



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 12:46 AM JST

PDB ID : 5XNN / pdb_00005xnn
EMDB ID : EMD-6743
Title : Structure of M-LHCII and CP24 complexes in the stacked C2S2M2-type PSII-LHCII supercomplex from *Pisum sativum*
Authors : Su, X.D.; Ma, J.; Wei, X.P.; Cao, P.; Zhu, D.J.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : 2017-05-23
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
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

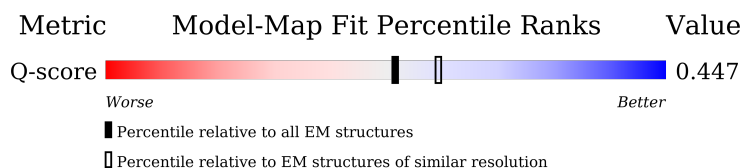
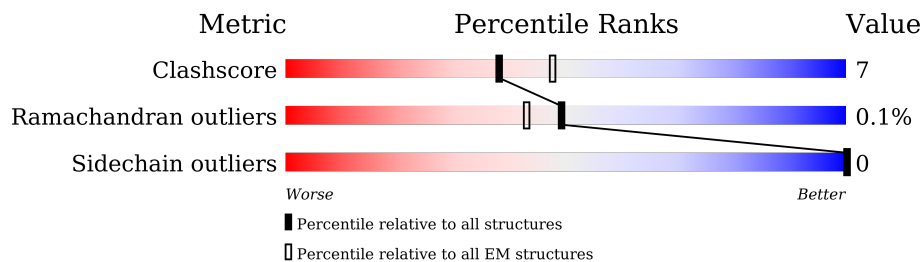
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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 $\leq 5\%$. 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	1	232	
1	2	232	
2	3	243	
3	4	210	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CHL	1	607	X	-	-	-
4	CHL	1	609	X	-	-	-
4	CHL	2	607	X	-	-	-
4	CHL	2	609	X	-	-	-
4	CHL	3	601	X	-	-	-
4	CHL	3	609	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10020 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 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	2	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		

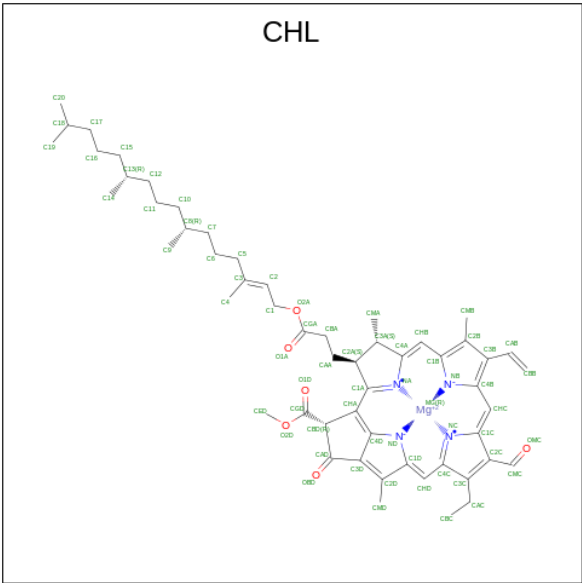
- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		

- Molecule 3 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

- Molecule 4 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



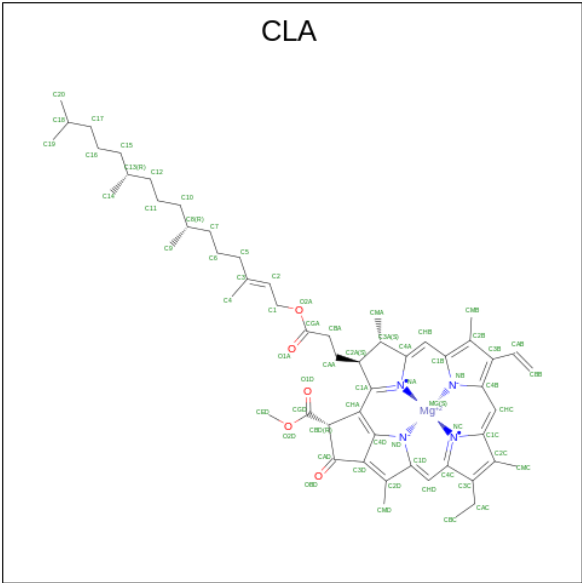
Mol	Chain	Residues	Atoms					AltConf
4	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1	1	Total 63	C 52	Mg 1	N 4	O 6	0
4	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1	1	Total 62	C 51	Mg 1	N 4	O 6	0
4	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	2	1	Total 61	C 50	Mg 1	N 4	O 6	0
4	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	2	1	Total 61	C 50	Mg 1	N 4	O 6	0
4	3	1	Total 64	C 53	Mg 1	N 4	O 6	0
4	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	3	1	Total 53	C 42	Mg 1	N 4	O 6	0
4	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	3	1	Total 61	C 50	Mg 1	N 4	O 6	0
4	4	1	Total 45	C 34	Mg 1	N 4	O 6	0
4	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	4	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
4	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 5 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



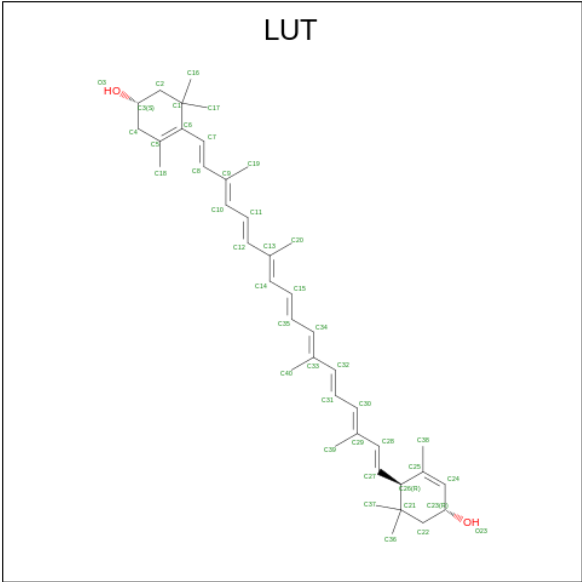
Mol	Chain	Residues	Atoms					AltConf
5	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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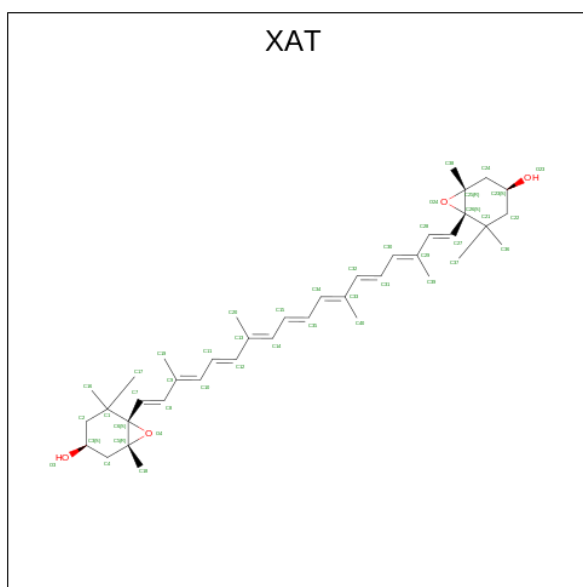
Mol	Chain	Residues	Atoms					AltConf
5	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 6 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3, 3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



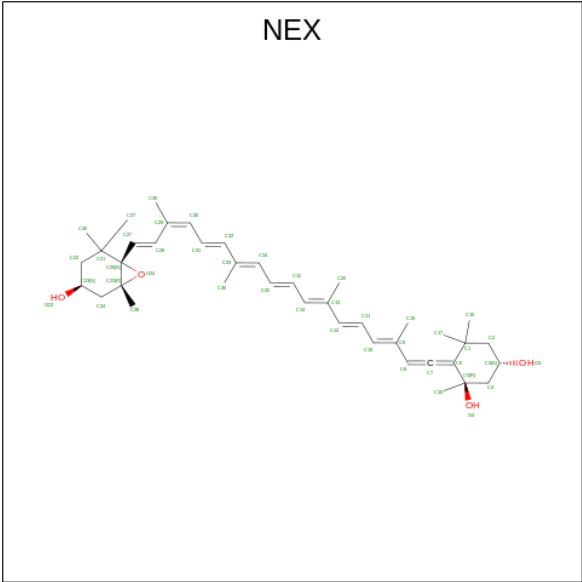
Mol	Chain	Residues	Atoms			AltConf
6	1	1	Total	C	O	0
			42	40	2	
6	1	1	Total	C	O	0
			42	40	2	
6	2	1	Total	C	O	0
			42	40	2	
6	2	1	Total	C	O	0
			42	40	2	
6	3	1	Total	C	O	0
			42	40	2	
6	3	1	Total	C	O	0
			42	40	2	
6	4	1	Total	C	O	0
			42	40	2	

- Molecule 7 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



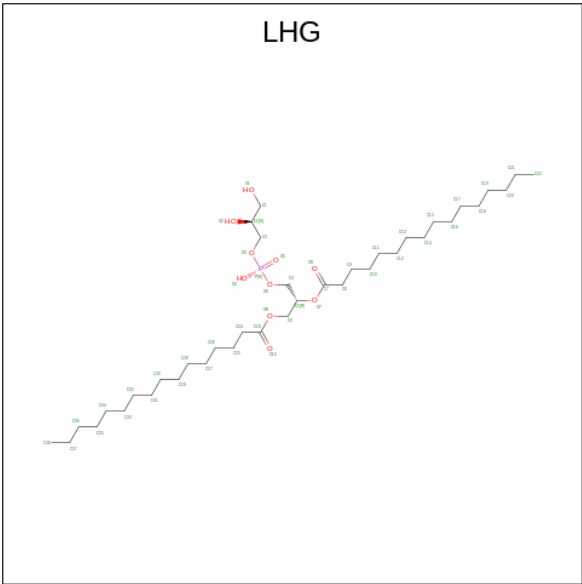
Mol	Chain	Residues	Atoms			AltConf
7	1	1	Total	C	O	0
			44	40	4	
7	2	1	Total	C	O	0
			44	40	4	
7	3	1	Total	C	O	0
			44	40	4	
7	4	1	Total	C	O	0
			44	40	4	

- Molecule 8 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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



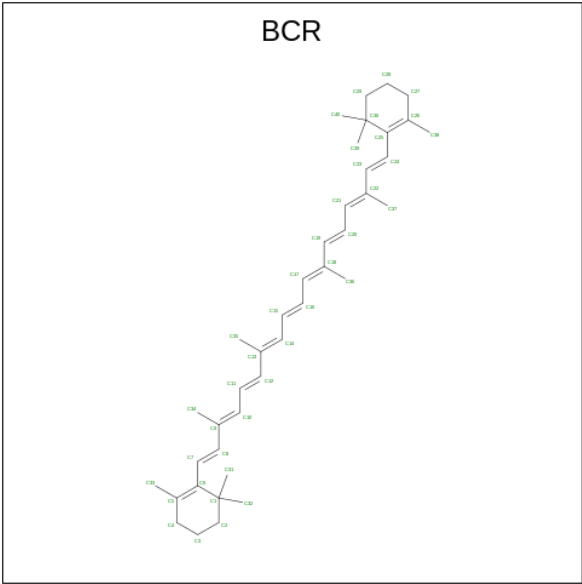
Mol	Chain	Residues	Atoms			AltConf
8	1	1	Total	C	O	0
			44	40	4	
8	2	1	Total	C	O	0
			44	40	4	
8	3	1	Total	C	O	0
			44	40	4	

- Molecule 9 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
9	1	1	Total	C	O	P	0
			41	30	10	1	
9	2	1	Total	C	O	P	0
			37	26	10	1	
9	3	1	Total	C	O	P	0
			47	36	10	1	
9	4	1	Total	C	O	P	0
			21	10	10	1	

- Molecule 10 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).

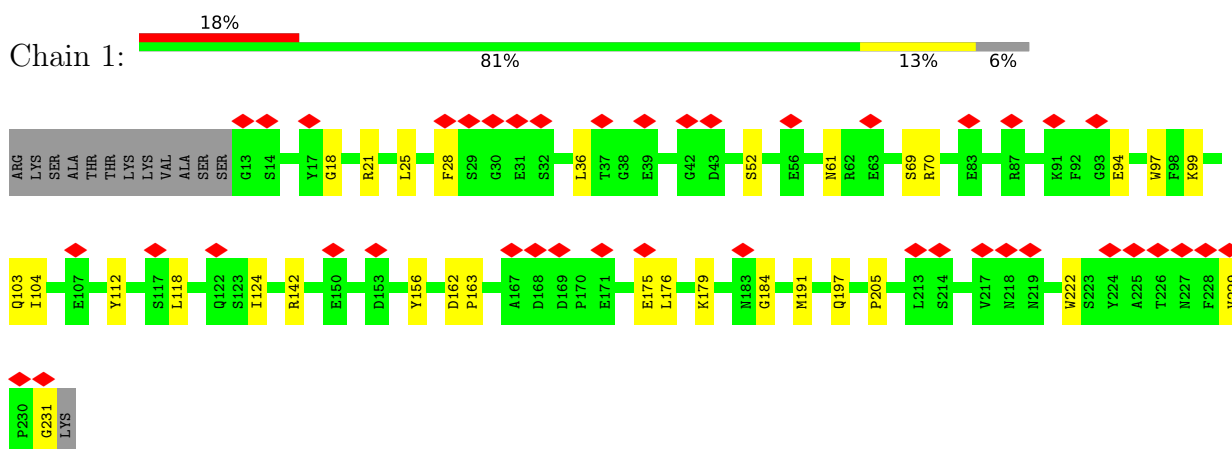


Mol	Chain	Residues	Atoms		AltConf
10	4	1	Total	C	0
			40	40	

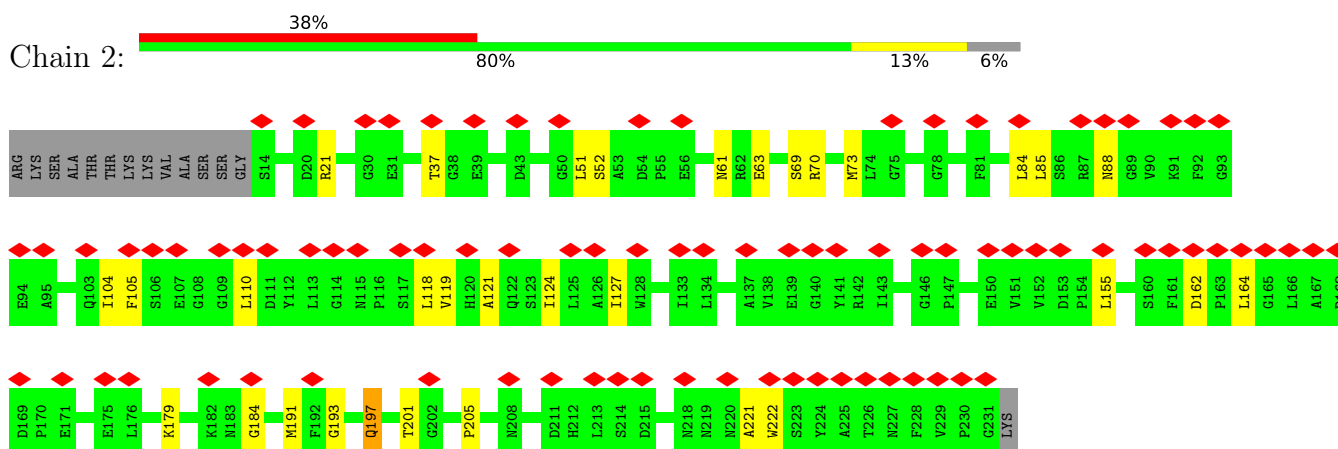
3 Residue-property plots

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.

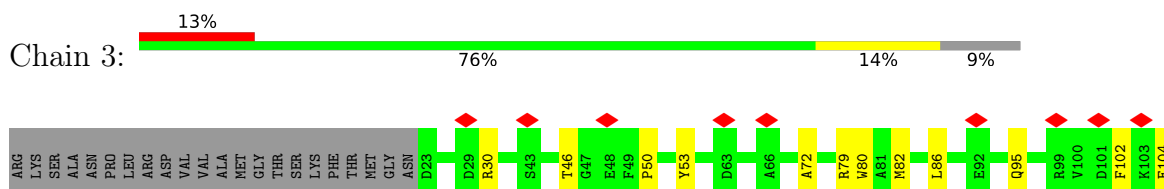
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

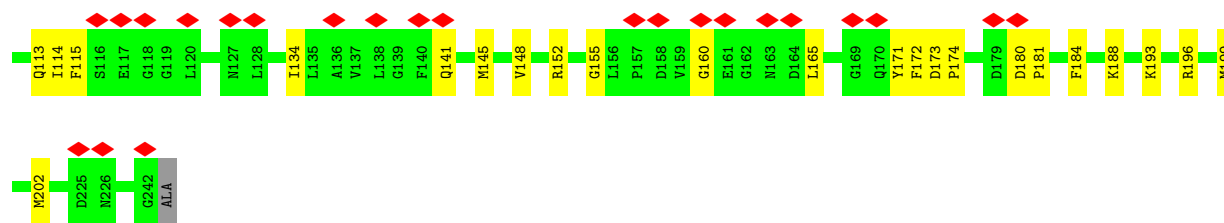


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



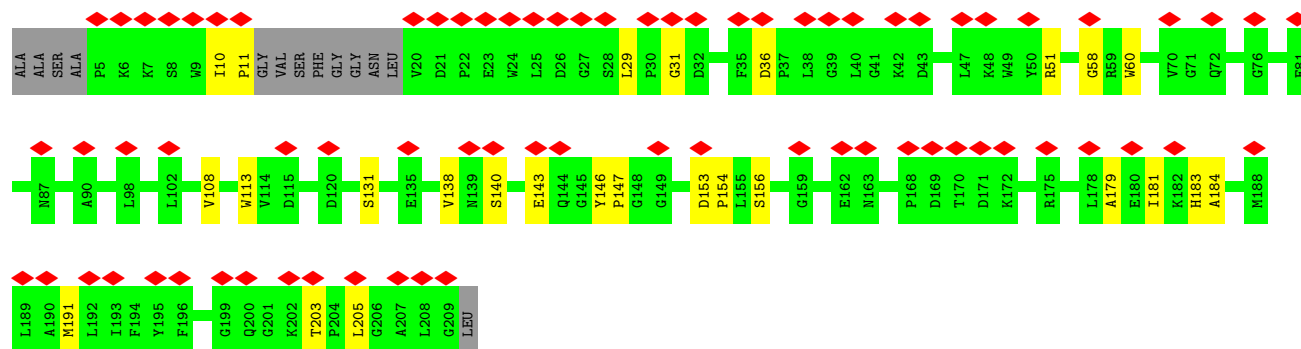
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic





- Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

Chain 4: 35% 81% 12% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	136521	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	156.0, 156.0, 156.0	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: XAT, CLA, NEX, BCR, CHL, LHG, 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	1	0.27	0/1720	0.46	0/2342
1	2	0.25	0/1716	0.49	1/2337 (0.0%)
2	3	0.31	0/1759	0.50	0/2396
3	4	0.27	0/1586	0.59	0/2158
All	All	0.28	0/6781	0.51	1/9233 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	197	GLN	CA-CB-CG	5.92	125.95	114.10

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	1	1668	0	1596	23	0
1	2	1664	0	1593	24	0
2	3	1707	0	1659	26	0
3	4	1534	0	1486	18	0
4	1	309	0	244	8	0
4	2	306	0	238	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	316	0	254	18	0
4	4	229	0	152	7	0
5	1	412	0	348	7	0
5	2	391	0	314	7	0
5	3	426	0	373	10	0
5	4	270	0	198	2	0
6	1	84	0	112	11	0
6	2	84	0	112	7	0
6	3	84	0	112	7	0
6	4	42	0	56	3	0
7	1	44	0	56	2	0
7	2	44	0	56	4	0
7	3	44	0	56	2	0
7	4	44	0	56	4	0
8	1	44	0	56	2	0
8	2	44	0	56	0	0
8	3	44	0	56	3	0
9	1	41	0	55	2	0
9	2	37	0	44	1	0
9	3	47	0	67	1	0
9	4	21	0	12	1	0
10	4	40	0	56	5	0
All	All	10020	0	9473	144	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 7.

All (144) 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)
1:2:191:MET:HE2	6:2:1621:LUT:H10	1.65	0.79
5:3:602:CLA:HAB	6:3:1621:LUT:H32	1.67	0.75
2:3:202:MET:HE2	6:3:1621:LUT:H10	1.71	0.73
5:1:602:CLA:HAB	6:1:1621:LUT:H32	1.72	0.72
1:1:191:MET:HE2	6:1:1621:LUT:H10	1.75	0.68
5:3:611:CLA:H3A	3:4:131:SER:HA	1.77	0.67
1:2:85:LEU:HD23	1:2:88:ASN:HD22	1.64	0.63
4:3:606:CHL:HBB2	4:3:607:CHL:HBB1	1.82	0.62
1:1:163:PRO:HD2	6:1:1620:LUT:H23	1.81	0.61
2:3:171:TYR:O	2:3:172:PHE:HB2	2.00	0.61
5:4:610:CLA:HAB	6:4:620:LUT:H32	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:607:CHL:HAA2	7:3:1622:XAT:H41	1.84	0.57
3:4:191:MET:HE2	7:4:622:XAT:H10	1.86	0.57
5:4:612:CLA:HED2	5:4:612:CLA:H2A	1.87	0.56
1:2:51:LEU:HD13	5:2:602:CLA:H42	1.86	0.56
1:1:99:LYS:HA	4:1:607:CHL:HED3	1.87	0.56
1:2:222:TRP:HB3	2:3:115:PHE:HZ	1.71	0.56
3:4:138:VAL:HG22	3:4:140:SER:H	1.71	0.56
1:2:21:ARG:NH1	1:2:37:THR:O	2.38	0.56
1:2:110:LEU:HD21	5:2:604:CLA:HAA2	1.88	0.55
1:1:21:ARG:NH2	1:1:36:LEU:O	2.40	0.55
1:1:103:GLN:HE22	5:1:604:CLA:HED3	1.72	0.55
1:1:104:ILE:HG21	1:1:124:ILE:HD13	1.88	0.54
2:3:114:ILE:HG21	2:3:134:ILE:HD13	1.89	0.54
1:1:197:GLN:HE22	6:1:1620:LUT:H42	1.71	0.54
2:3:79:ARG:NH1	4:3:608:CHL:OBD	2.40	0.54
2:3:173:ASP:OD1	6:3:1620:LUT:O23	2.26	0.54
1:2:164:LEU:HD12	6:2:1620:LUT:H222	1.90	0.54
5:3:603:CLA:HED2	4:3:609:CHL:H93	1.90	0.53
3:4:58:GLY:HA3	3:4:184:ALA:HB1	1.89	0.53
4:2:606:CHL:HMB2	4:2:609:CHL:HMC	1.90	0.53
3:4:191:MET:HG2	7:4:622:XAT:H12	1.90	0.53
2:3:141:GLN:HE22	4:3:607:CHL:HMC	1.74	0.53
4:4:606:CHL:HAA1	10:4:623:BCR:H19C	1.92	0.52
1:1:162:ASP:OD1	6:1:1620:LUT:O23	2.28	0.51
2:3:30:ARG:NH1	2:3:46:THR:O	2.43	0.51
3:4:29:LEU:HD11	3:4:51:ARG:HD3	1.92	0.51
4:1:607:CHL:HBB1	4:3:601:CHL:H141	1.92	0.51
7:2:1622:XAT:H41	4:3:607:CHL:HAA2	1.93	0.51
2:3:104:GLU:O	2:3:113:GLN:NE2	2.44	0.51
1:2:69:SER:HB3	1:2:184:GLY:HA3	1.93	0.51
1:2:104:ILE:HG21	1:2:124:ILE:HD13	1.92	0.51
4:3:606:CHL:HBA2	8:3:1623:NEX:H403	1.93	0.51
2:3:95:GLN:HE22	2:3:102:PHE:H	1.59	0.50
4:1:601:CHL:HMA3	9:1:2630:LHG:H121	1.92	0.50
1:1:69:SER:HB3	1:1:184:GLY:HA3	1.94	0.50
5:2:603:CLA:HMD3	4:2:609:CHL:HBA2	1.94	0.50
1:2:85:LEU:HA	1:2:88:ASN:HB2	1.94	0.50
5:3:603:CLA:HMD3	4:3:609:CHL:HBA2	1.94	0.50
1:1:176:LEU:HD23	1:1:179:LYS:HD2	1.93	0.49
1:2:162:ASP:OD1	6:2:1620:LUT:O23	2.29	0.49
1:1:52:SER:OG	1:1:61:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:18:GLY:O	1:1:21:ARG:NH1	2.41	0.49
4:4:606:CHL:HAA1	10:4:623:BCR:H21C	1.94	0.49
1:2:205:PRO:O	6:2:1620:LUT:O3	2.31	0.48
7:2:1622:XAT:H393	9:2:2630:LHG:HC92	1.94	0.48
3:4:154:PRO:HD2	6:4:620:LUT:H23	1.94	0.48
2:3:50:PRO:HG3	2:3:188:LYS:HD3	1.95	0.48
1:1:156:TYR:HB3	5:1:610:CLA:HED2	1.94	0.48
5:1:603:CLA:HMD3	4:1:609:CHL:HBA2	1.95	0.48
1:2:121:ALA:HB1	1:2:127:ILE:HD11	1.95	0.48
3:4:113:TRP:HB2	4:4:609:CHL:HMA1	1.96	0.48
1:2:52:SER:OG	1:2:61:ASN:ND2	2.47	0.47
1:2:179:LYS:HD3	5:2:612:CLA:HAA2	1.96	0.47
2:3:72:ALA:HA	2:3:165:LEU:HD11	1.96	0.47
1:1:97:TRP:O	6:1:1621:LUT:O3	2.32	0.47
1:1:94:GLU:N	1:1:103:GLN:OE1	2.45	0.47
1:2:118:LEU:HD23	4:2:605:CHL:HED2	1.96	0.47
3:4:203:THR:HG22	3:4:205:LEU:H	1.79	0.47
4:4:601:CHL:HBA1	4:4:601:CHL:H3A	1.66	0.47
1:1:222:TRP:HB3	1:2:105:PHE:HZ	1.80	0.46
1:1:112:TYR:HD2	1:1:118:LEU:HD13	1.79	0.46
2:3:181:PRO:HA	2:3:184:PHE:HB3	1.98	0.46
1:1:142:ARG:NH2	4:1:609:CHL:O1D	2.45	0.46
1:1:205:PRO:O	6:1:1620:LUT:O3	2.31	0.46
7:2:1622:XAT:H15	7:2:1622:XAT:H201	1.79	0.46
10:4:623:BCR:H341	10:4:623:BCR:H11C	1.69	0.46
5:1:613:CLA:H2	5:1:613:CLA:H61	1.67	0.46
1:1:229:VAL:HG22	1:1:231:GLY:H	1.80	0.45
4:2:607:CHL:H91	4:2:607:CHL:H112	1.80	0.45
3:4:31:GLY:HA3	3:4:181:ILE:HG21	1.98	0.45
3:4:36:ASP:OD1	7:4:622:XAT:O23	2.34	0.45
4:4:601:CHL:HBC1	9:4:2630:LHG:HC2	1.99	0.45
1:2:84:LEU:O	1:2:88:ASN:N	2.48	0.45
1:2:197:GLN:O	1:2:201:THR:OG1	2.31	0.45
7:3:1622:XAT:H31	7:3:1622:XAT:H391	1.72	0.45
6:3:1620:LUT:H35	6:3:1620:LUT:H401	1.86	0.45
1:1:70:ARG:NH1	4:1:608:CHL:OBD	2.42	0.44
2:3:79:ARG:HA	2:3:82:MET:HE3	1.99	0.44
2:3:174:PRO:HD2	6:3:1620:LUT:H23	1.99	0.44
2:3:196:ARG:HA	2:3:199:MET:HE3	1.99	0.44
4:3:609:CHL:H112	4:3:609:CHL:H91	1.83	0.44
6:1:1620:LUT:H35	6:1:1620:LUT:H401	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:221:ALA:N	5:2:613:CLA:O1A	2.49	0.44
7:1:1622:XAT:H12	9:1:2630:LHG:H182	1.99	0.44
2:3:155:GLY:HA2	4:3:608:CHL:HAC1	1.98	0.44
4:3:606:CHL:HMC	4:3:607:CHL:C4C	2.48	0.44
1:2:51:LEU:HD12	6:2:1621:LUT:H221	2.00	0.44
5:1:602:CLA:HBA1	6:1:1621:LUT:H382	1.99	0.44
7:1:1622:XAT:H11	7:1:1622:XAT:H191	1.79	0.44
2:3:160:GLY:HA3	4:3:608:CHL:HBC3	1.99	0.44
4:2:607:CHL:HMB1	4:2:607:CHL:H61	1.99	0.44
2:3:80:TRP:CE2	4:3:608:CHL:HED2	2.52	0.44
5:2:611:CLA:HBA2	5:2:612:CLA:HMD3	2.00	0.43
6:3:1621:LUT:H35	6:3:1621:LUT:H401	1.90	0.43
1:1:25:LEU:HB3	1:1:28:PHE:HB2	1.99	0.43
6:1:1621:LUT:H15	6:1:1621:LUT:H201	1.79	0.43
5:3:611:CLA:C4D	5:3:612:CLA:HMD2	2.49	0.43
3:4:153:ASP:HB3	3:4:156:SER:HA	1.99	0.43
5:3:603:CLA:H91	4:3:609:CHL:H121	1.99	0.43
7:4:622:XAT:H15	7:4:622:XAT:H201	1.87	0.43
2:3:145:MET:HA	2:3:148:VAL:HG22	2.01	0.43
2:3:193:LYS:NZ	9:3:2630:LHG:O5	2.52	0.43
4:3:601:CHL:H92	4:3:601:CHL:H62	1.86	0.43
1:2:63:GLU:HA	1:2:155:LEU:HD11	2.00	0.43
5:1:603:CLA:H8	5:3:602:CLA:H91	2.01	0.42
3:4:143:GLU:H	3:4:146:TYR:HB2	1.84	0.42
4:1:607:CHL:H142	4:1:609:CHL:H101	1.99	0.42
8:1:1623:NEX:H11	8:1:1623:NEX:H191	1.88	0.42
8:3:1623:NEX:H35	8:3:1623:NEX:H401	1.90	0.42
3:4:108:VAL:HG21	10:4:623:BCR:H16C	2.02	0.42
3:4:147:PRO:HB3	4:4:608:CHL:HBC2	2.01	0.42
3:4:179:ALA:O	3:4:183:HIS:ND1	2.38	0.42
2:3:152:ARG:NH2	4:3:609:CHL:O1D	2.52	0.42
2:3:180:ASP:HA	2:3:181:PRO:HD3	1.93	0.42
1:1:175:GLU:HG2	1:1:179:LYS:HE3	2.01	0.41
6:3:1621:LUT:H15	6:3:1621:LUT:H201	1.80	0.41
3:4:60:TRP:CE2	4:4:608:CHL:HED2	2.55	0.41
8:3:1623:NEX:H191	8:3:1623:NEX:H11	1.75	0.41
6:2:1620:LUT:H401	6:2:1620:LUT:H35	1.82	0.41
7:2:1622:XAT:H391	7:2:1622:XAT:H31	1.75	0.41
2:3:53:TYR:OH	2:3:193:LYS:NZ	2.41	0.41
3:4:10:ILE:HG23	3:4:11:PRO:HD3	2.02	0.41
8:1:1623:NEX:H15	8:1:1623:NEX:H201	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:152:ARG:HH21	4:3:609:CHL:HMA3	1.86	0.41
5:3:602:CLA:H93	5:3:602:CLA:H111	1.91	0.41
6:4:620:LUT:H15	6:4:620:LUT:H201	1.86	0.41
1:2:193:GLY:O	1:2:197:GLN:HG2	2.22	0.40
6:1:1621:LUT:H35	6:1:1621:LUT:H401	1.87	0.40
2:3:86:LEU:HB3	5:3:604:CLA:HMC2	2.03	0.40
5:3:603:CLA:HBC1	4:3:609:CHL:HBC2	2.03	0.40
10:4:623:BCR:H15C	10:4:623:BCR:H351	1.72	0.40
5:2:602:CLA:HBA1	6:2:1621:LUT:H382	2.02	0.40
1:2:70:ARG:HA	1:2:73:MET:HE3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1	217/232 (94%)	209 (96%)	8 (4%)	0	100	100
1	2	216/232 (93%)	210 (97%)	5 (2%)	1 (0%)	24	57
2	3	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
3	4	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
All	All	844/917 (92%)	807 (96%)	36 (4%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	119	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	171/182 (94%)	171 (100%)	0	100	100
1	2	171/182 (94%)	171 (100%)	0	100	100
2	3	175/193 (91%)	175 (100%)	0	100	100
3	4	154/162 (95%)	154 (100%)	0	100	100
All	All	671/719 (93%)	671 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	2	61	ASN
1	2	88	ASN
2	3	95	GLN
2	3	113	GLN
2	3	219	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

72 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$
6	LUT	2	1621	-	42,43,43	0.84	1 (2%)	51,60,60	1.68	15 (29%)
4	CHL	2	607	-	65,69,74	1.96	18 (27%)	74,108,114	2.95	24 (32%)
4	CHL	2	601	1	50,54,74	2.27	18 (36%)	56,90,114	3.47	26 (46%)
4	CHL	2	608	-	50,54,74	2.21	18 (36%)	56,90,114	3.36	21 (37%)
4	CHL	4	608	-	50,54,74	2.16	17 (34%)	56,90,114	3.42	21 (37%)
5	CLA	1	612	1	49,53,73	1.48	9 (18%)	59,89,113	1.45	10 (16%)
5	CLA	1	614	1	49,53,73	1.47	7 (14%)	59,89,113	1.29	6 (10%)
9	LHG	3	2630	5	46,46,48	0.70	1 (2%)	49,52,54	1.24	5 (10%)
4	CHL	2	606	-	50,54,74	2.26	18 (36%)	56,90,114	3.22	22 (39%)
7	XAT	3	1622	-	39,47,47	1.03	3 (7%)	54,74,74	2.85	24 (44%)
4	CHL	1	608	-	50,54,74	2.18	17 (34%)	56,90,114	3.36	19 (33%)
4	CHL	1	607	-	67,71,74	1.92	19 (28%)	76,110,114	3.11	24 (31%)
4	CHL	2	609	1	65,69,74	1.99	18 (27%)	74,108,114	2.87	24 (32%)
5	CLA	1	603	1	59,63,73	1.32	10 (16%)	71,101,113	1.44	7 (9%)
5	CLA	2	611	9	49,53,73	1.46	7 (14%)	59,89,113	1.38	7 (11%)
4	CHL	4	609	3	50,54,74	2.31	19 (38%)	56,90,114	3.26	20 (35%)
5	CLA	4	612	3	49,53,73	1.47	7 (14%)	59,89,113	1.35	6 (10%)
6	LUT	2	1620	-	42,43,43	0.80	0	51,60,60	1.80	15 (29%)
4	CHL	1	609	1	66,70,74	1.95	18 (27%)	75,109,114	2.86	22 (29%)
8	NEX	3	1623	-	38,46,46	0.87	1 (2%)	50,70,70	2.40	16 (32%)
5	CLA	2	602	1	65,69,73	1.30	10 (15%)	78,108,113	1.19	8 (10%)
5	CLA	3	613	2	62,66,73	1.32	9 (14%)	74,104,113	1.28	7 (9%)
9	LHG	2	2630	5	36,36,48	0.74	0	39,42,54	1.27	4 (10%)
9	LHG	4	2630	5	20,20,48	0.91	0	23,26,54	1.30	2 (8%)
5	CLA	4	602	3	49,53,73	1.45	9 (18%)	59,89,113	1.41	6 (10%)
4	CHL	3	606	-	50,54,74	2.19	18 (36%)	56,90,114	3.24	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CLA	2	603	1	59,63,73	1.34	9 (15%)	71,101,113	1.40	8 (11%)
5	CLA	4	603	3	49,53,73	1.49	10 (20%)	59,89,113	1.44	6 (10%)
5	CLA	1	604	-	54,58,73	1.43	10 (18%)	65,95,113	1.37	10 (15%)
4	CHL	3	605	2	50,54,74	2.27	18 (36%)	56,90,114	3.31	24 (42%)
5	CLA	3	611	9	59,63,73	1.38	9 (15%)	71,101,113	1.45	10 (14%)
6	LUT	1	1620	-	42,43,43	0.80	0	51,60,60	1.66	15 (29%)
7	XAT	2	1622	-	39,47,47	0.91	1 (2%)	54,74,74	2.81	21 (38%)
5	CLA	3	604	-	49,53,73	1.48	9 (18%)	59,89,113	1.32	6 (10%)
5	CLA	3	614	2	52,56,73	1.42	8 (15%)	62,92,113	1.16	5 (8%)
5	CLA	3	610	2	64,68,73	1.28	7 (10%)	77,107,113	1.18	7 (9%)
8	NEX	2	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.39	16 (32%)
7	XAT	4	622	-	39,47,47	0.92	1 (2%)	54,74,74	2.62	22 (40%)
5	CLA	1	611	9	49,53,73	1.47	9 (18%)	59,89,113	1.28	6 (10%)
4	CHL	4	607	-	50,54,74	2.30	18 (36%)	56,90,114	3.17	21 (37%)
9	LHG	1	2630	5	40,40,48	0.72	1 (2%)	43,46,54	1.33	6 (13%)
5	CLA	2	613	1	49,53,73	1.47	9 (18%)	59,89,113	1.29	6 (10%)
8	NEX	1	1623	-	38,46,46	0.98	2 (5%)	50,70,70	2.42	15 (30%)
10	BCR	4	623	-	41,41,41	0.74	0	56,56,56	2.31	17 (30%)
5	CLA	3	603	2	59,63,73	1.31	10 (16%)	71,101,113	1.46	8 (11%)
4	CHL	4	606	-	50,54,74	2.29	18 (36%)	56,90,114	3.30	25 (44%)
4	CHL	3	608	-	50,54,74	2.19	18 (36%)	56,90,114	3.42	21 (37%)
5	CLA	3	612	2	49,53,73	1.47	10 (20%)	59,89,113	1.39	9 (15%)
4	CHL	2	605	1	50,54,74	2.28	18 (36%)	56,90,114	3.31	22 (39%)
7	XAT	1	1622	-	39,47,47	0.90	0	54,74,74	2.77	22 (40%)
4	CHL	1	601	1	50,54,74	2.32	18 (36%)	56,90,114	3.26	24 (42%)
6	LUT	4	620	-	42,43,43	0.81	0	51,60,60	1.87	17 (33%)
5	CLA	4	611	9	49,53,73	1.49	7 (14%)	59,89,113	1.31	4 (6%)
5	CLA	1	613	1	59,63,73	1.36	9 (15%)	71,101,113	1.23	5 (7%)
5	CLA	2	604	-	49,53,73	1.47	9 (18%)	59,89,113	1.36	6 (10%)
6	LUT	3	1621	-	42,43,43	0.84	1 (2%)	51,60,60	1.60	11 (21%)
5	CLA	2	610	1	54,58,73	1.36	8 (14%)	65,95,113	1.22	8 (12%)
4	CHL	3	601	2	68,72,74	1.95	16 (23%)	77,111,114	3.10	27 (35%)
5	CLA	4	610	3	49,53,73	1.48	9 (18%)	59,89,113	1.18	6 (10%)
4	CHL	1	606	-	50,54,74	2.24	17 (34%)	56,90,114	3.15	22 (39%)
4	CHL	3	607	-	57,61,74	2.25	19 (33%)	64,98,114	3.11	26 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CHL	3	609	2	65,69,74	2.04	17 (26%)	74,108,114	2.72	24 (32%)
4	CHL	1	605	1	50,54,74	2.23	18 (36%)	56,90,114	3.37	24 (42%)
5	CLA	1	602	1	65,69,73	1.28	10 (15%)	78,108,113	1.19	8 (10%)
6	LUT	1	1621	-	42,43,43	0.90	2 (4%)	51,60,60	1.74	15 (29%)
4	CHL	4	601	3	48,53,74	2.38	19 (39%)	53,89,114	3.18	19 (35%)
5	CLA	2	614	1	49,53,73	1.48	7 (14%)	59,89,113	1.27	4 (6%)
5	CLA	3	602	2	64,68,73	1.30	8 (12%)	77,107,113	1.21	8 (10%)
5	CLA	2	612	1	49,53,73	1.51	8 (16%)	59,89,113	1.37	6 (10%)
5	CLA	4	604	-	49,53,73	1.50	8 (16%)	59,89,113	1.28	5 (8%)
5	CLA	1	610	1	60,64,73	1.30	8 (13%)	72,102,113	1.16	6 (8%)
6	LUT	3	1620	-	42,43,43	0.85	0	51,60,60	1.72	12 (23%)

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
6	LUT	2	1621	-	-	3/29/67/67	0/2/2/2
4	CHL	2	607	-	1/1/14/21	16/35/111/117	-
4	CHL	2	601	1	-	6/17/93/117	-
4	CHL	2	608	-	-	7/17/93/117	-
4	CHL	4	608	-	-	7/17/93/117	-
5	CLA	1	612	1	-	5/15/91/115	-
5	CLA	1	614	1	-	4/15/91/115	-
9	LHG	3	2630	5	-	24/51/51/53	-
4	CHL	2	606	-	-	6/17/93/117	-
7	XAT	3	1622	-	-	2/31/93/93	0/4/4/4
4	CHL	1	608	-	-	7/17/93/117	-
4	CHL	1	607	-	1/1/14/21	22/38/114/117	-
4	CHL	2	609	1	1/1/14/21	13/35/111/117	-
5	CLA	1	603	1	-	14/27/103/115	-
5	CLA	2	611	9	-	5/15/91/115	-
4	CHL	4	609	3	-	6/17/93/117	-
5	CLA	4	612	3	-	7/15/91/115	-
6	LUT	2	1620	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHL	1	609	1	1/1/14/21	18/37/113/117	-
8	NEX	3	1623	-	-	4/27/83/83	0/3/3/3
5	CLA	2	602	1	-	12/35/111/115	-
5	CLA	3	613	2	-	11/31/107/115	-
9	LHG	2	2630	5	-	16/41/41/53	-
9	LHG	4	2630	5	-	8/23/23/53	-
5	CLA	4	602	3	-	9/15/91/115	-
4	CHL	3	606	-	-	9/17/93/117	-
5	CLA	2	603	1	-	13/27/103/115	-
5	CLA	4	603	3	-	6/15/91/115	-
5	CLA	1	604	-	-	12/21/97/115	-
4	CHL	3	605	2	-	11/17/93/117	-
5	CLA	3	611	9	-	9/27/103/115	-
6	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
7	XAT	2	1622	-	-	3/31/93/93	0/4/4/4
5	CLA	3	604	-	-	11/15/91/115	-
5	CLA	3	614	2	-	11/19/95/115	-
5	CLA	3	610	2	-	9/33/109/115	-
8	NEX	2	1623	-	-	7/27/83/83	0/3/3/3
7	XAT	4	622	-	-	2/31/93/93	0/4/4/4
5	CLA	1	611	9	-	8/15/91/115	-
4	CHL	4	607	-	-	10/17/93/117	-
9	LHG	1	2630	5	-	15/45/45/53	-
5	CLA	2	613	1	-	7/15/91/115	-
8	NEX	1	1623	-	-	6/27/83/83	0/3/3/3
10	BCR	4	623	-	-	9/29/63/63	0/2/2/2
5	CLA	3	603	2	-	15/27/103/115	-
4	CHL	4	606	-	-	8/17/93/117	-
4	CHL	3	608	-	-	5/17/93/117	-
5	CLA	3	612	2	-	10/15/91/115	-
4	CHL	2	605	1	-	11/17/93/117	-
7	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
4	CHL	1	601	1	-	6/17/93/117	-
6	LUT	4	620	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	4	611	9	-	6/15/91/115	-
5	CLA	1	613	1	-	10/27/103/115	-
5	CLA	2	604	-	-	10/15/91/115	-
6	LUT	3	1621	-	-	3/29/67/67	0/2/2/2
5	CLA	2	610	1	-	6/21/97/115	-
4	CHL	3	601	2	1/1/14/21	18/39/115/117	-
5	CLA	4	610	3	-	6/15/91/115	-
4	CHL	1	606	-	-	10/17/93/117	-
4	CHL	3	607	-	-	8/26/102/117	-
4	CHL	3	609	2	1/1/14/21	15/35/111/117	-
4	CHL	1	605	1	-	10/17/93/117	-
5	CLA	1	602	1	-	14/35/111/115	-
6	LUT	1	1621	-	-	3/29/67/67	0/2/2/2
4	CHL	4	601	3	-	9/15/91/117	-
5	CLA	2	614	1	-	7/15/91/115	-
5	CLA	3	602	2	-	16/33/109/115	-
5	CLA	2	612	1	-	5/15/91/115	-
5	CLA	4	604	-	-	10/15/91/115	-
5	CLA	1	610	1	-	7/29/105/115	-
6	LUT	3	1620	-	-	2/29/67/67	0/2/2/2

