Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 09:08 PM JST

PDB ID	:	8IX1 / pdb_00008ix1
EMDB ID	:	EMD-35786
Title	:	Cryo-EM structure of protonated LHCII nanodisc at low pH value
Authors	:	Ruan, M.X.; Ding, W.
Deposited on	:	2023-03-31
Resolution	:	2.63 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 (i) 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 (i)) were used in the production of this report:

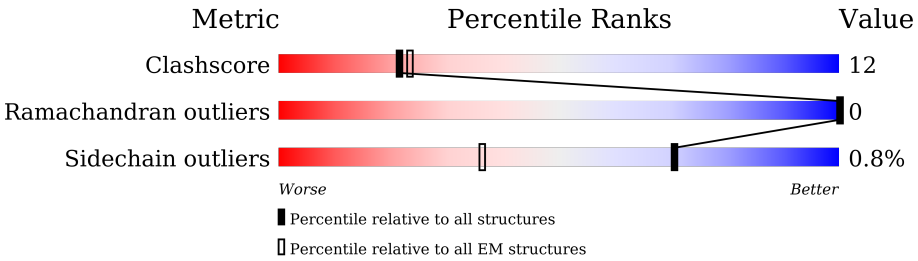
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

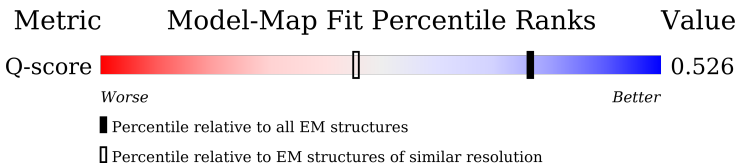
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.63 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8888 (2.13 - 3.13)

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	83% 17% •
1	N	218	83% 17%
1	Y	218	86% 13% •

2 Entry composition (i)

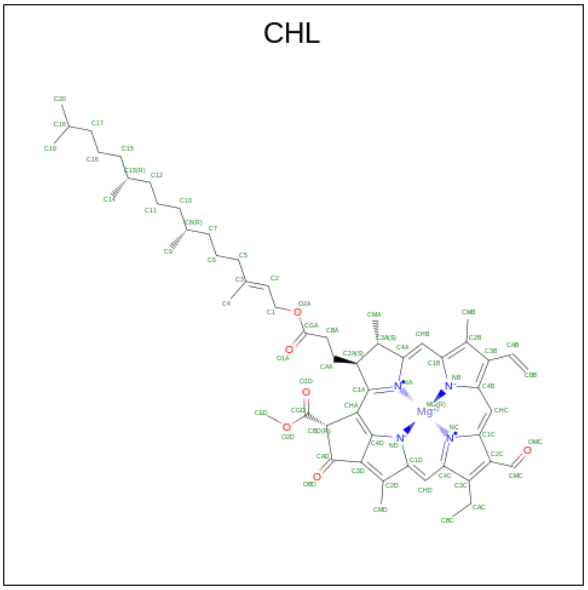
There are 7 unique types of molecules in this entry. The entry contains 7896 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S		
1	G	218	1661	1079	270	305	7	0	0
1	N	218	1661	1079	270	305	7	0	0
1	Y	218	1661	1079	270	305	7	0	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
2	G	1	51	40	1	4	6	0
2	G	1	48	37	1	4	6	0
2	G	1	50	39	1	4	6	0

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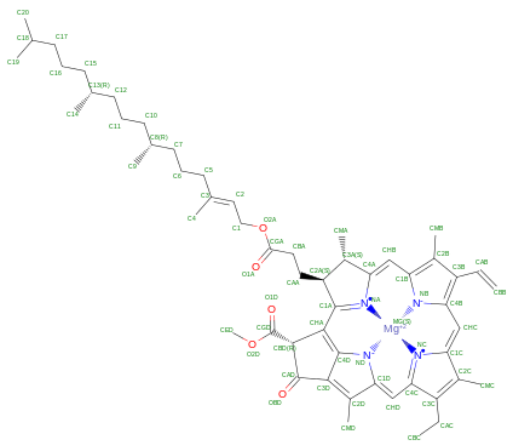
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
2	G	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
2	G	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
2	G	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
2	N	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
2	N	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
2	N	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
2	N	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
2	N	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
2	N	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
2	N	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
2	Y	1	49	38	1	4	6	0
			Total	C	Mg	N	O	
2	Y	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
2	Y	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
2	Y	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
2	Y	1	53	42	1	4	6	0

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

CLA



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

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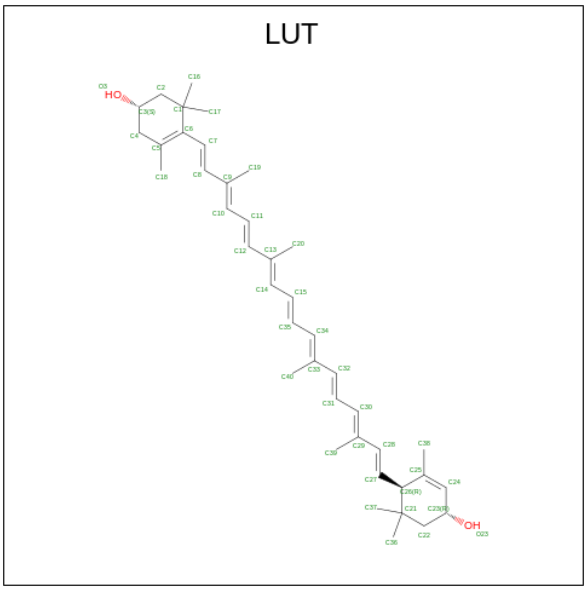
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
3	N	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
3	N	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
3	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
3	Y	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
3	Y	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
3	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
3	Y	1	65	55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

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



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

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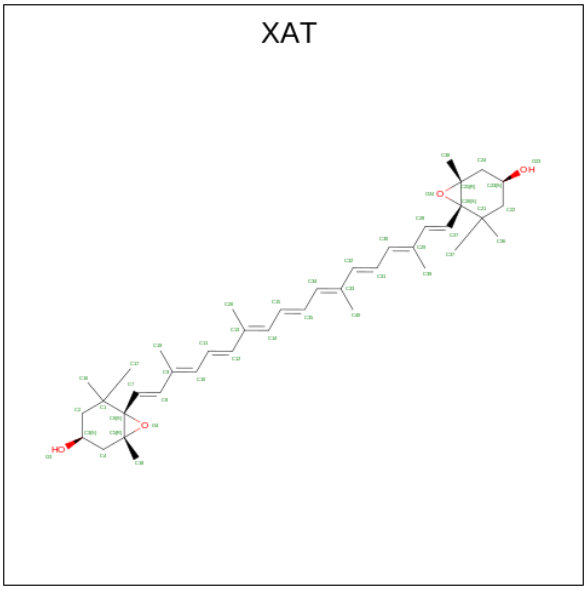
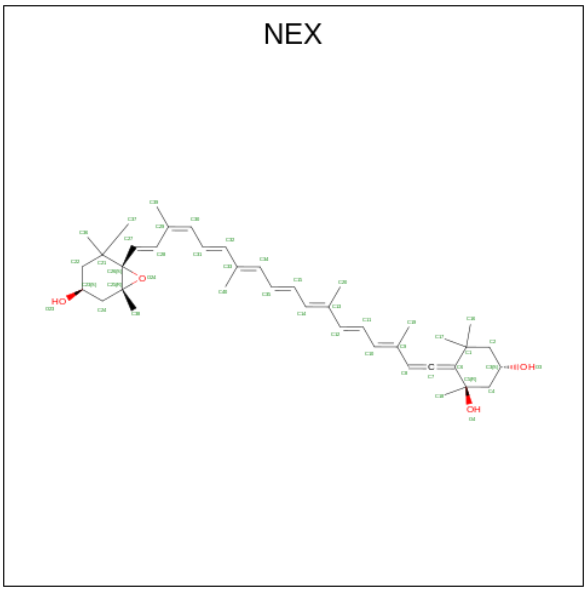
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
4	G	1	42	40	2	0
4	N	1	42	40	2	0
4	N	1	42	40	2	0
4	Y	1	42	40	2	0
4	Y	1	42	40	2	0

- Molecule 5 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 (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



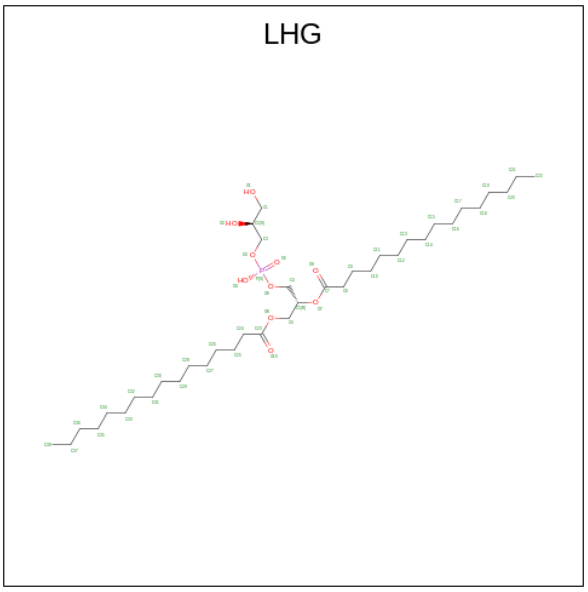
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	G	1	44	40	4	0
5	N	1	44	40	4	0
5	N	1	44	40	4	0

- Molecule 6 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 (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



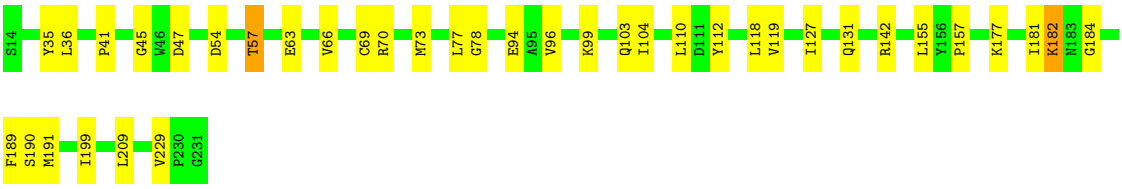
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
7	G	1	49	38	10	1	0
			Total	C	O	P	
7	N	1	49	38	10	1	0
			Total	C	O	P	
7	Y	1	49	38	10	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

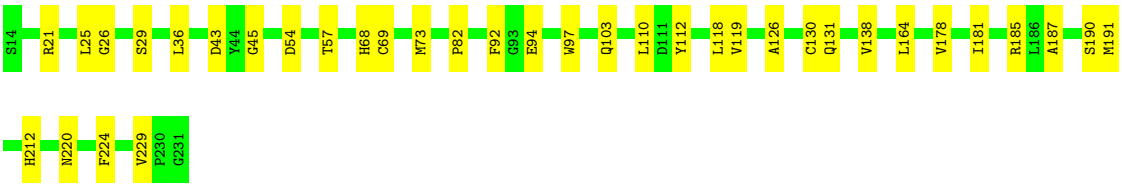
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain G: 83% 17%



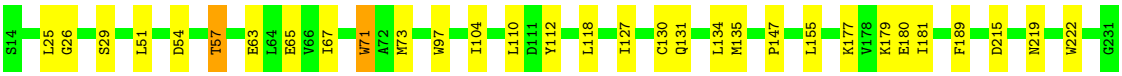
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain N: 83% 17%



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

Chain Y: 86% 13%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	860690	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	0.570	Depositor
Minimum map value	-0.196	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	220.0, 220.0, 220.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, XAT, LHG, CHL, NEX, LUT

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	0.36	0/1713	0.64	0/2333
1	N	0.36	0/1713	0.64	0/2333
1	Y	0.36	0/1713	0.66	0/2333
All	All	0.36	0/5139	0.65	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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1661	0	1591	41	0
1	N	1661	0	1592	28	0
1	Y	1661	0	1592	38	0
2	G	299	0	218	15	0
2	N	349	0	255	8	0
2	Y	250	0	182	14	0
3	G	440	0	411	23	0
3	N	440	0	411	6	0
3	Y	472	0	477	25	0
4	G	84	0	112	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	84	0	112	11	0
4	Y	84	0	112	12	0
5	G	44	0	56	4	0
5	N	88	0	112	6	0
6	G	44	0	56	4	0
6	N	44	0	56	3	0
6	Y	44	0	56	5	0
7	G	49	0	74	4	0
7	N	49	0	74	1	0
7	Y	49	0	74	2	0
All	All	7896	0	7623	182	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (182) 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:Y:54:ASP:HB2	1:Y:57:THR:CG2	1.51	1.39
1:G:54:ASP:HB2	1:G:57:THR:CG2	1.67	1.22
1:Y:54:ASP:HB2	1:Y:57:THR:HG21	1.38	1.04
1:Y:54:ASP:CB	1:Y:57:THR:CG2	2.40	0.99
3:Y:610:CLA:H122	3:Y:611:CLA:HBB1	1.46	0.97
1:Y:135:MET:HE3	2:Y:606:CHL:HMB3	1.49	0.95
1:Y:54:ASP:HB2	1:Y:57:THR:HG23	1.50	0.91
3:Y:609:CLA:H52	4:Y:614:LUT:H30	1.52	0.90
1:G:54:ASP:HB2	1:G:57:THR:HG23	1.50	0.90
1:G:127:ILE:O	1:G:131:GLN:HB2	1.76	0.86
1:Y:54:ASP:HB2	1:Y:57:THR:HG22	1.61	0.82
1:G:54:ASP:HB2	1:G:57:THR:HG21	1.67	0.76
1:Y:135:MET:HE3	2:Y:606:CHL:CMB	2.16	0.75
1:N:164:LEU:HD12	4:N:316:LUT:H222	1.70	0.73
1:G:54:ASP:HB2	1:G:57:THR:HG22	1.71	0.72
3:Y:612:CLA:C2B	4:Y:614:LUT:H183	2.20	0.71
3:Y:612:CLA:HMA3	4:Y:614:LUT:O3	1.91	0.69
1:Y:134:LEU:HD13	2:Y:606:CHL:H12	1.76	0.68
1:N:112:TYR:HB2	1:N:119:VAL:HG22	1.76	0.67
1:N:220:ASN:OD1	1:N:224:PHE:HB2	1.93	0.67
2:G:601:CHL:H42	7:G:618:LHG:H171	1.77	0.67
3:G:609:CLA:HAB	4:G:614:LUT:H32	1.77	0.66
1:N:94:GLU:HB2	1:N:103:GLN:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:187:ALA:O	1:N:191:MET:HG2	1.95	0.66
1:G:131:GLN:HE21	2:G:606:CHL:C4A	2.11	0.64
1:Y:54:ASP:CB	1:Y:57:THR:HG23	2.18	0.63
1:N:126:ALA:HB3	2:N:306:CHL:HMC	1.81	0.63
2:N:301:CHL:HAA2	5:N:321:XAT:H41	1.80	0.63
7:G:618:LHG:H281	7:G:618:LHG:HC91	1.81	0.62
1:Y:135:MET:CE	2:Y:606:CHL:HHB	2.30	0.62
1:Y:147:PRO:HG3	6:Y:616:NEX:H182	1.82	0.61
5:N:318:XAT:H393	7:Y:617:LHG:H101	1.81	0.61
3:G:609:CLA:H2	4:G:614:LUT:H28	1.81	0.60
1:Y:127:ILE:CD1	2:Y:605:CHL:HAC1	2.30	0.60
1:G:41:PRO:HG2	1:G:177:LYS:HD2	1.82	0.60
1:Y:179:LYS:HE2	3:Y:610:CLA:HED1	1.83	0.60
1:Y:135:MET:HE2	2:Y:606:CHL:HHB	1.84	0.59
3:N:311:CLA:H52	4:N:316:LUT:H30	1.85	0.59
1:G:94:GLU:HB2	1:G:103:GLN:HB2	1.84	0.58
1:G:77:LEU:HD22	3:G:609:CLA:H142	1.84	0.57
3:G:611:CLA:HMB3	3:G:611:CLA:H151	1.86	0.57
1:Y:71:TRP:HZ2	6:Y:616:NEX:H391	1.69	0.57
3:G:609:CLA:H122	4:G:614:LUT:H403	1.85	0.57
1:G:157:PRO:HB3	2:G:607:CHL:HBC2	1.86	0.57
1:G:54:ASP:CB	1:G:57:THR:HG23	2.30	0.56
1:N:164:LEU:HD12	4:N:316:LUT:C22	2.34	0.56
1:Y:51:LEU:HD12	3:Y:602:CLA:H11	1.88	0.56
1:Y:54:ASP:CB	1:Y:57:THR:HG22	2.28	0.56
3:G:609:CLA:H2A	3:G:609:CLA:O2D	2.06	0.56
1:G:73:MET:HB2	4:G:614:LUT:C35	2.35	0.56
3:G:602:CLA:H2	4:G:615:LUT:H26	1.88	0.56
1:Y:215:ASP:O	1:Y:219:ASN:ND2	2.39	0.55
3:Y:602:CLA:HAB	4:Y:615:LUT:H30	1.87	0.55
3:Y:610:CLA:HED3	3:Y:610:CLA:HAA1	1.88	0.54
1:G:104:ILE:HB	1:G:110:LEU:HD13	1.90	0.54
1:N:212:HIS:HD1	3:N:314:CLA:HAA2	1.72	0.54
3:Y:609:CLA:H2	4:Y:614:LUT:H28	1.88	0.54
2:G:607:CHL:H11	3:G:609:CLA:HMD2	1.89	0.54
1:G:73:MET:HB2	4:G:614:LUT:C34	2.38	0.53
1:G:110:LEU:HD21	3:G:604:CLA:HAA1	1.90	0.53
1:G:199:ILE:HG22	2:N:301:CHL:H42	1.91	0.53
3:G:604:CLA:H42	6:G:617:NEX:O24	2.09	0.53
1:N:181:ILE:O	1:N:185:ARG:HG3	2.09	0.52
1:G:112:TYR:HB2	1:G:119:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:26:GLY:O	1:N:29:SER:HB3	2.09	0.52
1:G:63:GLU:HA	1:G:155:LEU:HD11	1.92	0.52
3:G:612:CLA:H2A	3:G:612:CLA:HED3	1.92	0.52
1:G:70:ARG:HD2	3:G:609:CLA:C4C	2.40	0.52
1:Y:189:PHE:HE2	3:Y:612:CLA:H93	1.75	0.52
1:Y:63:GLU:HA	1:Y:155:LEU:HD11	1.92	0.52
1:G:209:LEU:HD13	4:G:614:LUT:H163	1.92	0.51
1:Y:54:ASP:O	1:Y:57:THR:HG23	2.10	0.51
1:N:69:CYS:O	1:N:73:MET:HG3	2.11	0.51
1:G:190:SER:HA	3:G:612:CLA:HBB1	1.91	0.50
3:N:313:CLA:HBB1	4:N:316:LUT:C14	2.41	0.50
1:G:96:VAL:HB	1:G:99:LYS:HB2	1.94	0.50
1:G:142:ARG:HA	2:G:607:CHL:C2C	2.41	0.50
1:Y:135:MET:HE1	6:Y:616:NEX:H30	1.94	0.50
1:Y:127:ILE:HD13	2:Y:605:CHL:HAC1	1.94	0.49
1:Y:26:GLY:O	1:Y:29:SER:HB3	2.12	0.49
1:N:164:LEU:CD1	4:N:316:LUT:H222	2.40	0.49
1:G:182:LYS:HB3	3:G:610:CLA:HMD1	1.95	0.49
2:G:608:CHL:H43	2:N:302:CHL:H11	1.95	0.48
1:N:21:ARG:NH1	1:N:43:ASP:O	2.45	0.48
2:N:302:CHL:HHC	2:N:302:CHL:HBB1	1.95	0.48
1:N:112:TYR:HB3	1:N:118:LEU:HD13	1.94	0.48
3:N:312:CLA:H3A	3:N:312:CLA:O1A	2.13	0.47
3:G:602:CLA:H92	3:G:603:CLA:HHB	1.96	0.47
3:N:311:CLA:H141	3:N:311:CLA:H162	1.57	0.47
1:Y:65:GLU:OE1	3:Y:602:CLA:NB	2.47	0.47
6:N:319:NEX:H191	6:N:319:NEX:H11	1.68	0.47
1:G:35:TYR:OH	1:G:47:ASP:OD2	2.30	0.47
1:G:36:LEU:HD12	1:G:45:GLY:HA2	1.96	0.47
1:G:229:VAL:HG11	2:G:619:CHL:HBD	1.96	0.47
1:G:54:ASP:O	1:G:57:THR:HG23	2.14	0.47
1:G:191:MET:HE2	4:G:615:LUT:H10	1.97	0.47
5:N:318:XAT:H15	5:N:318:XAT:H201	1.74	0.47
3:Y:609:CLA:CBB	4:Y:614:LUT:H32	2.44	0.47
1:Y:130:CYS:SG	1:Y:131:GLN:N	2.88	0.47
1:N:54:ASP:HB2	1:N:57:THR:HG23	1.97	0.46
1:G:104:ILE:HG21	2:G:606:CHL:HBC1	1.96	0.46
1:G:131:GLN:HG2	2:G:606:CHL:HMA3	1.96	0.46
1:N:97:TRP:HZ3	4:N:317:LUT:H173	1.81	0.46
1:Y:25:LEU:HB2	1:Y:29:SER:HA	1.97	0.46
1:Y:104:ILE:HB	1:Y:110:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:602:CLA:H93	3:G:602:CLA:H111	1.84	0.46
3:Y:610:CLA:H2	3:Y:611:CLA:C2D	2.46	0.46
3:Y:610:CLA:H92	3:Y:610:CLA:H61	1.71	0.46
7:N:320:LHG:H111	7:N:320:LHG:H281	1.97	0.45
2:Y:605:CHL:CHA	2:Y:605:CHL:HBA1	2.46	0.45
3:Y:612:CLA:H111	3:Y:612:CLA:H152	1.70	0.45
1:N:190:SER:HB3	4:N:316:LUT:H182	1.98	0.45
2:G:601:CHL:HMA1	5:G:616:XAT:H403	1.99	0.45
3:G:609:CLA:H52	4:G:614:LUT:H30	1.99	0.45
1:Y:73:MET:SD	3:Y:609:CLA:HAB	2.57	0.45
3:Y:612:CLA:CMB	4:Y:614:LUT:H183	2.46	0.45
2:G:605:CHL:HBB1	2:G:605:CHL:HHC	1.99	0.45
1:N:229:VAL:HG11	2:N:301:CHL:HBD	1.99	0.45
3:Y:602:CLA:H2	4:Y:615:LUT:H26	1.98	0.45
5:G:616:XAT:H12	7:G:618:LHG:H211	1.98	0.45
1:G:131:GLN:HE21	2:G:606:CHL:CHB	2.29	0.45
1:N:36:LEU:HD12	1:N:45:GLY:HA2	1.99	0.45
1:N:178:VAL:HA	1:N:181:ILE:HG22	1.99	0.44
5:G:616:XAT:H201	5:G:616:XAT:H15	1.65	0.44
1:Y:181:ILE:HD12	1:Y:181:ILE:HA	1.87	0.44
1:Y:222:TRP:HE1	3:Y:613:CLA:HED2	1.83	0.44
1:G:112:TYR:HB3	1:G:118:LEU:HD23	1.98	0.44
1:G:131:GLN:NE2	2:G:606:CHL:CHB	2.80	0.44
2:G:619:CHL:HHD	2:Y:606:CHL:HBC2	1.99	0.44
1:N:68:HIS:HD2	2:N:310:CHL:HMD1	1.82	0.44
4:Y:614:LUT:H31	4:Y:614:LUT:H391	1.85	0.44
3:Y:610:CLA:H171	3:Y:610:CLA:H13	1.47	0.44
1:N:97:TRP:H	1:N:97:TRP:CD1	2.36	0.44
4:N:316:LUT:H31	4:N:316:LUT:H391	1.85	0.44
5:N:321:XAT:H31	5:N:321:XAT:H391	1.81	0.44
2:Y:606:CHL:HMB1	2:Y:608:CHL:HAC1	2.00	0.43
1:G:127:ILE:HD13	1:G:127:ILE:HA	1.76	0.43
4:Y:615:LUT:H15	4:Y:615:LUT:H201	1.88	0.43
1:N:25:LEU:HB2	1:N:29:SER:HA	2.00	0.43
6:Y:616:NEX:H191	6:Y:616:NEX:H11	1.72	0.43
1:G:78:GLY:HA3	3:G:604:CLA:C1C	2.48	0.43
3:G:609:CLA:H62	3:G:609:CLA:H41	1.84	0.43
6:G:617:NEX:H191	6:G:617:NEX:H11	1.67	0.43
3:Y:609:CLA:HBA1	4:Y:614:LUT:H382	2.00	0.43
1:Y:135:MET:CE	2:Y:606:CHL:HMB3	2.34	0.43
5:G:616:XAT:H11	5:G:616:XAT:H191	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:ILE:HD12	1:G:181:ILE:HA	1.91	0.42
1:N:97:TRP:CZ3	4:N:317:LUT:H173	2.54	0.42
4:N:317:LUT:H15	4:N:317:LUT:H201	1.74	0.42
2:Y:606:CHL:HAA1	6:Y:616:NEX:C28	2.48	0.42
1:G:66:VAL:O	1:G:70:ARG:HB2	2.19	0.42
1:G:78:GLY:HA3	3:G:604:CLA:C2C	2.49	0.42
5:N:318:XAT:H35	5:N:318:XAT:H401	1.94	0.42
3:G:609:CLA:H61	3:G:611:CLA:H91	2.00	0.42
7:Y:617:LHG:H242	7:Y:617:LHG:H272	1.71	0.42
3:N:305:CLA:C1C	6:N:319:NEX:H222	2.50	0.42
1:Y:54:ASP:C	1:Y:57:THR:HG23	2.45	0.42
3:Y:610:CLA:HBA2	3:Y:611:CLA:HMD3	2.02	0.42
1:N:103:GLN:HG2	1:N:110:LEU:HA	2.02	0.42
4:G:615:LUT:H35	4:G:615:LUT:H401	1.83	0.42
2:Y:607:CHL:HBB1	2:Y:607:CHL:HHC	2.02	0.42
1:G:69:CYS:HB3	1:G:184:GLY:HA3	2.02	0.41
6:G:617:NEX:H35	6:G:617:NEX:H401	1.82	0.41
1:G:189:PHE:HZ	7:G:618:LHG:H141	1.85	0.41
3:G:609:CLA:H121	3:G:611:CLA:H203	2.03	0.41
1:N:138:VAL:HG23	6:N:319:NEX:H201	2.01	0.41
1:N:82:PRO:HB3	1:N:92:PHE:HE2	1.85	0.41
1:N:130:CYS:SG	1:N:131:GLN:N	2.93	0.41
3:Y:609:CLA:H141	3:Y:609:CLA:H161	1.84	0.41
1:Y:67:ILE:HD13	1:Y:67:ILE:HA	1.94	0.41
1:Y:127:ILE:HD11	2:Y:605:CHL:HAC1	2.01	0.41
5:N:318:XAT:H11	5:N:318:XAT:H191	1.85	0.41
1:Y:97:TRP:CD1	1:Y:97:TRP:H	2.38	0.41
1:Y:177:LYS:HA	1:Y:180:GLU:HG2	2.03	0.41
4:G:614:LUT:H31	4:G:614:LUT:H391	1.85	0.41
1:Y:112:TYR:HB3	1:Y:118:LEU:HD23	2.03	0.41
3:Y:610:CLA:H152	3:Y:611:CLA:CBB	2.51	0.40
4:N:317:LUT:H35	4:N:317:LUT:H401	1.83	0.40
3:Y:602:CLA:H52	4:Y:615:LUT:H28	2.04	0.40
3:G:602:CLA:HBA1	4:G:615:LUT:H382	2.03	0.40
2:G:606:CHL:HMC	2:N:301:CHL:CHD	2.51	0.40
6:G:617:NEX:H201	6:G:617:NEX:H15	1.74	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%)	208 (96%)	8 (4%)	0	100	100
1	N	216/218 (99%)	205 (95%)	11 (5%)	0	100	100
1	Y	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
All	All	648/654 (99%)	620 (96%)	28 (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%)	166 (99%)	2 (1%)	63	78
1	N	168/168 (100%)	168 (100%)	0	100	100
1	Y	168/168 (100%)	166 (99%)	2 (1%)	63	78
All	All	504/504 (100%)	500 (99%)	4 (1%)	70	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	57	THR
1	G	182	LYS
1	Y	57	THR
1	Y	71	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	131	GLN
1	N	88	ASN
1	N	120	HIS
1	N	197	GLN
1	N	208	ASN
1	Y	61	ASN
1	Y	68	HIS
1	Y	197	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	LUT	G	615	-	42,43,43	0.78	0	51,60,60	1.77	17 (33%)
2	CHL	G	608	1	54,58,74	1.47	10 (18%)	59,94,114	1.67	12 (20%)
2	CHL	N	309	-	54,58,74	1.41	7 (12%)	59,94,114	1.34	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	XAT	G	616	-	39,47,47	0.96	2 (5%)	54,74,74	2.79	17 (31%)
3	CLA	Y	602	1	69,73,73	1.26	6 (8%)	83,113,113	1.23	10 (12%)
5	XAT	N	318	-	39,47,47	0.92	0	54,74,74	2.81	22 (40%)
5	XAT	N	321	-	39,47,47	0.98	2 (5%)	54,74,74	2.83	19 (35%)
3	CLA	Y	613	-	53,57,73	1.43	6 (11%)	62,93,113	1.41	9 (14%)
6	NEX	G	617	-	38,46,46	1.10	2 (5%)	50,70,70	2.98	17 (34%)
2	CHL	Y	608	1	57,61,74	1.34	9 (15%)	64,98,114	1.57	6 (9%)
3	CLA	G	610	-	53,57,73	1.39	9 (16%)	62,93,113	1.43	6 (9%)
3	CLA	N	311	1	69,73,73	1.26	7 (10%)	83,113,113	1.15	5 (6%)
2	CHL	Y	605	-	52,56,74	1.41	8 (15%)	58,92,114	1.49	7 (12%)
2	CHL	Y	601	-	53,57,74	1.42	7 (13%)	59,93,114	1.27	7 (11%)
2	CHL	N	301	-	54,58,74	1.43	7 (12%)	59,94,114	1.41	10 (16%)
6	NEX	N	319	-	38,46,46	0.91	1 (2%)	50,70,70	2.35	17 (34%)
3	CLA	G	602	1	69,73,73	1.26	6 (8%)	83,113,113	1.22	6 (7%)
3	CLA	Y	609	1	69,73,73	1.26	7 (10%)	83,113,113	1.36	10 (12%)
2	CHL	G	601	-	55,59,74	1.40	7 (12%)	62,96,114	1.19	7 (11%)
3	CLA	Y	610	7	69,73,73	1.23	8 (11%)	83,113,113	1.19	9 (10%)
2	CHL	N	310	-	54,58,74	1.40	7 (12%)	59,94,114	1.34	7 (11%)
2	CHL	G	606	-	54,58,74	1.39	8 (14%)	59,94,114	1.39	6 (10%)
2	CHL	N	302	-	54,58,74	1.43	8 (14%)	59,94,114	1.23	7 (11%)
3	CLA	Y	611	-	69,73,73	1.38	8 (11%)	83,113,113	1.15	5 (6%)
3	CLA	G	604	-	53,57,73	1.42	7 (13%)	62,93,113	1.33	8 (12%)
7	LHG	Y	617	3	48,48,48	0.88	2 (4%)	51,54,54	1.03	1 (1%)
3	CLA	G	609	1	69,73,73	1.23	9 (13%)	83,113,113	1.33	8 (9%)
3	CLA	N	314	-	53,57,73	1.42	9 (16%)	62,93,113	1.30	6 (9%)
3	CLA	Y	603	-	53,57,73	1.43	8 (15%)	62,93,113	1.45	6 (9%)
3	CLA	Y	604	-	53,57,73	1.42	9 (16%)	62,93,113	1.38	8 (12%)
2	CHL	Y	606	-	54,58,74	1.39	9 (16%)	59,94,114	1.26	4 (6%)
4	LUT	Y	615	-	42,43,43	0.79	0	51,60,60	1.70	15 (29%)
2	CHL	Y	607	-	54,58,74	1.45	8 (14%)	59,94,114	1.44	6 (10%)
7	LHG	G	618	-	48,48,48	0.93	2 (4%)	51,54,54	0.93	2 (3%)
2	CHL	G	605	1	52,56,74	1.41	7 (13%)	58,92,114	1.74	11 (18%)
6	NEX	Y	616	-	38,46,46	0.91	1 (2%)	50,70,70	2.48	16 (32%)
3	CLA	N	303	1	69,73,73	1.28	8 (11%)	83,113,113	1.12	7 (8%)
3	CLA	N	315	1	53,57,73	1.44	7 (13%)	62,93,113	1.18	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CLA	G	603	-	53,57,73	1.43	7 (13%)	62,93,113	1.47	5 (8%)
4	LUT	N	316	-	42,43,43	1.58	8 (19%)	51,60,60	1.48	10 (19%)
2	CHL	N	306	-	52,56,74	1.40	7 (13%)	58,92,114	1.51	9 (15%)
4	LUT	Y	614	-	42,43,43	1.58	8 (19%)	51,60,60	1.49	10 (19%)
2	CHL	G	607	-	54,58,74	1.41	9 (16%)	59,94,114	1.66	8 (13%)
3	CLA	G	613	1	53,57,73	1.46	8 (15%)	62,93,113	1.18	7 (11%)
3	CLA	N	305	-	53,57,73	1.43	9 (16%)	62,93,113	1.32	7 (11%)
4	LUT	N	317	-	42,43,43	0.97	1 (2%)	51,60,60	2.08	11 (21%)
3	CLA	G	611	1	69,73,73	1.25	10 (14%)	83,113,113	1.27	10 (12%)
4	LUT	G	614	-	42,43,43	1.58	8 (19%)	51,60,60	1.50	10 (19%)
7	LHG	N	320	3	48,48,48	0.88	2 (4%)	51,54,54	1.12	4 (7%)
2	CHL	N	308	-	55,59,74	1.42	6 (10%)	62,96,114	1.29	5 (8%)
2	CHL	G	619	-	54,58,74	1.42	8 (14%)	59,94,114	1.38	8 (13%)
3	CLA	G	612	-	53,57,73	1.42	8 (15%)	62,93,113	1.30	7 (11%)
3	CLA	N	304	-	53,57,73	1.45	7 (13%)	62,93,113	1.40	6 (9%)
3	CLA	N	312	7	53,57,73	1.41	7 (13%)	62,93,113	1.38	5 (8%)
3	CLA	Y	612	-	69,73,73	1.28	9 (13%)	83,113,113	1.20	7 (8%)
2	CHL	N	307	-	54,58,74	1.46	8 (14%)	59,94,114	1.47	7 (11%)
3	CLA	N	313	1	69,73,73	1.24	9 (13%)	83,113,113	1.20	8 (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
4	LUT	G	615	-	-	2/29/67/67	0/2/2/2
2	CHL	G	608	1	-	8/22/98/117	-
2	CHL	N	309	-	-	6/22/98/117	-
5	XAT	G	616	-	-	2/31/93/93	0/4/4/4
3	CLA	Y	602	1	-	14/39/115/115	-
5	XAT	N	318	-	-	1/31/93/93	0/4/4/4
5	XAT	N	321	-	-	6/31/93/93	0/4/4/4
3	CLA	Y	613	-	-	10/20/96/115	-
6	NEX	G	617	-	-	7/27/83/83	0/3/3/3
2	CHL	Y	608	1	-	12/26/102/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	G	610	-	-	9/20/96/115	-
3	CLA	N	311	1	-	13/39/115/115	-
2	CHL	Y	605	-	-	14/20/96/117	-
2	CHL	Y	601	-	-	3/21/97/117	-
2	CHL	N	301	-	-	10/22/98/117	-
6	NEX	N	319	-	-	6/27/83/83	0/3/3/3
3	CLA	G	602	1	-	15/39/115/115	-
3	CLA	Y	609	1	-	12/39/115/115	-
2	CHL	G	601	-	-	3/23/99/117	-
3	CLA	Y	610	7	-	16/39/115/115	-
2	CHL	N	310	-	-	7/22/98/117	-
2	CHL	G	606	-	-	6/22/98/117	-
2	CHL	N	302	-	-	6/22/98/117	-
3	CLA	Y	611	-	-	13/39/115/115	-
3	CLA	G	604	-	-	10/20/96/115	-
7	LHG	Y	617	3	-	22/53/53/53	-
3	CLA	G	609	1	-	15/39/115/115	-
3	CLA	N	314	-	-	10/20/96/115	-
3	CLA	Y	603	-	-	5/20/96/115	-
3	CLA	Y	604	-	-	8/20/96/115	-
2	CHL	Y	606	-	-	14/22/98/117	-
4	LUT	Y	615	-	-	1/29/67/67	0/2/2/2
2	CHL	Y	607	-	-	9/22/98/117	-
7	LHG	G	618	-	-	7/53/53/53	-
2	CHL	G	605	1	-	6/20/96/117	-
6	NEX	Y	616	-	-	3/27/83/83	0/3/3/3
3	CLA	N	303	1	-	11/39/115/115	-
3	CLA	N	315	1	-	12/20/96/115	-
3	CLA	G	603	-	-	6/20/96/115	-
4	LUT	N	316	-	-	7/29/67/67	0/2/2/2
2	CHL	N	306	-	-	6/20/96/117	-
4	LUT	Y	614	-	-	7/29/67/67	0/2/2/2
2	CHL	G	607	-	-	8/22/98/117	-
3	CLA	G	613	1	-	8/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	N	305	-	-	8/20/96/115	-
4	LUT	N	317	-	-	3/29/67/67	0/2/2/2
3	CLA	G	611	1	-	22/39/115/115	-
4	LUT	G	614	-	-	7/29/67/67	0/2/2/2
7	LHG	N	320	3	-	27/53/53/53	-
2	CHL	N	308	-	-	5/23/99/117	-
2	CHL	G	619	-	-	8/22/98/117	-
3	CLA	G	612	-	-	10/20/96/115	-
3	CLA	N	304	-	-	12/20/96/115	-
3	CLA	N	312	7	-	10/20/96/115	-
3	CLA	Y	612	-	-	15/39/115/115	-
2	CHL	N	307	-	-	4/22/98/117	-
3	CLA	N	313	1	-	12/39/115/115	-

