



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 07:11 PM JST

PDB ID : 8JP3 / pdb_00008jp3
EMDB ID : EMD-36466
Title : FCP trimer in diatom *Thalassiosira pseudonana*
Authors : Feng, Y.; Li, Z.; Zhou, C.C.; Liu, C.; Shen, J.R.; Wang, W.
Deposited on : 2023-06-10
Resolution : 2.73 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

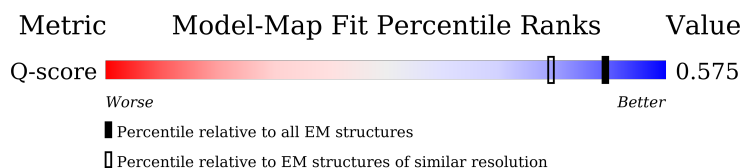
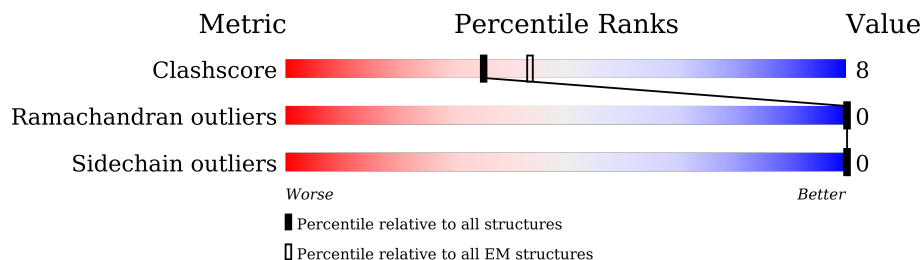
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 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	10432 (2.23 - 3.23)

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	A	180	
1	B	180	
1	C	180	

2 Entry composition [i](#)

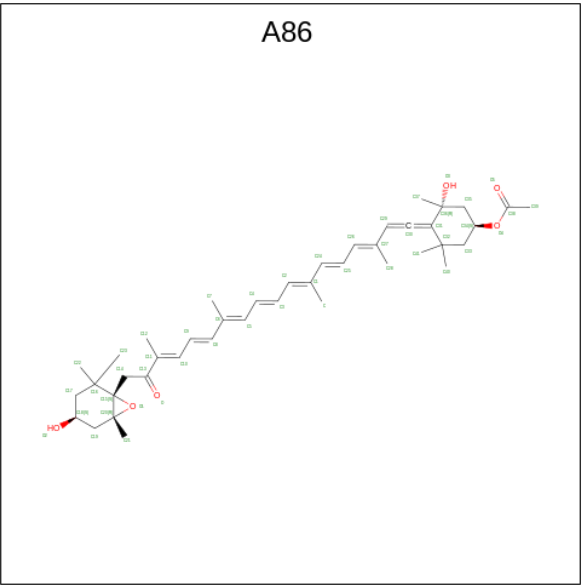
There are 6 unique types of molecules in this entry. The entry contains 7104 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fucoxanthin chlorophyll a/c protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	180	Total	C	N	O	S	0	0
			1384	886	233	258	7		
1	B	180	Total	C	N	O	S	0	0
			1384	886	233	258	7		
1	C	180	Total	C	N	O	S	0	0
			1384	886	233	258	7		

- Molecule 2 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆) (labeled as "Ligand of Interest" by depositor).



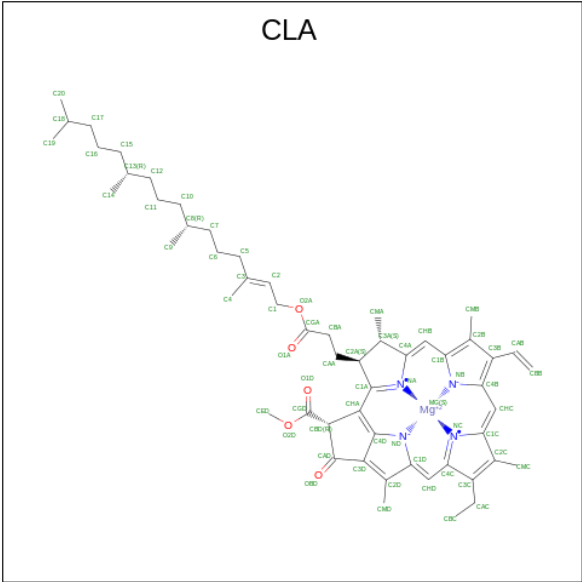
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			48	42	6	
2	A	1	Total	C	O	0
			48	42	6	
2	A	1	Total	C	O	0
			48	42	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			48	42	6	
2	A	1	Total	C	O	0
			48	42	6	
2	A	1	Total	C	O	0
			48	42	6	
2	A	1	Total	C	O	0
			48	42	6	
2	B	1	Total	C	O	0
			48	42	6	
2	B	1	Total	C	O	0
			48	42	6	
2	B	1	Total	C	O	0
			48	42	6	
2	B	1	Total	C	O	0
			48	42	6	
2	B	1	Total	C	O	0
			48	42	6	
2	B	1	Total	C	O	0
			48	42	6	
2	C	1	Total	C	O	0
			48	42	6	
2	C	1	Total	C	O	0
			48	42	6	
2	C	1	Total	C	O	0
			48	42	6	
2	C	1	Total	C	O	0
			48	42	6	
2	C	1	Total	C	O	0
			48	42	6	
2	C	1	Total	C	O	0
			48	42	6	

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



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
3	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

Continued on next page...

Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
3	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	C	1	Total 58	C 48	Mg 1	N 4	O 5	0
3	C	1	Total 53	C 43	Mg 1	N 4	O 5	0
3	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	C	1	Total 59	C 49	Mg 1	N 4	O 5	0
3	C	1	Total 53	C 43	Mg 1	N 4	O 5	0
3	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
3	C	1	Total 61	C 51	Mg 1	N 4	O 5	0

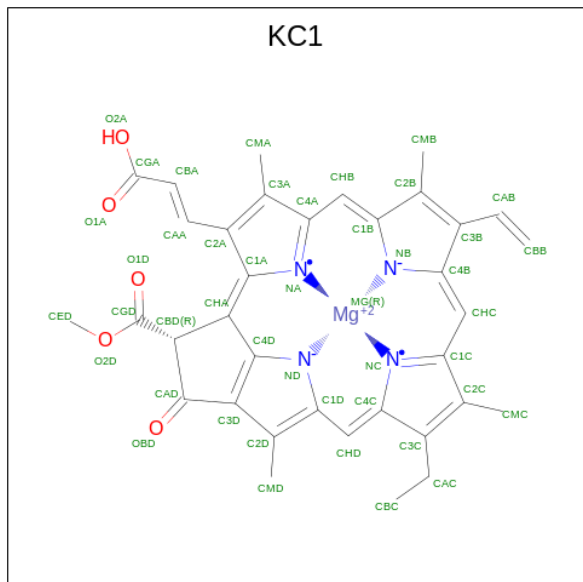
- ## KC2



Continued from previous page...

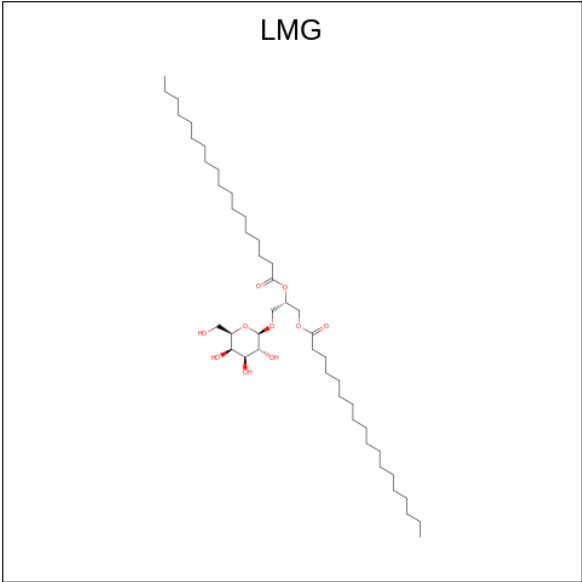
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 5 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 6 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).

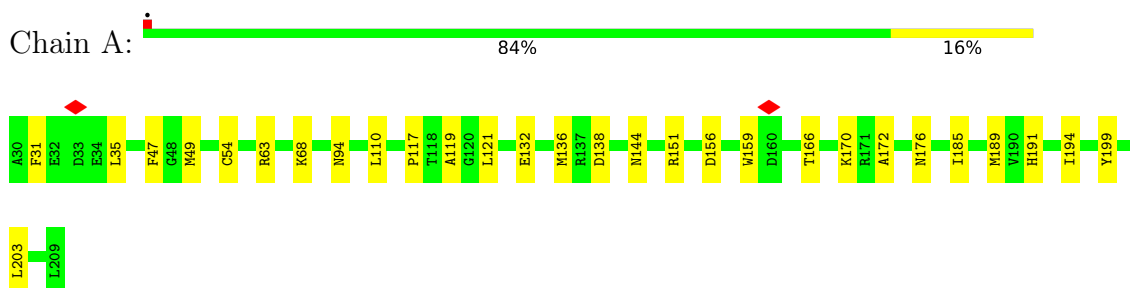


Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			34	24	10	
6	B	1	Total	C	O	0
			34	24	10	
6	C	1	Total	C	O	0
			34	24	10	

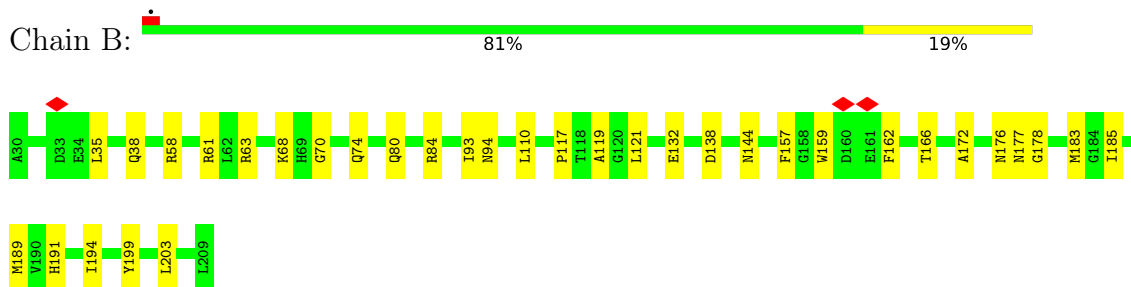
3 Residue-property plots

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.

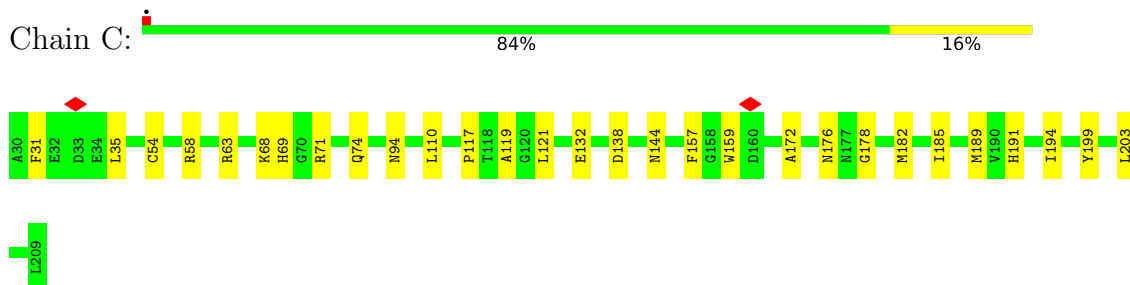
- Molecule 1: Fucoxanthin chlorophyll a/c protein 8



- Molecule 1: Fucoxanthin chlorophyll a/c protein 8



- Molecule 1: Fucoxanthin chlorophyll a/c protein 8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103596	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)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.775	Depositor
Minimum map value	-0.290	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.253	Depositor
Map size ($\text{\AA}$)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: CLA, KC1, KC2, A86, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/1417	0.24	0/1917
1	B	0.13	0/1417	0.24	0/1917
1	C	0.13	0/1417	0.25	0/1917
All	All	0.13	0/4251	0.24	0/5751

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1384	0	1335	18	0
1	B	1384	0	1335	25	0
1	C	1384	0	1335	19	0
2	A	336	0	0	0	0
2	B	336	0	0	2	0
2	C	336	0	0	3	0
3	A	479	0	480	17	0
3	B	414	0	408	10	0
3	C	544	0	552	18	0
4	A	90	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	90	0	0	1	0
4	C	90	0	0	2	0
5	A	45	0	0	0	0
5	B	45	0	0	0	0
5	C	45	0	0	0	0
6	A	34	0	38	5	0
6	B	34	0	38	7	0
6	C	34	0	38	6	0
All	All	7104	0	5559	100	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 8.

All (100) 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)
4:C:313:KC2:O2A	6:C:320:LMG:HC91	1.66	0.92
1:C:94:ASN:HD21	1:C:117:PRO:HG2	1.50	0.76
1:A:119:ALA:HA	3:C:318:CLA:H12	1.72	0.72
6:A:319:LMG:H152	3:C:318:CLA:H43	1.74	0.68
1:B:94:ASN:HD21	1:B:117:PRO:HG2	1.57	0.68
1:B:58:ARG:NH2	2:B:306:A86:O3	2.27	0.68
1:B:138:ASP:OD1	1:B:144:ASN:ND2	2.27	0.67
1:C:138:ASP:OD1	1:C:144:ASN:ND2	2.26	0.67
1:A:94:ASN:HD21	1:A:117:PRO:HG2	1.59	0.67
6:A:319:LMG:HC62	3:C:318:CLA:H12	1.77	0.67
1:C:119:ALA:HA	3:C:301:CLA:H12	1.77	0.67
3:A:317:CLA:H12	1:B:119:ALA:HA	1.77	0.66
1:A:176:ASN:ND2	3:A:308:CLA:O1D	2.30	0.64
1:B:176:ASN:ND2	3:B:308:CLA:O1D	2.31	0.64
1:C:176:ASN:ND2	3:C:309:CLA:O1D	2.32	0.62
1:C:172:ALA:O	1:C:176:ASN:ND2	2.33	0.61
1:A:138:ASP:OD1	1:A:144:ASN:ND2	2.28	0.61
3:C:301:CLA:HBA2	6:C:320:LMG:HC4	1.82	0.60
1:A:172:ALA:O	1:A:176:ASN:ND2	2.35	0.59
3:A:314:CLA:HBD	3:A:314:CLA:HBA1	1.85	0.59
1:B:183:MET:HE3	3:B:309:CLA:HMC3	1.84	0.58
3:C:315:CLA:HBA1	3:C:315:CLA:HBD	1.85	0.58
3:A:317:CLA:H42	6:B:318:LMG:H291	1.84	0.58
3:B:314:CLA:HBD	3:B:314:CLA:HBA1	1.86	0.57
1:C:71:ARG:HA	1:C:74:GLN:HE21	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LEU:HD22	1:C:121:LEU:HD13	1.88	0.56
4:B:312:KC2:O2A	6:B:318:LMG:HC91	2.06	0.56
1:B:38:GLN:NE2	1:B:172:ALA:HB1	2.22	0.54
1:B:194:ILE:HB	1:B:199:TYR:HB2	1.88	0.54
6:A:319:LMG:HC4	3:C:318:CLA:HBA2	1.90	0.53
3:C:301:CLA:H43	6:C:320:LMG:H131	1.91	0.53
1:B:110:LEU:HD22	1:B:121:LEU:HD13	1.89	0.53
3:A:317:CLA:H2	6:B:318:LMG:H112	1.90	0.53
3:C:301:CLA:H43	6:C:320:LMG:H152	1.89	0.53
4:C:313:KC2:O2A	6:C:320:LMG:C9	2.49	0.53
1:B:74:GLN:HE21	1:B:178:GLY:N	2.06	0.52
1:B:93:ILE:HG23	1:B:94:ASN:ND2	2.26	0.51
3:A:317:CLA:HBA2	6:B:318:LMG:HC4	1.92	0.51
3:A:316:CLA:HMD1	3:A:317:CLA:HAB	1.93	0.50
1:C:157:PHE:HB2	3:C:315:CLA:H12	1.93	0.50
3:C:301:CLA:H2	6:C:320:LMG:H112	1.92	0.50
1:A:194:ILE:HB	1:A:199:TYR:HB2	1.93	0.49
1:B:185:ILE:O	1:B:189:MET:HG3	2.13	0.49
3:C:317:CLA:HMD1	3:C:318:CLA:HAB	1.96	0.48
1:B:157:PHE:HB2	3:B:314:CLA:H12	1.95	0.48
1:C:178:GLY:O	1:C:182:MET:HG3	2.13	0.48
3:A:311:CLA:HED3	3:A:311:CLA:H2A	1.95	0.48
1:C:69:HIS:HB3	1:C:182:MET:SD	2.54	0.48
6:B:318:LMG:H171	6:B:318:LMG:H141	1.44	0.48
3:A:316:CLA:H2A	3:A:316:CLA:O1D	2.14	0.47
3:B:316:CLA:H2A	3:B:316:CLA:O1D	2.14	0.47
3:A:318:CLA:H91	3:A:318:CLA:H112	1.64	0.47
1:A:35:LEU:HB3	1:A:63:ARG:HH12	1.80	0.47
1:B:68:LYS:NZ	1:B:132:GLU:OE1	2.48	0.47
1:B:61:ARG:HE	3:B:313:CLA:HED1	1.80	0.47
3:B:317:CLA:H112	3:B:317:CLA:H91	1.65	0.46
1:A:110:LEU:HD22	1:A:121:LEU:HD13	1.97	0.46
3:B:317:CLA:H62	3:B:317:CLA:H92	1.77	0.46
3:B:308:CLA:H92	3:B:308:CLA:H61	1.68	0.46
1:A:159:TRP:CE3	3:A:314:CLA:HBA2	2.51	0.46
1:C:68:LYS:NZ	1:C:132:GLU:OE1	2.50	0.45
1:A:68:LYS:NZ	1:A:132:GLU:OE1	2.49	0.45
1:B:35:LEU:HB3	1:B:63:ARG:HH12	1.82	0.45
1:A:185:ILE:O	1:A:189:MET:HG3	2.17	0.45
6:A:319:LMG:O10	2:C:302:A86:C39	2.65	0.45
1:B:80:GLN:HG2	1:B:84:ARG:HE	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:301:CLA:HBA2	3:C:301:CLA:H3A	1.42	0.45
1:B:74:GLN:HE21	1:B:177:ASN:C	2.25	0.44
1:C:31:PHE:HE2	1:C:54:CYS:HB3	1.83	0.44
1:C:194:ILE:HB	1:C:199:TYR:HB2	1.99	0.44
1:C:191:HIS:NE2	1:C:203:LEU:HD21	2.32	0.44
1:C:159:TRP:CE3	3:C:315:CLA:HBA2	2.53	0.43
3:A:317:CLA:HBA2	3:A:317:CLA:H3A	1.40	0.43
1:B:94:ASN:ND2	1:B:117:PRO:HG2	2.31	0.43
1:A:31:PHE:HE2	1:A:54:CYS:HB3	1.84	0.43
1:B:191:HIS:NE2	1:B:203:LEU:HD21	2.34	0.43
3:A:308:CLA:H92	3:A:308:CLA:H61	1.77	0.43
1:B:159:TRP:CE3	3:B:314:CLA:HBA2	2.54	0.43
3:A:318:CLA:H2	3:A:318:CLA:ND	2.34	0.43
3:A:317:CLA:HBA2	6:B:318:LMG:HC5	2.00	0.43
1:B:70:GLY:O	1:B:74:GLN:HG3	2.19	0.42
1:A:191:HIS:NE2	1:A:203:LEU:HD21	2.33	0.42
1:B:183:MET:HG3	2:B:301:A86:C10	2.49	0.42
1:B:172:ALA:O	1:B:176:ASN:ND2	2.52	0.42
1:C:58:ARG:NH2	2:C:307:A86:O3	2.32	0.42
1:B:162:PHE:HB3	1:B:166:THR:HB	2.02	0.42
3:C:312:CLA:H162	3:C:312:CLA:H141	1.82	0.42
3:A:316:CLA:H61	3:A:316:CLA:H41	1.76	0.41
3:C:318:CLA:HBA2	3:C:318:CLA:H3A	1.41	0.41
3:C:319:CLA:H91	3:C:319:CLA:H112	1.66	0.41
6:B:318:LMG:H122	6:B:318:LMG:H152	1.42	0.41
1:C:74:GLN:HG2	2:C:306:A86:C4	2.51	0.41
1:C:35:LEU:HB3	1:C:63:ARG:HH12	1.85	0.41
1:A:94:ASN:ND2	1:A:117:PRO:HG2	2.32	0.41
6:A:319:LMG:H152	6:A:319:LMG:H122	1.91	0.41
1:C:185:ILE:O	1:C:189:MET:HG3	2.21	0.41
1:A:47:PHE:HB3	1:A:49:MET:HE3	2.03	0.40
1:A:166:THR:O	1:A:170:LYS:HG2	2.21	0.40
1:A:151:ARG:HD2	1:A:156:ASP:CG	2.47	0.40
1:A:136:MET:HE1	3:A:314:CLA:HMD1	2.03	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	A	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
1	B	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
1	C	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
All	All	534/540 (99%)	520 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/142 (100%)	142 (100%)	0	100	100
1	B	142/142 (100%)	142 (100%)	0	100	100
1	C	142/142 (100%)	142 (100%)	0	100	100
All	All	426/426 (100%)	426 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	B	38	GLN
1	B	94	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	38	GLN
1	C	56	GLN
1	C	74	GLN
1	C	80	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

57 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CLA	B	308	-	62,66,73	1.33	9 (14%)	74,104,113	1.32	7 (9%)
2	A86	B	303	-	44,50,50	1.25	4 (9%)	51,76,76	3.24	16 (31%)
2	A86	C	306	-	44,50,50	1.23	3 (6%)	51,76,76	2.96	10 (19%)
3	CLA	A	318	1	65,69,73	1.30	9 (13%)	78,108,113	1.30	5 (6%)
2	A86	A	302	-	44,50,50	1.26	4 (9%)	51,76,76	2.68	15 (29%)
3	CLA	A	309	1	57,61,73	1.37	9 (15%)	68,98,113	1.37	7 (10%)
3	CLA	A	317	-	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
3	CLA	B	309	1	57,61,73	1.37	9 (15%)	68,98,113	1.39	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLA	C	310	-	57,61,73	1.36	8 (14%)	68,98,113	1.38	6 (8%)
4	KC2	A	312	1	49,53,53	1.78	11 (22%)	62,89,89	2.17	18 (29%)
3	CLA	B	311	-	69,73,73	1.24	8 (11%)	83,113,113	1.30	7 (8%)
2	A86	A	304	-	44,50,50	1.24	3 (6%)	51,76,76	3.14	15 (29%)
3	CLA	B	314	-	63,67,73	1.31	8 (12%)	75,105,113	1.37	10 (13%)
2	A86	A	301	-	44,50,50	1.22	3 (6%)	51,76,76	2.93	14 (27%)
2	A86	C	302	-	44,50,50	1.23	3 (6%)	51,76,76	2.88	15 (29%)
2	A86	C	305	-	44,50,50	1.24	3 (6%)	51,76,76	3.14	16 (31%)
3	CLA	B	317	1	65,69,73	1.29	8 (12%)	78,108,113	1.31	5 (6%)
3	CLA	C	309	-	62,66,73	1.32	8 (12%)	74,104,113	1.33	6 (8%)
3	CLA	C	315	-	63,67,73	1.31	10 (15%)	75,105,113	1.37	10 (13%)
3	CLA	C	317	1	57,61,73	1.37	9 (15%)	68,98,113	1.41	6 (8%)
2	A86	B	304	-	44,50,50	1.24	3 (6%)	51,76,76	3.13	17 (33%)
4	KC2	A	310	1	49,53,53	1.79	12 (24%)	62,89,89	2.18	17 (27%)
5	KC1	C	316	-	49,53,53	1.41	7 (14%)	63,89,89	1.98	14 (22%)
4	KC2	B	310	1	49,53,53	1.81	11 (22%)	62,89,89	2.20	17 (27%)
3	CLA	A	313	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	5 (6%)
3	CLA	C	301	-	69,73,73	1.24	8 (11%)	83,113,113	1.29	8 (9%)
4	KC2	C	313	1	49,53,53	1.78	11 (22%)	62,89,89	2.17	18 (29%)
6	LMG	C	320	-	34,34,55	1.10	2 (5%)	42,42,63	1.09	2 (4%)
2	A86	C	304	-	44,50,50	1.25	4 (9%)	51,76,76	3.13	13 (25%)
3	CLA	A	314	-	63,67,73	1.31	10 (15%)	75,105,113	1.37	10 (13%)
6	LMG	A	319	-	34,34,55	1.11	2 (5%)	42,42,63	1.13	2 (4%)
2	A86	A	305	-	44,50,50	1.22	3 (6%)	51,76,76	2.96	10 (19%)
3	CLA	C	314	-	69,73,73	1.25	9 (13%)	83,113,113	1.26	4 (4%)
2	A86	B	301	-	44,50,50	1.24	3 (6%)	51,76,76	2.88	16 (31%)
3	CLA	B	316	1	57,61,73	1.36	9 (15%)	68,98,113	1.44	6 (8%)
3	CLA	A	308	-	62,66,73	1.32	9 (14%)	74,104,113	1.32	6 (8%)
4	KC2	B	312	1	49,53,53	1.78	10 (20%)	62,89,89	2.16	18 (29%)
2	A86	A	303	-	44,50,50	1.24	4 (9%)	51,76,76	3.29	13 (25%)
2	A86	B	307	-	44,50,50	1.23	3 (6%)	51,76,76	3.38	16 (31%)
5	KC1	A	315	-	49,53,53	1.40	7 (14%)	63,89,89	1.99	14 (22%)
2	A86	B	306	-	44,50,50	1.25	4 (9%)	51,76,76	4.68	19 (37%)
3	CLA	C	318	-	69,73,73	1.24	8 (11%)	83,113,113	1.29	5 (6%)
3	CLA	A	316	1	57,61,73	1.37	9 (15%)	68,98,113	1.44	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLA	C	312	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
6	LMG	B	318	-	34,34,55	1.13	2 (5%)	42,42,63	1.14	4 (9%)
5	KC1	B	315	-	49,53,53	1.40	7 (14%)	63,89,89	1.99	14 (22%)
2	A86	B	302	-	44,50,50	1.25	3 (6%)	51,76,76	2.79	15 (29%)
2	A86	A	306	-	44,50,50	1.24	4 (9%)	51,76,76	4.72	18 (35%)
3	CLA	A	311	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	8 (9%)
3	CLA	B	313	-	69,73,73	1.25	9 (13%)	83,113,113	1.27	4 (4%)
3	CLA	C	319	1	65,69,73	1.30	9 (13%)	78,108,113	1.31	5 (6%)
2	A86	A	307	-	44,50,50	1.23	3 (6%)	51,76,76	3.50	16 (31%)
2	A86	C	303	-	44,50,50	1.25	3 (6%)	51,76,76	2.74	15 (29%)
2	A86	C	308	-	44,50,50	1.23	3 (6%)	51,76,76	3.40	16 (31%)
2	A86	B	305	-	44,50,50	1.22	3 (6%)	51,76,76	2.97	10 (19%)
4	KC2	C	311	1	49,53,53	1.79	11 (22%)	62,89,89	2.19	17 (27%)
2	A86	C	307	-	44,50,50	1.25	4 (9%)	51,76,76	4.78	18 (35%)

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
3	CLA	B	308	-	-	12/31/107/115	-
2	A86	B	303	-	-	9/34/90/90	0/3/3/3
2	A86	C	306	-	-	13/34/90/90	0/3/3/3
3	CLA	A	318	1	-	7/35/111/115	-
2	A86	A	302	-	-	9/34/90/90	0/3/3/3
3	CLA	A	309	1	-	7/25/101/115	-
3	CLA	A	317	-	-	15/39/115/115	-
3	CLA	B	309	1	-	8/25/101/115	-
3	CLA	C	310	-	-	7/25/101/115	-
4	KC2	A	312	1	-	7/15/71/71	-
3	CLA	B	311	-	-	9/39/115/115	-
2	A86	A	304	-	-	8/34/90/90	0/3/3/3
3	CLA	B	314	-	-	8/32/108/115	-
2	A86	A	301	-	-	10/34/90/90	0/3/3/3
2	A86	C	302	-	-	10/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A86	C	305	-	-	10/34/90/90	0/3/3/3
3	CLA	B	317	1	-	8/35/111/115	-
3	CLA	C	309	-	-	11/31/107/115	-
3	CLA	C	315	-	-	6/32/108/115	-
3	CLA	C	317	1	-	15/25/101/115	-
2	A86	B	304	-	-	8/34/90/90	0/3/3/3
4	KC2	A	310	1	-	6/15/71/71	-
5	KC1	C	316	-	-	5/15/71/71	-
4	KC2	B	310	1	-	7/15/71/71	-
3	CLA	A	313	-	-	9/39/115/115	-
3	CLA	C	301	-	-	16/39/115/115	-
4	KC2	C	313	1	-	7/15/71/71	-
6	LMG	C	320	-	-	13/29/49/70	0/1/1/1
2	A86	C	304	-	-	9/34/90/90	0/3/3/3
3	CLA	A	314	-	-	8/32/108/115	-
6	LMG	A	319	-	-	18/29/49/70	0/1/1/1
2	A86	A	305	-	-	13/34/90/90	0/3/3/3
3	CLA	C	314	-	-	11/39/115/115	-
2	A86	B	301	-	-	9/34/90/90	0/3/3/3
3	CLA	B	316	1	-	11/25/101/115	-
3	CLA	A	308	-	-	11/31/107/115	-
4	KC2	B	312	1	-	5/15/71/71	-
2	A86	A	303	-	-	9/34/90/90	0/3/3/3
2	A86	B	307	-	-	10/34/90/90	0/3/3/3
5	KC1	A	315	-	-	6/15/71/71	-
2	A86	B	306	-	-	11/34/90/90	1/3/3/3
3	CLA	C	318	-	-	18/39/115/115	-
3	CLA	A	316	1	-	13/25/101/115	-
3	CLA	C	312	-	-	9/39/115/115	-
6	LMG	B	318	-	-	11/29/49/70	0/1/1/1
5	KC1	B	315	-	-	6/15/71/71	-
2	A86	B	302	-	-	9/34/90/90	0/3/3/3
2	A86	A	306	-	-	11/34/90/90	1/3/3/3
3	CLA	A	311	-	-	11/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	B	313	-	-	8/39/115/115	-
3	CLA	C	319	1	-	7/35/111/115	-
2	A86	A	307	-	-	9/34/90/90	0/3/3/3
2	A86	C	303	-	-	9/34/90/90	0/3/3/3
2	A86	C	308	-	-	9/34/90/90	0/3/3/3
2	A86	B	305	-	-	13/34/90/90	0/3/3/3
4	KC2	C	311	1	-	8/15/71/71	-
2	A86	C	307	-	-	11/34/90/90	1/3/3/3

