligand CLA L 305



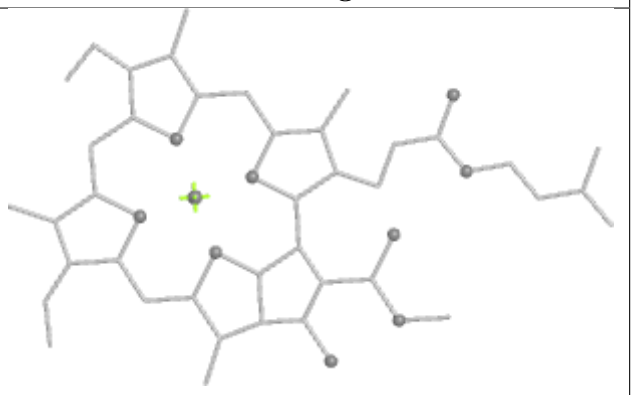
Bond lengths



Bond angles

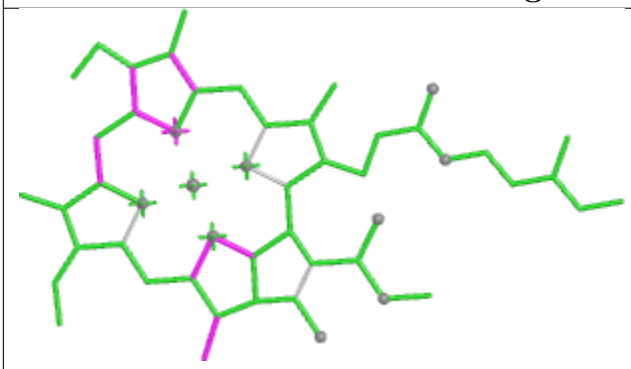


Torsions

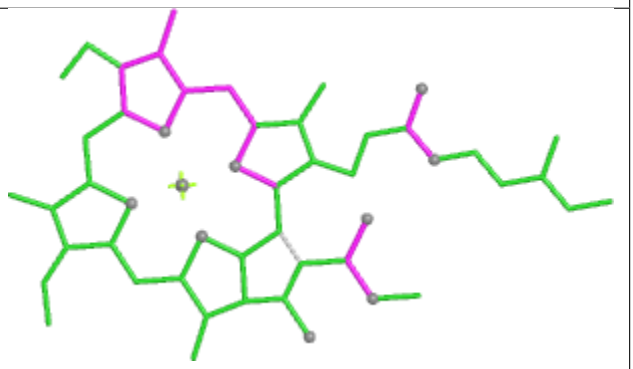


Rings

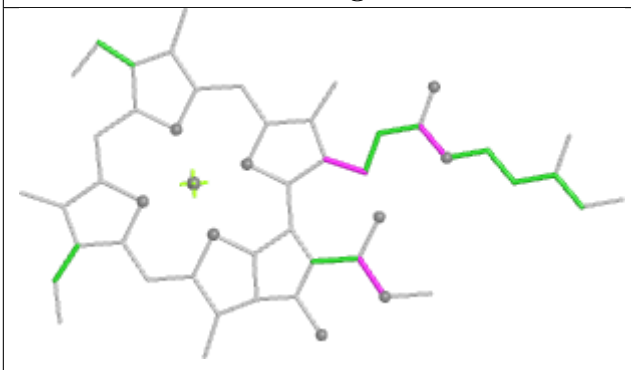
Ligand CLA B 828



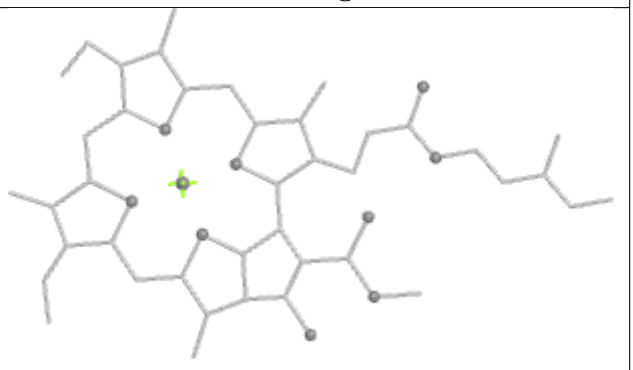
Bond lengths



Bond angles

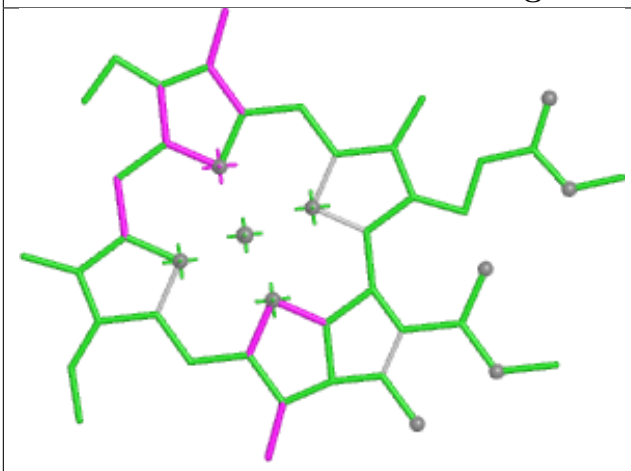


Torsions

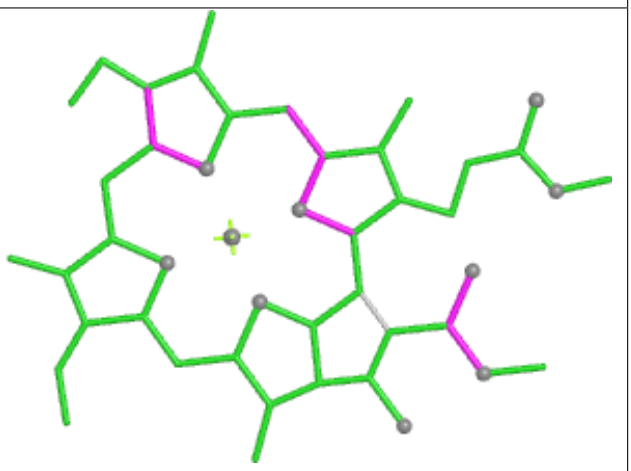


Rings

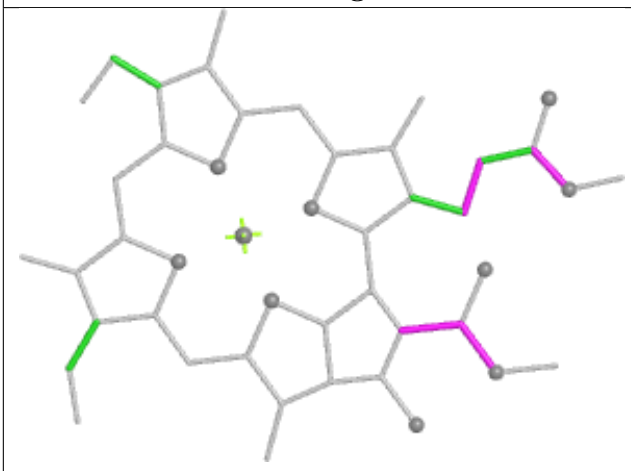
Ligand CLA B 816



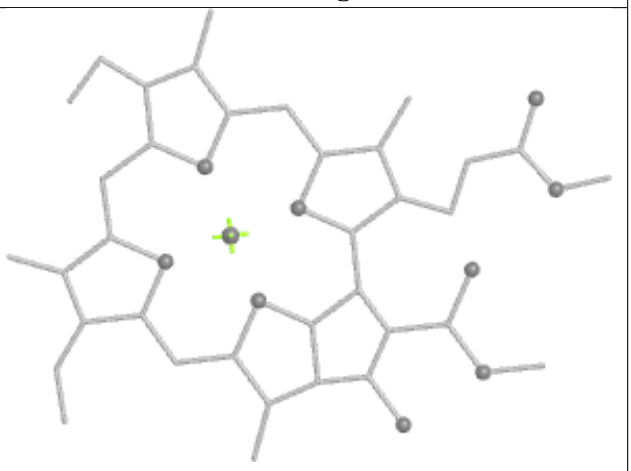
Bond lengths



Bond angles

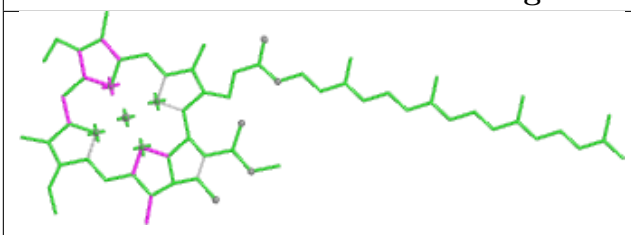


Torsions

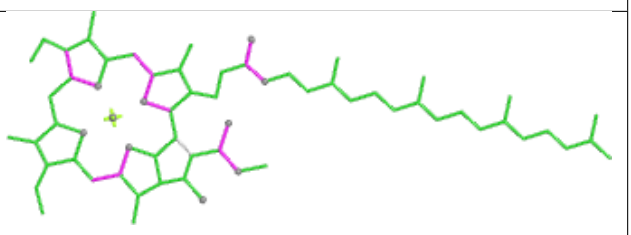


Rings

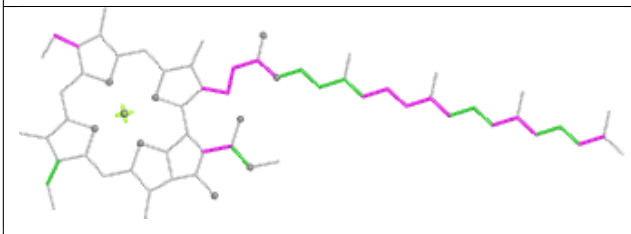
Ligand CLA A 816



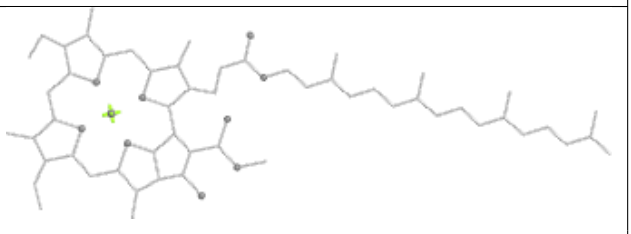
Bond lengths



Bond angles

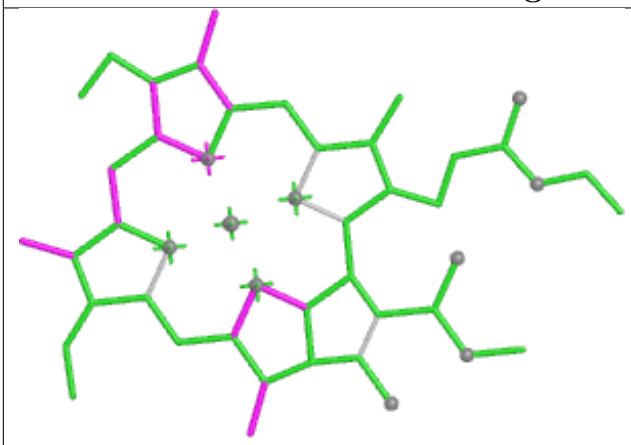


Torsions

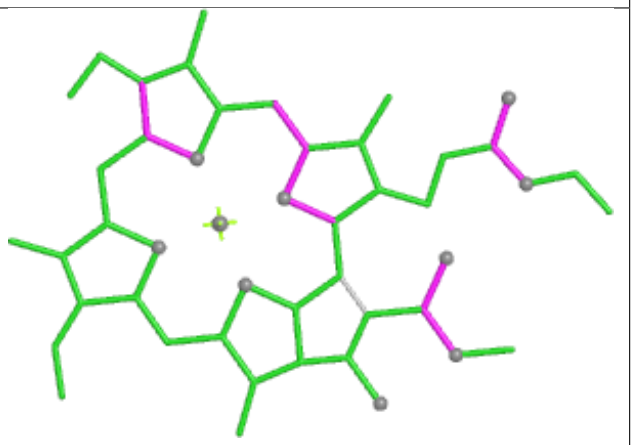


Rings

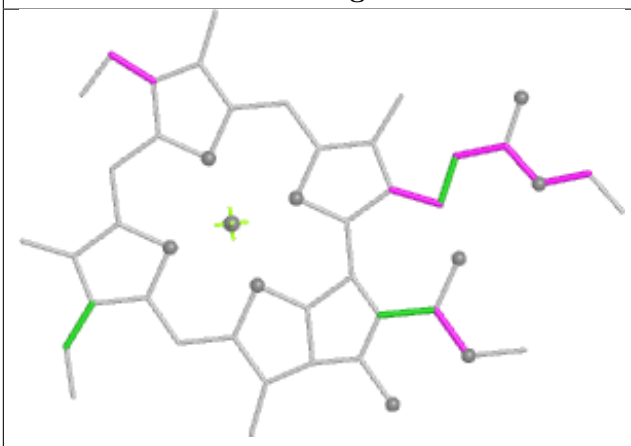
Ligand CLA B 822



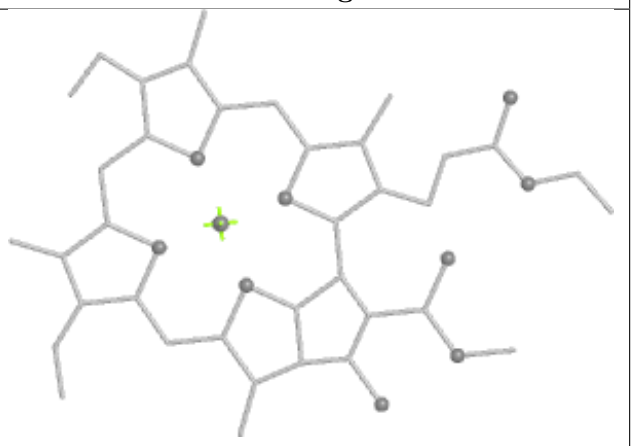
Bond lengths



Bond angles

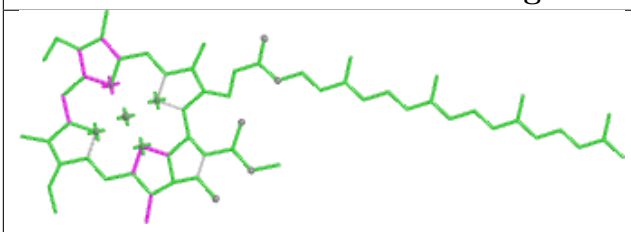


Torsions

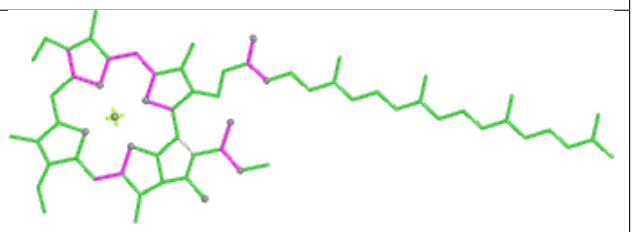


Rings

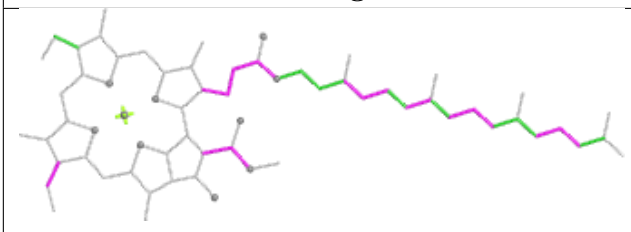
Ligand CLA A 831



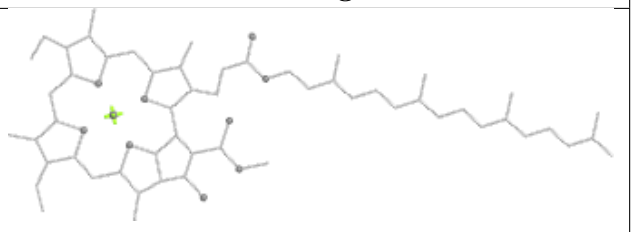
Bond lengths



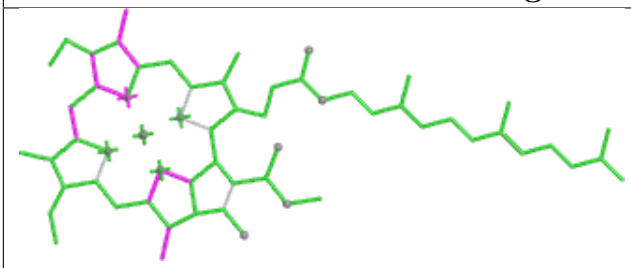
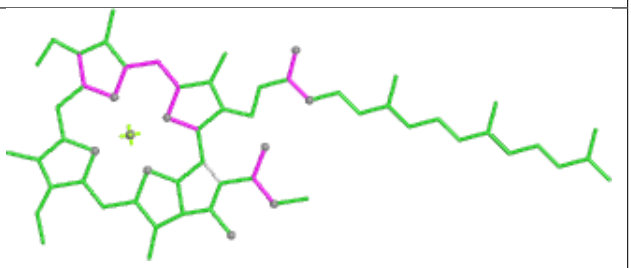
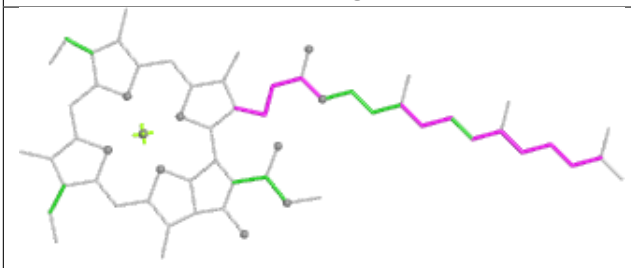
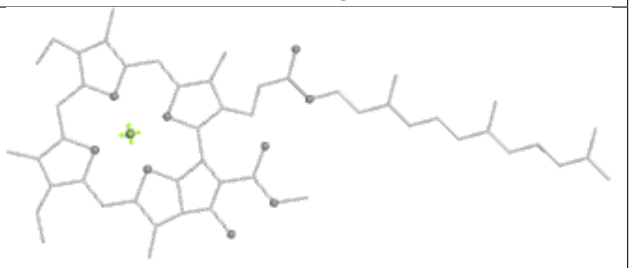
Bond angles

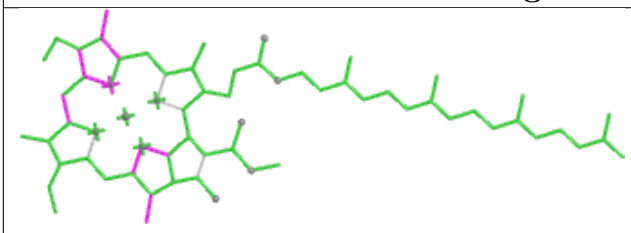
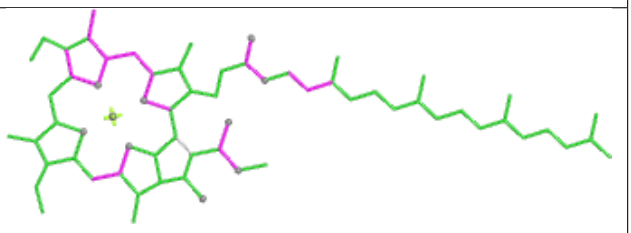
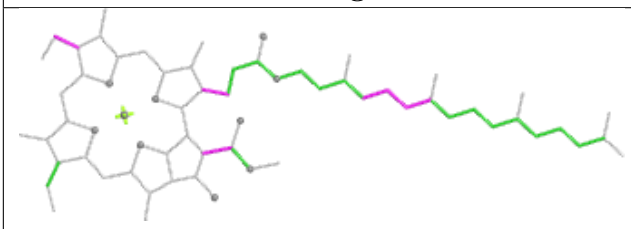
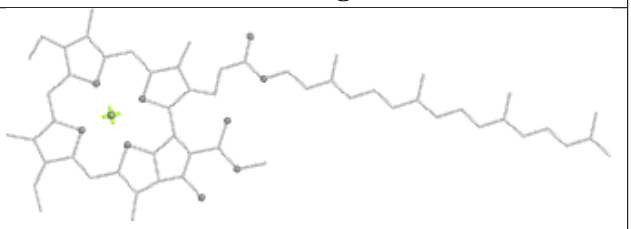


Torsions

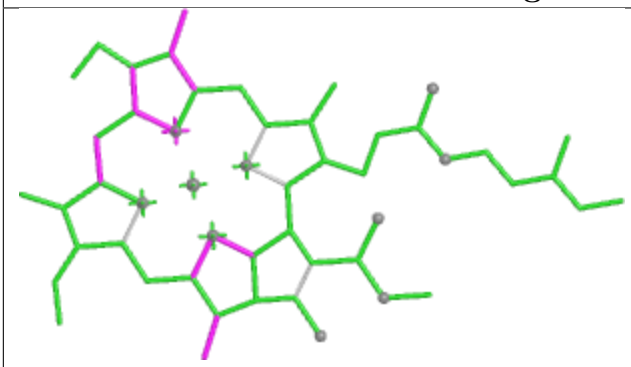


Rings

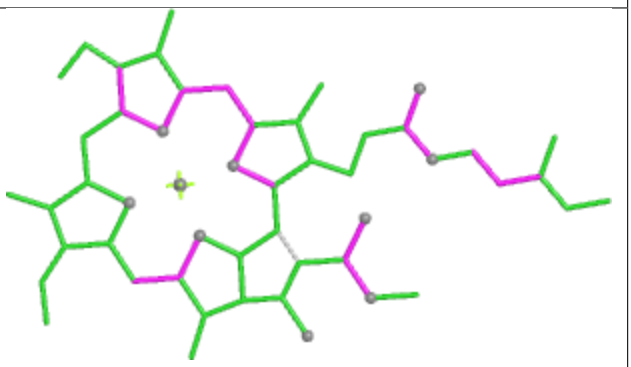
Ligand CLA B 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

