Full wwPDB EM Validation Report ⓘ

Sep 24, 2023 – 12:12 AM JST

PDB ID	:	8IWZ
EMDB ID	:	EMD-35784
Title	:	Cryo-EM structure of unprotonated LHCII in detergent solution at low pH value
Authors	:	Ruan, M.X.; Ding, W.
Deposited on	:	2023-03-31
Resolution	:	2.52 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:

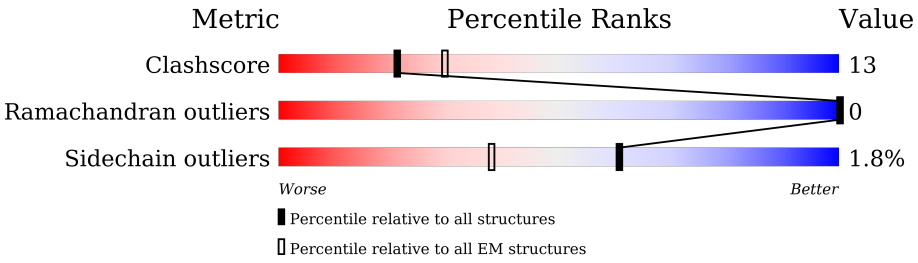
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.52 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	G	218	79% 20%
1	N	218	87% 13%
1	Y	218	81% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CHL	G	601	X	-	-	-
2	CHL	G	605	X	-	-	-
2	CHL	G	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CHL	G	607	X	-	-	-
2	CHL	G	608	X	-	-	-
2	CHL	G	609	X	-	-	-
2	CHL	N	601	X	-	-	-
2	CHL	N	605	X	-	-	-
2	CHL	N	606	X	-	-	-
2	CHL	N	607	X	-	-	-
2	CHL	N	608	X	-	-	-
2	CHL	N	609	X	-	-	-
2	CHL	Y	302	X	-	-	-
2	CHL	Y	306	X	-	-	-
2	CHL	Y	307	X	-	-	-
2	CHL	Y	308	X	-	-	-
2	CHL	Y	309	X	-	-	-
2	CHL	Y	310	X	-	-	-
3	CLA	G	602	X	-	-	-
3	CLA	G	603	X	-	-	-
3	CLA	G	610	X	-	-	-
3	CLA	G	612	X	-	-	-
3	CLA	G	614	X	-	-	-
3	CLA	N	602	X	-	-	-
3	CLA	N	603	X	-	-	-
3	CLA	N	604	X	-	-	-
3	CLA	N	610	X	-	-	-
3	CLA	N	611	X	-	-	-
3	CLA	N	612	X	-	-	-
3	CLA	N	613	X	-	-	-
3	CLA	N	614	X	-	-	-
3	CLA	Y	303	X	-	-	-
3	CLA	Y	304	X	-	-	-
3	CLA	Y	305	X	-	-	-
3	CLA	Y	311	X	-	-	-
3	CLA	Y	313	X	-	-	-
3	CLA	Y	314	X	-	-	-
3	CLA	Y	315	X	-	-	-

2 Entry composition

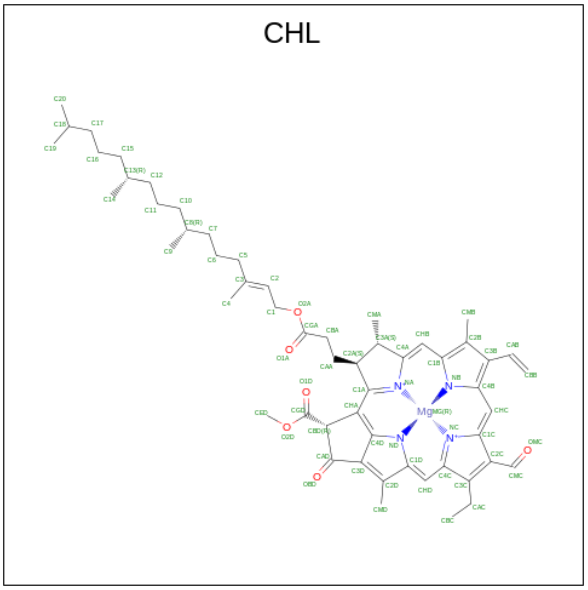
There are 7 unique types of molecules in this entry. The entry contains 8238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
1	G	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
1	Y	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		

- Molecule 2 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
2	N	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

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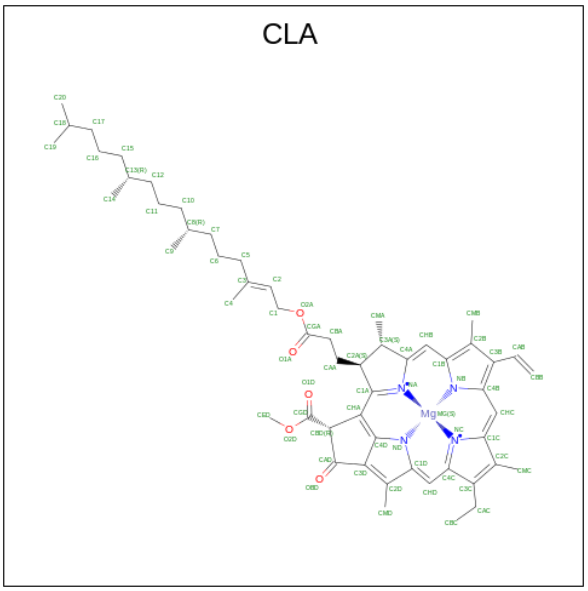
Mol	Chain	Residues	Atoms					AltConf
2	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	Y	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
2	Y	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
2	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
2	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 3 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	N	1	Total 62	C 52	Mg 1	N 4	O 5	0
3	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
3	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	G	1	Total 62	C 52	Mg 1	N 4	O 5	0
3	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	G	1	Total 65	C 55	Mg 1	N 4	O 5	0

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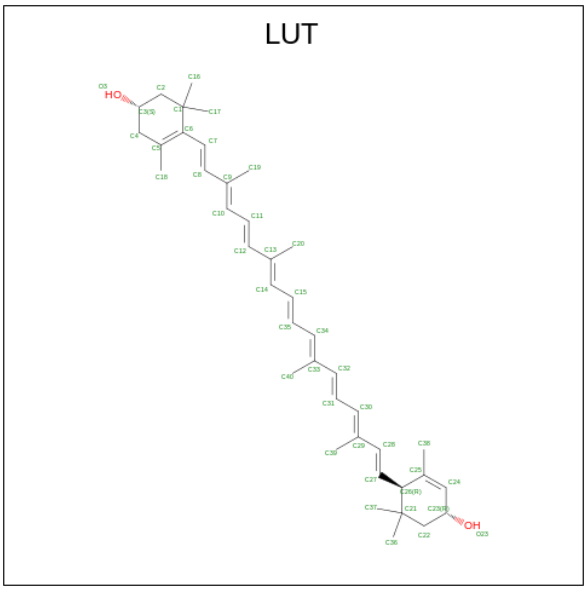
Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	Y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

- Molecule 4 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3, 3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
4	N	1	Total	C	O	0
			42	40	2	

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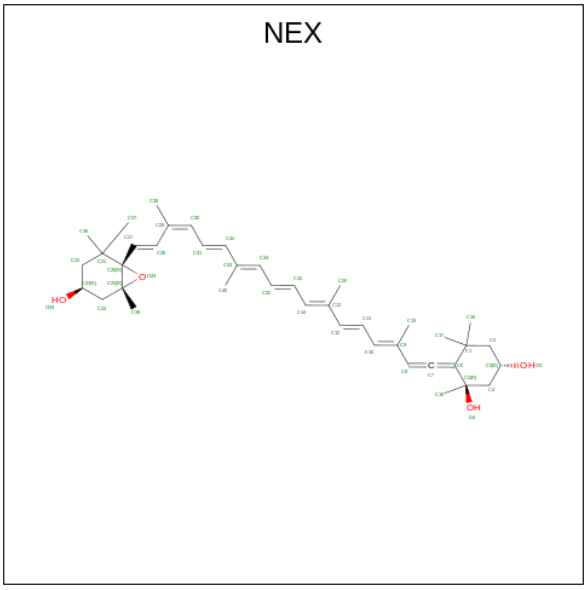
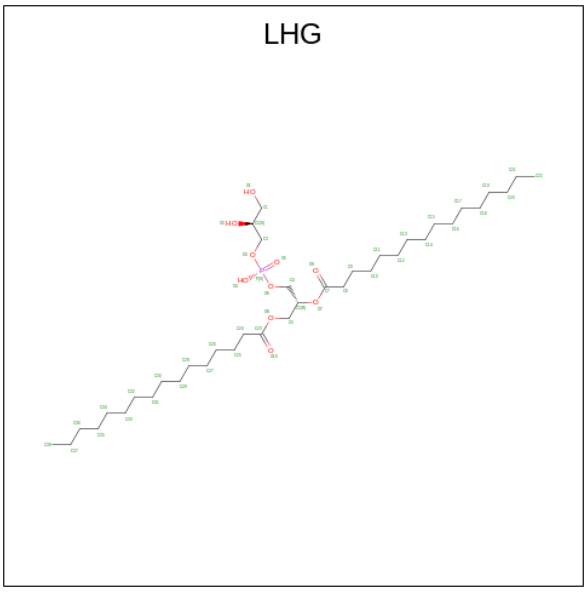
Mol	Chain	Residues	Atoms	AltConf
4	N	1	Total C O 42 40 2	0
4	G	1	Total C O 42 40 2	0
4	G	1	Total C O 42 40 2	0
4	Y	1	Total C O 42 40 2	0
4	Y	1	Total C O 42 40 2	0

- Molecule 5 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



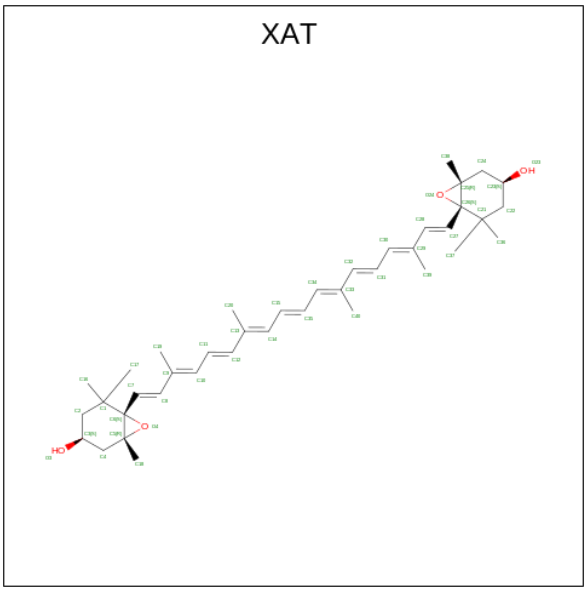
Mol	Chain	Residues	Atoms	AltConf
5	N	1	Total C O 44 40 4	0
5	G	1	Total C O 44 40 4	0
5	Y	1	Total C O 44 40 4	0

- Molecule 6 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
6	N	1	Total	C	O	P	0
			49	38	10	1	
6	G	1	Total	C	O	P	0
			49	38	10	1	
6	Y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 7 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
7	N	1	Total	C	O	0
			44	40	4	
7	G	1	Total	C	O	0
			44	40	4	
7	Y	1	Total	C	O	0
			44	40	4	

3 Residue-property plots (i)

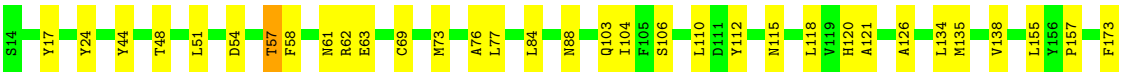
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Chlorophyll a-b binding protein, chloroplastic

Chain N:

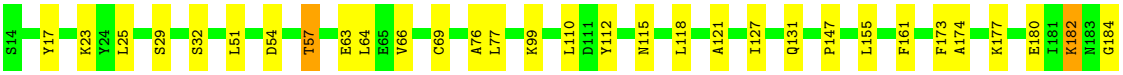
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

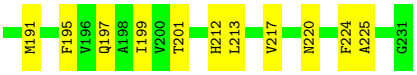
Chain G:



- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain Y:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	879190	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.506	Depositor
Minimum map value	-0.199	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LUT, LHG, CHL, NEX, XAT, 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	G	0.35	0/1713	0.59	0/2333
1	N	0.38	0/1713	0.58	0/2333
1	Y	0.35	0/1713	0.63	0/2333
All	All	0.36	0/5139	0.60	0/6999

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	G	1661	0	1590	41	0
1	N	1661	0	1591	29	0
1	Y	1661	0	1592	35	0
2	G	363	0	350	27	0
2	N	363	0	350	22	0
2	Y	363	0	350	21	0
3	G	501	0	534	19	0
3	N	501	0	534	19	0
3	Y	501	0	534	25	0
4	G	84	0	112	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	84	0	112	5	0
4	Y	84	0	112	9	0
5	G	44	0	56	4	0
5	N	44	0	56	3	0
5	Y	44	0	56	2	0
6	G	49	0	74	6	0
6	N	49	0	74	7	0
6	Y	49	0	74	5	0
7	G	44	0	56	6	0
7	N	44	0	56	5	0
7	Y	44	0	56	7	0
All	All	8238	0	8319	218	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 13.

All (218) 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:G:54:ASP:HB3	1:G:57:THR:CG2	1.66	1.23
1:Y:54:ASP:HB3	1:Y:57:THR:CG2	1.75	1.14
1:Y:54:ASP:HB3	1:Y:57:THR:HG22	1.30	1.12
1:G:54:ASP:HB3	1:G:57:THR:HG22	1.30	1.05
1:G:54:ASP:CB	1:G:57:THR:CG2	2.45	0.93
1:Y:54:ASP:O	1:Y:57:THR:HG23	1.73	0.88
1:G:54:ASP:O	1:G:57:THR:HG23	1.74	0.86
3:N:602:CLA:HAB	4:N:616:LUT:H32	1.62	0.82
1:N:46:TRP:HZ3	3:N:602:CLA:HBC2	1.46	0.80
1:Y:54:ASP:CB	1:Y:57:THR:CG2	2.63	0.75
2:G:601:CHL:HAC1	6:G:618:LHG:HC12	1.67	0.74
2:G:601:CHL:H8	7:G:619:XAT:H14	1.69	0.74
3:N:611:CLA:H152	3:N:612:CLA:HBB1	1.71	0.73
1:N:46:TRP:CZ3	3:N:602:CLA:HBC2	2.25	0.71
1:N:48:THR:HG21	2:G:609:CHL:HAA1	1.73	0.71
1:G:54:ASP:HB3	1:G:57:THR:HG23	1.71	0.70
1:N:191:MET:HG2	4:N:616:LUT:H12	1.75	0.68
1:G:44:TYR:CD2	2:G:601:CHL:HMD2	2.29	0.67
3:N:603:CLA:HBB1	2:N:609:CHL:H13	1.77	0.66
2:N:601:CHL:HMC	7:N:619:XAT:H242	1.78	0.65
1:Y:110:LEU:HB3	1:Y:121:ALA:HB3	1.78	0.65
1:Y:191:MET:HG2	4:Y:317:LUT:H12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:311:CLA:H52	3:Y:311:CLA:HBB1	1.80	0.64
3:N:613:CLA:H93	6:N:618:LHG:H131	1.79	0.63
3:Y:305:CLA:HBA1	5:Y:318:NEX:H241	1.81	0.63
1:Y:182:LYS:HE3	6:Y:319:LHG:HC42	1.80	0.63
7:Y:301:XAT:H242	2:Y:302:CHL:HMC	1.80	0.62
2:G:601:CHL:CHC	7:G:619:XAT:H383	2.31	0.61
1:G:185:ARG:HG2	6:G:618:LHG:H252	1.81	0.61
1:N:131:GLN:HG3	2:N:606:CHL:HMA3	1.81	0.61
6:G:618:LHG:H281	6:G:618:LHG:HC91	1.82	0.61
3:G:610:CLA:HBB1	4:G:615:LUT:H30	1.81	0.61
1:Y:213:LEU:HD23	3:Y:315:CLA:HBB1	1.81	0.60
2:N:609:CHL:HHC	2:Y:302:CHL:H52	1.83	0.60
1:N:173:PHE:CZ	1:N:177:LYS:HD3	2.37	0.60
2:G:601:CHL:HHD	6:G:618:LHG:HC41	1.84	0.59
2:G:608:CHL:H13	2:G:608:CHL:HMB2	1.83	0.59
3:Y:303:CLA:H92	3:Y:304:CLA:HMA1	1.84	0.59
1:N:63:GLU:HA	1:N:155:LEU:HD11	1.83	0.59
1:N:46:TRP:HE3	3:N:602:CLA:HMD2	1.67	0.59
3:G:602:CLA:H52	4:G:616:LUT:H28	1.85	0.59
3:Y:303:CLA:HAB	4:Y:317:LUT:H32	1.85	0.58
1:Y:69:CYS:HB3	1:Y:184:GLY:HA3	1.86	0.58
2:N:601:CHL:H52	2:G:609:CHL:HHC	1.85	0.58
1:G:110:LEU:HB3	1:G:121:ALA:HB3	1.86	0.58
1:G:135:MET:HA	1:G:138:VAL:HG22	1.85	0.57
1:N:173:PHE:HE2	1:N:177:LYS:HZ3	1.51	0.57
1:G:84:LEU:O	1:G:88:ASN:ND2	2.33	0.57
2:N:601:CHL:HHB	2:G:609:CHL:HMB1	1.87	0.57
3:Y:314:CLA:H71	6:Y:319:LHG:H151	1.86	0.57
1:N:70:ARG:NH1	2:N:608:CHL:OBD	2.38	0.56
1:N:173:PHE:CE2	1:N:177:LYS:HD3	2.40	0.56
1:Y:201:THR:HG22	1:Y:224:PHE:HE2	1.70	0.56
6:Y:319:LHG:H281	6:Y:319:LHG:HC91	1.86	0.56
2:G:607:CHL:H18	2:G:609:CHL:H52	1.87	0.56
1:Y:197:GLN:O	1:Y:201:THR:OG1	2.21	0.55
1:Y:51:LEU:HD13	3:Y:303:CLA:H42	1.88	0.55
1:N:177:LYS:HA	1:N:180:GLU:HG2	1.89	0.55
1:Y:115:ASN:HB3	1:Y:118:LEU:HB2	1.88	0.55
1:G:54:ASP:CB	1:G:57:THR:HG21	2.33	0.54
1:G:201:THR:HG22	1:G:203:LYS:HG3	1.89	0.54
2:G:608:CHL:HHC	2:G:608:CHL:HBB1	1.90	0.54
2:N:609:CHL:HMC	2:Y:302:CHL:H72	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:CYS:O	1:G:73:MET:HG3	2.08	0.53
1:N:115:ASN:HD22	1:N:118:LEU:HD13	1.71	0.53
3:N:610:CLA:CBB	4:N:615:LUT:H32	2.39	0.53
1:N:42:GLY:HA3	1:N:181:ILE:HG21	1.91	0.53
1:N:174:ALA:HA	1:N:177:LYS:HE2	1.91	0.53
1:N:112:TYR:HD2	1:N:118:LEU:HD23	1.75	0.52
3:N:613:CLA:H141	3:N:614:CLA:H2	1.91	0.52
1:Y:217:VAL:O	1:Y:220:ASN:ND2	2.43	0.52
3:Y:311:CLA:H61	4:Y:316:LUT:H371	1.91	0.52
3:Y:304:CLA:HBC2	2:Y:310:CHL:HMD2	1.92	0.52
3:G:610:CLA:H61	4:G:615:LUT:H371	1.91	0.51
2:N:609:CHL:HMB1	2:Y:302:CHL:HHB	1.91	0.51
1:G:126:ALA:HB3	2:G:605:CHL:HMC	1.93	0.51
1:N:63:GLU:HG2	2:N:609:CHL:HED2	1.92	0.51
3:G:610:CLA:H51	3:G:612:CLA:HMA1	1.93	0.50
1:Y:112:TYR:HB3	1:Y:118:LEU:HB3	1.94	0.50
6:N:618:LHG:HC91	6:N:618:LHG:H282	1.92	0.50
2:N:601:CHL:HMA3	6:N:618:LHG:H121	1.94	0.50
1:Y:173:PHE:O	1:Y:177:LYS:HG3	2.11	0.49
3:G:610:CLA:CBB	4:G:615:LUT:H32	2.42	0.49
3:G:611:CLA:HBB1	7:G:619:XAT:H221	1.95	0.49
1:G:120:HIS:ND1	1:G:121:ALA:N	2.60	0.49
3:G:612:CLA:H2A	3:G:612:CLA:H12	1.95	0.49
3:Y:303:CLA:HAB	4:Y:317:LUT:H30	1.95	0.48
2:N:601:CHL:H202	6:N:618:LHG:H221	1.94	0.48
1:G:77:LEU:HD21	3:G:612:CLA:H18	1.94	0.48
3:N:611:CLA:HBD	3:N:612:CLA:OBD	2.13	0.48
1:G:61:ASN:HB3	3:G:602:CLA:HHB	1.94	0.48
1:N:115:ASN:HB3	1:N:118:LEU:HB2	1.96	0.48
1:Y:195:PHE:O	1:Y:199:ILE:HG13	2.14	0.48
3:Y:312:CLA:H152	3:Y:313:CLA:HBB1	1.96	0.48
1:G:193:GLY:O	1:G:197:GLN:HG3	2.13	0.48
2:G:608:CHL:H162	2:G:608:CHL:H121	1.62	0.48
1:Y:99:LYS:HA	2:Y:308:CHL:HED3	1.95	0.48
2:N:609:CHL:CHC	2:Y:302:CHL:H2	2.44	0.47
2:G:601:CHL:H202	2:G:601:CHL:H161	1.65	0.47
1:Y:63:GLU:HA	1:Y:155:LEU:HD11	1.95	0.47
1:N:51:LEU:HB2	3:N:602:CLA:O1A	2.14	0.47
1:G:54:ASP:C	1:G:57:THR:HG23	2.33	0.47
3:Y:303:CLA:H52	4:Y:317:LUT:H28	1.97	0.47
6:Y:319:LHG:HC62	6:Y:319:LHG:H262	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:161:PHE:HD1	2:Y:309:CHL:H61	1.78	0.47
2:N:609:CHL:H93	2:N:609:CHL:H112	1.81	0.47
2:G:608:CHL:H171	2:G:608:CHL:HAA2	1.97	0.46
1:N:185:ARG:HG2	6:N:618:LHG:H252	1.98	0.46
1:G:76:ALA:HB1	4:G:615:LUT:H12	1.98	0.46
2:N:609:CHL:H202	2:N:609:CHL:H161	1.66	0.46
2:N:601:CHL:H2	2:G:609:CHL:CHC	2.46	0.46
1:G:44:TYR:HD2	2:G:601:CHL:HMD2	1.75	0.46
1:G:205:PRO:HB2	4:G:615:LUT:H173	1.98	0.46
4:G:616:LUT:H15	4:G:616:LUT:H201	1.81	0.46
1:G:44:TYR:CE2	2:G:601:CHL:HMD2	2.51	0.46
1:G:63:GLU:HA	1:G:155:LEU:HD11	1.98	0.46
1:Y:76:ALA:HB1	4:Y:316:LUT:H12	1.98	0.46
1:G:48:THR:HG21	2:Y:310:CHL:H2A	1.97	0.45
1:G:115:ASN:HB3	1:G:118:LEU:HB2	1.98	0.45
2:Y:302:CHL:H202	2:Y:302:CHL:H161	1.82	0.45
1:Y:225:ALA:O	7:Y:301:XAT:O3	2.32	0.45
1:Y:64:LEU:HD11	3:Y:304:CLA:HAA2	1.99	0.45
1:G:54:ASP:CB	1:G:57:THR:HG23	2.39	0.45
3:Y:311:CLA:H51	3:Y:313:CLA:HMA1	1.97	0.45
6:N:618:LHG:H202	7:N:619:XAT:H10	1.99	0.45
2:G:601:CHL:H62	6:G:618:LHG:H171	1.99	0.45
2:N:608:CHL:H152	5:N:617:NEX:H402	1.99	0.45
2:N:609:CHL:H62	2:N:609:CHL:H2	1.69	0.45
7:N:619:XAT:H15	7:N:619:XAT:H201	1.69	0.45
3:N:602:CLA:H92	3:N:603:CLA:HMA1	1.99	0.44
3:G:613:CLA:H61	3:G:613:CLA:H2	1.68	0.44
1:N:51:LEU:HB2	3:N:602:CLA:H11	1.99	0.44
1:G:51:LEU:HD13	3:G:602:CLA:H42	2.00	0.44
3:N:603:CLA:H72	3:N:603:CLA:H112	1.79	0.44
1:G:176:LEU:O	1:G:180:GLU:HG2	2.18	0.44
1:Y:25:LEU:HB2	1:Y:29:SER:HA	2.00	0.44
1:Y:213:LEU:CD2	3:Y:315:CLA:CBB	2.96	0.44
2:N:601:CHL:HBA1	2:N:601:CHL:H3A	1.63	0.43
3:N:611:CLA:H112	3:N:611:CLA:H91	1.65	0.43
5:N:617:NEX:H11	5:N:617:NEX:H191	1.82	0.43
2:G:601:CHL:HHC	7:G:619:XAT:H383	2.00	0.43
5:G:617:NEX:H11	5:G:617:NEX:H191	1.81	0.43
6:G:618:LHG:H212	3:Y:304:CLA:H201	2.00	0.43
3:Y:304:CLA:H2	3:Y:304:CLA:H61	1.76	0.43
1:G:58:PHE:O	1:G:62:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:301:XAT:H35	7:Y:301:XAT:H401	1.81	0.43
1:N:174:ALA:O	1:N:178:VAL:HG23	2.18	0.43
1:N:217:VAL:O	1:N:220:ASN:ND2	2.51	0.43
2:G:601:CHL:H2	2:Y:310:CHL:C3B	2.48	0.43
3:G:611:CLA:H143	3:G:611:CLA:H111	1.81	0.43
4:G:615:LUT:H11	4:G:615:LUT:H191	1.91	0.43
2:Y:308:CHL:HBB2	2:Y:310:CHL:HBC1	2.01	0.43
4:N:616:LUT:H201	4:N:616:LUT:H15	1.82	0.43
5:N:617:NEX:H35	5:N:617:NEX:H401	1.81	0.43
2:G:607:CHL:H143	2:G:607:CHL:H111	1.81	0.43
1:Y:66:VAL:HG21	1:Y:155:LEU:HD13	2.01	0.43
1:Y:147:PRO:HB3	5:Y:318:NEX:H183	2.01	0.43
1:N:56:GLU:O	1:N:60:LYS:HG2	2.19	0.43
1:Y:17:TYR:CE2	1:Y:174:ALA:HB1	2.54	0.43
1:Y:213:LEU:HD23	3:Y:315:CLA:CBB	2.47	0.43
1:G:180:GLU:OE1	3:G:610:CLA:C2B	2.67	0.43
2:Y:309:CHL:H171	2:Y:309:CHL:HAA2	2.00	0.43
3:Y:312:CLA:H143	3:Y:312:CLA:H111	1.84	0.43
4:Y:317:LUT:H15	4:Y:317:LUT:H201	1.86	0.43
3:N:611:CLA:HMB1	3:N:611:CLA:HBB1	2.01	0.42
6:N:618:LHG:H282	6:N:618:LHG:H312	1.78	0.42
5:G:617:NEX:H15	5:G:617:NEX:H201	1.78	0.42
1:N:157:PRO:HB3	2:N:608:CHL:HBC2	2.01	0.42
7:Y:301:XAT:H201	7:Y:301:XAT:H15	1.75	0.42
4:N:615:LUT:H15	4:N:615:LUT:H201	1.90	0.42
7:N:619:XAT:H35	7:N:619:XAT:H401	1.78	0.42
3:G:602:CLA:CBB	4:G:616:LUT:H32	2.50	0.42
1:N:17:TYR:CE2	1:N:174:ALA:HB1	2.55	0.42
1:G:180:GLU:OE1	3:G:610:CLA:HMB3	2.18	0.42
2:Y:308:CHL:H93	2:Y:308:CHL:H61	1.79	0.42
2:G:608:CHL:H152	5:G:617:NEX:H402	2.00	0.42
3:Y:314:CLA:H151	3:Y:315:CLA:HBA2	2.02	0.42
7:N:619:XAT:H11	7:N:619:XAT:H191	1.92	0.42
1:G:134:LEU:HD21	2:G:606:CHL:H42	2.01	0.42
7:Y:301:XAT:H11	7:Y:301:XAT:H191	1.91	0.42
1:N:85:LEU:HD23	1:N:85:LEU:HA	1.93	0.41
3:Y:304:CLA:H102	2:Y:310:CHL:H143	2.01	0.41
3:Y:311:CLA:CBB	4:Y:316:LUT:H32	2.50	0.41
1:N:112:TYR:HB3	1:N:118:LEU:HB3	2.01	0.41
2:N:608:CHL:HHB	2:N:608:CHL:H13	2.03	0.41
4:Y:316:LUT:H31	4:Y:316:LUT:H391	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:64:LEU:HD11	3:N:603:CLA:HAA2	2.03	0.41
1:Y:77:LEU:HD21	3:Y:313:CLA:H202	2.02	0.41
2:Y:308:CHL:H12	2:Y:308:CHL:HMA2	2.01	0.41
3:G:602:CLA:H161	3:G:602:CLA:H141	1.85	0.41
3:G:602:CLA:H93	3:G:602:CLA:H111	1.84	0.41
1:G:112:TYR:HB3	1:G:118:LEU:HB3	2.02	0.41
1:G:217:VAL:HG23	1:G:218:ASN:OD1	2.21	0.41
2:G:601:CHL:H141	2:G:601:CHL:H162	1.77	0.41
7:G:619:XAT:H35	7:G:619:XAT:H401	1.87	0.41
1:Y:54:ASP:HB3	1:Y:57:THR:HG21	1.83	0.41
7:Y:301:XAT:H14	2:Y:302:CHL:H8	2.03	0.41
2:Y:308:CHL:H111	2:Y:308:CHL:H143	1.82	0.41
2:Y:308:CHL:H18	2:Y:310:CHL:H52	2.03	0.41
1:G:180:GLU:OE1	3:G:610:CLA:C1B	2.69	0.41
1:G:157:PRO:HB3	2:G:608:CHL:HBC2	2.03	0.40
1:G:222:TRP:CZ2	3:G:614:CLA:HED2	2.55	0.40
2:G:607:CHL:H93	2:G:607:CHL:H61	1.82	0.40
1:Y:23:LYS:HE2	1:Y:32:SER:HB3	2.04	0.40
7:Y:301:XAT:H12	2:Y:302:CHL:H111	2.03	0.40
3:Y:305:CLA:HMB1	3:Y:305:CLA:HBB1	2.03	0.40
3:N:613:CLA:H61	3:N:613:CLA:H2	1.58	0.40
5:G:617:NEX:H35	5:G:617:NEX:H401	1.85	0.40
2:N:607:CHL:H143	2:N:607:CHL:H111	1.80	0.40
3:N:611:CLA:H62	3:N:611:CLA:H101	1.47	0.40
1:G:104:ILE:HD12	1:G:104:ILE:HA	1.87	0.40
1:Y:127:ILE:O	1:Y:131:GLN:HG2	2.22	0.40
2:Y:302:CHL:H202	6:Y:319:LHG:H221	2.03	0.40
1:G:17:TYR:CE2	1:G:174:ALA:HB1	2.57	0.40
1:G:103:GLN:O	1:G:106:SER:OG	2.25	0.40
7:G:619:XAT:H31	7:G:619:XAT:H391	1.82	0.40
1:Y:17:TYR:HE2	1:Y:174:ALA:HB1	1.86	0.40
1:Y:212:HIS:ND1	3:Y:314:CLA:HAA2	2.36	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	G	216/218 (99%)	210 (97%)	6 (3%)	0	100	100
1	N	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
1	Y	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
All	All	648/654 (99%)	624 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	G	168/168 (100%)	165 (98%)	3 (2%)	59	80
1	N	168/168 (100%)	165 (98%)	3 (2%)	59	80
1	Y	168/168 (100%)	165 (98%)	3 (2%)	59	80
All	All	504/504 (100%)	495 (98%)	9 (2%)	61	80

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	131	GLN
1	N	135	MET
1	N	139	GLU
1	G	24	TYR
1	G	57	THR
1	G	173	PHE
1	Y	57	THR
1	Y	180	GLU
1	Y	182	LYS

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

sidechains are listed below:

Mol	Chain	Res	Type
1	N	131	GLN
1	G	61	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

57 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	$\#\|Z\| > 2$
2	CHL	N	607	-	66,74,74	1.46	6 (9%)	73,114,114	1.54	9 (12%)
3	CLA	G	611	6	65,73,73	1.51	7 (10%)	76,113,113	1.34	9 (11%)
2	CHL	N	609	1	66,74,74	1.41	7 (10%)	73,114,114	1.62	12 (16%)
5	NEX	N	617	-	38,46,46	0.96	2 (5%)	50,70,70	2.39	16 (32%)
3	CLA	Y	315	-	49,57,73	1.77	7 (14%)	55,93,113	1.31	8 (14%)
3	CLA	N	613	1	65,73,73	1.48	5 (7%)	76,113,113	1.41	8 (10%)
5	NEX	Y	318	-	38,46,46	1.56	7 (18%)	50,70,70	1.59	10 (20%)
2	CHL	Y	306	1	48,56,74	1.69	6 (12%)	51,92,114	1.48	12 (23%)
3	CLA	N	614	-	49,57,73	1.77	7 (14%)	55,93,113	1.28	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CLA	G	612	-	65,73,73	1.47	6 (9%)	76,113,113	1.34	8 (10%)
3	CLA	G	603	-	65,73,73	1.57	8 (12%)	76,113,113	1.30	7 (9%)
3	CLA	Y	304	-	65,73,73	1.52	8 (12%)	76,113,113	1.44	8 (10%)
4	LUT	G	615	-	42,43,43	0.77	0	51,60,60	1.58	13 (25%)
2	CHL	Y	309	-	66,74,74	1.48	6 (9%)	73,114,114	1.30	7 (9%)
6	LHG	N	618	3	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
3	CLA	N	602	1	65,73,73	1.49	5 (7%)	76,113,113	1.32	8 (10%)
3	CLA	G	604	-	62,70,73	1.54	6 (9%)	72,109,113	1.40	8 (11%)
3	CLA	Y	313	-	65,73,73	1.53	7 (10%)	76,113,113	1.33	10 (13%)
3	CLA	Y	314	1	65,73,73	1.51	6 (9%)	76,113,113	1.32	7 (9%)
2	CHL	G	608	-	66,74,74	1.51	6 (9%)	73,114,114	1.27	7 (9%)
2	CHL	N	601	1	66,74,74	1.50	6 (9%)	73,114,114	1.33	9 (12%)
3	CLA	Y	311	1	65,73,73	1.49	10 (15%)	76,113,113	1.31	10 (13%)
2	CHL	N	606	-	51,59,74	1.65	6 (11%)	55,96,114	1.78	10 (18%)
3	CLA	N	612	-	65,73,73	1.54	9 (13%)	76,113,113	1.30	8 (10%)
2	CHL	Y	302	1	66,74,74	1.49	6 (9%)	73,114,114	1.32	9 (12%)
2	CHL	Y	308	-	66,74,74	1.47	6 (9%)	73,114,114	1.61	11 (15%)
4	LUT	N	615	-	42,43,43	0.75	0	51,60,60	1.58	9 (17%)
4	LUT	N	616	-	42,43,43	0.76	0	51,60,60	1.51	10 (19%)
3	CLA	N	610	1	65,73,73	1.56	8 (12%)	76,113,113	1.26	7 (9%)
3	CLA	N	611	6	65,73,73	1.43	7 (10%)	76,113,113	1.37	7 (9%)
3	CLA	G	602	-	65,73,73	1.59	7 (10%)	76,113,113	1.29	7 (9%)
3	CLA	G	614	-	49,57,73	1.78	7 (14%)	55,93,113	1.33	8 (14%)
7	XAT	G	619	-	39,47,47	0.89	2 (5%)	54,74,74	2.67	21 (38%)
2	CHL	N	608	-	66,74,74	1.46	6 (9%)	73,114,114	1.34	7 (9%)
2	CHL	N	605	1	48,56,74	1.68	6 (12%)	51,92,114	1.53	10 (19%)
5	NEX	G	617	-	38,46,46	0.95	2 (5%)	50,70,70	2.37	14 (28%)
4	LUT	Y	316	-	42,43,43	0.80	0	51,60,60	1.55	12 (23%)
2	CHL	G	601	-	66,74,74	1.45	7 (10%)	73,114,114	1.37	12 (16%)
7	XAT	N	619	-	39,47,47	0.90	2 (5%)	54,74,74	2.71	20 (37%)
2	CHL	Y	310	1	66,74,74	1.50	5 (7%)	73,114,114	1.66	14 (19%)
3	CLA	Y	305	-	62,70,73	1.52	6 (9%)	72,109,113	1.50	10 (13%)
2	CHL	G	607	-	66,74,74	1.45	5 (7%)	73,114,114	1.54	8 (10%)
4	LUT	G	616	-	42,43,43	0.73	0	51,60,60	1.56	10 (19%)
2	CHL	G	606	-	51,59,74	1.68	5 (9%)	55,96,114	1.66	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CHL	Y	307	1	51,59,74	1.63	7 (13%)	55,96,114	1.76	11 (20%)
3	CLA	Y	312	6	65,73,73	1.54	8 (12%)	76,113,113	1.39	8 (10%)
7	XAT	Y	301	-	39,47,47	0.89	2 (5%)	54,74,74	2.66	19 (35%)
2	CHL	G	609	1	66,74,74	1.43	6 (9%)	73,114,114	1.84	15 (20%)
3	CLA	G	610	-	65,73,73	1.55	9 (13%)	76,113,113	1.32	9 (11%)
3	CLA	Y	303	1	65,73,73	1.53	6 (9%)	76,113,113	1.29	6 (7%)
3	CLA	N	604	-	62,70,73	1.55	6 (9%)	72,109,113	1.40	8 (11%)
4	LUT	Y	317	-	42,43,43	0.76	0	51,60,60	1.54	11 (21%)
2	CHL	G	605	1	48,56,74	1.70	6 (12%)	51,92,114	1.41	8 (15%)
3	CLA	N	603	-	65,73,73	1.55	8 (12%)	76,113,113	1.31	7 (9%)
6	LHG	G	618	3	48,48,48	0.92	2 (4%)	51,54,54	1.07	3 (5%)
6	LHG	Y	319	3	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
3	CLA	G	613	1	65,73,73	1.48	5 (7%)	76,113,113	1.40	7 (9%)