All (367) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	611	CLA	MG-NB	-4.80	1.96	2.05
2	Y	607	CHL	C1D-ND	4.19	1.42	1.37
7	G	618	LHG	O8-C23	4.15	1.45	1.33
7	G	618	LHG	O7-C7	4.12	1.45	1.34
3	Y	602	CLA	C1D-ND	4.06	1.42	1.37
3	G	613	CLA	C1D-ND	4.04	1.42	1.37
3	Y	611	CLA	C1D-ND	4.04	1.42	1.37
2	G	605	CHL	C4B-NB	3.97	1.42	1.37
2	G	608	CHL	C1D-ND	3.97	1.42	1.37
2	N	308	CHL	C1D-ND	3.96	1.42	1.37
3	N	304	CLA	C1D-ND	3.94	1.42	1.37
3	N	315	CLA	C1D-ND	3.90	1.42	1.37
7	N	320	LHG	O8-C23	3.89	1.44	1.33
2	N	302	CHL	C1D-ND	3.89	1.42	1.37
2	N	309	CHL	C1D-ND	3.88	1.42	1.37
3	G	613	CLA	C4B-NB	3.87	1.42	1.37
2	N	307	CHL	C4B-NB	3.87	1.42	1.37
7	Y	617	LHG	O8-C23	3.85	1.44	1.33
2	N	306	CHL	C1D-ND	3.85	1.42	1.37
3	Y	603	CLA	C1D-ND	3.82	1.42	1.37
2	G	601	CHL	C4B-NB	3.81	1.42	1.37
3	N	303	CLA	C1D-ND	3.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	612	CLA	C4B-NB	3.81	1.42	1.37
7	N	320	LHG	O7-C7	3.78	1.45	1.34
2	N	301	CHL	C1D-ND	3.78	1.42	1.37
3	N	304	CLA	C4B-NB	3.78	1.42	1.37
7	Y	617	LHG	O7-C7	3.77	1.44	1.34
3	Y	613	CLA	C1D-ND	3.76	1.42	1.37
3	G	602	CLA	C1D-ND	3.75	1.42	1.37
2	Y	601	CHL	C1D-ND	3.74	1.42	1.37
3	G	603	CLA	C4B-NB	3.74	1.42	1.37
2	Y	601	CHL	C4B-NB	3.74	1.42	1.37
3	N	303	CLA	C4B-NB	3.74	1.42	1.37
2	G	607	CHL	C1D-ND	3.72	1.42	1.37
3	N	305	CLA	C1D-ND	3.72	1.42	1.37
2	G	606	CHL	C1D-ND	3.71	1.42	1.37
3	G	612	CLA	C1D-ND	3.71	1.42	1.37
3	Y	609	CLA	C1D-ND	3.69	1.42	1.37
3	N	313	CLA	C1D-ND	3.68	1.42	1.37
2	G	619	CHL	C1D-ND	3.68	1.42	1.37
3	G	604	CLA	C1D-ND	3.67	1.42	1.37
2	N	307	CHL	C3B-C4B	3.65	1.51	1.42
2	N	302	CHL	C3B-C4B	3.65	1.51	1.42
3	N	305	CLA	C4B-NB	3.65	1.42	1.37
3	Y	603	CLA	C4B-NB	3.65	1.42	1.37
3	N	315	CLA	C4B-NB	3.64	1.42	1.37
3	Y	610	CLA	C4D-ND	-3.64	1.32	1.37
2	N	308	CHL	C4B-NB	3.63	1.42	1.37
2	G	607	CHL	C3B-C4B	3.62	1.51	1.42
3	G	609	CLA	C1D-ND	3.62	1.42	1.37
3	Y	604	CLA	C1D-ND	3.62	1.42	1.37
3	G	603	CLA	C1D-ND	3.61	1.42	1.37
3	Y	612	CLA	C1D-ND	3.61	1.42	1.37
2	N	302	CHL	C4B-NB	3.61	1.42	1.37
2	N	307	CHL	C1D-ND	3.61	1.42	1.37
2	N	309	CHL	C3B-C4B	3.60	1.51	1.42
2	G	605	CHL	C1D-ND	3.60	1.42	1.37
2	Y	606	CHL	C1D-ND	3.60	1.42	1.37
3	G	612	CLA	C4B-NB	3.60	1.42	1.37
2	G	601	CHL	C1D-ND	3.60	1.42	1.37
2	G	619	CHL	C3B-C4B	3.58	1.51	1.42
3	Y	611	CLA	C4B-NB	3.56	1.42	1.37
3	G	611	CLA	C1D-ND	3.55	1.42	1.37
3	N	312	CLA	C1D-ND	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	308	CHL	C3B-C4B	3.52	1.51	1.42
3	N	314	CLA	C1D-ND	3.51	1.42	1.37
3	Y	604	CLA	C4B-NB	3.51	1.42	1.37
2	N	301	CHL	C3B-C4B	3.50	1.50	1.42
3	Y	602	CLA	C4B-NB	3.50	1.42	1.37
3	Y	613	CLA	C4B-NB	3.50	1.42	1.37
2	Y	605	CHL	C4D-ND	-3.48	1.32	1.37
2	G	601	CHL	C3B-C4B	3.48	1.50	1.42
2	N	309	CHL	C4B-NB	3.46	1.42	1.37
3	N	312	CLA	C4B-NB	3.45	1.42	1.37
2	Y	607	CHL	C3B-C4B	3.45	1.50	1.42
3	N	311	CLA	C4D-ND	-3.44	1.33	1.37
3	G	602	CLA	C4B-NB	3.44	1.42	1.37
4	Y	614	LUT	C10-C9	3.43	1.40	1.35
2	N	301	CHL	C4B-NB	3.43	1.42	1.37
2	G	605	CHL	C3B-C4B	3.41	1.50	1.42
3	N	303	CLA	C3B-C4B	3.41	1.50	1.42
2	Y	601	CHL	C3B-C4B	3.40	1.50	1.42
4	N	316	LUT	C10-C9	3.40	1.40	1.35
4	G	614	LUT	C10-C9	3.39	1.40	1.35
3	N	311	CLA	C1D-ND	3.39	1.41	1.37
2	N	310	CHL	C1D-ND	3.38	1.41	1.37
3	N	314	CLA	C4D-ND	-3.38	1.33	1.37
2	Y	605	CHL	C1D-ND	3.37	1.41	1.37
3	G	610	CLA	C1D-ND	3.37	1.41	1.37
3	N	311	CLA	C4B-NB	3.36	1.41	1.37
2	Y	608	CHL	C4D-ND	-3.35	1.33	1.37
6	G	617	NEX	C7-C8	-3.35	1.26	1.32
2	Y	606	CHL	C4B-NB	3.34	1.41	1.37
3	G	604	CLA	C4B-NB	3.34	1.41	1.37
3	N	313	CLA	C4B-NB	3.33	1.41	1.37
2	G	607	CHL	C4B-NB	3.33	1.41	1.37
4	G	614	LUT	C30-C29	3.32	1.40	1.35
2	G	619	CHL	C4B-NB	3.29	1.41	1.37
2	N	306	CHL	C4B-NB	3.28	1.41	1.37
4	N	316	LUT	C30-C29	3.28	1.40	1.35
3	N	314	CLA	C4B-NB	3.26	1.41	1.37
2	Y	605	CHL	C4B-NB	3.25	1.41	1.37
3	G	613	CLA	C3B-C4B	3.25	1.50	1.42
4	Y	614	LUT	C30-C29	3.25	1.40	1.35
3	Y	609	CLA	C4B-NB	3.23	1.41	1.37
3	G	610	CLA	C4D-ND	-3.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	614	LUT	C34-C33	3.21	1.40	1.35
2	G	606	CHL	C4D-ND	-3.20	1.33	1.37
2	G	608	CHL	C3B-C4B	3.20	1.50	1.42
3	N	315	CLA	C3B-C4B	3.19	1.50	1.42
4	N	316	LUT	C14-C13	3.17	1.40	1.35
2	Y	608	CHL	C1D-ND	3.17	1.41	1.37
3	N	304	CLA	C3B-C4B	3.16	1.50	1.42
2	Y	606	CHL	C4D-ND	-3.15	1.33	1.37
4	N	317	LUT	C35-C15	3.15	1.44	1.36
4	G	614	LUT	C14-C13	3.15	1.40	1.35
4	N	316	LUT	C34-C33	3.14	1.40	1.35
3	G	611	CLA	C4B-NB	3.14	1.41	1.37
3	G	603	CLA	C3B-C4B	3.14	1.50	1.42
4	Y	614	LUT	C14-C13	3.13	1.39	1.35
4	G	614	LUT	C34-C33	3.13	1.39	1.35
3	Y	611	CLA	C3B-C4B	3.12	1.50	1.42
2	N	310	CHL	C3B-C4B	3.11	1.50	1.42
2	N	310	CHL	C4B-NB	3.11	1.41	1.37
4	Y	614	LUT	C8-C9	-3.10	1.39	1.45
2	N	307	CHL	C4D-ND	-3.10	1.33	1.37
3	Y	612	CLA	C4D-ND	-3.10	1.33	1.37
3	Y	603	CLA	C3B-C4B	3.10	1.50	1.42
3	Y	610	CLA	C1D-ND	3.09	1.41	1.37
4	G	614	LUT	C8-C9	-3.08	1.39	1.45
4	N	316	LUT	C8-C9	-3.08	1.39	1.45
3	Y	610	CLA	C4B-NB	3.07	1.41	1.37
2	G	608	CHL	C4B-NB	3.06	1.41	1.37
3	G	610	CLA	C4B-NB	3.06	1.41	1.37
2	G	619	CHL	C4D-ND	-3.05	1.33	1.37
2	G	607	CHL	C4D-ND	-3.05	1.33	1.37
3	N	312	CLA	C3B-C4B	3.03	1.49	1.42
3	N	315	CLA	C4D-ND	-3.03	1.33	1.37
2	Y	607	CHL	C4D-ND	-3.02	1.33	1.37
3	Y	609	CLA	C3B-C4B	3.00	1.49	1.42
3	N	305	CLA	C4D-ND	-2.99	1.33	1.37
2	G	608	CHL	C4D-ND	-2.98	1.33	1.37
3	N	303	CLA	C4D-ND	-2.98	1.33	1.37
3	G	611	CLA	C4D-ND	-2.96	1.33	1.37
2	Y	607	CHL	C4B-NB	2.94	1.41	1.37
3	Y	609	CLA	MG-NA	2.94	2.13	2.06
3	G	612	CLA	C4D-ND	-2.94	1.33	1.37
3	Y	604	CLA	C4D-ND	-2.93	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	301	CHL	C4D-ND	-2.93	1.33	1.37
3	G	612	CLA	C3B-C4B	2.93	1.49	1.42
2	G	601	CHL	C4D-ND	-2.92	1.33	1.37
3	G	604	CLA	C4D-ND	-2.92	1.33	1.37
3	Y	612	CLA	C3B-C4B	2.91	1.49	1.42
2	G	606	CHL	C1B-C2B	2.91	1.50	1.43
3	Y	602	CLA	C3B-C4B	2.91	1.49	1.42
6	N	319	NEX	C7-C8	-2.91	1.27	1.32
3	N	305	CLA	C3B-C4B	2.88	1.49	1.42
3	Y	602	CLA	C4D-ND	-2.87	1.33	1.37
2	N	310	CHL	C4D-ND	-2.87	1.33	1.37
3	Y	609	CLA	C4D-ND	-2.86	1.33	1.37
3	G	602	CLA	C4D-ND	-2.86	1.33	1.37
3	Y	603	CLA	C4D-ND	-2.86	1.33	1.37
2	Y	606	CHL	C3B-C4B	2.85	1.49	1.42
4	Y	614	LUT	C28-C29	-2.85	1.39	1.45
4	G	614	LUT	C28-C29	-2.84	1.39	1.45
4	N	316	LUT	C28-C29	-2.84	1.39	1.45
2	N	306	CHL	C3B-C4B	2.84	1.49	1.42
2	Y	608	CHL	C4B-NB	2.82	1.41	1.37
3	G	604	CLA	C3B-C4B	2.82	1.49	1.42
3	G	602	CLA	C3B-C4B	2.81	1.49	1.42
2	N	309	CHL	C4D-ND	-2.81	1.33	1.37
2	Y	601	CHL	C4D-ND	-2.81	1.33	1.37
2	G	606	CHL	C4B-NB	2.78	1.41	1.37
3	N	304	CLA	C4D-ND	-2.78	1.33	1.37
3	Y	613	CLA	C4D-ND	-2.78	1.33	1.37
3	N	313	CLA	C4D-ND	-2.76	1.33	1.37
4	G	614	LUT	C32-C33	-2.75	1.40	1.45
3	N	314	CLA	C3B-C4B	2.75	1.49	1.42
4	Y	614	LUT	C32-C33	-2.75	1.40	1.45
4	G	614	LUT	C12-C13	-2.75	1.40	1.45
3	Y	613	CLA	C3B-C4B	2.75	1.49	1.42
2	N	302	CHL	C4D-ND	-2.74	1.33	1.37
4	N	316	LUT	C32-C33	-2.74	1.40	1.45
4	N	316	LUT	C12-C13	-2.74	1.40	1.45
6	Y	616	NEX	C7-C8	-2.74	1.27	1.32
3	N	313	CLA	C3B-C4B	2.73	1.49	1.42
3	G	609	CLA	C3B-C4B	2.73	1.49	1.42
3	G	603	CLA	C1B-C2B	2.73	1.49	1.43
2	Y	608	CHL	C3B-C4B	2.72	1.49	1.42
3	G	603	CLA	C4D-ND	-2.72	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	CLA	C1B-C2B	2.72	1.49	1.43
3	Y	613	CLA	CMD-C2D	-2.71	1.45	1.50
3	Y	610	CLA	C3B-C4B	2.71	1.49	1.42
3	G	611	CLA	C3B-C4B	2.71	1.49	1.42
4	Y	614	LUT	C12-C13	-2.71	1.40	1.45
2	N	306	CHL	C1B-C2B	2.69	1.49	1.43
2	N	306	CHL	C4D-ND	-2.69	1.34	1.37
3	Y	613	CLA	C1B-C2B	2.67	1.49	1.43
2	Y	605	CHL	C3B-C4B	2.65	1.49	1.42
3	N	312	CLA	C4D-ND	-2.65	1.34	1.37
3	Y	611	CLA	C4D-ND	-2.64	1.34	1.37
3	G	610	CLA	C3B-C4B	2.64	1.48	1.42
3	G	609	CLA	C4D-ND	-2.62	1.34	1.37
2	G	605	CHL	C1B-C2B	2.60	1.49	1.43
3	Y	604	CLA	CMB-C2B	-2.59	1.45	1.50
3	G	609	CLA	C4B-NB	2.59	1.41	1.37
2	N	310	CHL	C1B-C2B	2.59	1.49	1.43
2	Y	606	CHL	C1B-C2B	2.59	1.49	1.43
3	N	304	CLA	C1B-C2B	2.58	1.49	1.43
3	Y	611	CLA	MG-NC	2.58	2.12	2.06
3	N	311	CLA	C3B-C4B	2.58	1.48	1.42
2	N	307	CHL	CHC-C1C	2.57	1.43	1.38
3	Y	604	CLA	C3B-C4B	2.56	1.48	1.42
5	N	321	XAT	O4-C5	-2.56	1.42	1.46
3	Y	612	CLA	C1B-C2B	2.56	1.49	1.43
3	G	613	CLA	C4D-ND	-2.56	1.34	1.37
2	Y	605	CHL	C1B-C2B	2.56	1.49	1.43
3	Y	603	CLA	C1B-C2B	2.55	1.49	1.43
3	N	315	CLA	C1B-C2B	2.53	1.49	1.43
3	Y	611	CLA	C1B-C2B	2.52	1.49	1.43
2	G	605	CHL	C4D-ND	-2.52	1.34	1.37
3	N	305	CLA	C1B-C2B	2.51	1.49	1.43
3	G	612	CLA	C1B-C2B	2.51	1.49	1.43
2	N	308	CHL	C4D-ND	-2.49	1.34	1.37
2	Y	608	CHL	C1B-C2B	2.48	1.49	1.43
3	N	312	CLA	CMD-C2D	-2.47	1.45	1.50
3	N	314	CLA	C1B-C2B	2.47	1.49	1.43
3	N	312	CLA	C1B-C2B	2.47	1.49	1.43
2	Y	601	CHL	C1B-C2B	2.47	1.49	1.43
3	G	613	CLA	C1B-C2B	2.46	1.49	1.43
3	G	604	CLA	C1B-C2B	2.46	1.49	1.43
2	Y	607	CHL	C1B-C2B	2.44	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	311	CLA	CMD-C2D	-2.44	1.45	1.50
3	Y	610	CLA	CMD-C2D	-2.44	1.45	1.50
2	N	302	CHL	C1B-C2B	2.44	1.49	1.43
3	N	303	CLA	C1B-C2B	2.44	1.49	1.43
3	G	611	CLA	C1B-C2B	2.42	1.49	1.43
2	G	601	CHL	C1B-C2B	2.40	1.48	1.43
2	G	608	CHL	C1B-C2B	2.40	1.48	1.43
3	Y	602	CLA	C1B-C2B	2.39	1.48	1.43
2	N	308	CHL	CHC-C1C	2.39	1.43	1.38
2	Y	607	CHL	MG-NB	-2.38	2.01	2.05
3	Y	612	CLA	CMB-C2B	-2.38	1.45	1.50
3	N	311	CLA	CMB-C2B	-2.38	1.45	1.50
2	N	308	CHL	C1B-C2B	2.38	1.48	1.43
2	G	607	CHL	CHC-C1C	2.38	1.43	1.38
3	Y	609	CLA	CMD-C2D	-2.37	1.45	1.50
2	N	307	CHL	CMB-C2B	-2.36	1.45	1.50
3	G	610	CLA	C1B-C2B	2.34	1.48	1.43
2	N	301	CHL	CHC-C1C	2.34	1.43	1.38
3	N	313	CLA	C1B-C2B	2.33	1.48	1.43
3	G	609	CLA	CMB-C2B	-2.33	1.45	1.50
6	G	617	NEX	O24-C25	-2.32	1.42	1.46
2	G	606	CHL	C3B-C4B	2.32	1.48	1.42
3	N	313	CLA	CMC-C2C	-2.32	1.45	1.50
2	N	301	CHL	C1B-C2B	2.29	1.48	1.43
2	N	310	CHL	CMD-C2D	-2.29	1.45	1.50
3	N	314	CLA	CMB-C2B	-2.29	1.45	1.50
2	N	309	CHL	C1B-C2B	2.29	1.48	1.43
2	Y	608	CHL	MG-ND	-2.28	2.01	2.05
3	G	609	CLA	MG-NA	2.28	2.11	2.06
2	N	302	CHL	CHC-C1C	2.27	1.43	1.38
2	G	608	CHL	CMB-C2B	-2.27	1.46	1.50
2	G	601	CHL	CHC-C1C	2.26	1.43	1.38
3	Y	610	CLA	C1B-C2B	2.26	1.48	1.43
3	Y	604	CLA	C1B-C2B	2.26	1.48	1.43
2	G	606	CHL	MG-NB	-2.25	2.01	2.05
3	G	602	CLA	CMD-C2D	-2.24	1.46	1.50
5	N	321	XAT	O24-C25	-2.24	1.43	1.46
2	N	309	CHL	CHC-C1C	2.22	1.43	1.38
2	Y	608	CHL	CMD-C2D	-2.21	1.46	1.50
3	N	313	CLA	CMB-C2B	-2.20	1.46	1.50
3	G	611	CLA	CMB-C2B	-2.19	1.46	1.50
3	G	613	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	603	CLA	CMD-C2D	-2.18	1.46	1.50
3	N	305	CLA	CMC-C2C	-2.18	1.46	1.50
3	N	313	CLA	CMD-C2D	-2.18	1.46	1.50
3	G	610	CLA	CMD-C2D	-2.18	1.46	1.50
3	G	610	CLA	MG-NB	-2.18	2.01	2.05
3	Y	610	CLA	CMC-C2C	-2.18	1.46	1.50
2	G	606	CHL	CMD-C2D	-2.17	1.46	1.50
3	G	609	CLA	C1B-C2B	2.17	1.48	1.43
2	Y	601	CHL	CHC-C1C	2.17	1.42	1.38
3	G	613	CLA	MG-NA	2.17	2.11	2.06
3	G	603	CLA	CMD-C2D	-2.17	1.46	1.50
2	Y	607	CHL	CHC-C1C	2.16	1.42	1.38
3	N	305	CLA	CMD-C2D	-2.16	1.46	1.50
3	N	314	CLA	MG-NB	-2.16	2.01	2.05
3	N	311	CLA	C1B-C2B	2.16	1.48	1.43
3	N	315	CLA	CMD-C2D	-2.16	1.46	1.50
2	Y	605	CHL	MG-NB	-2.15	2.01	2.05
2	Y	605	CHL	CMB-C2B	-2.15	1.46	1.50
3	N	314	CLA	CMC-C2C	-2.15	1.46	1.50
3	Y	610	CLA	MG-NB	-2.15	2.01	2.05
3	G	613	CLA	CHC-C1C	2.15	1.42	1.38
2	Y	608	CHL	MG-NB	-2.15	2.01	2.05
2	Y	605	CHL	CMD-C2D	-2.15	1.46	1.50
2	Y	606	CHL	MG-NB	-2.15	2.01	2.05
2	G	607	CHL	MG-NB	-2.15	2.01	2.05
3	G	609	CLA	CMC-C2C	-2.14	1.46	1.50
3	N	313	CLA	MG-NA	2.14	2.11	2.06
3	Y	603	CLA	CMB-C2B	-2.13	1.46	1.50
2	G	608	CHL	MG-NB	-2.13	2.01	2.05
3	Y	612	CLA	CMD-C2D	-2.13	1.46	1.50
2	Y	608	CHL	CMB-C2B	-2.13	1.46	1.50
3	G	603	CLA	CMB-C2B	-2.13	1.46	1.50
3	G	610	CLA	CMB-C2B	-2.13	1.46	1.50
2	G	607	CHL	C1B-NB	-2.13	1.35	1.37
3	G	611	CLA	CMD-C2D	-2.12	1.46	1.50
3	N	314	CLA	CMD-C2D	-2.12	1.46	1.50
2	G	606	CHL	CMB-C2B	-2.12	1.46	1.50
3	Y	602	CLA	CHC-C1C	2.12	1.42	1.38
3	G	604	CLA	CMB-C2B	-2.12	1.46	1.50
2	G	619	CHL	CHC-C1C	2.12	1.42	1.38
2	Y	606	CHL	CHC-C1C	2.11	1.42	1.38
3	G	610	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	607	CHL	CMB-C2B	-2.11	1.46	1.50
3	Y	612	CLA	CMC-C2C	-2.11	1.46	1.50
2	N	309	CHL	CMD-C2D	-2.11	1.46	1.50
2	G	619	CHL	C1B-C2B	2.10	1.48	1.43
3	Y	612	CLA	CHC-C1C	2.10	1.42	1.38
2	Y	606	CHL	CMB-C2B	-2.10	1.46	1.50
2	N	307	CHL	C1B-C2B	2.10	1.48	1.43
3	Y	609	CLA	C1B-C2B	2.10	1.48	1.43
3	G	612	CLA	CHC-C1C	2.09	1.42	1.38
3	G	609	CLA	CMD-C2D	-2.09	1.46	1.50
3	G	611	CLA	MG-NB	-2.09	2.01	2.05
3	N	303	CLA	CHC-C1C	2.09	1.42	1.38
3	N	304	CLA	CMD-C2D	-2.09	1.46	1.50
3	N	305	CLA	CHC-C1C	2.08	1.42	1.38
2	G	619	CHL	CMB-C2B	-2.08	1.46	1.50
3	Y	604	CLA	CMC-C2C	-2.08	1.46	1.50
3	N	305	CLA	CMB-C2B	-2.07	1.46	1.50
3	Y	604	CLA	CMD-C2D	-2.07	1.46	1.50
2	G	608	CHL	CMD-C2D	-2.07	1.46	1.50
5	G	616	XAT	O4-C5	-2.07	1.43	1.46
2	N	307	CHL	CMD-C2D	-2.06	1.46	1.50
2	Y	606	CHL	CMD-C2D	-2.06	1.46	1.50
3	Y	604	CLA	MG-NB	-2.06	2.01	2.05
5	G	616	XAT	O24-C25	-2.06	1.43	1.46
3	N	312	CLA	CMB-C2B	-2.06	1.46	1.50
2	G	608	CHL	C1D-C2D	2.05	1.49	1.45
3	G	604	CLA	CHC-C1C	2.05	1.42	1.38
2	Y	601	CHL	CMD-C2D	-2.05	1.46	1.50
2	G	601	CHL	CMD-C2D	-2.05	1.46	1.50
3	G	612	CLA	CMD-C2D	-2.05	1.46	1.50
3	G	611	CLA	CHC-C1C	2.04	1.42	1.38
3	N	303	CLA	CMB-C2B	-2.04	1.46	1.50
3	N	304	CLA	CMB-C2B	-2.04	1.46	1.50
2	N	306	CHL	C3D-C4D	2.04	1.48	1.44
2	N	302	CHL	CMD-C2D	-2.04	1.46	1.50
2	G	607	CHL	CMD-C2D	-2.03	1.46	1.50
3	G	611	CLA	CMC-C2C	-2.02	1.46	1.50
3	Y	611	CLA	CMD-C2D	-2.02	1.46	1.50
3	G	612	CLA	CMB-C2B	-2.02	1.46	1.50
2	G	607	CHL	MG-ND	-2.02	2.01	2.05
2	G	608	CHL	C2C-C3C	2.02	1.41	1.36
2	N	302	CHL	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	315	CLA	CMB-C2B	-2.02	1.46	1.50
2	N	306	CHL	CMD-C2D	-2.02	1.46	1.50
2	G	605	CHL	C3D-C4D	2.02	1.48	1.44
3	N	303	CLA	CMC-C2C	-2.02	1.46	1.50
2	N	310	CHL	CMB-C2B	-2.01	1.46	1.50
2	G	605	CHL	CAC-C3C	-2.01	1.46	1.51
3	Y	603	CLA	CAC-C3C	-2.01	1.46	1.51
2	N	301	CHL	CMB-C2B	-2.01	1.46	1.50
2	G	619	CHL	CMD-C2D	-2.01	1.46	1.50