All (686) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	601	CHL	C3D-C4D	-5.50	1.31	1.44
4	1	601	CHL	C3D-C4D	-5.38	1.32	1.44
4	2	601	CHL	C3D-C4D	-5.34	1.32	1.44
4	3	606	CHL	C3D-C4D	-5.17	1.32	1.44
4	3	605	CHL	O2D-CGD	5.16	1.45	1.33
4	1	608	CHL	C3D-C4D	-5.15	1.32	1.44
4	3	608	CHL	C3D-C4D	-5.15	1.32	1.44
4	2	605	CHL	O2D-CGD	5.14	1.45	1.33
4	1	609	CHL	C3D-C4D	-5.13	1.32	1.44
4	2	601	CHL	O2D-CGD	5.13	1.45	1.33
4	4	608	CHL	C3D-C4D	-5.12	1.32	1.44
4	1	606	CHL	C3D-C4D	-5.12	1.32	1.44
4	4	609	CHL	C3D-C4D	-5.11	1.32	1.44
4	4	607	CHL	O2D-CGD	5.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1	606	CHL	O2D-CGD	5.10	1.45	1.33
4	4	606	CHL	C3D-C4D	-5.08	1.32	1.44
4	1	601	CHL	O2D-CGD	5.08	1.45	1.33
4	2	606	CHL	O2D-CGD	5.08	1.45	1.33
4	2	608	CHL	C3D-C4D	-5.08	1.32	1.44
4	3	609	CHL	C3D-C4D	-5.08	1.32	1.44
4	3	607	CHL	C3D-C4D	-5.06	1.32	1.44
4	3	607	CHL	O2D-CGD	5.06	1.45	1.33
4	3	606	CHL	O2D-CGD	5.04	1.45	1.33
4	4	606	CHL	O2D-CGD	5.03	1.45	1.33
4	2	607	CHL	O2D-CGD	5.03	1.45	1.33
4	1	605	CHL	C3D-C4D	-5.01	1.32	1.44
4	2	606	CHL	C3D-C4D	-4.99	1.32	1.44
4	2	609	CHL	C3D-C4D	-4.99	1.32	1.44
4	1	605	CHL	O2D-CGD	4.98	1.45	1.33
4	4	609	CHL	O2D-CGD	4.98	1.45	1.33
4	4	608	CHL	O2D-CGD	4.97	1.45	1.33
4	3	601	CHL	O2D-CGD	4.97	1.45	1.33
4	3	609	CHL	O2D-CGD	4.95	1.45	1.33
4	4	607	CHL	C3D-C4D	-4.94	1.33	1.44
4	2	609	CHL	O2D-CGD	4.90	1.45	1.33
4	1	607	CHL	C3D-C4D	-4.88	1.33	1.44
4	1	607	CHL	O2D-CGD	4.86	1.45	1.33
4	2	608	CHL	O2D-CGD	4.84	1.45	1.33
4	1	608	CHL	O2D-CGD	4.83	1.45	1.33
4	1	609	CHL	O2D-CGD	4.82	1.45	1.33
4	4	601	CHL	C2C-C3C	4.82	1.47	1.36
4	3	607	CHL	O2A-CGA	4.81	1.47	1.33
4	3	605	CHL	C3D-C4D	-4.81	1.33	1.44
4	4	601	CHL	C3D-C4D	-4.80	1.33	1.44
4	3	608	CHL	O2D-CGD	4.80	1.44	1.33
4	3	607	CHL	C2C-C3C	4.79	1.47	1.36
4	2	607	CHL	C3D-C4D	-4.77	1.33	1.44
4	2	605	CHL	C3D-C4D	-4.72	1.33	1.44
4	4	601	CHL	O2D-CGD	4.71	1.46	1.30
4	1	601	CHL	CHD-C1D	4.67	1.47	1.38
4	4	601	CHL	CHD-C1D	4.65	1.47	1.38
4	3	609	CHL	CHD-C1D	4.64	1.47	1.38
4	2	606	CHL	C2C-C3C	4.63	1.46	1.36
4	3	609	CHL	C2C-C3C	4.62	1.46	1.36
4	3	607	CHL	CHD-C1D	4.62	1.47	1.38
4	4	601	CHL	CHC-C1C	4.61	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	605	CHL	C2C-C3C	4.60	1.46	1.36
4	4	608	CHL	CHC-C1C	4.58	1.47	1.38
4	4	606	CHL	C2C-C3C	4.57	1.46	1.36
4	2	609	CHL	C2C-C3C	4.55	1.46	1.36
4	2	608	CHL	O2A-CGA	4.54	1.46	1.30
4	4	609	CHL	CHD-C1D	4.53	1.47	1.38
4	3	605	CHL	O2A-CGA	4.52	1.45	1.30
4	1	608	CHL	O2A-CGA	4.51	1.45	1.30
4	1	601	CHL	O2A-CGA	4.50	1.45	1.30
4	4	601	CHL	O2A-CGA	4.50	1.45	1.30
4	1	605	CHL	O2A-CGA	4.50	1.45	1.30
4	3	606	CHL	O2A-CGA	4.50	1.45	1.30
4	3	601	CHL	CHC-C1C	4.48	1.47	1.38
4	2	606	CHL	O2A-CGA	4.48	1.45	1.30
4	4	609	CHL	O2A-CGA	4.48	1.45	1.30
4	1	606	CHL	O2A-CGA	4.48	1.45	1.30
4	2	605	CHL	CHC-C1C	4.47	1.47	1.38
4	3	605	CHL	C2C-C3C	4.47	1.46	1.36
4	4	607	CHL	O2A-CGA	4.47	1.45	1.30
4	4	608	CHL	O2A-CGA	4.47	1.45	1.30
4	4	607	CHL	C2C-C3C	4.47	1.46	1.36
4	2	605	CHL	O2A-CGA	4.46	1.45	1.30
4	4	606	CHL	O2A-CGA	4.46	1.45	1.30
4	3	608	CHL	O2A-CGA	4.45	1.45	1.30
4	3	609	CHL	O2A-CGA	4.45	1.46	1.33
4	3	607	CHL	CHC-C1C	4.44	1.47	1.38
4	1	607	CHL	C2C-C3C	4.44	1.46	1.36
4	1	609	CHL	C2C-C3C	4.44	1.46	1.36
4	1	601	CHL	C2C-C3C	4.43	1.46	1.36
4	2	601	CHL	O2A-CGA	4.43	1.45	1.30
4	4	609	CHL	C2C-C3C	4.43	1.46	1.36
4	4	607	CHL	CHD-C1D	4.42	1.47	1.38
4	4	609	CHL	CHC-C1C	4.42	1.47	1.38
4	1	601	CHL	CHC-C1C	4.41	1.47	1.38
4	3	608	CHL	C2C-C3C	4.39	1.46	1.36
4	3	608	CHL	CHC-C1C	4.38	1.47	1.38
4	2	607	CHL	CHC-C1C	4.38	1.47	1.38
4	2	608	CHL	C2C-C3C	4.37	1.46	1.36
4	2	607	CHL	C2C-C3C	4.36	1.46	1.36
4	3	605	CHL	CHC-C1C	4.35	1.47	1.38
4	2	608	CHL	CHC-C1C	4.34	1.47	1.38
4	1	605	CHL	CHC-C1C	4.32	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1	607	CHL	CHC-C1C	4.32	1.47	1.38
4	1	609	CHL	O2A-CGA	4.31	1.45	1.33
4	4	607	CHL	CHC-C1C	4.30	1.47	1.38
4	1	606	CHL	C2C-C3C	4.30	1.46	1.36
4	1	606	CHL	CHC-C1C	4.29	1.47	1.38
4	2	601	CHL	CHD-C1D	4.25	1.46	1.38
4	2	607	CHL	O2A-CGA	4.25	1.45	1.33
4	4	606	CHL	CHD-C1D	4.23	1.46	1.38
4	2	606	CHL	CHD-C1D	4.22	1.46	1.38
4	2	609	CHL	O2A-CGA	4.21	1.45	1.33
4	1	605	CHL	C2C-C3C	4.21	1.45	1.36
4	1	608	CHL	C2C-C3C	4.20	1.45	1.36
4	1	609	CHL	CHD-C1D	4.20	1.46	1.38
4	1	601	CHL	CHD-C4C	4.20	1.48	1.39
4	2	601	CHL	C2C-C3C	4.19	1.45	1.36
4	4	608	CHL	C2C-C3C	4.19	1.45	1.36
4	2	607	CHL	CHD-C1D	4.19	1.46	1.38
4	2	609	CHL	CHC-C1C	4.19	1.47	1.38
4	4	606	CHL	CHC-C1C	4.17	1.47	1.38
4	3	609	CHL	CHC-C1C	4.17	1.47	1.38
4	2	601	CHL	CHC-C1C	4.17	1.47	1.38
4	1	605	CHL	CHD-C1D	4.16	1.46	1.38
4	3	601	CHL	O2A-CGA	4.16	1.45	1.33
4	3	605	CHL	CHD-C1D	4.14	1.46	1.38
4	1	608	CHL	CHC-C1C	4.14	1.46	1.38
4	2	605	CHL	CHD-C1D	4.12	1.46	1.38
4	3	606	CHL	CHD-C1D	4.11	1.46	1.38
4	1	607	CHL	O2A-CGA	4.09	1.45	1.33
4	2	609	CHL	CHD-C1D	4.09	1.46	1.38
4	1	606	CHL	CHD-C1D	4.08	1.46	1.38
4	3	601	CHL	C2C-C3C	4.08	1.45	1.36
4	1	607	CHL	CHD-C1D	4.06	1.46	1.38
4	4	601	CHL	CHD-C4C	4.04	1.48	1.39
4	2	601	CHL	CHD-C4C	4.00	1.48	1.39
4	3	606	CHL	CHC-C1C	4.00	1.46	1.38
4	2	606	CHL	CHC-C1C	3.97	1.46	1.38
4	4	607	CHL	CHD-C4C	3.97	1.48	1.39
4	3	609	CHL	CHD-C4C	3.95	1.48	1.39
4	3	607	CHL	CHD-C4C	3.95	1.48	1.39
4	3	601	CHL	CHD-C1D	3.93	1.46	1.38
4	3	601	CHL	CHD-C4C	3.93	1.48	1.39
4	4	609	CHL	CHD-C4C	3.92	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	608	CHL	CHD-C1D	3.90	1.46	1.38
4	1	609	CHL	CHC-C1C	3.82	1.46	1.38
4	3	606	CHL	C2C-C3C	3.82	1.45	1.36
5	4	611	CLA	C1D-ND	3.78	1.42	1.37
4	4	606	CHL	CHD-C4C	3.78	1.47	1.39
4	1	609	CHL	CHD-C4C	3.77	1.47	1.39
5	2	612	CLA	C1D-ND	3.75	1.42	1.37
5	2	612	CLA	C4B-NB	3.75	1.42	1.37
4	2	607	CHL	CHD-C4C	3.73	1.47	1.39
4	2	609	CHL	CHD-C4C	3.73	1.47	1.39
5	1	612	CLA	C1D-ND	3.72	1.42	1.37
4	2	609	CHL	CHB-C1B	3.70	1.47	1.39
5	4	610	CLA	C4D-ND	-3.69	1.32	1.37
5	2	614	CLA	C1D-ND	3.69	1.42	1.37
5	4	603	CLA	C1D-ND	3.69	1.42	1.37
4	1	608	CHL	CHD-C1D	3.69	1.45	1.38
4	4	607	CHL	CHB-C1B	3.67	1.47	1.39
4	2	605	CHL	CHD-C4C	3.67	1.47	1.39
4	1	607	CHL	CHD-C4C	3.66	1.47	1.39
4	3	605	CHL	CHD-C4C	3.66	1.47	1.39
4	2	606	CHL	CHD-C4C	3.64	1.47	1.39
4	2	605	CHL	OBD-CAD	3.61	1.28	1.22
5	1	614	CLA	C1D-ND	3.61	1.42	1.37
4	4	601	CHL	CHC-C4B	3.61	1.47	1.39
4	2	609	CHL	OBD-CAD	3.60	1.28	1.22
4	4	601	CHL	OBD-CAD	3.60	1.28	1.22
4	3	605	CHL	CHC-C4B	3.59	1.47	1.39
5	4	604	CLA	C1D-ND	3.58	1.42	1.37
4	3	605	CHL	OBD-CAD	3.58	1.28	1.22
5	1	613	CLA	C4D-ND	-3.58	1.32	1.37
4	4	607	CHL	OBD-CAD	3.57	1.28	1.22
4	3	608	CHL	CHD-C1D	3.57	1.45	1.38
4	2	606	CHL	OBD-CAD	3.57	1.28	1.22
4	2	607	CHL	OBD-CAD	3.56	1.28	1.22
4	2	605	CHL	CHC-C4B	3.55	1.47	1.39
5	3	604	CLA	C1D-ND	3.55	1.42	1.37
5	3	613	CLA	C4D-ND	-3.54	1.32	1.37
4	4	606	CHL	OBD-CAD	3.54	1.28	1.22
4	1	605	CHL	CHD-C4C	3.54	1.47	1.39
4	3	601	CHL	CHC-C4B	3.54	1.47	1.39
4	1	606	CHL	CHD-C4C	3.54	1.47	1.39
5	3	611	CLA	C4D-ND	-3.54	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	608	CHL	CHC-C4B	3.53	1.47	1.39
4	4	601	CHL	CHB-C1B	3.52	1.47	1.39
4	3	607	CHL	OBD-CAD	3.52	1.28	1.22
5	4	604	CLA	C4D-ND	-3.52	1.32	1.37
4	3	609	CHL	OBD-CAD	3.51	1.28	1.22
4	4	608	CHL	CHB-C1B	3.51	1.47	1.39
5	2	602	CLA	C4D-ND	-3.51	1.32	1.37
5	4	610	CLA	C1D-ND	3.51	1.42	1.37
4	3	606	CHL	CHD-C4C	3.51	1.47	1.39
5	3	610	CLA	C1D-ND	3.50	1.42	1.37
5	3	612	CLA	C4D-ND	-3.50	1.32	1.37
5	3	602	CLA	C1D-ND	3.50	1.42	1.37
4	2	605	CHL	CHB-C1B	3.50	1.47	1.39
4	4	608	CHL	CHC-C4B	3.50	1.47	1.39
5	2	613	CLA	C4B-NB	3.50	1.42	1.37
4	2	608	CHL	CHB-C1B	3.49	1.47	1.39
4	1	608	CHL	CHB-C1B	3.49	1.47	1.39
5	4	612	CLA	C1D-ND	3.49	1.42	1.37
4	2	608	CHL	CHD-C4C	3.47	1.47	1.39
5	3	602	CLA	C4D-ND	-3.47	1.32	1.37
4	3	605	CHL	CHB-C1B	3.47	1.47	1.39
4	1	605	CHL	OBD-CAD	3.47	1.28	1.22
4	1	607	CHL	OBD-CAD	3.47	1.28	1.22
5	2	604	CLA	C1D-ND	3.46	1.42	1.37
5	1	602	CLA	C4D-ND	-3.44	1.33	1.37
5	1	604	CLA	C4D-ND	-3.44	1.33	1.37
4	1	606	CHL	OBD-CAD	3.43	1.28	1.22
5	3	614	CLA	C4D-ND	-3.43	1.33	1.37
4	1	608	CHL	CHC-C4B	3.42	1.47	1.39
4	4	606	CHL	CHC-C4B	3.42	1.47	1.39
5	4	602	CLA	C1D-ND	3.42	1.42	1.37
4	4	608	CHL	CHD-C1D	3.41	1.45	1.38
5	2	611	CLA	C1D-ND	3.40	1.42	1.37
4	4	606	CHL	CHB-C1B	3.40	1.47	1.39
4	3	606	CHL	CHC-C4B	3.40	1.47	1.39
4	3	608	CHL	CHD-C4C	3.40	1.47	1.39
4	1	601	CHL	CHC-C4B	3.40	1.47	1.39
4	2	606	CHL	CHC-C4B	3.39	1.47	1.39
5	2	614	CLA	C4B-NB	3.39	1.42	1.37
4	3	607	CHL	CHC-C4B	3.39	1.47	1.39
5	1	611	CLA	C1D-ND	3.39	1.41	1.37
5	3	613	CLA	C1D-ND	3.39	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	604	CLA	C4B-NB	3.38	1.41	1.37
4	1	609	CHL	OBD-CAD	3.37	1.28	1.22
5	2	610	CLA	C1D-ND	3.36	1.41	1.37
4	1	605	CHL	CHC-C4B	3.36	1.46	1.39
5	2	611	CLA	C4B-NB	3.36	1.41	1.37
5	4	611	CLA	C4B-NB	3.35	1.41	1.37
4	4	609	CHL	OBD-CAD	3.35	1.28	1.22
4	1	601	CHL	OBD-CAD	3.34	1.28	1.22
5	1	613	CLA	C1D-ND	3.34	1.41	1.37
5	3	614	CLA	C1D-ND	3.33	1.41	1.37
5	1	612	CLA	C4B-NB	3.33	1.41	1.37
5	3	604	CLA	C4D-ND	-3.32	1.33	1.37
4	3	609	CHL	CHB-C1B	3.32	1.46	1.39
4	3	608	CHL	CHC-C4B	3.32	1.46	1.39
4	2	606	CHL	CHB-C1B	3.32	1.46	1.39
4	4	608	CHL	CHD-C4C	3.32	1.46	1.39
5	2	602	CLA	C1D-ND	3.31	1.41	1.37
4	4	609	CHL	CHB-C1B	3.31	1.46	1.39
4	3	607	CHL	C1B-NB	-3.31	1.33	1.37
4	4	609	CHL	CHC-C4B	3.31	1.46	1.39
4	3	608	CHL	CHB-C1B	3.30	1.46	1.39
4	2	601	CHL	CHC-C4B	3.30	1.46	1.39
4	1	605	CHL	CHB-C1B	3.30	1.46	1.39
5	2	611	CLA	C4D-ND	-3.30	1.33	1.37
4	1	601	CHL	CHB-C1B	3.29	1.46	1.39
4	3	607	CHL	CHB-C1B	3.29	1.46	1.39
5	2	612	CLA	C3B-C4B	3.28	1.50	1.42
4	1	608	CHL	CHD-C4C	3.28	1.46	1.39
4	4	607	CHL	CHC-C4B	3.28	1.46	1.39
5	1	613	CLA	C4B-NB	3.27	1.41	1.37
4	1	606	CHL	CHB-C1B	3.27	1.46	1.39
4	3	606	CHL	CHB-C1B	3.27	1.46	1.39
4	1	609	CHL	CHB-C1B	3.26	1.46	1.39
5	1	611	CLA	C4D-ND	-3.26	1.33	1.37
5	1	611	CLA	C4B-NB	3.26	1.41	1.37
4	1	606	CHL	CHC-C4B	3.25	1.46	1.39
5	1	604	CLA	C4B-NB	3.25	1.41	1.37
5	2	613	CLA	C4D-ND	-3.25	1.33	1.37
5	4	602	CLA	C4D-ND	-3.23	1.33	1.37
5	4	603	CLA	C4B-NB	3.23	1.41	1.37
5	3	613	CLA	C4B-NB	3.23	1.41	1.37
4	1	606	CHL	C1B-NB	-3.23	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	604	CLA	C4B-NB	3.22	1.41	1.37
5	1	610	CLA	C4D-ND	-3.21	1.33	1.37
4	2	607	CHL	CHC-C4B	3.21	1.46	1.39
5	2	603	CLA	C1D-ND	3.20	1.41	1.37
4	2	609	CHL	CHC-C4B	3.20	1.46	1.39
5	1	614	CLA	C4D-ND	-3.20	1.33	1.37
5	3	604	CLA	C4B-NB	3.19	1.41	1.37
4	2	607	CHL	CHB-C1B	3.18	1.46	1.39
5	4	611	CLA	C4D-ND	-3.18	1.33	1.37
4	1	609	CHL	C1B-NB	-3.17	1.33	1.37
5	3	611	CLA	C1D-ND	3.17	1.41	1.37
5	1	614	CLA	C4B-NB	3.17	1.41	1.37
8	1	1623	NEX	C7-C8	-3.17	1.26	1.32
4	3	609	CHL	C1B-NB	-3.17	1.33	1.37
5	3	610	CLA	C4D-ND	-3.17	1.33	1.37
4	3	607	CHL	MG-NA	-3.17	1.98	2.06
5	1	603	CLA	C4D-ND	-3.16	1.33	1.37
4	3	609	CHL	CHC-C4B	3.16	1.46	1.39
5	4	612	CLA	C4B-NB	3.16	1.41	1.37
5	3	603	CLA	C4D-ND	-3.16	1.33	1.37
5	1	610	CLA	C1D-ND	3.15	1.41	1.37
5	2	610	CLA	C4D-ND	-3.15	1.33	1.37
4	3	606	CHL	OBD-CAD	3.14	1.27	1.22
5	4	603	CLA	C4D-ND	-3.12	1.33	1.37
4	3	601	CHL	C1B-NB	-3.12	1.33	1.37
5	2	603	CLA	C4B-NB	3.12	1.41	1.37
5	2	613	CLA	C1D-ND	3.11	1.41	1.37
4	2	601	CHL	OBD-CAD	3.11	1.27	1.22
5	2	614	CLA	C4D-ND	-3.10	1.33	1.37
5	3	614	CLA	C4B-NB	3.10	1.41	1.37
5	2	603	CLA	C4D-ND	-3.10	1.33	1.37
4	3	601	CHL	OBD-CAD	3.10	1.27	1.22
4	1	607	CHL	CHC-C4B	3.09	1.46	1.39
5	4	612	CLA	C4D-ND	-3.09	1.33	1.37
5	3	610	CLA	C4B-NB	3.07	1.41	1.37
5	1	604	CLA	C1D-ND	3.06	1.41	1.37
5	3	603	CLA	C1D-ND	3.06	1.41	1.37
5	2	610	CLA	C4B-NB	3.05	1.41	1.37
4	2	608	CHL	OBD-CAD	3.05	1.27	1.22
5	3	611	CLA	C4B-NB	3.03	1.41	1.37
4	2	601	CHL	CHB-C1B	3.02	1.46	1.39
5	2	604	CLA	C4D-ND	-3.02	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	607	CHL	C4B-NB	-3.01	1.34	1.37
4	1	608	CHL	OBD-CAD	3.01	1.27	1.22
5	1	603	CLA	C4B-NB	3.01	1.41	1.37
4	3	606	CHL	C1B-NB	-3.01	1.34	1.37
4	2	601	CHL	C1B-NB	-3.01	1.34	1.37
5	1	603	CLA	C1D-ND	3.00	1.41	1.37
5	3	612	CLA	C4B-NB	2.99	1.41	1.37
8	2	1623	NEX	C7-C8	-2.99	1.27	1.32
5	1	602	CLA	C1D-ND	2.99	1.41	1.37
4	2	609	CHL	C1B-NB	-2.98	1.34	1.37
5	2	602	CLA	C4B-NB	2.98	1.41	1.37
5	3	612	CLA	C1D-ND	2.97	1.41	1.37
5	4	602	CLA	C4B-NB	2.97	1.41	1.37
5	4	610	CLA	C4B-NB	2.97	1.41	1.37
5	1	604	CLA	CMB-C2B	-2.96	1.44	1.50
5	1	610	CLA	C4B-NB	2.95	1.41	1.37
4	1	609	CHL	C4B-NB	-2.94	1.34	1.37
4	4	609	CHL	C1D-C2D	2.93	1.51	1.45
4	1	609	CHL	CHC-C4B	2.93	1.46	1.39
5	3	614	CLA	C3B-C4B	2.91	1.49	1.42
4	3	601	CHL	CHB-C1B	2.91	1.45	1.39
4	1	601	CHL	C1D-C2D	2.91	1.51	1.45
4	2	601	CHL	C1D-C2D	2.90	1.51	1.45
4	4	601	CHL	C1D-C2D	2.90	1.51	1.45
4	3	601	CHL	C3B-C4B	2.90	1.49	1.42
5	3	611	CLA	CMB-C2B	-2.89	1.44	1.50
4	4	607	CHL	C1D-C2D	2.89	1.51	1.45
5	2	612	CLA	C4D-ND	-2.89	1.33	1.37
5	4	611	CLA	C3B-C4B	2.88	1.49	1.42
5	4	604	CLA	C3B-C4B	2.86	1.49	1.42
4	1	607	CHL	CHB-C1B	2.86	1.45	1.39
4	4	606	CHL	C1B-NB	-2.86	1.34	1.37
5	2	611	CLA	C3B-C4B	2.85	1.49	1.42
4	2	606	CHL	C1B-NB	-2.84	1.34	1.37
4	3	609	CHL	C4B-NB	-2.82	1.34	1.37
5	2	614	CLA	C3B-C4B	2.82	1.49	1.42
4	3	601	CHL	C1D-C2D	2.82	1.50	1.45
4	3	607	CHL	C1D-C2D	2.82	1.50	1.45
4	4	601	CHL	MG-NA	-2.82	1.99	2.06
4	1	607	CHL	MG-NA	-2.82	1.99	2.06
4	4	607	CHL	C1B-NB	-2.82	1.34	1.37
5	3	602	CLA	C4B-NB	2.81	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	609	CHL	MG-NA	-2.81	1.99	2.06
4	2	601	CHL	C3B-C4B	2.80	1.49	1.42
4	3	609	CHL	MG-NA	-2.80	1.99	2.06
4	1	607	CHL	C1D-C2D	2.80	1.50	1.45
4	4	601	CHL	C3D-C2D	2.79	1.46	1.39
4	3	609	CHL	C1D-C2D	2.79	1.50	1.45
4	4	606	CHL	MG-NA	-2.78	1.99	2.06
5	2	613	CLA	C3B-C4B	2.77	1.49	1.42
4	2	607	CHL	C1B-NB	-2.76	1.34	1.37
4	1	608	CHL	C3B-C4B	2.75	1.49	1.42
4	4	609	CHL	C1B-NB	-2.74	1.34	1.37
4	4	607	CHL	MG-NA	-2.74	1.99	2.06
5	3	603	CLA	C4B-NB	2.73	1.41	1.37
4	1	607	CHL	C1B-NB	-2.73	1.34	1.37
5	3	610	CLA	C3B-C4B	2.73	1.49	1.42
4	4	608	CHL	OBD-CAD	2.72	1.27	1.22
4	1	607	CHL	C4B-NB	-2.72	1.34	1.37
5	4	602	CLA	C3B-C4B	2.72	1.49	1.42
5	2	610	CLA	C3B-C4B	2.70	1.49	1.42
5	1	612	CLA	C3B-C4B	2.70	1.49	1.42
5	3	602	CLA	C3B-C4B	2.70	1.49	1.42
5	2	603	CLA	C3B-C4B	2.70	1.49	1.42
5	1	612	CLA	C4D-ND	-2.70	1.34	1.37
4	2	605	CHL	C1D-C2D	2.69	1.50	1.45
5	4	603	CLA	C3B-C4B	2.69	1.49	1.42
4	3	605	CHL	C1D-C2D	2.69	1.50	1.45
4	4	609	CHL	C4B-NB	-2.69	1.34	1.37
4	4	606	CHL	C1D-C2D	2.69	1.50	1.45
4	3	608	CHL	C4B-NB	-2.69	1.34	1.37
4	2	605	CHL	MG-NA	-2.68	1.99	2.06
5	3	604	CLA	C3B-C4B	2.68	1.49	1.42
4	3	608	CHL	OBD-CAD	2.68	1.27	1.22
4	1	608	CHL	C1B-NB	-2.67	1.34	1.37
4	4	606	CHL	C3B-C4B	2.67	1.49	1.42
5	4	612	CLA	C3B-C4B	2.67	1.49	1.42
4	4	608	CHL	MG-NA	-2.67	1.99	2.06
4	3	607	CHL	C3D-C2D	2.67	1.46	1.39
5	1	604	CLA	C3B-C4B	2.66	1.49	1.42
4	1	609	CHL	MG-NA	-2.65	2.00	2.06
5	1	602	CLA	C4B-NB	2.65	1.41	1.37
5	1	614	CLA	C3B-C4B	2.65	1.49	1.42
5	2	602	CLA	C3B-C4B	2.64	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	601	CHL	C4B-NB	-2.64	1.34	1.37
4	2	609	CHL	MG-NA	-2.63	2.00	2.06
4	2	605	CHL	C3D-C2D	2.63	1.46	1.39
4	1	609	CHL	C1D-C2D	2.61	1.50	1.45
5	1	603	CLA	C3B-C4B	2.61	1.48	1.42
4	2	608	CHL	C3B-C4B	2.61	1.48	1.42
5	1	613	CLA	C3B-C4B	2.61	1.48	1.42
5	4	610	CLA	C3B-C4B	2.61	1.48	1.42
4	1	601	CHL	C3B-C4B	2.60	1.48	1.42
5	3	613	CLA	C3B-C4B	2.60	1.48	1.42
4	2	601	CHL	C4B-NB	-2.60	1.34	1.37
5	3	602	CLA	CMC-C2C	-2.60	1.45	1.50
4	3	609	CHL	C3D-C2D	2.59	1.46	1.39
4	4	609	CHL	C3D-C2D	2.59	1.46	1.39
4	3	605	CHL	C3D-C2D	2.59	1.46	1.39
5	4	611	CLA	C1B-C2B	2.59	1.49	1.43
4	2	605	CHL	C1B-NB	-2.59	1.34	1.37
5	1	611	CLA	C3B-C4B	2.58	1.48	1.42
4	3	607	CHL	C3B-C4B	2.58	1.48	1.42
5	3	612	CLA	C3B-C4B	2.57	1.48	1.42
5	3	611	CLA	C1B-C2B	2.57	1.49	1.43
4	4	607	CHL	C3D-C2D	2.57	1.46	1.39
4	1	605	CHL	C1D-C2D	2.57	1.50	1.45
4	3	608	CHL	C1B-NB	-2.57	1.34	1.37
4	3	605	CHL	C1B-C2B	2.56	1.49	1.43
4	1	601	CHL	C1B-NB	-2.55	1.34	1.37
4	2	607	CHL	C4B-NB	-2.55	1.34	1.37
4	2	608	CHL	C1D-C2D	2.55	1.50	1.45
4	2	606	CHL	C1D-C2D	2.55	1.50	1.45
4	4	601	CHL	C3B-C4B	2.55	1.48	1.42
5	1	602	CLA	C3B-C4B	2.55	1.48	1.42
4	2	607	CHL	MG-NA	-2.55	2.00	2.06
4	2	606	CHL	C4B-NB	-2.55	1.34	1.37
9	1	2630	LHG	O7-C5	-2.54	1.40	1.46
4	1	601	CHL	C4B-NB	-2.53	1.34	1.37
4	4	606	CHL	C3D-C2D	2.53	1.46	1.39
4	2	607	CHL	C1D-C2D	2.53	1.50	1.45
5	1	611	CLA	C1B-C2B	2.53	1.49	1.43
5	3	611	CLA	CMD-C2D	-2.53	1.45	1.50
4	3	601	CHL	MG-NA	-2.52	2.00	2.06
4	2	609	CHL	C3D-C2D	2.52	1.46	1.39
4	4	608	CHL	C4B-NB	-2.52	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	605	CHL	MG-NA	-2.51	2.00	2.06
4	4	601	CHL	C1B-C2B	2.51	1.49	1.43
4	4	607	CHL	C4B-NB	-2.51	1.34	1.37
5	2	613	CLA	CMD-C2D	-2.51	1.45	1.50
4	1	606	CHL	MG-NA	-2.51	2.00	2.06
4	4	601	CHL	C1B-NB	-2.50	1.34	1.37
4	3	606	CHL	C3B-C4B	2.50	1.48	1.42
5	1	613	CLA	C1B-C2B	2.50	1.49	1.43
4	1	601	CHL	MG-NA	-2.50	2.00	2.06
4	3	601	CHL	C4B-NB	-2.49	1.34	1.37
4	2	609	CHL	C4B-NB	-2.49	1.34	1.37
5	3	612	CLA	CMD-C2D	-2.49	1.45	1.50
4	2	601	CHL	MG-NA	-2.49	2.00	2.06
4	2	605	CHL	C3B-C4B	2.48	1.48	1.42
4	2	607	CHL	C3D-C2D	2.48	1.45	1.39
4	1	608	CHL	MG-NA	-2.47	2.00	2.06
4	1	605	CHL	C3D-C2D	2.47	1.45	1.39
5	1	610	CLA	C3B-C4B	2.47	1.48	1.42
5	2	604	CLA	C3B-C4B	2.47	1.48	1.42
5	3	613	CLA	C1B-C2B	2.47	1.49	1.43
5	2	602	CLA	CMC-C2C	-2.47	1.45	1.50
4	1	606	CHL	C4B-NB	-2.46	1.34	1.37
4	2	606	CHL	C3B-C4B	2.46	1.48	1.42
4	2	609	CHL	C1B-C2B	2.46	1.49	1.43
4	2	605	CHL	C4B-NB	-2.46	1.34	1.37
5	2	604	CLA	CMB-C2B	-2.45	1.45	1.50
5	1	602	CLA	CMC-C2C	-2.45	1.45	1.50
5	3	614	CLA	C1B-C2B	2.45	1.49	1.43
5	2	602	CLA	CMD-C2D	-2.45	1.45	1.50
4	3	605	CHL	C3B-C4B	2.44	1.48	1.42
5	2	614	CLA	C1B-C2B	2.44	1.49	1.43
5	2	611	CLA	C1B-C2B	2.44	1.49	1.43
9	3	2630	LHG	O7-C5	-2.44	1.40	1.46
5	1	613	CLA	CMD-C2D	-2.44	1.45	1.50
5	4	612	CLA	C1B-C2B	2.43	1.49	1.43
4	3	605	CHL	C1B-NB	-2.43	1.34	1.37
4	3	608	CHL	MG-NA	-2.43	2.00	2.06
5	2	603	CLA	CMD-C2D	-2.43	1.45	1.50
5	1	603	CLA	C1B-C2B	2.42	1.49	1.43
4	2	605	CHL	C1B-C2B	2.42	1.48	1.43
4	1	605	CHL	MG-NA	-2.41	2.00	2.06
5	2	613	CLA	C1B-C2B	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3	603	CLA	C1B-C2B	2.41	1.48	1.43
5	3	612	CLA	CMC-C2C	-2.40	1.45	1.50
4	1	605	CHL	C3B-C4B	2.40	1.48	1.42
4	2	609	CHL	C1D-C2D	2.40	1.50	1.45
5	4	604	CLA	C1B-C2B	2.40	1.48	1.43
5	4	602	CLA	C1B-C2B	2.40	1.48	1.43
4	2	606	CHL	C3D-C2D	2.40	1.45	1.39
4	1	605	CHL	C1B-NB	-2.40	1.34	1.37
5	1	610	CLA	CMB-C2B	-2.39	1.45	1.50
5	3	614	CLA	CMD-C2D	-2.38	1.45	1.50
4	2	606	CHL	C4C-C3C	2.38	1.49	1.45
5	4	603	CLA	C1B-C2B	2.38	1.48	1.43
5	4	604	CLA	CMB-C2B	-2.37	1.45	1.50
5	3	604	CLA	CMB-C2B	-2.37	1.45	1.50
4	1	605	CHL	C1B-C2B	2.37	1.48	1.43
5	1	602	CLA	C1B-C2B	2.37	1.48	1.43
4	2	608	CHL	MG-NA	-2.37	2.00	2.06
5	3	610	CLA	CMB-C2B	-2.36	1.45	1.50
4	4	607	CHL	C1B-C2B	2.36	1.48	1.43
4	2	607	CHL	C3B-C4B	2.36	1.48	1.42
4	3	601	CHL	CHB-C4A	-2.36	1.32	1.37
5	2	604	CLA	C1B-C2B	2.36	1.48	1.43
4	1	606	CHL	C3D-C2D	2.36	1.45	1.39
4	3	605	CHL	C4B-NB	-2.36	1.34	1.37
5	2	602	CLA	C1B-C2B	2.36	1.48	1.43
4	4	608	CHL	C1D-C2D	2.35	1.50	1.45
4	3	606	CHL	MG-NA	-2.35	2.00	2.06
4	4	607	CHL	C3B-C4B	2.35	1.48	1.42
5	3	603	CLA	MG-ND	-2.35	2.01	2.05
4	3	608	CHL	C1B-C2B	2.34	1.48	1.43
5	1	604	CLA	MG-NB	-2.34	2.01	2.05
4	3	606	CHL	C4B-NB	-2.34	1.34	1.37
6	2	1621	LUT	C22-C21	-2.34	1.51	1.54
4	1	605	CHL	C4B-NB	-2.34	1.34	1.37
4	1	606	CHL	C1D-C2D	2.34	1.49	1.45
4	1	601	CHL	C1B-C2B	2.34	1.48	1.43
4	1	607	CHL	C1B-C2B	2.34	1.48	1.43
5	1	604	CLA	CMD-C2D	-2.34	1.45	1.50
4	4	607	CHL	C4C-C3C	2.33	1.49	1.45
5	2	613	CLA	MG-ND	-2.33	2.01	2.05
4	2	607	CHL	C4C-C3C	2.33	1.49	1.45
4	2	607	CHL	C1B-C2B	2.33	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	609	CHL	C3B-C4B	2.33	1.48	1.42
4	3	606	CHL	C3D-C2D	2.32	1.45	1.39
5	1	614	CLA	C1B-C2B	2.32	1.48	1.43
5	4	610	CLA	CMD-C2D	-2.32	1.45	1.50
4	4	609	CHL	C4C-C3C	2.32	1.49	1.45
4	2	606	CHL	MG-NA	-2.32	2.00	2.06
4	3	608	CHL	C1D-C2D	2.31	1.49	1.45
4	4	606	CHL	C4B-NB	-2.31	1.34	1.37
4	4	608	CHL	C1B-C2B	2.31	1.48	1.43
5	2	603	CLA	C1B-C2B	2.31	1.48	1.43
4	1	609	CHL	C3D-C2D	2.31	1.45	1.39
4	1	607	CHL	C3D-C2D	2.31	1.45	1.39
4	1	607	CHL	C3B-C4B	2.31	1.48	1.42
5	2	610	CLA	C1B-C2B	2.30	1.48	1.43
5	2	612	CLA	C1B-C2B	2.30	1.48	1.43
5	3	603	CLA	CMD-C2D	-2.30	1.45	1.50
4	3	609	CHL	C4C-C3C	2.30	1.49	1.45
4	1	608	CHL	C1D-C2D	2.30	1.49	1.45
4	3	607	CHL	C1B-C2B	2.29	1.48	1.43
5	3	603	CLA	C3B-C4B	2.29	1.48	1.42
4	3	607	CHL	C4C-C3C	2.29	1.49	1.45
4	1	601	CHL	C4C-C3C	2.28	1.49	1.45
5	1	613	CLA	MG-ND	-2.28	2.01	2.05
4	2	608	CHL	C4B-NB	-2.28	1.35	1.37
5	1	612	CLA	CMD-C2D	-2.27	1.46	1.50
5	2	614	CLA	CMD-C2D	-2.27	1.46	1.50
4	4	608	CHL	C3D-C2D	2.27	1.45	1.39
4	4	609	CHL	C3B-C4B	2.27	1.48	1.42
5	2	603	CLA	CMB-C2B	-2.26	1.46	1.50
4	3	606	CHL	C1D-C2D	2.26	1.49	1.45
5	4	610	CLA	C1B-C2B	2.26	1.48	1.43
5	2	604	CLA	CMD-C2D	-2.26	1.46	1.50
5	1	602	CLA	CMD-C2D	-2.25	1.46	1.50
4	2	608	CHL	C3D-C2D	2.25	1.45	1.39
5	1	604	CLA	C1B-NB	-2.25	1.35	1.37
5	4	610	CLA	CMC-C2C	-2.25	1.46	1.50
4	4	608	CHL	C1B-NB	-2.25	1.35	1.37
5	3	612	CLA	CMB-C2B	-2.25	1.46	1.50
5	3	611	CLA	MG-ND	-2.25	2.01	2.05
4	3	608	CHL	C3B-C4B	2.24	1.48	1.42
4	2	608	CHL	C1B-NB	-2.24	1.35	1.37
5	1	603	CLA	MG-ND	-2.24	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3	613	CLA	CMD-C2D	-2.24	1.46	1.50
5	1	614	CLA	CMD-C2D	-2.24	1.46	1.50
4	4	606	CHL	C4C-C3C	2.24	1.48	1.45
5	1	602	CLA	MG-NB	-2.24	2.01	2.05
4	2	609	CHL	C3B-C4B	2.24	1.48	1.42
5	2	603	CLA	MG-ND	-2.23	2.01	2.05
4	1	601	CHL	C3D-C2D	2.23	1.45	1.39
4	2	608	CHL	C1B-C2B	2.23	1.48	1.43
5	4	603	CLA	MG-ND	-2.23	2.01	2.05
4	4	606	CHL	C1B-C2B	2.23	1.48	1.43
5	3	610	CLA	CMC-C2C	-2.23	1.46	1.50
4	2	601	CHL	C1B-C2B	2.23	1.48	1.43
5	3	613	CLA	CMC-C2C	-2.23	1.46	1.50
4	3	608	CHL	C3D-C2D	2.22	1.45	1.39
5	1	610	CLA	CMD-C2D	-2.22	1.46	1.50
5	3	602	CLA	C1B-C2B	2.21	1.48	1.43
5	4	603	CLA	CMB-C2B	-2.21	1.46	1.50
5	1	612	CLA	C1B-C2B	2.21	1.48	1.43
5	1	603	CLA	CMD-C2D	-2.21	1.46	1.50
4	1	608	CHL	C1B-C2B	2.21	1.48	1.43
5	3	610	CLA	CMD-C2D	-2.20	1.46	1.50
4	1	608	CHL	C4B-NB	-2.19	1.35	1.37
5	3	612	CLA	C1B-C2B	2.19	1.48	1.43
5	3	611	CLA	MG-NB	-2.19	2.01	2.05
5	3	613	CLA	CMB-C2B	-2.19	1.46	1.50
4	1	606	CHL	C3B-C4B	2.18	1.47	1.42
5	2	602	CLA	MG-NB	-2.18	2.01	2.05
5	4	603	CLA	CMD-C2D	-2.18	1.46	1.50
5	3	614	CLA	CMB-C2B	-2.18	1.46	1.50
5	3	602	CLA	CMD-C2D	-2.18	1.46	1.50
6	1	1621	LUT	C22-C21	-2.17	1.52	1.54
4	1	609	CHL	C1B-C2B	2.17	1.48	1.43
4	4	608	CHL	C3B-C4B	2.17	1.47	1.42
5	3	602	CLA	CMB-C2B	-2.16	1.46	1.50
5	2	610	CLA	CMB-C2B	-2.16	1.46	1.50
5	3	611	CLA	CHC-C4B	-2.16	1.34	1.39
5	4	610	CLA	CMB-C2B	-2.16	1.46	1.50
5	1	602	CLA	MG-ND	-2.16	2.01	2.05
5	1	610	CLA	CMC-C2C	-2.16	1.46	1.50
4	2	609	CHL	C4C-C3C	2.16	1.48	1.45
7	3	1622	XAT	C34-C33	-2.15	1.32	1.35
4	3	605	CHL	C4C-C3C	2.15	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	602	CLA	CMB-C2B	-2.15	1.46	1.50
5	1	611	CLA	CMD-C2D	-2.15	1.46	1.50
5	4	602	CLA	CMC-C2C	-2.14	1.46	1.50
4	4	601	CHL	C4C-C3C	2.14	1.48	1.45
5	1	612	CLA	CMB-C2B	-2.13	1.46	1.50
5	4	602	CLA	CMD-C2D	-2.13	1.46	1.50
5	4	612	CLA	CMD-C2D	-2.13	1.46	1.50
4	2	601	CHL	CHB-C4A	-2.13	1.32	1.37
4	4	609	CHL	CHB-C4A	-2.13	1.32	1.37
6	3	1621	LUT	C22-C21	-2.13	1.52	1.54
5	1	603	CLA	CMB-C2B	-2.13	1.46	1.50
4	3	606	CHL	C4C-C3C	2.13	1.48	1.45
5	3	603	CLA	CMB-C2B	-2.12	1.46	1.50
5	1	604	CLA	MG-ND	-2.12	2.01	2.05
5	1	614	CLA	CMB-C2B	-2.12	1.46	1.50
5	3	613	CLA	MG-ND	-2.12	2.01	2.05
5	2	612	CLA	CMD-C2D	-2.11	1.46	1.50
4	2	601	CHL	C3D-C2D	2.11	1.44	1.39
7	4	622	XAT	O4-C5	-2.11	1.43	1.46
5	3	603	CLA	CAC-C3C	-2.11	1.45	1.51
5	1	613	CLA	CMC-C2C	-2.11	1.46	1.50
5	1	604	CLA	CMC-C2C	-2.11	1.46	1.50
5	3	604	CLA	CMC-C2C	-2.11	1.46	1.50
7	3	1622	XAT	O4-C5	-2.10	1.43	1.46
5	2	611	CLA	CMD-C2D	-2.10	1.46	1.50
4	4	609	CHL	C1B-C2B	2.10	1.48	1.43
5	3	604	CLA	C1B-C2B	2.10	1.48	1.43
5	1	611	CLA	CMB-C2B	-2.09	1.46	1.50
8	1	1623	NEX	O24-C25	-2.09	1.43	1.46
5	1	613	CLA	CMB-C2B	-2.09	1.46	1.50
5	2	613	CLA	CMC-C2C	-2.09	1.46	1.50
5	4	610	CLA	MG-NB	-2.09	2.01	2.05
4	2	606	CHL	C1B-C2B	2.09	1.48	1.43
5	1	611	CLA	MG-NB	-2.09	2.01	2.05
5	2	612	CLA	CMB-C2B	-2.08	1.46	1.50
5	3	612	CLA	MG-ND	-2.08	2.01	2.05
4	3	607	CHL	C4D-CHA	2.08	1.45	1.38
6	1	1621	LUT	C1-C6	-2.08	1.50	1.53
4	4	601	CHL	C4D-CHA	2.08	1.45	1.38
4	1	606	CHL	C4C-C3C	2.08	1.48	1.45
5	3	614	CLA	CMC-C2C	-2.08	1.46	1.50
5	4	604	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1	608	CHL	C3D-C2D	2.07	1.44	1.39
5	4	603	CLA	CMC-C2C	-2.07	1.46	1.50
5	2	610	CLA	CMD-C2D	-2.07	1.46	1.50
5	1	603	CLA	CMC-C2C	-2.07	1.46	1.50
4	1	607	CHL	CHB-C4A	-2.07	1.32	1.37
5	4	612	CLA	CMB-C2B	-2.07	1.46	1.50
5	2	613	CLA	CMB-C2B	-2.07	1.46	1.50
5	3	603	CLA	CHC-C4B	-2.07	1.34	1.39
4	3	608	CHL	C2C-C1C	2.06	1.49	1.44
5	1	611	CLA	MG-ND	-2.06	2.01	2.05
5	2	602	CLA	MG-ND	-2.06	2.01	2.05
4	1	607	CHL	C4C-C3C	2.06	1.48	1.45
5	1	612	CLA	MG-ND	-2.06	2.01	2.05
5	1	610	CLA	MG-NB	-2.06	2.01	2.05
5	4	611	CLA	MG-ND	-2.06	2.01	2.05
5	4	603	CLA	MG-NB	-2.05	2.01	2.05
8	3	1623	NEX	O24-C25	-2.05	1.43	1.46
5	2	614	CLA	CMB-C2B	-2.05	1.46	1.50
5	1	612	CLA	CMC-C2C	-2.05	1.46	1.50
5	4	611	CLA	CMD-C2D	-2.05	1.46	1.50
5	2	604	CLA	MG-NB	-2.05	2.01	2.05
5	3	612	CLA	C1B-NB	-2.05	1.35	1.37
4	2	605	CHL	C2C-C1C	2.04	1.48	1.44
5	3	604	CLA	CMD-C2D	-2.04	1.46	1.50
5	2	610	CLA	CMC-C2C	-2.04	1.46	1.50
7	3	1622	XAT	C14-C13	-2.03	1.33	1.35
5	1	602	CLA	CMB-C2B	-2.03	1.46	1.50
5	2	611	CLA	CMB-C2B	-2.03	1.46	1.50
5	4	604	CLA	CMC-C2C	-2.03	1.46	1.50
5	1	603	CLA	CAC-C3C	-2.03	1.45	1.51
5	4	602	CLA	MG-NB	-2.03	2.01	2.05
4	2	608	CHL	C2C-C1C	2.02	1.48	1.44
5	4	602	CLA	CMB-C2B	-2.01	1.46	1.50
4	1	609	CHL	C4C-C3C	2.01	1.48	1.45
4	1	605	CHL	C4C-C3C	2.01	1.48	1.45
5	2	612	CLA	CMC-C2C	-2.01	1.46	1.50
4	3	606	CHL	CHB-C4A	-2.01	1.32	1.37
5	2	603	CLA	CAC-C3C	-2.01	1.46	1.51
5	2	604	CLA	CMC-C2C	-2.01	1.46	1.50
4	1	609	CHL	C3B-C4B	2.00	1.47	1.42
7	2	1622	XAT	O4-C5	-2.00	1.43	1.46
5	3	604	CLA	MG-NB	-2.00	2.01	2.05