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
2	CHL	N	607	-	3/3/20/26	14/39/137/137	-
3	CLA	G	611	6	-	11/37/115/115	-
2	CHL	N	609	1	3/3/20/26	18/39/137/137	-
5	NEX	N	617	-	-	6/27/83/83	0/3/3/3
3	CLA	Y	315	-	1/1/11/20	7/18/96/115	-
3	CLA	N	613	1	1/1/15/20	12/37/115/115	-
5	NEX	Y	318	-	-	13/27/83/83	0/3/3/3
2	CHL	Y	306	1	3/3/16/26	8/18/116/137	-
3	CLA	N	614	-	1/1/11/20	9/18/96/115	-
3	CLA	G	612	-	1/1/15/20	13/37/115/115	-
3	CLA	G	603	-	1/1/15/20	15/37/115/115	-
3	CLA	Y	304	-	1/1/15/20	17/37/115/115	-
4	LUT	G	615	-	-	4/29/67/67	0/2/2/2
2	CHL	Y	309	-	3/3/20/26	19/39/137/137	-
6	LHG	N	618	3	-	30/53/53/53	-
3	CLA	N	602	1	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	G	604	-	-	16/34/112/115	-
3	CLA	Y	313	-	1/1/15/20	19/37/115/115	-
3	CLA	Y	314	1	1/1/15/20	8/37/115/115	-
2	CHL	G	608	-	3/3/20/26	14/39/137/137	-
2	CHL	N	601	1	3/3/20/26	10/39/137/137	-
3	CLA	Y	311	1	1/1/15/20	3/37/115/115	-
2	CHL	N	606	-	3/3/17/26	6/21/119/137	-
3	CLA	N	612	-	1/1/15/20	15/37/115/115	-
2	CHL	Y	302	1	3/3/20/26	11/39/137/137	-
2	CHL	Y	308	-	3/3/20/26	13/39/137/137	-
4	LUT	N	615	-	-	5/29/67/67	0/2/2/2
4	LUT	N	616	-	-	3/29/67/67	0/2/2/2
3	CLA	N	610	1	1/1/15/20	3/37/115/115	-
3	CLA	N	611	6	1/1/15/20	16/37/115/115	-
3	CLA	G	602	-	1/1/15/20	10/37/115/115	-
3	CLA	G	614	-	1/1/11/20	10/18/96/115	-
7	XAT	G	619	-	-	7/31/93/93	0/4/4/4
2	CHL	N	608	-	3/3/20/26	13/39/137/137	-
2	CHL	N	605	1	3/3/16/26	8/18/116/137	-
5	NEX	G	617	-	-	6/27/83/83	0/3/3/3
4	LUT	Y	316	-	-	4/29/67/67	0/2/2/2
2	CHL	G	601	-	3/3/20/26	13/39/137/137	-
7	XAT	N	619	-	-	7/31/93/93	0/4/4/4
2	CHL	Y	310	1	3/3/20/26	15/39/137/137	-
3	CLA	Y	305	-	1/1/14/20	12/34/112/115	-
2	CHL	G	607	-	3/3/20/26	16/39/137/137	-
4	LUT	G	616	-	-	3/29/67/67	0/2/2/2
2	CHL	G	606	-	3/3/17/26	4/21/119/137	-
2	CHL	Y	307	1	3/3/17/26	7/21/119/137	-
3	CLA	Y	312	6	-	13/37/115/115	-
7	XAT	Y	301	-	-	7/31/93/93	0/4/4/4
2	CHL	G	609	1	3/3/20/26	15/39/137/137	-
3	CLA	G	610	-	1/1/15/20	2/37/115/115	-
3	CLA	Y	303	1	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	N	604	-	1/1/14/20	12/34/112/115	-
4	LUT	Y	317	-	-	3/29/67/67	0/2/2/2
2	CHL	G	605	1	3/3/16/26	5/18/116/137	-
3	CLA	N	603	-	1/1/15/20	15/37/115/115	-
6	LHG	G	618	3	-	30/53/53/53	-
6	LHG	Y	319	3	-	30/53/53/53	-
3	CLA	G	613	1	-	11/37/115/115	-

All (299) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	CLA	C4B-NB	8.29	1.42	1.35
3	G	603	CLA	C4B-NB	8.17	1.42	1.35
3	Y	312	CLA	C4B-NB	8.05	1.42	1.35
2	G	608	CHL	C4B-NB	8.04	1.42	1.35
3	Y	313	CLA	C4B-NB	7.99	1.42	1.35
3	N	612	CLA	C4B-NB	7.96	1.42	1.35
3	N	614	CLA	C4B-NB	7.96	1.42	1.35
3	Y	314	CLA	C4B-NB	7.89	1.42	1.35
2	N	601	CHL	C4B-NB	7.88	1.42	1.35
3	G	614	CLA	C4B-NB	7.87	1.42	1.35
2	Y	310	CHL	C4B-NB	7.87	1.42	1.35
2	Y	302	CHL	C4B-NB	7.86	1.42	1.35
3	Y	303	CLA	C4B-NB	7.85	1.42	1.35
3	N	603	CLA	C4B-NB	7.84	1.42	1.35
2	Y	309	CHL	C4B-NB	7.81	1.42	1.35
3	G	611	CLA	C4B-NB	7.80	1.42	1.35
3	Y	315	CLA	C4B-NB	7.78	1.42	1.35
3	N	610	CLA	C4B-NB	7.72	1.42	1.35
3	G	610	CLA	C4B-NB	7.71	1.42	1.35
3	G	604	CLA	C4B-NB	7.70	1.42	1.35
3	N	604	CLA	C4B-NB	7.69	1.42	1.35
3	Y	305	CLA	C4B-NB	7.68	1.42	1.35
2	N	608	CHL	C4B-NB	7.66	1.42	1.35
2	G	606	CHL	C4B-NB	7.65	1.42	1.35
3	Y	304	CLA	C4B-NB	7.64	1.42	1.35
3	G	613	CLA	C4B-NB	7.49	1.41	1.35
3	N	613	CLA	C4B-NB	7.44	1.41	1.35
3	N	602	CLA	C4B-NB	7.42	1.41	1.35
2	Y	306	CHL	C4B-NB	7.42	1.41	1.35
2	G	605	CHL	C4B-NB	7.41	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	607	CHL	C4B-NB	7.27	1.41	1.35
3	G	612	CLA	C4B-NB	7.26	1.41	1.35
2	N	606	CHL	C4B-NB	7.26	1.41	1.35
2	Y	307	CHL	C4B-NB	7.22	1.41	1.35
2	G	607	CHL	C4B-NB	7.17	1.41	1.35
2	Y	308	CHL	C4B-NB	7.15	1.41	1.35
2	N	605	CHL	C4B-NB	7.13	1.41	1.35
2	G	601	CHL	C4B-NB	7.11	1.41	1.35
3	N	611	CLA	C4B-NB	6.88	1.41	1.35
2	G	609	CHL	C4B-NB	6.70	1.41	1.35
2	N	609	CHL	C4B-NB	6.67	1.41	1.35
3	Y	311	CLA	C4B-NB	6.53	1.41	1.35
6	Y	319	LHG	O8-C23	4.37	1.46	1.33
6	G	618	LHG	O8-C23	4.16	1.45	1.33
2	G	608	CHL	C1D-ND	4.13	1.42	1.37
6	N	618	LHG	O8-C23	4.12	1.45	1.33
3	Y	315	CLA	C1D-ND	4.04	1.42	1.37
6	N	618	LHG	O7-C7	4.04	1.45	1.34
6	G	618	LHG	O7-C7	4.03	1.45	1.34
3	N	603	CLA	C1D-ND	4.01	1.42	1.37
3	N	612	CLA	C1D-ND	4.00	1.42	1.37
2	Y	309	CHL	C1D-ND	3.99	1.42	1.37
3	N	610	CLA	C1D-ND	3.98	1.42	1.37
3	N	602	CLA	C1D-ND	3.96	1.42	1.37
3	G	603	CLA	C1D-ND	3.94	1.42	1.37
3	Y	303	CLA	C1D-ND	3.94	1.42	1.37
2	N	605	CHL	C1D-ND	3.93	1.42	1.37
2	N	608	CHL	C1D-ND	3.92	1.42	1.37
3	N	614	CLA	C1D-ND	3.89	1.42	1.37
2	Y	302	CHL	C1D-ND	3.89	1.42	1.37
2	G	605	CHL	C1D-ND	3.88	1.42	1.37
3	G	614	CLA	C1D-ND	3.88	1.42	1.37
6	Y	319	LHG	O7-C7	3.87	1.45	1.34
2	N	601	CHL	C1D-ND	3.85	1.42	1.37
3	Y	304	CLA	C1D-ND	3.83	1.42	1.37
2	Y	308	CHL	C1D-ND	3.82	1.42	1.37
3	Y	311	CLA	C1D-ND	3.79	1.42	1.37
3	N	604	CLA	C1D-ND	3.78	1.42	1.37
3	Y	313	CLA	C1D-ND	3.76	1.42	1.37
3	N	613	CLA	C1D-ND	3.76	1.42	1.37
3	G	604	CLA	C1D-ND	3.76	1.42	1.37
5	Y	318	NEX	C14-C13	3.71	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	607	CHL	C1D-ND	3.70	1.42	1.37
3	G	602	CLA	C1D-ND	3.69	1.42	1.37
2	Y	306	CHL	C1D-ND	3.68	1.42	1.37
3	Y	314	CLA	C1D-ND	3.65	1.42	1.37
2	G	609	CHL	C1D-ND	3.65	1.42	1.37
2	G	606	CHL	C1D-ND	3.64	1.42	1.37
2	N	607	CHL	C1D-ND	3.63	1.42	1.37
2	Y	310	CHL	C1D-ND	3.61	1.42	1.37
5	Y	318	NEX	C30-C29	3.60	1.40	1.35
5	Y	318	NEX	C34-C33	3.60	1.40	1.35
2	Y	307	CHL	C1D-ND	3.59	1.42	1.37
3	G	612	CLA	C1D-ND	3.58	1.42	1.37
2	Y	310	CHL	CHC-C1C	3.55	1.44	1.35
3	G	613	CLA	C1D-ND	3.53	1.42	1.37
2	N	606	CHL	C1D-ND	3.52	1.42	1.37
3	G	610	CLA	C1D-ND	3.46	1.42	1.37
3	N	611	CLA	C4D-ND	-3.45	1.33	1.37
2	N	609	CHL	C4D-ND	-3.35	1.33	1.37
2	G	609	CHL	C4D-ND	-3.34	1.33	1.37
3	N	611	CLA	C1D-ND	3.31	1.41	1.37
2	N	609	CHL	C1D-ND	3.31	1.41	1.37
3	Y	312	CLA	C4D-ND	-3.30	1.33	1.37
3	Y	305	CLA	C1D-ND	3.29	1.41	1.37
2	G	601	CHL	C1D-ND	3.26	1.41	1.37
3	Y	312	CLA	C1D-ND	3.24	1.41	1.37
3	G	611	CLA	C1D-ND	3.23	1.41	1.37
2	N	606	CHL	C4D-ND	-3.22	1.33	1.37
3	G	602	CLA	CHC-C1C	3.20	1.43	1.35
2	Y	308	CHL	CHC-C1C	3.19	1.43	1.35
3	Y	311	CLA	C4D-ND	-3.18	1.33	1.37
3	N	602	CLA	CHC-C1C	3.17	1.43	1.35
2	N	607	CHL	CHC-C1C	3.17	1.43	1.35
3	G	612	CLA	C4D-ND	-3.16	1.33	1.37
3	N	610	CLA	C3B-C2B	-3.14	1.36	1.40
3	G	614	CLA	CHC-C1C	3.14	1.43	1.35
2	N	609	CHL	CHC-C1C	3.12	1.43	1.35
3	G	610	CLA	CMB-C2B	-3.11	1.45	1.51
2	Y	310	CHL	C4D-ND	-3.10	1.33	1.37
3	Y	305	CLA	CHC-C1C	3.10	1.42	1.35
2	Y	307	CHL	CHC-C1C	3.10	1.42	1.35
2	G	606	CHL	CHC-C1C	3.08	1.42	1.35
2	N	607	CHL	C4D-ND	-3.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	315	CLA	CHC-C1C	3.07	1.42	1.35
2	N	601	CHL	CHC-C1C	3.06	1.42	1.35
3	N	604	CLA	CHC-C1C	3.04	1.42	1.35
2	G	607	CHL	C4D-ND	-3.03	1.33	1.37
2	Y	306	CHL	CHC-C1C	3.02	1.42	1.35
2	G	607	CHL	CHC-C1C	3.02	1.42	1.35
2	Y	308	CHL	C4D-ND	-3.02	1.33	1.37
2	G	609	CHL	CHC-C1C	3.02	1.42	1.35
3	G	610	CLA	C4D-ND	-3.01	1.33	1.37
2	G	605	CHL	CHC-C1C	3.01	1.42	1.35
3	G	610	CLA	CHC-C1C	3.00	1.42	1.35
3	Y	303	CLA	CHC-C1C	2.99	1.42	1.35
3	N	604	CLA	C4D-ND	-2.99	1.33	1.37
2	Y	302	CHL	CHC-C1C	2.98	1.42	1.35
3	G	602	CLA	C4D-ND	-2.96	1.33	1.37
3	G	604	CLA	CHC-C1C	2.96	1.42	1.35
3	Y	314	CLA	CHC-C1C	2.96	1.42	1.35
2	N	605	CHL	CHC-C1C	2.96	1.42	1.35
2	N	608	CHL	CHC-C1C	2.95	1.42	1.35
5	N	617	NEX	C7-C8	-2.94	1.27	1.32
3	Y	303	CLA	C4D-ND	-2.94	1.33	1.37
3	G	613	CLA	C4D-ND	-2.93	1.33	1.37
3	G	611	CLA	C4D-ND	-2.93	1.33	1.37
3	Y	314	CLA	C4D-ND	-2.93	1.33	1.37
3	N	613	CLA	C4D-ND	-2.92	1.33	1.37
5	Y	318	NEX	C10-C9	2.92	1.39	1.35
3	G	602	CLA	CMB-C2B	-2.92	1.45	1.51
3	N	610	CLA	CMB-C2B	-2.91	1.45	1.51
3	N	614	CLA	CHC-C1C	2.91	1.42	1.35
3	G	612	CLA	CHC-C1C	2.90	1.42	1.35
3	G	613	CLA	CHC-C1C	2.90	1.42	1.35
3	Y	305	CLA	C4D-ND	-2.90	1.33	1.37
3	N	613	CLA	CHC-C1C	2.90	1.42	1.35
2	G	601	CHL	CHC-C1C	2.90	1.42	1.35
3	Y	315	CLA	C4D-ND	-2.88	1.33	1.37
2	G	608	CHL	CHC-C1C	2.88	1.42	1.35
2	N	606	CHL	CHC-C1C	2.88	1.42	1.35
2	G	609	CHL	CMB-C2B	-2.88	1.45	1.51
3	G	604	CLA	C4D-ND	-2.88	1.33	1.37
3	Y	313	CLA	C4D-ND	-2.87	1.33	1.37
2	N	606	CHL	CMB-C2B	-2.87	1.45	1.51
3	N	610	CLA	CHC-C1C	2.86	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	617	NEX	C7-C8	-2.86	1.27	1.32
3	Y	313	CLA	CHC-C1C	2.86	1.42	1.35
3	Y	312	CLA	CHC-C1C	2.85	1.42	1.35
3	G	614	CLA	C4D-ND	-2.83	1.33	1.37
3	G	603	CLA	CHC-C1C	2.82	1.42	1.35
3	N	612	CLA	CHC-C1C	2.82	1.42	1.35
2	Y	309	CHL	CHC-C1C	2.81	1.42	1.35
2	G	601	CHL	C4D-ND	-2.81	1.33	1.37
3	N	602	CLA	C4D-ND	-2.81	1.33	1.37
3	N	611	CLA	CHC-C1C	2.78	1.42	1.35
2	G	606	CHL	C4D-ND	-2.77	1.33	1.37
3	G	611	CLA	CHC-C1C	2.76	1.42	1.35
3	N	612	CLA	C4D-ND	-2.75	1.33	1.37
3	Y	304	CLA	C4D-ND	-2.74	1.33	1.37
3	N	603	CLA	C4D-ND	-2.73	1.33	1.37
3	G	603	CLA	C4D-ND	-2.73	1.33	1.37
2	Y	306	CHL	C4D-ND	-2.72	1.34	1.37
2	N	608	CHL	C4D-ND	-2.71	1.34	1.37
3	Y	305	CLA	CMB-C2B	-2.69	1.46	1.51
2	Y	302	CHL	C4D-ND	-2.68	1.34	1.37
2	G	601	CHL	CMD-C2D	-2.68	1.45	1.50
2	N	609	CHL	CMB-C2B	-2.68	1.46	1.51
2	Y	307	CHL	C4D-ND	-2.67	1.34	1.37
3	G	604	CLA	CMB-C2B	-2.66	1.46	1.51
3	Y	312	CLA	CMD-C2D	-2.66	1.45	1.50
3	N	614	CLA	C4D-ND	-2.66	1.34	1.37
3	N	603	CLA	CMB-C2B	-2.66	1.46	1.51
2	Y	309	CHL	C4D-ND	-2.66	1.34	1.37
3	N	603	CLA	CHC-C1C	2.65	1.41	1.35
3	N	604	CLA	CMB-C2B	-2.63	1.46	1.51
2	G	608	CHL	CMB-C2B	-2.63	1.46	1.51
3	G	610	CLA	C3B-C2B	-2.62	1.36	1.40
2	N	605	CHL	C4D-ND	-2.62	1.34	1.37
2	G	605	CHL	C4D-ND	-2.60	1.34	1.37
2	Y	310	CHL	CMB-C2B	-2.60	1.46	1.51
3	G	611	CLA	CMB-C2B	-2.56	1.46	1.51
3	Y	311	CLA	CHC-C1C	2.54	1.41	1.35
5	Y	318	NEX	C32-C33	-2.53	1.40	1.45
2	G	608	CHL	C4D-ND	-2.53	1.34	1.37
3	N	610	CLA	C4D-ND	-2.53	1.34	1.37
2	N	601	CHL	C4D-ND	-2.53	1.34	1.37
2	N	608	CHL	CMB-C2B	-2.51	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	612	CLA	CMB-C2B	-2.51	1.46	1.51
7	Y	301	XAT	O4-C5	-2.50	1.42	1.46
2	G	607	CHL	CMB-C2B	-2.50	1.46	1.51
2	Y	302	CHL	CMB-C2B	-2.50	1.46	1.51
2	G	601	CHL	CMB-C2B	-2.49	1.46	1.51
5	Y	318	NEX	C12-C13	-2.49	1.40	1.45
2	N	605	CHL	CMB-C2B	-2.49	1.46	1.51
3	Y	304	CLA	CHC-C1C	2.48	1.41	1.35
3	Y	304	CLA	CMB-C2B	-2.48	1.46	1.51
2	G	606	CHL	CMB-C2B	-2.47	1.46	1.51
2	Y	308	CHL	CMB-C2B	-2.47	1.46	1.51
2	N	601	CHL	CMB-C2B	-2.47	1.46	1.51
2	Y	307	CHL	CMB-C2B	-2.47	1.46	1.51
3	G	603	CLA	CMB-C2B	-2.47	1.46	1.51
3	G	613	CLA	CMB-C2B	-2.47	1.46	1.51
3	Y	312	CLA	CMB-C2B	-2.46	1.46	1.51
2	Y	306	CHL	CMB-C2B	-2.46	1.46	1.51
3	N	612	CLA	CMB-C2B	-2.45	1.46	1.51
3	Y	311	CLA	C3B-CAB	-2.45	1.42	1.47
3	N	611	CLA	CMB-C2B	-2.45	1.46	1.51
5	Y	318	NEX	C28-C29	-2.44	1.40	1.45
5	N	617	NEX	O24-C25	-2.44	1.42	1.46
2	N	607	CHL	CMB-C2B	-2.44	1.46	1.51
3	Y	314	CLA	CMB-C2B	-2.43	1.46	1.51
3	Y	313	CLA	CMB-C2B	-2.42	1.46	1.51
3	Y	315	CLA	CMB-C2B	-2.41	1.46	1.51
2	Y	309	CHL	CMB-C2B	-2.39	1.46	1.51
2	G	605	CHL	CMB-C2B	-2.39	1.46	1.51
3	N	614	CLA	CMB-C2B	-2.38	1.46	1.51
3	Y	303	CLA	CMB-C2B	-2.38	1.46	1.51
3	Y	311	CLA	CMB-C2B	-2.36	1.46	1.51
2	G	608	CHL	CMD-C2D	-2.35	1.45	1.50
3	N	613	CLA	CMB-C2B	-2.35	1.46	1.51
3	Y	315	CLA	CMD-C2D	-2.35	1.45	1.50
7	N	619	XAT	O24-C25	-2.34	1.42	1.46
3	Y	311	CLA	C3B-C2B	-2.34	1.37	1.40
3	Y	304	CLA	CMD-C2D	-2.34	1.45	1.50
3	N	602	CLA	CMB-C2B	-2.33	1.46	1.51
5	G	617	NEX	O24-C25	-2.32	1.42	1.46
3	G	614	CLA	CMB-C2B	-2.31	1.46	1.51
3	N	610	CLA	C3B-CAB	-2.31	1.43	1.47
7	G	619	XAT	O24-C25	-2.29	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	610	CLA	C3B-CAB	-2.28	1.43	1.47
3	Y	313	CLA	C3B-C2B	-2.27	1.37	1.40
7	N	619	XAT	O4-C5	-2.26	1.43	1.46
2	Y	302	CHL	CMD-C2D	-2.25	1.46	1.50
3	G	603	CLA	C3B-C2B	-2.24	1.37	1.40
3	G	611	CLA	CMD-C2D	-2.24	1.46	1.50
3	G	602	CLA	C3B-C2B	-2.23	1.37	1.40
2	Y	308	CHL	CMD-C2D	-2.22	1.46	1.50
3	G	610	CLA	CMD-C2D	-2.21	1.46	1.50
3	G	614	CLA	CMD-C2D	-2.21	1.46	1.50
3	N	603	CLA	C3B-C2B	-2.20	1.37	1.40
2	N	601	CHL	CMD-C2D	-2.19	1.46	1.50
7	Y	301	XAT	O24-C25	-2.19	1.43	1.46
3	Y	304	CLA	C3B-C2B	-2.18	1.37	1.40
3	G	614	CLA	C3B-C2B	-2.18	1.37	1.40
2	G	605	CHL	CMD-C2D	-2.18	1.46	1.50
3	N	614	CLA	CMD-C2D	-2.18	1.46	1.50
3	G	611	CLA	C3B-C2B	-2.17	1.37	1.40
3	N	611	CLA	CMC-C2C	-2.15	1.46	1.50
2	N	605	CHL	CMD-C2D	-2.15	1.46	1.50
3	Y	311	CLA	MG-ND	-2.15	2.01	2.05
3	N	611	CLA	CMD-C2D	-2.13	1.46	1.50
3	Y	313	CLA	C3D-C4D	2.13	1.49	1.44
3	Y	303	CLA	CMD-C2D	-2.13	1.46	1.50
7	G	619	XAT	O4-C5	-2.12	1.43	1.46
3	G	612	CLA	CMD-C2D	-2.12	1.46	1.50
3	Y	305	CLA	CMD-C2D	-2.11	1.46	1.50
2	G	601	CHL	CAC-C3C	-2.11	1.45	1.51
3	N	612	CLA	C3B-C2B	-2.10	1.37	1.40
3	Y	311	CLA	C4B-CHC	-2.10	1.35	1.41
3	N	612	CLA	C3D-C4D	2.10	1.48	1.44
3	N	604	CLA	CMD-C2D	-2.08	1.46	1.50
2	N	609	CHL	MG-ND	-2.08	2.01	2.05
3	Y	314	CLA	CMD-C2D	-2.07	1.46	1.50
3	G	603	CLA	CMD-C2D	-2.07	1.46	1.50
2	N	609	CHL	CMD-C2D	-2.06	1.46	1.50
2	N	608	CHL	CMD-C2D	-2.06	1.46	1.50
2	G	609	CHL	CMD-C2D	-2.06	1.46	1.50
3	N	603	CLA	CMD-C2D	-2.06	1.46	1.50
3	N	612	CLA	CMC-C2C	-2.06	1.46	1.50
3	Y	311	CLA	CMD-C2D	-2.06	1.46	1.50
3	Y	312	CLA	C3D-C4D	2.05	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	606	CHL	CMD-C2D	-2.05	1.46	1.50
3	N	614	CLA	C3B-C2B	-2.04	1.37	1.40
3	N	610	CLA	CMD-C2D	-2.04	1.46	1.50
2	Y	307	CHL	CMD-C2D	-2.04	1.46	1.50
3	G	602	CLA	CMC-C2C	-2.04	1.46	1.50
3	Y	315	CLA	C3B-C2B	-2.04	1.37	1.40
3	Y	304	CLA	C4B-CHC	-2.04	1.35	1.41
3	G	603	CLA	CMC-C2C	-2.03	1.46	1.50
2	Y	309	CHL	CMD-C2D	-2.02	1.46	1.50
2	Y	306	CHL	CMD-C2D	-2.02	1.46	1.50
3	Y	312	CLA	CMC-C2C	-2.01	1.46	1.50
2	Y	307	CHL	C3D-C4D	2.00	1.48	1.44
3	G	604	CLA	CMD-C2D	-2.00	1.46	1.50
3	G	610	CLA	CMC-C2C	-2.00	1.46	1.50
2	N	607	CHL	CMD-C2D	-2.00	1.46	1.50
3	N	603	CLA	CMC-C2C	-2.00	1.46	1.50
3	N	612	CLA	CMD-C2D	-2.00	1.46	1.50