All (493) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	617	NEX	O24-C25-C24	10.71	121.42	113.38
5	G	616	XAT	O24-C25-C24	9.66	120.64	113.38
5	N	321	XAT	O24-C25-C24	9.22	120.31	113.38
6	G	617	NEX	C38-C25-C26	-8.91	107.33	122.26
5	N	318	XAT	O4-C5-C4	8.61	119.85	113.38
5	G	616	XAT	O4-C5-C4	8.58	119.83	113.38
5	N	321	XAT	O4-C5-C4	8.30	119.62	113.38
2	G	607	CHL	C4A-NA-C1A	7.43	110.05	106.71
6	N	319	NEX	O24-C25-C24	7.36	118.91	113.38
2	Y	608	CHL	C4A-NA-C1A	7.34	110.00	106.71
4	N	317	LUT	C15-C14-C13	-7.24	116.97	127.31
6	Y	616	NEX	O24-C25-C24	7.18	118.78	113.38
2	G	608	CHL	C4A-NA-C1A	7.16	109.92	106.71
5	N	318	XAT	O24-C25-C24	6.96	118.61	113.38
3	G	603	CLA	C4A-NA-C1A	6.91	109.81	106.71
2	G	605	CHL	C4A-NA-C1A	6.68	109.71	106.71
2	Y	607	CHL	C4A-NA-C1A	6.48	109.62	106.71
5	N	318	XAT	C31-C30-C29	-6.45	118.11	127.31
3	N	312	CLA	C4A-NA-C1A	6.37	109.57	106.71
4	N	317	LUT	C35-C15-C14	-6.25	110.67	123.47
2	Y	605	CHL	C4A-NA-C1A	6.23	109.51	106.71
3	Y	603	CLA	C4A-NA-C1A	6.20	109.50	106.71
6	N	319	NEX	C11-C10-C9	-6.10	118.61	127.31
6	G	617	NEX	C11-C10-C9	-6.09	118.61	127.31
5	G	616	XAT	C15-C14-C13	-6.09	118.62	127.31
2	G	606	CHL	C4A-NA-C1A	5.95	109.38	106.71
3	G	610	CLA	C4A-NA-C1A	5.94	109.38	106.71
6	Y	616	NEX	C27-C28-C29	-5.90	116.37	125.53
2	N	306	CHL	C4A-NA-C1A	5.87	109.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	617	NEX	O24-C25-C38	5.69	121.87	115.06
6	G	617	NEX	C15-C14-C13	-5.68	119.21	127.31
5	N	321	XAT	C35-C34-C33	-5.67	119.22	127.31
6	Y	616	NEX	C15-C14-C13	-5.63	119.28	127.31
3	Y	604	CLA	C4A-NA-C1A	5.61	109.23	106.71
3	N	304	CLA	C4A-NA-C1A	5.60	109.22	106.71
5	N	318	XAT	C15-C14-C13	-5.39	119.62	127.31
3	Y	612	CLA	C4A-NA-C1A	5.37	109.12	106.71
3	N	305	CLA	C4A-NA-C1A	5.36	109.11	106.71
6	G	617	NEX	C35-C34-C33	-5.23	119.84	127.31
2	N	307	CHL	C4A-NA-C1A	5.19	109.04	106.71
2	N	310	CHL	C4A-NA-C1A	5.17	109.03	106.71
3	N	314	CLA	C4A-NA-C1A	5.17	109.03	106.71
3	G	612	CLA	C4A-NA-C1A	5.13	109.01	106.71
6	N	319	NEX	C38-C25-C26	-5.12	113.68	122.26
5	N	318	XAT	C38-C25-C26	-5.02	113.84	122.26
3	Y	613	CLA	C4A-NA-C1A	5.02	108.96	106.71
6	Y	616	NEX	C38-C25-C26	-4.97	113.93	122.26
6	Y	616	NEX	C31-C30-C29	-4.96	120.23	127.31
5	N	321	XAT	C6-C7-C8	-4.91	115.61	125.99
3	G	611	CLA	C4A-NA-C1A	4.88	108.90	106.71
5	G	616	XAT	C38-C25-C26	-4.83	114.17	122.26
2	G	605	CHL	O2D-CGD-O1D	-4.79	114.47	123.84
6	N	319	NEX	C15-C14-C13	-4.78	120.49	127.31
5	N	318	XAT	O24-C25-C38	4.76	120.76	115.06
5	N	321	XAT	C31-C30-C29	-4.72	120.57	127.31
5	G	616	XAT	C18-C5-C6	-4.69	114.39	122.26
6	Y	616	NEX	C11-C10-C9	-4.68	120.64	127.31
5	N	321	XAT	C11-C10-C9	-4.68	120.64	127.31
6	Y	616	NEX	O24-C25-C38	4.67	120.65	115.06
3	G	602	CLA	C4A-NA-C1A	4.65	108.80	106.71
6	G	617	NEX	C27-C28-C29	-4.63	118.34	125.53
3	G	609	CLA	O2D-CGD-O1D	-4.48	115.07	123.84
3	Y	602	CLA	C4A-NA-C1A	4.46	108.71	106.71
2	G	619	CHL	C4A-NA-C1A	4.40	108.68	106.71
3	Y	610	CLA	C4A-NA-C1A	4.39	108.68	106.71
2	Y	606	CHL	C4A-NA-C1A	4.34	108.66	106.71
3	G	604	CLA	C4A-NA-C1A	4.33	108.65	106.71
6	Y	616	NEX	C35-C34-C33	-4.31	121.15	127.31
3	Y	609	CLA	C4A-NA-C1A	-4.31	104.77	106.71
2	Y	601	CHL	C4A-NA-C1A	4.31	108.64	106.71
5	G	616	XAT	C6-C7-C8	-4.28	116.94	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	303	CLA	C4A-NA-C1A	4.27	108.62	106.71
5	N	318	XAT	C18-C5-C6	-4.24	115.15	122.26
5	N	318	XAT	C27-C28-C29	-4.23	118.97	125.53
6	N	319	NEX	O24-C25-C38	4.20	120.09	115.06
5	N	318	XAT	O4-C5-C18	4.12	120.00	115.06
4	G	615	LUT	C35-C34-C33	-4.12	121.43	127.31
5	N	321	XAT	C15-C14-C13	-4.08	121.49	127.31
4	G	614	LUT	C39-C29-C30	-4.08	117.21	122.92
3	N	315	CLA	C4A-NA-C1A	4.07	108.54	106.71
4	Y	614	LUT	C39-C29-C30	-4.07	117.22	122.92
5	N	318	XAT	C6-C7-C8	-4.05	117.43	125.99
4	N	316	LUT	C39-C29-C30	-4.05	117.25	122.92
2	N	309	CHL	C4A-NA-C1A	4.03	108.52	106.71
6	N	319	NEX	C35-C34-C33	-4.02	121.58	127.31
5	G	616	XAT	C31-C30-C29	-4.01	121.59	127.31
4	G	614	LUT	C19-C9-C10	-4.01	117.31	122.92
4	Y	614	LUT	C19-C9-C10	-3.99	117.33	122.92
2	N	308	CHL	C4A-NA-C1A	3.98	108.50	106.71
4	N	316	LUT	C19-C9-C10	-3.96	117.38	122.92
4	N	317	LUT	C35-C34-C33	-3.95	121.67	127.31
5	N	318	XAT	C15-C35-C34	-3.95	115.38	123.47
5	N	321	XAT	O4-C5-C18	3.92	119.75	115.06
5	G	616	XAT	O4-C5-C18	3.90	119.73	115.06
2	N	302	CHL	C4A-NA-C1A	3.86	108.44	106.71
2	N	307	CHL	C3B-C4B-NB	-3.85	106.94	110.52
3	Y	611	CLA	C4A-NA-C1A	3.83	108.43	106.71
2	G	607	CHL	CMB-C2B-C1B	-3.81	119.57	125.37
3	G	609	CLA	O2D-CGD-CBD	3.77	117.97	111.27
2	G	619	CHL	C3B-C4B-NB	-3.76	107.03	110.52
5	N	321	XAT	C4-C3-C2	-3.75	103.53	110.77
5	G	616	XAT	O24-C25-C38	3.67	119.45	115.06
2	N	301	CHL	C4A-NA-C1A	3.62	108.33	106.71
4	G	614	LUT	C35-C15-C14	3.62	130.88	123.47
4	Y	614	LUT	C35-C15-C14	3.61	130.88	123.47
4	N	316	LUT	C35-C15-C14	3.61	130.87	123.47
5	N	318	XAT	C11-C10-C9	-3.61	122.16	127.31
3	Y	609	CLA	O2D-CGD-O1D	-3.61	116.79	123.84
5	N	321	XAT	O24-C25-C38	3.59	119.36	115.06
3	Y	609	CLA	CHB-C1B-NB	3.57	128.04	124.26
3	N	313	CLA	CHB-C1B-NB	3.57	128.04	124.26
4	G	615	LUT	C15-C14-C13	-3.56	122.23	127.31
6	N	319	NEX	C11-C12-C13	-3.52	116.53	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	617	NEX	C24-C23-C22	-3.51	103.99	110.77
3	G	609	CLA	C1-C2-C3	-3.50	119.98	126.04
2	N	301	CHL	O2D-CGD-O1D	-3.50	116.99	123.84
7	G	618	LHG	O7-C7-C8	3.50	119.04	111.50
5	G	616	XAT	C15-C35-C34	-3.50	116.31	123.47
2	G	608	CHL	CHD-C1D-ND	-3.49	121.25	124.45
2	G	605	CHL	CHD-C1D-ND	-3.45	121.28	124.45
5	N	321	XAT	C18-C5-C6	-3.43	116.51	122.26
3	G	610	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
5	N	321	XAT	C38-C25-C26	-3.40	116.56	122.26
3	N	314	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
4	G	615	LUT	C31-C30-C29	-3.35	122.53	127.31
2	N	307	CHL	CAA-C2A-C3A	-3.34	103.62	112.78
4	Y	615	LUT	C2-C3-C4	3.34	114.88	110.30
3	G	611	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
5	G	616	XAT	C35-C34-C33	-3.33	122.56	127.31
2	G	607	CHL	C3B-C4B-NB	-3.28	107.47	110.52
2	N	301	CHL	C3B-C4B-NB	-3.28	107.48	110.52
6	G	617	NEX	C11-C12-C13	-3.27	117.23	126.42
6	N	319	NEX	C27-C28-C29	-3.25	120.48	125.53
4	Y	615	LUT	C15-C14-C13	-3.25	122.67	127.31
5	N	321	XAT	C26-C27-C28	-3.24	119.13	125.99
4	N	317	LUT	C15-C35-C34	-3.21	116.90	123.47
2	N	308	CHL	O2D-CGD-O1D	-3.21	117.57	123.84
3	N	312	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
2	N	306	CHL	CHB-C4A-NA	3.18	128.92	124.51
4	G	615	LUT	C10-C11-C12	-3.18	113.28	123.22
4	G	614	LUT	C40-C33-C34	-3.18	118.47	122.92
6	N	319	NEX	C16-C1-C6	3.17	113.31	110.47
2	N	308	CHL	C3B-C4B-NB	-3.16	107.58	110.52
4	Y	614	LUT	C40-C33-C34	-3.16	118.50	122.92
3	G	613	CLA	C4A-NA-C1A	3.16	108.12	106.71
4	G	614	LUT	C20-C13-C14	-3.16	118.50	122.92
3	Y	609	CLA	O2D-CGD-CBD	3.15	116.87	111.27
4	N	316	LUT	C20-C13-C14	-3.15	118.51	122.92
7	N	320	LHG	O7-C7-C8	3.15	118.29	111.50
6	G	617	NEX	C15-C35-C34	-3.15	117.02	123.47
3	G	604	CLA	CMB-C2B-C1B	-3.13	120.61	125.37
4	Y	615	LUT	C11-C10-C9	-3.13	122.85	127.31
4	Y	614	LUT	C20-C13-C14	-3.12	118.55	122.92
2	Y	607	CHL	C3B-C4B-NB	-3.12	107.62	110.52
4	N	316	LUT	C40-C33-C34	-3.11	118.56	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	609	CLA	CHB-C1B-NB	3.08	127.51	124.26
2	G	619	CHL	O2D-CGD-CBD	3.07	116.73	111.27
6	G	617	NEX	C39-C29-C30	-3.07	118.63	122.92
6	N	319	NEX	C31-C30-C29	-3.05	122.96	127.31
3	N	305	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
3	G	610	CLA	O2D-CGD-CBD	3.04	116.67	111.27
7	Y	617	LHG	O7-C7-C8	3.04	118.04	111.50
2	N	306	CHL	C2A-C1A-CHA	3.02	129.13	123.86
5	G	616	XAT	C26-C27-C28	-3.00	119.65	125.99
4	Y	615	LUT	C10-C11-C12	-3.00	113.86	123.22
5	G	616	XAT	C11-C10-C9	-3.00	123.03	127.31
2	N	307	CHL	CHB-C1B-NB	3.00	127.43	124.26
2	G	601	CHL	C4A-NA-C1A	2.99	108.05	106.71
3	Y	602	CLA	CHB-C1B-NB	2.99	127.42	124.26
2	G	608	CHL	C2D-C1D-ND	-2.98	107.91	110.10
3	G	604	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
3	Y	613	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
3	Y	611	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
5	N	321	XAT	C35-C15-C14	-2.96	117.41	123.47
2	G	608	CHL	O2D-CGD-O1D	-2.95	118.07	123.84
2	G	601	CHL	C3B-C4B-NB	-2.95	107.78	110.52
5	N	321	XAT	C27-C28-C29	-2.94	120.97	125.53
3	Y	612	CLA	CHD-C1D-ND	-2.93	121.76	124.45
2	N	310	CHL	O2D-CGD-O1D	-2.92	118.13	123.84
3	N	304	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
3	G	602	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
2	G	605	CHL	O2D-CGD-CBD	2.88	116.38	111.27
2	G	619	CHL	O2D-CGD-O1D	-2.87	118.23	123.84
2	G	601	CHL	O2D-CGD-O1D	-2.87	118.23	123.84
2	N	301	CHL	O2D-CGD-CBD	2.86	116.35	111.27
3	Y	604	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
3	G	613	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
3	Y	604	CLA	CMB-C2B-C1B	-2.84	121.04	125.37
5	N	318	XAT	C4-C3-C2	-2.84	105.29	110.77
6	Y	616	NEX	C15-C35-C34	-2.83	117.67	123.47
3	N	303	CLA	C3B-C4B-NB	-2.83	107.89	110.52
3	Y	612	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
4	N	317	LUT	C10-C11-C12	-2.82	114.42	123.22
4	N	317	LUT	C31-C30-C29	-2.82	123.29	127.31
5	N	321	XAT	C31-C32-C33	-2.82	118.50	126.42
3	G	612	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
2	G	607	CHL	O2D-CGD-O1D	-2.82	118.33	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	602	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
3	Y	603	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
3	Y	604	CLA	CHB-C1B-NB	2.81	127.23	124.26
2	Y	607	CHL	O2D-CGD-O1D	-2.81	118.34	123.84
2	N	306	CHL	O2D-CGD-O1D	-2.80	118.37	123.84
5	N	321	XAT	C7-C8-C9	-2.79	121.20	125.53
2	G	605	CHL	C3A-C2A-C1A	2.78	105.50	101.34
2	G	607	CHL	CMB-C2B-C3B	2.78	133.32	126.59
6	N	319	NEX	C39-C29-C30	-2.78	119.03	122.92
2	G	607	CHL	C2A-C1A-CHA	2.78	128.71	123.86
6	G	617	NEX	C26-C27-C28	-2.77	120.14	125.99
2	Y	605	CHL	OMC-CMC-C2C	-2.76	119.45	125.69
4	Y	615	LUT	C7-C8-C9	-2.75	122.07	126.23
4	Y	615	LUT	C35-C34-C33	-2.74	123.39	127.31
2	N	307	CHL	O2D-CGD-O1D	-2.74	118.49	123.84
4	G	614	LUT	C32-C33-C34	2.74	123.14	118.94
3	N	313	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
4	G	615	LUT	C7-C8-C9	-2.73	122.11	126.23
2	N	301	CHL	CHB-C1B-NB	2.73	127.15	124.26
4	N	317	LUT	C30-C31-C32	-2.73	114.70	123.22
2	Y	601	CHL	O2D-CGD-O1D	-2.73	118.50	123.84
2	G	605	CHL	CAA-CBA-CGA	-2.72	105.30	113.25
2	Y	608	CHL	O2D-CGD-O1D	-2.72	118.52	123.84
2	N	302	CHL	O2D-CGD-O1D	-2.71	118.53	123.84
2	Y	606	CHL	C3B-C4B-NB	-2.70	108.01	110.52
3	G	610	CLA	CHB-C4A-NA	2.69	128.24	124.51
3	N	311	CLA	C2D-C1D-ND	-2.69	108.12	110.10
3	Y	613	CLA	C2D-C1D-ND	-2.69	108.12	110.10
3	N	304	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
2	Y	608	CHL	C3B-C4B-NB	-2.69	108.02	110.52
4	N	316	LUT	C32-C33-C34	2.69	123.07	118.94
5	G	616	XAT	C27-C28-C29	-2.69	121.36	125.53
4	Y	614	LUT	C32-C33-C34	2.69	123.06	118.94
4	N	317	LUT	C38-C25-C24	-2.68	117.81	123.56
3	Y	609	CLA	C1-C2-C3	-2.68	121.41	126.04
7	N	320	LHG	O8-C6-C5	-2.67	100.67	108.43
3	Y	613	CLA	CMB-C2B-C1B	-2.66	121.32	125.37
2	Y	607	CHL	C2A-C1A-CHA	2.64	128.48	123.86
2	G	619	CHL	CHB-C1B-NB	2.64	127.06	124.26
2	N	309	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
2	Y	605	CHL	CHD-C1D-ND	-2.63	122.03	124.45
3	Y	603	CLA	CHB-C4A-NA	2.63	128.15	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	303	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
2	Y	608	CHL	CHD-C1D-ND	-2.62	122.04	124.45
3	Y	609	CLA	C2B-C1B-NB	2.62	111.99	110.23
5	N	318	XAT	C24-C23-C22	-2.62	105.72	110.77
4	G	615	LUT	C38-C25-C24	-2.62	117.96	123.56
3	N	313	CLA	CHC-C4B-NB	2.62	127.03	124.26
2	Y	608	CHL	OMC-CMC-C2C	-2.61	119.79	125.69
2	G	606	CHL	O2D-CGD-O1D	-2.61	118.74	123.84
3	G	609	CLA	CMB-C2B-C1B	-2.61	121.40	125.37
3	N	305	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
2	Y	601	CHL	C3B-C4B-NB	-2.60	108.10	110.52
6	Y	616	NEX	C11-C12-C13	-2.60	119.12	126.42
5	N	318	XAT	C26-C27-C28	-2.60	120.50	125.99
3	N	311	CLA	CHB-C1B-NB	2.59	127.00	124.26
3	Y	609	CLA	CHB-C1B-C2B	-2.59	119.91	127.24
2	N	301	CHL	CHD-C1D-ND	-2.59	122.07	124.45
3	Y	612	CLA	CHB-C1B-NB	2.59	127.00	124.26
6	G	617	NEX	O24-C25-C26	-2.58	56.82	58.96
3	Y	612	CLA	C3B-C4B-NB	-2.58	108.12	110.52
3	N	314	CLA	O2D-CGD-CBD	2.58	115.85	111.27
4	G	614	LUT	C12-C13-C14	2.58	122.89	118.94
4	G	615	LUT	C19-C9-C8	2.58	122.14	118.08
2	G	605	CHL	CHB-C4A-NA	2.57	128.07	124.51
2	N	309	CHL	CHB-C1B-NB	2.57	126.98	124.26
4	N	316	LUT	C12-C13-C14	2.57	122.88	118.94
2	G	619	CHL	CHD-C1D-ND	-2.57	122.09	124.45
6	G	617	NEX	C19-C9-C10	-2.57	119.33	122.92
4	Y	615	LUT	C15-C35-C34	-2.56	118.22	123.47
6	Y	616	NEX	C24-C23-C22	-2.56	105.83	110.77
4	G	615	LUT	C36-C21-C26	2.56	113.42	109.55
3	G	612	CLA	CHD-C1D-ND	-2.56	122.10	124.45
3	G	611	CLA	CHB-C1B-NB	2.56	126.97	124.26
3	G	603	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
3	Y	611	CLA	CHB-C4A-NA	2.55	128.04	124.51
4	G	615	LUT	C30-C31-C32	-2.55	115.25	123.22
2	G	608	CHL	CHD-C1D-C2D	2.55	130.84	125.48
2	G	608	CHL	C3B-C4B-NB	-2.55	108.15	110.52
2	Y	605	CHL	O2D-CGD-O1D	-2.55	118.85	123.84
2	Y	606	CHL	O2D-CGD-O1D	-2.55	118.86	123.84
2	N	306	CHL	CMB-C2B-C1B	-2.54	121.50	125.37
4	Y	614	LUT	C12-C13-C14	2.54	122.84	118.94
3	G	604	CLA	CHB-C1B-NB	2.54	126.94	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	319	NEX	C24-C23-C22	-2.54	105.88	110.77
5	N	318	XAT	C35-C34-C33	-2.53	123.70	127.31
2	G	605	CHL	C1C-C2C-C3C	-2.53	105.11	107.11
6	Y	616	NEX	C17-C1-C6	-2.52	108.22	110.47
2	Y	606	CHL	CHB-C1B-NB	2.52	126.93	124.26
3	N	312	CLA	CHB-C4A-NA	2.52	128.00	124.51
3	N	313	CLA	CHB-C1B-C2B	-2.52	120.12	127.24
3	Y	613	CLA	CHB-C4A-NA	2.52	127.99	124.51
5	N	321	XAT	C10-C11-C12	-2.51	115.37	123.22
3	G	611	CLA	C3B-C4B-NB	-2.51	108.18	110.52
3	Y	602	CLA	CHD-C1D-ND	-2.51	122.15	124.45
2	N	302	CHL	C3B-C4B-NB	-2.51	108.19	110.52
2	Y	605	CHL	C3B-C4B-NB	-2.50	108.19	110.52
3	N	304	CLA	CHB-C4A-NA	2.50	127.97	124.51
3	N	313	CLA	CHB-C4A-NA	2.50	127.97	124.51
3	G	611	CLA	CHB-C4A-NA	2.50	127.97	124.51
2	N	308	CHL	CHB-C4A-NA	2.50	127.97	124.51
2	N	309	CHL	CHB-C4A-NA	2.49	127.96	124.51
3	N	311	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
3	N	311	CLA	CHB-C4A-NA	2.49	127.95	124.51
3	G	604	CLA	CHB-C4A-NA	2.48	127.95	124.51
2	G	601	CHL	CHB-C1B-NB	2.48	126.88	124.26
3	G	604	CLA	CHD-C1D-ND	-2.48	122.17	124.45
4	G	615	LUT	C3-C4-C5	-2.48	106.91	111.85
3	G	604	CLA	CMB-C2B-C3B	2.48	132.59	126.59
3	G	612	CLA	C3B-C4B-NB	-2.47	108.22	110.52
3	N	315	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
3	G	613	CLA	C3B-C4B-NB	-2.46	108.23	110.52
4	Y	615	LUT	C38-C25-C24	-2.46	118.31	123.56
3	N	303	CLA	CHB-C1B-NB	2.45	126.85	124.26
3	Y	604	CLA	CHC-C4B-NB	2.45	126.85	124.26
4	N	317	LUT	C36-C21-C26	2.45	113.25	109.55
3	G	611	CLA	O2D-CGD-CBD	2.44	115.60	111.27
2	N	302	CHL	CHB-C1B-NB	2.44	126.84	124.26
6	G	617	NEX	C28-C29-C30	2.42	122.66	118.94
2	Y	601	CHL	CHB-C1B-NB	2.42	126.82	124.26
3	Y	610	CLA	CMB-C2B-C1B	-2.42	121.69	125.37
2	N	310	CHL	C3B-C4B-NB	-2.41	108.28	110.52
2	Y	601	CHL	O2A-CGA-O1A	-2.41	117.52	123.59
2	Y	601	CHL	CHD-C1D-ND	-2.40	122.24	124.45
2	Y	601	CHL	CHB-C4A-NA	2.40	127.83	124.51
3	Y	604	CLA	CHD-C1D-ND	-2.40	122.25	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	301	CHL	CHB-C4A-NA	2.39	127.82	124.51
2	N	309	CHL	CHD-C1D-ND	-2.39	122.26	124.45
6	Y	616	NEX	C2-C1-C6	2.38	111.52	109.21
3	Y	602	CLA	CHC-C4B-NB	2.38	126.78	124.26
5	G	616	XAT	C4-C3-C2	-2.38	106.18	110.77
3	N	313	CLA	C1-C2-C3	-2.37	121.94	126.04
3	Y	610	CLA	CHB-C1B-NB	2.37	126.77	124.26
2	G	619	CHL	CHB-C4A-NA	2.37	127.79	124.51
3	G	602	CLA	CHB-C4A-NA	2.37	127.79	124.51
3	G	611	CLA	C1-C2-C3	-2.37	121.95	126.04
3	Y	610	CLA	CHB-C4A-NA	2.36	127.78	124.51
4	N	317	LUT	C3-C4-C5	-2.36	107.15	111.85
4	G	615	LUT	C15-C35-C34	-2.36	118.64	123.47
3	G	609	CLA	C1D-ND-C4D	-2.36	104.66	106.33
4	Y	615	LUT	C19-C9-C8	2.36	121.79	118.08
2	N	302	CHL	CHB-C4A-NA	2.35	127.77	124.51
2	N	306	CHL	CAA-C2A-C3A	-2.35	106.35	112.78
3	G	609	CLA	CAA-CBA-CGA	-2.35	106.39	113.25
2	N	308	CHL	CHB-C1B-NB	2.35	126.74	124.26
2	G	608	CHL	O2A-CGA-O1A	-2.34	117.68	123.59
3	G	612	CLA	CHB-C4A-NA	2.34	127.75	124.51
2	N	309	CHL	C3B-C4B-NB	-2.34	108.34	110.52
2	N	310	CHL	CHD-C1D-ND	-2.34	122.31	124.45
5	N	318	XAT	C7-C8-C9	-2.34	121.91	125.53
3	Y	604	CLA	CHB-C4A-NA	2.33	127.74	124.51
2	N	307	CHL	CHD-C1D-ND	-2.33	122.31	124.45
3	G	612	CLA	CHB-C1B-NB	2.33	126.72	124.26
3	G	610	CLA	C3B-C4B-NB	-2.32	108.36	110.52
3	N	304	CLA	CHB-C1B-NB	2.32	126.72	124.26
4	Y	615	LUT	C36-C21-C26	2.32	113.06	109.55
3	Y	610	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
7	G	618	LHG	O8-C23-C24	2.31	119.17	111.91
4	G	615	LUT	C11-C10-C9	-2.31	124.01	127.31
4	G	615	LUT	C22-C23-C24	-2.30	109.12	111.74
3	Y	613	CLA	CMB-C2B-C3B	2.30	132.16	126.59
4	N	316	LUT	C15-C35-C34	2.30	128.19	123.47
4	G	614	LUT	C15-C35-C34	2.30	128.18	123.47
4	Y	614	LUT	C15-C35-C34	2.30	128.18	123.47
6	Y	616	NEX	C19-C9-C10	-2.30	119.71	122.92
3	Y	611	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
2	Y	607	CHL	CHA-C4D-ND	2.29	137.30	132.50
3	G	602	CLA	CMB-C2B-C1B	-2.29	121.88	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	319	NEX	C26-C27-C28	-2.29	121.15	125.99
3	Y	602	CLA	C1-C2-C3	-2.29	122.08	126.04
3	N	305	CLA	CHD-C1D-ND	-2.29	122.35	124.45
3	G	603	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
4	G	615	LUT	C35-C15-C14	-2.28	118.80	123.47
2	G	608	CHL	O2D-CGD-CBD	2.28	115.32	111.27
2	N	306	CHL	CHA-C1A-NA	-2.28	121.19	126.40
3	Y	609	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
4	G	615	LUT	C21-C26-C27	-2.27	109.83	112.70
2	Y	607	CHL	CHA-C1A-NA	-2.26	121.21	126.40
3	Y	610	CLA	C3B-C4B-NB	-2.26	108.42	110.52
2	G	605	CHL	O1D-CGD-CBD	2.26	129.10	124.48
2	N	302	CHL	CHD-C1D-ND	-2.26	122.38	124.45
3	G	603	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
2	N	306	CHL	O2A-CGA-O1A	-2.25	117.91	123.59
3	G	603	CLA	CHB-C4A-NA	2.25	127.62	124.51
7	N	320	LHG	O8-C23-C24	2.24	118.95	111.91
3	G	612	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
3	N	313	CLA	C2B-C1B-NB	2.24	111.73	110.23
3	N	314	CLA	C3B-C4B-NB	-2.23	108.44	110.52
6	G	617	NEX	C40-C33-C34	-2.23	119.80	122.92
2	G	606	CHL	CHC-C4B-NB	2.22	126.61	124.26
3	Y	613	CLA	CAC-C3C-C4C	2.21	127.68	124.81
3	G	602	CLA	C4-C3-C5	2.21	119.00	115.27
2	N	310	CHL	O2D-CGD-CBD	2.21	115.19	111.27
3	G	613	CLA	CHB-C1B-NB	2.20	126.59	124.26
4	G	615	LUT	C20-C13-C12	2.20	121.55	118.08
2	N	301	CHL	O2A-C1-C2	-2.20	103.82	108.97
2	G	606	CHL	C3A-C2A-C1A	2.20	104.64	101.34
3	N	315	CLA	CHB-C4A-NA	2.20	127.56	124.51
6	Y	616	NEX	C31-C32-C33	-2.20	120.23	126.42
2	N	307	CHL	O2D-CGD-CBD	2.20	115.18	111.27
4	N	317	LUT	C19-C9-C8	2.20	121.54	118.08
3	Y	603	CLA	CAA-C2A-C3A	-2.20	106.77	112.78
2	N	306	CHL	CMB-C2B-C3B	2.19	131.90	126.59
3	N	314	CLA	CHB-C4A-NA	2.19	127.54	124.51
3	Y	610	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
2	Y	605	CHL	CHC-C4B-NB	2.18	126.57	124.26
5	N	318	XAT	C40-C33-C32	2.18	121.51	118.08
4	Y	615	LUT	C8-C7-C6	-2.18	121.08	127.20
4	Y	615	LUT	C31-C30-C29	-2.18	124.20	127.31
4	Y	615	LUT	C3-C4-C5	-2.17	107.53	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	609	CLA	CMB-C2B-C3B	2.17	131.84	126.59
3	Y	602	CLA	CHB-C4A-NA	2.17	127.51	124.51
3	N	315	CLA	O2D-CGD-CBD	2.17	115.12	111.27
2	Y	605	CHL	CHB-C4A-NA	2.17	127.51	124.51
3	G	613	CLA	CHB-C4A-NA	2.17	127.51	124.51
3	N	303	CLA	CHB-C4A-NA	2.17	127.51	124.51
2	G	608	CHL	C3C-C4C-NC	-2.16	108.15	110.57
3	N	305	CLA	CHB-C4A-NA	2.15	127.49	124.51
3	N	312	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
3	G	609	CLA	CMB-C2B-C3B	2.15	131.79	126.59
3	Y	612	CLA	CHB-C4A-NA	2.15	127.48	124.51
7	N	320	LHG	C5-O7-C7	-2.14	112.51	117.79
3	G	613	CLA	CHD-C1D-ND	-2.14	122.48	124.45
2	G	608	CHL	CHD-C4C-C3C	2.14	127.99	124.84
3	Y	610	CLA	CMB-C2B-C3B	2.14	131.76	126.59
4	Y	615	LUT	C21-C26-C27	-2.14	110.00	112.70
3	Y	612	CLA	C11-C10-C8	-2.14	109.02	115.92
5	G	616	XAT	O24-C25-C26	-2.13	57.19	58.96
3	N	312	CLA	C3B-C4B-NB	-2.13	108.54	110.52
3	Y	611	CLA	CHB-C1B-NB	2.13	126.51	124.26
3	G	611	CLA	C3A-C2A-C1A	2.13	104.52	101.34
4	Y	615	LUT	C40-C33-C32	2.12	121.42	118.08
3	G	611	CLA	CHC-C4B-NB	2.12	126.50	124.26
3	N	313	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
3	G	602	CLA	CHD-C1D-ND	-2.12	122.50	124.45
2	N	309	CHL	O2A-CGA-O1A	-2.12	118.25	123.59
5	N	321	XAT	C24-C23-C22	-2.11	106.69	110.77
3	N	303	CLA	C1-C2-C3	-2.11	122.39	126.04
4	G	614	LUT	C8-C9-C10	2.11	122.18	118.94
3	N	315	CLA	CHB-C1B-NB	2.11	126.49	124.26
2	N	310	CHL	O2A-CGA-O1A	-2.10	118.28	123.59
3	N	315	CLA	C3B-C4B-NB	-2.10	108.56	110.52
5	N	318	XAT	C10-C11-C12	-2.10	116.66	123.22
6	N	319	NEX	C15-C35-C34	-2.09	119.18	123.47
2	G	601	CHL	O2A-CGA-O1A	-2.09	118.32	123.59
3	N	303	CLA	CHD-C1D-ND	-2.09	122.53	124.45
3	Y	610	CLA	C1-C2-C3	-2.09	122.43	126.04
3	N	311	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
4	Y	614	LUT	C8-C9-C10	2.09	122.15	118.94
2	Y	608	CHL	C3C-C4C-NC	-2.09	108.23	110.57
5	N	318	XAT	C30-C31-C32	-2.08	116.71	123.22
3	Y	602	CLA	O2A-CGA-O1A	-2.08	118.33	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	609	CLA	CHD-C1D-ND	-2.08	122.54	124.45
4	N	316	LUT	C8-C9-C10	2.08	122.13	118.94
2	N	301	CHL	C2A-C1A-CHA	2.08	127.49	123.86
3	Y	603	CLA	CBC-CAC-C3C	-2.08	106.71	112.43
4	Y	614	LUT	C28-C29-C30	2.07	122.12	118.94
2	N	301	CHL	C1-O2A-CGA	2.07	121.87	116.44
3	N	305	CLA	CHB-C1B-NB	2.07	126.45	124.26
3	Y	613	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
3	G	611	CLA	CHD-C1D-ND	-2.06	122.56	124.45
4	G	614	LUT	C28-C29-C30	2.06	122.10	118.94
5	N	318	XAT	C19-C9-C8	2.06	121.32	118.08
2	G	605	CHL	C2C-C3C-C4C	2.05	107.95	106.49
3	N	305	CLA	CMB-C2B-C3B	2.05	131.56	126.59
6	N	319	NEX	C40-C33-C34	-2.05	120.05	122.92
2	N	302	CHL	O2A-CGA-O1A	-2.05	118.42	123.59
2	G	606	CHL	O2A-CGA-O1A	-2.05	118.42	123.59
5	N	318	XAT	C39-C29-C30	-2.05	120.06	122.92
6	N	319	NEX	O24-C25-C26	-2.05	57.27	58.96
4	N	316	LUT	C28-C29-C30	2.04	122.08	118.94
2	G	607	CHL	CHD-C1D-ND	-2.04	122.58	124.45
2	G	606	CHL	CHB-C4A-NA	2.04	127.33	124.51
3	Y	603	CLA	C3C-C4C-NC	-2.04	108.28	110.57
6	G	617	NEX	C31-C30-C29	-2.04	124.40	127.31
3	Y	602	CLA	C3B-C4B-NB	-2.03	108.63	110.52
5	G	616	XAT	O4-C5-C6	-2.03	57.28	58.96
3	Y	604	CLA	CMB-C2B-C3B	2.03	131.51	126.59
3	Y	602	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
3	G	613	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
3	N	304	CLA	C3B-C4B-NB	-2.03	108.63	110.52
2	G	608	CHL	CMB-C2B-C1B	-2.03	122.28	125.37
3	G	610	CLA	CAA-CBA-CGA	-2.02	107.34	113.25
6	Y	616	NEX	O24-C25-C26	-2.01	57.29	58.96
6	N	319	NEX	C31-C32-C33	-2.01	120.76	126.42
2	G	601	CHL	CHD-C1D-ND	-2.01	122.61	124.45
2	G	619	CHL	C2A-C1A-CHA	2.01	127.37	123.86
2	G	608	CHL	C1C-C2C-C3C	-2.01	105.52	107.11
2	G	601	CHL	C2A-C1A-CHA	2.01	127.37	123.86
2	G	607	CHL	CHA-C1A-NA	-2.01	121.80	126.40
3	Y	613	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
2	N	310	CHL	C1C-C2C-C3C	-2.00	105.52	107.11
3	N	314	CLA	CHB-C1B-NB	2.00	126.38	124.26
4	G	615	LUT	C8-C9-C10	-2.00	115.87	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	604	CLA	CHC-C4B-NB	2.00	126.38	124.26
2	G	605	CHL	C3C-C4C-NC	-2.00	108.33	110.57

There are no chirality outliers.

All (519) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	601	CHL	CHA-CBD-CGD-O1D
2	G	601	CHL	CHA-CBD-CGD-O2D
2	G	605	CHL	CAD-CBD-CGD-O1D
2	G	605	CHL	CAD-CBD-CGD-O2D
2	G	606	CHL	C1C-C2C-CMC-OMC
2	G	606	CHL	C3C-C2C-CMC-OMC
2	G	607	CHL	C1C-C2C-CMC-OMC
2	G	607	CHL	C3C-C2C-CMC-OMC
2	G	607	CHL	CBD-CGD-O2D-CED
2	N	302	CHL	CHA-CBD-CGD-O1D
2	N	302	CHL	CHA-CBD-CGD-O2D
2	N	306	CHL	C1C-C2C-CMC-OMC
2	N	306	CHL	C3C-C2C-CMC-OMC
2	N	307	CHL	C1A-C2A-CAA-CBA
2	N	308	CHL	C1C-C2C-CMC-OMC
2	N	308	CHL	C3C-C2C-CMC-OMC
2	N	309	CHL	C1A-C2A-CAA-CBA
2	Y	605	CHL	C1A-C2A-CAA-CBA
2	Y	605	CHL	C2B-C3B-CAB-CBB
2	Y	605	CHL	C4B-C3B-CAB-CBB
2	Y	605	CHL	C1C-C2C-CMC-OMC
2	Y	605	CHL	C3C-C2C-CMC-OMC
2	Y	606	CHL	C2B-C3B-CAB-CBB
2	Y	606	CHL	C4B-C3B-CAB-CBB
2	Y	606	CHL	C1C-C2C-CMC-OMC
2	Y	606	CHL	C3C-C2C-CMC-OMC
2	Y	608	CHL	C1A-C2A-CAA-CBA
2	Y	608	CHL	C3A-C2A-CAA-CBA
2	Y	608	CHL	C2B-C3B-CAB-CBB
2	Y	608	CHL	C4B-C3B-CAB-CBB
2	Y	608	CHL	C1C-C2C-CMC-OMC
2	Y	608	CHL	C3C-C2C-CMC-OMC
3	G	609	CLA	C1A-C2A-CAA-CBA
3	G	609	CLA	CBD-CGD-O2D-CED
3	G	609	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
3	G	609	CLA	C4-C3-C5-C6
3	G	610	CLA	C2B-C3B-CAB-CBB
3	G	610	CLA	C4B-C3B-CAB-CBB
3	G	611	CLA	C2B-C3B-CAB-CBB
3	G	611	CLA	C4B-C3B-CAB-CBB
3	G	611	CLA	CBD-CGD-O2D-CED
3	G	611	CLA	C11-C12-C13-C15
3	G	612	CLA	C4B-C3B-CAB-CBB
3	G	612	CLA	CHA-CBD-CGD-O1D
3	G	612	CLA	CHA-CBD-CGD-O2D
3	N	312	CLA	CAD-CBD-CGD-O1D
3	N	312	CLA	CAD-CBD-CGD-O2D
3	N	313	CLA	C2B-C3B-CAB-CBB
3	N	313	CLA	C4B-C3B-CAB-CBB
3	N	314	CLA	CHA-CBD-CGD-O1D
3	N	314	CLA	CHA-CBD-CGD-O2D
3	N	314	CLA	CBD-CGD-O2D-CED
3	N	315	CLA	CHA-CBD-CGD-O1D
3	N	315	CLA	CHA-CBD-CGD-O2D
3	N	315	CLA	CAD-CBD-CGD-O1D
3	N	315	CLA	CAD-CBD-CGD-O2D
3	N	315	CLA	CBD-CGD-O2D-CED
3	Y	610	CLA	CBD-CGD-O2D-CED
3	Y	612	CLA	C2B-C3B-CAB-CBB
3	Y	612	CLA	C4B-C3B-CAB-CBB
3	Y	612	CLA	CBD-CGD-O2D-CED
4	G	614	LUT	C6-C7-C8-C9
4	N	316	LUT	C6-C7-C8-C9
4	N	317	LUT	C1-C6-C7-C8
4	Y	614	LUT	C6-C7-C8-C9
5	N	321	XAT	O4-C6-C7-C8
5	N	321	XAT	O24-C26-C27-C28
5	N	321	XAT	C31-C32-C33-C34
5	N	321	XAT	C31-C32-C33-C40
6	G	617	NEX	C7-C8-C9-C10
6	G	617	NEX	C7-C8-C9-C19
6	G	617	NEX	O24-C26-C27-C28
6	N	319	NEX	C11-C12-C13-C20
7	G	618	LHG	C3-O3-P-O6
7	G	618	LHG	C4-O6-P-O3
7	G	618	LHG	C4-O6-P-O4
7	G	618	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
7	N	320	LHG	O1-C1-C2-C3
7	N	320	LHG	C3-O3-P-O4
7	N	320	LHG	C4-O6-P-O3
7	Y	617	LHG	O1-C1-C2-C3
7	Y	617	LHG	O7-C5-C6-O8
2	G	607	CHL	O1D-CGD-O2D-CED
3	G	604	CLA	O1D-CGD-O2D-CED
3	G	611	CLA	O1D-CGD-O2D-CED
3	N	314	CLA	O1D-CGD-O2D-CED
3	Y	610	CLA	O1D-CGD-O2D-CED
3	G	602	CLA	CBD-CGD-O2D-CED
3	G	604	CLA	CBD-CGD-O2D-CED
3	G	613	CLA	CBD-CGD-O2D-CED
3	N	303	CLA	CBD-CGD-O2D-CED
3	N	311	CLA	CBD-CGD-O2D-CED
3	Y	604	CLA	CBD-CGD-O2D-CED
3	Y	609	CLA	CBD-CGD-O2D-CED
3	G	613	CLA	O1D-CGD-O2D-CED
3	G	609	CLA	O1D-CGD-O2D-CED
3	G	604	CLA	CBA-CGA-O2A-C1
7	N	320	LHG	C24-C23-O8-C6
2	N	301	CHL	CBD-CGD-O2D-CED
2	N	306	CHL	CBD-CGD-O2D-CED
2	Y	605	CHL	CBD-CGD-O2D-CED
3	G	612	CLA	CBD-CGD-O2D-CED
3	Y	602	CLA	CBD-CGD-O2D-CED
3	Y	603	CLA	CBD-CGD-O2D-CED
3	Y	613	CLA	CBD-CGD-O2D-CED
2	N	306	CHL	O1A-CGA-O2A-C1
2	Y	605	CHL	O1A-CGA-O2A-C1
3	G	604	CLA	O1A-CGA-O2A-C1
3	G	612	CLA	O1A-CGA-O2A-C1
3	G	613	CLA	O1A-CGA-O2A-C1
3	N	312	CLA	O1A-CGA-O2A-C1
7	N	320	LHG	O10-C23-O8-C6
3	N	315	CLA	O1D-CGD-O2D-CED
3	Y	612	CLA	O1D-CGD-O2D-CED
2	G	619	CHL	CBD-CGD-O2D-CED
3	G	611	CLA	C3-C5-C6-C7
3	Y	612	CLA	C3-C5-C6-C7
2	N	306	CHL	CBA-CGA-O2A-C1
2	Y	605	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
3	G	613	CLA	CBA-CGA-O2A-C1
7	Y	617	LHG	C24-C23-O8-C6
3	G	602	CLA	O1D-CGD-O2D-CED
2	G	619	CHL	C2A-CAA-CBA-CGA
2	N	309	CHL	C2A-CAA-CBA-CGA
3	G	609	CLA	C2A-CAA-CBA-CGA
3	G	602	CLA	C3-C5-C6-C7
3	N	313	CLA	C3-C5-C6-C7
3	G	612	CLA	CBA-CGA-O2A-C1
3	N	312	CLA	CBA-CGA-O2A-C1
3	N	303	CLA	O1D-CGD-O2D-CED
3	N	311	CLA	O1D-CGD-O2D-CED
3	Y	604	CLA	O1D-CGD-O2D-CED
3	N	305	CLA	CBD-CGD-O2D-CED
2	N	308	CHL	CBA-CGA-O2A-C1
7	Y	617	LHG	O10-C23-O8-C6
2	Y	606	CHL	CBD-CGD-O2D-CED
3	N	304	CLA	CBD-CGD-O2D-CED
3	Y	609	CLA	O1D-CGD-O2D-CED
2	Y	607	CHL	C2A-CAA-CBA-CGA
2	N	308	CHL	O1A-CGA-O2A-C1
3	G	612	CLA	O1D-CGD-O2D-CED
3	Y	602	CLA	O1D-CGD-O2D-CED
3	Y	613	CLA	O1D-CGD-O2D-CED
3	Y	611	CLA	C3-C5-C6-C7
2	G	605	CHL	CBA-CGA-O2A-C1
3	N	305	CLA	CBA-CGA-O2A-C1
2	Y	605	CHL	O1D-CGD-O2D-CED
3	G	611	CLA	C15-C16-C17-C18
3	N	303	CLA	C10-C11-C12-C13
2	Y	601	CHL	O2A-C1-C2-C3
3	G	602	CLA	C6-C7-C8-C9
3	N	311	CLA	C11-C12-C13-C14
2	N	301	CHL	O1D-CGD-O2D-CED
7	Y	617	LHG	C24-C25-C26-C27
2	G	605	CHL	O1A-CGA-O2A-C1
2	N	306	CHL	O1D-CGD-O2D-CED
3	G	602	CLA	C8-C10-C11-C12
3	Y	609	CLA	C5-C6-C7-C8
3	G	602	CLA	C5-C6-C7-C8
7	Y	617	LHG	C23-C24-C25-C26
3	N	313	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
3	Y	610	CLA	C5-C6-C7-C8
3	Y	603	CLA	O1D-CGD-O2D-CED
3	N	305	CLA	O1A-CGA-O2A-C1
4	G	614	LUT	C9-C10-C11-C12
4	N	316	LUT	C9-C10-C11-C12
4	Y	614	LUT	C9-C10-C11-C12
5	N	318	XAT	C29-C30-C31-C32
3	Y	604	CLA	C2A-CAA-CBA-CGA
3	Y	613	CLA	C2A-CAA-CBA-CGA
4	G	614	LUT	C10-C11-C12-C13
4	N	316	LUT	C10-C11-C12-C13
4	Y	614	LUT	C10-C11-C12-C13
3	N	311	CLA	C15-C16-C17-C18
2	G	619	CHL	O1D-CGD-O2D-CED
3	G	611	CLA	C8-C10-C11-C12
7	N	320	LHG	C3-O3-P-O6
3	G	611	CLA	CBA-CGA-O2A-C1
3	Y	602	CLA	C10-C11-C12-C13
3	Y	610	CLA	C8-C10-C11-C12
3	G	602	CLA	C4-C3-C5-C6
3	Y	611	CLA	C4-C3-C5-C6
3	N	311	CLA	C5-C6-C7-C8
2	G	607	CHL	C2A-CAA-CBA-CGA
2	N	301	CHL	C2A-CAA-CBA-CGA
3	G	604	CLA	C2A-CAA-CBA-CGA
3	Y	609	CLA	C2A-CAA-CBA-CGA
2	G	607	CHL	CBA-CGA-O2A-C1
3	N	304	CLA	CBA-CGA-O2A-C1
7	Y	617	LHG	C29-C30-C31-C32
3	N	311	CLA	C13-C15-C16-C17
3	Y	610	CLA	C13-C15-C16-C17
3	N	312	CLA	C2A-CAA-CBA-CGA
3	N	315	CLA	C2A-CAA-CBA-CGA
3	Y	602	CLA	C8-C10-C11-C12
7	N	320	LHG	C32-C33-C34-C35
3	G	611	CLA	C5-C6-C7-C8
3	N	305	CLA	O1D-CGD-O2D-CED
3	Y	611	CLA	CBA-CGA-O2A-C1
3	G	603	CLA	C3A-C2A-CAA-CBA
3	G	609	CLA	C3A-C2A-CAA-CBA
3	N	304	CLA	C3A-C2A-CAA-CBA
7	N	320	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	G	611	CLA	O1A-CGA-O2A-C1
3	N	313	CLA	C2-C3-C5-C6
3	Y	611	CLA	C2-C3-C5-C6
3	Y	612	CLA	C2-C3-C5-C6
7	Y	617	LHG	C34-C35-C36-C37
3	N	304	CLA	O1D-CGD-O2D-CED
7	N	320	LHG	O1-C1-C2-O2
7	Y	617	LHG	O1-C1-C2-O2
3	N	304	CLA	O1A-CGA-O2A-C1
3	G	612	CLA	C2B-C3B-CAB-CBB
7	G	618	LHG	C9-C10-C11-C12
7	Y	617	LHG	C15-C16-C17-C18
3	N	311	CLA	C16-C17-C18-C20
7	Y	617	LHG	C14-C15-C16-C17
2	Y	606	CHL	O1D-CGD-O2D-CED
2	G	607	CHL	O1A-CGA-O2A-C1
3	Y	611	CLA	O1A-CGA-O2A-C1
3	G	602	CLA	C11-C10-C8-C7
3	N	311	CLA	C11-C12-C13-C15
2	G	608	CHL	C2C-C3C-CAC-CBC
3	Y	612	CLA	C5-C6-C7-C8
7	N	320	LHG	O9-C7-O7-C5
2	N	301	CHL	C2C-C3C-CAC-CBC
2	G	606	CHL	C2A-CAA-CBA-CGA
3	G	612	CLA	C2A-CAA-CBA-CGA
3	Y	602	CLA	C2A-CAA-CBA-CGA
3	N	313	CLA	C5-C6-C7-C8
7	Y	617	LHG	C32-C33-C34-C35
2	Y	608	CHL	CBD-CGD-O2D-CED
3	Y	612	CLA	C16-C17-C18-C19
3	Y	609	CLA	C8-C10-C11-C12
3	Y	611	CLA	C15-C16-C17-C18
7	N	320	LHG	C8-C7-O7-C5
7	Y	617	LHG	O2-C2-C3-O3
3	N	313	CLA	C4-C3-C5-C6
3	Y	612	CLA	C4-C3-C5-C6
3	G	602	CLA	C2-C3-C5-C6
3	Y	602	CLA	C6-C7-C8-C9
3	Y	610	CLA	C14-C13-C15-C16
7	Y	617	LHG	C28-C29-C30-C31
3	G	602	CLA	C2A-CAA-CBA-CGA
3	N	303	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	N	320	LHG	C13-C14-C15-C16
3	G	603	CLA	C1A-C2A-CAA-CBA
3	G	604	CLA	C1A-C2A-CAA-CBA
3	N	304	CLA	C1A-C2A-CAA-CBA
3	Y	609	CLA	C1A-C2A-CAA-CBA
3	Y	610	CLA	C1A-C2A-CAA-CBA
3	N	311	CLA	C16-C17-C18-C19
3	N	313	CLA	C16-C17-C18-C20
2	Y	601	CHL	CBA-CGA-O2A-C1
3	Y	613	CLA	CBA-CGA-O2A-C1
7	N	320	LHG	O6-C4-C5-C6
7	Y	617	LHG	C13-C14-C15-C16
7	N	320	LHG	C28-C29-C30-C31
3	Y	613	CLA	O1A-CGA-O2A-C1
7	Y	617	LHG	C11-C10-C9-C8
7	N	320	LHG	C24-C25-C26-C27
3	Y	610	CLA	C4-C3-C5-C6
7	N	320	LHG	C15-C16-C17-C18
4	G	614	LUT	C26-C27-C28-C29
4	N	316	LUT	C26-C27-C28-C29
4	Y	614	LUT	C26-C27-C28-C29
2	Y	601	CHL	O1A-CGA-O2A-C1
3	G	611	CLA	C10-C11-C12-C13
3	G	611	CLA	C6-C7-C8-C10
3	Y	602	CLA	C6-C7-C8-C10
3	Y	610	CLA	C12-C13-C15-C16
3	G	602	CLA	C11-C10-C8-C9
3	G	611	CLA	C11-C10-C8-C9
3	Y	610	CLA	C2-C3-C5-C6
2	G	608	CHL	C4C-C3C-CAC-CBC
3	Y	604	CLA	CBA-CGA-O2A-C1
2	N	307	CHL	C3A-C2A-CAA-CBA
2	N	309	CHL	C3A-C2A-CAA-CBA
3	Y	611	CLA	C5-C6-C7-C8
2	G	605	CHL	C3C-C2C-CMC-OMC
2	G	608	CHL	C3C-C2C-CMC-OMC
2	N	301	CHL	C3C-C2C-CMC-OMC
2	Y	607	CHL	C3C-C2C-CMC-OMC
3	N	313	CLA	C16-C17-C18-C19
3	Y	612	CLA	C16-C17-C18-C20
3	Y	602	CLA	C15-C16-C17-C18
3	G	611	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	N	303	CLA	C6-C7-C8-C9
3	N	311	CLA	C14-C13-C15-C16
3	Y	610	CLA	C11-C12-C13-C14
4	N	317	LUT	C5-C6-C7-C8
7	N	320	LHG	C30-C31-C32-C33
4	G	614	LUT	C27-C28-C29-C39
4	N	316	LUT	C27-C28-C29-C39
4	Y	614	LUT	C27-C28-C29-C39
6	N	319	NEX	C11-C12-C13-C14
2	Y	608	CHL	O1D-CGD-O2D-CED
7	N	320	LHG	C11-C10-C9-C8
3	G	611	CLA	C11-C10-C8-C7
3	G	611	CLA	C12-C13-C15-C16
3	N	303	CLA	C6-C7-C8-C10
3	Y	612	CLA	C8-C10-C11-C12
3	G	609	CLA	CBA-CGA-O2A-C1
2	G	606	CHL	CAD-CBD-CGD-O2D
3	G	609	CLA	CAD-CBD-CGD-O2D
3	N	303	CLA	CAD-CBD-CGD-O2D
3	N	304	CLA	CAD-CBD-CGD-O2D
6	N	319	NEX	C7-C8-C9-C19
2	Y	606	CHL	CBA-CGA-O2A-C1
7	Y	617	LHG	C4-C5-C6-O8
3	G	604	CLA	O2A-C1-C2-C3
3	N	314	CLA	O2A-C1-C2-C3
3	G	610	CLA	CHA-CBD-CGD-O1D
3	G	611	CLA	CHA-CBD-CGD-O1D
3	G	611	CLA	CHA-CBD-CGD-O2D
3	Y	609	CLA	CHA-CBD-CGD-O1D
3	Y	609	CLA	CHA-CBD-CGD-O2D
3	Y	613	CLA	CHA-CBD-CGD-O1D
3	Y	613	CLA	CHA-CBD-CGD-O2D
3	Y	604	CLA	O1A-CGA-O2A-C1
3	G	611	CLA	C11-C12-C13-C14
5	G	616	XAT	C31-C32-C33-C40
2	N	310	CHL	C4B-C3B-CAB-CBB
3	N	312	CLA	C4B-C3B-CAB-CBB
3	N	314	CLA	C4B-C3B-CAB-CBB
3	Y	611	CLA	C4B-C3B-CAB-CBB
7	G	618	LHG	C3-O3-P-O4
7	N	320	LHG	C4-O6-P-O4
3	G	613	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	Y	612	CLA	C2A-CAA-CBA-CGA
3	Y	613	CLA	CAD-CBD-CGD-O1D
2	Y	606	CHL	C3A-C2A-CAA-CBA
3	G	609	CLA	C11-C12-C13-C15
7	N	320	LHG	O6-C4-C5-O7
6	G	617	NEX	C29-C30-C31-C32
2	Y	606	CHL	O1A-CGA-O2A-C1
7	Y	617	LHG	C33-C34-C35-C36
2	G	608	CHL	C1C-C2C-CMC-OMC
2	N	301	CHL	C1C-C2C-CMC-OMC
2	Y	607	CHL	C1C-C2C-CMC-OMC
3	G	609	CLA	O1A-CGA-O2A-C1
3	G	611	CLA	C14-C13-C15-C16
2	G	608	CHL	O1A-CGA-O2A-C1
2	N	301	CHL	C4C-C3C-CAC-CBC
3	Y	603	CLA	C2A-CAA-CBA-CGA
3	N	311	CLA	C2B-C3B-CAB-CBB
3	Y	602	CLA	C2B-C3B-CAB-CBB
2	G	606	CHL	C1-C2-C3-C4
2	G	607	CHL	C1-C2-C3-C4
2	G	608	CHL	C1-C2-C3-C4
2	G	619	CHL	C1-C2-C3-C4
2	N	301	CHL	C1-C2-C3-C4
2	N	302	CHL	C1-C2-C3-C4
2	N	307	CHL	C1-C2-C3-C4
2	N	309	CHL	C1-C2-C3-C4
2	N	310	CHL	C1-C2-C3-C4
2	Y	606	CHL	C1-C2-C3-C4
2	Y	607	CHL	C1-C2-C3-C4
3	G	603	CLA	C1-C2-C3-C4
3	G	604	CLA	C1-C2-C3-C4
3	G	610	CLA	C1-C2-C3-C4
3	G	612	CLA	C1-C2-C3-C4
3	G	613	CLA	C1-C2-C3-C4
3	N	304	CLA	C1-C2-C3-C4
3	N	305	CLA	C1-C2-C3-C4
3	N	312	CLA	C1-C2-C3-C4
3	N	314	CLA	C1-C2-C3-C4
3	N	315	CLA	C1-C2-C3-C4
3	Y	603	CLA	C1-C2-C3-C4
3	Y	604	CLA	C1-C2-C3-C4
3	Y	613	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	Y	606	CHL	C2A-CAA-CBA-CGA
3	N	313	CLA	C2A-CAA-CBA-CGA
3	Y	611	CLA	C2A-CAA-CBA-CGA
2	G	606	CHL	C2-C1-O2A-CGA
2	N	302	CHL	C2-C1-O2A-CGA
2	N	310	CHL	C2-C1-O2A-CGA
3	G	602	CLA	C2-C1-O2A-CGA
2	G	608	CHL	CBA-CGA-O2A-C1
4	Y	615	LUT	C1-C6-C7-C8
3	Y	610	CLA	C11-C12-C13-C15
3	N	314	CLA	CBA-CGA-O2A-C1
7	N	320	LHG	C5-C4-O6-P
4	G	614	LUT	C27-C28-C29-C30
4	N	316	LUT	C27-C28-C29-C30
3	G	610	CLA	O2A-C1-C2-C3
3	Y	612	CLA	CBA-CGA-O2A-C1
3	Y	612	CLA	C13-C15-C16-C17
2	N	302	CHL	O1A-CGA-O2A-C1
3	N	304	CLA	C4B-C3B-CAB-CBB
3	N	311	CLA	C4B-C3B-CAB-CBB
3	N	315	CLA	C4B-C3B-CAB-CBB
4	N	317	LUT	C29-C30-C31-C32
2	Y	608	CHL	C4-C3-C5-C6
2	Y	605	CHL	C2A-CAA-CBA-CGA
3	N	303	CLA	C2A-CAA-CBA-CGA
7	N	320	LHG	C33-C34-C35-C36
2	N	301	CHL	O2A-C1-C2-C3
3	N	304	CLA	O2A-C1-C2-C3
6	G	617	NEX	C33-C34-C35-C15
3	Y	609	CLA	C13-C15-C16-C17
4	G	614	LUT	C11-C10-C9-C19
4	N	316	LUT	C11-C10-C9-C19
4	Y	614	LUT	C11-C10-C9-C19
6	G	617	NEX	C39-C29-C30-C31
6	N	319	NEX	C39-C29-C30-C31
6	Y	616	NEX	C39-C29-C30-C31
4	Y	614	LUT	C27-C28-C29-C30
2	Y	606	CHL	C1A-C2A-CAA-CBA
2	Y	607	CHL	C1A-C2A-CAA-CBA
2	G	619	CHL	C3C-C2C-CMC-OMC
2	N	308	CHL	C2A-CAA-CBA-CGA
3	Y	611	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
2	Y	608	CHL	C2-C3-C5-C6
2	N	310	CHL	C2B-C3B-CAB-CBB
3	N	312	CLA	C2B-C3B-CAB-CBB
3	N	315	CLA	C2B-C3B-CAB-CBB
3	Y	611	CLA	C2B-C3B-CAB-CBB
6	G	617	NEX	C28-C29-C30-C31
6	N	319	NEX	C28-C29-C30-C31
6	Y	616	NEX	C28-C29-C30-C31
3	N	313	CLA	CBA-CGA-O2A-C1
2	G	619	CHL	C2-C1-O2A-CGA
2	G	608	CHL	O2A-C1-C2-C3
2	N	309	CHL	O2A-C1-C2-C3
3	N	313	CLA	O1A-CGA-O2A-C1
4	G	615	LUT	C1-C6-C7-C8
3	N	314	CLA	O1A-CGA-O2A-C1
3	Y	612	CLA	O1A-CGA-O2A-C1
2	N	302	CHL	CBA-CGA-O2A-C1
5	N	321	XAT	C33-C34-C35-C15
2	N	307	CHL	O2A-C1-C2-C3
2	N	310	CHL	O2A-C1-C2-C3
2	Y	607	CHL	O2A-C1-C2-C3
2	Y	607	CHL	O1D-CGD-O2D-CED
2	Y	605	CHL	C3A-C2A-CAA-CBA
2	Y	607	CHL	C3A-C2A-CAA-CBA
3	Y	609	CLA	C3A-C2A-CAA-CBA
3	G	610	CLA	O1A-CGA-O2A-C1
2	Y	606	CHL	CAD-CBD-CGD-O2D
3	G	602	CLA	CAD-CBD-CGD-O2D
3	G	613	CLA	CAD-CBD-CGD-O2D
3	N	311	CLA	CAD-CBD-CGD-O2D
3	G	609	CLA	CAA-CBA-CGA-O2A
3	G	603	CLA	CAA-CBA-CGA-O2A
5	G	616	XAT	C31-C32-C33-C34
6	N	319	NEX	O24-C26-C27-C28
6	Y	616	NEX	O24-C26-C27-C28
3	N	303	CLA	C13-C15-C16-C17
2	Y	605	CHL	CAA-CBA-CGA-O2A
3	Y	613	CLA	O2A-C1-C2-C3
2	G	601	CHL	O2A-C1-C2-C3
3	G	610	CLA	CBA-CGA-O2A-C1
2	N	309	CHL	O1D-CGD-O2D-CED
3	G	604	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
3	G	604	CLA	CHA-CBD-CGD-O2D
3	G	609	CLA	CHA-CBD-CGD-O2D
3	G	610	CLA	CHA-CBD-CGD-O2D
3	N	305	CLA	CHA-CBD-CGD-O1D
3	N	305	CLA	CHA-CBD-CGD-O2D
3	N	312	CLA	CHA-CBD-CGD-O1D
3	N	312	CLA	CHA-CBD-CGD-O2D
3	Y	603	CLA	CHA-CBD-CGD-O1D
3	Y	604	CLA	CHA-CBD-CGD-O1D
3	Y	611	CLA	CHA-CBD-CGD-O2D
5	N	321	XAT	C13-C14-C15-C35
3	G	602	CLA	CAA-CBA-CGA-O2A
3	Y	609	CLA	CAA-CBA-CGA-O2A
7	N	320	LHG	O7-C5-C6-O8
2	Y	608	CHL	CAA-CBA-CGA-O2A
3	Y	602	CLA	CAA-CBA-CGA-O2A
7	Y	617	LHG	O8-C23-C24-C25
3	Y	610	CLA	CAA-CBA-CGA-O2A
3	Y	602	CLA	C11-C12-C13-C15
7	N	320	LHG	O8-C23-C24-C25
4	G	615	LUT	C29-C30-C31-C32
2	G	619	CHL	O2A-C1-C2-C3
3	G	603	CLA	O2A-C1-C2-C3
2	N	310	CHL	CBA-CGA-O2A-C1
3	N	304	CLA	CAA-CBA-CGA-O2A
3	N	314	CLA	C2A-CAA-CBA-CGA
3	Y	610	CLA	C16-C17-C18-C20
3	Y	611	CLA	C16-C17-C18-C19
7	G	618	LHG	C26-C27-C28-C29
3	Y	602	CLA	C1A-C2A-CAA-CBA
7	N	320	LHG	O10-C23-C24-C25
3	G	609	CLA	CAA-CBA-CGA-O1A
2	Y	605	CHL	CAA-CBA-CGA-O1A
3	G	602	CLA	CAA-CBA-CGA-O1A
3	G	609	CLA	C5-C6-C7-C8
7	Y	617	LHG	C5-C4-O6-P
2	Y	608	CHL	CAA-CBA-CGA-O1A
3	G	603	CLA	CAA-CBA-CGA-O1A
3	G	613	CLA	C4B-C3B-CAB-CBB
2	Y	607	CHL	C4C-C3C-CAC-CBC
3	N	305	CLA	O2A-C1-C2-C3
3	N	315	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	N	304	CLA	CAA-CBA-CGA-O1A
3	Y	602	CLA	CAA-CBA-CGA-O1A
3	Y	610	CLA	CAA-CBA-CGA-O1A
3	Y	609	CLA	CAA-CBA-CGA-O1A
7	Y	617	LHG	C30-C31-C32-C33
2	Y	605	CHL	CAD-CBD-CGD-O1D
3	G	610	CLA	CAD-CBD-CGD-O1D
3	Y	604	CLA	CAD-CBD-CGD-O1D
2	N	310	CHL	O1A-CGA-O2A-C1
7	N	320	LHG	O2-C2-C3-O3
3	Y	602	CLA	C11-C12-C13-C14
2	Y	606	CHL	CAA-CBA-CGA-O2A
3	N	303	CLA	CAA-CBA-CGA-O2A
7	N	320	LHG	C1-C2-C3-O3
3	G	611	CLA	C16-C17-C18-C20
2	G	605	CHL	CAA-CBA-CGA-O2A
2	G	619	CHL	CAA-CBA-CGA-O2A
2	N	301	CHL	CAA-CBA-CGA-O2A
3	N	303	CLA	CAA-CBA-CGA-O1A
7	Y	617	LHG	O10-C23-C24-C25
3	N	315	CLA	O1A-CGA-O2A-C1
3	Y	610	CLA	O1A-CGA-O2A-C1