All (999) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	601	CHL	CMD-C2D-C1D	10.43	143.09	124.71
7	2	1622	XAT	O24-C25-C24	10.30	121.12	113.38
4	1	607	CHL	C2B-C1B-NB	10.15	117.04	110.23
4	2	601	CHL	CMD-C2D-C1D	9.97	142.28	124.71
4	3	601	CHL	C2B-C1B-NB	9.95	116.90	110.23
4	2	601	CHL	C2B-C1B-NB	9.87	116.85	110.23
4	1	601	CHL	CMD-C2D-C1D	9.75	141.90	124.71
4	2	607	CHL	C2B-C1B-NB	9.43	116.56	110.23
4	1	607	CHL	C2C-C3C-C4C	-9.33	99.84	106.49
4	1	605	CHL	C2B-C1B-NB	9.31	116.47	110.23
8	1	1623	NEX	O24-C25-C24	9.19	120.28	113.38
4	1	601	CHL	C2B-C1B-NB	9.15	116.37	110.23
7	1	1622	XAT	O24-C25-C24	9.13	120.24	113.38
4	4	609	CHL	C2B-C1B-NB	9.06	116.30	110.23
7	2	1622	XAT	O4-C5-C4	9.01	120.15	113.38
4	4	608	CHL	C1D-ND-C4D	-8.96	99.97	106.33
8	2	1623	NEX	O24-C25-C24	8.95	120.11	113.38
4	3	608	CHL	C2B-C1B-NB	8.89	116.19	110.23
4	3	605	CHL	C2B-C1B-NB	8.86	116.17	110.23
4	2	606	CHL	C2B-C1B-NB	8.80	116.13	110.23
4	2	605	CHL	C2B-C1B-NB	8.78	116.12	110.23
4	1	608	CHL	CMD-C2D-C1D	8.78	140.18	124.71
4	4	608	CHL	CMD-C2D-C1D	8.75	140.14	124.71
4	2	608	CHL	CMD-C2D-C1D	8.74	140.11	124.71
4	3	601	CHL	C1D-ND-C4D	-8.73	100.13	106.33
4	3	607	CHL	C2B-C1B-NB	8.68	116.05	110.23
4	1	609	CHL	CMD-C2D-C1D	8.66	139.97	124.71
4	4	601	CHL	C2B-C1B-NB	8.65	116.03	110.23
4	3	608	CHL	CMD-C2D-C1D	8.65	139.96	124.71
4	1	607	CHL	CMD-C2D-C1D	8.61	139.90	124.71
4	2	608	CHL	C1D-ND-C4D	-8.59	100.24	106.33
4	1	608	CHL	C1D-ND-C4D	-8.57	100.24	106.33
4	2	608	CHL	C2B-C1B-NB	8.51	115.94	110.23
4	3	606	CHL	C2B-C1B-NB	8.51	115.94	110.23
4	4	609	CHL	CMD-C2D-C1D	8.50	139.70	124.71
4	3	607	CHL	CMD-C2D-C1D	8.49	139.68	124.71
4	4	607	CHL	CMD-C2D-C1D	8.49	139.67	124.71
4	1	608	CHL	C2C-C3C-C4C	-8.48	100.45	106.49
4	1	607	CHL	C1D-ND-C4D	-8.46	100.33	106.33
4	4	608	CHL	C2B-C1B-NB	8.43	115.89	110.23
4	1	605	CHL	CMD-C2D-C1D	8.42	139.56	124.71
4	2	606	CHL	CMD-C2D-C1D	8.38	139.47	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	606	CHL	C2B-C1B-NB	8.37	115.84	110.23
4	3	605	CHL	CMD-C2D-C1D	8.36	139.45	124.71
4	3	608	CHL	C1D-ND-C4D	-8.35	100.41	106.33
4	4	606	CHL	CMD-C2D-C1D	8.29	139.33	124.71
4	3	609	CHL	CMD-C2D-C1D	8.29	139.32	124.71
4	2	605	CHL	C1D-ND-C4D	-8.29	100.45	106.33
4	4	601	CHL	CMD-C2D-C1D	8.26	139.26	124.71
4	2	601	CHL	C1D-ND-C4D	-8.24	100.48	106.33
4	3	606	CHL	C2C-C3C-C4C	-8.24	100.62	106.49
4	1	608	CHL	C2B-C1B-NB	8.22	115.74	110.23
4	2	609	CHL	CMD-C2D-C1D	8.22	139.19	124.71
4	2	607	CHL	CMD-C2D-C1D	8.20	139.16	124.71
4	2	605	CHL	CMD-C2D-C1D	8.18	139.12	124.71
4	2	606	CHL	C2C-C3C-C4C	-8.15	100.68	106.49
4	2	607	CHL	C2C-C3C-C4C	-8.11	100.71	106.49
4	3	606	CHL	CMD-C2D-C1D	8.08	138.96	124.71
4	1	606	CHL	CMD-C2D-C1D	8.06	138.92	124.71
4	1	606	CHL	C2B-C1B-NB	8.03	115.62	110.23
4	1	609	CHL	C2B-C1B-NB	8.00	115.60	110.23
4	1	606	CHL	C2C-C3C-C4C	-7.94	100.83	106.49
4	4	608	CHL	C2D-C1D-ND	7.92	115.94	110.10
4	1	605	CHL	C1D-ND-C4D	-7.90	100.72	106.33
4	3	608	CHL	C2C-C3C-C4C	-7.89	100.87	106.49
4	3	609	CHL	C2B-C1B-NB	7.84	115.48	110.23
4	4	606	CHL	C1D-ND-C4D	-7.82	100.78	106.33
4	4	607	CHL	C2B-C1B-NB	7.79	115.45	110.23
4	3	608	CHL	C2D-C1D-ND	7.75	115.82	110.10
4	3	601	CHL	CHD-C1D-ND	-7.73	117.35	124.45
4	2	608	CHL	C2C-C3C-C4C	-7.71	100.99	106.49
4	4	609	CHL	CHD-C1D-ND	-7.71	117.37	124.45
8	3	1623	NEX	O24-C25-C24	7.67	119.14	113.38
4	3	607	CHL	C2C-C3C-C4C	-7.64	101.04	106.49
4	4	606	CHL	C2C-C3C-C4C	-7.63	101.05	106.49
4	3	607	CHL	CHD-C1D-ND	-7.62	117.45	124.45
4	1	609	CHL	C1D-ND-C4D	-7.60	100.93	106.33
7	4	622	XAT	O24-C25-C24	7.60	119.09	113.38
4	3	605	CHL	C1D-ND-C4D	-7.58	100.95	106.33
10	4	623	BCR	C24-C23-C22	-7.55	114.83	126.23
4	1	606	CHL	C1D-ND-C4D	-7.53	100.99	106.33
4	1	605	CHL	C2C-C3C-C4C	-7.53	101.12	106.49
4	4	601	CHL	CHD-C1D-ND	-7.52	117.55	124.45
4	4	608	CHL	C2C-C3C-C4C	-7.48	101.16	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	608	CHL	C2D-C1D-ND	7.46	115.60	110.10
4	2	606	CHL	C1D-ND-C4D	-7.46	101.04	106.33
7	3	1622	XAT	O4-C5-C4	7.45	118.97	113.38
4	3	606	CHL	C1D-ND-C4D	-7.44	101.05	106.33
4	2	607	CHL	C1D-ND-C4D	-7.39	101.09	106.33
4	2	605	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
4	2	609	CHL	C1D-ND-C4D	-7.33	101.13	106.33
4	2	609	CHL	C2B-C1B-NB	7.31	115.13	110.23
4	4	609	CHL	C2C-C3C-C4C	-7.31	101.28	106.49
4	3	605	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
4	4	607	CHL	C1D-ND-C4D	-7.25	101.18	106.33
4	2	608	CHL	C2D-C1D-ND	7.25	115.45	110.10
4	2	609	CHL	C2C-C3C-C4C	-7.22	101.34	106.49
4	2	601	CHL	CHD-C1D-ND	-7.16	117.87	124.45
4	1	609	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
4	4	609	CHL	C1D-ND-C4D	-6.99	101.37	106.33
4	4	607	CHL	CHD-C1D-ND	-6.92	118.10	124.45
4	2	605	CHL	C2D-C1D-ND	6.87	115.17	110.10
4	3	609	CHL	C2C-C3C-C4C	-6.85	101.60	106.49
4	1	601	CHL	CHD-C1D-ND	-6.85	118.16	124.45
4	4	607	CHL	C2C-C3C-C4C	-6.84	101.61	106.49
4	1	601	CHL	C1D-ND-C4D	-6.83	101.48	106.33
4	1	607	CHL	C2D-C1D-ND	6.81	115.12	110.10
4	3	609	CHL	CHD-C1D-ND	-6.73	118.27	124.45
4	1	609	CHL	CHD-C1D-ND	-6.72	118.28	124.45
4	4	601	CHL	C2C-C3C-C4C	-6.71	101.70	106.49
4	4	606	CHL	CHD-C1D-ND	-6.55	118.44	124.45
4	3	609	CHL	C1D-ND-C4D	-6.54	101.69	106.33
4	4	608	CHL	CHD-C1D-ND	-6.54	118.45	124.45
4	3	607	CHL	CHB-C1B-NB	-6.49	117.39	124.26
4	2	609	CHL	CHD-C1D-ND	-6.45	118.52	124.45
4	3	605	CHL	C2D-C1D-ND	6.43	114.84	110.10
4	1	605	CHL	C2D-C1D-ND	6.43	114.84	110.10
4	3	601	CHL	C2D-C1D-ND	6.41	114.83	110.10
4	4	606	CHL	C2D-C1D-ND	6.40	114.82	110.10
7	1	1622	XAT	O4-C5-C4	6.37	118.17	113.38
4	1	601	CHL	C2C-C3C-C4C	-6.36	101.95	106.49
7	4	622	XAT	O4-C5-C4	6.33	118.14	113.38
4	1	605	CHL	CHD-C1D-ND	-6.32	118.64	124.45
4	4	601	CHL	C1D-ND-C4D	-6.29	101.87	106.33
5	3	611	CLA	C4A-NA-C1A	6.23	109.51	106.71
4	1	607	CHL	CHD-C1D-ND	-6.19	118.76	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	609	CHL	C2D-C1D-ND	6.17	114.65	110.10
4	3	605	CHL	CHD-C1D-ND	-6.15	118.80	124.45
7	3	1622	XAT	O24-C25-C24	6.15	118.00	113.38
4	3	608	CHL	CHD-C1D-ND	-6.15	118.80	124.45
4	2	607	CHL	C2D-C1D-ND	6.12	114.62	110.10
10	4	623	BCR	C11-C10-C9	-6.12	118.58	127.31
4	3	601	CHL	C2C-C3C-C4C	-6.10	102.14	106.49
4	1	609	CHL	C2D-C1D-ND	6.08	114.58	110.10
4	2	607	CHL	CHD-C1D-ND	-6.05	118.89	124.45
4	2	605	CHL	CHD-C1D-ND	-6.02	118.92	124.45
4	3	606	CHL	C2D-C1D-ND	5.99	114.52	110.10
4	2	601	CHL	C2D-C1D-ND	5.98	114.51	110.10
4	2	608	CHL	CHD-C1D-ND	-5.98	118.96	124.45
4	4	601	CHL	CHB-C1B-NB	-5.94	117.97	124.26
4	3	608	CHL	C3D-C2D-C1D	-5.91	97.76	105.83
5	1	603	CLA	C4A-NA-C1A	5.88	109.35	106.71
4	3	608	CHL	C3C-C4C-NC	5.85	117.13	110.57
4	4	607	CHL	C2D-C1D-ND	5.84	114.41	110.10
4	2	606	CHL	C2D-C1D-ND	5.81	114.39	110.10
4	1	608	CHL	C3C-C4C-NC	5.78	117.06	110.57
8	3	1623	NEX	C15-C14-C13	-5.78	119.06	127.31
4	4	608	CHL	C3D-C2D-C1D	-5.77	97.96	105.83
4	1	606	CHL	C2D-C1D-ND	5.76	114.35	110.10
4	2	608	CHL	C3C-C4C-NC	5.76	117.03	110.57
5	2	611	CLA	C4A-NA-C1A	5.74	109.28	106.71
4	1	608	CHL	CHD-C1D-ND	-5.70	119.22	124.45
4	1	607	CHL	C3B-C2B-C1B	-5.69	100.29	107.16
4	2	606	CHL	CHD-C1D-ND	-5.69	119.23	124.45
7	3	1622	XAT	C6-C7-C8	-5.68	113.98	125.99
4	3	607	CHL	C1D-ND-C4D	-5.67	102.31	106.33
4	1	608	CHL	C3D-C2D-C1D	-5.65	98.12	105.83
5	3	603	CLA	C4A-NA-C1A	5.63	109.24	106.71
4	2	609	CHL	O2D-CGD-CBD	5.61	121.25	111.27
5	4	603	CLA	C4A-NA-C1A	5.53	109.19	106.71
4	2	601	CHL	C2C-C3C-C4C	-5.52	102.55	106.49
7	4	622	XAT	C6-C7-C8	-5.52	114.32	125.99
4	1	606	CHL	CHD-C1D-ND	-5.51	119.39	124.45
4	2	608	CHL	C3D-C2D-C1D	-5.50	98.32	105.83
4	4	601	CHL	C2D-C1D-ND	5.50	114.16	110.10
7	3	1622	XAT	C31-C30-C29	-5.46	119.51	127.31
4	4	608	CHL	C3C-C4C-NC	5.46	116.69	110.57
4	4	601	CHL	C3B-C2B-C1B	-5.45	100.58	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	607	CHL	C3B-C2B-C1B	-5.45	100.59	107.16
4	1	606	CHL	C3C-C4C-NC	5.43	116.66	110.57
10	4	623	BCR	C16-C17-C18	-5.43	119.56	127.31
4	2	609	CHL	CHB-C1B-NB	-5.42	118.52	124.26
4	2	606	CHL	C3C-C4C-NC	5.42	116.64	110.57
4	4	609	CHL	C2D-C1D-ND	5.40	114.09	110.10
4	3	609	CHL	O2D-CGD-CBD	5.40	120.86	111.27
4	1	605	CHL	C3C-C4C-NC	5.40	116.62	110.57
4	3	608	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
4	3	606	CHL	C3C-C4C-NC	5.36	116.58	110.57
4	4	609	CHL	C3B-C2B-C1B	-5.34	100.71	107.16
4	3	605	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
4	4	606	CHL	O2D-CGD-CBD	5.34	120.75	111.27
4	2	605	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
4	4	608	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
4	1	605	CHL	C3B-C2B-C1B	-5.30	100.77	107.16
4	2	605	CHL	C3C-C4C-NC	5.29	116.50	110.57
4	3	605	CHL	O2D-CGD-CBD	5.27	120.63	111.27
7	3	1622	XAT	C15-C14-C13	-5.26	119.80	127.31
4	1	607	CHL	C3C-C4C-NC	5.26	116.47	110.57
4	1	601	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
4	3	606	CHL	O2D-CGD-CBD	5.25	120.61	111.27
7	3	1622	XAT	C38-C25-C26	-5.25	113.46	122.26
7	4	622	XAT	C18-C5-C6	-5.23	113.49	122.26
4	2	607	CHL	O2D-CGD-CBD	5.21	120.53	111.27
4	3	601	CHL	C3D-C2D-C1D	-5.21	98.72	105.83
7	1	1622	XAT	C31-C30-C29	-5.20	119.89	127.31
7	1	1622	XAT	C15-C14-C13	-5.18	119.92	127.31
4	1	607	CHL	C3D-C2D-C1D	-5.16	98.79	105.83
10	4	623	BCR	C28-C27-C26	-5.15	104.88	114.08
4	4	608	CHL	CHD-C4C-C3C	-5.14	117.29	124.84
4	2	601	CHL	C3B-C2B-C1B	-5.13	100.97	107.16
4	3	607	CHL	C3B-C2B-C1B	-5.13	100.97	107.16
8	3	1623	NEX	C38-C25-C26	-5.10	113.72	122.26
7	1	1622	XAT	C38-C25-C26	-5.10	113.72	122.26
4	2	609	CHL	C3C-C4C-NC	5.09	116.28	110.57
8	2	1623	NEX	C15-C14-C13	-5.09	120.05	127.31
4	2	607	CHL	C3C-C4C-NC	5.07	116.26	110.57
4	3	606	CHL	CHD-C1D-ND	-5.06	119.80	124.45
4	2	605	CHL	C3D-C2D-C1D	-5.05	98.94	105.83
4	4	606	CHL	C3D-C2D-C1D	-5.05	98.94	105.83
4	3	601	CHL	C3B-C2B-C1B	-5.04	101.08	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	604	CLA	C4A-NA-C1A	5.03	108.97	106.71
4	3	601	CHL	C3D-C4D-ND	5.03	118.37	110.24
8	1	1623	NEX	C27-C28-C29	-5.03	117.73	125.53
4	1	609	CHL	O2D-CGD-CBD	5.02	120.20	111.27
4	1	605	CHL	O2D-CGD-CBD	5.02	120.18	111.27
4	3	605	CHL	C3C-C4C-NC	5.01	116.19	110.57
4	1	609	CHL	C3D-C2D-C1D	-5.00	99.01	105.83
4	1	605	CHL	C3D-C2D-C1D	-5.00	99.01	105.83
4	2	601	CHL	C3D-C2D-C1D	-4.99	99.02	105.83
4	3	605	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
7	4	622	XAT	O4-C5-C18	4.96	121.00	115.06
5	4	602	CLA	C4A-NA-C1A	4.95	108.93	106.71
10	4	623	BCR	C15-C14-C13	-4.95	120.24	127.31
4	3	609	CHL	C2D-C1D-ND	4.95	113.75	110.10
5	3	613	CLA	C4A-NA-C1A	4.94	108.93	106.71
4	2	606	CHL	C3B-C2B-C1B	-4.93	101.21	107.16
4	2	601	CHL	C3D-C4D-ND	4.93	118.21	110.24
4	4	601	CHL	C3D-C2D-C1D	-4.91	99.12	105.83
4	3	606	CHL	CAC-C3C-C4C	4.91	131.18	124.81
4	4	606	CHL	C3C-C4C-NC	4.91	116.07	110.57
4	2	605	CHL	C3D-C4D-ND	4.89	118.15	110.24
4	3	607	CHL	O2D-CGD-CBD	4.89	119.95	111.27
4	2	608	CHL	C3B-C2B-C1B	-4.88	101.27	107.16
4	1	607	CHL	C3D-C4D-ND	4.88	118.13	110.24
8	2	1623	NEX	C38-C25-C26	-4.87	114.09	122.26
4	4	607	CHL	O2D-CGD-CBD	4.87	119.92	111.27
4	4	609	CHL	C3D-C4D-ND	4.85	118.09	110.24
7	4	622	XAT	C26-C27-C28	-4.85	115.73	125.99
4	4	606	CHL	C3D-C4D-ND	4.85	118.08	110.24
4	1	605	CHL	C3D-C4D-ND	4.84	118.07	110.24
4	1	609	CHL	C3C-C4C-NC	4.84	116.00	110.57
4	3	606	CHL	C3D-C2D-C1D	-4.84	99.23	105.83
4	2	609	CHL	C3D-C2D-C1D	-4.83	99.24	105.83
4	4	607	CHL	C3D-C2D-C1D	-4.83	99.24	105.83
4	3	607	CHL	C2D-C1D-ND	4.83	113.66	110.10
4	1	609	CHL	C3D-C4D-ND	4.83	118.05	110.24
6	2	1620	LUT	C35-C34-C33	-4.83	120.42	127.31
4	3	607	CHL	C3D-C2D-C1D	-4.82	99.25	105.83
8	3	1623	NEX	C11-C10-C9	-4.82	120.44	127.31
7	3	1622	XAT	O24-C25-C38	4.80	120.81	115.06
4	1	606	CHL	C3D-C4D-ND	4.79	117.99	110.24
7	1	1622	XAT	C6-C7-C8	-4.78	115.88	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	601	CHL	C3D-C4D-ND	4.78	117.97	110.24
4	4	609	CHL	C3D-C2D-C1D	-4.77	99.32	105.83
4	4	609	CHL	O2D-CGD-CBD	4.76	119.72	111.27
4	2	607	CHL	C3D-C2D-C1D	-4.76	99.34	105.83
4	4	608	CHL	C3D-C4D-ND	4.75	117.93	110.24
7	2	1622	XAT	C38-C25-C26	-4.75	114.30	122.26
7	2	1622	XAT	C31-C30-C29	-4.75	120.54	127.31
4	2	606	CHL	C3D-C4D-ND	4.74	117.91	110.24
10	4	623	BCR	C7-C8-C9	-4.74	119.07	126.23
4	4	607	CHL	C3D-C4D-ND	4.74	117.91	110.24
4	3	601	CHL	O2D-CGD-CBD	4.74	119.69	111.27
4	2	608	CHL	C3D-C4D-ND	4.73	117.89	110.24
4	1	601	CHL	O2D-CGD-CBD	4.73	119.67	111.27
4	3	609	CHL	C3D-C4D-ND	4.73	117.88	110.24
4	1	609	CHL	C3B-C2B-C1B	-4.72	101.46	107.16
4	4	606	CHL	C3B-C2B-C1B	-4.72	101.46	107.16
4	4	607	CHL	C3B-C2B-C1B	-4.71	101.47	107.16
4	1	608	CHL	CHD-C4C-C3C	-4.70	117.93	124.84
4	3	608	CHL	O2D-CGD-CBD	4.69	119.60	111.27
4	2	605	CHL	O2D-CGD-CBD	4.69	119.60	111.27
8	1	1623	NEX	C38-C25-C26	-4.67	114.43	122.26
4	3	605	CHL	C3D-C4D-ND	4.65	117.76	110.24
5	1	613	CLA	C4A-NA-C1A	4.65	108.80	106.71
5	2	612	CLA	C4A-NA-C1A	4.65	108.80	106.71
4	4	609	CHL	C3C-C4C-NC	4.65	115.78	110.57
7	3	1622	XAT	C18-C5-C6	-4.64	114.48	122.26
4	2	606	CHL	C3D-C2D-C1D	-4.64	99.49	105.83
7	2	1622	XAT	C18-C5-C6	-4.64	114.49	122.26
4	3	609	CHL	C3C-C4C-NC	4.63	115.77	110.57
4	2	606	CHL	O2D-CGD-CBD	4.63	119.49	111.27
4	3	605	CHL	CHB-C1B-NB	-4.62	119.37	124.26
4	4	607	CHL	CHB-C1B-NB	-4.62	119.37	124.26
4	2	608	CHL	CHD-C4C-C3C	-4.61	118.06	124.84
5	4	612	CLA	C4A-NA-C1A	4.61	108.78	106.71
4	1	609	CHL	CHB-C1B-NB	-4.61	119.38	124.26
4	2	609	CHL	C3D-C4D-ND	4.60	117.68	110.24
5	2	603	CLA	C4A-NA-C1A	4.60	108.77	106.71
8	1	1623	NEX	C31-C30-C29	-4.58	120.77	127.31
4	3	606	CHL	C3B-C2B-C1B	-4.57	101.65	107.16
4	1	606	CHL	O2D-CGD-CBD	4.56	119.37	111.27
4	3	606	CHL	C3D-C4D-ND	4.56	117.61	110.24
5	4	611	CLA	C4A-NA-C1A	4.56	108.75	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	607	CHL	CHB-C1B-NB	-4.55	119.44	124.26
4	1	601	CHL	C2D-C1D-ND	4.55	113.45	110.10
7	1	1622	XAT	C18-C5-C6	-4.54	114.66	122.26
4	2	607	CHL	C3D-C4D-ND	4.53	117.57	110.24
7	4	622	XAT	C38-C25-C26	-4.53	114.67	122.26
4	2	609	CHL	C3B-C2B-C1B	-4.53	101.69	107.16
4	3	609	CHL	C3D-C2D-C1D	-4.52	99.67	105.83
8	3	1623	NEX	C27-C28-C29	-4.51	118.53	125.53
4	2	601	CHL	O2D-CGD-CBD	4.49	119.25	111.27
4	1	608	CHL	C3D-C4D-ND	4.49	117.50	110.24
4	1	608	CHL	C3B-C2B-C1B	-4.46	101.78	107.16
4	2	608	CHL	O2D-CGD-CBD	4.46	119.19	111.27
8	1	1623	NEX	C35-C34-C33	-4.45	120.96	127.31
4	1	606	CHL	C3D-C2D-C1D	-4.43	99.79	105.83
6	1	1620	LUT	C35-C34-C33	-4.42	121.00	127.31
4	3	608	CHL	C3D-C4D-ND	4.41	117.37	110.24
4	3	609	CHL	C3B-C2B-C1B	-4.41	101.84	107.16
4	1	601	CHL	C3D-C2D-C1D	-4.40	99.82	105.83
4	4	607	CHL	C3C-C4C-NC	4.40	115.51	110.57
7	2	1622	XAT	C15-C14-C13	-4.36	121.09	127.31
4	4	601	CHL	C3D-C4D-ND	4.36	117.29	110.24
4	1	606	CHL	C3B-C2B-C1B	-4.35	101.91	107.16
8	3	1623	NEX	O24-C25-C38	4.34	120.26	115.06
4	3	601	CHL	C3C-C4C-NC	4.33	115.43	110.57
7	3	1622	XAT	C15-C35-C34	-4.31	114.64	123.47
8	2	1623	NEX	C27-C28-C29	-4.31	118.84	125.53
4	1	607	CHL	O2D-CGD-CBD	4.30	118.92	111.27
7	1	1622	XAT	C11-C10-C9	-4.30	121.17	127.31
9	4	2630	LHG	O4-P-O5	4.30	133.50	112.24
4	3	607	CHL	C3C-C4C-NC	4.29	115.38	110.57
5	4	602	CLA	O2D-CGD-O1D	-4.27	115.48	123.84
5	1	614	CLA	C4A-NA-C1A	4.26	108.62	106.71
5	3	604	CLA	C4A-NA-C1A	4.26	108.62	106.71
4	3	608	CHL	CHD-C4C-C3C	-4.26	118.58	124.84
4	4	601	CHL	C3C-C4C-NC	4.26	115.35	110.57
5	4	604	CLA	C4A-NA-C1A	4.25	108.62	106.71
4	2	605	CHL	CHB-C1B-NB	-4.24	119.77	124.26
4	2	605	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
9	1	2630	LHG	O4-P-O5	4.20	133.00	112.24
5	2	613	CLA	C4A-NA-C1A	4.17	108.58	106.71
4	3	607	CHL	C3D-C4D-ND	4.17	116.98	110.24
8	2	1623	NEX	C11-C10-C9	-4.14	121.41	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	2630	LHG	O4-P-O5	4.13	132.65	112.24
6	1	1621	LUT	C15-C14-C13	-4.13	121.42	127.31
4	3	607	CHL	CHC-C4B-NB	-4.12	119.89	124.26
6	2	1620	LUT	C35-C15-C14	-4.12	115.04	123.47
4	2	601	CHL	CHC-C4B-NB	-4.12	119.90	124.26
4	4	609	CHL	CHB-C1B-NB	-4.11	119.91	124.26
6	2	1621	LUT	C15-C14-C13	-4.10	121.45	127.31
4	3	601	CHL	CMD-C2D-C3D	-4.10	118.19	127.61
5	1	611	CLA	C4A-NA-C1A	4.07	108.54	106.71
9	3	2630	LHG	O4-P-O5	4.07	132.35	112.24
4	2	607	CHL	CAC-C3C-C4C	4.06	130.08	124.81
4	1	601	CHL	CMD-C2D-C3D	-4.06	118.28	127.61
4	3	601	CHL	CHC-C4B-NB	-4.05	119.97	124.26
7	3	1622	XAT	C27-C28-C29	-4.01	119.30	125.53
5	1	612	CLA	C4A-NA-C1A	3.97	108.49	106.71
7	1	1622	XAT	O4-C5-C18	3.96	119.80	115.06
5	3	614	CLA	C4A-NA-C1A	3.95	108.48	106.71
4	1	605	CHL	CHD-C4C-C3C	-3.93	119.06	124.84
4	1	601	CHL	CHB-C1B-NB	-3.92	120.10	124.26
4	1	601	CHL	C3C-C4C-NC	3.91	114.96	110.57
4	4	608	CHL	O2D-CGD-CBD	3.89	118.17	111.27
7	4	622	XAT	C35-C34-C33	-3.88	121.77	127.31
4	2	601	CHL	CMD-C2D-C3D	-3.88	118.69	127.61
4	1	608	CHL	O2D-CGD-CBD	3.85	118.11	111.27
4	1	607	CHL	CHB-C1B-NB	-3.85	120.18	124.26
6	3	1621	LUT	C15-C14-C13	-3.84	121.83	127.31
4	2	601	CHL	C3C-C4C-NC	3.84	114.88	110.57
4	4	609	CHL	CAC-C3C-C4C	3.82	129.77	124.81
7	3	1622	XAT	C26-C27-C28	-3.82	117.92	125.99
4	3	606	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
4	1	606	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
5	2	614	CLA	C4A-NA-C1A	3.81	108.42	106.71
4	1	609	CHL	C3B-C4B-NB	3.80	114.04	110.52
4	1	601	CHL	CAC-C3C-C4C	3.77	129.71	124.81
4	4	606	CHL	CHB-C1B-NB	-3.77	120.27	124.26
4	4	608	CHL	CHB-C1B-NB	-3.76	120.28	124.26
4	1	607	CHL	CHD-C4C-C3C	-3.76	119.32	124.84
4	1	607	CHL	CHB-C4A-NA	3.75	129.69	124.51
6	1	1620	LUT	C30-C31-C32	-3.74	111.53	123.22
4	2	601	CHL	CHB-C1B-NB	-3.74	120.30	124.26
4	2	601	CHL	C3B-C4B-NB	3.74	113.98	110.52
6	4	620	LUT	C15-C14-C13	-3.72	122.01	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1	1622	XAT	C27-C28-C29	-3.70	119.79	125.53
4	1	607	CHL	C3B-C4B-NB	3.70	113.95	110.52
6	4	620	LUT	C7-C8-C9	-3.70	120.65	126.23
6	3	1620	LUT	C35-C34-C33	-3.69	122.04	127.31
6	2	1621	LUT	C35-C34-C33	-3.68	122.06	127.31
8	2	1623	NEX	O24-C25-C38	3.68	119.46	115.06
7	2	1622	XAT	C11-C10-C9	-3.67	122.07	127.31
6	3	1620	LUT	C15-C14-C13	-3.66	122.08	127.31
8	2	1623	NEX	C31-C30-C29	-3.64	122.11	127.31
4	1	605	CHL	C3B-C4B-NB	3.63	113.88	110.52
7	3	1622	XAT	C4-C3-C2	-3.62	103.78	110.77
8	1	1623	NEX	C15-C14-C13	-3.62	122.14	127.31
6	1	1621	LUT	C2-C3-C4	3.60	115.23	110.30
4	2	601	CHL	C1C-C2C-C3C	-3.59	104.26	107.11
6	3	1620	LUT	C10-C11-C12	-3.58	112.05	123.22
4	3	608	CHL	CAC-C3C-C4C	3.57	129.44	124.81
8	1	1623	NEX	O24-C25-C38	3.56	119.33	115.06
4	3	601	CHL	CAC-C3C-C4C	3.54	129.41	124.81
4	3	605	CHL	CHD-C4C-C3C	-3.54	119.64	124.84
4	2	606	CHL	CHD-C4C-C3C	-3.53	119.65	124.84
5	1	604	CLA	CHB-C1B-NB	3.51	127.97	124.26
6	2	1620	LUT	C30-C31-C32	-3.50	112.30	123.22
7	3	1622	XAT	O4-C5-C18	3.49	119.23	115.06
5	4	602	CLA	O2D-CGD-CBD	3.48	117.45	111.27
4	4	607	CHL	CAC-C3C-C4C	3.47	129.31	124.81
6	1	1620	LUT	C10-C11-C12	-3.45	112.46	123.22
7	1	1622	XAT	O24-C25-C38	3.44	119.18	115.06
4	3	609	CHL	CHB-C1B-NB	-3.44	120.62	124.26
5	1	604	CLA	CMB-C2B-C1B	-3.43	120.14	125.37
4	1	605	CHL	CAC-C3C-C4C	3.43	129.25	124.81
8	2	1623	NEX	C16-C1-C6	3.42	113.53	110.47
4	4	606	CHL	CHD-C4C-C3C	-3.42	119.81	124.84
6	1	1620	LUT	C35-C15-C14	-3.42	116.48	123.47
4	2	607	CHL	C3B-C4B-NB	3.40	113.67	110.52
4	3	608	CHL	C3B-C4B-NB	3.40	113.67	110.52
5	3	612	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
4	2	607	CHL	CHD-C4C-C3C	-3.39	119.86	124.84
4	3	609	CHL	C1C-C2C-C3C	-3.38	104.43	107.11
4	2	609	CHL	C3B-C4B-NB	3.38	113.65	110.52
4	1	608	CHL	CHB-C1B-NB	-3.38	120.68	124.26
4	3	605	CHL	C3B-C4B-NB	3.37	113.64	110.52
6	1	1621	LUT	C35-C34-C33	-3.36	122.52	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	606	CHL	C3B-C4B-NB	3.36	113.63	110.52
5	1	604	CLA	C4A-NA-C1A	3.35	108.21	106.71
4	3	605	CHL	CAC-C3C-C4C	3.35	129.16	124.81
7	3	1622	XAT	C24-C23-C22	-3.34	104.32	110.77
4	1	607	CHL	CAC-C3C-C4C	3.34	129.14	124.81
4	2	601	CHL	CAC-C3C-C4C	3.33	129.13	124.81
5	3	603	CLA	CHB-C4A-NA	3.33	129.12	124.51
4	2	609	CHL	CMB-C2B-C1B	3.32	130.43	125.37
4	2	609	CHL	CAC-C3C-C4C	3.32	129.12	124.81
6	3	1620	LUT	C30-C31-C32	-3.32	112.86	123.22
8	3	1623	NEX	C39-C29-C30	-3.32	118.27	122.92
4	3	601	CHL	CHB-C1B-NB	-3.31	120.76	124.26
8	3	1623	NEX	C11-C12-C13	-3.30	117.14	126.42
4	3	608	CHL	CHB-C1B-NB	-3.30	120.77	124.26
7	4	622	XAT	O24-C25-C38	3.30	119.00	115.06
4	1	609	CHL	C1C-C2C-C3C	-3.29	104.50	107.11
6	4	620	LUT	C11-C10-C9	-3.29	122.61	127.31
4	1	607	CHL	CMB-C2B-C1B	3.29	130.38	125.37
7	2	1622	XAT	C27-C28-C29	-3.29	120.43	125.53
5	3	602	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
8	3	1623	NEX	C24-C23-C22	-3.28	104.44	110.77
4	1	601	CHL	C3B-C4B-NB	3.28	113.56	110.52
7	2	1622	XAT	C7-C8-C9	-3.28	120.44	125.53
4	3	609	CHL	C3B-C4B-NB	3.27	113.55	110.52
4	1	601	CHL	CHC-C4B-NB	-3.27	120.80	124.26
5	2	611	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
7	1	1622	XAT	C35-C34-C33	-3.26	122.66	127.31
4	2	608	CHL	CAC-C3C-C4C	3.26	129.03	124.81
4	3	607	CHL	C4A-NA-C1A	3.25	108.17	106.71
4	1	608	CHL	CAC-C3C-C4C	3.25	129.03	124.81
4	4	607	CHL	C3B-C4B-NB	3.24	113.53	110.52
4	3	609	CHL	CAC-C3C-C4C	3.23	129.01	124.81
6	4	620	LUT	C18-C5-C4	3.22	120.33	114.36
5	3	614	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
6	4	620	LUT	C18-C5-C6	-3.21	120.92	124.53
7	4	622	XAT	C4-C3-C2	-3.20	104.59	110.77
5	2	603	CLA	CHB-C4A-NA	3.20	128.93	124.51
4	2	606	CHL	C3B-C4B-NB	3.20	113.48	110.52
8	1	1623	NEX	C11-C10-C9	-3.19	122.76	127.31
5	1	610	CLA	CHB-C1B-NB	3.18	127.63	124.26
7	4	622	XAT	C15-C14-C13	-3.18	122.77	127.31
6	4	620	LUT	C35-C34-C33	-3.18	122.77	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	608	CHL	C3B-C4B-NB	3.18	113.46	110.52
8	2	1623	NEX	C15-C35-C34	-3.17	116.97	123.47
5	2	602	CLA	C4A-NA-C1A	3.17	108.13	106.71
4	1	605	CHL	CHB-C1B-NB	-3.17	120.91	124.26
4	4	606	CHL	CHC-C4B-NB	-3.16	120.91	124.26
4	3	607	CHL	CAC-C3C-C4C	3.14	128.89	124.81
4	3	601	CHL	CHD-C4C-C3C	-3.14	120.23	124.84
4	2	608	CHL	C3B-C4B-NB	3.14	113.43	110.52
4	3	601	CHL	C3B-C4B-NB	3.13	113.42	110.52
7	3	1622	XAT	C11-C10-C9	-3.13	122.84	127.31
4	3	601	CHL	C4A-NA-C1A	-3.13	105.30	106.71
6	3	1621	LUT	C15-C35-C34	-3.13	117.07	123.47
4	3	601	CHL	C1C-C2C-C3C	-3.12	104.64	107.11
4	1	606	CHL	CAC-C3C-C4C	3.11	128.84	124.81
4	3	607	CHL	CMB-C2B-C1B	3.11	130.10	125.37
5	2	610	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
7	2	1622	XAT	C35-C34-C33	-3.11	122.88	127.31
5	3	603	CLA	CBC-CAC-C3C	-3.10	103.88	112.43
5	1	603	CLA	CHB-C4A-NA	3.10	128.80	124.51
5	3	610	CLA	CHB-C1B-NB	3.10	127.54	124.26
6	4	620	LUT	C30-C31-C32	-3.10	113.55	123.22
4	3	607	CHL	C3B-C4B-NB	3.10	113.39	110.52
7	4	622	XAT	C24-C23-C22	-3.09	104.80	110.77
10	4	623	BCR	C11-C12-C13	-3.09	117.74	126.42
4	2	607	CHL	CMB-C2B-C1B	3.08	130.06	125.37
4	2	609	CHL	CHD-C4C-C3C	-3.08	120.31	124.84
4	2	609	CHL	C1C-C2C-C3C	-3.07	104.67	107.11
4	1	609	CHL	CHD-C4C-C3C	-3.07	120.32	124.84
4	2	601	CHL	CHD-C4C-C3C	-3.05	120.36	124.84
5	1	610	CLA	C3B-C4B-NB	-3.04	107.69	110.52
6	4	620	LUT	C8-C7-C6	-3.04	118.67	127.20
4	2	601	CHL	C4A-NA-C1A	-3.04	105.34	106.71
7	3	1622	XAT	C31-C32-C33	-3.04	117.89	126.42
4	2	605	CHL	C3B-C4B-NB	3.03	113.33	110.52
4	4	609	CHL	C3B-C4B-NB	3.03	113.33	110.52
4	3	606	CHL	C3B-C4B-NB	3.03	113.33	110.52
5	2	610	CLA	C4A-NA-C1A	3.03	108.07	106.71
4	1	608	CHL	CHC-C4B-NB	-3.03	121.05	124.26
4	3	605	CHL	CMB-C2B-C1B	3.02	129.97	125.37
8	1	1623	NEX	C24-C23-C22	-3.02	104.94	110.77
4	4	608	CHL	CMB-C2B-C1B	3.02	129.96	125.37
4	2	601	CHL	C4D-CHA-C1A	-3.00	117.60	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	606	CHL	CAC-C3C-C4C	2.97	128.67	124.81
6	2	1620	LUT	C10-C11-C12	-2.97	113.94	123.22
4	4	601	CHL	C3B-C4B-NB	2.96	113.26	110.52
4	2	606	CHL	CHB-C1B-NB	-2.96	121.12	124.26
5	3	611	CLA	CHC-C4B-NB	2.96	127.39	124.26
4	4	606	CHL	C3B-C4B-NB	2.95	113.25	110.52
5	1	604	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
6	1	1621	LUT	C18-C5-C6	-2.95	121.22	124.53
7	2	1622	XAT	C6-C7-C8	-2.94	119.77	125.99
5	1	614	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
6	2	1621	LUT	C10-C11-C12	-2.92	114.09	123.22
6	3	1621	LUT	C35-C34-C33	-2.92	123.14	127.31
4	4	608	CHL	C3B-C4B-NB	2.92	113.22	110.52
7	1	1622	XAT	C31-C32-C33	-2.92	118.22	126.42
5	1	612	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
4	3	606	CHL	OMC-CMC-C2C	-2.90	119.12	125.69
10	4	623	BCR	C3-C4-C5	-2.90	108.90	114.08
6	3	1621	LUT	C10-C11-C12	-2.90	114.18	123.22
7	2	1622	XAT	O24-C25-C38	2.90	118.53	115.06
8	1	1623	NEX	C26-C27-C28	-2.89	119.88	125.99
7	1	1622	XAT	C4-C3-C2	-2.89	105.19	110.77
4	4	606	CHL	CAC-C3C-C4C	2.89	128.56	124.81
4	4	609	CHL	CMD-C2D-C3D	-2.88	120.98	127.61
5	4	612	CLA	CHB-C4A-NA	2.88	128.50	124.51
4	4	607	CHL	CHD-C4C-C3C	-2.88	120.61	124.84
7	4	622	XAT	C10-C11-C12	-2.87	114.25	123.22
4	3	609	CHL	CMD-C2D-C3D	-2.87	121.01	127.61
4	3	608	CHL	CMB-C2B-C1B	2.87	129.74	125.37
4	1	609	CHL	CMD-C2D-C3D	-2.87	121.02	127.61
6	1	1621	LUT	C22-C23-C24	-2.87	108.48	111.74
4	2	606	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
7	4	622	XAT	C38-C25-C24	2.86	117.50	114.28
6	4	620	LUT	C31-C30-C29	-2.85	123.24	127.31
4	3	607	CHL	CMD-C2D-C3D	-2.85	121.06	127.61
6	3	1621	LUT	C22-C23-C24	-2.85	108.50	111.74
7	2	1622	XAT	O4-C5-C18	2.85	118.47	115.06
4	3	601	CHL	CMB-C2B-C1B	2.84	129.69	125.37
4	3	607	CHL	O2A-CGA-CBA	2.83	120.80	111.91
4	4	607	CHL	CMD-C2D-C3D	-2.83	121.09	127.61
4	4	601	CHL	CAC-C3C-C4C	2.83	128.49	124.81
5	4	604	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
5	2	613	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	1620	LUT	C15-C14-C13	-2.83	123.27	127.31
5	3	603	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
5	2	602	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
4	1	601	CHL	C1C-C2C-C3C	-2.83	104.87	107.11
4	4	606	CHL	CAA-C2A-C3A	-2.82	105.05	112.78
5	2	612	CLA	CHB-C4A-NA	2.82	128.41	124.51
4	4	607	CHL	C1C-C2C-C3C	-2.82	104.88	107.11
4	2	605	CHL	C1C-C2C-C3C	-2.81	104.88	107.11
5	3	613	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
5	1	602	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
4	3	601	CHL	C2A-C1A-CHA	-2.80	118.97	123.86
7	1	1622	XAT	C18-C5-C4	2.80	117.43	114.28
6	3	1620	LUT	C7-C8-C9	-2.80	122.01	126.23
5	1	603	CLA	CBC-CAC-C3C	-2.79	104.75	112.43
5	1	603	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
8	3	1623	NEX	C15-C35-C34	-2.78	117.77	123.47
5	3	603	CLA	C2A-C1A-CHA	2.78	128.71	123.86
5	1	612	CLA	CHB-C1B-NB	2.78	127.20	124.26
4	4	608	CHL	OMC-CMC-C2C	-2.78	119.41	125.69
4	4	609	CHL	CMB-C2B-C1B	2.77	129.59	125.37
5	2	612	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
5	3	611	CLA	CHB-C4A-NA	2.76	128.34	124.51
5	1	612	CLA	C2B-C1B-NB	2.76	112.08	110.23
5	2	603	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
5	3	610	CLA	C3B-C4B-NB	-2.76	107.95	110.52
5	2	612	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
4	4	607	CHL	CMB-C2B-C1B	2.76	129.57	125.37
4	4	601	CHL	CHC-C4B-NB	-2.76	121.34	124.26
4	2	605	CHL	CMB-C2B-C1B	2.75	129.56	125.37
5	3	613	CLA	CHB-C4A-NA	2.75	128.32	124.51
6	2	1620	LUT	C20-C13-C12	2.75	122.41	118.08
4	1	606	CHL	CMD-C2D-C3D	-2.75	121.29	127.61
7	3	1622	XAT	C40-C33-C32	2.74	122.40	118.08
4	1	609	CHL	CMB-C2B-C1B	2.74	129.54	125.37
7	2	1622	XAT	C4-C3-C2	-2.74	105.48	110.77
4	2	609	CHL	C1-C2-C3	-2.74	121.30	126.04
10	4	623	BCR	C29-C30-C25	2.74	114.70	110.48
4	1	607	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
4	3	601	CHL	O2A-CGA-CBA	2.74	120.50	111.91
4	3	605	CHL	C1C-C2C-C3C	-2.74	104.94	107.11
5	4	610	CLA	CHB-C1B-NB	2.74	127.15	124.26
4	2	608	CHL	CHB-C1B-NB	-2.73	121.36	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	603	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
9	2	2630	LHG	O8-C23-C24	2.73	120.47	111.91
5	4	603	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
5	2	614	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
4	4	601	CHL	C1C-C2C-C3C	-2.72	104.96	107.11
4	1	608	CHL	CMB-C2B-C1B	2.72	129.51	125.37
5	4	611	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
4	1	609	CHL	CAC-C3C-C4C	2.72	128.33	124.81
6	4	620	LUT	C10-C11-C12	-2.72	114.74	123.22
4	2	606	CHL	C1C-C2C-C3C	-2.71	104.96	107.11
7	2	1622	XAT	C26-C27-C28	-2.71	120.26	125.99
4	1	605	CHL	CMB-C2B-C1B	2.71	129.50	125.37
4	3	601	CHL	C4D-CHA-C1A	-2.71	117.95	121.25
5	3	602	CLA	CHB-C1B-NB	2.71	127.12	124.26
6	3	1621	LUT	C19-C9-C8	2.71	122.34	118.08
5	1	612	CLA	CHC-C4B-NB	2.70	127.12	124.26
5	4	602	CLA	CHB-C4A-NA	2.70	128.25	124.51
4	4	601	CHL	CMB-C2B-C1B	2.70	129.48	125.37
4	3	607	CHL	C4-C3-C5	2.70	119.81	115.27
4	2	608	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
5	2	604	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
6	2	1621	LUT	C19-C9-C8	2.69	122.32	118.08
7	3	1622	XAT	C10-C11-C12	-2.69	114.81	123.22
5	1	602	CLA	C4A-NA-C1A	2.69	107.92	106.71
4	1	605	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
4	3	609	CHL	O2A-CGA-CBA	2.68	120.32	111.91
4	3	605	CHL	CAA-C2A-C3A	-2.68	105.44	112.78
7	3	1622	XAT	C35-C34-C33	-2.68	123.49	127.31
5	3	603	CLA	CHC-C4B-NB	2.68	127.09	124.26
7	2	1622	XAT	C15-C35-C34	-2.68	117.99	123.47
4	2	601	CHL	CMB-C2B-C1B	2.68	129.44	125.37
6	2	1620	LUT	C11-C10-C9	-2.68	123.49	127.31
5	3	612	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
5	3	610	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
8	1	1623	NEX	C5-C4-C3	-2.66	108.59	111.75
4	1	601	CHL	C4D-CHA-C1A	-2.66	118.01	121.25
4	4	606	CHL	CMB-C2B-C1B	2.66	129.42	125.37
6	2	1620	LUT	C39-C29-C28	2.66	122.27	118.08
4	2	607	CHL	CMD-C2D-C3D	-2.66	121.50	127.61
5	1	613	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
4	3	608	CHL	CHB-C4A-NA	2.65	128.18	124.51
5	2	612	CLA	CHB-C1B-NB	2.65	127.06	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	605	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
4	2	606	CHL	CMB-C2B-C1B	2.65	129.40	125.37
4	1	605	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
4	1	606	CHL	CHB-C1B-NB	-2.65	121.45	124.26
5	4	611	CLA	CHB-C4A-NA	2.65	128.17	124.51
8	2	1623	NEX	C26-C27-C28	-2.64	120.40	125.99
4	1	601	CHL	CHD-C4C-C3C	-2.64	120.96	124.84
4	3	608	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
5	1	612	CLA	CHB-C4A-NA	2.64	128.16	124.51
4	3	605	CHL	CHC-C4B-NB	-2.64	121.47	124.26
7	1	1622	XAT	C26-C27-C28	-2.64	120.42	125.99
4	4	606	CHL	C1C-C2C-C3C	-2.63	105.02	107.11
5	1	602	CLA	C3B-C4B-NB	-2.63	108.07	110.52
5	3	604	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
4	2	609	CHL	CMD-C2D-C3D	-2.63	121.56	127.61
4	2	608	CHL	CMD-C2D-C3D	-2.63	121.57	127.61
5	3	604	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
4	1	601	CHL	C4A-NA-C1A	-2.62	105.53	106.71
4	1	609	CHL	O2A-CGA-CBA	2.62	120.14	111.91
6	2	1621	LUT	C39-C29-C28	2.62	122.21	118.08
5	4	610	CLA	C3B-C4B-NB	-2.62	108.09	110.52
4	4	601	CHL	CMD-C2D-C3D	-2.61	121.61	127.61
5	1	603	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
8	3	1623	NEX	C30-C31-C32	-2.61	115.07	123.22
7	3	1622	XAT	C18-C5-C4	2.61	117.22	114.28
4	2	605	CHL	CAC-C3C-C4C	2.61	128.19	124.81
4	2	601	CHL	C2A-C1A-CHA	-2.61	119.30	123.86
5	4	603	CLA	CHB-C4A-NA	2.61	128.12	124.51
5	1	611	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
4	4	607	CHL	CHC-C4B-NB	-2.60	121.50	124.26
4	4	609	CHL	CHD-C4C-C3C	-2.60	121.02	124.84
5	2	611	CLA	CHB-C4A-NA	2.60	128.10	124.51
5	1	614	CLA	CHB-C4A-NA	2.60	128.10	124.51
4	1	607	CHL	CHC-C4B-NB	-2.60	121.51	124.26
4	1	609	CHL	C1-C2-C3	-2.59	121.56	126.04
5	2	613	CLA	CHB-C4A-NA	2.59	128.09	124.51
5	3	604	CLA	CHB-C1B-NB	2.58	126.99	124.26
5	3	602	CLA	C4A-NA-C1A	2.58	107.87	106.71
6	3	1620	LUT	C35-C15-C14	-2.58	118.19	123.47
5	2	604	CLA	CHB-C1B-NB	2.58	126.98	124.26
5	3	611	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
6	4	620	LUT	C15-C35-C34	-2.57	118.20	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	608	CHL	CMD-C2D-C3D	-2.57	121.69	127.61
5	2	614	CLA	CHB-C4A-NA	2.57	128.07	124.51
6	1	1621	LUT	C10-C11-C12	-2.57	115.20	123.22
9	3	2630	LHG	C11-C10-C9	-2.57	101.38	114.42
4	3	601	CHL	CHB-C4A-NA	2.57	128.06	124.51
8	1	1623	NEX	C15-C35-C34	-2.57	118.22	123.47
5	4	603	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
6	3	1620	LUT	C15-C35-C34	-2.56	118.23	123.47
5	3	604	CLA	CHB-C4A-NA	2.56	128.05	124.51
4	1	606	CHL	CHB-C4A-NA	2.56	128.05	124.51
6	4	620	LUT	C35-C15-C14	-2.56	118.23	123.47
4	4	606	CHL	CMD-C2D-C3D	-2.56	121.73	127.61
5	1	613	CLA	CHB-C4A-NA	2.55	128.04	124.51
7	4	622	XAT	C35-C15-C14	-2.55	118.24	123.47
4	1	607	CHL	CAA-C2A-C3A	-2.55	105.79	112.78
4	2	609	CHL	C4-C3-C5	2.55	119.56	115.27
4	2	607	CHL	CAA-C2A-C3A	-2.55	105.81	112.78
8	3	1623	NEX	C20-C13-C14	-2.54	119.36	122.92
6	3	1621	LUT	C38-C25-C24	-2.54	118.12	123.56
4	1	601	CHL	CMB-C2B-C1B	2.54	129.24	125.37
5	1	613	CLA	CHC-C4B-NB	2.54	126.94	124.26
4	1	605	CHL	CHB-C4A-NA	2.53	128.02	124.51
4	2	607	CHL	O2A-CGA-CBA	2.53	119.86	111.91
5	2	602	CLA	C1-C2-C3	-2.53	121.66	126.04
5	2	613	CLA	CHD-C1D-ND	-2.53	122.13	124.45
6	1	1620	LUT	C15-C14-C13	-2.53	123.70	127.31
4	4	601	CHL	CHD-C4C-C3C	-2.53	121.12	124.84
6	3	1620	LUT	C3-C4-C5	2.53	116.89	111.85
8	2	1623	NEX	C24-C23-C22	-2.53	105.89	110.77
7	1	1622	XAT	C11-C12-C13	-2.53	119.31	126.42
8	2	1623	NEX	C39-C29-C30	-2.53	119.38	122.92
5	1	613	CLA	CHB-C1B-NB	2.52	126.93	124.26
6	2	1620	LUT	C38-C25-C24	-2.52	118.16	123.56
7	2	1622	XAT	C18-C5-C4	2.52	117.12	114.28
5	2	604	CLA	CHC-C4B-NB	2.52	126.93	124.26
4	1	609	CHL	C4-C3-C5	2.52	119.51	115.27
4	3	606	CHL	CMD-C2D-C3D	-2.52	121.81	127.61
4	3	609	CHL	CHD-C4C-C3C	-2.52	121.14	124.84
4	2	607	CHL	CHC-C4B-NB	-2.51	121.60	124.26
5	2	610	CLA	CHB-C4A-NA	2.51	127.98	124.51
5	1	611	CLA	CHC-C4B-NB	2.51	126.91	124.26
4	1	605	CHL	O2D-CGD-O1D	-2.50	118.94	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	604	CLA	CHB-C1B-NB	2.50	126.91	124.26
6	1	1621	LUT	C38-C25-C24	-2.50	118.21	123.56
8	2	1623	NEX	C11-C12-C13	-2.50	119.39	126.42
6	1	1621	LUT	C7-C8-C9	-2.49	122.47	126.23
5	3	612	CLA	CHB-C4A-NA	2.48	127.94	124.51
4	4	608	CHL	CMD-C2D-C3D	-2.48	121.91	127.61
4	1	605	CHL	C4A-NA-C1A	-2.48	105.59	106.71
7	1	1622	XAT	C15-C35-C34	-2.48	118.40	123.47
5	4	612	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
6	3	1621	LUT	C3-C4-C5	-2.47	106.92	111.85
5	4	604	CLA	CHD-C1D-ND	-2.47	122.18	124.45
6	2	1620	LUT	C7-C8-C9	-2.47	122.50	126.23
4	4	606	CHL	O2D-CGD-O1D	-2.47	119.01	123.84
5	2	603	CLA	CHB-C1B-NB	2.47	126.87	124.26
4	2	605	CHL	CMD-C2D-C3D	-2.47	121.94	127.61
4	4	606	CHL	CAA-CBA-CGA	-2.47	105.96	112.51
6	4	620	LUT	C21-C26-C27	-2.46	109.59	112.70
7	3	1622	XAT	C32-C33-C34	-2.46	115.17	118.94
4	2	601	CHL	CHB-C4A-NA	2.46	127.91	124.51
5	4	612	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
5	3	611	CLA	C2A-C1A-CHA	2.45	128.15	123.86
4	3	606	CHL	CHC-C4B-NB	-2.45	121.66	124.26
9	1	2630	LHG	C11-C10-C9	-2.45	101.98	114.42
4	3	609	CHL	O2D-CGD-O1D	-2.45	119.05	123.84
6	1	1621	LUT	C30-C31-C32	-2.45	115.58	123.22
4	1	607	CHL	O2A-CGA-CBA	2.45	119.59	111.91
5	3	611	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
6	3	1621	LUT	C31-C30-C29	-2.44	123.82	127.31
5	2	602	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
5	1	610	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
4	2	609	CHL	O2A-CGA-CBA	2.44	119.56	111.91
4	3	606	CHL	C4A-NA-C1A	-2.44	105.61	106.71
10	4	623	BCR	C20-C19-C18	-2.43	119.58	126.42
5	3	614	CLA	CHB-C4A-NA	2.43	127.87	124.51
8	2	1623	NEX	C35-C34-C33	-2.43	123.84	127.31
7	3	1622	XAT	C19-C9-C8	2.43	121.90	118.08
6	2	1621	LUT	C16-C1-C6	-2.42	106.37	110.30
4	3	609	CHL	CHC-C4B-NB	-2.42	121.70	124.26
4	1	606	CHL	C1C-C2C-C3C	-2.42	105.20	107.11
6	2	1620	LUT	C28-C29-C30	-2.41	115.24	118.94
5	2	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
6	1	1620	LUT	C39-C29-C28	2.41	121.88	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	609	CHL	O1D-CGD-CBD	-2.41	119.56	124.48
4	2	607	CHL	O1D-CGD-CBD	-2.40	119.56	124.48
5	2	610	CLA	CHB-C1B-NB	2.40	126.80	124.26
5	1	612	CLA	C2A-C1A-CHA	2.40	128.06	123.86
7	4	622	XAT	C30-C31-C32	-2.40	115.72	123.22
9	1	2630	LHG	C20-C19-C18	-2.40	102.24	114.42
5	4	604	CLA	CHB-C4A-NA	2.40	127.83	124.51
5	1	610	CLA	CHB-C4A-NA	2.39	127.82	124.51
4	2	605	CHL	CHC-C4B-NB	-2.39	121.72	124.26
9	1	2630	LHG	O8-C23-C24	2.39	119.41	111.91
10	4	623	BCR	C27-C26-C25	-2.38	119.27	122.73
8	3	1623	NEX	C35-C34-C33	-2.38	123.91	127.31
4	3	605	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
4	3	606	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
8	3	1623	NEX	C28-C29-C30	2.38	122.59	118.94
5	2	603	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
4	4	609	CHL	C1C-C2C-C3C	-2.38	105.23	107.11
4	2	609	CHL	O2D-CGD-O1D	-2.37	119.20	123.84
7	1	1622	XAT	C24-C23-C22	-2.37	106.19	110.77
4	2	606	CHL	CHC-C4B-NB	-2.37	121.75	124.26
6	2	1621	LUT	C38-C25-C24	-2.37	118.48	123.56
6	3	1620	LUT	C39-C29-C28	2.37	121.81	118.08
9	3	2630	LHG	O8-C23-C24	2.37	119.34	111.91
4	3	607	CHL	CHD-C4C-C3C	-2.37	121.36	124.84
4	1	606	CHL	CED-O2D-CGD	2.37	121.29	115.94
4	1	607	CHL	C4-C3-C5	2.37	119.25	115.27
5	3	602	CLA	CHB-C4A-NA	2.36	127.77	124.51
5	2	602	CLA	CHB-C1B-NB	2.36	126.75	124.26
6	3	1620	LUT	C20-C13-C12	2.36	121.79	118.08
8	3	1623	NEX	C26-C27-C28	-2.35	121.01	125.99
5	3	603	CLA	CHA-C1A-NA	-2.35	121.01	126.40
6	1	1620	LUT	C19-C9-C8	2.35	121.78	118.08
6	4	620	LUT	C39-C29-C28	2.35	121.78	118.08
5	4	610	CLA	CHC-C4B-NB	2.35	126.74	124.26
7	2	1622	XAT	C31-C32-C33	-2.35	119.82	126.42
6	2	1620	LUT	C21-C26-C27	-2.35	109.73	112.70
5	3	610	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
5	3	602	CLA	O2D-CGD-CBD	2.34	115.42	111.27
5	3	612	CLA	CHB-C1B-NB	2.34	126.73	124.26
5	3	613	CLA	CHB-C1B-NB	2.34	126.73	124.26
8	3	1623	NEX	C12-C13-C14	2.33	122.52	118.94
4	2	606	CHL	CHB-C4A-NA	2.33	127.74	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	3	602	CLA	CHD-C1D-ND	-2.33	122.31	124.45
5	1	602	CLA	CHB-C1B-NB	2.33	126.72	124.26
5	3	612	CLA	C4A-NA-C1A	2.33	107.75	106.71
5	4	603	CLA	CHB-C1B-NB	2.32	126.72	124.26
6	2	1620	LUT	C12-C13-C14	-2.32	115.38	118.94
4	3	608	CHL	CMD-C2D-C3D	-2.32	122.28	127.61
5	1	612	CLA	CHB-C1B-C2B	-2.32	120.69	127.24
4	2	608	CHL	CHB-C4A-NA	2.32	127.72	124.51
4	1	606	CHL	C4D-CHA-C1A	-2.32	118.43	121.25
10	4	623	BCR	C37-C22-C23	2.32	121.73	118.08
5	1	612	CLA	CHA-C1A-NA	-2.32	121.09	126.40
6	4	620	LUT	C1-C6-C5	-2.31	119.35	122.61
5	2	610	CLA	C1-C2-C3	-2.31	123.01	126.75
5	4	610	CLA	C4A-NA-C1A	2.31	107.75	106.71
7	4	622	XAT	C19-C9-C8	2.31	121.72	118.08
4	1	601	CHL	C2A-C1A-CHA	-2.31	119.82	123.86
6	2	1621	LUT	C18-C5-C6	-2.31	121.94	124.53
4	2	608	CHL	C2A-C1A-CHA	-2.31	119.83	123.86
4	2	608	CHL	CMB-C2B-C1B	2.30	128.87	125.37
5	2	611	CLA	CHB-C1B-NB	2.30	126.69	124.26
4	3	607	CHL	C1-O2A-CGA	2.29	122.46	116.44
5	1	611	CLA	CHB-C1B-NB	2.29	126.69	124.26
6	2	1621	LUT	C8-C9-C10	-2.29	115.42	118.94
6	2	1621	LUT	C30-C31-C32	-2.29	116.07	123.22
5	3	614	CLA	C3B-C4B-NB	-2.29	108.39	110.52
4	4	609	CHL	CHC-C4B-NB	-2.29	121.84	124.26
4	2	608	CHL	CHC-C4B-NB	-2.28	121.85	124.26
4	4	608	CHL	CHB-C4A-NA	2.28	127.66	124.51
9	2	2630	LHG	C11-C10-C9	-2.28	102.87	114.42
5	1	603	CLA	CHD-C1D-ND	-2.27	122.36	124.45
6	2	1621	LUT	C21-C26-C27	-2.27	109.83	112.70
7	1	1622	XAT	C19-C9-C8	2.27	121.65	118.08
5	2	613	CLA	CHB-C1B-NB	2.27	126.66	124.26
10	4	623	BCR	C20-C21-C22	-2.26	124.08	127.31
4	4	601	CHL	O2D-CGD-O1D	-2.26	118.95	124.09
4	3	608	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
6	1	1621	LUT	C19-C9-C8	2.26	121.64	118.08
4	1	609	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
5	1	602	CLA	CAC-C3C-C4C	2.26	127.74	124.81
4	3	606	CHL	CHB-C1B-NB	-2.26	121.87	124.26
7	4	622	XAT	C20-C13-C12	2.26	121.63	118.08
4	3	609	CHL	C1-C2-C3	-2.25	122.14	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	606	CHL	CBA-CAA-C2A	-2.25	107.23	113.86
6	1	1621	LUT	C8-C7-C6	-2.25	120.89	127.20
6	1	1621	LUT	C39-C29-C28	2.24	121.61	118.08
4	3	606	CHL	CHB-C4A-NA	2.24	127.61	124.51
9	1	2630	LHG	C18-C17-C16	-2.24	103.04	114.42
5	3	612	CLA	CHC-C4B-NB	2.24	126.63	124.26
9	1	2630	LHG	C27-C26-C25	-2.23	103.08	114.42
5	1	603	CLA	CHC-C4B-NB	2.23	126.62	124.26
9	2	2630	LHG	C27-C26-C25	-2.23	103.10	114.42
4	3	608	CHL	O2A-CGA-CBA	2.23	121.20	114.03
7	2	1622	XAT	C10-C11-C12	-2.23	116.26	123.22
4	1	607	CHL	OMC-CMC-C2C	-2.23	120.65	125.69
5	1	604	CLA	C3B-C4B-NB	-2.23	108.45	110.52
4	2	601	CHL	C4D-C3D-CAD	2.22	110.72	108.10
4	1	607	CHL	C1-C2-C3	-2.22	122.20	126.04
5	3	610	CLA	CHB-C4A-NA	2.22	127.58	124.51
4	3	607	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
4	1	601	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
5	2	610	CLA	CHD-C1D-ND	-2.22	122.42	124.45
7	4	622	XAT	C25-C24-C23	-2.22	108.36	112.75
6	2	1621	LUT	C8-C7-C6	-2.22	120.98	127.20
6	3	1620	LUT	C18-C5-C6	-2.21	122.04	124.53
10	4	623	BCR	C2-C3-C4	-2.21	106.45	111.38
7	1	1622	XAT	C5-C4-C3	-2.20	108.39	112.75
5	3	611	CLA	CHA-C1A-NA	-2.20	121.36	126.40
5	3	610	CLA	CHD-C1D-ND	-2.20	122.43	124.45
5	1	612	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
4	3	607	CHL	C1C-C2C-C3C	-2.19	105.37	107.11
4	1	605	CHL	CAA-C2A-C3A	-2.19	106.77	112.78
5	4	602	CLA	C3B-C4B-NB	-2.19	108.48	110.52
4	4	607	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
5	2	610	CLA	C3B-C4B-NB	-2.19	108.49	110.52
5	3	610	CLA	C4A-NA-C1A	2.18	107.69	106.71
6	1	1620	LUT	C28-C29-C30	-2.18	115.59	118.94
5	3	603	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
8	1	1623	NEX	C11-C12-C13	-2.18	120.31	126.42
5	1	604	CLA	CHB-C4A-NA	2.17	127.52	124.51
7	4	622	XAT	C39-C29-C28	2.17	121.50	118.08
5	2	612	CLA	C2A-C1A-CHA	2.17	127.66	123.86
4	2	609	CHL	CHC-C4B-NB	-2.17	121.96	124.26
5	1	611	CLA	CHB-C4A-NA	2.17	127.51	124.51
6	2	1621	LUT	C35-C15-C14	-2.16	119.05	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	603	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
4	1	606	CHL	C2A-C1A-CHA	-2.16	120.08	123.86
4	3	607	CHL	OMC-CMC-C2C	-2.15	120.82	125.69
4	3	609	CHL	C4-C3-C5	2.15	118.89	115.27
6	1	1620	LUT	C8-C7-C6	-2.15	121.17	127.20
4	3	609	CHL	O1D-CGD-CBD	-2.15	120.09	124.48
5	2	603	CLA	C3C-C4C-NC	-2.15	108.16	110.57
4	3	607	CHL	CAA-C2A-C3A	-2.14	106.91	112.78
4	4	608	CHL	C1C-C2C-C3C	-2.14	105.41	107.11
4	2	606	CHL	O2D-CGD-O1D	-2.14	119.65	123.84
6	1	1621	LUT	C21-C26-C27	-2.14	110.00	112.70
4	4	608	CHL	O2A-CGA-CBA	2.13	120.89	114.03
4	2	607	CHL	CHB-C4A-NA	2.13	127.46	124.51
5	3	611	CLA	C2C-C1C-NC	2.13	111.97	109.97
5	2	613	CLA	CHC-C4B-NB	2.13	126.51	124.26
6	1	1620	LUT	C8-C9-C10	-2.13	115.67	118.94
5	4	610	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
5	3	612	CLA	CHA-C1A-NA	-2.13	121.53	126.40
6	2	1620	LUT	C19-C9-C8	2.13	121.43	118.08
6	1	1621	LUT	C15-C35-C34	-2.12	119.12	123.47
4	2	605	CHL	O2D-CGD-O1D	-2.12	119.69	123.84
5	1	610	CLA	CHC-C4B-NB	2.12	126.50	124.26
4	1	605	CHL	C2A-C1A-CHA	-2.12	120.16	123.86
4	2	607	CHL	C4-C3-C5	2.12	118.83	115.27
4	4	606	CHL	C4D-CHA-C1A	-2.11	118.68	121.25
5	1	614	CLA	CHD-C1D-ND	-2.11	122.51	124.45
5	2	611	CLA	CHC-C4B-NB	2.11	126.49	124.26
9	3	2630	LHG	C18-C17-C16	-2.11	103.72	114.42
6	3	1620	LUT	C8-C9-C10	-2.11	115.71	118.94
5	1	604	CLA	CHD-C1D-ND	-2.11	122.52	124.45
5	3	612	CLA	CMD-C2D-C3D	2.10	132.46	127.61
5	3	611	CLA	C2D-C1D-ND	-2.10	108.55	110.10
5	1	614	CLA	CHB-C1B-NB	2.10	126.48	124.26
5	2	611	CLA	O2D-CGD-CBD	2.10	115.00	111.27
10	4	623	BCR	C38-C26-C27	2.10	117.65	113.62
4	4	608	CHL	C2A-C1A-CHA	-2.10	120.19	123.86
4	3	605	CHL	O1D-CGD-CBD	-2.10	120.19	124.48
5	4	612	CLA	O2A-CGA-O1A	-2.10	118.07	123.30
6	4	620	LUT	C3-C4-C5	-2.10	107.68	111.85
5	1	604	CLA	CMB-C2B-C3B	2.10	131.66	126.59
4	3	601	CHL	C4D-C3D-CAD	2.09	110.56	108.10
4	3	606	CHL	O1D-CGD-CBD	-2.09	120.20	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	601	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
6	1	1620	LUT	C20-C13-C12	2.09	121.37	118.08
6	1	1620	LUT	C7-C8-C9	-2.09	123.08	126.23
4	2	601	CHL	CED-O2D-CGD	2.09	120.66	115.94
6	2	1621	LUT	C3-C4-C5	-2.09	107.69	111.85
5	3	613	CLA	CHD-C1D-ND	-2.09	122.53	124.45
4	4	609	CHL	O1D-CGD-CBD	-2.09	120.21	124.48
5	3	602	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
10	4	623	BCR	C35-C13-C14	-2.09	120.00	122.92
6	2	1620	LUT	C8-C7-C6	-2.08	121.35	127.20
8	1	1623	NEX	C10-C11-C12	-2.08	116.71	123.22
5	1	610	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
4	4	607	CHL	OMC-CMC-C2C	-2.08	120.97	125.69
5	1	604	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
6	4	620	LUT	C19-C9-C8	2.08	121.36	118.08
4	2	605	CHL	CAA-C2A-C3A	-2.08	107.08	112.78
6	1	1621	LUT	C31-C30-C29	-2.08	124.34	127.31
4	4	606	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
4	1	601	CHL	C4D-C3D-CAD	2.07	110.54	108.10
5	4	611	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
5	1	611	CLA	C3B-C4B-NB	-2.07	108.60	110.52
5	1	602	CLA	CHC-C4B-NB	2.07	126.45	124.26
4	3	601	CHL	O2D-CGD-O1D	-2.07	119.80	123.84
4	1	605	CHL	O2A-CGA-CBA	2.06	120.66	114.03
7	3	1622	XAT	O24-C25-C26	-2.06	57.25	58.96
7	2	1622	XAT	C39-C29-C30	-2.06	120.03	122.92
6	2	1621	LUT	C28-C29-C30	-2.06	115.78	118.94
5	3	614	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
5	1	604	CLA	C1-C2-C3	-2.06	123.42	126.75
5	2	602	CLA	CHB-C4A-NA	2.06	127.36	124.51
5	4	602	CLA	CHB-C1B-NB	2.05	126.43	124.26
5	2	602	CLA	CMB-C2B-C3B	2.05	131.56	126.59
6	3	1621	LUT	C30-C31-C32	-2.05	116.81	123.22
5	2	602	CLA	CHD-C1D-ND	-2.05	122.57	124.45
5	2	611	CLA	C3B-C4B-NB	-2.05	108.62	110.52
5	3	613	CLA	CHC-C4B-NB	2.04	126.42	124.26
4	3	605	CHL	OMC-CMC-C2C	-2.04	121.07	125.69
8	2	1623	NEX	C19-C9-C10	-2.04	120.06	122.92
5	1	602	CLA	CHB-C4A-NA	2.04	127.33	124.51
9	4	2630	LHG	C5-O7-C7	-2.04	114.10	117.90
6	1	1620	LUT	C11-C10-C9	-2.04	124.40	127.31
5	3	613	CLA	O2A-C1-C2	-2.04	103.28	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	1623	NEX	O24-C25-C26	-2.04	57.27	58.96
5	4	610	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
4	2	607	CHL	O2D-CGD-O1D	-2.04	119.86	123.84
5	4	612	CLA	CHA-C1A-NA	-2.03	121.74	126.40
7	2	1622	XAT	C24-C23-C22	-2.03	106.85	110.77
10	4	623	BCR	C2-C1-C6	2.03	113.61	110.48
5	1	614	CLA	C3B-C4B-NB	-2.03	108.63	110.52
9	3	2630	LHG	C27-C26-C25	-2.03	104.12	114.42
6	3	1621	LUT	C8-C7-C6	-2.03	121.50	127.20
6	1	1620	LUT	C38-C25-C24	-2.03	119.22	123.56
5	4	603	CLA	C2A-C1A-CHA	2.03	127.40	123.86
7	4	622	XAT	C15-C35-C34	-2.02	119.33	123.47
4	3	609	CHL	C2A-C1A-CHA	-2.02	120.32	123.86
5	2	604	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
7	3	1622	XAT	C38-C25-C24	2.02	116.55	114.28
4	4	606	CHL	O2A-CGA-O1A	-2.02	118.27	123.30
5	3	602	CLA	CMB-C2B-C3B	2.02	131.47	126.59
5	3	612	CLA	CMD-C2D-C1D	-2.02	121.16	124.71
4	3	605	CHL	C4D-CHA-C1A	-2.02	118.80	121.25
5	2	614	CLA	CHD-C1D-ND	-2.02	122.60	124.45
4	3	601	CHL	CGD-CBD-CAD	-2.02	104.21	110.73
5	3	604	CLA	CMB-C2B-C3B	2.01	131.47	126.59
7	4	622	XAT	O4-C5-C6	-2.01	57.29	58.96
4	3	606	CHL	CMB-C2B-C1B	2.01	128.44	125.37
5	2	610	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
5	3	611	CLA	CAA-C2A-C1A	2.01	118.56	111.97
4	1	608	CHL	CHB-C4A-NA	2.01	127.29	124.51
6	1	1620	LUT	C21-C26-C27	-2.01	110.16	112.70
7	1	1622	XAT	O24-C25-C26	-2.01	57.30	58.96
4	2	605	CHL	C4D-CHA-C1A	-2.00	118.81	121.25
8	2	1623	NEX	O24-C25-C26	-2.00	57.30	58.96
5	1	602	CLA	CHA-C1A-NA	-2.00	121.81	126.40
4	2	606	CHL	C2A-C1A-CHA	-2.00	120.36	123.86