All (545) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	617	NEX	O24-C25-C24	9.08	120.20	113.38
5	G	617	NEX	O24-C25-C24	8.88	120.05	113.38
2	Y	307	CHL	C4A-NA-C1A	8.64	110.59	106.71
2	N	606	CHL	C4A-NA-C1A	8.31	110.44	106.71
7	G	619	XAT	O4-C5-C4	8.27	119.59	113.38
7	Y	301	XAT	O4-C5-C4	7.86	119.28	113.38
7	G	619	XAT	O24-C25-C24	7.73	119.19	113.38
7	N	619	XAT	O4-C5-C4	7.73	119.19	113.38
2	Y	310	CHL	C4A-NA-C1A	7.71	110.17	106.71
7	N	619	XAT	O24-C25-C24	7.41	118.95	113.38
7	Y	301	XAT	O24-C25-C24	7.26	118.84	113.38
2	Y	308	CHL	C4A-NA-C1A	6.74	109.73	106.71
2	G	607	CHL	C4A-NA-C1A	6.73	109.73	106.71
2	N	607	CHL	C4A-NA-C1A	6.61	109.68	106.71
3	Y	312	CLA	C4A-NA-C1A	6.58	109.67	106.71
2	G	609	CHL	C1B-CHB-C4A	-6.44	117.37	130.12
2	G	606	CHL	C4A-NA-C1A	6.43	109.60	106.71
2	G	609	CHL	C4A-NA-C1A	6.31	109.54	106.71
3	G	613	CLA	C4A-NA-C1A	6.07	109.43	106.71
2	N	609	CHL	C4A-NA-C1A	5.64	109.24	106.71
2	G	609	CHL	CMB-C2B-C1B	-5.54	119.95	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	619	XAT	C15-C14-C13	-5.44	119.55	127.31
3	Y	305	CLA	CMB-C2B-C1B	-5.43	120.12	128.46
3	Y	314	CLA	C4A-NA-C1A	5.40	109.13	106.71
3	N	613	CLA	C4A-NA-C1A	5.37	109.12	106.71
3	G	604	CLA	C4A-NA-C1A	5.34	109.11	106.71
3	Y	304	CLA	C4A-NA-C1A	5.26	109.07	106.71
5	N	617	NEX	C27-C28-C29	-5.18	117.49	125.53
3	N	604	CLA	C4A-NA-C1A	5.02	108.97	106.71
2	N	609	CHL	C1B-CHB-C4A	-4.96	120.29	130.12
2	G	608	CHL	C4A-NA-C1A	4.91	108.92	106.71
3	Y	313	CLA	C4A-NA-C1A	4.84	108.88	106.71
2	Y	309	CHL	C4A-NA-C1A	4.82	108.87	106.71
3	N	612	CLA	C4A-NA-C1A	4.82	108.87	106.71
3	N	613	CLA	CMB-C2B-C1B	-4.78	121.12	128.46
2	N	608	CHL	C4A-NA-C1A	4.76	108.84	106.71
2	Y	308	CHL	C1B-CHB-C4A	-4.70	120.81	130.12
3	G	612	CLA	C4A-NA-C1A	4.68	108.81	106.71
7	N	619	XAT	C18-C5-C6	-4.66	114.44	122.26
7	Y	301	XAT	C15-C14-C13	-4.65	120.67	127.31
3	G	604	CLA	CMB-C2B-C1B	-4.65	121.32	128.46
7	G	619	XAT	C18-C5-C6	-4.61	114.53	122.26
3	N	604	CLA	CMB-C2B-C1B	-4.60	121.39	128.46
7	Y	301	XAT	O24-C25-C38	4.60	120.57	115.06
7	G	619	XAT	C11-C10-C9	-4.59	120.76	127.31
3	Y	305	CLA	C4A-NA-C1A	4.58	108.76	106.71
3	N	611	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
3	N	611	CLA	C4A-NA-C1A	4.51	108.73	106.71
3	G	602	CLA	CMB-C2B-C1B	-4.49	121.57	128.46
5	N	617	NEX	C15-C14-C13	-4.48	120.91	127.31
7	Y	301	XAT	C38-C25-C26	-4.45	114.81	122.26
3	N	602	CLA	C4A-NA-C1A	4.44	108.70	106.71
7	N	619	XAT	C38-C25-C26	-4.44	114.82	122.26
7	G	619	XAT	C38-C25-C26	-4.40	114.89	122.26
7	N	619	XAT	O24-C25-C38	4.40	120.32	115.06
3	Y	303	CLA	C4A-NA-C1A	4.37	108.67	106.71
2	N	607	CHL	C1B-CHB-C4A	-4.36	121.49	130.12
5	G	617	NEX	C15-C14-C13	-4.36	121.09	127.31
7	N	619	XAT	C35-C34-C33	-4.36	121.09	127.31
7	Y	301	XAT	C18-C5-C6	-4.34	114.98	122.26
7	N	619	XAT	C11-C10-C9	-4.26	121.24	127.31
7	Y	301	XAT	C11-C10-C9	-4.24	121.26	127.31
7	G	619	XAT	O4-C5-C18	4.24	120.13	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	617	NEX	C38-C25-C26	-4.23	115.17	122.26
3	G	611	CLA	C4A-NA-C1A	4.23	108.61	106.71
2	Y	310	CHL	C1B-CHB-C4A	-4.23	121.75	130.12
2	G	609	CHL	CMB-C2B-C3B	4.22	132.57	124.68
3	Y	305	CLA	CMB-C2B-C3B	4.22	132.57	124.68
2	N	609	CHL	CMB-C2B-C1B	-4.20	122.01	128.46
5	N	617	NEX	C38-C25-C26	-4.20	115.22	122.26
5	Y	318	NEX	C39-C29-C30	-4.19	117.05	122.92
3	G	613	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
3	G	610	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
2	G	607	CHL	C1B-CHB-C4A	-4.16	121.88	130.12
2	N	609	CHL	CHD-C1D-ND	-4.15	120.64	124.45
7	G	619	XAT	O24-C25-C38	4.14	120.02	115.06
3	Y	303	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
4	N	615	LUT	C35-C34-C33	-4.13	121.41	127.31
4	G	616	LUT	C2-C3-C4	-4.13	104.65	110.30
2	G	609	CHL	CHD-C1D-ND	-4.12	120.66	124.45
3	N	613	CLA	CMB-C2B-C3B	4.12	132.39	124.68
3	Y	314	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
3	N	603	CLA	C4A-NA-C1A	4.05	108.53	106.71
3	N	602	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
5	G	617	NEX	C11-C10-C9	-4.04	121.54	127.31
5	G	617	NEX	C27-C28-C29	-4.03	119.27	125.53
7	N	619	XAT	O4-C5-C18	4.03	119.89	115.06
5	G	617	NEX	C17-C1-C6	-4.02	106.88	110.47
3	G	612	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
7	Y	301	XAT	C31-C30-C29	-3.98	121.62	127.31
7	Y	301	XAT	O4-C5-C18	3.93	119.76	115.06
5	N	617	NEX	C35-C34-C33	-3.86	121.80	127.31
7	Y	301	XAT	C35-C34-C33	-3.85	121.81	127.31
2	N	608	CHL	C1B-CHB-C4A	-3.85	122.49	130.12
7	G	619	XAT	C31-C30-C29	-3.85	121.81	127.31
3	N	611	CLA	CMB-C2B-C3B	3.85	131.87	124.68
2	G	601	CHL	CMB-C2B-C1B	-3.79	122.63	128.46
2	G	606	CHL	CMB-C2B-C1B	-3.78	122.65	128.46
5	N	617	NEX	C11-C10-C9	-3.77	121.93	127.31
2	Y	310	CHL	CMB-C2B-C1B	-3.77	122.67	128.46
2	Y	302	CHL	C4A-NA-C1A	3.75	108.39	106.71
5	Y	318	NEX	C15-C35-C34	3.75	131.16	123.47
2	Y	306	CHL	C1B-CHB-C4A	-3.74	122.72	130.12
2	N	606	CHL	CMB-C2B-C1B	-3.73	122.73	128.46
2	G	605	CHL	C1B-CHB-C4A	-3.72	122.75	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	617	NEX	O24-C25-C38	3.70	119.50	115.06
3	N	604	CLA	CMB-C2B-C3B	3.70	131.60	124.68
2	N	605	CHL	C4A-NA-C1A	3.70	108.37	106.71
4	G	616	LUT	C15-C14-C13	-3.68	122.05	127.31
7	N	619	XAT	C31-C30-C29	-3.67	122.07	127.31
3	G	604	CLA	CMB-C2B-C3B	3.66	131.52	124.68
3	G	603	CLA	C4A-NA-C1A	3.64	108.34	106.71
5	G	617	NEX	O24-C25-C38	3.63	119.40	115.06
3	G	610	CLA	C1B-CHB-C4A	-3.61	122.97	130.12
3	G	611	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
2	Y	309	CHL	CMB-C2B-C1B	-3.57	122.97	128.46
4	Y	317	LUT	C7-C8-C9	-3.57	120.84	126.23
7	G	619	XAT	C15-C14-C13	-3.56	122.22	127.31
2	N	608	CHL	CMB-C2B-C1B	-3.53	123.04	128.46
4	N	616	LUT	C35-C34-C33	-3.52	122.29	127.31
3	N	612	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
3	G	612	CLA	CMB-C2B-C3B	3.51	131.24	124.68
3	G	613	CLA	CMB-C2B-C3B	3.49	131.21	124.68
3	N	602	CLA	CMB-C2B-C3B	3.49	131.21	124.68
4	G	616	LUT	C35-C34-C33	-3.49	122.33	127.31
2	N	605	CHL	CMB-C2B-C1B	-3.48	123.11	128.46
2	Y	308	CHL	CMB-C2B-C1B	-3.48	123.12	128.46
3	Y	303	CLA	CMB-C2B-C3B	3.47	131.17	124.68
6	Y	319	LHG	O8-C23-C24	3.47	122.80	111.91
4	N	616	LUT	C15-C14-C13	-3.47	122.36	127.31
2	N	607	CHL	CMB-C2B-C1B	-3.46	123.14	128.46
2	N	609	CHL	CMB-C2B-C3B	3.46	131.15	124.68
6	G	618	LHG	O8-C23-C24	3.46	122.76	111.91
2	N	605	CHL	C1B-CHB-C4A	-3.46	123.27	130.12
2	N	601	CHL	CMB-C2B-C1B	-3.45	123.16	128.46
3	G	603	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
2	Y	302	CHL	CMB-C2B-C1B	-3.42	123.21	128.46
7	G	619	XAT	C26-C27-C28	-3.42	118.77	125.99
5	Y	318	NEX	C40-C33-C34	-3.41	118.14	122.92
4	N	615	LUT	C11-C10-C9	-3.40	122.45	127.31
2	Y	310	CHL	CHD-C1D-ND	-3.40	121.33	124.45
3	Y	312	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
5	G	617	NEX	C31-C30-C29	-3.39	122.48	127.31
2	G	607	CHL	CMB-C2B-C1B	-3.38	123.27	128.46
3	N	610	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
2	Y	306	CHL	C4A-NA-C1A	3.37	108.22	106.71
2	Y	310	CHL	CAC-C3C-C4C	3.36	129.17	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	615	LUT	C35-C15-C14	-3.36	116.59	123.47
2	Y	307	CHL	CMB-C2B-C1B	-3.35	123.31	128.46
3	G	610	CLA	CMB-C2B-C3B	3.35	130.94	124.68
3	Y	314	CLA	CMB-C2B-C3B	3.33	130.90	124.68
3	G	602	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
2	Y	309	CHL	C1B-CHB-C4A	-3.32	123.55	130.12
2	Y	306	CHL	CMB-C2B-C1B	-3.31	123.38	128.46
3	Y	304	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
3	Y	311	CLA	C1B-CHB-C4A	-3.30	123.57	130.12
4	Y	316	LUT	C7-C8-C9	-3.30	121.25	126.23
5	Y	318	NEX	C20-C13-C14	-3.29	118.31	122.92
3	G	602	CLA	CMB-C2B-C3B	3.28	130.82	124.68
3	N	610	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
3	G	614	CLA	C4A-NA-C1A	3.28	108.18	106.71
7	N	619	XAT	C26-C27-C28	-3.28	119.07	125.99
3	N	611	CLA	C1B-CHB-C4A	-3.27	123.65	130.12
3	G	610	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
3	G	611	CLA	CMD-C2D-C1D	-3.26	118.97	124.71
3	Y	305	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
6	G	618	LHG	O7-C7-C8	3.25	118.51	111.50
2	N	601	CHL	C4A-NA-C1A	3.25	108.17	106.71
3	Y	313	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
5	Y	318	NEX	C35-C15-C14	3.24	130.11	123.47
3	N	612	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
2	G	606	CHL	CMB-C2B-C3B	3.23	130.72	124.68
3	Y	311	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
3	Y	311	CLA	CMA-C3A-C4A	3.22	120.43	111.77
4	G	615	LUT	C35-C34-C33	-3.22	122.72	127.31
3	N	611	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
4	G	615	LUT	C21-C26-C27	-3.20	108.65	112.70
3	N	603	CLA	CAA-C2A-C3A	-3.20	104.02	112.78
3	G	611	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
3	G	611	CLA	C1B-CHB-C4A	-3.19	123.79	130.12
3	N	610	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
5	G	617	NEX	C35-C34-C33	-3.18	122.77	127.31
7	G	619	XAT	C17-C1-C2	-3.18	103.47	108.98
2	N	605	CHL	O2D-CGD-O1D	-3.16	117.65	123.84
3	G	602	CLA	C4A-NA-C1A	3.16	108.13	106.71
2	G	601	CHL	C1B-CHB-C4A	-3.16	123.86	130.12
3	N	602	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
5	Y	318	NEX	C32-C33-C34	3.15	123.77	118.94
3	N	614	CLA	C4A-NA-C1A	3.15	108.12	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Y	301	XAT	C7-C8-C9	-3.14	120.66	125.53
2	G	607	CHL	CHD-C1D-ND	-3.14	121.57	124.45
7	N	619	XAT	C11-C12-C13	-3.13	117.61	126.42
7	G	619	XAT	C35-C34-C33	-3.13	122.84	127.31
2	G	605	CHL	CMB-C2B-C1B	-3.13	123.65	128.46
3	Y	315	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
3	Y	312	CLA	C1B-CHB-C4A	-3.13	123.91	130.12
3	G	602	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
4	Y	317	LUT	C15-C14-C13	-3.12	122.85	127.31
3	G	614	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
3	G	614	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
7	Y	301	XAT	C27-C28-C29	-3.11	120.71	125.53
2	G	601	CHL	CMB-C2B-C3B	3.10	130.49	124.68
2	Y	308	CHL	CMB-C2B-C3B	3.10	130.48	124.68
3	Y	315	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
2	N	607	CHL	CMB-C2B-C3B	3.09	130.46	124.68
2	G	608	CHL	CMB-C2B-C1B	-3.08	123.72	128.46
6	N	618	LHG	O7-C7-C8	3.08	118.14	111.50
3	G	604	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
4	G	615	LUT	C7-C8-C9	-3.07	121.59	126.23
3	Y	305	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
5	Y	318	NEX	C19-C9-C10	-3.06	118.63	122.92
3	Y	304	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
2	G	607	CHL	O2D-CGD-O1D	-3.05	117.88	123.84
2	Y	306	CHL	O2D-CGD-O1D	-3.05	117.88	123.84
2	G	606	CHL	O2D-CGD-O1D	-3.04	117.89	123.84
3	Y	305	CLA	C4-C3-C5	3.03	120.37	115.27
3	Y	311	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
3	N	602	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
3	G	614	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
3	N	613	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
2	N	607	CHL	CHD-C1D-ND	-3.01	121.69	124.45
4	N	615	LUT	C30-C31-C32	-3.01	113.84	123.22
5	Y	318	NEX	C12-C13-C14	3.00	123.55	118.94
7	G	619	XAT	C7-C8-C9	-3.00	120.88	125.53
3	G	612	CLA	C1B-CHB-C4A	-3.00	124.19	130.12
7	Y	301	XAT	C26-C27-C28	-2.99	119.66	125.99
6	Y	319	LHG	O7-C7-C8	2.99	117.94	111.50
7	G	619	XAT	C15-C35-C34	-2.98	117.36	123.47
3	Y	303	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
3	G	611	CLA	CMD-C2D-C3D	2.97	134.45	127.61
3	N	603	CLA	CMB-C2B-C1B	-2.97	123.90	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	607	CHL	CMB-C2B-C3B	2.96	130.22	124.68
4	N	615	LUT	C7-C8-C9	-2.96	121.77	126.23
4	N	616	LUT	C31-C30-C29	-2.95	123.10	127.31
2	G	608	CHL	O2D-CGD-O1D	-2.94	118.08	123.84
5	N	617	NEX	C39-C29-C30	-2.94	118.81	122.92
4	N	615	LUT	C15-C14-C13	-2.94	123.12	127.31
3	N	604	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
7	Y	301	XAT	C11-C12-C13	-2.94	118.17	126.42
3	Y	304	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
3	Y	311	CLA	CMB-C2B-C3B	2.93	130.17	124.68
2	N	601	CHL	CMB-C2B-C3B	2.93	130.16	124.68
3	N	614	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
3	N	614	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
2	N	606	CHL	C1-C2-C3	-2.92	122.03	126.75
2	G	601	CHL	O2D-CGD-O1D	-2.91	118.15	123.84
3	N	614	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
3	Y	314	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
2	G	606	CHL	C2A-C1A-CHA	2.90	128.93	123.86
5	Y	318	NEX	C28-C29-C30	2.89	123.38	118.94
7	N	619	XAT	C17-C1-C2	-2.89	103.96	108.98
4	Y	317	LUT	C38-C25-C24	-2.89	117.38	123.56
3	G	603	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
3	Y	304	CLA	CHB-C4A-NA	2.89	128.50	124.51
2	Y	302	CHL	CMB-C2B-C3B	2.89	130.08	124.68
2	G	605	CHL	O2D-CGD-O1D	-2.89	118.20	123.84
7	N	619	XAT	C18-C5-C4	2.88	117.52	114.28
3	N	603	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
2	Y	302	CHL	O2D-CGD-O1D	-2.88	118.22	123.84
3	N	604	CLA	C1-C2-C3	-2.87	121.08	126.04
3	G	613	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
2	Y	302	CHL	C1B-CHB-C4A	-2.86	124.44	130.12
3	G	604	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
3	N	611	CLA	O2D-CGD-CBD	2.86	116.34	111.27
3	N	610	CLA	C4A-NA-C1A	2.84	107.98	106.71
4	Y	317	LUT	C11-C10-C9	-2.84	123.25	127.31
2	G	609	CHL	C1D-CHD-C4C	-2.84	119.93	126.06
5	G	617	NEX	C24-C23-C22	-2.83	105.30	110.77
3	G	603	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
2	G	609	CHL	CHD-C4C-C3C	2.82	128.99	124.84
3	G	613	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
3	Y	314	CLA	CHD-C1D-ND	-2.82	121.87	124.45
3	G	611	CLA	CMB-C2B-C3B	2.81	129.94	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Y	301	XAT	C17-C1-C2	-2.81	104.10	108.98
3	N	612	CLA	CMB-C2B-C3B	2.81	129.93	124.68
2	N	606	CHL	O2D-CGD-O1D	-2.80	118.36	123.84
2	G	605	CHL	C4A-NA-C1A	2.80	107.97	106.71
3	G	603	CLA	CHB-C4A-NA	2.80	128.38	124.51
2	N	605	CHL	CMB-C2B-C3B	2.80	129.92	124.68
3	G	603	CLA	CMB-C2B-C3B	2.80	129.92	124.68
5	N	617	NEX	C24-C23-C22	-2.79	105.38	110.77
3	Y	303	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
7	G	619	XAT	C11-C12-C13	-2.79	118.59	126.42
2	G	601	CHL	C3C-C4C-NC	-2.78	107.45	110.57
5	N	617	NEX	C31-C30-C29	-2.78	123.34	127.31
2	G	608	CHL	C1B-CHB-C4A	-2.78	124.61	130.12
3	Y	313	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
2	N	601	CHL	O2D-CGD-O1D	-2.78	118.41	123.84
3	G	612	CLA	C1-C2-C3	-2.78	121.24	126.04
4	G	616	LUT	C38-C25-C24	-2.77	117.62	123.56
3	Y	304	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
3	Y	315	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
7	N	619	XAT	C5-C4-C3	-2.76	107.28	112.75
5	N	617	NEX	C31-C32-C33	-2.76	118.66	126.42
3	G	610	CLA	C4A-NA-C1A	2.75	107.94	106.71
4	G	615	LUT	C11-C10-C9	-2.75	123.38	127.31
2	Y	309	CHL	O2D-CGD-O1D	-2.74	118.47	123.84
4	Y	316	LUT	C18-C5-C6	-2.74	121.45	124.53
3	N	604	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
4	G	616	LUT	C7-C8-C9	-2.74	122.09	126.23
2	N	601	CHL	O2A-C1-C2	-2.74	101.44	108.64
2	G	606	CHL	C1B-CHB-C4A	-2.73	124.71	130.12
3	N	613	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
3	N	603	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
2	Y	310	CHL	CMB-C2B-C3B	2.72	129.78	124.68
4	N	615	LUT	C21-C26-C27	-2.72	109.26	112.70
5	G	617	NEX	C26-C27-C28	-2.72	120.24	125.99
2	Y	307	CHL	CHB-C4A-NA	2.72	128.27	124.51
3	N	603	CLA	CHB-C4A-NA	2.72	128.27	124.51
2	N	606	CHL	C1B-CHB-C4A	-2.72	124.74	130.12
2	Y	308	CHL	CHD-C1D-ND	-2.71	121.96	124.45
7	G	619	XAT	C27-C28-C29	-2.71	121.33	125.53
7	Y	301	XAT	C15-C35-C34	-2.70	117.94	123.47
5	N	617	NEX	C15-C35-C34	-2.70	117.95	123.47
4	N	616	LUT	C21-C26-C27	-2.69	109.30	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	613	CLA	CHD-C1D-ND	-2.68	121.99	124.45
7	Y	301	XAT	C18-C5-C4	2.68	117.29	114.28
2	Y	308	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
2	N	606	CHL	CMB-C2B-C3B	2.67	129.68	124.68
7	Y	301	XAT	C24-C23-C22	-2.67	105.61	110.77
2	Y	307	CHL	CMB-C2B-C3B	2.67	129.68	124.68
2	N	608	CHL	O2D-CGD-O1D	-2.67	118.62	123.84
2	N	608	CHL	CMB-C2B-C3B	2.67	129.67	124.68
3	Y	315	CLA	CMB-C2B-C3B	2.67	129.67	124.68
7	N	619	XAT	C27-C28-C29	-2.67	121.39	125.53
3	N	610	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
3	Y	313	CLA	CMB-C2B-C3B	2.65	129.64	124.68
2	Y	306	CHL	CMB-C2B-C3B	2.65	129.63	124.68
5	G	617	NEX	C39-C29-C30	-2.65	119.22	122.92
3	G	612	CLA	CHB-C4A-NA	2.65	128.17	124.51
5	N	617	NEX	C17-C1-C6	-2.64	108.11	110.47
2	G	606	CHL	O2D-CGD-CBD	2.64	115.96	111.27
2	Y	310	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
3	G	614	CLA	CMB-C2B-C3B	2.62	129.59	124.68
4	G	615	LUT	C15-C14-C13	-2.62	123.57	127.31
3	G	611	CLA	O2D-CGD-CBD	2.61	115.91	111.27
2	N	607	CHL	O2D-CGD-O1D	-2.61	118.73	123.84
7	G	619	XAT	C5-C4-C3	-2.61	107.59	112.75
2	G	606	CHL	CHB-C4A-NA	2.60	128.11	124.51
3	Y	314	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
2	N	601	CHL	C1B-CHB-C4A	-2.60	124.97	130.12
3	G	613	CLA	CHB-C4A-NA	2.60	128.10	124.51
2	G	609	CHL	CHD-C1D-C2D	2.60	130.92	125.48
4	G	615	LUT	C38-C25-C24	-2.59	118.01	123.56
5	G	617	NEX	C15-C35-C34	-2.59	118.18	123.47
3	Y	312	CLA	CMB-C2B-C3B	2.59	129.52	124.68
5	N	617	NEX	C28-C29-C30	2.58	122.90	118.94
4	G	615	LUT	C18-C5-C6	-2.57	121.64	124.53
5	G	617	NEX	C5-C4-C3	2.57	114.79	111.75
3	N	610	CLA	CMB-C2B-C3B	2.56	129.47	124.68
2	Y	308	CHL	C2A-C1A-CHA	2.56	128.34	123.86
4	N	616	LUT	C38-C25-C24	-2.56	118.08	123.56
3	G	612	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
2	G	605	CHL	CMB-C2B-C3B	2.55	129.45	124.68
2	G	607	CHL	OMC-CMC-C2C	-2.55	119.92	125.69
2	Y	307	CHL	O2D-CGD-O1D	-2.54	118.87	123.84
7	N	619	XAT	C6-C7-C8	-2.54	120.62	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	313	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
5	N	617	NEX	C5-C4-C3	2.54	114.75	111.75
4	Y	316	LUT	C11-C10-C9	-2.53	123.69	127.31
7	N	619	XAT	C15-C35-C34	-2.53	118.30	123.47
4	Y	317	LUT	C21-C26-C27	-2.52	109.51	112.70
4	Y	316	LUT	C37-C21-C22	-2.52	104.67	109.44
2	G	601	CHL	CHD-C1D-ND	-2.51	122.14	124.45
2	Y	309	CHL	CMB-C2B-C3B	2.51	129.38	124.68
2	Y	310	CHL	OMC-CMC-C2C	-2.51	120.01	125.69
2	N	608	CHL	C2A-C1A-CHA	2.50	128.22	123.86
2	G	601	CHL	O2A-CGA-O1A	-2.49	117.30	123.59
2	Y	302	CHL	CHD-C1D-ND	-2.49	122.17	124.45
2	Y	302	CHL	C1-C2-C3	-2.49	121.74	126.04
3	Y	305	CLA	C1-C2-C3	-2.48	121.75	126.04
3	N	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
3	G	603	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
3	Y	313	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
4	G	615	LUT	C30-C31-C32	-2.48	115.48	123.22
2	N	606	CHL	CHB-C4A-NA	2.46	127.92	124.51
3	Y	315	CLA	C4A-NA-C1A	2.46	107.81	106.71
3	N	604	CLA	CHD-C1D-ND	-2.46	122.19	124.45
3	Y	305	CLA	O2D-CGD-CBD	2.46	115.63	111.27
4	N	615	LUT	C38-C25-C24	-2.45	118.31	123.56
2	N	609	CHL	C1D-CHD-C4C	-2.45	120.77	126.06
4	G	616	LUT	C21-C26-C27	-2.45	109.61	112.70
3	Y	313	CLA	C1-C2-C3	-2.45	121.81	126.04
2	N	609	CHL	O2D-CGD-O1D	-2.44	119.06	123.84
3	Y	304	CLA	CMB-C2B-C3B	2.44	129.25	124.68
4	Y	316	LUT	C15-C14-C13	-2.44	123.83	127.31
2	Y	309	CHL	C2A-C1A-CHA	2.44	128.12	123.86
4	Y	317	LUT	C35-C34-C33	-2.44	123.83	127.31
2	N	601	CHL	CHD-C1D-ND	-2.43	122.22	124.45
2	N	609	CHL	C1-C2-C3	-2.43	121.84	126.04
4	Y	316	LUT	C2-C3-C4	2.43	113.63	110.30
2	G	609	CHL	O2D-CGD-O1D	-2.43	119.08	123.84
3	N	604	CLA	CHB-C4A-NA	2.43	127.87	124.51
2	Y	307	CHL	C2A-C1A-CHA	2.42	128.09	123.86
3	G	604	CLA	CHB-C4A-NA	2.42	127.85	124.51
3	N	613	CLA	CHB-C4A-NA	2.41	127.85	124.51
2	G	608	CHL	CAC-C3C-C4C	2.41	127.94	124.81
2	Y	309	CHL	CHB-C4A-NA	2.41	127.85	124.51
3	Y	305	CLA	CHB-C4A-NA	2.41	127.84	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Y	317	LUT	C31-C30-C29	-2.40	123.88	127.31
3	N	602	CLA	O2D-CGD-CBD	2.40	115.53	111.27
4	N	616	LUT	C18-C5-C6	-2.40	121.83	124.53
3	Y	313	CLA	CMD-C2D-C3D	2.40	133.13	127.61
4	N	616	LUT	C7-C8-C9	-2.40	122.61	126.23
2	Y	307	CHL	C1-C2-C3	-2.39	122.88	126.75
2	N	605	CHL	CHB-C4A-NA	2.38	127.81	124.51
3	Y	303	CLA	CHB-C4A-NA	2.38	127.80	124.51
4	N	616	LUT	C16-C1-C6	-2.37	106.45	110.30
4	Y	316	LUT	C38-C25-C24	-2.37	118.48	123.56
2	N	609	CHL	CHD-C1D-C2D	2.37	130.46	125.48
2	G	601	CHL	OMC-CMC-C2C	-2.37	120.32	125.69
6	Y	319	LHG	O8-C23-O10	-2.37	117.62	123.59
3	N	614	CLA	CMB-C2B-C3B	2.36	129.10	124.68
3	Y	311	CLA	C2D-C1D-ND	-2.36	108.36	110.10
7	G	619	XAT	C18-C5-C4	2.36	116.94	114.28
6	G	618	LHG	O8-C23-O10	-2.35	117.66	123.59
5	Y	318	NEX	C27-C28-C29	-2.34	121.89	125.53
3	G	610	CLA	O2D-CGD-CBD	2.34	115.43	111.27
3	N	612	CLA	CHB-C4A-NA	2.34	127.74	124.51
2	G	605	CHL	CHD-C1D-ND	-2.34	122.31	124.45
2	N	609	CHL	OMC-CMC-C2C	-2.33	120.42	125.69
3	Y	315	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
2	G	609	CHL	C2D-C1D-ND	-2.33	108.39	110.10
2	Y	310	CHL	C2A-C1A-CHA	2.33	127.92	123.86
2	Y	308	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
6	N	618	LHG	O8-C23-C24	2.32	119.19	111.91
7	Y	301	XAT	C5-C4-C3	-2.32	108.16	112.75
2	N	601	CHL	CHB-C4A-NA	2.32	127.72	124.51
4	G	616	LUT	C31-C30-C29	-2.32	124.00	127.31
3	G	610	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
7	N	619	XAT	C7-C8-C9	-2.31	121.94	125.53
3	N	613	CLA	CHD-C1D-ND	-2.31	122.33	124.45
2	Y	302	CHL	OMC-CMC-C2C	-2.31	120.47	125.69
3	N	603	CLA	CMB-C2B-C3B	2.31	129.00	124.68
2	Y	302	CHL	CHB-C4A-NA	2.31	127.70	124.51
4	G	616	LUT	C16-C1-C6	-2.31	106.56	110.30
3	G	604	CLA	CHD-C1D-ND	-2.30	122.34	124.45
3	Y	312	CLA	CMD-C2D-C3D	2.30	132.91	127.61
2	N	606	CHL	C2A-C1A-CHA	2.30	127.89	123.86
3	G	614	CLA	CAA-CBA-CGA	-2.30	106.53	113.25
3	Y	305	CLA	CHD-C1D-ND	-2.30	122.34	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	605	CHL	C2A-C1A-CHA	2.29	127.87	123.86
2	Y	308	CHL	CAA-C2A-C3A	-2.29	106.50	112.78
3	N	610	CLA	C1D-ND-C4D	-2.28	104.71	106.33
3	N	614	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
3	G	614	CLA	CHB-C4A-NA	2.28	127.67	124.51
4	G	615	LUT	C10-C11-C12	-2.28	116.10	123.22
3	N	611	CLA	CHB-C4A-NA	2.28	127.66	124.51
2	G	608	CHL	CHB-C4A-NA	2.27	127.65	124.51
3	Y	313	CLA	CHB-C4A-NA	2.27	127.65	124.51
4	N	616	LUT	C30-C31-C32	-2.27	116.14	123.22
2	G	601	CHL	O2D-CGD-CBD	2.27	115.30	111.27
2	Y	307	CHL	C3A-C2A-C1A	2.27	104.74	101.34
3	N	614	CLA	CHB-C4A-NA	2.26	127.64	124.51
3	Y	314	CLA	CHB-C4A-NA	2.26	127.64	124.51
3	N	602	CLA	CHD-C1D-ND	-2.26	122.38	124.45
2	G	609	CHL	O2A-CGA-O1A	-2.26	117.89	123.59
2	Y	307	CHL	C1B-CHB-C4A	-2.26	125.65	130.12
2	N	607	CHL	O2D-CGD-CBD	2.26	115.28	111.27
2	N	607	CHL	C2A-C1A-CHA	2.25	127.80	123.86
3	Y	312	CLA	CMD-C2D-C1D	-2.25	120.74	124.71
4	Y	316	LUT	C21-C26-C27	-2.24	109.87	112.70
3	Y	311	CLA	O2D-CGD-CBD	2.24	115.24	111.27
2	Y	306	CHL	C2A-C1A-CHA	2.24	127.77	123.86
2	N	605	CHL	CHD-C1D-ND	-2.23	122.41	124.45
2	Y	310	CHL	C3C-C4C-NC	-2.23	108.07	110.57
2	Y	306	CHL	C2C-C3C-C4C	2.23	108.08	106.49
2	Y	306	CHL	CHD-C1D-ND	-2.22	122.41	124.45
3	G	610	CLA	CHB-C4A-NA	2.22	127.58	124.51
3	N	612	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
4	Y	317	LUT	C18-C5-C6	-2.19	122.07	124.53
3	G	602	CLA	CHD-C1D-ND	-2.19	122.44	124.45
2	N	608	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
2	Y	310	CHL	CHD-C1D-C2D	2.18	130.06	125.48
2	G	609	CHL	OMC-CMC-C2C	-2.18	120.75	125.69
2	Y	307	CHL	CBA-CAA-C2A	-2.18	107.43	113.86
4	Y	316	LUT	C22-C23-C24	-2.17	109.27	111.74
3	G	611	CLA	CHB-C4A-NA	2.17	127.51	124.51
2	G	605	CHL	C2A-C1A-CHA	2.16	127.63	123.86
4	N	615	LUT	C22-C23-C24	-2.16	109.29	111.74
2	G	605	CHL	O2A-CGA-O1A	-2.15	118.16	123.59
4	N	616	LUT	C10-C11-C12	-2.15	116.51	123.22
3	Y	312	CLA	C1D-ND-C4D	-2.15	104.81	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	619	XAT	C38-C25-C24	2.14	116.69	114.28
2	N	601	CHL	C7-C6-C5	-2.14	107.54	113.36
3	Y	311	CLA	C2A-C3A-C4A	-2.14	98.41	101.87
5	N	617	NEX	C11-C12-C13	-2.14	120.41	126.42
4	Y	316	LUT	C10-C11-C12	-2.14	116.55	123.22
2	G	606	CHL	CHA-C1A-NA	-2.13	121.53	126.40
3	Y	315	CLA	CHB-C4A-NA	2.12	127.45	124.51
2	Y	307	CHL	O2A-CGA-O1A	-2.12	118.24	123.59
2	G	601	CHL	CHB-C4A-NA	2.12	127.44	124.51
3	G	602	CLA	CHB-C4A-NA	2.12	127.44	124.51
2	N	606	CHL	C3A-C2A-C1A	2.11	104.50	101.34
4	Y	317	LUT	C10-C11-C12	-2.11	116.63	123.22
3	G	604	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
3	N	612	CLA	O2D-CGD-CBD	2.11	115.02	111.27
2	G	606	CHL	CHD-C1D-ND	-2.10	122.52	124.45
2	N	607	CHL	OMC-CMC-C2C	-2.10	120.93	125.69
4	G	615	LUT	C8-C7-C6	-2.10	121.31	127.20
2	Y	306	CHL	CHB-C4A-NA	2.10	127.41	124.51
4	Y	316	LUT	C35-C34-C33	-2.09	124.33	127.31
2	G	609	CHL	CAC-C3C-C4C	2.08	127.51	124.81
4	G	615	LUT	C35-C15-C14	-2.08	119.21	123.47
3	Y	304	CLA	C1-C2-C3	-2.08	122.44	126.04
2	Y	308	CHL	C2D-C1D-ND	-2.08	108.57	110.10
3	Y	315	CLA	CHD-C1D-ND	-2.08	122.54	124.45
2	Y	306	CHL	O2A-CGA-O1A	-2.08	118.35	123.59
2	G	609	CHL	C3C-C4C-NC	-2.08	108.24	110.57
2	Y	310	CHL	O1D-CGD-CBD	2.08	128.73	124.48
2	G	608	CHL	CHD-C1D-ND	-2.07	122.55	124.45
2	Y	306	CHL	C1C-C2C-C3C	-2.06	105.48	107.11
2	N	605	CHL	C3C-C4C-NC	-2.06	108.26	110.57
2	G	606	CHL	C1-C2-C3	-2.06	123.42	126.75
3	Y	313	CLA	C2A-C1A-CHA	2.06	127.45	123.86
2	Y	306	CHL	C3C-C4C-NC	-2.05	108.27	110.57
2	G	601	CHL	C2C-C3C-C4C	2.05	107.95	106.49
3	Y	311	CLA	CMA-C3A-C2A	-2.05	105.55	113.83
2	G	609	CHL	C2A-C1A-CHA	2.05	127.45	123.86
4	G	616	LUT	C3-C4-C5	-2.05	107.77	111.85
4	Y	317	LUT	C19-C9-C10	-2.05	120.05	122.92
4	G	615	LUT	C2-C3-C4	2.05	113.11	110.30
3	N	613	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
7	G	619	XAT	C40-C33-C32	2.05	121.30	118.08
2	Y	310	CHL	C2D-C1D-ND	-2.04	108.60	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	308	CHL	CHA-C1A-NA	-2.04	121.72	126.40
3	G	614	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
4	Y	316	LUT	C1-C2-C3	2.04	118.25	113.64
2	N	605	CHL	CAA-C2A-C3A	-2.04	107.19	112.78
7	G	619	XAT	C24-C23-C22	-2.04	106.84	110.77
2	G	607	CHL	C2A-C1A-CHA	2.03	127.41	123.86
7	G	619	XAT	C38-C25-C24	2.03	116.56	114.28
2	G	601	CHL	CHA-C4D-ND	2.03	136.75	132.50
2	N	609	CHL	C2A-C1A-CHA	2.03	127.41	123.86
3	G	612	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
4	Y	317	LUT	C1-C2-C3	2.03	118.22	113.64
3	Y	311	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
4	G	615	LUT	C1-C2-C3	2.02	118.21	113.64
4	G	616	LUT	C30-C31-C32	-2.02	116.91	123.22
2	Y	310	CHL	C16-C15-C13	-2.02	109.40	115.92
3	G	610	CLA	CAC-C3C-C4C	2.02	127.43	124.81
2	N	606	CHL	O2A-CGA-O1A	-2.01	118.51	123.59
2	N	609	CHL	C3C-C4C-NC	-2.01	108.32	110.57
3	N	612	CLA	C2A-C1A-CHA	2.01	127.37	123.86
3	Y	312	CLA	CHB-C4A-NA	2.00	127.28	124.51

All (74) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	N	601	CHL	NC
2	N	601	CHL	ND
2	N	601	CHL	NA
2	N	605	CHL	NC
2	N	605	CHL	ND
2	N	605	CHL	NA
2	N	606	CHL	NC
2	N	606	CHL	ND
2	N	606	CHL	NA
2	N	607	CHL	NC
2	N	607	CHL	ND
2	N	607	CHL	NA
2	N	608	CHL	NC
2	N	608	CHL	ND
2	N	608	CHL	NA
2	N	609	CHL	NC
2	N	609	CHL	ND
2	N	609	CHL	NA

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Mol	Chain	Res	Type	Atom
2	G	601	CHL	NC
2	G	601	CHL	ND
2	G	601	CHL	NA
2	G	605	CHL	NC
2	G	605	CHL	ND
2	G	605	CHL	NA
2	G	606	CHL	NC
2	G	606	CHL	ND
2	G	606	CHL	NA
2	G	607	CHL	NC
2	G	607	CHL	ND
2	G	607	CHL	NA
2	G	608	CHL	NC
2	G	608	CHL	ND
2	G	608	CHL	NA
2	G	609	CHL	NC
2	G	609	CHL	ND
2	G	609	CHL	NA
2	Y	302	CHL	NC
2	Y	302	CHL	ND
2	Y	302	CHL	NA
2	Y	306	CHL	NC
2	Y	306	CHL	ND
2	Y	306	CHL	NA
2	Y	307	CHL	NC
2	Y	307	CHL	ND
2	Y	307	CHL	NA
2	Y	308	CHL	NC
2	Y	308	CHL	ND
2	Y	308	CHL	NA
2	Y	309	CHL	NC
2	Y	309	CHL	ND
2	Y	309	CHL	NA
2	Y	310	CHL	NC
2	Y	310	CHL	ND
2	Y	310	CHL	NA
3	N	602	CLA	ND
3	N	603	CLA	ND
3	N	604	CLA	ND
3	N	610	CLA	ND
3	N	611	CLA	ND
3	N	612	CLA	ND

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Mol	Chain	Res	Type	Atom
3	N	613	CLA	ND
3	N	614	CLA	ND
3	G	602	CLA	ND
3	G	603	CLA	ND
3	G	610	CLA	ND
3	G	612	CLA	ND
3	G	614	CLA	ND
3	Y	303	CLA	ND
3	Y	304	CLA	ND
3	Y	305	CLA	ND
3	Y	311	CLA	ND
3	Y	313	CLA	ND
3	Y	314	CLA	ND
3	Y	315	CLA	ND