All (372) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	312	KC2	CHD-C4C	5.13	1.48	1.38
4	C	313	KC2	CHD-C4C	5.12	1.48	1.38
4	B	312	KC2	CHD-C4C	5.12	1.48	1.38
4	B	310	KC2	CHD-C4C	5.10	1.48	1.38
4	C	311	KC2	CHD-C4C	5.06	1.48	1.38
4	A	310	KC2	CHD-C4C	5.06	1.48	1.38
5	B	315	KC1	MG-ND	-5.01	1.95	2.05
5	C	316	KC1	MG-ND	-5.00	1.95	2.05
5	A	315	KC1	MG-ND	-4.97	1.95	2.05
2	A	307	A86	O4-C38	4.72	1.45	1.35
2	B	306	A86	O4-C38	4.72	1.45	1.35
2	B	307	A86	O4-C38	4.71	1.45	1.35
2	B	302	A86	O4-C38	4.70	1.45	1.35
2	A	302	A86	O4-C38	4.70	1.45	1.35
2	C	307	A86	O4-C38	4.69	1.45	1.35
2	B	301	A86	O4-C38	4.68	1.45	1.35
2	C	303	A86	O4-C38	4.68	1.45	1.35
2	B	304	A86	O4-C38	4.68	1.45	1.35
2	C	308	A86	O4-C38	4.68	1.45	1.35
2	A	306	A86	O4-C38	4.68	1.45	1.35
2	C	302	A86	O4-C38	4.67	1.45	1.35
2	C	306	A86	O4-C38	4.66	1.45	1.35
2	A	304	A86	O4-C38	4.66	1.45	1.35
2	A	305	A86	O4-C38	4.66	1.45	1.35
5	B	315	KC1	MG-NB	-4.65	1.96	2.05
5	C	316	KC1	MG-NB	-4.65	1.96	2.05
2	B	305	A86	O4-C38	4.65	1.45	1.35
2	C	305	A86	O4-C38	4.65	1.45	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	A86	O4-C38	4.64	1.45	1.35
5	A	315	KC1	MG-NB	-4.62	1.96	2.05
2	B	303	A86	O4-C38	4.62	1.45	1.35
2	A	303	A86	O4-C38	4.59	1.45	1.35
2	C	304	A86	O4-C38	4.58	1.45	1.35
4	B	310	KC2	MG-ND	-4.50	1.96	2.05
4	B	312	KC2	MG-ND	-4.47	1.96	2.05
4	C	311	KC2	MG-ND	-4.47	1.96	2.05
4	A	310	KC2	MG-ND	-4.46	1.96	2.05
4	A	312	KC2	MG-ND	-4.43	1.97	2.05
4	C	313	KC2	MG-ND	-4.42	1.97	2.05
6	A	319	LMG	O8-C28	4.23	1.45	1.33
4	B	310	KC2	MG-NB	-4.23	1.97	2.05
4	A	310	KC2	MG-NB	-4.22	1.97	2.05
6	B	318	LMG	O8-C28	4.19	1.45	1.33
6	C	320	LMG	O8-C28	4.15	1.45	1.33
4	C	311	KC2	MG-NB	-4.13	1.97	2.05
4	C	311	KC2	CHC-C1C	4.13	1.48	1.39
4	C	313	KC2	CHC-C1C	4.11	1.48	1.39
4	B	312	KC2	MG-NB	-4.11	1.97	2.05
4	A	312	KC2	MG-NB	-4.11	1.97	2.05
4	B	310	KC2	CHC-C1C	4.09	1.48	1.39
6	C	320	LMG	O7-C10	4.09	1.45	1.34
4	C	313	KC2	MG-NB	-4.08	1.97	2.05
4	B	312	KC2	CHC-C1C	4.08	1.48	1.39
4	A	310	KC2	CHC-C1C	4.08	1.48	1.39
4	A	312	KC2	CHC-C1C	4.06	1.48	1.39
6	A	319	LMG	O7-C10	4.06	1.45	1.34
6	B	318	LMG	O7-C10	4.06	1.45	1.34
4	B	310	KC2	CHC-C4B	4.02	1.46	1.38
4	B	312	KC2	CHC-C4B	4.02	1.46	1.38
4	C	313	KC2	CHC-C4B	3.98	1.46	1.38
4	A	310	KC2	CHC-C4B	3.98	1.46	1.38
4	A	312	KC2	CHC-C4B	3.97	1.46	1.38
4	C	311	KC2	CHC-C4B	3.95	1.46	1.38
3	B	308	CLA	C1D-ND	3.85	1.42	1.37
2	B	306	A86	C30-C29	-3.83	1.25	1.32
3	A	308	CLA	C1D-ND	3.82	1.42	1.37
3	B	317	CLA	C1D-ND	3.80	1.42	1.37
2	A	306	A86	C30-C29	-3.79	1.25	1.32
3	A	318	CLA	C1D-ND	3.77	1.42	1.37
2	C	307	A86	C30-C29	-3.77	1.25	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	316	CLA	C1D-ND	3.76	1.42	1.37
3	C	309	CLA	C1D-ND	3.76	1.42	1.37
3	C	317	CLA	C1D-ND	3.75	1.42	1.37
3	A	317	CLA	C1D-ND	3.74	1.42	1.37
3	C	301	CLA	C1D-ND	3.73	1.42	1.37
3	B	316	CLA	C1D-ND	3.72	1.42	1.37
3	C	319	CLA	C1D-ND	3.72	1.42	1.37
3	B	309	CLA	C1D-ND	3.72	1.42	1.37
3	A	309	CLA	C1D-ND	3.70	1.42	1.37
3	C	310	CLA	C1D-ND	3.70	1.42	1.37
3	C	318	CLA	C1D-ND	3.69	1.42	1.37
3	A	314	CLA	C1D-ND	3.68	1.42	1.37
3	C	315	CLA	C1D-ND	3.67	1.42	1.37
3	A	311	CLA	C1D-ND	3.66	1.42	1.37
3	C	312	CLA	C1D-ND	3.65	1.42	1.37
3	B	311	CLA	C1D-ND	3.65	1.42	1.37
3	B	314	CLA	C1D-ND	3.62	1.42	1.37
2	B	301	A86	C30-C29	-3.61	1.25	1.32
2	C	304	A86	C30-C29	-3.60	1.26	1.32
3	A	313	CLA	C1D-ND	3.58	1.42	1.37
2	A	307	A86	C30-C29	-3.56	1.26	1.32
2	C	308	A86	C30-C29	-3.54	1.26	1.32
2	B	303	A86	C30-C29	-3.54	1.26	1.32
2	C	303	A86	C30-C29	-3.54	1.26	1.32
2	B	302	A86	C30-C29	-3.54	1.26	1.32
2	B	307	A86	C30-C29	-3.54	1.26	1.32
2	C	302	A86	C30-C29	-3.53	1.26	1.32
2	A	301	A86	C30-C29	-3.52	1.26	1.32
2	A	302	A86	C30-C29	-3.52	1.26	1.32
2	A	303	A86	C30-C29	-3.52	1.26	1.32
2	A	305	A86	C30-C29	-3.52	1.26	1.32
2	B	305	A86	C30-C29	-3.51	1.26	1.32
3	C	314	CLA	C1D-ND	3.51	1.42	1.37
2	C	306	A86	C30-C29	-3.51	1.26	1.32
3	B	313	CLA	C1D-ND	3.50	1.42	1.37
2	A	304	A86	C30-C29	-3.49	1.26	1.32
2	C	305	A86	C30-C29	-3.45	1.26	1.32
2	B	304	A86	C30-C29	-3.44	1.26	1.32
3	C	319	CLA	C4B-NB	3.37	1.41	1.37
3	B	308	CLA	C4B-NB	3.36	1.41	1.37
4	C	313	KC2	CHD-C1D	3.33	1.46	1.39
3	A	318	CLA	C4B-NB	3.33	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	311	KC2	CHD-C1D	3.32	1.46	1.39
4	A	312	KC2	CHD-C1D	3.32	1.46	1.39
4	B	312	KC2	CHD-C1D	3.32	1.46	1.39
4	B	310	KC2	CHD-C1D	3.31	1.46	1.39
3	B	317	CLA	C4B-NB	3.30	1.41	1.37
4	A	310	KC2	CHD-C1D	3.30	1.46	1.39
3	C	314	CLA	C4B-NB	3.26	1.41	1.37
3	C	309	CLA	C4B-NB	3.25	1.41	1.37
3	A	308	CLA	C4B-NB	3.23	1.41	1.37
3	B	313	CLA	C4B-NB	3.21	1.41	1.37
3	A	313	CLA	C4B-NB	3.20	1.41	1.37
3	B	314	CLA	C4D-ND	-3.17	1.33	1.37
3	A	311	CLA	C4B-NB	3.16	1.41	1.37
3	C	312	CLA	C4B-NB	3.15	1.41	1.37
3	B	314	CLA	C4B-NB	3.15	1.41	1.37
3	B	311	CLA	C4B-NB	3.13	1.41	1.37
3	A	316	CLA	C4B-NB	3.13	1.41	1.37
3	C	317	CLA	C4B-NB	3.13	1.41	1.37
3	A	317	CLA	C4B-NB	3.11	1.41	1.37
3	A	314	CLA	C4B-NB	3.11	1.41	1.37
3	C	315	CLA	C4B-NB	3.11	1.41	1.37
3	B	316	CLA	C4B-NB	3.10	1.41	1.37
3	C	301	CLA	C4B-NB	3.10	1.41	1.37
3	B	309	CLA	C4B-NB	3.10	1.41	1.37
3	C	318	CLA	C4B-NB	3.09	1.41	1.37
3	A	309	CLA	C4B-NB	3.08	1.41	1.37
3	B	309	CLA	C4D-ND	-3.08	1.33	1.37
3	A	311	CLA	C4D-ND	-3.07	1.33	1.37
3	C	315	CLA	C4D-ND	-3.06	1.33	1.37
3	C	312	CLA	C4D-ND	-3.06	1.33	1.37
3	A	314	CLA	C4D-ND	-3.05	1.33	1.37
3	A	309	CLA	C4D-ND	-3.04	1.33	1.37
3	C	310	CLA	C4B-NB	3.03	1.41	1.37
3	C	310	CLA	C4D-ND	-3.01	1.33	1.37
3	C	314	CLA	C4D-ND	-3.00	1.33	1.37
3	A	313	CLA	C4D-ND	-2.99	1.33	1.37
3	B	308	CLA	C4D-ND	-2.98	1.33	1.37
3	A	317	CLA	C4D-ND	-2.97	1.33	1.37
3	C	319	CLA	C4D-ND	-2.97	1.33	1.37
3	A	318	CLA	C4D-ND	-2.97	1.33	1.37
3	B	313	CLA	C4D-ND	-2.97	1.33	1.37
3	B	311	CLA	C4D-ND	-2.97	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	317	CLA	C4D-ND	-2.96	1.33	1.37
3	C	309	CLA	C4D-ND	-2.95	1.33	1.37
3	B	317	CLA	C4D-ND	-2.93	1.33	1.37
3	B	314	CLA	C3B-C4B	2.93	1.49	1.42
3	C	318	CLA	C4D-ND	-2.91	1.33	1.37
3	C	301	CLA	C4D-ND	-2.91	1.33	1.37
3	A	308	CLA	C4D-ND	-2.91	1.33	1.37
3	A	316	CLA	C4D-ND	-2.89	1.33	1.37
3	C	315	CLA	C3B-C4B	2.89	1.49	1.42
3	B	308	CLA	C3B-C4B	2.88	1.49	1.42
3	C	301	CLA	C3B-C4B	2.87	1.49	1.42
5	C	316	KC1	CBA-CGA	-2.87	1.41	1.48
3	B	316	CLA	C4D-ND	-2.87	1.33	1.37
3	C	310	CLA	C3B-C4B	2.86	1.49	1.42
3	A	308	CLA	C3B-C4B	2.86	1.49	1.42
4	A	310	KC2	CBA-CGA	-2.86	1.41	1.48
3	C	319	CLA	C3B-C4B	2.86	1.49	1.42
5	B	315	KC1	CBA-CGA	-2.86	1.41	1.48
3	A	318	CLA	C3B-C4B	2.86	1.49	1.42
3	B	317	CLA	C3B-C4B	2.85	1.49	1.42
3	A	314	CLA	C3B-C4B	2.84	1.49	1.42
3	C	309	CLA	C3B-C4B	2.84	1.49	1.42
5	A	315	KC1	CBA-CGA	-2.84	1.41	1.48
5	A	315	KC1	C4B-NB	-2.84	1.34	1.37
3	B	309	CLA	C3B-C4B	2.83	1.49	1.42
4	C	311	KC2	CBA-CGA	-2.83	1.42	1.48
5	C	316	KC1	C4B-NB	-2.82	1.34	1.37
4	B	310	KC2	CBA-CGA	-2.82	1.42	1.48
3	C	312	CLA	C3B-C4B	2.81	1.49	1.42
3	A	309	CLA	C3B-C4B	2.81	1.49	1.42
3	C	318	CLA	C3B-C4B	2.80	1.49	1.42
3	C	317	CLA	C3B-C4B	2.79	1.49	1.42
3	B	316	CLA	C3B-C4B	2.79	1.49	1.42
4	A	312	KC2	CBA-CGA	-2.78	1.42	1.48
4	B	312	KC2	CBA-CGA	-2.78	1.42	1.48
4	C	313	KC2	CBA-CGA	-2.78	1.42	1.48
3	A	317	CLA	C3B-C4B	2.78	1.49	1.42
3	A	311	CLA	C3B-C4B	2.78	1.49	1.42
3	B	311	CLA	C3B-C4B	2.77	1.49	1.42
5	B	315	KC1	C4B-NB	-2.76	1.34	1.37
3	A	316	CLA	C3B-C4B	2.75	1.49	1.42
4	B	310	KC2	C4B-NB	-2.74	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	304	A86	O1-C20	-2.70	1.42	1.46
3	A	313	CLA	C3B-C4B	2.70	1.49	1.42
4	C	311	KC2	C4B-NB	-2.70	1.34	1.37
3	C	314	CLA	C3B-C4B	2.68	1.49	1.42
3	B	313	CLA	C3B-C4B	2.67	1.49	1.42
4	A	310	KC2	C4B-NB	-2.65	1.34	1.37
2	B	306	A86	O1-C20	-2.65	1.42	1.46
2	A	302	A86	O1-C20	-2.64	1.42	1.46
3	B	317	CLA	C1B-C2B	2.63	1.49	1.43
2	C	307	A86	O1-C20	-2.63	1.42	1.46
2	A	306	A86	O1-C20	-2.61	1.42	1.46
3	B	309	CLA	C1B-C2B	2.61	1.49	1.43
3	A	308	CLA	C1B-C2B	2.61	1.49	1.43
3	C	310	CLA	C1B-C2B	2.61	1.49	1.43
3	A	317	CLA	C1B-C2B	2.61	1.49	1.43
4	B	312	KC2	C4B-NB	-2.60	1.34	1.37
3	B	308	CLA	C1B-C2B	2.60	1.49	1.43
3	B	316	CLA	C1B-C2B	2.59	1.49	1.43
3	C	309	CLA	C1B-C2B	2.59	1.49	1.43
3	A	316	CLA	C1B-C2B	2.59	1.49	1.43
3	C	317	CLA	C1B-C2B	2.59	1.49	1.43
3	A	318	CLA	C1B-C2B	2.58	1.49	1.43
3	A	311	CLA	C1B-C2B	2.58	1.49	1.43
3	C	318	CLA	C1B-C2B	2.58	1.49	1.43
3	C	319	CLA	C1B-C2B	2.58	1.49	1.43
4	C	313	KC2	C4B-NB	-2.58	1.34	1.37
2	B	303	A86	O1-C20	-2.58	1.42	1.46
3	A	309	CLA	C1B-C2B	2.57	1.49	1.43
3	B	311	CLA	C1B-C2B	2.57	1.49	1.43
3	C	312	CLA	C1B-C2B	2.56	1.49	1.43
2	C	303	A86	O1-C20	-2.55	1.42	1.46
3	C	301	CLA	C1B-C2B	2.54	1.49	1.43
4	A	312	KC2	C4B-NB	-2.54	1.34	1.37
3	A	313	CLA	C1B-C2B	2.54	1.49	1.43
2	B	302	A86	O1-C20	-2.53	1.42	1.46
3	B	313	CLA	C1B-C2B	2.53	1.49	1.43
3	A	314	CLA	C1B-C2B	2.52	1.49	1.43
3	C	314	CLA	C1B-C2B	2.51	1.49	1.43
2	A	303	A86	O1-C20	-2.49	1.42	1.46
3	B	314	CLA	C1B-C2B	2.46	1.49	1.43
2	C	305	A86	O1-C20	-2.45	1.42	1.46
3	C	315	CLA	C1B-C2B	2.45	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	315	KC1	C1B-NB	-2.45	1.34	1.37
2	A	304	A86	O1-C20	-2.43	1.42	1.46
2	B	304	A86	O1-C20	-2.42	1.42	1.46
4	B	310	KC2	C4A-C3A	-2.40	1.39	1.44
5	C	316	KC1	C1B-NB	-2.40	1.34	1.37
3	B	313	CLA	CMB-C2B	-2.38	1.45	1.50
4	A	310	KC2	C4A-C3A	-2.37	1.40	1.44
5	B	315	KC1	C1B-NB	-2.35	1.34	1.37
4	C	311	KC2	C4A-C3A	-2.34	1.40	1.44
3	A	313	CLA	CMB-C2B	-2.32	1.45	1.50
2	C	306	A86	O1-C20	-2.31	1.42	1.46
2	B	301	A86	O1-C20	-2.29	1.42	1.46
2	A	301	A86	O1-C20	-2.29	1.42	1.46
3	C	314	CLA	CMB-C2B	-2.29	1.46	1.50
2	A	305	A86	O1-C20	-2.28	1.42	1.46
2	B	305	A86	O1-C20	-2.28	1.42	1.46
3	C	314	CLA	MG-NB	-2.27	2.01	2.05
2	C	302	A86	O1-C20	-2.27	1.43	1.46
3	B	313	CLA	MG-NB	-2.26	2.01	2.05
3	B	314	CLA	CHC-C1C	2.25	1.43	1.38
3	A	313	CLA	MG-NB	-2.24	2.01	2.05
3	A	314	CLA	CHC-C1C	2.22	1.43	1.38
2	B	307	A86	O1-C20	-2.22	1.43	1.46
4	B	312	KC2	C4A-C3A	-2.21	1.40	1.44
3	C	315	CLA	CHC-C1C	2.21	1.43	1.38
4	A	312	KC2	C4A-C3A	-2.21	1.40	1.44
3	A	314	CLA	CMD-C2D	-2.21	1.46	1.50
3	C	312	CLA	CHC-C1C	2.21	1.43	1.38
3	A	309	CLA	CHC-C1C	2.21	1.43	1.38
4	C	313	KC2	C4A-C3A	-2.20	1.40	1.44
3	A	311	CLA	CHC-C1C	2.19	1.43	1.38
3	C	318	CLA	CHC-C1C	2.19	1.43	1.38
3	C	312	CLA	MG-NB	-2.18	2.01	2.05
5	B	315	KC1	C4A-C3A	-2.18	1.40	1.44
3	B	311	CLA	CHC-C1C	2.17	1.42	1.38
3	B	309	CLA	CMD-C2D	-2.17	1.46	1.50
3	C	309	CLA	CHC-C1C	2.17	1.42	1.38
5	A	315	KC1	C4A-C3A	-2.17	1.40	1.44
5	C	316	KC1	C4A-C3A	-2.17	1.40	1.44
3	C	314	CLA	CMD-C2D	-2.16	1.46	1.50
3	B	309	CLA	CHC-C1C	2.16	1.42	1.38
3	A	317	CLA	MG-NB	-2.16	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	319	CLA	CHC-C1C	2.16	1.42	1.38
2	C	308	A86	O1-C20	-2.16	1.43	1.46
3	C	301	CLA	CHC-C1C	2.16	1.42	1.38
3	A	311	CLA	MG-NB	-2.15	2.01	2.05
3	B	317	CLA	CHC-C1C	2.15	1.42	1.38
3	A	313	CLA	CMD-C2D	-2.15	1.46	1.50
3	B	313	CLA	CMD-C2D	-2.15	1.46	1.50
3	C	317	CLA	CHC-C1C	2.15	1.42	1.38
3	B	311	CLA	MG-NB	-2.15	2.01	2.05
3	A	316	CLA	MG-NB	-2.15	2.01	2.05
3	A	314	CLA	MG-NB	-2.14	2.01	2.05
3	B	314	CLA	MG-NB	-2.14	2.01	2.05
3	C	301	CLA	MG-NB	-2.14	2.01	2.05
4	B	312	KC2	C1C-C2C	-2.14	1.40	1.44
3	A	317	CLA	CHC-C1C	2.14	1.42	1.38
3	B	308	CLA	CHC-C1C	2.14	1.42	1.38
4	B	310	KC2	C1B-NB	-2.13	1.35	1.37
3	A	316	CLA	CHC-C1C	2.13	1.42	1.38
3	B	316	CLA	MG-NB	-2.13	2.01	2.05
4	C	313	KC2	C1C-C2C	-2.13	1.40	1.44
4	A	312	KC2	C1C-C2C	-2.13	1.40	1.44
3	C	317	CLA	MG-NB	-2.13	2.01	2.05
5	A	315	KC1	C1D-ND	-2.12	1.35	1.37
3	A	318	CLA	CHC-C1C	2.12	1.42	1.38
5	C	316	KC1	C1D-ND	-2.12	1.35	1.37
3	A	308	CLA	CHC-C1C	2.12	1.42	1.38
2	A	303	A86	C13-C11	-2.12	1.45	1.49
5	B	315	KC1	C1D-ND	-2.12	1.35	1.37
3	C	310	CLA	CHC-C1C	2.12	1.42	1.38
3	C	315	CLA	MG-NB	-2.11	2.01	2.05
2	A	306	A86	C13-C11	-2.11	1.45	1.49
3	A	309	CLA	MG-NB	-2.11	2.01	2.05
2	B	306	A86	C13-C11	-2.11	1.45	1.49
3	B	316	CLA	CHC-C1C	2.11	1.42	1.38
3	A	316	CLA	CMD-C2D	-2.11	1.46	1.50
3	C	318	CLA	MG-NB	-2.10	2.01	2.05
4	C	311	KC2	C1C-C2C	-2.10	1.40	1.44
3	C	310	CLA	CMD-C2D	-2.10	1.46	1.50
3	B	309	CLA	MG-NB	-2.10	2.01	2.05
3	C	315	CLA	CMD-C2D	-2.09	1.46	1.50
3	B	308	CLA	MG-NB	-2.09	2.01	2.05
3	C	310	CLA	MG-NB	-2.09	2.01	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	303	A86	C13-C11	-2.09	1.45	1.49
3	B	317	CLA	CMB-C2B	-2.09	1.46	1.50
3	A	309	CLA	CMD-C2D	-2.08	1.46	1.50
3	B	309	CLA	CMC-C2C	-2.08	1.46	1.50
2	C	304	A86	C13-C11	-2.08	1.45	1.49
3	A	314	CLA	CMB-C2B	-2.08	1.46	1.50
3	B	317	CLA	MG-NB	-2.08	2.01	2.05
3	C	319	CLA	CMB-C2B	-2.07	1.46	1.50
3	A	308	CLA	MG-NB	-2.07	2.01	2.05
2	C	307	A86	C13-C11	-2.07	1.45	1.49
3	A	318	CLA	CMB-C2B	-2.07	1.46	1.50
3	C	314	CLA	CHC-C1C	2.07	1.42	1.38
3	C	319	CLA	MG-NB	-2.07	2.01	2.05
3	C	312	CLA	CMD-C2D	-2.06	1.46	1.50
4	B	310	KC2	C1C-C2C	-2.06	1.40	1.44
3	A	318	CLA	MG-NB	-2.06	2.01	2.05
4	A	310	KC2	C1B-NB	-2.06	1.35	1.37
3	B	311	CLA	CMD-C2D	-2.05	1.46	1.50
3	B	316	CLA	CMB-C2B	-2.05	1.46	1.50
3	C	309	CLA	MG-NB	-2.05	2.01	2.05
3	C	317	CLA	CMD-C2D	-2.05	1.46	1.50
3	B	316	CLA	CMD-C2D	-2.05	1.46	1.50
3	C	315	CLA	CMB-C2B	-2.05	1.46	1.50
4	A	312	KC2	C1D-ND	-2.04	1.35	1.37
3	B	313	CLA	CHC-C1C	2.04	1.42	1.38
2	A	307	A86	O1-C20	-2.04	1.43	1.46
3	A	308	CLA	CMD-C2D	-2.04	1.46	1.50
3	C	319	CLA	CMD-C2D	-2.04	1.46	1.50
3	A	311	CLA	CMD-C2D	-2.04	1.46	1.50
3	A	316	CLA	CMB-C2B	-2.04	1.46	1.50
3	B	308	CLA	CMB-C2B	-2.04	1.46	1.50
3	A	317	CLA	CMD-C2D	-2.04	1.46	1.50
3	A	318	CLA	CMD-C2D	-2.04	1.46	1.50
3	C	309	CLA	CMD-C2D	-2.03	1.46	1.50
2	A	302	A86	C13-C11	-2.03	1.45	1.49
4	A	310	KC2	C1C-C2C	-2.03	1.40	1.44
3	C	317	CLA	CMB-C2B	-2.03	1.46	1.50
3	B	314	CLA	CMD-C2D	-2.03	1.46	1.50
3	A	308	CLA	CMB-C2B	-2.03	1.46	1.50
3	C	301	CLA	CMD-C2D	-2.03	1.46	1.50
4	A	310	KC2	C1D-ND	-2.02	1.35	1.37
3	C	312	CLA	CMB-C2B	-2.02	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	313	CLA	CHC-C1C	2.02	1.42	1.38
4	C	311	KC2	C1B-NB	-2.02	1.35	1.37
3	A	314	CLA	CMC-C2C	-2.01	1.46	1.50
3	C	315	CLA	CMC-C2C	-2.01	1.46	1.50
3	B	308	CLA	CMD-C2D	-2.01	1.46	1.50
3	A	309	CLA	CMB-C2B	-2.01	1.46	1.50
3	C	318	CLA	CMD-C2D	-2.01	1.46	1.50
4	C	313	KC2	C1D-ND	-2.00	1.35	1.37