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	1	607	CHL	C8
4	1	609	CHL	C8
4	2	607	CHL	C8
4	2	609	CHL	C8
4	3	601	CHL	C8

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Mol	Chain	Res	Type	Atom
4	3	609	CHL	C8

All (630) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	1	601	CHL	C1C-C2C-CMC-OMC
4	1	601	CHL	C3C-C2C-CMC-OMC
4	1	601	CHL	CHA-CBD-CGD-O1D
4	1	601	CHL	CHA-CBD-CGD-O2D
4	1	605	CHL	C1C-C2C-CMC-OMC
4	1	605	CHL	C3C-C2C-CMC-OMC
4	1	606	CHL	C2B-C3B-CAB-CBB
4	1	606	CHL	C4B-C3B-CAB-CBB
4	1	606	CHL	C1C-C2C-CMC-OMC
4	1	607	CHL	C1C-C2C-CMC-OMC
4	1	607	CHL	C3C-C2C-CMC-OMC
4	1	608	CHL	C1A-C2A-CAA-CBA
4	1	608	CHL	C1C-C2C-CMC-OMC
4	1	608	CHL	C3C-C2C-CMC-OMC
4	1	608	CHL	CBD-CGD-O2D-CED
4	1	609	CHL	C1C-C2C-CMC-OMC
4	1	609	CHL	C3C-C2C-CMC-OMC
4	2	601	CHL	C1A-C2A-CAA-CBA
4	2	601	CHL	CHA-CBD-CGD-O1D
4	2	601	CHL	CHA-CBD-CGD-O2D
4	2	605	CHL	C3C-C2C-CMC-OMC
4	2	607	CHL	C1C-C2C-CMC-OMC
4	2	607	CHL	C3C-C2C-CMC-OMC
4	2	608	CHL	C3C-C2C-CMC-OMC
4	2	608	CHL	CBD-CGD-O2D-CED
4	2	609	CHL	C1C-C2C-CMC-OMC
4	2	609	CHL	C3C-C2C-CMC-OMC
4	3	605	CHL	C1C-C2C-CMC-OMC
4	3	605	CHL	C3C-C2C-CMC-OMC
4	3	606	CHL	C1C-C2C-CMC-OMC
4	3	606	CHL	C3C-C2C-CMC-OMC
4	3	607	CHL	C1C-C2C-CMC-OMC
4	3	607	CHL	C3C-C2C-CMC-OMC
4	3	608	CHL	CBD-CGD-O2D-CED
4	3	609	CHL	C1C-C2C-CMC-OMC
4	3	609	CHL	C3C-C2C-CMC-OMC
4	4	601	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
4	4	601	CHL	C3C-C2C-CMC-OMC
4	4	606	CHL	C1A-C2A-CAA-CBA
4	4	606	CHL	C1C-C2C-CMC-OMC
4	4	606	CHL	C3C-C2C-CMC-OMC
4	4	607	CHL	C1C-C2C-CMC-OMC
4	4	607	CHL	C3C-C2C-CMC-OMC
4	4	608	CHL	C2B-C3B-CAB-CBB
4	4	608	CHL	C4B-C3B-CAB-CBB
4	4	608	CHL	C1C-C2C-CMC-OMC
4	4	608	CHL	C3C-C2C-CMC-OMC
4	4	608	CHL	CBD-CGD-O2D-CED
4	4	609	CHL	C1C-C2C-CMC-OMC
4	4	609	CHL	C3C-C2C-CMC-OMC
5	1	603	CLA	CHA-CBD-CGD-O1D
5	1	603	CLA	CBD-CGD-O2D-CED
5	1	604	CLA	CHA-CBD-CGD-O1D
5	1	604	CLA	CHA-CBD-CGD-O2D
5	1	604	CLA	CAD-CBD-CGD-O1D
5	1	604	CLA	CAD-CBD-CGD-O2D
5	1	610	CLA	C2B-C3B-CAB-CBB
5	1	610	CLA	C4B-C3B-CAB-CBB
5	1	611	CLA	C2A-CAA-CBA-CGA
5	1	611	CLA	C2B-C3B-CAB-CBB
5	1	611	CLA	C4B-C3B-CAB-CBB
5	1	612	CLA	C2B-C3B-CAB-CBB
5	1	612	CLA	C4B-C3B-CAB-CBB
5	2	603	CLA	C2B-C3B-CAB-CBB
5	2	603	CLA	C4B-C3B-CAB-CBB
5	2	603	CLA	CBD-CGD-O2D-CED
5	2	604	CLA	C1A-C2A-CAA-CBA
5	2	604	CLA	CBD-CGD-O2D-CED
5	2	610	CLA	C4B-C3B-CAB-CBB
5	2	611	CLA	C2B-C3B-CAB-CBB
5	2	611	CLA	C4B-C3B-CAB-CBB
5	2	613	CLA	CHA-CBD-CGD-O1D
5	2	613	CLA	CHA-CBD-CGD-O2D
5	2	614	CLA	C1A-C2A-CAA-CBA
5	2	614	CLA	C3A-C2A-CAA-CBA
5	2	614	CLA	CBD-CGD-O2D-CED
5	3	603	CLA	CHA-CBD-CGD-O1D
5	3	603	CLA	CHA-CBD-CGD-O2D
5	3	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
5	3	604	CLA	CHA-CBD-CGD-O1D
5	3	610	CLA	C2B-C3B-CAB-CBB
5	3	610	CLA	C4B-C3B-CAB-CBB
5	3	611	CLA	C1A-C2A-CAA-CBA
5	3	611	CLA	C2B-C3B-CAB-CBB
5	3	611	CLA	C4B-C3B-CAB-CBB
5	3	612	CLA	C2B-C3B-CAB-CBB
5	3	612	CLA	C4B-C3B-CAB-CBB
5	3	612	CLA	CHA-CBD-CGD-O1D
5	3	612	CLA	CHA-CBD-CGD-O2D
5	3	612	CLA	CAD-CBD-CGD-O1D
5	3	613	CLA	CHA-CBD-CGD-O1D
5	3	613	CLA	CHA-CBD-CGD-O2D
5	3	613	CLA	CBD-CGD-O2D-CED
5	3	614	CLA	CHA-CBD-CGD-O1D
5	3	614	CLA	CHA-CBD-CGD-O2D
5	4	602	CLA	CBD-CGD-O2D-CED
5	4	603	CLA	C2B-C3B-CAB-CBB
5	4	603	CLA	C4B-C3B-CAB-CBB
5	4	603	CLA	CBD-CGD-O2D-CED
5	4	604	CLA	C2A-CAA-CBA-CGA
5	4	604	CLA	CHA-CBD-CGD-O1D
5	4	604	CLA	CHA-CBD-CGD-O2D
5	4	604	CLA	CBD-CGD-O2D-CED
5	4	610	CLA	C2B-C3B-CAB-CBB
5	4	610	CLA	C4B-C3B-CAB-CBB
5	4	611	CLA	C2B-C3B-CAB-CBB
5	4	611	CLA	C4B-C3B-CAB-CBB
5	4	612	CLA	C2B-C3B-CAB-CBB
5	4	612	CLA	C4B-C3B-CAB-CBB
6	1	1620	LUT	C1-C6-C7-C8
6	2	1620	LUT	C1-C6-C7-C8
7	1	1622	XAT	C31-C32-C33-C34
7	1	1622	XAT	C31-C32-C33-C40
7	2	1622	XAT	O4-C6-C7-C8
7	2	1622	XAT	C31-C32-C33-C34
7	2	1622	XAT	C31-C32-C33-C40
8	1	1623	NEX	C11-C12-C13-C14
8	1	1623	NEX	C11-C12-C13-C20
9	1	2630	LHG	C4-O6-P-O5
9	1	2630	LHG	O7-C5-C6-O8
9	2	2630	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
9	3	2630	LHG	C4-O6-P-O3
9	3	2630	LHG	C4-O6-P-O4
9	3	2630	LHG	C4-O6-P-O5
9	4	2630	LHG	C3-O3-P-O5
10	4	623	BCR	C7-C8-C9-C10
10	4	623	BCR	C7-C8-C9-C34
10	4	623	BCR	C21-C22-C23-C24
10	4	623	BCR	C37-C22-C23-C24
5	2	612	CLA	O1D-CGD-O2D-CED
5	2	613	CLA	O1D-CGD-O2D-CED
5	1	614	CLA	O1D-CGD-O2D-CED
5	4	604	CLA	O1D-CGD-O2D-CED
4	2	605	CHL	CBD-CGD-O2D-CED
5	1	614	CLA	CBD-CGD-O2D-CED
5	2	612	CLA	CBD-CGD-O2D-CED
5	2	613	CLA	CBD-CGD-O2D-CED
5	3	603	CLA	CBD-CGD-O2D-CED
5	3	614	CLA	CBD-CGD-O2D-CED
5	4	611	CLA	CBD-CGD-O2D-CED
5	4	612	CLA	CBD-CGD-O2D-CED
5	3	603	CLA	O1D-CGD-O2D-CED
5	4	611	CLA	O1D-CGD-O2D-CED
4	2	608	CHL	O1D-CGD-O2D-CED
4	3	608	CHL	O1D-CGD-O2D-CED
5	1	603	CLA	O1D-CGD-O2D-CED
5	2	603	CLA	O1D-CGD-O2D-CED
5	2	614	CLA	O1D-CGD-O2D-CED
5	3	613	CLA	O1D-CGD-O2D-CED
5	4	603	CLA	O1D-CGD-O2D-CED
4	1	606	CHL	CBD-CGD-O2D-CED
5	1	602	CLA	CBD-CGD-O2D-CED
5	2	602	CLA	CBD-CGD-O2D-CED
5	2	610	CLA	CBD-CGD-O2D-CED
5	3	612	CLA	CBD-CGD-O2D-CED
5	3	603	CLA	O1A-CGA-O2A-C1
4	4	608	CHL	O1D-CGD-O2D-CED
5	2	604	CLA	O1D-CGD-O2D-CED
4	1	608	CHL	O1D-CGD-O2D-CED
5	4	602	CLA	O1D-CGD-O2D-CED
5	1	604	CLA	CBD-CGD-O2D-CED
4	2	607	CHL	C3-C5-C6-C7
5	3	611	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	1	603	CLA	CBA-CGA-O2A-C1
5	3	603	CLA	CBA-CGA-O2A-C1
5	3	604	CLA	CBD-CGD-O2D-CED
4	3	605	CHL	C2A-CAA-CBA-CGA
5	2	604	CLA	C2A-CAA-CBA-CGA
5	3	603	CLA	C2A-CAA-CBA-CGA
5	1	613	CLA	C3-C5-C6-C7
5	2	602	CLA	C3-C5-C6-C7
5	2	603	CLA	CBA-CGA-O2A-C1
9	4	2630	LHG	C24-C23-O8-C6
5	4	612	CLA	O1D-CGD-O2D-CED
5	2	603	CLA	O1A-CGA-O2A-C1
4	2	605	CHL	O1D-CGD-O2D-CED
4	3	605	CHL	CBD-CGD-O2D-CED
5	3	602	CLA	CBD-CGD-O2D-CED
5	1	603	CLA	O1A-CGA-O2A-C1
9	3	2630	LHG	O10-C23-O8-C6
4	3	609	CHL	CBD-CGD-O2D-CED
5	3	614	CLA	O1D-CGD-O2D-CED
4	3	606	CHL	CBD-CGD-O2D-CED
9	4	2630	LHG	O10-C23-O8-C6
4	1	606	CHL	C2A-CAA-CBA-CGA
5	3	611	CLA	C2A-CAA-CBA-CGA
5	2	610	CLA	O1D-CGD-O2D-CED
4	3	601	CHL	C3-C5-C6-C7
5	3	612	CLA	O1D-CGD-O2D-CED
5	3	613	CLA	CBA-CGA-O2A-C1
9	3	2630	LHG	C24-C23-O8-C6
5	3	614	CLA	O2A-C1-C2-C3
9	3	2630	LHG	O7-C5-C6-O8
4	1	607	CHL	C11-C10-C8-C9
4	3	601	CHL	C6-C7-C8-C9
4	3	601	CHL	C14-C13-C15-C16
4	2	605	CHL	C2A-CAA-CBA-CGA
4	2	607	CHL	C2A-CAA-CBA-CGA
6	4	620	LUT	C27-C28-C29-C39
7	3	1622	XAT	C31-C32-C33-C40
8	2	1623	NEX	C31-C32-C33-C40
4	3	601	CHL	C5-C6-C7-C8
4	3	601	CHL	C10-C11-C12-C13
4	1	606	CHL	O1D-CGD-O2D-CED
5	1	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
4	1	609	CHL	C8-C10-C11-C12
4	3	601	CHL	C8-C10-C11-C12
5	2	602	CLA	O1D-CGD-O2D-CED
9	2	2630	LHG	O1-C1-C2-O2
9	1	2630	LHG	C23-C24-C25-C26
4	3	609	CHL	C10-C11-C12-C13
5	3	602	CLA	C10-C11-C12-C13
5	1	612	CLA	CBD-CGD-O2D-CED
4	1	607	CHL	C13-C15-C16-C17
5	3	613	CLA	C6-C7-C8-C10
5	3	613	CLA	O1A-CGA-O2A-C1
4	1	607	CHL	C2A-CAA-CBA-CGA
4	2	609	CHL	C8-C10-C11-C12
4	3	601	CHL	C13-C15-C16-C17
4	2	607	CHL	C5-C6-C7-C8
9	4	2630	LHG	C3-O3-P-O6
5	1	604	CLA	O1D-CGD-O2D-CED
5	3	614	CLA	CBA-CGA-O2A-C1
9	1	2630	LHG	C24-C23-O8-C6
9	2	2630	LHG	C23-C24-C25-C26
5	3	604	CLA	O1D-CGD-O2D-CED
4	2	607	CHL	C8-C10-C11-C12
5	1	613	CLA	C6-C7-C8-C10
4	1	607	CHL	CBD-CGD-O2D-CED
9	1	2630	LHG	C12-C13-C14-C15
9	2	2630	LHG	C7-C8-C9-C10
9	3	2630	LHG	C27-C28-C29-C30
5	1	603	CLA	C5-C6-C7-C8
4	2	609	CHL	C11-C12-C13-C15
4	3	601	CHL	C4-C3-C5-C6
9	3	2630	LHG	C31-C32-C33-C34
4	3	601	CHL	C2-C3-C5-C6
4	3	607	CHL	C2A-CAA-CBA-CGA
4	3	608	CHL	C2A-CAA-CBA-CGA
7	4	622	XAT	C27-C28-C29-C39
9	2	2630	LHG	O1-C1-C2-C3
9	4	2630	LHG	O1-C1-C2-C3
7	3	1622	XAT	C31-C32-C33-C34
5	1	603	CLA	C3-C5-C6-C7
9	3	2630	LHG	C28-C29-C30-C31
9	1	2630	LHG	C7-C8-C9-C10
5	3	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	2	2630	LHG	C24-C25-C26-C27
9	3	2630	LHG	C15-C16-C17-C18
4	1	607	CHL	C4B-C3B-CAB-CBB
5	1	614	CLA	C4B-C3B-CAB-CBB
5	3	603	CLA	C4B-C3B-CAB-CBB
5	3	614	CLA	O1A-CGA-O2A-C1
4	3	605	CHL	O1D-CGD-O2D-CED
4	1	605	CHL	C3A-C2A-CAA-CBA
4	1	607	CHL	C3A-C2A-CAA-CBA
4	2	601	CHL	C3A-C2A-CAA-CBA
4	2	605	CHL	C3A-C2A-CAA-CBA
4	3	605	CHL	C3A-C2A-CAA-CBA
4	3	606	CHL	C3A-C2A-CAA-CBA
4	4	606	CHL	C3A-C2A-CAA-CBA
5	1	611	CLA	C3A-C2A-CAA-CBA
5	3	611	CLA	C3A-C2A-CAA-CBA
5	2	602	CLA	C10-C11-C12-C13
9	2	2630	LHG	C12-C13-C14-C15
4	2	609	CHL	CBA-CGA-O2A-C1
4	3	601	CHL	C2A-CAA-CBA-CGA
4	2	609	CHL	C11-C12-C13-C14
4	1	607	CHL	C2B-C3B-CAB-CBB
5	1	614	CLA	C2B-C3B-CAB-CBB
5	2	610	CLA	C2B-C3B-CAB-CBB
5	2	613	CLA	C2B-C3B-CAB-CBB
5	3	603	CLA	C2B-C3B-CAB-CBB
4	1	607	CHL	C5-C6-C7-C8
9	1	2630	LHG	C11-C12-C13-C14
6	1	1620	LUT	C5-C6-C7-C8
6	2	1620	LUT	C5-C6-C7-C8
6	3	1620	LUT	C1-C6-C7-C8
6	3	1620	LUT	C5-C6-C7-C8
5	3	610	CLA	C10-C11-C12-C13
4	1	607	CHL	C8-C10-C11-C12
4	2	607	CHL	C4-C3-C5-C6
4	3	606	CHL	O1D-CGD-O2D-CED
4	3	601	CHL	C6-C7-C8-C10
4	1	609	CHL	C3-C5-C6-C7
5	3	602	CLA	C8-C10-C11-C12
9	3	2630	LHG	C30-C31-C32-C33
4	2	606	CHL	C2A-CAA-CBA-CGA
5	1	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
5	3	602	CLA	C2A-CAA-CBA-CGA
5	3	613	CLA	C2A-CAA-CBA-CGA
5	4	602	CLA	C2A-CAA-CBA-CGA
4	1	609	CHL	C2C-C3C-CAC-CBC
4	2	609	CHL	O1A-CGA-O2A-C1
9	2	2630	LHG	C8-C7-O7-C5
5	1	613	CLA	C6-C7-C8-C9
5	2	602	CLA	C4-C3-C5-C6
4	2	607	CHL	C2-C3-C5-C6
5	1	602	CLA	C6-C7-C8-C9
5	3	613	CLA	C6-C7-C8-C9
4	3	609	CHL	O1D-CGD-O2D-CED
4	3	606	CHL	C2A-CAA-CBA-CGA
4	1	605	CHL	C1A-C2A-CAA-CBA
4	2	605	CHL	C1A-C2A-CAA-CBA
4	2	608	CHL	C1A-C2A-CAA-CBA
4	3	605	CHL	C1A-C2A-CAA-CBA
4	3	606	CHL	C1A-C2A-CAA-CBA
4	4	607	CHL	C1A-C2A-CAA-CBA
4	4	608	CHL	C1A-C2A-CAA-CBA
5	1	602	CLA	C1A-C2A-CAA-CBA
5	1	604	CLA	C1A-C2A-CAA-CBA
5	1	610	CLA	C1A-C2A-CAA-CBA
5	1	611	CLA	C1A-C2A-CAA-CBA
5	3	604	CLA	C1A-C2A-CAA-CBA
5	3	614	CLA	C1A-C2A-CAA-CBA
5	4	604	CLA	C1A-C2A-CAA-CBA
5	4	610	CLA	C1A-C2A-CAA-CBA
9	1	2630	LHG	O9-C7-O7-C5
9	3	2630	LHG	C3-O3-P-O6
9	3	2630	LHG	C24-C25-C26-C27
9	3	2630	LHG	C13-C14-C15-C16
4	1	609	CHL	C10-C11-C12-C13
4	1	609	CHL	CBA-CGA-O2A-C1
4	1	607	CHL	C2C-C3C-CAC-CBC
5	2	613	CLA	C2A-CAA-CBA-CGA
9	3	2630	LHG	C35-C36-C37-C38
9	3	2630	LHG	C10-C11-C12-C13
4	3	609	CHL	C8-C10-C11-C12
4	1	607	CHL	C4-C3-C5-C6
4	1	609	CHL	C4-C3-C5-C6
5	1	603	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	1	2630	LHG	C27-C28-C29-C30
4	3	609	CHL	CBA-CGA-O2A-C1
9	3	2630	LHG	C29-C30-C31-C32
5	1	612	CLA	O1D-CGD-O2D-CED
9	3	2630	LHG	C17-C18-C19-C20
5	2	603	CLA	C4-C3-C5-C6
4	1	607	CHL	C6-C7-C8-C10
4	3	601	CHL	C11-C10-C8-C7
4	3	601	CHL	C12-C13-C15-C16
5	1	602	CLA	C6-C7-C8-C10
5	2	602	CLA	C11-C12-C13-C15
5	2	603	CLA	C2-C3-C5-C6
4	1	607	CHL	C6-C7-C8-C9
4	3	601	CHL	C11-C10-C8-C9
5	3	602	CLA	C6-C7-C8-C9
5	1	602	CLA	C4B-C3B-CAB-CBB
5	1	603	CLA	C4B-C3B-CAB-CBB
5	1	604	CLA	C4B-C3B-CAB-CBB
5	2	613	CLA	C4B-C3B-CAB-CBB
5	2	614	CLA	C4B-C3B-CAB-CBB
5	4	602	CLA	C4B-C3B-CAB-CBB
5	4	604	CLA	C4B-C3B-CAB-CBB
4	1	607	CHL	C2-C3-C5-C6
4	1	609	CHL	C2-C3-C5-C6
5	1	603	CLA	C2-C3-C5-C6
4	1	609	CHL	O1A-CGA-O2A-C1
4	4	601	CHL	C3A-C2A-CAA-CBA
5	2	604	CLA	C3A-C2A-CAA-CBA
6	1	1621	LUT	C29-C30-C31-C32
6	2	1621	LUT	C29-C30-C31-C32
9	1	2630	LHG	C18-C19-C20-C21
5	1	602	CLA	C10-C11-C12-C13
9	3	2630	LHG	C4-C5-C6-O8
4	3	609	CHL	O1A-CGA-O2A-C1
4	1	606	CHL	C3C-C2C-CMC-OMC
4	2	606	CHL	C3C-C2C-CMC-OMC
4	3	608	CHL	C2B-C3B-CAB-CBB
5	1	602	CLA	C2B-C3B-CAB-CBB
5	2	614	CLA	C2B-C3B-CAB-CBB
9	4	2630	LHG	O7-C5-C6-O8
9	2	2630	LHG	O9-C7-O7-C5
4	2	609	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
5	3	610	CLA	C2-C1-O2A-CGA
9	1	2630	LHG	C24-C25-C26-C27
4	2	607	CHL	C6-C7-C8-C9
4	3	601	CHL	C15-C16-C17-C18
6	1	1621	LUT	C5-C6-C7-C8
6	3	1621	LUT	C1-C6-C7-C8
6	3	1621	LUT	C5-C6-C7-C8
10	4	623	BCR	C5-C6-C7-C8
4	1	609	CHL	C5-C6-C7-C8
5	1	602	CLA	C8-C10-C11-C12
6	4	620	LUT	C27-C28-C29-C30
8	2	1623	NEX	C31-C32-C33-C34
4	1	609	CHL	C14-C13-C15-C16
4	2	607	CHL	C6-C7-C8-C10
5	3	602	CLA	C6-C7-C8-C10
6	3	1621	LUT	C29-C30-C31-C32
8	1	1623	NEX	C29-C30-C31-C32
10	4	623	BCR	C19-C20-C21-C22
9	1	2630	LHG	C8-C7-O7-C5
9	3	2630	LHG	C26-C27-C28-C29
4	1	606	CHL	CAD-CBD-CGD-O2D
5	1	602	CLA	CAD-CBD-CGD-O2D
5	1	610	CLA	CAD-CBD-CGD-O2D
5	3	612	CLA	CAD-CBD-CGD-O2D
9	3	2630	LHG	O9-C7-O7-C5
9	1	2630	LHG	C4-C5-C6-O8
5	3	611	CLA	C5-C6-C7-C8
5	3	610	CLA	C11-C12-C13-C14
5	1	603	CLA	CHA-CBD-CGD-O2D
5	2	603	CLA	CHA-CBD-CGD-O1D
5	2	603	CLA	CHA-CBD-CGD-O2D
5	3	604	CLA	CHA-CBD-CGD-O2D
4	4	606	CHL	O1D-CGD-O2D-CED
4	3	609	CHL	C2C-C3C-CAC-CBC
4	1	607	CHL	C1A-C2A-CAA-CBA
4	1	609	CHL	C1A-C2A-CAA-CBA
4	3	609	CHL	C1A-C2A-CAA-CBA
4	4	601	CHL	C1A-C2A-CAA-CBA
4	4	601	CHL	CHA-CBD-CGD-O2D
5	2	602	CLA	C1A-C2A-CAA-CBA
5	2	610	CLA	C1A-C2A-CAA-CBA
9	2	2630	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
9	1	2630	LHG	O10-C23-O8-C6
4	1	605	CHL	C4B-C3B-CAB-CBB
4	1	609	CHL	C4B-C3B-CAB-CBB
4	2	605	CHL	C4B-C3B-CAB-CBB
4	2	607	CHL	C4B-C3B-CAB-CBB
4	2	609	CHL	C4B-C3B-CAB-CBB
4	3	605	CHL	C4B-C3B-CAB-CBB
4	3	608	CHL	C4B-C3B-CAB-CBB
4	4	601	CHL	C4B-C3B-CAB-CBB
4	4	607	CHL	C4B-C3B-CAB-CBB
4	4	609	CHL	C4B-C3B-CAB-CBB
5	3	614	CLA	C4B-C3B-CAB-CBB
9	3	2630	LHG	C3-O3-P-O5
5	1	603	CLA	CAD-CBD-CGD-O1D
5	2	603	CLA	CAD-CBD-CGD-O1D
5	3	603	CLA	CAD-CBD-CGD-O1D
5	3	604	CLA	CAD-CBD-CGD-O1D
5	3	614	CLA	CAD-CBD-CGD-O1D
4	4	606	CHL	CBD-CGD-O2D-CED
4	1	607	CHL	C11-C10-C8-C7
4	1	607	CHL	C4C-C3C-CAC-CBC
5	1	603	CLA	C2A-CAA-CBA-CGA
5	2	602	CLA	C2A-CAA-CBA-CGA
4	2	605	CHL	C1C-C2C-CMC-OMC
4	2	608	CHL	C1C-C2C-CMC-OMC
4	1	609	CHL	C4C-C3C-CAC-CBC
5	2	602	CLA	C2-C3-C5-C6
10	4	623	BCR	C36-C18-C19-C20
5	3	610	CLA	C11-C12-C13-C15
4	1	609	CHL	C2B-C3B-CAB-CBB
4	2	607	CHL	C2B-C3B-CAB-CBB
4	4	609	CHL	C2B-C3B-CAB-CBB
5	1	603	CLA	C2B-C3B-CAB-CBB
5	1	604	CLA	C2B-C3B-CAB-CBB
5	1	613	CLA	C2B-C3B-CAB-CBB
5	2	604	CLA	C2B-C3B-CAB-CBB
5	3	602	CLA	C2B-C3B-CAB-CBB
5	3	604	CLA	C2B-C3B-CAB-CBB
5	3	613	CLA	C2B-C3B-CAB-CBB
5	4	602	CLA	C2B-C3B-CAB-CBB
5	4	604	CLA	C2B-C3B-CAB-CBB
5	4	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
5	4	612	CLA	C2A-CAA-CBA-CGA
4	1	609	CHL	C2-C1-O2A-CGA
9	2	2630	LHG	C5-C4-O6-P
5	1	604	CLA	CBA-CGA-O2A-C1
5	3	611	CLA	CBA-CGA-O2A-C1
6	1	1621	LUT	C1-C6-C7-C8
6	2	1621	LUT	C1-C6-C7-C8
10	4	623	BCR	C1-C6-C7-C8
4	1	605	CHL	O1D-CGD-O2D-CED
9	2	2630	LHG	C3-O3-P-O6
4	1	607	CHL	O1D-CGD-O2D-CED
5	2	602	CLA	C11-C12-C13-C14
5	1	604	CLA	O1A-CGA-O2A-C1
6	4	620	LUT	C7-C8-C9-C19
8	3	1623	NEX	C11-C12-C13-C20
9	3	2630	LHG	C5-C4-O6-P
5	1	610	CLA	C5-C6-C7-C8
4	4	607	CHL	O1D-CGD-O2D-CED
4	1	609	CHL	C12-C13-C15-C16
5	1	610	CLA	C11-C10-C8-C7
9	4	2630	LHG	O1-C1-C2-O2
5	1	613	CLA	C4B-C3B-CAB-CBB
5	2	604	CLA	C4B-C3B-CAB-CBB
5	3	602	CLA	C4B-C3B-CAB-CBB
5	3	604	CLA	C4B-C3B-CAB-CBB
8	1	1623	NEX	C33-C34-C35-C15
5	3	602	CLA	C4-C3-C5-C6
5	3	611	CLA	O1A-CGA-O2A-C1
5	1	613	CLA	C2A-CAA-CBA-CGA
8	1	1623	NEX	C39-C29-C30-C31
8	2	1623	NEX	C39-C29-C30-C31
8	3	1623	NEX	C39-C29-C30-C31
9	2	2630	LHG	C4-C5-C6-O8
5	3	604	CLA	CAA-CBA-CGA-O2A
5	4	603	CLA	CAA-CBA-CGA-O2A
4	1	608	CHL	C2A-CAA-CBA-CGA
5	4	603	CLA	CAA-CBA-CGA-O1A
4	2	607	CHL	C1A-C2A-CAA-CBA
5	3	602	CLA	C1A-C2A-CAA-CBA
5	3	610	CLA	C1A-C2A-CAA-CBA
5	3	604	CLA	CAA-CBA-CGA-O1A
5	4	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
4	2	609	CHL	C4-C3-C5-C6
4	3	609	CHL	C4-C3-C5-C6
4	1	605	CHL	C2B-C3B-CAB-CBB
4	2	605	CHL	C2B-C3B-CAB-CBB
4	2	609	CHL	C2B-C3B-CAB-CBB
4	3	605	CHL	C2B-C3B-CAB-CBB
4	3	609	CHL	C2B-C3B-CAB-CBB
4	4	601	CHL	C2B-C3B-CAB-CBB
4	4	607	CHL	C2B-C3B-CAB-CBB
5	3	614	CLA	C2B-C3B-CAB-CBB
4	2	605	CHL	CAA-CBA-CGA-O2A
8	1	1623	NEX	C28-C29-C30-C31
8	2	1623	NEX	C28-C29-C30-C31
8	3	1623	NEX	C28-C29-C30-C31
4	4	606	CHL	CAA-CBA-CGA-O1A
4	4	606	CHL	CAA-CBA-CGA-O2A
4	4	607	CHL	CAA-CBA-CGA-O2A
8	2	1623	NEX	C13-C14-C15-C35
5	1	604	CLA	C2-C1-O2A-CGA
4	3	607	CHL	C2C-C3C-CAC-CBC
5	4	602	CLA	CAA-CBA-CGA-O2A
4	4	601	CHL	CAA-CBA-CGA-O2A
6	2	1621	LUT	C5-C6-C7-C8
4	2	601	CHL	CAA-CBA-CGA-O1A
4	2	605	CHL	CAA-CBA-CGA-O1A
6	4	620	LUT	C7-C8-C9-C10
7	4	622	XAT	C27-C28-C29-C30
4	4	607	CHL	CAA-CBA-CGA-O1A
4	4	609	CHL	CAA-CBA-CGA-O1A
4	3	609	CHL	C4C-C3C-CAC-CBC
5	1	610	CLA	C11-C10-C8-C9
4	4	601	CHL	CAA-CBA-CGA-O1A
5	4	602	CLA	CAA-CBA-CGA-O1A
4	4	607	CHL	C2A-CAA-CBA-CGA
9	1	2630	LHG	C13-C14-C15-C16
4	3	605	CHL	CAA-CBA-CGA-O1A
5	4	612	CLA	CAA-CBA-CGA-O1A
5	3	613	CLA	C4B-C3B-CAB-CBB
5	4	611	CLA	CAA-CBA-CGA-O2A
5	4	612	CLA	CAA-CBA-CGA-O2A
9	2	2630	LHG	O7-C5-C6-O8
4	2	608	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
4	3	605	CHL	CAA-CBA-CGA-O2A
5	1	602	CLA	C4-C3-C5-C6
5	3	603	CLA	C4-C3-C5-C6
5	1	611	CLA	CAA-CBA-CGA-O2A
4	3	609	CHL	C2-C3-C5-C6
5	2	604	CLA	CAA-CBA-CGA-O1A
4	1	608	CHL	C3A-C2A-CAA-CBA
4	2	607	CHL	C3A-C2A-CAA-CBA
5	3	603	CLA	C3A-C2A-CAA-CBA
4	1	601	CHL	CAA-CBA-CGA-O2A
4	2	606	CHL	CAA-CBA-CGA-O2A
5	2	611	CLA	CAA-CBA-CGA-O2A
5	2	612	CLA	CAA-CBA-CGA-O2A
4	1	605	CHL	CAD-CBD-CGD-O2D
5	2	604	CLA	CAD-CBD-CGD-O2D
5	2	610	CLA	CAD-CBD-CGD-O2D
5	2	614	CLA	CAD-CBD-CGD-O2D
5	4	604	CLA	CAA-CBA-CGA-O2A
9	3	2630	LHG	O8-C23-C24-C25
4	2	609	CHL	C2-C3-C5-C6
8	3	1623	NEX	C11-C12-C13-C14
8	2	1623	NEX	O24-C26-C27-C28
4	1	606	CHL	CAA-CBA-CGA-O1A
4	2	608	CHL	CAA-CBA-CGA-O1A
4	3	601	CHL	O2A-C1-C2-C3
4	3	607	CHL	O2A-C1-C2-C3
4	1	607	CHL	CAA-CBA-CGA-O2A
4	1	606	CHL	CAA-CBA-CGA-O2A
5	2	611	CLA	CAA-CBA-CGA-O1A
5	2	612	CLA	CAA-CBA-CGA-O1A
5	4	611	CLA	CAA-CBA-CGA-O1A
4	2	606	CHL	CHA-CBD-CGD-O1D
4	2	606	CHL	CHA-CBD-CGD-O2D
5	1	613	CLA	CHA-CBD-CGD-O1D
5	1	613	CLA	CHA-CBD-CGD-O2D
5	2	602	CLA	CHA-CBD-CGD-O2D
5	2	612	CLA	CHA-CBD-CGD-O2D
5	3	602	CLA	CHA-CBD-CGD-O1D
5	3	602	CLA	CHA-CBD-CGD-O2D
5	4	602	CLA	CHA-CBD-CGD-O1D
5	4	602	CLA	CHA-CBD-CGD-O2D
4	1	601	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
4	1	605	CHL	CAA-CBA-CGA-O2A
4	2	606	CHL	CAA-CBA-CGA-O1A
5	2	604	CLA	CAA-CBA-CGA-O2A
5	4	604	CLA	CAA-CBA-CGA-O1A
5	3	610	CLA	C3-C5-C6-C7
5	1	602	CLA	CAA-CBA-CGA-O2A
5	1	613	CLA	CAA-CBA-CGA-O2A
5	2	603	CLA	CAA-CBA-CGA-O2A
4	3	601	CHL	CAA-CBA-CGA-O2A
5	3	610	CLA	C2A-CAA-CBA-CGA
4	3	606	CHL	CAA-CBA-CGA-O2A
5	3	612	CLA	CAA-CBA-CGA-O2A
4	4	607	CHL	CBD-CGD-O2D-CED
4	3	607	CHL	C2-C3-C5-C6
8	2	1623	NEX	C9-C10-C11-C12
9	2	2630	LHG	C16-C17-C18-C19
4	2	601	CHL	CAA-CBA-CGA-O2A
4	4	609	CHL	CAA-CBA-CGA-O2A
5	1	611	CLA	CAA-CBA-CGA-O1A
5	1	612	CLA	C2A-CAA-CBA-CGA
4	1	607	CHL	CAA-CBA-CGA-O1A
5	3	603	CLA	C5-C6-C7-C8
4	3	607	CHL	C1A-C2A-CAA-CBA
5	3	603	CLA	C1A-C2A-CAA-CBA
9	4	2630	LHG	C4-C5-C6-O8
5	1	602	CLA	CAA-CBA-CGA-O1A
4	3	609	CHL	C4B-C3B-CAB-CBB
9	2	2630	LHG	C3-O3-P-O5
4	1	605	CHL	CAA-CBA-CGA-O1A
5	4	610	CLA	C2A-CAA-CBA-CGA
5	3	612	CLA	CAA-CBA-CGA-O1A
4	3	606	CHL	CAA-CBA-CGA-O1A
5	2	611	CLA	CAD-CBD-CGD-O1D
5	1	611	CLA	CBD-CGD-O2D-CED
5	3	603	CLA	C3-C5-C6-C7
5	3	602	CLA	CAA-CBA-CGA-O2A
4	2	609	CHL	C5-C6-C7-C8
4	2	607	CHL	CAA-CBA-CGA-O2A
5	3	602	CLA	C2-C3-C5-C6
4	3	601	CHL	CAA-CBA-CGA-O1A
5	1	613	CLA	CAA-CBA-CGA-O1A
10	4	623	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
5	2	603	CLA	CAA-CBA-CGA-O1A
5	2	602	CLA	CAA-CBA-CGA-O2A
4	2	607	CHL	CAA-CBA-CGA-O1A
5	3	602	CLA	CAA-CBA-CGA-O1A
4	3	607	CHL	C4C-C3C-CAC-CBC

There are no ring outliers.

53 monomers are involved in 97 short contacts:

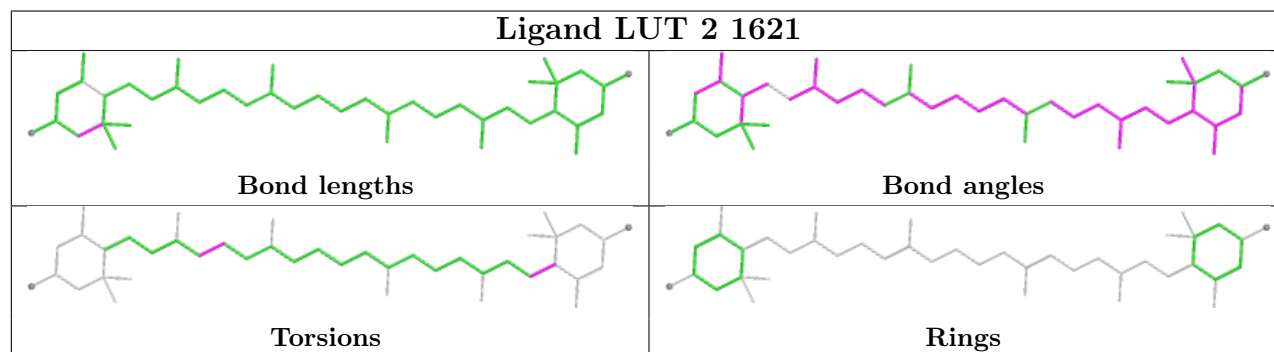
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	2	1621	LUT	3	0
4	2	607	CHL	2	0
4	4	608	CHL	2	0
9	3	2630	LHG	1	0
4	2	606	CHL	1	0
7	3	1622	XAT	2	0
4	1	608	CHL	1	0
4	1	607	CHL	4	0
4	2	609	CHL	2	0
5	1	603	CLA	2	0
5	2	611	CLA	1	0
4	4	609	CHL	1	0
5	4	612	CLA	1	0
6	2	1620	LUT	4	0
4	1	609	CHL	3	0
8	3	1623	NEX	3	0
5	2	602	CLA	2	0
9	2	2630	LHG	1	0
9	4	2630	LHG	1	0
4	3	606	CHL	3	0
5	2	603	CLA	1	0
5	1	604	CLA	1	0
5	3	611	CLA	2	0
6	1	1620	LUT	5	0
7	2	1622	XAT	4	0
5	3	604	CLA	1	0
7	4	622	XAT	4	0
9	1	2630	LHG	2	0
5	2	613	CLA	1	0
8	1	1623	NEX	2	0
10	4	623	BCR	5	0
5	3	603	CLA	4	0

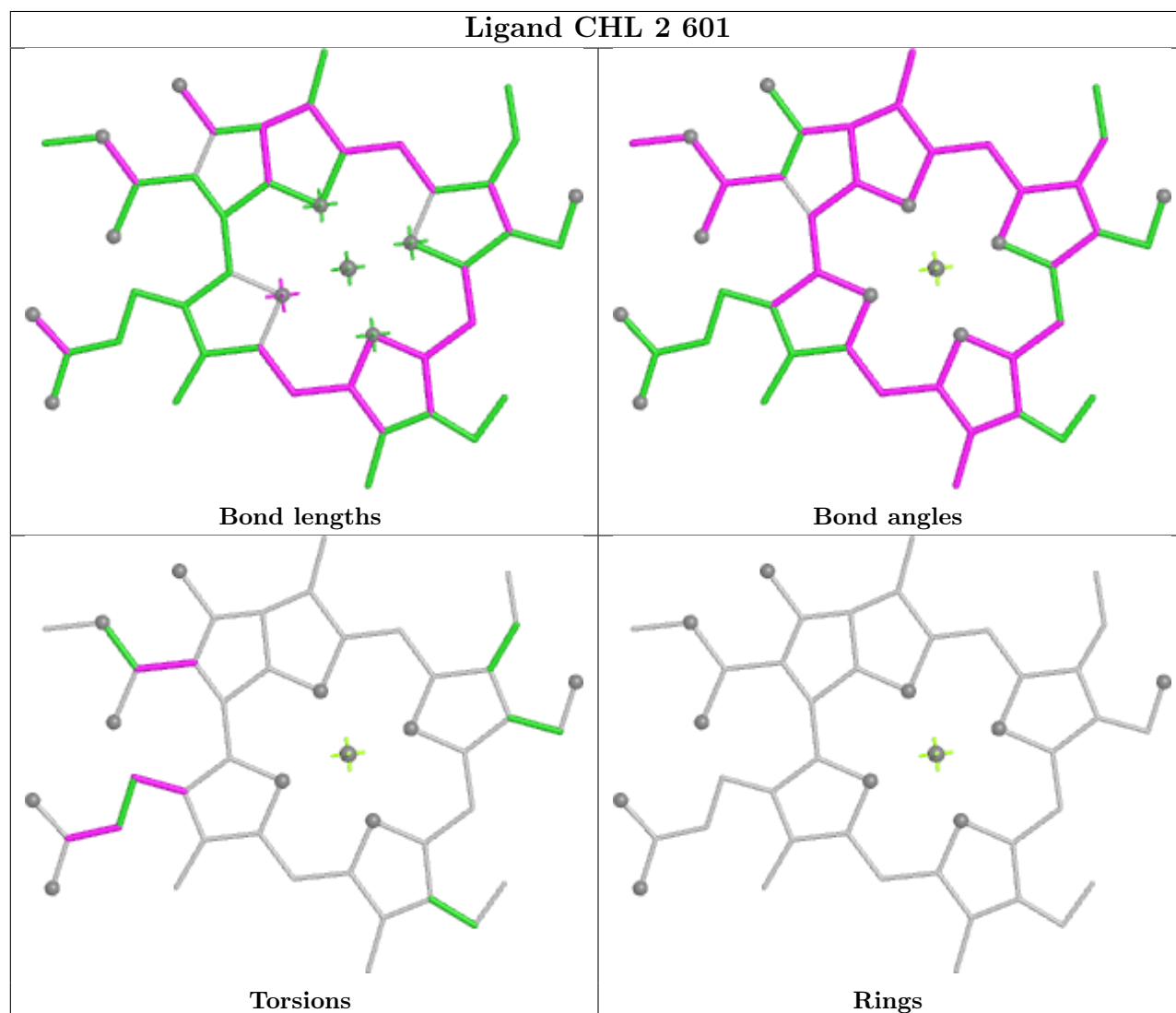
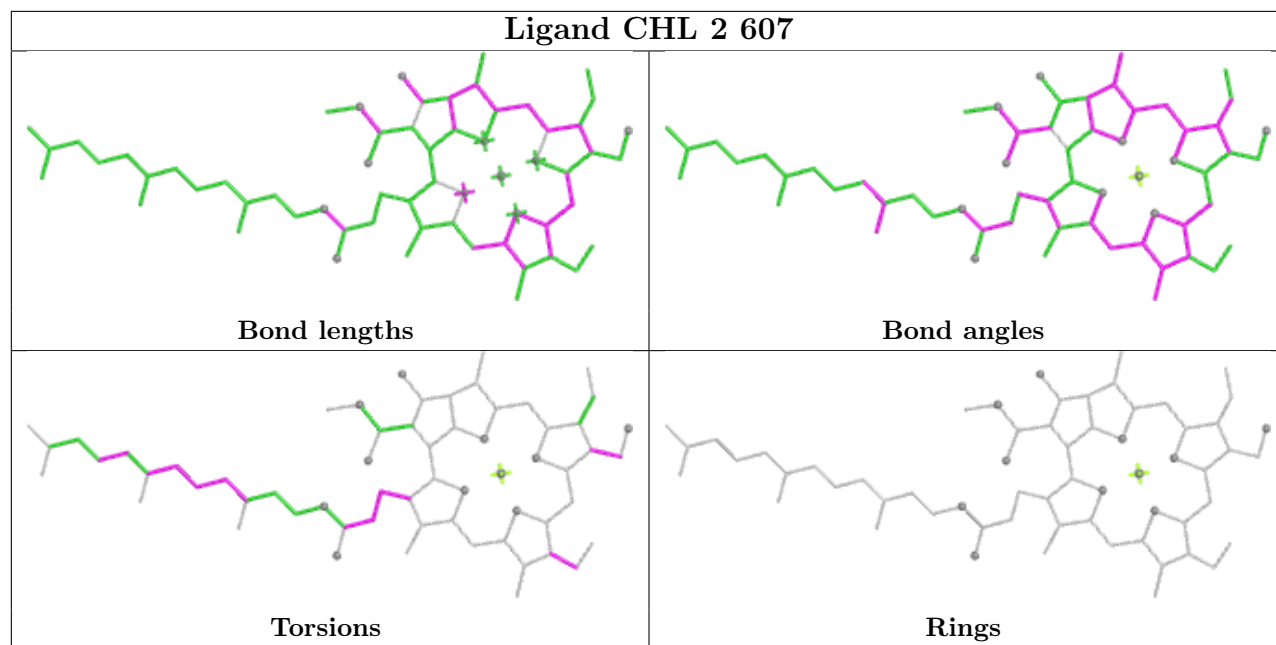
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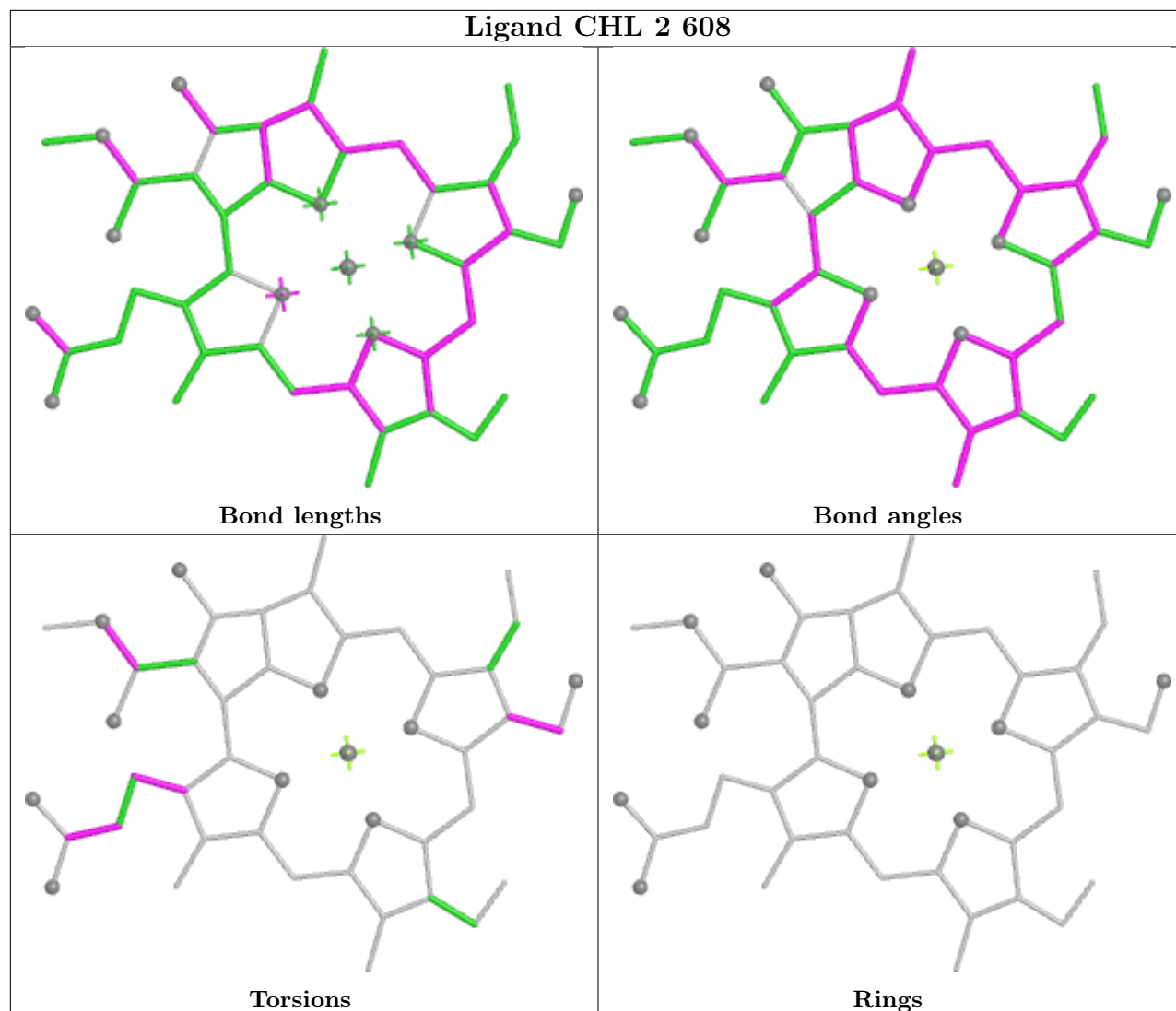
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	4	606	CHL	2	0
4	3	608	CHL	4	0
5	3	612	CLA	1	0
4	2	605	CHL	1	0
7	1	1622	XAT	2	0
4	1	601	CHL	1	0
6	4	620	LUT	3	0
5	1	613	CLA	1	0
5	2	604	CLA	1	0
6	3	1621	LUT	4	0
4	3	601	CHL	2	0
5	4	610	CLA	1	0
4	3	607	CHL	4	0
4	3	609	CHL	7	0
5	1	602	CLA	2	0
6	1	1621	LUT	6	0
4	4	601	CHL	2	0
5	3	602	CLA	3	0
5	2	612	CLA	2	0
5	1	610	CLA	1	0
6	3	1620	LUT	3	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 than 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.