There are no ring outliers.

47 monomers are involved in 125 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	615	LUT	4	0
2	G	608	CHL	1	0
5	G	616	XAT	4	0
3	Y	602	CLA	5	0
5	N	318	XAT	4	0
5	N	321	XAT	2	0
3	Y	613	CLA	1	0
6	G	617	NEX	4	0
2	Y	608	CHL	1	0
3	G	610	CLA	1	0
3	N	311	CLA	2	0
2	Y	605	CHL	4	0
2	N	301	CHL	4	0
6	N	319	NEX	3	0
3	G	602	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	609	CLA	6	0
2	G	601	CHL	2	0
3	Y	610	CLA	8	0
2	N	310	CHL	1	0
2	G	606	CHL	6	0
2	N	302	CHL	2	0
3	Y	611	CLA	4	0
3	G	604	CLA	4	0
7	Y	617	LHG	2	0
3	G	609	CLA	11	0
3	N	314	CLA	1	0
2	Y	606	CHL	9	0
4	Y	615	LUT	4	0
2	Y	607	CHL	1	0
7	G	618	LHG	4	0
2	G	605	CHL	1	0
6	Y	616	NEX	5	0
3	G	603	CLA	1	0
4	N	316	LUT	7	0
2	N	306	CHL	1	0
4	Y	614	LUT	8	0
2	G	607	CHL	3	0
3	N	305	CLA	1	0
4	N	317	LUT	4	0
3	G	611	CLA	3	0
4	G	614	LUT	8	0
7	N	320	LHG	1	0
2	G	619	CHL	2	0
3	G	612	CLA	2	0
3	N	312	CLA	1	0
3	Y	612	CLA	5	0
3	N	313	CLA	1	0

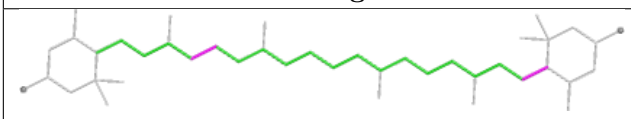
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

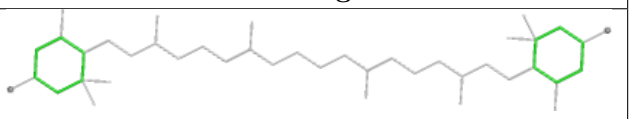
Ligand LUT G 615

Bond lengths

Bond angles

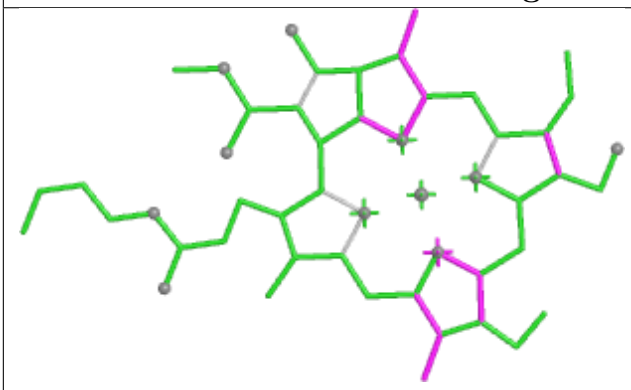


Torsions

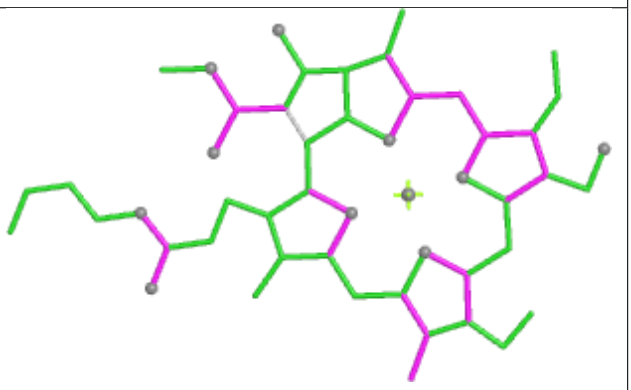


Rings

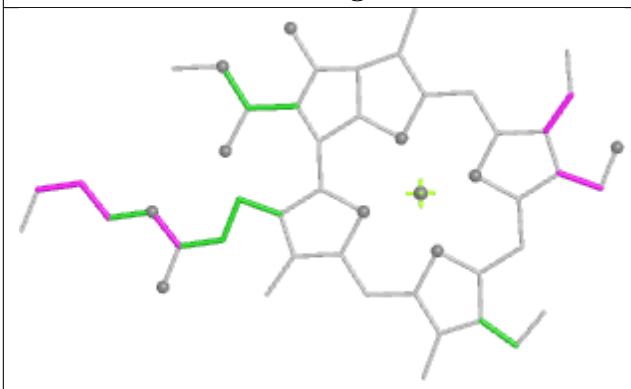
Ligand CHL G 608



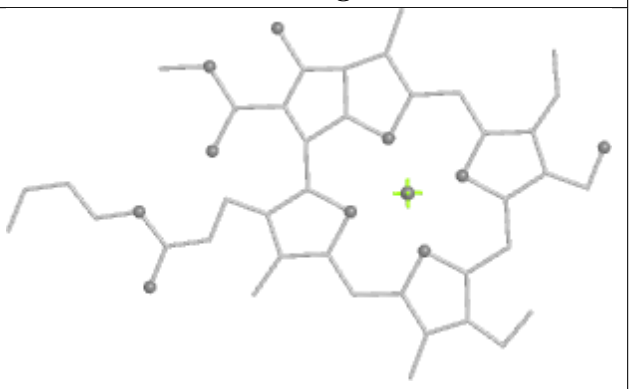
Bond lengths



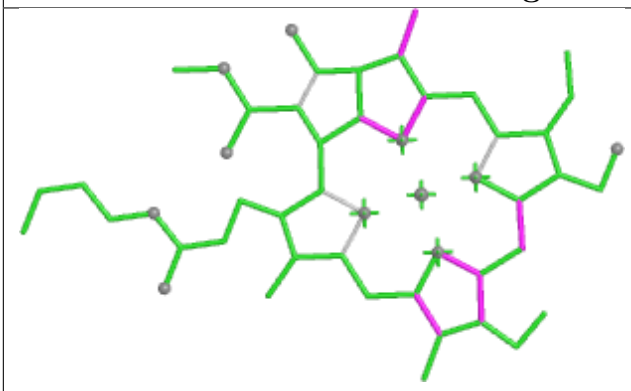
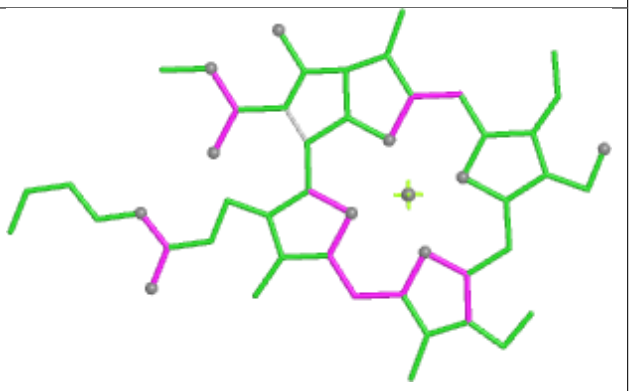
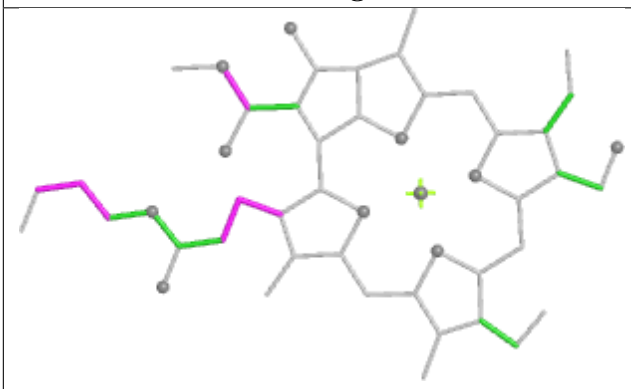
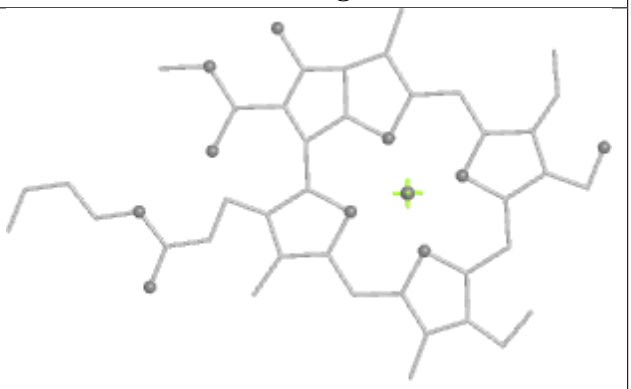
Bond angles

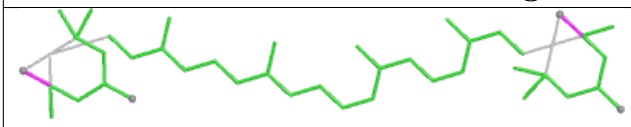
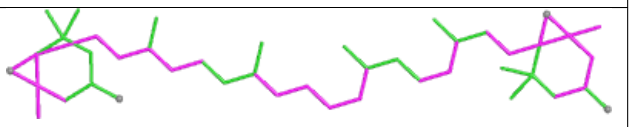
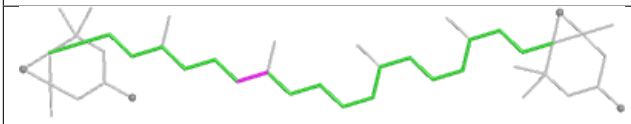
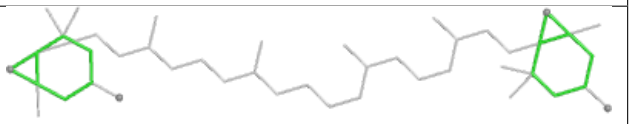


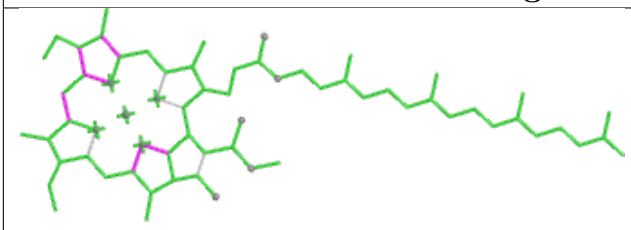
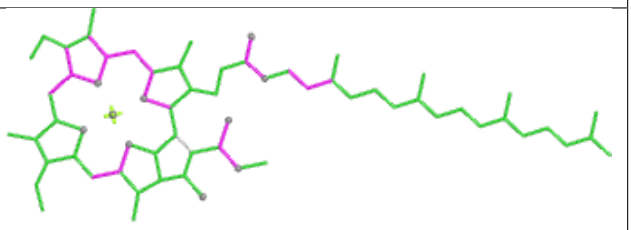
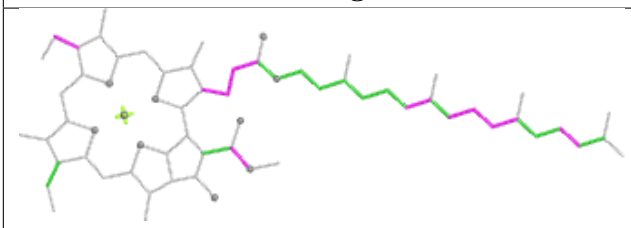
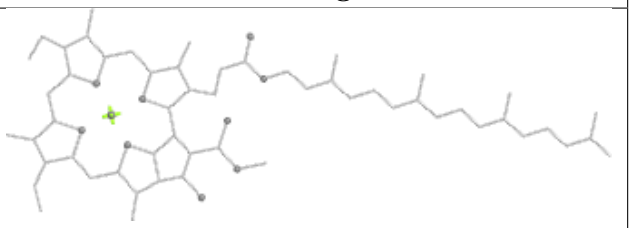
Torsions

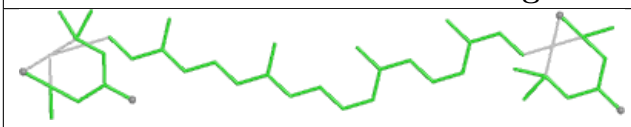
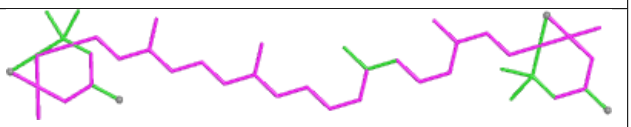
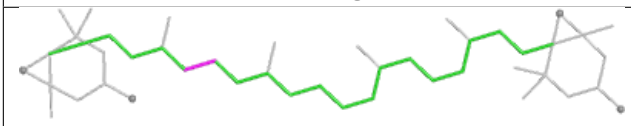
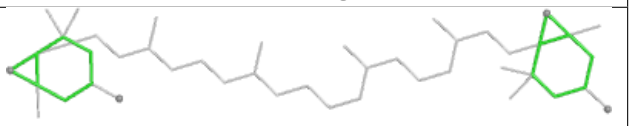


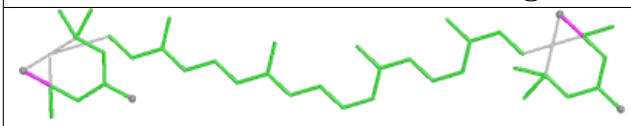
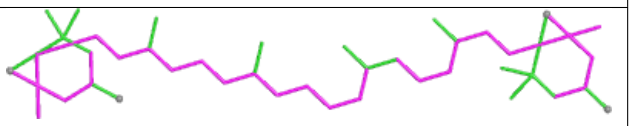
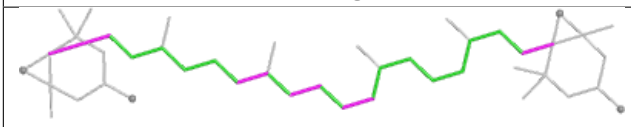
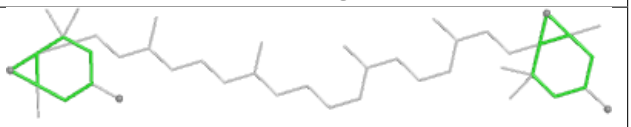
Rings

Ligand CHL N 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

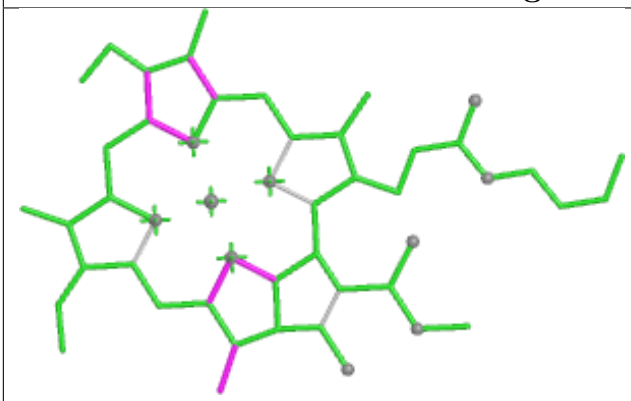
Ligand XAT G 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Y 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

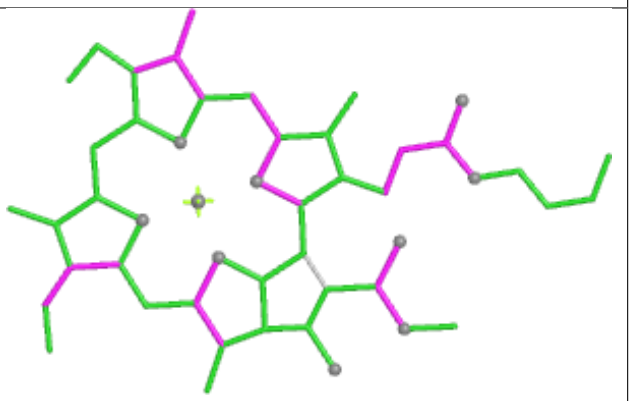
Ligand XAT N 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT N 321	
 Bond lengths	 Bond angles
 Torsions	 Rings

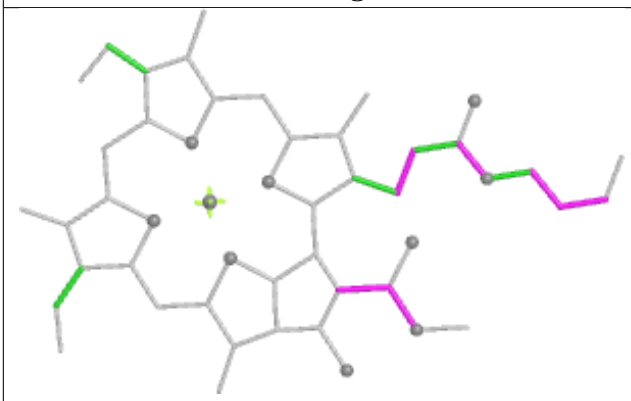
Ligand CLA Y 613



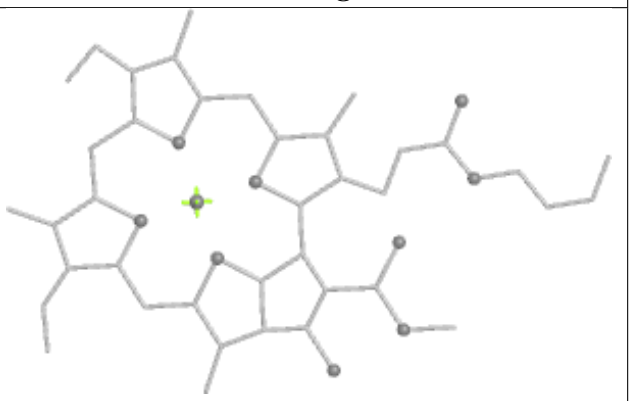
Bond lengths



Bond angles

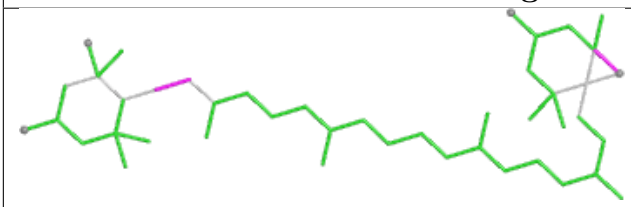


Torsions



Rings

Ligand NEX G 617



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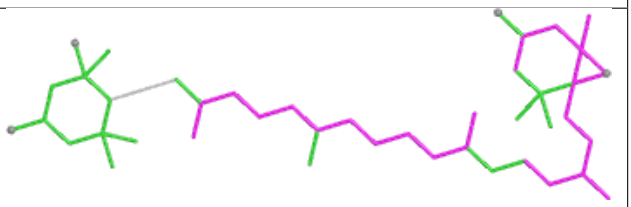
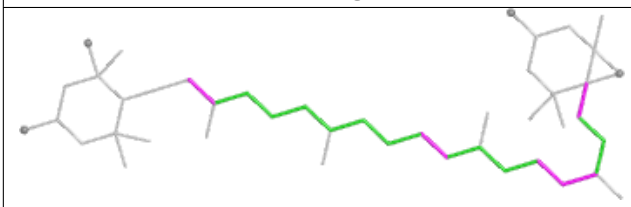
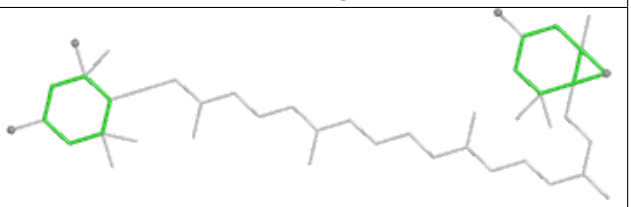


Bond angles

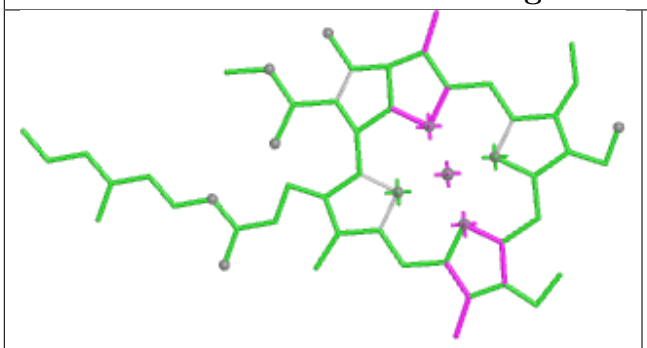


Torsions



Rings

Ligand CHL Y 608



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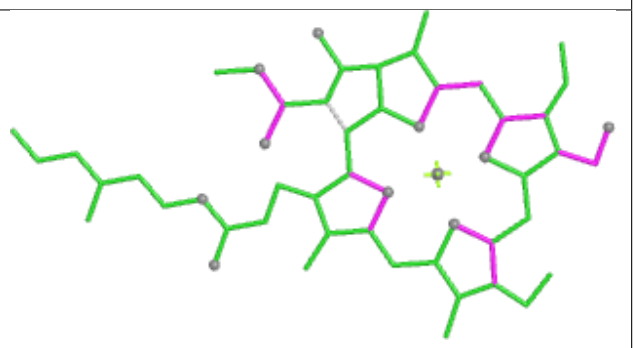
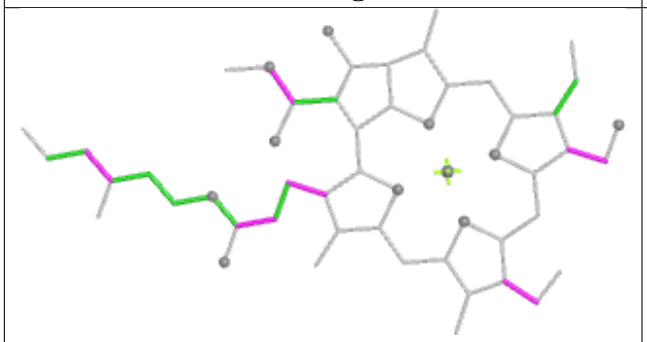
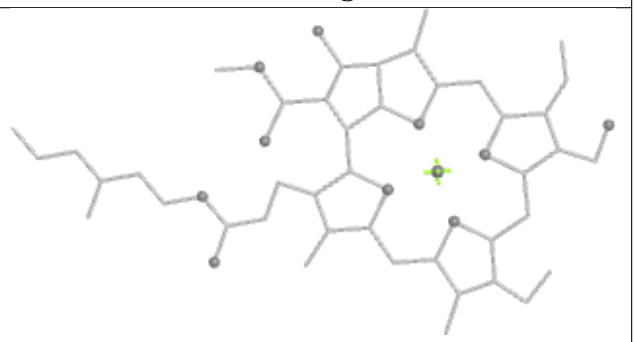


Bond angles

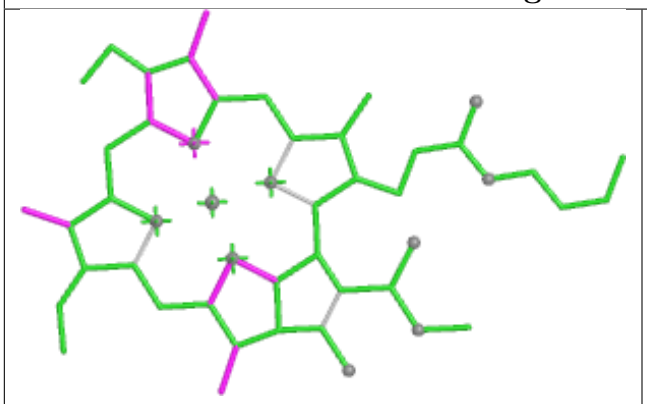


Torsions



Rings

Ligand CLA G 610



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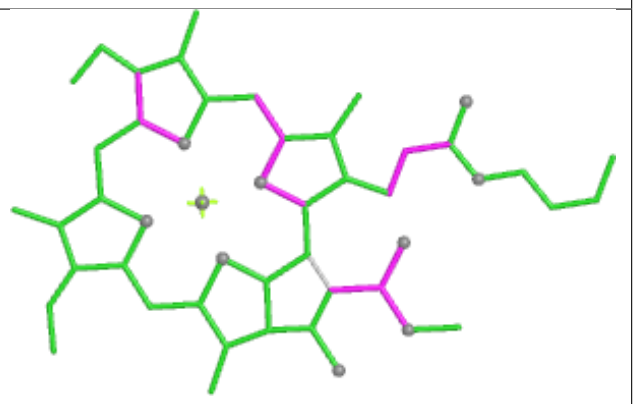
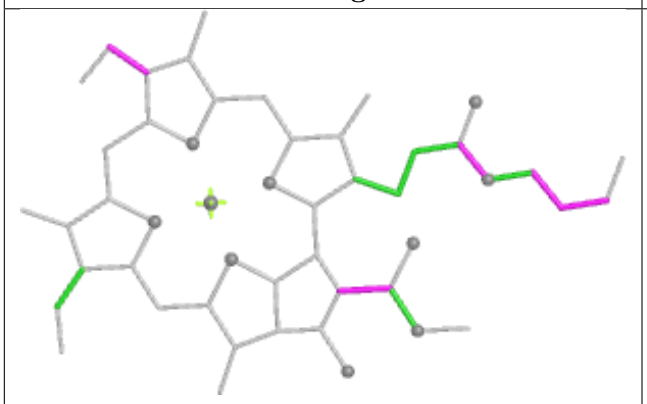
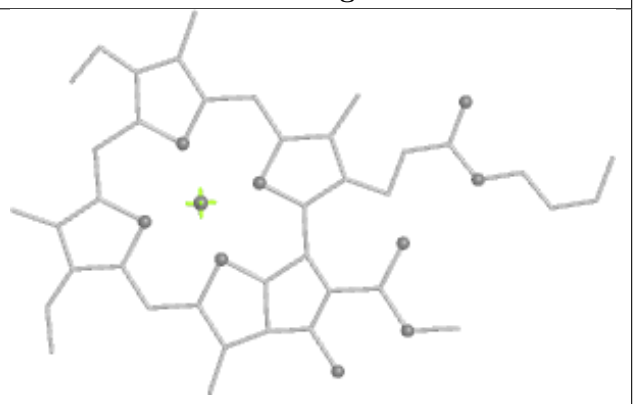


Bond angles

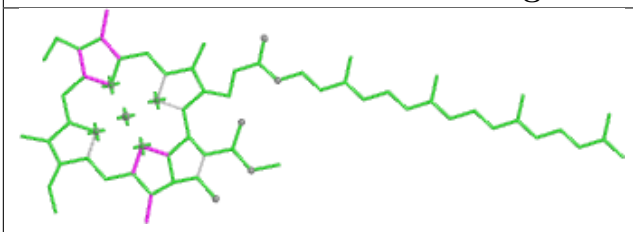


Torsions



Rings

Ligand CLA N 311



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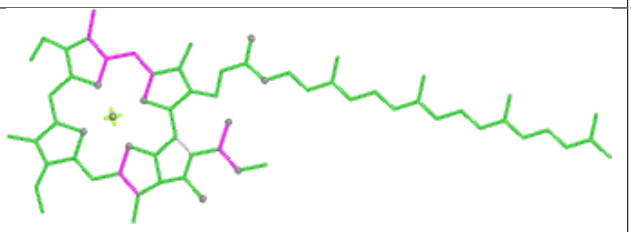
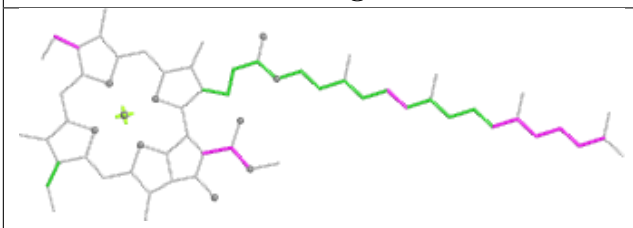


Bond angles



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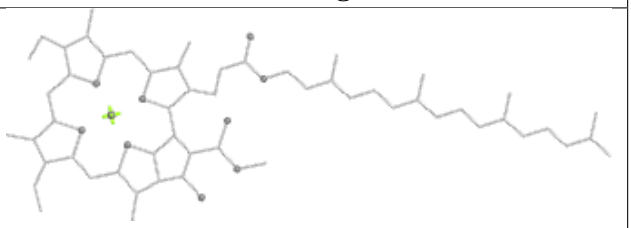
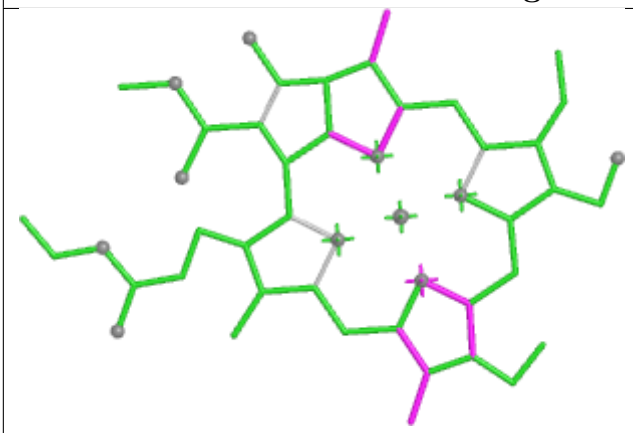
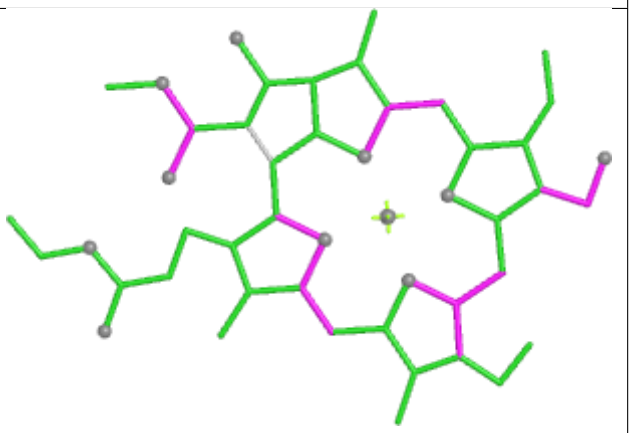