All (636) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	601	CHL	C1C-C2C-CMC-OMC
2	N	601	CHL	C3C-C2C-CMC-OMC
2	N	601	CHL	CHA-CBD-CGD-O1D
2	N	601	CHL	CHA-CBD-CGD-O2D
2	N	605	CHL	C1A-C2A-CAA-CBA
2	N	606	CHL	C3A-C2A-CAA-CBA
2	N	606	CHL	CBA-CGA-O2A-C1
2	N	606	CHL	O1A-CGA-O2A-C1
2	N	606	CHL	C1C-C2C-CMC-OMC
2	N	607	CHL	C1C-C2C-CMC-OMC
2	N	607	CHL	C3C-C2C-CMC-OMC
2	N	607	CHL	CBD-CGD-O2D-CED
2	N	608	CHL	C1C-C2C-CMC-OMC
2	N	608	CHL	C3C-C2C-CMC-OMC
2	N	609	CHL	C1A-C2A-CAA-CBA
2	N	609	CHL	C1C-C2C-CMC-OMC
2	N	609	CHL	C3C-C2C-CMC-OMC
2	N	609	CHL	C11-C10-C8-C9
2	G	601	CHL	C1A-C2A-CAA-CBA
2	G	601	CHL	C1C-C2C-CMC-OMC
2	G	601	CHL	C3C-C2C-CMC-OMC
2	G	601	CHL	CHA-CBD-CGD-O1D
2	G	601	CHL	CHA-CBD-CGD-O2D
2	G	606	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
2	G	607	CHL	C2A-CAA-CBA-CGA
2	G	607	CHL	C1C-C2C-CMC-OMC
2	G	607	CHL	C3C-C2C-CMC-OMC
2	G	608	CHL	C3C-C2C-CMC-OMC
2	G	609	CHL	C1C-C2C-CMC-OMC
2	G	609	CHL	C3C-C2C-CMC-OMC
2	Y	302	CHL	C1C-C2C-CMC-OMC
2	Y	302	CHL	C3C-C2C-CMC-OMC
2	Y	302	CHL	CHA-CBD-CGD-O1D
2	Y	302	CHL	CHA-CBD-CGD-O2D
2	Y	307	CHL	C3C-C2C-CMC-OMC
2	Y	308	CHL	C1C-C2C-CMC-OMC
2	Y	308	CHL	C3C-C2C-CMC-OMC
2	Y	309	CHL	C1C-C2C-CMC-OMC
2	Y	309	CHL	C3C-C2C-CMC-OMC
2	Y	310	CHL	C1C-C2C-CMC-OMC
2	Y	310	CHL	C3C-C2C-CMC-OMC
2	Y	310	CHL	CBD-CGD-O2D-CED
3	N	602	CLA	CHA-CBD-CGD-O1D
3	N	602	CLA	CHA-CBD-CGD-O2D
3	N	604	CLA	CBD-CGD-O2D-CED
3	N	613	CLA	CBD-CGD-O2D-CED
3	N	614	CLA	CBD-CGD-O2D-CED
3	G	604	CLA	C1A-C2A-CAA-CBA
3	G	604	CLA	C3A-C2A-CAA-CBA
3	G	613	CLA	CBD-CGD-O2D-CED
3	G	614	CLA	CBD-CGD-O2D-CED
3	Y	304	CLA	CBD-CGD-O2D-CED
3	Y	305	CLA	C1A-C2A-CAA-CBA
3	Y	305	CLA	CHA-CBD-CGD-O1D
3	Y	305	CLA	CHA-CBD-CGD-O2D
3	Y	312	CLA	CHA-CBD-CGD-O1D
3	Y	312	CLA	CHA-CBD-CGD-O2D
3	Y	314	CLA	CBD-CGD-O2D-CED
4	N	615	LUT	C27-C28-C29-C39
4	G	615	LUT	C27-C28-C29-C30
4	G	615	LUT	C27-C28-C29-C39
5	N	617	NEX	O24-C26-C27-C28
5	G	617	NEX	O24-C26-C27-C28
5	Y	318	NEX	C9-C10-C11-C12
5	Y	318	NEX	C28-C29-C30-C31
5	Y	318	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
6	G	618	LHG	C3-O3-P-O5
6	G	618	LHG	C4-O6-P-O4
6	Y	319	LHG	O1-C1-C2-C3
6	Y	319	LHG	C3-O3-P-O5
6	Y	319	LHG	C4-O6-P-O4
6	Y	319	LHG	O10-C23-O8-C6
6	Y	319	LHG	C24-C23-O8-C6
7	N	619	XAT	O4-C6-C7-C8
7	N	619	XAT	C7-C8-C9-C10
7	N	619	XAT	C7-C8-C9-C19
7	N	619	XAT	C31-C32-C33-C34
7	N	619	XAT	C31-C32-C33-C40
7	G	619	XAT	O4-C6-C7-C8
7	G	619	XAT	C7-C8-C9-C10
7	G	619	XAT	C7-C8-C9-C19
7	G	619	XAT	O24-C26-C27-C28
7	G	619	XAT	C31-C32-C33-C34
7	G	619	XAT	C31-C32-C33-C40
7	Y	301	XAT	O4-C6-C7-C8
7	Y	301	XAT	C7-C8-C9-C10
7	Y	301	XAT	C7-C8-C9-C19
3	Y	305	CLA	O1D-CGD-O2D-CED
2	G	608	CHL	O1D-CGD-O2D-CED
2	G	608	CHL	CBD-CGD-O2D-CED
2	G	609	CHL	CBD-CGD-O2D-CED
2	Y	306	CHL	CBD-CGD-O2D-CED
3	N	610	CLA	CBD-CGD-O2D-CED
3	Y	303	CLA	CBD-CGD-O2D-CED
3	Y	305	CLA	CBD-CGD-O2D-CED
3	Y	315	CLA	CBD-CGD-O2D-CED
2	Y	307	CHL	O1A-CGA-O2A-C1
6	G	618	LHG	O10-C23-O8-C6
2	N	607	CHL	O1D-CGD-O2D-CED
2	Y	310	CHL	O1D-CGD-O2D-CED
3	N	614	CLA	O1D-CGD-O2D-CED
3	G	613	CLA	O1D-CGD-O2D-CED
3	G	614	CLA	O1D-CGD-O2D-CED
3	Y	303	CLA	O1D-CGD-O2D-CED
3	Y	314	CLA	O1D-CGD-O2D-CED
2	Y	307	CHL	CBA-CGA-O2A-C1
2	N	605	CHL	CBD-CGD-O2D-CED
2	N	608	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	Y	313	CLA	CBD-CGD-O2D-CED
2	N	607	CHL	O1A-CGA-O2A-C1
2	G	607	CHL	O1A-CGA-O2A-C1
2	Y	308	CHL	O1A-CGA-O2A-C1
3	Y	315	CLA	O1A-CGA-O2A-C1
6	N	618	LHG	O10-C23-O8-C6
3	N	604	CLA	O1D-CGD-O2D-CED
3	N	613	CLA	O1D-CGD-O2D-CED
3	Y	304	CLA	O1D-CGD-O2D-CED
3	G	604	CLA	CBD-CGD-O2D-CED
2	G	601	CHL	C3-C5-C6-C7
2	G	606	CHL	CBA-CGA-O2A-C1
3	Y	315	CLA	CBA-CGA-O2A-C1
6	N	618	LHG	C24-C23-O8-C6
6	G	618	LHG	C24-C23-O8-C6
2	Y	306	CHL	O1D-CGD-O2D-CED
3	G	603	CLA	CBD-CGD-O2D-CED
2	N	607	CHL	C2A-CAA-CBA-CGA
2	Y	308	CHL	C2A-CAA-CBA-CGA
2	G	607	CHL	C3-C5-C6-C7
3	G	604	CLA	C3-C5-C6-C7
3	Y	312	CLA	C3-C5-C6-C7
3	Y	313	CLA	C3-C5-C6-C7
2	N	607	CHL	CBA-CGA-O2A-C1
2	G	607	CHL	CBA-CGA-O2A-C1
2	Y	308	CHL	CBA-CGA-O2A-C1
3	G	612	CLA	CBA-CGA-O2A-C1
2	G	609	CHL	O1D-CGD-O2D-CED
3	Y	315	CLA	O1D-CGD-O2D-CED
4	G	616	LUT	C29-C30-C31-C32
2	N	609	CHL	CBD-CGD-O2D-CED
2	G	607	CHL	CBD-CGD-O2D-CED
3	N	611	CLA	C3-C5-C6-C7
3	N	614	CLA	CBA-CGA-O2A-C1
3	G	612	CLA	O1A-CGA-O2A-C1
3	Y	311	CLA	CBD-CGD-O2D-CED
3	N	610	CLA	O1D-CGD-O2D-CED
3	N	604	CLA	C3-C5-C6-C7
3	N	614	CLA	O1A-CGA-O2A-C1
3	G	614	CLA	CBA-CGA-O2A-C1
3	Y	313	CLA	O1D-CGD-O2D-CED
6	N	618	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
3	G	614	CLA	O1A-CGA-O2A-C1
2	Y	308	CHL	C3-C5-C6-C7
2	N	609	CHL	C2C-C3C-CAC-CBC
2	N	608	CHL	O1D-CGD-O2D-CED
2	Y	302	CHL	C15-C16-C17-C18
3	Y	314	CLA	C13-C15-C16-C17
6	Y	319	LHG	O2-C2-C3-O3
2	Y	309	CHL	C11-C12-C13-C14
2	Y	310	CHL	C6-C7-C8-C9
4	Y	316	LUT	C27-C28-C29-C39
5	N	617	NEX	C11-C12-C13-C20
5	G	617	NEX	C11-C12-C13-C20
7	Y	301	XAT	C11-C12-C13-C20
2	G	605	CHL	CBA-CGA-O2A-C1
3	G	611	CLA	CBA-CGA-O2A-C1
2	G	601	CHL	C15-C16-C17-C18
3	G	612	CLA	C15-C16-C17-C18
3	N	603	CLA	C13-C15-C16-C17
3	G	603	CLA	C5-C6-C7-C8
2	G	607	CHL	C5-C6-C7-C8
3	N	611	CLA	C10-C11-C12-C13
3	G	602	CLA	C10-C11-C12-C13
2	N	605	CHL	O1D-CGD-O2D-CED
3	G	612	CLA	C13-C15-C16-C17
6	Y	319	LHG	C23-C24-C25-C26
2	N	608	CHL	C12-C13-C15-C16
3	N	611	CLA	C6-C7-C8-C10
3	G	612	CLA	C12-C13-C15-C16
3	G	613	CLA	C3-C5-C6-C7
2	Y	309	CHL	C2A-CAA-CBA-CGA
2	N	609	CHL	C15-C16-C17-C18
2	Y	308	CHL	C5-C6-C7-C8
3	G	612	CLA	C8-C10-C11-C12
5	Y	318	NEX	C30-C31-C32-C33
3	N	612	CLA	C3-C5-C6-C7
3	Y	312	CLA	C8-C10-C11-C12
3	Y	305	CLA	CBA-CGA-O2A-C1
3	N	611	CLA	C5-C6-C7-C8
3	G	603	CLA	O1D-CGD-O2D-CED
3	G	603	CLA	C15-C16-C17-C18
3	Y	312	CLA	C10-C11-C12-C13
6	G	618	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
6	Y	319	LHG	C4-O6-P-O3
6	N	618	LHG	C23-C24-C25-C26
3	G	611	CLA	C3-C5-C6-C7
3	G	603	CLA	C10-C11-C12-C13
3	G	611	CLA	O1A-CGA-O2A-C1
3	G	604	CLA	C13-C15-C16-C17
3	G	604	CLA	O1D-CGD-O2D-CED
6	Y	319	LHG	C1-C2-C3-O3
2	N	601	CHL	C15-C16-C17-C18
3	G	612	CLA	C5-C6-C7-C8
2	N	608	CHL	C2A-CAA-CBA-CGA
3	N	612	CLA	CBA-CGA-O2A-C1
3	Y	313	CLA	CBA-CGA-O2A-C1
2	G	605	CHL	O1A-CGA-O2A-C1
6	Y	319	LHG	C26-C27-C28-C29
6	N	618	LHG	C25-C26-C27-C28
6	Y	319	LHG	C32-C33-C34-C35
3	N	611	CLA	C8-C10-C11-C12
6	G	618	LHG	C23-C24-C25-C26
2	G	607	CHL	O1D-CGD-O2D-CED
6	G	618	LHG	C9-C10-C11-C12
3	N	613	CLA	C3-C5-C6-C7
3	Y	305	CLA	O1A-CGA-O2A-C1
3	N	611	CLA	C16-C17-C18-C19
2	Y	310	CHL	C14-C13-C15-C16
3	Y	312	CLA	C14-C13-C15-C16
3	Y	313	CLA	C11-C10-C8-C9
3	Y	304	CLA	C2A-CAA-CBA-CGA
6	Y	319	LHG	C15-C16-C17-C18
6	G	618	LHG	C32-C33-C34-C35
3	G	612	CLA	C16-C17-C18-C20
6	N	618	LHG	C15-C16-C17-C18
6	G	618	LHG	C14-C15-C16-C17
3	Y	311	CLA	O1D-CGD-O2D-CED
3	Y	313	CLA	O1A-CGA-O2A-C1
2	N	605	CHL	C3A-C2A-CAA-CBA
2	G	601	CHL	C3A-C2A-CAA-CBA
2	G	605	CHL	C3A-C2A-CAA-CBA
2	G	606	CHL	C3A-C2A-CAA-CBA
2	Y	306	CHL	C3A-C2A-CAA-CBA
2	Y	307	CHL	C3A-C2A-CAA-CBA
3	N	603	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
3	Y	304	CLA	C3A-C2A-CAA-CBA
3	Y	304	CLA	C10-C11-C12-C13
2	N	609	CHL	O1D-CGD-O2D-CED
3	G	612	CLA	C16-C17-C18-C19
6	N	618	LHG	C32-C33-C34-C35
5	Y	318	NEX	C14-C15-C35-C34
2	N	609	CHL	C3-C5-C6-C7
3	Y	314	CLA	C3-C5-C6-C7
6	Y	319	LHG	O1-C1-C2-O2
2	N	609	CHL	C4C-C3C-CAC-CBC
3	N	604	CLA	C13-C15-C16-C17
3	N	612	CLA	O1A-CGA-O2A-C1
3	N	611	CLA	C16-C17-C18-C20
2	N	605	CHL	CBA-CGA-O2A-C1
6	Y	319	LHG	C29-C30-C31-C32
3	Y	305	CLA	C2-C1-O2A-CGA
6	Y	319	LHG	C28-C29-C30-C31
3	G	613	CLA	C13-C15-C16-C17
4	G	615	LUT	C1-C6-C7-C8
4	G	615	LUT	C5-C6-C7-C8
4	Y	316	LUT	C1-C6-C7-C8
4	Y	316	LUT	C5-C6-C7-C8
2	G	601	CHL	C10-C11-C12-C13
6	G	618	LHG	C29-C30-C31-C32
2	Y	310	CHL	C12-C13-C15-C16
3	N	602	CLA	C6-C7-C8-C10
3	N	612	CLA	C11-C10-C8-C7
3	N	613	CLA	C11-C12-C13-C15
3	G	602	CLA	C6-C7-C8-C10
3	G	603	CLA	C12-C13-C15-C16
3	G	611	CLA	C12-C13-C15-C16
3	Y	313	CLA	C11-C10-C8-C7
3	Y	313	CLA	C11-C12-C13-C15
5	Y	318	NEX	C33-C34-C35-C15
6	N	618	LHG	O9-C7-O7-C5
6	G	618	LHG	O9-C7-O7-C5
2	N	609	CHL	C8-C10-C11-C12
3	N	611	CLA	C13-C15-C16-C17
6	G	618	LHG	C25-C26-C27-C28
3	G	612	CLA	C10-C11-C12-C13
6	N	618	LHG	C14-C15-C16-C17
6	G	618	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
6	N	618	LHG	C8-C7-O7-C5
6	G	618	LHG	C8-C7-O7-C5
2	N	601	CHL	C13-C15-C16-C17
2	Y	302	CHL	CBD-CGD-O2D-CED
3	N	612	CLA	CBD-CGD-O2D-CED
3	G	603	CLA	C3-C5-C6-C7
2	N	607	CHL	C14-C13-C15-C16
2	Y	308	CHL	C14-C13-C15-C16
3	N	602	CLA	C6-C7-C8-C9
3	N	612	CLA	C11-C10-C8-C9
3	N	613	CLA	C11-C12-C13-C14
3	G	602	CLA	C6-C7-C8-C9
3	G	603	CLA	C11-C10-C8-C9
3	G	611	CLA	C14-C13-C15-C16
3	Y	313	CLA	C11-C12-C13-C14
3	Y	305	CLA	C3-C5-C6-C7
3	Y	303	CLA	C2A-CAA-CBA-CGA
6	G	618	LHG	C10-C11-C12-C13
2	N	605	CHL	O1A-CGA-O2A-C1
2	N	606	CHL	C1A-C2A-CAA-CBA
2	G	605	CHL	C1A-C2A-CAA-CBA
2	G	606	CHL	C1A-C2A-CAA-CBA
2	G	609	CHL	C1A-C2A-CAA-CBA
2	Y	307	CHL	C1A-C2A-CAA-CBA
3	N	603	CLA	C1A-C2A-CAA-CBA
3	N	604	CLA	C1A-C2A-CAA-CBA
3	N	611	CLA	C1A-C2A-CAA-CBA
3	G	611	CLA	C1A-C2A-CAA-CBA
3	Y	304	CLA	C1A-C2A-CAA-CBA
3	Y	315	CLA	C1A-C2A-CAA-CBA
5	G	617	NEX	C29-C30-C31-C32
2	N	607	CHL	C15-C16-C17-C18
2	G	608	CHL	C5-C6-C7-C8
3	N	611	CLA	C15-C16-C17-C18
3	N	612	CLA	C8-C10-C11-C12
3	Y	303	CLA	C15-C16-C17-C18
3	Y	313	CLA	C10-C11-C12-C13
6	N	618	LHG	C4-O6-P-O3
3	N	612	CLA	C10-C11-C12-C13
6	Y	319	LHG	C30-C31-C32-C33
3	G	611	CLA	C8-C10-C11-C12
6	G	618	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
3	G	602	CLA	C15-C16-C17-C18
3	N	604	CLA	CBA-CGA-O2A-C1
6	Y	319	LHG	C27-C28-C29-C30
6	G	618	LHG	C33-C34-C35-C36
3	Y	304	CLA	C8-C10-C11-C12
6	N	618	LHG	C24-C25-C26-C27
2	G	609	CHL	C4-C3-C5-C6
2	N	607	CHL	C12-C13-C15-C16
2	N	608	CHL	C11-C10-C8-C7
2	N	609	CHL	C6-C7-C8-C10
2	G	607	CHL	C12-C13-C15-C16
2	Y	308	CHL	C12-C13-C15-C16
2	Y	309	CHL	C11-C12-C13-C15
3	N	603	CLA	C6-C7-C8-C10
3	N	613	CLA	C6-C7-C8-C10
3	G	603	CLA	C11-C10-C8-C7
3	G	611	CLA	C11-C10-C8-C7
3	G	613	CLA	C12-C13-C15-C16
3	Y	303	CLA	C6-C7-C8-C10
3	Y	304	CLA	C6-C7-C8-C10
3	Y	312	CLA	C12-C13-C15-C16
2	N	609	CHL	C6-C7-C8-C9
2	G	607	CHL	C14-C13-C15-C16
2	G	609	CHL	C14-C13-C15-C16
2	Y	308	CHL	C11-C10-C8-C9
3	N	603	CLA	C6-C7-C8-C9
3	N	611	CLA	C6-C7-C8-C9
3	N	613	CLA	C6-C7-C8-C9
3	G	603	CLA	C14-C13-C15-C16
3	G	611	CLA	C11-C10-C8-C9
3	G	612	CLA	C14-C13-C15-C16
3	G	613	CLA	C14-C13-C15-C16
3	Y	304	CLA	C6-C7-C8-C9
5	N	617	NEX	C29-C30-C31-C32
2	G	605	CHL	C2A-CAA-CBA-CGA
2	G	609	CHL	CBA-CGA-O2A-C1
6	G	618	LHG	O6-C4-C5-C6
2	G	609	CHL	C2-C3-C5-C6
6	G	618	LHG	C15-C16-C17-C18
3	Y	304	CLA	CBA-CGA-O2A-C1
6	G	618	LHG	C26-C27-C28-C29
6	Y	319	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	G	604	CLA	CBA-CGA-O2A-C1
3	N	602	CLA	C10-C11-C12-C13
3	Y	313	CLA	C4-C3-C5-C6
2	N	606	CHL	C3C-C2C-CMC-OMC
2	Y	306	CHL	C3C-C2C-CMC-OMC
6	N	618	LHG	C27-C28-C29-C30
6	Y	319	LHG	C34-C35-C36-C37
6	G	618	LHG	O1-C1-C2-O2
3	Y	313	CLA	C8-C10-C11-C12
3	N	604	CLA	O1A-CGA-O2A-C1
2	N	609	CHL	C16-C17-C18-C20
2	G	609	CHL	C2-C1-O2A-CGA
3	Y	313	CLA	C2-C3-C5-C6
2	N	607	CHL	C10-C11-C12-C13
2	N	608	CHL	C11-C10-C8-C9
2	N	608	CHL	C14-C13-C15-C16
2	G	608	CHL	C6-C7-C8-C9
2	G	608	CHL	C11-C12-C13-C14
2	Y	310	CHL	C11-C12-C13-C14
3	G	611	CLA	C13-C15-C16-C17
3	Y	312	CLA	C5-C6-C7-C8
4	N	615	LUT	C1-C6-C7-C8
4	N	615	LUT	C5-C6-C7-C8
4	G	616	LUT	C1-C6-C7-C8
4	G	616	LUT	C5-C6-C7-C8
4	Y	317	LUT	C1-C6-C7-C8
4	Y	317	LUT	C5-C6-C7-C8
4	N	615	LUT	C27-C28-C29-C30
5	N	617	NEX	C11-C12-C13-C14
5	G	617	NEX	C11-C12-C13-C14
7	Y	301	XAT	C11-C12-C13-C14
3	N	613	CLA	C16-C17-C18-C20
6	Y	319	LHG	O6-C4-C5-C6
2	N	607	CHL	C11-C10-C8-C7
2	N	609	CHL	C11-C10-C8-C7
2	G	607	CHL	C11-C10-C8-C7
2	G	609	CHL	C12-C13-C15-C16
2	Y	308	CHL	C11-C10-C8-C7
3	N	603	CLA	C11-C12-C13-C15
3	N	604	CLA	C11-C12-C13-C15
3	G	604	CLA	C12-C13-C15-C16
3	Y	303	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
4	Y	317	LUT	C29-C30-C31-C32
2	G	608	CHL	C2A-CAA-CBA-CGA
5	Y	318	NEX	C11-C10-C9-C19
6	N	618	LHG	C29-C30-C31-C32
3	G	604	CLA	O1A-CGA-O2A-C1
3	G	603	CLA	C13-C15-C16-C17
2	N	605	CHL	CAD-CBD-CGD-O2D
2	Y	306	CHL	CAD-CBD-CGD-O2D
3	G	603	CLA	CAD-CBD-CGD-O2D
6	N	618	LHG	C30-C31-C32-C33
3	G	612	CLA	C4-C3-C5-C6
3	G	612	CLA	C2-C3-C5-C6
6	G	618	LHG	C4-C5-C6-O8
6	Y	319	LHG	O6-C4-C5-O7
2	Y	309	CHL	C3-C5-C6-C7
3	N	614	CLA	O2A-C1-C2-C3
3	G	614	CLA	O2A-C1-C2-C3
3	G	602	CLA	C2A-CAA-CBA-CGA
6	Y	319	LHG	C33-C34-C35-C36
3	N	614	CLA	CHA-CBD-CGD-O1D
3	N	614	CLA	CHA-CBD-CGD-O2D
3	G	614	CLA	CHA-CBD-CGD-O1D
3	Y	304	CLA	O1A-CGA-O2A-C1
6	N	618	LHG	O7-C5-C6-O8
6	G	618	LHG	O7-C5-C6-O8
6	Y	319	LHG	O7-C5-C6-O8
3	N	611	CLA	CBD-CGD-O2D-CED
3	N	612	CLA	O1D-CGD-O2D-CED
6	N	618	LHG	O1-C1-C2-O2
2	G	607	CHL	C11-C10-C8-C9
3	G	604	CLA	C14-C13-C15-C16
3	Y	303	CLA	C6-C7-C8-C9
3	G	604	CLA	C2A-CAA-CBA-CGA
5	Y	318	NEX	C11-C12-C13-C20
4	Y	316	LUT	C27-C28-C29-C30
2	G	609	CHL	C2C-C3C-CAC-CBC
2	Y	306	CHL	C1A-C2A-CAA-CBA
3	G	602	CLA	C1A-C2A-CAA-CBA
2	Y	310	CHL	C16-C17-C18-C20
4	N	616	LUT	C29-C30-C31-C32
5	Y	318	NEX	C13-C14-C15-C35
6	G	618	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
6	G	618	LHG	C30-C31-C32-C33
6	Y	319	LHG	C25-C26-C27-C28
2	G	609	CHL	O1A-CGA-O2A-C1
6	N	618	LHG	O6-C4-C5-C6
2	G	609	CHL	C4C-C3C-CAC-CBC
3	N	614	CLA	CAD-CBD-CGD-O1D
5	Y	318	NEX	C7-C8-C9-C10
3	Y	313	CLA	C5-C6-C7-C8
3	Y	312	CLA	O1D-CGD-O2D-CED
2	N	601	CHL	C11-C10-C8-C7
2	G	608	CHL	C12-C13-C15-C16
2	Y	309	CHL	C6-C7-C8-C10
3	N	603	CLA	C12-C13-C15-C16
3	N	612	CLA	C11-C12-C13-C15
3	N	613	CLA	C12-C13-C15-C16
3	G	602	CLA	C11-C12-C13-C15
3	Y	312	CLA	C11-C10-C8-C7
3	Y	314	CLA	C12-C13-C15-C16
6	G	618	LHG	O6-C4-C5-O7
6	N	618	LHG	C13-C14-C15-C16
6	Y	319	LHG	C7-C8-C9-C10
2	G	608	CHL	C1C-C2C-CMC-OMC
2	Y	306	CHL	C1C-C2C-CMC-OMC
2	Y	307	CHL	C1C-C2C-CMC-OMC
6	N	618	LHG	C4-C5-C6-O8
6	Y	319	LHG	C4-C5-C6-O8
2	N	601	CHL	C11-C10-C8-C9
2	N	607	CHL	C11-C10-C8-C9
2	Y	310	CHL	C11-C10-C8-C9
3	N	603	CLA	C11-C12-C13-C14
3	N	604	CLA	C11-C12-C13-C14
3	Y	303	CLA	C11-C12-C13-C14
2	Y	302	CHL	C13-C15-C16-C17
7	N	619	XAT	C9-C10-C11-C12
3	G	603	CLA	C8-C10-C11-C12
2	Y	302	CHL	O1D-CGD-O2D-CED
3	Y	304	CLA	C5-C6-C7-C8
3	N	614	CLA	C1-C2-C3-C4
3	G	614	CLA	C1-C2-C3-C4
3	Y	315	CLA	C1-C2-C3-C4
6	G	618	LHG	C4-C5-O7-C7
2	G	601	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
3	N	604	CLA	C2-C1-O2A-CGA
3	G	611	CLA	C2-C1-O2A-CGA
6	N	618	LHG	O6-C4-C5-O7
3	G	602	CLA	C8-C10-C11-C12
6	N	618	LHG	C3-O3-P-O6
6	Y	319	LHG	C3-O3-P-O6
3	N	610	CLA	C5-C6-C7-C8
2	Y	309	CHL	C12-C13-C15-C16
3	N	602	CLA	C11-C12-C13-C15
3	N	603	CLA	C14-C13-C15-C16
3	N	612	CLA	C11-C12-C13-C14
3	Y	313	CLA	C16-C17-C18-C20
3	N	603	CLA	CBA-CGA-O2A-C1
3	N	603	CLA	O1A-CGA-O2A-C1
7	Y	301	XAT	C9-C10-C11-C12
2	G	607	CHL	C15-C16-C17-C18
3	N	602	CLA	C2A-CAA-CBA-CGA
3	Y	314	CLA	C2A-CAA-CBA-CGA
2	N	601	CHL	C3A-C2A-CAA-CBA
2	Y	302	CHL	C3A-C2A-CAA-CBA
3	N	613	CLA	C16-C17-C18-C19
2	G	601	CHL	C11-C10-C8-C9
2	G	607	CHL	C6-C7-C8-C9
2	Y	308	CHL	C6-C7-C8-C9
2	Y	309	CHL	C14-C13-C15-C16
3	N	611	CLA	C11-C10-C8-C9
5	N	617	NEX	C39-C29-C30-C31
5	G	617	NEX	C39-C29-C30-C31
5	Y	318	NEX	C11-C12-C13-C14
6	N	618	LHG	C4-C5-O7-C7
6	G	618	LHG	C6-C5-O7-C7
3	N	612	CLA	C4-C3-C5-C6
2	G	608	CHL	C1A-C2A-CAA-CBA
3	G	610	CLA	C1A-C2A-CAA-CBA
3	G	614	CLA	C1A-C2A-CAA-CBA
2	G	608	CHL	C6-C7-C8-C10
2	Y	310	CHL	C6-C7-C8-C10
3	Y	304	CLA	C12-C13-C15-C16
2	N	605	CHL	C3C-C2C-CMC-OMC
2	N	608	CHL	C16-C17-C18-C20
2	N	609	CHL	C16-C17-C18-C19
3	G	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
3	N	612	CLA	C5-C6-C7-C8
3	G	604	CLA	C4-C3-C5-C6
3	G	613	CLA	C15-C16-C17-C18
5	N	617	NEX	C28-C29-C30-C31
5	G	617	NEX	C28-C29-C30-C31
7	G	619	XAT	C9-C10-C11-C12
2	G	608	CHL	C16-C17-C18-C19
2	G	609	CHL	C16-C17-C18-C19
2	Y	309	CHL	C4-C3-C5-C6
2	Y	302	CHL	C2-C1-O2A-CGA
3	G	604	CLA	C2-C1-O2A-CGA
3	N	603	CLA	C10-C11-C12-C13
4	N	616	LUT	C1-C6-C7-C8
6	G	618	LHG	O1-C1-C2-C3
3	Y	314	CLA	C15-C16-C17-C18
3	G	602	CLA	C13-C15-C16-C17
3	N	612	CLA	C2-C3-C5-C6
4	N	615	LUT	C29-C30-C31-C32
6	N	618	LHG	C34-C35-C36-C37
2	N	607	CHL	C5-C6-C7-C8
3	Y	315	CLA	O2A-C1-C2-C3
3	Y	313	CLA	C16-C17-C18-C19
3	G	613	CLA	CBA-CGA-O2A-C1
3	N	611	CLA	O1D-CGD-O2D-CED
6	Y	319	LHG	C13-C14-C15-C16
2	Y	309	CHL	C6-C7-C8-C9
3	N	602	CLA	C11-C12-C13-C14
3	G	602	CLA	C11-C12-C13-C14
3	Y	312	CLA	C11-C10-C8-C9
3	Y	314	CLA	C14-C13-C15-C16
2	N	609	CHL	C3A-C2A-CAA-CBA
3	Y	305	CLA	C3A-C2A-CAA-CBA
2	N	609	CHL	CAD-CBD-CGD-O2D
2	Y	307	CHL	CAD-CBD-CGD-O2D
3	Y	303	CLA	CAD-CBD-CGD-O2D
3	Y	304	CLA	CAD-CBD-CGD-O2D
5	Y	318	NEX	C7-C8-C9-C19
2	Y	309	CHL	C2-C3-C5-C6
3	G	604	CLA	C2-C3-C5-C6
2	Y	309	CHL	CAA-CBA-CGA-O2A
6	Y	319	LHG	O8-C23-C24-C25
7	N	619	XAT	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
2	N	608	CHL	CAA-CBA-CGA-O2A
2	N	608	CHL	O2A-C1-C2-C3
2	G	608	CHL	O2A-C1-C2-C3
2	Y	309	CHL	O2A-C1-C2-C3
2	Y	310	CHL	O2A-C1-C2-C3
2	Y	309	CHL	C16-C17-C18-C19
2	Y	309	CHL	CHA-CBD-CGD-O1D
2	Y	309	CHL	CHA-CBD-CGD-O2D
2	Y	310	CHL	CHA-CBD-CGD-O1D
2	Y	310	CHL	CHA-CBD-CGD-O2D
3	G	604	CLA	CHA-CBD-CGD-O1D
3	G	604	CLA	CHA-CBD-CGD-O2D
3	G	614	CLA	CHA-CBD-CGD-O2D
3	Y	313	CLA	CHA-CBD-CGD-O1D
3	Y	312	CLA	C4-C3-C5-C6
3	Y	304	CLA	CAA-CBA-CGA-O2A
6	N	618	LHG	C9-C10-C11-C12
3	N	611	CLA	C4-C3-C5-C6
3	G	603	CLA	C16-C17-C18-C20
3	N	613	CLA	C14-C13-C15-C16
3	G	603	CLA	C16-C17-C18-C19
6	N	618	LHG	O1-C1-C2-C3
2	N	608	CHL	CAA-CBA-CGA-O1A
6	Y	319	LHG	O10-C23-C24-C25
2	N	601	CHL	C1A-C2A-CAA-CBA
2	Y	302	CHL	C1A-C2A-CAA-CBA
2	Y	310	CHL	C1A-C2A-CAA-CBA
3	Y	303	CLA	C1A-C2A-CAA-CBA
3	Y	311	CLA	C1A-C2A-CAA-CBA
2	G	601	CHL	C16-C17-C18-C20
2	G	601	CHL	CAA-CBA-CGA-O2A
3	Y	303	CLA	C13-C15-C16-C17
6	N	618	LHG	C3-O3-P-O5
6	N	618	LHG	C4-O6-P-O4
2	Y	309	CHL	CAA-CBA-CGA-O1A
4	N	616	LUT	C5-C6-C7-C8
3	Y	304	CLA	CAA-CBA-CGA-O1A
3	N	603	CLA	C2A-CAA-CBA-CGA
2	Y	309	CHL	CAD-CBD-CGD-O1D
3	N	604	CLA	CAD-CBD-CGD-O1D
3	G	614	CLA	CAD-CBD-CGD-O1D
3	Y	313	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
6	N	618	LHG	C6-C5-O7-C7
6	G	618	LHG	O8-C23-C24-C25
2	G	608	CHL	C14-C13-C15-C16
3	N	604	CLA	C14-C13-C15-C16
3	N	611	CLA	C14-C13-C15-C16
3	Y	304	CLA	C14-C13-C15-C16
3	G	613	CLA	C8-C10-C11-C12
3	Y	305	CLA	CAA-CBA-CGA-O2A
2	Y	308	CHL	C15-C16-C17-C18
3	N	603	CLA	CAA-CBA-CGA-O2A
2	G	607	CHL	C6-C7-C8-C10
3	G	610	CLA	C11-C10-C8-C7
3	G	613	CLA	C11-C12-C13-C15
6	N	618	LHG	O8-C23-C24-C25
5	Y	318	NEX	C31-C32-C33-C34
7	Y	301	XAT	C31-C32-C33-C34
3	Y	313	CLA	CAA-CBA-CGA-O2A
3	N	613	CLA	C13-C15-C16-C17
3	Y	303	CLA	C8-C10-C11-C12
2	Y	306	CHL	O1A-CGA-O2A-C1
3	Y	305	CLA	CAA-CBA-CGA-O1A
3	N	612	CLA	CAA-CBA-CGA-O2A
3	N	603	CLA	CAA-CBA-CGA-O1A
3	Y	312	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

51 monomers are involved in 157 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	607	CHL	1	0
3	G	611	CLA	2	0
2	N	609	CHL	9	0
5	N	617	NEX	3	0
3	Y	315	CLA	4	0
3	N	613	CLA	3	0
5	Y	318	NEX	2	0
3	N	614	CLA	1	0
3	G	612	CLA	3	0
3	Y	304	CLA	6	0
4	G	615	LUT	6	0
2	Y	309	CHL	2	0
6	N	618	LHG	7	0

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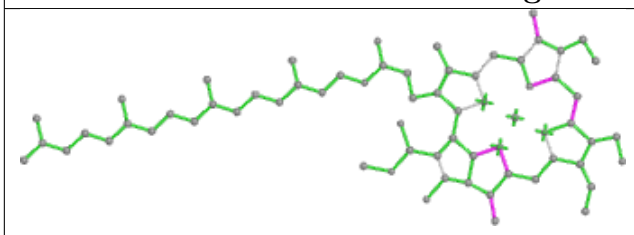
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	602	CLA	7	0
3	Y	313	CLA	3	0
3	Y	314	CLA	3	0
2	G	608	CHL	6	0
2	N	601	CHL	7	0
3	Y	311	CLA	4	0
2	N	606	CHL	1	0
3	N	612	CLA	2	0
2	Y	302	CHL	9	0
2	Y	308	CHL	6	0
4	N	615	LUT	2	0
4	N	616	LUT	3	0
3	N	610	CLA	1	0
3	N	611	CLA	5	0
3	G	602	CLA	6	0
3	G	614	CLA	1	0
7	G	619	XAT	6	0
2	N	608	CHL	4	0
5	G	617	NEX	4	0
4	Y	316	LUT	4	0
2	G	601	CHL	12	0
7	N	619	XAT	5	0
2	Y	310	CHL	6	0
3	Y	305	CLA	2	0
2	G	607	CHL	3	0
4	G	616	LUT	3	0
2	G	606	CHL	1	0
3	Y	312	CLA	2	0
7	Y	301	XAT	7	0
2	G	609	CHL	5	0
3	G	610	CLA	7	0
3	Y	303	CLA	5	0
4	Y	317	LUT	5	0
2	G	605	CHL	1	0
3	N	603	CLA	4	0
6	G	618	LHG	6	0
6	Y	319	LHG	5	0
3	G	613	CLA	1	0

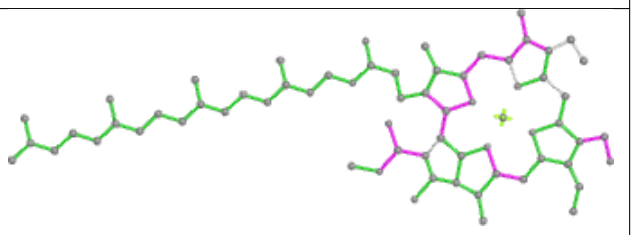
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