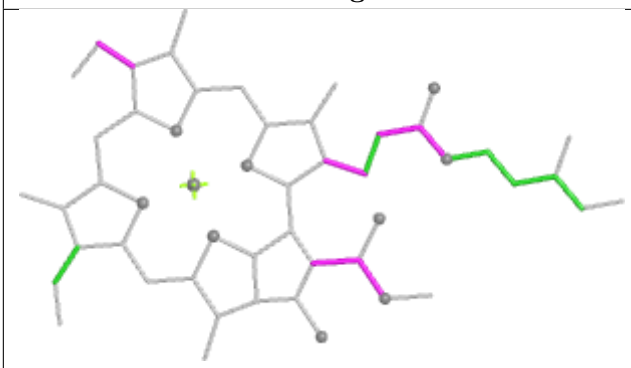
Ligand CLA A 834



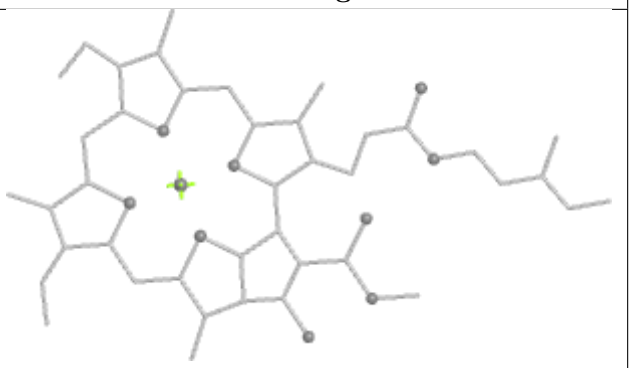
Bond lengths



Bond angles

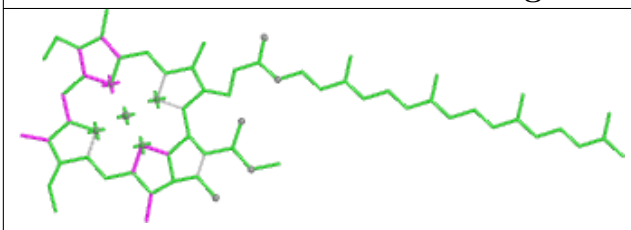


Torsions

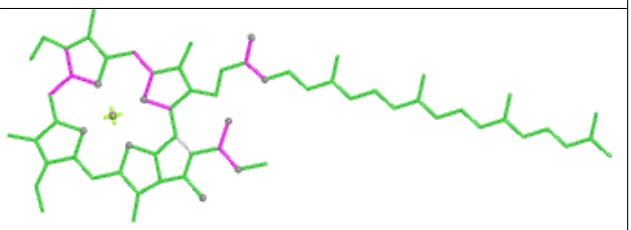


Rings

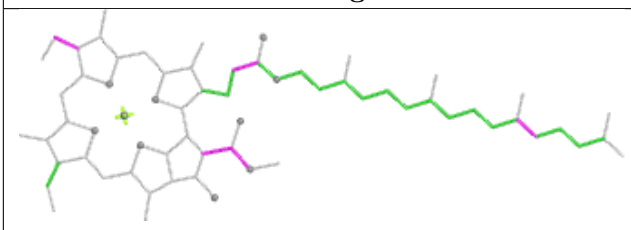
Ligand CLA B 803



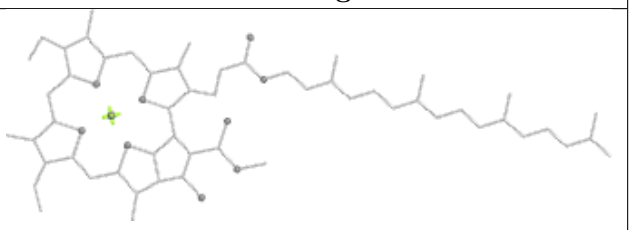
Bond lengths



Bond angles

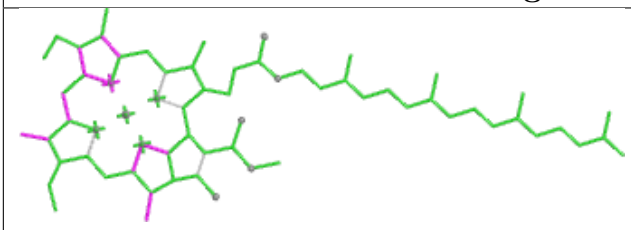


Torsions

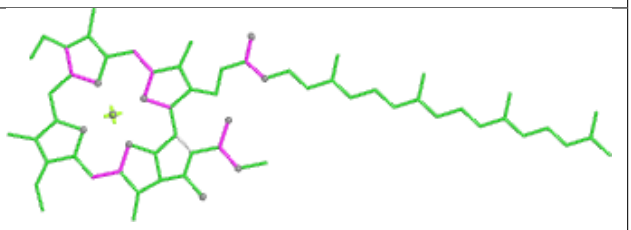


Rings

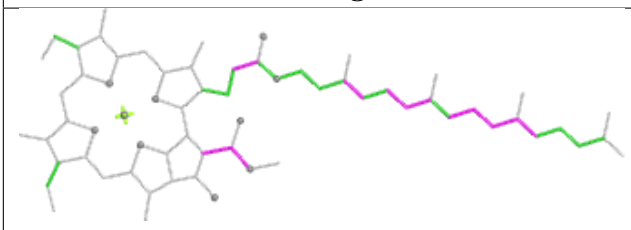
Ligand CLA A 808



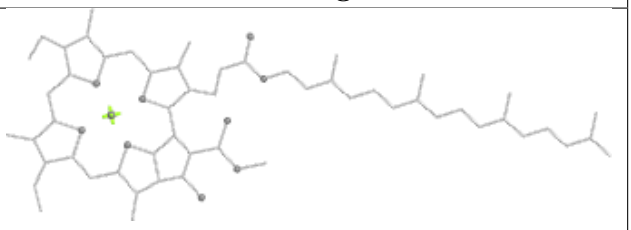
Bond lengths



Bond angles

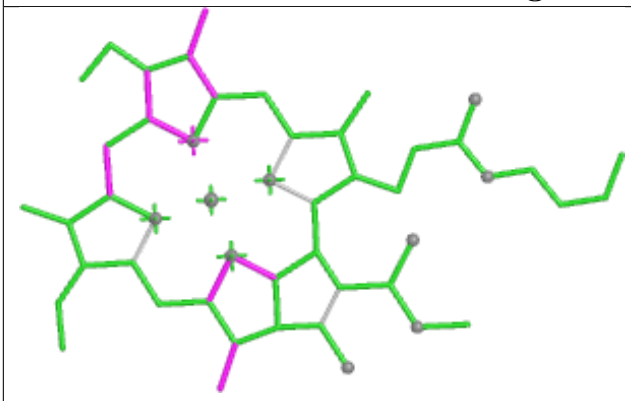


Torsions

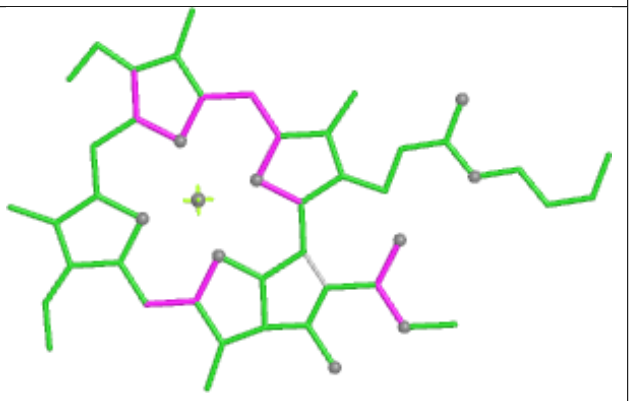


Rings

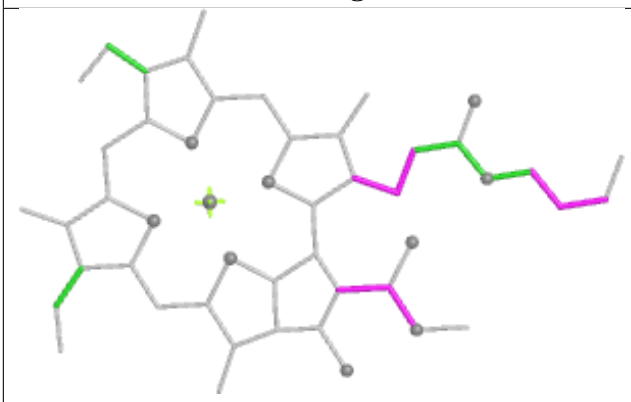
Ligand CLA L 303



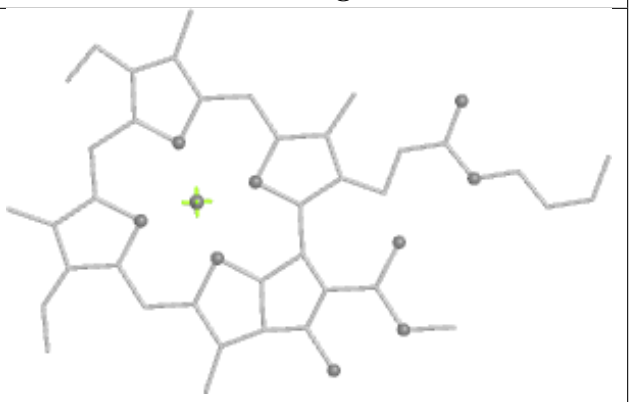
Bond lengths



Bond angles

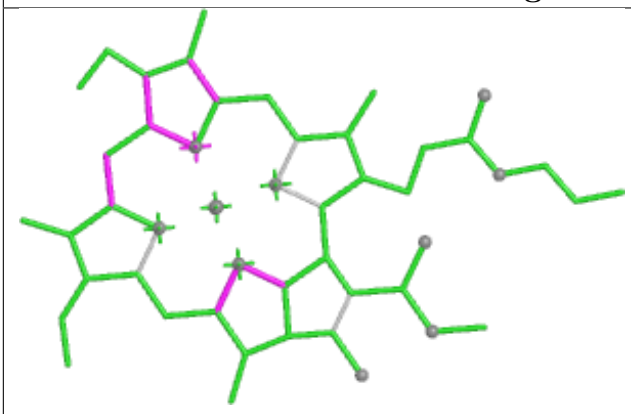


Torsions

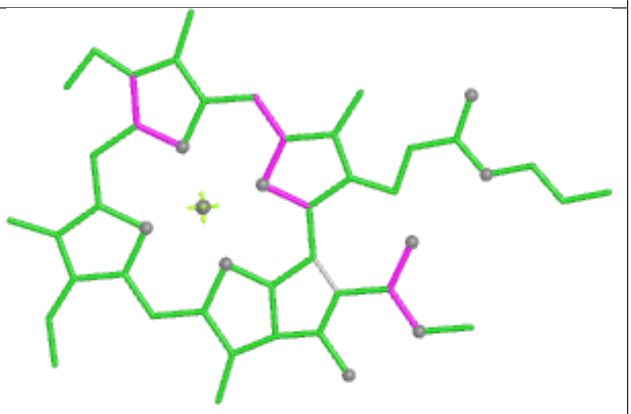


Rings

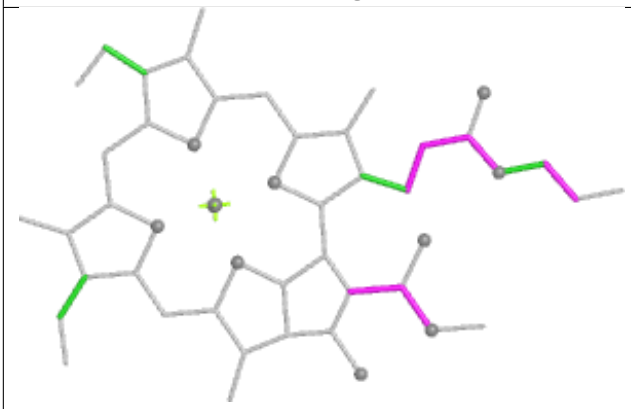
Ligand CLA B 840



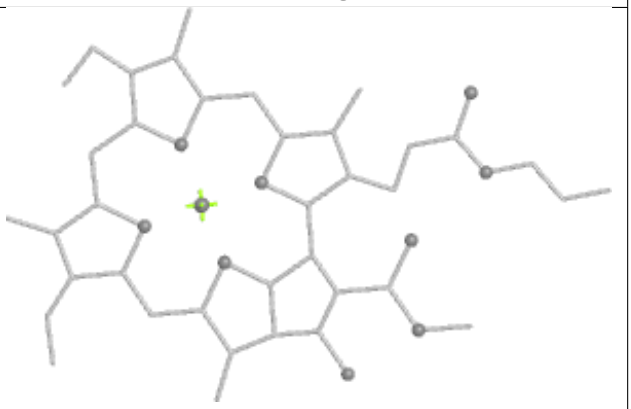
Bond lengths



Bond angles

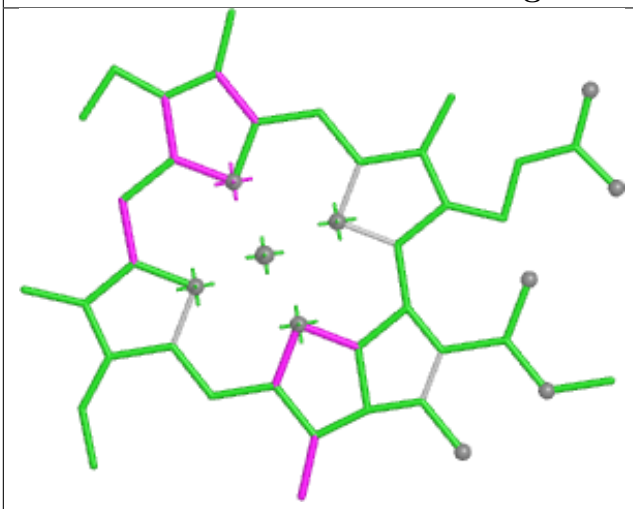


Torsions

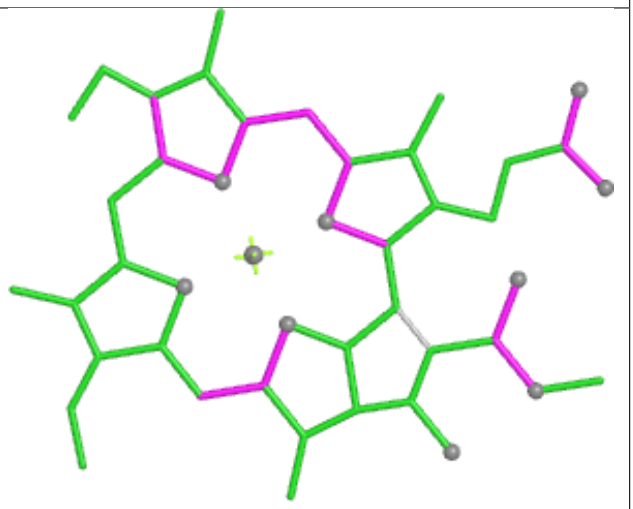


Rings

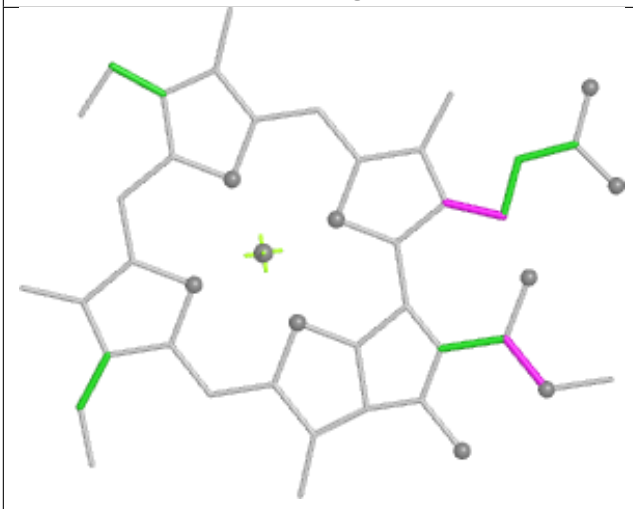
Ligand CLA A 812



Bond lengths



Bond angles

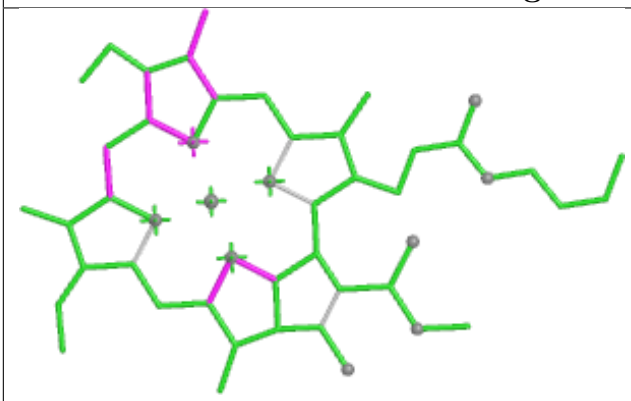


Torsions

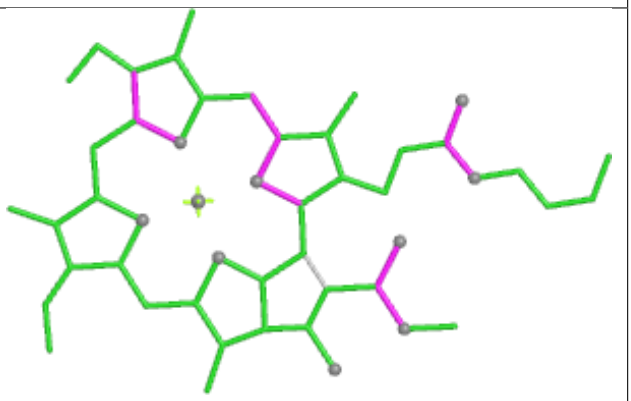


Rings

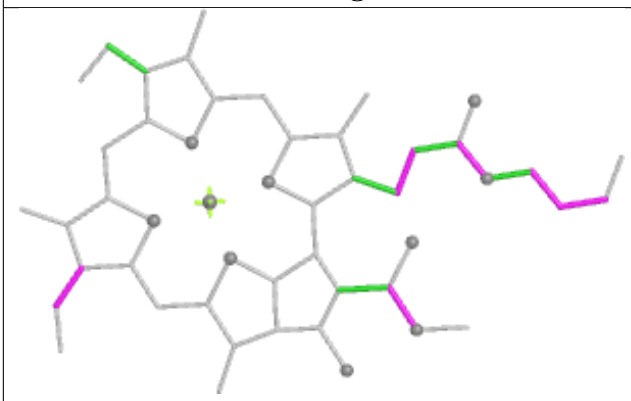
Ligand CLA A 820



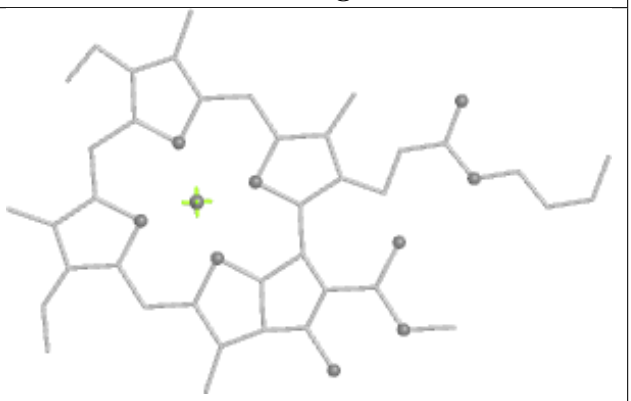
Bond lengths



Bond angles

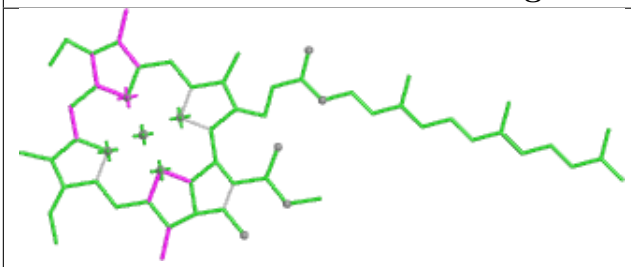


Torsions

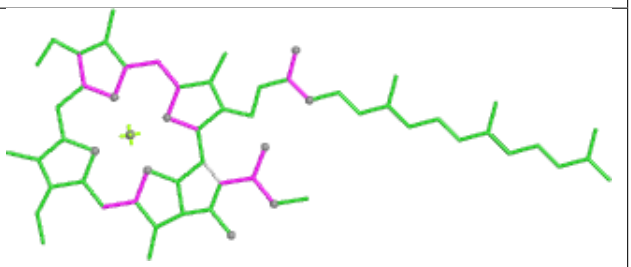


Rings

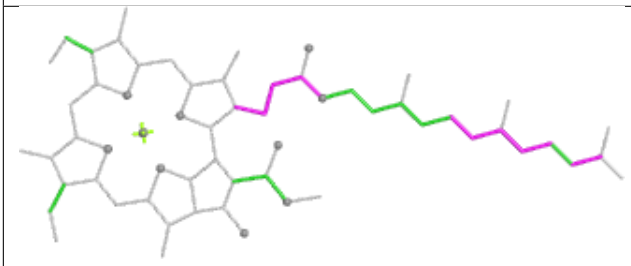
Ligand CLA B 819



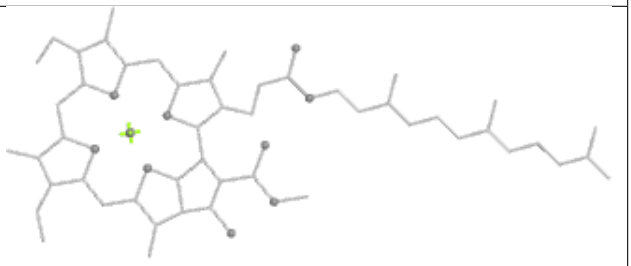
Bond lengths



Bond angles

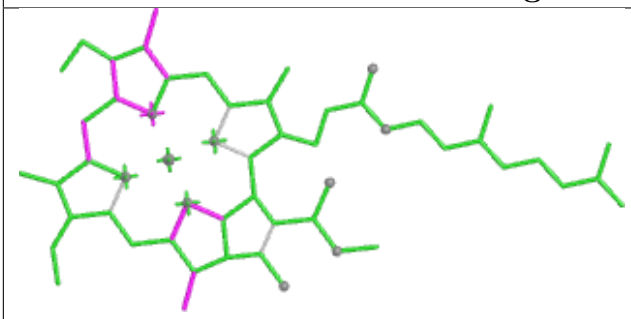


Torsions

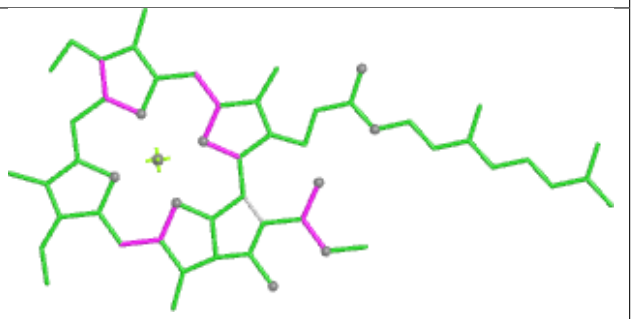


Rings

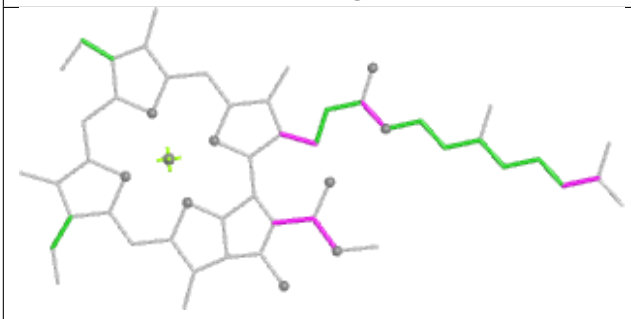
Ligand CLA A 822



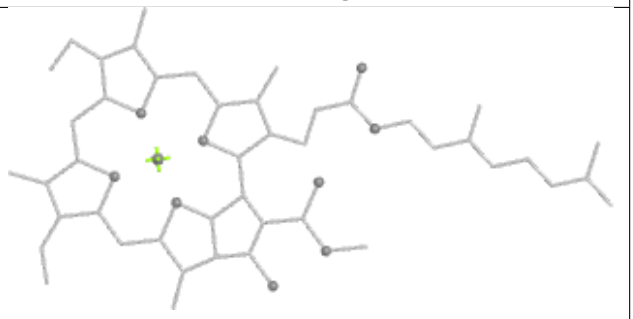
Bond lengths



Bond angles

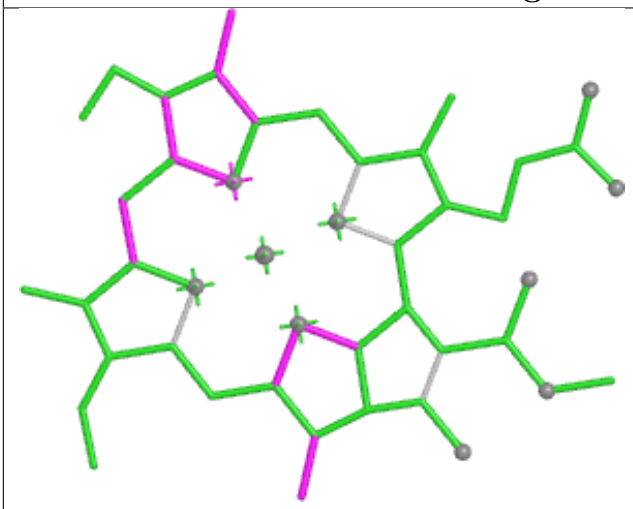


Torsions

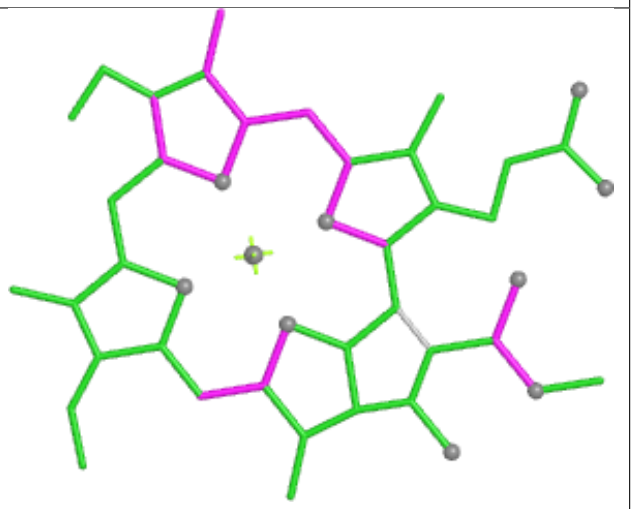


Rings

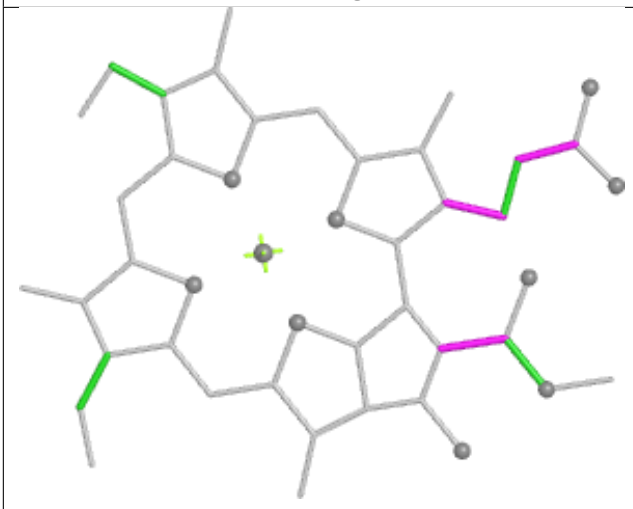
Ligand CLA A 833



Bond lengths



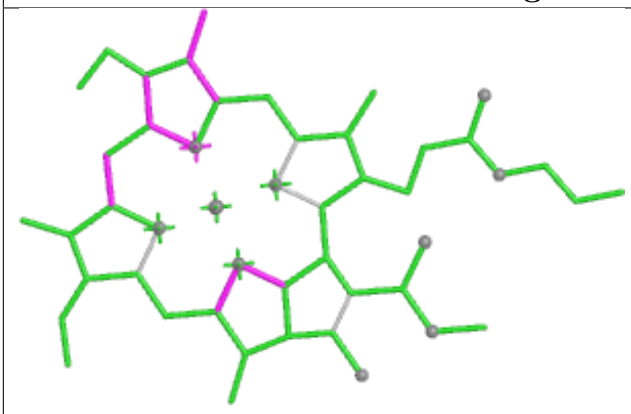
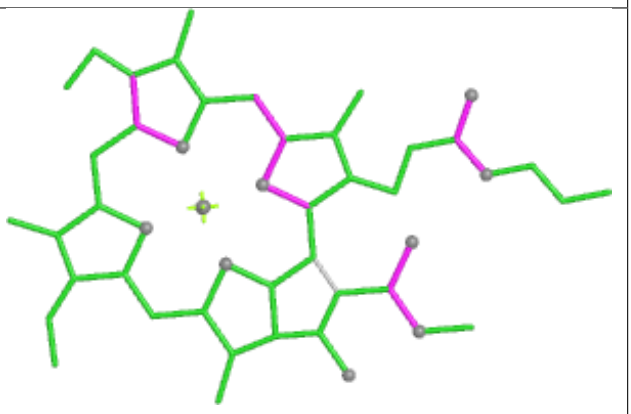
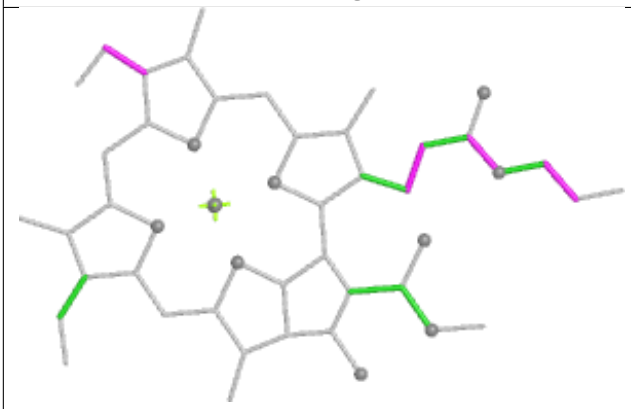
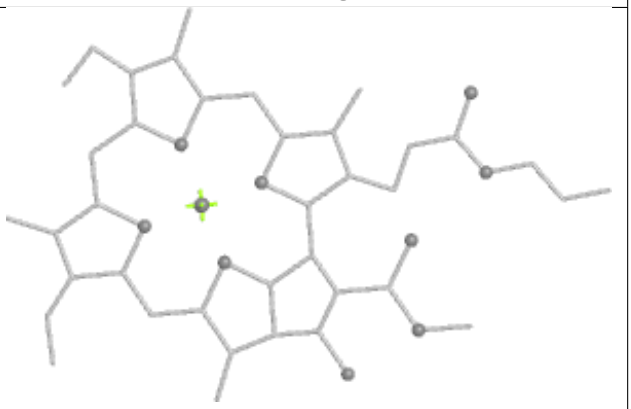
Bond angles

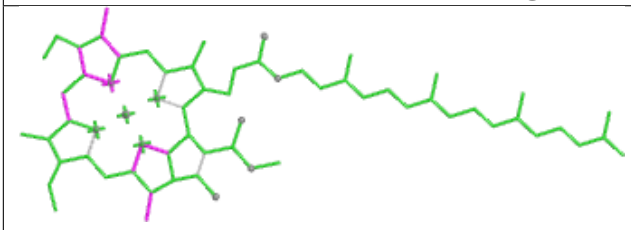
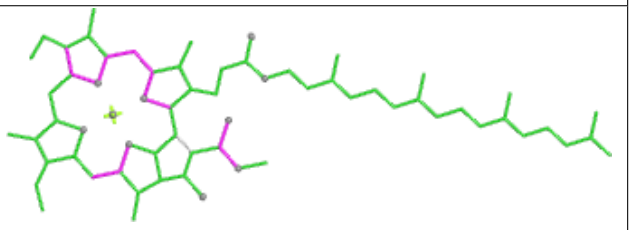
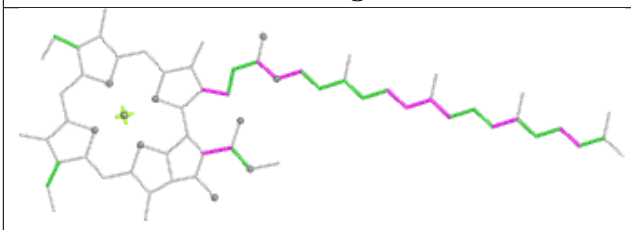
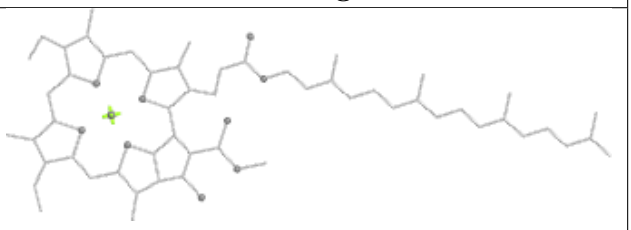


Torsions

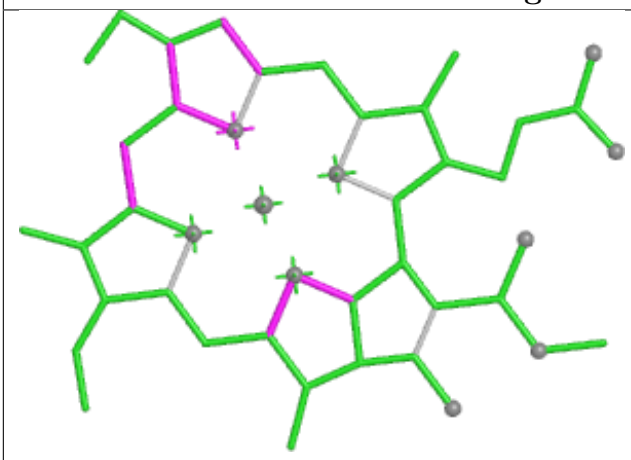


Rings

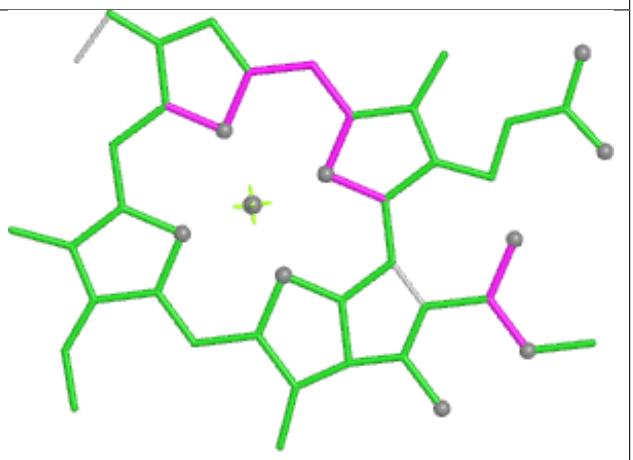
Ligand CLA A 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