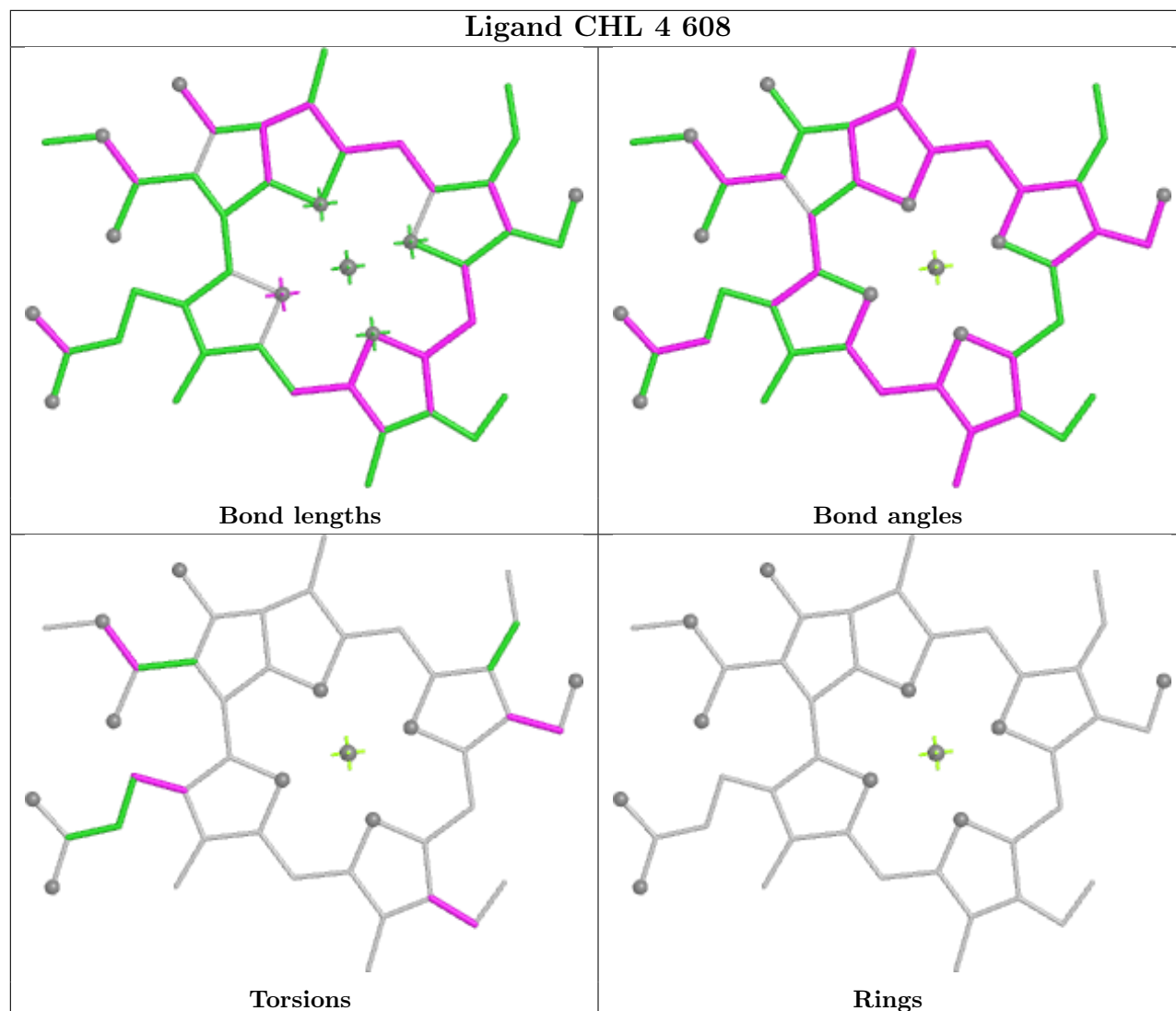




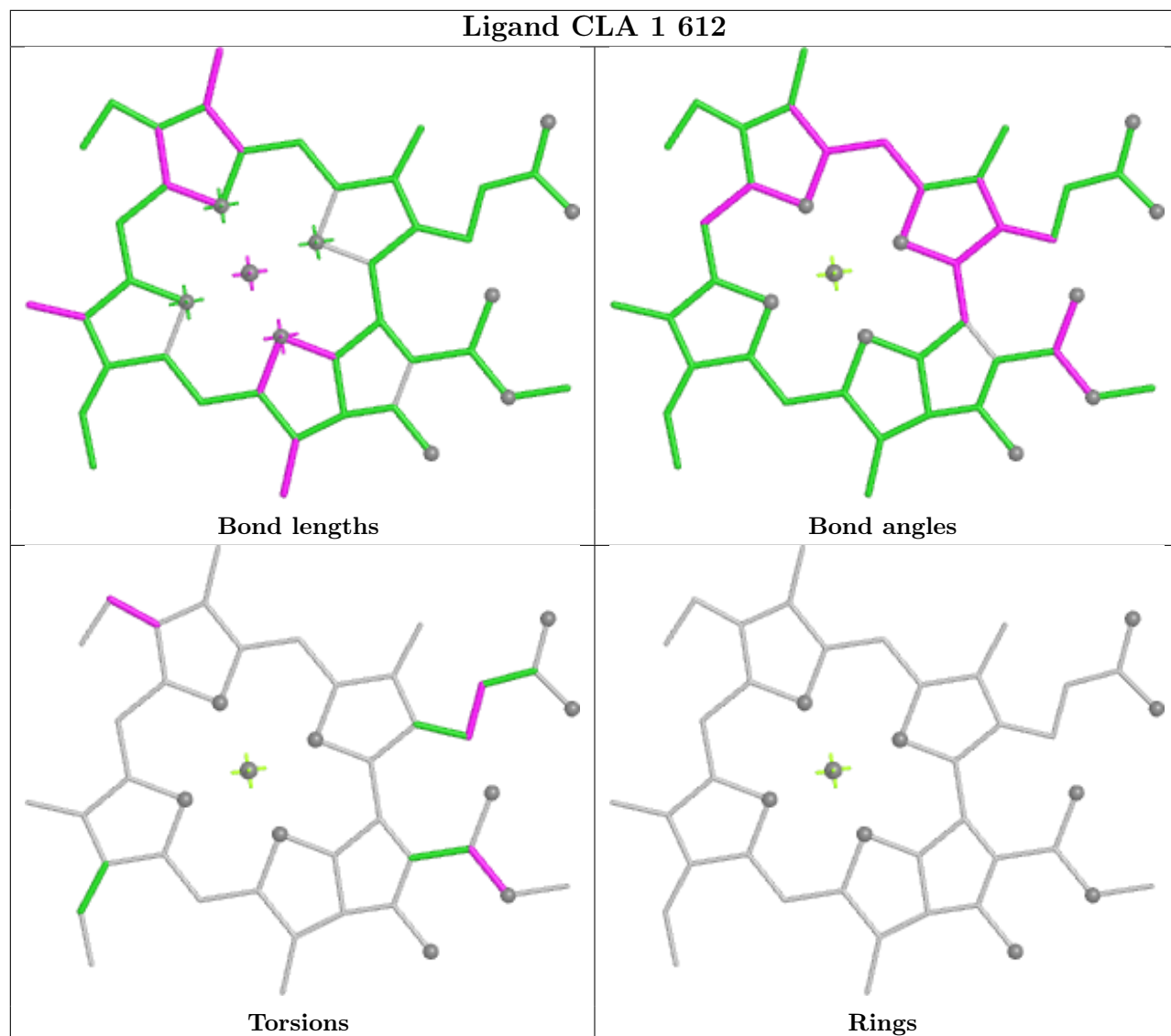
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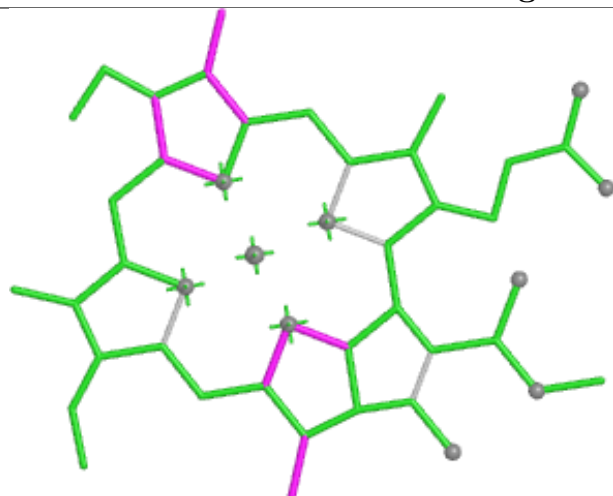
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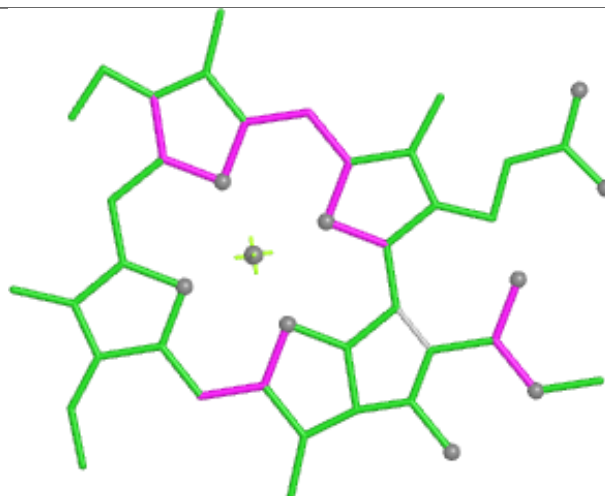
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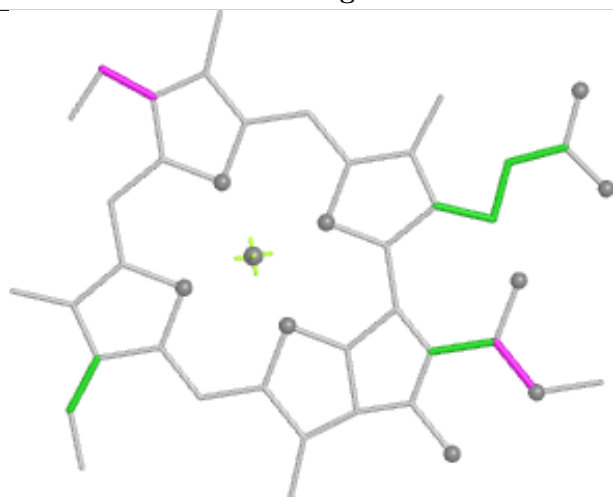
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Bond lengths



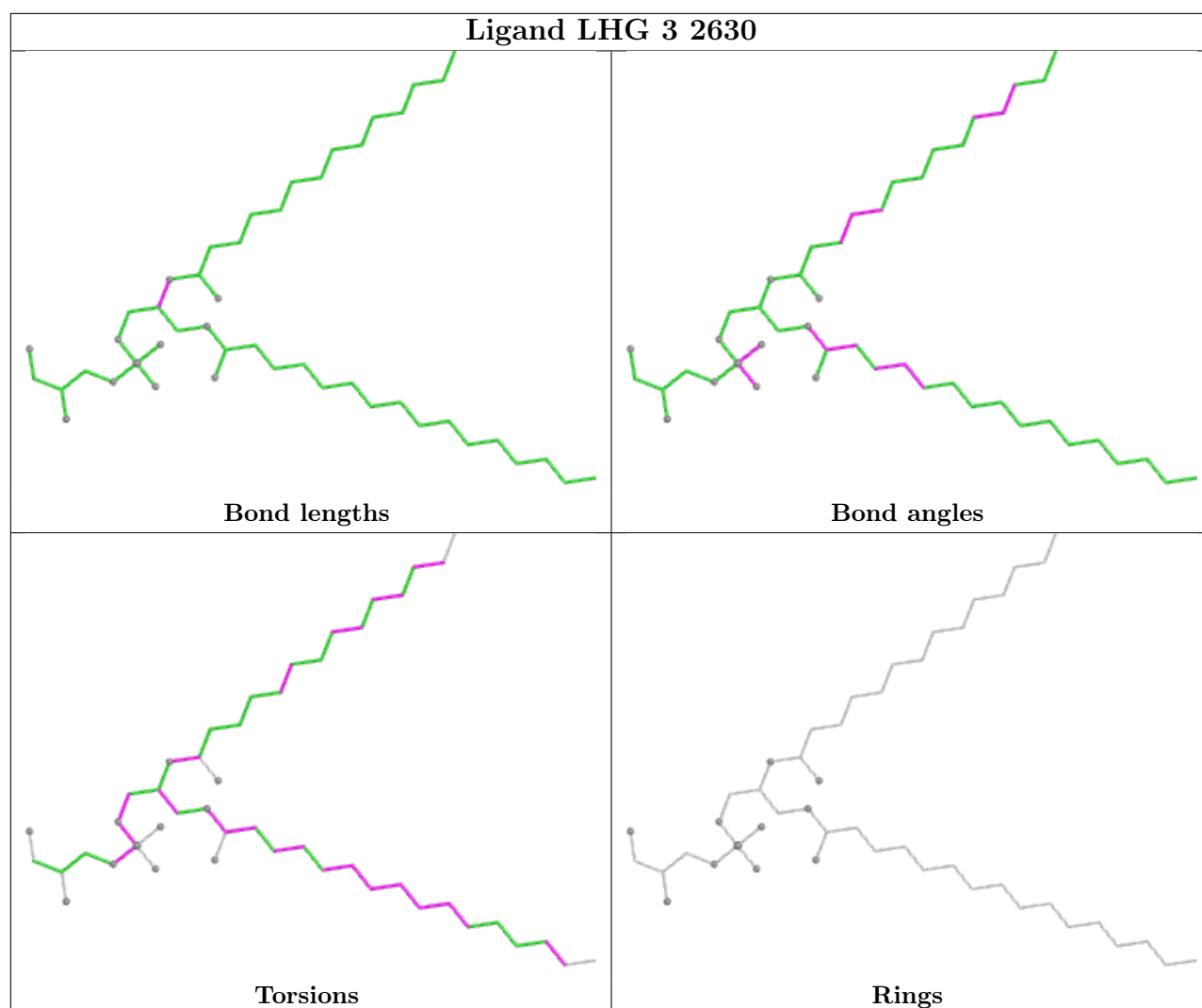
Bond angles



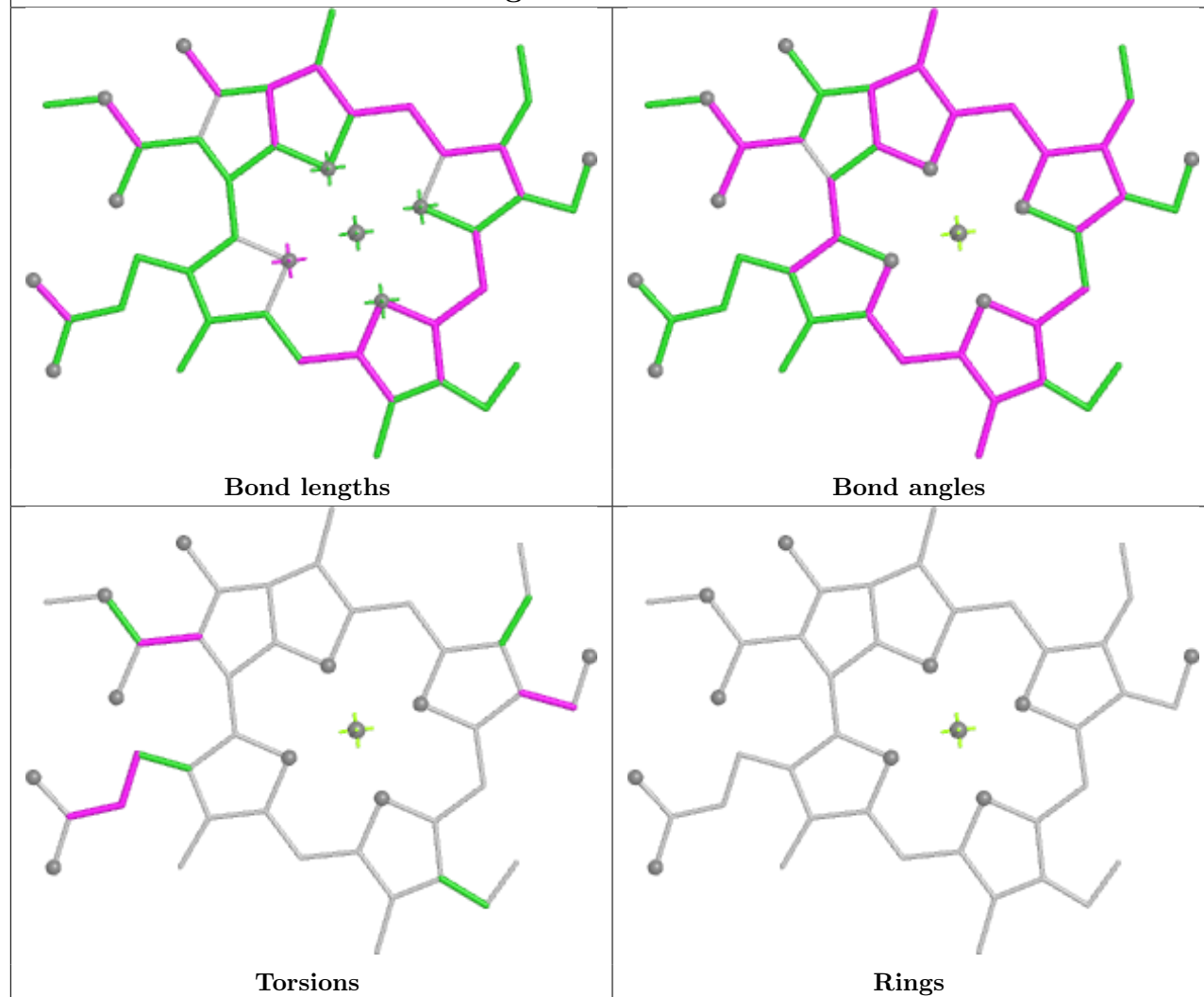
Torsions



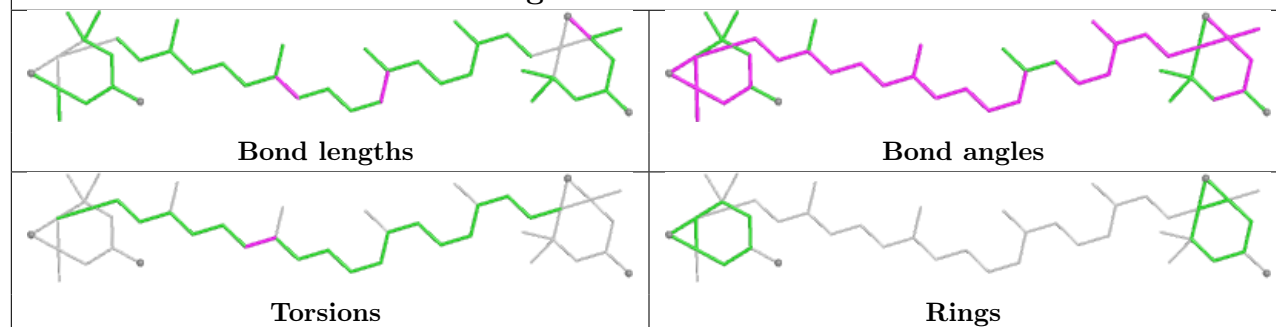
Rings

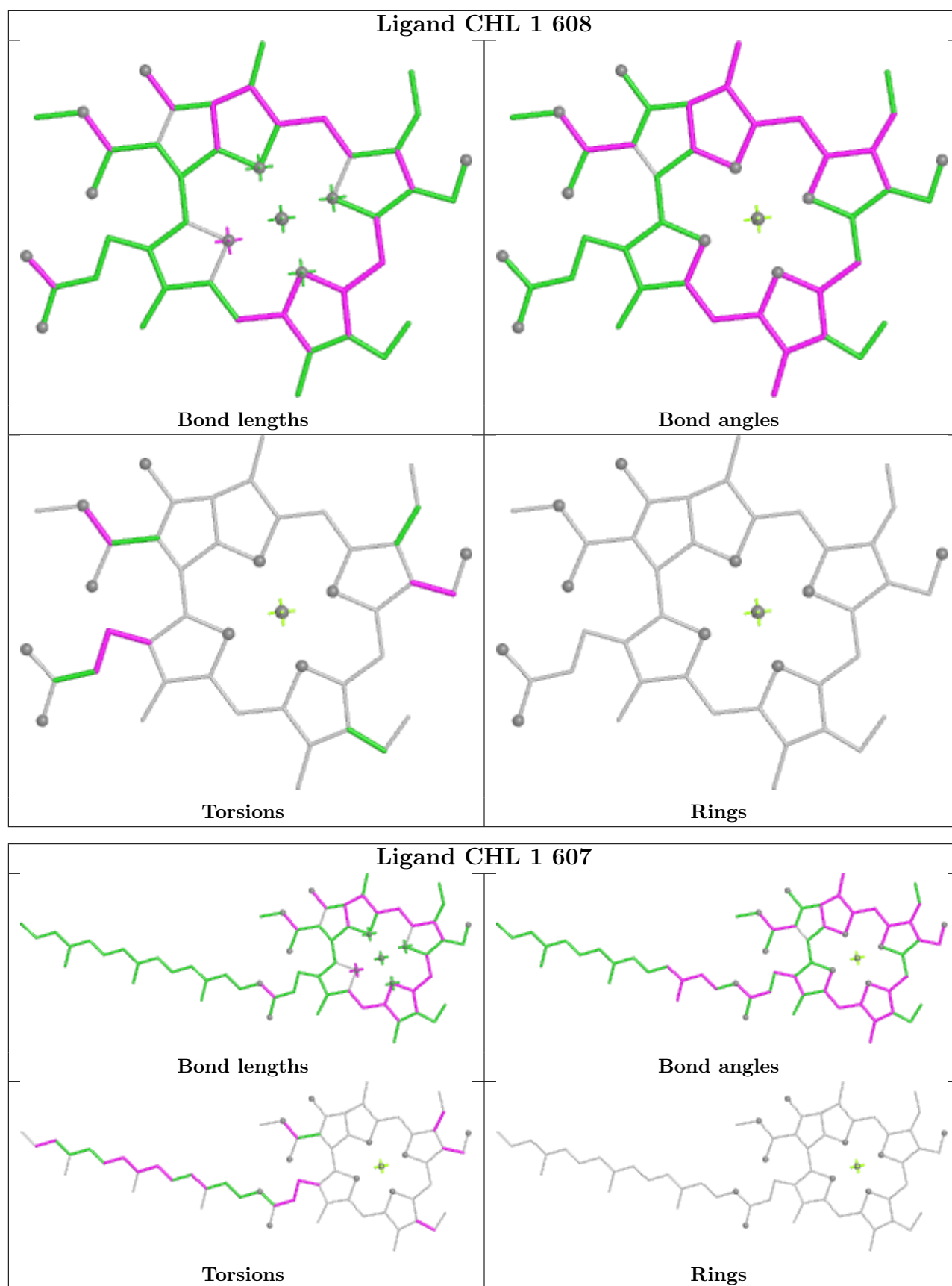


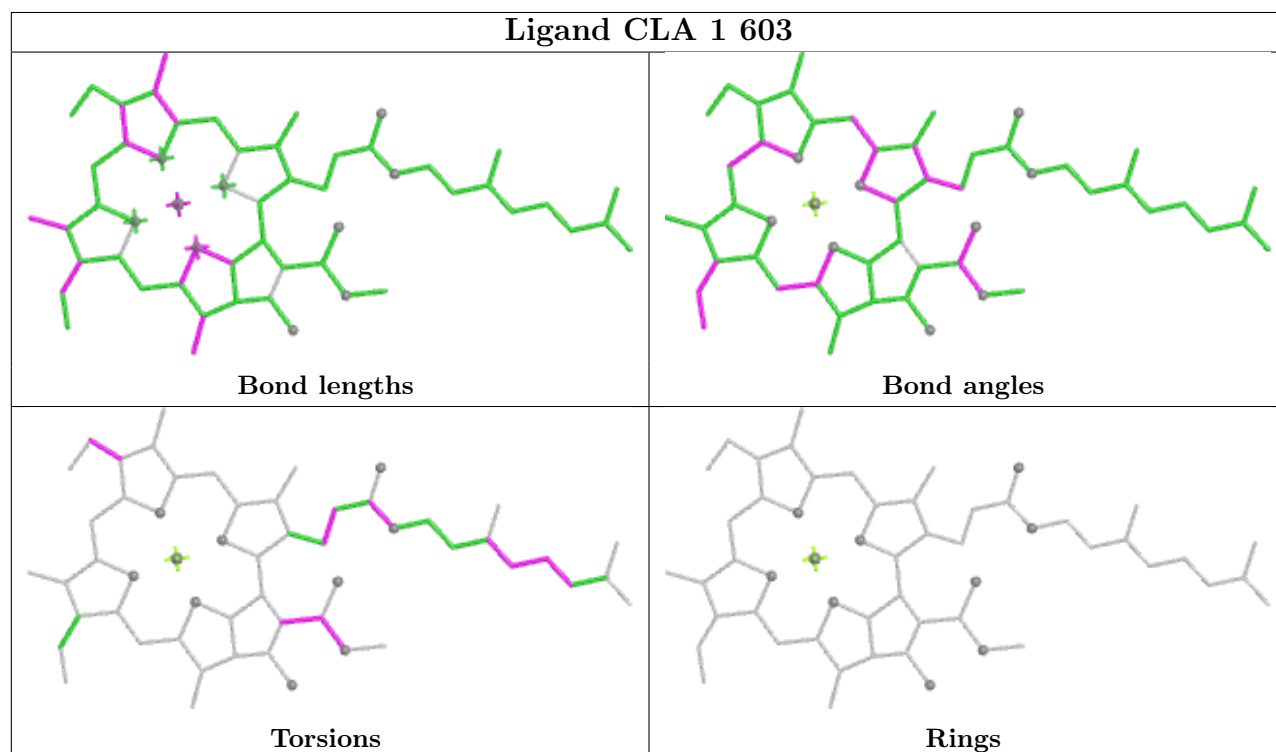
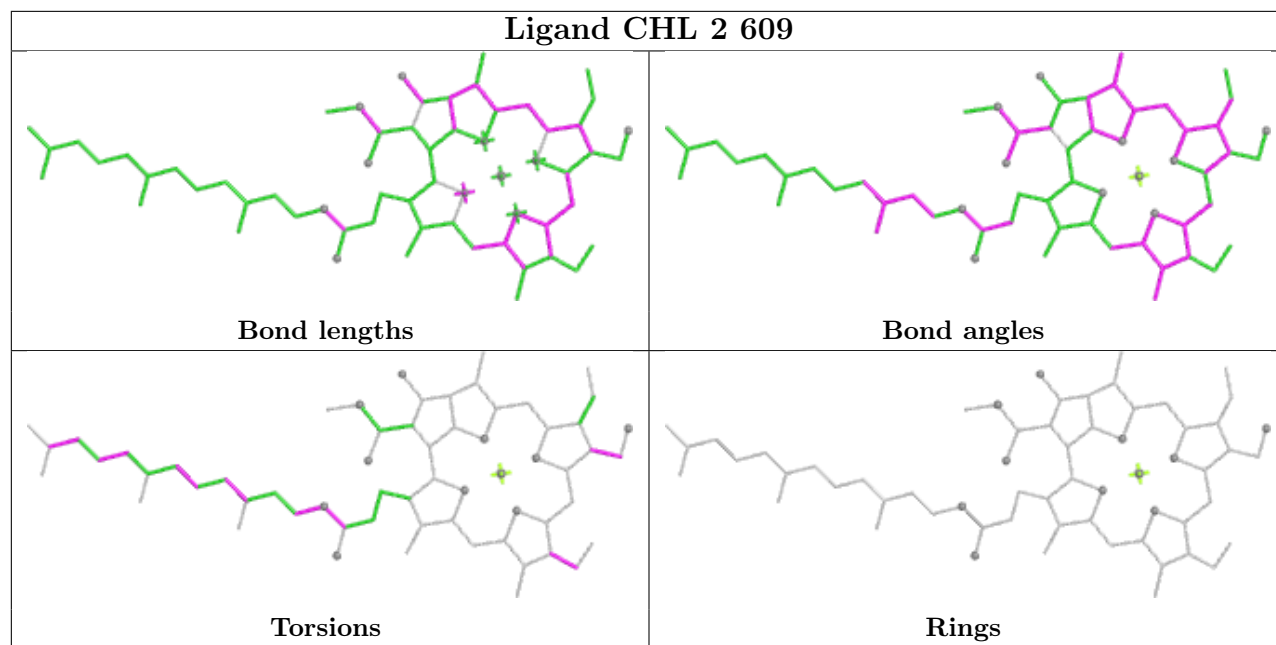
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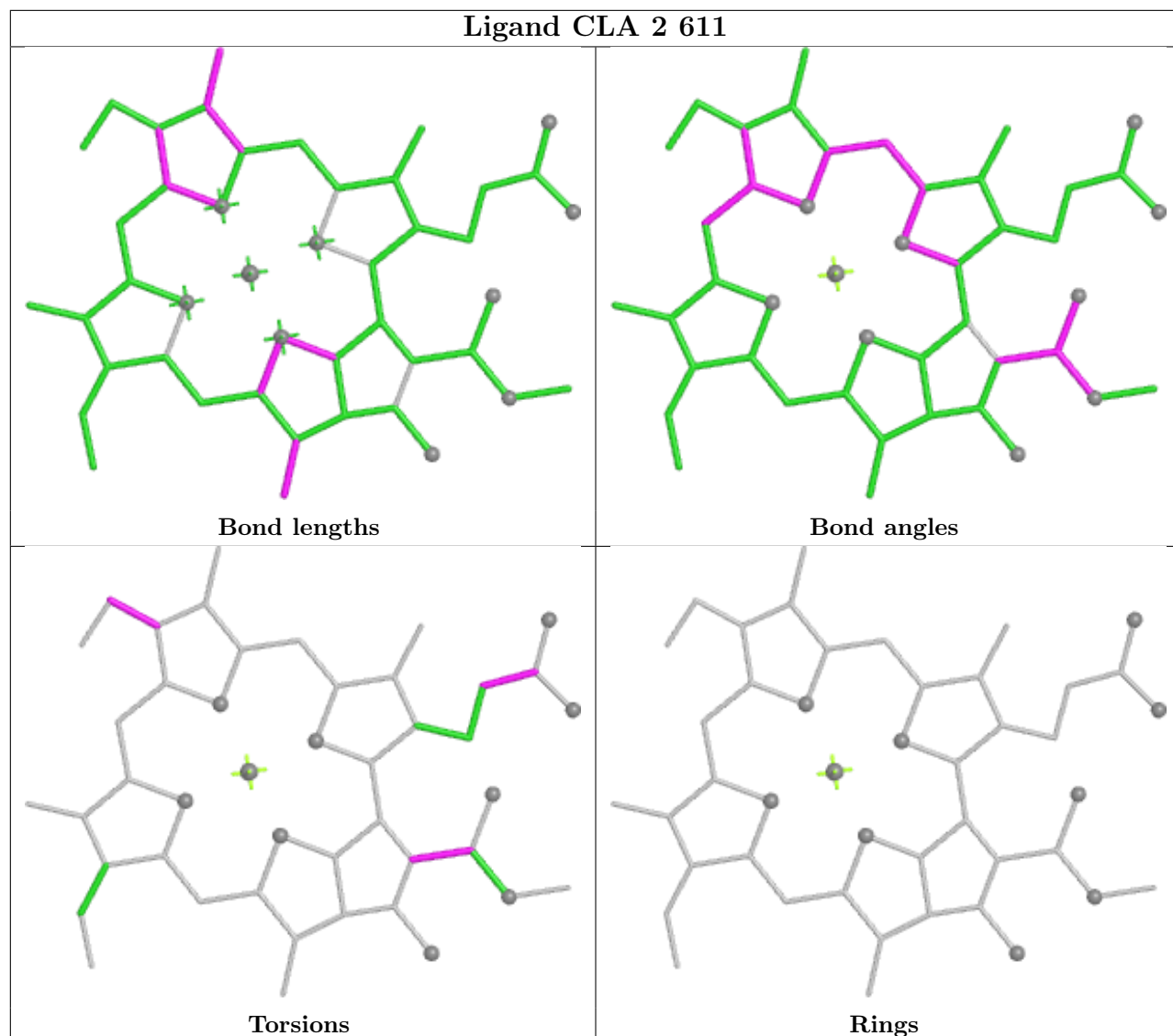
Ligand XAT 3 1622



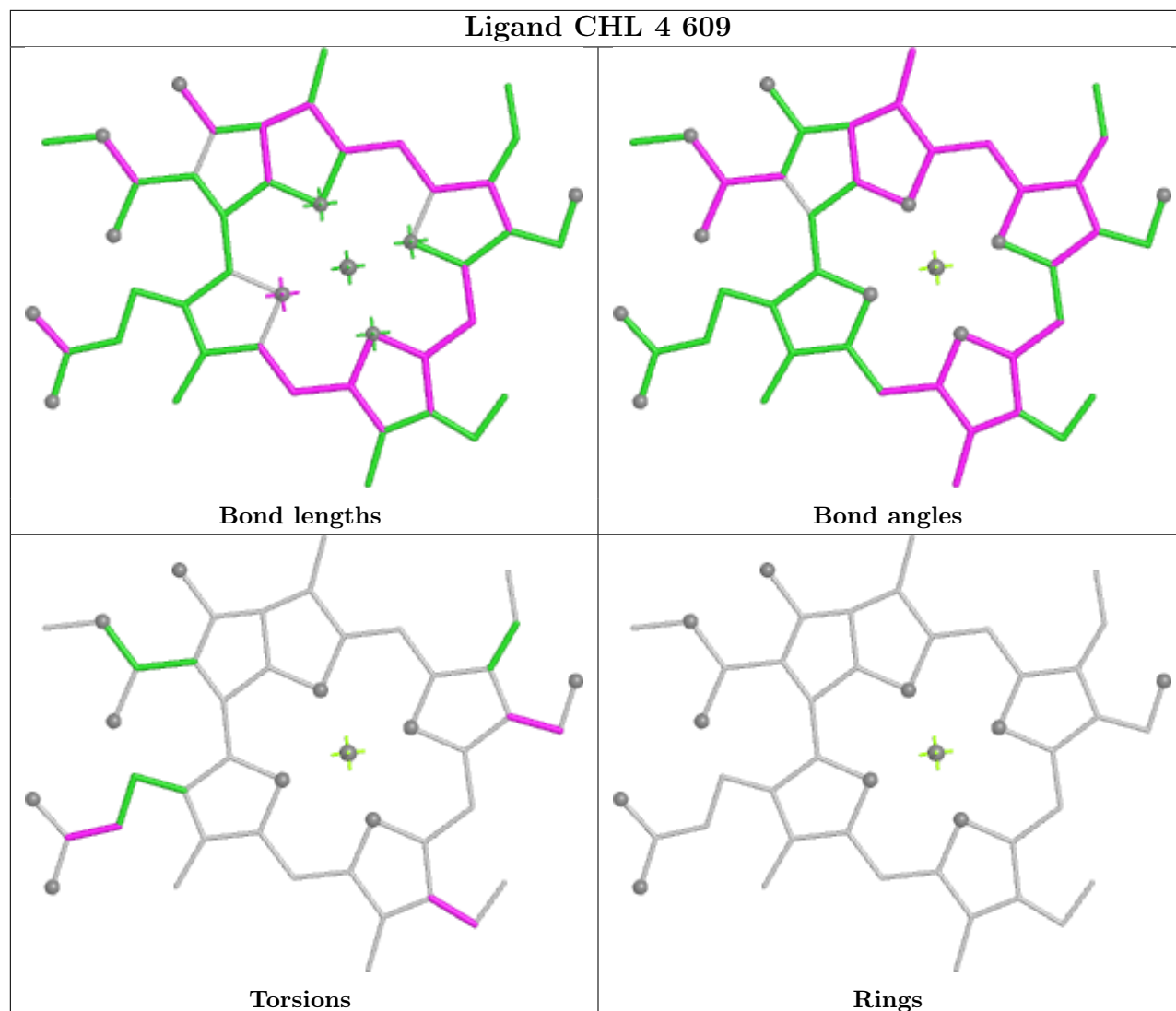




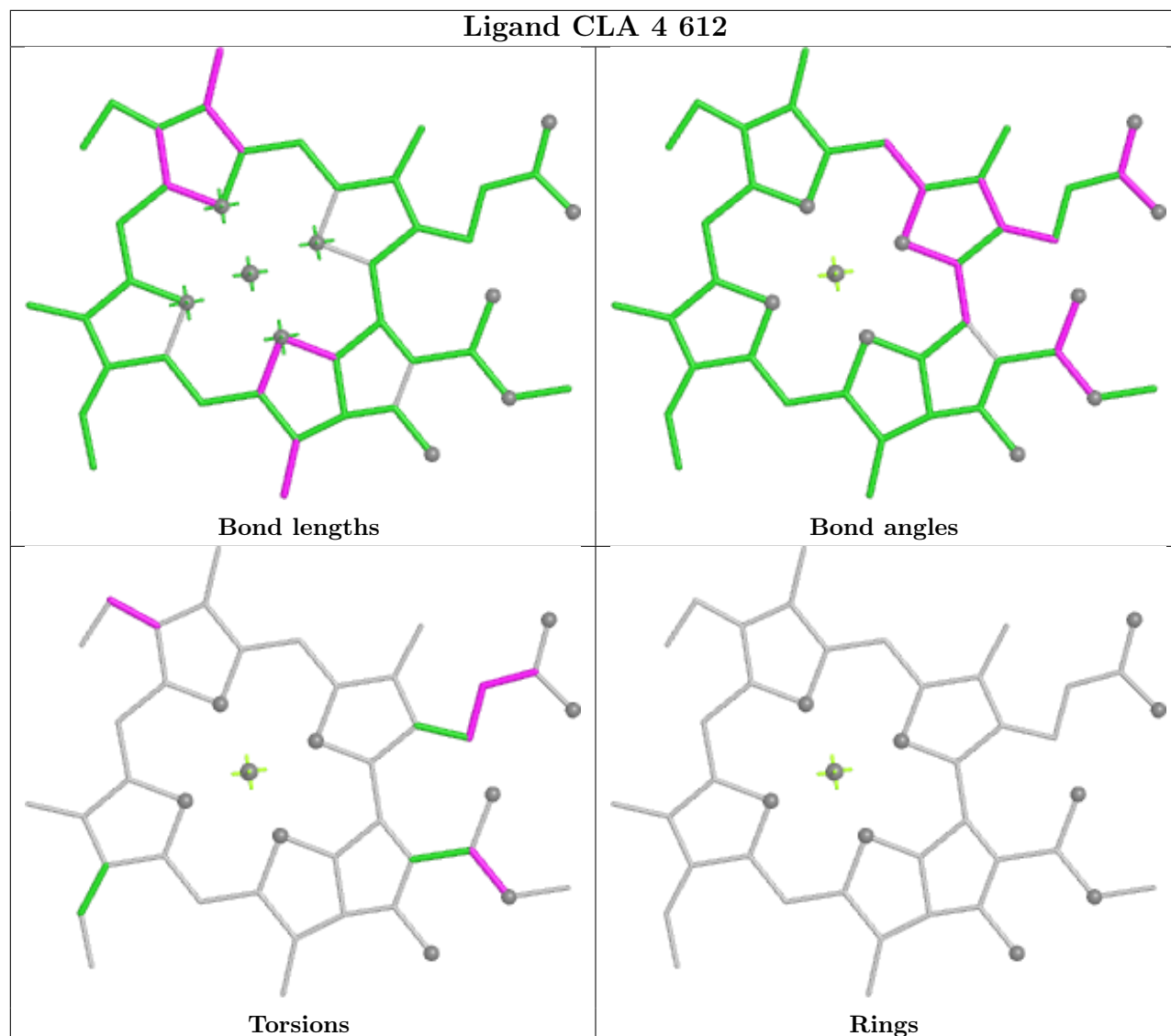
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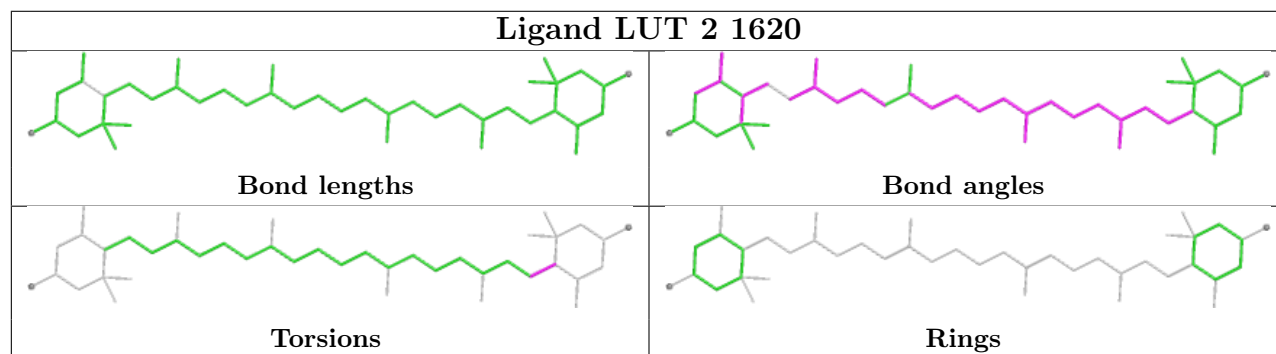
Ligand CHL 4 609