Rings

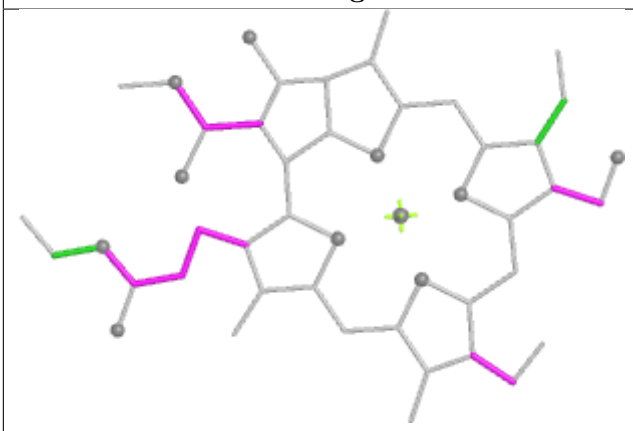
Ligand CHL Y 605



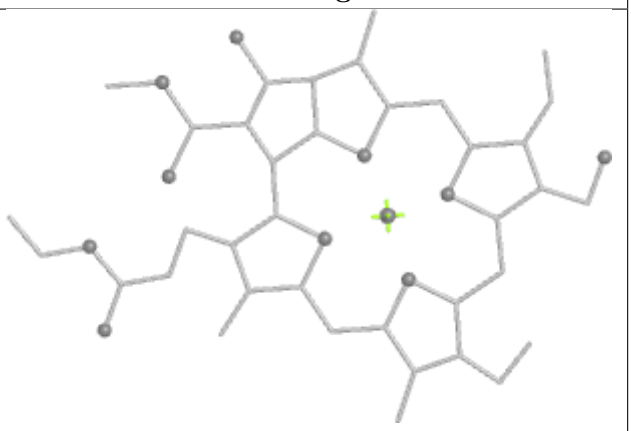
Bond lengths



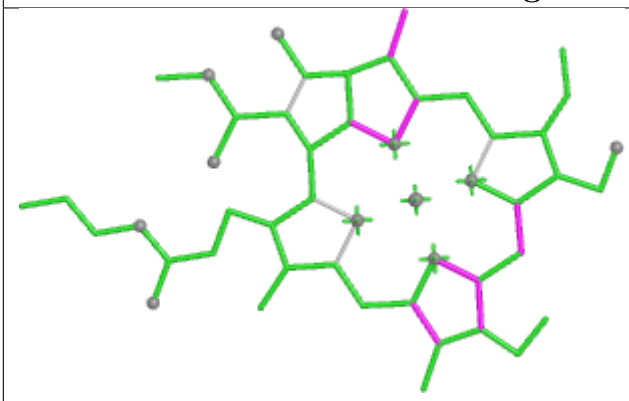
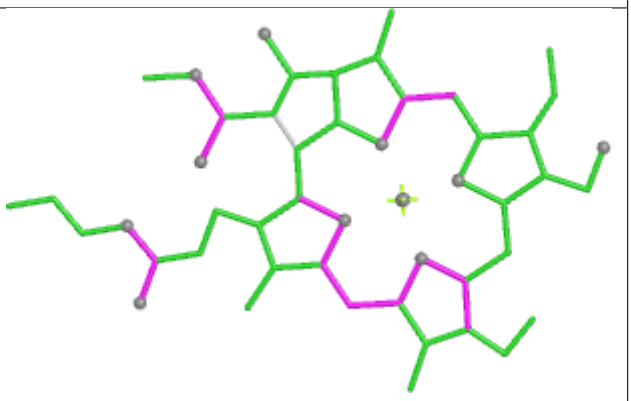
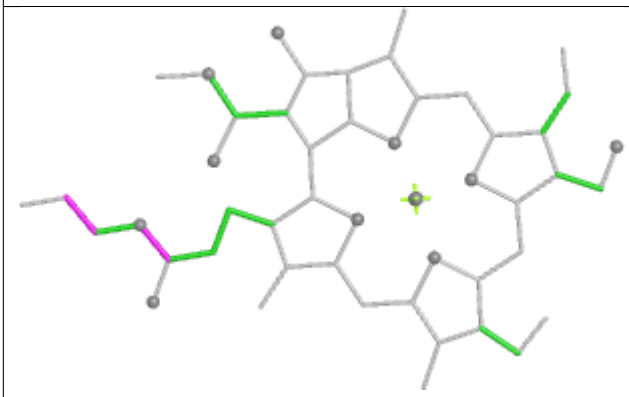
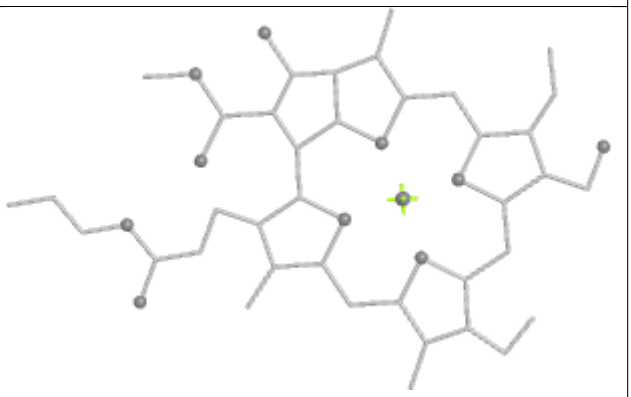
Bond angles

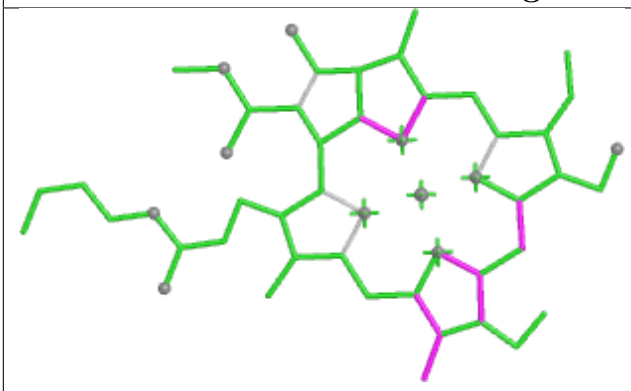
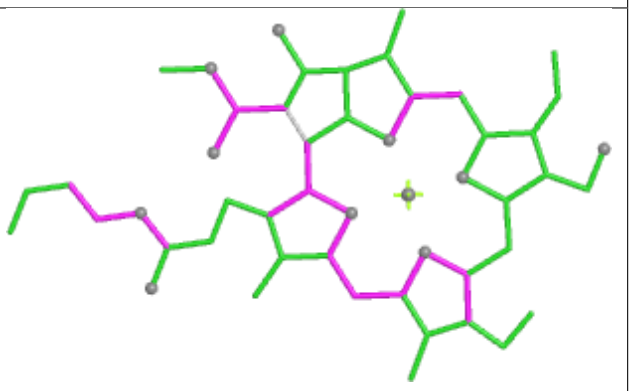
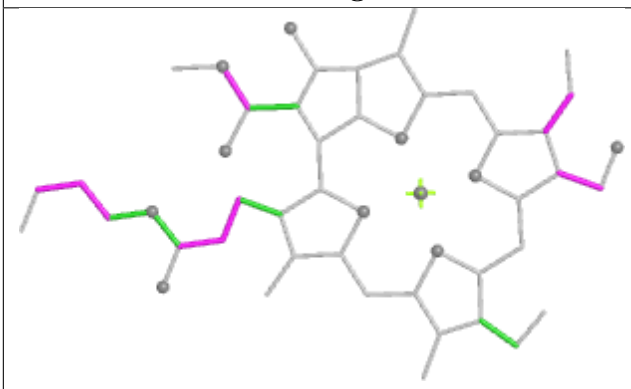
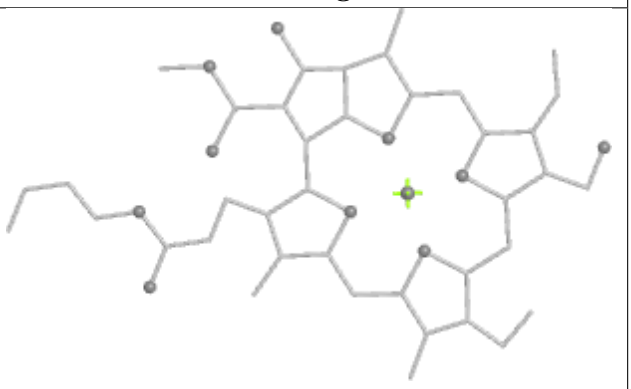


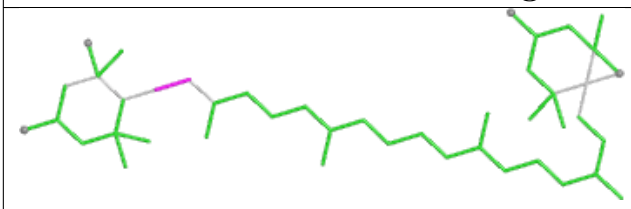
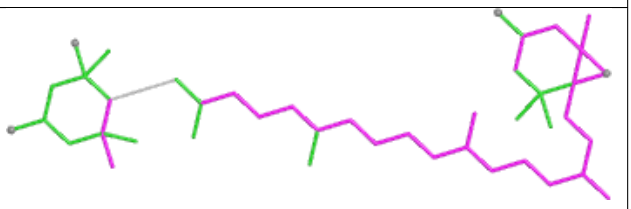
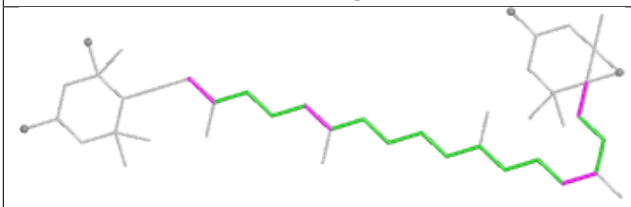
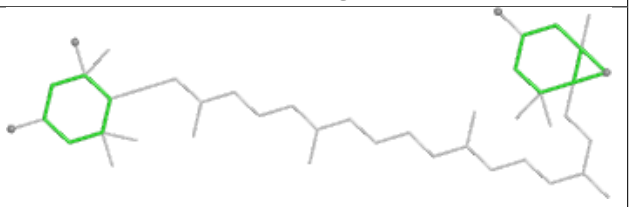
Torsions

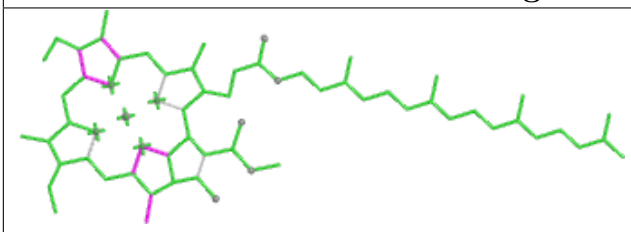
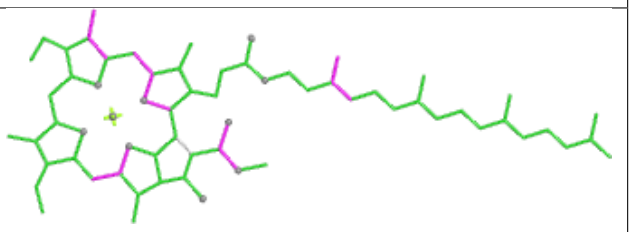
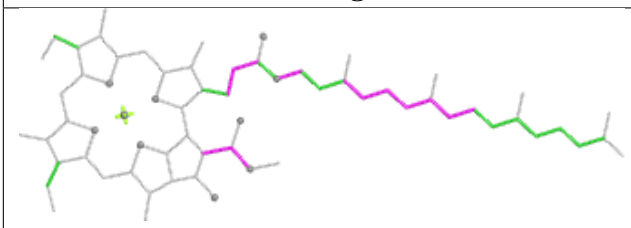
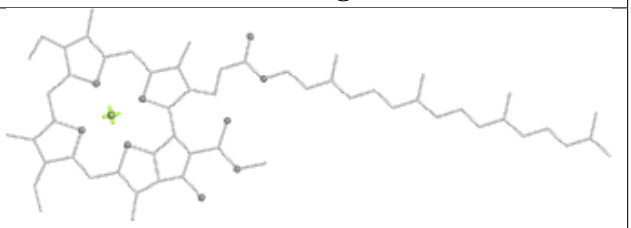


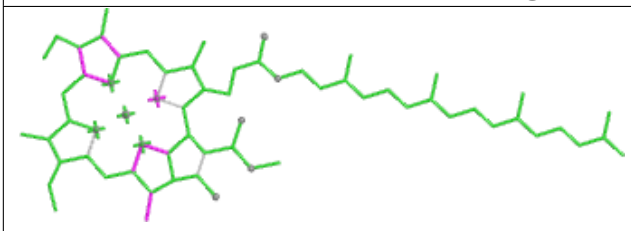
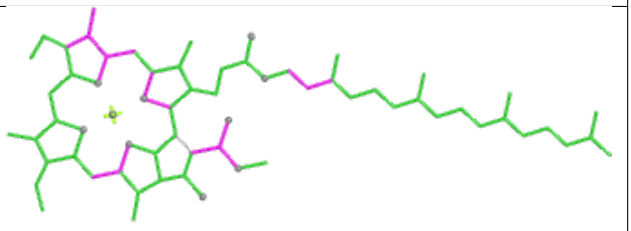
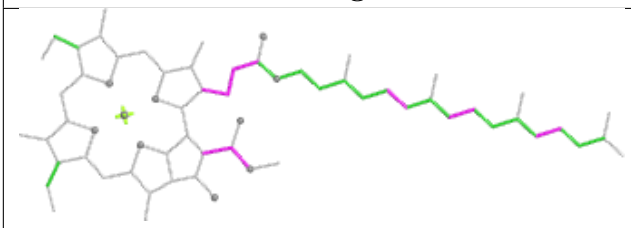
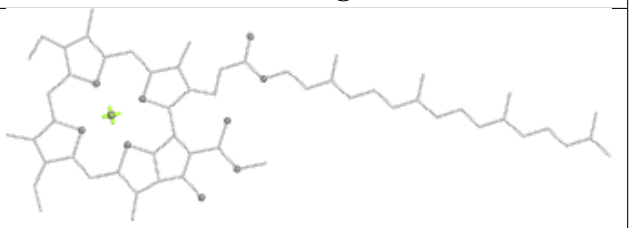
Rings

Ligand CHL Y 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL N 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX N 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Y 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

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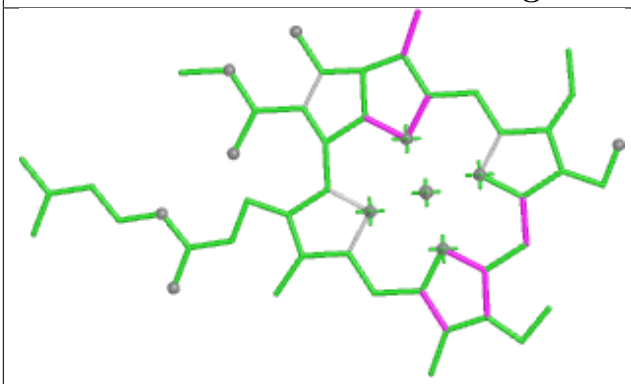
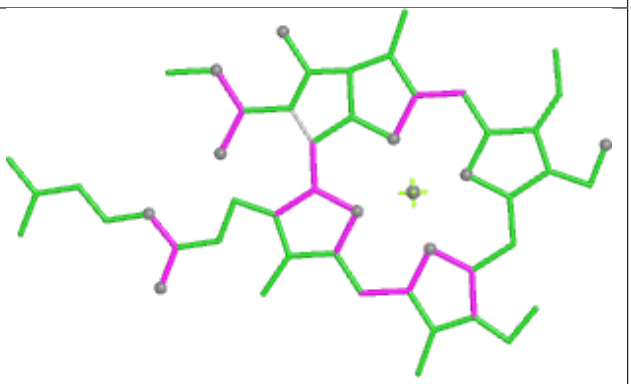
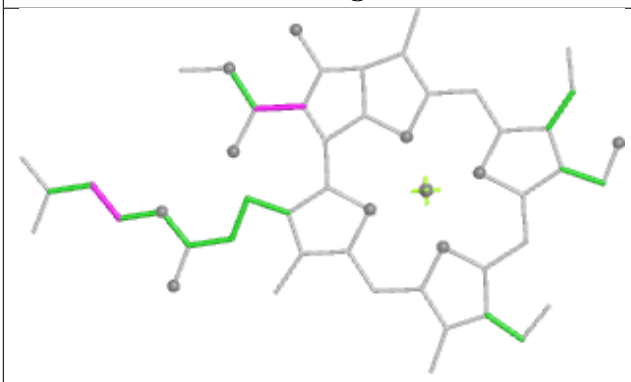
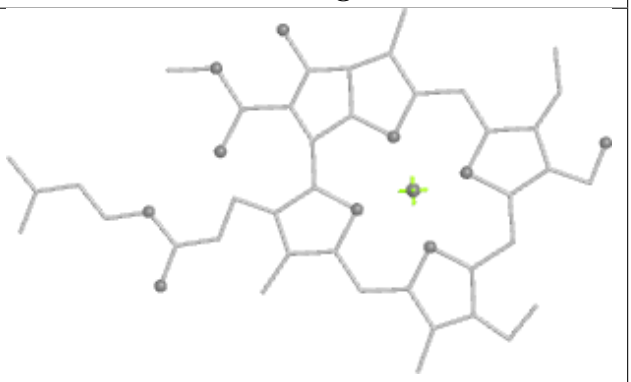
 Bond lengths	 Bond angles
 Torsions	 Rings

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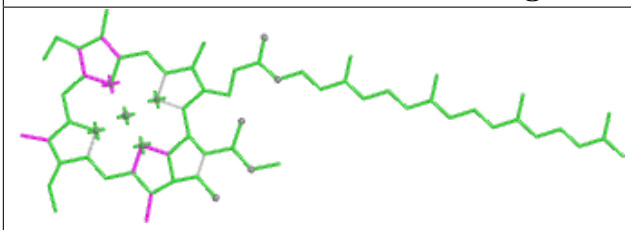
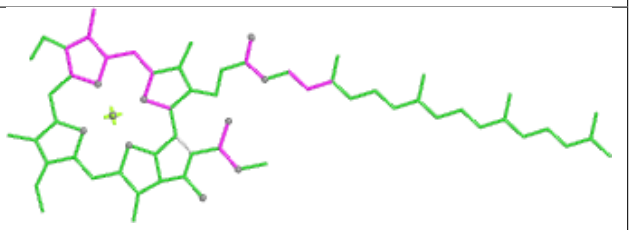
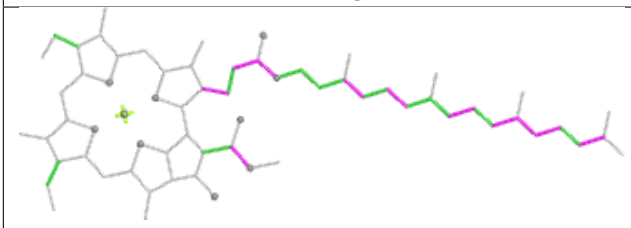
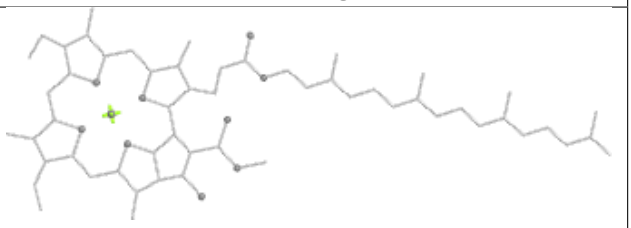
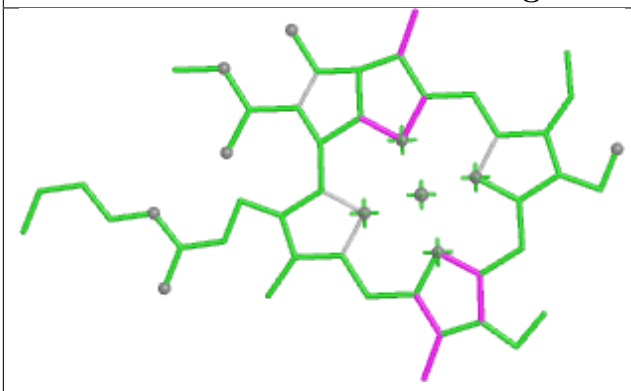
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL N 310



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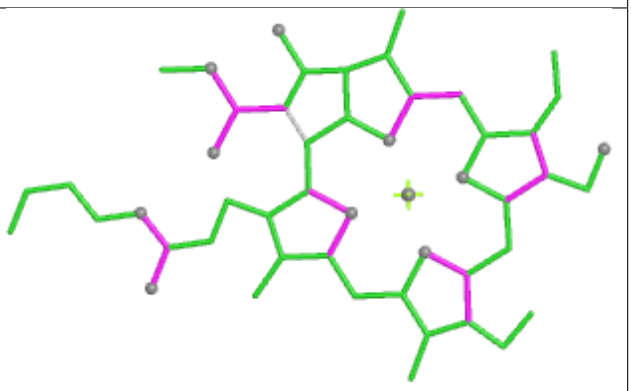
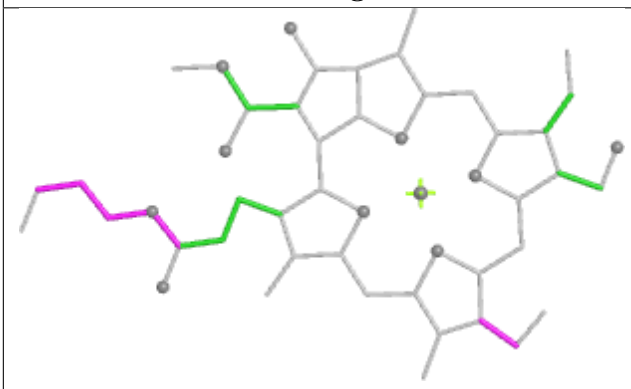
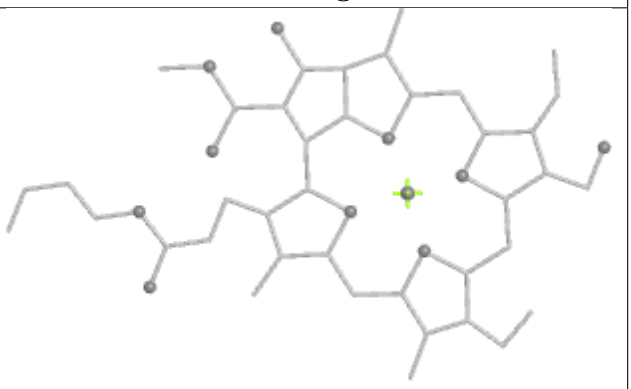


Bond angles

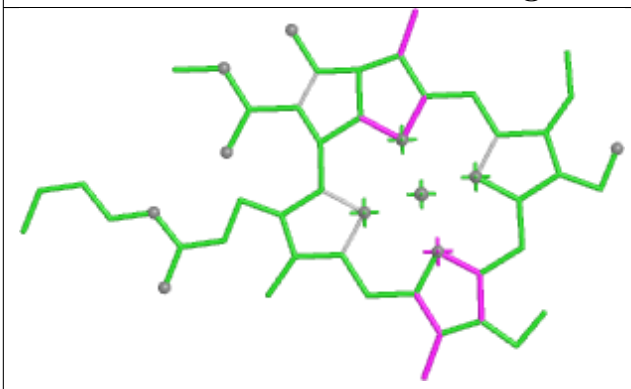


Torsions



Rings

Ligand CHL G 606



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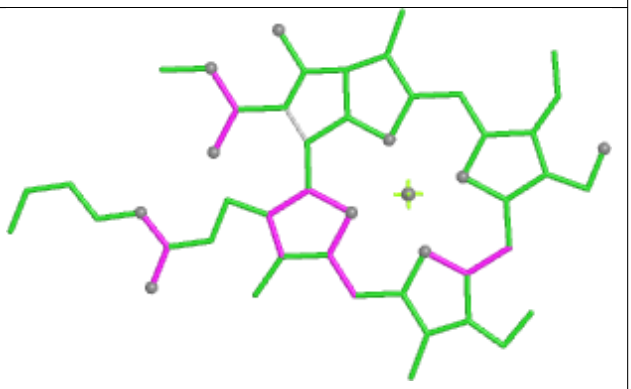
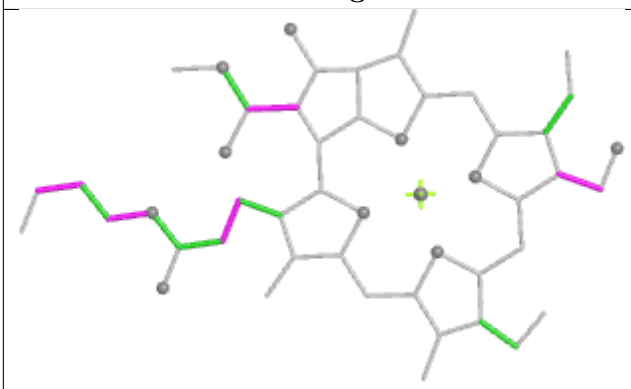


Bond angles



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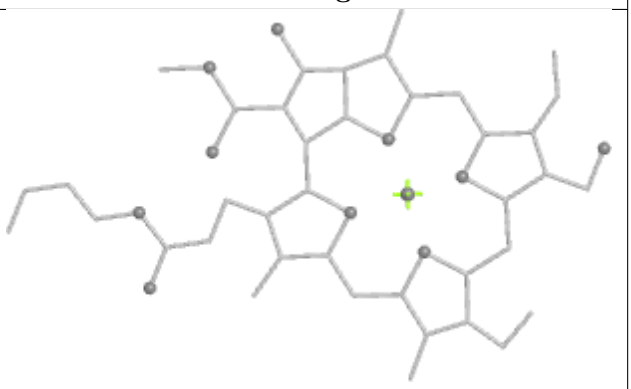
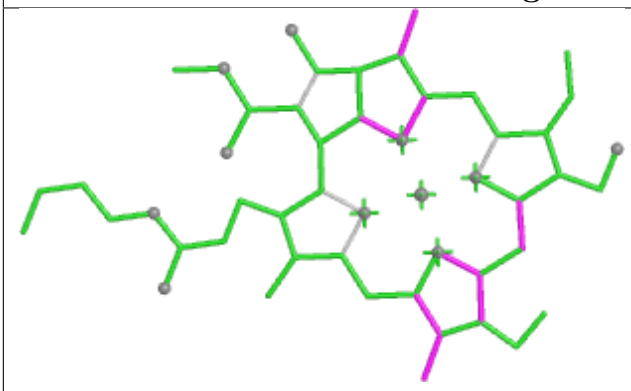
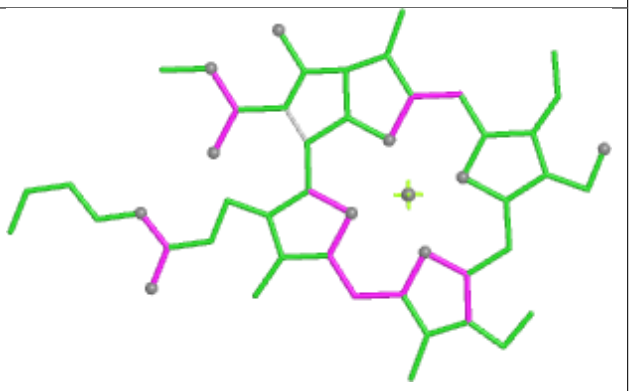
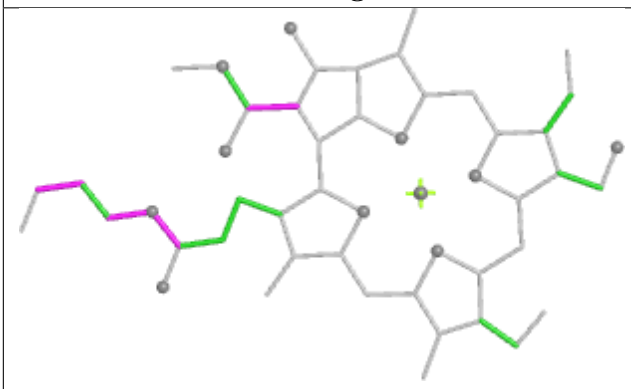
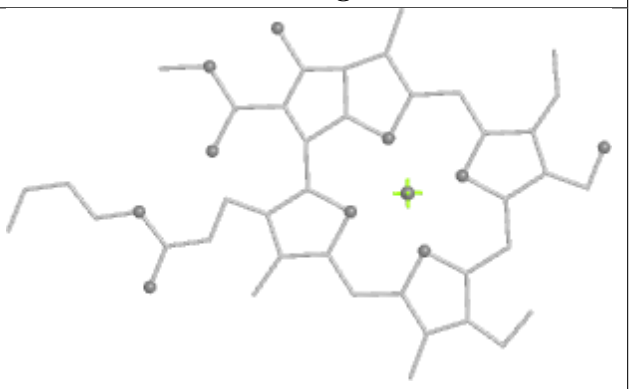
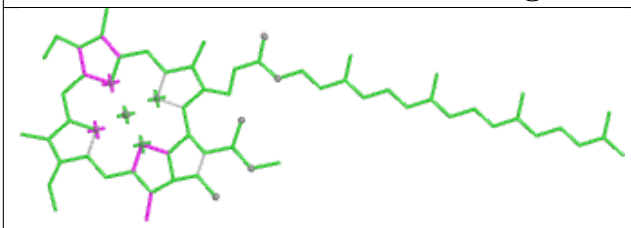
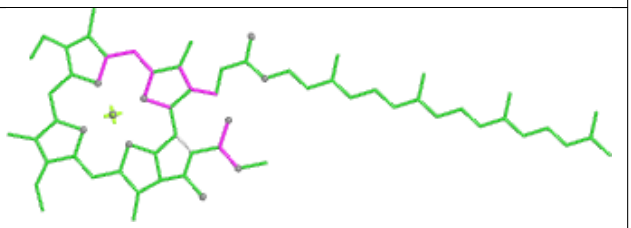
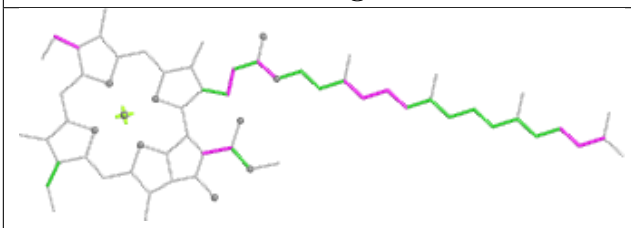
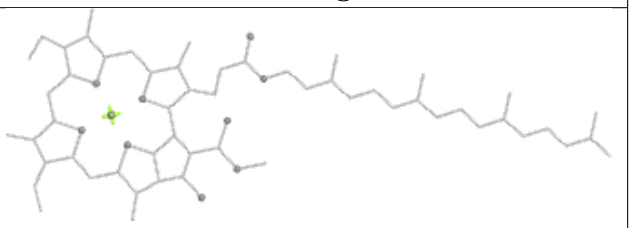
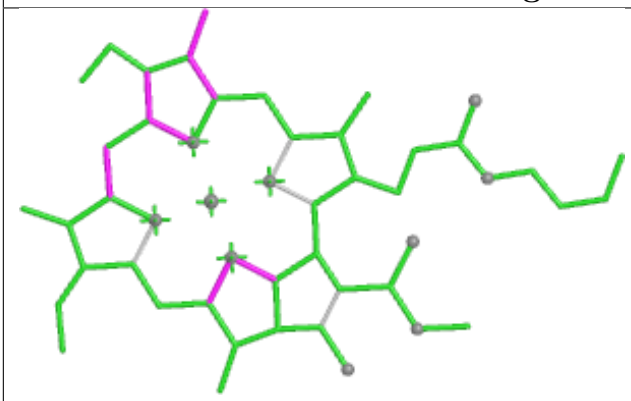
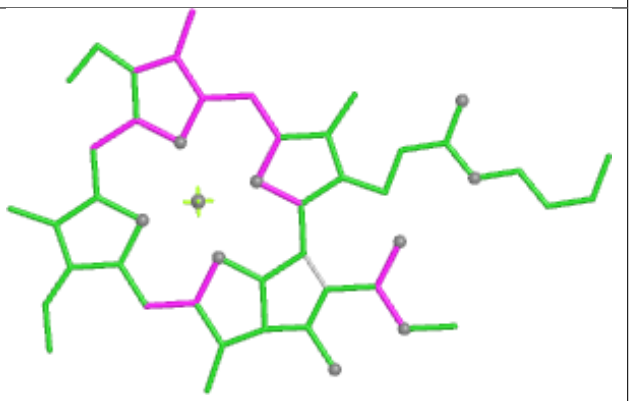
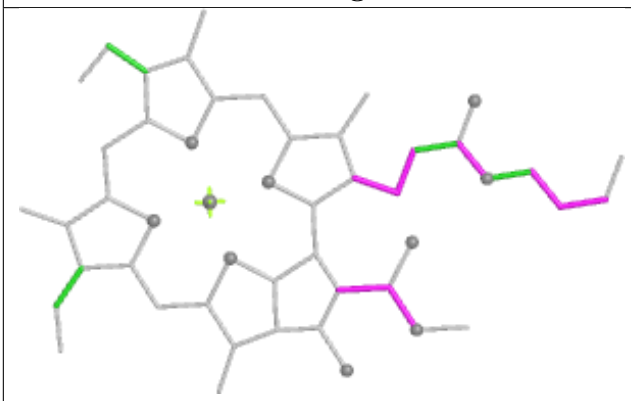
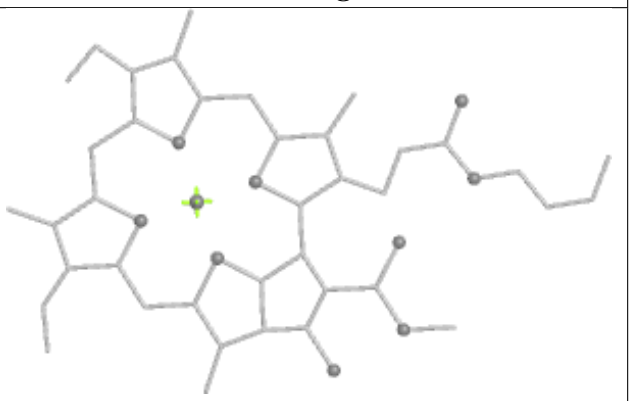


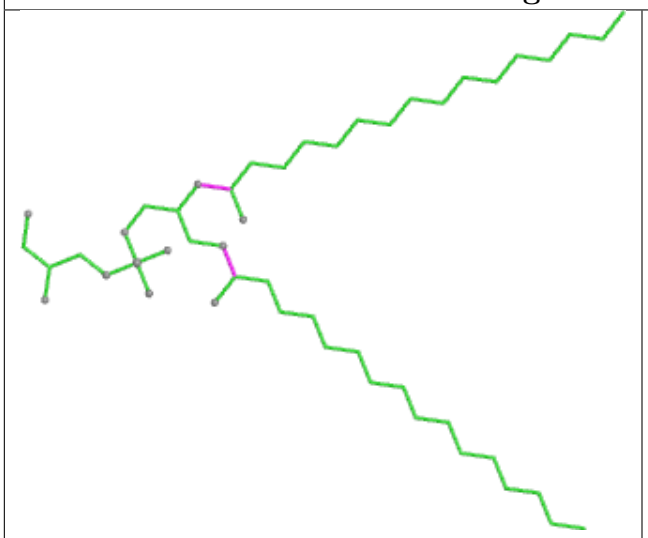
Rings

Ligand CHL N 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Y 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG Y 617



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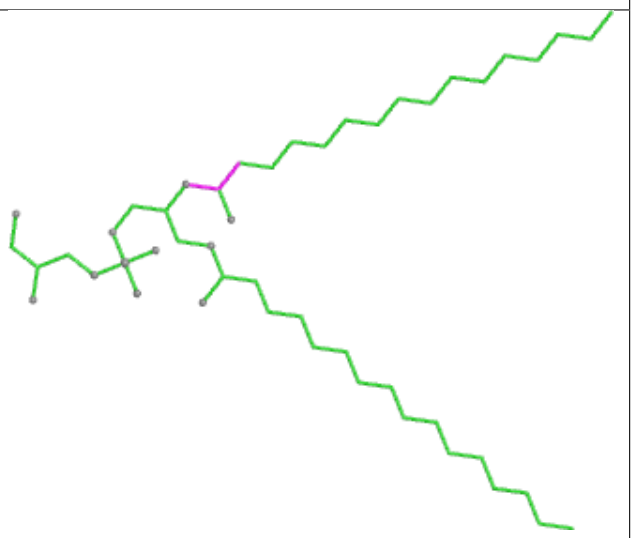
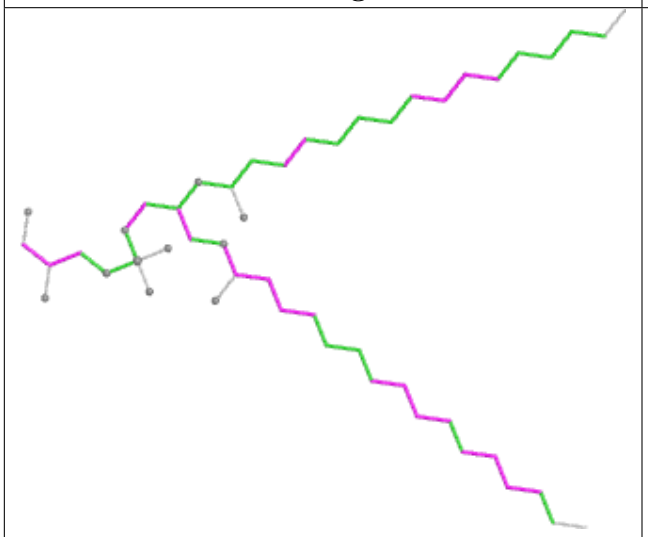


Bond angles



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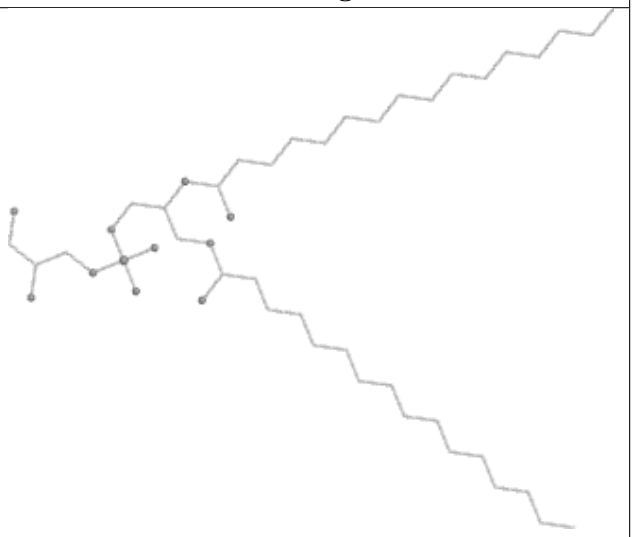
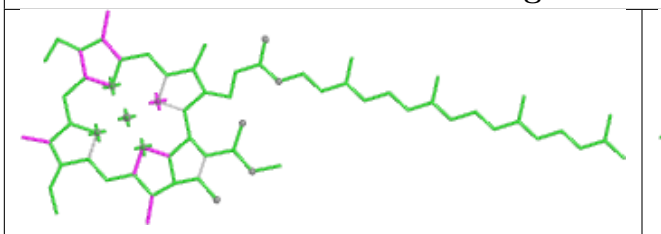


Rings

Ligand CLA G 609



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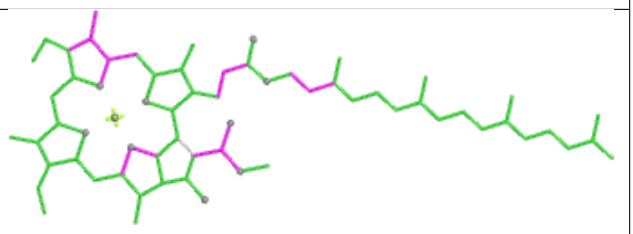
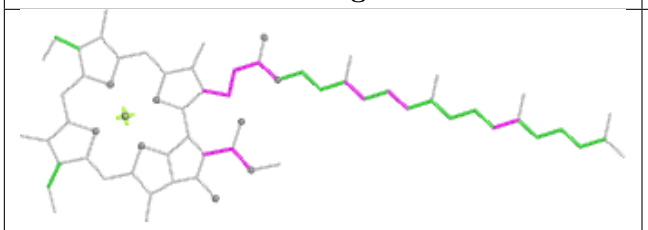


Bond angles



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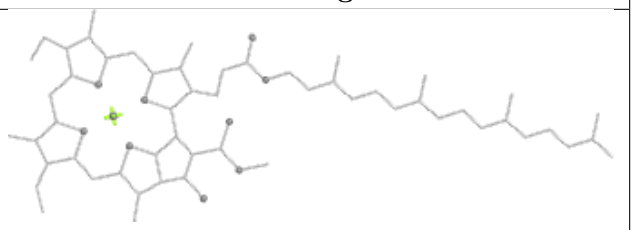
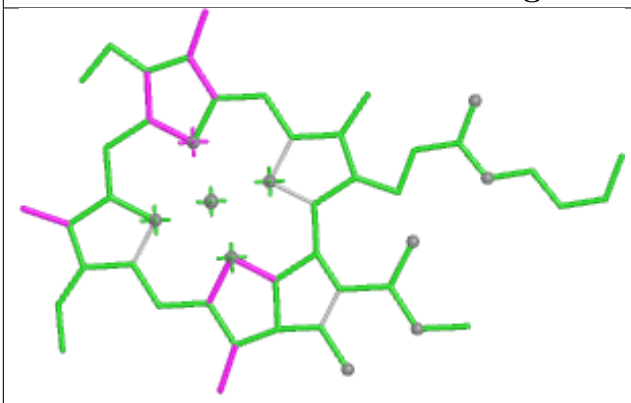
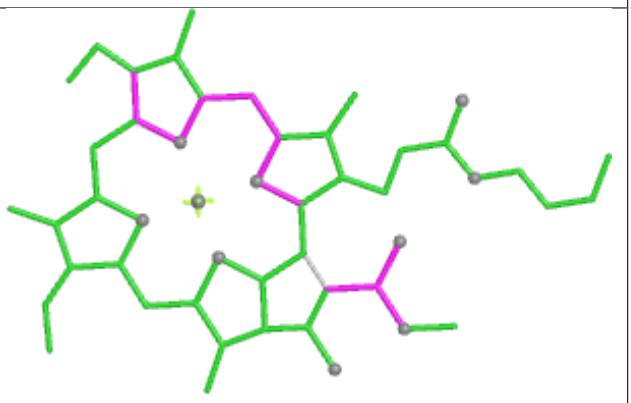
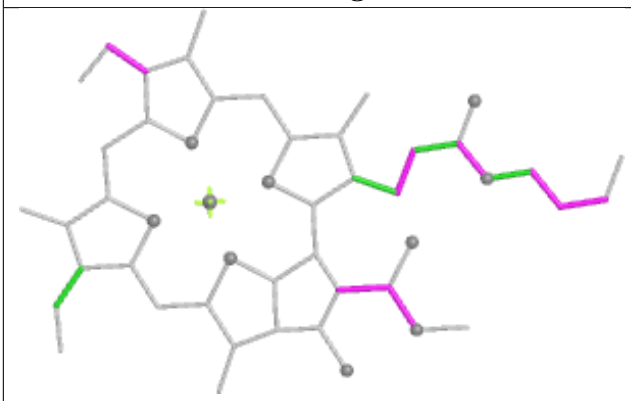
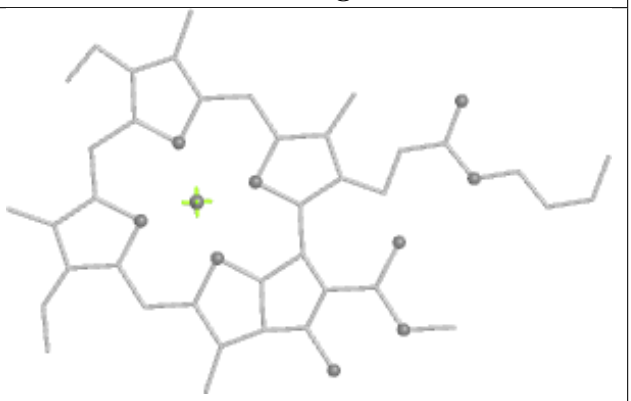