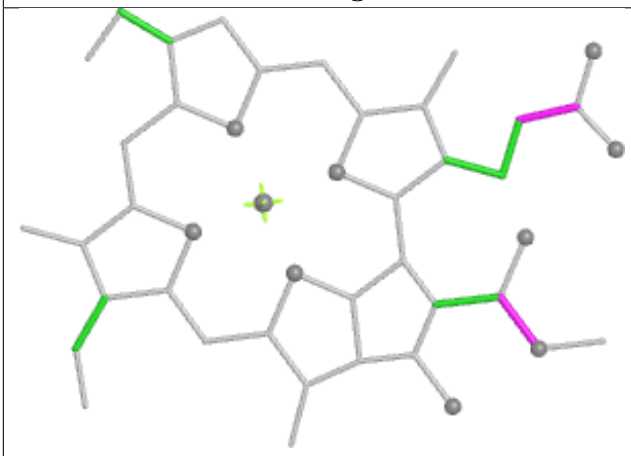
Ligand CLA B 813



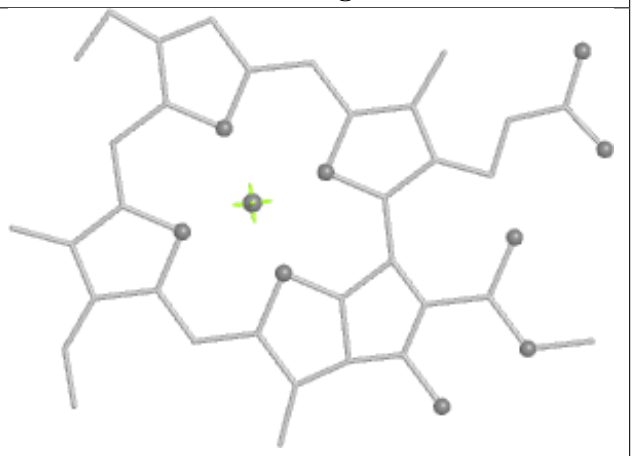
Bond lengths



Bond angles

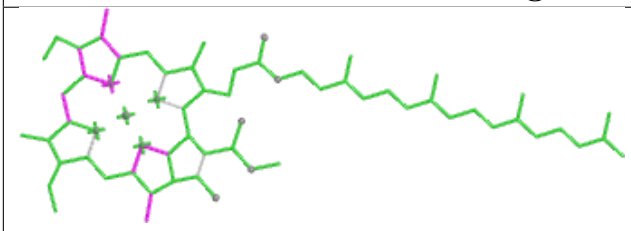


Torsions

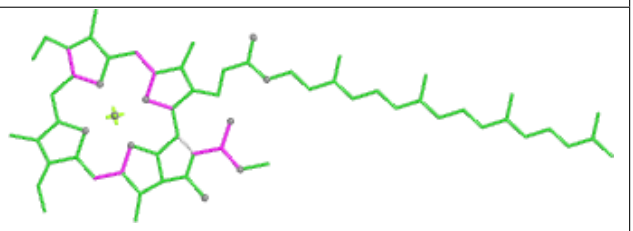


Rings

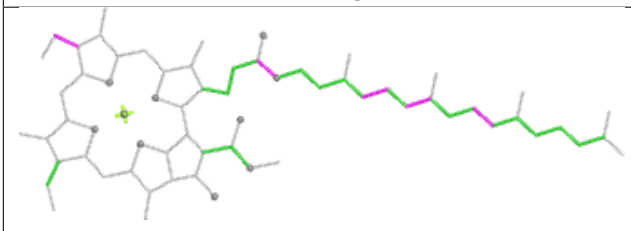
Ligand CLA L 304



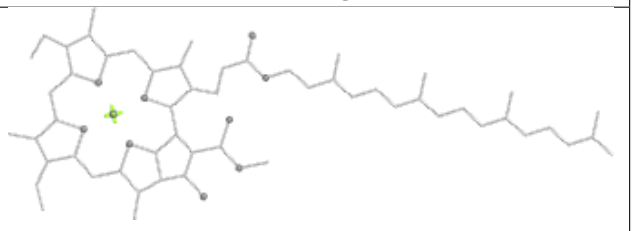
Bond lengths



Bond angles

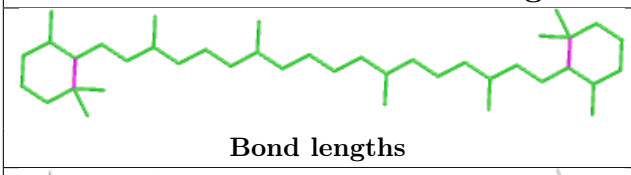


Torsions

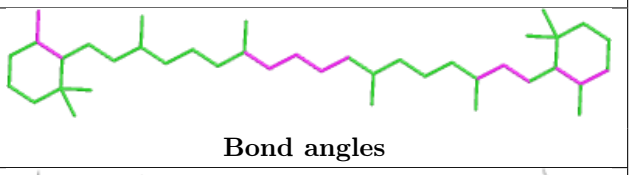


Rings

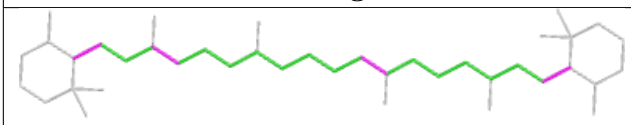
Ligand BCR L 302



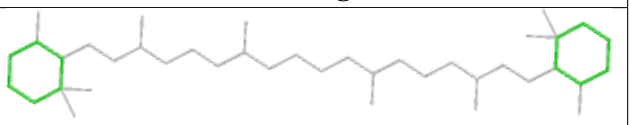
Bond lengths



Bond angles

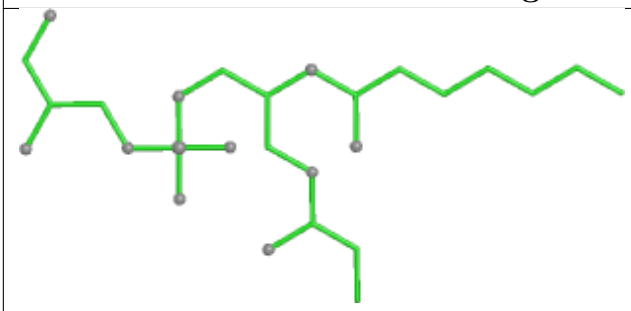


Torsions

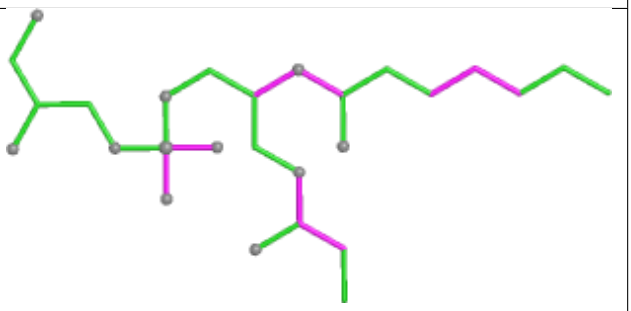


Rings

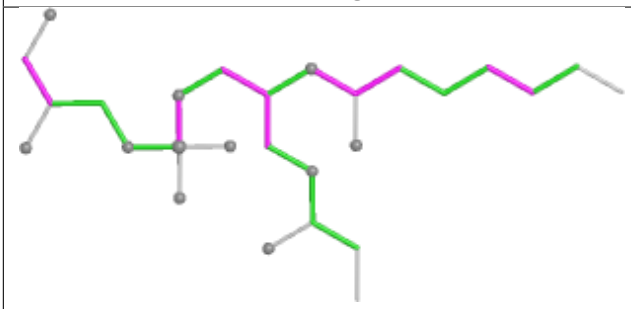
Ligand LHG A 843



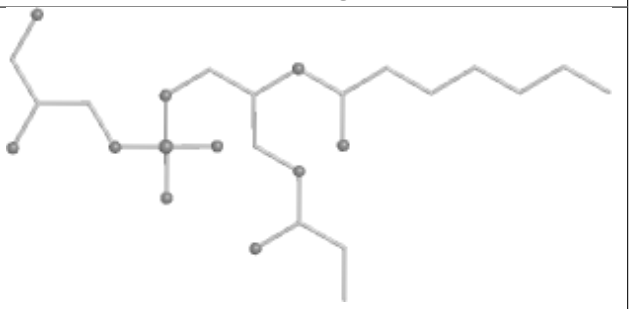
Bond lengths



Bond angles

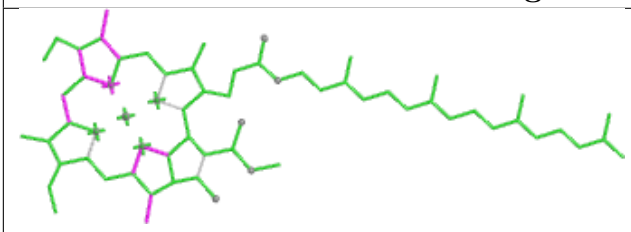


Torsions

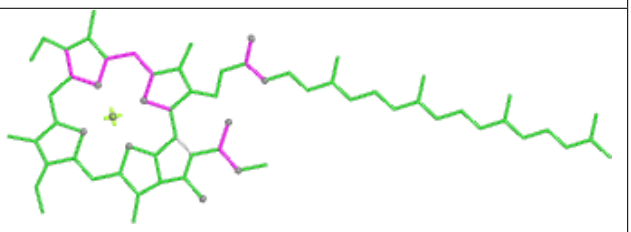


Rings

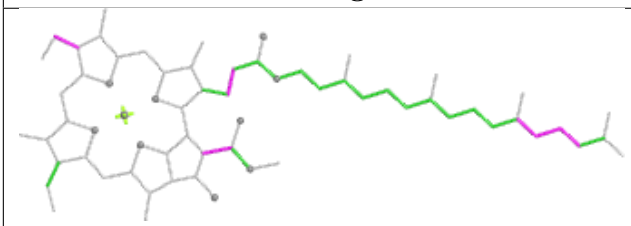
Ligand CLA B 831



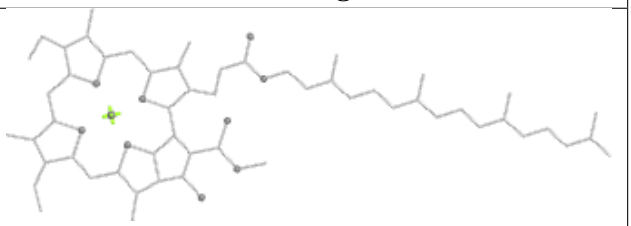
Bond lengths



Bond angles

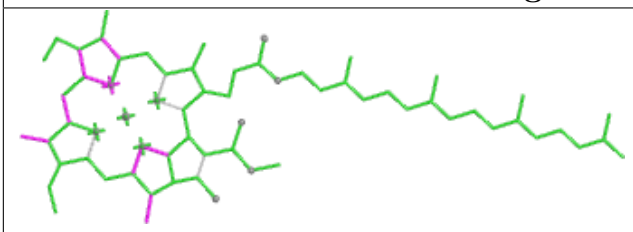


Torsions

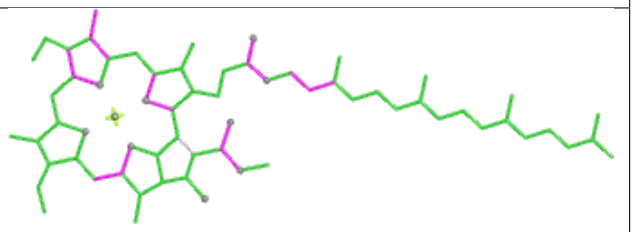


Rings

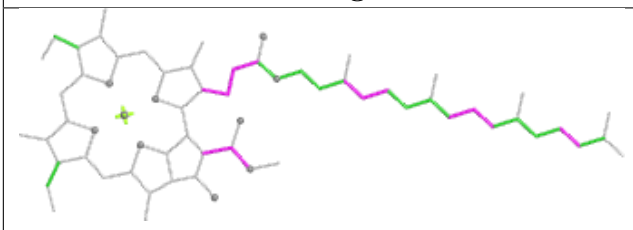
Ligand CLA B 802



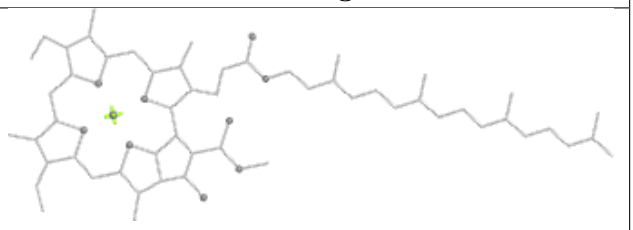
Bond lengths



Bond angles

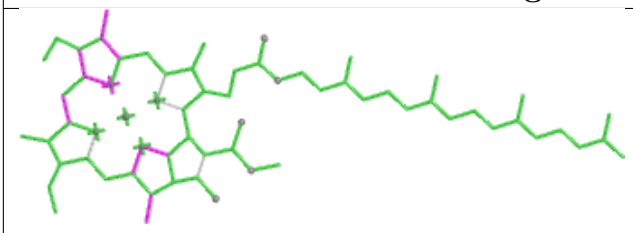


Torsions

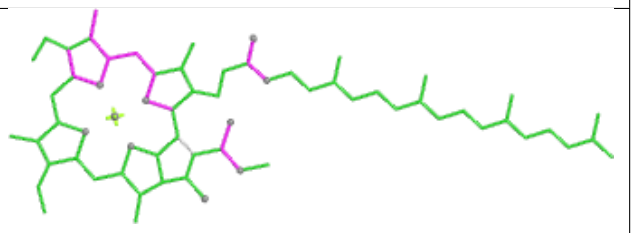


Rings

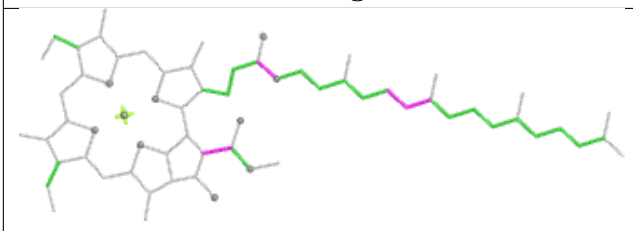
Ligand CLA B 825



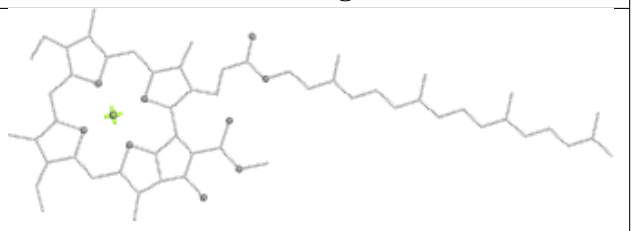
Bond lengths



Bond angles

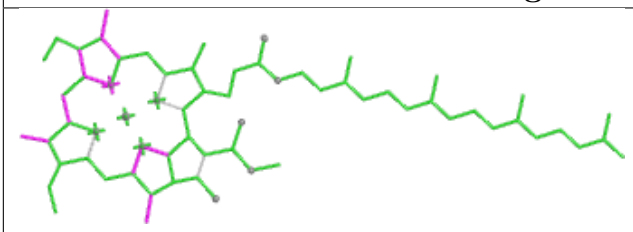


Torsions

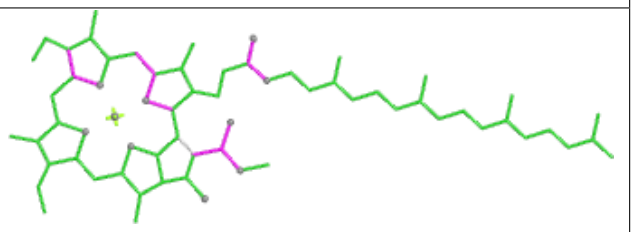


Rings

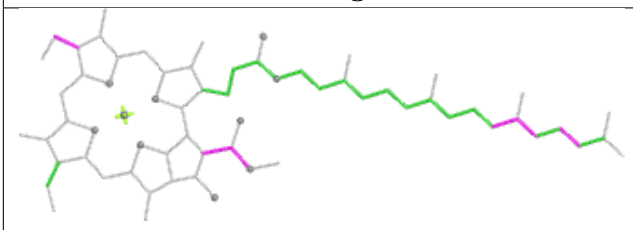
Ligand CLA B 809



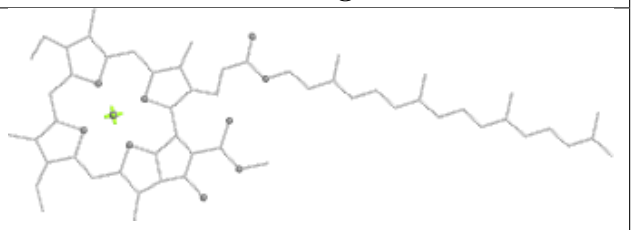
Bond lengths



Bond angles

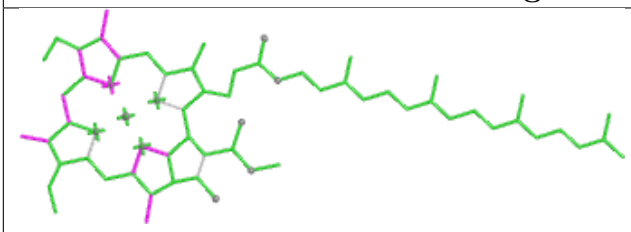


Torsions

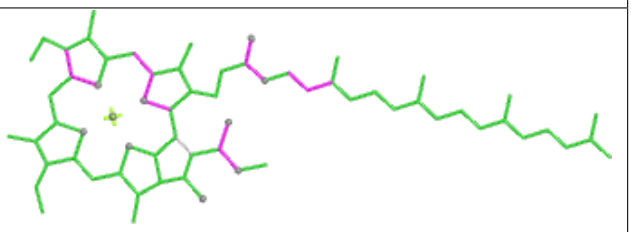


Rings

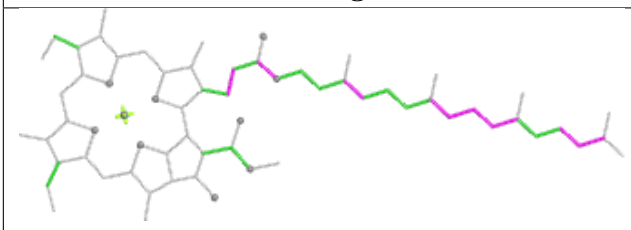
Ligand CLA A 827



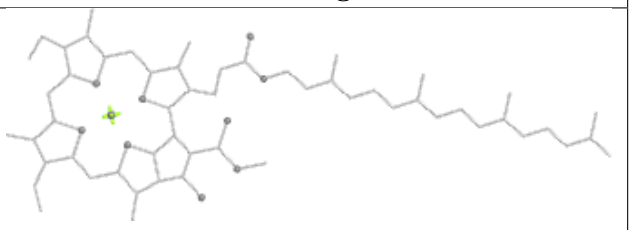
Bond lengths



Bond angles

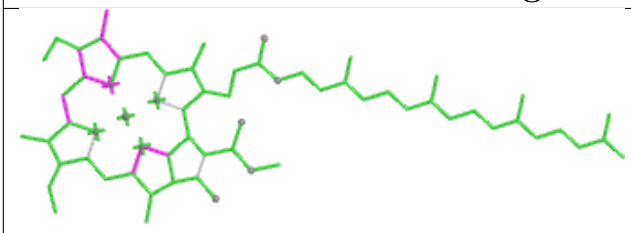


Torsions

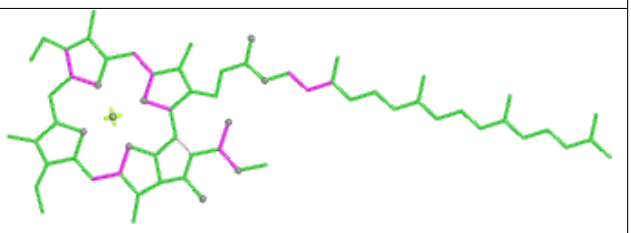


Rings

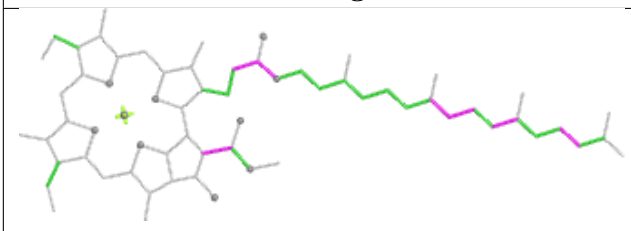
Ligand CLA H 201



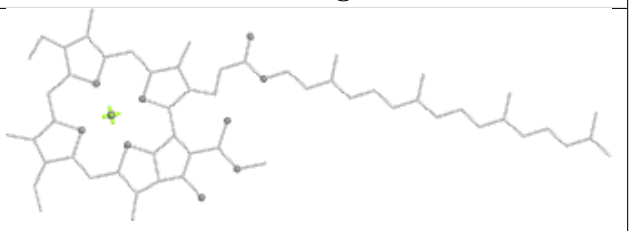
Bond lengths



Bond angles

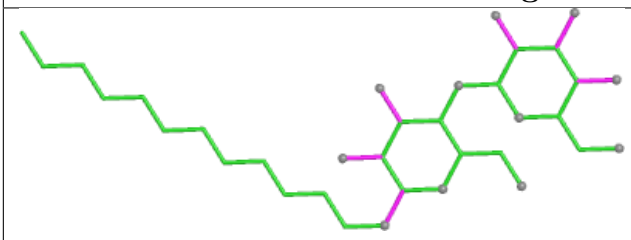


Torsions

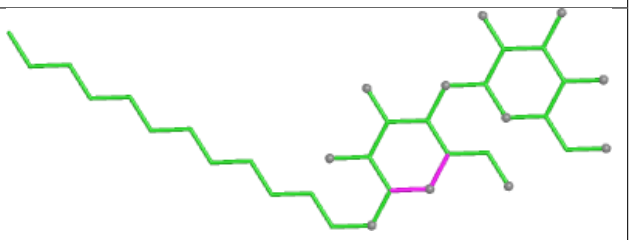


Rings

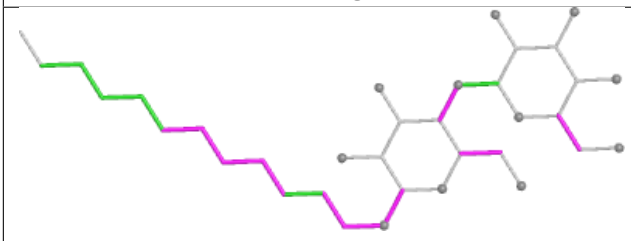
Ligand LMT B 838



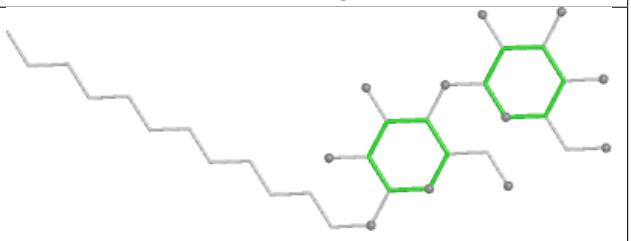
Bond lengths



Bond angles

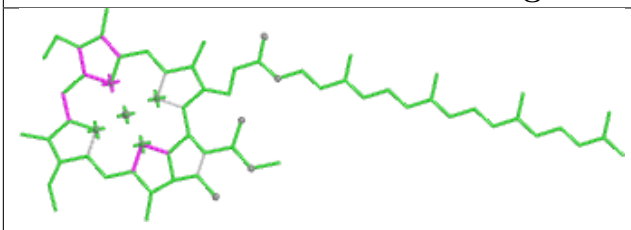


Torsions

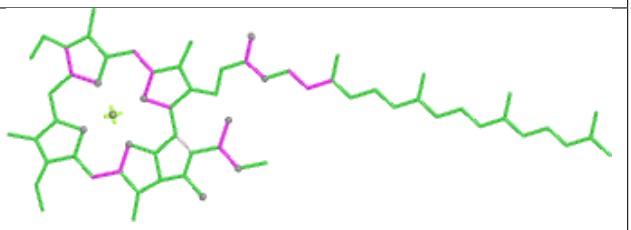


Rings

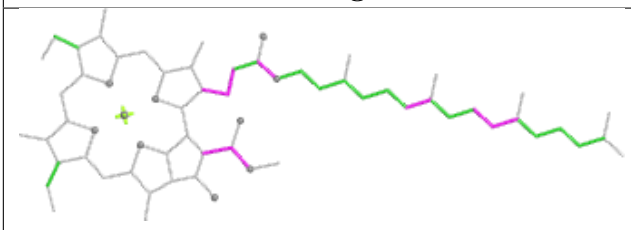
Ligand CLA A 811



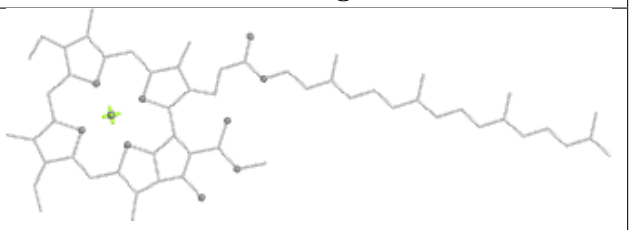
Bond lengths



Bond angles

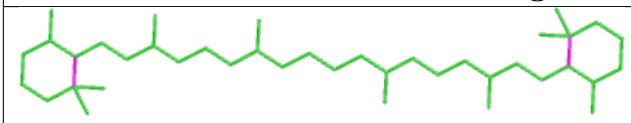


Torsions

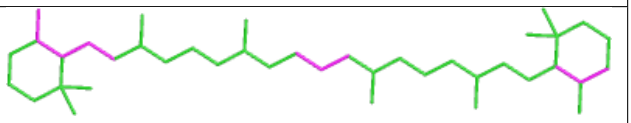


Rings

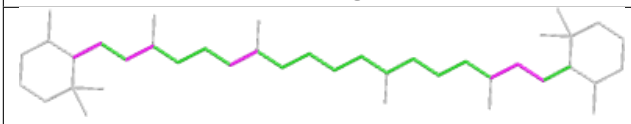
Ligand BCR I 101



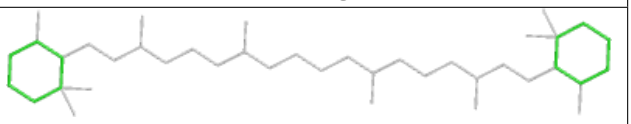
Bond lengths



Bond angles

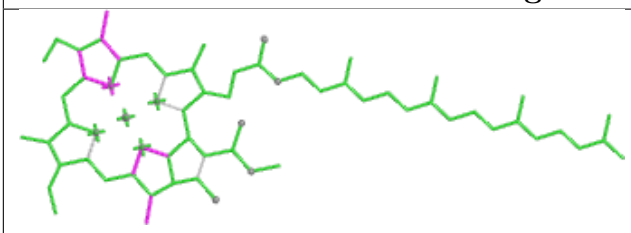


Torsions

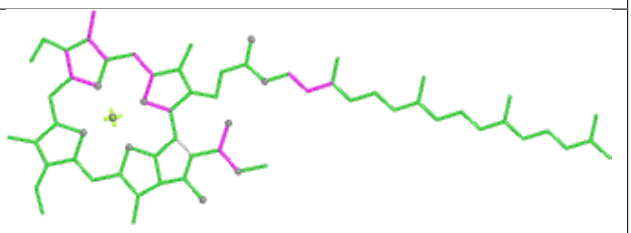


Rings

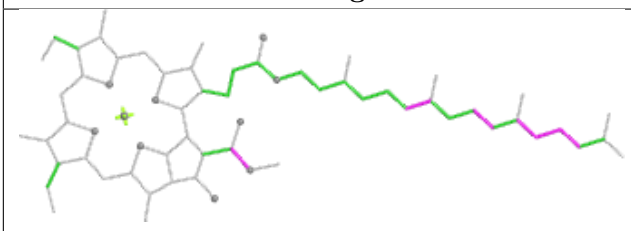
Ligand CLA B 810



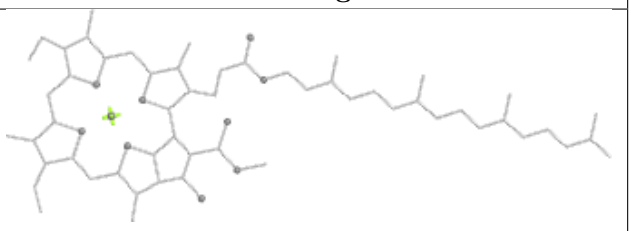
Bond lengths



Bond angles

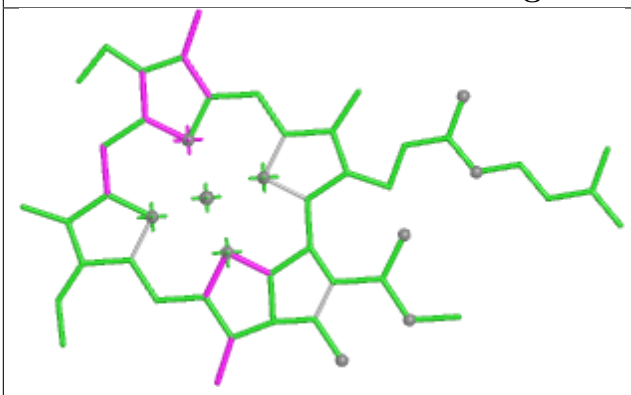


Torsions

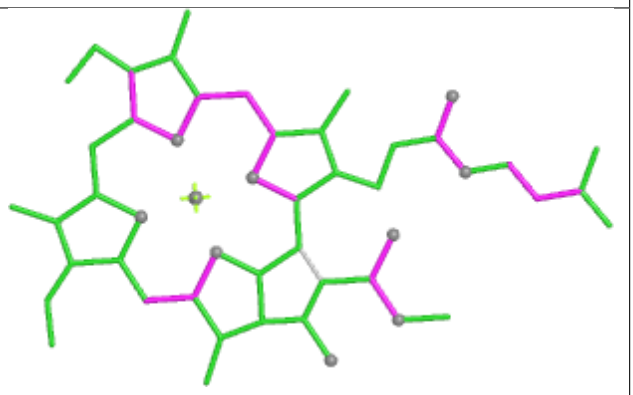


Rings

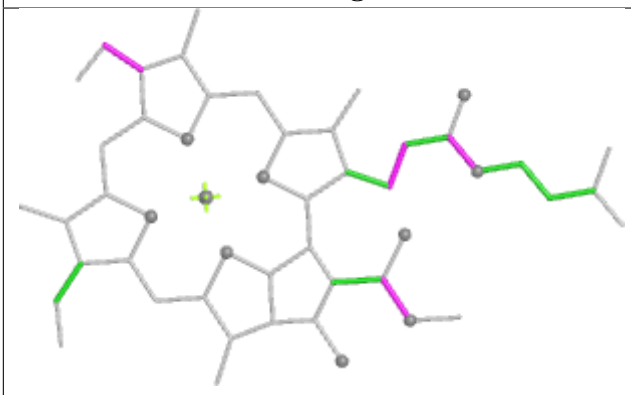
Ligand CLA A 813



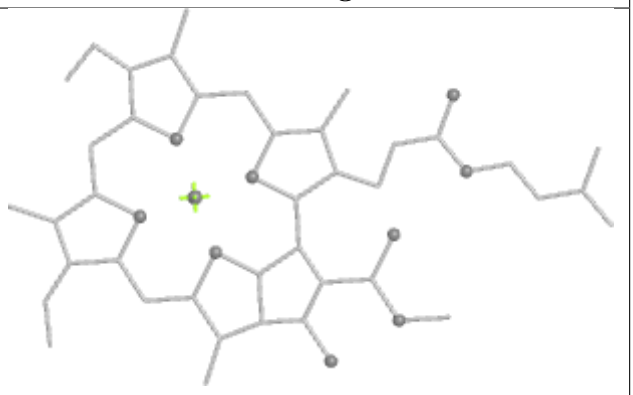