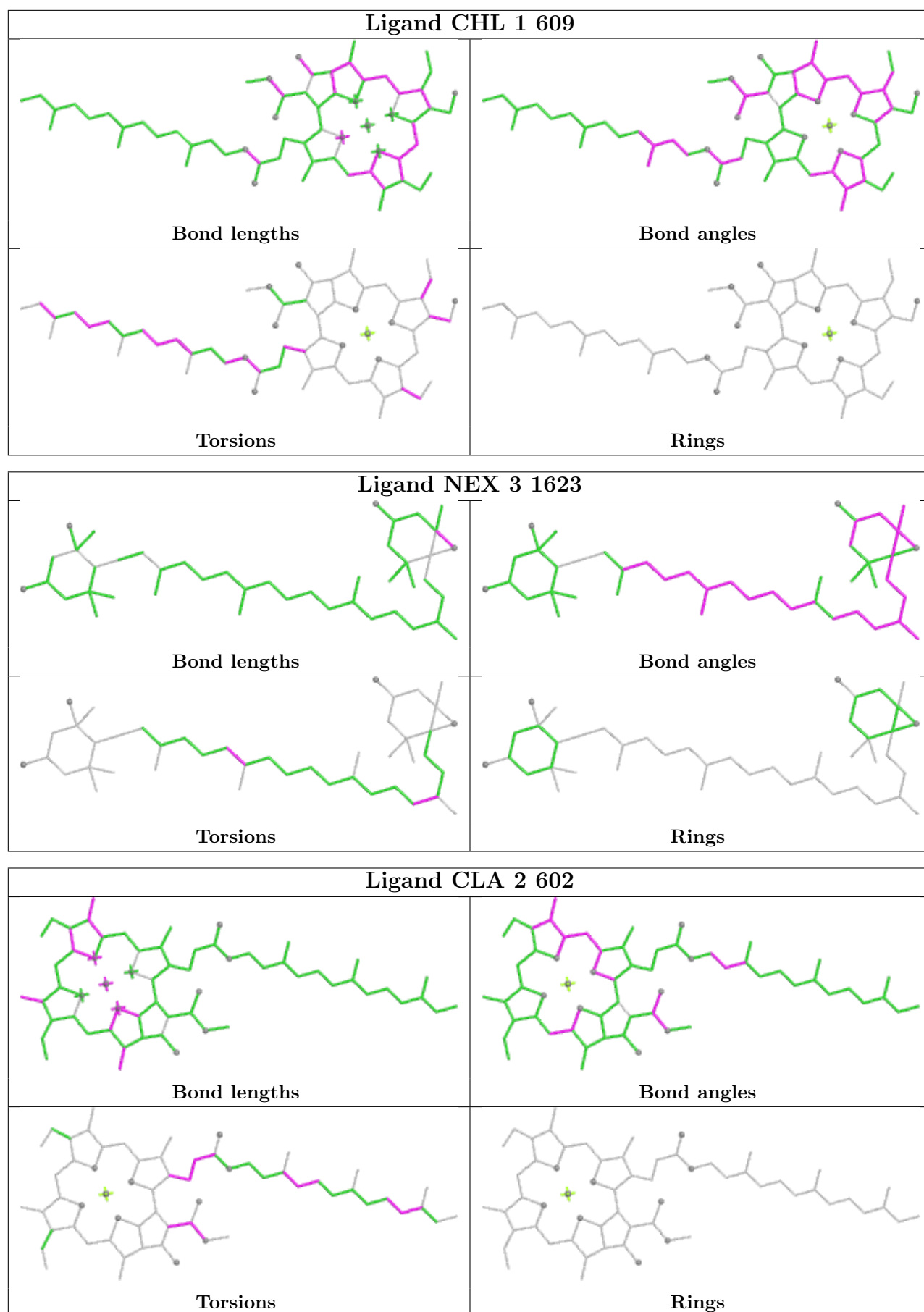


Ligand CLA 4 612

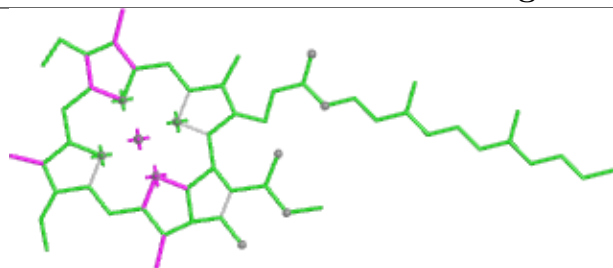


Ligand LUT 2 1620

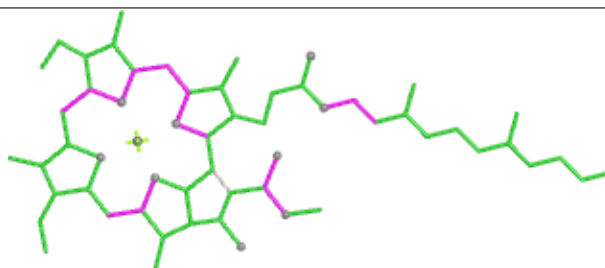




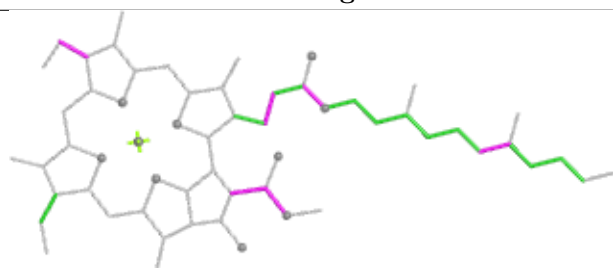
Ligand CLA 3 613



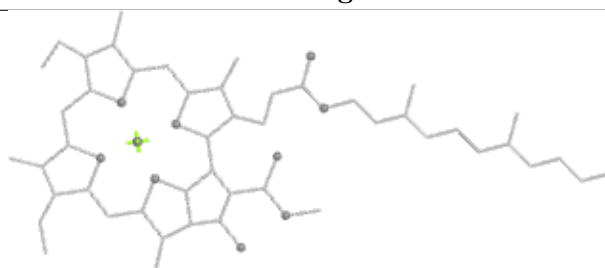
Bond lengths



Bond angles

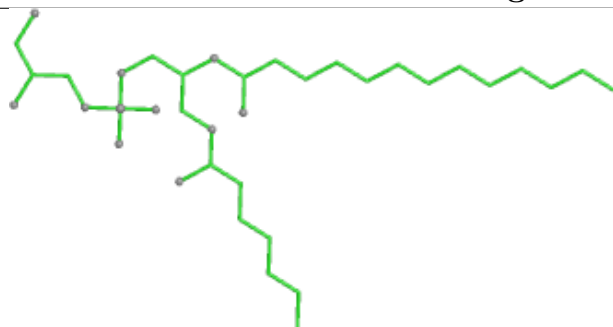


Torsions

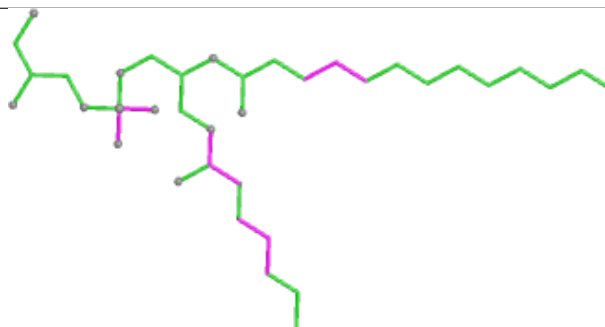


Rings

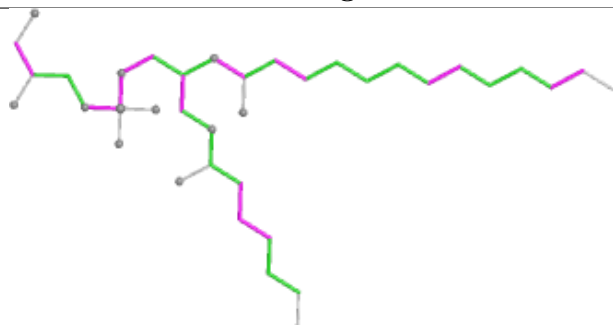
Ligand LHG 2 2630



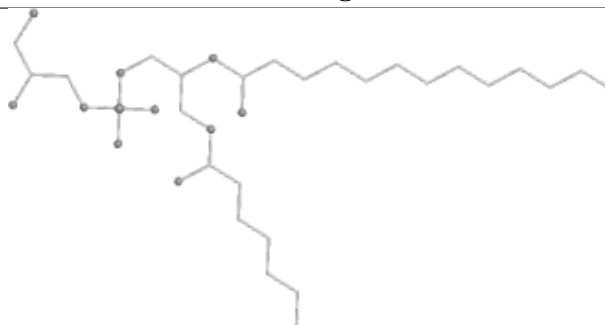
Bond lengths



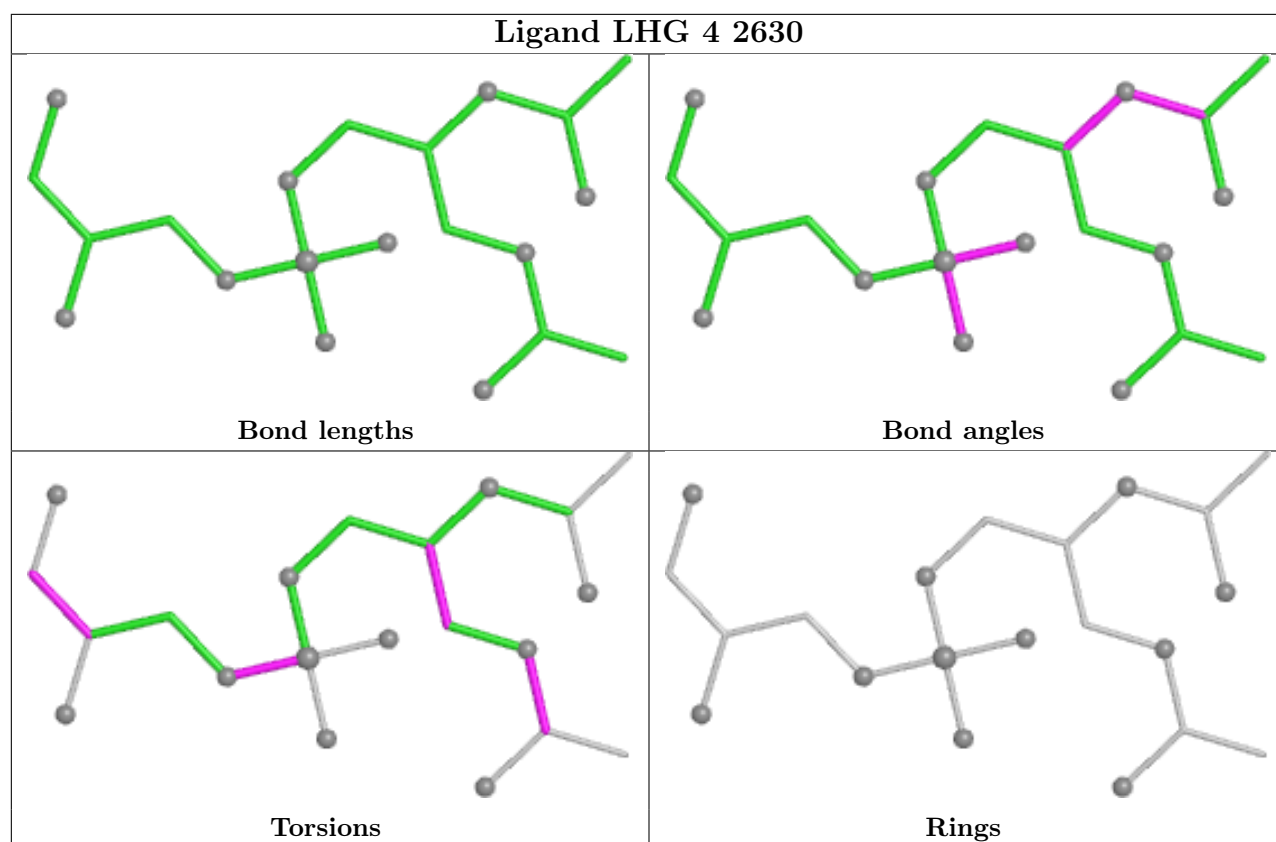
Bond angles



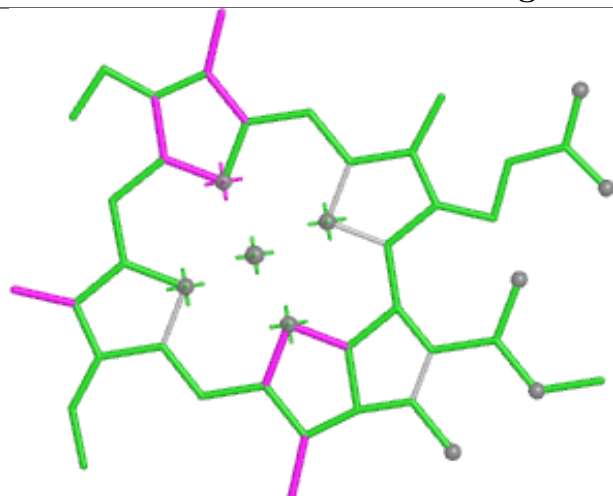
Torsions



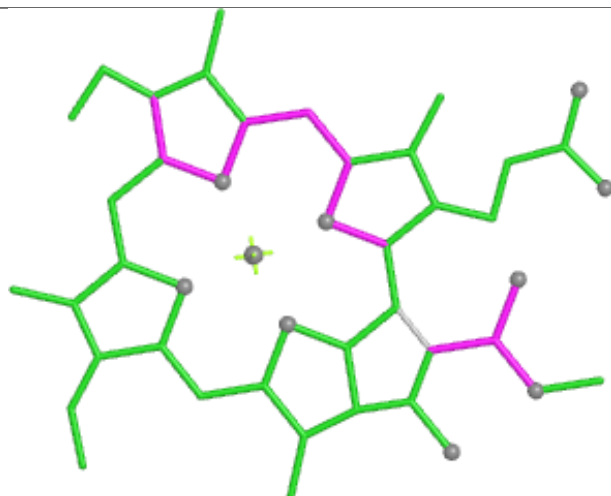
Rings



Ligand CLA 4 602



Bond lengths



Bond angles

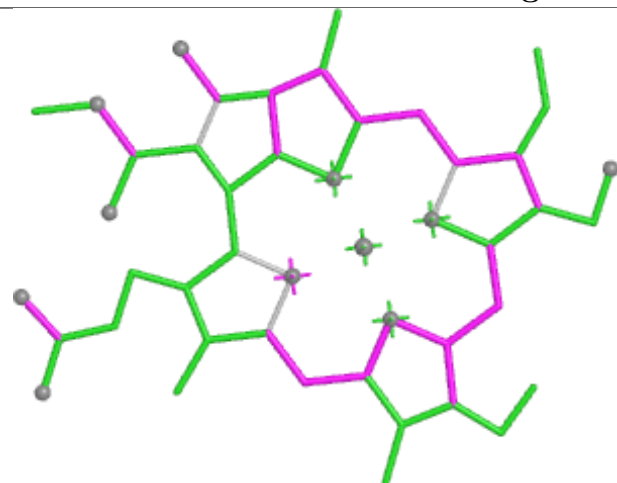


Torsions

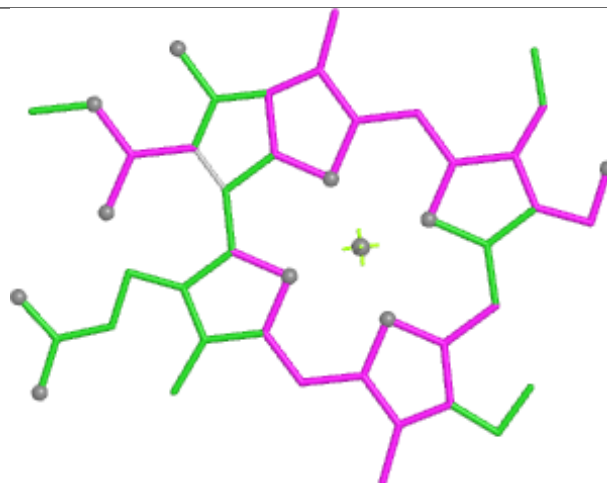


Rings

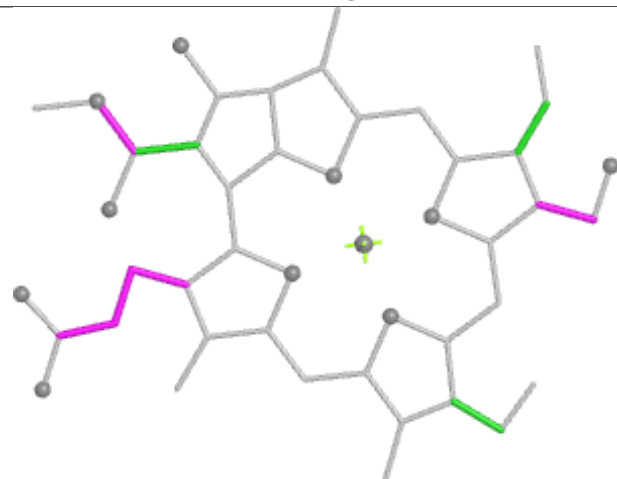
Ligand CHL 3 606



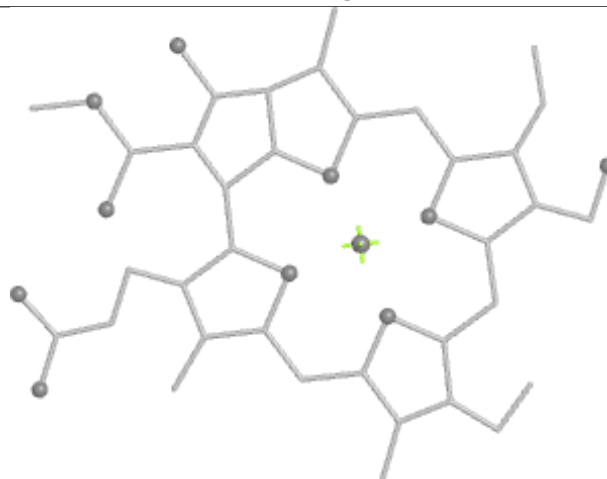
Bond lengths



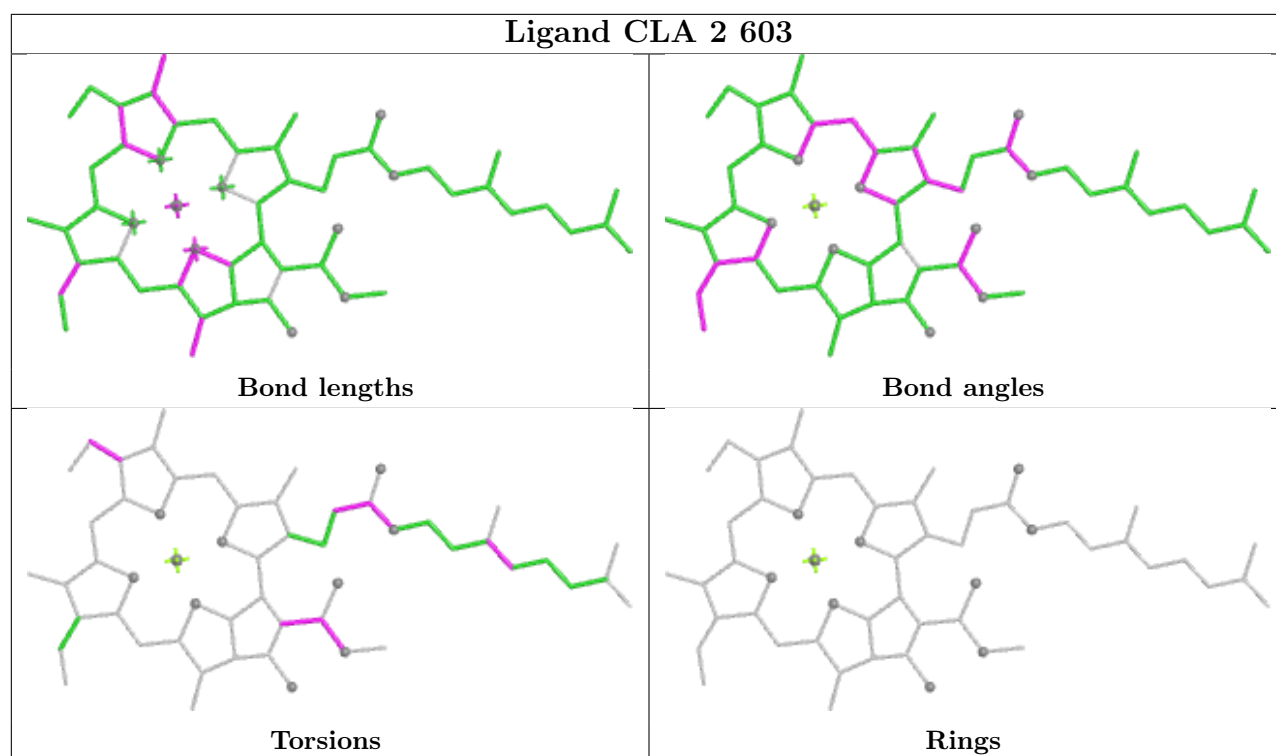
Bond angles



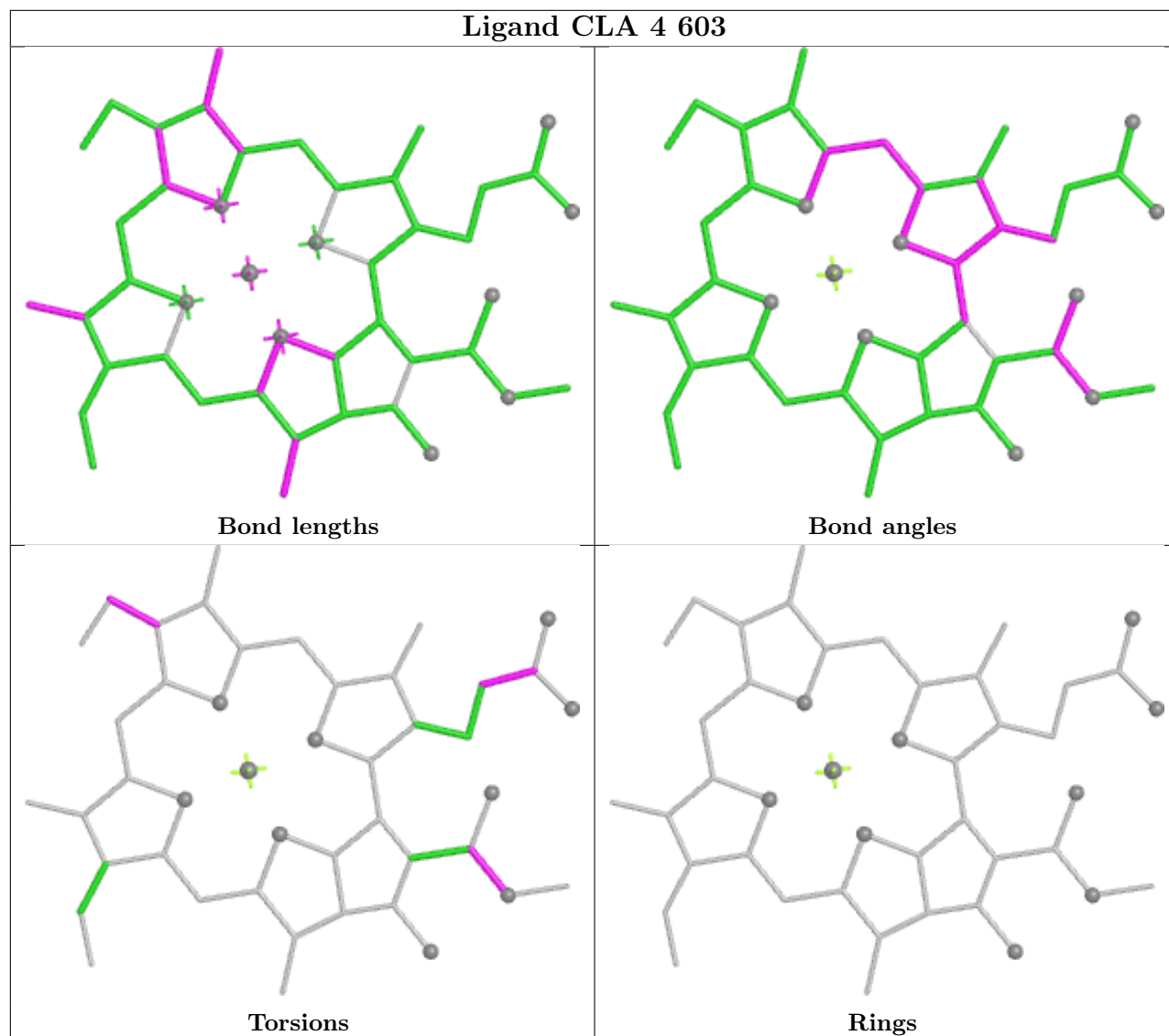
Torsions

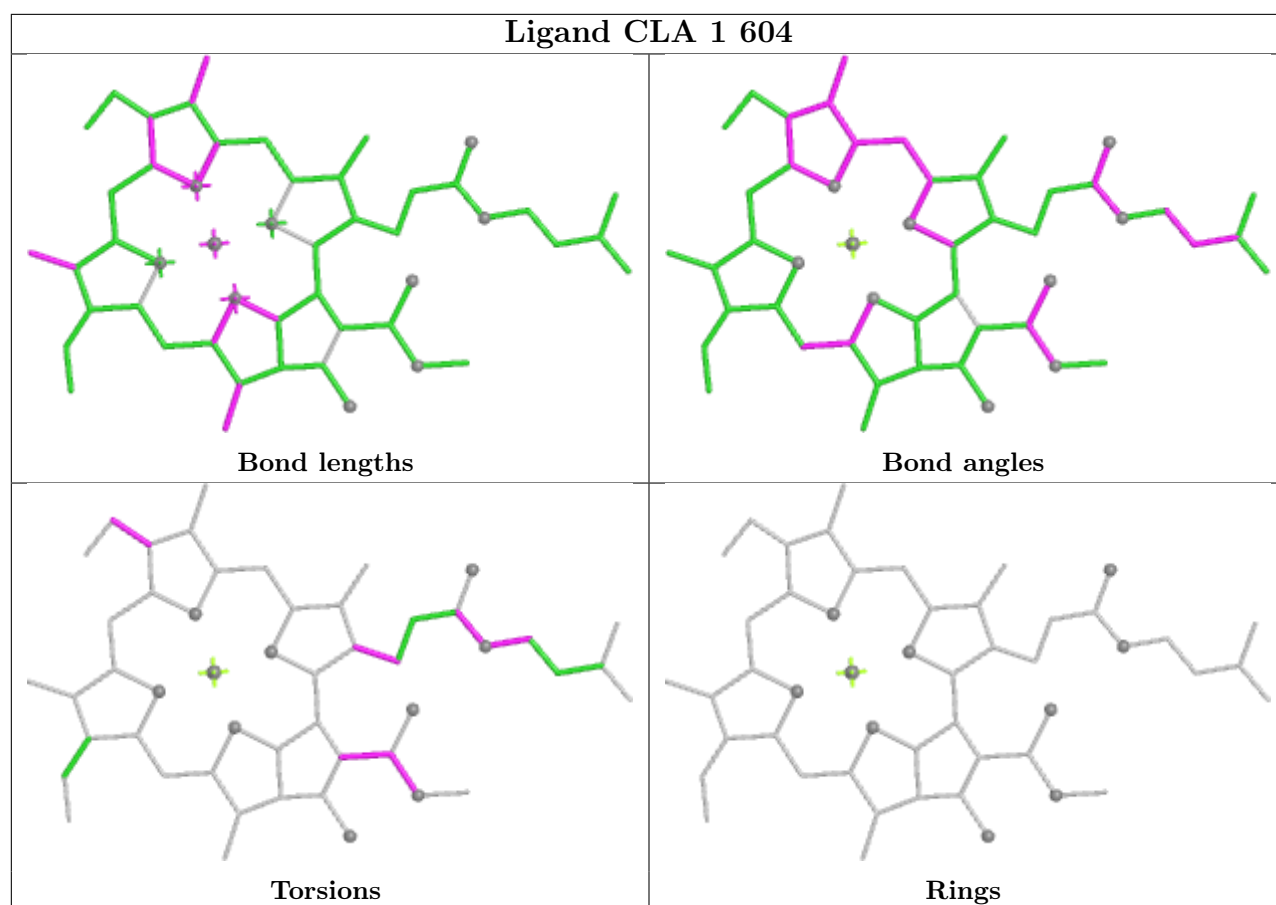


Rings

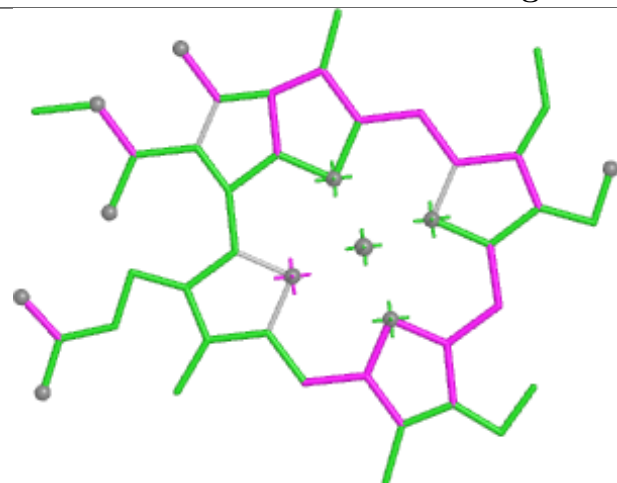


Ligand CLA 4 603

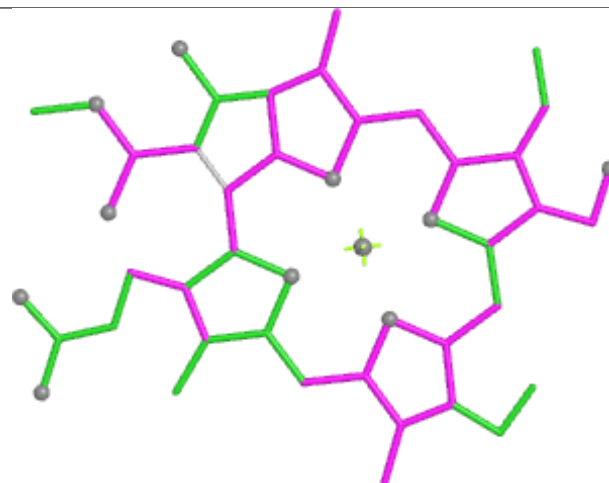




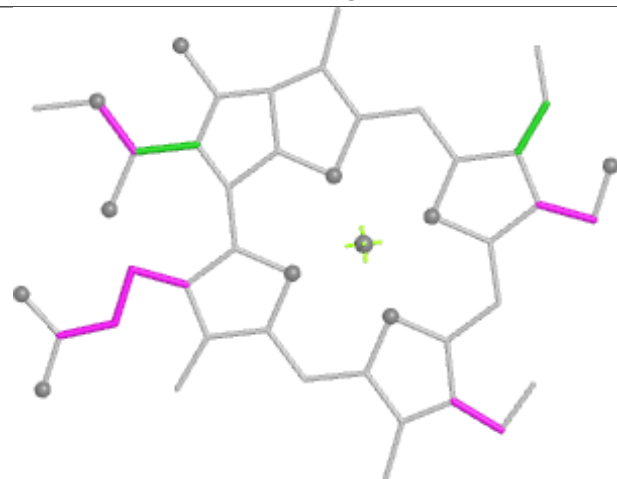
Ligand CHL 3 605



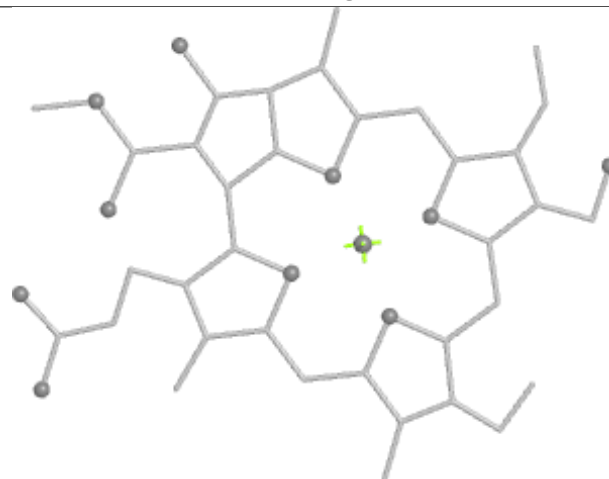
Bond lengths



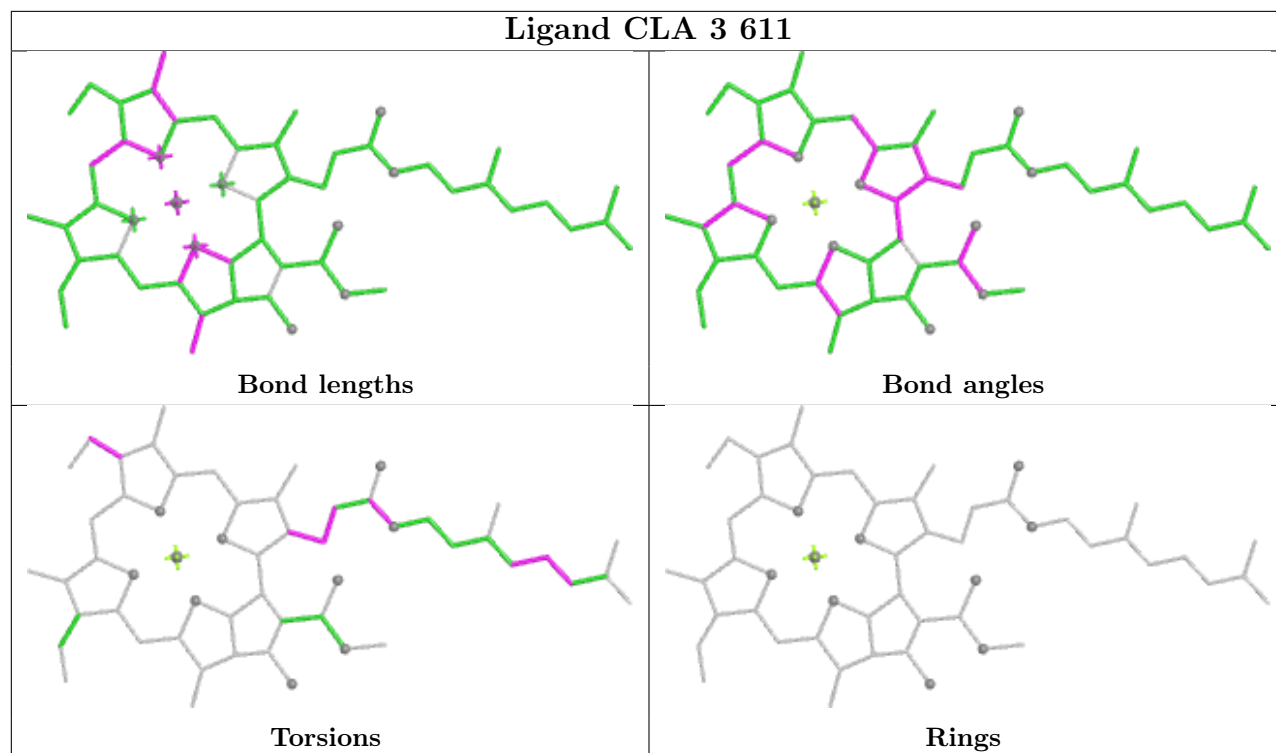
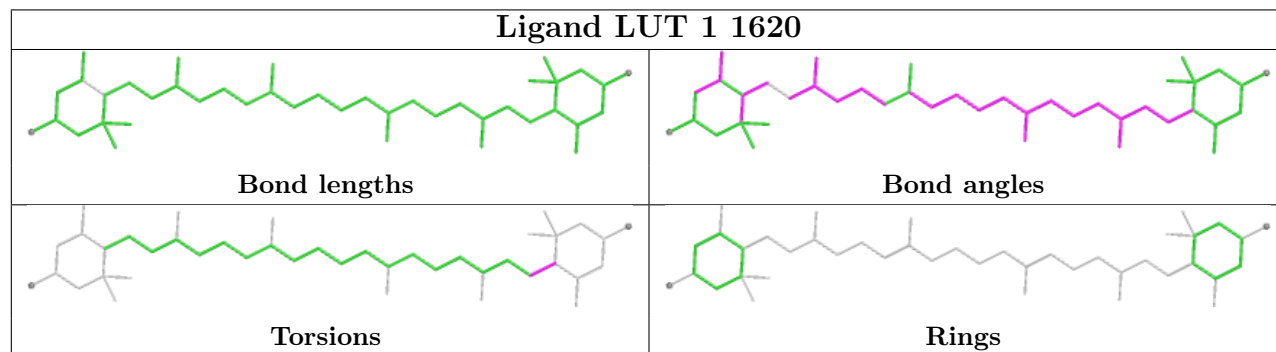
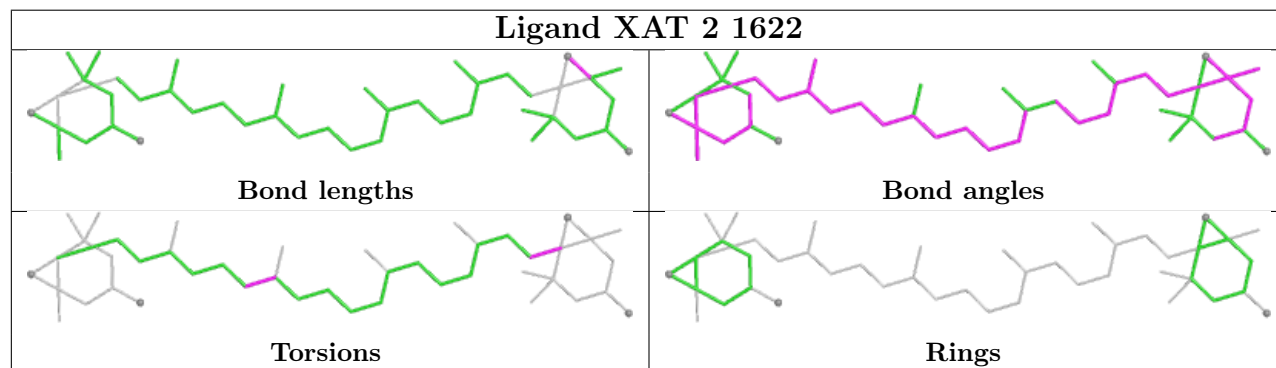
Bond angles



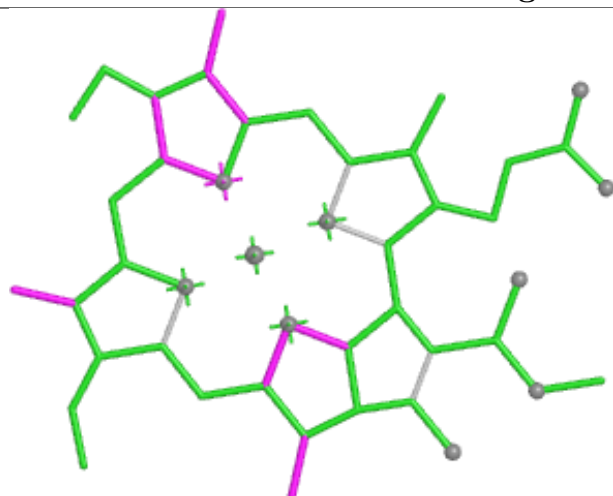
Torsions



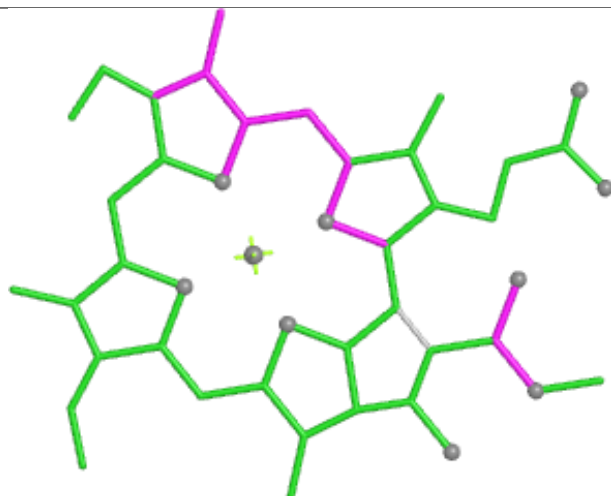
Rings

Ligand CLA 3 611**Ligand LUT 1 1620****Ligand XAT 2 1622**

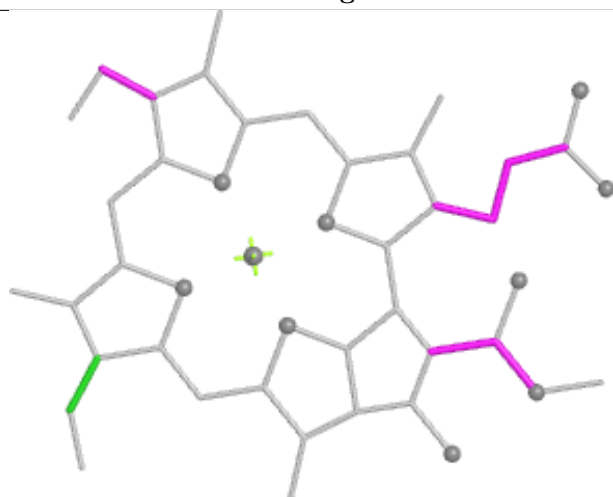
Ligand CLA 3 604



Bond lengths



Bond angles

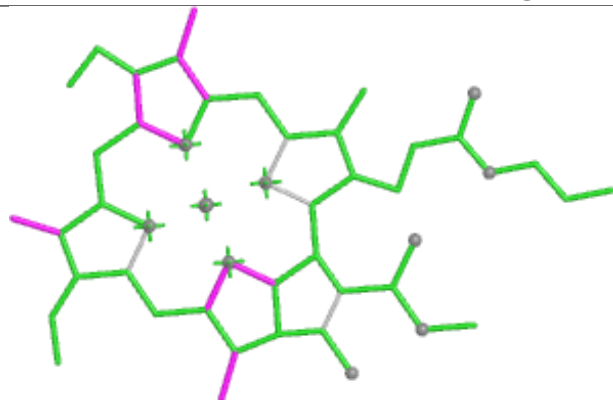


Torsions

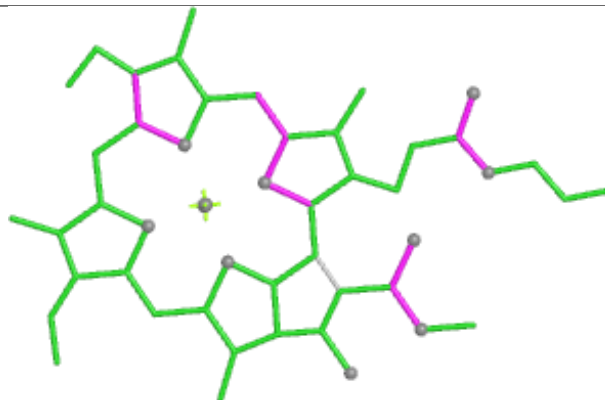


Rings

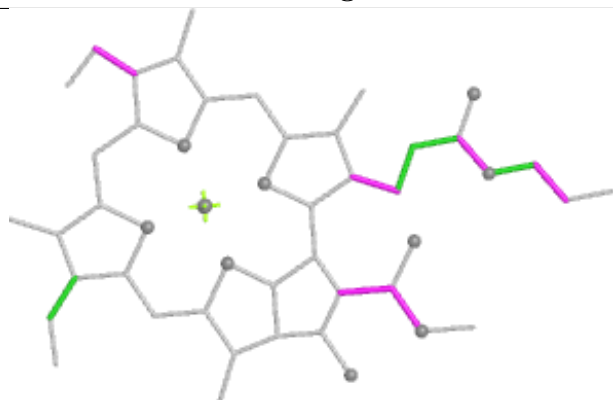
Ligand CLA 3 614



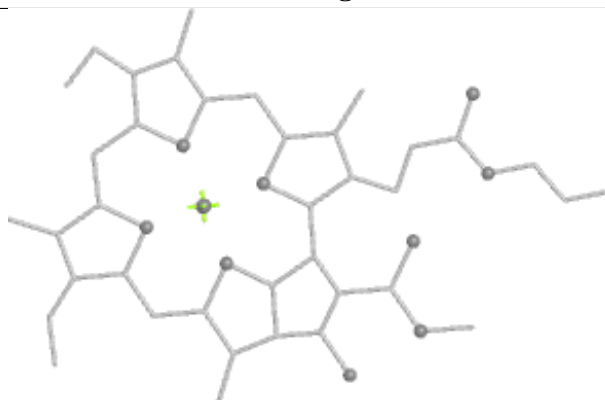
Bond lengths



Bond angles

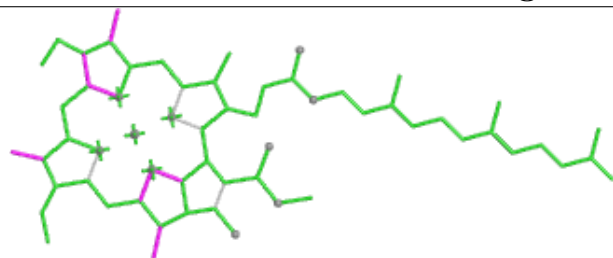


Torsions

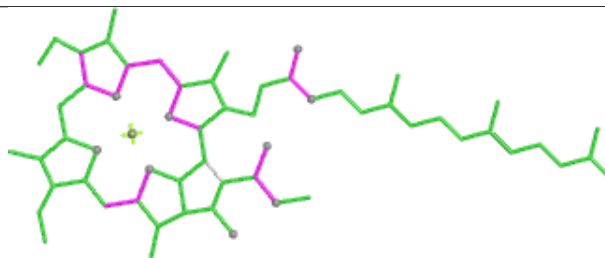


Rings

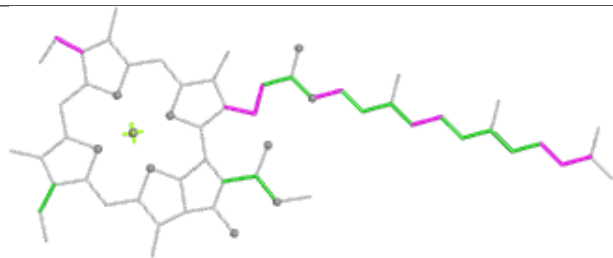
Ligand CLA 3 610



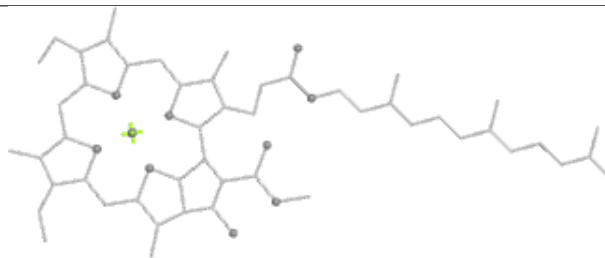
Bond lengths



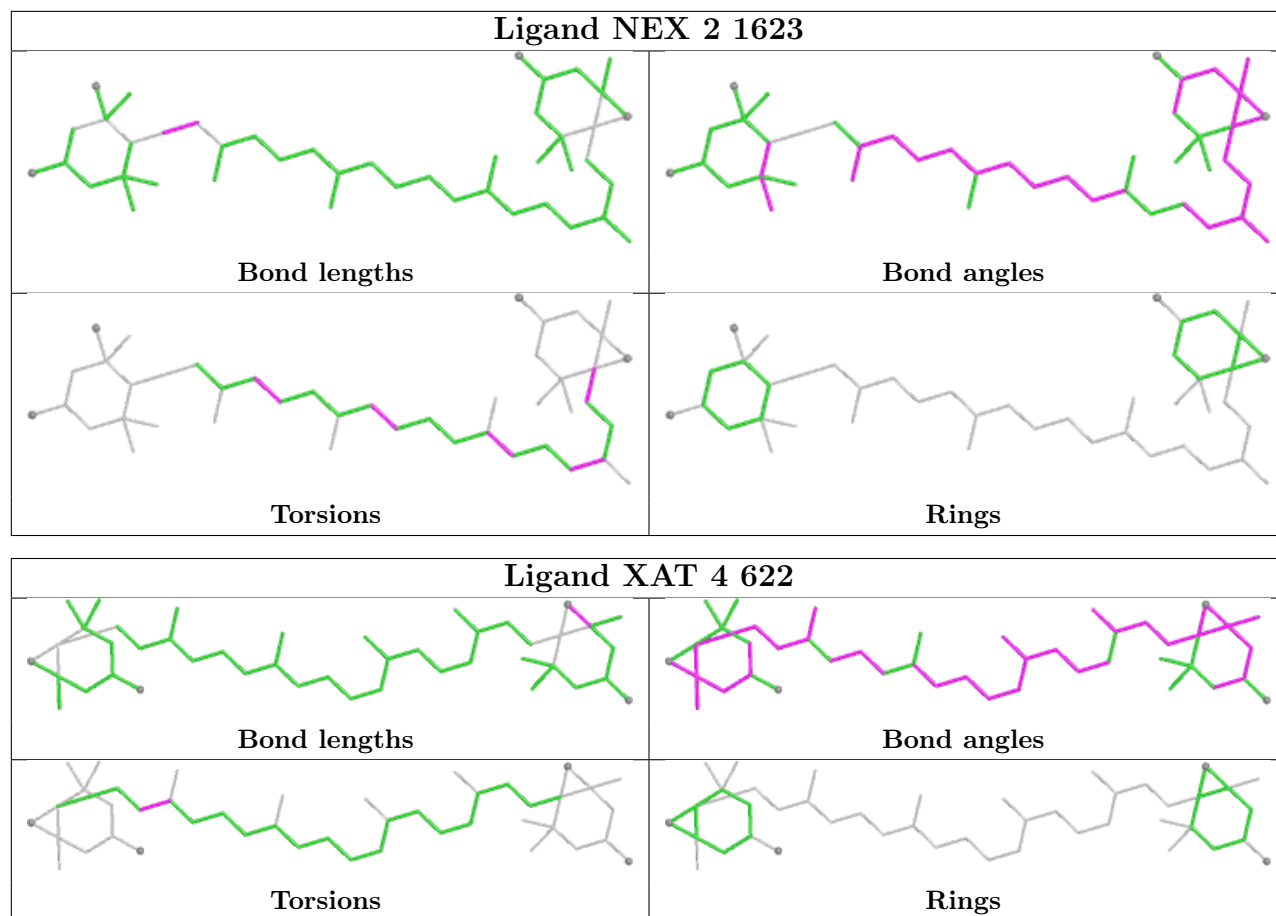
Bond angles



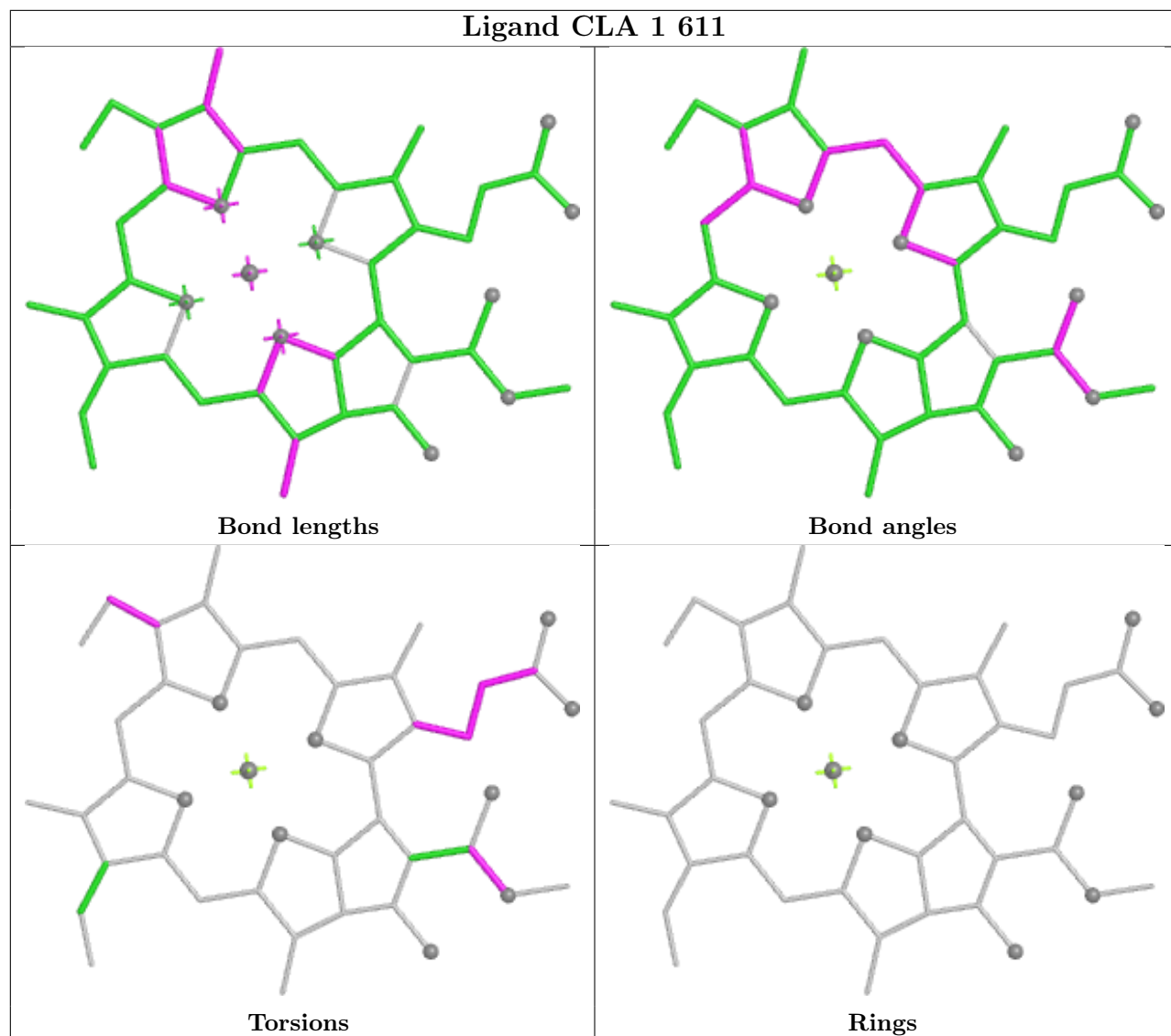
Torsions



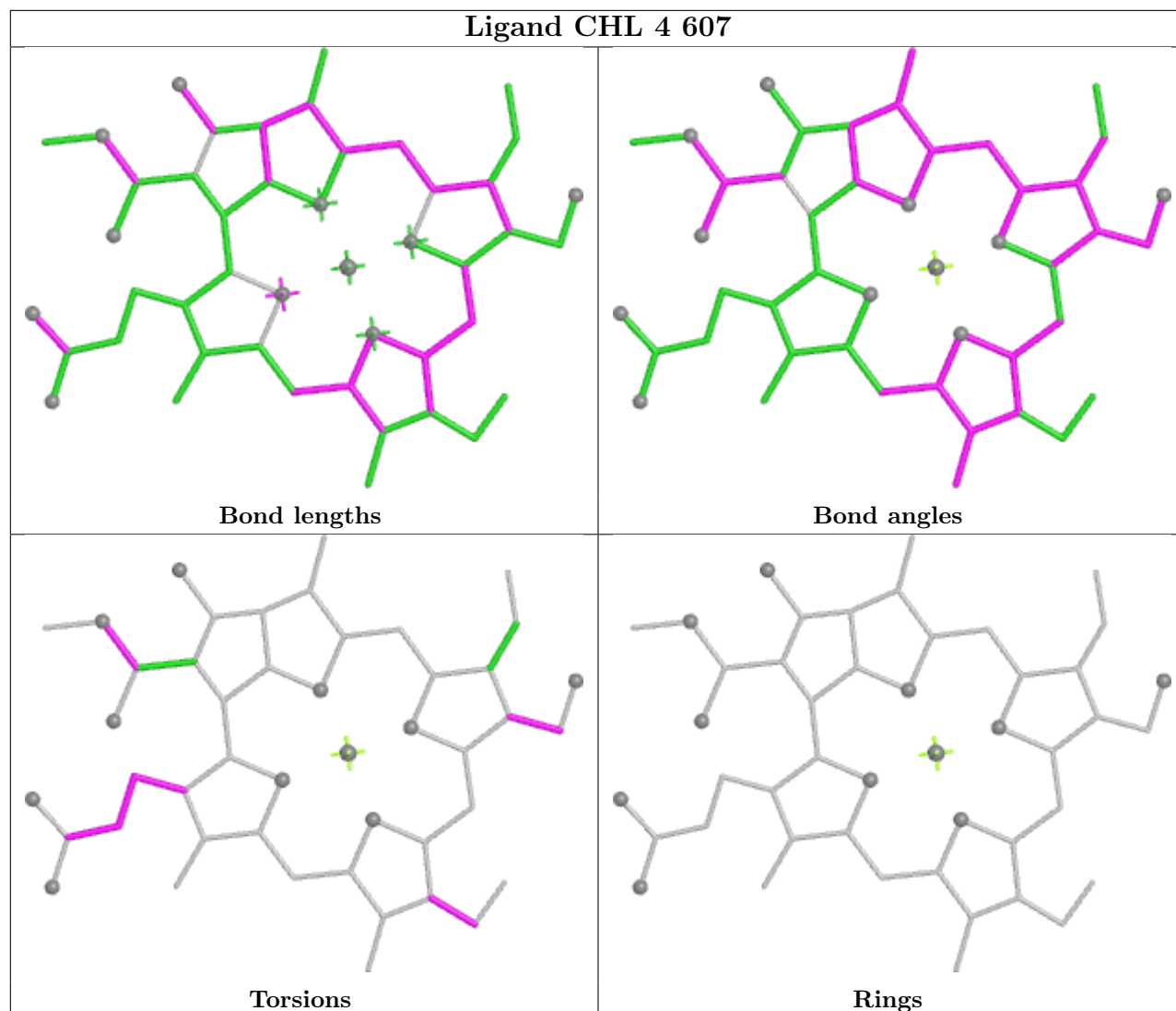
Rings

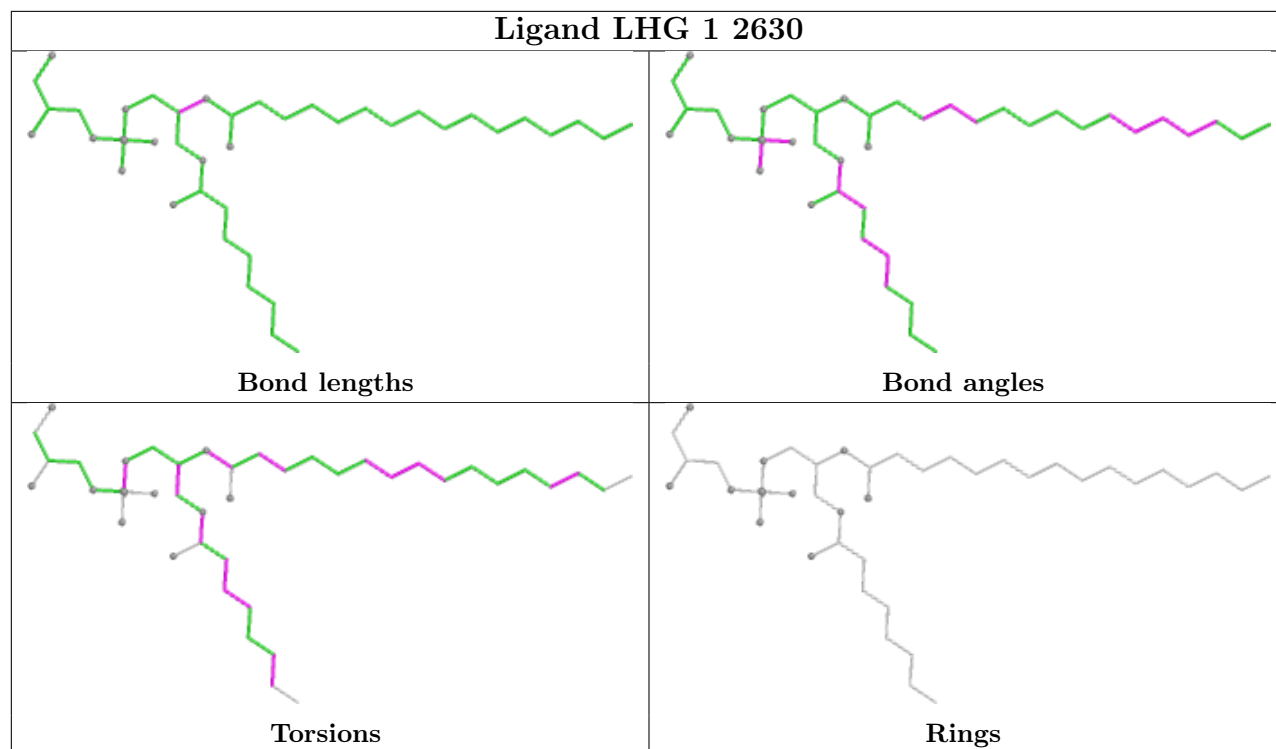


Ligand CLA 1 611

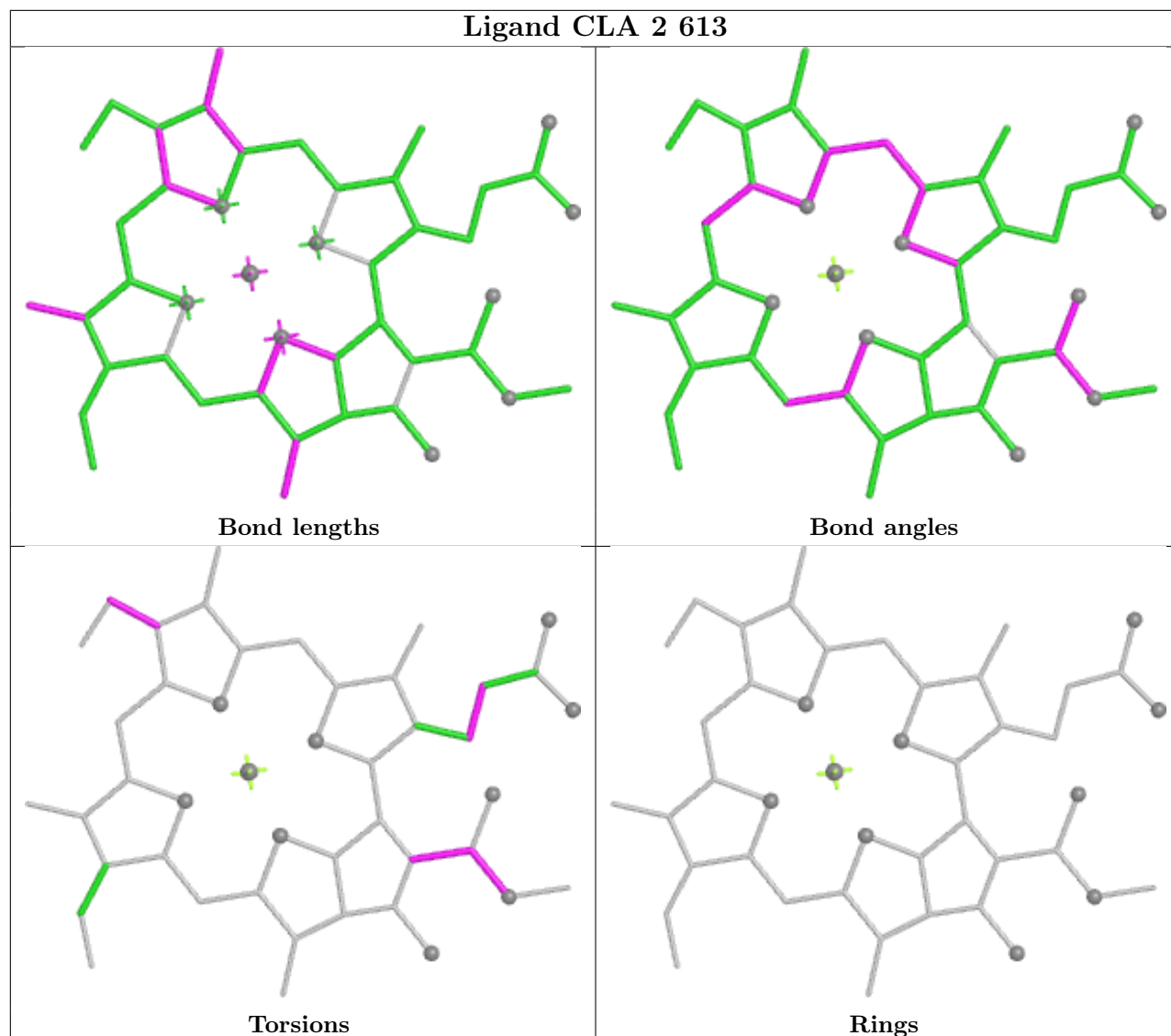


Ligand CHL 4 607

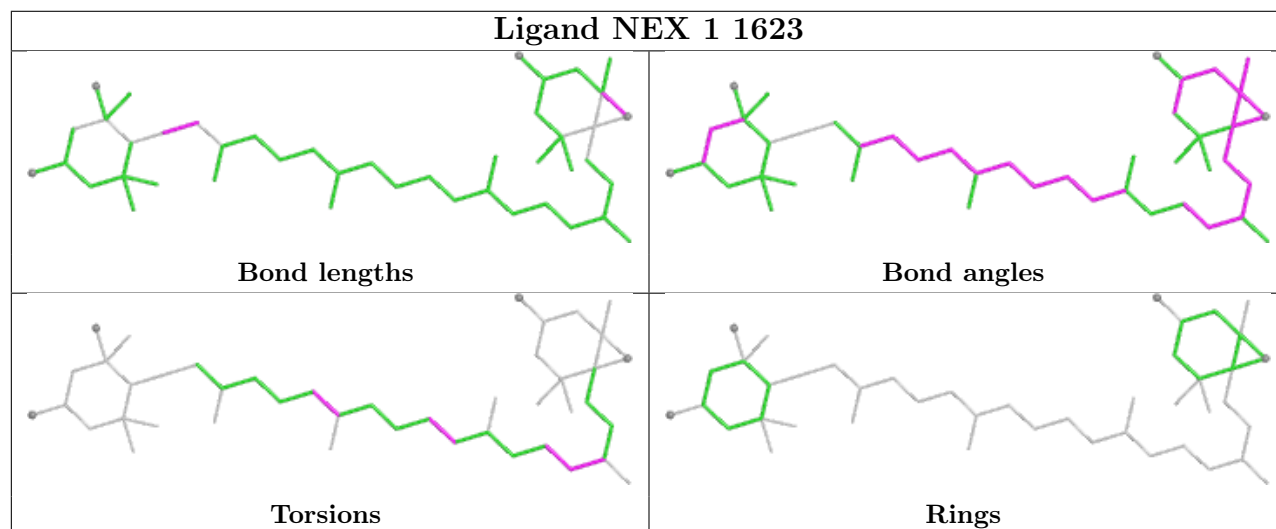


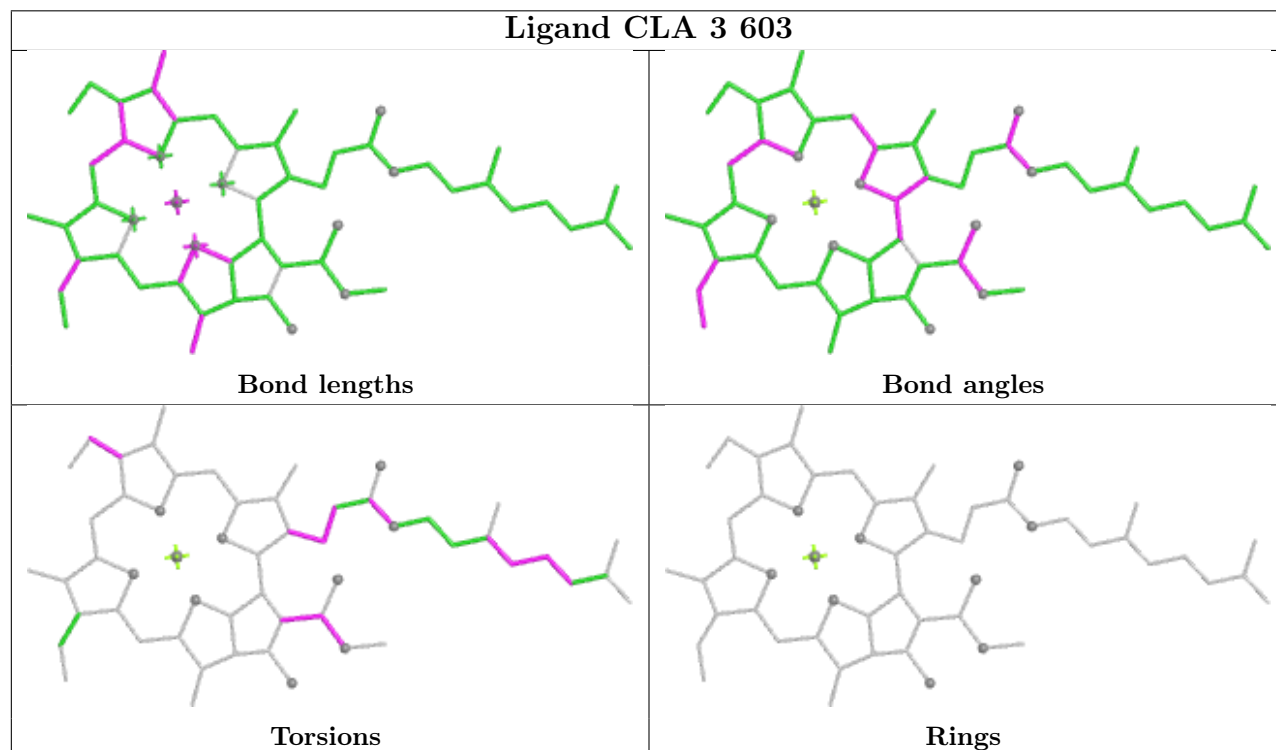
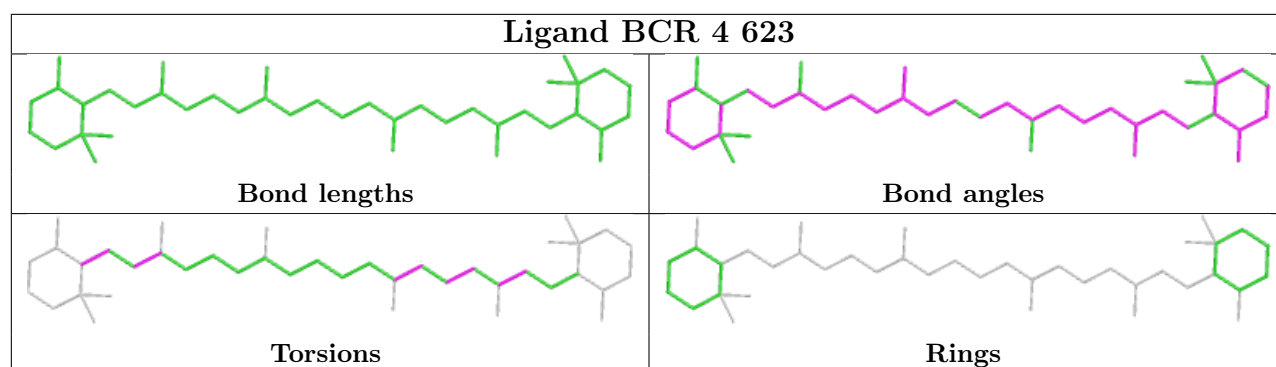