Rings

Ligand CLA N 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

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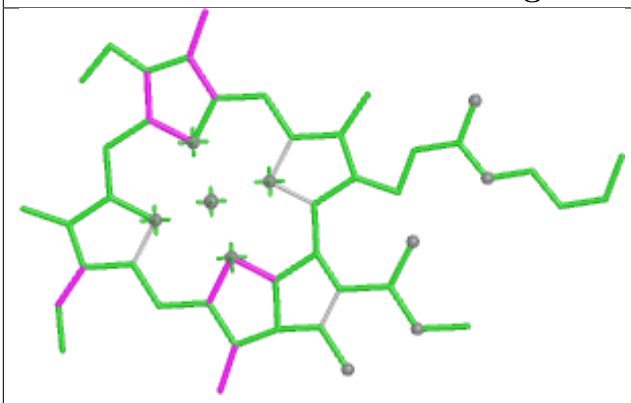
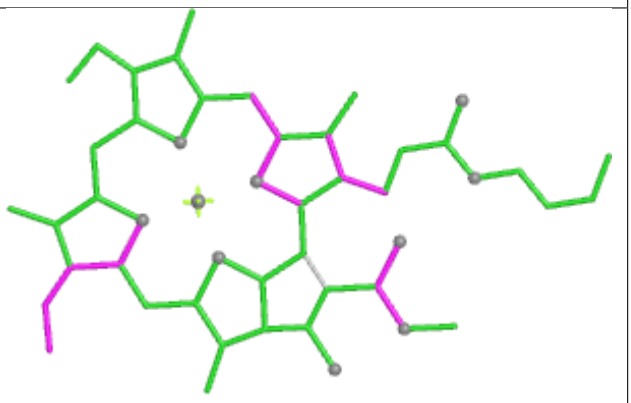
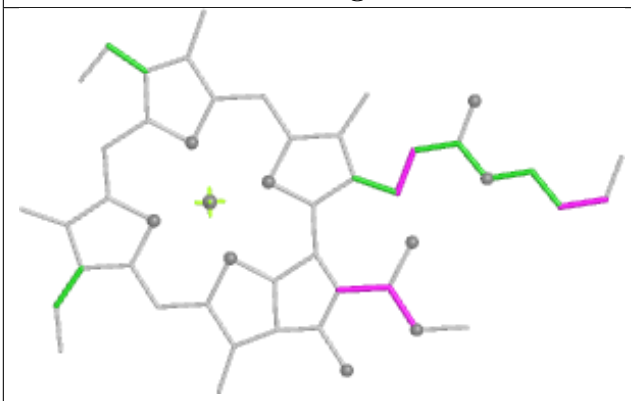
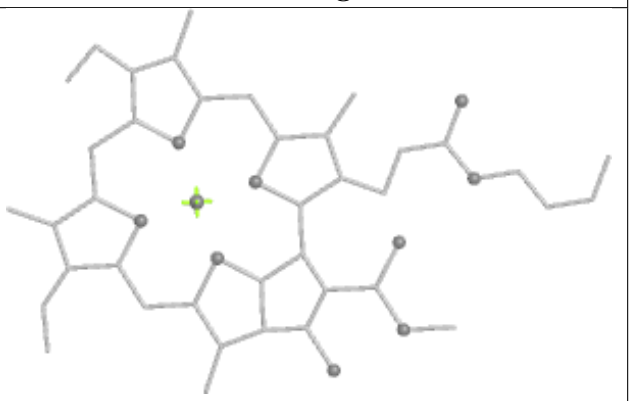
 Bond lengths	 Bond angles
 Torsions	 Rings

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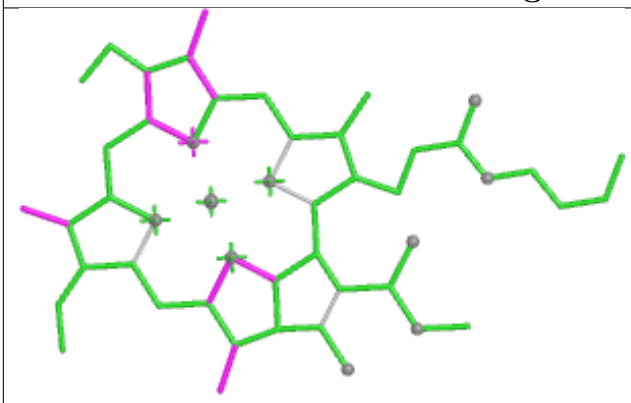
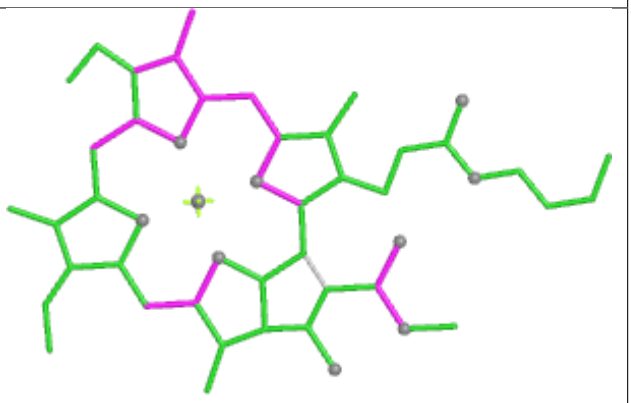
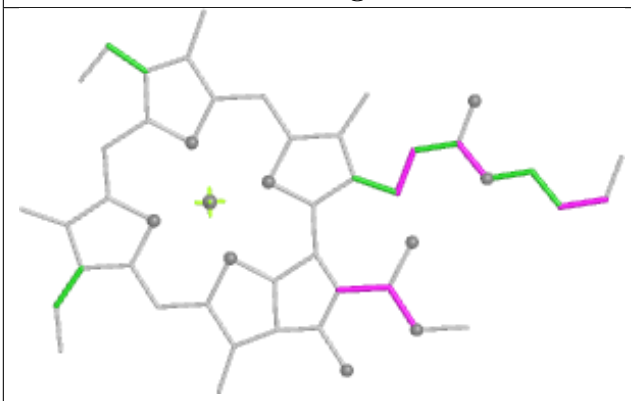
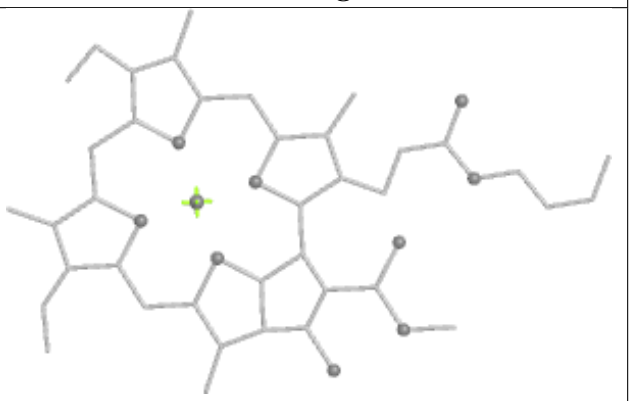
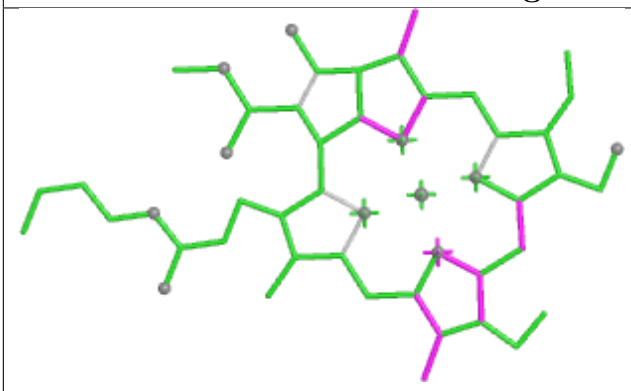
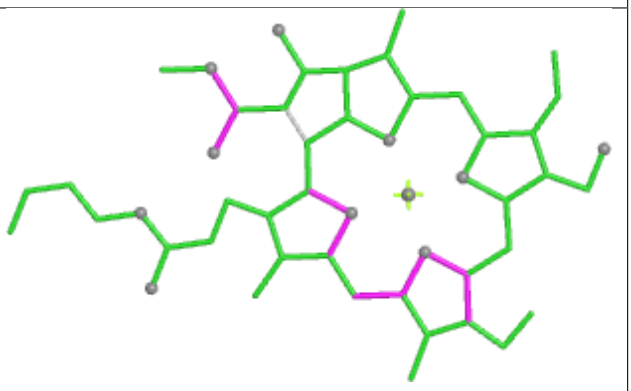
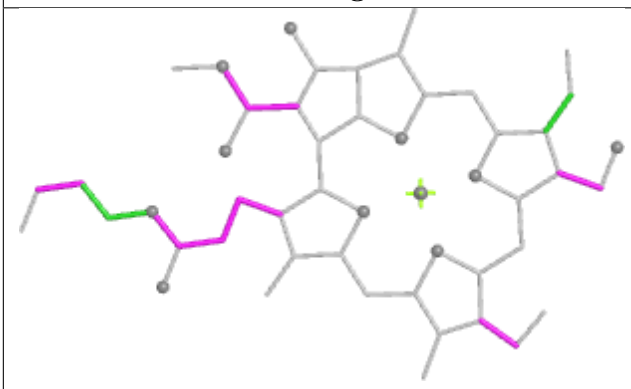
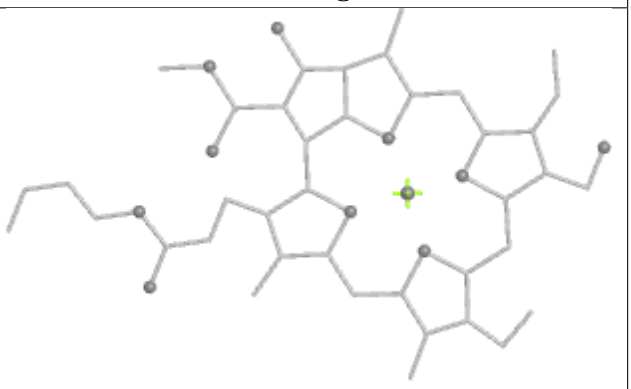
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL Y 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

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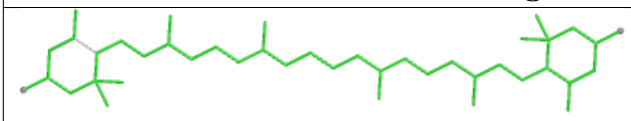
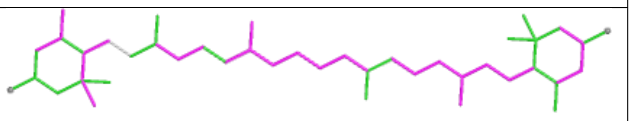
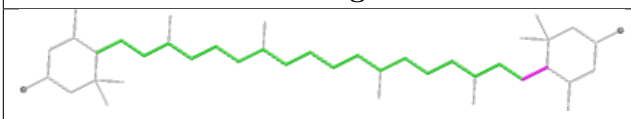
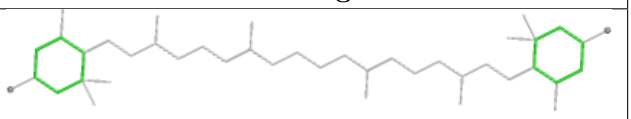
 Bond lengths	 Bond angles
 Torsions	 Rings

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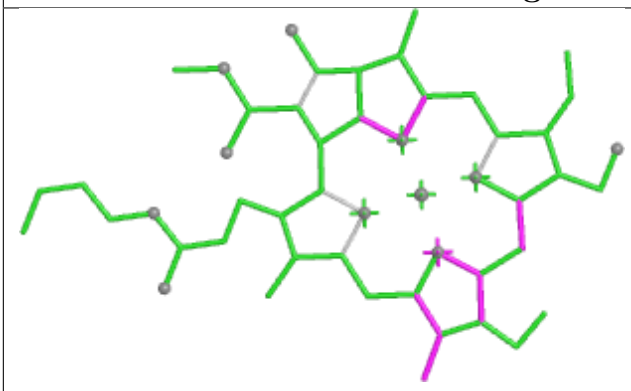
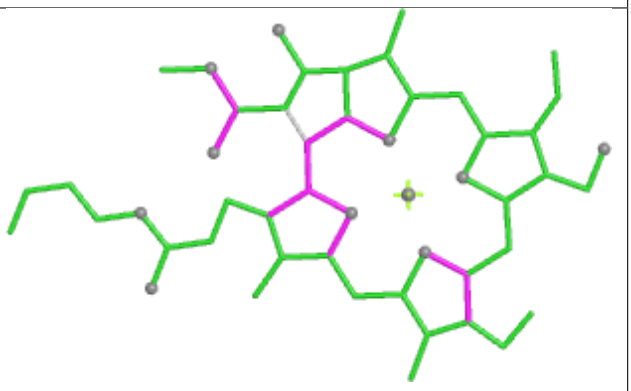
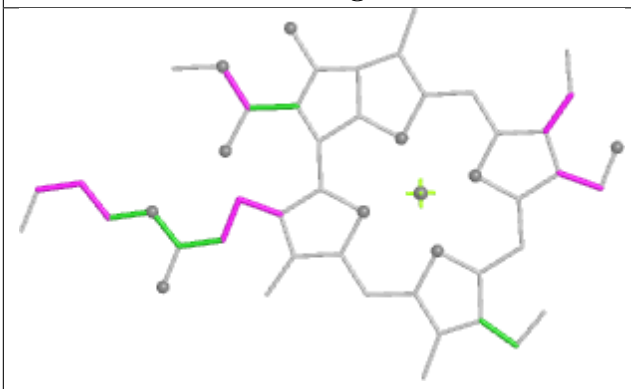
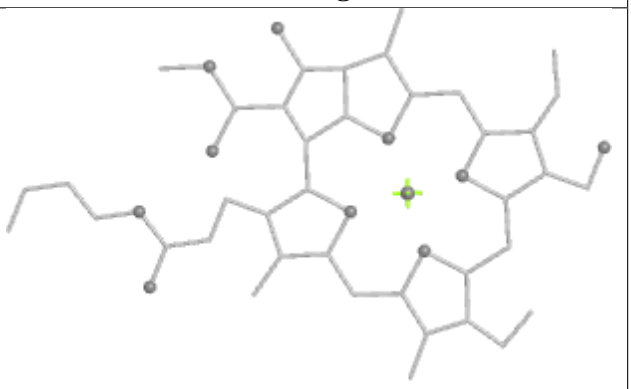
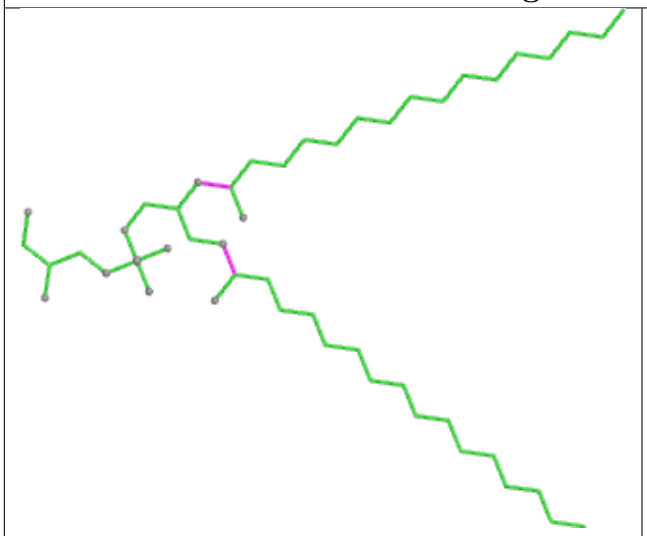
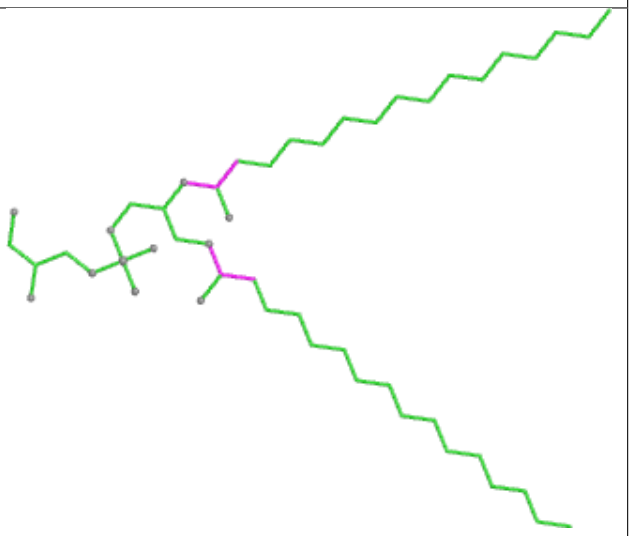
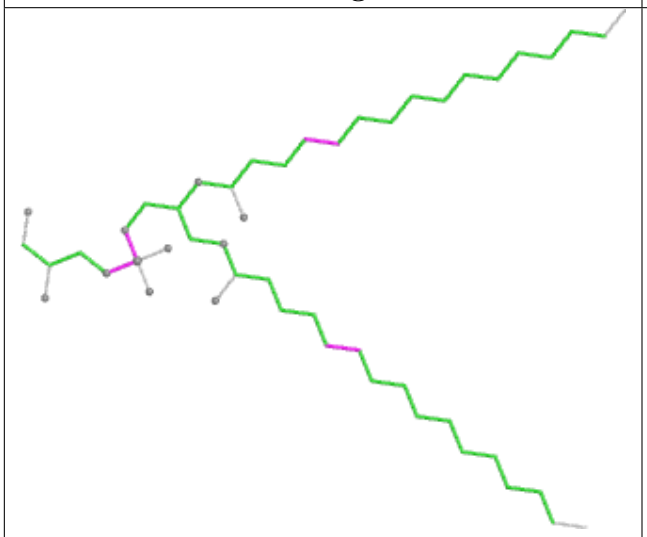
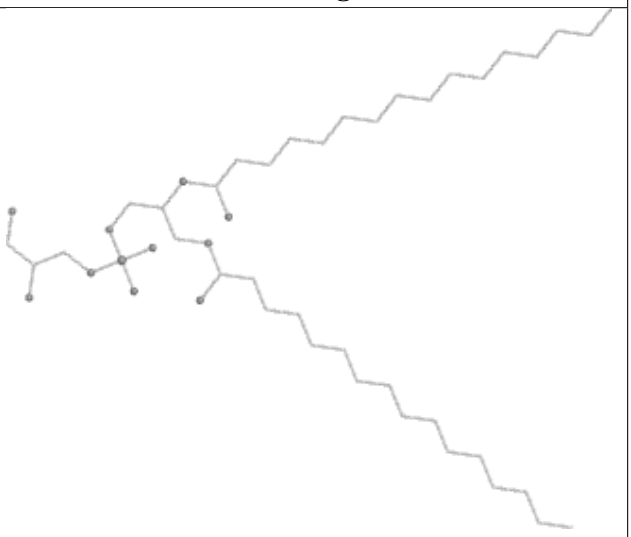
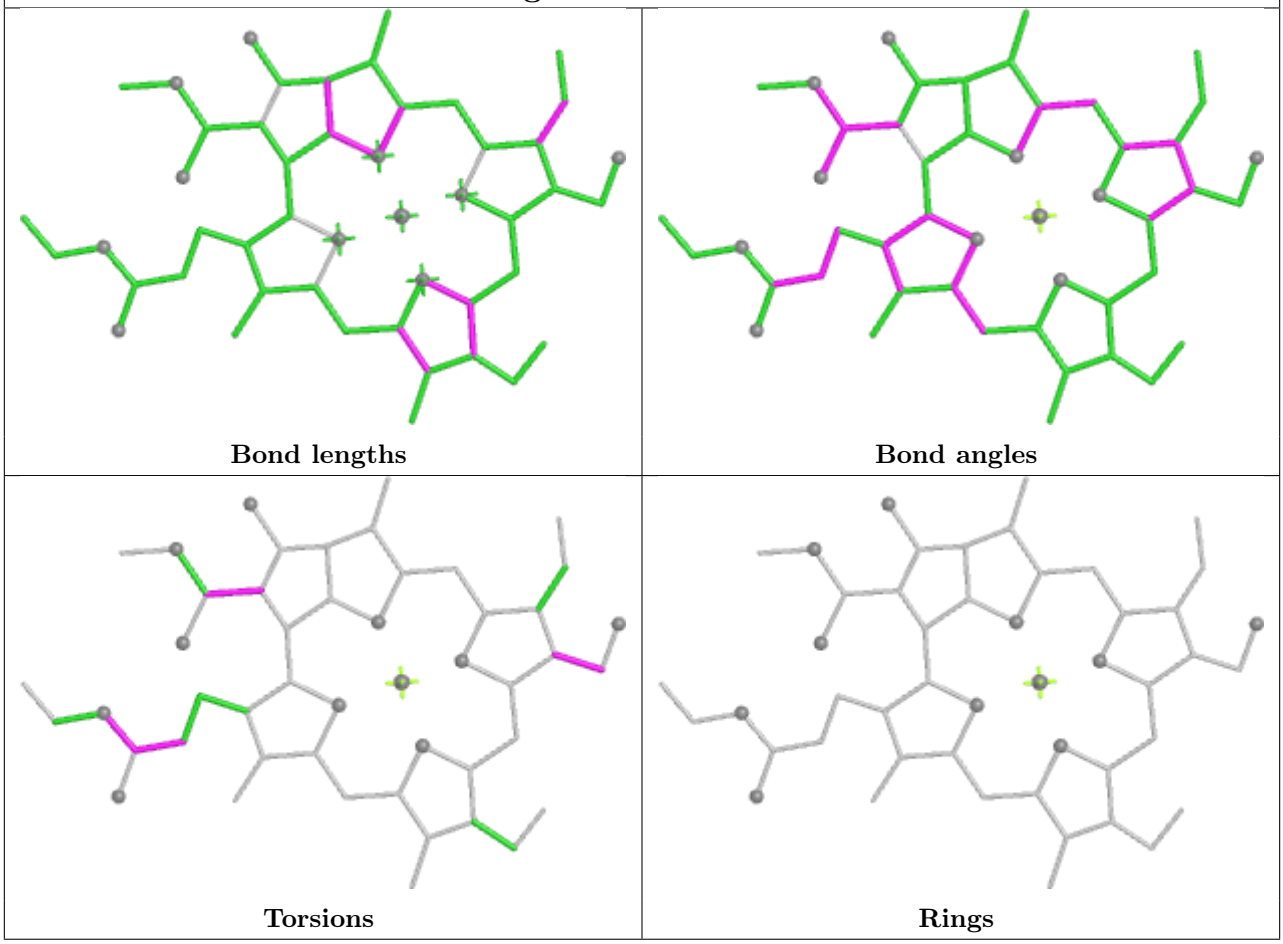
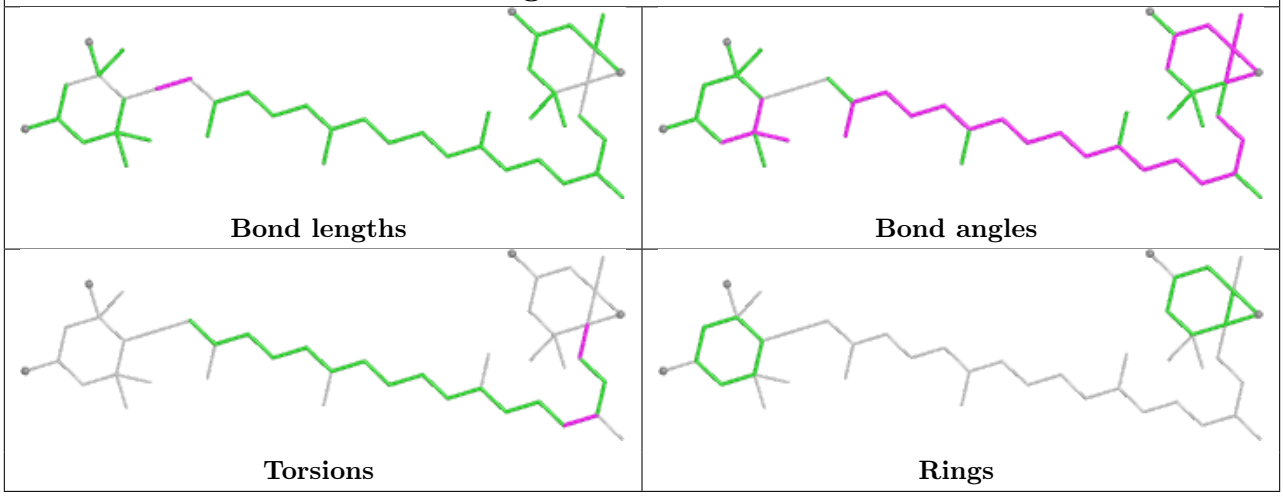
 Bond lengths	 Bond angles
 Torsions	 Rings

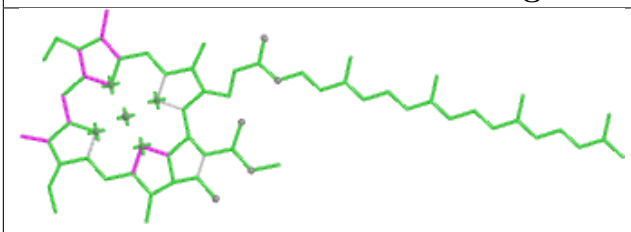
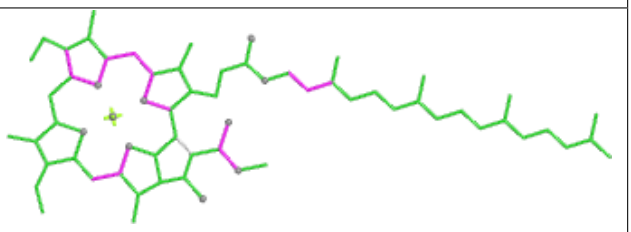
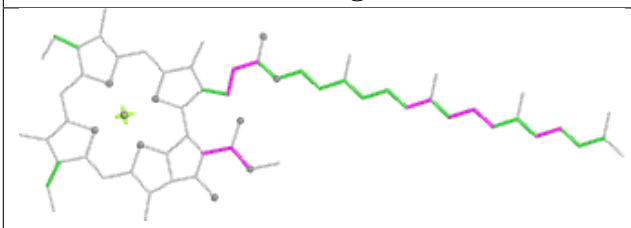
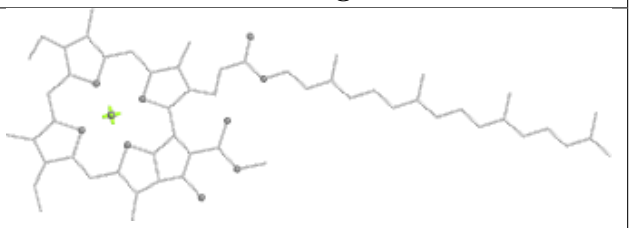
Ligand LHG G 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

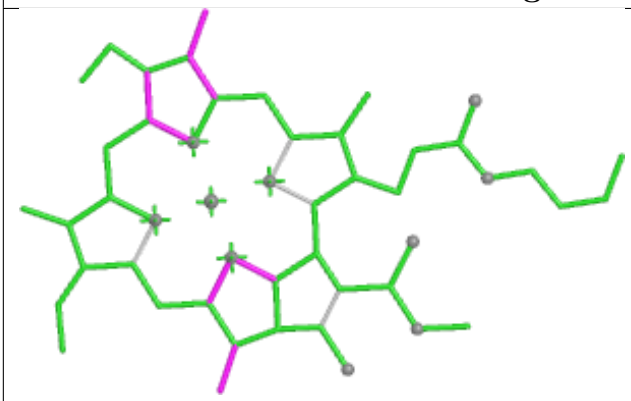
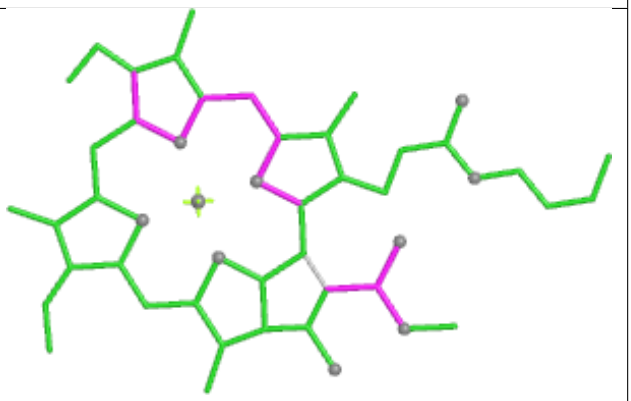
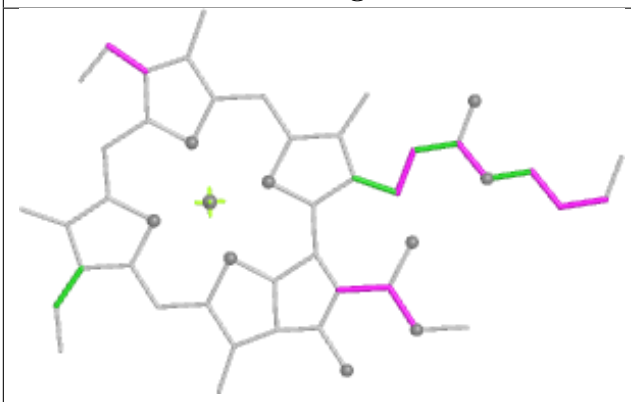
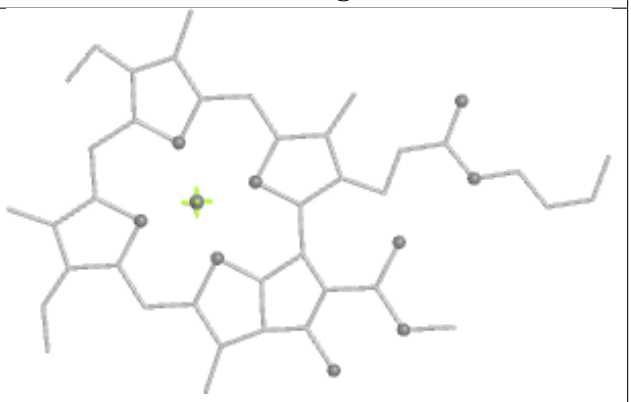
Ligand CHL G 605

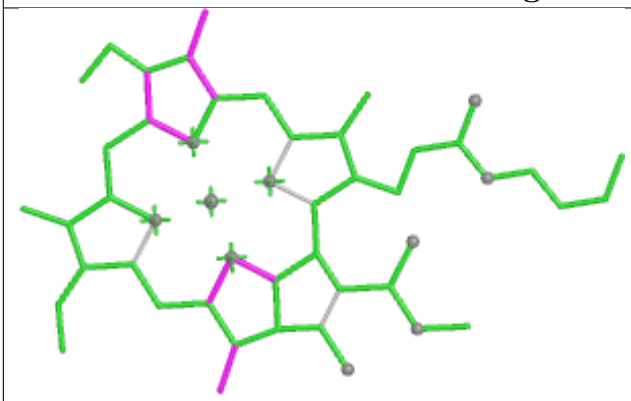
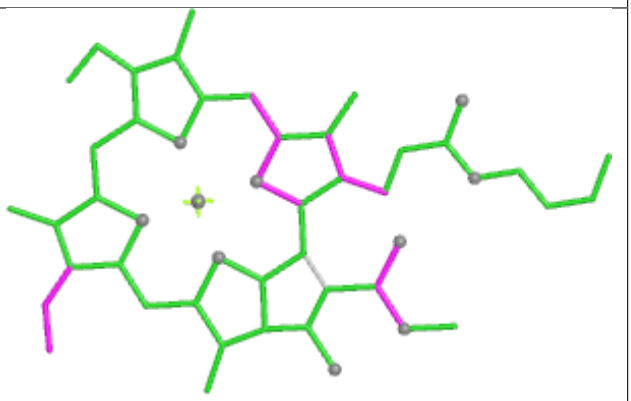
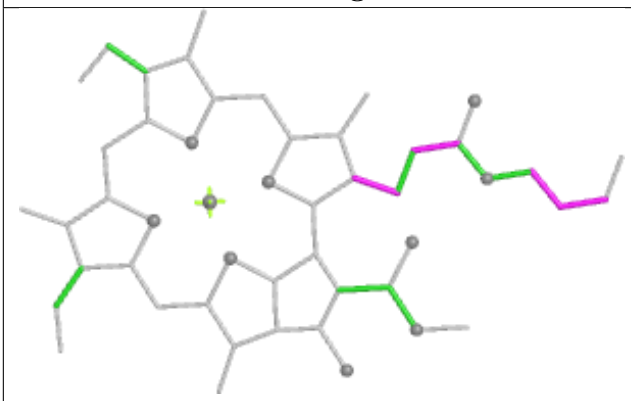
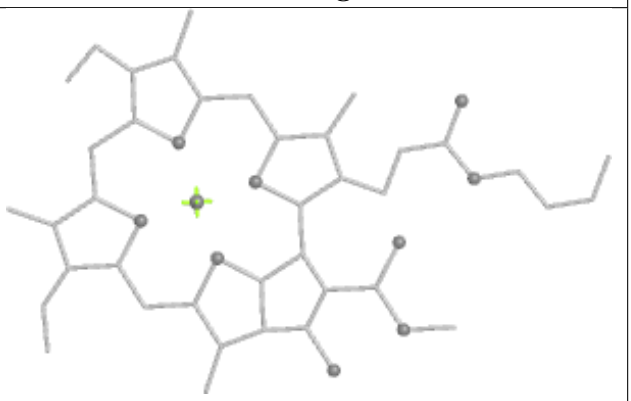


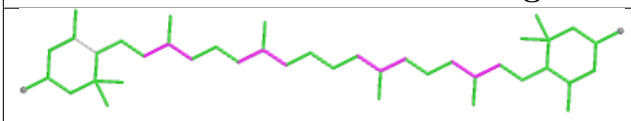
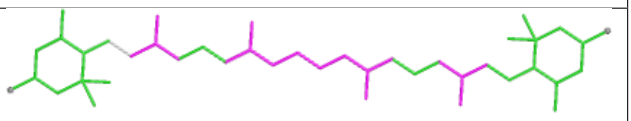
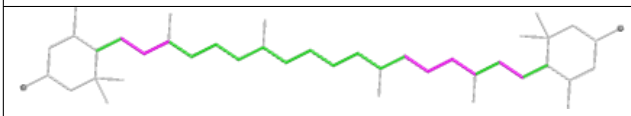
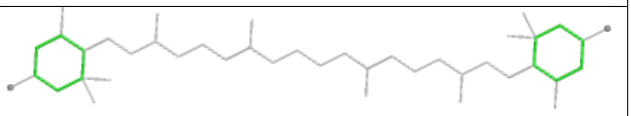
Ligand NEX Y 616



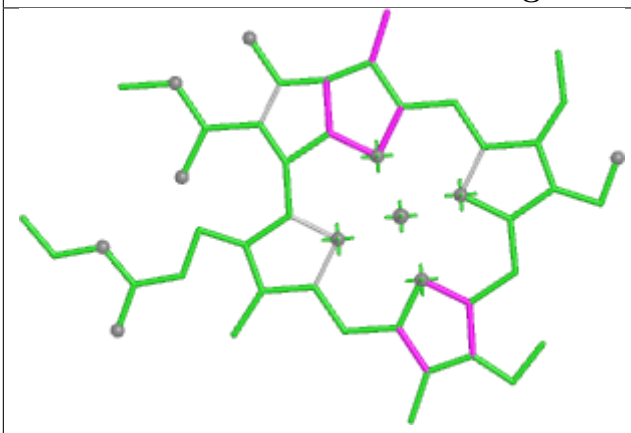
Ligand CLA N 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

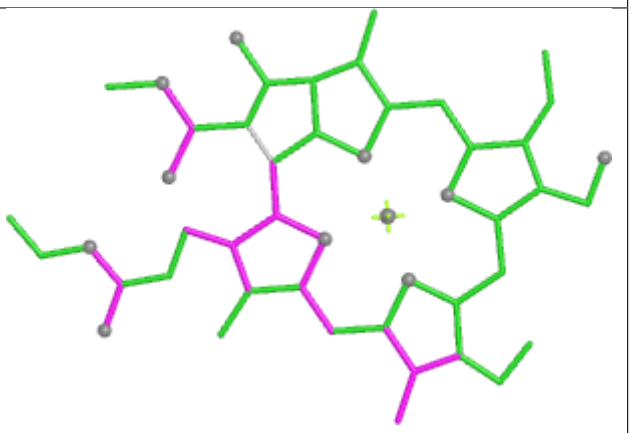
Ligand CLA G 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT N 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

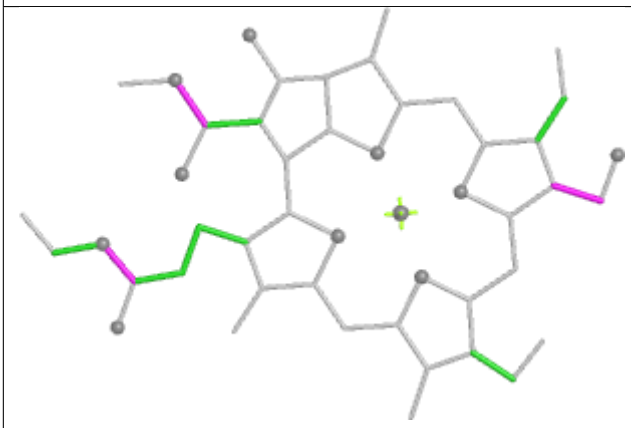
Ligand CHL N 306



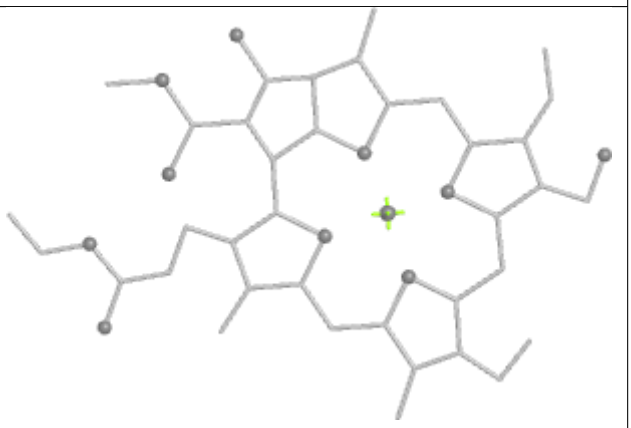
Bond lengths



Bond angles

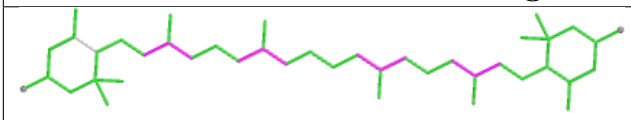


Torsions

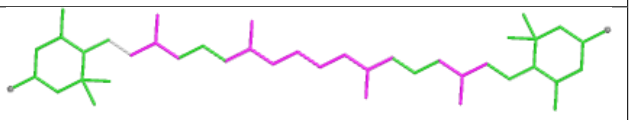


Rings

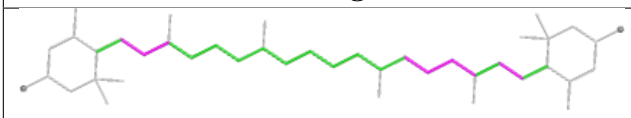
Ligand LUT Y 614



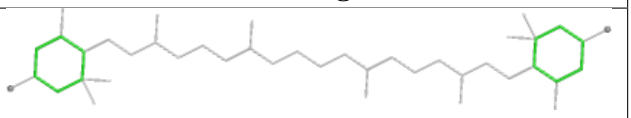
Bond lengths



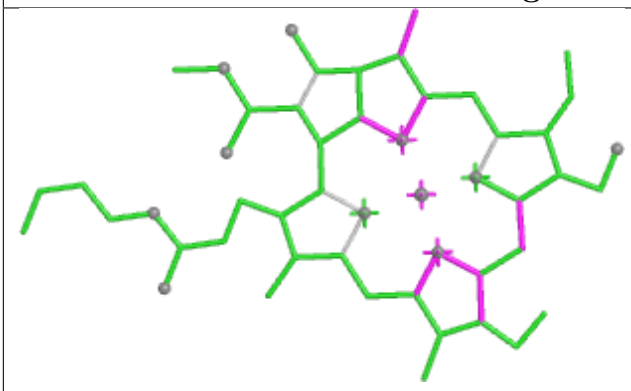
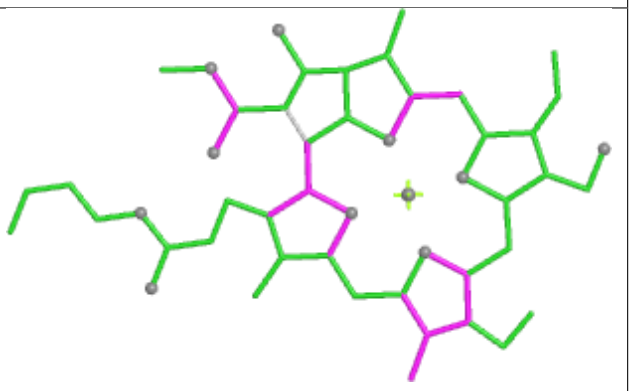
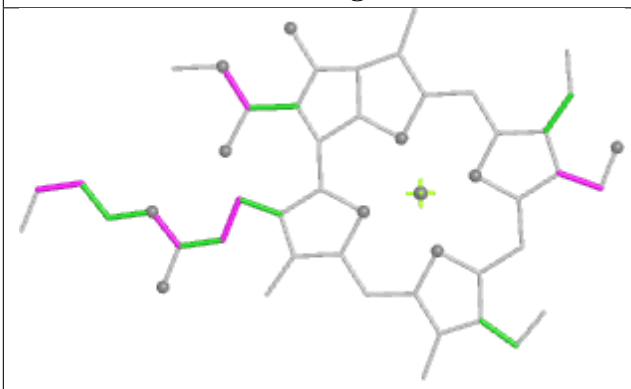
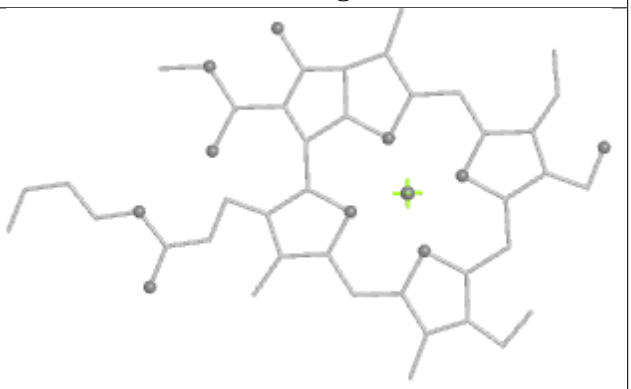
Bond angles