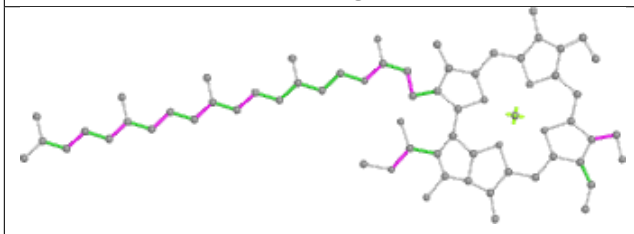
Ligand CHL N 607



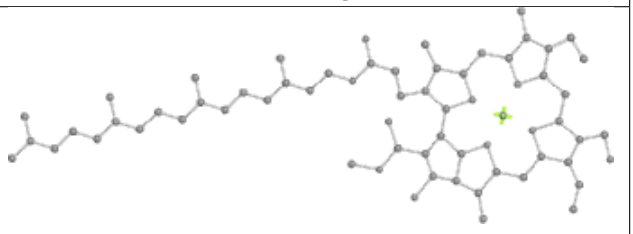
Bond lengths



Bond angles

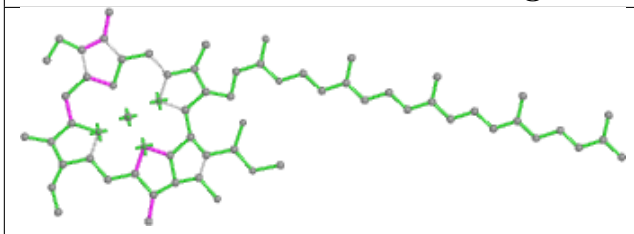


Torsions

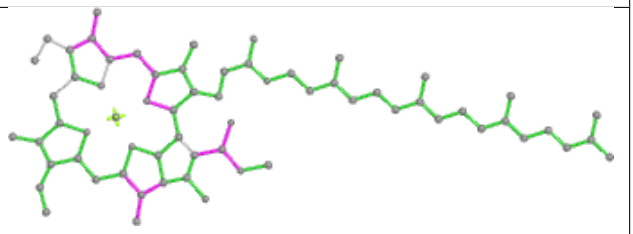


Rings

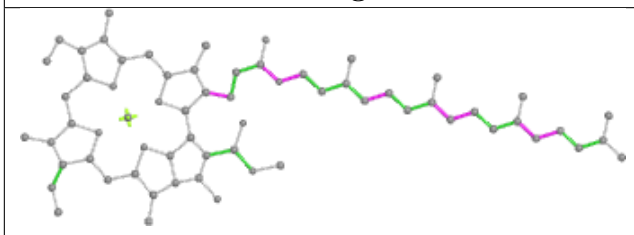
Ligand CLA G 611



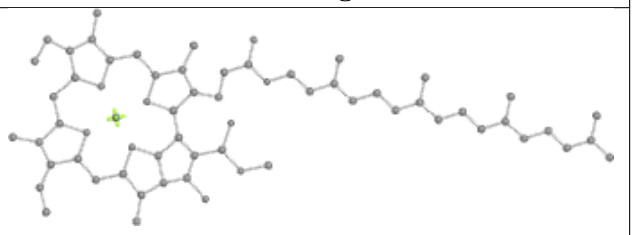
Bond lengths



Bond angles

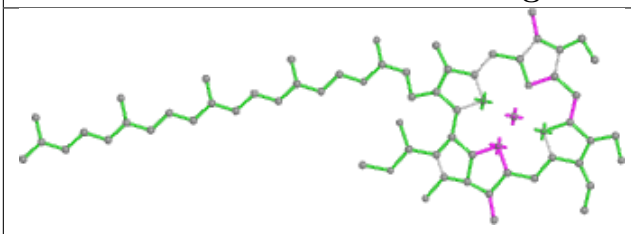


Torsions

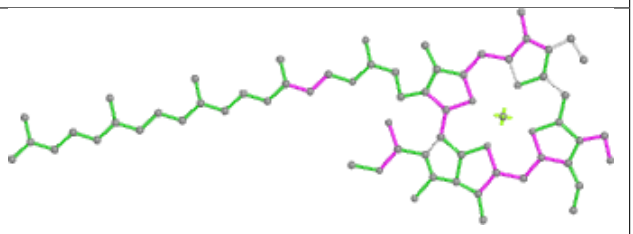


Rings

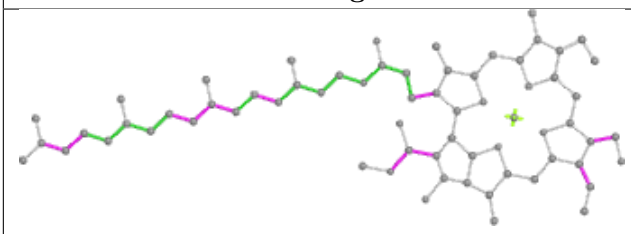
Ligand CHL N 609



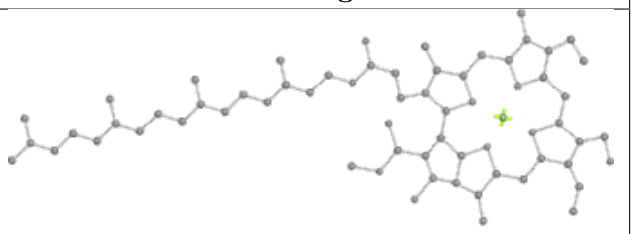
Bond lengths



Bond angles

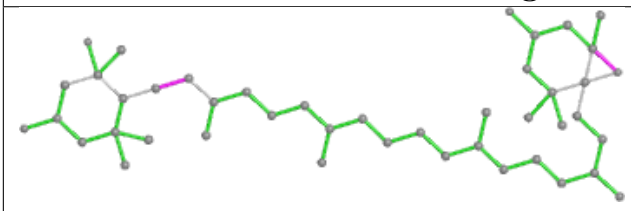


Torsions

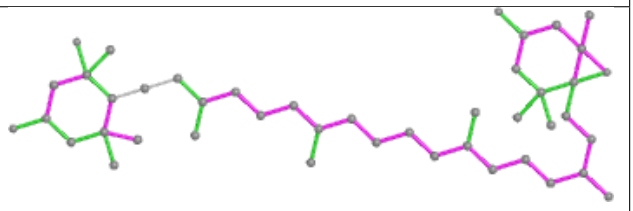


Rings

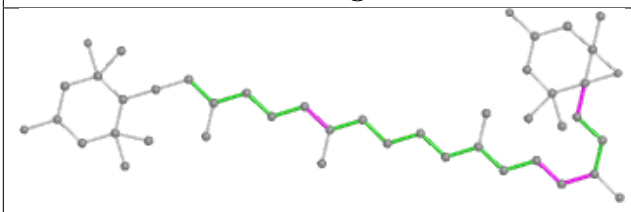
Ligand NEX N 617



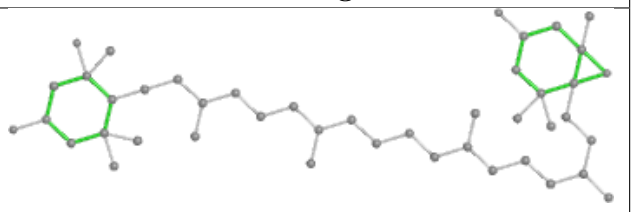
Bond lengths



Bond angles

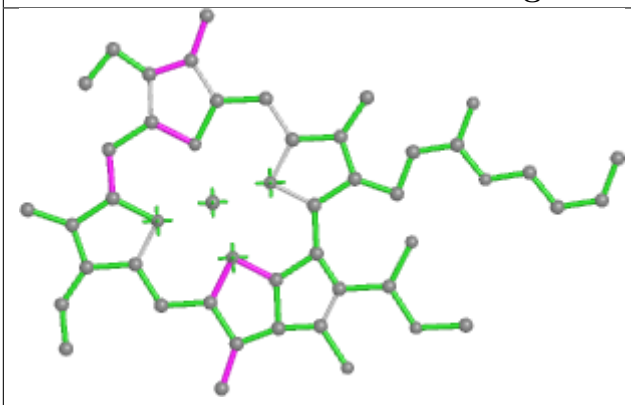


Torsions

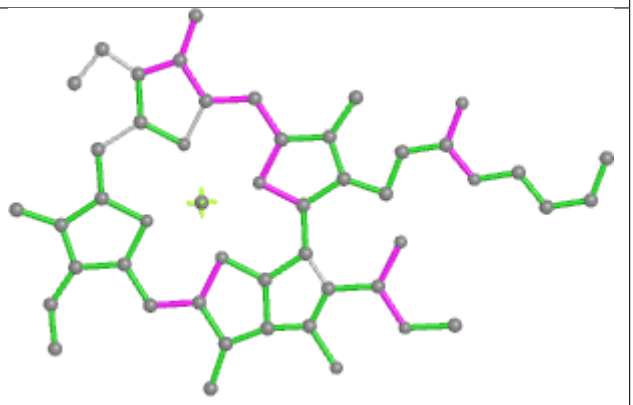


Rings

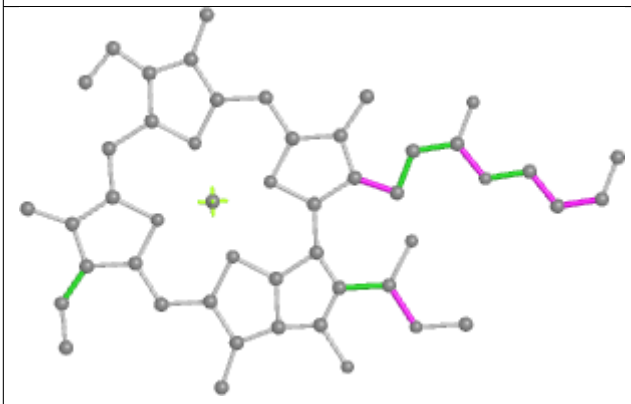
Ligand CLA Y 315



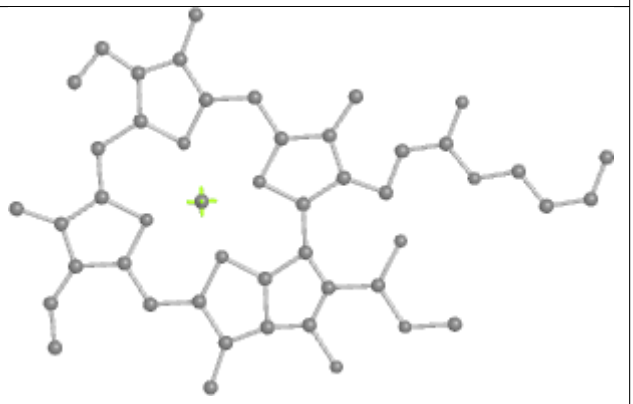
Bond lengths



Bond angles

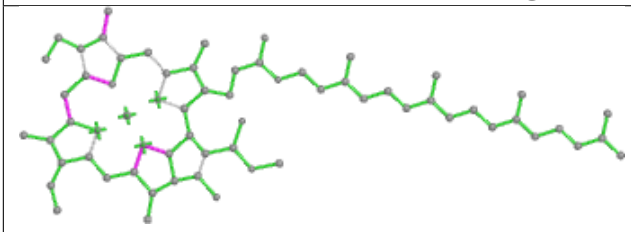


Torsions

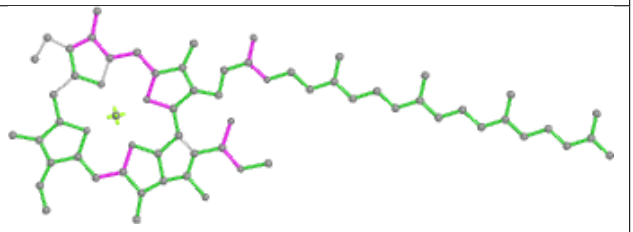


Rings

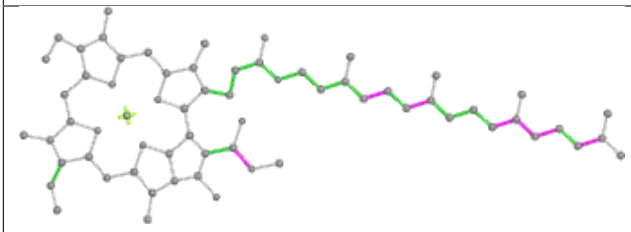
Ligand CLA N 613



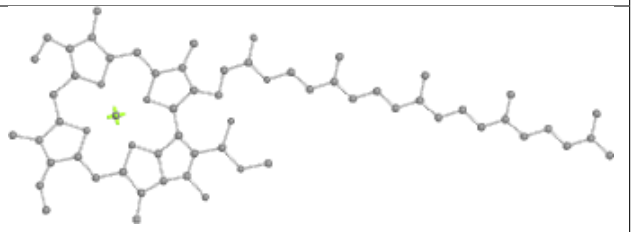
Bond lengths



Bond angles

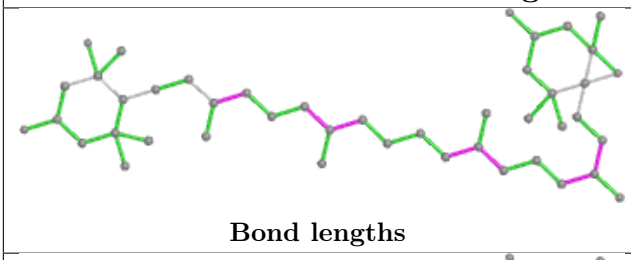


Torsions

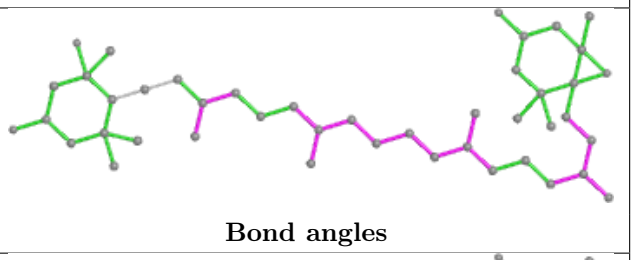


Rings

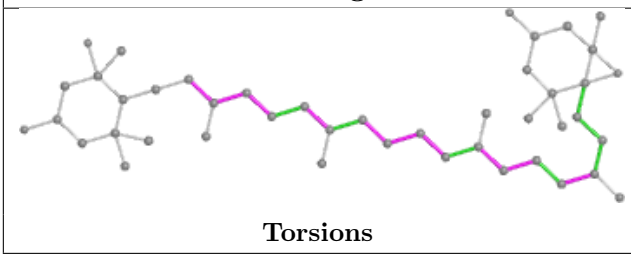
Ligand NEX Y 318



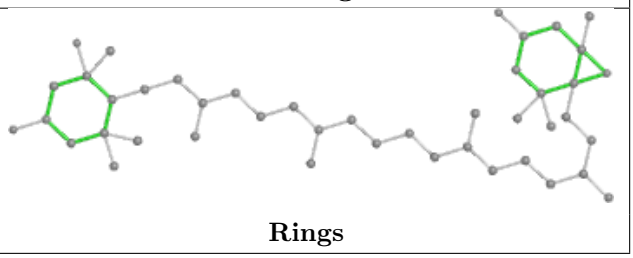
Bond lengths



Bond angles

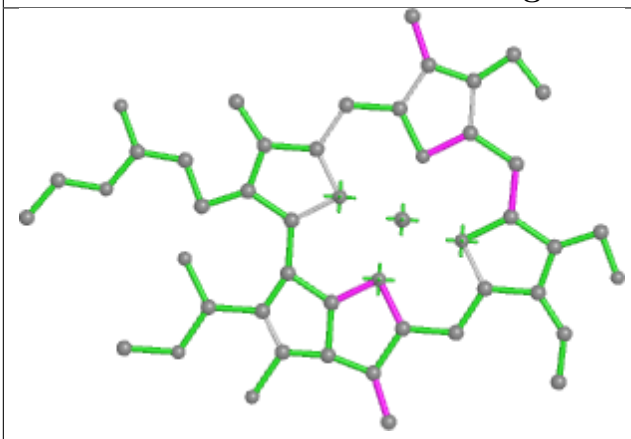


Torsions

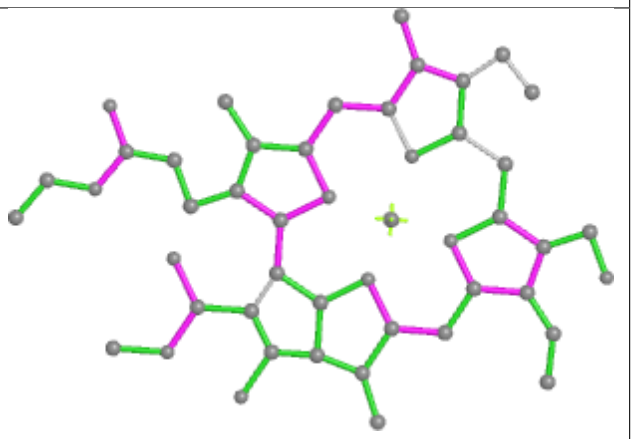


Rings

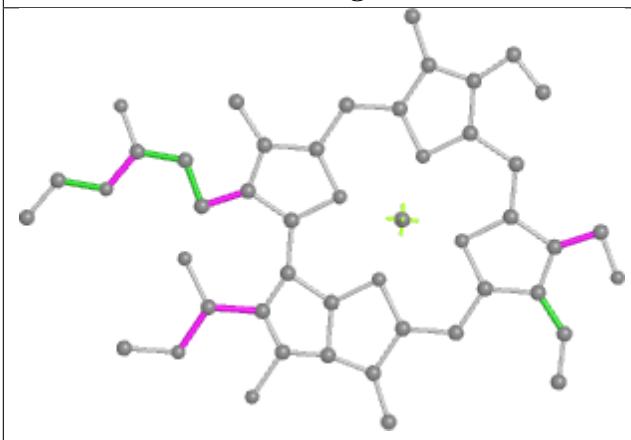
Ligand CHL Y 306



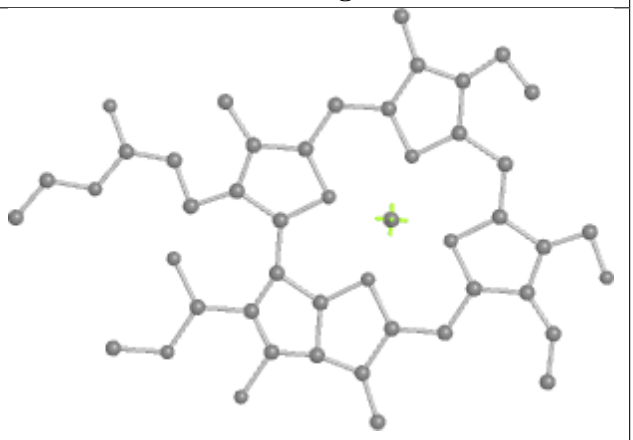
Bond lengths



Bond angles

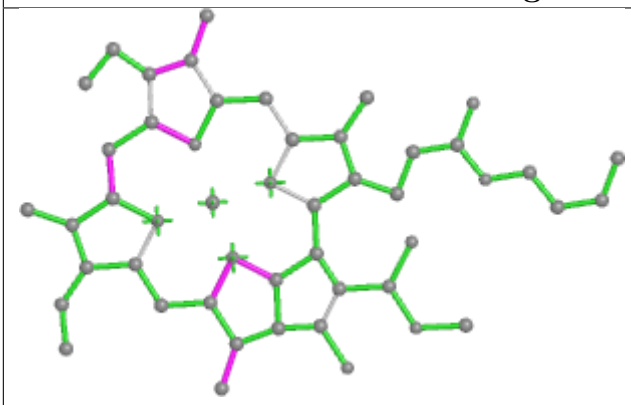


Torsions

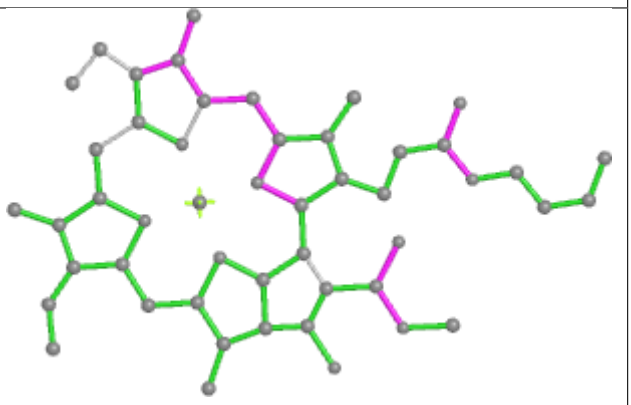


Rings

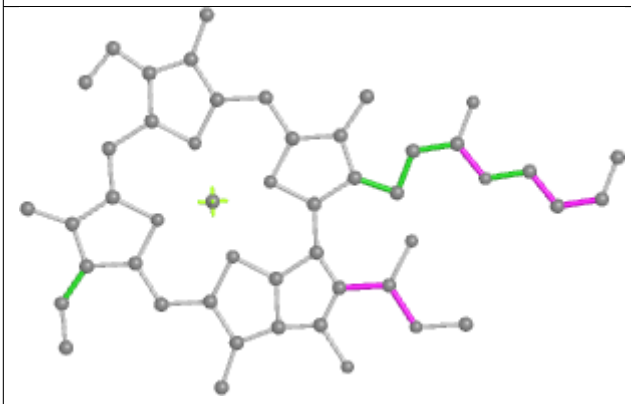
Ligand CLA N 614



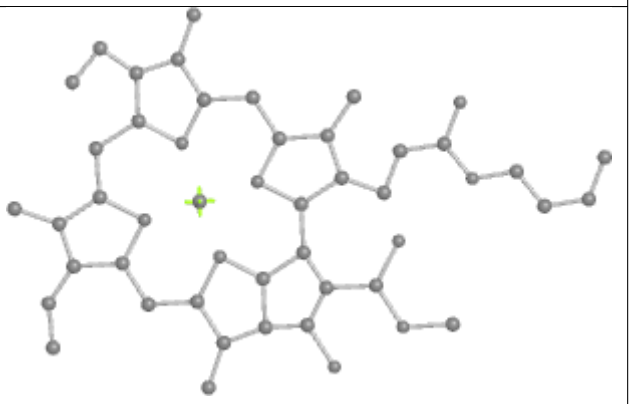
Bond lengths



Bond angles

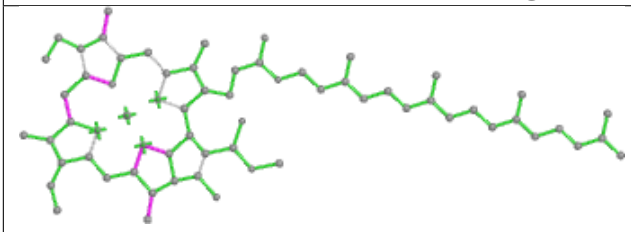


Torsions

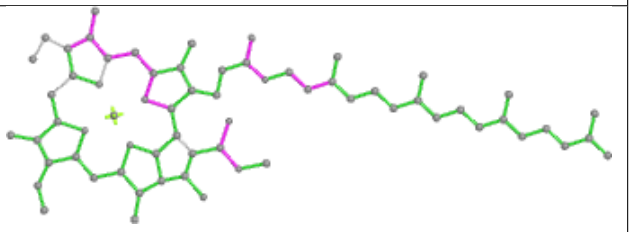


Rings

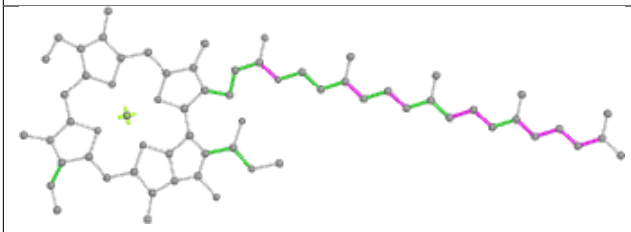
Ligand CLA G 612



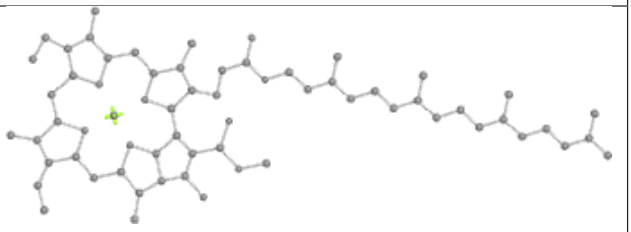
Bond lengths



Bond angles

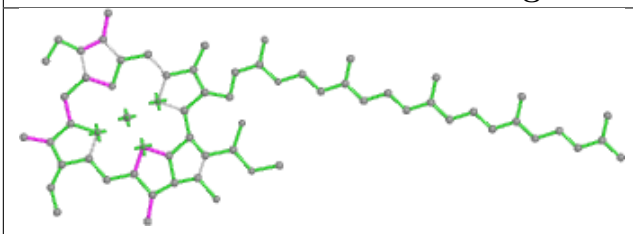


Torsions

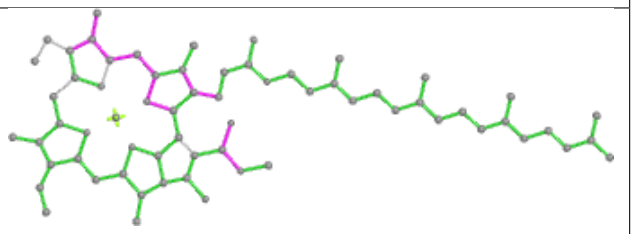


Rings

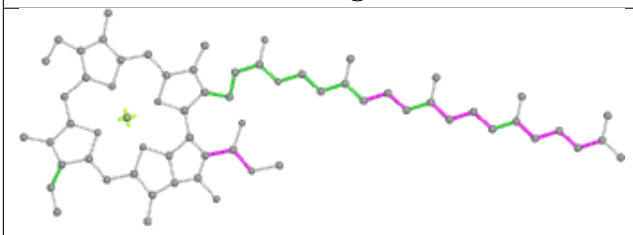
Ligand CLA G 603



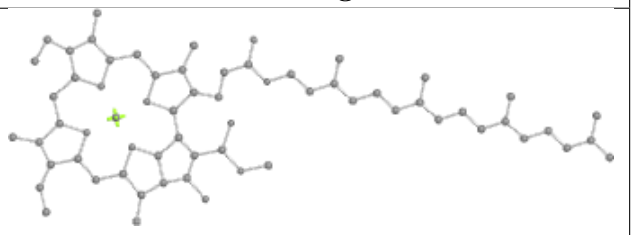
Bond lengths



Bond angles

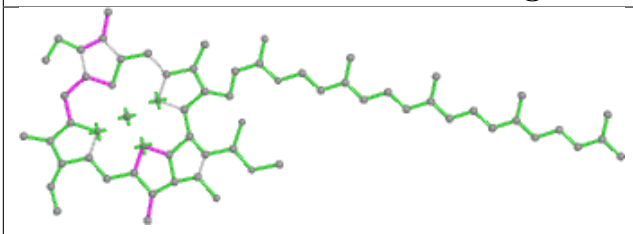


Torsions

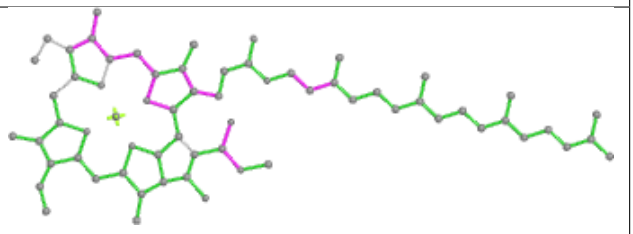


Rings

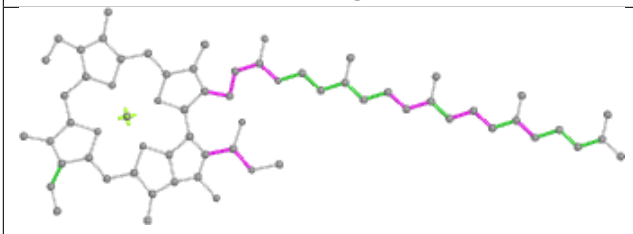
Ligand CLA Y 304



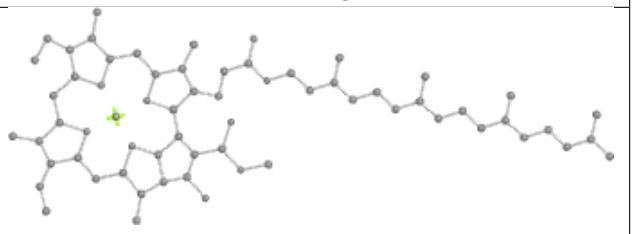
Bond lengths



Bond angles

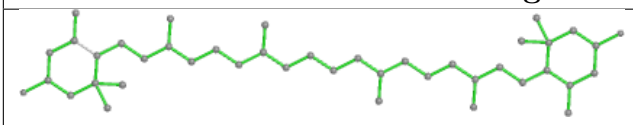


Torsions

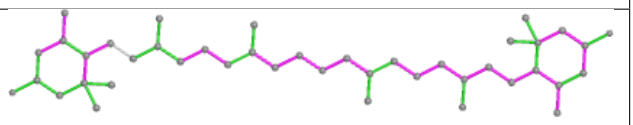


Rings

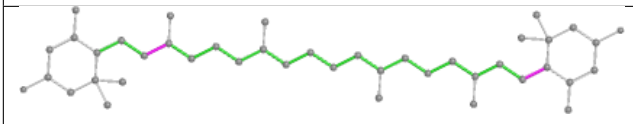
Ligand LUT G 615



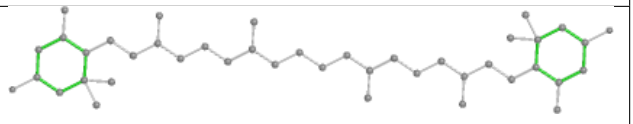
Bond lengths



Bond angles

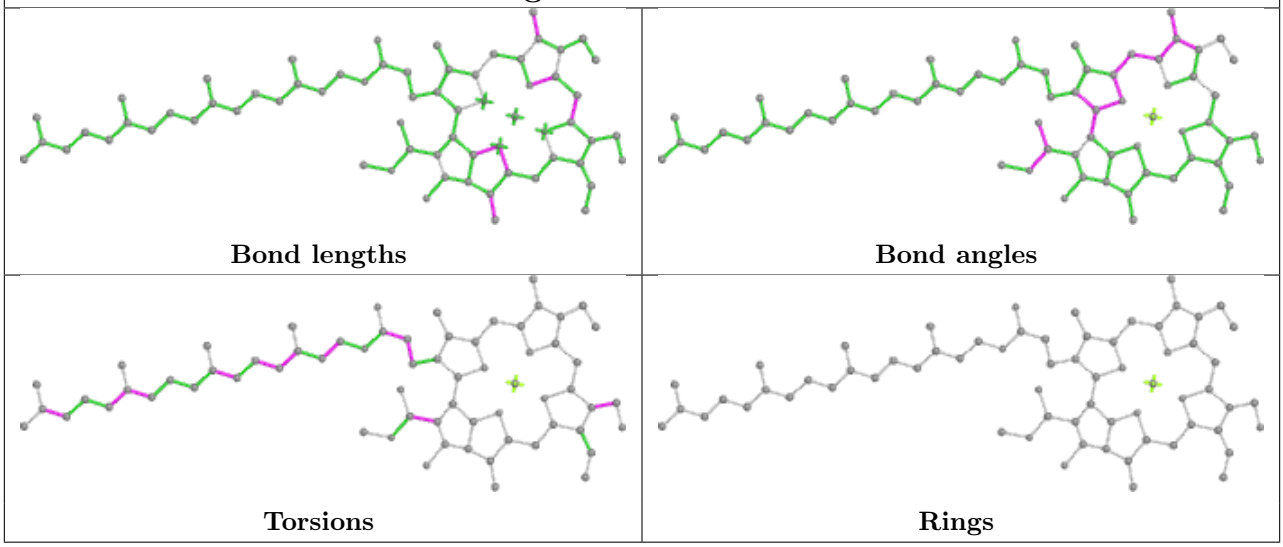


Torsions

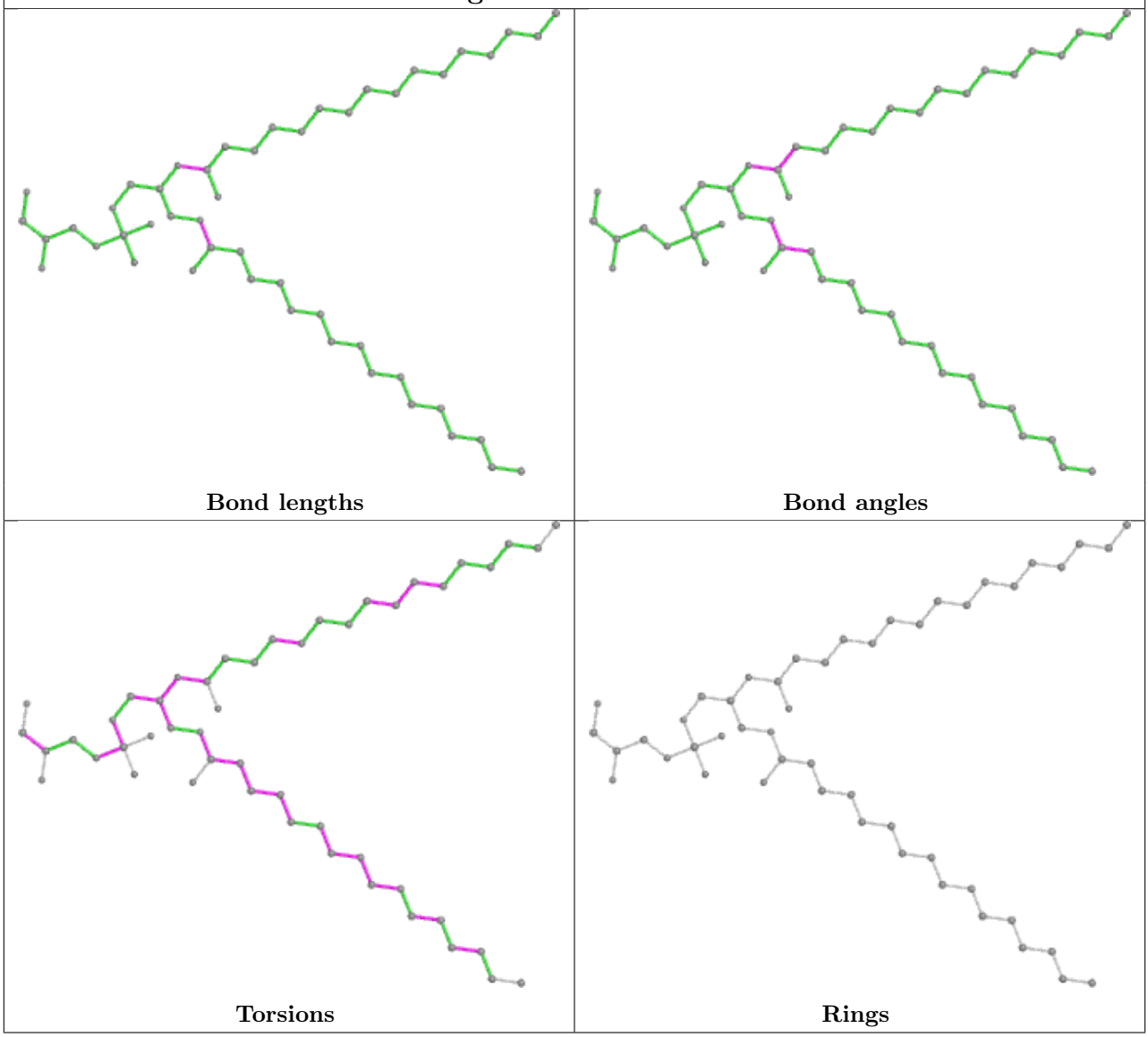


Rings

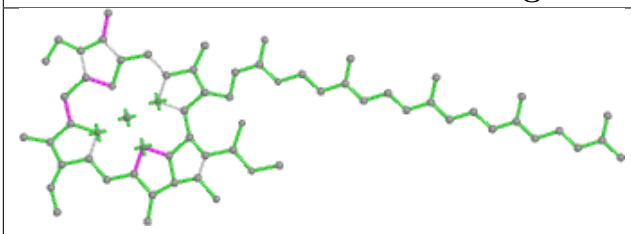
Ligand CHL Y 309



Ligand LHG N 618



Ligand CLA N 602



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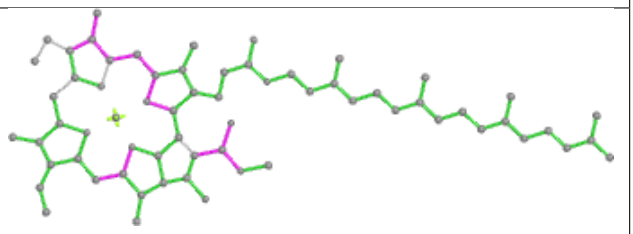
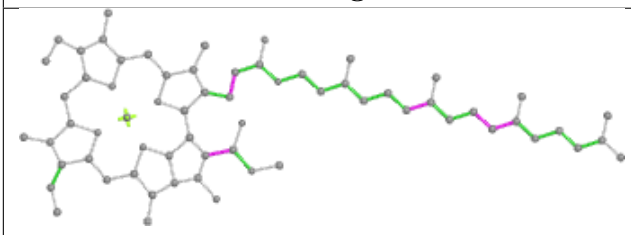
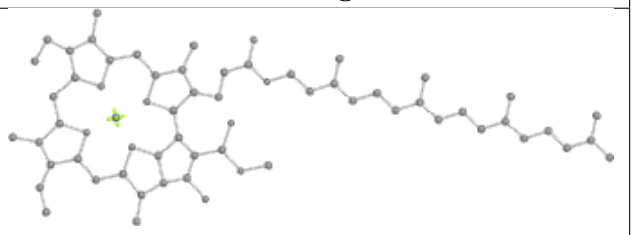


Bond angles

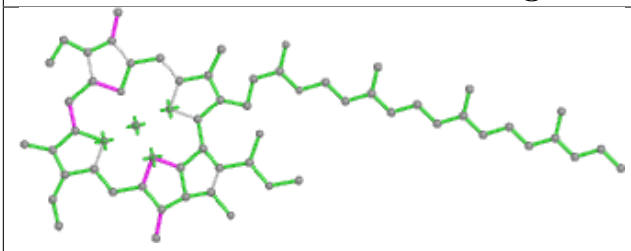


Torsions



Rings

Ligand CLA G 604



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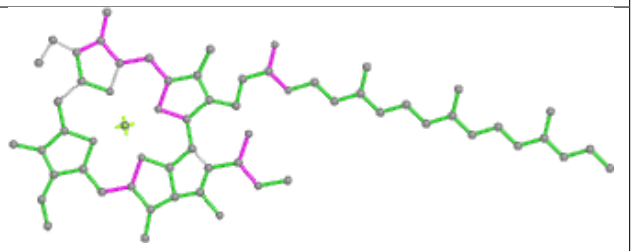
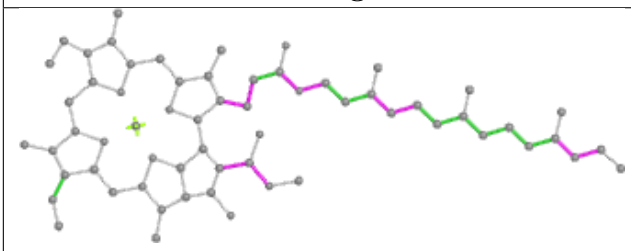
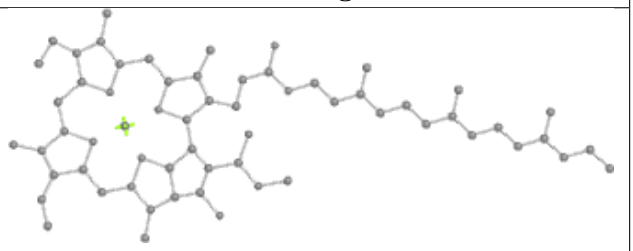