Bond lengths



Bond angles

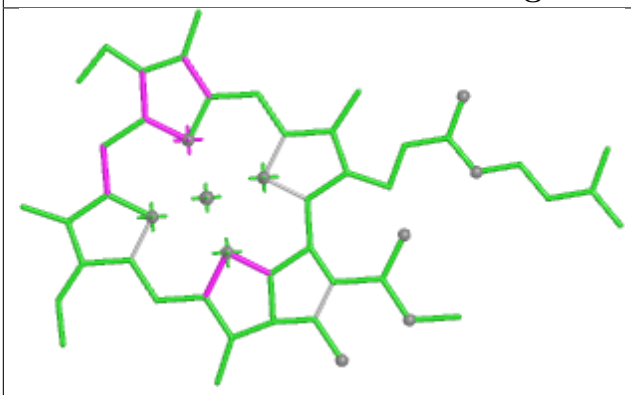


Torsions

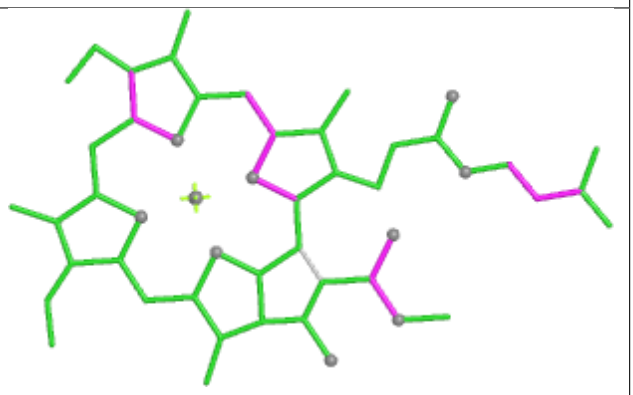


Rings

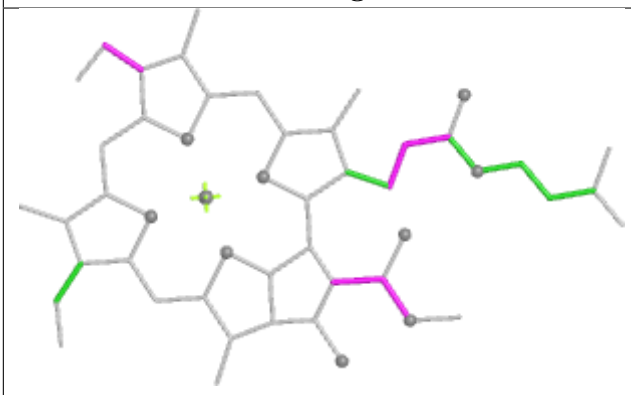
Ligand CLA B 820



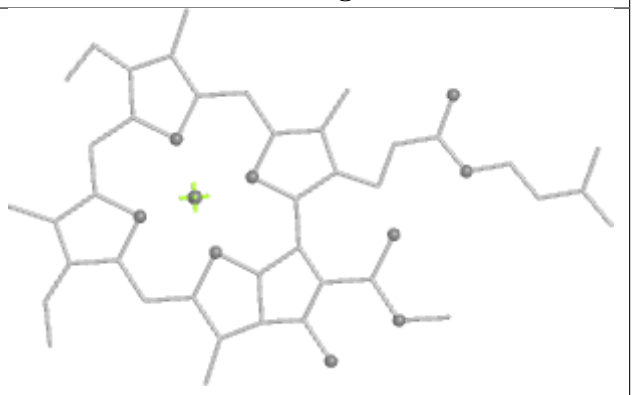
Bond lengths



Bond angles

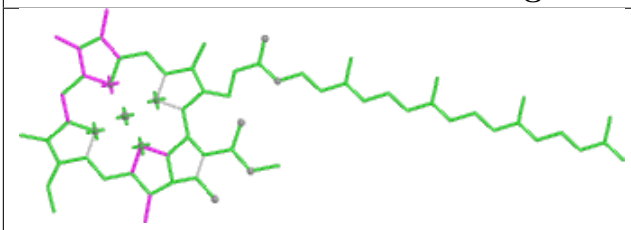


Torsions

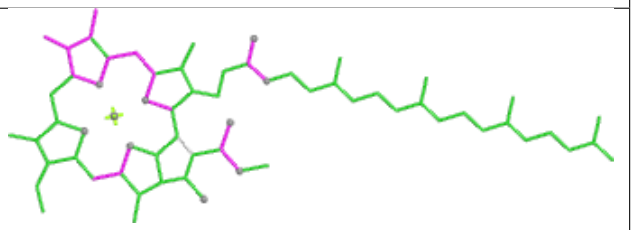


Rings

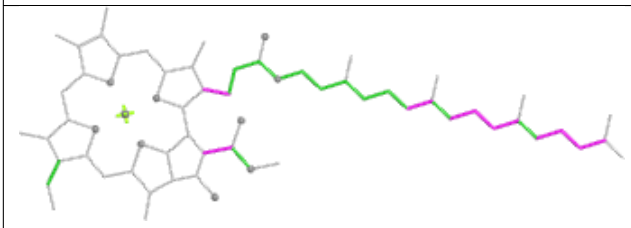
Ligand CLA B 821



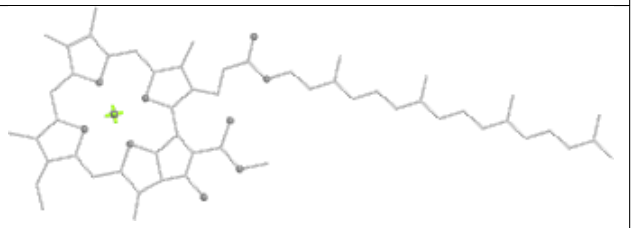
Bond lengths



Bond angles

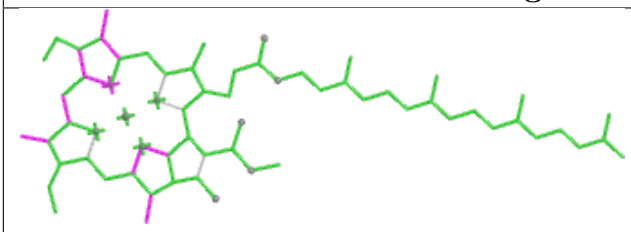


Torsions

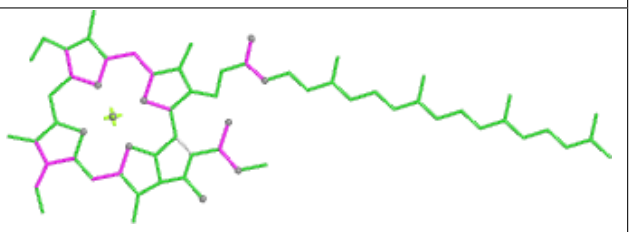


Rings

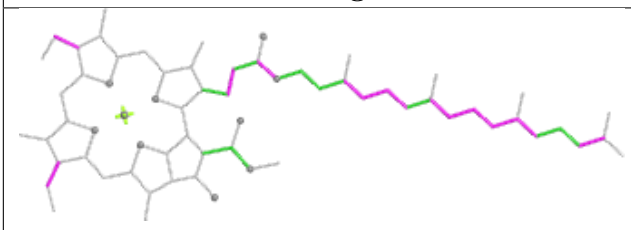
Ligand CLA B 801



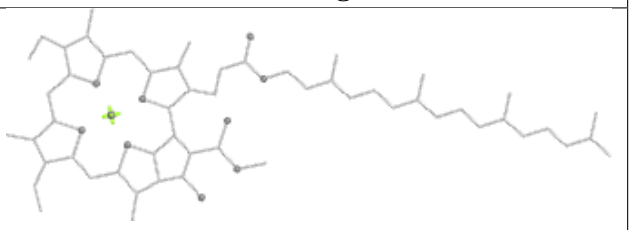
Bond lengths



Bond angles

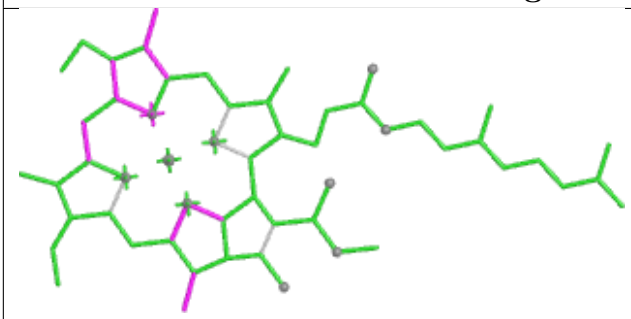


Torsions

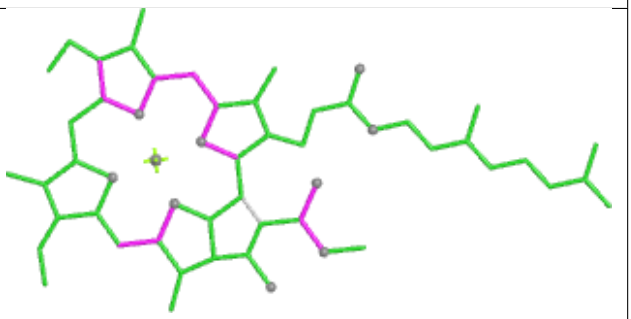


Rings

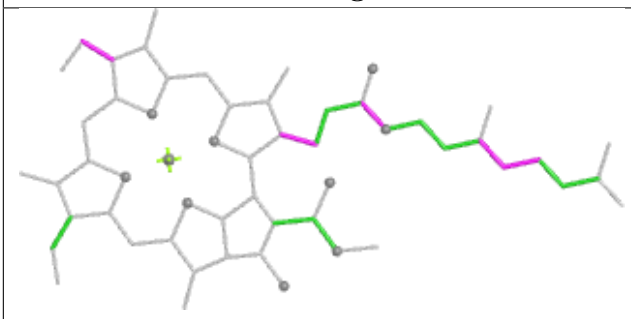
Ligand CLA B 817



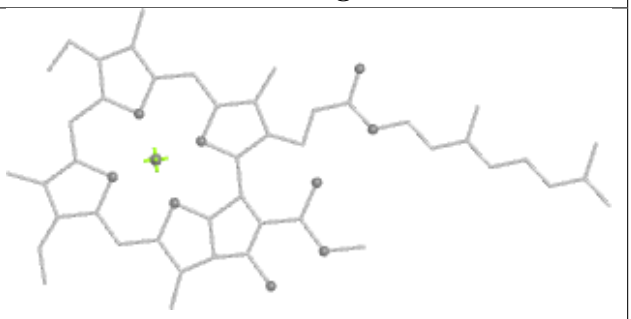
Bond lengths



Bond angles

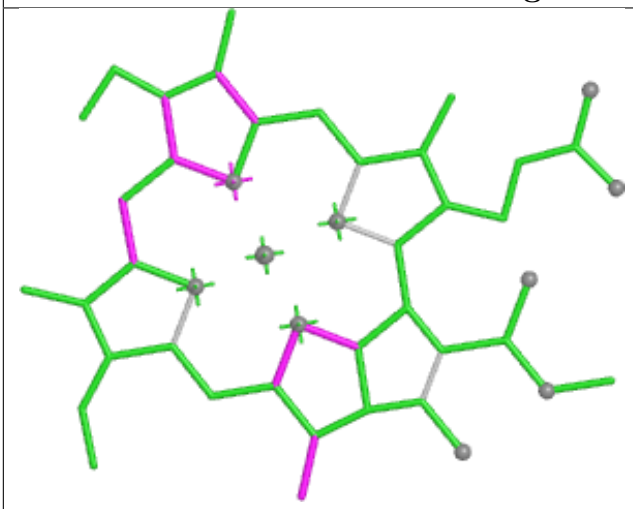


Torsions

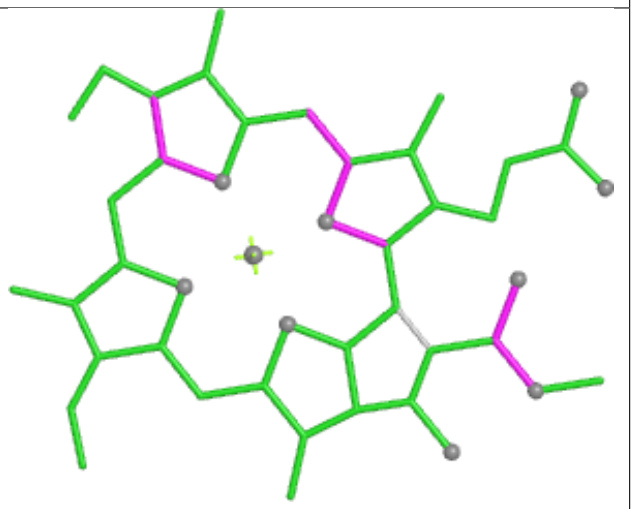


Rings

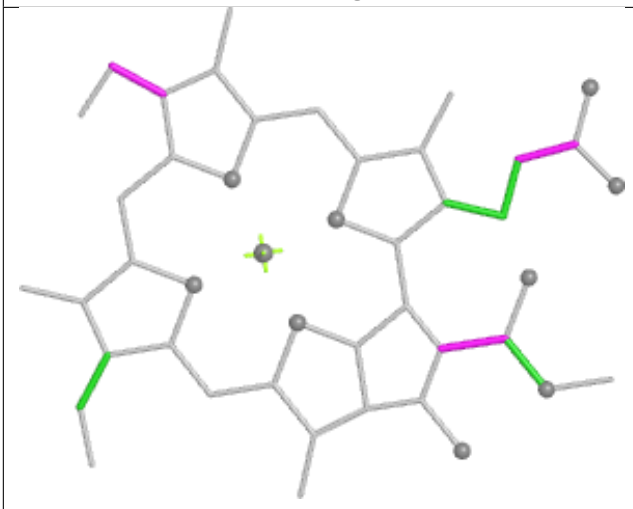
Ligand CLA A 818



Bond lengths



Bond angles

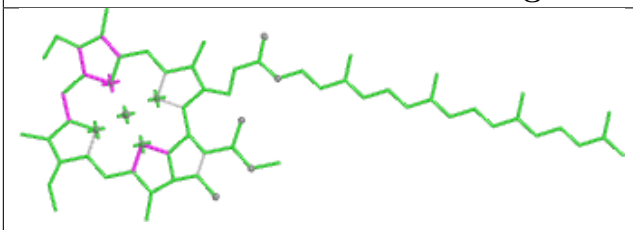


Torsions

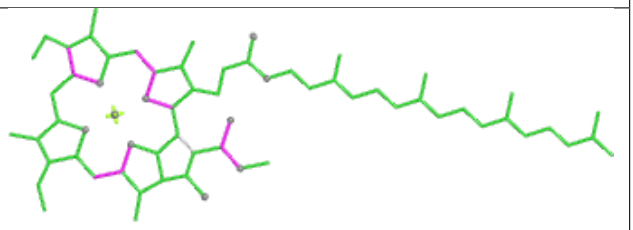


Rings

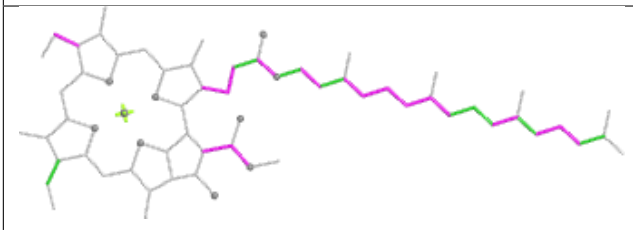
Ligand CLA A 807



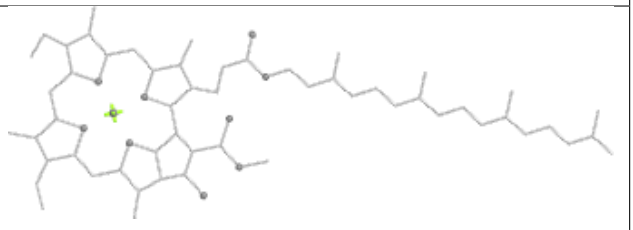
Bond lengths



Bond angles

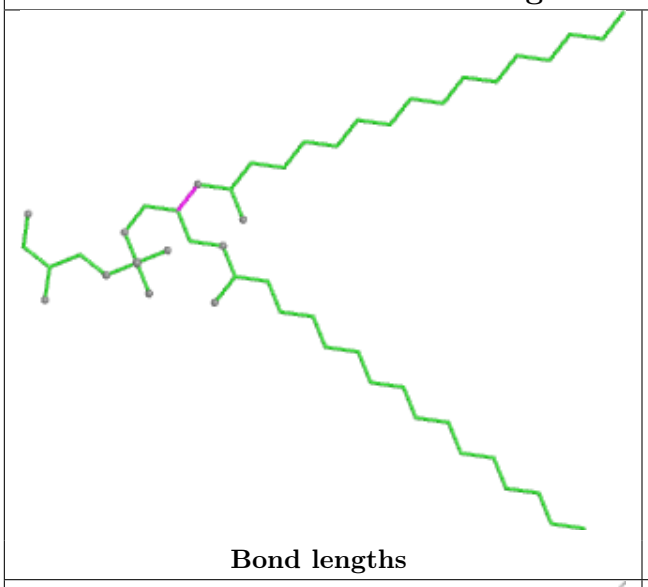


Torsions

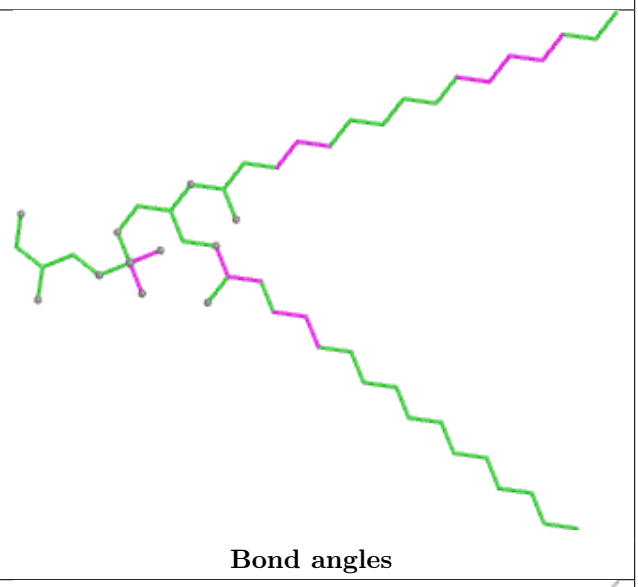


Rings

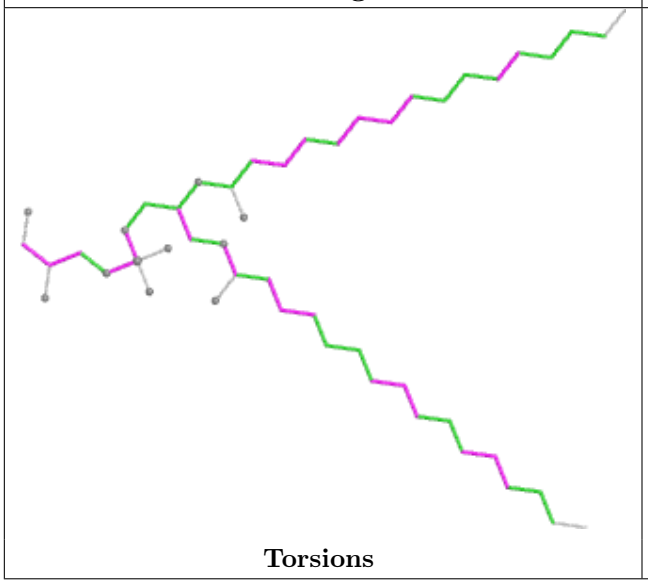
Ligand LHG L 301



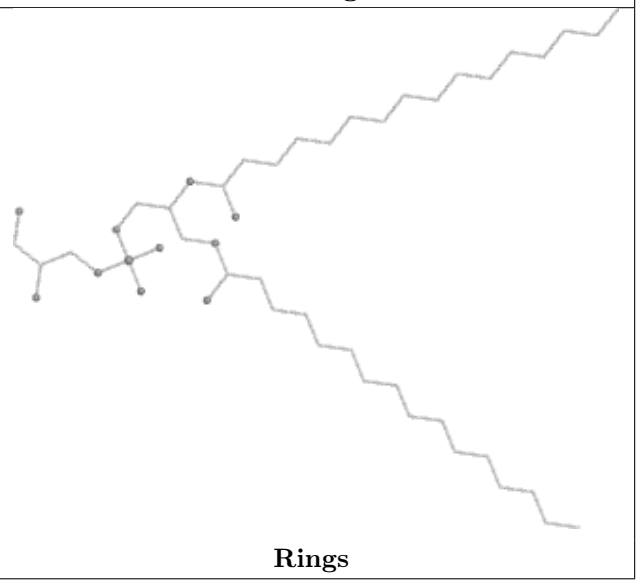
Bond lengths



Bond angles

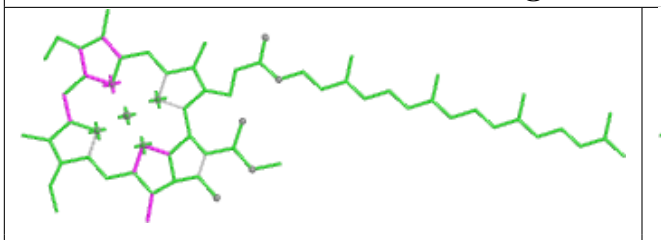


Torsions

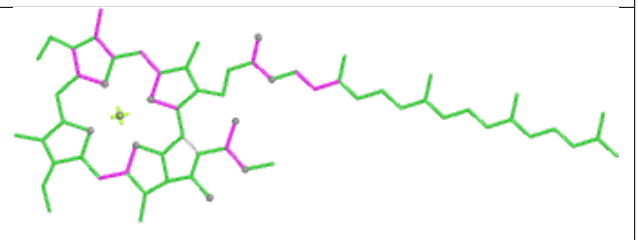


Rings

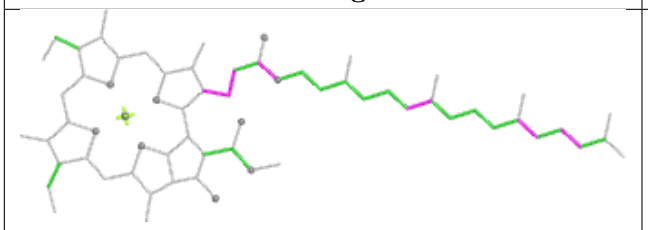
Ligand CLA A 805



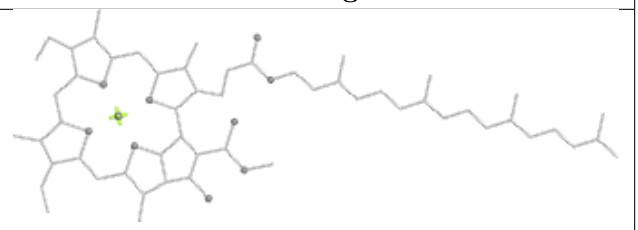
Bond lengths



Bond angles

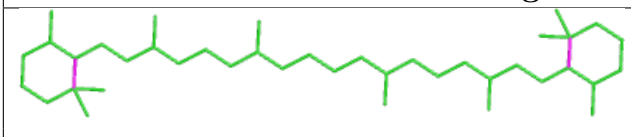


Torsions

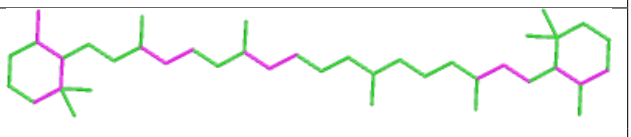


Rings

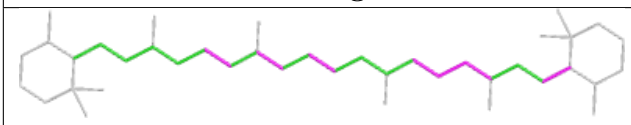
Ligand BCR A 845



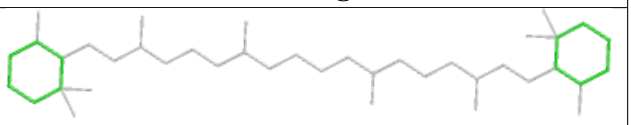
Bond lengths



Bond angles

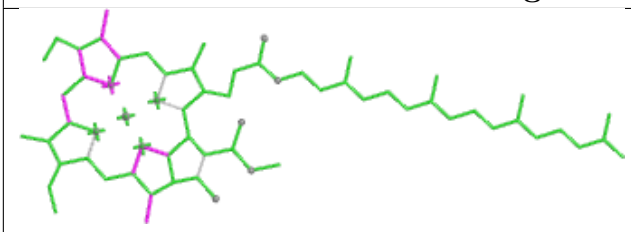


Torsions

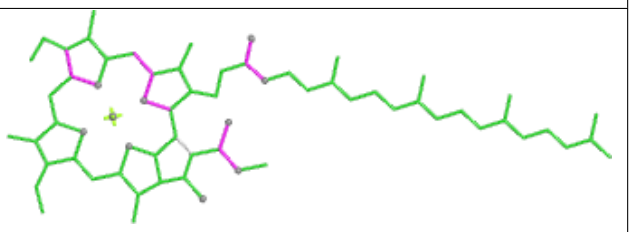


Rings

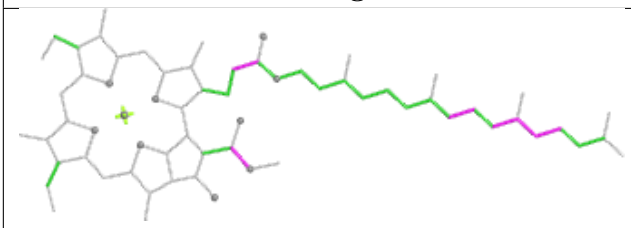
Ligand CLA A 823



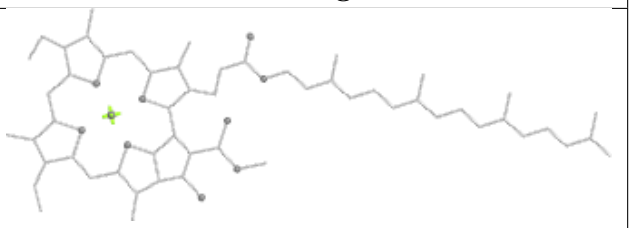
Bond lengths



Bond angles

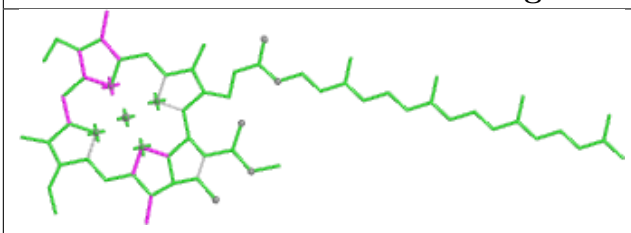


Torsions

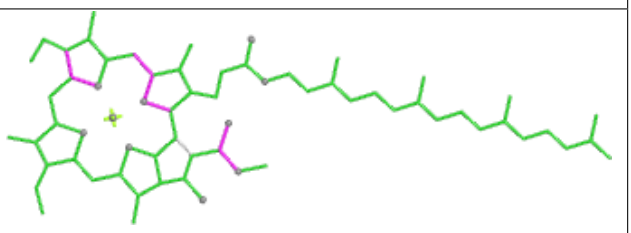


Rings

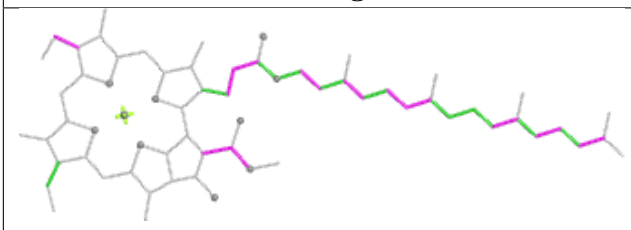
Ligand CLA B 811



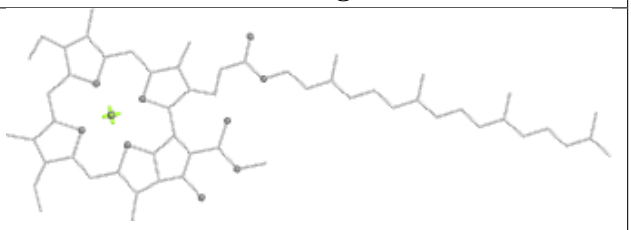
Bond lengths



Bond angles

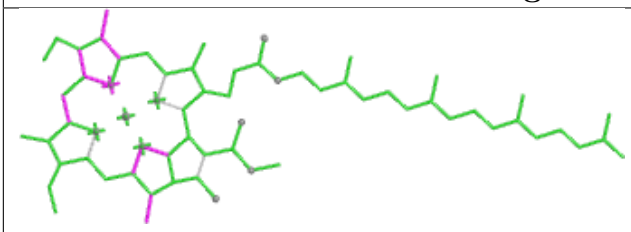


Torsions

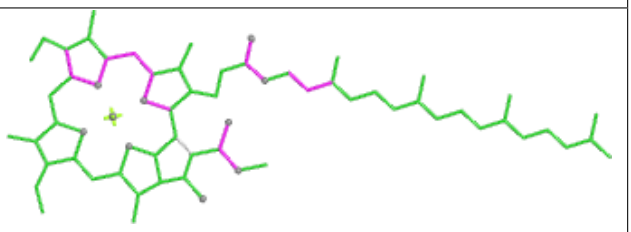


Rings

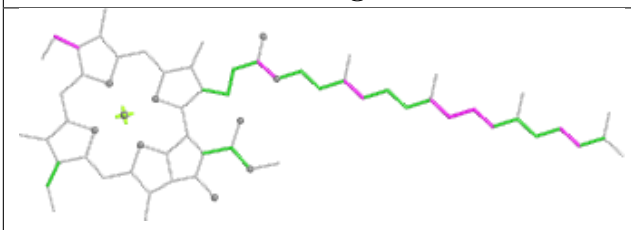
Ligand CLA A 835



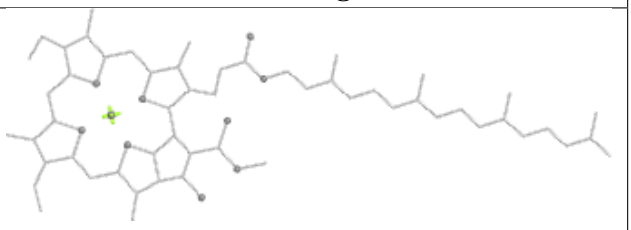
Bond lengths



Bond angles

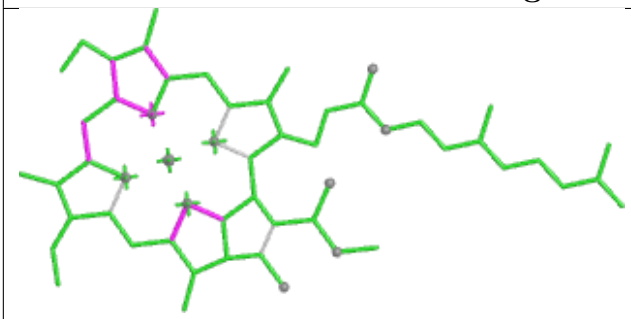


Torsions

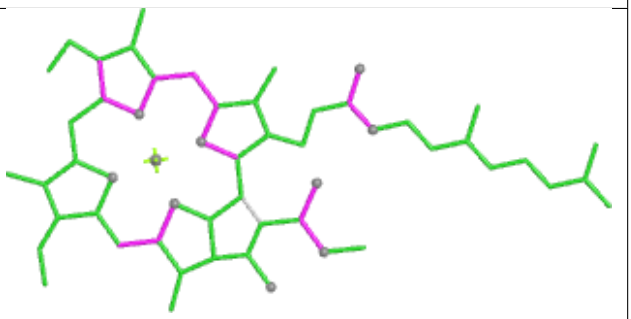


Rings

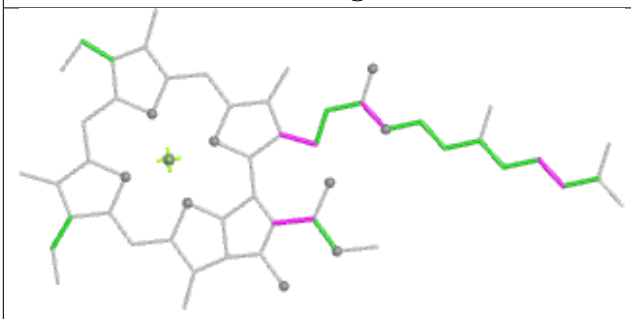
Ligand CLA A 803



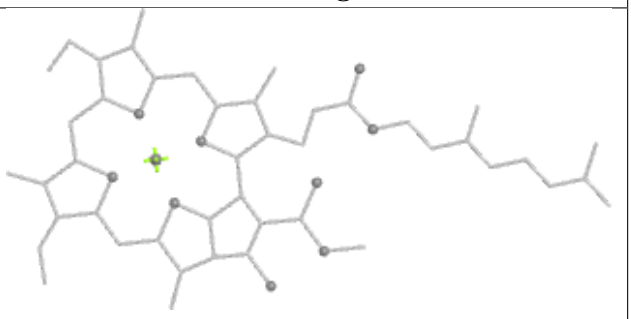
Bond lengths



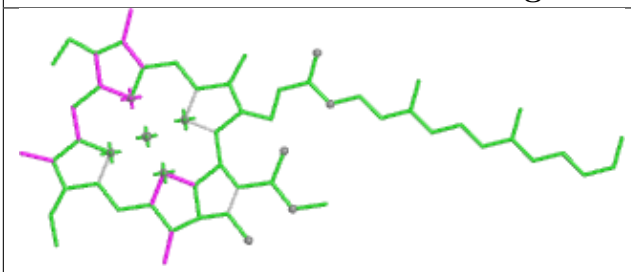
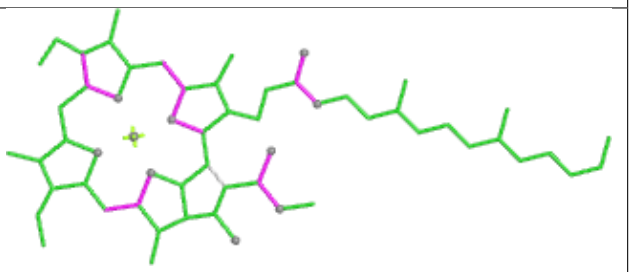
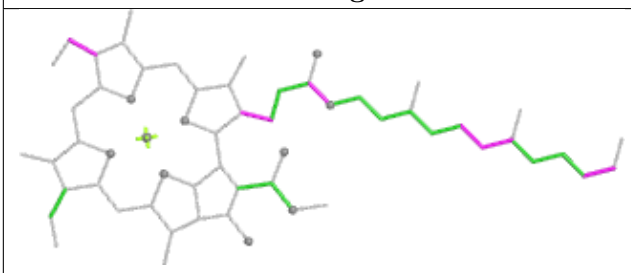
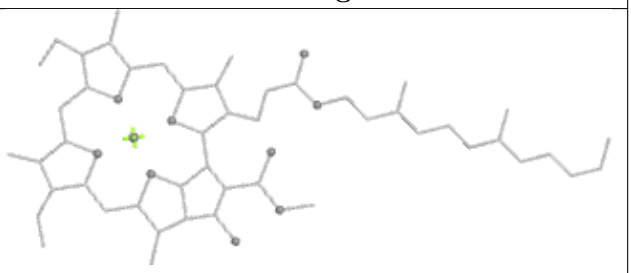
Bond angles

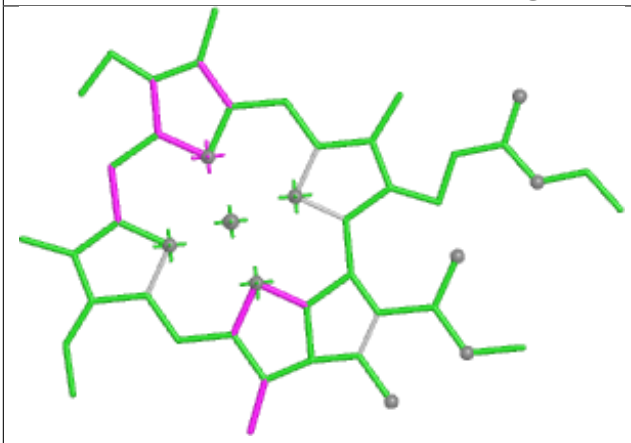
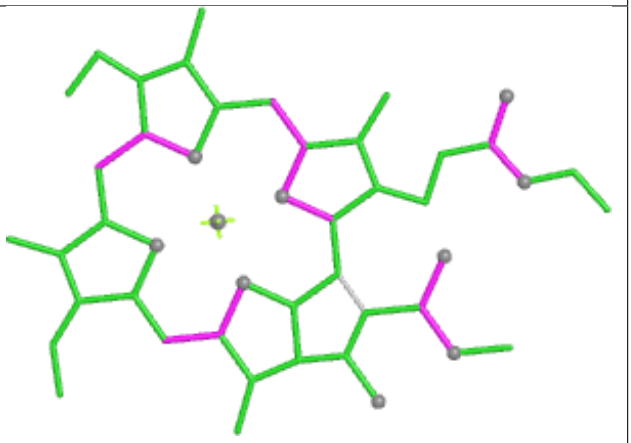
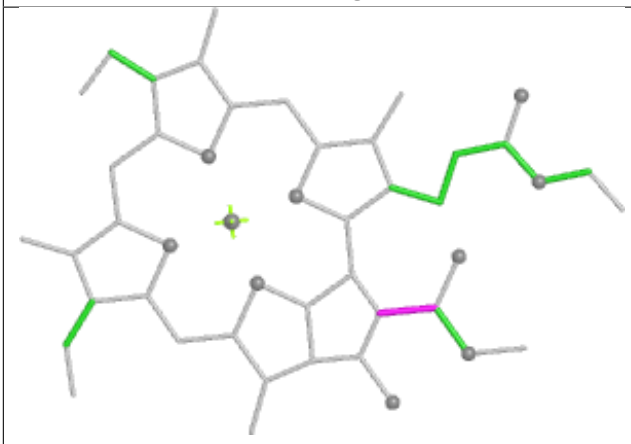
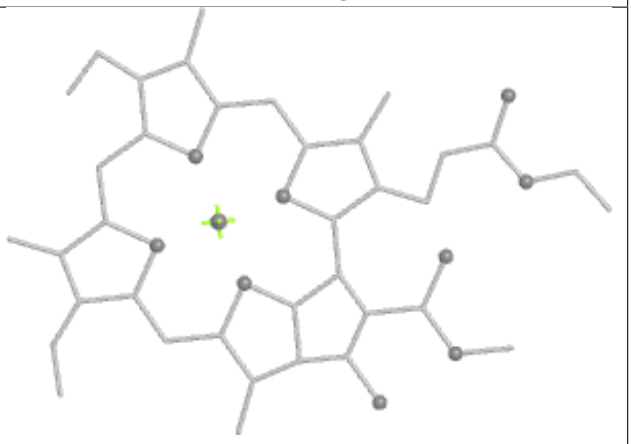