All (625) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	307	A86	C34-O4-C38	17.56	150.62	117.90
2	C	307	A86	O1-C15-C14	-17.22	78.65	113.21
2	A	306	A86	C34-O4-C38	17.19	149.94	117.90
2	A	304	A86	O1-C15-C14	-17.05	78.99	113.21
2	C	307	A86	C33-C32-C31	-17.00	92.69	109.21
2	C	305	A86	O1-C15-C14	-16.99	79.11	113.21
2	B	304	A86	O1-C15-C14	-16.96	79.17	113.21
2	B	306	A86	O1-C15-C14	-16.93	79.24	113.21
2	A	306	A86	O1-C15-C14	-16.89	79.32	113.21
2	A	306	A86	C33-C32-C31	-16.83	92.85	109.21
2	A	303	A86	O1-C15-C14	-16.79	79.53	113.21
2	B	306	A86	C34-O4-C38	16.76	149.12	117.90
2	B	306	A86	C33-C32-C31	-16.57	93.11	109.21
2	A	307	A86	O1-C15-C14	-16.42	80.25	113.21
2	B	303	A86	O1-C15-C14	-16.35	80.40	113.21
2	C	304	A86	O1-C15-C14	-16.29	80.51	113.21
2	C	308	A86	O1-C15-C14	-15.88	81.33	113.21
2	A	305	A86	C34-O4-C38	15.72	147.20	117.90
2	B	305	A86	C34-O4-C38	15.70	147.15	117.90
2	B	307	A86	O1-C15-C14	-15.67	81.75	113.21
2	C	306	A86	C34-O4-C38	15.61	146.98	117.90
2	C	302	A86	O1-C15-C14	-14.16	84.79	113.21
2	A	301	A86	O1-C15-C14	-13.88	85.36	113.21
2	B	301	A86	O1-C15-C14	-13.49	86.14	113.21
2	B	302	A86	O1-C15-C14	-13.30	86.52	113.21
2	C	303	A86	O1-C15-C14	-12.64	87.85	113.21
2	A	302	A86	O1-C15-C14	-11.60	89.94	113.21
2	A	307	A86	C34-O4-C38	10.89	138.19	117.90
2	B	307	A86	C34-O4-C38	10.62	137.69	117.90
2	C	308	A86	C34-O4-C38	10.44	137.35	117.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	306	A86	O1-C15-C14	9.01	131.29	113.21
2	A	303	A86	C34-O4-C38	8.97	134.60	117.90
2	B	305	A86	O1-C15-C14	8.94	131.16	113.21
2	A	305	A86	O1-C15-C14	8.81	130.89	113.21
2	B	303	A86	C34-O4-C38	8.24	133.25	117.90
4	B	310	KC2	CHB-C1B-NB	7.50	131.35	124.45
4	C	311	KC2	CHB-C1B-NB	7.47	131.32	124.45
2	A	301	A86	C34-O4-C38	7.36	131.61	117.90
4	A	310	KC2	CHB-C1B-NB	7.35	131.21	124.45
4	A	312	KC2	CHB-C1B-NB	7.15	131.03	124.45
4	C	313	KC2	CHB-C1B-NB	7.13	131.01	124.45
4	B	312	KC2	CHB-C1B-NB	7.10	130.98	124.45
3	A	316	CLA	C4A-NA-C1A	6.74	109.74	106.71
3	B	316	CLA	C4A-NA-C1A	6.73	109.73	106.71
3	C	318	CLA	C4A-NA-C1A	6.69	109.71	106.71
3	B	309	CLA	C4A-NA-C1A	6.68	109.71	106.71
3	A	317	CLA	C4A-NA-C1A	6.68	109.71	106.71
3	C	312	CLA	C4A-NA-C1A	6.67	109.70	106.71
2	C	304	A86	C34-O4-C38	6.65	130.30	117.90
3	C	317	CLA	C4A-NA-C1A	6.59	109.67	106.71
3	C	301	CLA	C4A-NA-C1A	6.58	109.66	106.71
3	A	311	CLA	C4A-NA-C1A	6.57	109.66	106.71
3	B	311	CLA	C4A-NA-C1A	6.55	109.65	106.71
4	C	311	KC2	CHC-C4B-NB	6.54	130.47	124.45
3	C	319	CLA	C4A-NA-C1A	6.54	109.65	106.71
3	C	310	CLA	C4A-NA-C1A	6.53	109.64	106.71
3	A	309	CLA	C4A-NA-C1A	6.50	109.63	106.71
3	B	317	CLA	C4A-NA-C1A	6.50	109.63	106.71
3	C	309	CLA	C4A-NA-C1A	6.49	109.62	106.71
3	A	318	CLA	C4A-NA-C1A	6.49	109.62	106.71
4	A	312	KC2	CHC-C4B-NB	6.49	130.41	124.45
3	A	313	CLA	C4A-NA-C1A	6.48	109.62	106.71
4	C	313	KC2	CHC-C4B-NB	6.48	130.41	124.45
4	B	310	KC2	CHC-C4B-NB	6.46	130.39	124.45
3	A	308	CLA	C4A-NA-C1A	6.44	109.60	106.71
4	A	310	KC2	CHC-C4B-NB	6.44	130.37	124.45
4	B	312	KC2	CHC-C4B-NB	6.43	130.36	124.45
3	B	313	CLA	C4A-NA-C1A	6.41	109.59	106.71
3	C	314	CLA	C4A-NA-C1A	6.41	109.59	106.71
3	B	308	CLA	C4A-NA-C1A	6.41	109.59	106.71
2	B	306	A86	O4-C34-C33	6.37	123.46	107.59
2	B	301	A86	C34-O4-C38	6.30	129.63	117.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	306	A86	O4-C34-C33	6.29	123.25	107.59
5	C	316	KC1	CHC-C4B-NB	6.28	130.23	124.45
5	A	315	KC1	CHC-C4B-NB	6.24	130.19	124.45
5	A	315	KC1	CHB-C1B-NB	6.24	130.18	124.45
5	B	315	KC1	CHC-C4B-NB	6.23	130.18	124.45
2	C	307	A86	O4-C34-C33	6.23	123.11	107.59
5	C	316	KC1	CHB-C1B-NB	6.16	130.12	124.45
3	B	314	CLA	C4A-NA-C1A	6.11	109.45	106.71
5	B	315	KC1	CHB-C1B-NB	6.10	130.06	124.45
3	C	315	CLA	C4A-NA-C1A	6.06	109.43	106.71
2	C	307	A86	C41-C32-C31	6.05	115.89	110.47
3	A	314	CLA	C4A-NA-C1A	6.03	109.42	106.71
2	C	304	A86	O1-C20-C21	-5.95	107.93	115.06
2	B	306	A86	C41-C32-C31	5.92	115.77	110.47
2	A	306	A86	C41-C32-C31	5.86	115.72	110.47
2	B	301	A86	C4-C5-C6	-5.76	119.10	127.31
2	A	302	A86	C4-C5-C6	-5.74	119.11	127.31
2	C	308	A86	C4-C5-C6	-5.74	119.12	127.31
2	B	307	A86	C4-C5-C6	-5.67	119.21	127.31
2	A	302	A86	O1-C20-C21	-5.67	108.27	115.06
2	C	303	A86	C4-C5-C6	-5.64	119.25	127.31
2	B	303	A86	O1-C20-C21	-5.63	108.31	115.06
2	A	307	A86	C4-C5-C6	-5.63	119.27	127.31
2	B	302	A86	C4-C5-C6	-5.57	119.37	127.31
2	C	302	A86	C34-O4-C38	5.55	128.24	117.90
2	C	303	A86	O1-C20-C21	-5.50	108.47	115.06
2	B	302	A86	O1-C20-C21	-5.47	108.50	115.06
2	A	306	A86	O1-C20-C21	-5.38	108.61	115.06
2	A	303	A86	C3-C2-C1	-5.38	119.64	127.31
2	A	307	A86	O1-C20-C19	-5.37	109.35	113.38
2	B	303	A86	C3-C2-C1	-5.36	119.67	127.31
2	A	301	A86	C4-C5-C6	-5.27	119.80	127.31
2	B	306	A86	O1-C20-C21	-5.25	108.76	115.06
2	C	307	A86	O1-C20-C21	-5.14	108.89	115.06
2	C	302	A86	C4-C5-C6	-5.08	120.06	127.31
2	B	304	A86	C3-C2-C1	-5.06	120.08	127.31
2	C	305	A86	O1-C20-C21	-5.04	109.02	115.06
2	C	305	A86	C3-C2-C1	-5.01	120.16	127.31
2	A	304	A86	C3-C2-C1	-5.00	120.17	127.31
2	A	306	A86	C25-C26-C27	-5.00	120.17	127.31
2	B	304	A86	O1-C20-C21	-5.00	109.06	115.06
2	C	307	A86	C25-C26-C27	-4.98	120.20	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	304	A86	O1-C20-C21	-4.97	109.10	115.06
2	A	302	A86	C25-C26-C27	-4.95	120.25	127.31
2	C	303	A86	C25-C26-C27	-4.94	120.27	127.31
2	C	307	A86	C36-C31-C32	4.93	124.59	119.70
2	A	306	A86	C36-C31-C32	4.90	124.56	119.70
2	B	302	A86	C25-C26-C27	-4.88	120.34	127.31
2	B	304	A86	C25-C26-C27	-4.88	120.34	127.31
2	B	306	A86	C36-C31-C32	4.87	124.53	119.70
2	A	303	A86	O1-C20-C21	-4.87	109.22	115.06
2	A	304	A86	C25-C26-C27	-4.84	120.40	127.31
2	B	307	A86	C25-C26-C27	-4.81	120.45	127.31
2	A	307	A86	C25-C26-C27	-4.79	120.47	127.31
2	B	306	A86	C25-C26-C27	-4.78	120.49	127.31
4	C	311	KC2	O2D-CGD-CBD	4.77	119.75	111.27
2	B	306	A86	O4-C38-C39	4.77	119.86	111.09
2	C	304	A86	C3-C2-C1	-4.77	120.51	127.31
2	C	308	A86	C25-C26-C27	-4.77	120.51	127.31
2	A	307	A86	O1-C20-C21	-4.74	109.37	115.06
5	C	316	KC1	C1D-ND-C4D	4.71	109.68	106.33
4	B	310	KC2	O2D-CGD-CBD	4.71	119.64	111.27
2	A	306	A86	O4-C38-C39	4.71	119.75	111.09
5	B	315	KC1	C1D-ND-C4D	4.69	109.67	106.33
4	B	312	KC2	O2D-CGD-CBD	4.69	119.60	111.27
5	A	315	KC1	C1D-ND-C4D	4.69	109.66	106.33
5	B	315	KC1	CHD-C1D-ND	4.66	129.19	124.26
2	C	307	A86	O4-C38-C39	4.63	119.61	111.09
4	B	310	KC2	CHD-C1D-ND	4.63	129.16	124.26
4	A	310	KC2	O2D-CGD-CBD	4.63	119.49	111.27
5	A	315	KC1	CHD-C1D-ND	4.62	129.15	124.26
2	C	305	A86	C25-C26-C27	-4.60	120.74	127.31
5	C	316	KC1	CHD-C1D-ND	4.60	129.13	124.26
4	C	313	KC2	O2D-CGD-CBD	4.60	119.44	111.27
2	A	303	A86	O4-C38-C39	4.58	119.51	111.09
4	C	311	KC2	CHD-C1D-ND	4.58	129.10	124.26
2	A	302	A86	O4-C38-C39	4.58	119.51	111.09
2	C	305	A86	C34-O4-C38	4.57	126.41	117.90
2	C	303	A86	O4-C38-C39	4.57	119.50	111.09
4	A	312	KC2	CHD-C1D-ND	4.56	129.08	124.26
2	B	302	A86	O4-C38-C39	4.55	119.45	111.09
4	A	310	KC2	CHD-C1D-ND	4.54	129.06	124.26
2	C	304	A86	O4-C38-C39	4.53	119.42	111.09
2	C	308	A86	O1-C20-C19	-4.53	109.98	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	305	A86	O4-C38-C39	4.52	119.40	111.09
2	B	303	A86	O4-C38-C39	4.51	119.39	111.09
2	C	306	A86	O4-C38-C39	4.50	119.37	111.09
2	C	302	A86	O4-C38-C39	4.50	119.37	111.09
2	B	307	A86	O1-C20-C21	-4.50	109.67	115.06
2	C	308	A86	O1-C20-C21	-4.49	109.67	115.06
2	A	305	A86	O4-C38-C39	4.49	119.35	111.09
2	B	301	A86	O1-C20-C21	-4.49	109.68	115.06
4	B	312	KC2	CHD-C1D-ND	4.48	129.00	124.26
4	C	313	KC2	CHD-C1D-ND	4.47	128.99	124.26
2	C	305	A86	O4-C38-C39	4.47	119.31	111.09
2	A	301	A86	O1-C20-C21	-4.46	109.71	115.06
2	A	304	A86	C34-O4-C38	4.45	126.20	117.90
2	B	304	A86	O4-C38-C39	4.45	119.27	111.09
2	A	304	A86	O4-C38-C39	4.44	119.25	111.09
2	C	308	A86	O4-C38-C39	4.43	119.25	111.09
2	B	304	A86	C4-C5-C6	-4.43	120.98	127.31
2	A	307	A86	O4-C38-C39	4.43	119.23	111.09
2	A	301	A86	C25-C26-C27	-4.42	121.00	127.31
2	A	301	A86	O4-C38-C39	4.42	119.23	111.09
2	B	307	A86	O4-C38-C39	4.42	119.22	111.09
4	A	312	KC2	O2D-CGD-CBD	4.42	119.12	111.27
2	A	304	A86	C4-C5-C6	-4.42	121.01	127.31
2	B	301	A86	O4-C38-C39	4.42	119.21	111.09
5	C	316	KC1	O2D-CGD-CBD	4.40	119.08	111.27
2	C	305	A86	C4-C5-C6	-4.39	121.04	127.31
2	A	307	A86	C3-C2-C1	-4.35	121.11	127.31
2	C	302	A86	O1-C20-C21	-4.34	109.85	115.06
5	B	315	KC1	O2D-CGD-CBD	4.34	118.97	111.27
2	B	301	A86	C25-C26-C27	-4.33	121.14	127.31
5	A	315	KC1	O2D-CGD-CBD	4.32	118.94	111.27
2	C	308	A86	C3-C2-C1	-4.30	121.17	127.31
2	B	307	A86	C3-C2-C1	-4.30	121.17	127.31
2	C	302	A86	C25-C26-C27	-4.27	121.21	127.31
5	A	315	KC1	C2D-C1D-ND	-4.27	107.37	110.23
2	A	305	A86	C25-C26-C27	-4.25	121.24	127.31
2	B	302	A86	C3-C2-C1	-4.24	121.26	127.31
5	B	315	KC1	C2D-C1D-ND	-4.23	107.40	110.23
2	C	303	A86	C3-C2-C1	-4.21	121.30	127.31
2	A	303	A86	C4-C5-C6	-4.20	121.32	127.31
2	A	302	A86	C3-C2-C1	-4.19	121.33	127.31
2	B	305	A86	C25-C26-C27	-4.19	121.33	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	307	A86	O1-C20-C19	-4.19	110.23	113.38
2	B	303	A86	C4-C5-C6	-4.19	121.33	127.31
5	C	316	KC1	C2D-C1D-ND	-4.17	107.44	110.23
2	C	304	A86	C4-C5-C6	-4.13	121.42	127.31
2	C	306	A86	O1-C20-C21	-4.11	110.13	115.06
2	B	305	A86	O1-C20-C21	-4.08	110.17	115.06
2	A	301	A86	C3-C2-C1	-4.08	121.49	127.31
2	C	306	A86	C25-C26-C27	-4.05	121.53	127.31
2	A	305	A86	O1-C20-C21	-4.01	110.25	115.06
6	C	320	LMG	O7-C10-C11	4.00	120.12	111.50
2	B	301	A86	C3-C2-C1	-3.96	121.65	127.31
4	A	310	KC2	C4B-CHC-C1C	-3.96	117.52	126.06
2	C	302	A86	C3-C2-C1	-3.95	121.67	127.31
2	B	306	A86	O4-C34-C35	-3.94	97.78	107.59
4	C	311	KC2	C4B-CHC-C1C	-3.92	117.59	126.06
4	B	310	KC2	C4B-CHC-C1C	-3.91	117.62	126.06
6	A	319	LMG	O7-C10-C11	3.91	119.92	111.50
4	C	313	KC2	C4B-CHC-C1C	-3.86	117.73	126.06
4	B	310	KC2	C1D-CHD-C4C	-3.85	117.21	126.34
4	B	312	KC2	C4B-CHC-C1C	-3.85	117.76	126.06
4	C	311	KC2	C1D-CHD-C4C	-3.83	117.25	126.34
4	A	312	KC2	C4B-CHC-C1C	-3.83	117.80	126.06
2	A	306	A86	O4-C34-C35	-3.80	98.13	107.59
4	A	310	KC2	C1D-CHD-C4C	-3.80	117.34	126.34
2	C	307	A86	O4-C34-C35	-3.79	98.15	107.59
2	B	304	A86	C34-O4-C38	3.78	124.94	117.90
4	B	312	KC2	C1D-CHD-C4C	-3.77	117.40	126.34
4	A	312	KC2	C1D-CHD-C4C	-3.76	117.41	126.34
2	C	304	A86	C25-C26-C27	-3.74	121.97	127.31
4	C	313	KC2	C1D-CHD-C4C	-3.74	117.47	126.34
2	B	303	A86	C25-C26-C27	-3.72	122.00	127.31
3	B	316	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
4	B	310	KC2	CHB-C1B-C2B	-3.62	117.88	125.48
3	A	316	CLA	O2D-CGD-O1D	-3.60	116.81	123.84
4	C	311	KC2	CHB-C1B-C2B	-3.55	118.03	125.48
2	B	307	A86	C40-C32-C31	-3.55	107.29	110.47
4	A	310	KC2	CHB-C1B-C2B	-3.55	118.03	125.48
2	A	307	A86	C40-C32-C31	-3.53	107.31	110.47
2	C	308	A86	C40-C32-C31	-3.46	107.37	110.47
4	C	313	KC2	CHC-C4B-C3B	-3.43	119.38	125.26
4	A	312	KC2	CHC-C4B-C3B	-3.42	119.42	125.26
4	C	313	KC2	CHB-C1B-C2B	-3.41	118.33	125.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	312	KC2	CHC-C4B-C3B	-3.41	119.43	125.26
4	A	312	KC2	CHB-C1B-C2B	-3.38	118.38	125.48
4	C	311	KC2	CHC-C4B-C3B	-3.37	119.50	125.26
4	B	312	KC2	CHB-C1B-C2B	-3.36	118.44	125.48
6	B	318	LMG	O7-C10-C11	3.35	118.73	111.50
4	A	310	KC2	CHC-C4B-C3B	-3.35	119.53	125.26
4	B	310	KC2	CHC-C4B-C3B	-3.34	119.55	125.26
4	B	310	KC2	C1D-ND-C4D	3.31	108.69	106.33
2	A	303	A86	C25-C26-C27	-3.29	122.62	127.31
3	C	317	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
2	C	307	A86	C12-C11-C13	3.23	121.45	116.02
2	B	306	A86	C12-C11-C13	3.23	121.45	116.02
4	A	310	KC2	C1D-ND-C4D	3.23	108.63	106.33
4	C	311	KC2	C1D-ND-C4D	3.20	108.61	106.33
2	A	302	A86	C40-C32-C31	-3.20	107.61	110.47
2	A	306	A86	C12-C11-C13	3.19	121.38	116.02
2	B	302	A86	C40-C32-C31	-3.14	107.66	110.47
2	C	302	A86	O1-C20-C19	-3.12	111.04	113.38
2	C	303	A86	C40-C32-C31	-3.11	107.69	110.47
2	B	306	A86	C35-C34-C33	-3.10	104.47	109.88
4	B	312	KC2	C1D-ND-C4D	3.09	108.53	106.33
2	B	301	A86	O1-C20-C19	-3.01	111.12	113.38
3	C	310	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
3	C	319	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
3	B	317	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
3	B	309	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
4	A	312	KC2	C1D-ND-C4D	2.96	108.44	106.33
4	C	313	KC2	C1D-ND-C4D	2.96	108.44	106.33
2	A	302	A86	C17-C16-C15	2.96	112.18	109.16
3	A	318	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
2	A	306	A86	C35-C34-C33	-2.95	104.72	109.88
4	B	310	KC2	C1A-NA-C4A	-2.94	105.39	106.71
3	A	317	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
3	A	309	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
5	C	316	KC1	CHC-C4B-C3B	-2.91	120.27	125.26
4	B	310	KC2	C2D-C1D-ND	-2.91	108.28	110.23
5	B	315	KC1	CHC-C4B-C3B	-2.90	120.29	125.26
4	C	313	KC2	C1A-NA-C4A	-2.90	105.40	106.71
3	C	318	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
4	A	312	KC2	CBD-CHA-C1A	2.90	134.28	128.88
2	C	307	A86	C35-C34-C33	-2.90	104.82	109.88
5	A	315	KC1	CHC-C4B-C3B	-2.89	120.32	125.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	306	A86	C40-C32-C31	-2.88	107.89	110.47
2	B	303	A86	C3-C4-C5	-2.88	117.57	123.47
3	B	314	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
4	C	313	KC2	CBD-CHA-C1A	2.87	134.24	128.88
4	B	312	KC2	CBD-CHA-C1A	2.87	134.23	128.88
3	C	301	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
6	B	318	LMG	O8-C28-C29	2.87	120.90	111.91
4	A	310	KC2	C2D-C1D-ND	-2.86	108.31	110.23
3	C	309	CLA	C3B-C4B-NB	-2.86	107.86	110.52
3	C	312	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
4	A	310	KC2	CBD-CHA-C1A	2.85	134.20	128.88
3	B	313	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
3	C	315	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
3	B	311	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
2	B	301	A86	C9-C10-C11	-2.84	118.25	126.61
3	B	314	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
3	A	311	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
4	C	311	KC2	CBD-CHA-C1A	2.83	134.16	128.88
2	A	302	A86	C9-C10-C11	-2.83	118.28	126.61
4	B	310	KC2	CBD-CHA-C1A	2.82	134.13	128.88
3	A	313	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
3	A	308	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
4	C	311	KC2	C2D-C1D-ND	-2.81	108.35	110.23
3	C	314	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
3	B	308	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
4	A	312	KC2	C1A-NA-C4A	-2.80	105.45	106.71
3	A	314	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
3	A	308	CLA	C3B-C4B-NB	-2.79	107.93	110.52
3	C	309	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
2	A	301	A86	O1-C20-C19	-2.78	111.29	113.38
6	C	320	LMG	O8-C28-C29	2.78	120.64	111.91
3	B	314	CLA	C3B-C4B-NB	-2.78	107.94	110.52
3	B	311	CLA	C3B-C4B-NB	-2.77	107.94	110.52
2	B	307	A86	C9-C10-C11	-2.77	118.46	126.61
3	B	308	CLA	C3B-C4B-NB	-2.77	107.94	110.52
4	B	312	KC2	C1A-NA-C4A	-2.77	105.46	106.71
2	A	307	A86	C9-C10-C11	-2.77	118.47	126.61
2	C	303	A86	C9-C10-C11	-2.76	118.49	126.61
3	C	319	CLA	C3B-C4B-NB	-2.76	107.95	110.52
3	C	312	CLA	C3B-C4B-NB	-2.75	107.97	110.52
2	C	308	A86	C9-C10-C11	-2.75	118.53	126.61
3	A	311	CLA	C3B-C4B-NB	-2.74	107.97	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	302	A86	C9-C10-C11	-2.74	118.55	126.61
4	A	312	KC2	O1D-CGD-CBD	-2.74	118.89	124.48
2	B	301	A86	C4-C3-C2	-2.74	117.87	123.47
3	A	318	CLA	C3B-C4B-NB	-2.73	107.98	110.52
2	B	307	A86	C9-C8-C6	-2.72	118.78	126.42
3	C	315	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
6	A	319	LMG	O8-C28-C29	2.72	120.43	111.91
4	C	311	KC2	C1A-NA-C4A	-2.71	105.49	106.71
2	A	307	A86	C9-C8-C6	-2.71	118.81	126.42
3	B	317	CLA	C3B-C4B-NB	-2.70	108.01	110.52
2	C	308	A86	C9-C8-C6	-2.70	118.83	126.42
2	C	307	A86	C40-C32-C31	-2.70	108.06	110.47
3	A	314	CLA	C3B-C4B-NB	-2.70	108.01	110.52
3	C	315	CLA	C3B-C4B-NB	-2.70	108.01	110.52
4	B	312	KC2	C2D-C1D-ND	-2.69	108.43	110.23
2	A	303	A86	C3-C4-C5	-2.69	117.96	123.47
2	B	301	A86	C9-C8-C6	-2.69	118.86	126.42
2	B	302	A86	C9-C10-C11	-2.68	118.72	126.61
3	B	316	CLA	C3B-C4B-NB	-2.68	108.03	110.52
2	A	302	A86	C9-C8-C6	-2.68	118.89	126.42
5	A	315	KC1	CHB-C1B-C2B	-2.68	119.87	125.48
2	C	303	A86	C17-C16-C15	2.66	111.88	109.16
4	C	313	KC2	O1D-CGD-CBD	-2.65	119.05	124.48
5	C	316	KC1	CHB-C1B-C2B	-2.65	119.91	125.48
5	B	315	KC1	C1D-CHD-C4C	-2.65	120.05	126.34
2	A	302	A86	C4-C3-C2	-2.65	118.05	123.47
5	A	315	KC1	O1D-CGD-CBD	-2.65	119.07	124.48
5	A	315	KC1	C1D-CHD-C4C	-2.63	120.10	126.34
4	A	310	KC2	CHD-C4C-NC	2.63	128.19	124.20
4	C	311	KC2	CHD-C4C-NC	2.63	128.19	124.20
2	A	301	A86	C9-C10-C11	-2.62	118.89	126.61
2	A	306	A86	C40-C32-C31	-2.62	108.13	110.47
5	B	315	KC1	CHB-C1B-C2B	-2.62	119.98	125.48
5	B	315	KC1	CBD-CHA-C1A	2.62	133.76	128.88
5	B	315	KC1	O1D-CGD-CBD	-2.62	119.13	124.48
4	A	310	KC2	C1A-NA-C4A	-2.62	105.53	106.71
5	C	316	KC1	C1D-CHD-C4C	-2.62	120.14	126.34
3	A	316	CLA	C3B-C4B-NB	-2.61	108.09	110.52
3	C	317	CLA	C3B-C4B-NB	-2.61	108.09	110.52
5	A	315	KC1	CBD-CHA-C1A	2.61	133.75	128.88
2	B	302	A86	C4-C3-C2	-2.61	118.14	123.47
2	C	303	A86	C4-C3-C2	-2.60	118.14	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	316	KC1	CBD-CHA-C1A	2.60	133.73	128.88
6	B	318	LMG	O1-C1-C2	2.60	112.36	108.30
3	A	309	CLA	C3B-C4B-NB	-2.60	108.10	110.52
4	B	310	KC2	CHD-C4C-NC	2.60	128.14	124.20
2	C	303	A86	C9-C8-C6	-2.59	119.13	126.42
3	C	318	CLA	C3B-C4B-NB	-2.59	108.11	110.52
3	C	310	CLA	CHB-C4A-NA	2.57	128.07	124.51
4	C	313	KC2	C2D-C1D-ND	-2.57	108.51	110.23
3	A	314	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
2	C	304	A86	C3-C4-C5	-2.56	118.22	123.47
3	A	316	CLA	CHB-C4A-NA	2.56	128.05	124.51
3	A	314	CLA	CHB-C4A-NA	2.55	128.04	124.51
3	C	310	CLA	C3B-C4B-NB	-2.55	108.15	110.52
3	B	311	CLA	C1-C2-C3	-2.55	121.63	126.04
4	A	312	KC2	C2D-C1D-ND	-2.55	108.52	110.23
3	B	316	CLA	CHB-C4A-NA	2.54	128.03	124.51
3	C	301	CLA	C3B-C4B-NB	-2.54	108.16	110.52
3	B	309	CLA	CHB-C4A-NA	2.54	128.03	124.51
3	C	315	CLA	CHB-C4A-NA	2.54	128.03	124.51
3	C	318	CLA	CHB-C4A-NA	2.54	128.02	124.51
3	C	319	CLA	CHB-C4A-NA	2.53	128.01	124.51
4	B	312	KC2	O1D-CGD-CBD	-2.53	119.31	124.48
3	B	309	CLA	C3B-C4B-NB	-2.53	108.17	110.52
3	A	311	CLA	CHB-C4A-NA	2.52	128.00	124.51
2	A	301	A86	C4-C3-C2	-2.52	118.31	123.47
3	A	309	CLA	CHB-C4A-NA	2.52	127.99	124.51
3	B	314	CLA	CHB-C4A-NA	2.52	127.99	124.51
3	A	317	CLA	CHB-C4A-NA	2.52	127.99	124.51
3	C	312	CLA	CHB-C4A-NA	2.52	127.99	124.51
2	B	302	A86	C9-C8-C6	-2.51	119.36	126.42
3	B	317	CLA	CHB-C4A-NA	2.51	127.98	124.51
3	C	314	CLA	C3B-C4B-NB	-2.51	108.19	110.52
2	C	308	A86	C4-C3-C2	-2.51	118.34	123.47
3	C	301	CLA	CHB-C4A-NA	2.50	127.97	124.51
3	A	317	CLA	C3B-C4B-NB	-2.50	108.20	110.52
3	B	311	CLA	CHB-C4A-NA	2.49	127.95	124.51
2	C	302	A86	C4-C3-C2	-2.48	118.40	123.47
3	B	313	CLA	C3B-C4B-NB	-2.47	108.22	110.52
5	C	316	KC1	O1D-CGD-CBD	-2.47	119.42	124.48
2	C	302	A86	C9-C8-C6	-2.47	119.47	126.42
3	C	309	CLA	CHB-C4A-NA	2.47	127.93	124.51
3	A	311	CLA	C1-C2-C3	-2.47	121.77	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	307	A86	C4-C3-C2	-2.47	118.42	123.47
3	A	318	CLA	CHB-C4A-NA	2.47	127.92	124.51
3	A	313	CLA	C3B-C4B-NB	-2.46	108.23	110.52
3	A	314	CLA	C1-C2-C3	-2.46	121.79	126.04
2	B	306	A86	O4-C38-O5	-2.46	118.07	122.96
3	A	308	CLA	CHB-C4A-NA	2.46	127.91	124.51
3	C	317	CLA	CHB-C4A-NA	2.46	127.91	124.51
4	A	310	KC2	O1D-CGD-CBD	-2.45	119.47	124.48
4	B	312	KC2	CHD-C4C-NC	2.44	127.91	124.20
3	B	308	CLA	CHB-C4A-NA	2.44	127.89	124.51
2	A	303	A86	C9-C10-C11	-2.44	119.43	126.61
3	C	312	CLA	C1-C2-C3	-2.44	121.82	126.04
5	C	316	KC1	C4B-CHC-C1C	-2.44	120.80	126.06
4	A	312	KC2	CHD-C4C-NC	2.44	127.90	124.20
3	C	315	CLA	C1-C2-C3	-2.43	121.83	126.04
3	B	314	CLA	C1-C2-C3	-2.43	121.84	126.04
2	A	306	A86	O4-C38-O5	-2.43	118.14	122.96
5	A	315	KC1	C4B-CHC-C1C	-2.43	120.82	126.06
2	A	307	A86	C4-C3-C2	-2.43	118.50	123.47
4	C	313	KC2	CHD-C4C-NC	2.43	127.88	124.20
2	B	304	A86	C12-C11-C13	2.42	120.09	116.02
2	B	306	A86	C10-C9-C8	-2.42	115.68	123.22
2	A	303	A86	O4-C38-O5	-2.41	118.17	122.96
5	B	315	KC1	C4B-CHC-C1C	-2.41	120.85	126.06
4	B	310	KC2	O1D-CGD-CBD	-2.41	119.55	124.48
2	C	304	A86	C40-C32-C31	-2.41	108.31	110.47
2	A	302	A86	O4-C38-O5	-2.41	118.17	122.96
2	A	305	A86	O4-C38-O5	-2.41	118.18	122.96
2	B	305	A86	O4-C38-O5	-2.40	118.19	122.96
2	A	304	A86	C12-C11-C13	2.40	120.06	116.02
2	C	305	A86	C12-C11-C13	2.40	120.06	116.02
2	C	306	A86	O4-C38-O5	-2.40	118.19	122.96
4	A	310	KC2	CHB-C4A-C3A	-2.40	121.23	124.98
2	C	304	A86	O4-C38-O5	-2.40	118.19	122.96
2	B	303	A86	C9-C10-C11	-2.40	119.55	126.61
2	C	307	A86	C10-C9-C8	-2.40	115.73	123.22
2	C	303	A86	O4-C38-O5	-2.40	118.20	122.96
2	C	307	A86	O4-C38-O5	-2.39	118.21	122.96
2	B	307	A86	C17-C16-C15	2.38	111.59	109.16
2	B	302	A86	O4-C38-O5	-2.38	118.23	122.96
2	B	303	A86	O4-C38-O5	-2.37	118.25	122.96
5	B	315	KC1	O2D-CGD-O1D	-2.37	119.21	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	315	KC1	O2D-CGD-O1D	-2.36	119.22	123.84
4	B	310	KC2	CHB-C4A-C3A	-2.36	121.30	124.98
4	C	311	KC2	O1D-CGD-CBD	-2.35	119.67	124.48
4	C	311	KC2	CHB-C4A-C3A	-2.35	121.31	124.98
2	C	308	A86	C17-C16-C15	2.33	111.55	109.16
2	B	307	A86	C20-C19-C18	2.32	117.34	112.75
2	A	306	A86	C28-C27-C26	-2.32	119.67	122.92
2	B	304	A86	O4-C38-O5	-2.32	118.36	122.96
2	A	301	A86	C9-C8-C6	-2.32	119.90	126.42
2	C	307	A86	C28-C27-C26	-2.32	119.68	122.92
2	A	306	A86	C10-C9-C8	-2.32	115.99	123.22
2	C	302	A86	O4-C38-O5	-2.31	118.37	122.96
2	C	308	A86	C20-C19-C18	2.31	117.32	112.75
2	C	305	A86	C3-C4-C5	-2.31	118.74	123.47
2	B	303	A86	C40-C32-C31	-2.31	108.41	110.47
2	B	304	A86	C28-C27-C26	-2.31	119.69	122.92
4	B	310	KC2	C1B-CHB-C4A	-2.30	121.09	126.06
4	C	311	KC2	C1B-CHB-C4A	-2.30	121.09	126.06
2	B	304	A86	C3-C4-C5	-2.30	118.76	123.47
4	A	310	KC2	C1B-CHB-C4A	-2.30	121.10	126.06
5	B	315	KC1	C2A-C3A-C4A	2.30	108.19	106.49
2	A	307	A86	O4-C38-O5	-2.29	118.41	122.96
2	C	306	A86	C12-C11-C13	2.28	119.86	116.02
2	B	304	A86	C40-C32-C31	-2.28	108.43	110.47
2	A	305	A86	C12-C11-C13	2.28	119.85	116.02
2	A	304	A86	C40-C32-C31	-2.28	108.44	110.47
3	C	310	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
2	C	308	A86	O4-C38-O5	-2.27	118.45	122.96
4	A	312	KC2	O2D-CGD-O1D	-2.27	119.39	123.84
2	B	307	A86	O4-C38-O5	-2.27	118.45	122.96
2	C	305	A86	O4-C38-O5	-2.27	118.46	122.96
2	B	301	A86	O4-C38-O5	-2.27	118.46	122.96
2	B	302	A86	O1-C20-C19	-2.27	111.68	113.38
3	B	313	CLA	CHB-C4A-NA	2.26	127.64	124.51
2	B	306	A86	C41-C32-C33	2.26	119.20	109.05
2	A	304	A86	C28-C27-C26	-2.26	119.76	122.92
2	A	301	A86	O4-C38-O5	-2.26	118.47	122.96
2	A	304	A86	O4-C38-O5	-2.26	118.48	122.96
2	C	304	A86	O1-C15-C20	-2.26	57.20	59.40
3	A	313	CLA	CHB-C4A-NA	2.25	127.63	124.51
2	A	302	A86	O1-C15-C20	-2.25	57.20	59.40
3	C	314	CLA	CHB-C4A-NA	2.25	127.63	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	307	A86	C17-C16-C15	2.25	111.46	109.16
3	C	315	CLA	CMB-C2B-C1B	-2.25	121.95	125.37
3	B	309	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
3	B	316	CLA	O2D-CGD-CBD	2.24	115.25	111.27
2	B	305	A86	C12-C11-C13	2.24	119.79	116.02
2	C	307	A86	C41-C32-C33	2.24	119.11	109.05
2	A	303	A86	C33-C32-C31	-2.24	107.03	109.21
2	A	307	A86	C20-C19-C18	2.24	117.17	112.75
5	C	316	KC1	C2A-C3A-C4A	2.23	108.14	106.49
4	B	312	KC2	C1B-CHB-C4A	-2.23	121.25	126.06
2	A	302	A86	O1-C20-C19	-2.23	111.71	113.38
2	A	306	A86	C41-C32-C33	2.23	119.05	109.05
2	C	304	A86	C9-C10-C11	-2.22	120.07	126.61
2	A	303	A86	C40-C32-C31	-2.22	108.48	110.47
2	C	305	A86	C40-C32-C31	-2.22	108.48	110.47
2	A	304	A86	C3-C4-C5	-2.22	118.93	123.47
2	C	305	A86	C33-C32-C31	-2.22	107.05	109.21
4	C	313	KC2	C1B-CHB-C4A	-2.22	121.27	126.06
4	A	312	KC2	C1B-CHB-C4A	-2.22	121.27	126.06
4	A	312	KC2	C4D-C3D-CAD	2.22	108.92	107.42
4	B	310	KC2	O2D-CGD-O1D	-2.22	119.51	123.84
3	A	316	CLA	O2D-CGD-CBD	2.21	115.20	111.27
2	B	302	A86	C17-C16-C15	2.21	111.42	109.16
4	A	310	KC2	O2D-CGD-O1D	-2.21	119.52	123.84
3	C	301	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
3	B	314	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
3	A	314	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
5	C	316	KC1	O2D-CGD-O1D	-2.19	119.56	123.84
2	C	303	A86	O1-C15-C20	-2.19	57.26	59.40
2	B	303	A86	O1-C15-C20	-2.19	57.26	59.40
2	C	305	A86	C28-C27-C26	-2.19	119.86	122.92
5	A	315	KC1	C2A-C3A-C4A	2.19	108.11	106.49
3	B	314	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
3	C	315	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
6	B	318	LMG	C1-O6-C5	-2.17	109.42	113.69
2	C	302	A86	C20-C19-C18	2.17	117.04	112.75
2	B	301	A86	C20-C19-C18	2.17	117.04	112.75
2	B	306	A86	C28-C27-C26	-2.17	119.88	122.92
3	A	314	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
4	C	313	KC2	CHB-C4A-C3A	-2.16	121.60	124.98
2	B	302	A86	O1-C15-C20	-2.16	57.29	59.40
3	A	311	CLA	O2A-CGA-O1A	-2.15	118.16	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	315	CLA	CHB-C1B-NB	2.15	126.53	124.26
2	A	301	A86	C20-C19-C18	2.14	116.99	112.75
3	C	312	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
4	A	312	KC2	CHB-C4A-C3A	-2.14	121.64	124.98
2	B	303	A86	C12-C11-C13	2.14	119.62	116.02
2	C	303	A86	C28-C27-C26	-2.14	119.93	122.92
3	C	309	CLA	CHB-C1B-NB	2.14	126.52	124.26
2	B	306	A86	O1-C15-C20	-2.14	57.31	59.40
4	C	313	KC2	O2D-CGD-O1D	-2.14	119.66	123.84
3	A	317	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
2	B	305	A86	C17-C16-C15	2.13	111.34	109.16
3	A	309	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
3	B	311	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
2	A	306	A86	O1-C15-C20	-2.13	57.32	59.40
3	A	308	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
3	B	314	CLA	CHB-C1B-NB	2.11	126.50	124.26
4	B	312	KC2	CHB-C4A-C3A	-2.11	121.68	124.98
2	A	301	A86	O1-C15-C20	-2.11	57.34	59.40
2	A	302	A86	C28-C27-C26	-2.11	119.97	122.92
2	B	304	A86	C9-C10-C11	-2.11	120.41	126.61
2	A	303	A86	O1-C15-C20	-2.11	57.34	59.40
4	C	313	KC2	C4D-C3D-CAD	2.11	108.84	107.42
2	C	307	A86	O1-C15-C20	-2.10	57.34	59.40
3	C	309	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
4	B	312	KC2	C4D-C3D-CAD	2.10	108.84	107.42
3	C	301	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
2	B	303	A86	C33-C32-C31	-2.10	107.17	109.21
4	C	311	KC2	O2D-CGD-O1D	-2.10	119.74	123.84
3	B	308	CLA	CHB-C1B-NB	2.09	126.47	124.26
2	B	305	A86	O2-C18-C17	2.09	113.96	109.80
2	A	305	A86	C17-C16-C15	2.09	111.29	109.16
2	B	301	A86	O1-C15-C20	-2.09	57.36	59.40
3	C	301	CLA	CHB-C1B-NB	2.09	126.47	124.26
3	A	308	CLA	CHB-C1B-NB	2.08	126.46	124.26
3	A	309	CLA	CHD-C1D-ND	-2.08	122.54	124.45
3	B	308	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
3	A	311	CLA	CHB-C1B-NB	2.08	126.46	124.26
2	C	305	A86	O1-C15-C20	-2.07	57.37	59.40
3	A	314	CLA	CHD-C1D-ND	-2.07	122.55	124.45
2	C	303	A86	O1-C20-C19	-2.07	111.83	113.38
2	A	304	A86	C20-C19-C18	2.07	116.84	112.75
3	C	301	CLA	CHD-C1D-ND	-2.07	122.56	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	305	A86	C9-C10-C11	-2.07	120.53	126.61
2	B	303	A86	C26-C25-C24	-2.06	116.78	123.22
2	B	304	A86	C33-C32-C31	-2.06	107.21	109.21
2	B	305	A86	C20-C19-C18	2.06	116.82	112.75
3	A	317	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
2	C	304	A86	C26-C25-C24	-2.06	116.79	123.22
2	C	305	A86	C20-C19-C18	2.06	116.82	112.75
2	B	301	A86	C21-C20-C19	-2.05	111.97	114.28
2	C	308	A86	C7-C6-C5	-2.05	120.05	122.92
2	C	306	A86	C17-C16-C15	2.05	111.25	109.16
2	B	304	A86	O1-C15-C20	-2.05	57.40	59.40
3	B	317	CLA	CHB-C1B-NB	2.05	126.43	124.26
2	C	302	A86	C21-C20-C19	-2.05	111.97	114.28
3	C	315	CLA	CHD-C1D-ND	-2.05	122.57	124.45
2	B	304	A86	C20-C19-C18	2.05	116.80	112.75
2	C	306	A86	O2-C18-C17	2.05	113.87	109.80
4	B	312	KC2	O2D-CGD-O1D	-2.05	119.84	123.84
2	B	302	A86	C28-C27-C26	-2.05	120.06	122.92
3	A	316	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
2	A	304	A86	O1-C15-C20	-2.04	57.40	59.40
3	C	310	CLA	CHD-C1D-ND	-2.04	122.58	124.45
2	B	304	A86	C-C1-C2	-2.04	120.06	122.92
2	A	305	A86	O2-C18-C17	2.04	113.86	109.80
2	A	304	A86	C-C1-C2	-2.04	120.07	122.92
3	C	312	CLA	CHB-C1B-NB	2.04	126.42	124.26
2	C	302	A86	O1-C15-C20	-2.04	57.41	59.40
2	A	305	A86	C20-C19-C18	2.04	116.78	112.75
3	C	318	CLA	CHD-C1D-ND	-2.04	122.58	124.45
2	C	306	A86	C20-C19-C18	2.03	116.77	112.75
3	A	314	CLA	CHB-C1B-NB	2.03	126.41	124.26
3	A	313	CLA	CHB-C1B-NB	2.03	126.40	124.26
3	A	311	CLA	CHD-C1D-ND	-2.03	122.59	124.45
3	C	317	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
3	B	311	CLA	CHB-C1B-NB	2.02	126.40	124.26
3	C	319	CLA	CHB-C1B-NB	2.02	126.40	124.26
3	A	316	CLA	CHB-C1B-NB	2.02	126.39	124.26
3	C	317	CLA	CHB-C1B-NB	2.02	126.39	124.26
3	B	309	CLA	CHD-C1D-ND	-2.02	122.60	124.45
3	B	308	CLA	CHD-C1D-ND	-2.01	122.60	124.45
2	B	306	A86	C26-C25-C24	-2.01	116.94	123.22
3	B	314	CLA	CHD-C1D-ND	-2.01	122.61	124.45
2	A	307	A86	C7-C6-C5	-2.01	120.11	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	307	A86	C7-C6-C5	-2.01	120.11	122.92
2	B	301	A86	C17-C16-C15	2.01	111.22	109.16
3	A	309	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
3	A	318	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
3	A	317	CLA	CHD-C1D-ND	-2.00	122.61	124.45
3	B	316	CLA	CHB-C1B-NB	2.00	126.38	124.26
2	B	303	A86	C-C1-C2	-2.00	120.12	122.92