Ligand CLA 2 613

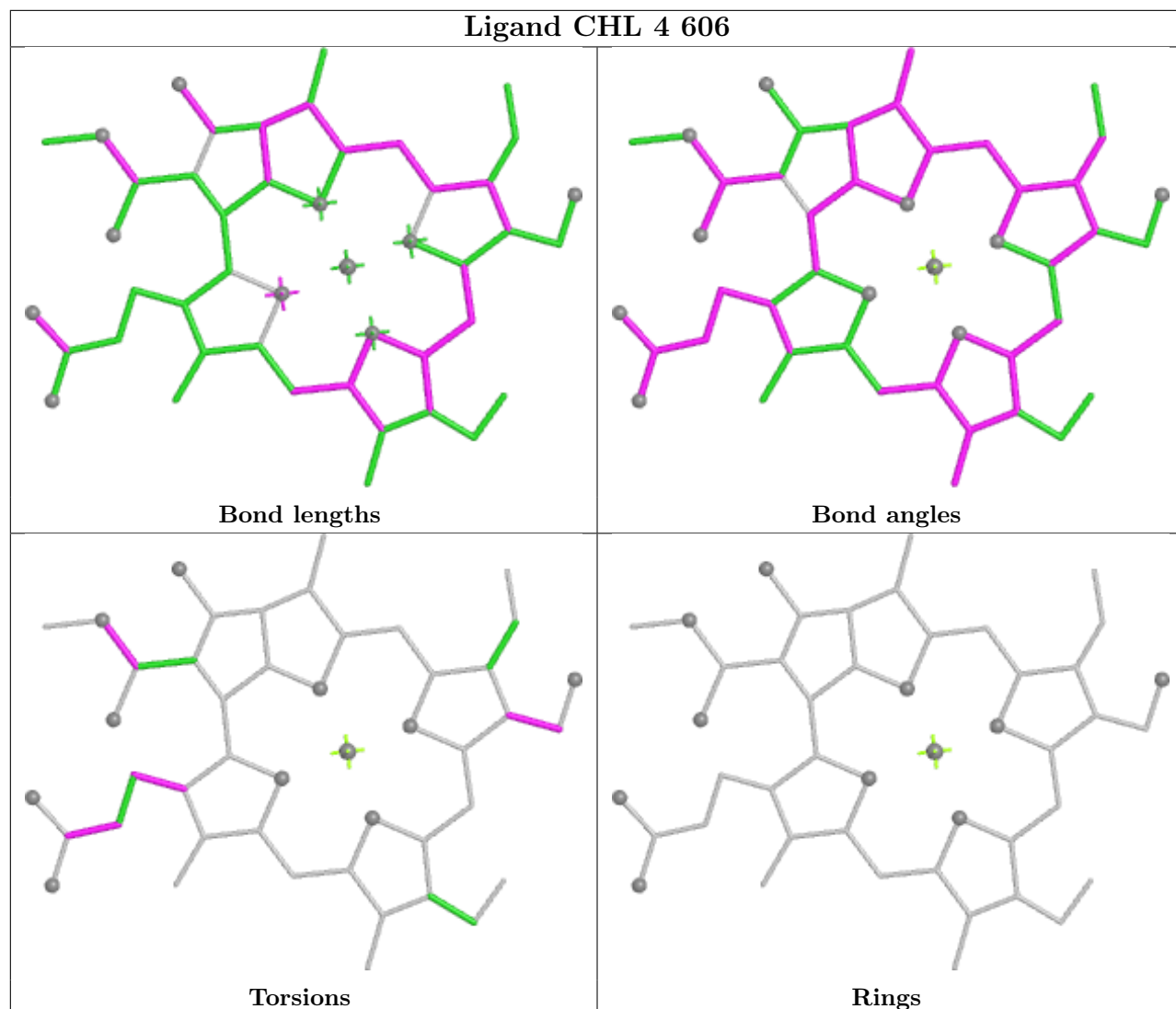


Ligand NEX 1 1623

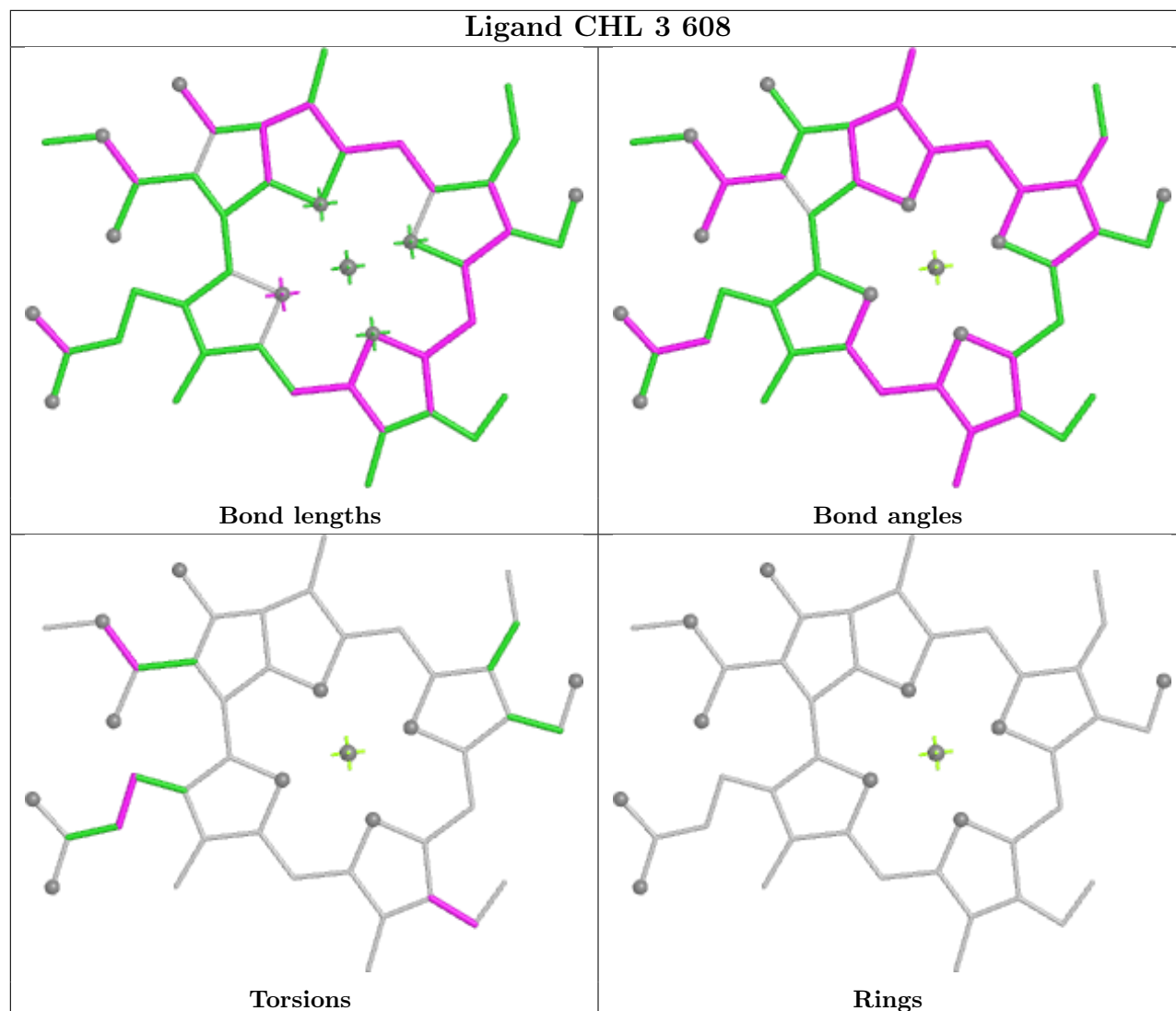




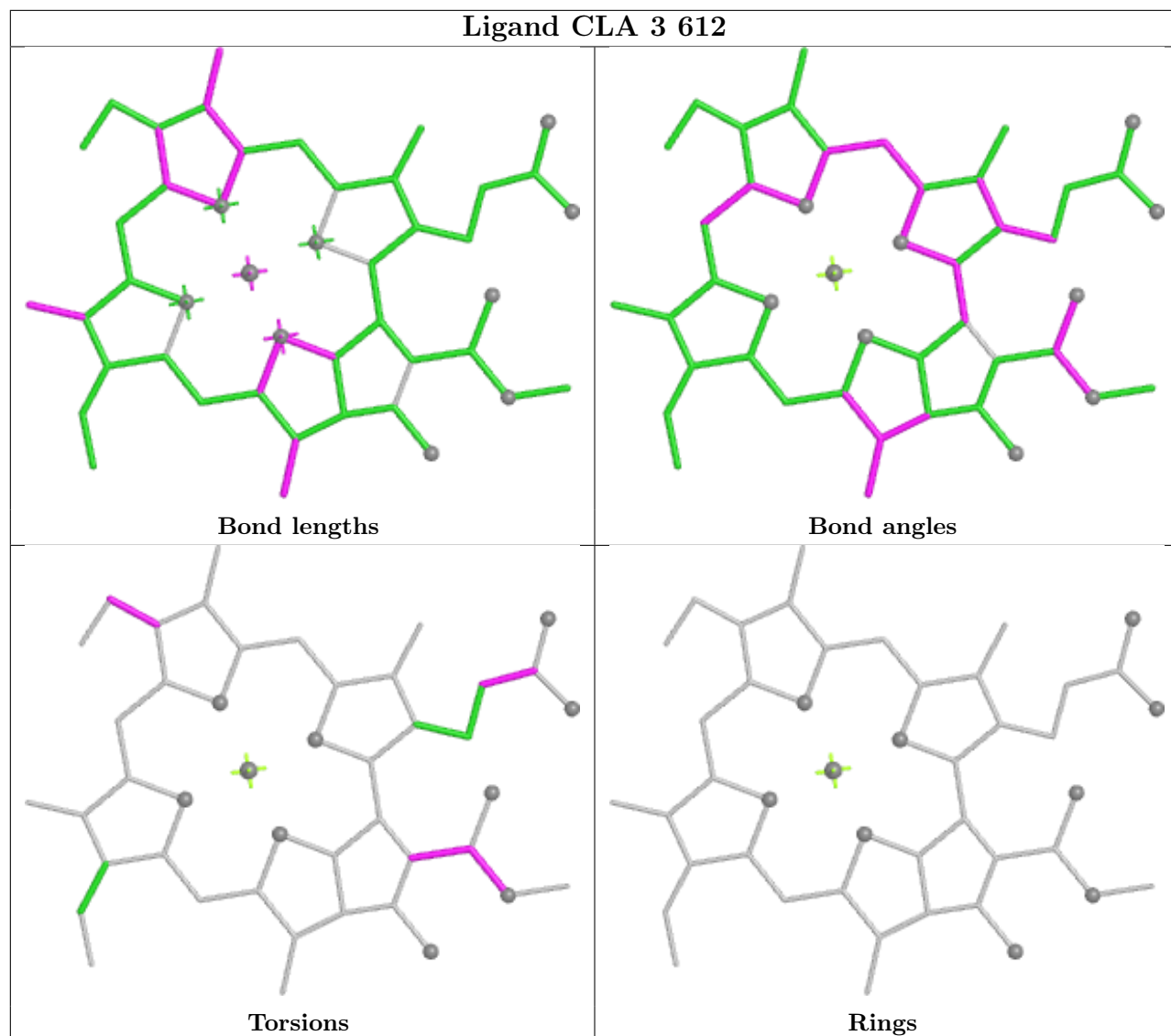
Ligand CHL 4 606



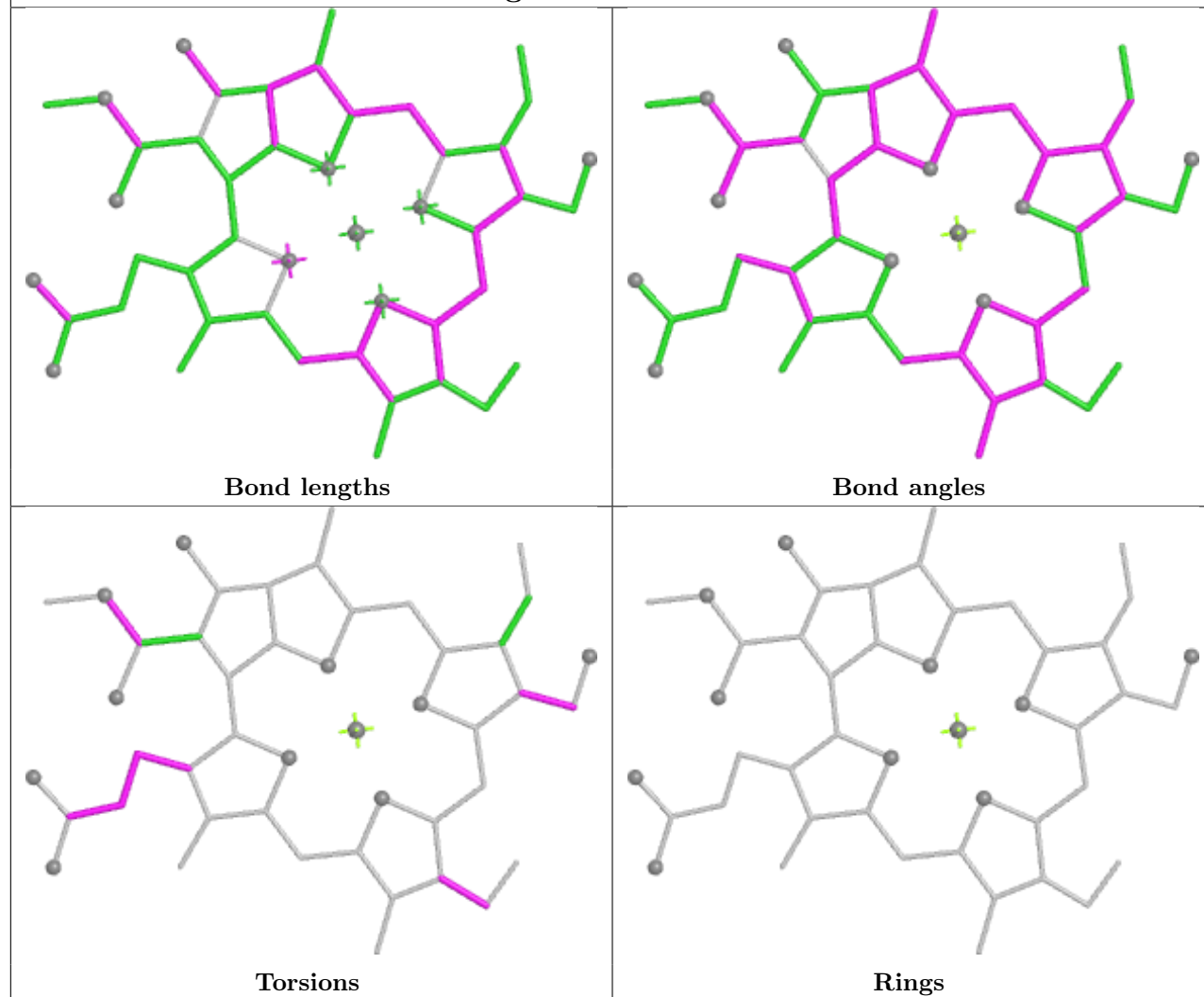
Ligand CHL 3 608



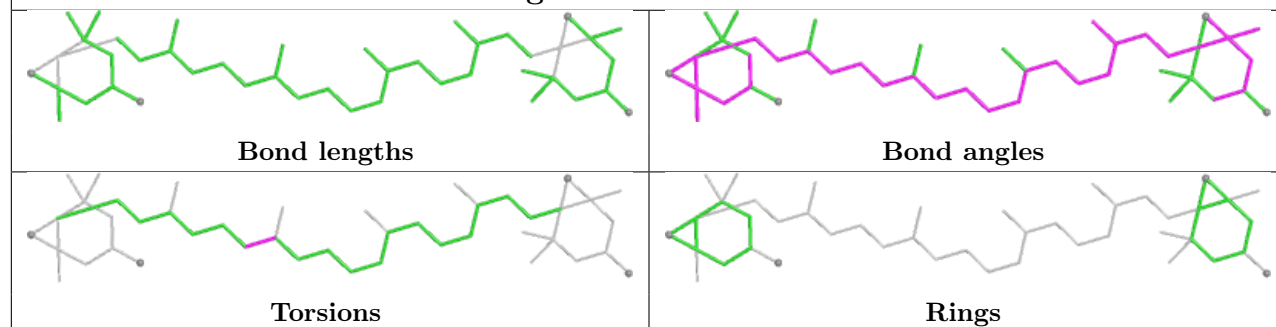
Ligand CLA 3 612



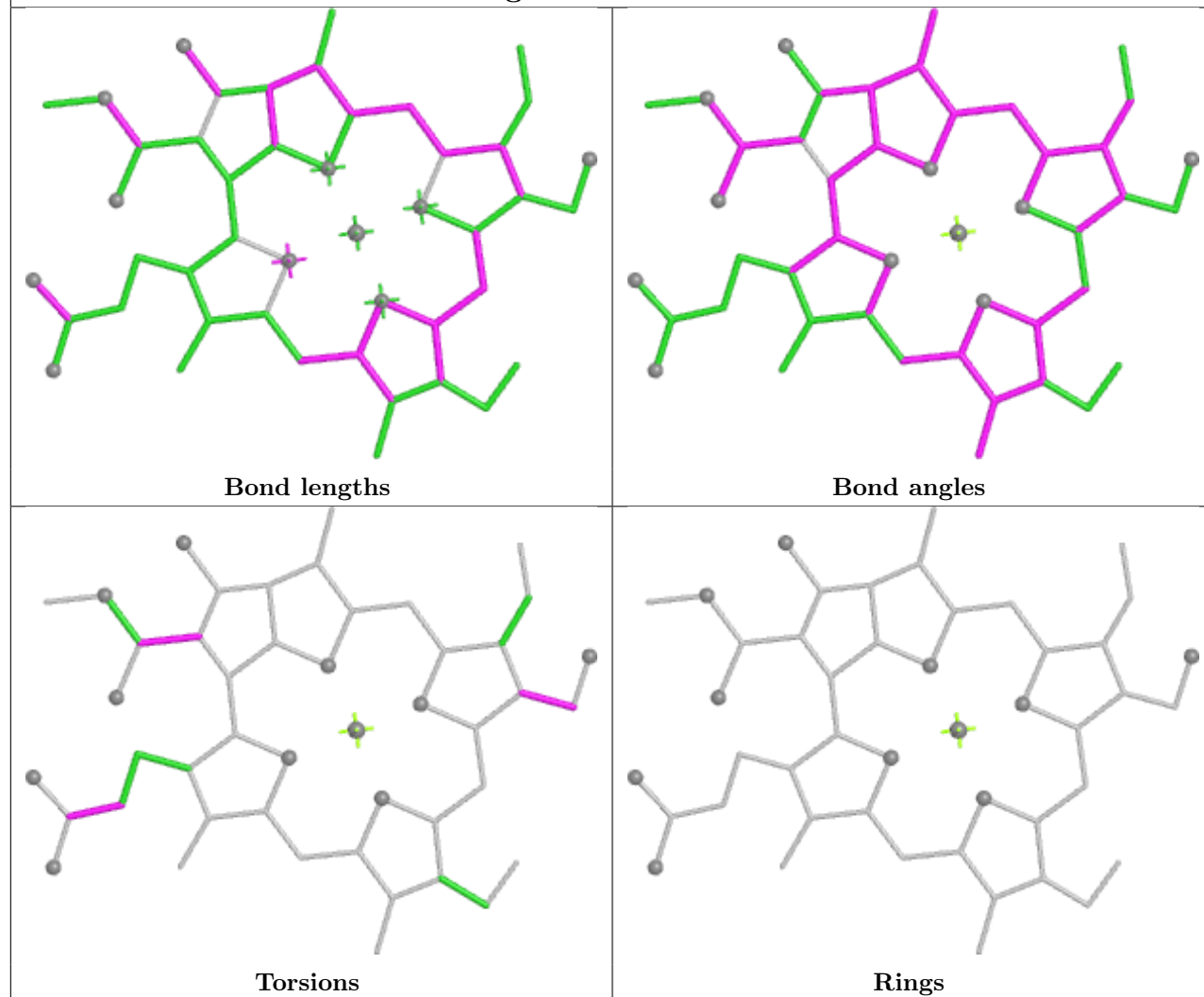
Ligand CHL 2 605



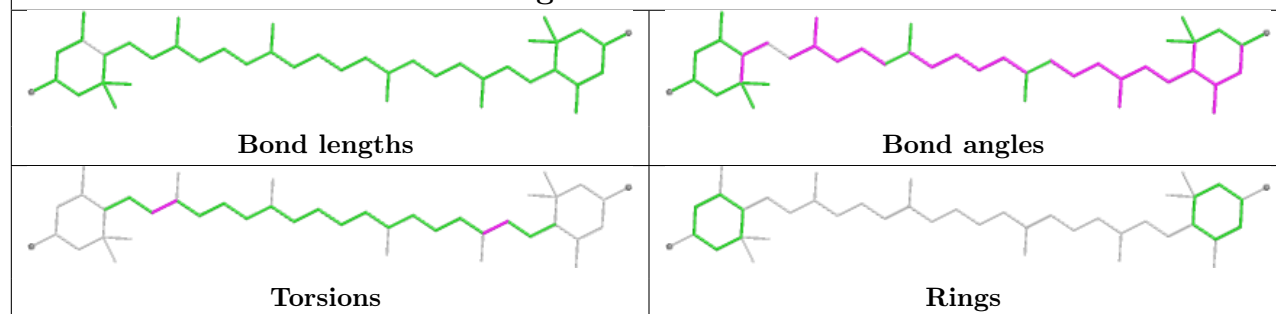
Ligand XAT 1 1622



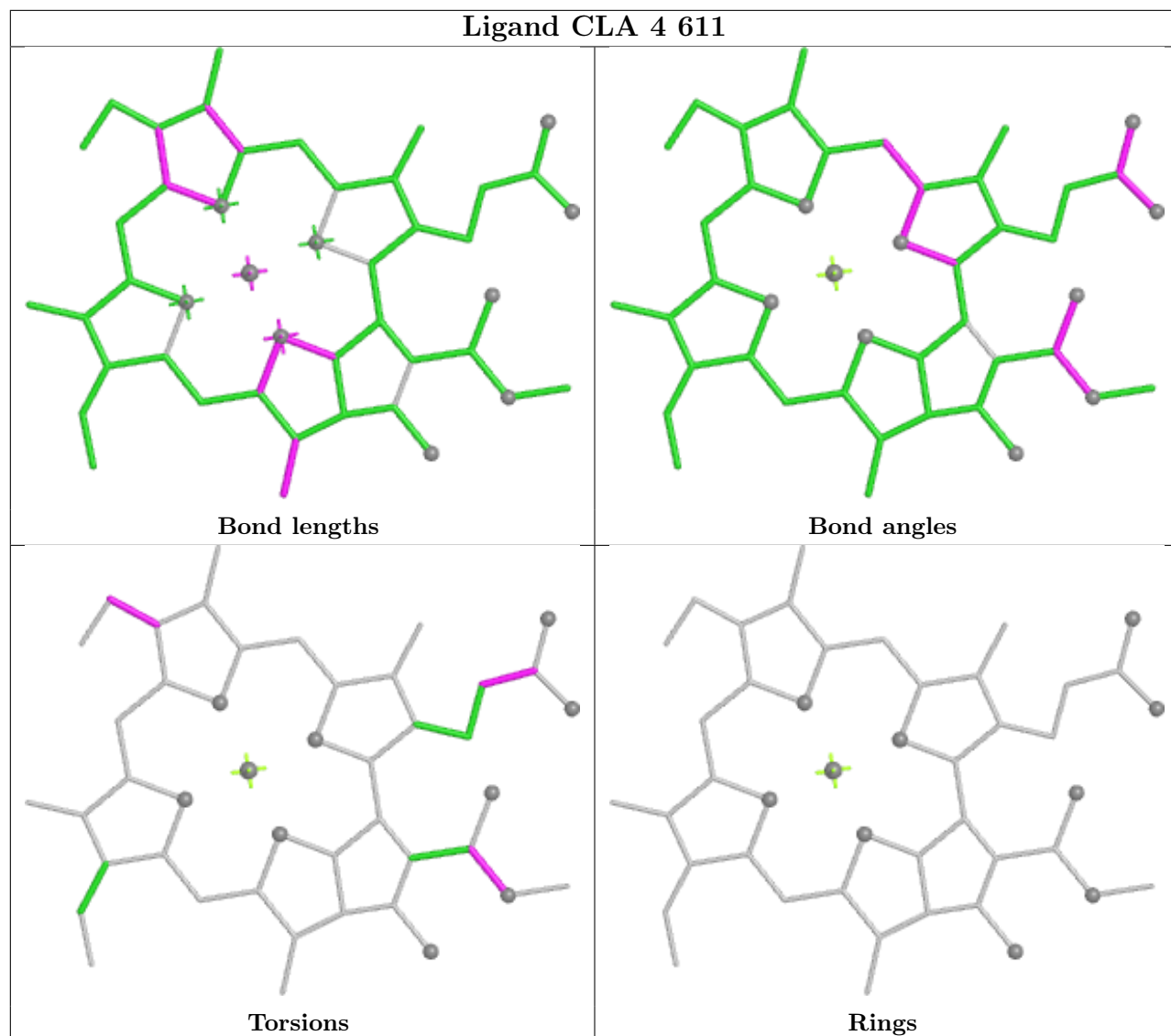
Ligand CHL 1 601

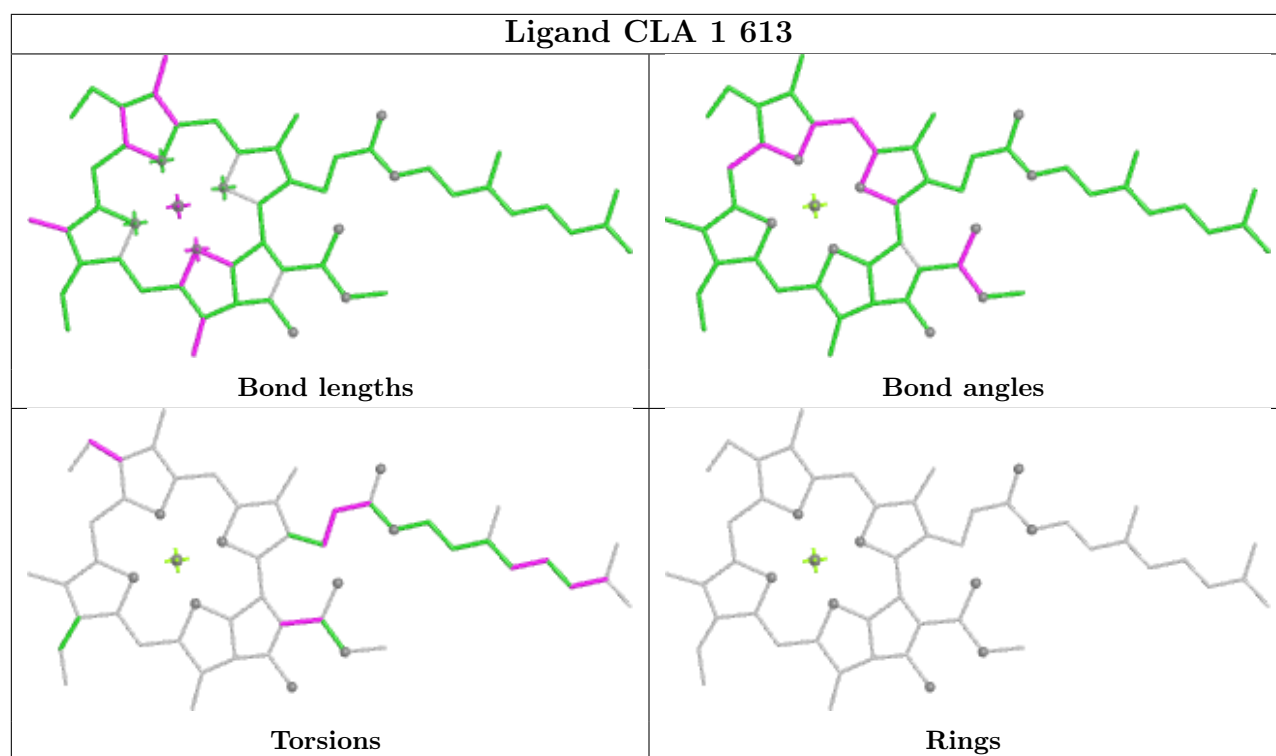


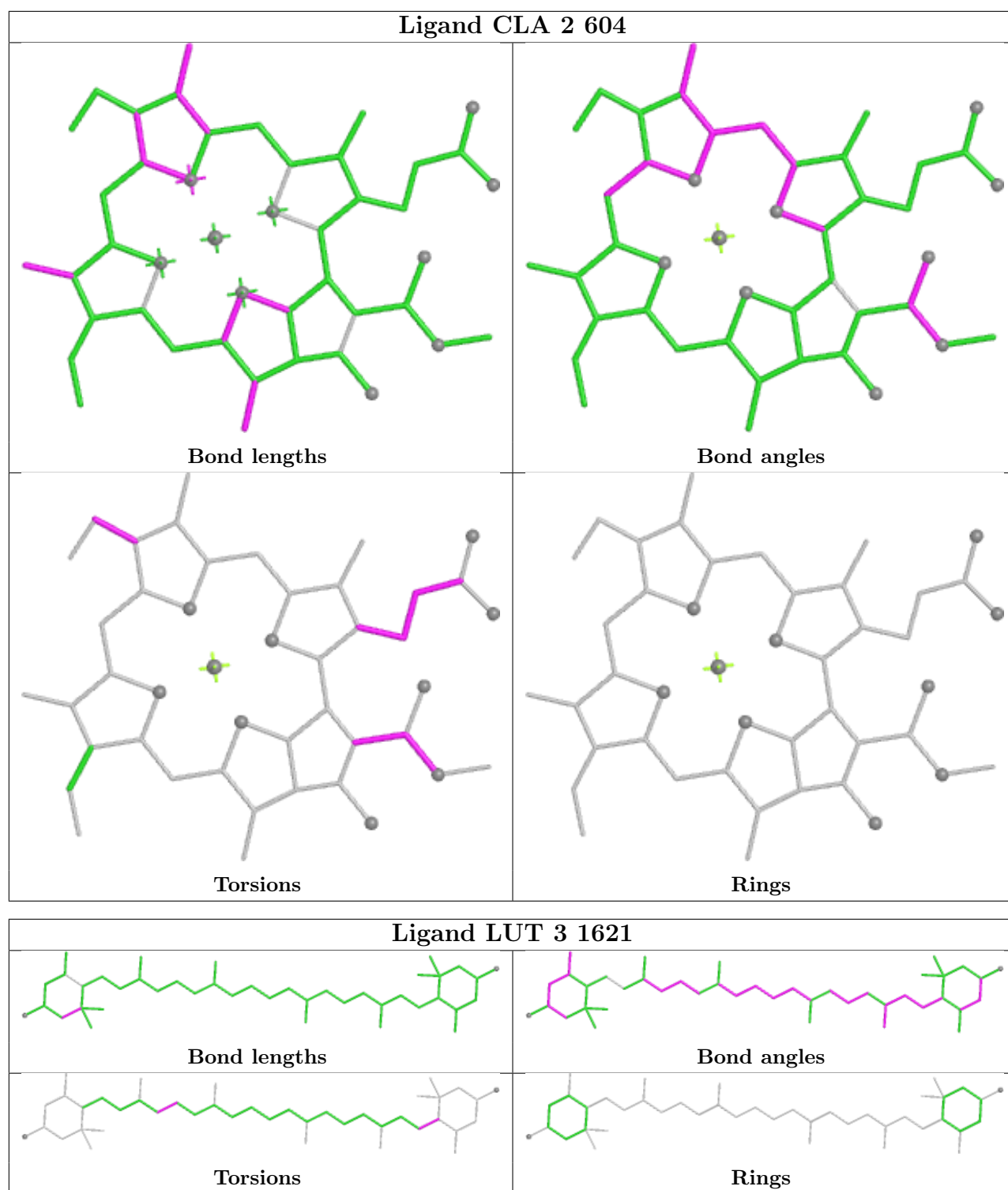
Ligand LUT 4 620



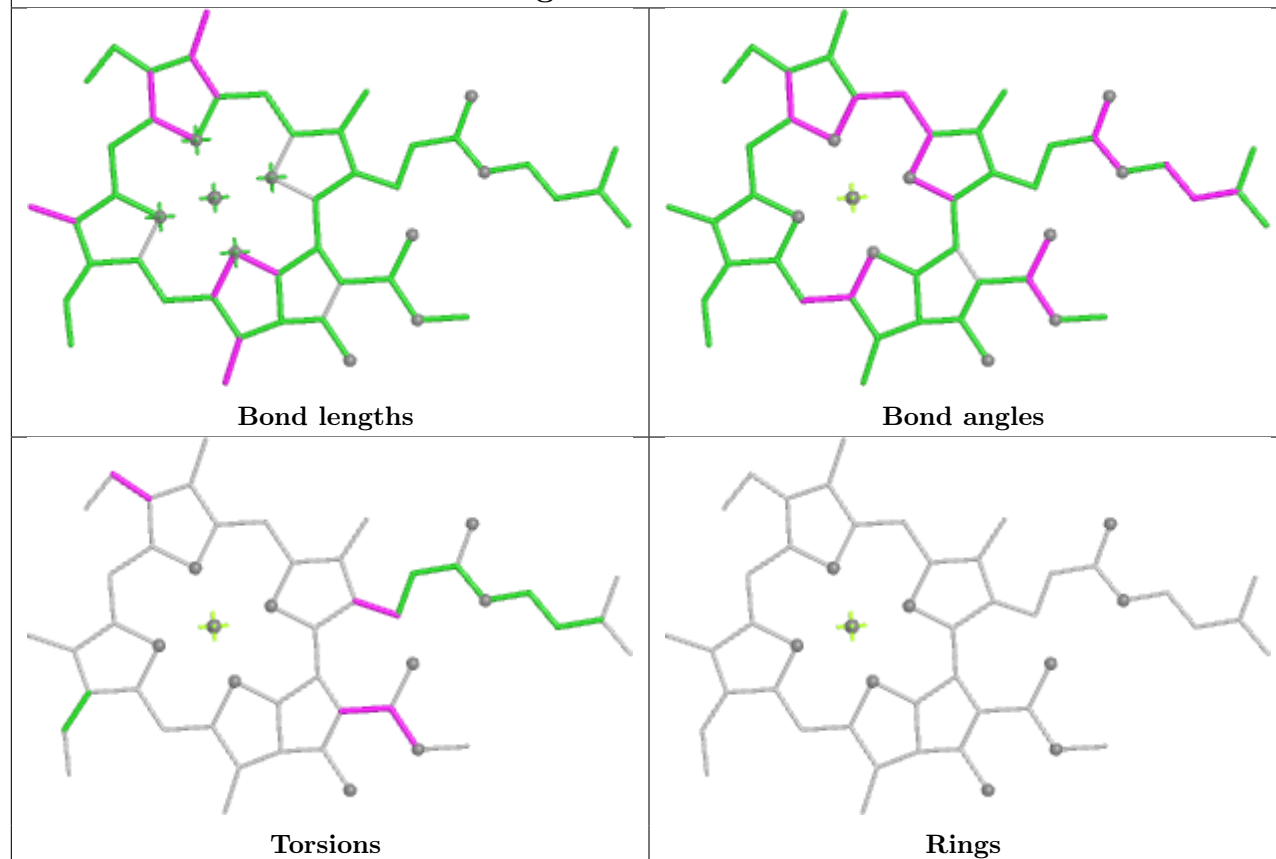
Ligand CLA 4 611



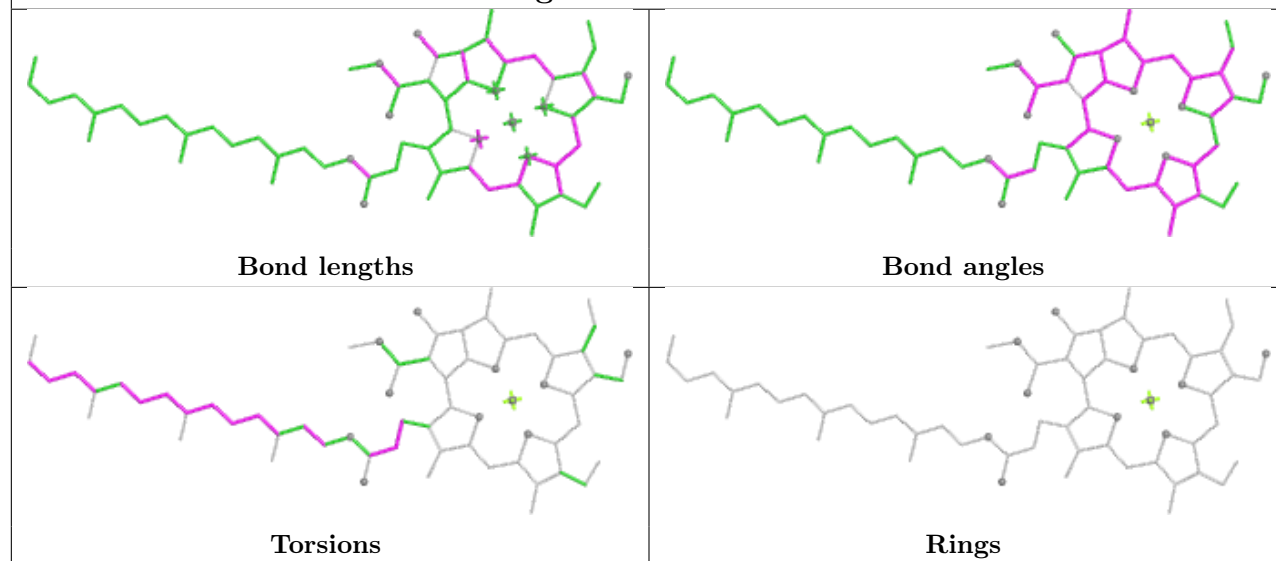




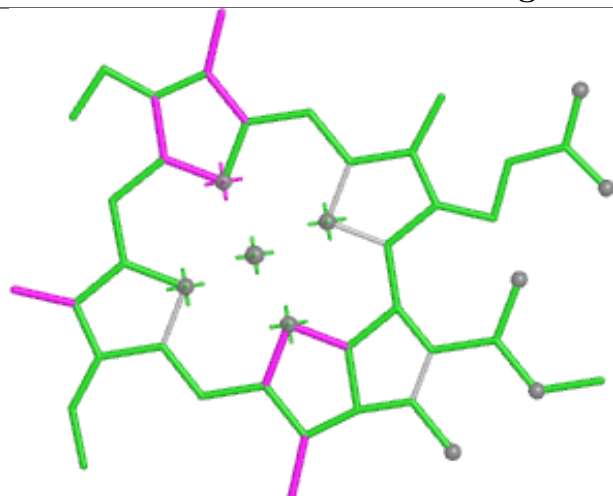
Ligand CLA 2 610



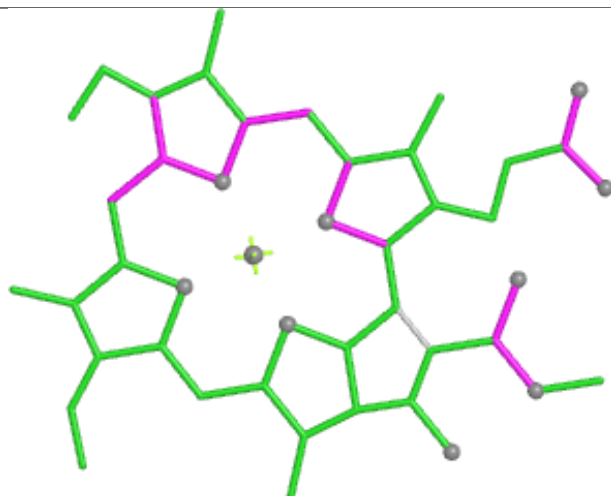
Ligand CHL 3 601



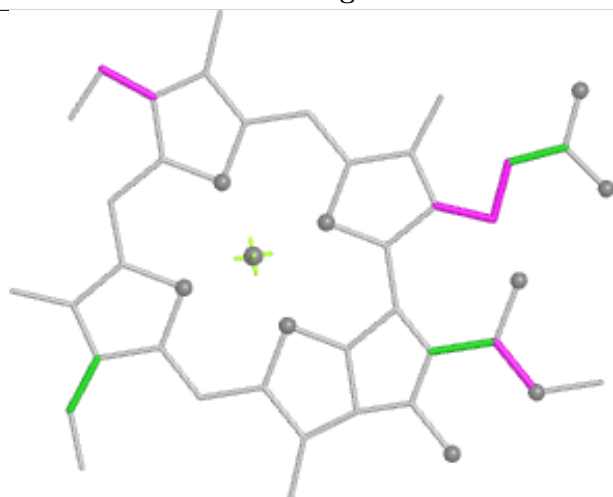
Ligand CLA 4 610



Bond lengths



Bond angles

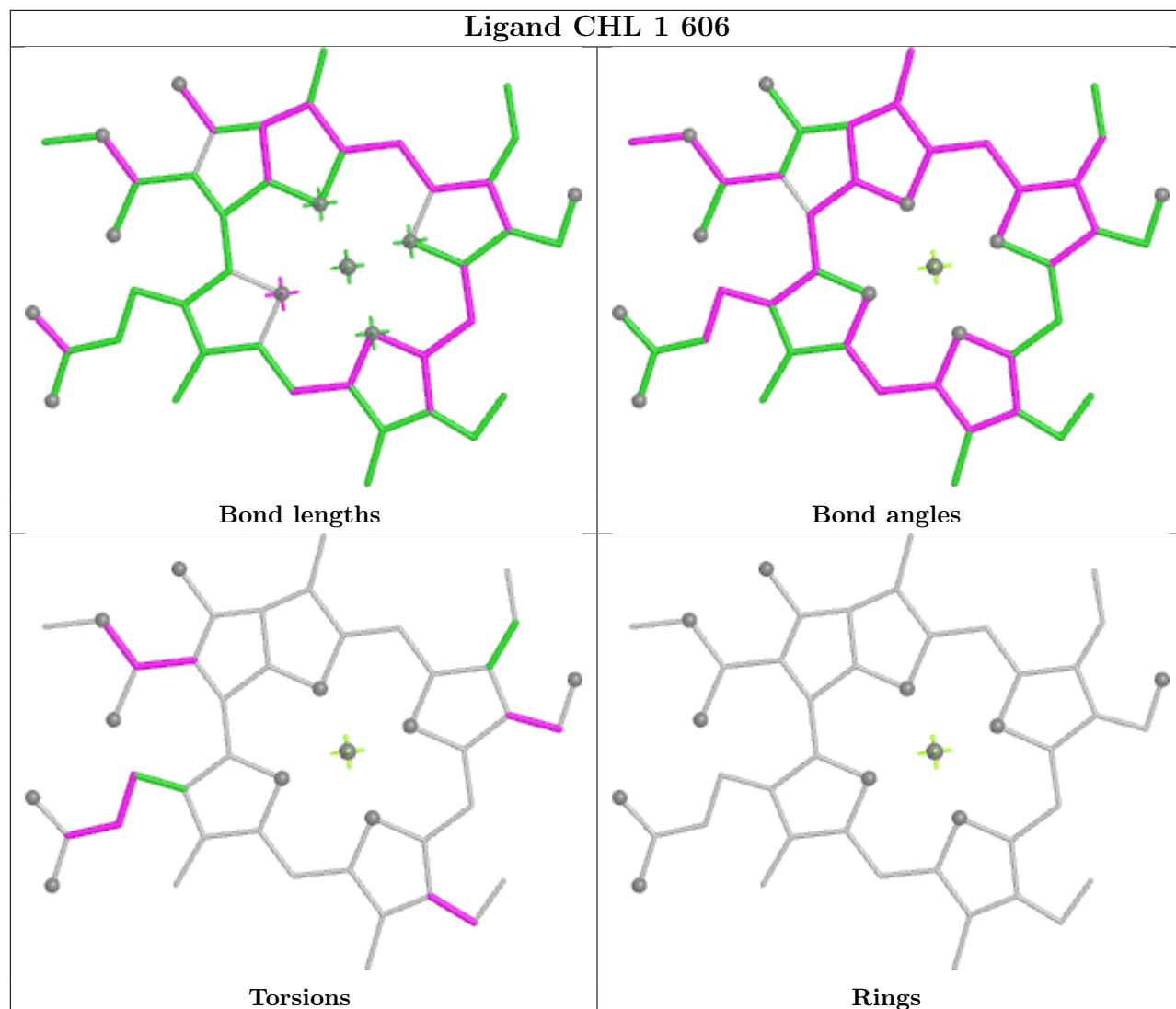


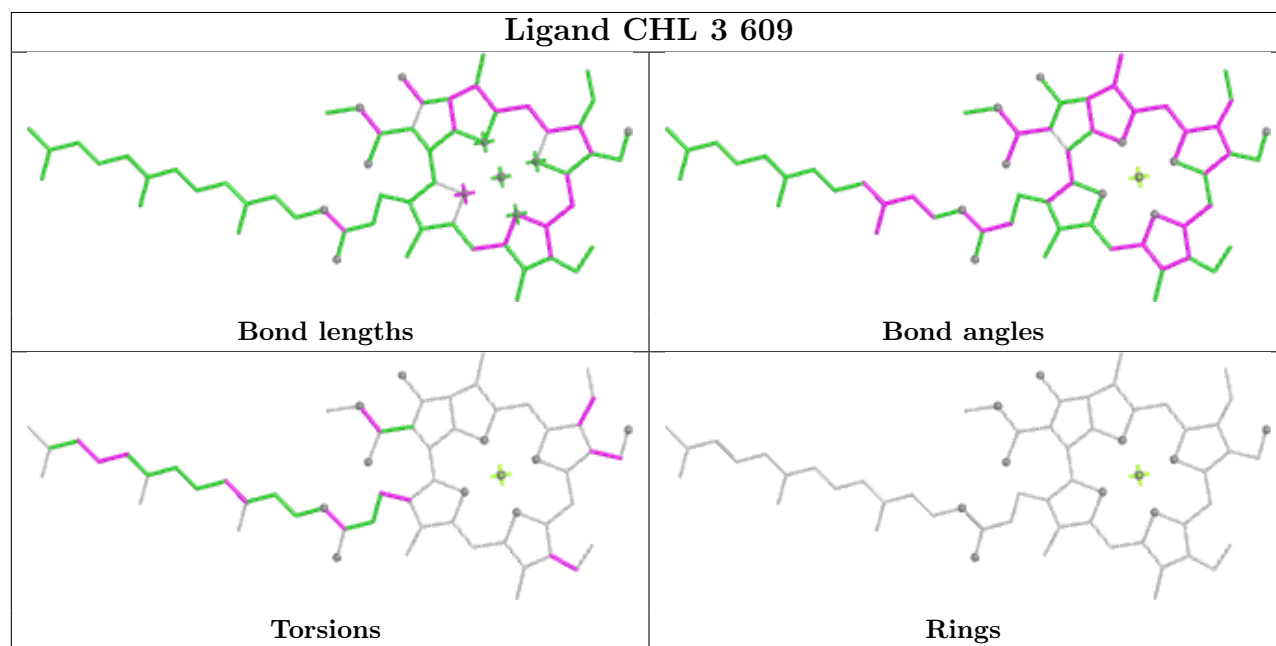
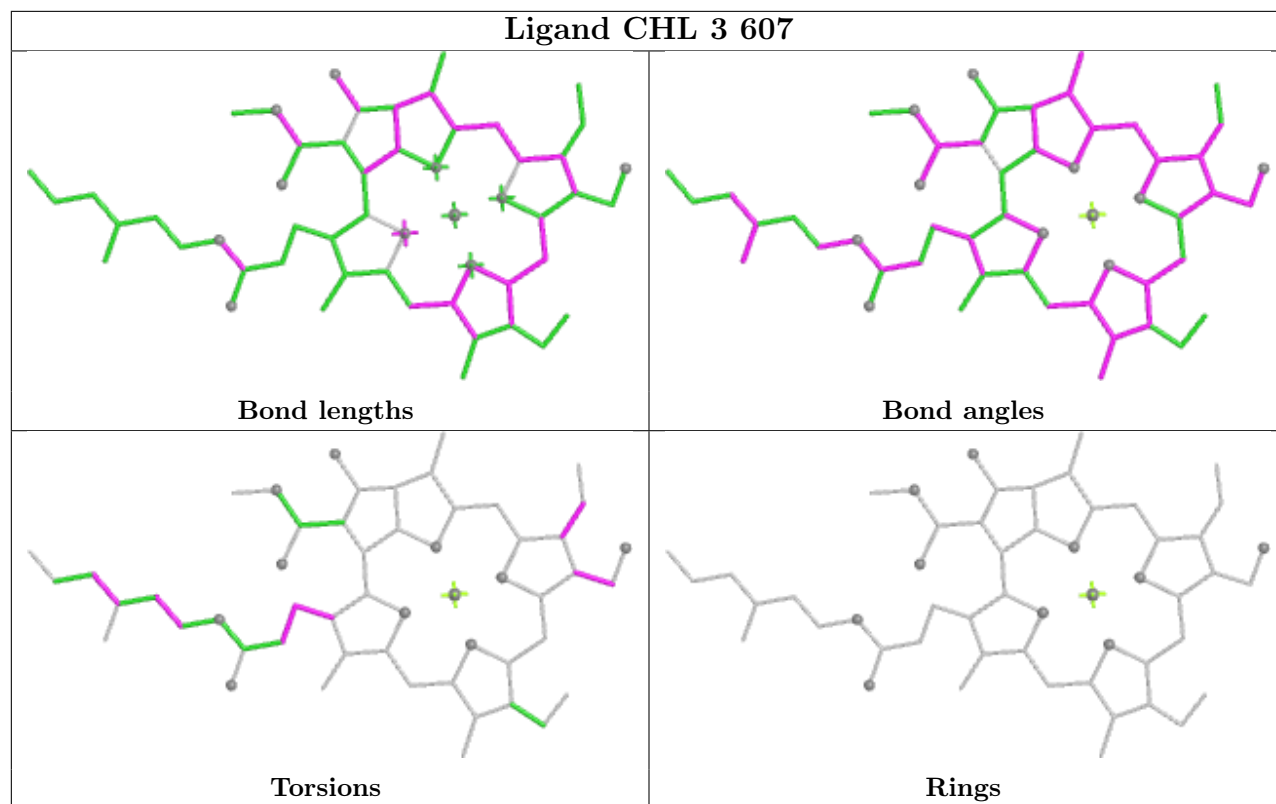
Torsions