Torsions

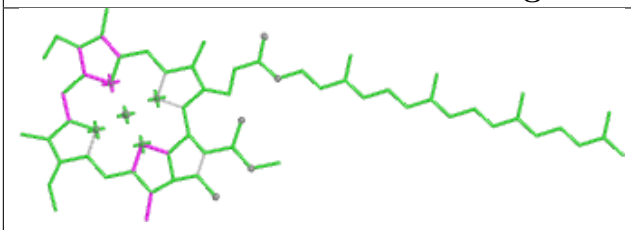


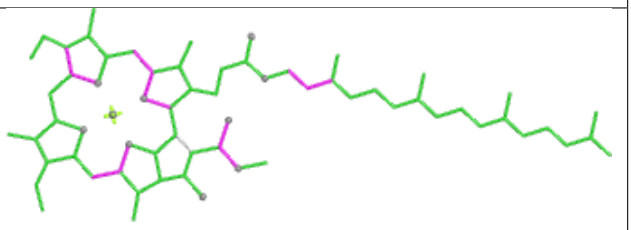
Rings

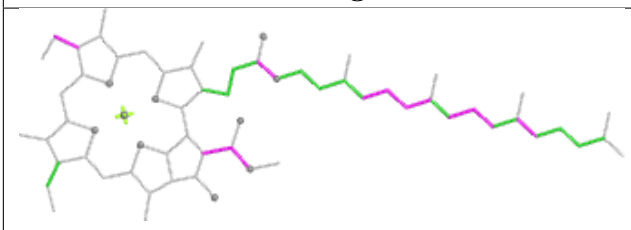
Ligand CLA B 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

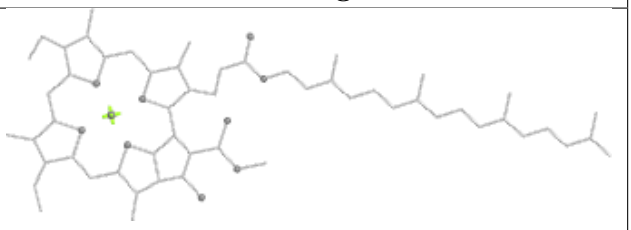
Ligand CLA B 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 806