There are no chirality outliers.

All (553) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	A86	C12-C11-C13-C14
2	A	301	A86	C13-C14-C15-C20
2	A	301	A86	C13-C14-C15-O1
2	A	302	A86	C12-C11-C13-C14
2	A	302	A86	C13-C14-C15-C16
2	A	303	A86	C10-C11-C13-O
2	A	303	A86	C12-C11-C13-O
2	A	304	A86	C10-C11-C13-O
2	A	304	A86	C12-C11-C13-O
2	A	305	A86	C12-C11-C13-C14
2	A	305	A86	C13-C14-C15-C16
2	A	305	A86	C13-C14-C15-C20
2	A	305	A86	C13-C14-C15-O1
2	A	305	A86	C1-C2-C3-C4
2	A	305	A86	C3-C4-C5-C6
2	A	306	A86	C1-C2-C3-C4
2	A	306	A86	C3-C4-C5-C6
2	A	307	A86	C12-C11-C13-C14
2	A	307	A86	C13-C14-C15-C20
2	B	301	A86	C12-C11-C13-C14
2	B	301	A86	C13-C14-C15-C20
2	B	302	A86	C12-C11-C13-C14
2	B	302	A86	C13-C14-C15-C16
2	B	303	A86	C10-C11-C13-O
2	B	303	A86	C12-C11-C13-O
2	B	304	A86	C10-C11-C13-O
2	B	304	A86	C12-C11-C13-O
2	B	305	A86	C12-C11-C13-C14
2	B	305	A86	C13-C14-C15-C16
2	B	305	A86	C13-C14-C15-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	305	A86	C13-C14-C15-O1
2	B	305	A86	C1-C2-C3-C4
2	B	305	A86	C3-C4-C5-C6
2	B	306	A86	C1-C2-C3-C4
2	B	306	A86	C3-C4-C5-C6
2	B	307	A86	C12-C11-C13-C14
2	B	307	A86	C13-C14-C15-C20
2	C	302	A86	C12-C11-C13-C14
2	C	302	A86	C13-C14-C15-C20
2	C	302	A86	C13-C14-C15-O1
2	C	303	A86	C12-C11-C13-C14
2	C	303	A86	C13-C14-C15-C16
2	C	304	A86	C10-C11-C13-O
2	C	304	A86	C12-C11-C13-O
2	C	305	A86	C10-C11-C13-O
2	C	305	A86	C12-C11-C13-O
2	C	306	A86	C12-C11-C13-C14
2	C	306	A86	C13-C14-C15-C16
2	C	306	A86	C13-C14-C15-C20
2	C	306	A86	C13-C14-C15-O1
2	C	306	A86	C1-C2-C3-C4
2	C	306	A86	C3-C4-C5-C6
2	C	307	A86	C1-C2-C3-C4
2	C	307	A86	C3-C4-C5-C6
2	C	308	A86	C12-C11-C13-C14
2	C	308	A86	C13-C14-C15-C20
3	A	308	CLA	CHA-CBD-CGD-O1D
3	A	308	CLA	CHA-CBD-CGD-O2D
3	A	309	CLA	C1A-C2A-CAA-CBA
3	A	314	CLA	C1A-C2A-CAA-CBA
3	A	314	CLA	C2-C3-C5-C6
3	A	314	CLA	C4-C3-C5-C6
3	A	316	CLA	CAD-CBD-CGD-O1D
3	A	316	CLA	CAD-CBD-CGD-O2D
3	A	317	CLA	C1A-C2A-CAA-CBA
3	A	317	CLA	C3A-C2A-CAA-CBA
3	A	317	CLA	CHA-CBD-CGD-O1D
3	A	317	CLA	CHA-CBD-CGD-O2D
3	A	317	CLA	CAD-CBD-CGD-O1D
3	B	308	CLA	CHA-CBD-CGD-O1D
3	B	308	CLA	CHA-CBD-CGD-O2D
3	B	309	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	313	CLA	CBD-CGD-O2D-CED
3	B	314	CLA	C1A-C2A-CAA-CBA
3	B	316	CLA	CAD-CBD-CGD-O1D
3	B	316	CLA	CAD-CBD-CGD-O2D
3	C	301	CLA	C1A-C2A-CAA-CBA
3	C	301	CLA	C3A-C2A-CAA-CBA
3	C	301	CLA	CHA-CBD-CGD-O1D
3	C	301	CLA	CHA-CBD-CGD-O2D
3	C	301	CLA	CAD-CBD-CGD-O1D
3	C	309	CLA	CHA-CBD-CGD-O1D
3	C	310	CLA	C1A-C2A-CAA-CBA
3	C	315	CLA	C1A-C2A-CAA-CBA
3	C	317	CLA	CHA-CBD-CGD-O1D
3	C	317	CLA	CAD-CBD-CGD-O1D
3	C	317	CLA	CAD-CBD-CGD-O2D
3	C	318	CLA	C1A-C2A-CAA-CBA
3	C	318	CLA	C3A-C2A-CAA-CBA
3	C	318	CLA	CHA-CBD-CGD-O1D
3	C	318	CLA	CHA-CBD-CGD-O2D
3	C	318	CLA	CAD-CBD-CGD-O1D
4	A	310	KC2	C1A-C2A-CAA-CBA
4	A	310	KC2	C2C-C3C-CAC-CBC
4	A	312	KC2	C1A-C2A-CAA-CBA
4	A	312	KC2	C2B-C3B-CAB-CBB
4	A	312	KC2	C4B-C3B-CAB-CBB
4	B	310	KC2	C2C-C3C-CAC-CBC
4	B	312	KC2	C1A-C2A-CAA-CBA
4	B	312	KC2	C2B-C3B-CAB-CBB
4	B	312	KC2	C4B-C3B-CAB-CBB
4	C	311	KC2	C1A-C2A-CAA-CBA
4	C	311	KC2	C2C-C3C-CAC-CBC
4	C	313	KC2	C1A-C2A-CAA-CBA
4	C	313	KC2	C2B-C3B-CAB-CBB
5	A	315	KC1	C1A-C2A-CAA-CBA
5	B	315	KC1	C1A-C2A-CAA-CBA
5	B	315	KC1	C2B-C3B-CAB-CBB
5	C	316	KC1	C1A-C2A-CAA-CBA
5	C	316	KC1	C2B-C3B-CAB-CBB
6	A	319	LMG	C8-C7-O1-C1
2	A	301	A86	C39-C38-O4-C34
2	A	302	A86	C39-C38-O4-C34
2	A	303	A86	C39-C38-O4-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	304	A86	C39-C38-O4-C34
2	A	307	A86	C39-C38-O4-C34
2	B	301	A86	C39-C38-O4-C34
2	B	302	A86	C39-C38-O4-C34
2	B	303	A86	C39-C38-O4-C34
2	B	304	A86	C39-C38-O4-C34
2	B	307	A86	C39-C38-O4-C34
2	C	302	A86	C39-C38-O4-C34
2	C	303	A86	C39-C38-O4-C34
2	C	304	A86	C39-C38-O4-C34
2	C	305	A86	C39-C38-O4-C34
2	C	308	A86	C39-C38-O4-C34
3	A	311	CLA	CBD-CGD-O2D-CED
3	B	311	CLA	CBD-CGD-O2D-CED
3	C	312	CLA	CBD-CGD-O2D-CED
3	B	316	CLA	CBD-CGD-O2D-CED
3	A	309	CLA	O1A-CGA-O2A-C1
2	A	301	A86	O5-C38-O4-C34
2	A	302	A86	O5-C38-O4-C34
2	A	303	A86	O5-C38-O4-C34
2	A	304	A86	O5-C38-O4-C34
2	A	307	A86	O5-C38-O4-C34
2	B	301	A86	O5-C38-O4-C34
2	B	302	A86	O5-C38-O4-C34
2	B	303	A86	O5-C38-O4-C34
2	B	304	A86	O5-C38-O4-C34
2	B	307	A86	O5-C38-O4-C34
2	C	302	A86	O5-C38-O4-C34
2	C	303	A86	O5-C38-O4-C34
2	C	304	A86	O5-C38-O4-C34
2	C	305	A86	O5-C38-O4-C34
2	C	308	A86	O5-C38-O4-C34
3	B	313	CLA	O1D-CGD-O2D-CED
3	B	311	CLA	O1D-CGD-O2D-CED
3	A	317	CLA	C3-C5-C6-C7
3	B	308	CLA	C3-C5-C6-C7
3	C	301	CLA	C3-C5-C6-C7
3	C	309	CLA	C3-C5-C6-C7
3	C	318	CLA	C3-C5-C6-C7
3	C	319	CLA	C3-C5-C6-C7
3	C	309	CLA	CBA-CGA-O2A-C1
3	A	313	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	314	CLA	CBD-CGD-O2D-CED
3	A	308	CLA	C3-C5-C6-C7
3	A	318	CLA	C3-C5-C6-C7
3	B	317	CLA	C3-C5-C6-C7
3	A	308	CLA	CBA-CGA-O2A-C1
3	A	309	CLA	CBA-CGA-O2A-C1
3	B	308	CLA	CBA-CGA-O2A-C1
3	C	310	CLA	CBA-CGA-O2A-C1
3	C	312	CLA	O1D-CGD-O2D-CED
3	A	308	CLA	O1A-CGA-O2A-C1
3	A	313	CLA	O1A-CGA-O2A-C1
3	A	316	CLA	O1A-CGA-O2A-C1
3	B	309	CLA	O1A-CGA-O2A-C1
3	B	316	CLA	O1A-CGA-O2A-C1
3	C	310	CLA	O1A-CGA-O2A-C1
3	C	314	CLA	O1A-CGA-O2A-C1
6	B	318	LMG	C12-C13-C14-C15
2	A	305	A86	C39-C38-O4-C34
2	A	306	A86	C39-C38-O4-C34
2	B	305	A86	C39-C38-O4-C34
2	B	306	A86	C39-C38-O4-C34
2	C	306	A86	C39-C38-O4-C34
2	C	307	A86	C39-C38-O4-C34
3	A	316	CLA	CBD-CGD-O2D-CED
3	B	316	CLA	C3-C5-C6-C7
3	A	313	CLA	CBA-CGA-O2A-C1
3	B	309	CLA	CBA-CGA-O2A-C1
3	B	313	CLA	CBA-CGA-O2A-C1
3	C	314	CLA	CBA-CGA-O2A-C1
2	A	305	A86	O5-C38-O4-C34
2	A	306	A86	O5-C38-O4-C34
2	B	305	A86	O5-C38-O4-C34
2	B	306	A86	O5-C38-O4-C34
2	C	306	A86	O5-C38-O4-C34
2	C	307	A86	O5-C38-O4-C34
3	B	308	CLA	O1A-CGA-O2A-C1
3	B	313	CLA	O1A-CGA-O2A-C1
3	C	309	CLA	O1A-CGA-O2A-C1
3	C	317	CLA	O1A-CGA-O2A-C1
5	B	315	KC1	CBD-CGD-O2D-CED
3	A	316	CLA	CBA-CGA-O2A-C1
3	B	316	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	317	CLA	CBA-CGA-O2A-C1
3	A	311	CLA	O1D-CGD-O2D-CED
6	B	318	LMG	C14-C15-C16-C17
6	A	319	LMG	O6-C5-C6-O5
2	A	305	A86	C35-C34-O4-C38
2	A	307	A86	C35-C34-O4-C38
2	B	305	A86	C35-C34-O4-C38
2	B	307	A86	C35-C34-O4-C38
2	C	306	A86	C35-C34-O4-C38
2	C	308	A86	C35-C34-O4-C38
3	A	314	CLA	CBA-CGA-O2A-C1
2	A	304	A86	C35-C34-O4-C38
2	B	304	A86	C35-C34-O4-C38
2	C	305	A86	C35-C34-O4-C38
3	C	309	CLA	C5-C6-C7-C8
6	A	319	LMG	C12-C13-C14-C15
6	A	319	LMG	C4-C5-C6-O5
3	B	308	CLA	C5-C6-C7-C8
3	C	318	CLA	CBD-CGD-O2D-CED
3	A	317	CLA	C8-C10-C11-C12
3	C	301	CLA	C8-C10-C11-C12
3	C	318	CLA	C8-C10-C11-C12
3	C	301	CLA	CBA-CGA-O2A-C1
2	A	301	A86	C35-C34-O4-C38
2	A	303	A86	C35-C34-O4-C38
2	B	301	A86	C35-C34-O4-C38
2	B	303	A86	C35-C34-O4-C38
2	C	302	A86	C35-C34-O4-C38
2	C	304	A86	C35-C34-O4-C38
3	A	308	CLA	C5-C6-C7-C8
2	A	302	A86	C35-C34-O4-C38
2	B	302	A86	C35-C34-O4-C38
2	C	303	A86	C35-C34-O4-C38
3	B	316	CLA	O1D-CGD-O2D-CED
3	B	317	CLA	C8-C10-C11-C12
3	A	318	CLA	C8-C10-C11-C12
3	A	314	CLA	O1A-CGA-O2A-C1
3	C	301	CLA	O1A-CGA-O2A-C1
3	C	319	CLA	C8-C10-C11-C12
3	A	316	CLA	C3-C5-C6-C7
3	A	317	CLA	CBA-CGA-O2A-C1
3	A	313	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	314	CLA	O1D-CGD-O2D-CED
6	B	318	LMG	O9-C10-O7-C8
5	A	315	KC1	CBD-CGD-O2D-CED
3	A	309	CLA	C2A-CAA-CBA-CGA
3	B	309	CLA	C2A-CAA-CBA-CGA
3	C	310	CLA	C2A-CAA-CBA-CGA
6	A	319	LMG	C29-C28-O8-C9
3	A	314	CLA	CBD-CGD-O2D-CED
6	B	318	LMG	C11-C10-O7-C8
3	A	311	CLA	C8-C10-C11-C12
6	A	319	LMG	C11-C12-C13-C14
6	C	320	LMG	C13-C14-C15-C16
2	B	306	A86	C35-C34-O4-C38
2	C	307	A86	C35-C34-O4-C38
6	A	319	LMG	C15-C16-C17-C18
3	A	317	CLA	O1A-CGA-O2A-C1
3	B	317	CLA	C2A-CAA-CBA-CGA
3	C	319	CLA	C2A-CAA-CBA-CGA
3	A	318	CLA	C4B-C3B-CAB-CBB
3	B	317	CLA	C4B-C3B-CAB-CBB
3	C	319	CLA	C4B-C3B-CAB-CBB
2	A	303	A86	C33-C34-O4-C38
2	B	301	A86	C33-C34-O4-C38
2	C	302	A86	C33-C34-O4-C38
6	B	318	LMG	C28-C29-C30-C31
6	C	320	LMG	C10-C11-C12-C13
3	C	319	CLA	C5-C6-C7-C8
6	A	319	LMG	O10-C28-O8-C9
6	C	320	LMG	C29-C28-O8-C9
3	C	310	CLA	C3A-C2A-CAA-CBA
2	A	301	A86	C33-C34-O4-C38
2	A	306	A86	C35-C34-O4-C38
2	C	304	A86	C33-C34-O4-C38
3	C	301	CLA	CBD-CGD-O2D-CED
3	A	318	CLA	C2B-C3B-CAB-CBB
3	B	317	CLA	C2B-C3B-CAB-CBB
3	C	319	CLA	C2B-C3B-CAB-CBB
2	A	302	A86	C33-C34-O4-C38
2	B	302	A86	C33-C34-O4-C38
2	B	303	A86	C33-C34-O4-C38
2	C	303	A86	C33-C34-O4-C38
3	B	317	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	320	LMG	O10-C28-O8-C9
6	B	318	LMG	C13-C14-C15-C16
3	C	317	CLA	C3-C5-C6-C7
3	A	316	CLA	O1D-CGD-O2D-CED
3	A	318	CLA	C5-C6-C7-C8
3	A	311	CLA	C4-C3-C5-C6
3	B	314	CLA	CBA-CGA-O2A-C1
3	C	315	CLA	CBA-CGA-O2A-C1
3	C	318	CLA	CBA-CGA-O2A-C1
3	A	318	CLA	C2A-CAA-CBA-CGA
3	C	312	CLA	C8-C10-C11-C12
4	A	310	KC2	C2B-C3B-CAB-CBB
4	A	312	KC2	C2C-C3C-CAC-CBC
4	B	312	KC2	C2C-C3C-CAC-CBC
4	C	311	KC2	C2B-C3B-CAB-CBB
4	C	313	KC2	C2C-C3C-CAC-CBC
5	A	315	KC1	C2B-C3B-CAB-CBB
4	A	310	KC2	C4C-C3C-CAC-CBC
4	A	312	KC2	C4C-C3C-CAC-CBC
4	B	310	KC2	C4C-C3C-CAC-CBC
4	B	312	KC2	C4C-C3C-CAC-CBC
4	C	311	KC2	C4B-C3B-CAB-CBB
4	C	311	KC2	C4C-C3C-CAC-CBC
4	C	313	KC2	C4B-C3B-CAB-CBB
4	C	313	KC2	C4C-C3C-CAC-CBC
5	A	315	KC1	C4B-C3B-CAB-CBB
5	B	315	KC1	C4B-C3B-CAB-CBB
5	C	316	KC1	C4B-C3B-CAB-CBB
3	C	314	CLA	C10-C11-C12-C13
6	A	319	LMG	C28-C29-C30-C31
3	A	311	CLA	C2-C3-C5-C6
3	A	311	CLA	C11-C12-C13-C14
3	B	311	CLA	C11-C12-C13-C14
3	C	312	CLA	C11-C12-C13-C14
6	C	320	LMG	C12-C13-C14-C15
3	A	316	CLA	C1A-C2A-CAA-CBA
3	B	316	CLA	C1A-C2A-CAA-CBA
3	C	317	CLA	C1A-C2A-CAA-CBA
6	C	320	LMG	C15-C16-C17-C18
3	B	311	CLA	C8-C10-C11-C12
3	B	314	CLA	O1A-CGA-O2A-C1
3	C	318	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	320	LMG	C8-C7-O1-C1
4	A	312	KC2	CBD-CGD-O2D-CED
3	C	315	CLA	O1A-CGA-O2A-C1
3	B	313	CLA	C10-C11-C12-C13
2	A	304	A86	C33-C34-O4-C38
6	B	318	LMG	C9-C8-O7-C10
3	C	318	CLA	O1D-CGD-O2D-CED
2	A	305	A86	C33-C34-O4-C38
2	B	304	A86	C33-C34-O4-C38
2	B	305	A86	C33-C34-O4-C38
2	C	306	A86	C33-C34-O4-C38
3	C	318	CLA	C4-C3-C5-C6
3	A	311	CLA	C11-C12-C13-C15
3	B	311	CLA	C11-C12-C13-C15
3	C	312	CLA	C11-C12-C13-C15
3	C	314	CLA	C6-C7-C8-C9
3	C	312	CLA	C2A-CAA-CBA-CGA
6	A	319	LMG	C16-C17-C18-C19
3	C	317	CLA	CBD-CGD-O2D-CED
3	A	308	CLA	C4B-C3B-CAB-CBB
3	B	308	CLA	C4B-C3B-CAB-CBB
3	C	309	CLA	C4B-C3B-CAB-CBB
3	B	314	CLA	C4-C3-C5-C6
2	C	305	A86	C33-C34-O4-C38
3	A	314	CLA	O1D-CGD-O2D-CED
6	C	320	LMG	O1-C7-C8-C9
3	B	311	CLA	C2A-CAA-CBA-CGA
2	A	307	A86	C33-C34-O4-C38
3	C	309	CLA	C2B-C3B-CAB-CBB
6	B	318	LMG	C29-C30-C31-C32
3	C	301	CLA	O1D-CGD-O2D-CED
6	A	319	LMG	C11-C10-O7-C8
2	B	307	A86	C33-C34-O4-C38
2	C	308	A86	C33-C34-O4-C38
2	A	301	A86	C10-C11-C13-C14
2	A	305	A86	C10-C11-C13-C14
2	A	307	A86	C10-C11-C13-C14
2	B	301	A86	C10-C11-C13-C14
2	B	305	A86	C10-C11-C13-C14
2	B	307	A86	C10-C11-C13-C14
2	C	302	A86	C10-C11-C13-C14
2	C	306	A86	C10-C11-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	308	A86	C10-C11-C13-C14
3	A	313	CLA	C6-C7-C8-C9
3	A	318	CLA	C11-C10-C8-C9
3	B	308	CLA	C6-C7-C8-C9
3	C	309	CLA	CBD-CGD-O2D-CED
3	C	315	CLA	CBD-CGD-O2D-CED
4	B	310	KC2	C1A-C2A-CAA-CBA
3	A	311	CLA	C2A-CAA-CBA-CGA
6	A	319	LMG	O9-C10-O7-C8
3	C	314	CLA	C12-C13-C15-C16
3	A	313	CLA	C10-C11-C12-C13
3	A	313	CLA	CAD-CBD-CGD-O2D
3	A	317	CLA	CAD-CBD-CGD-O2D
3	C	314	CLA	CAD-CBD-CGD-O2D
3	C	318	CLA	CAD-CBD-CGD-O2D
4	B	310	KC2	C2B-C3B-CAB-CBB
5	B	315	KC1	CAD-CBD-CGD-O2D
5	C	316	KC1	CAD-CBD-CGD-O2D
2	A	306	A86	C33-C34-O4-C38
6	C	320	LMG	O6-C1-O1-C7
2	A	301	A86	C12-C11-C13-O
2	A	302	A86	C12-C11-C13-O
2	A	305	A86	C12-C11-C13-O
2	A	306	A86	C12-C11-C13-O
2	A	307	A86	C12-C11-C13-O
2	B	301	A86	C12-C11-C13-O
2	B	302	A86	C12-C11-C13-O
2	B	305	A86	C12-C11-C13-O
2	B	306	A86	C12-C11-C13-O
2	B	307	A86	C12-C11-C13-O
2	C	302	A86	C12-C11-C13-O
2	C	303	A86	C12-C11-C13-O
2	C	306	A86	C12-C11-C13-O
2	C	307	A86	C12-C11-C13-O
2	C	308	A86	C12-C11-C13-O
6	A	319	LMG	O1-C7-C8-C9
3	A	308	CLA	CBD-CGD-O2D-CED
3	C	318	CLA	CAA-CBA-CGA-O2A
4	A	310	KC2	C4B-C3B-CAB-CBB
3	C	309	CLA	CHA-CBD-CGD-O2D
4	C	311	KC2	CHA-CBD-CGD-O2D
2	C	307	A86	C33-C34-O4-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	320	LMG	C2-C1-O1-C7
6	C	320	LMG	C28-C29-C30-C31
2	A	301	A86	C10-C11-C13-O
2	A	302	A86	C10-C11-C13-O
2	A	305	A86	C10-C11-C13-O
2	A	306	A86	C10-C11-C13-O
2	A	307	A86	C10-C11-C13-O
2	B	301	A86	C10-C11-C13-O
2	B	302	A86	C10-C11-C13-O
2	B	305	A86	C10-C11-C13-O
2	B	306	A86	C10-C11-C13-O
2	B	307	A86	C10-C11-C13-O
2	C	302	A86	C10-C11-C13-O
2	C	303	A86	C10-C11-C13-O
2	C	306	A86	C10-C11-C13-O
2	C	307	A86	C10-C11-C13-O
2	C	308	A86	C10-C11-C13-O
3	C	301	CLA	C4-C3-C5-C6
3	C	314	CLA	C14-C13-C15-C16
3	B	308	CLA	CBD-CGD-O2D-CED
3	B	314	CLA	CBD-CGD-O2D-CED
3	A	317	CLA	C4-C3-C5-C6
6	A	319	LMG	O6-C1-O1-C7
3	A	317	CLA	C16-C17-C18-C19
6	A	319	LMG	C10-C11-C12-C13
4	C	311	KC2	CAA-CBA-CGA-O1A
6	A	319	LMG	O1-C7-C8-O7
6	C	320	LMG	O1-C7-C8-O7
6	B	318	LMG	C8-C7-O1-C1
3	C	301	CLA	CAA-CBA-CGA-O2A
2	B	306	A86	C33-C34-O4-C38
2	A	303	A86	C13-C14-C15-C20
2	A	306	A86	C13-C14-C15-C20
2	B	303	A86	C13-C14-C15-C20
2	B	306	A86	C13-C14-C15-C20
2	C	304	A86	C13-C14-C15-C20
2	C	305	A86	C13-C14-C15-C20
2	C	307	A86	C13-C14-C15-C20
3	A	308	CLA	O1D-CGD-O2D-CED
3	C	309	CLA	O1D-CGD-O2D-CED
3	B	313	CLA	C6-C7-C8-C9
3	A	308	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	308	CLA	C2B-C3B-CAB-CBB
3	C	318	CLA	C2-C3-C5-C6
3	C	315	CLA	O1D-CGD-O2D-CED
3	A	317	CLA	CAA-CBA-CGA-O2A
6	C	320	LMG	C29-C30-C31-C32
3	C	317	CLA	O1D-CGD-O2D-CED
2	A	303	A86	C12-C11-C13-C14
2	A	304	A86	C12-C11-C13-C14
2	A	306	A86	C12-C11-C13-C14
2	B	303	A86	C12-C11-C13-C14
2	B	304	A86	C12-C11-C13-C14
2	B	306	A86	C12-C11-C13-C14
2	C	304	A86	C12-C11-C13-C14
2	C	305	A86	C12-C11-C13-C14
2	C	307	A86	C12-C11-C13-C14
3	A	316	CLA	C4-C3-C5-C6
3	B	308	CLA	O1D-CGD-O2D-CED
6	A	319	LMG	C2-C1-O1-C7
3	B	314	CLA	C2-C3-C5-C6
3	B	311	CLA	C10-C11-C12-C13
3	C	301	CLA	C16-C17-C18-C19
3	B	314	CLA	O1D-CGD-O2D-CED
6	B	318	LMG	O6-C1-O1-C7
4	B	310	KC2	C4B-C3B-CAB-CBB
3	C	317	CLA	C4-C3-C5-C6
6	A	319	LMG	C13-C14-C15-C16
3	A	314	CLA	C3A-C2A-CAA-CBA
3	B	309	CLA	C3A-C2A-CAA-CBA
3	B	314	CLA	C3A-C2A-CAA-CBA
3	C	315	CLA	C3A-C2A-CAA-CBA
3	B	317	CLA	C11-C10-C8-C9
3	C	309	CLA	C6-C7-C8-C9
3	C	318	CLA	C16-C17-C18-C19
3	A	317	CLA	C16-C17-C18-C20
3	C	312	CLA	C10-C11-C12-C13
5	A	315	KC1	C3A-C2A-CAA-CBA
5	B	315	KC1	C3A-C2A-CAA-CBA
5	C	316	KC1	C3A-C2A-CAA-CBA
4	A	310	KC2	CAA-CBA-CGA-O2A
3	C	312	CLA	C2-C3-C5-C6
2	C	305	A86	C13-C14-C15-C16
2	A	302	A86	C10-C11-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	303	A86	C10-C11-C13-C14
2	A	304	A86	C10-C11-C13-C14
2	A	306	A86	C10-C11-C13-C14
2	B	302	A86	C10-C11-C13-C14
2	B	303	A86	C10-C11-C13-C14
2	B	304	A86	C10-C11-C13-C14
2	B	306	A86	C10-C11-C13-C14
2	C	303	A86	C10-C11-C13-C14
2	C	304	A86	C10-C11-C13-C14
2	C	305	A86	C10-C11-C13-C14
2	C	307	A86	C10-C11-C13-C14
4	B	310	KC2	CAA-CBA-CGA-O2A
3	B	313	CLA	C16-C17-C18-C20
3	C	319	CLA	C11-C10-C8-C9
3	C	312	CLA	C4-C3-C5-C6
3	A	313	CLA	C16-C17-C18-C20
3	A	311	CLA	C10-C11-C12-C13
6	B	318	LMG	C2-C1-O1-C7
3	A	316	CLA	C2-C3-C5-C6
3	A	317	CLA	C2-C3-C5-C6
3	C	301	CLA	C2-C3-C5-C6
3	A	308	CLA	C6-C7-C8-C9
3	B	313	CLA	CAD-CBD-CGD-O2D
5	A	315	KC1	CAD-CBD-CGD-O2D
3	A	316	CLA	CAA-CBA-CGA-O2A
3	A	309	CLA	O2A-C1-C2-C3
3	A	316	CLA	O2A-C1-C2-C3
3	B	309	CLA	O2A-C1-C2-C3
3	C	310	CLA	O2A-C1-C2-C3
3	C	301	CLA	C16-C17-C18-C20
3	B	309	CLA	O1D-CGD-O2D-CED
3	A	311	CLA	CHA-CBD-CGD-O2D
3	B	317	CLA	CHA-CBD-CGD-O2D
3	C	317	CLA	CHA-CBD-CGD-O2D
4	A	312	KC2	CHA-CBD-CGD-O1D
4	B	310	KC2	CHA-CBD-CGD-O2D
4	C	311	KC2	CHA-CBD-CGD-O1D
4	C	313	KC2	CHA-CBD-CGD-O1D
3	C	317	CLA	CAA-CBA-CGA-O2A
2	B	307	A86	C13-C14-C15-O1
3	B	309	CLA	CBD-CGD-O2D-CED
3	B	311	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	314	CLA	C15-C16-C17-C18
3	B	316	CLA	CAA-CBA-CGA-O2A
3	A	313	CLA	C1A-C2A-CAA-CBA
3	B	316	CLA	CAA-CBA-CGA-O1A
3	C	317	CLA	C2-C3-C5-C6
3	C	318	CLA	C16-C17-C18-C20
3	C	317	CLA	CAA-CBA-CGA-O1A
3	A	316	CLA	CAA-CBA-CGA-O1A
3	A	309	CLA	CAA-CBA-CGA-O2A
3	B	316	CLA	C4-C3-C5-C6
3	A	311	CLA	CAD-CBD-CGD-O1D
4	C	313	KC2	CAD-CBD-CGD-O1D
3	C	314	CLA	C11-C10-C8-C9
3	C	318	CLA	CAA-CBA-CGA-O1A
3	A	309	CLA	C3A-C2A-CAA-CBA
3	C	317	CLA	C3A-C2A-CAA-CBA
3	B	308	CLA	C4-C3-C5-C6
3	B	311	CLA	C4-C3-C5-C6
3	C	310	CLA	O1D-CGD-O2D-CED