Bond angles

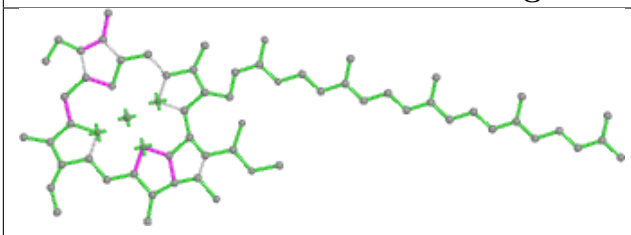


Torsions

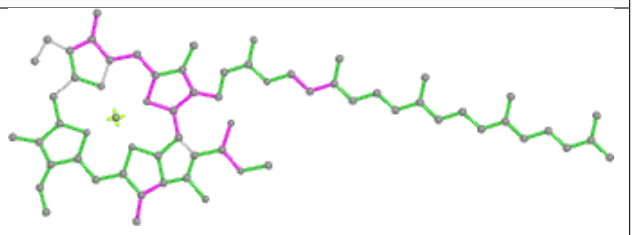


Rings

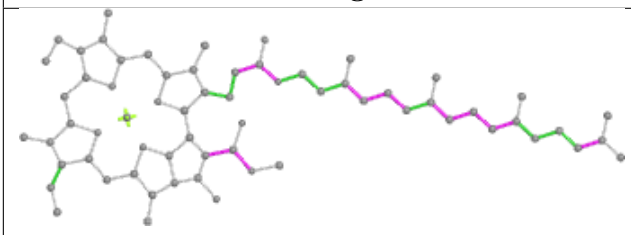
Ligand CLA Y 313



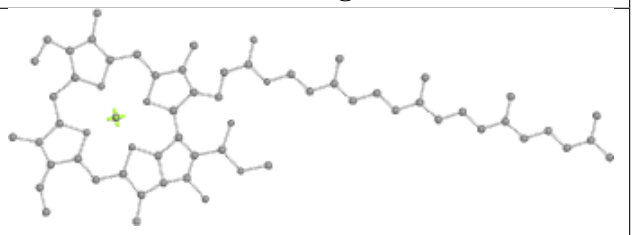
Bond lengths



Bond angles

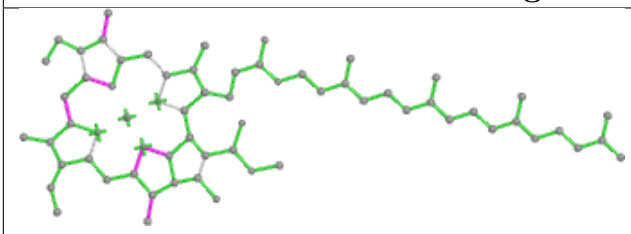


Torsions

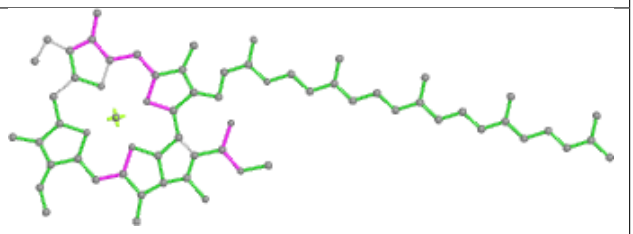


Rings

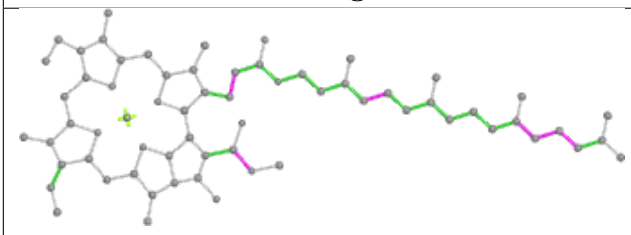
Ligand CLA Y 314



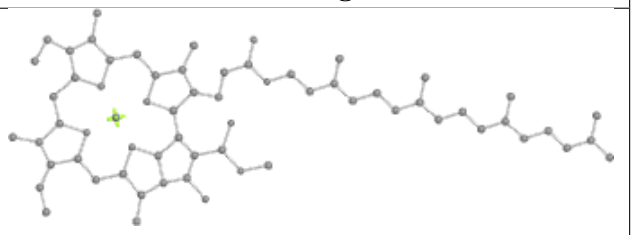
Bond lengths



Bond angles

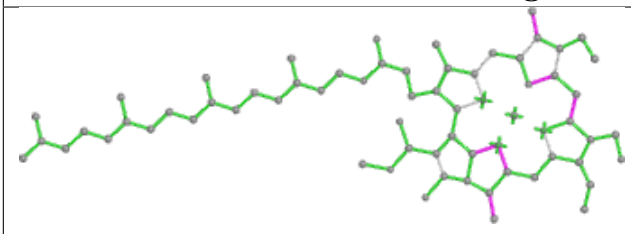


Torsions

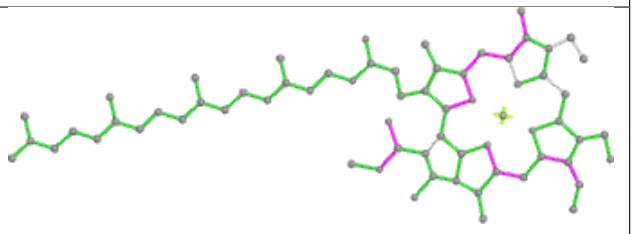


Rings

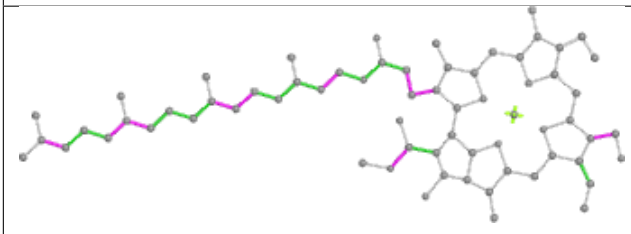
Ligand CHL G 608



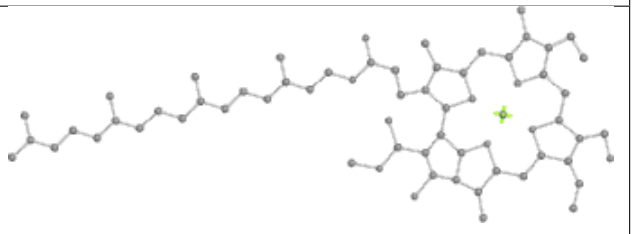
Bond lengths



Bond angles

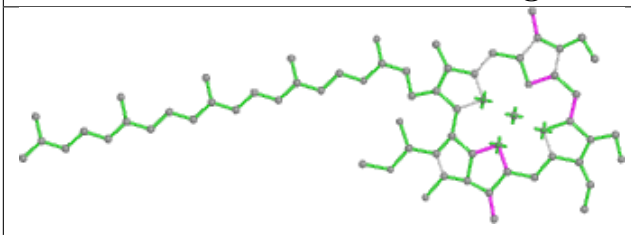


Torsions

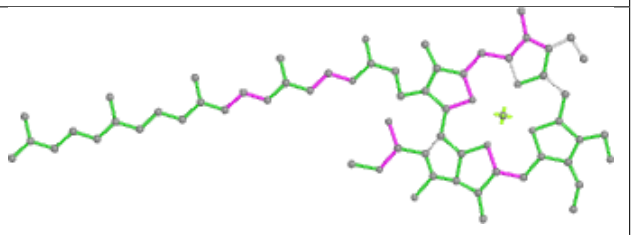


Rings

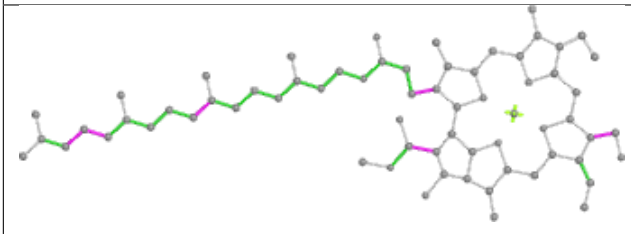
Ligand CHL N 601



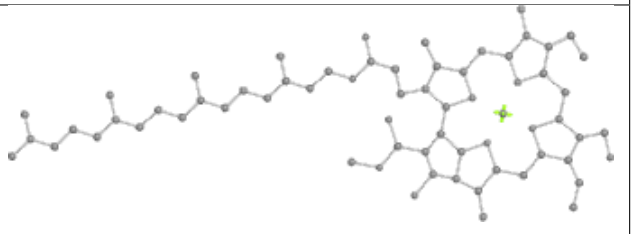
Bond lengths



Bond angles

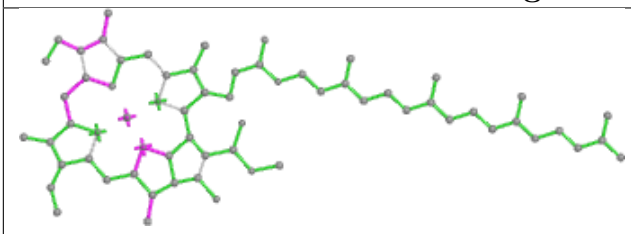


Torsions

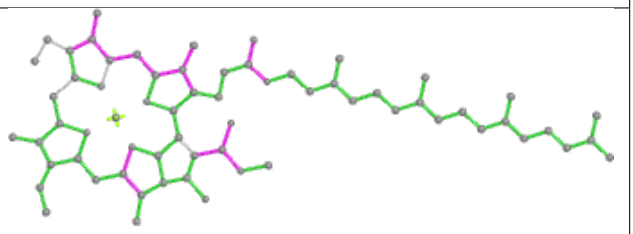


Rings

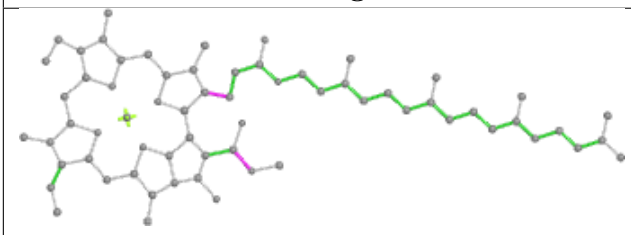
Ligand CLA Y 311



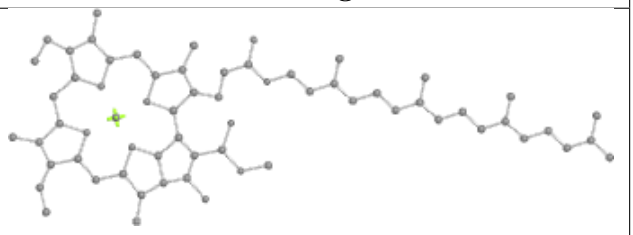
Bond lengths



Bond angles

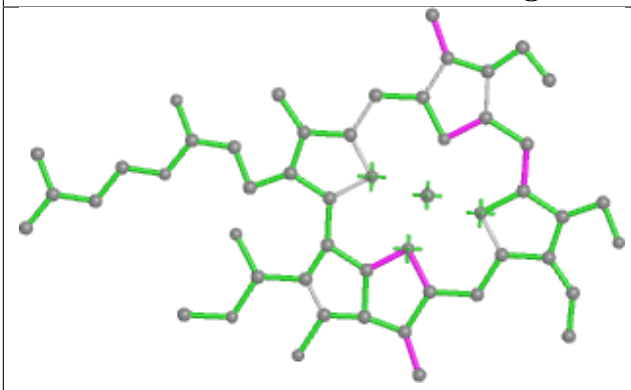


Torsions

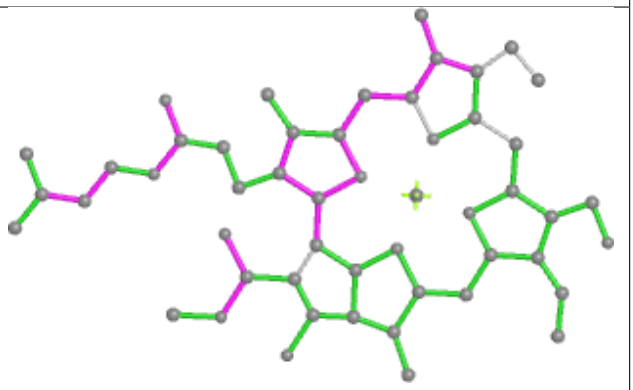


Rings

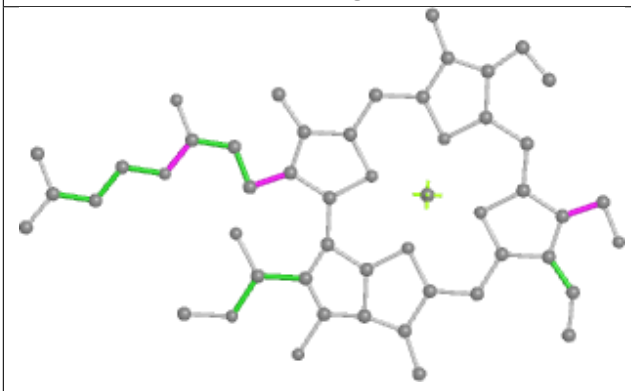
Ligand CHL N 606



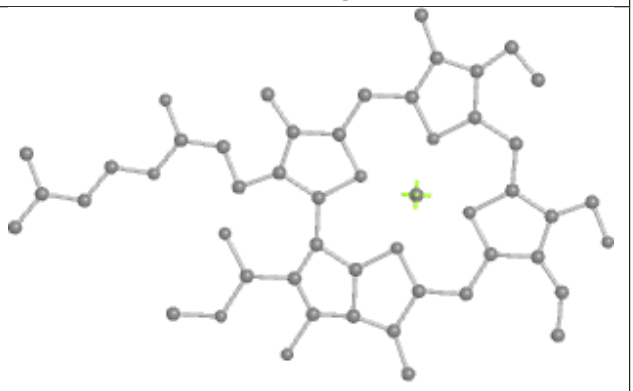
Bond lengths



Bond angles

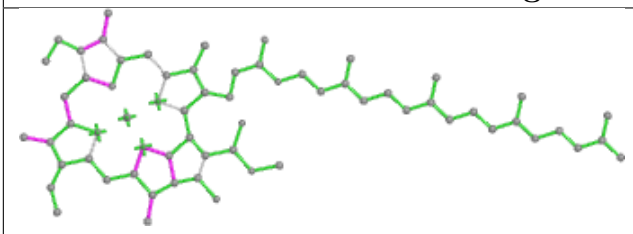


Torsions

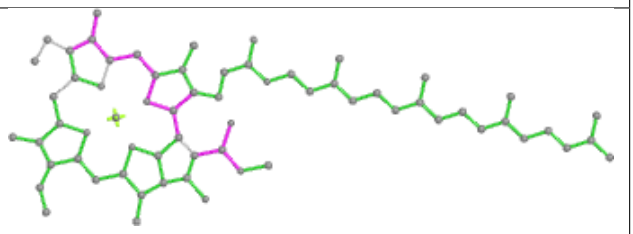


Rings

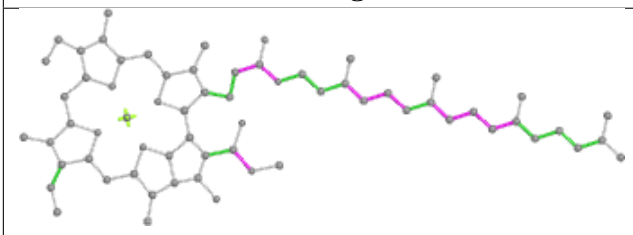
Ligand CLA N 612



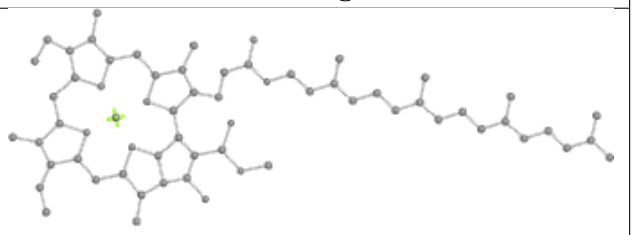
Bond lengths



Bond angles

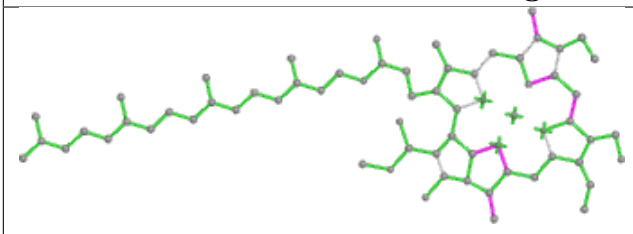


Torsions

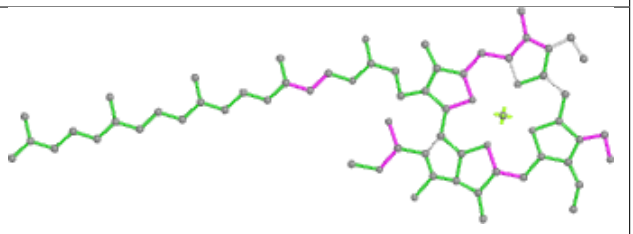


Rings

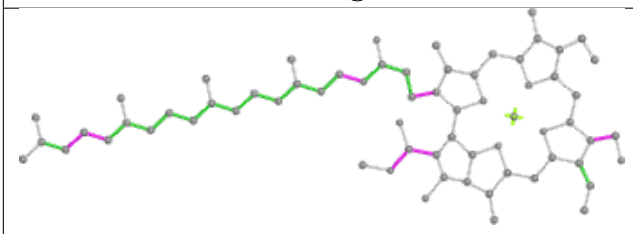
Ligand CHL Y 302



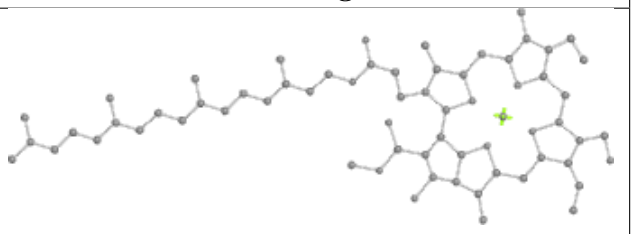
Bond lengths



Bond angles

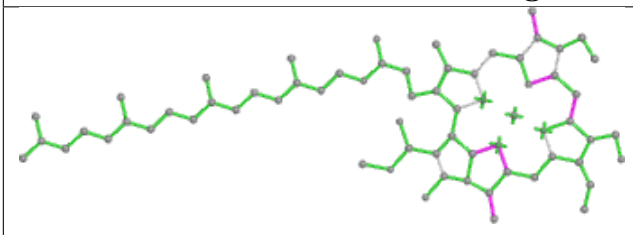


Torsions

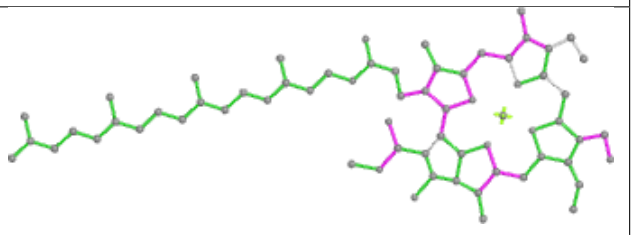


Rings

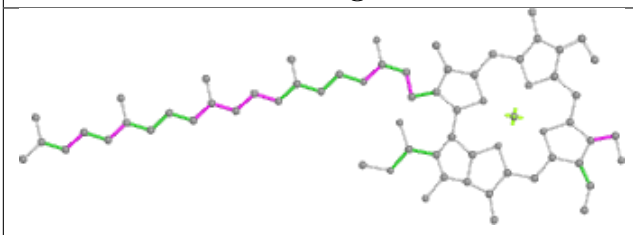
Ligand CHL Y 308



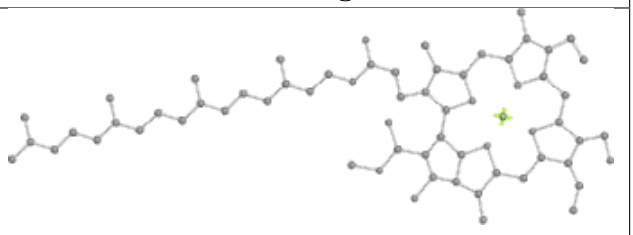
Bond lengths



Bond angles

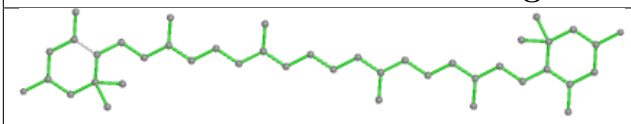


Torsions

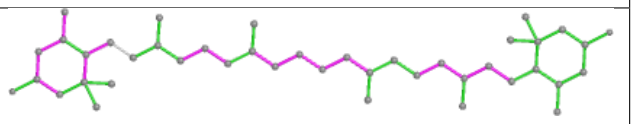


Rings

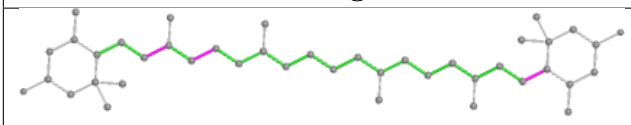
Ligand LUT N 615



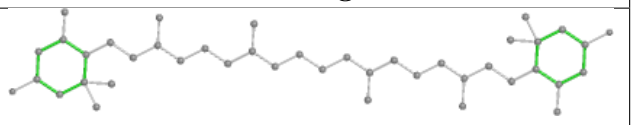
Bond lengths



Bond angles

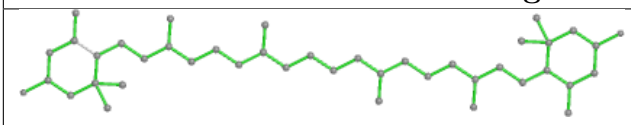


Torsions

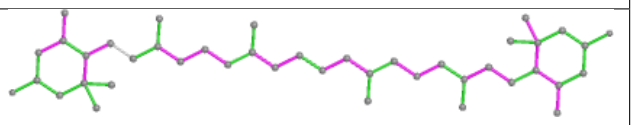


Rings

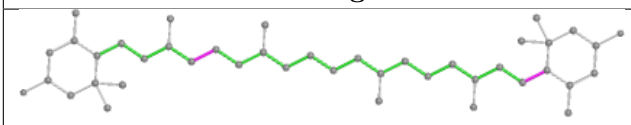
Ligand LUT N 616



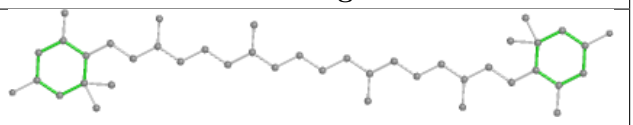
Bond lengths



Bond angles

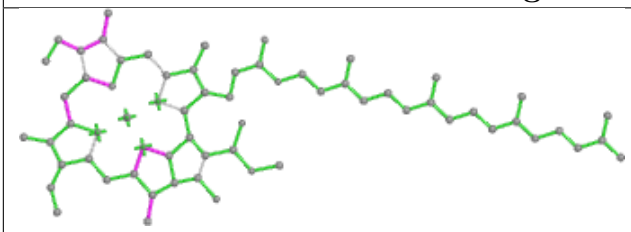


Torsions

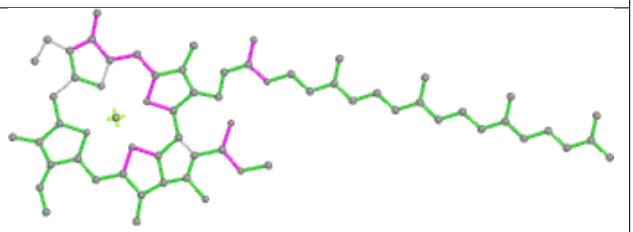


Rings

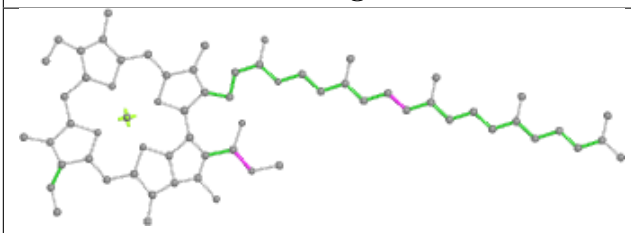
Ligand CLA N 610



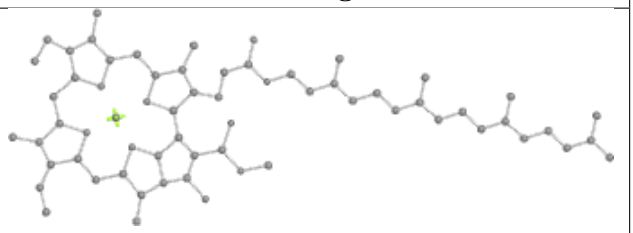
Bond lengths



Bond angles

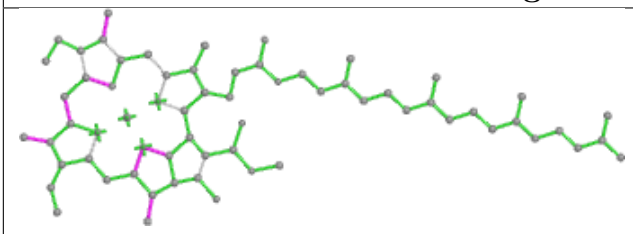


Torsions

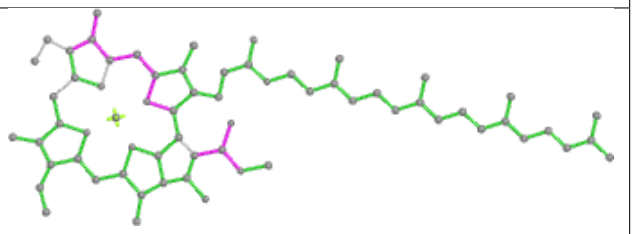


Rings

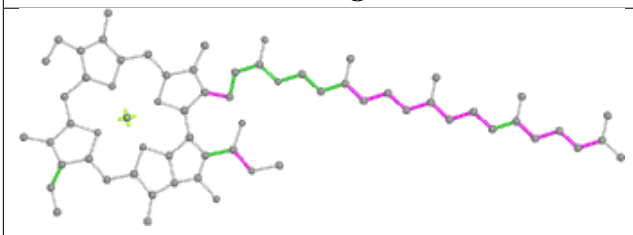
Ligand CLA N 611



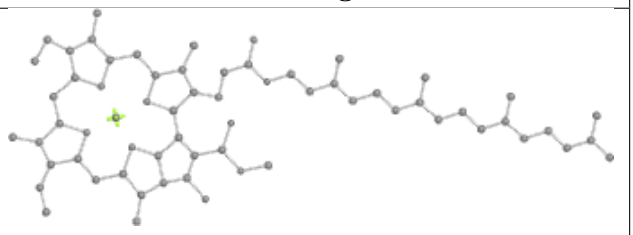
Bond lengths



Bond angles

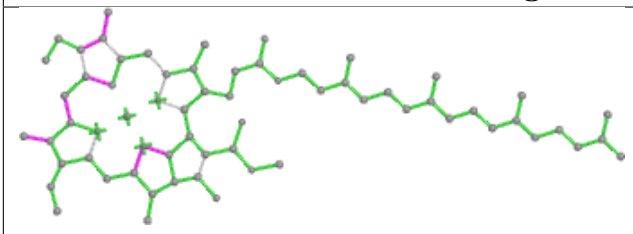


Torsions

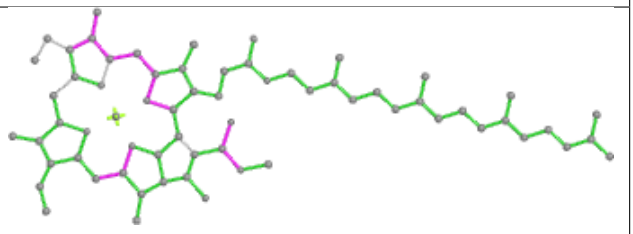


Rings

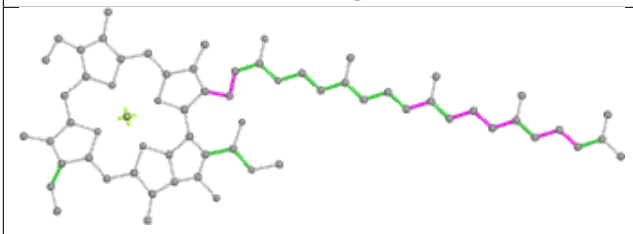
Ligand CLA G 602



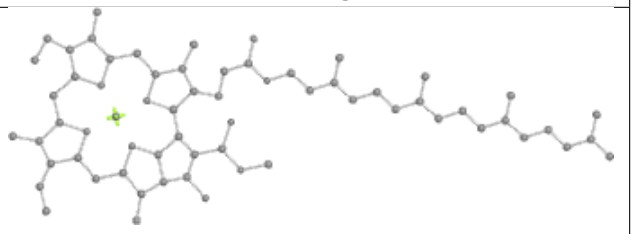
Bond lengths



Bond angles

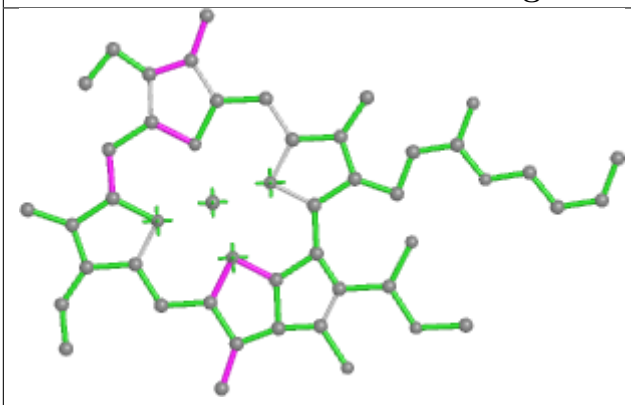


Torsions

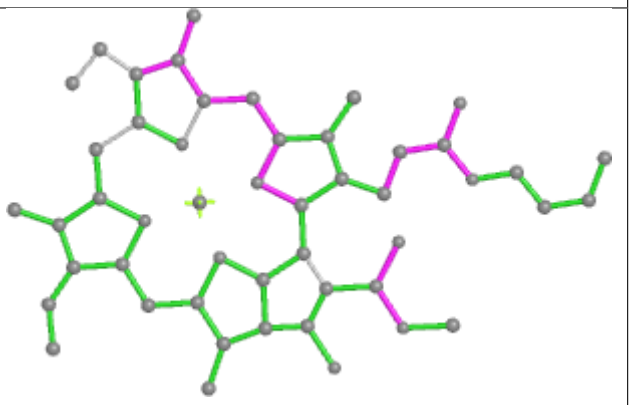


Rings

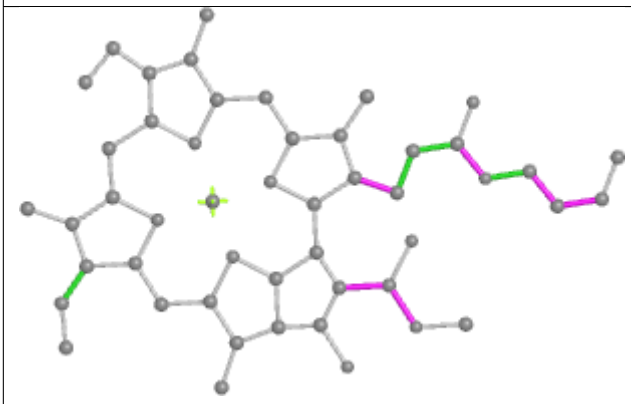
Ligand CLA G 614



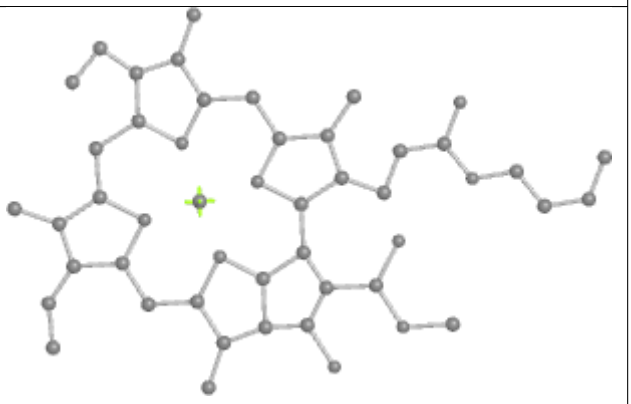
Bond lengths



Bond angles

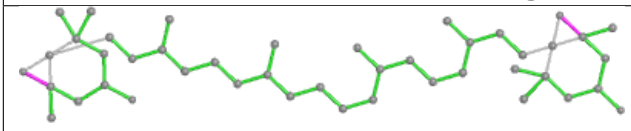


Torsions

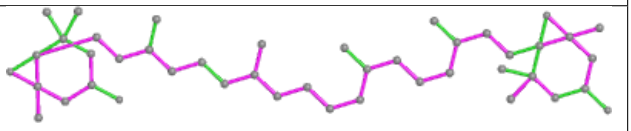


Rings

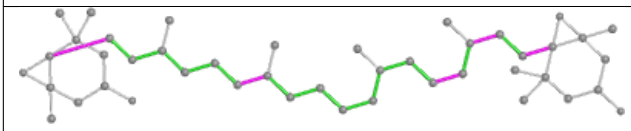
Ligand XAT G 619



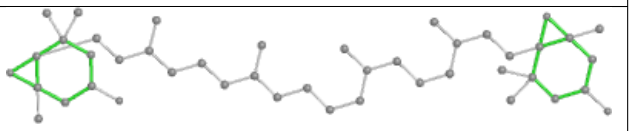
Bond lengths



Bond angles

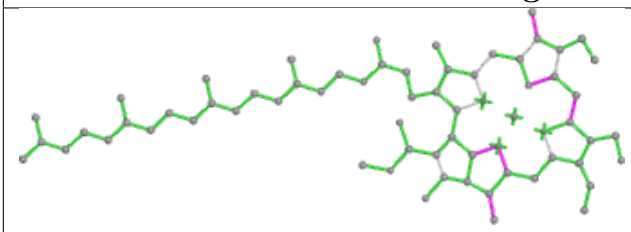


Torsions

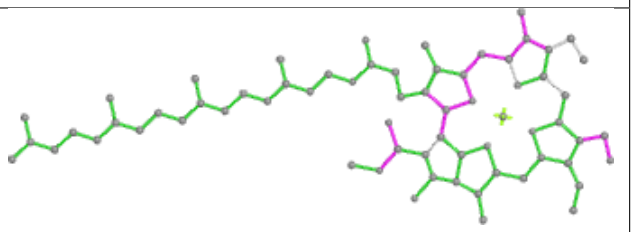


Rings

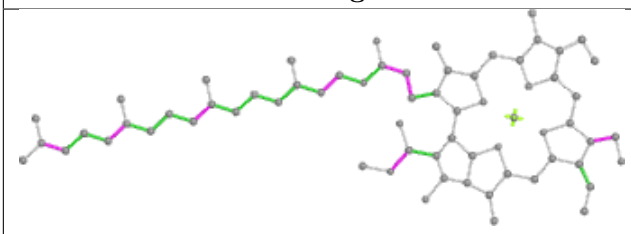
Ligand CHL N 608



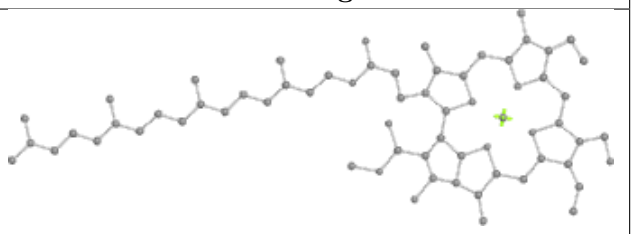
Bond lengths



Bond angles

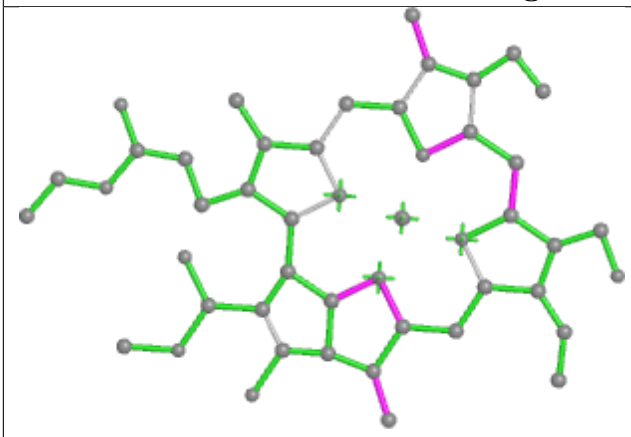


Torsions

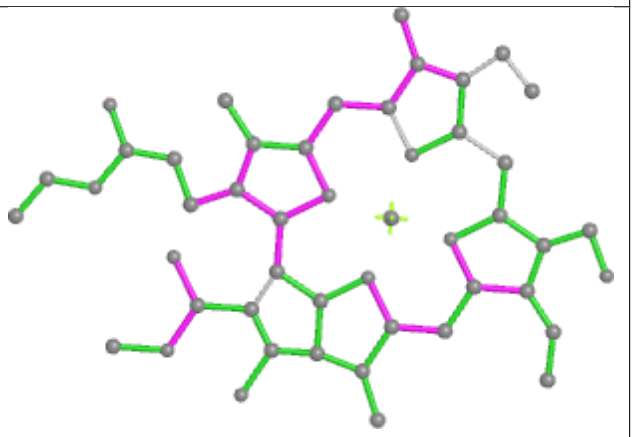


Rings

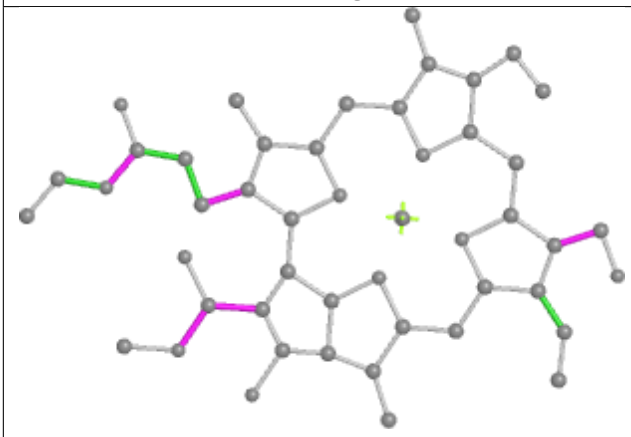
Ligand CHL N 605



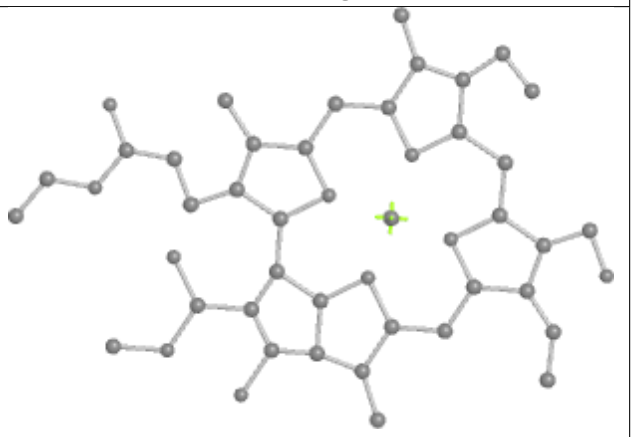
Bond lengths



Bond angles

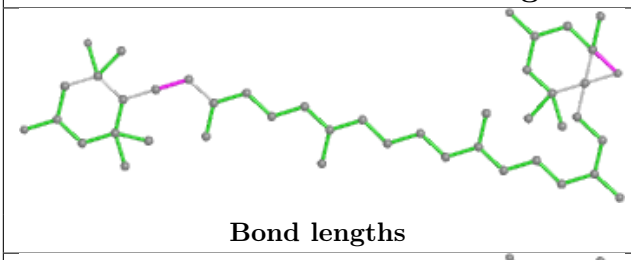


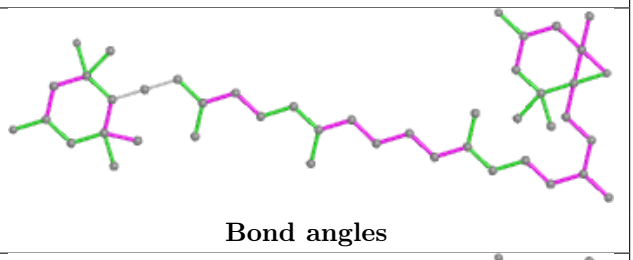
Torsions

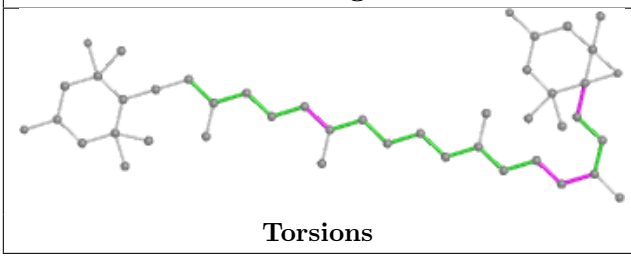


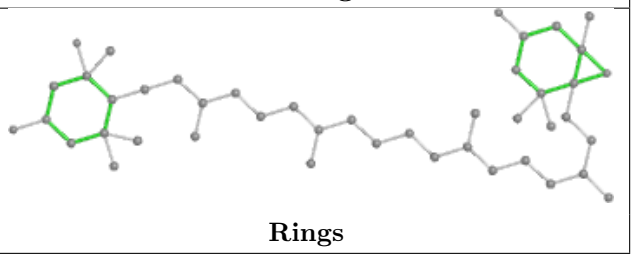
Rings

Ligand NEX G 617

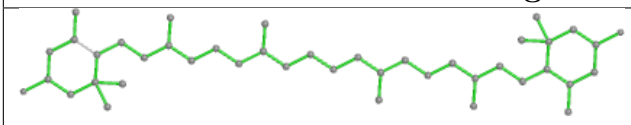

Bond lengths

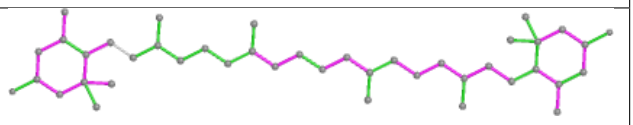

Bond angles

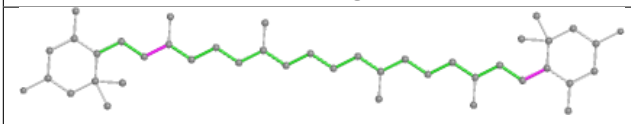

Torsions

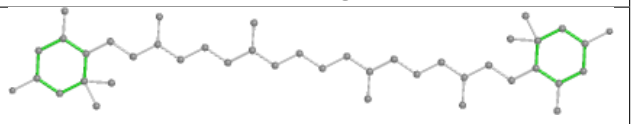

Rings

Ligand LUT Y 316

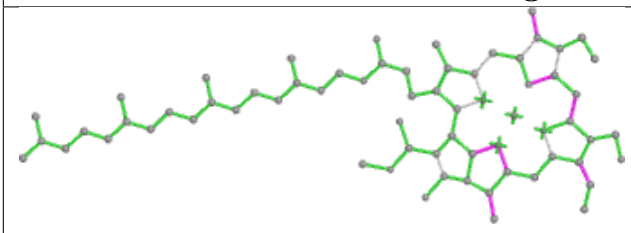

Bond lengths

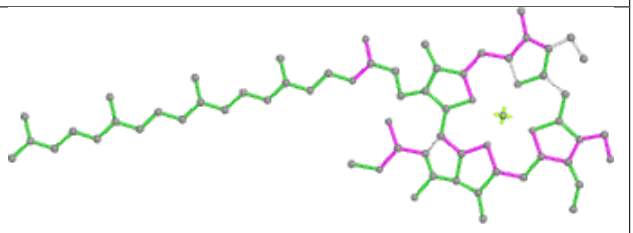

Bond angles

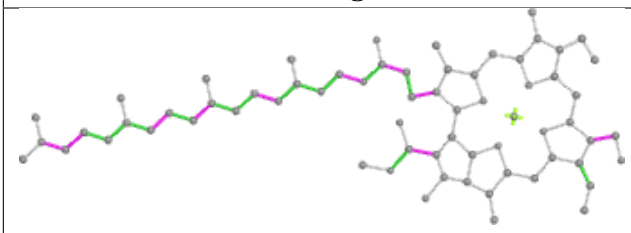