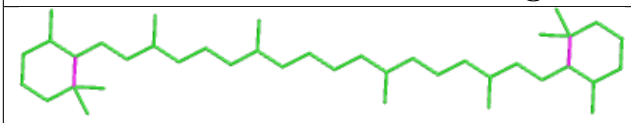

Bond lengths

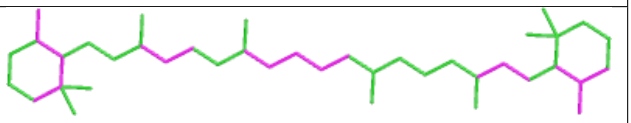

Bond angles


Torsions

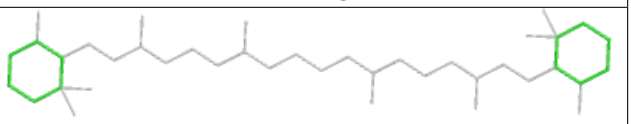

Rings

Ligand BCR L 306

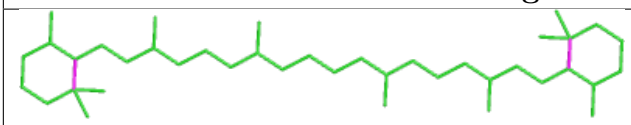

Bond lengths

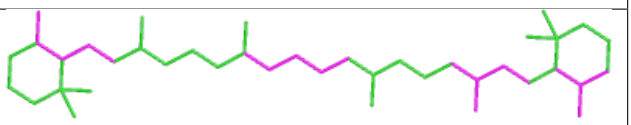

Bond angles

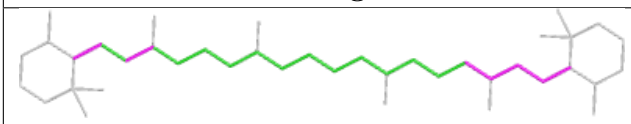

Torsions

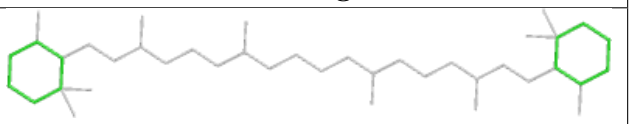

Rings

Ligand BCR A 847

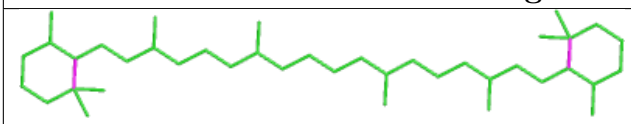

Bond lengths

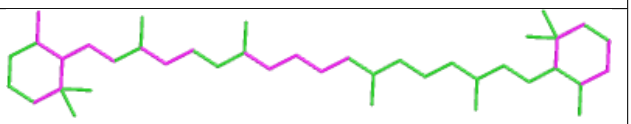

Bond angles

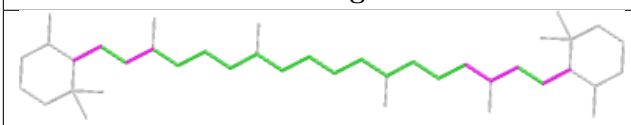

Torsions

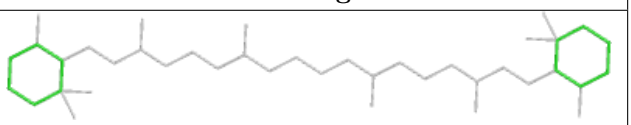

Rings

Ligand BCR L 308

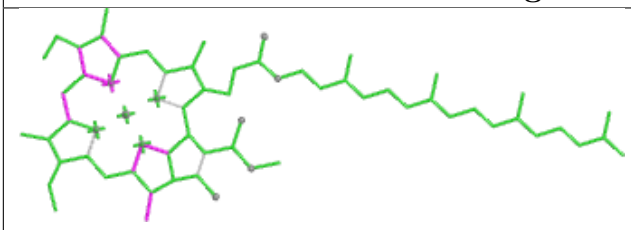

Bond lengths


Bond angles

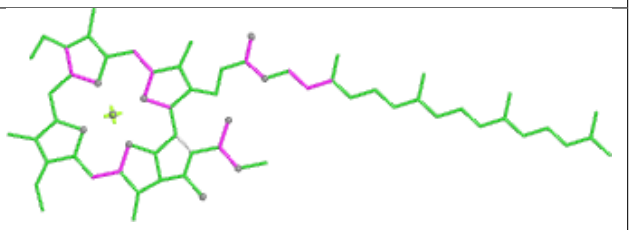

Torsions


Rings

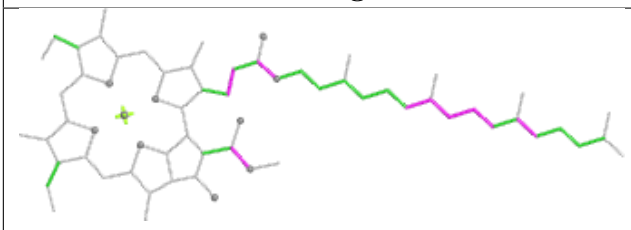
Ligand CLA B 823



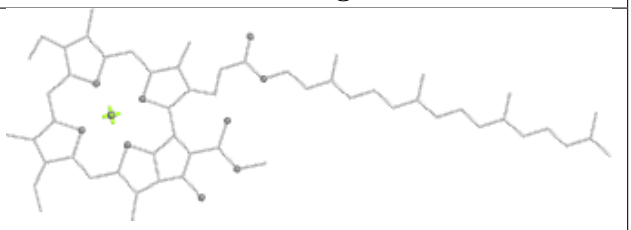
Bond lengths



Bond angles

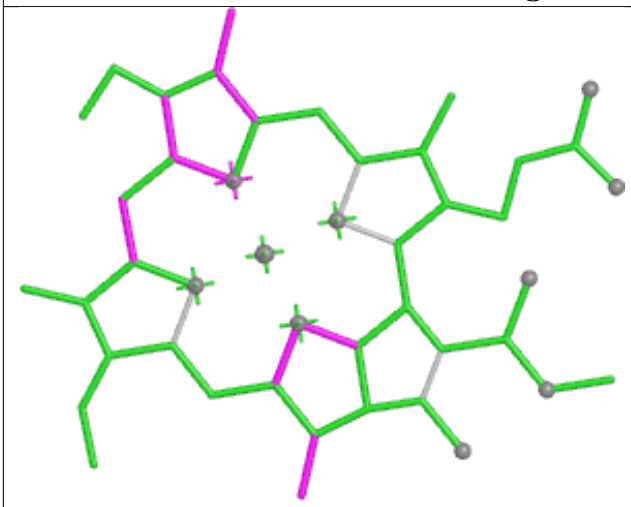


Torsions

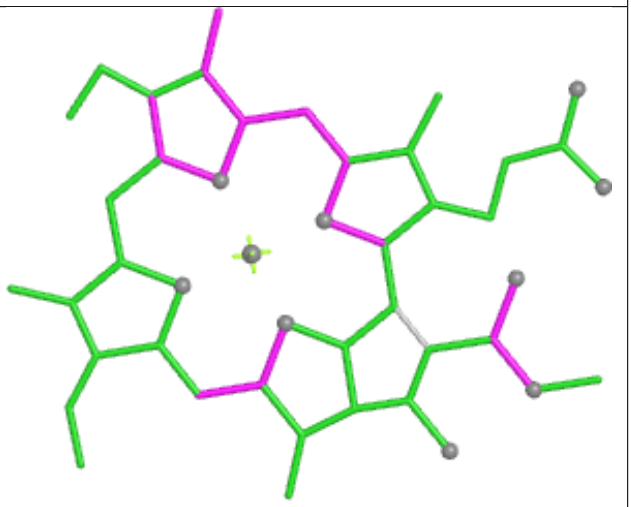


Rings

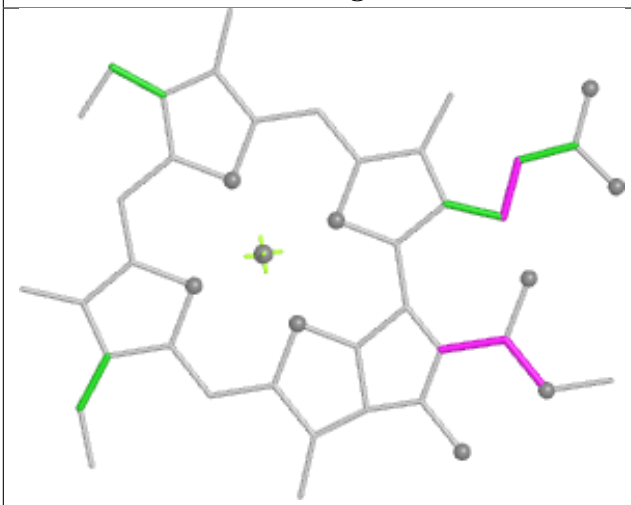
Ligand CLA B 827



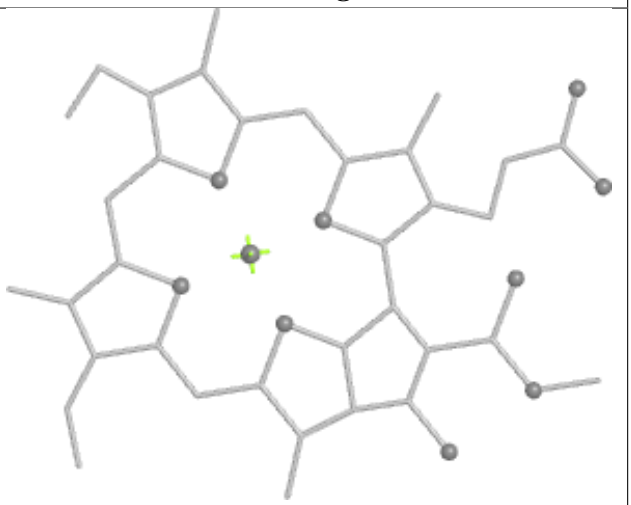
Bond lengths



Bond angles

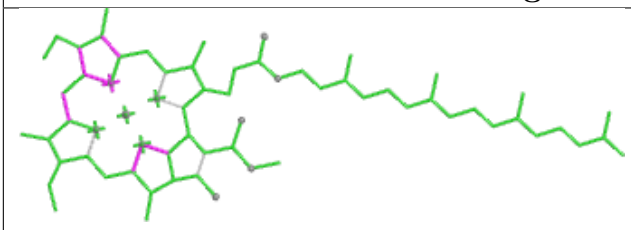


Torsions

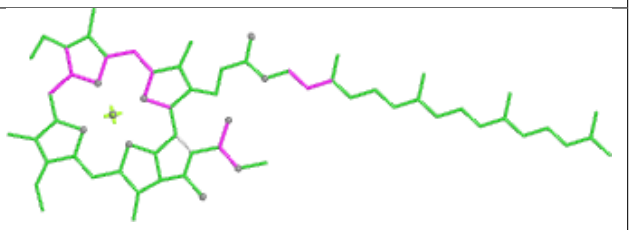


Rings

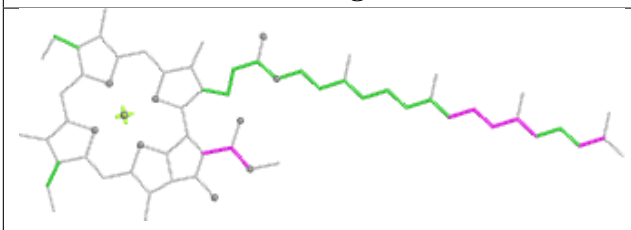
Ligand CLA A 836



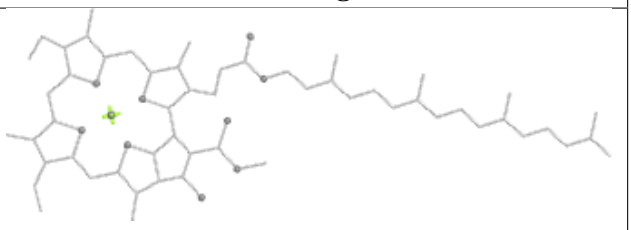
Bond lengths



Bond angles

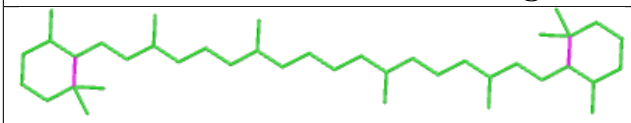


Torsions

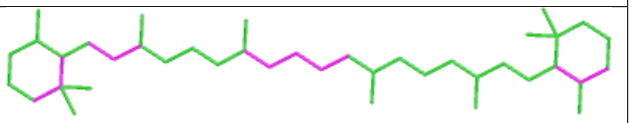


Rings

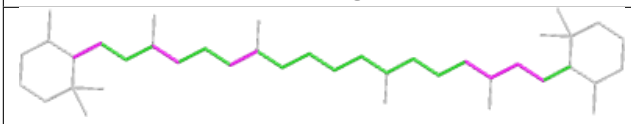
Ligand BCR B 834



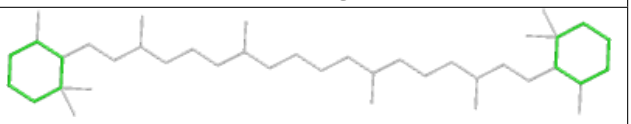
Bond lengths



Bond angles

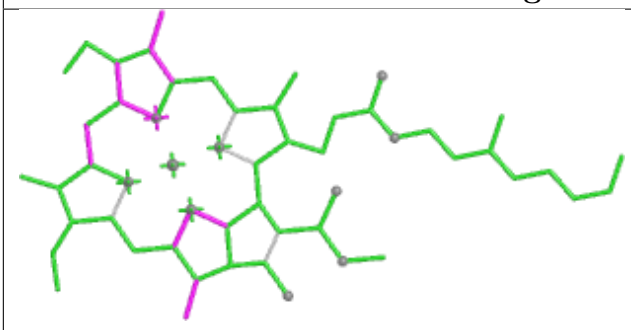


Torsions

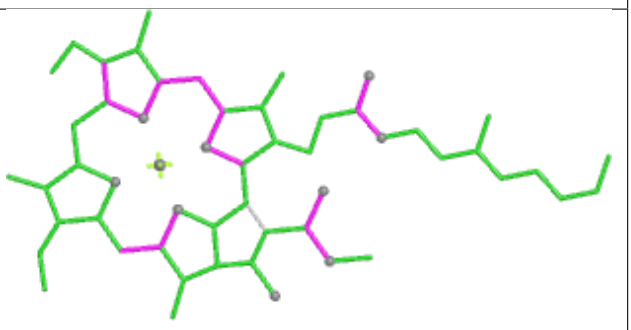


Rings

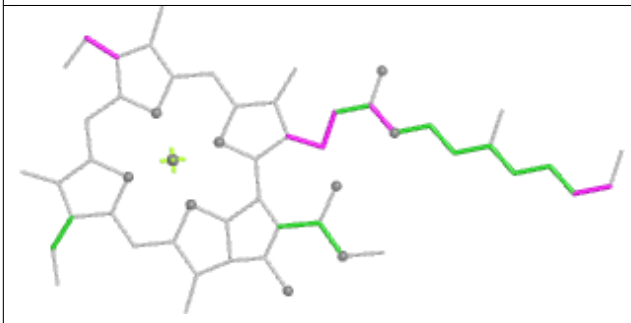
Ligand CLA A 810



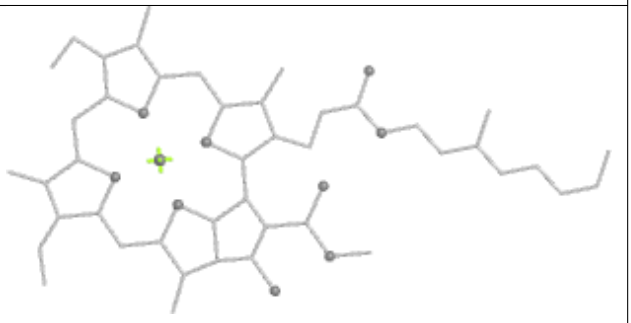
Bond lengths



Bond angles

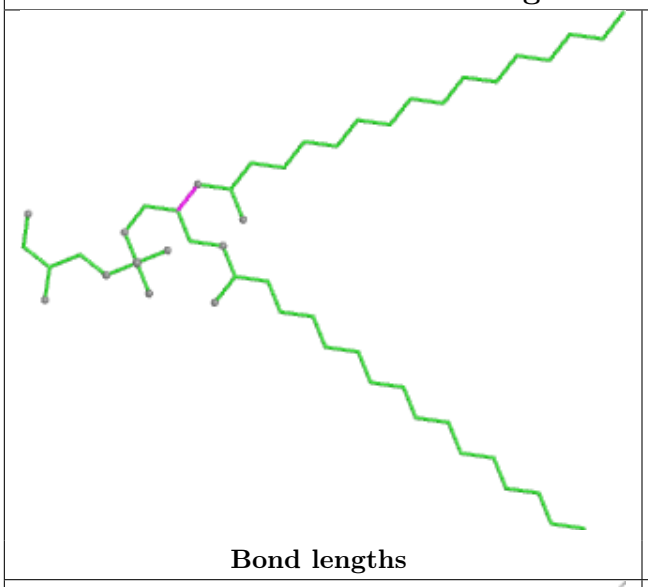


Torsions

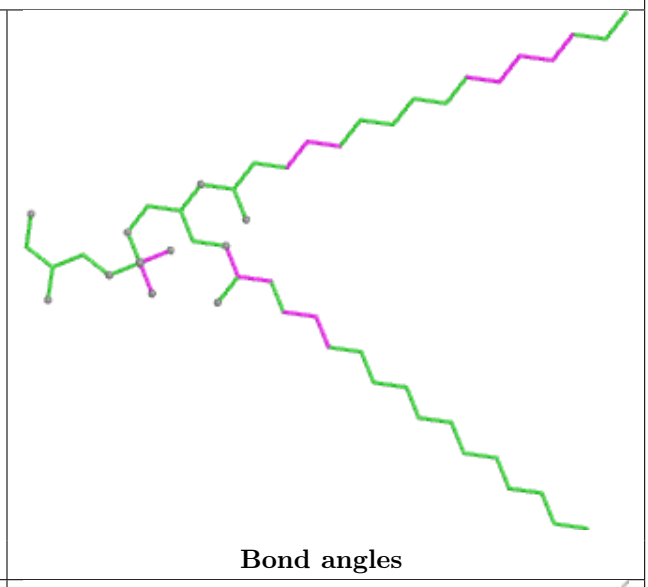


Rings

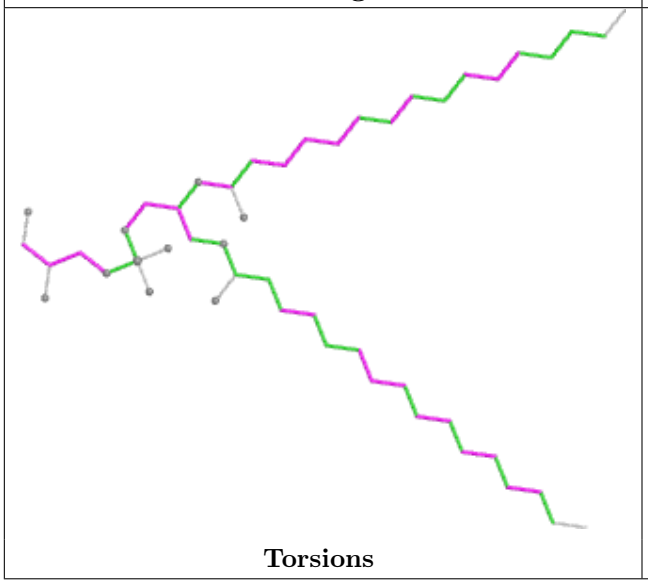
Ligand LHG A 842



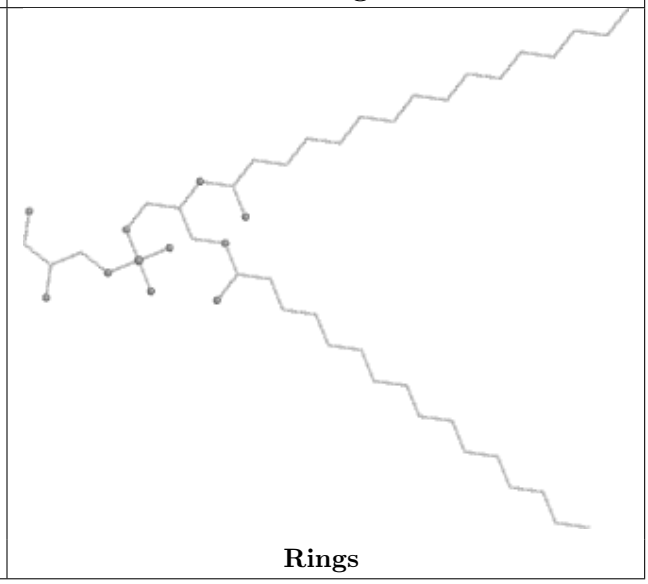
Bond lengths



Bond angles

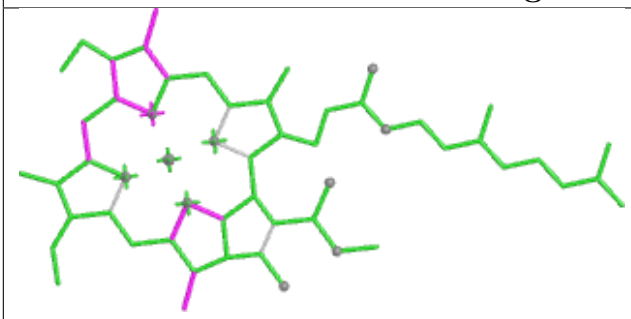


Torsions

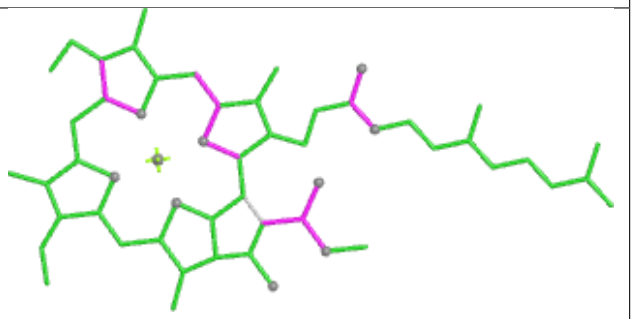


Rings

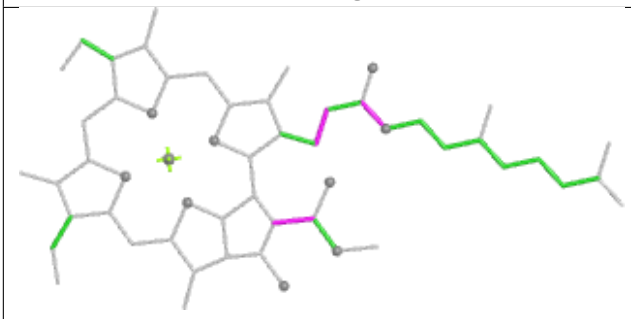
Ligand CLA B 808



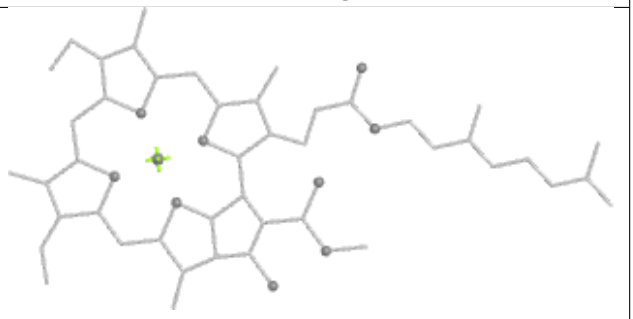
Bond lengths



Bond angles

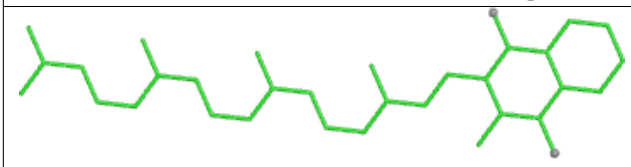


Torsions

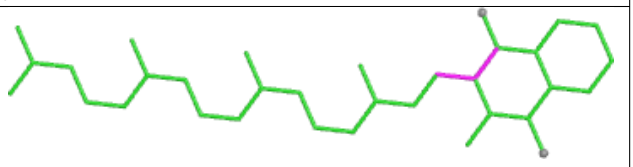


Rings

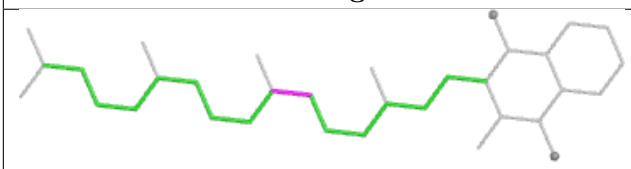
Ligand PQN B 833



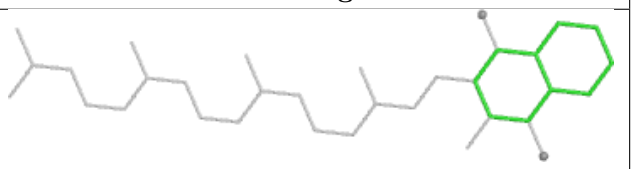
Bond lengths



Bond angles

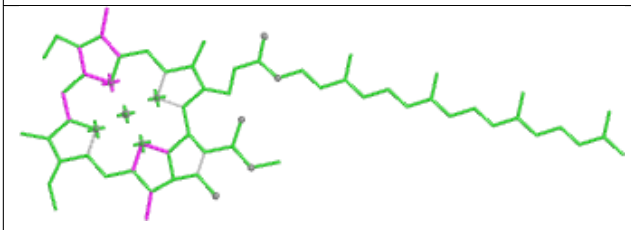


Torsions

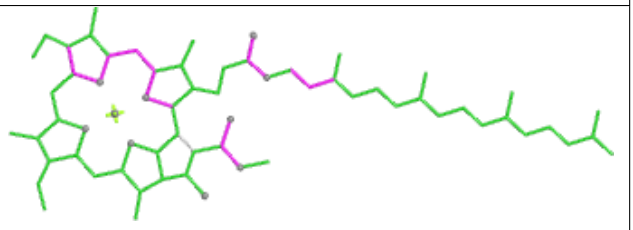


Rings

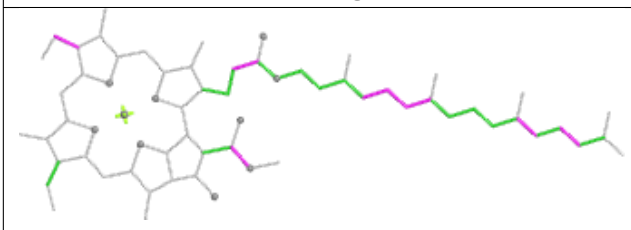
Ligand CLA B 807



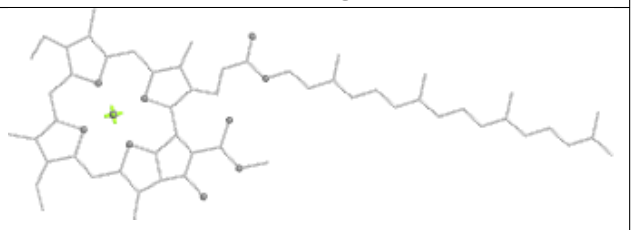
Bond lengths



Bond angles

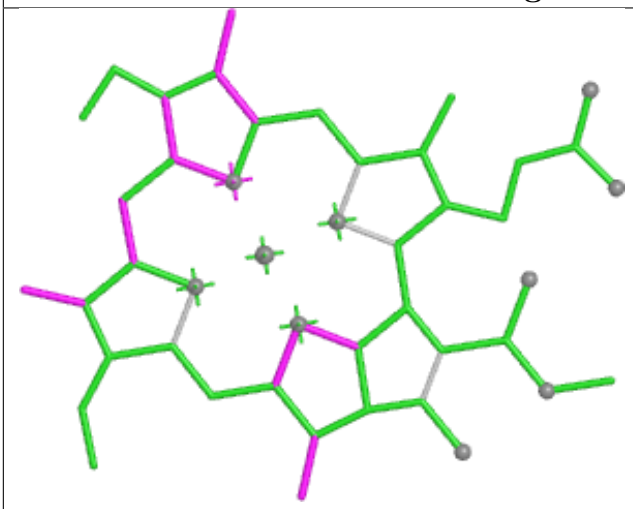


Torsions

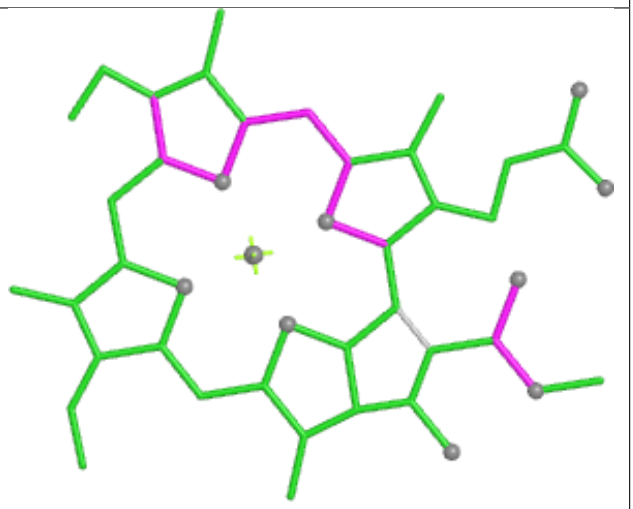


Rings

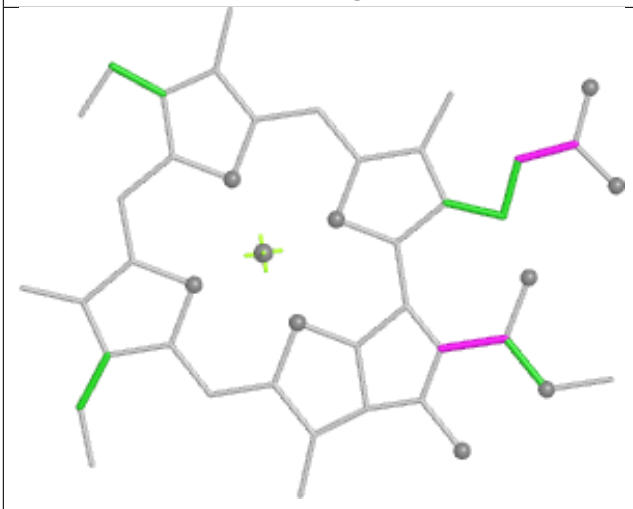
Ligand CLA B 805



Bond lengths



Bond angles

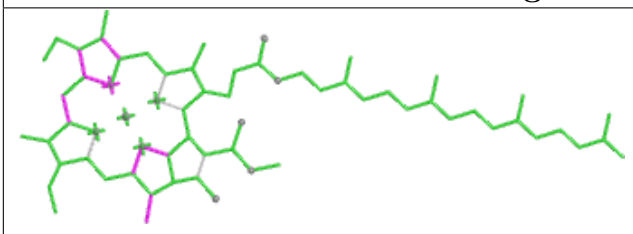


Torsions

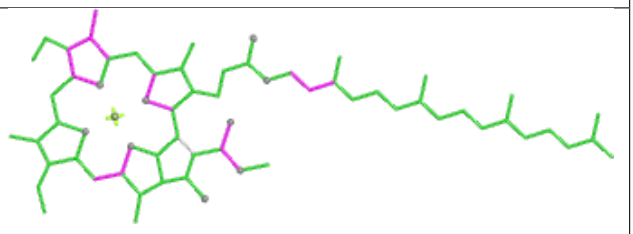


Rings

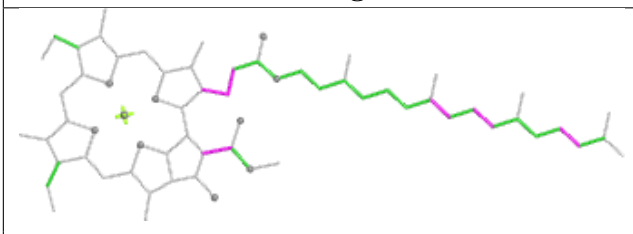
Ligand CLA A 802



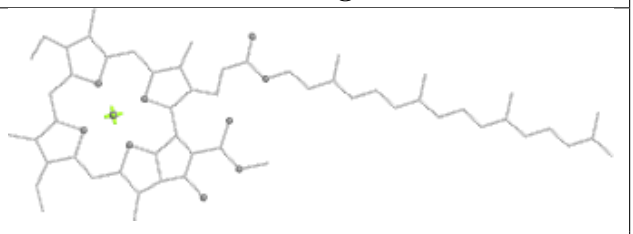
Bond lengths



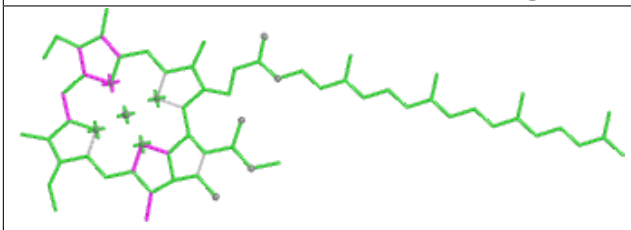
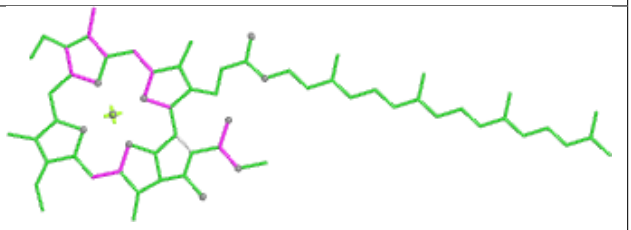
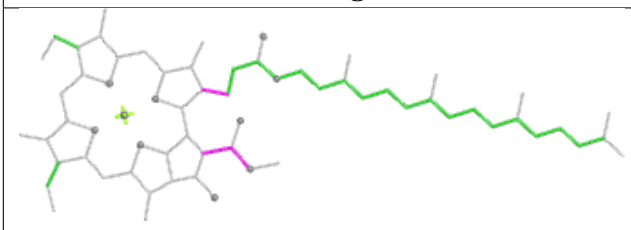
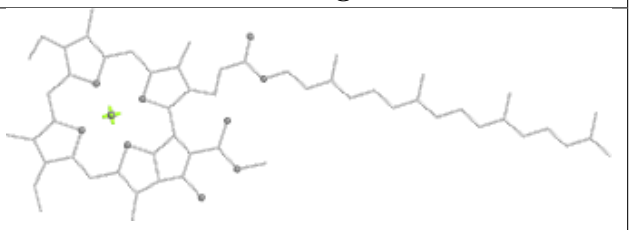
Bond angles

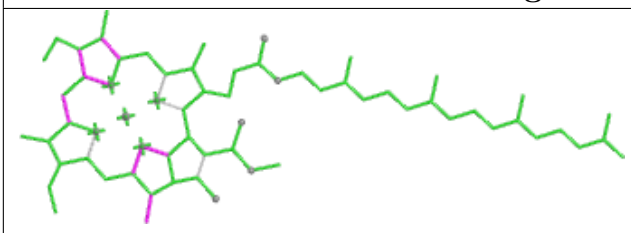
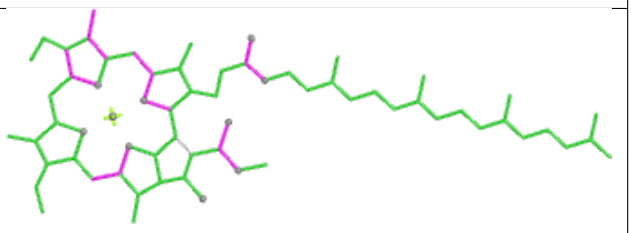
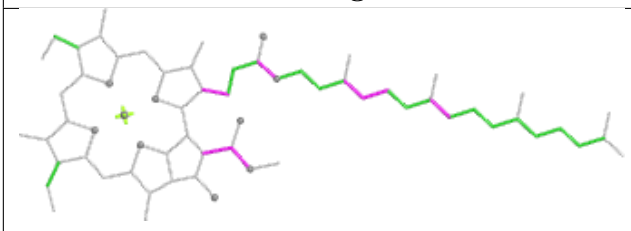
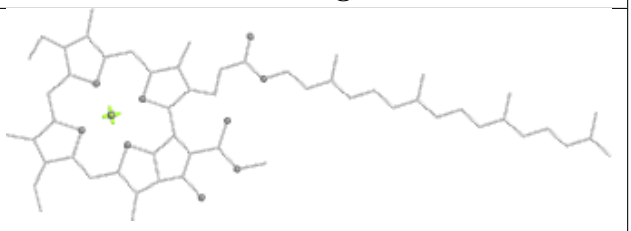


Torsions

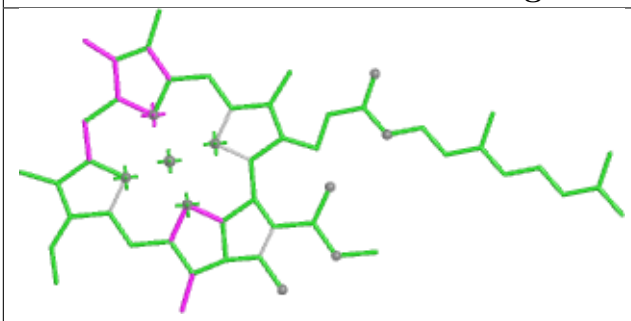


Rings

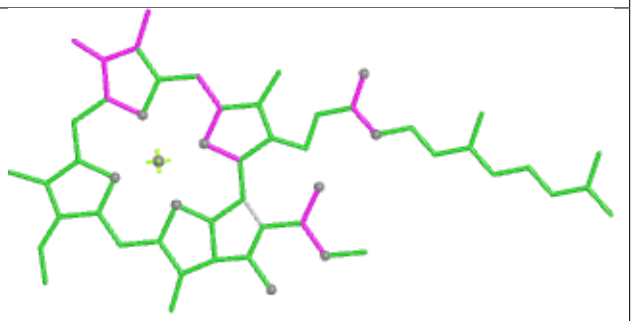
Ligand CLA A 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

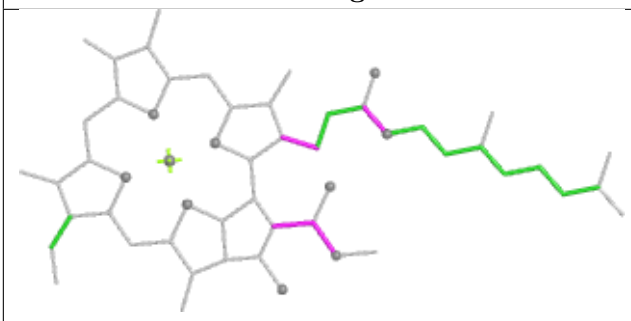
Ligand CLA B 812



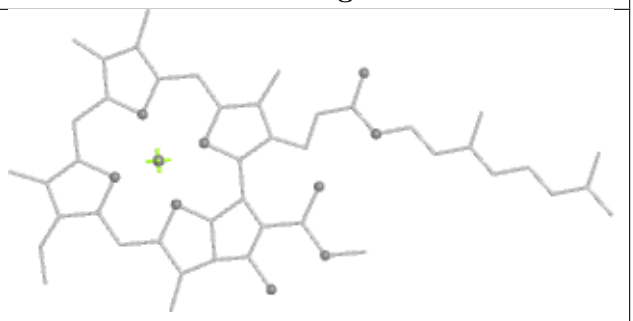
Bond lengths



Bond angles

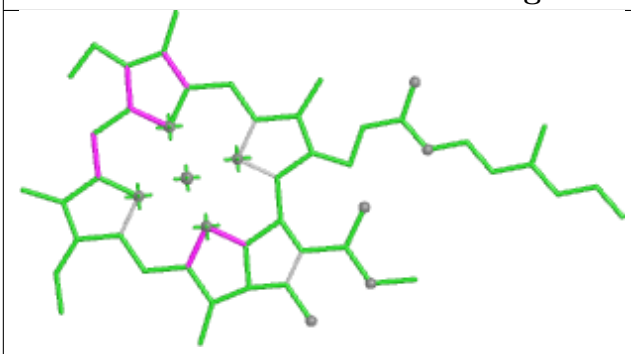


Torsions

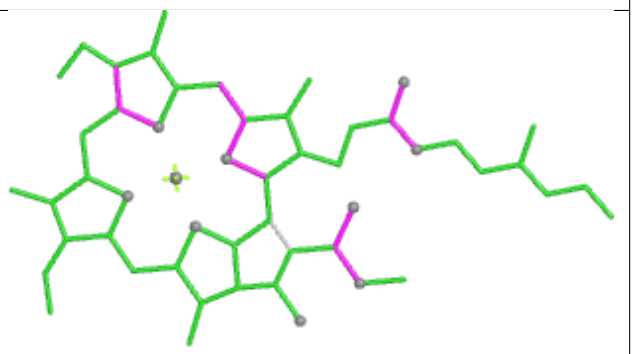


Rings

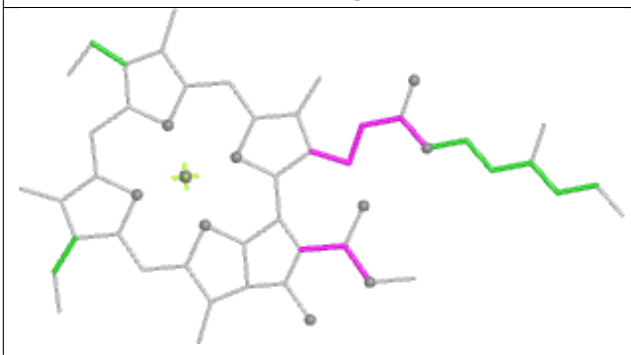
Ligand CLA A 841



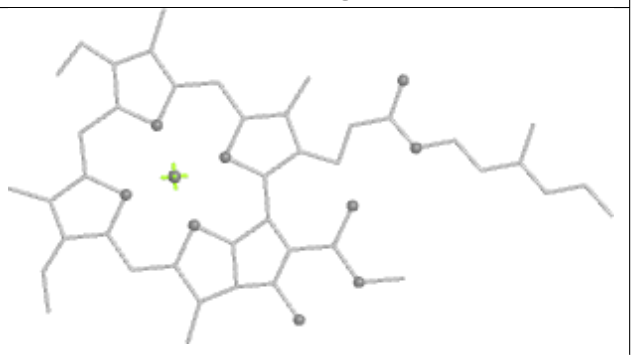
Bond lengths



Bond angles

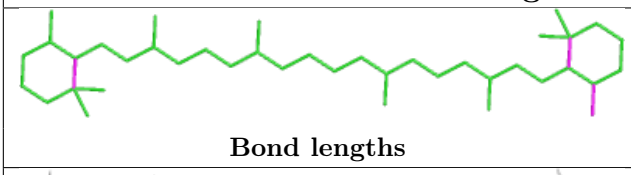


Torsions

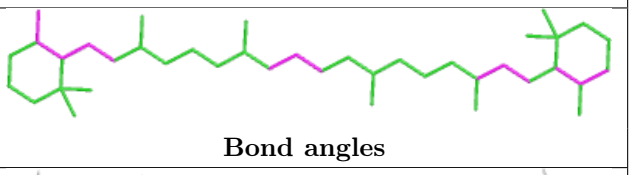


Rings

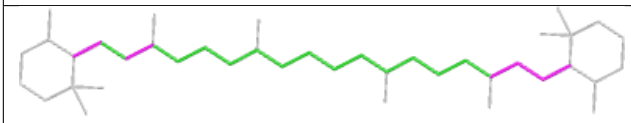
Ligand BCR B 836



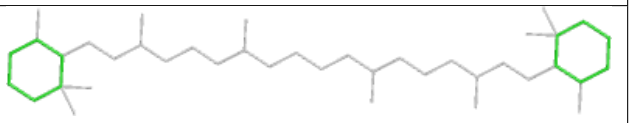
Bond lengths



Bond angles

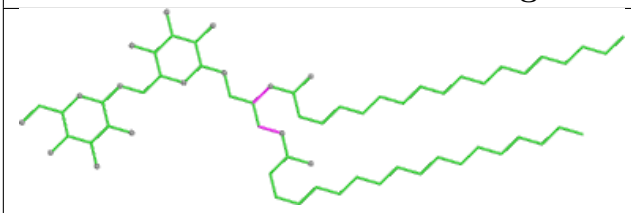


Torsions

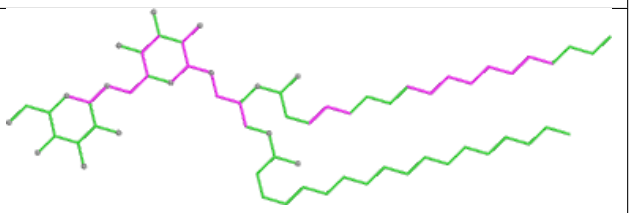


Rings

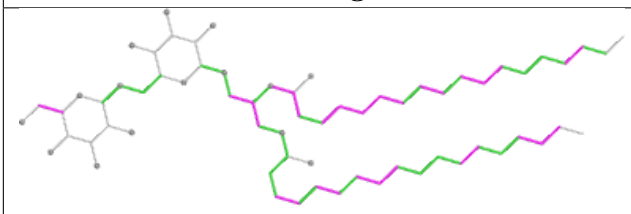
Ligand DGD B 837



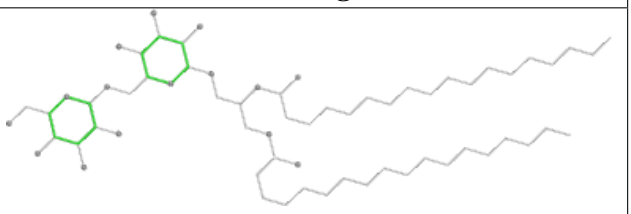
Bond lengths



Bond angles

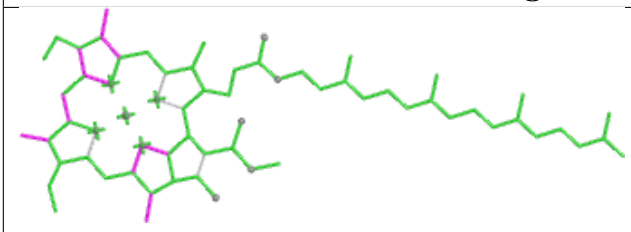


Torsions

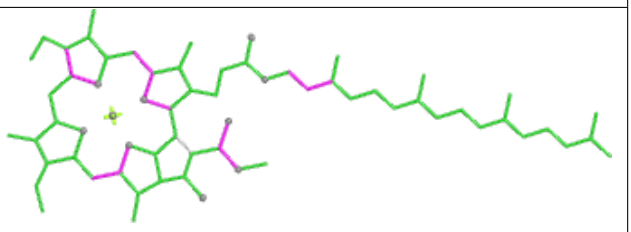


Rings

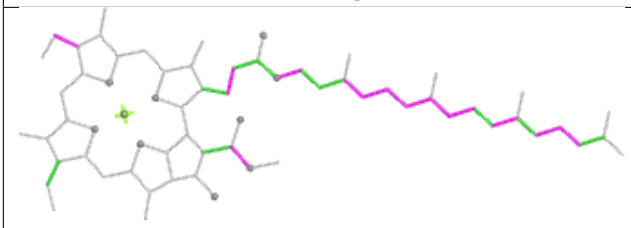
Ligand CLA A 849



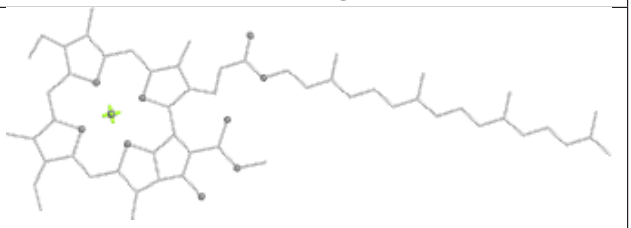
Bond lengths



Bond angles

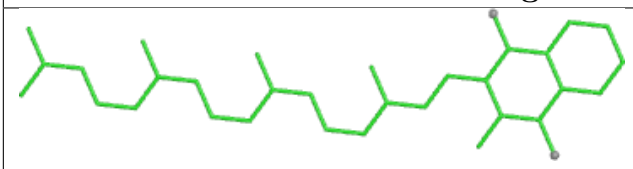


Torsions

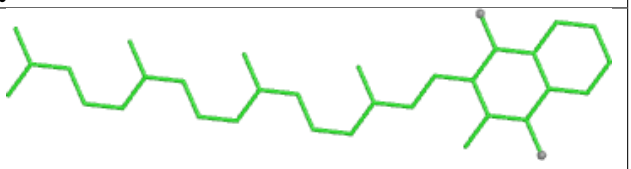


Rings

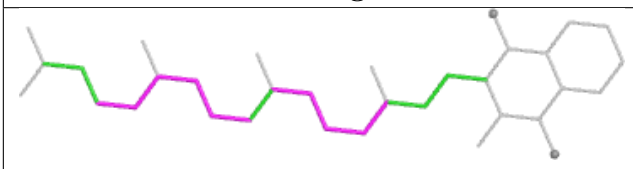
Ligand PQN A 840



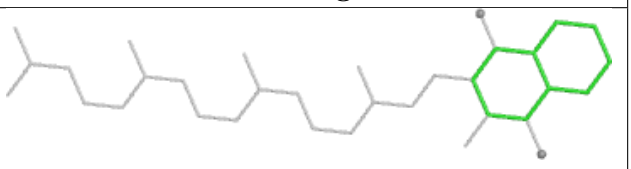
Bond lengths



Bond angles



Torsions

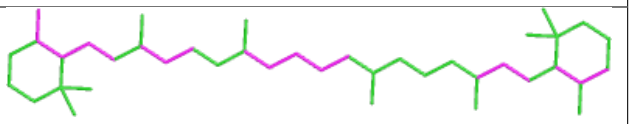


Rings

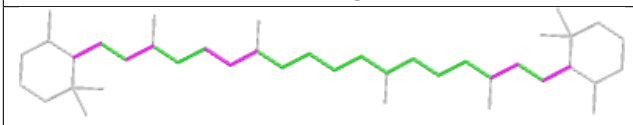
Ligand BCR L 307



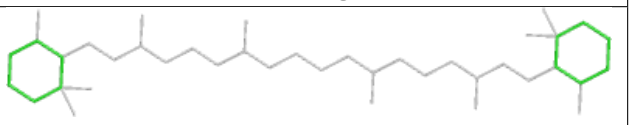
Bond lengths



Bond angles

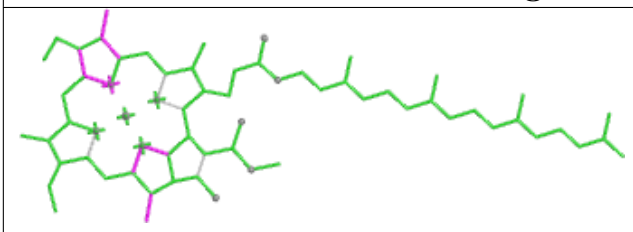


Torsions

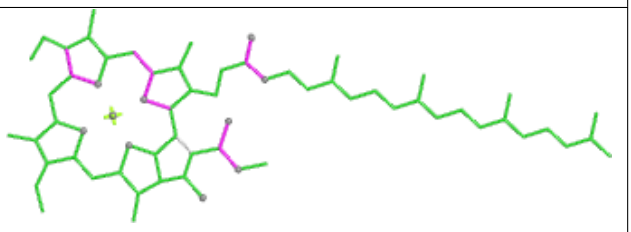


Rings

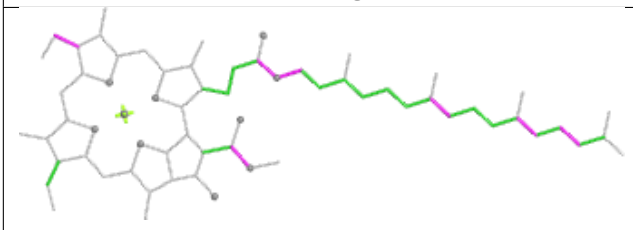
Ligand CLA B 832



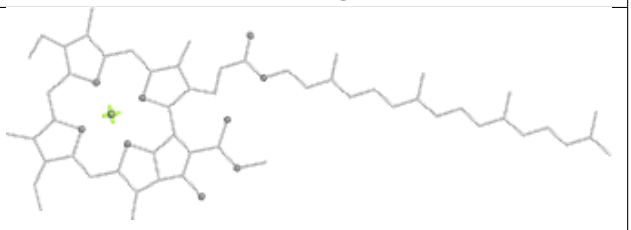
Bond lengths



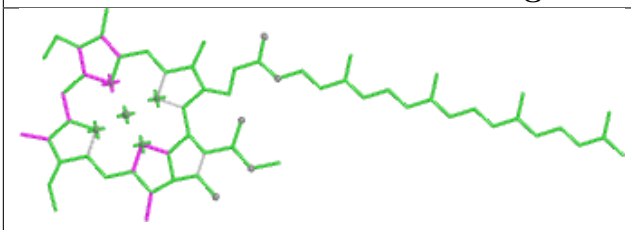
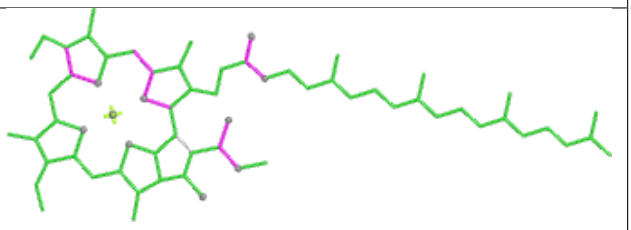
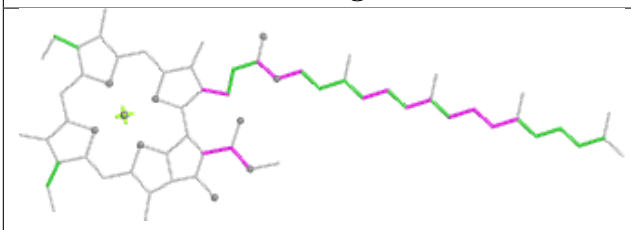
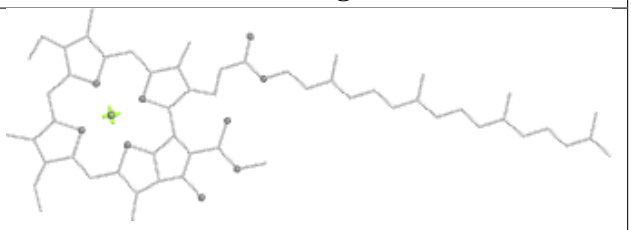
Bond angles

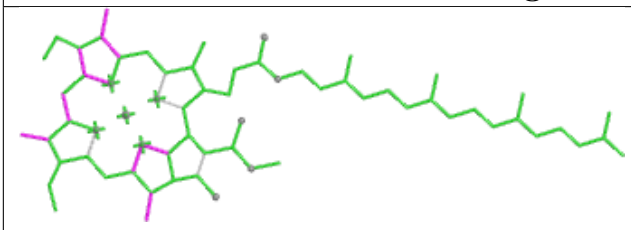
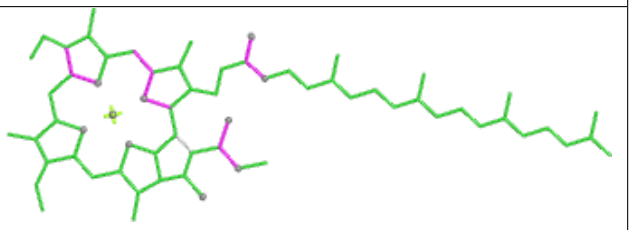
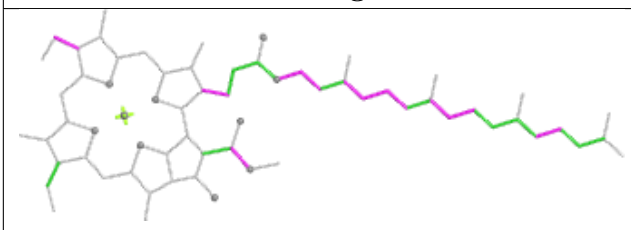
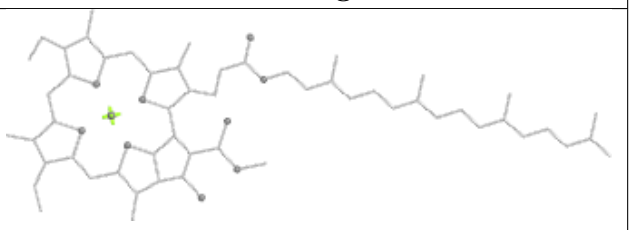


Torsions

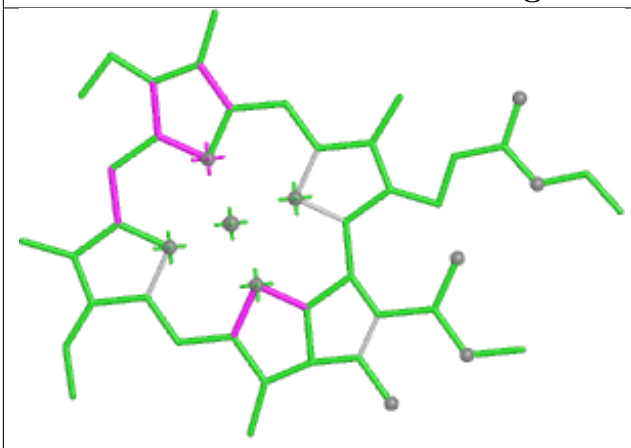


Rings

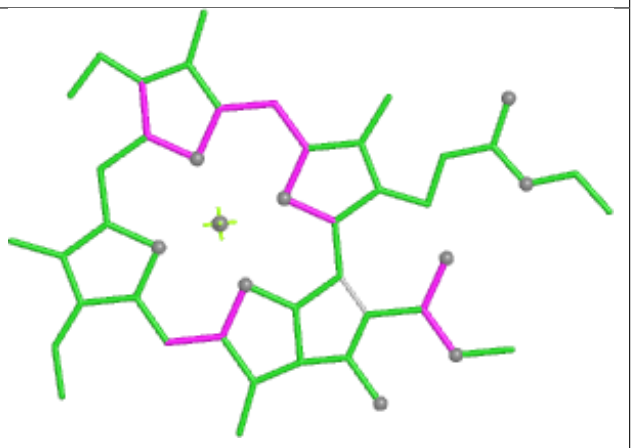
Ligand CLA B 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