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	307	A86	C31-C32-C33-C34-C35-C36
2	A	306	A86	C31-C32-C33-C34-C35-C36
2	B	306	A86	C31-C32-C33-C34-C35-C36

29 monomers are involved in 56 short contacts:

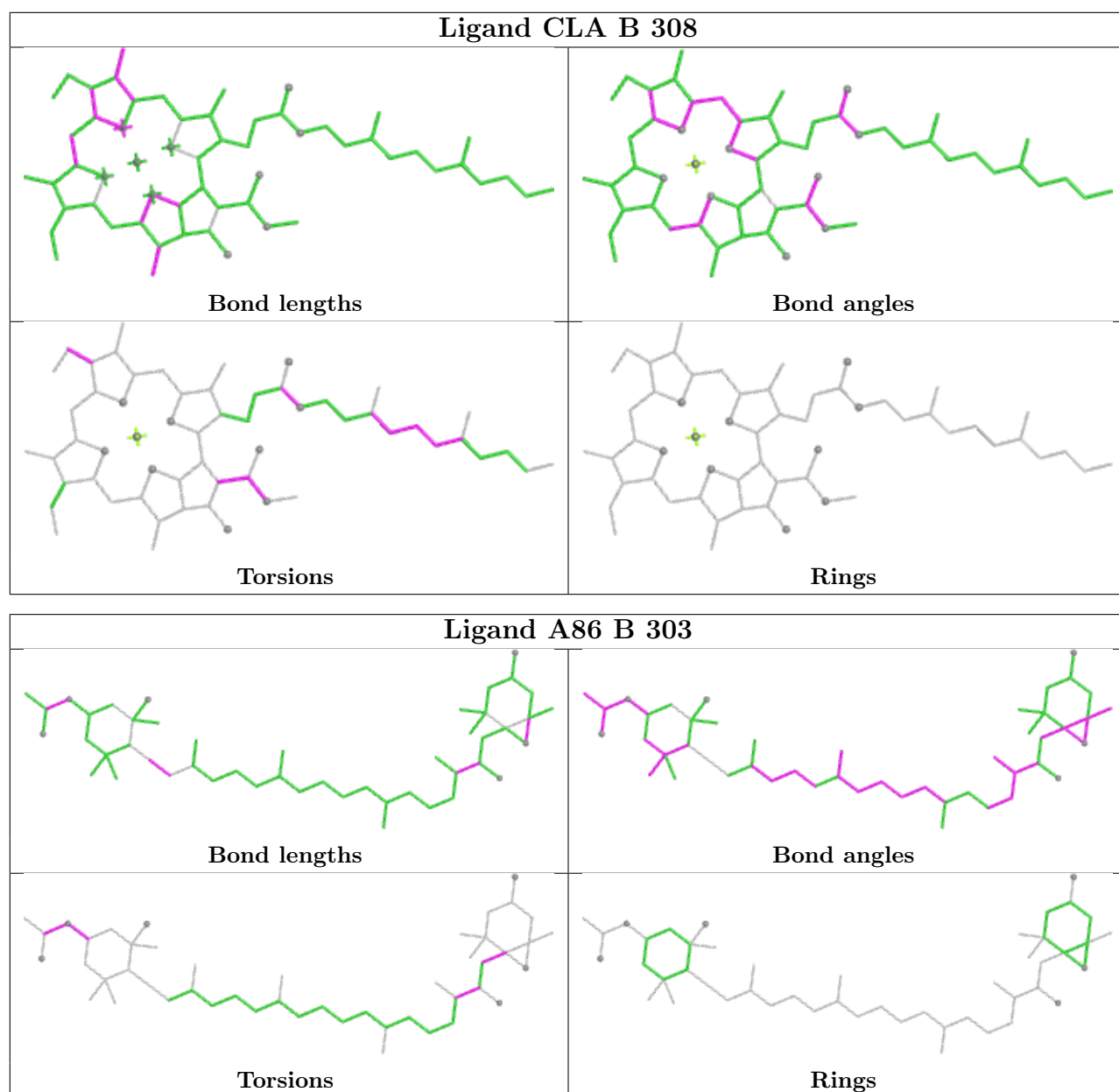
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	308	CLA	2	0
2	C	306	A86	1	0
3	A	318	CLA	2	0
3	A	317	CLA	7	0
3	B	309	CLA	1	0
3	B	314	CLA	3	0
2	C	302	A86	1	0
3	B	317	CLA	2	0
3	C	309	CLA	1	0
3	C	315	CLA	3	0
3	C	317	CLA	1	0
3	C	301	CLA	6	0

Continued on next page...

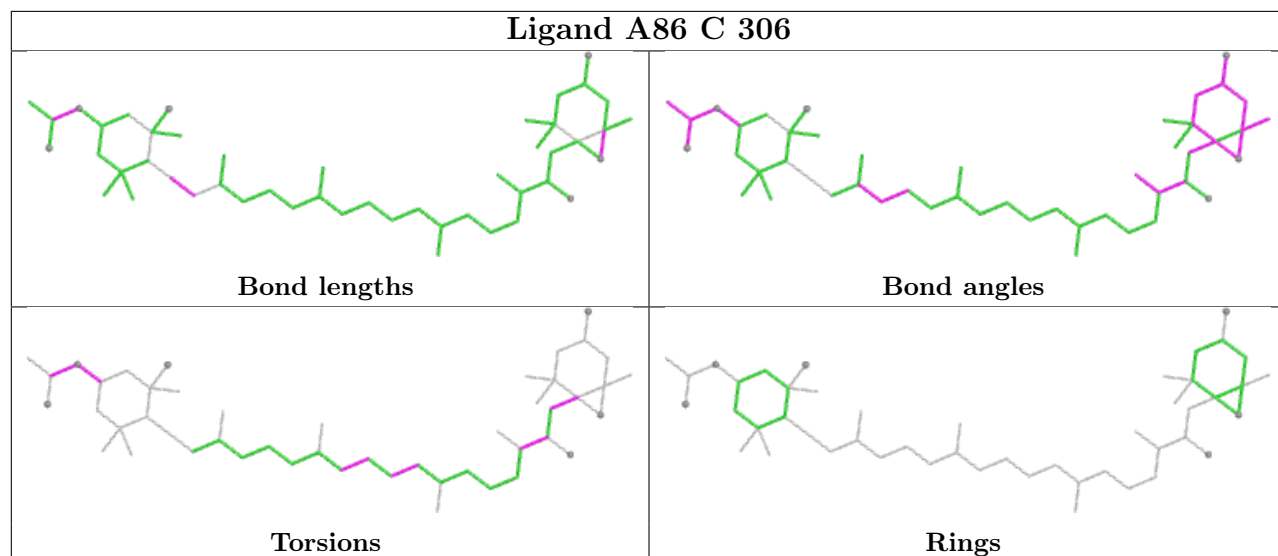
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	313	KC2	2	0
6	C	320	LMG	6	0
3	A	314	CLA	3	0
6	A	319	LMG	5	0
2	B	301	A86	1	0
3	B	316	CLA	1	0
3	A	308	CLA	2	0
4	B	312	KC2	1	0
2	B	306	A86	1	0
3	C	318	CLA	6	0
3	A	316	CLA	3	0
3	C	312	CLA	1	0
6	B	318	LMG	7	0
3	A	311	CLA	1	0
3	B	313	CLA	1	0
3	C	319	CLA	1	0
2	C	307	A86	1	0

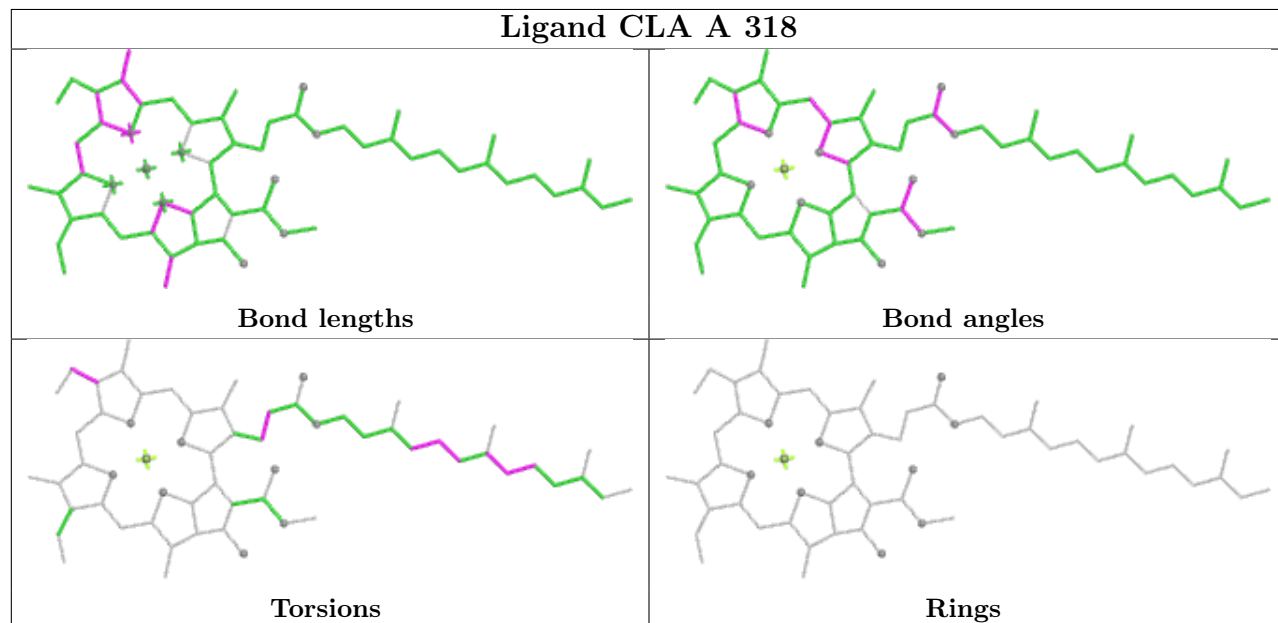
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