Torsions

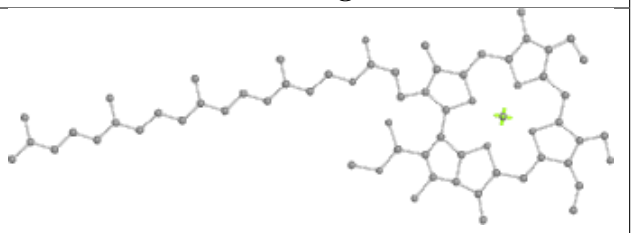

Rings

Ligand CHL G 601

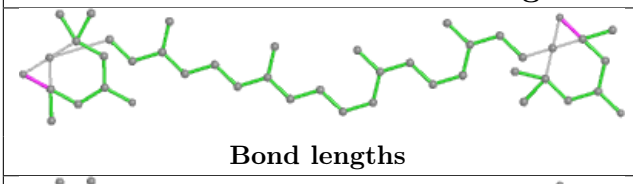

Bond lengths

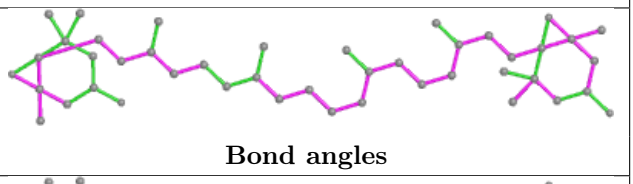

Bond angles

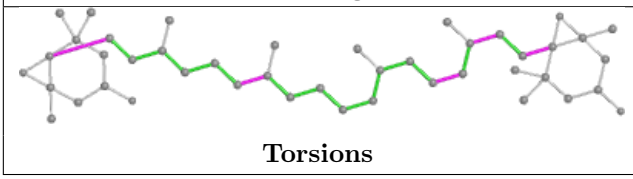

Torsions

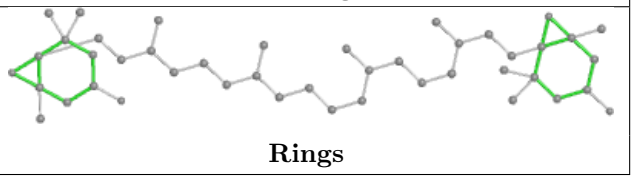

Rings

Ligand XAT N 619

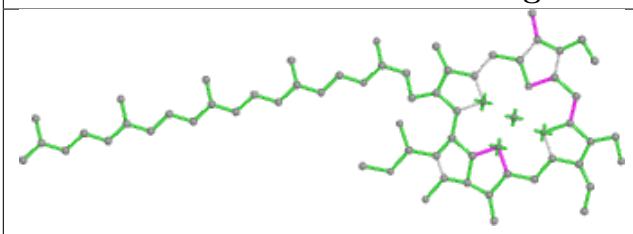

Bond lengths

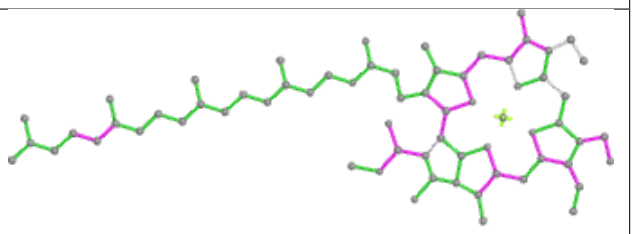

Bond angles

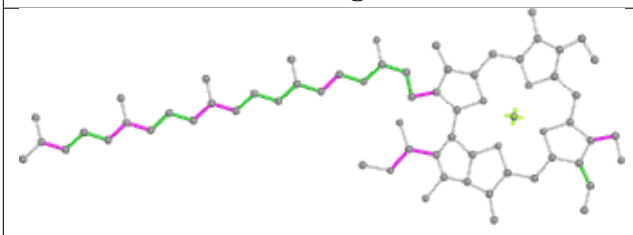

Torsions

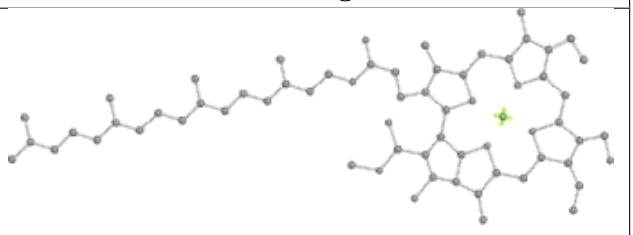

Rings

Ligand CHL Y 310

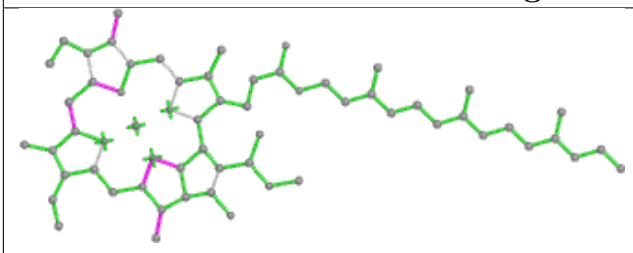

Bond lengths

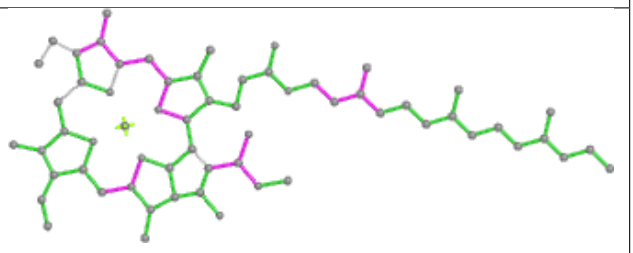

Bond angles

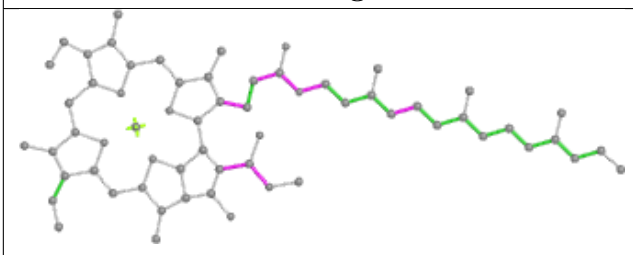

Torsions

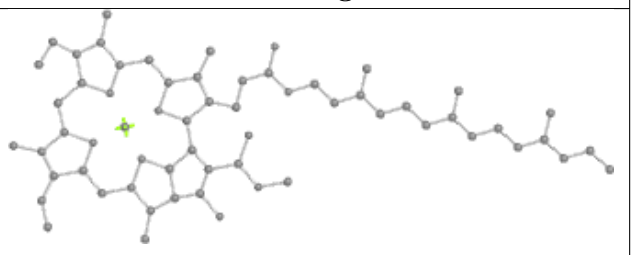

Rings

Ligand CLA Y 305

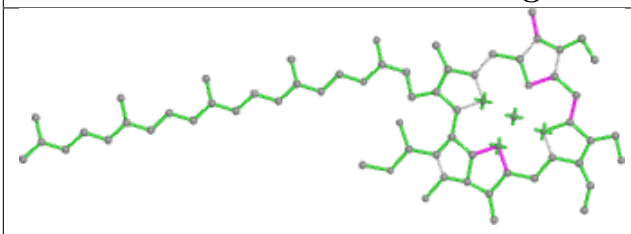

Bond lengths


Bond angles

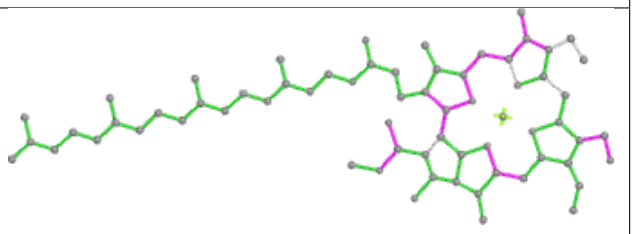

Torsions


Rings

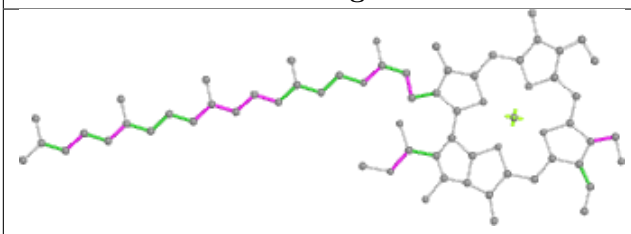
Ligand CHL G 607



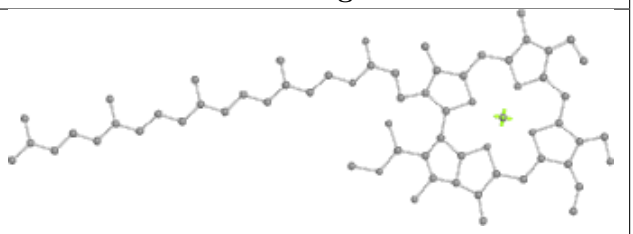
Bond lengths



Bond angles

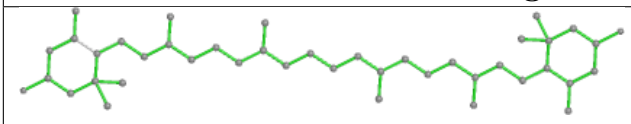


Torsions

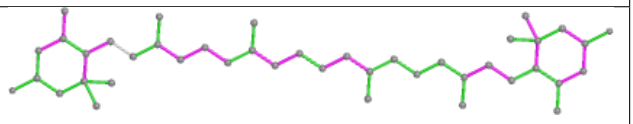


Rings

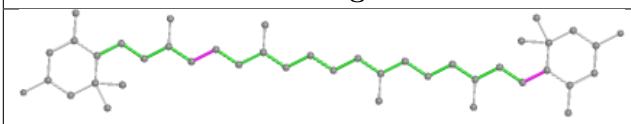
Ligand LUT G 616



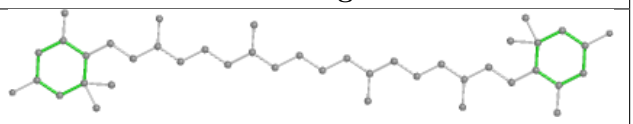
Bond lengths



Bond angles

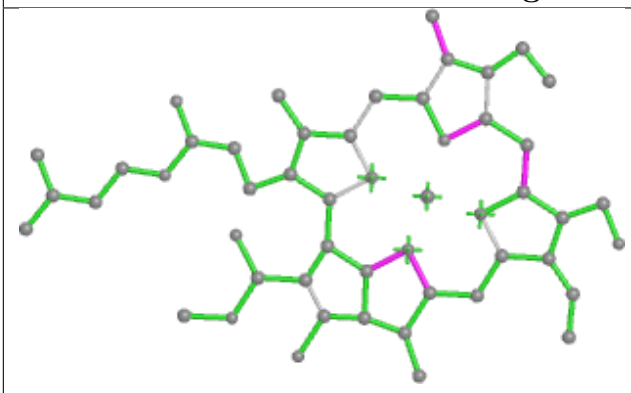


Torsions

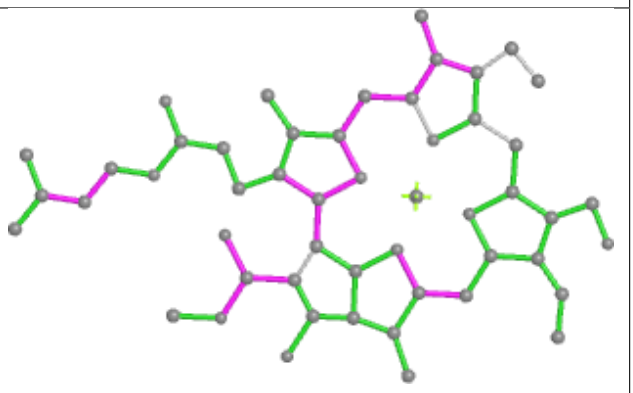


Rings

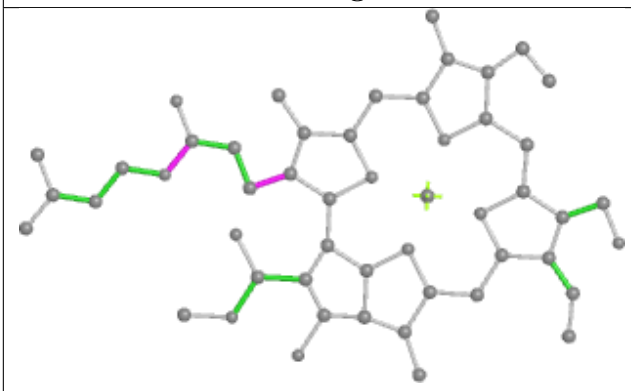
Ligand CHL G 606



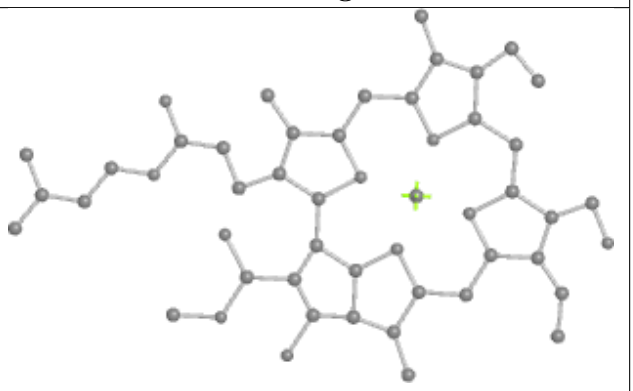
Bond lengths



Bond angles

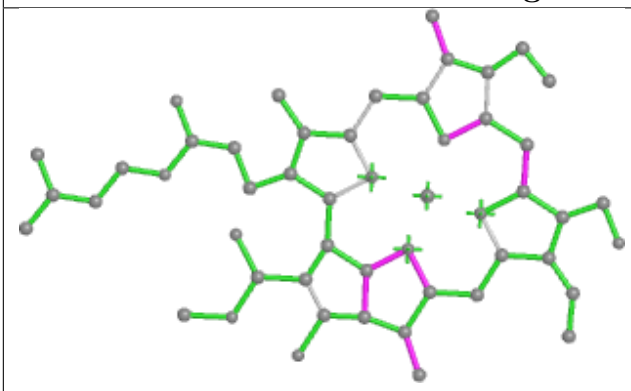


Torsions



Rings

Ligand CHL Y 307



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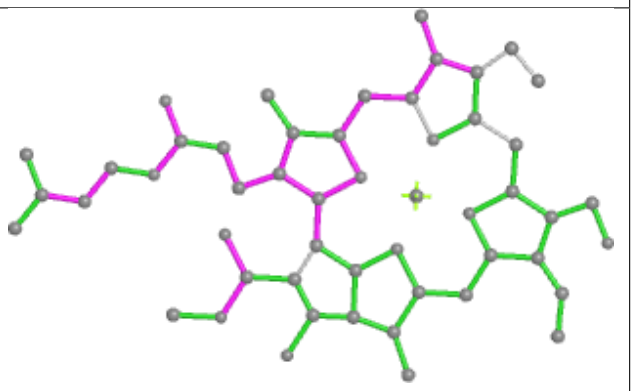
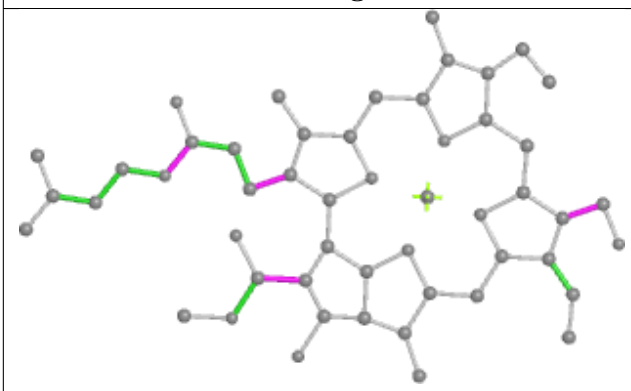
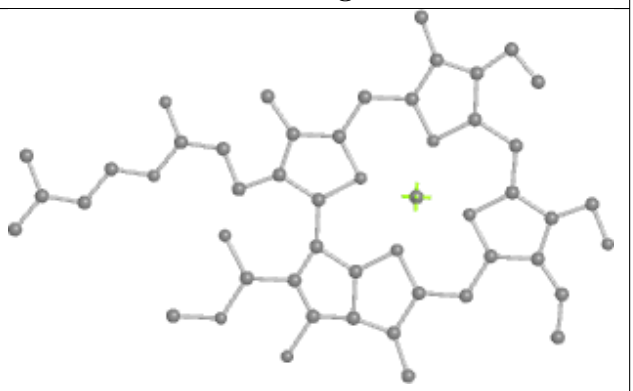


Bond angles

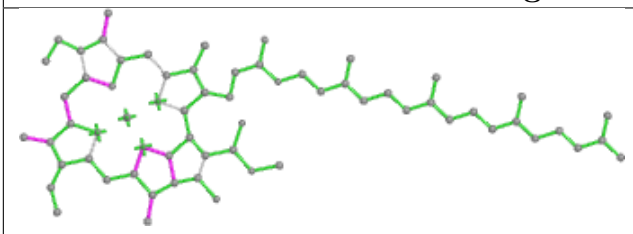


Torsions

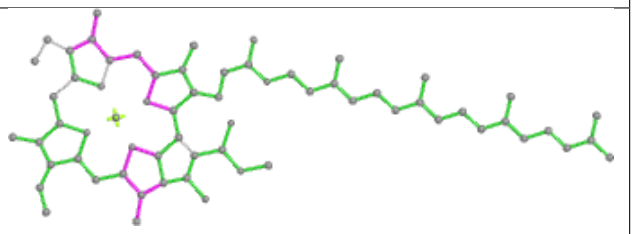


Rings

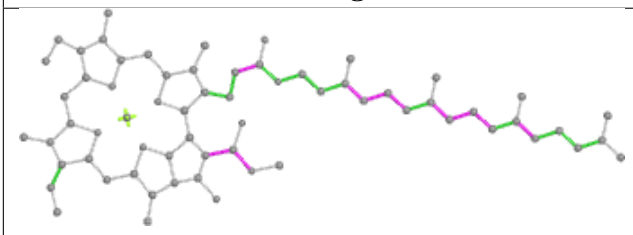
Ligand CLA Y 312



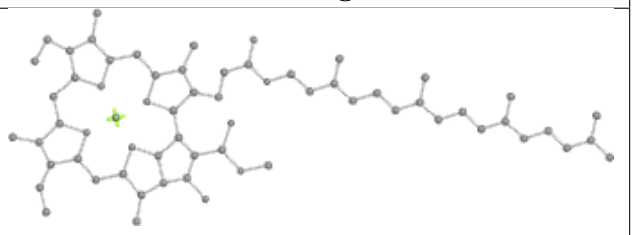
Bond lengths



Bond angles

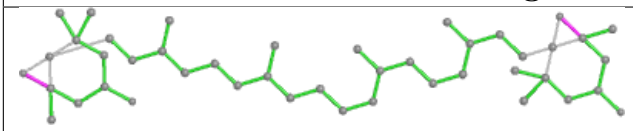


Torsions

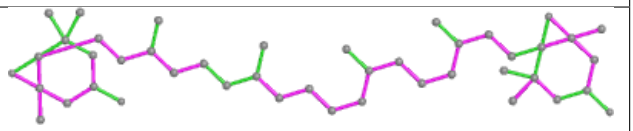


Rings

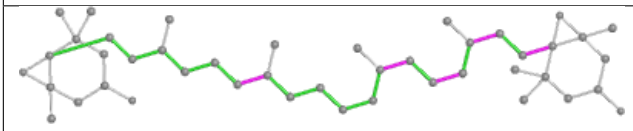
Ligand XAT Y 301



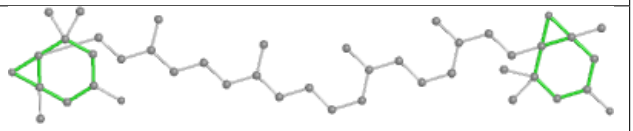
Bond lengths



Bond angles

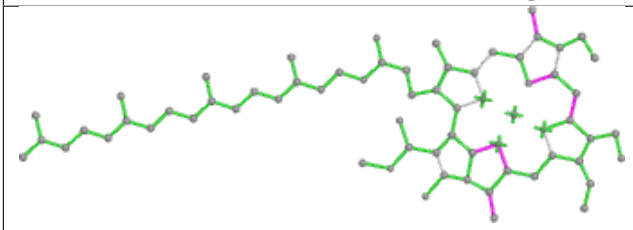


Torsions

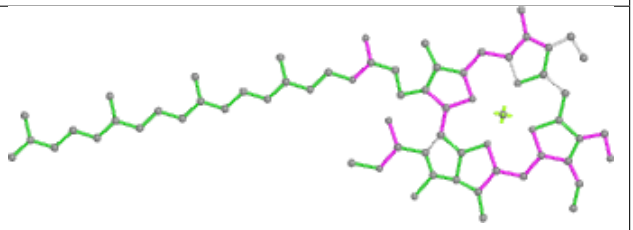


Rings

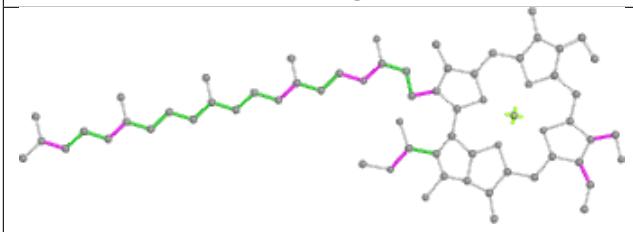
Ligand CHL G 609



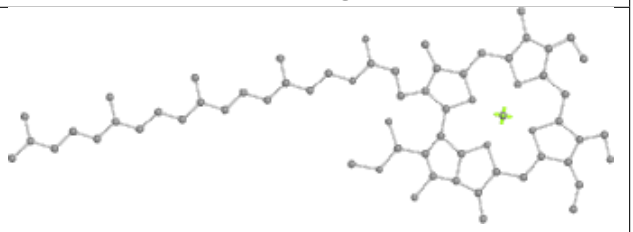
Bond lengths



Bond angles

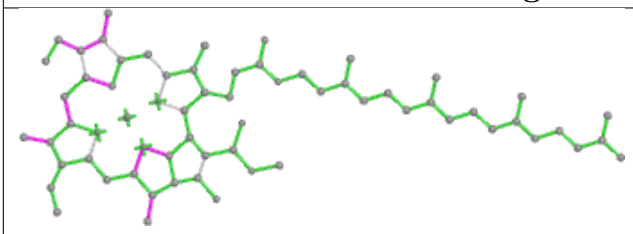


Torsions

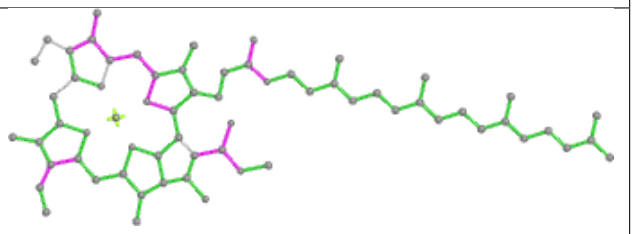


Rings

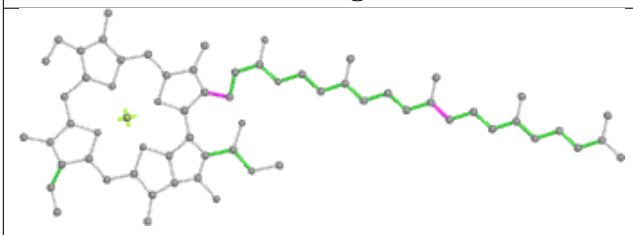
Ligand CLA G 610



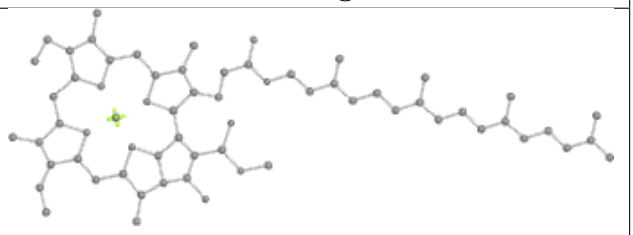
Bond lengths



Bond angles

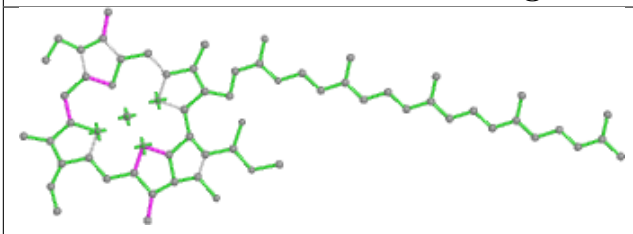


Torsions

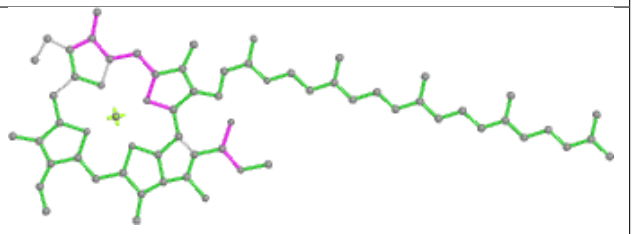


Rings

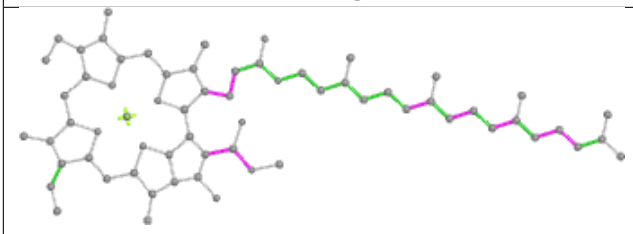
Ligand CLA Y 303



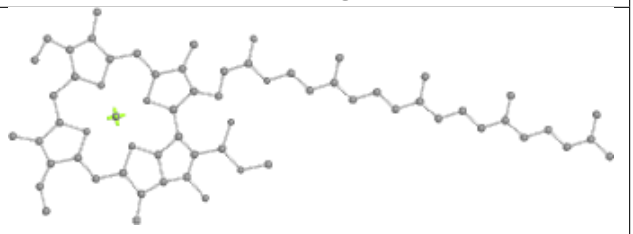
Bond lengths



Bond angles

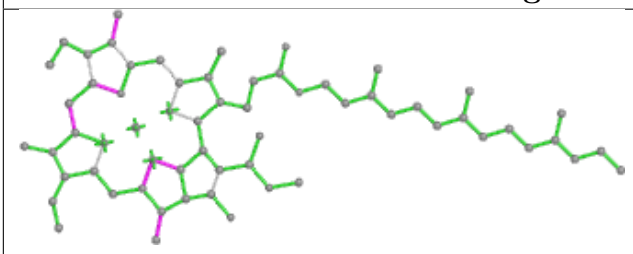


Torsions

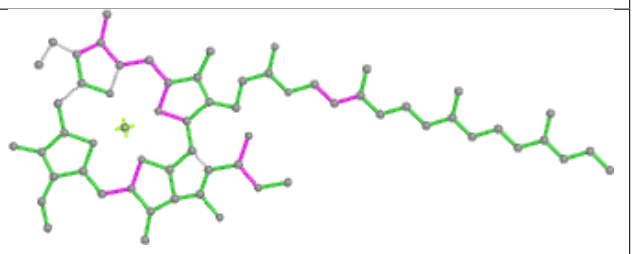


Rings

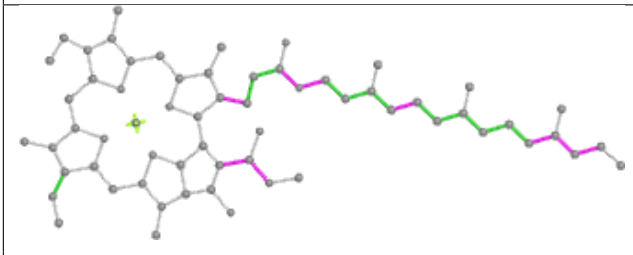
Ligand CLA N 604



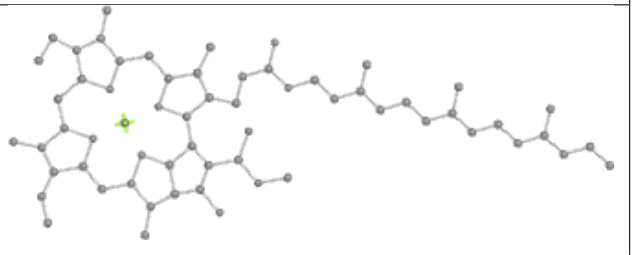
Bond lengths



Bond angles

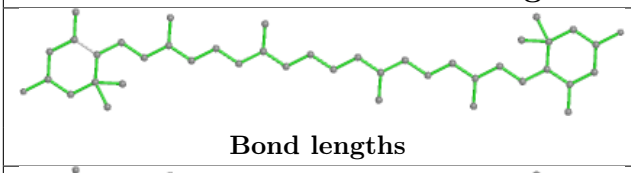


Torsions

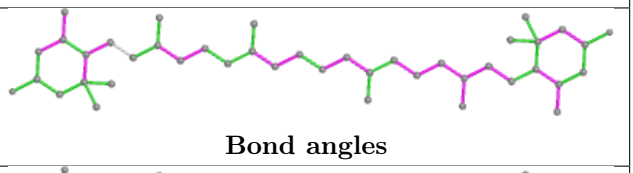


Rings

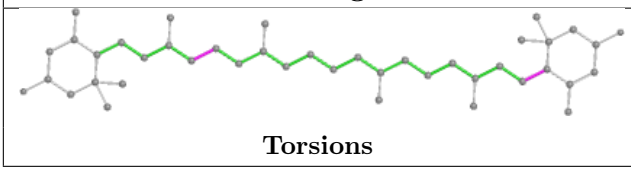
Ligand LUT Y 317



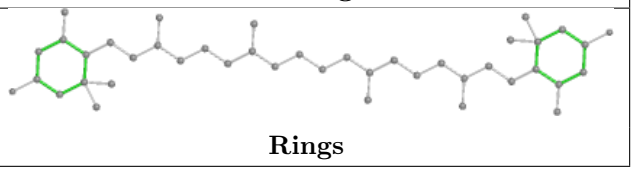
Bond lengths



Bond angles

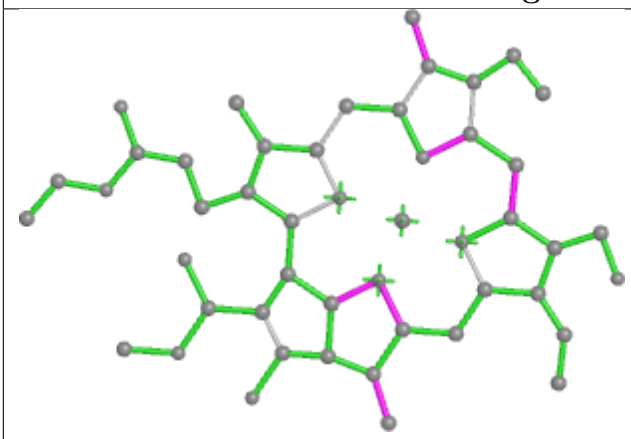


Torsions

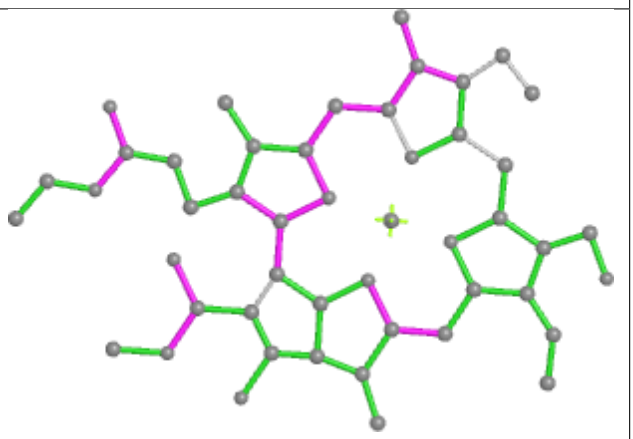


Rings

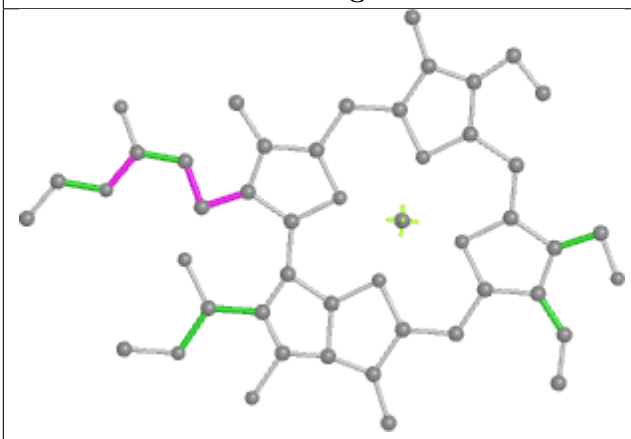
Ligand CHL G 605



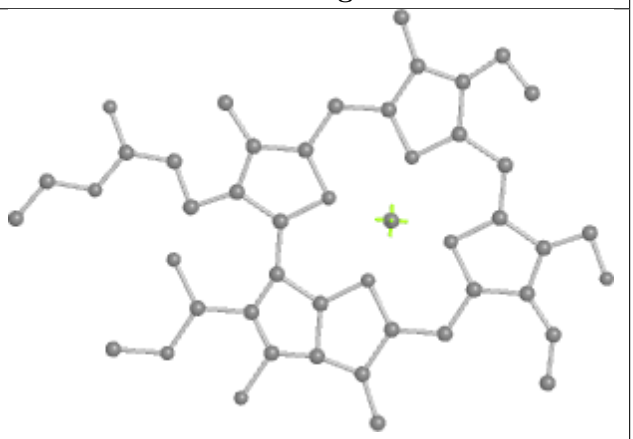
Bond lengths



Bond angles

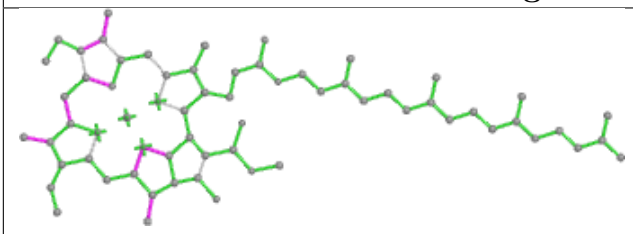


Torsions

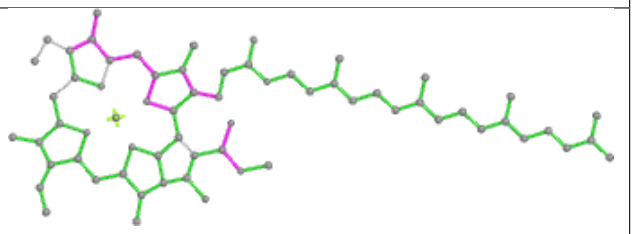


Rings

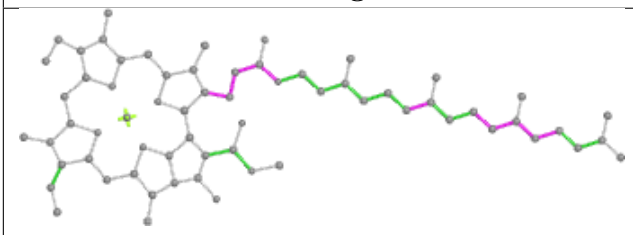
Ligand CLA N 603



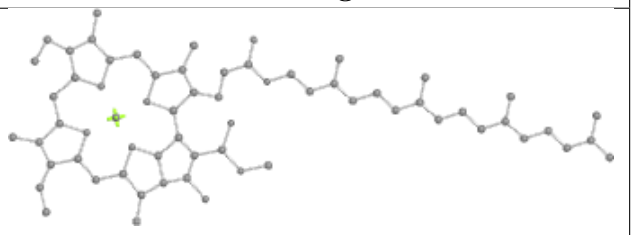
Bond lengths



Bond angles

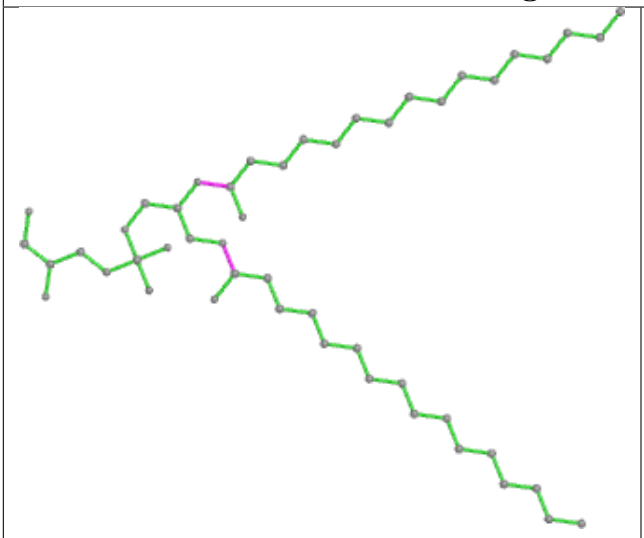


Torsions

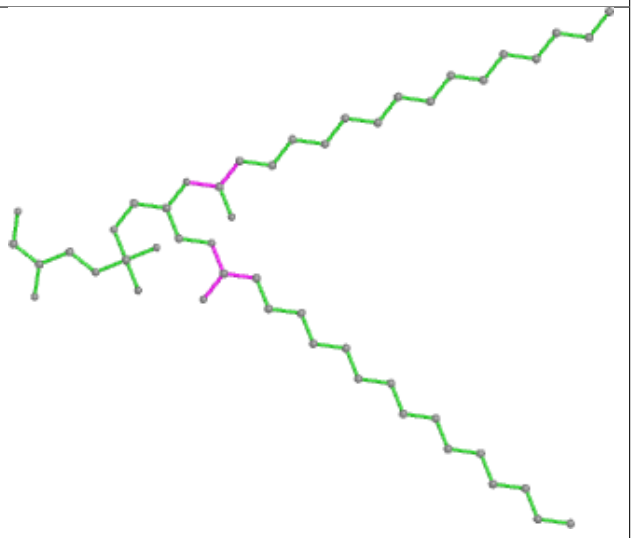


Rings

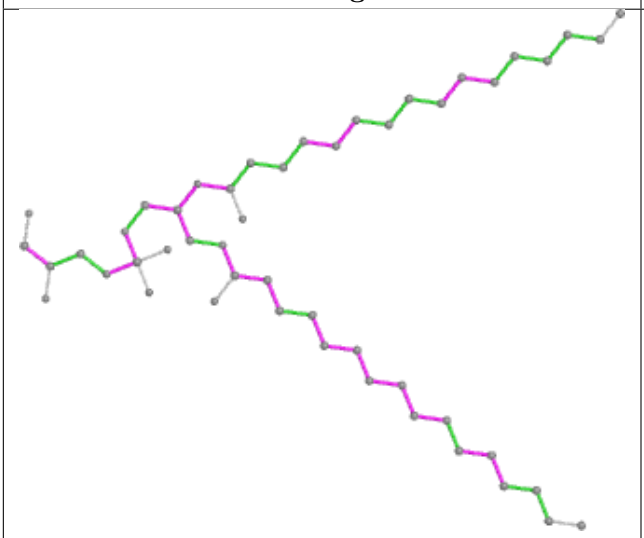
Ligand LHG G 618



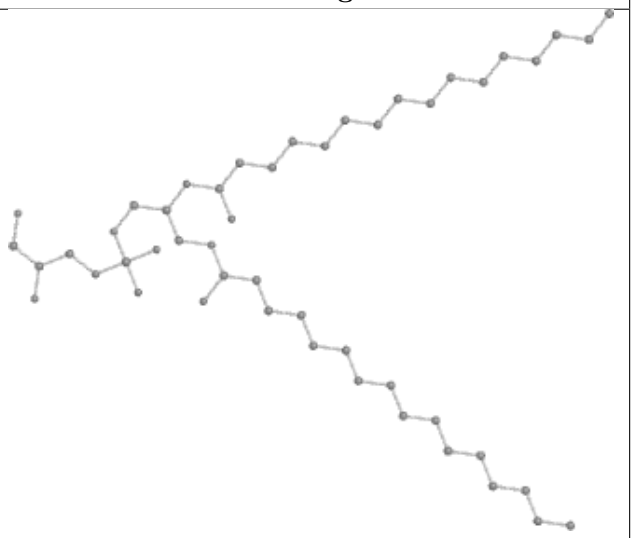
Bond lengths



Bond angles

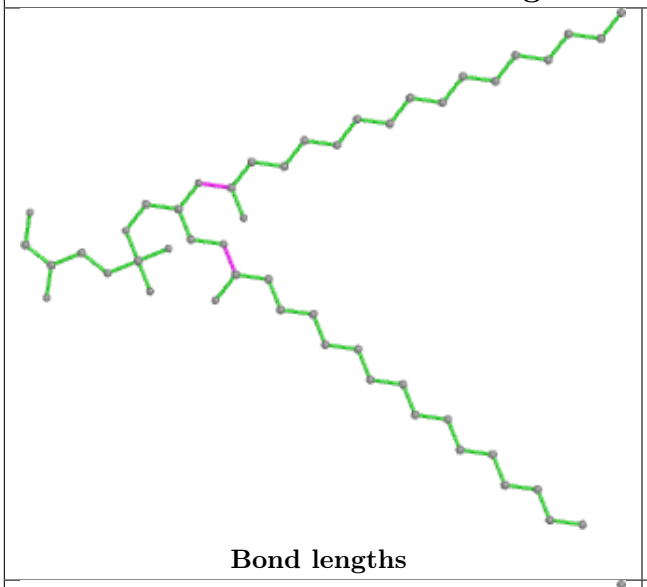


Torsions

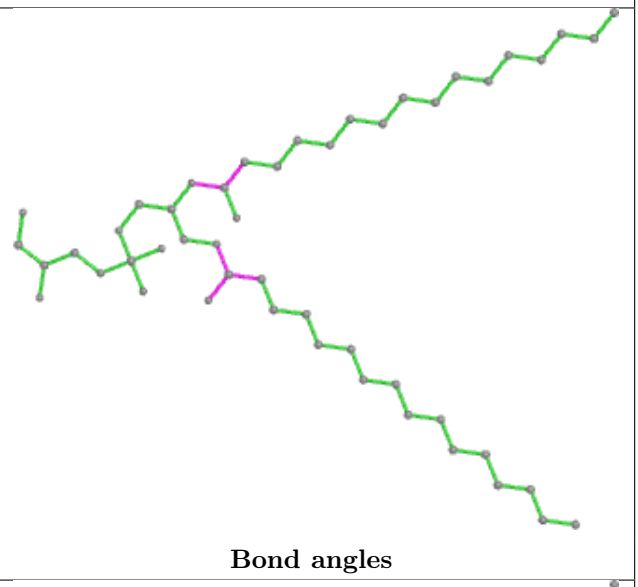


Rings

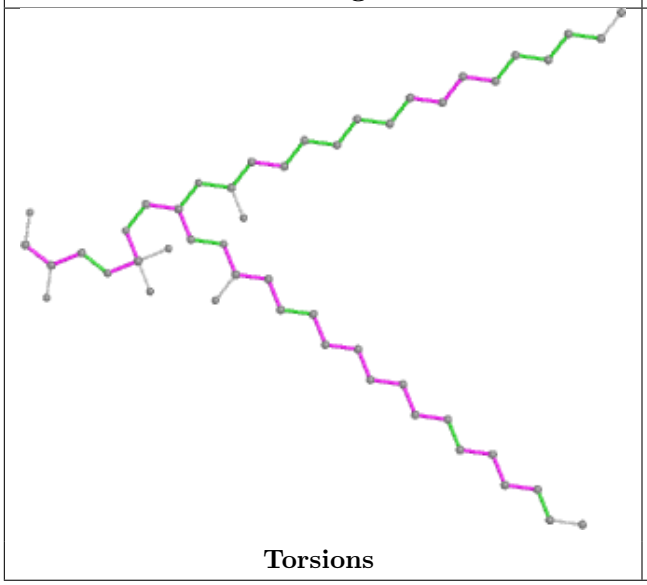
Ligand LHG Y 319



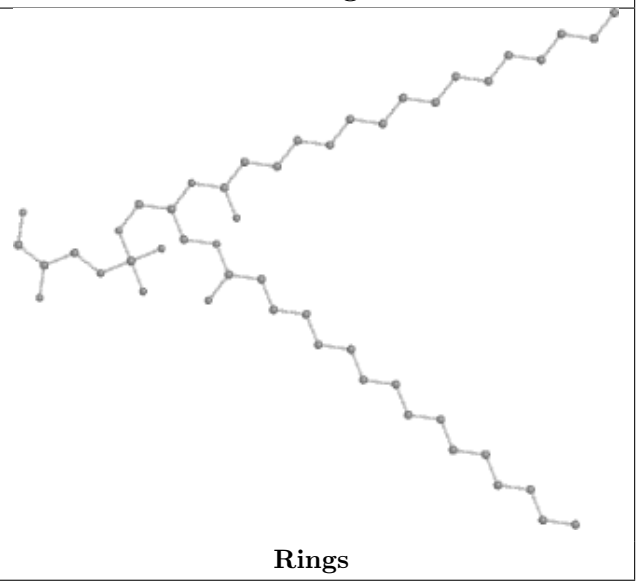
Bond lengths



Bond angles

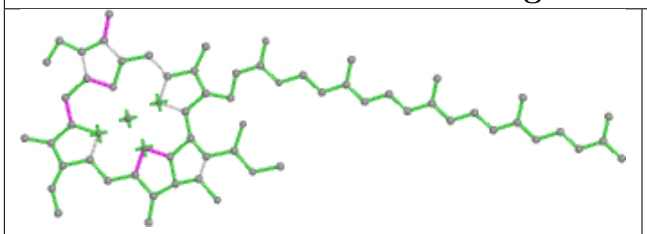


Torsions

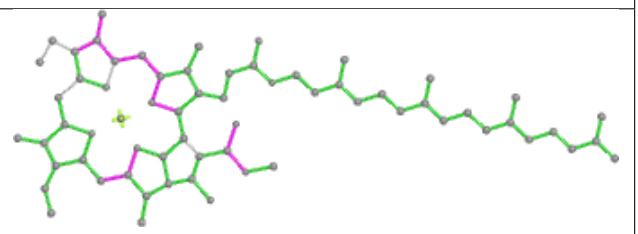


Rings

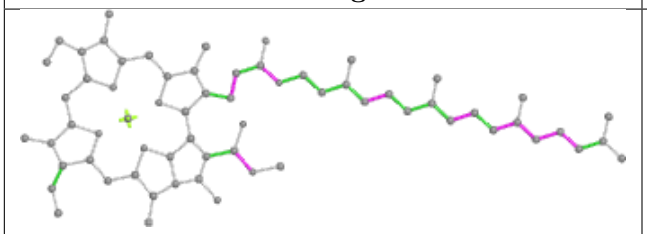
Ligand CLA G 613



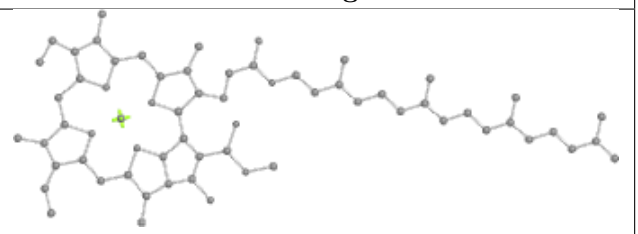
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

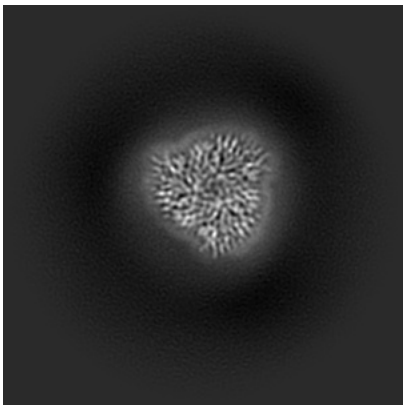
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35784. These allow visual inspection of the internal detail of the map and identification of artifacts.