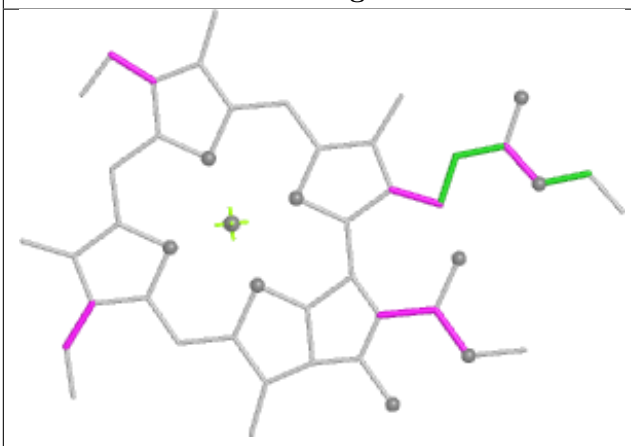
Ligand CLA A 837



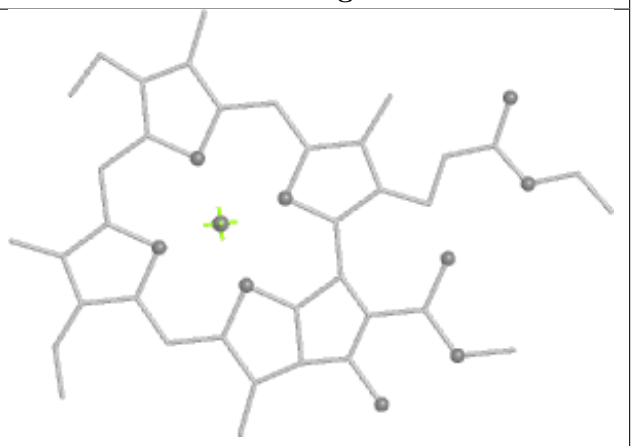
Bond lengths



Bond angles

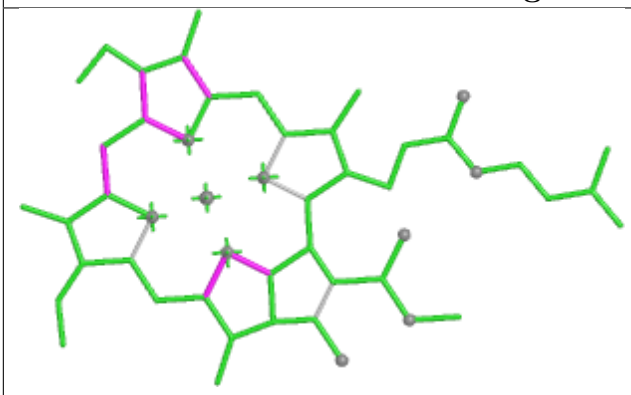


Torsions

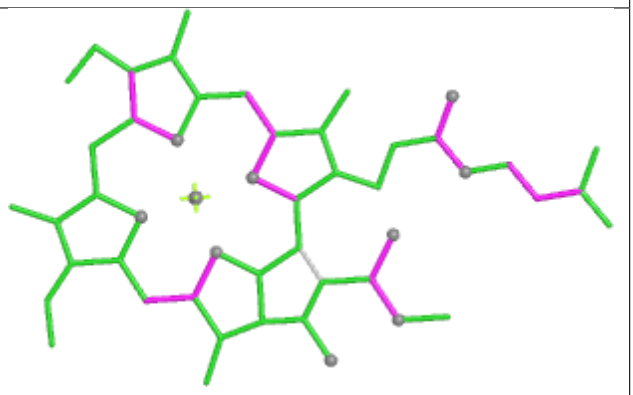


Rings

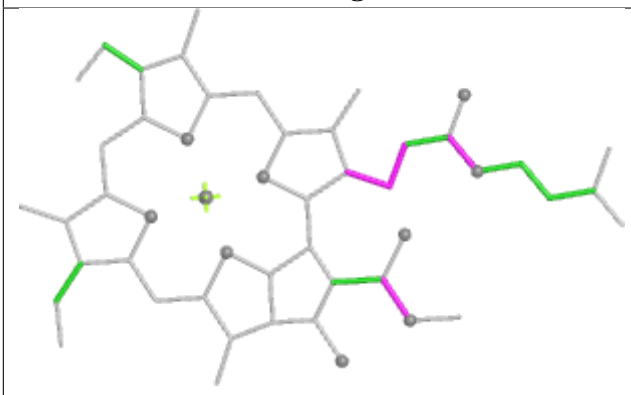
Ligand CLA A 832



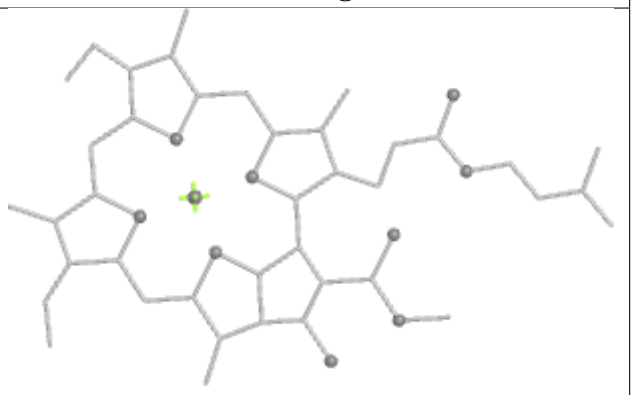
Bond lengths



Bond angles

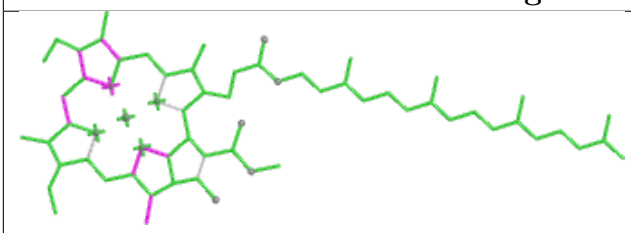


Torsions

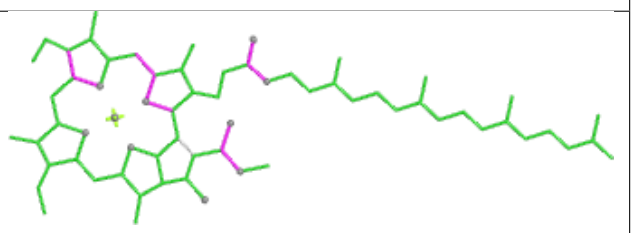


Rings

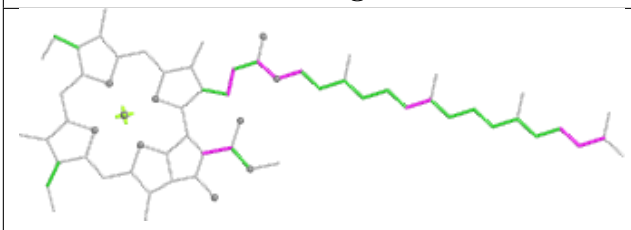
Ligand CLA B 815



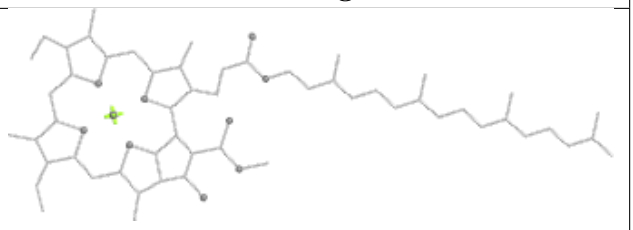
Bond lengths



Bond angles

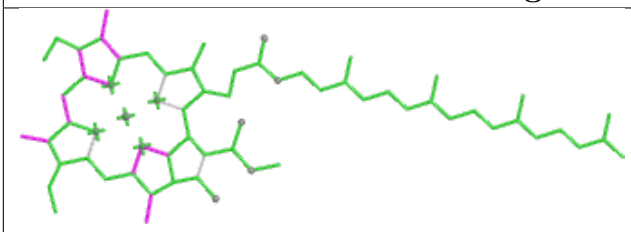


Torsions

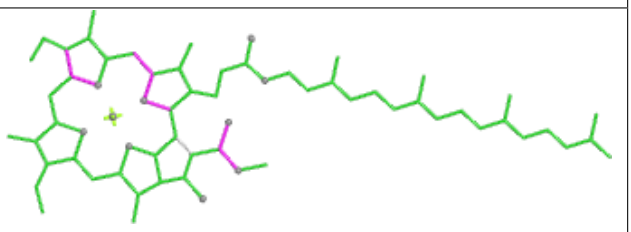


Rings

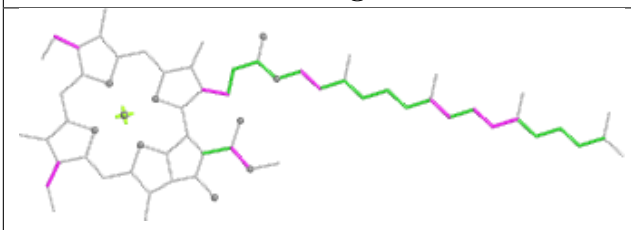
Ligand CLA B 804



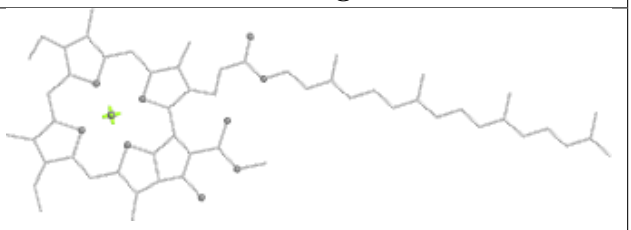
Bond lengths



Bond angles

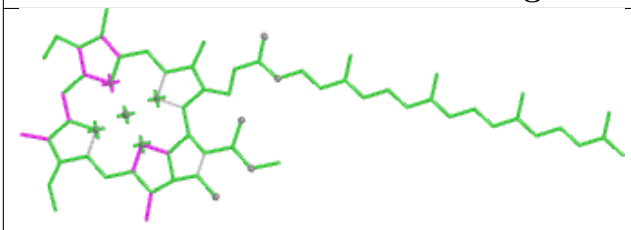


Torsions

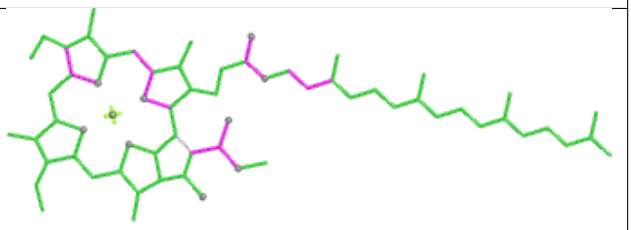


Rings

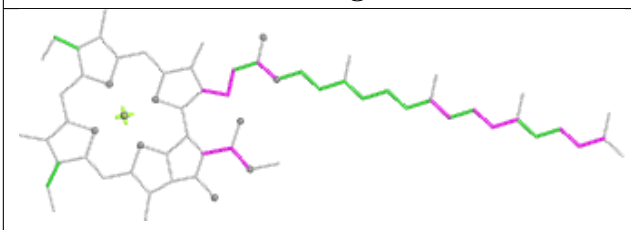
Ligand CLA A 815



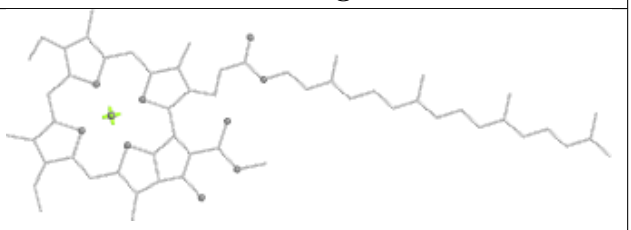
Bond lengths



Bond angles

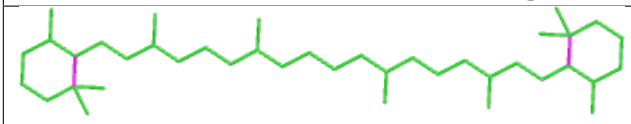


Torsions

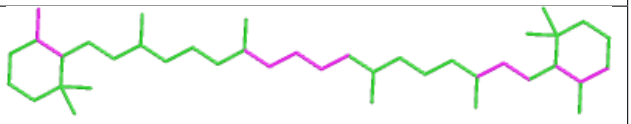


Rings

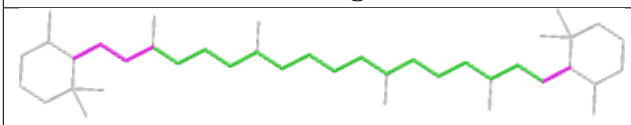
Ligand BCR A 844



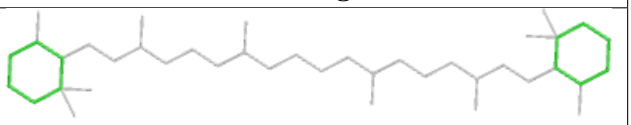
Bond lengths



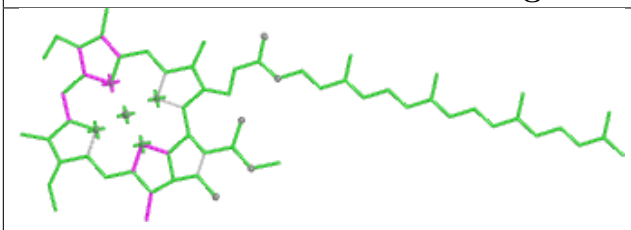
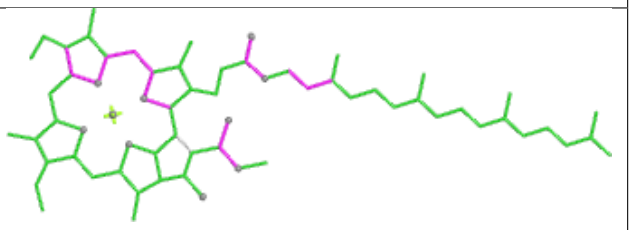
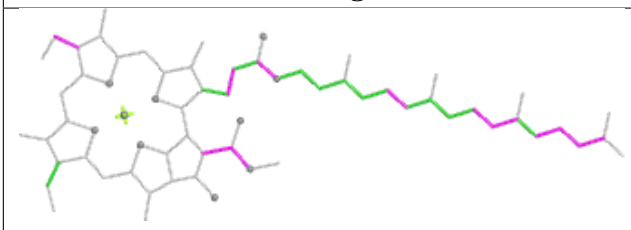
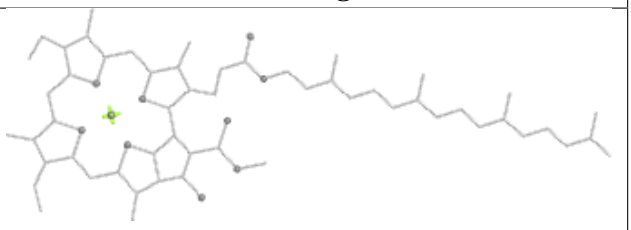
Bond angles

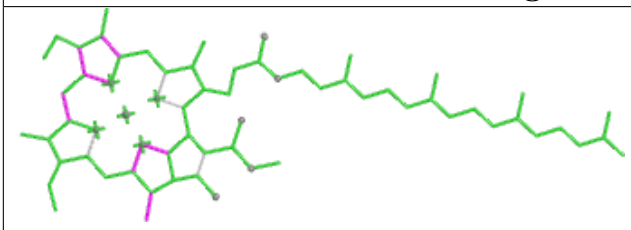
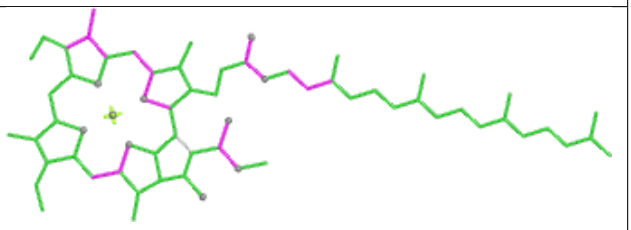
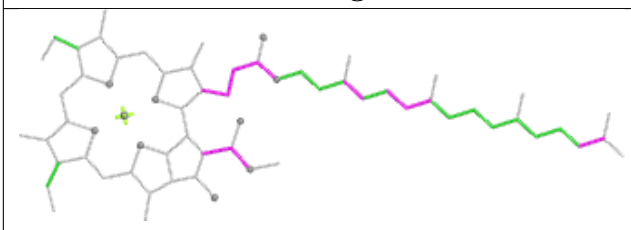
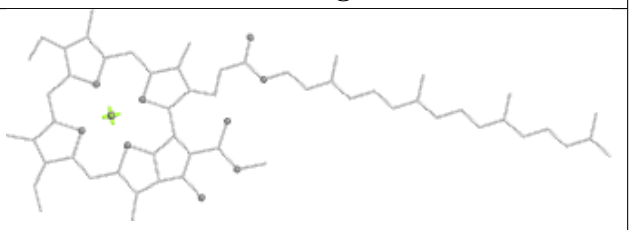


Torsions

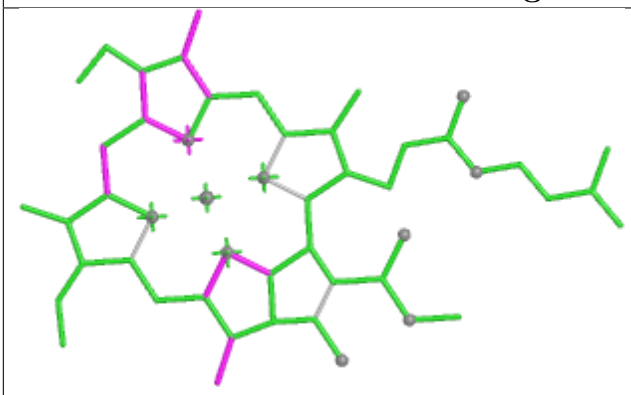


Rings

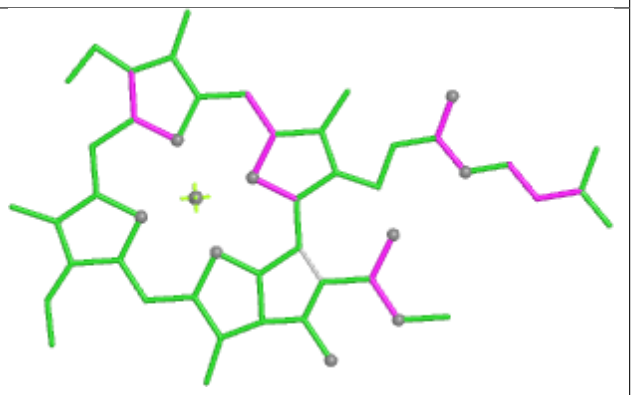
Ligand CLA A 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

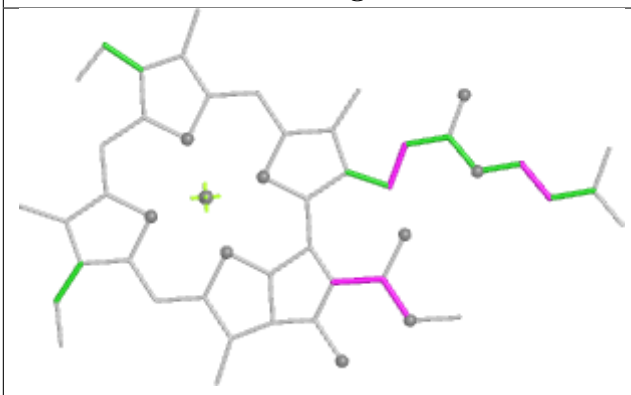
Ligand CLA A 829



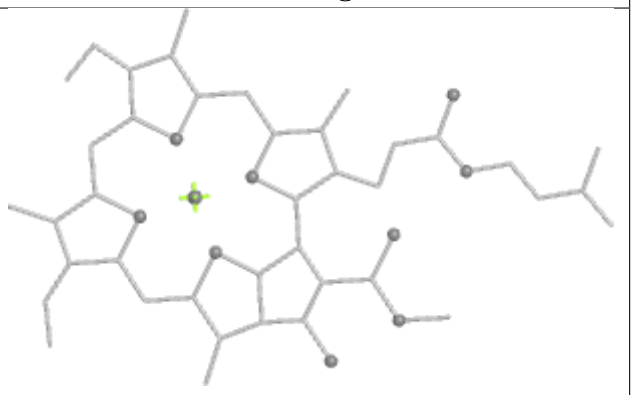
Bond lengths



Bond angles

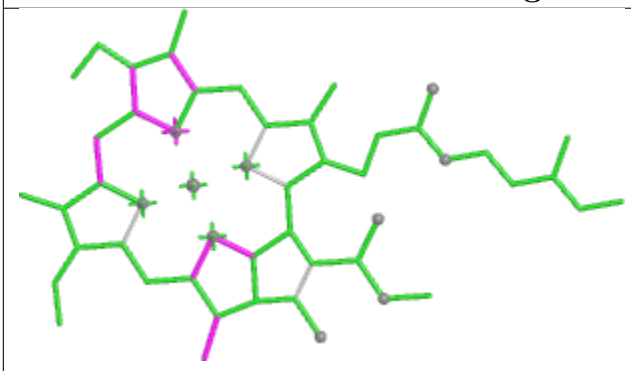


Torsions

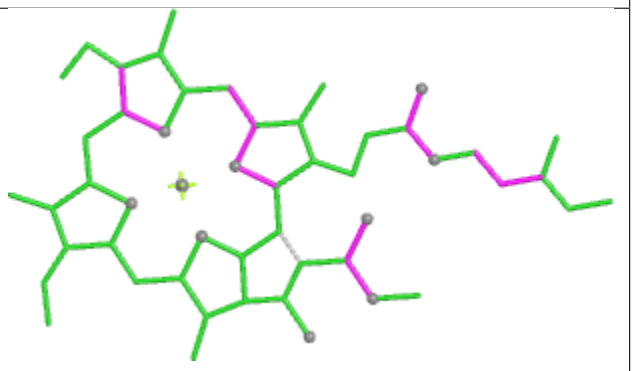


Rings

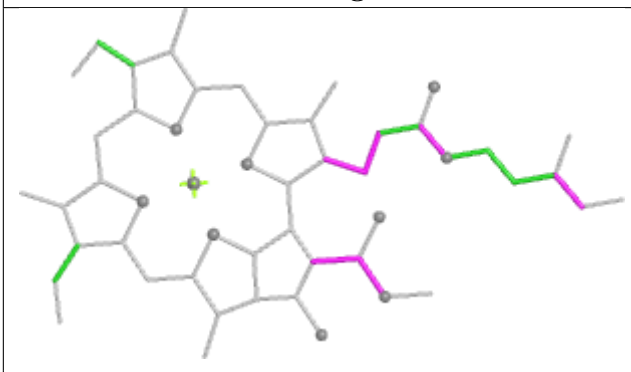
Ligand CLA A 821



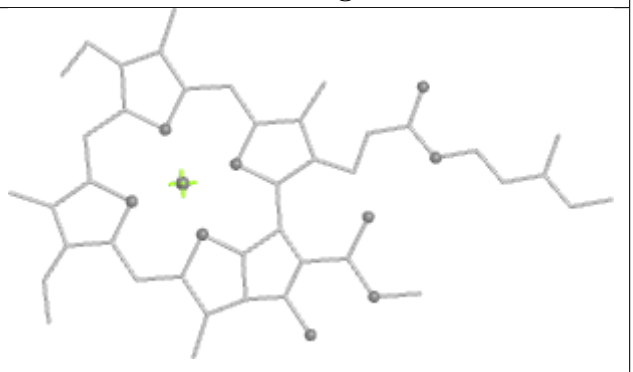
Bond lengths



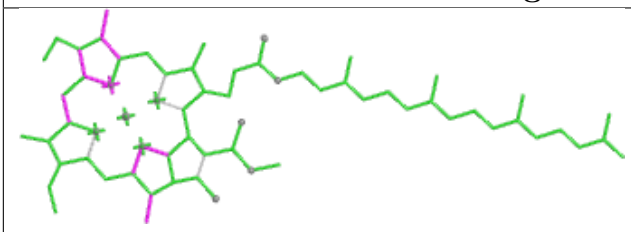
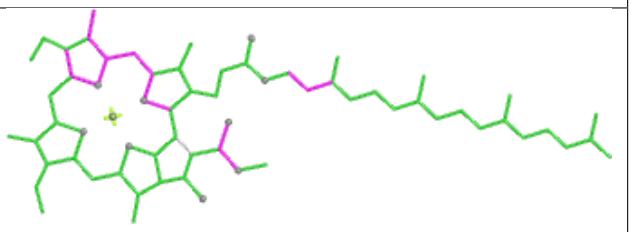
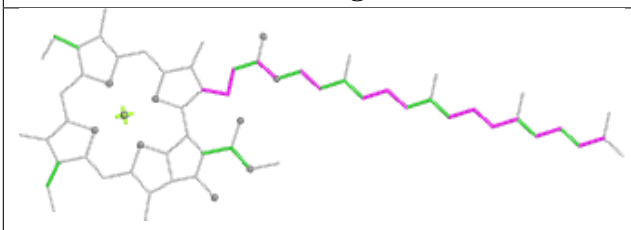
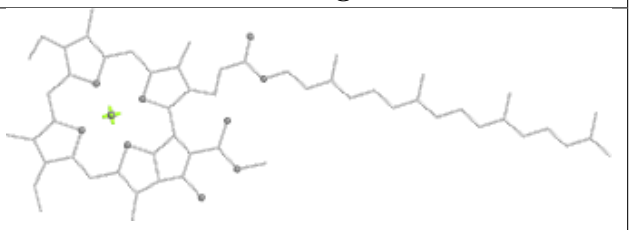
Bond angles



Torsions



Rings

Ligand CLA A 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

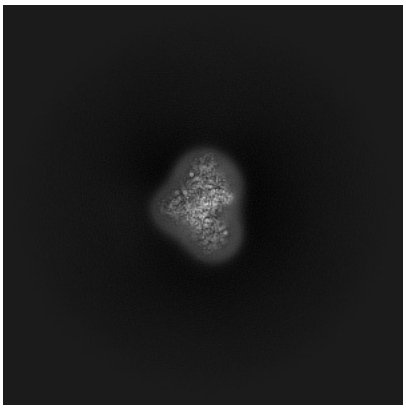
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66967. These allow visual inspection of the internal detail of the map and identification of artifacts.

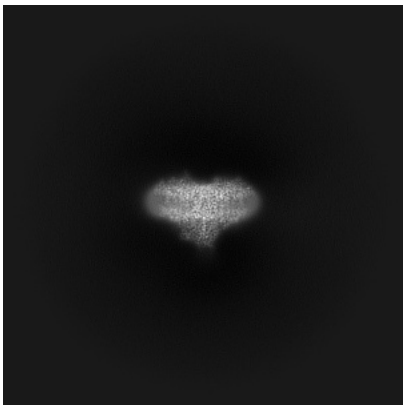
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

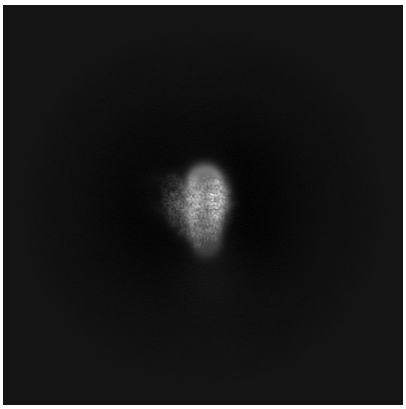
6.1.1 Primary map



X

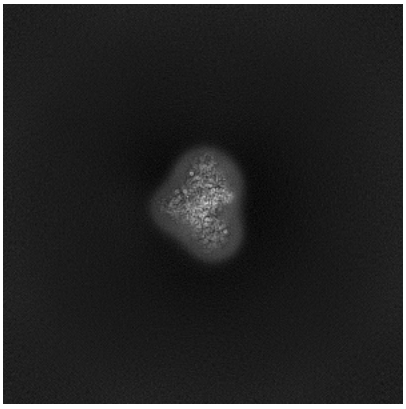


Y

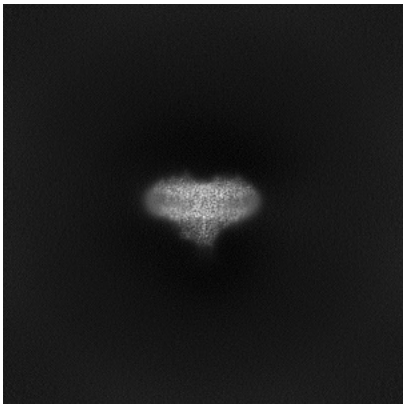


Z

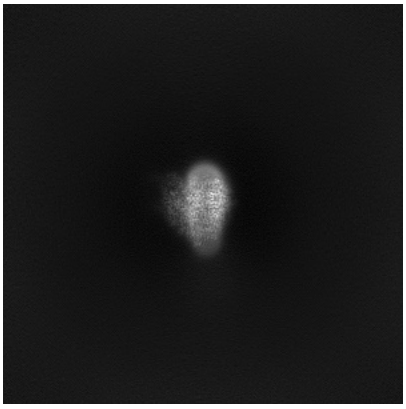
6.1.2 Raw map



X



Y

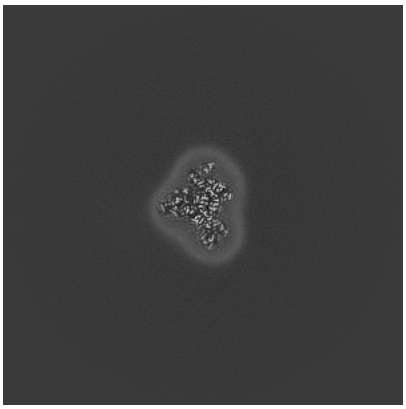


Z

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

6.2 Central slices (i)

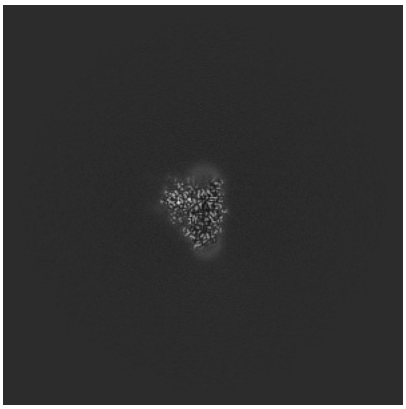
6.2.1 Primary map



X Index: 256

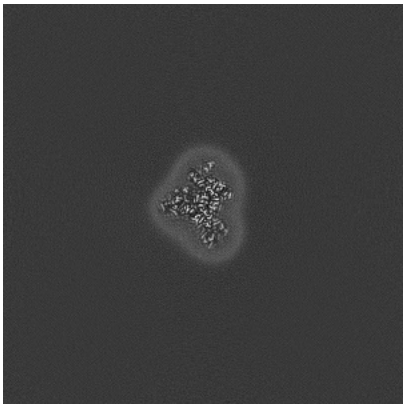


Y Index: 256



Z Index: 256

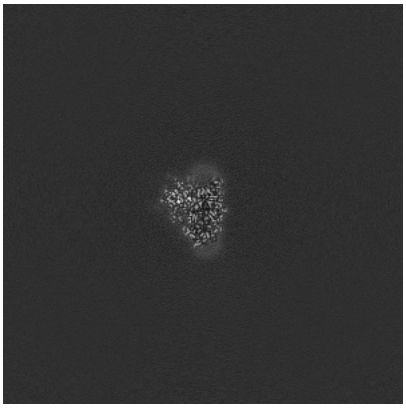
6.2.2 Raw map



X Index: 256



Y Index: 256

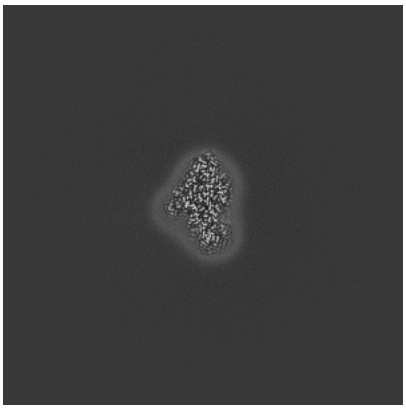


Z Index: 256

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

6.3 Largest variance slices (i)

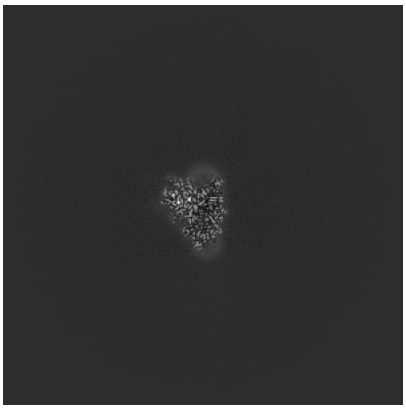
6.3.1 Primary map



X Index: 268

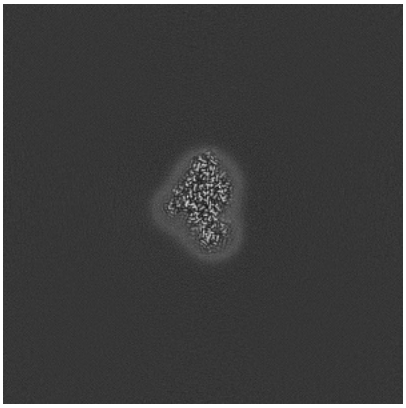


Y Index: 258

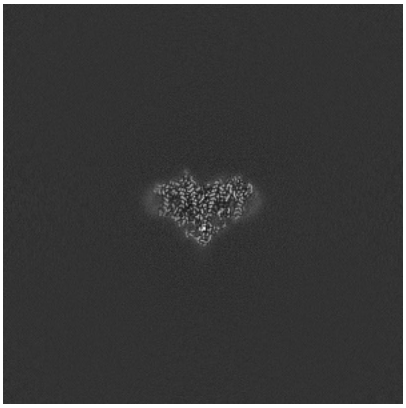


Z Index: 257

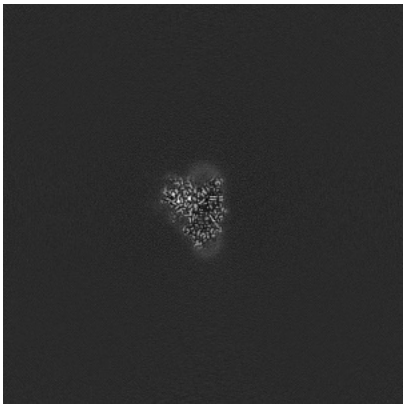
6.3.2 Raw map



X Index: 268



Y Index: 258

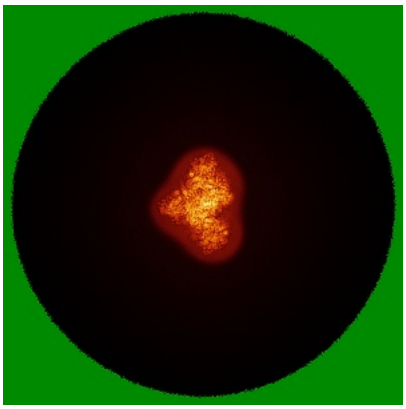


Z Index: 257

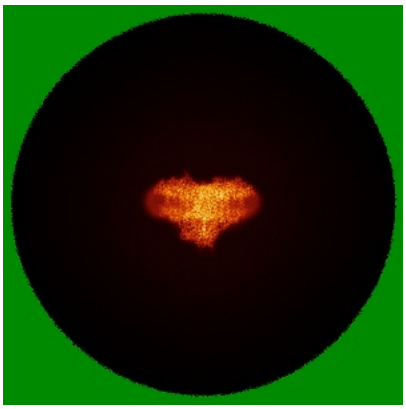
The images above show the largest variance slices of the map in three orthogonal directions.