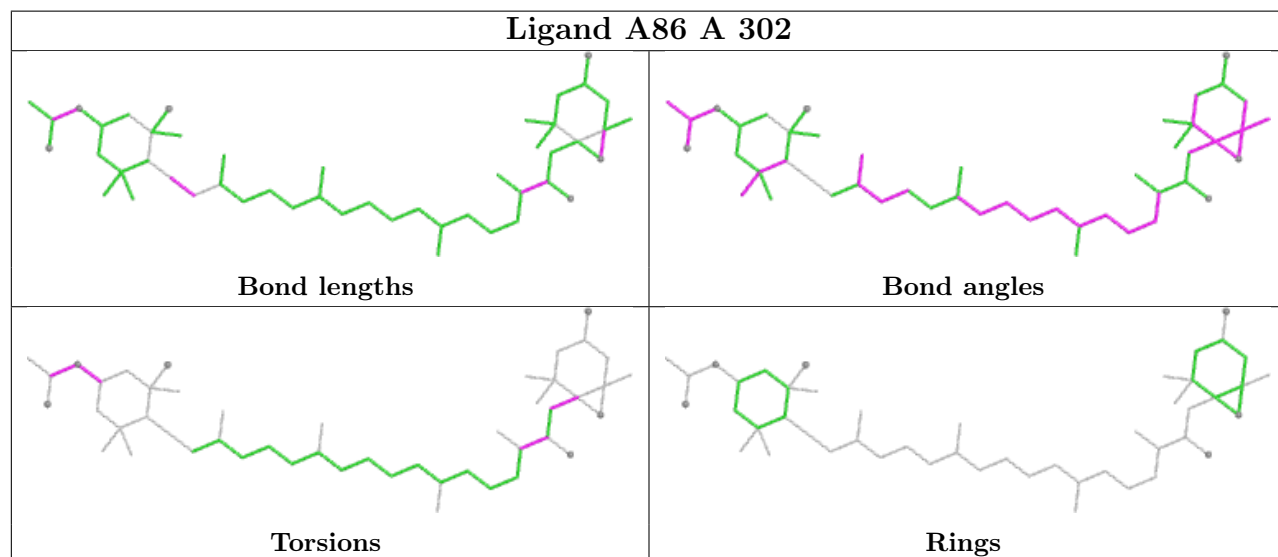
Ligand A86 C 306

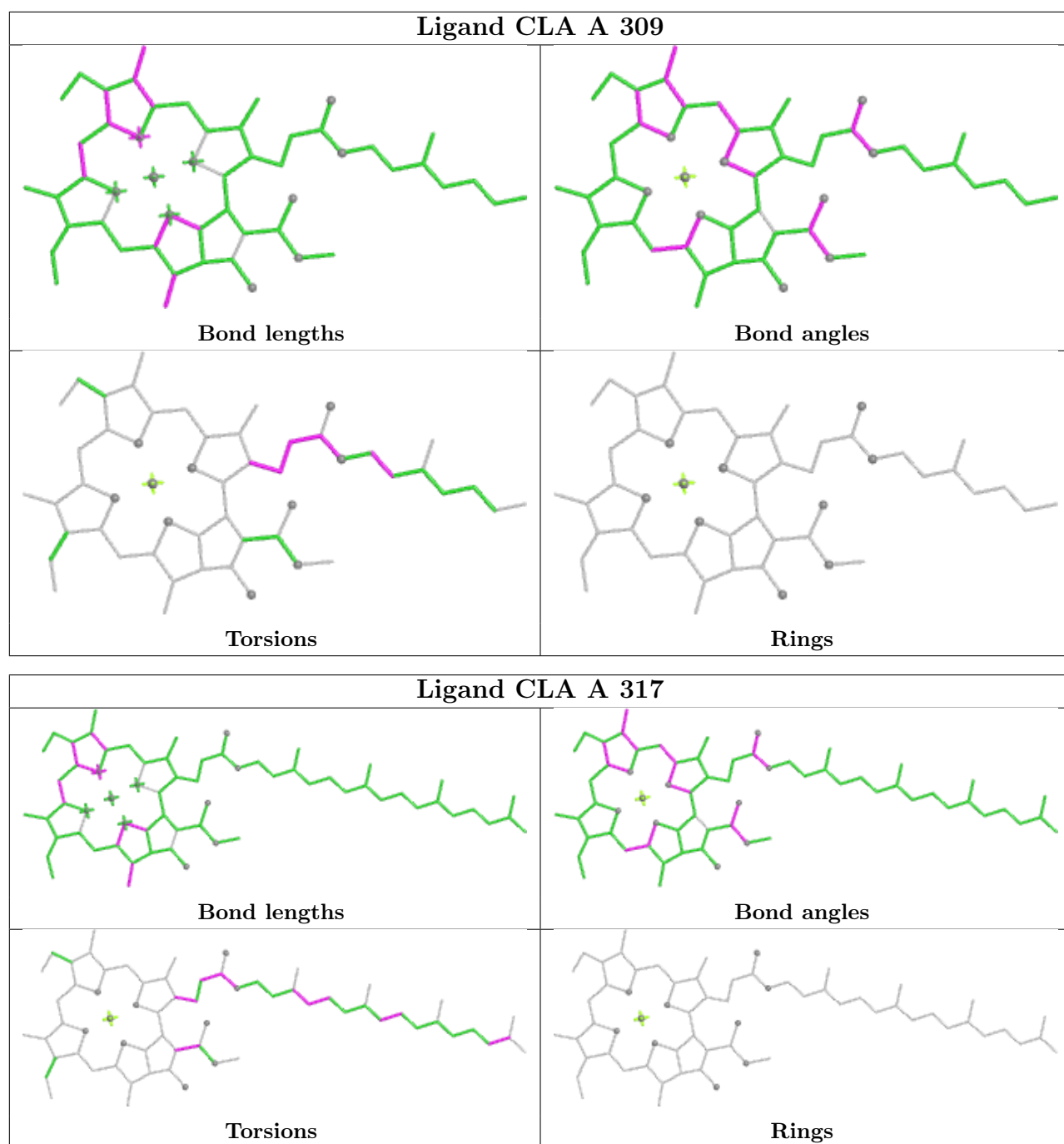


Ligand CLA A 318

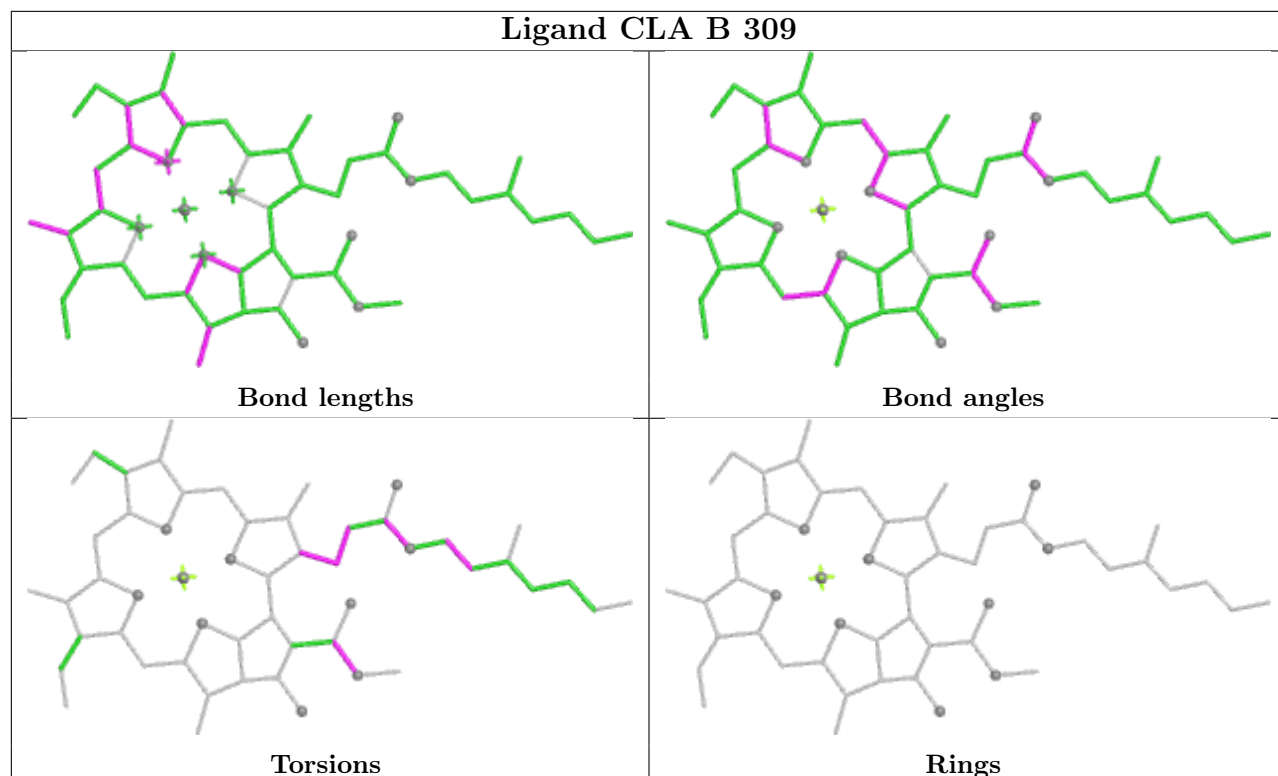


Ligand A86 A 302

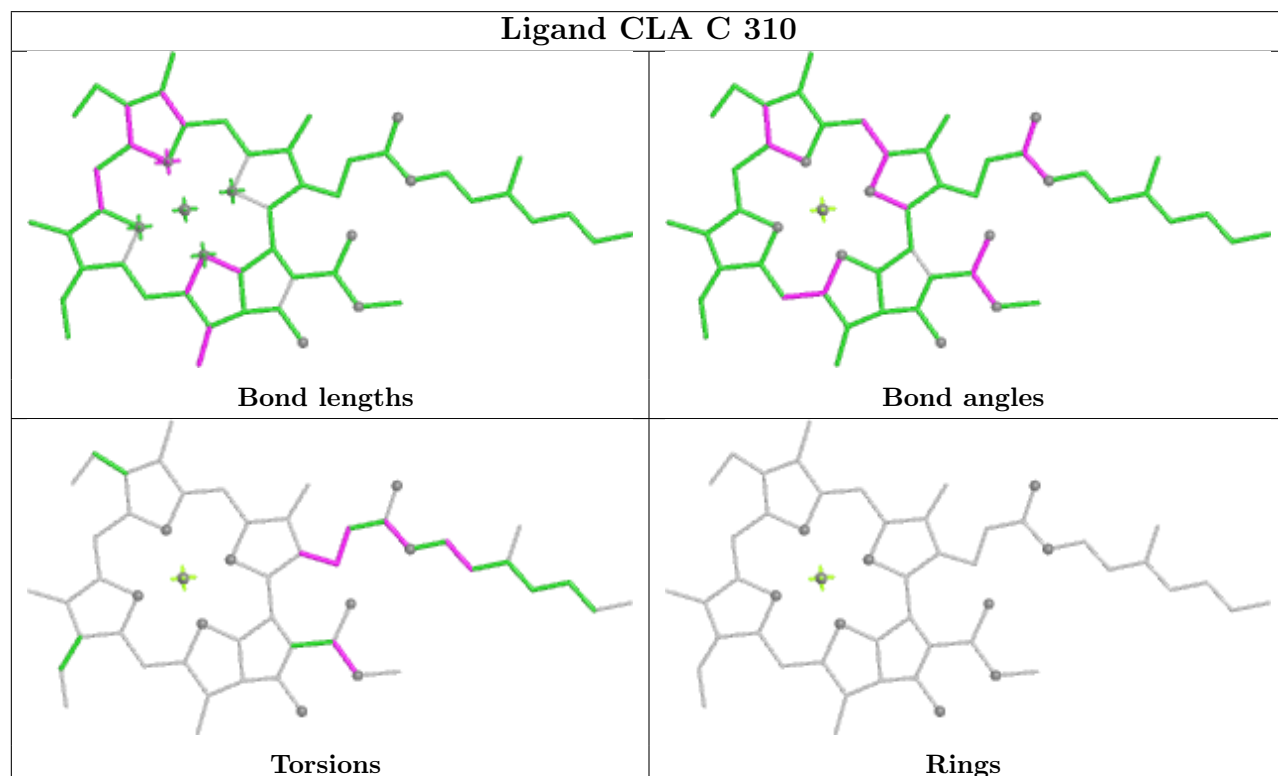




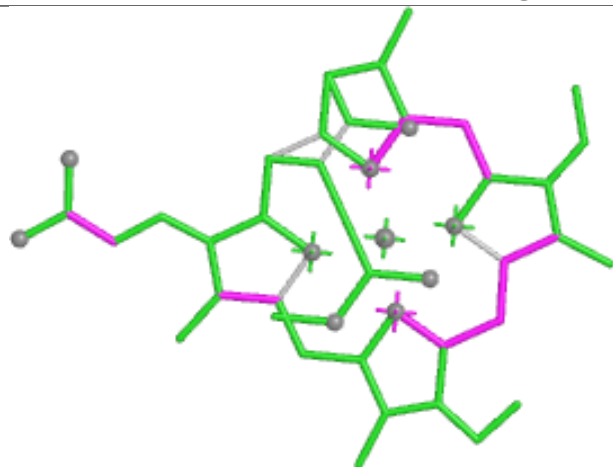
Ligand CLA B 309



Ligand CLA C 310



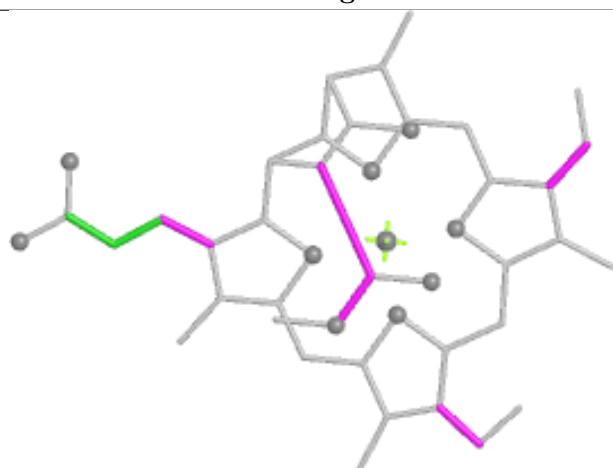
Ligand KC2 A 312



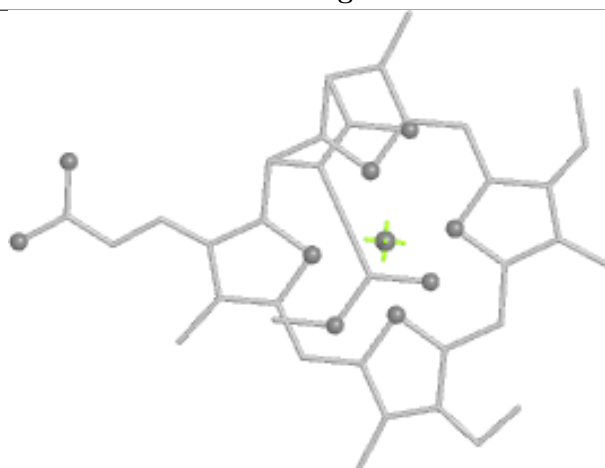
Bond lengths



Bond angles

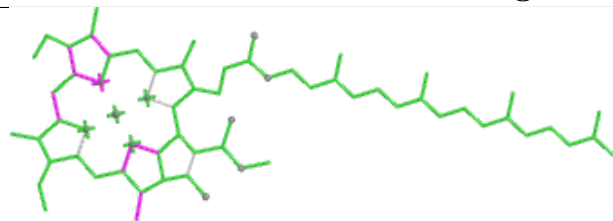


Torsions

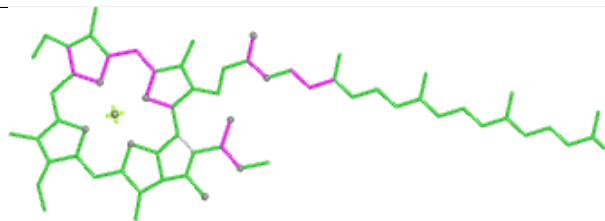


Rings

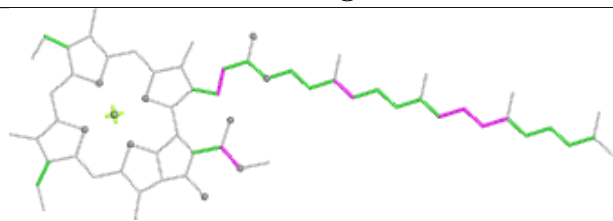
Ligand CLA B 311



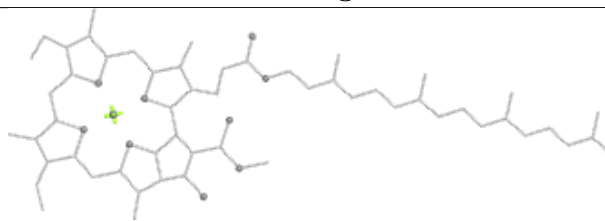
Bond lengths



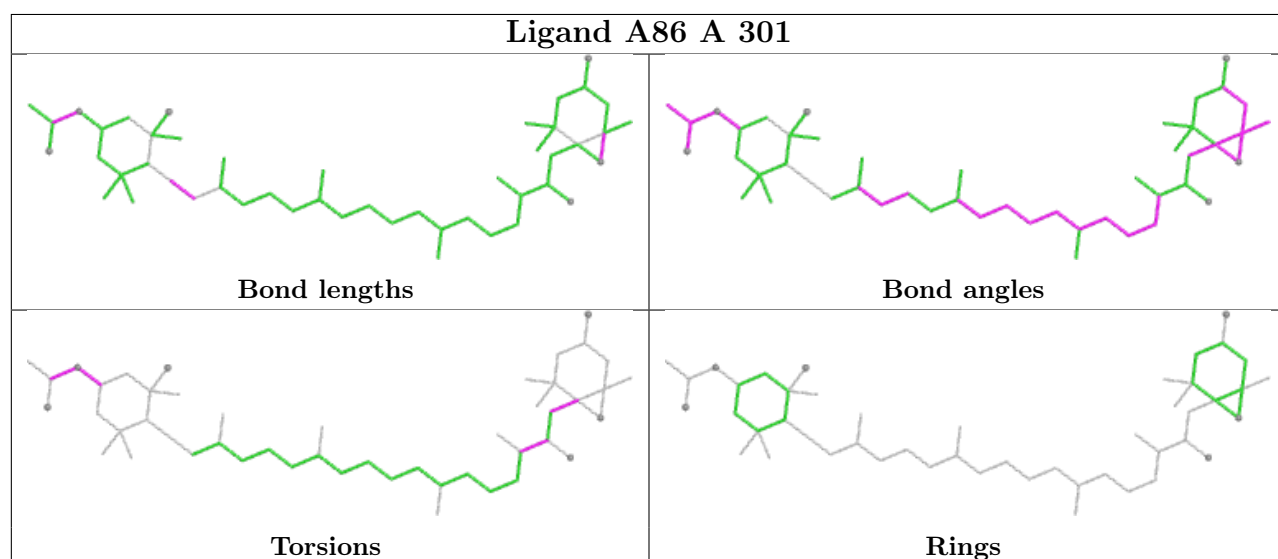
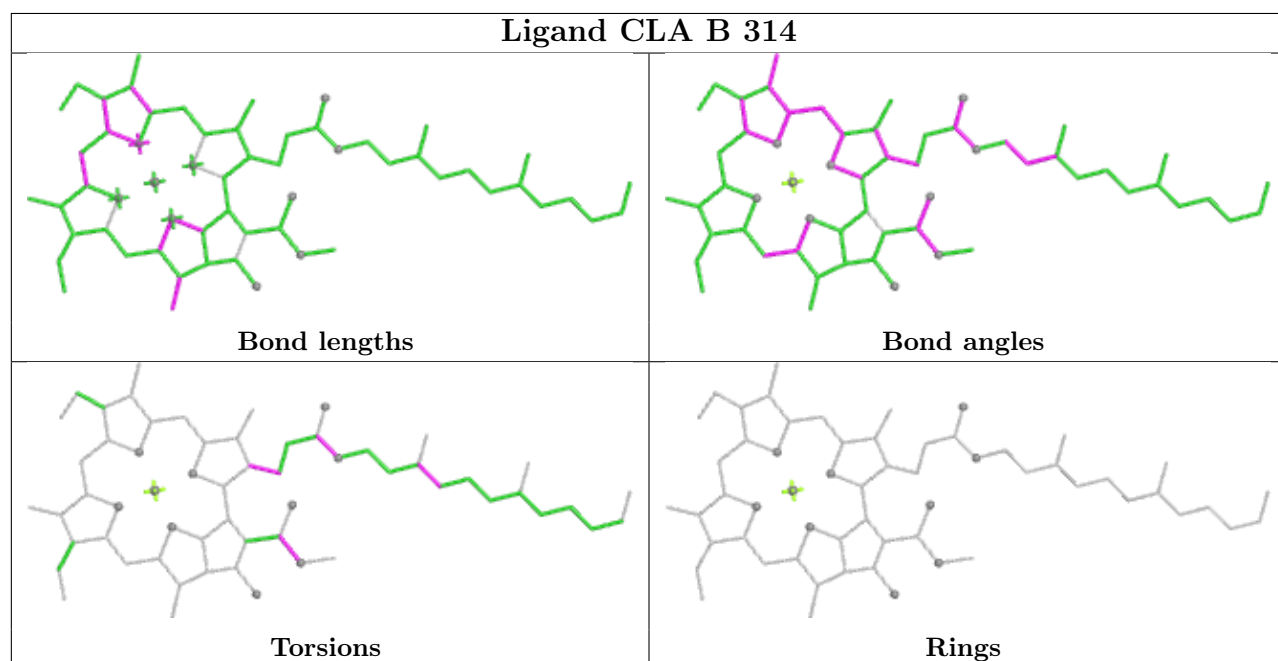
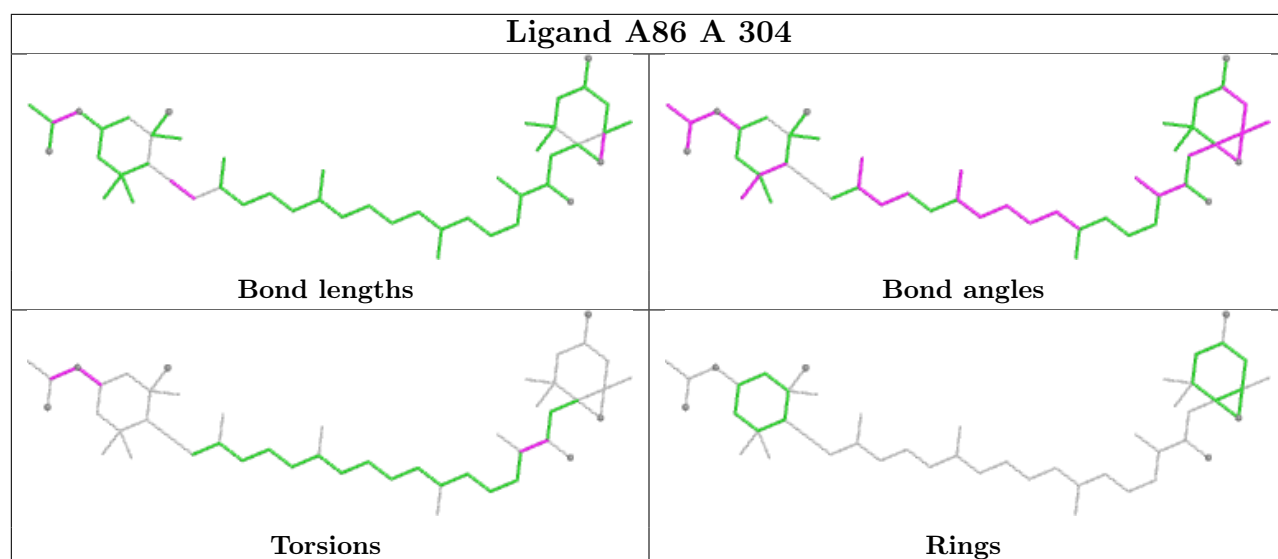
Bond angles