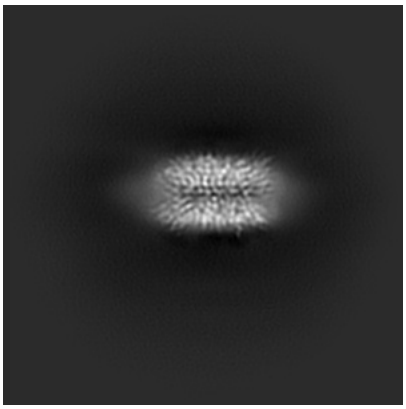
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

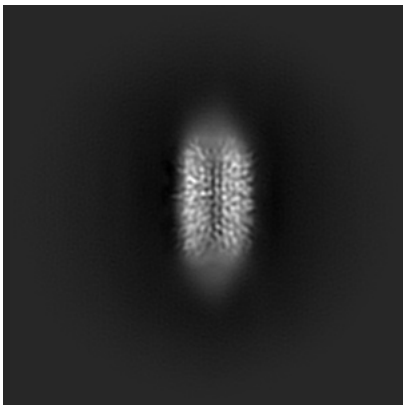
6.1.1 Primary map



X

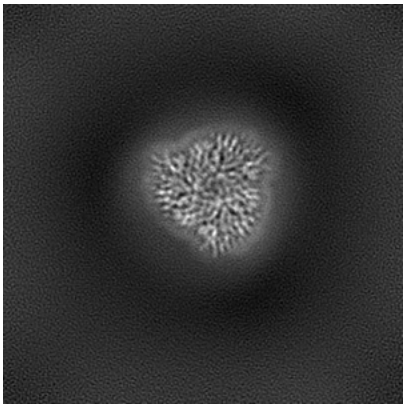


Y

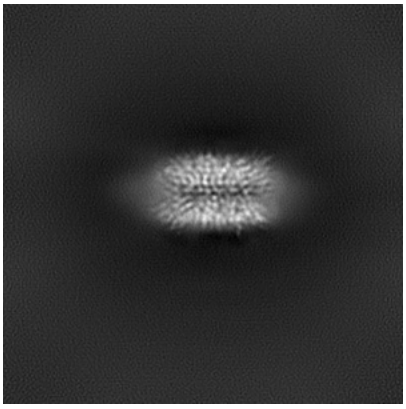


Z

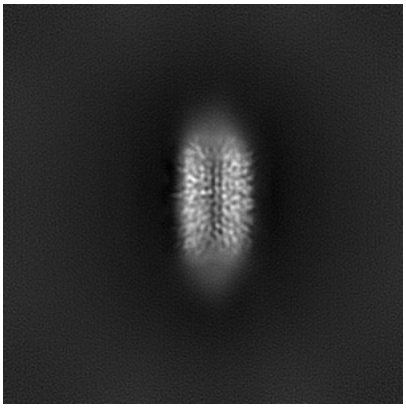
6.1.2 Raw map



X



Y

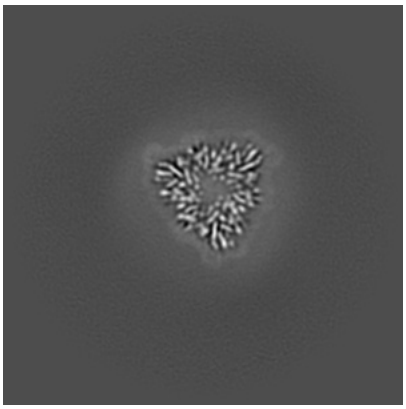


Z

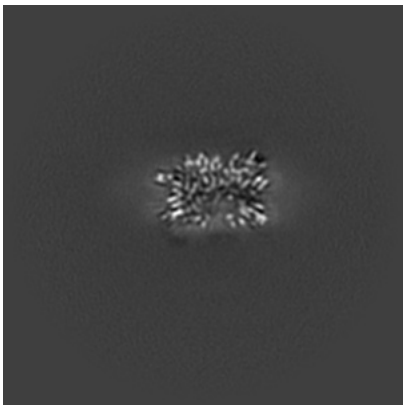
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

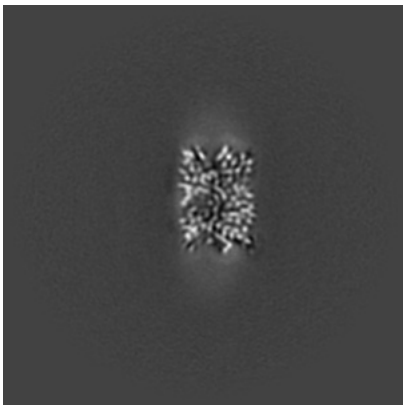
6.2.1 Primary map



X Index: 128

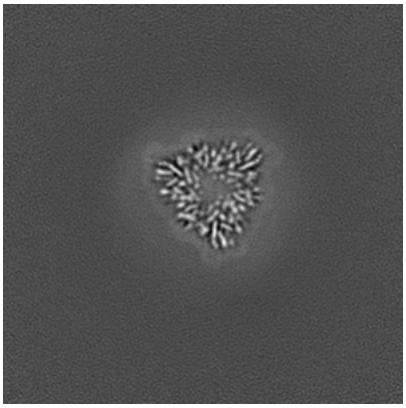


Y Index: 128

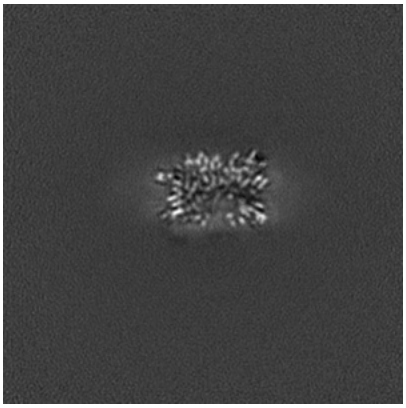


Z Index: 128

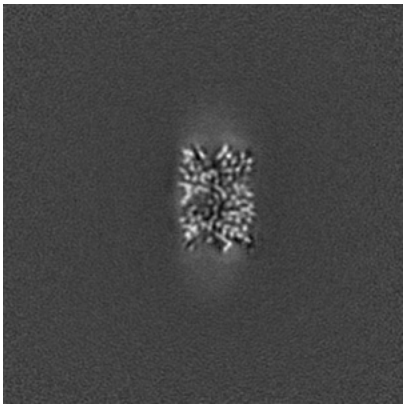
6.2.2 Raw map



X Index: 128



Y Index: 128

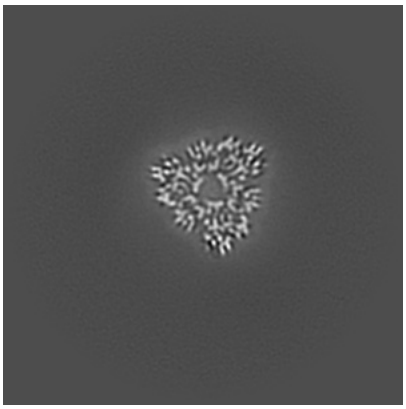


Z Index: 128

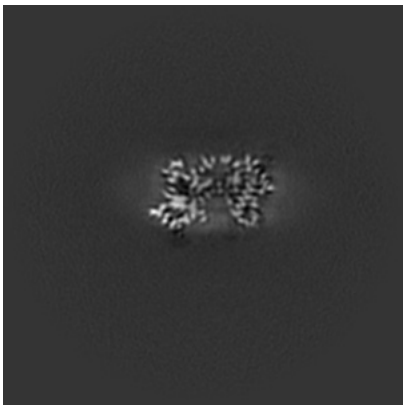
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

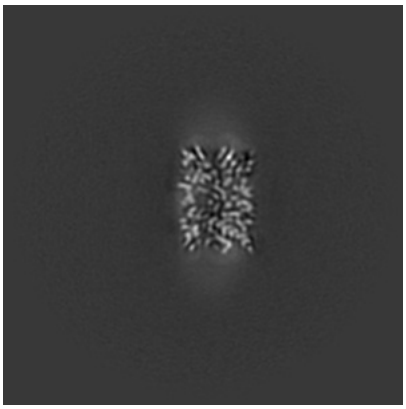
6.3.1 Primary map



X Index: 118

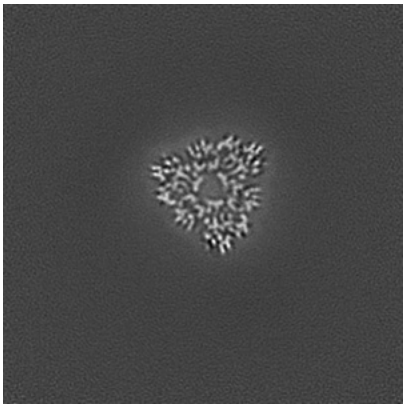


Y Index: 135

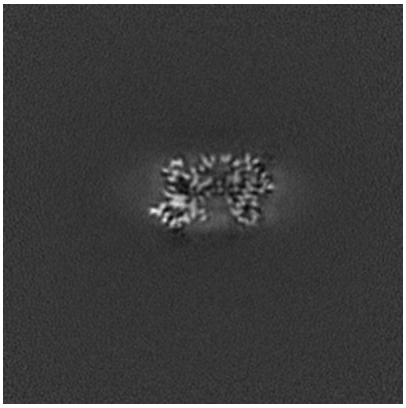


Z Index: 129

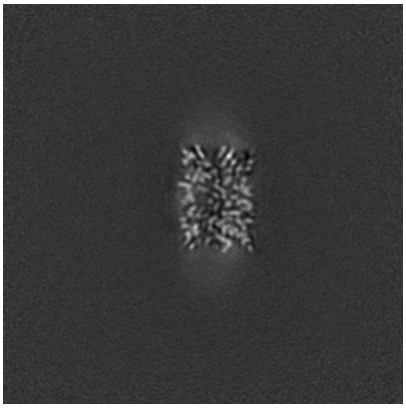
6.3.2 Raw map



X Index: 118



Y Index: 135

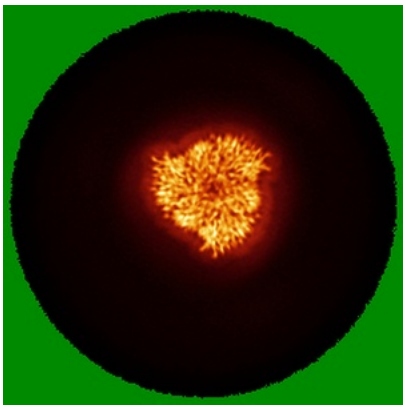


Z Index: 129

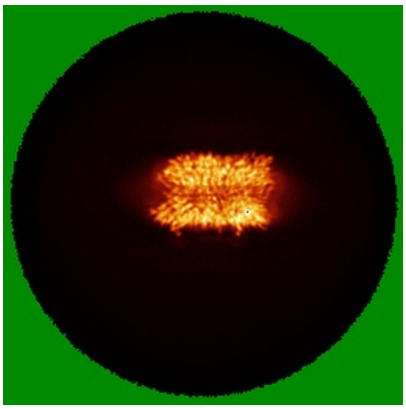
The images above show the largest variance slices of the map in three orthogonal directions.

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

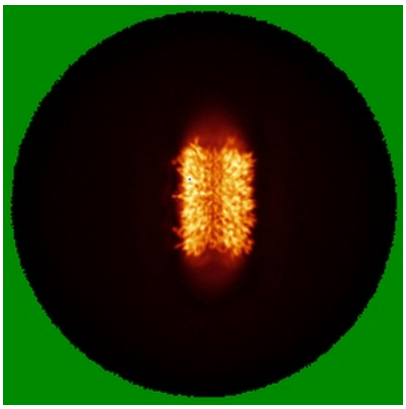
6.4.1 Primary map



X

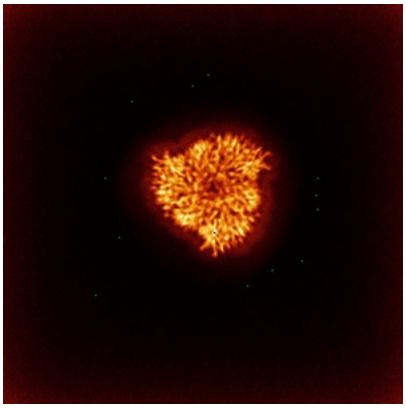


Y

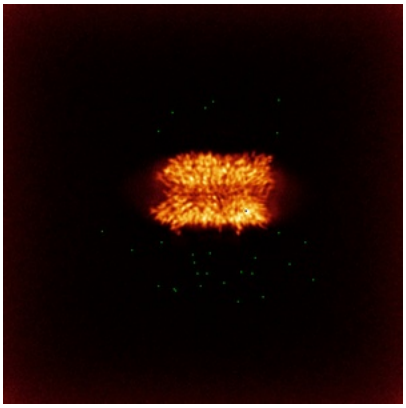


Z

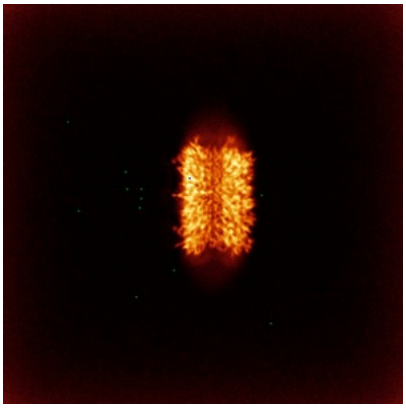
6.4.2 Raw map



X



Y

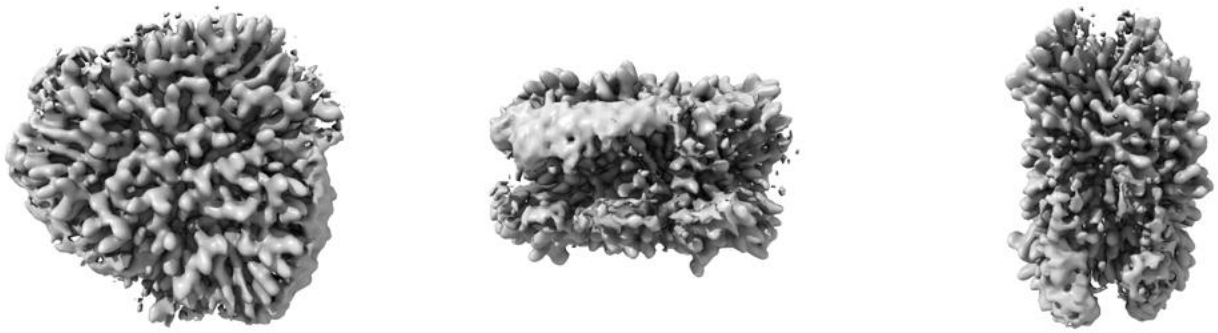


Z

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 0.06. 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.

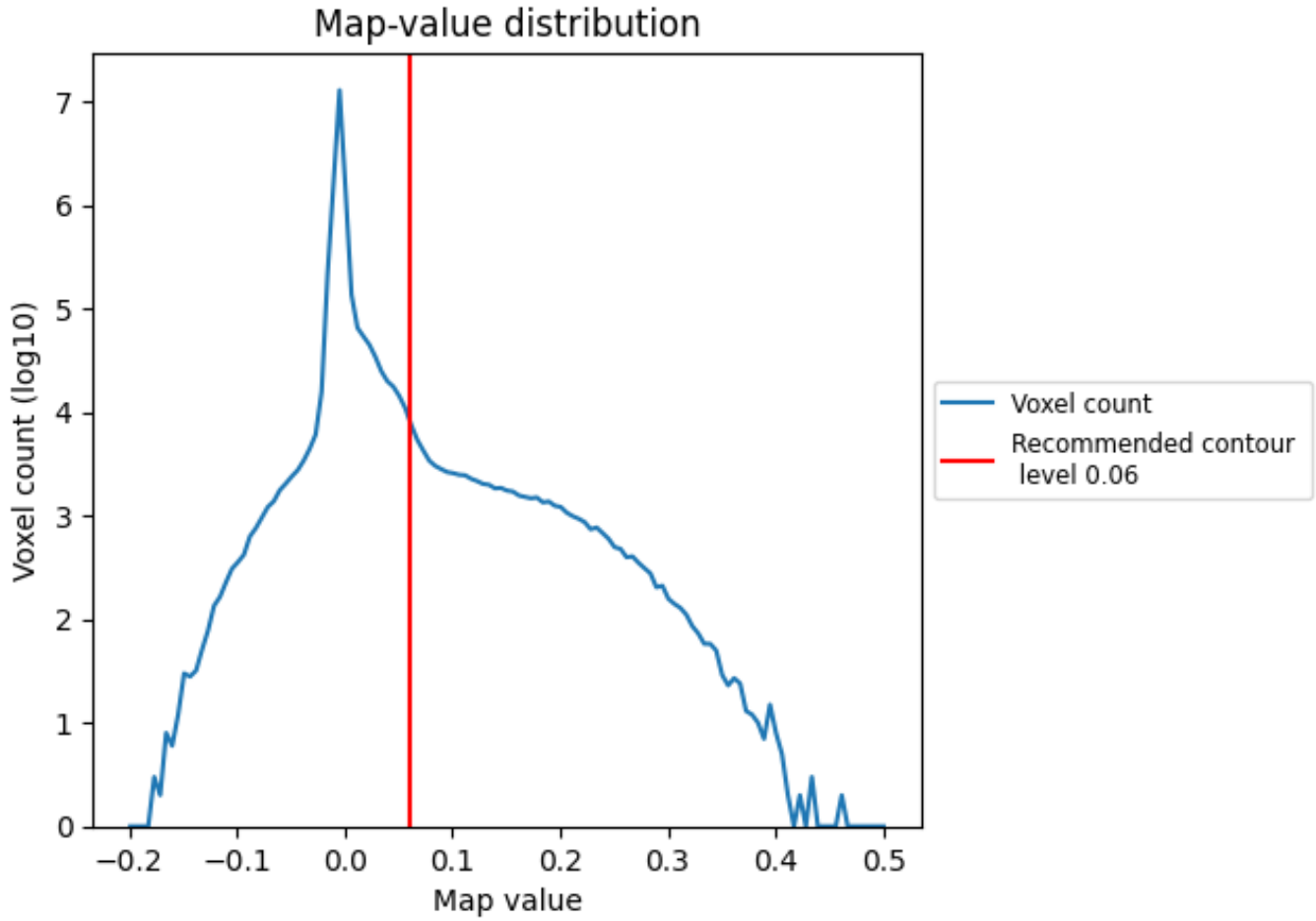
6.6 Mask visualisation (i)

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

7 Map analysis

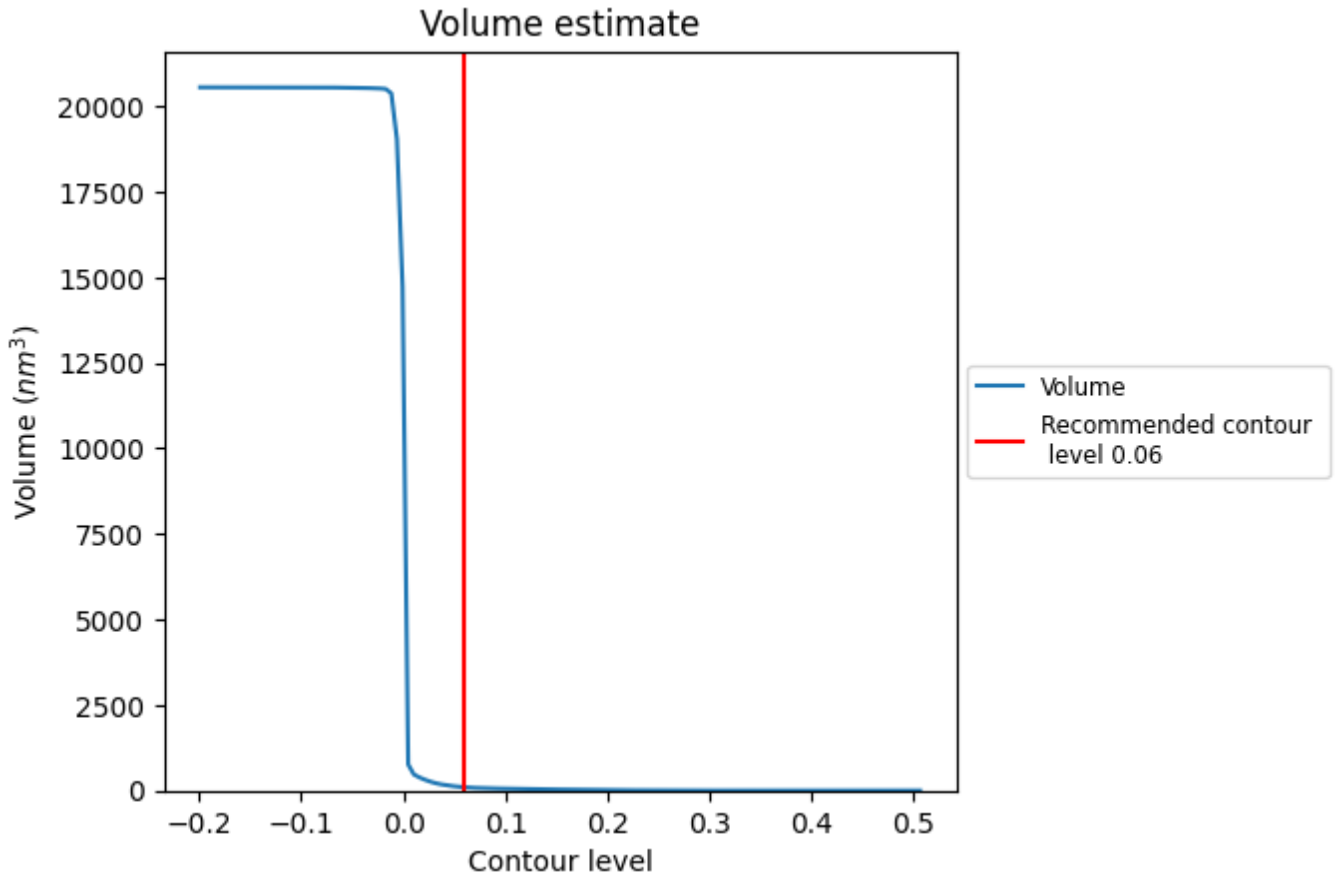
This section contains the results of statistical analysis of the map.

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.

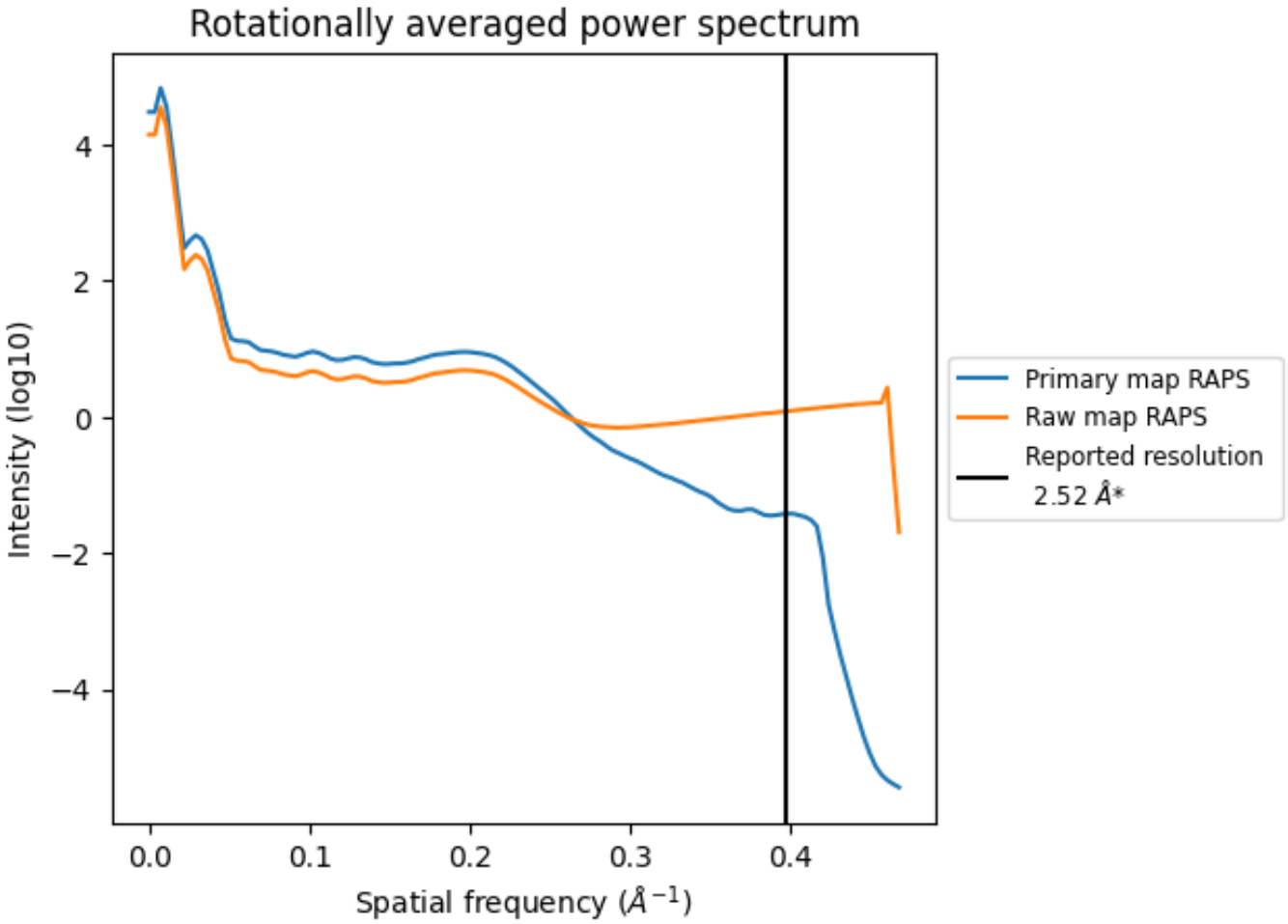
7.2 Volume estimate



The volume at the recommended contour level is 95 nm^3; this corresponds to an approximate mass of 86 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)

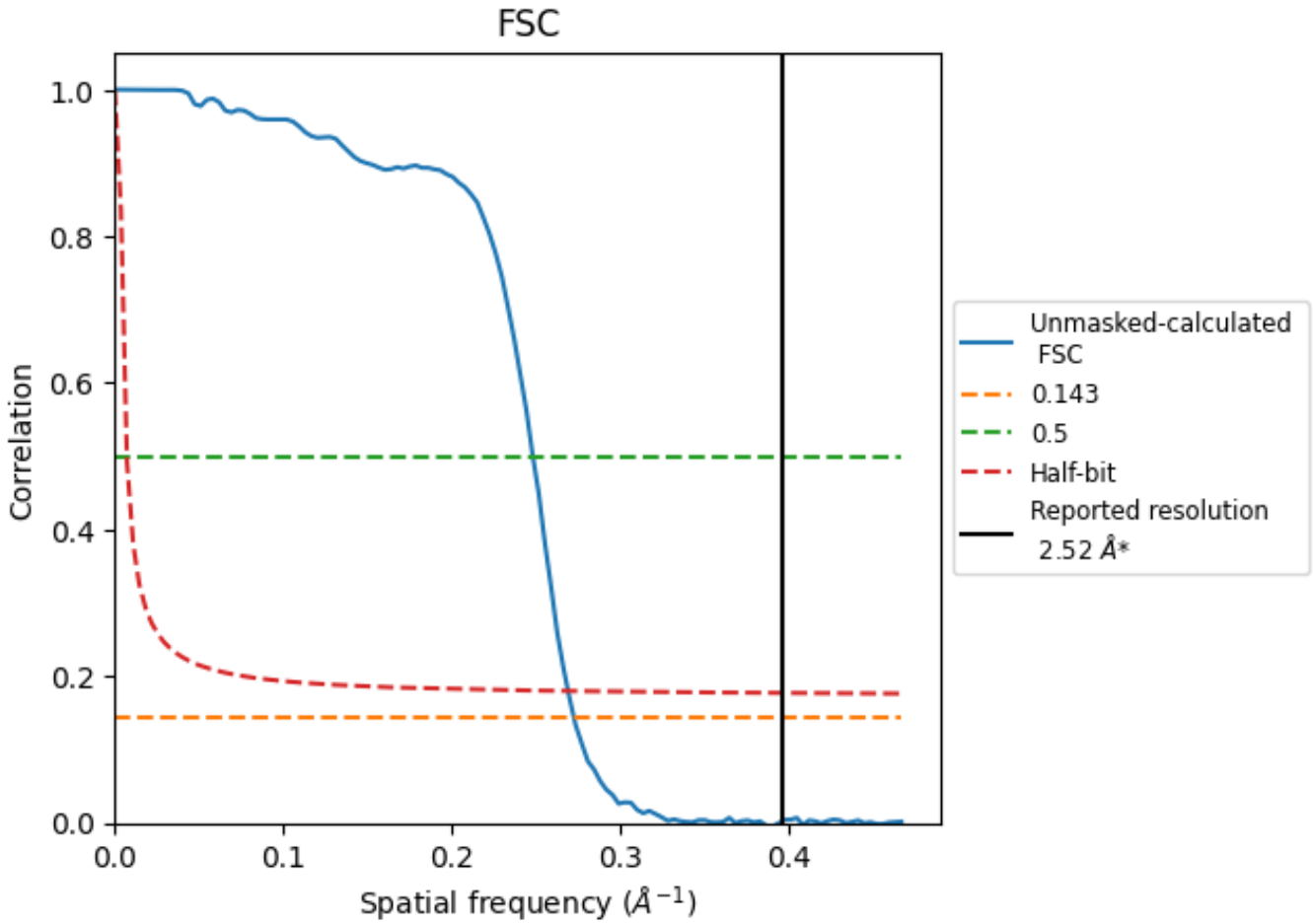


*Reported resolution corresponds to spatial frequency of 0.397 $Å^{-1}$

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 0.397 Å^{-1}

8.2 Resolution estimates (i)

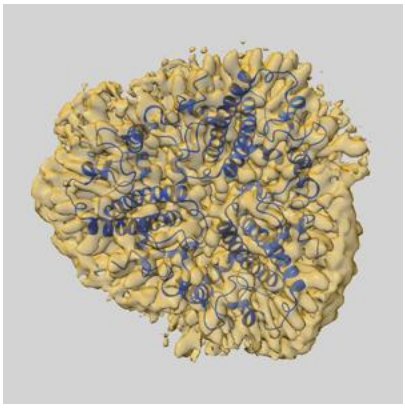
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.67	4.03	3.71

*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 3.67 differs from the reported value 2.52 by more than 10 %

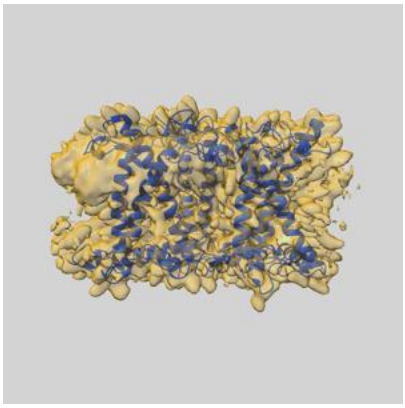
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35784 and PDB model 8IWZ. Per-residue inclusion information can be found in section 3 on page 11.

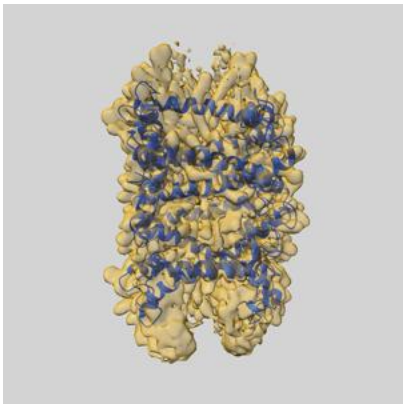
9.1 Map-model overlay



X



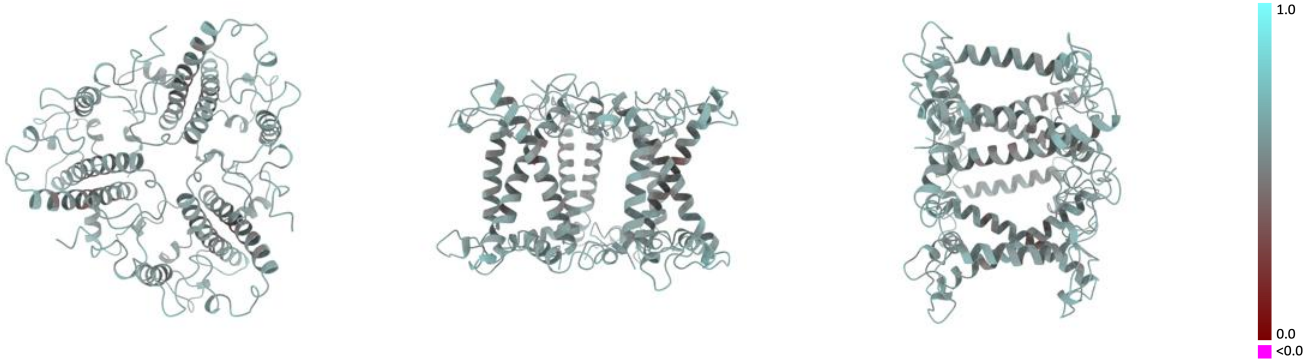
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

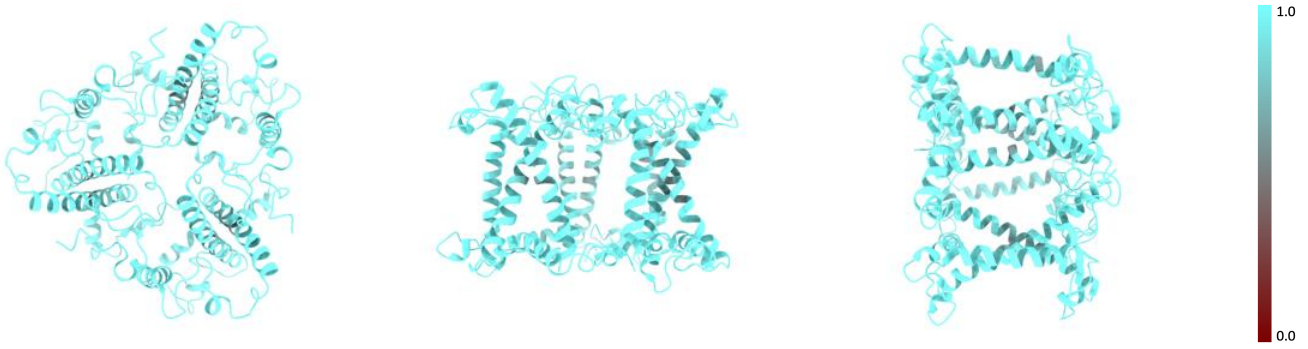
9.2 Q-score mapped to coordinate model



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.

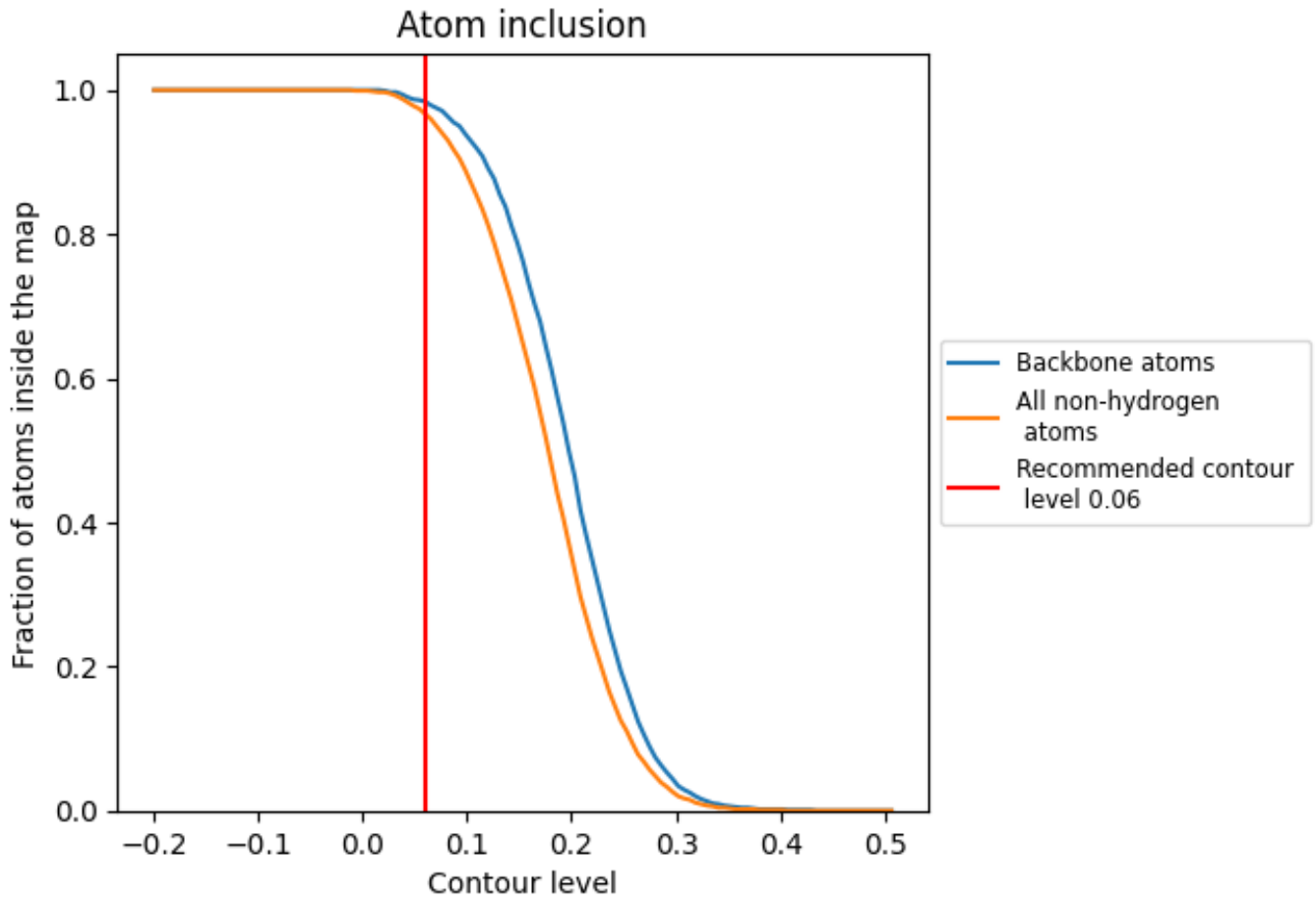
9.3 Atom inclusion mapped to coordinate model



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9670	0.5630
G	0.9630	0.5630
N	0.9710	0.5610
Y	0.9660	0.5650