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

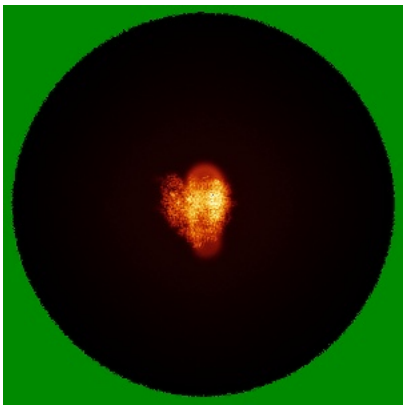
6.4.1 Primary map



X

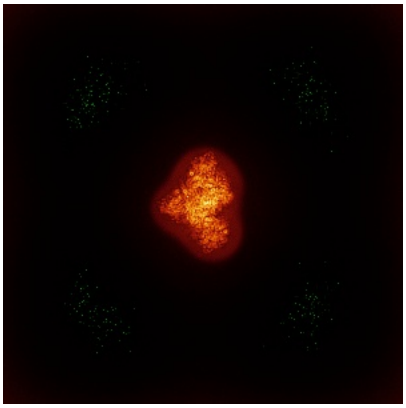


Y

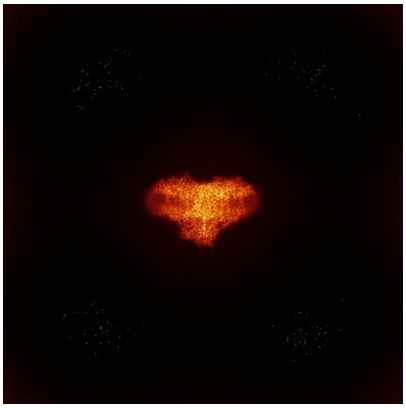


Z

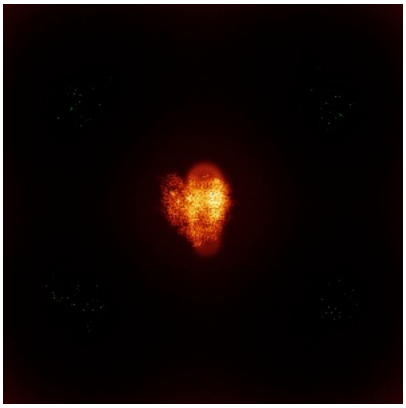
6.4.2 Raw map



X



Y

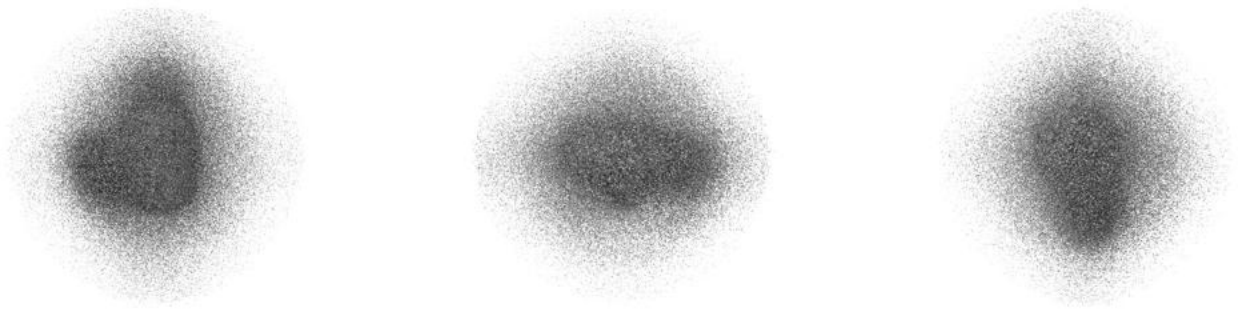


Z

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)

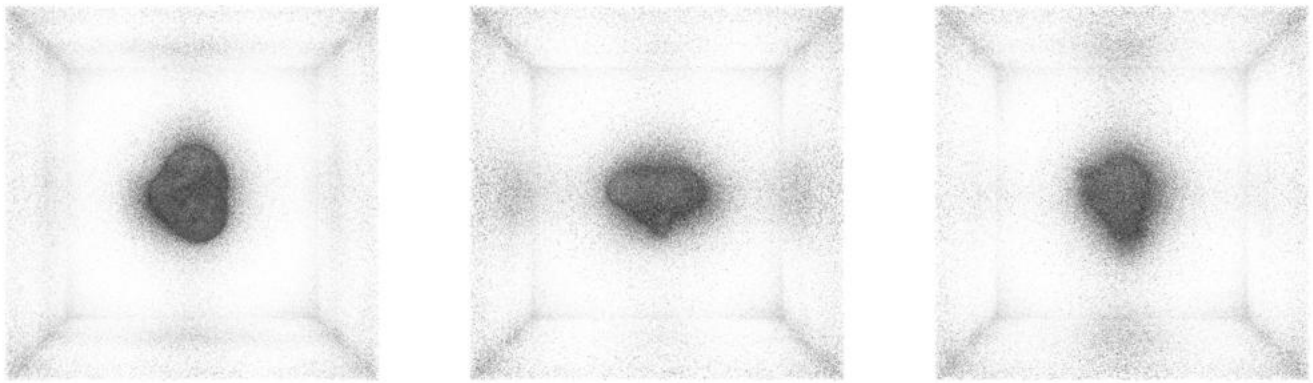
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0233. 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.

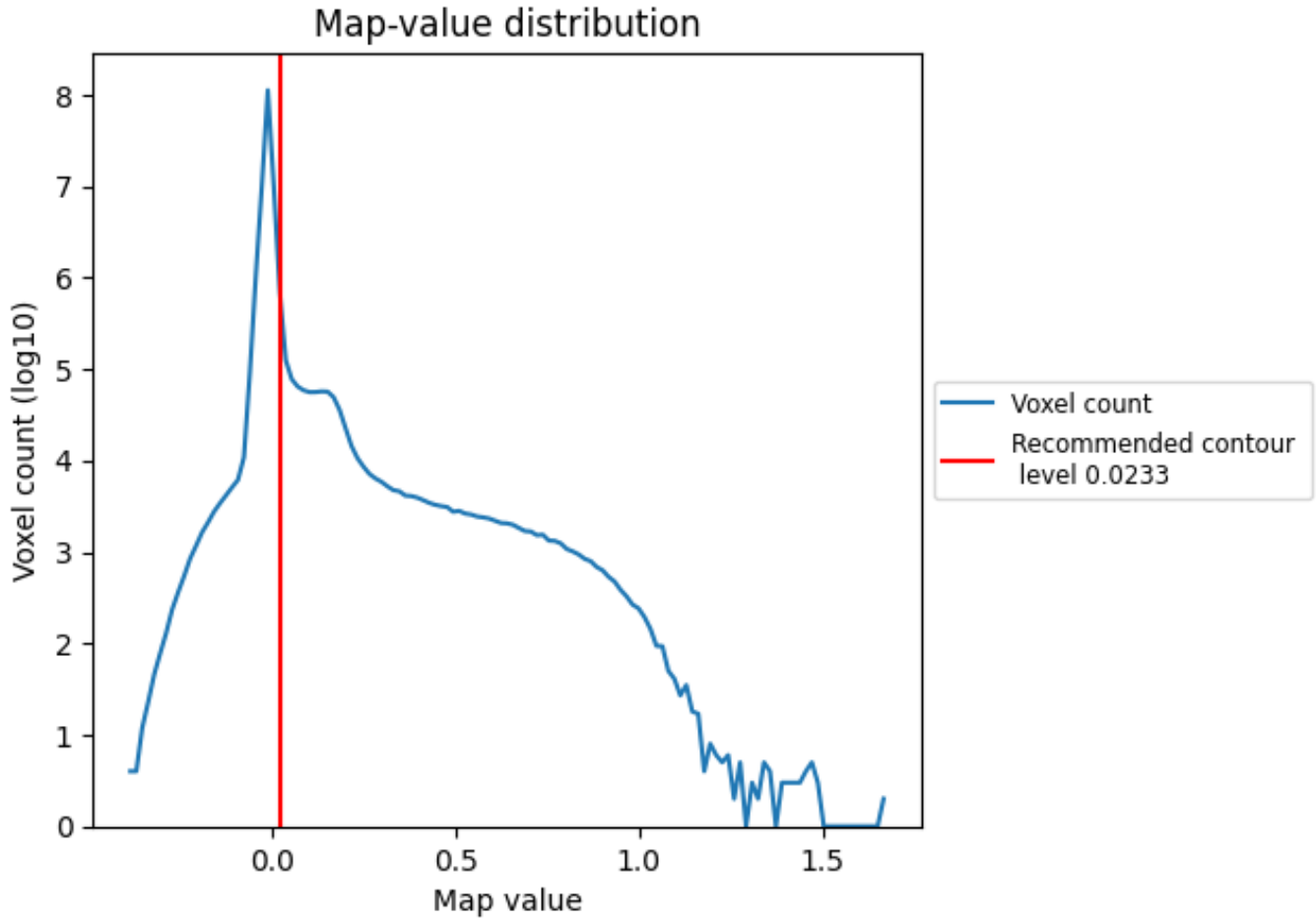
6.6 Mask visualisation (i)

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

7 Map analysis

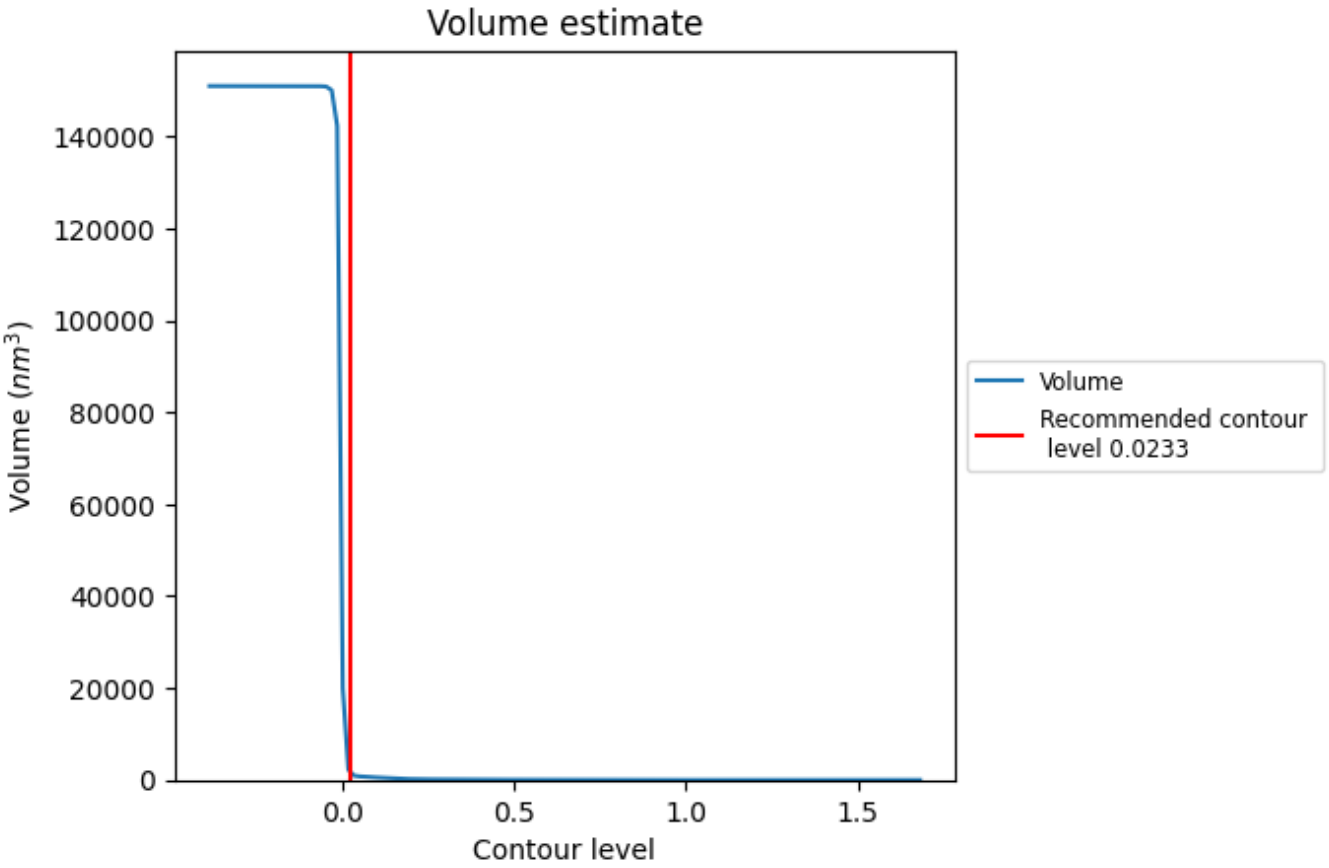
This section contains the results of statistical analysis of the map.

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.

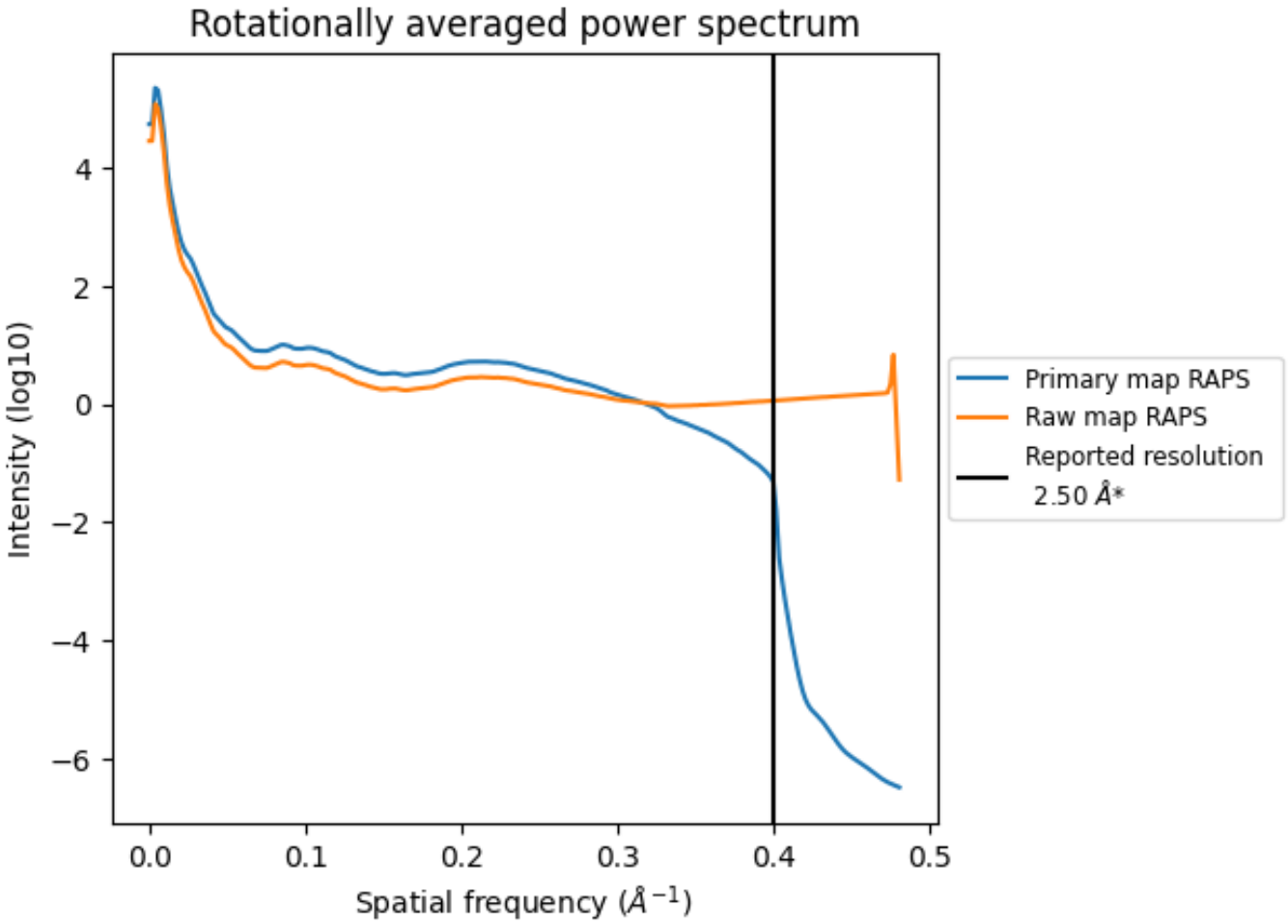
7.2 Volume estimate



The volume at the recommended contour level is 1872 nm^3; this corresponds to an approximate mass of 1691 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)

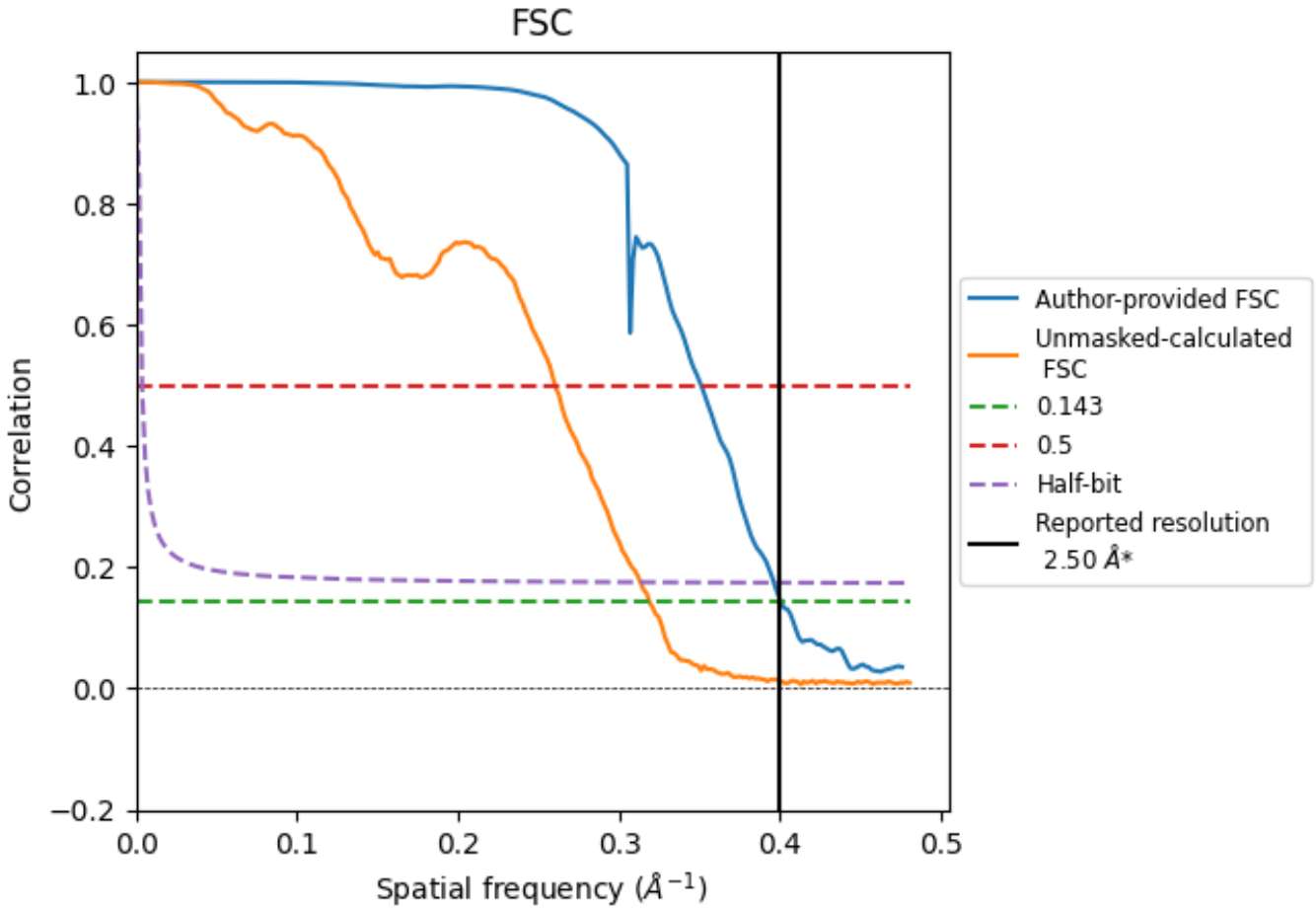


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

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 0.400 Å^{-1}

8.2 Resolution estimates (i)

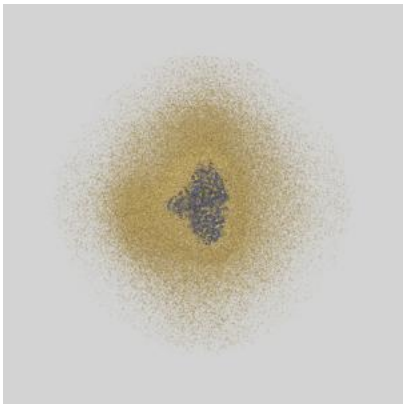
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.50	2.85	2.52
Unmasked-calculated*	3.13	3.84	3.19

*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 3.13 differs from the reported value 2.5 by more than 10 %

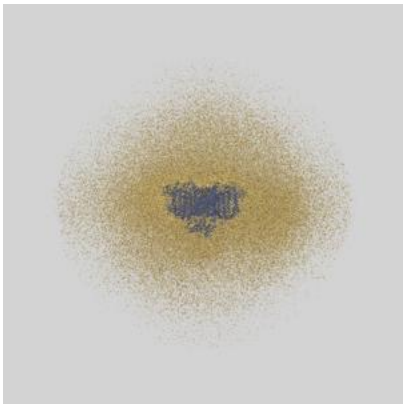
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66967 and PDB model 9XKK. Per-residue inclusion information can be found in section 3 on page 14.

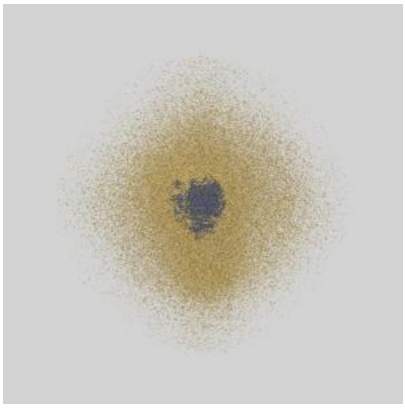
9.1 Map-model overlay



X



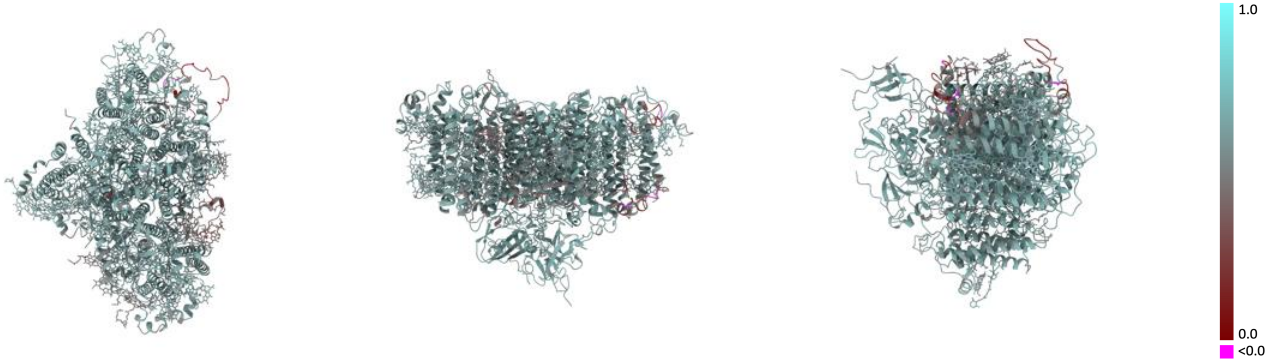
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0233 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.

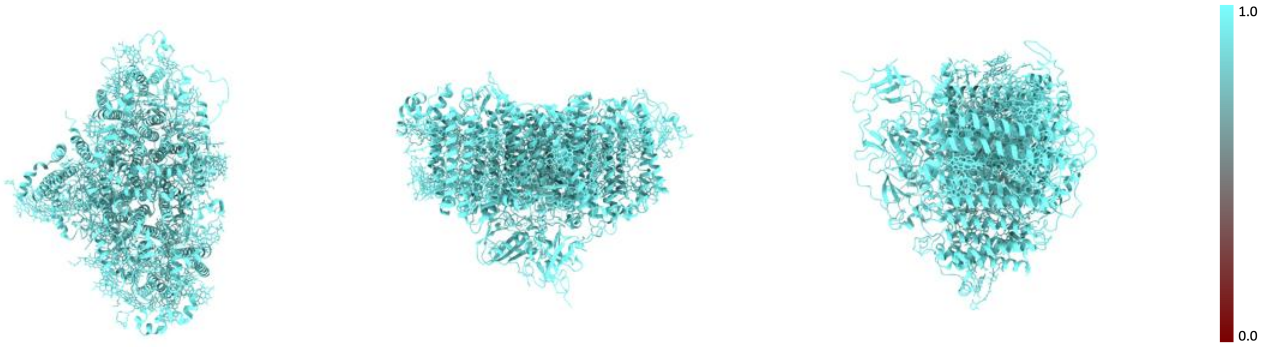
9.2 Q-score mapped to coordinate model (i)



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.

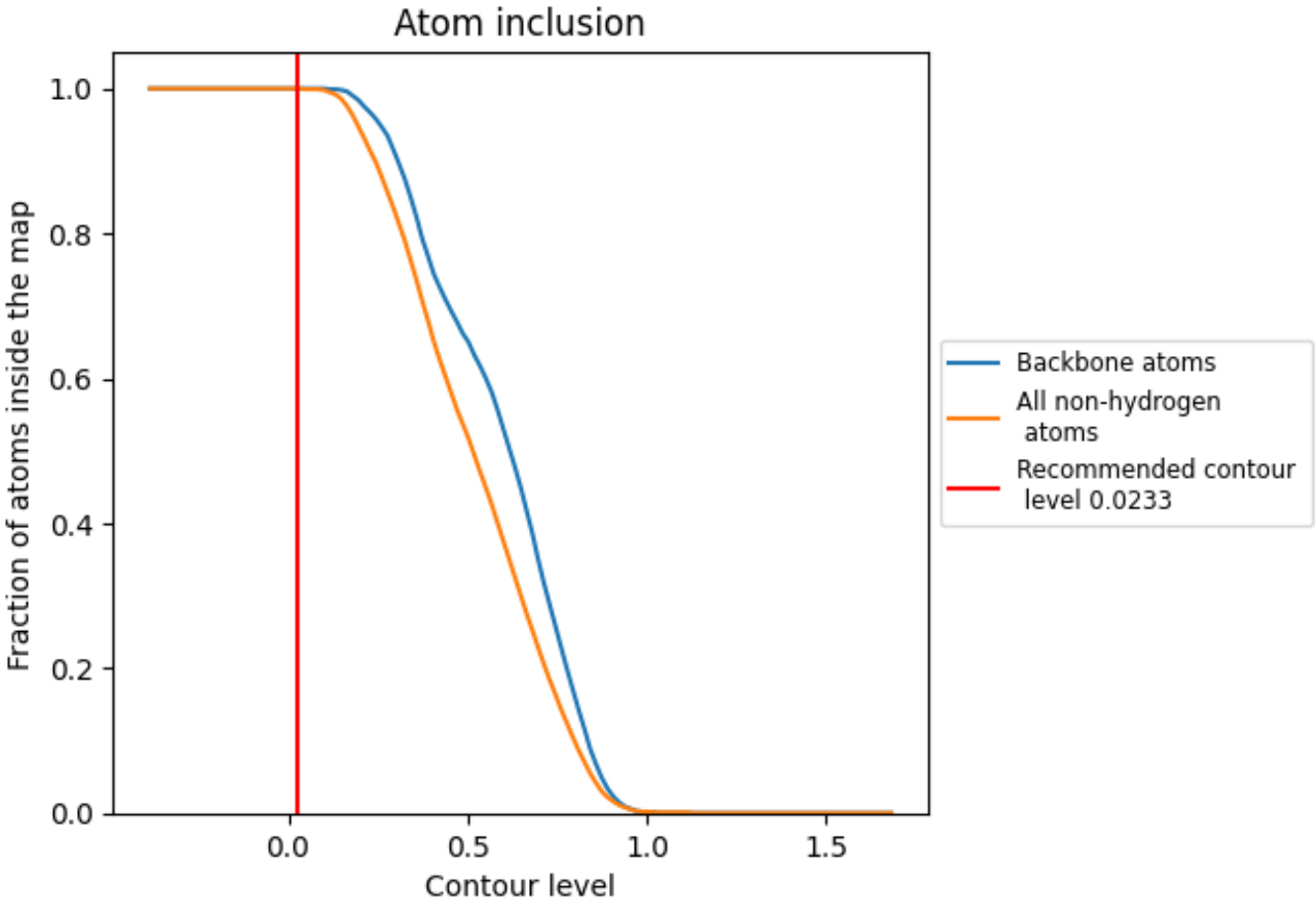
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0233).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0233) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	1.0000	0.5930
A	0.9990	0.5840
B	1.0000	0.5960
C	0.9980	0.6180
D	1.0000	0.6210
E	1.0000	0.5930
H	1.0000	0.5990
I	1.0000	0.5890
L	1.0000	0.5960