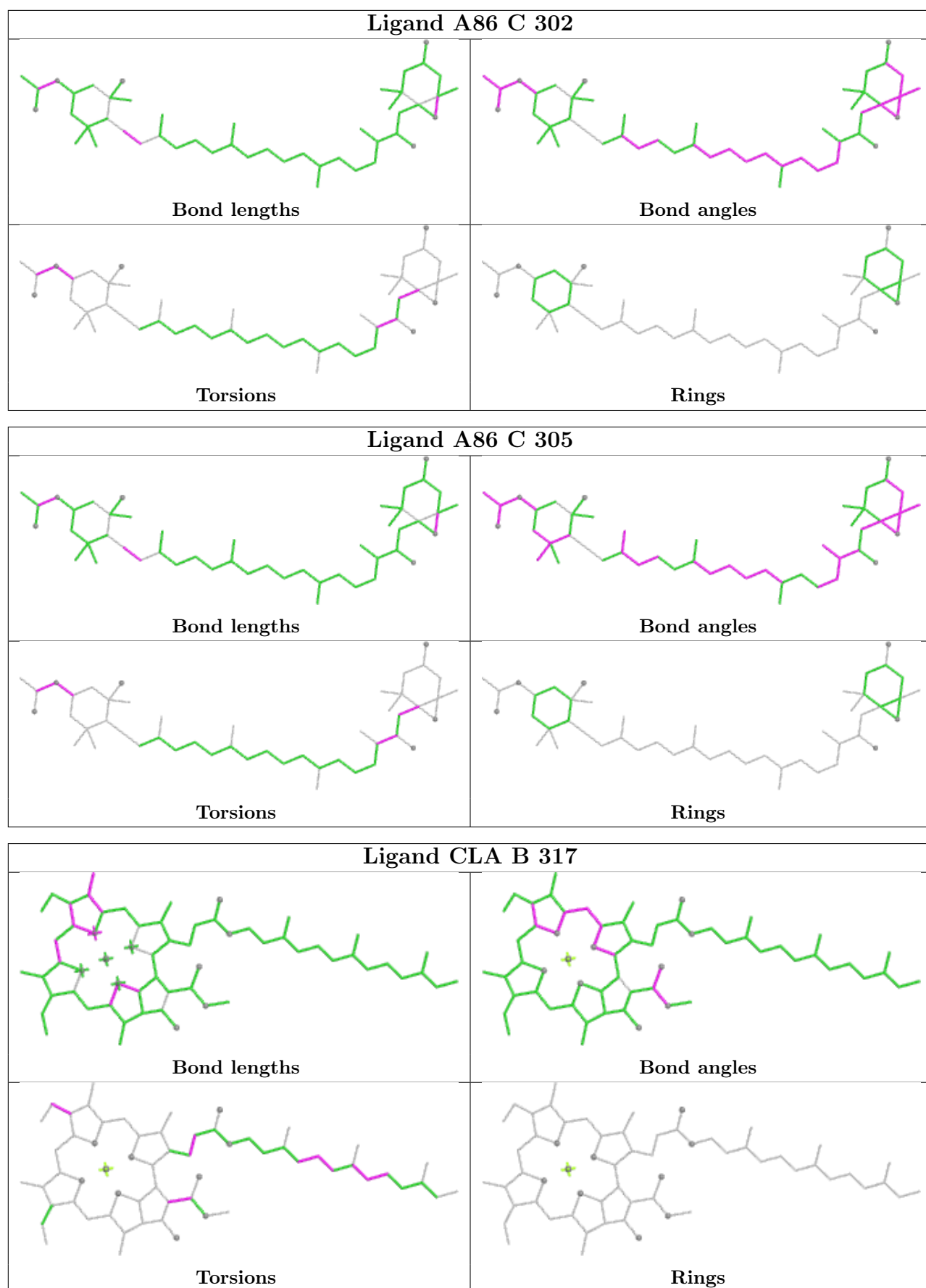


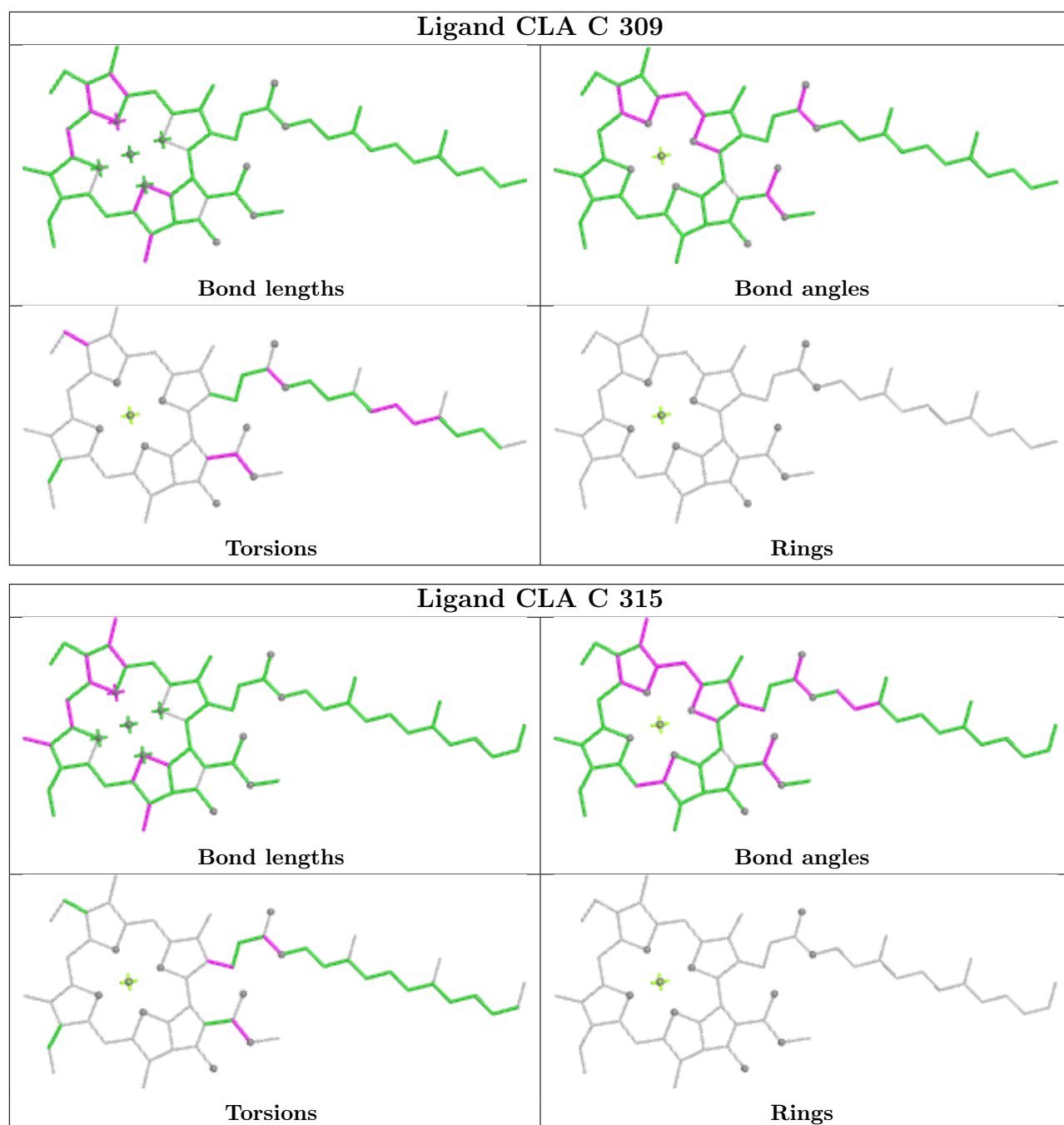
Torsions

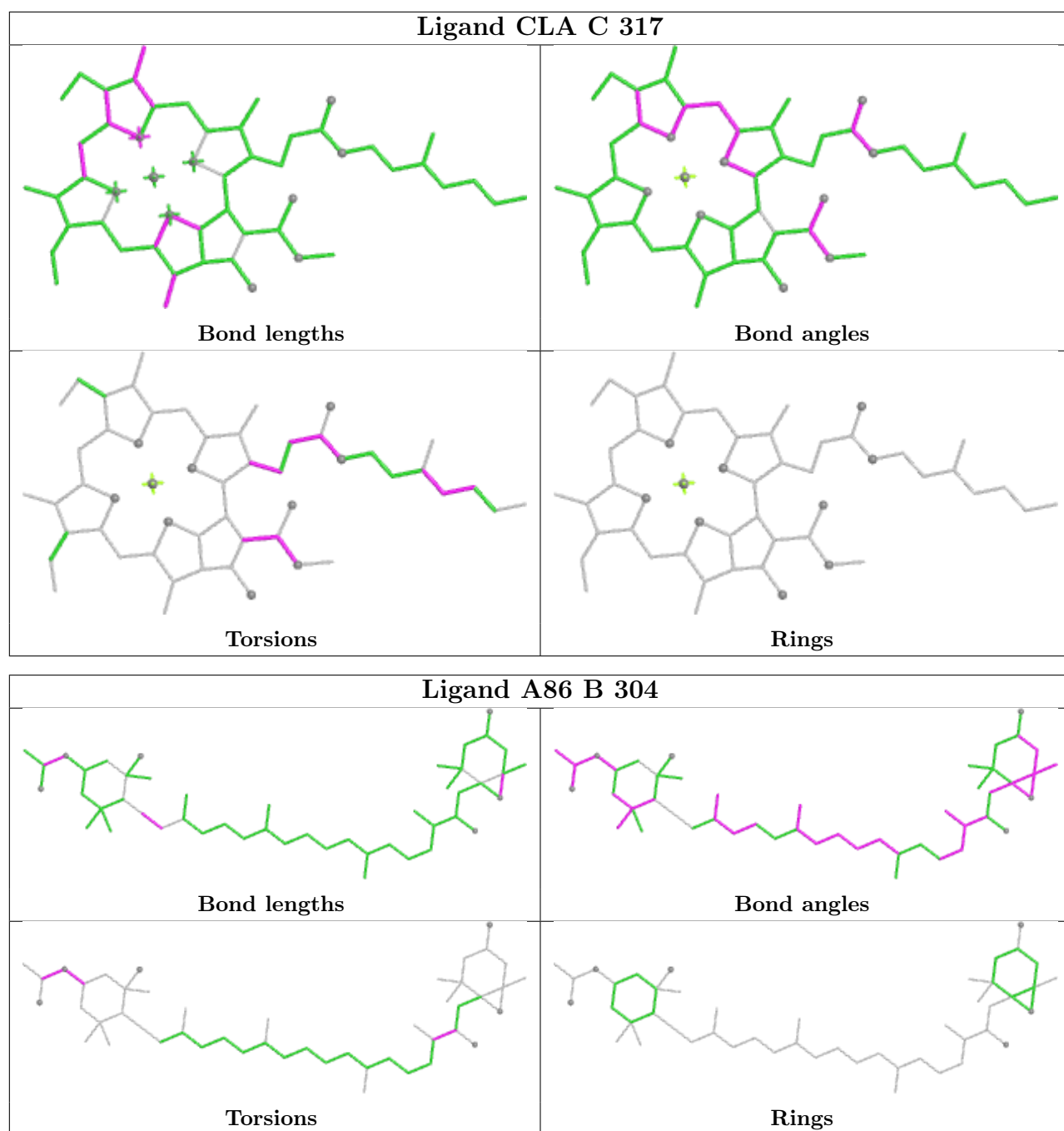


Rings

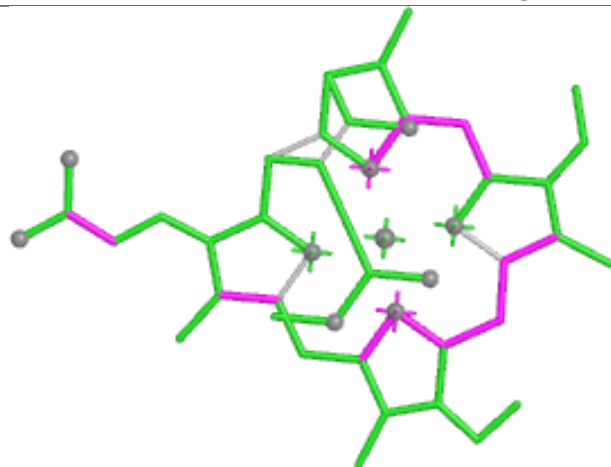








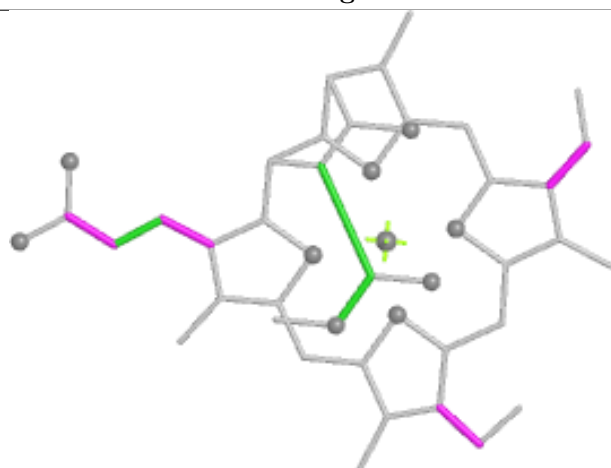
Ligand KC2 A 310



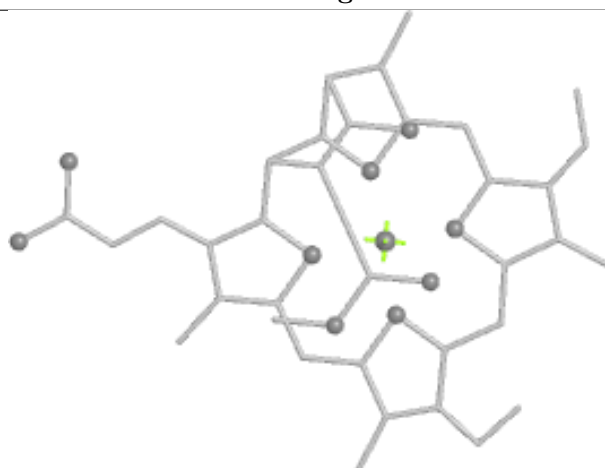
Bond lengths



Bond angles

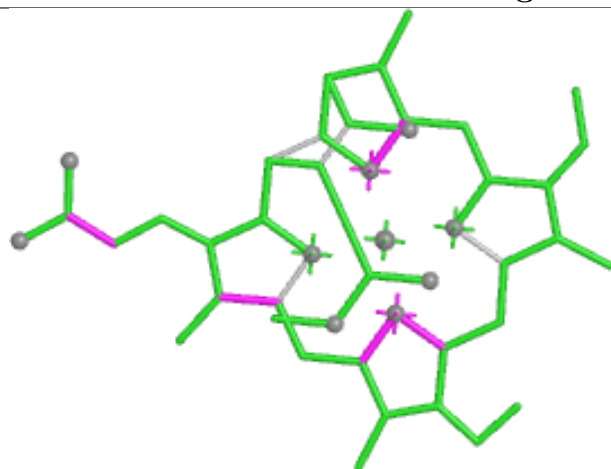


Torsions

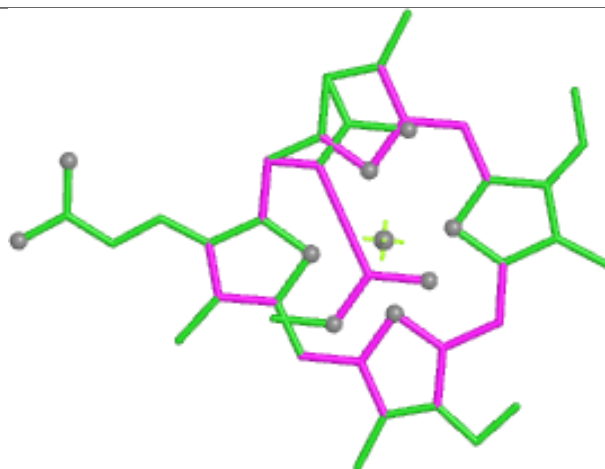


Rings

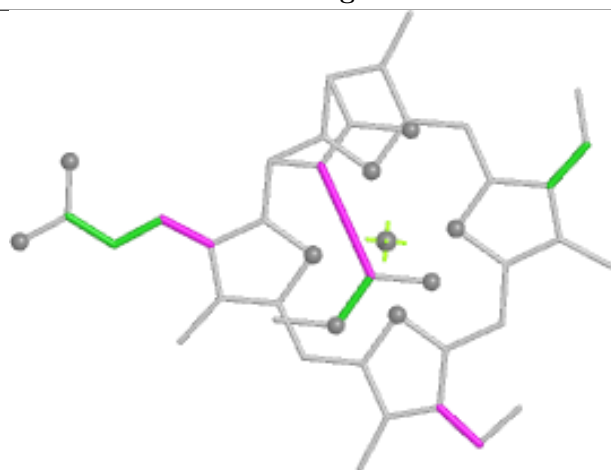
Ligand KC1 C 316



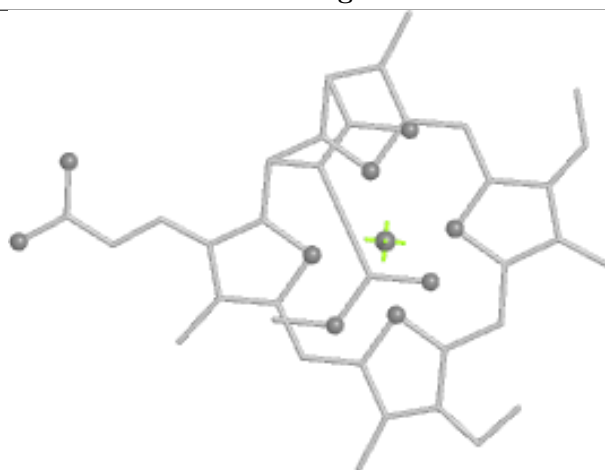
Bond lengths



Bond angles

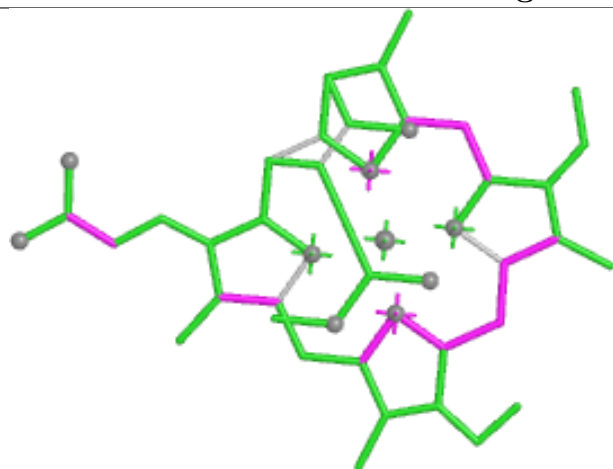


Torsions

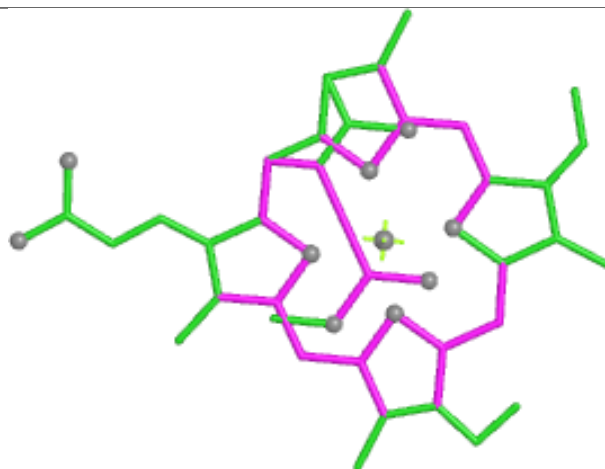


Rings

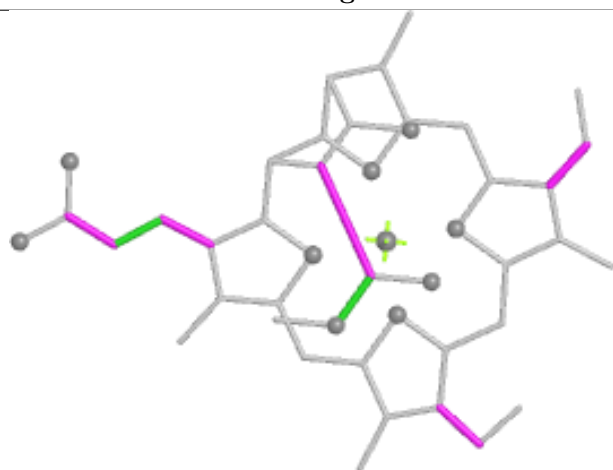
Ligand KC2 B 310



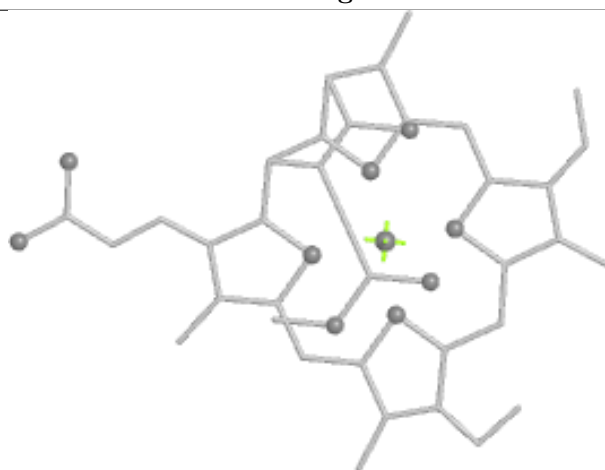
Bond lengths



Bond angles

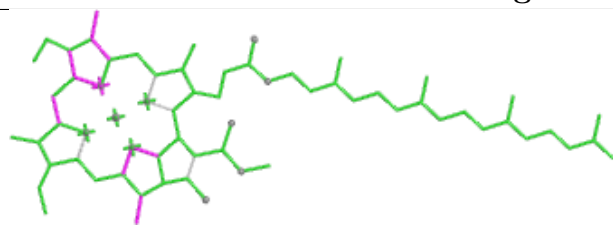


Torsions

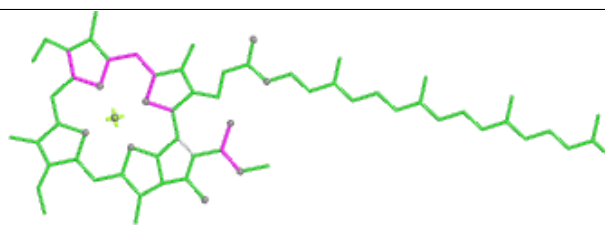


Rings

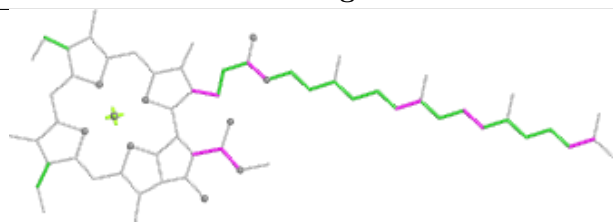
Ligand CLA A 313



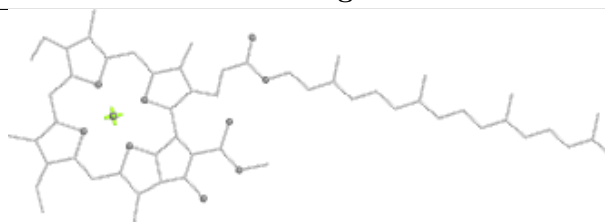
Bond lengths



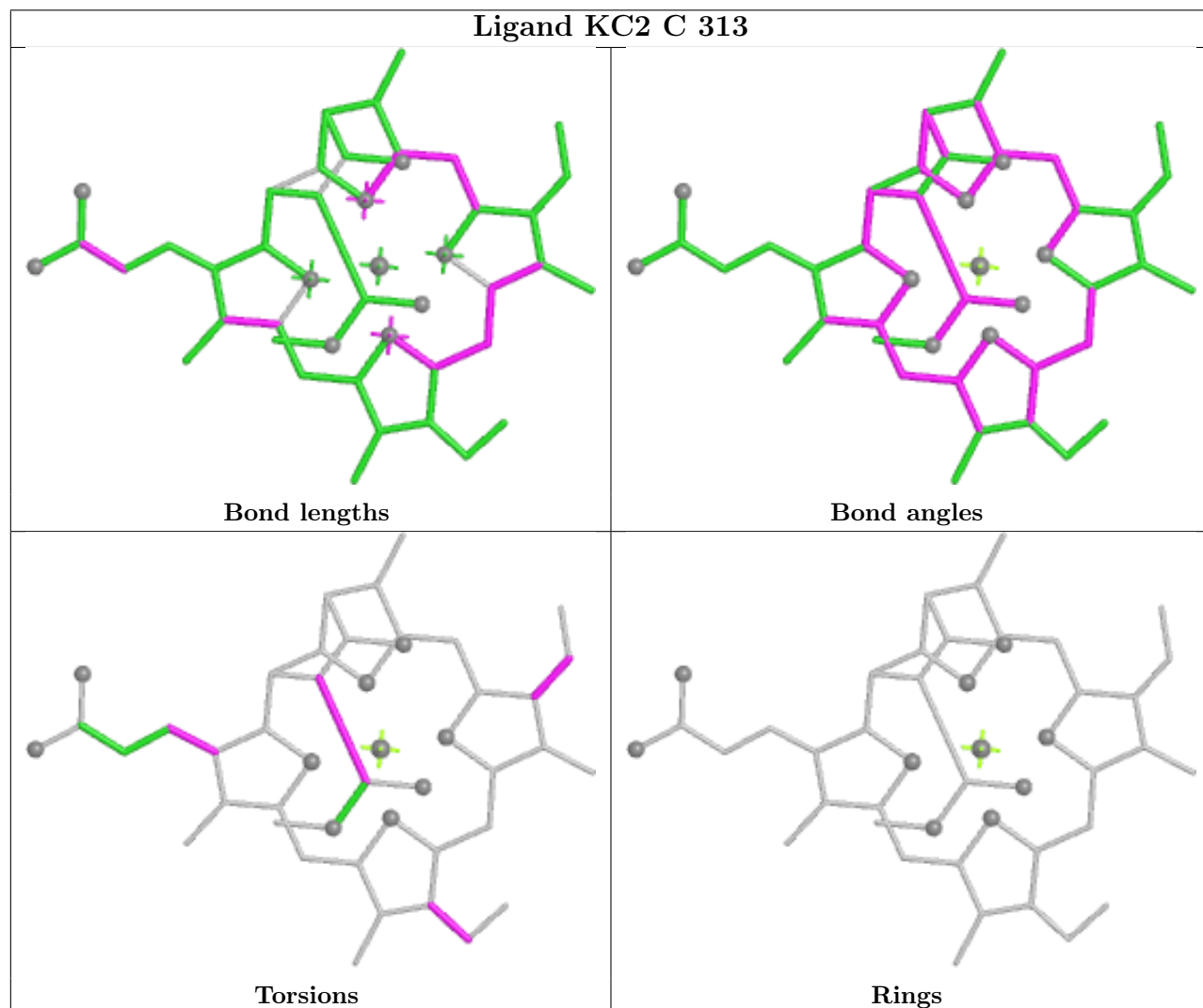
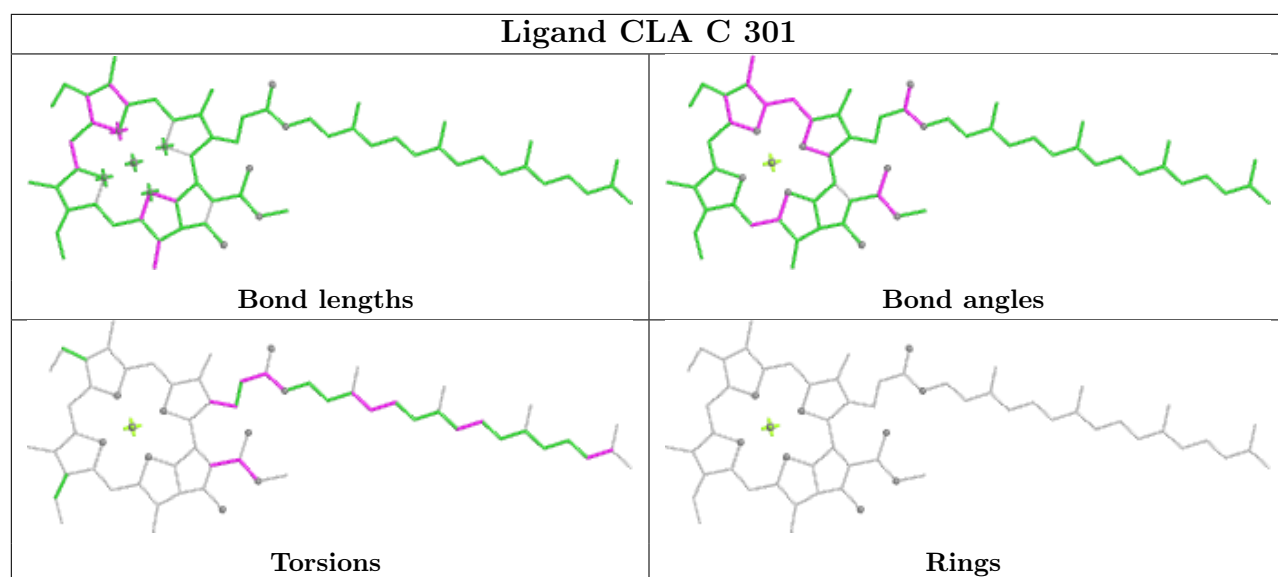
Bond angles

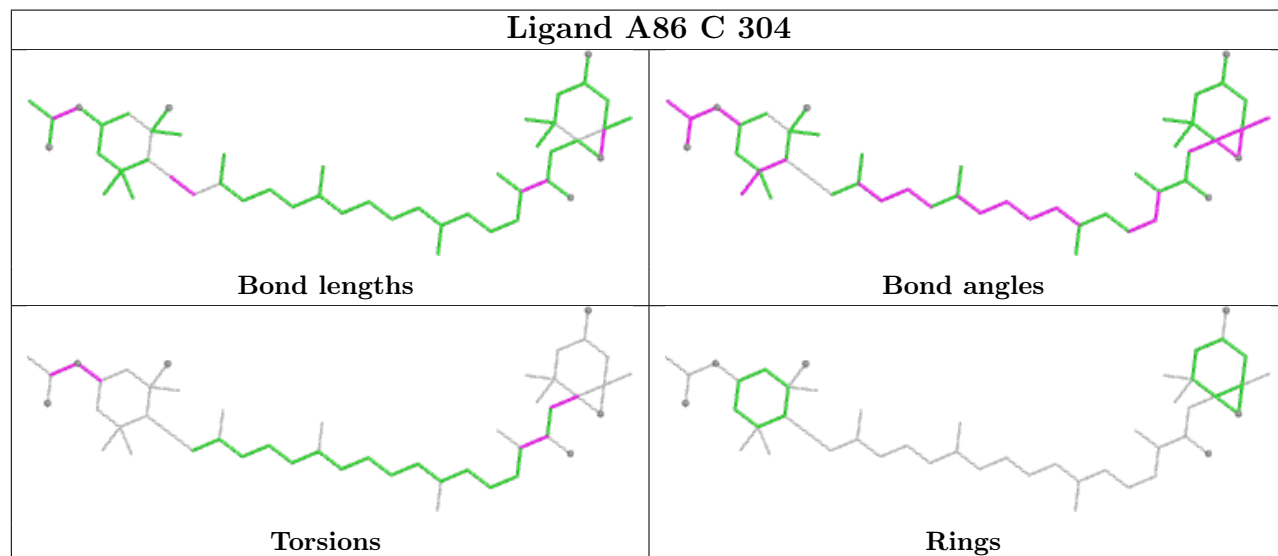
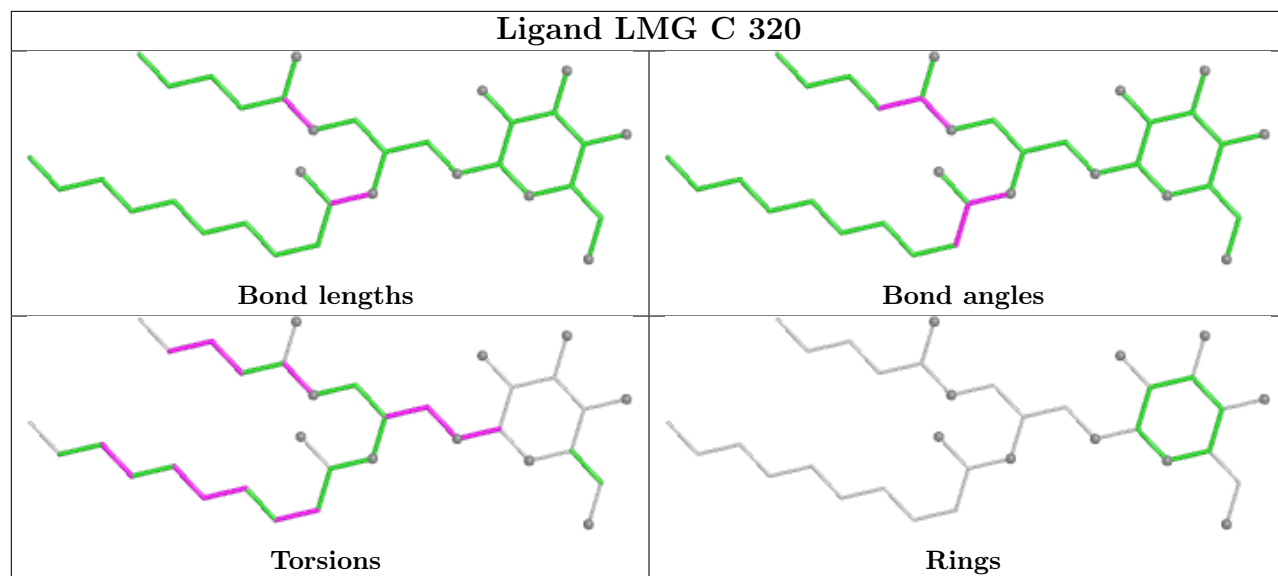