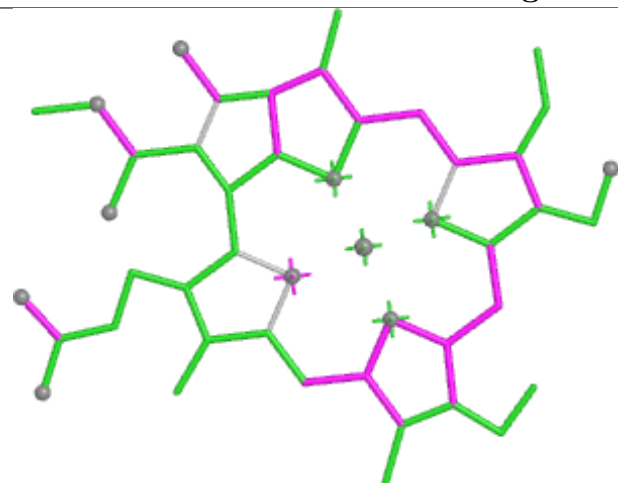
Rings

Ligand CHL 1 606

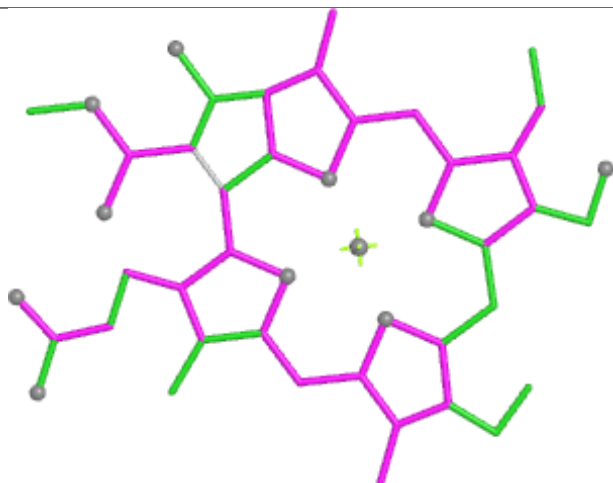




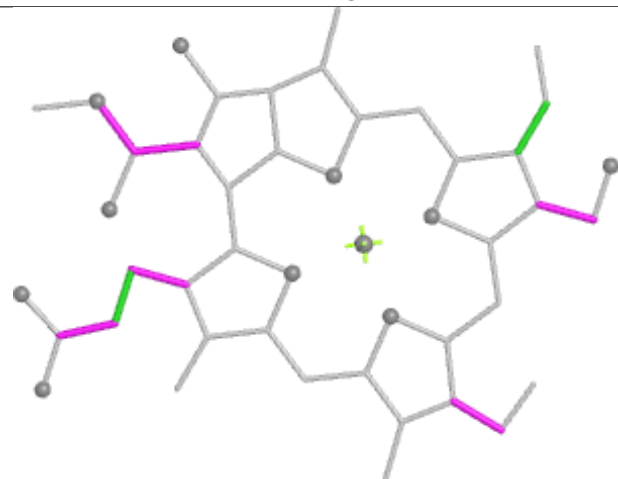
Ligand CHL 1 605



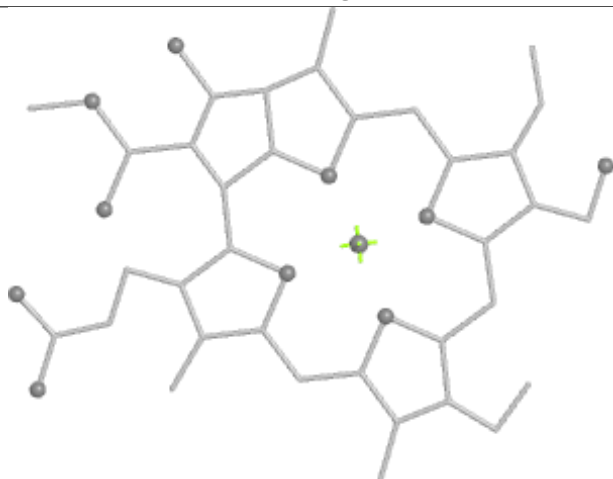
Bond lengths



Bond angles

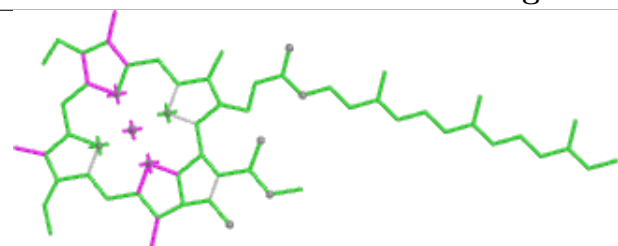


Torsions

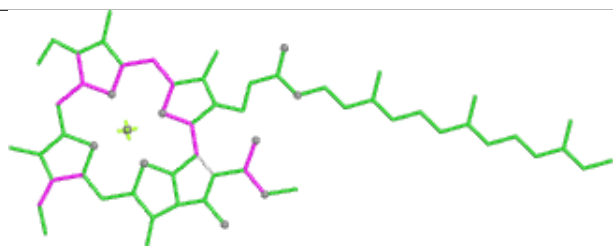


Rings

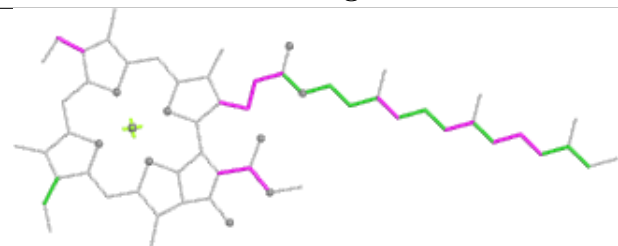
Ligand CLA 1 602



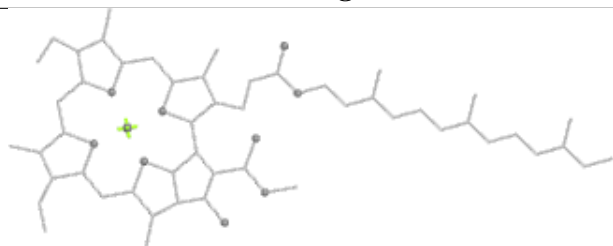
Bond lengths



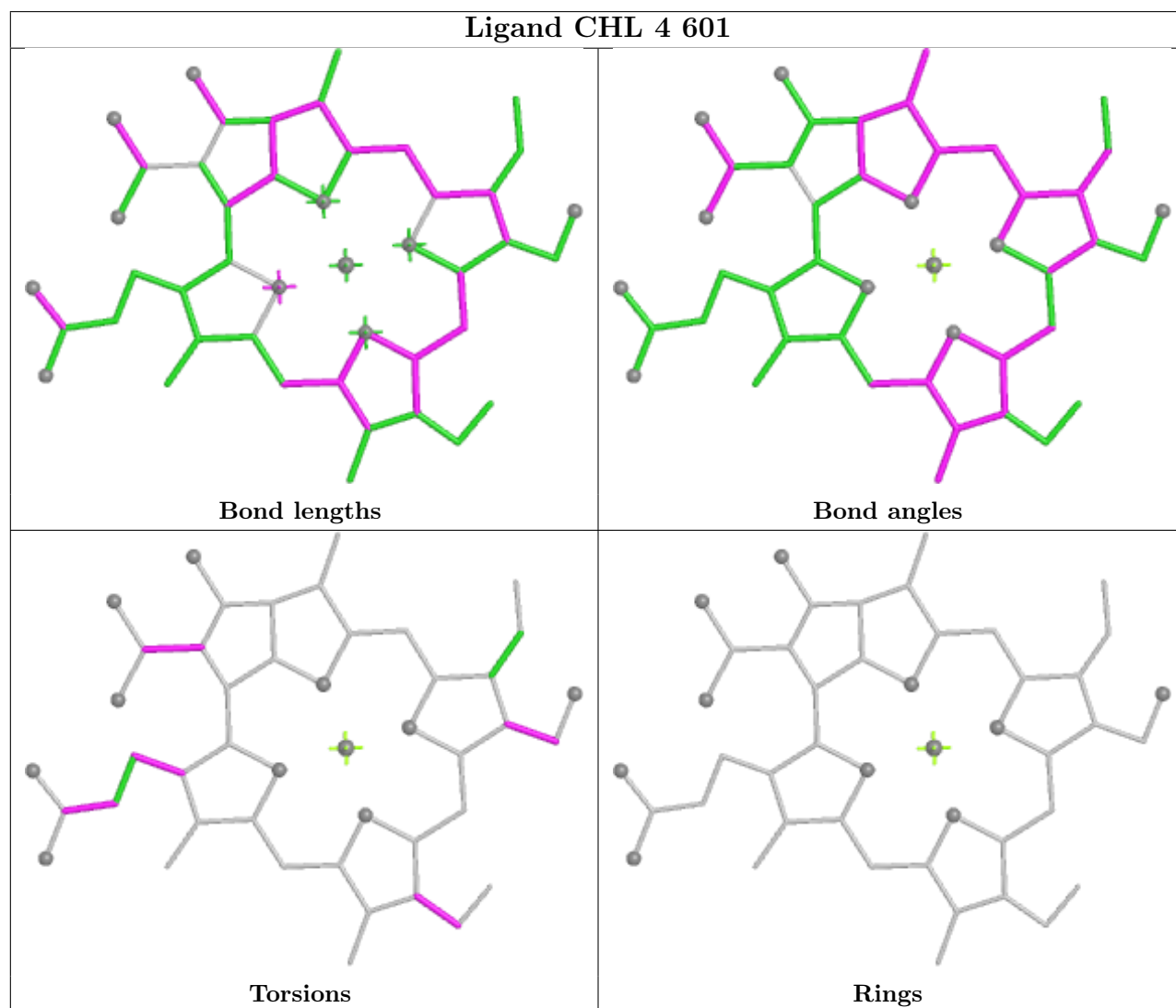
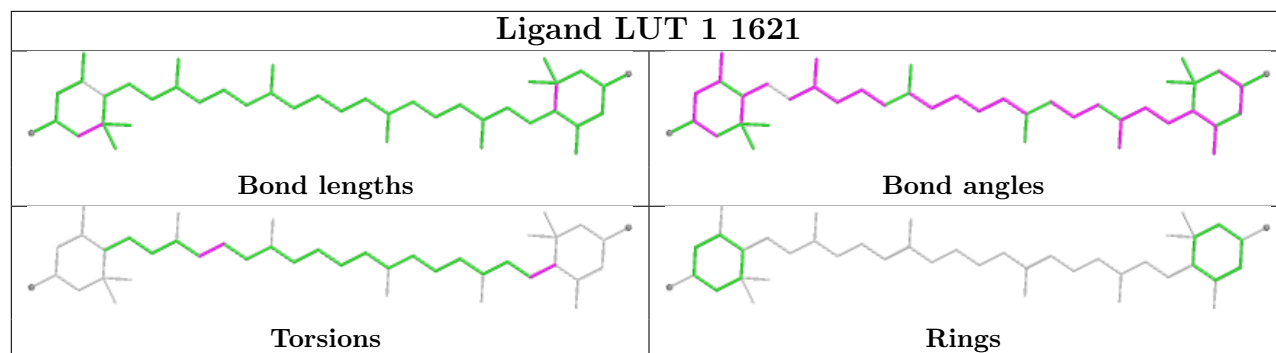
Bond angles



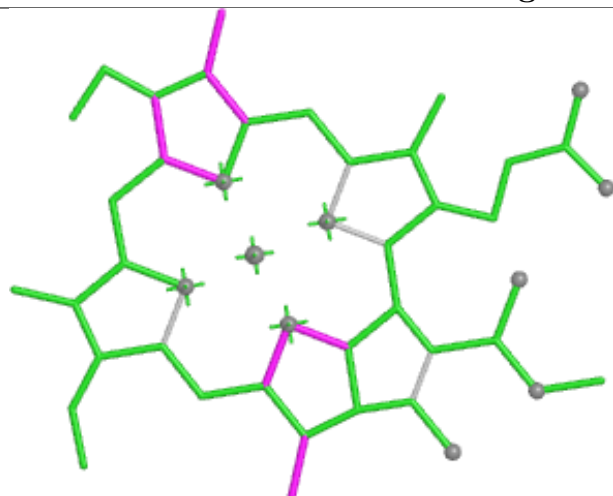
Torsions



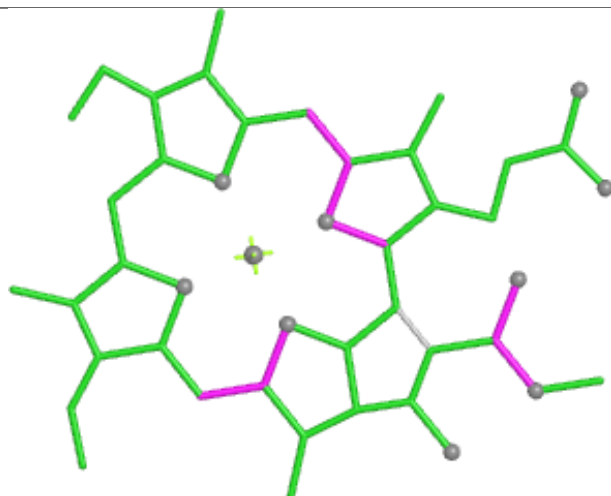
Rings



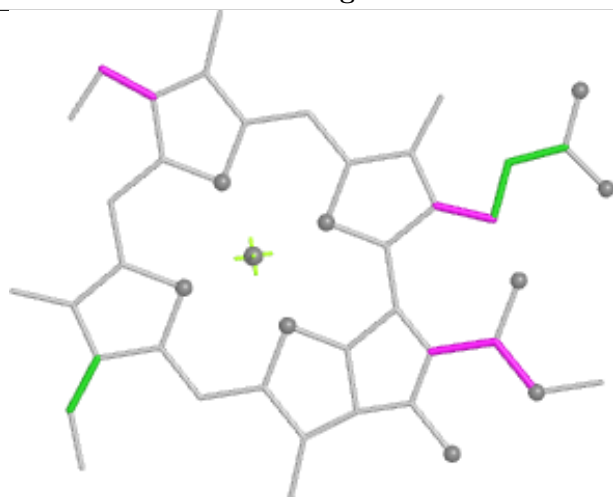
Ligand CLA 2 614



Bond lengths



Bond angles

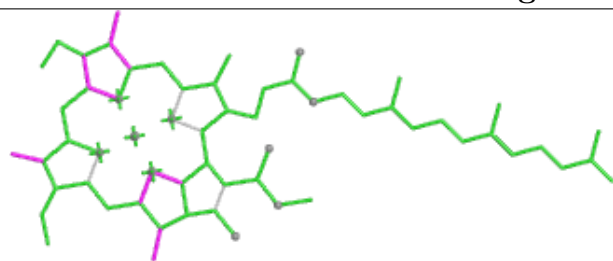


Torsions

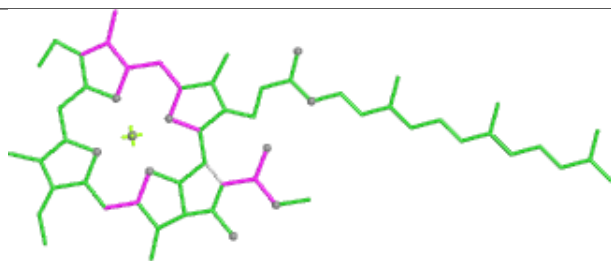


Rings

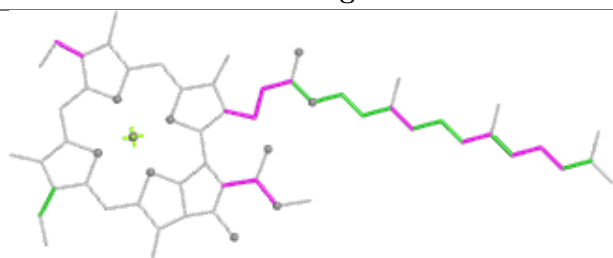
Ligand CLA 3 602



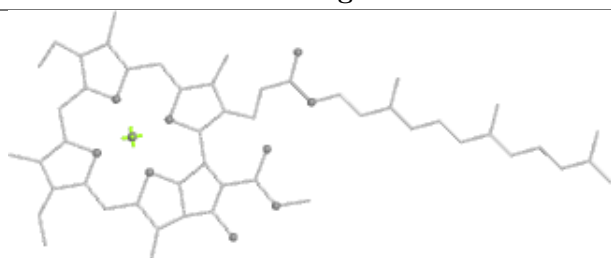
Bond lengths



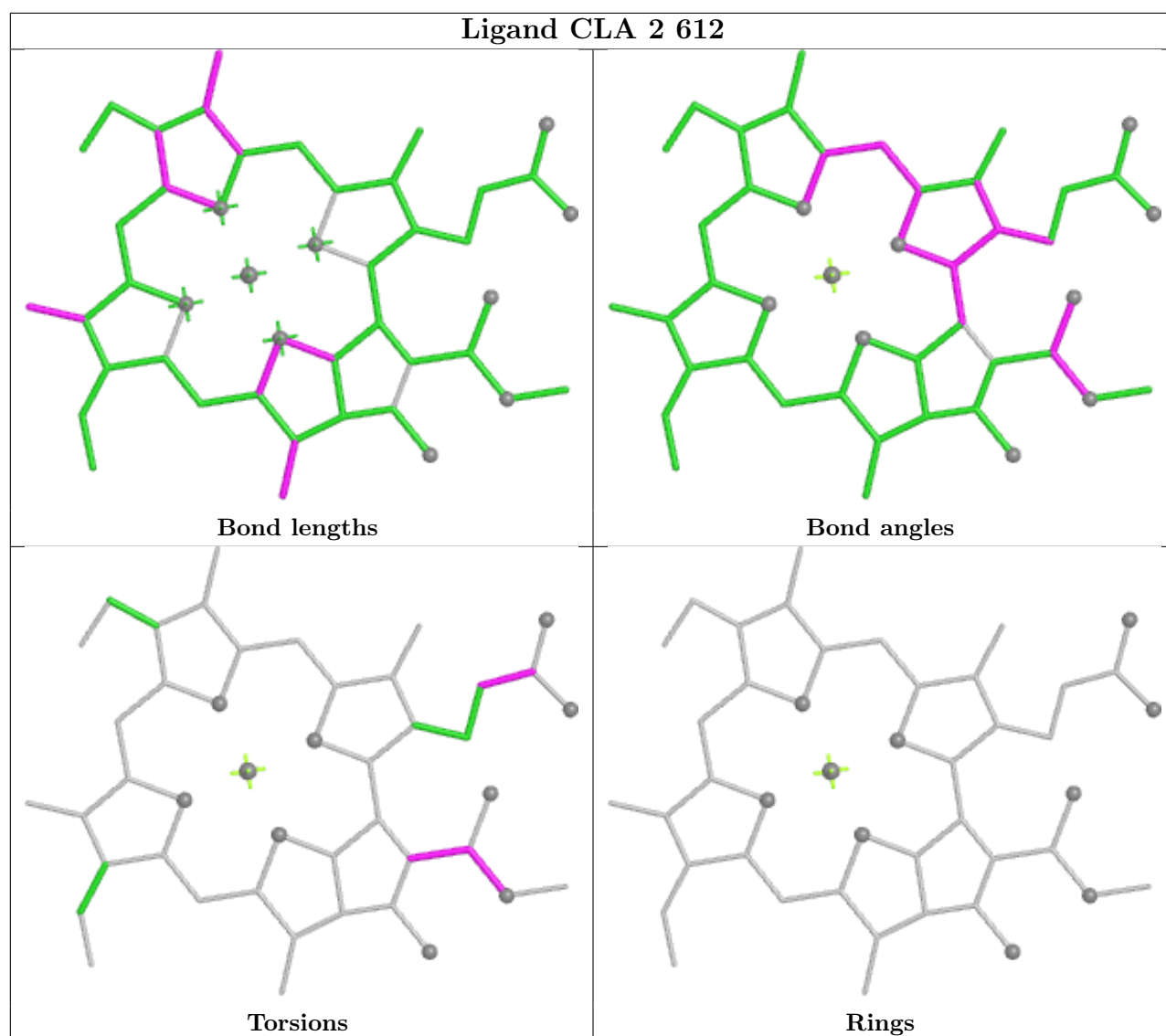
Bond angles



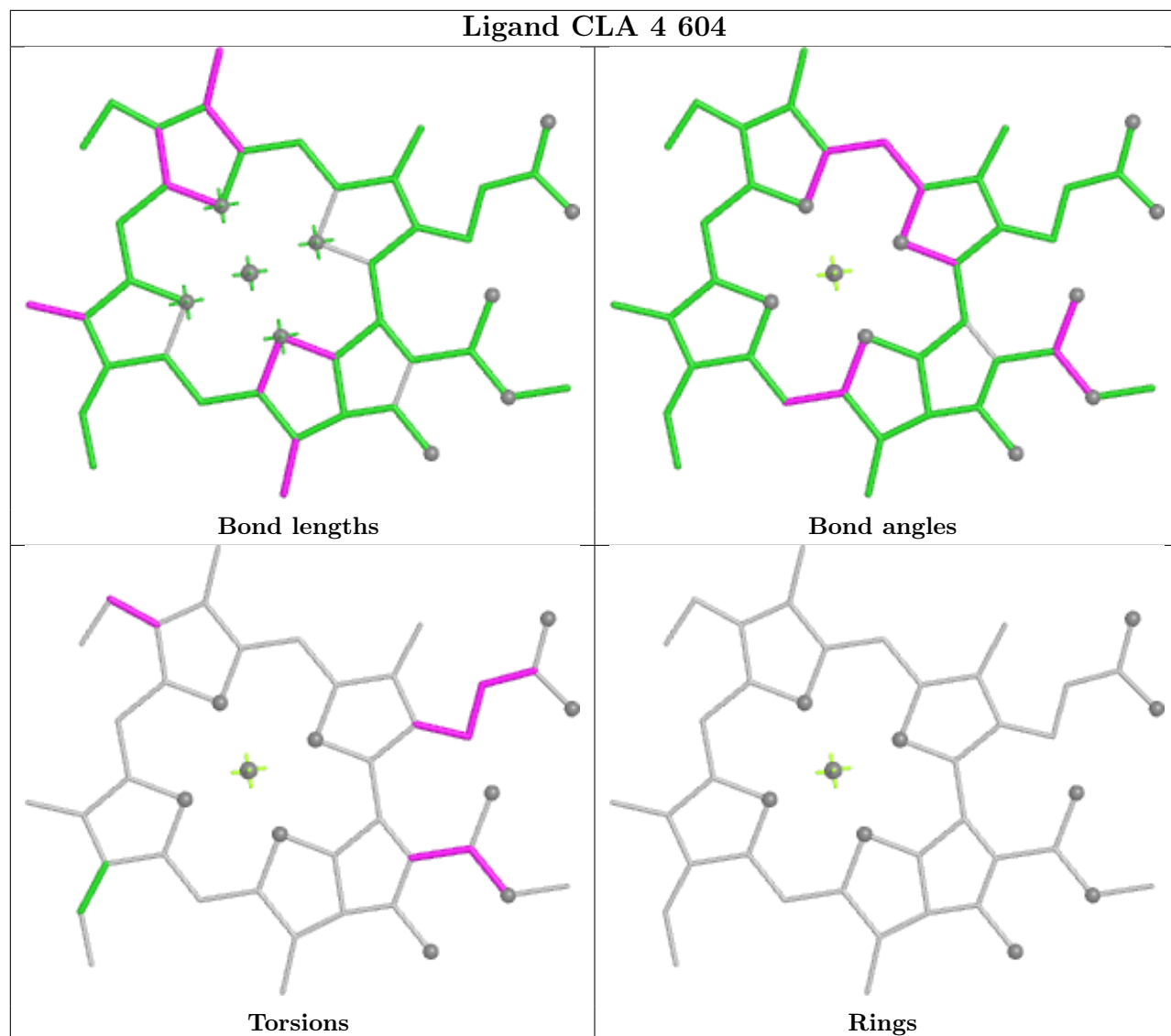
Torsions

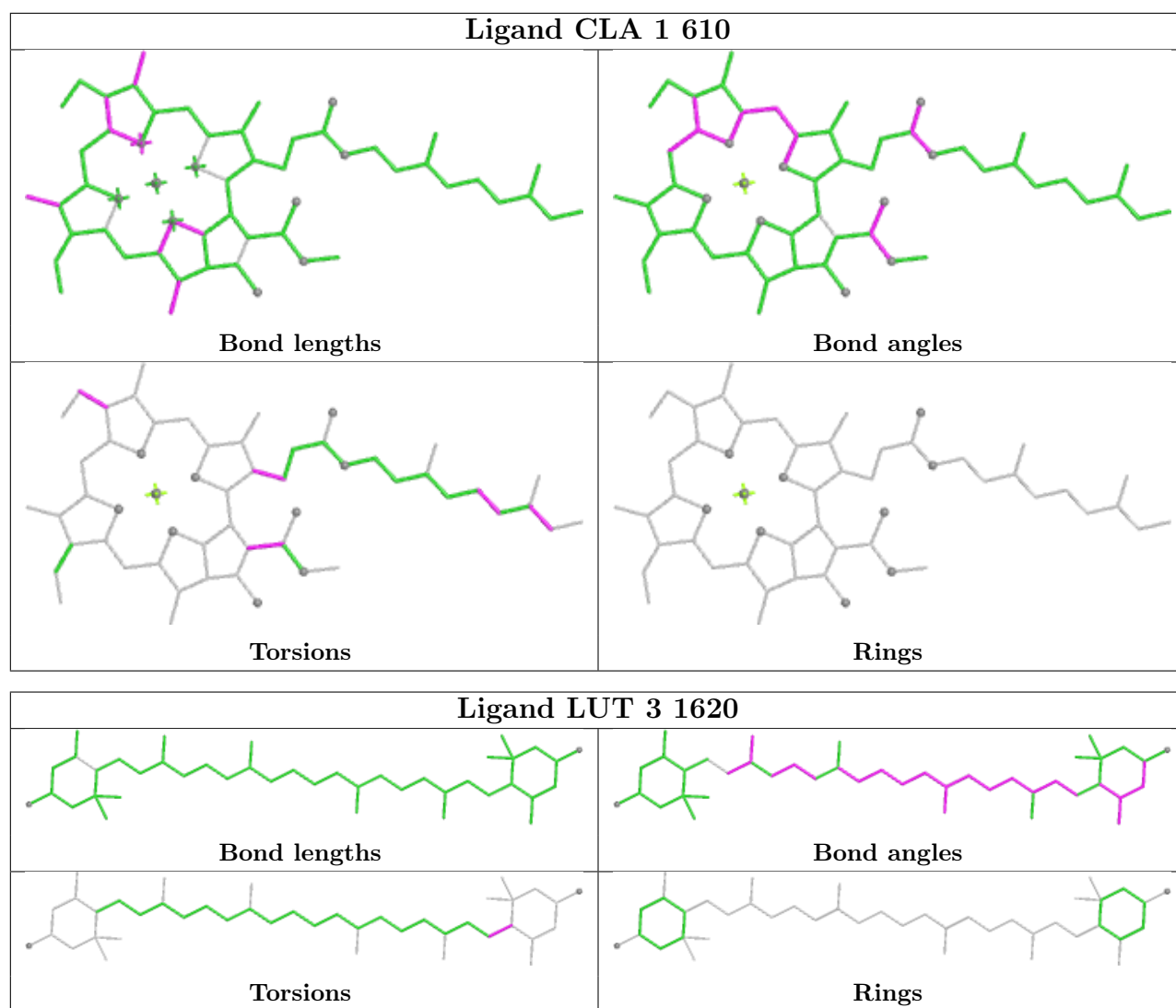


Rings



Ligand CLA 4 604





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.

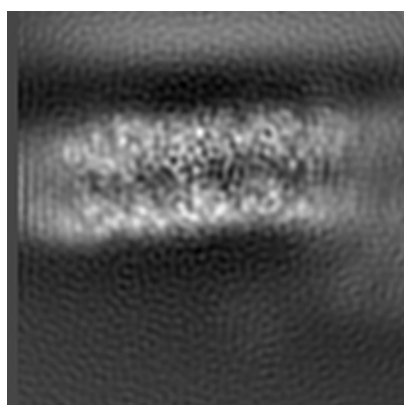
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6743. These allow visual inspection of the internal detail of the map and identification of artifacts.

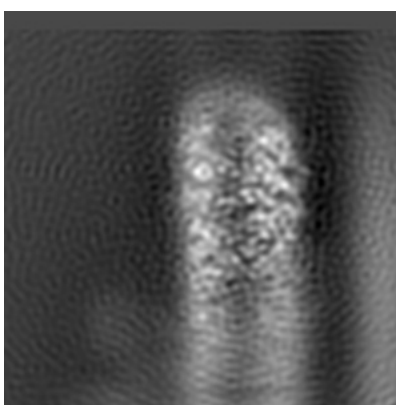
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

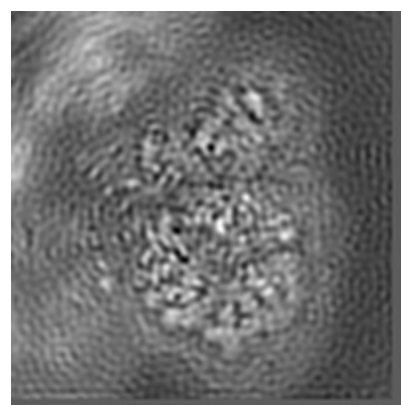
6.1.1 Primary map



X



Y

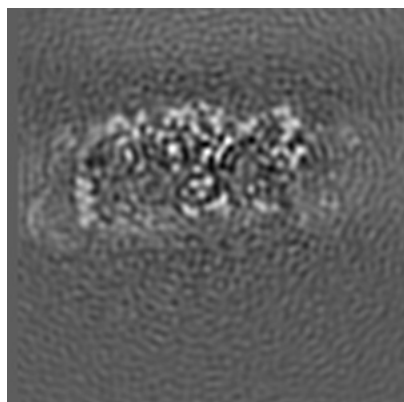


Z

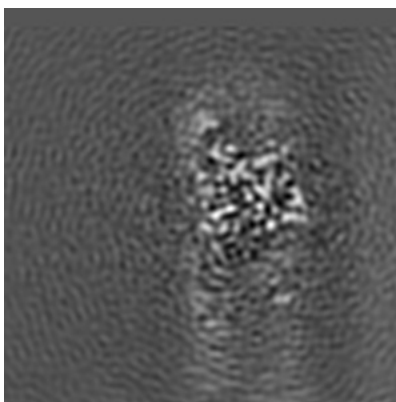
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

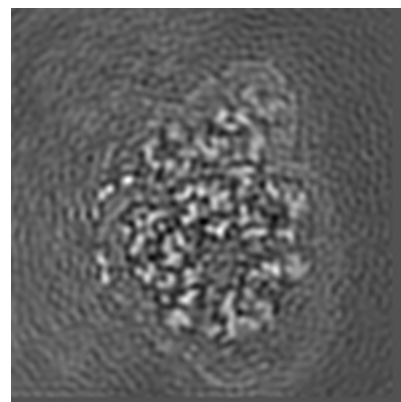
6.2.1 Primary map



X Index: 75



Y Index: 75

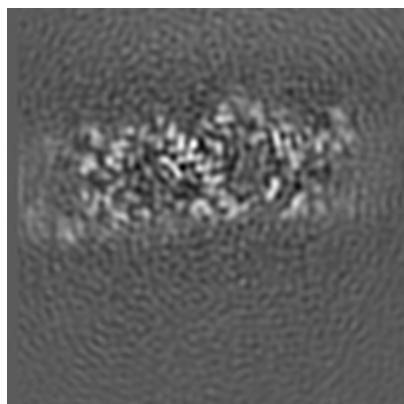


Z Index: 75

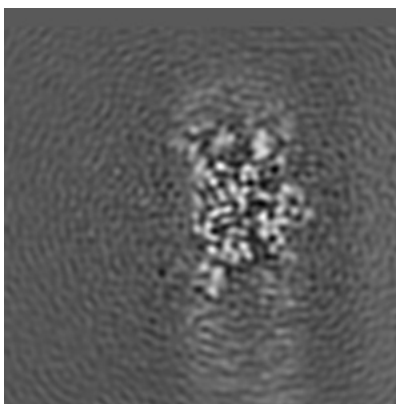
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

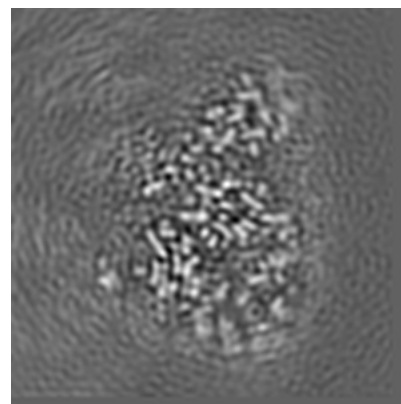
6.3.1 Primary map



X Index: 87



Y Index: 71

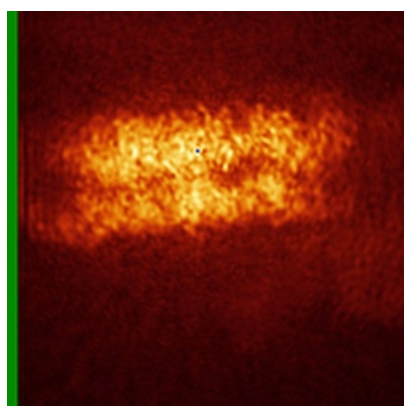


Z Index: 97

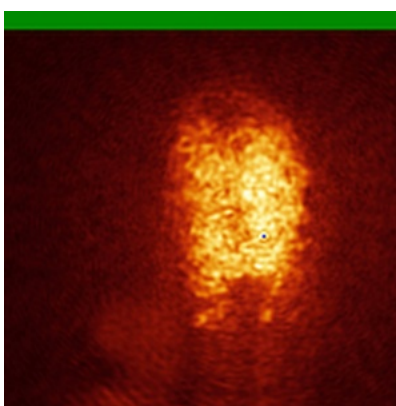
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

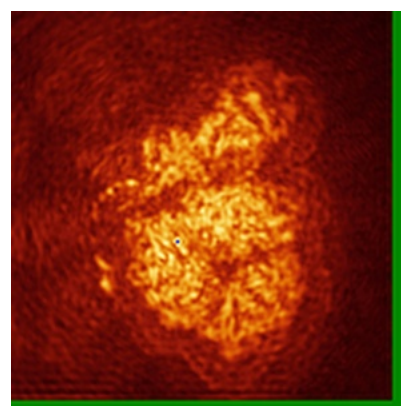
6.4.1 Primary map



X



Y

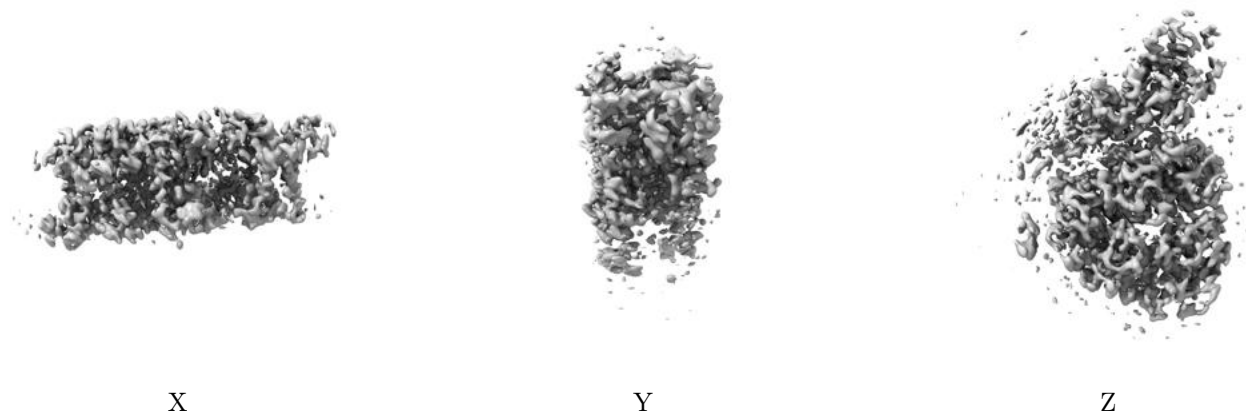


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

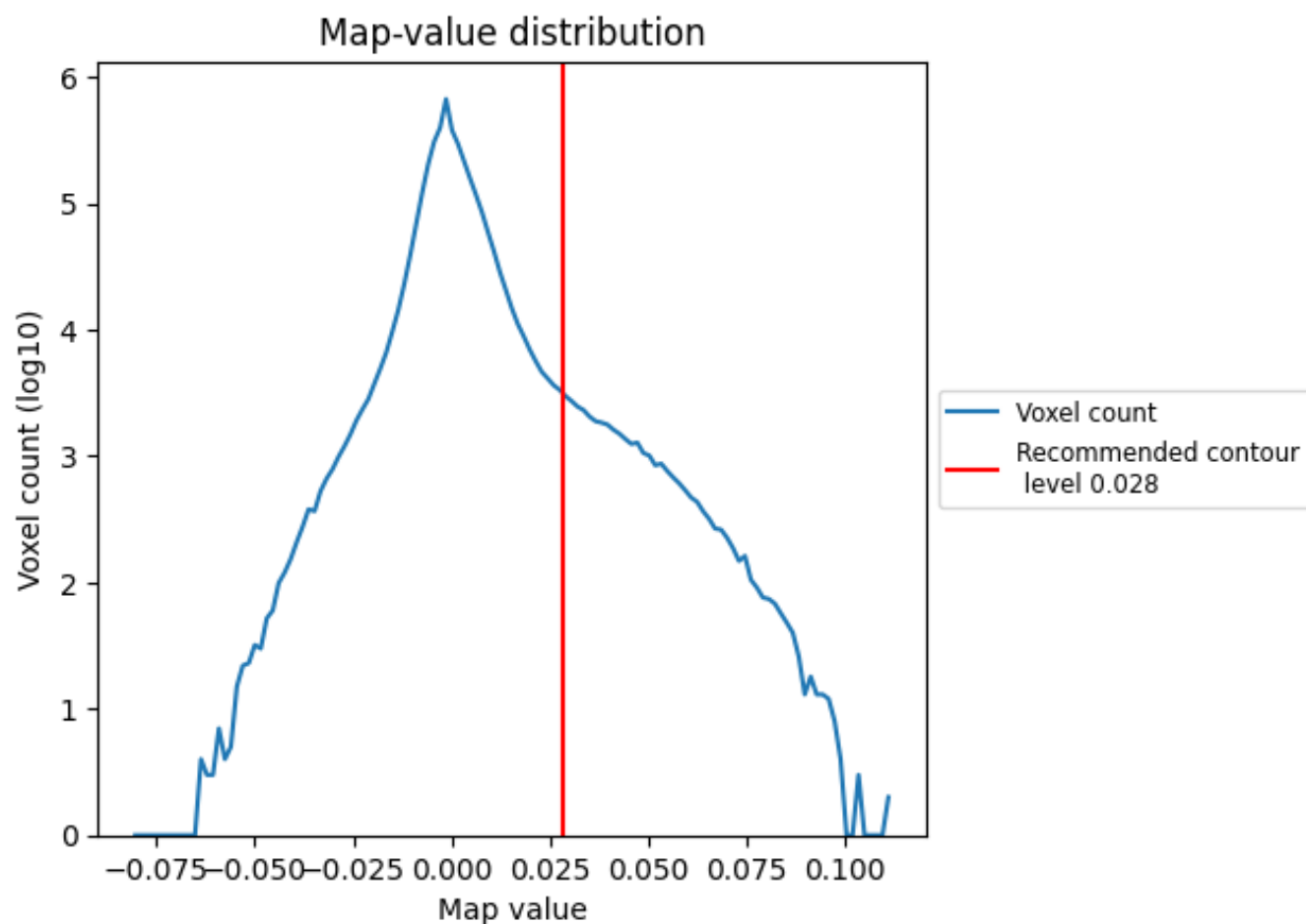
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

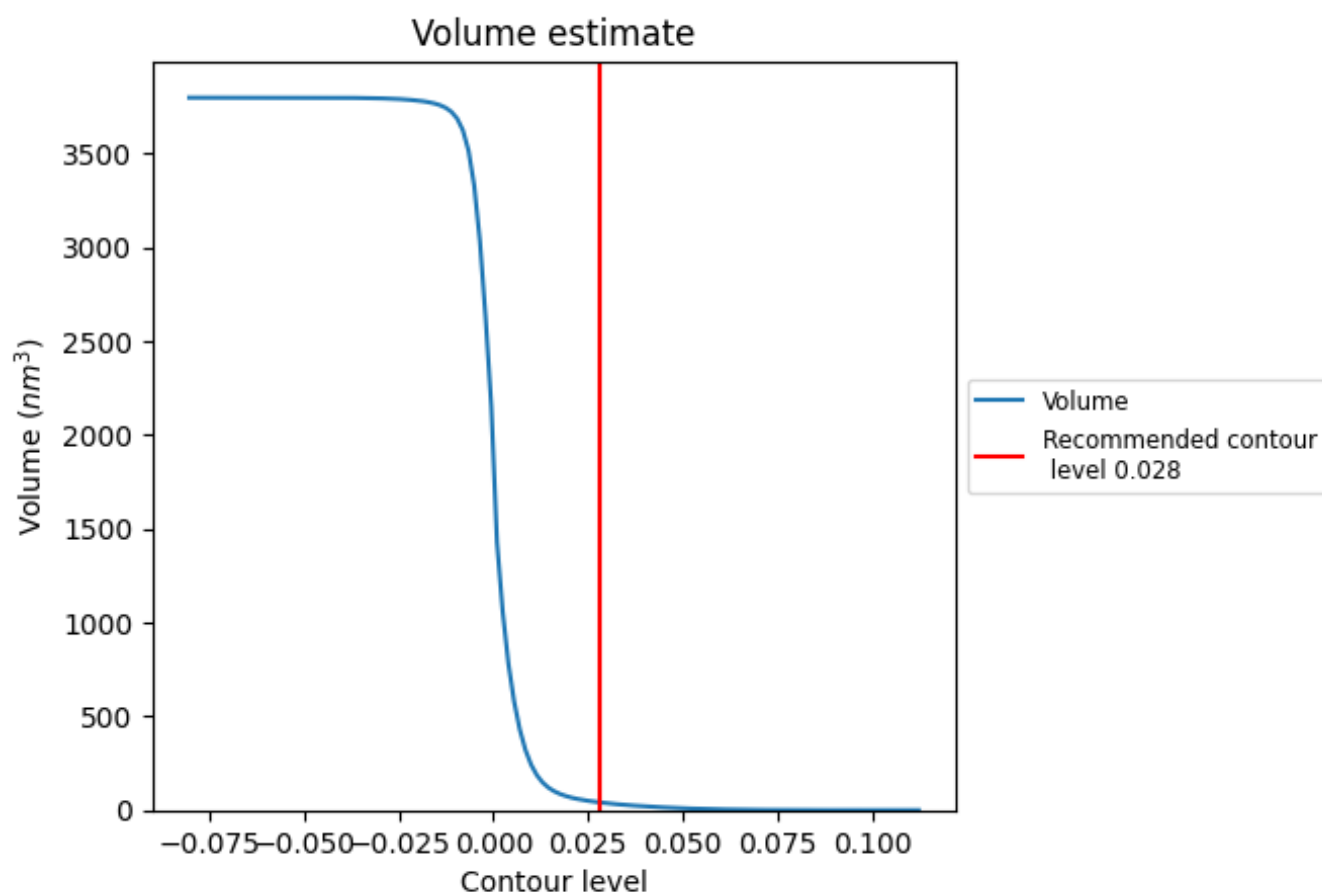
This section contains the results of statistical analysis of the map.

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.

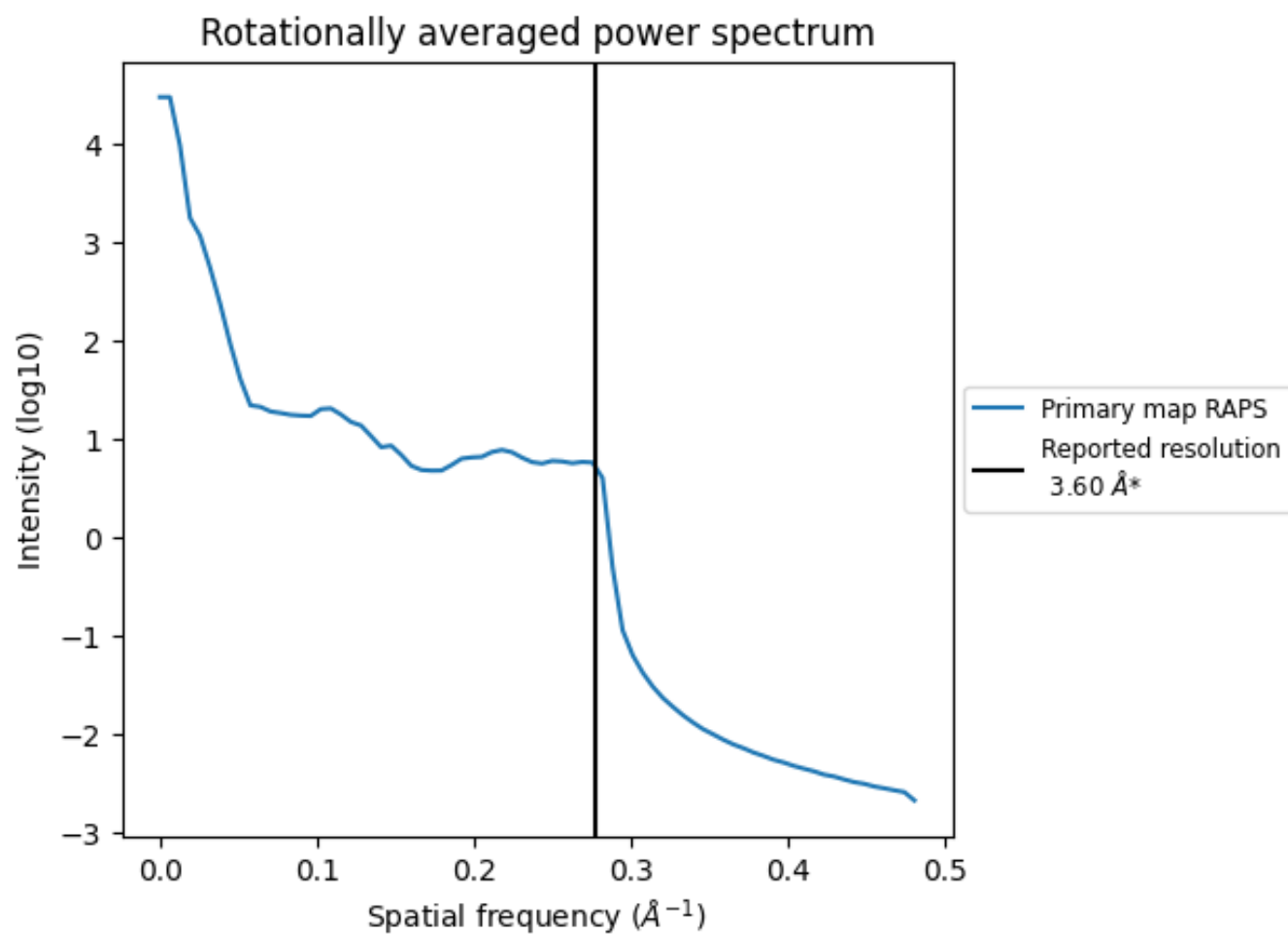
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 42 nm³; this corresponds to an approximate mass of 38 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

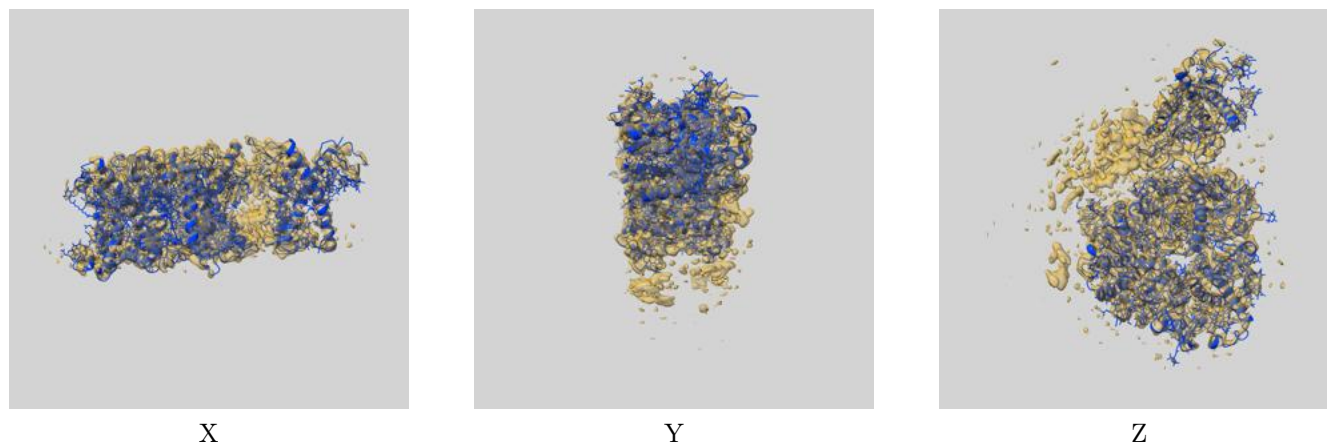
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

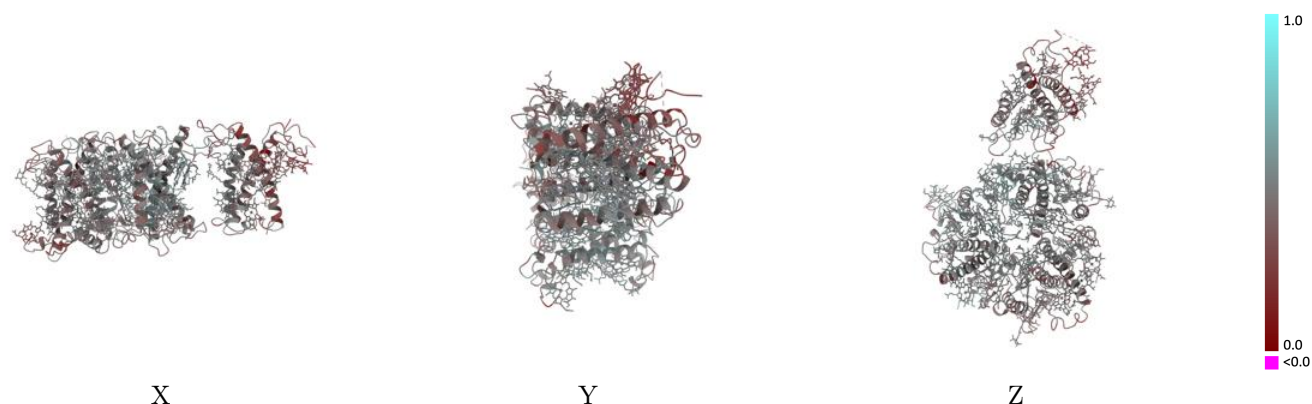
This section contains information regarding the fit between EMDB map EMD-6743 and PDB model 5XNN. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



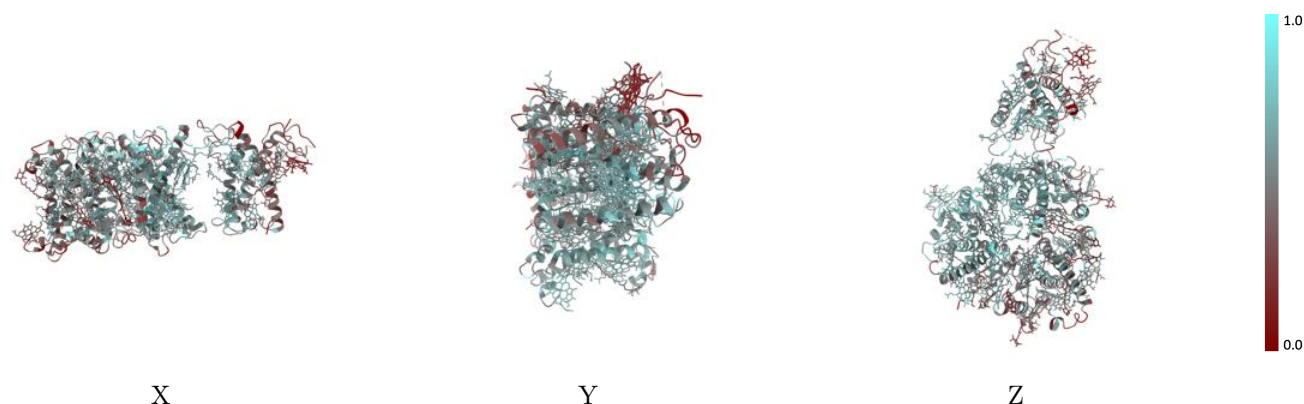
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



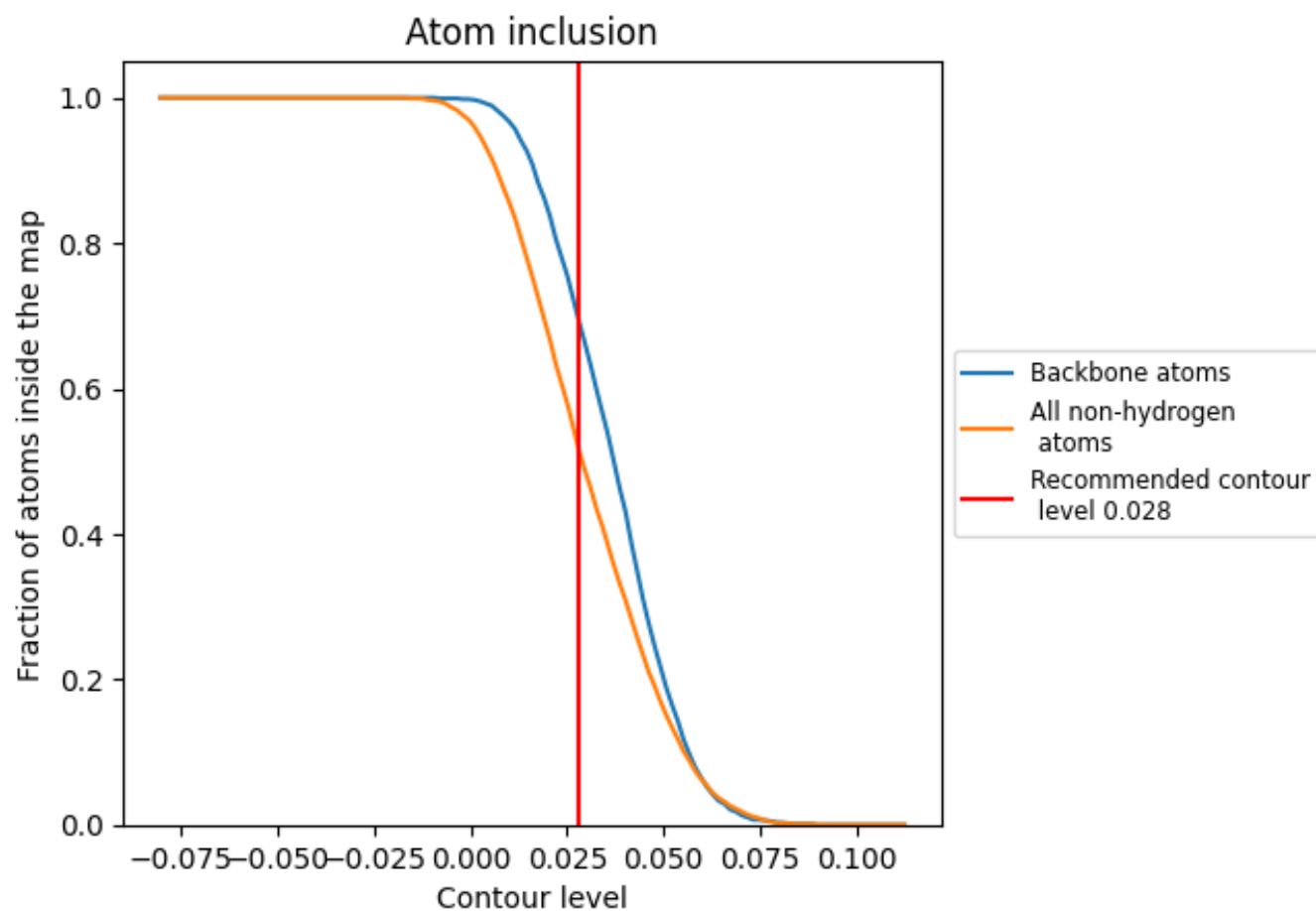
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.028).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5160	0.4470
1	0.5560	0.4700
2	0.4450	0.4310
3	0.5820	0.4800
4	0.4720	0.4010