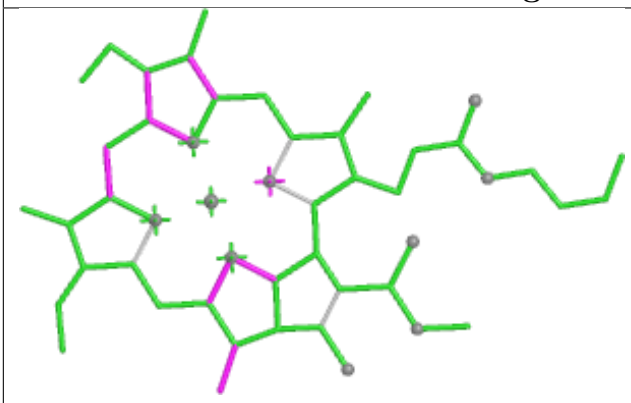
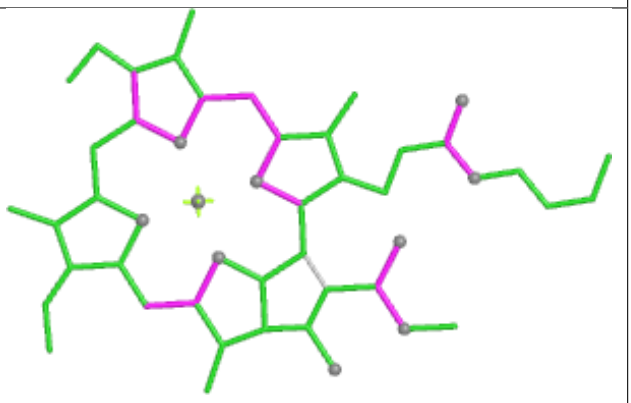
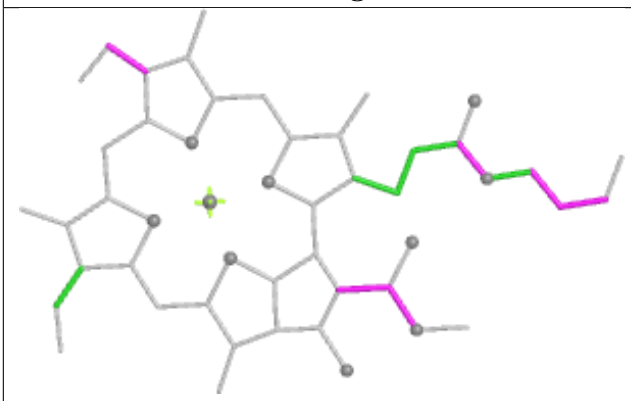
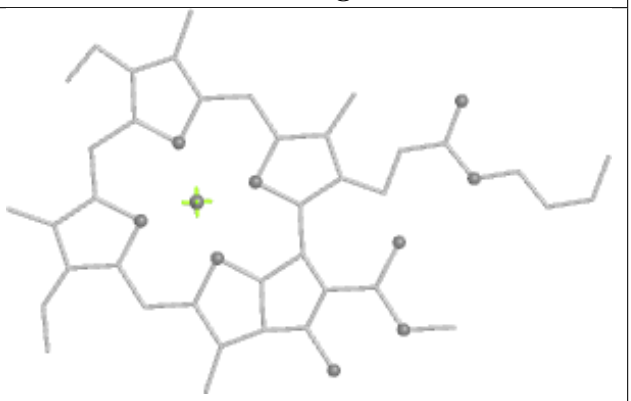


Torsions



Rings

Ligand CHL G 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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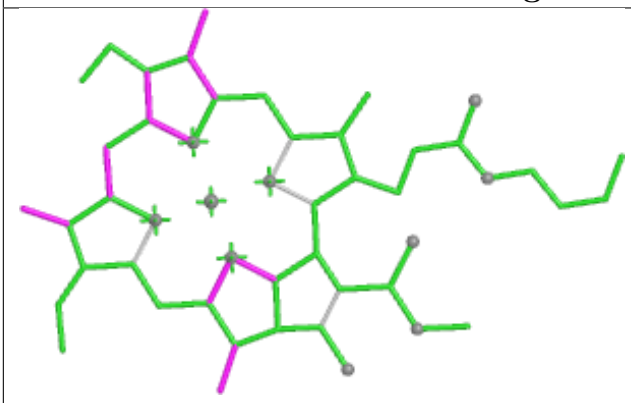
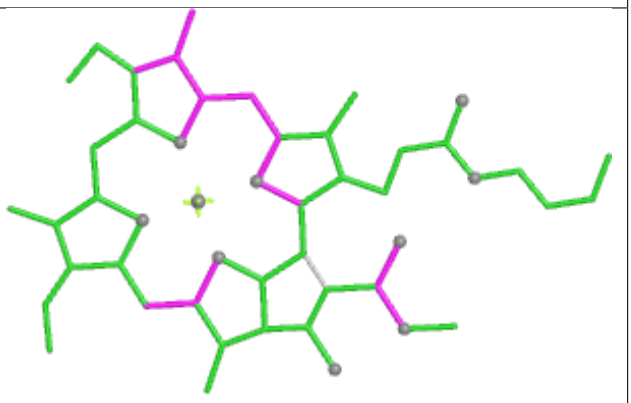
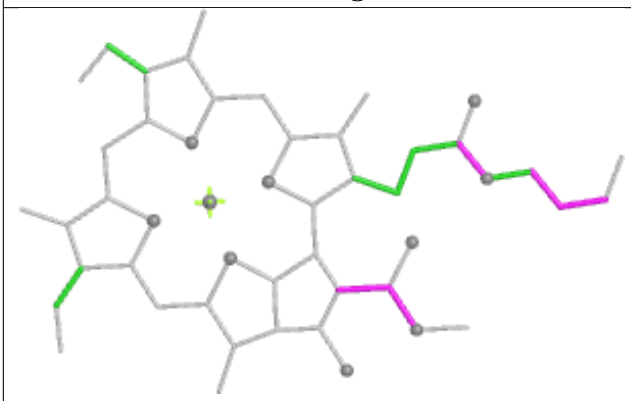
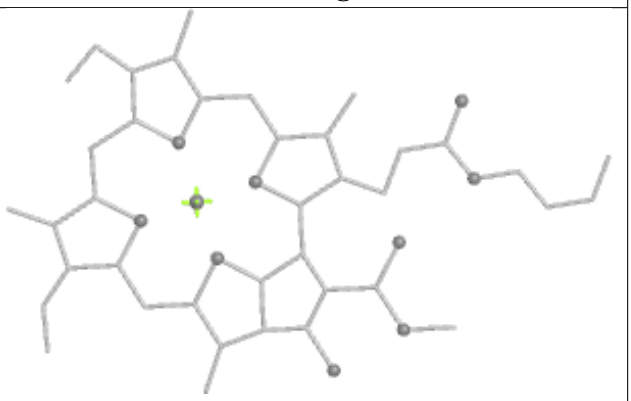
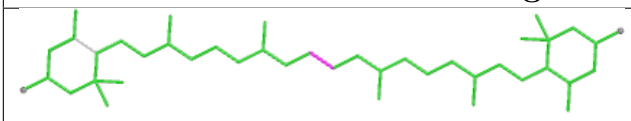
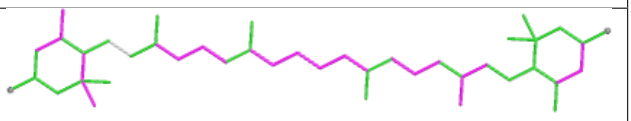
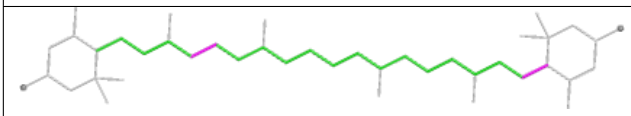
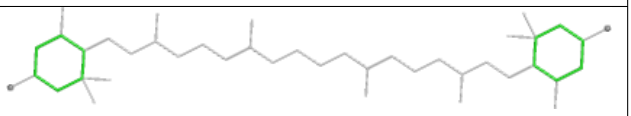
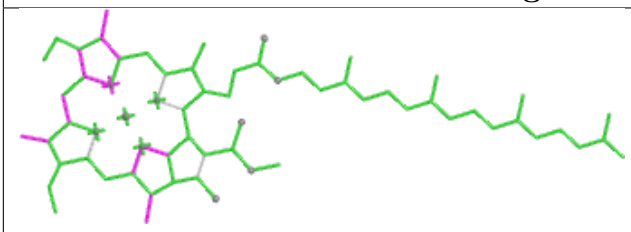
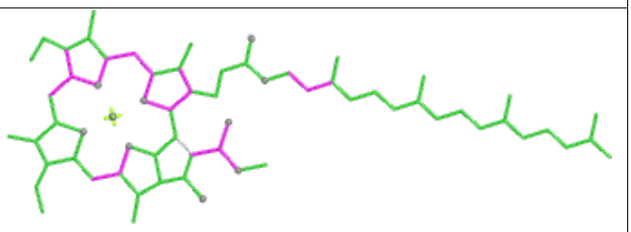
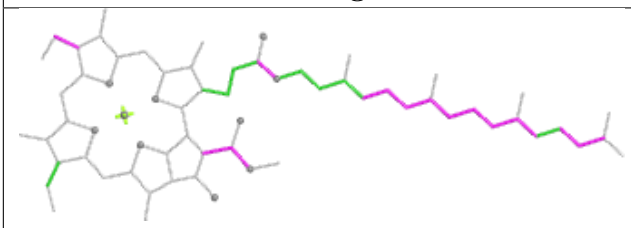
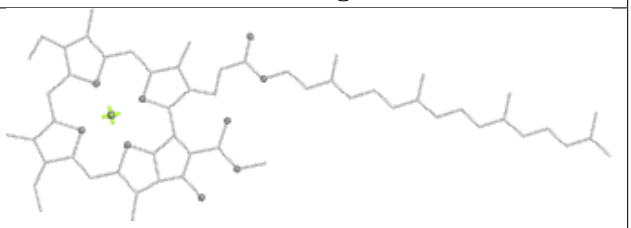
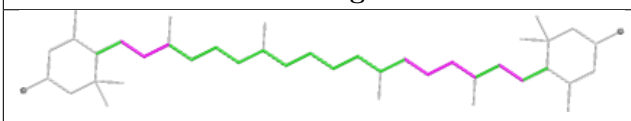
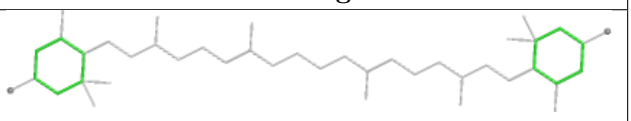
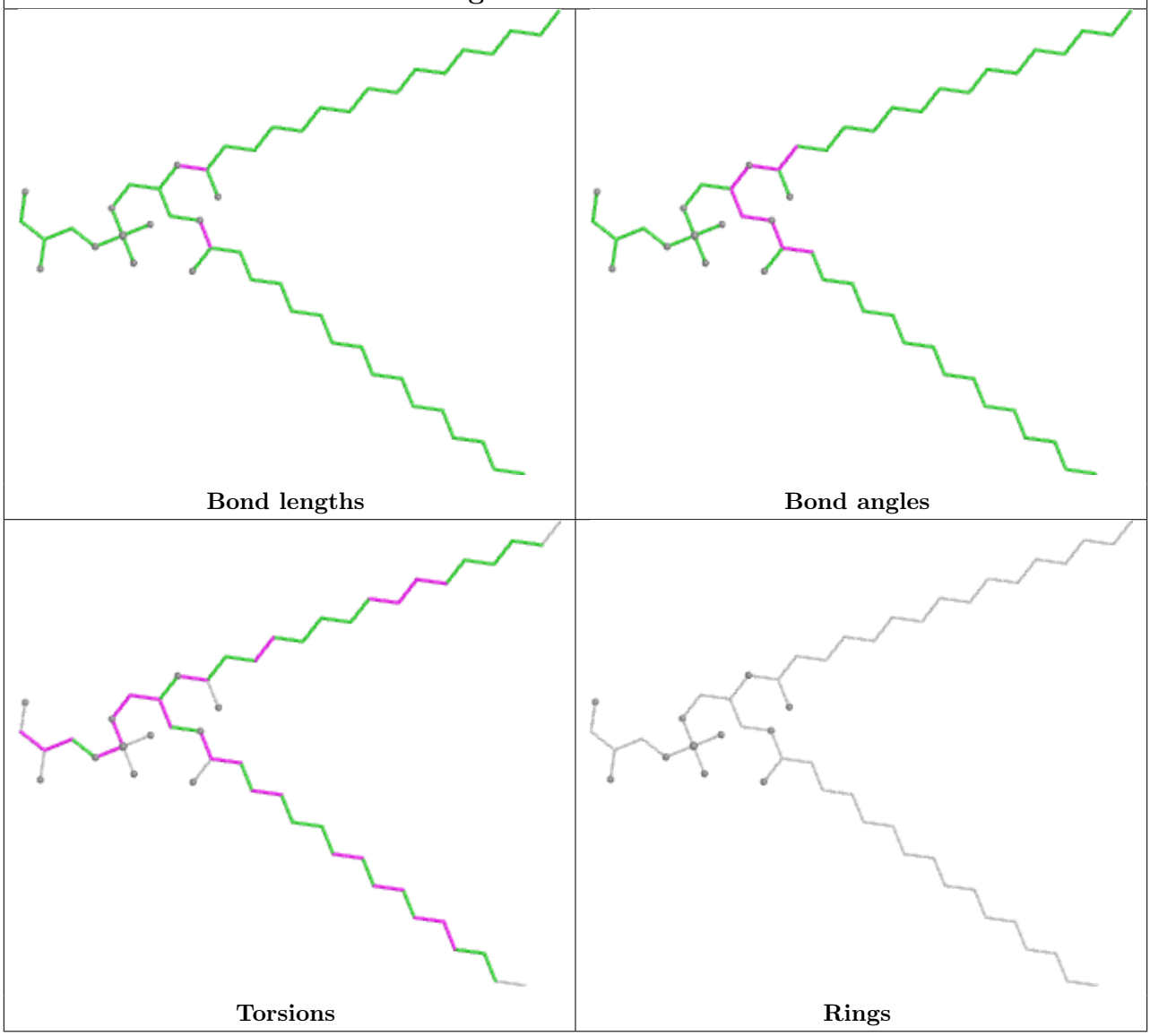
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT N 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

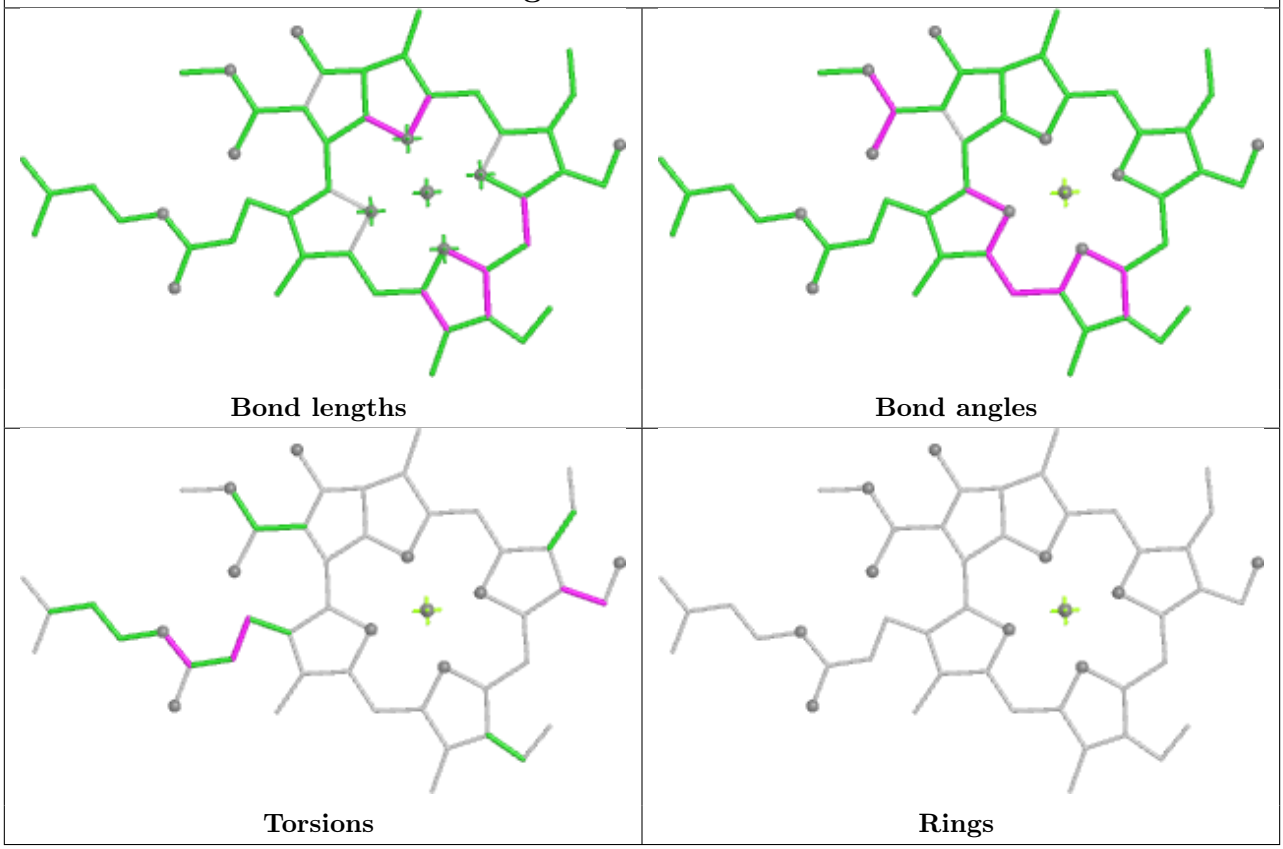
Ligand CLA G 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT G 614	
Bond lengths	Bond angles
 Torsions	 Rings

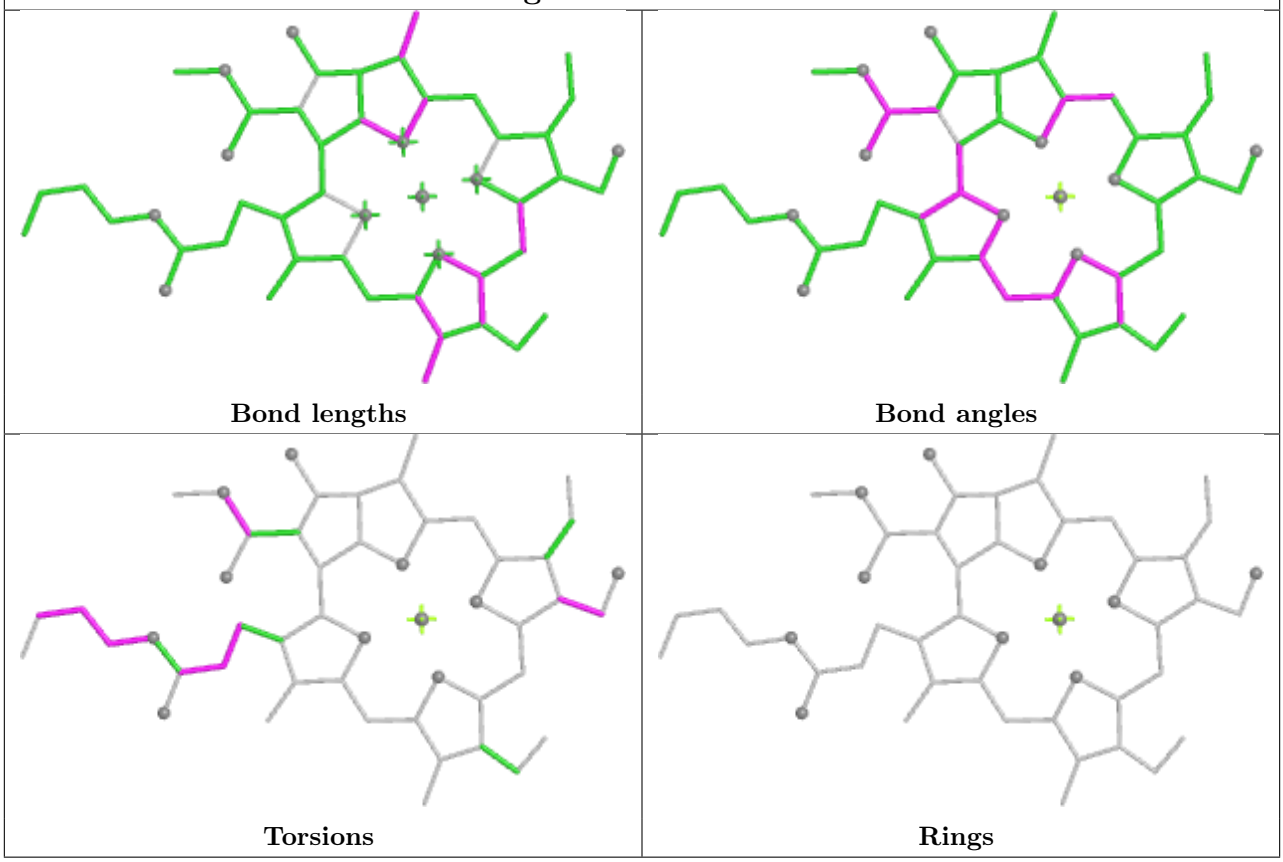
Ligand LHG N 320

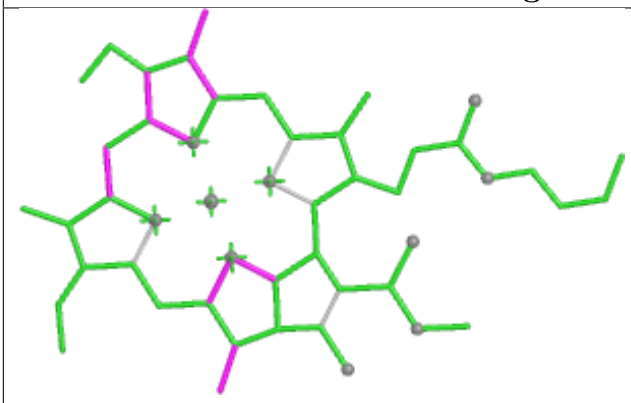
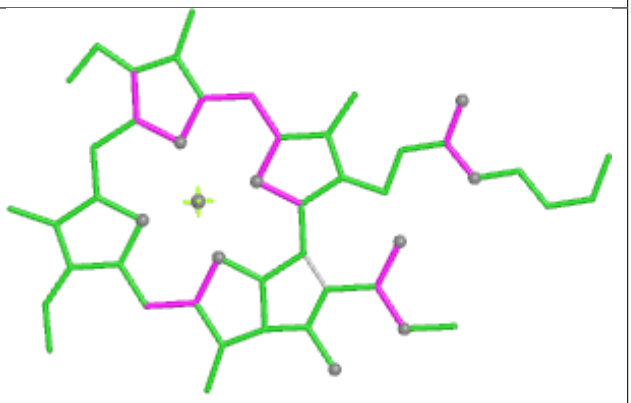
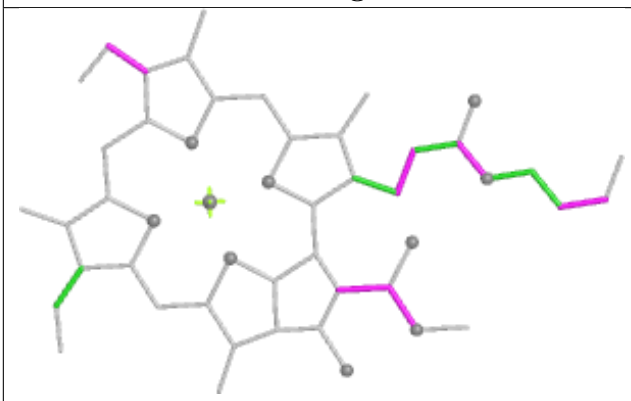
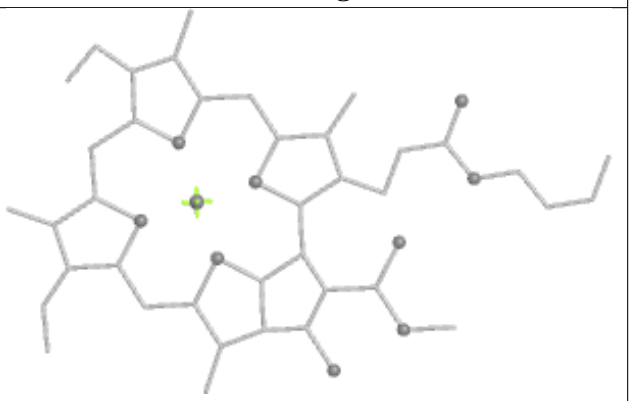


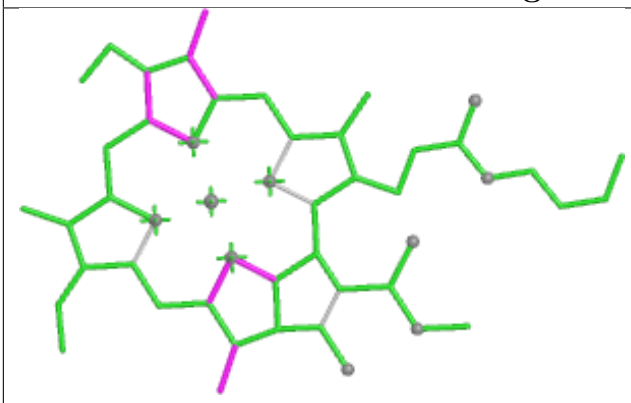
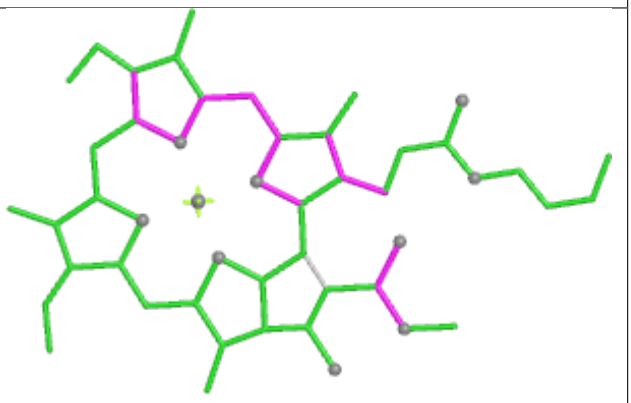
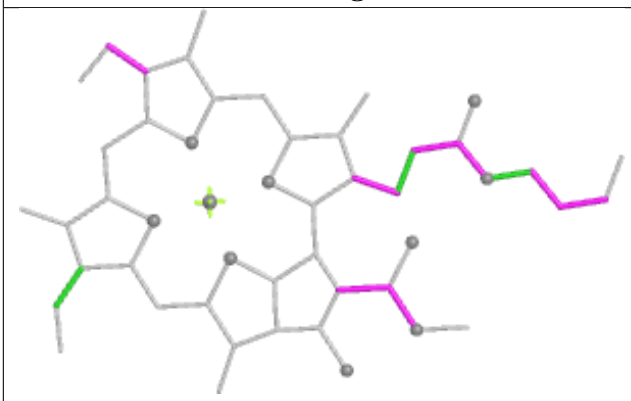
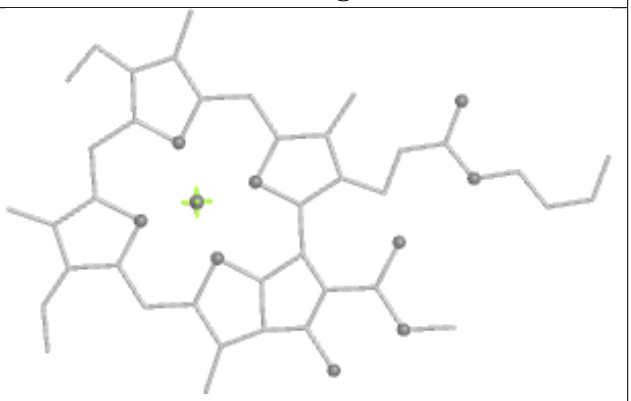
Ligand CHL N 308

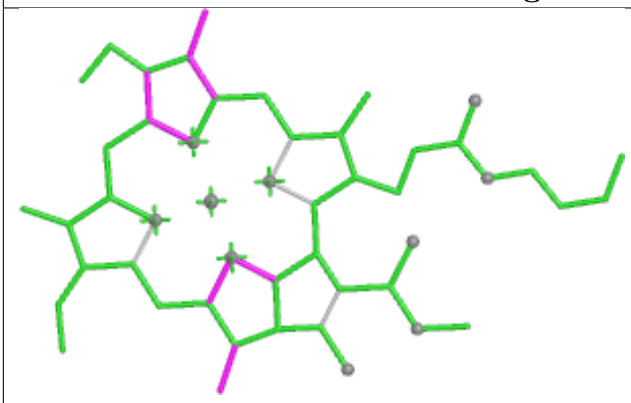
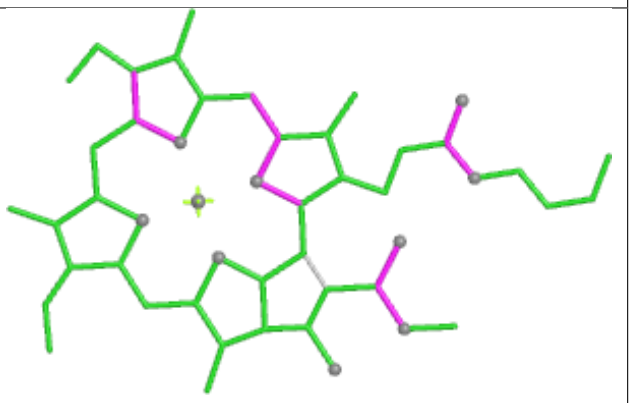
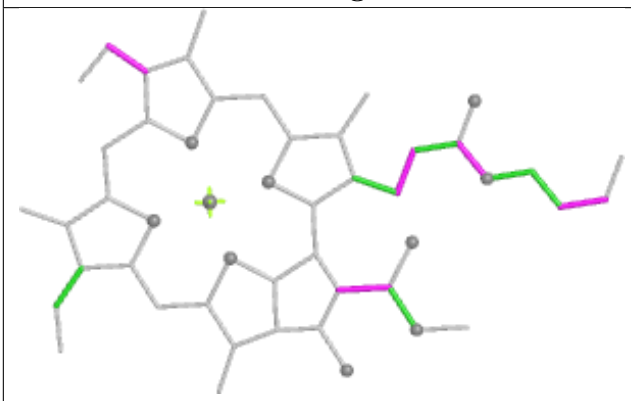
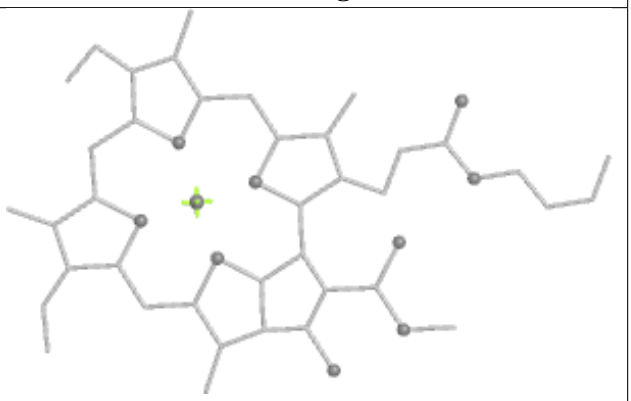


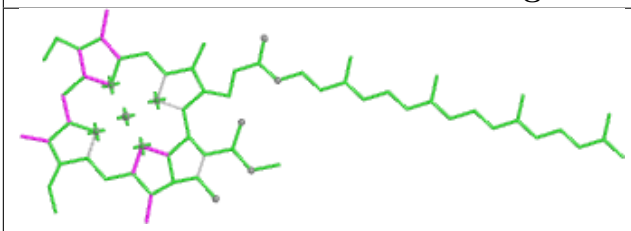
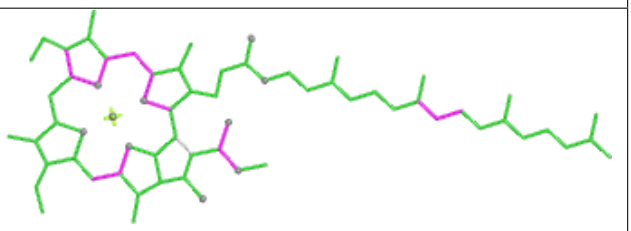
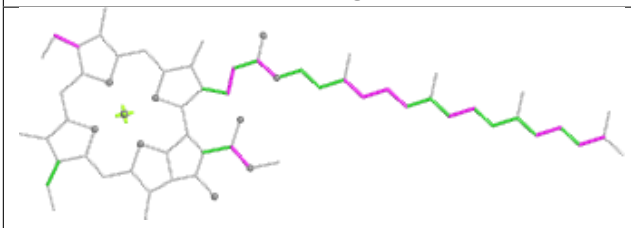
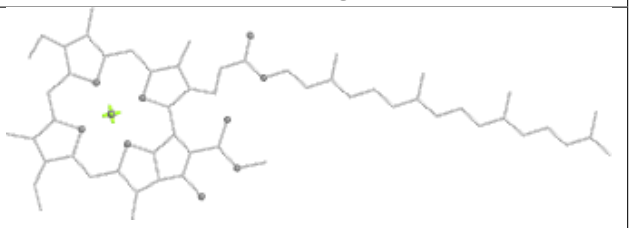
Ligand CHL G 619

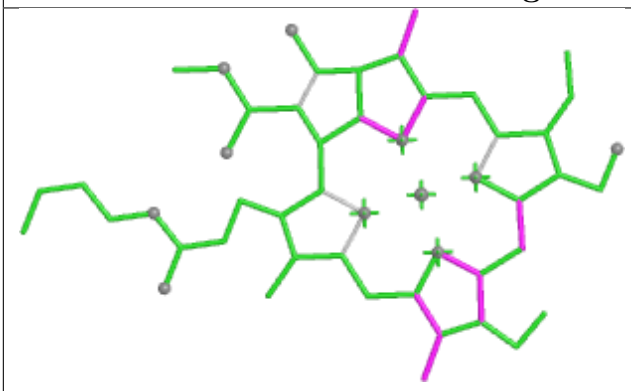
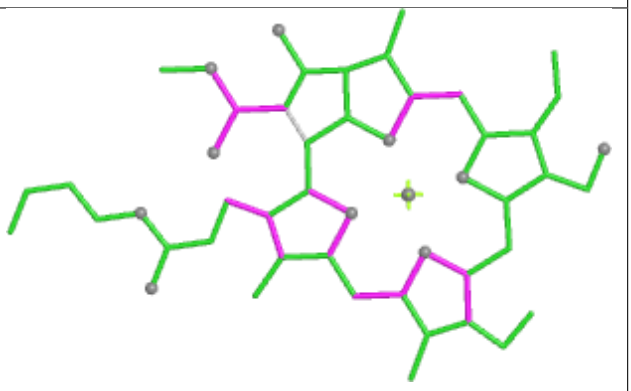
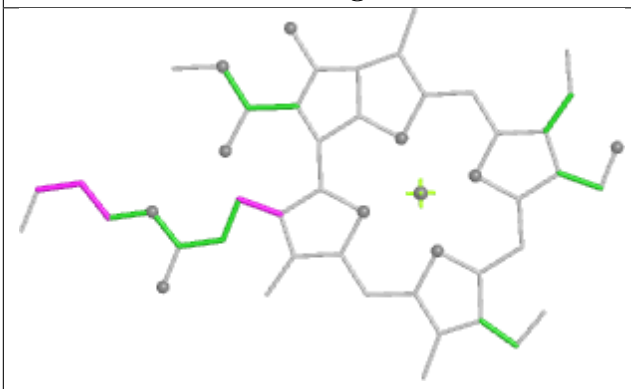
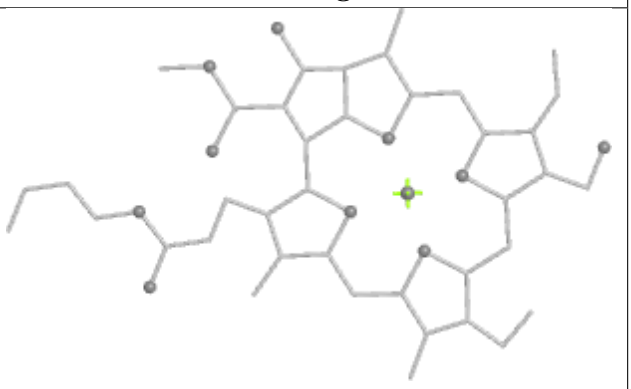


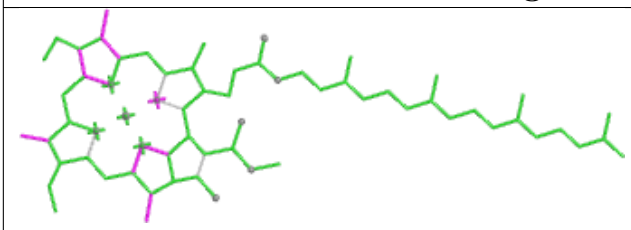
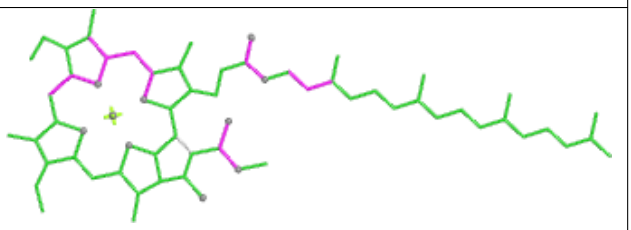
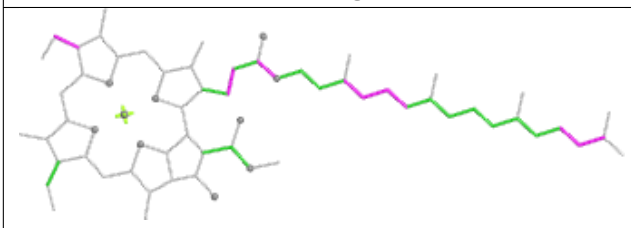
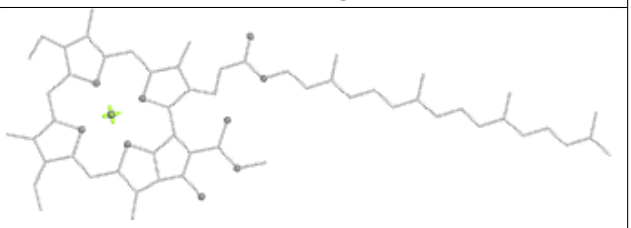
Ligand CLA G 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Y 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL N 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 313	
 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.

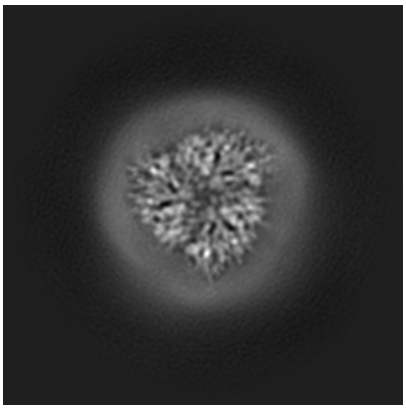
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-35786. These allow visual inspection of the internal detail of the map and identification of artifacts.

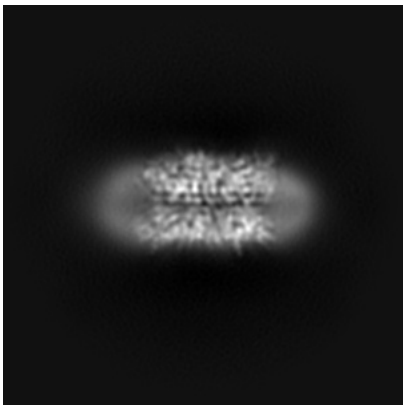
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

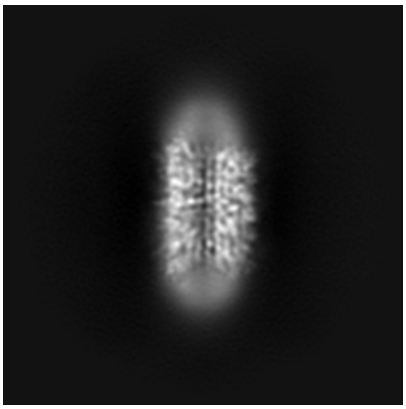
6.1.1 Primary map



X

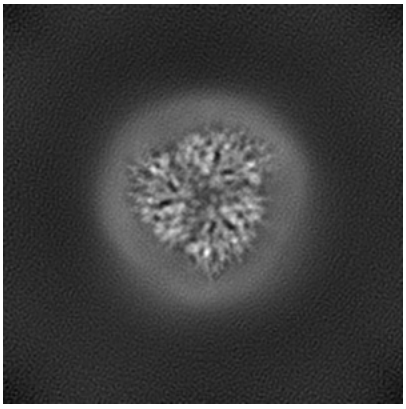


Y



Z

6.1.2 Raw map



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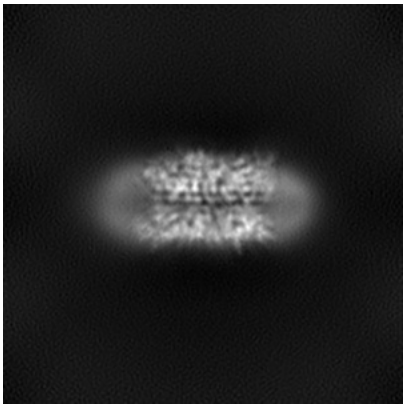

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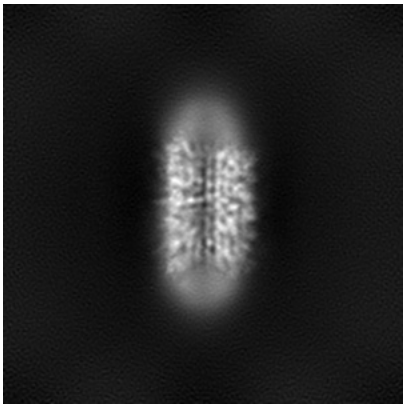
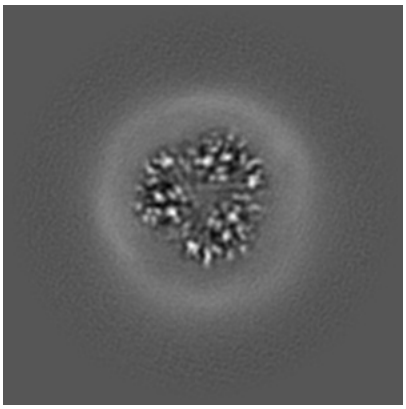


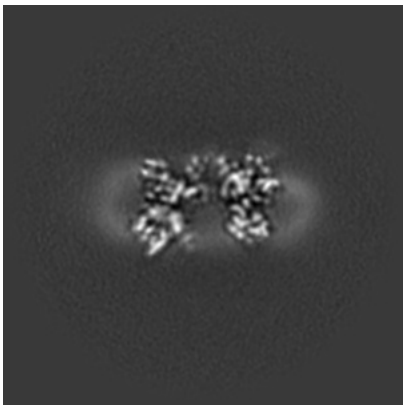
Z

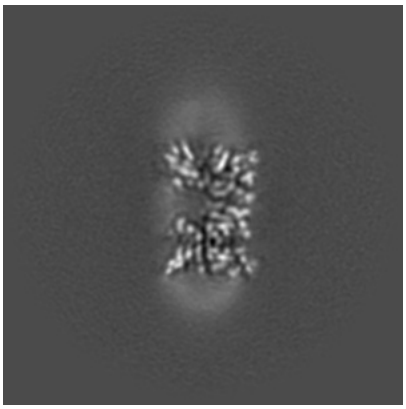
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

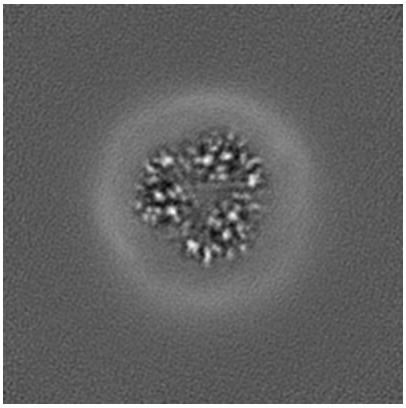
6.2.1 Primary map

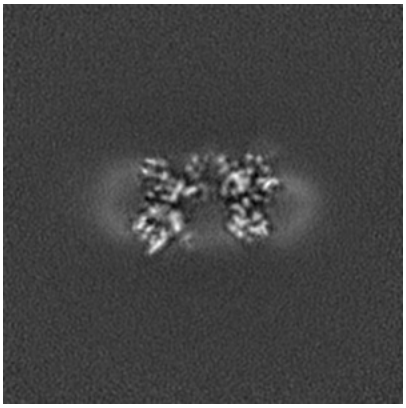

X Index: 100

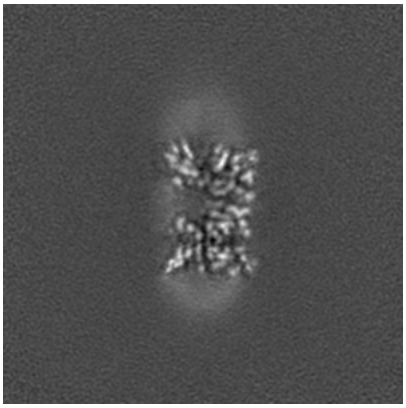

Y Index: 100


Z Index: 100

6.2.2 Raw map


X Index: 100

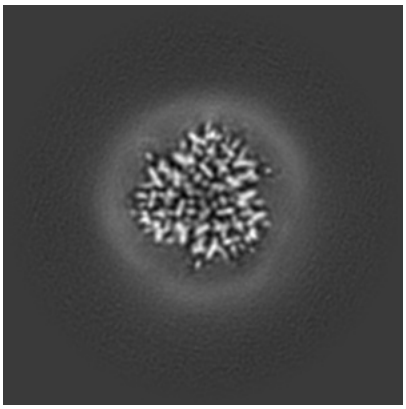

Y Index: 100

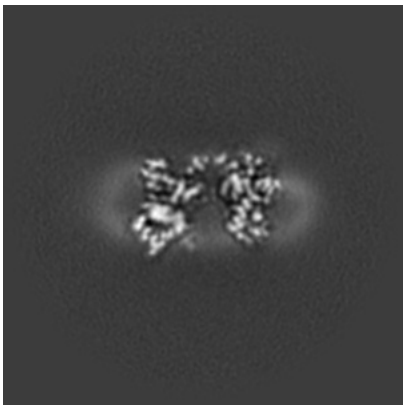

Z Index: 100

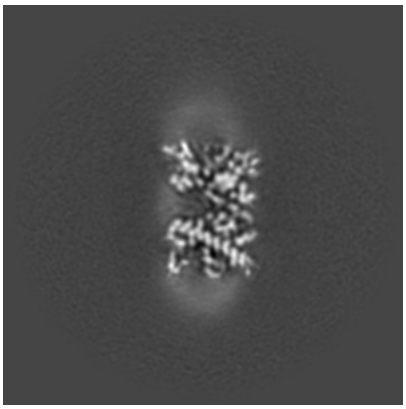
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

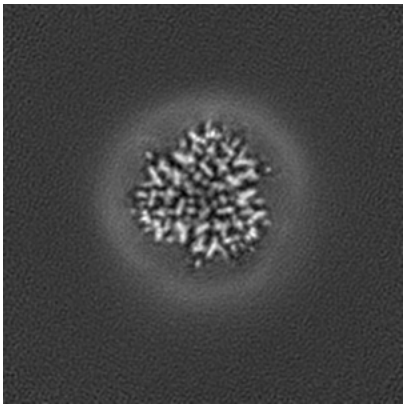
6.3.1 Primary map

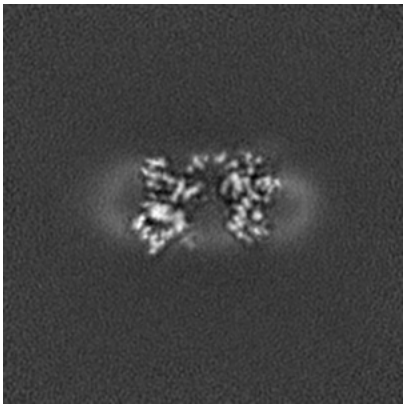

X Index: 108

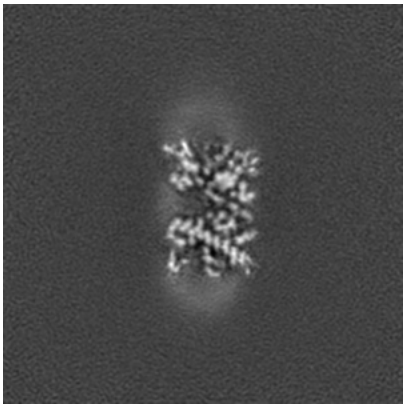

Y Index: 101


Z Index: 97

6.3.2 Raw map


X Index: 108

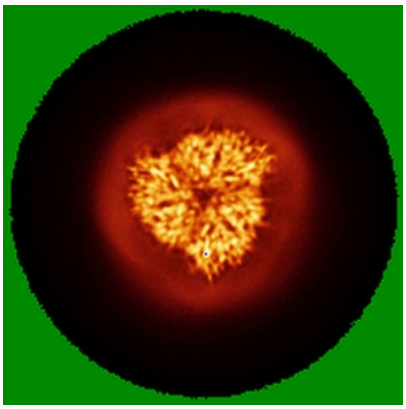

Y Index: 101

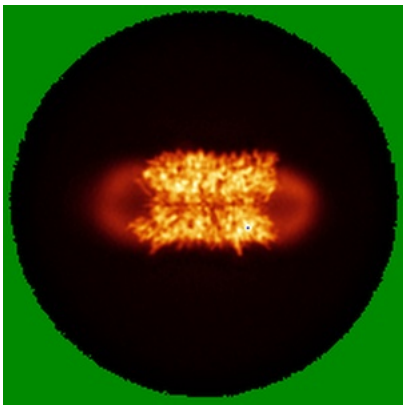

Z Index: 97

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

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

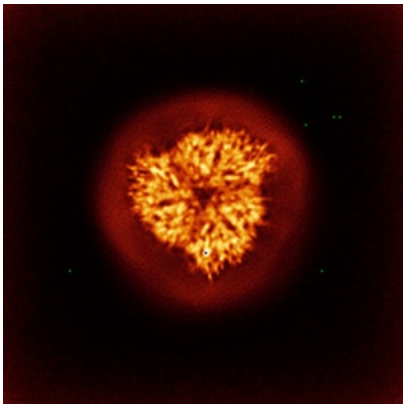
6.4.1 Primary map

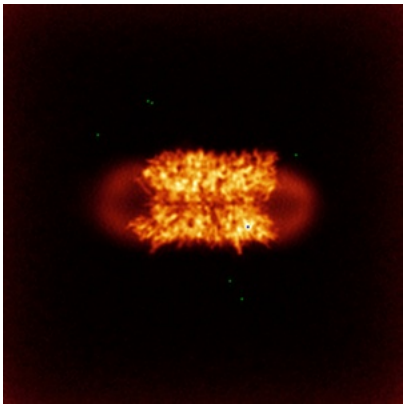

X

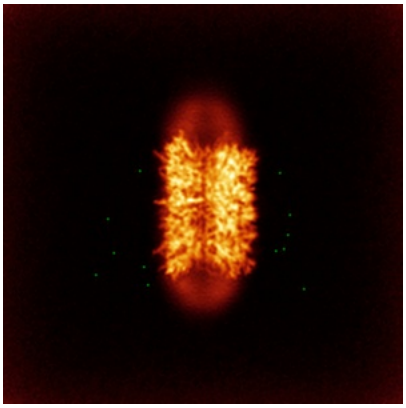

Y

Z

6.4.2 Raw map


X

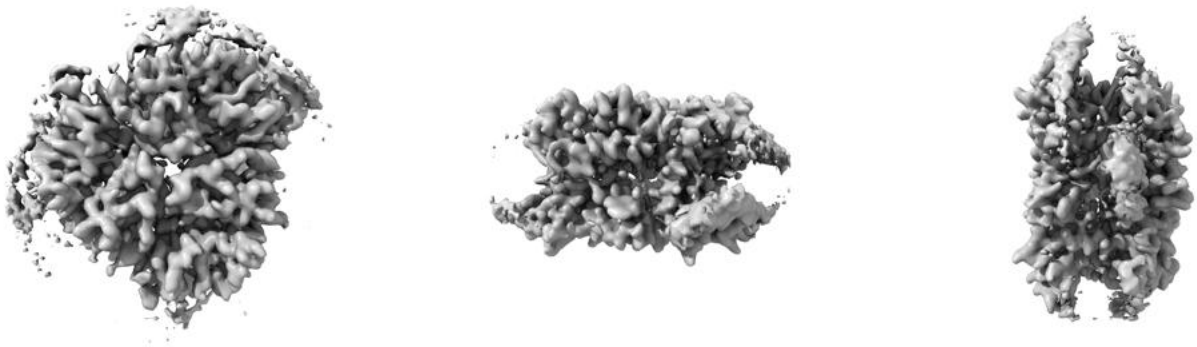

Y


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 0.1. 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.

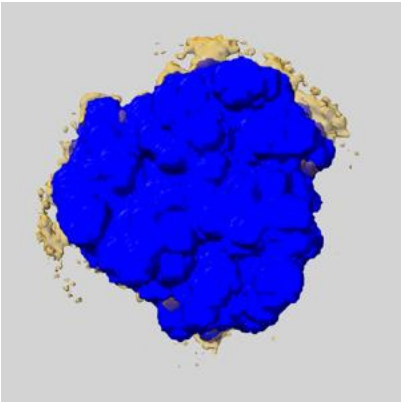
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

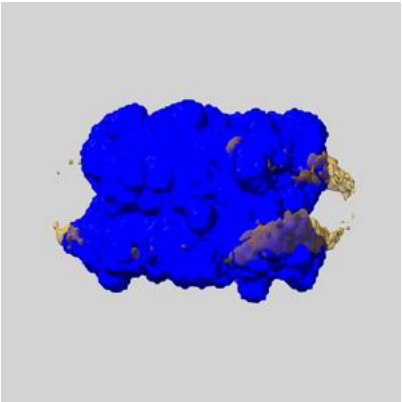
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

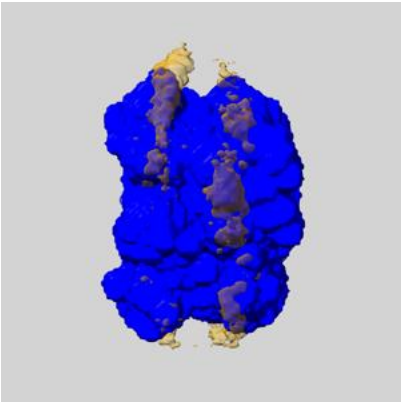
6.6.1 emd_35786_msk_1.map (i)



X



Y

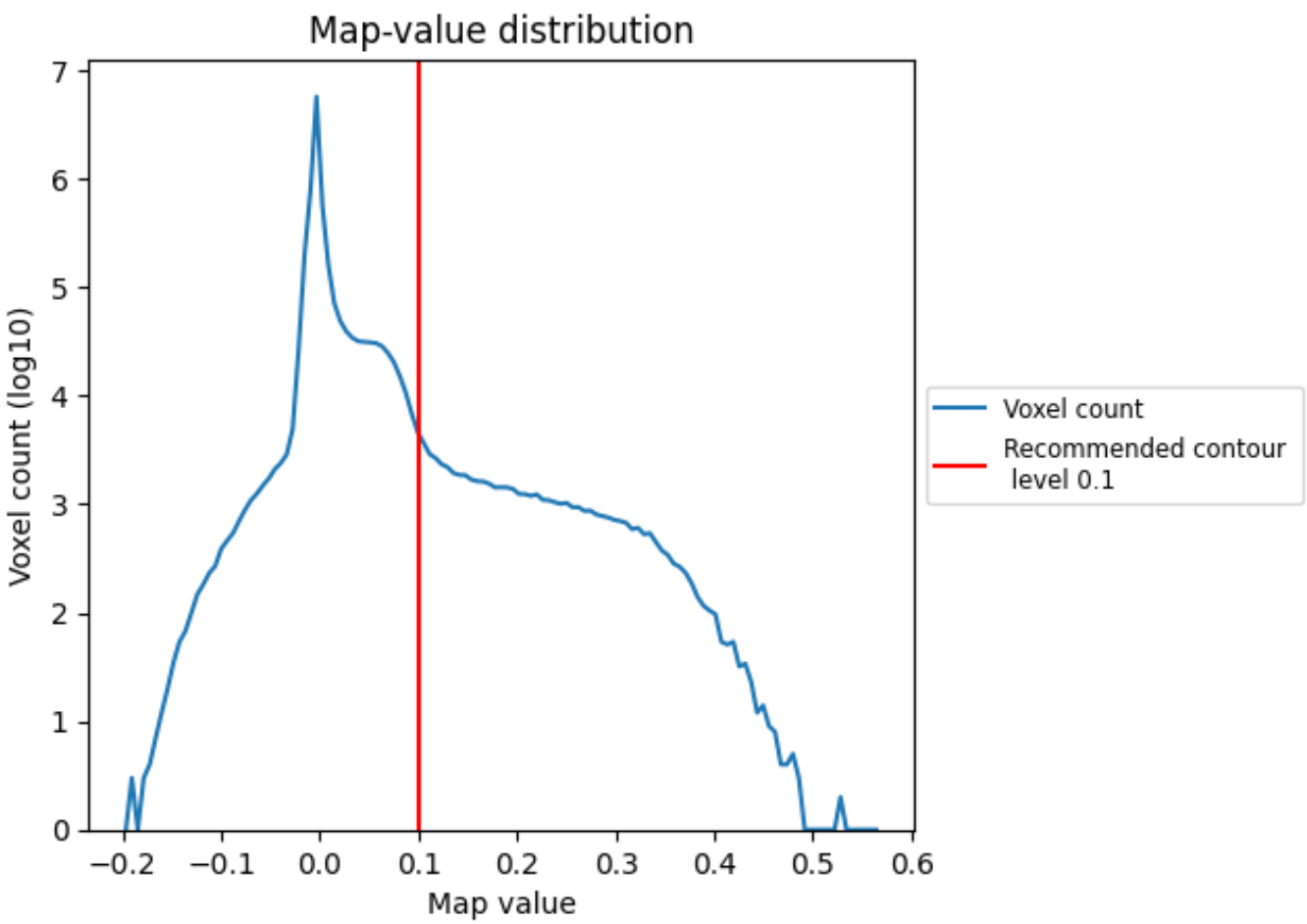


Z

7 Map analysis (i)

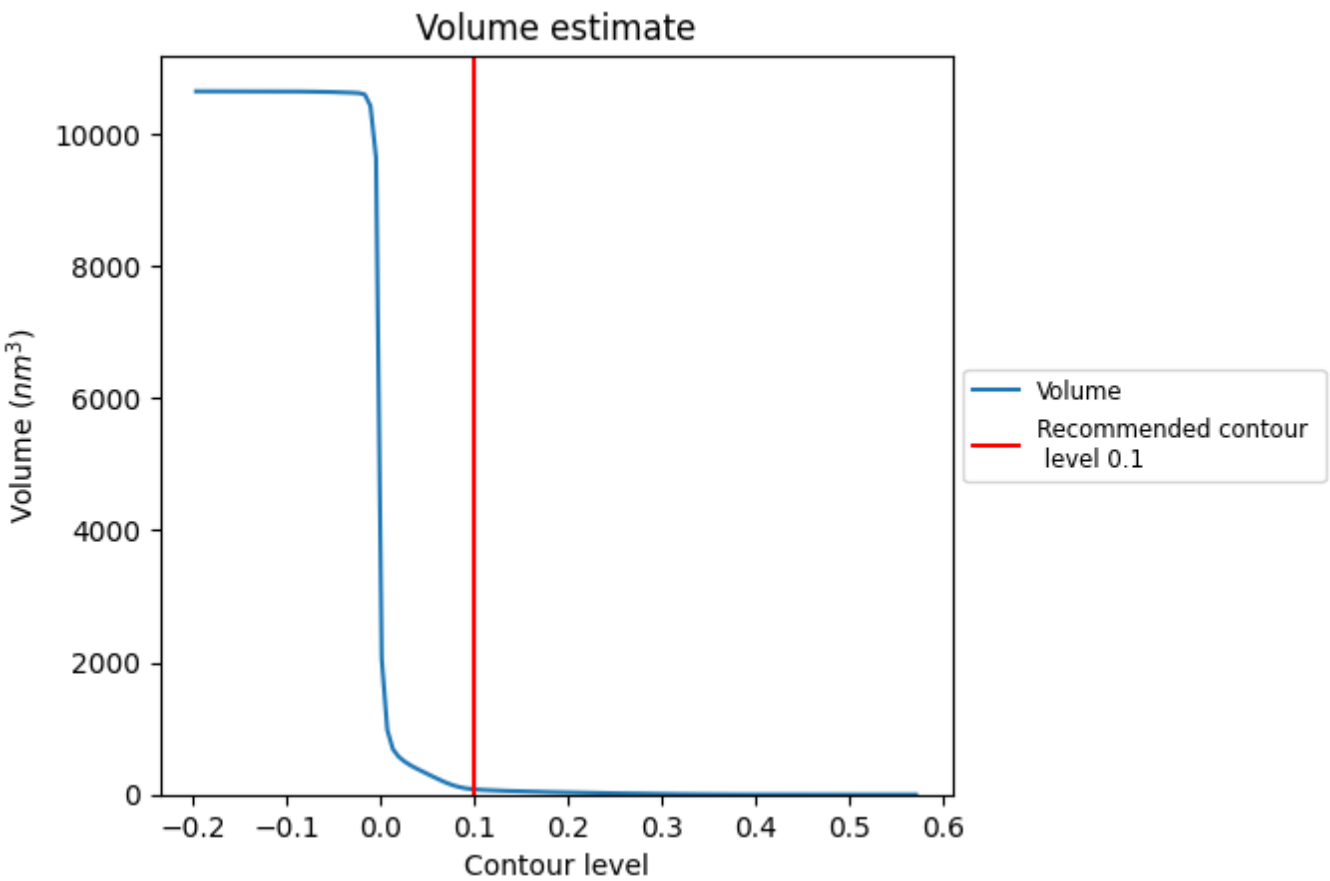
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

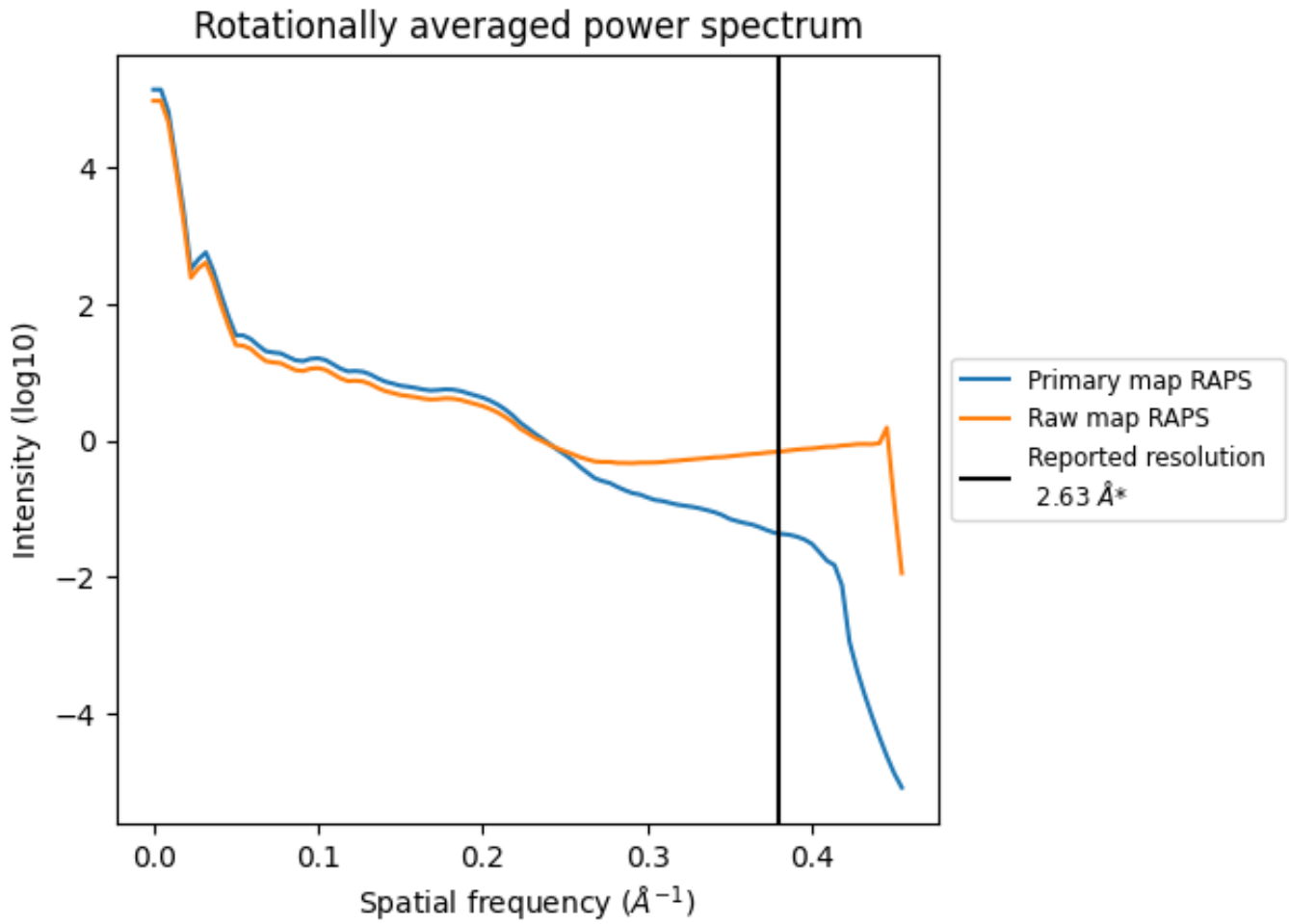
7.2 Volume estimate (i)



The volume at the recommended contour level is 79 nm^3; this corresponds to an approximate mass of 72 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)

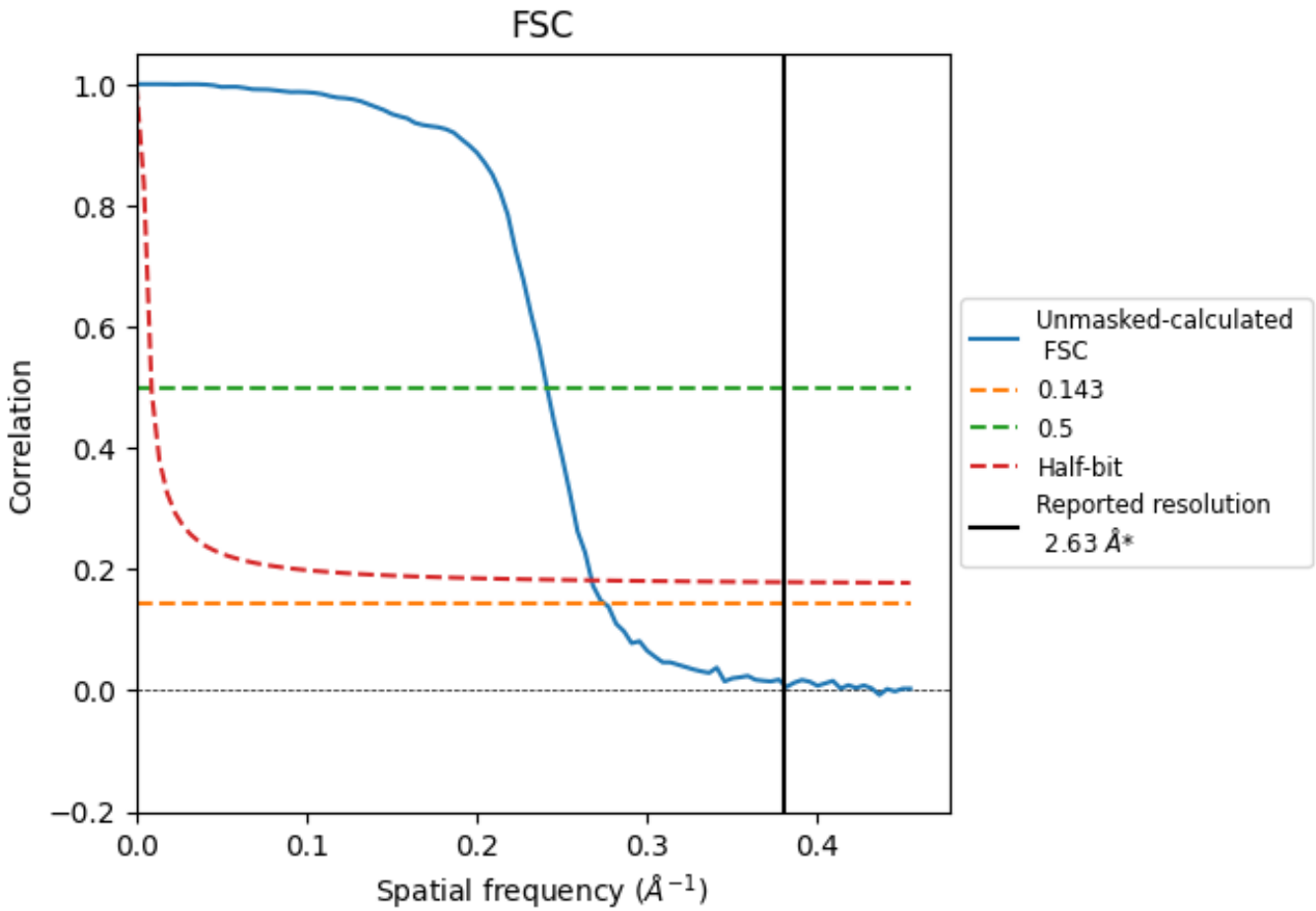


*Reported resolution corresponds to spatial frequency of 0.380 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.380 Å^{-1}

8.2 Resolution estimates (i)

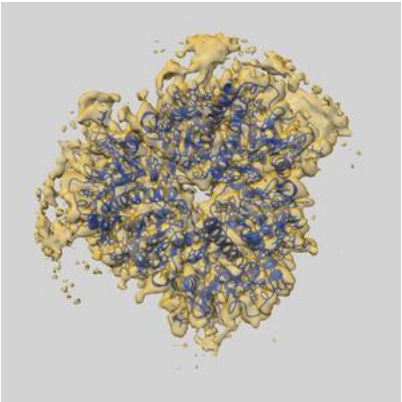
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.64	4.15	3.74

*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 3.64 differs from the reported value 2.63 by more than 10 %

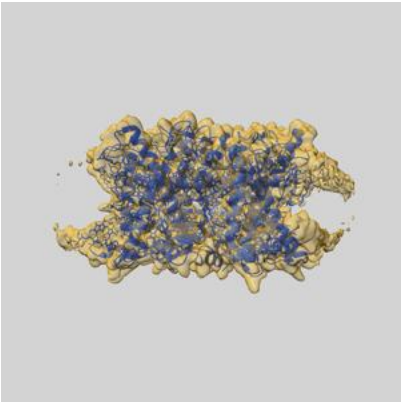
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-35786 and PDB model 8IX1. Per-residue inclusion information can be found in section 3 on page 10.

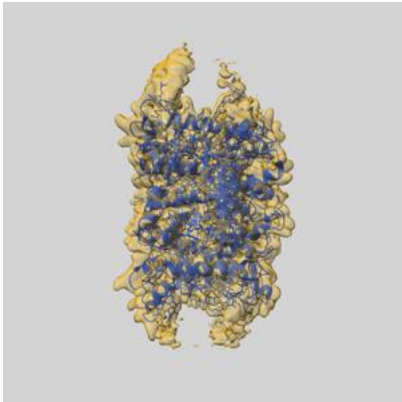
9.1 Map-model overlay (i)



X



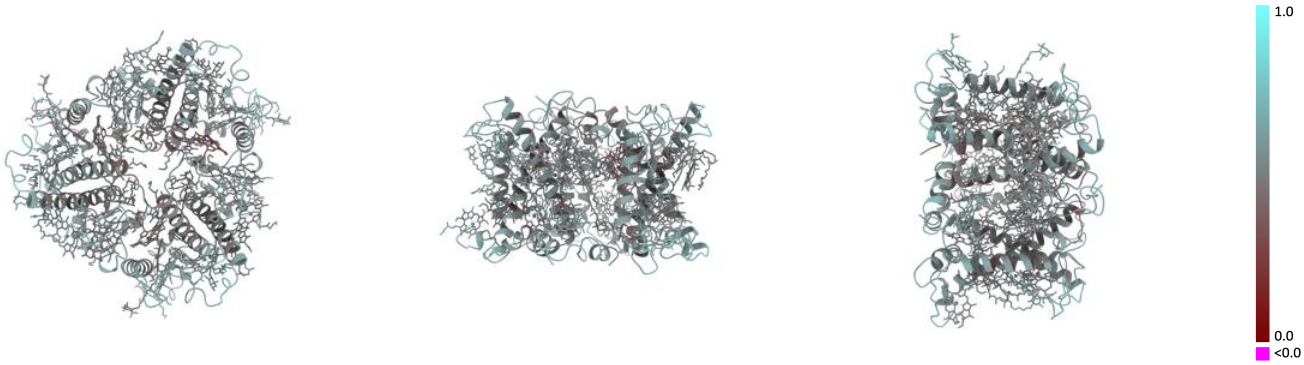
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

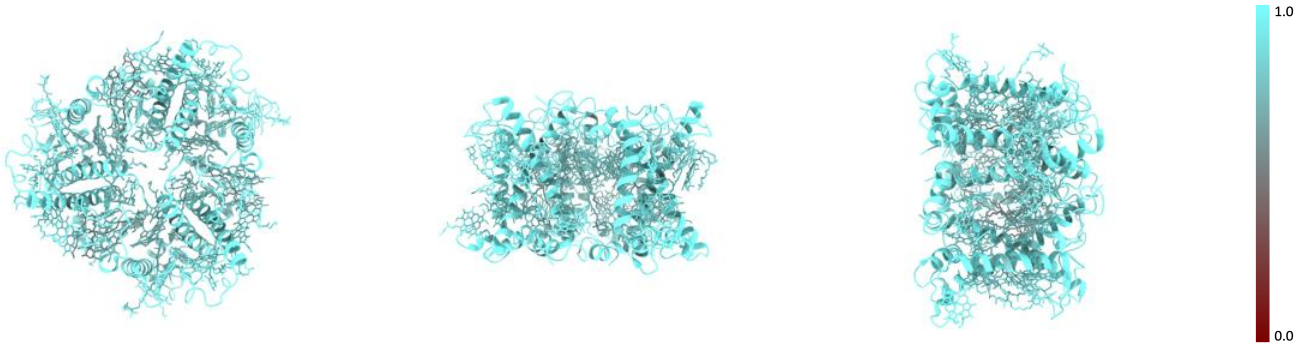
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

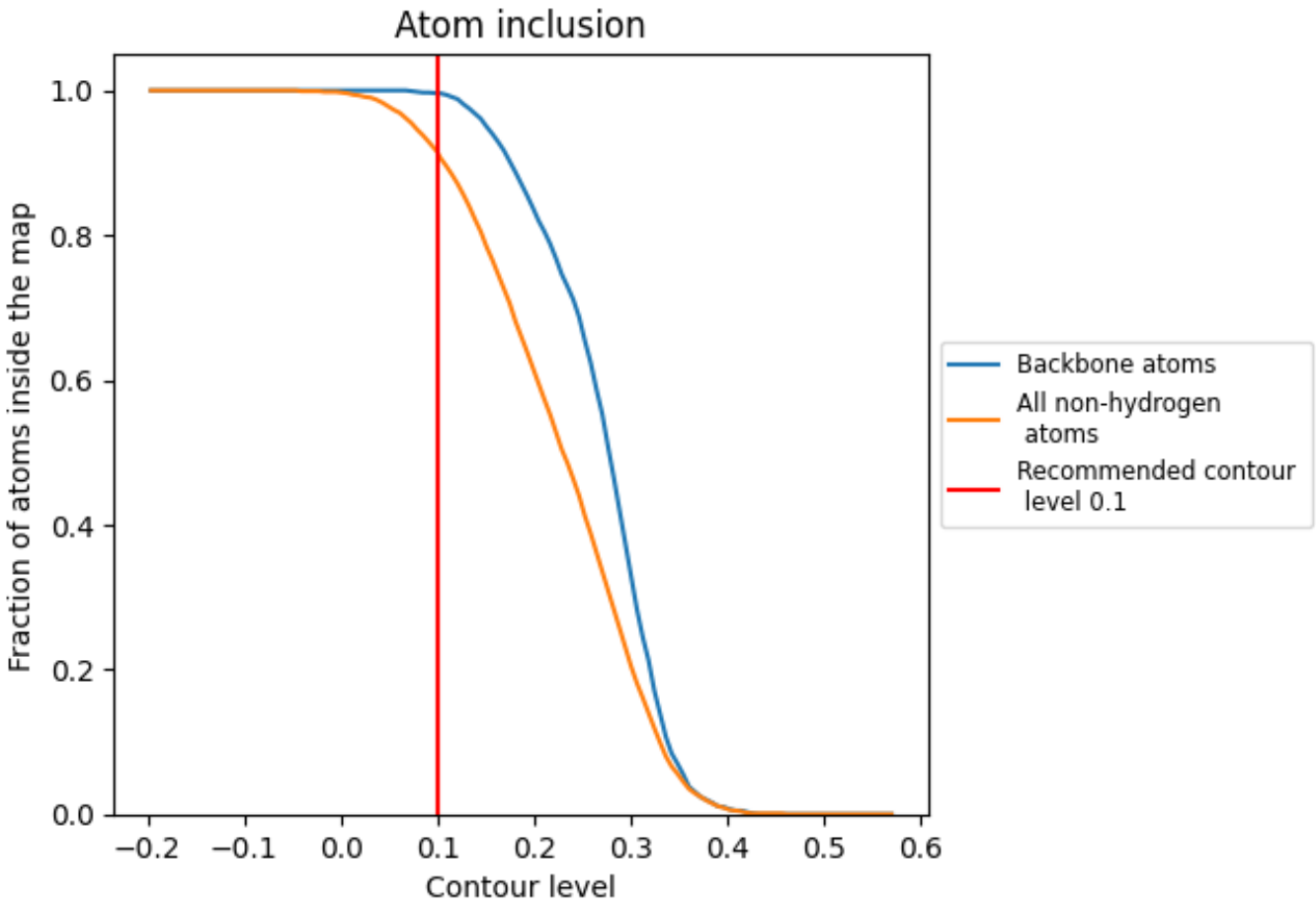
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 92% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9150	0.5260
G	0.9130	0.5280
N	0.9080	0.5190
Y	0.9230	0.5300