Torsions

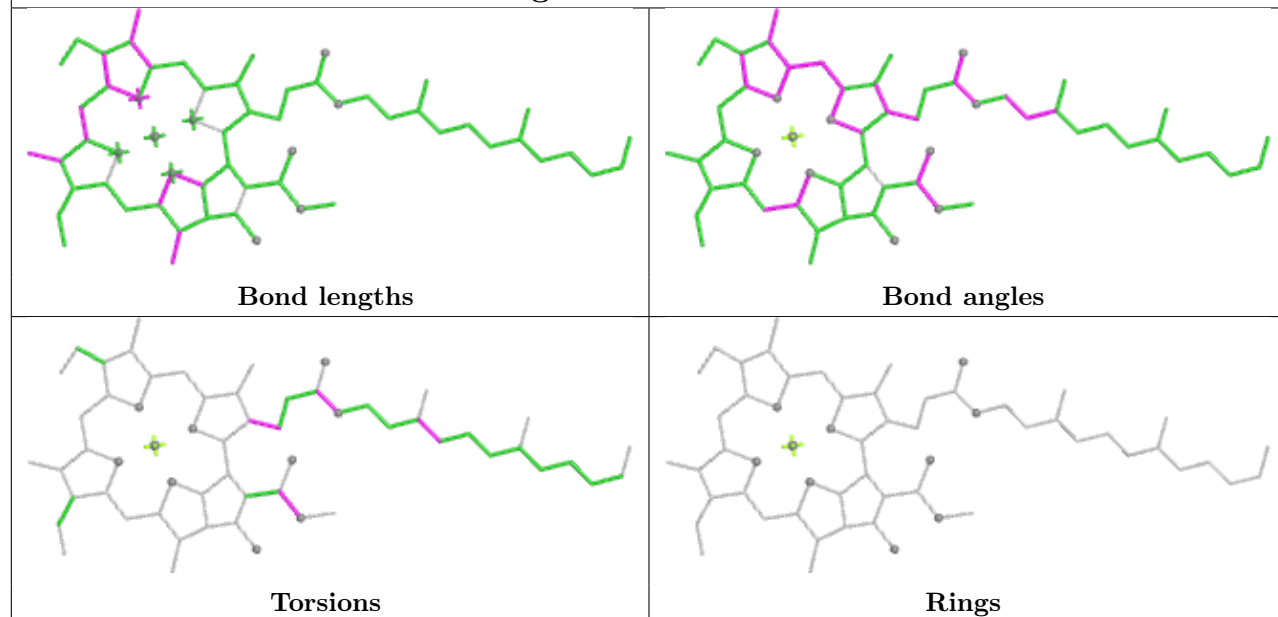


Rings

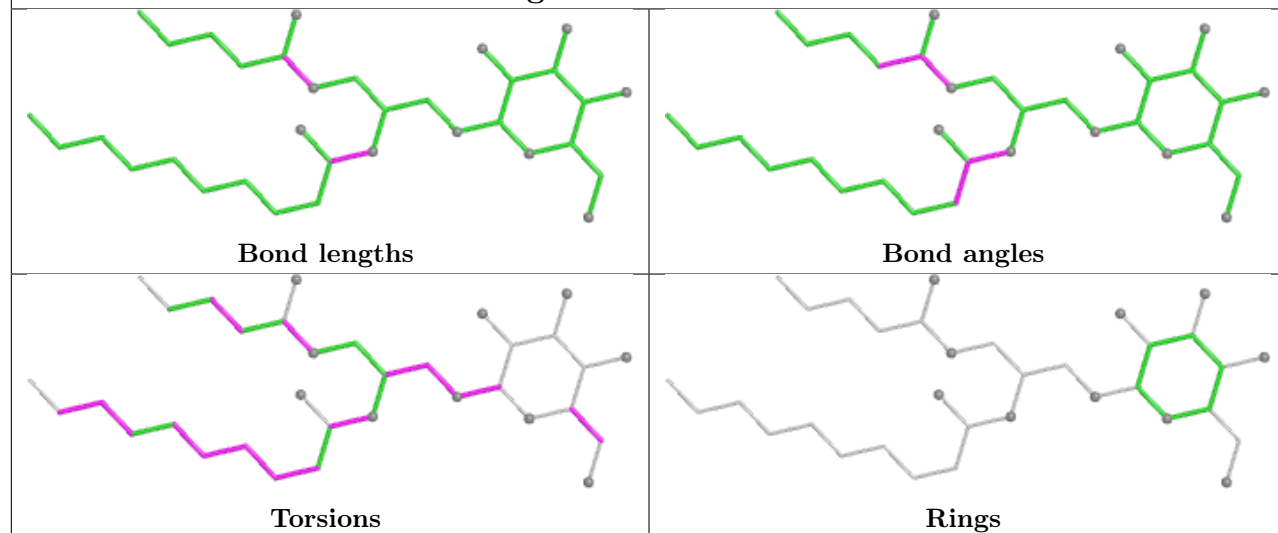


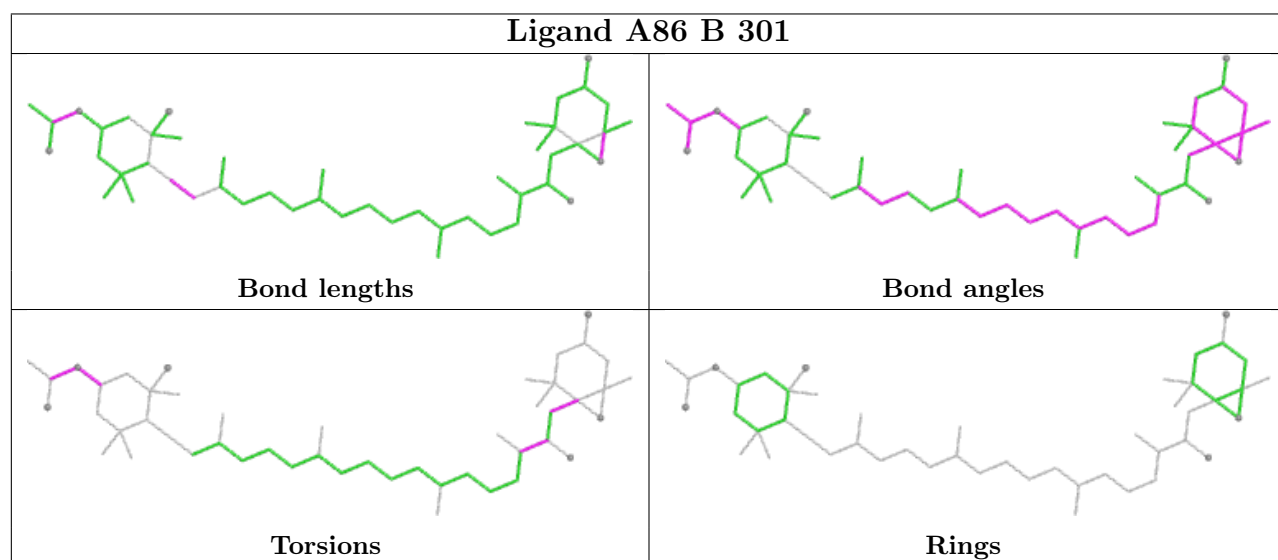
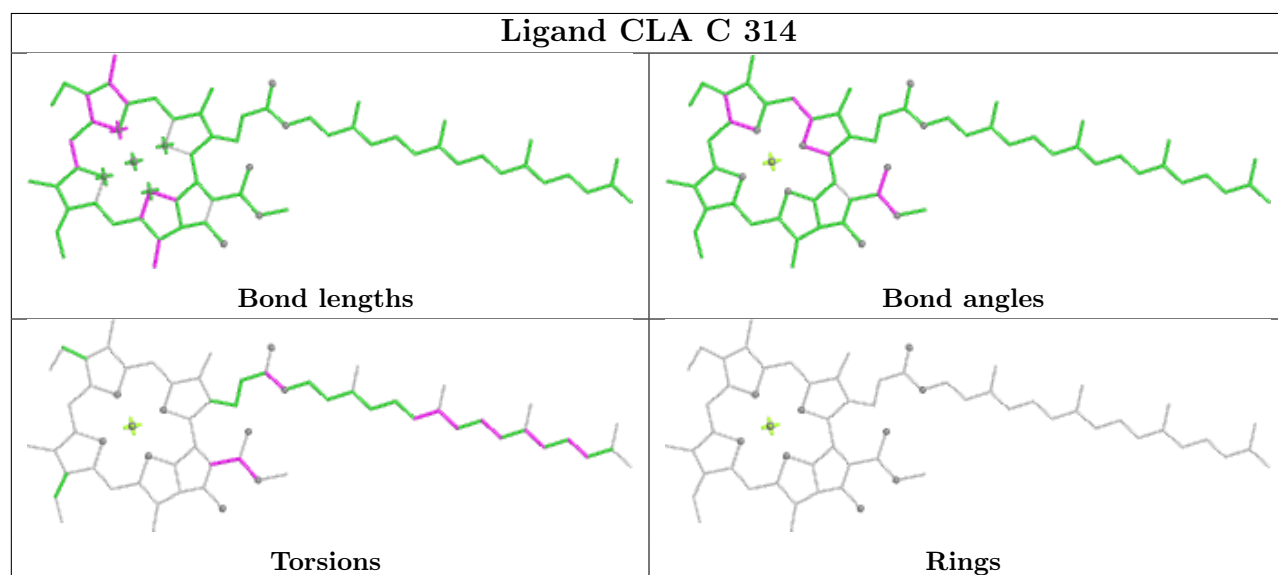
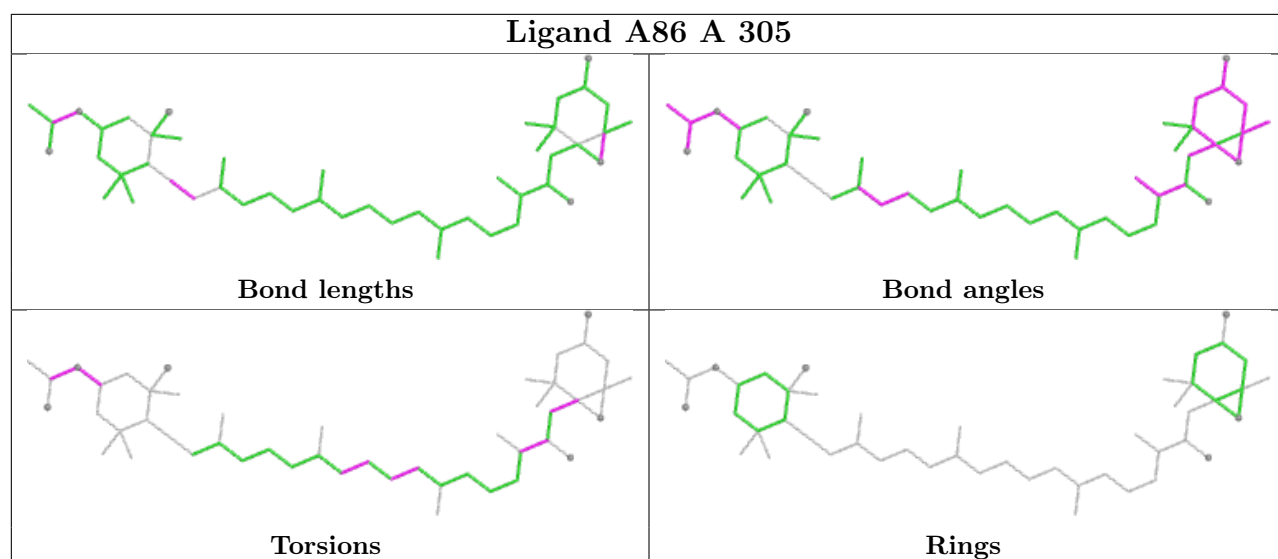


Ligand CLA A 314

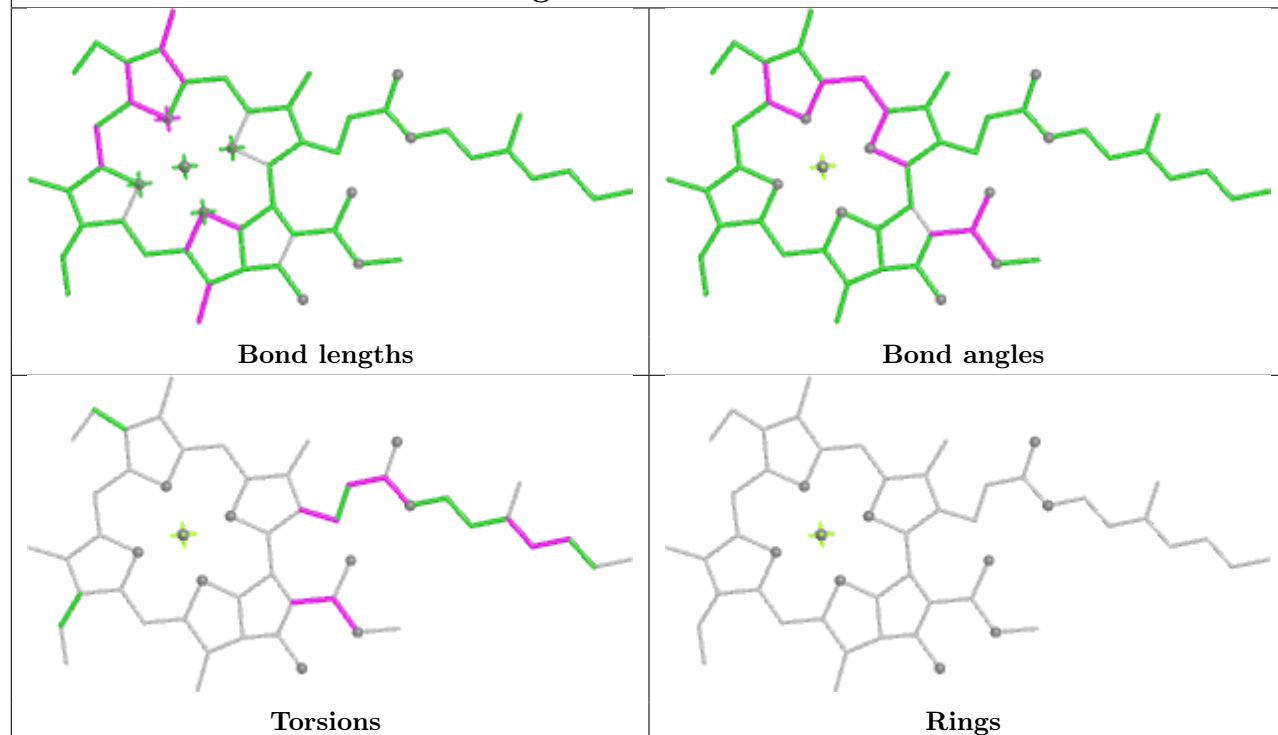


Ligand LMG A 319

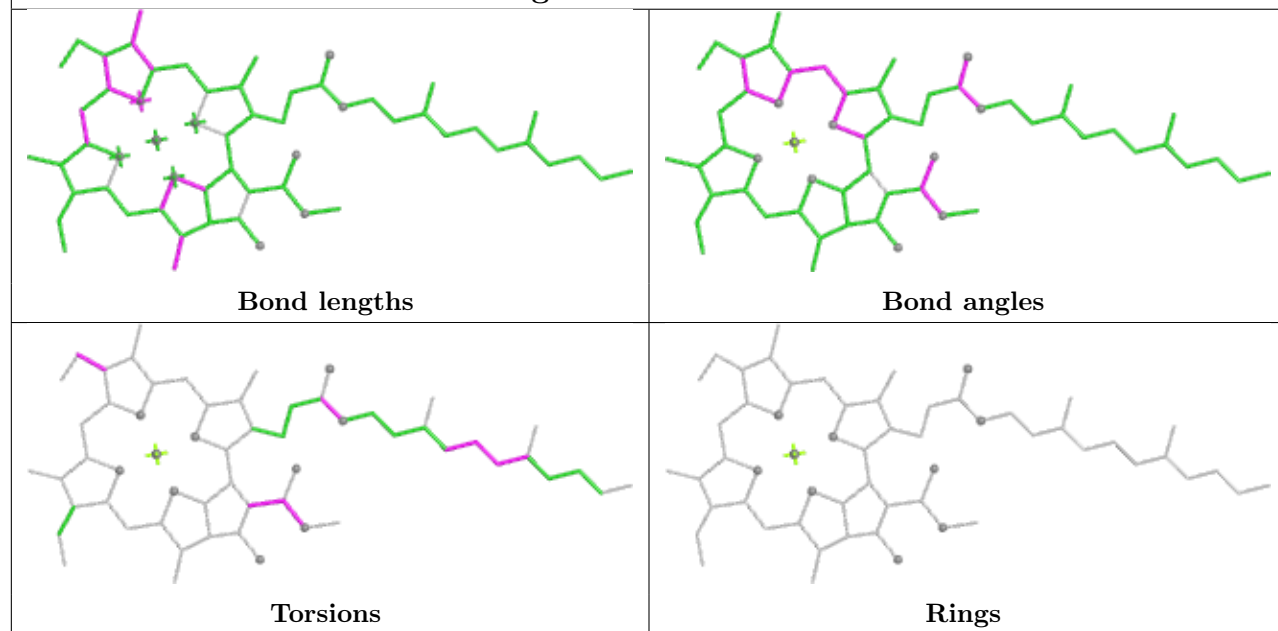




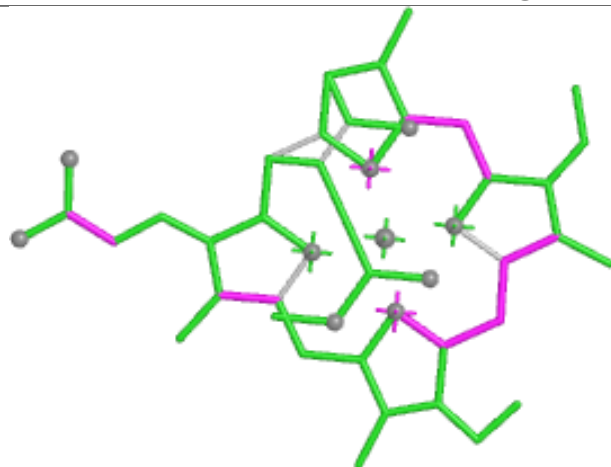
Ligand CLA B 316



Ligand CLA A 308



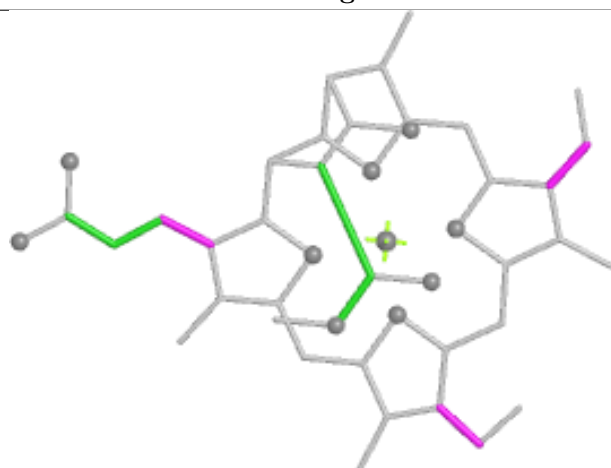
Ligand KC2 B 312



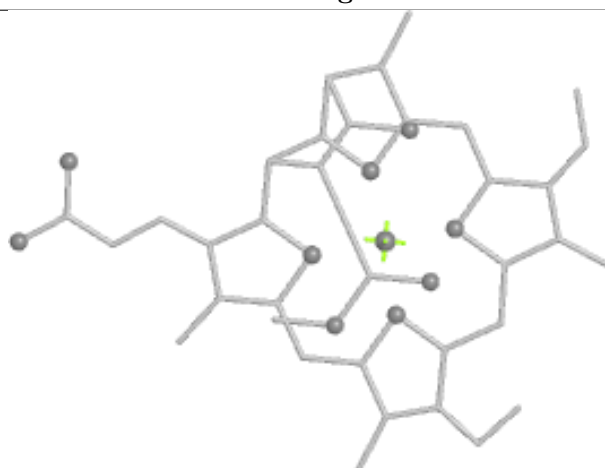
Bond lengths



Bond angles



Torsions

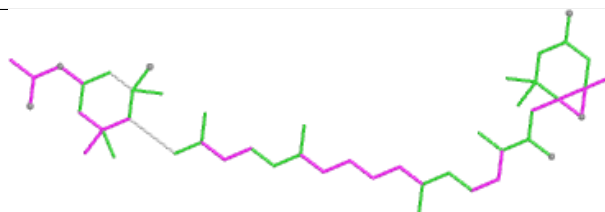


Rings

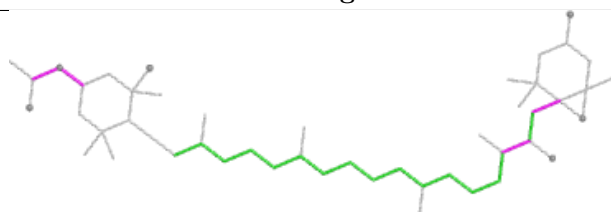
Ligand A86 A 303



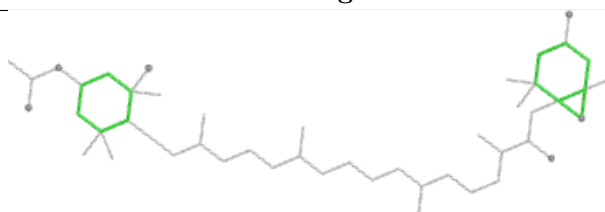
Bond lengths



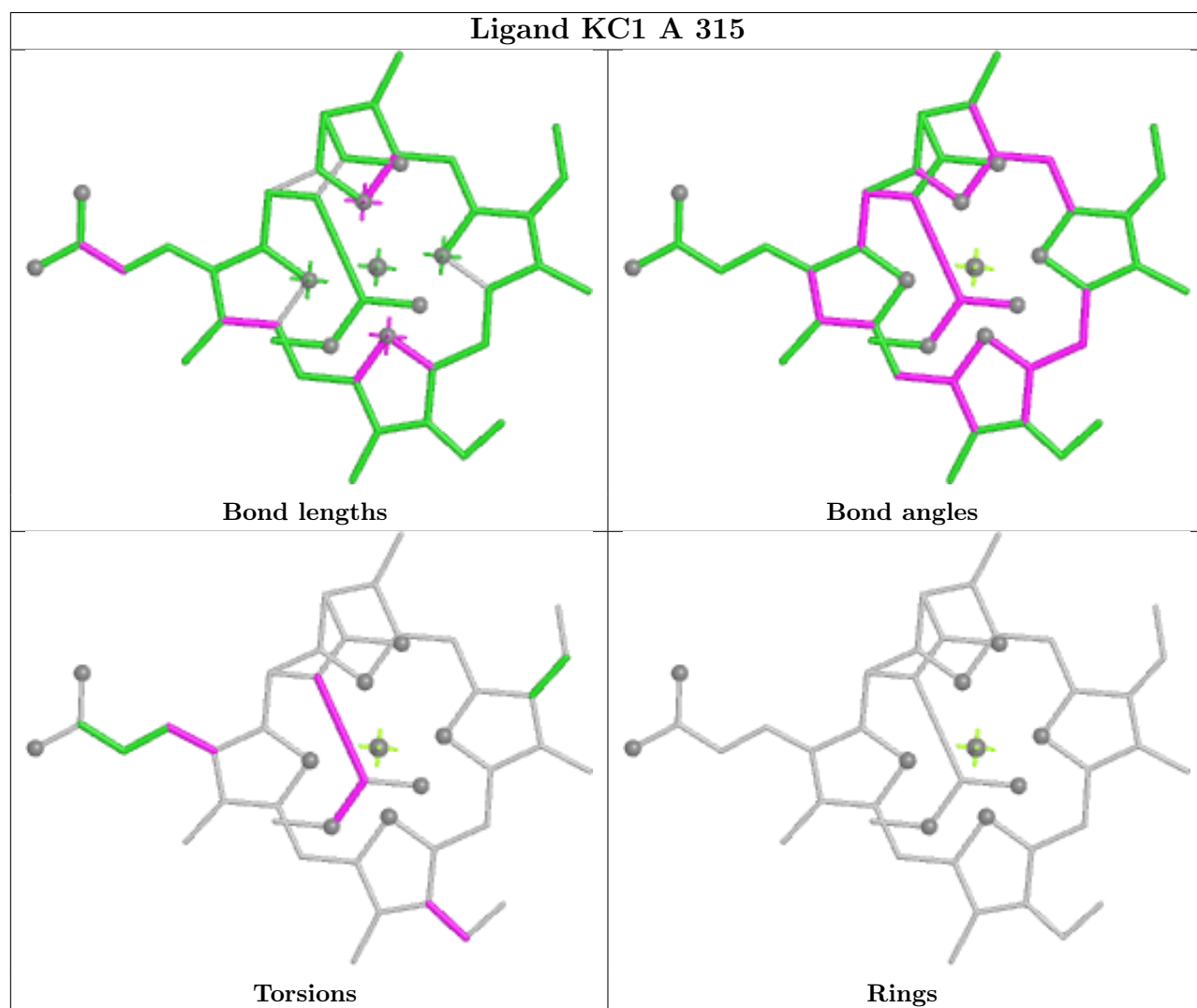
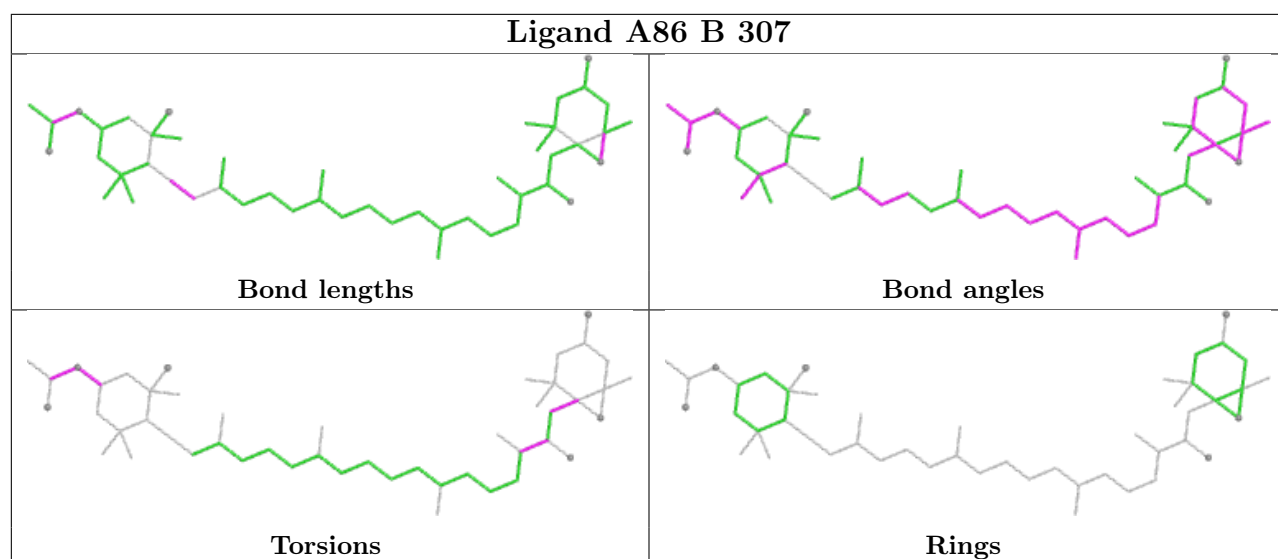
Bond angles

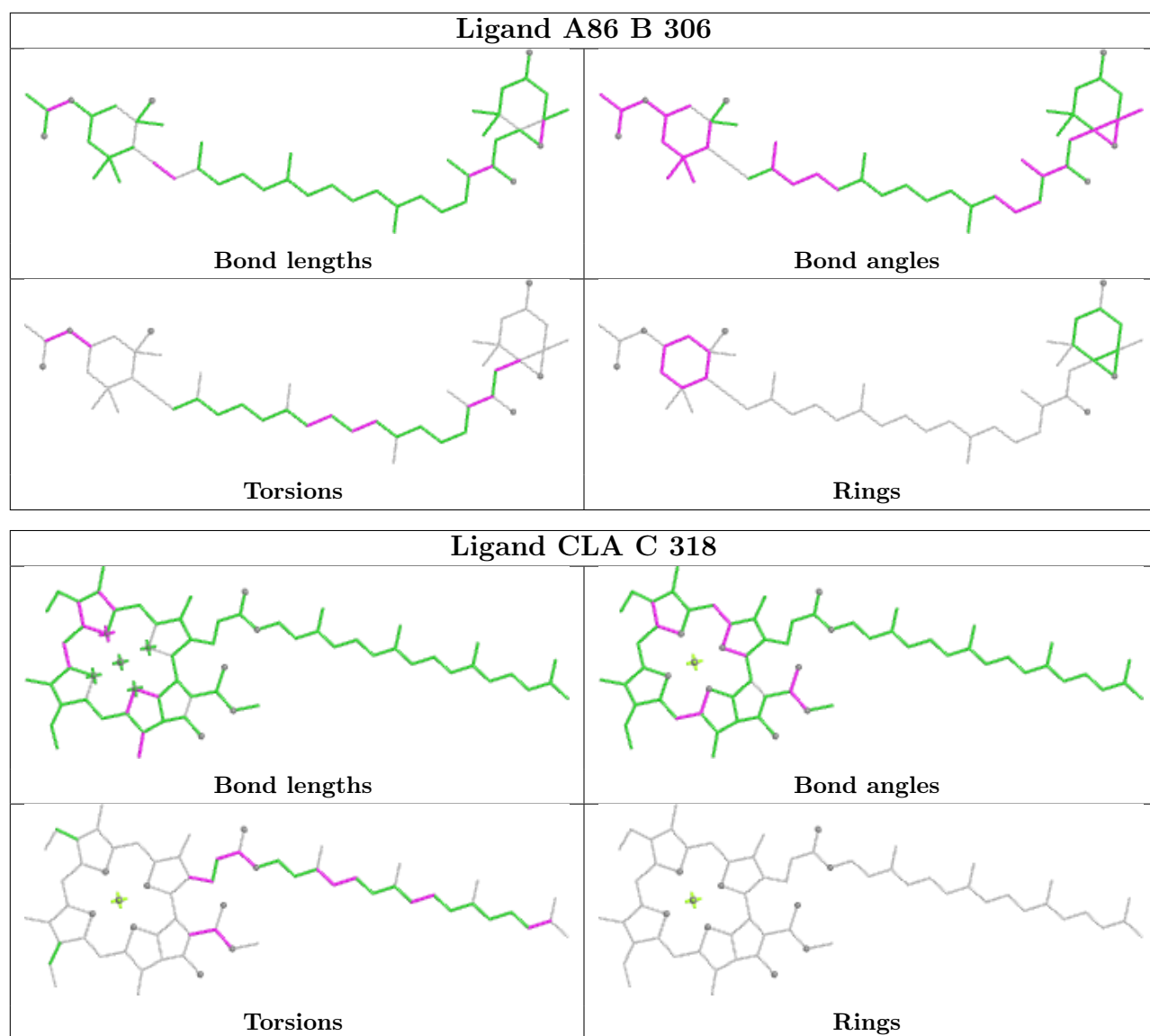


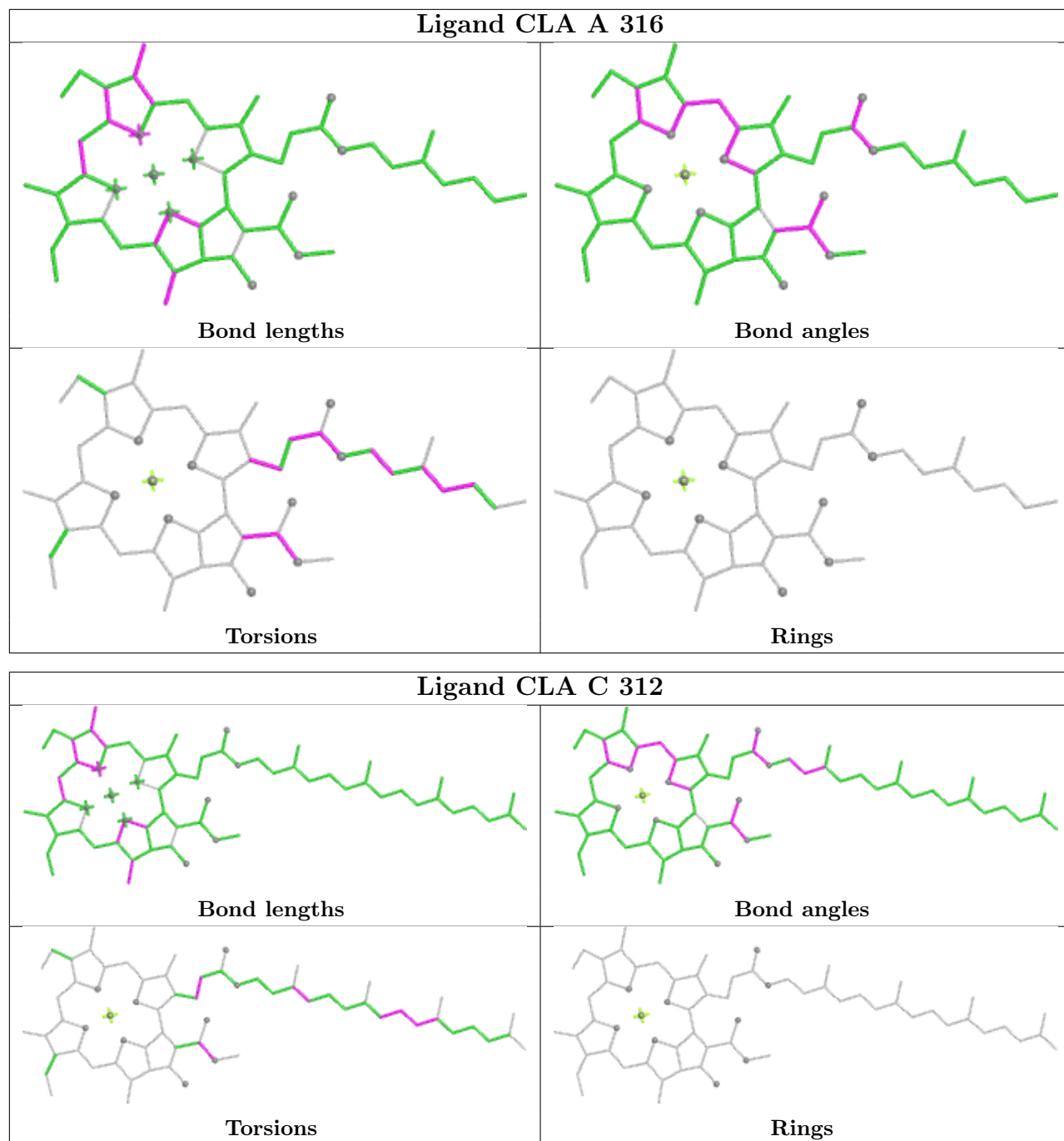
Torsions

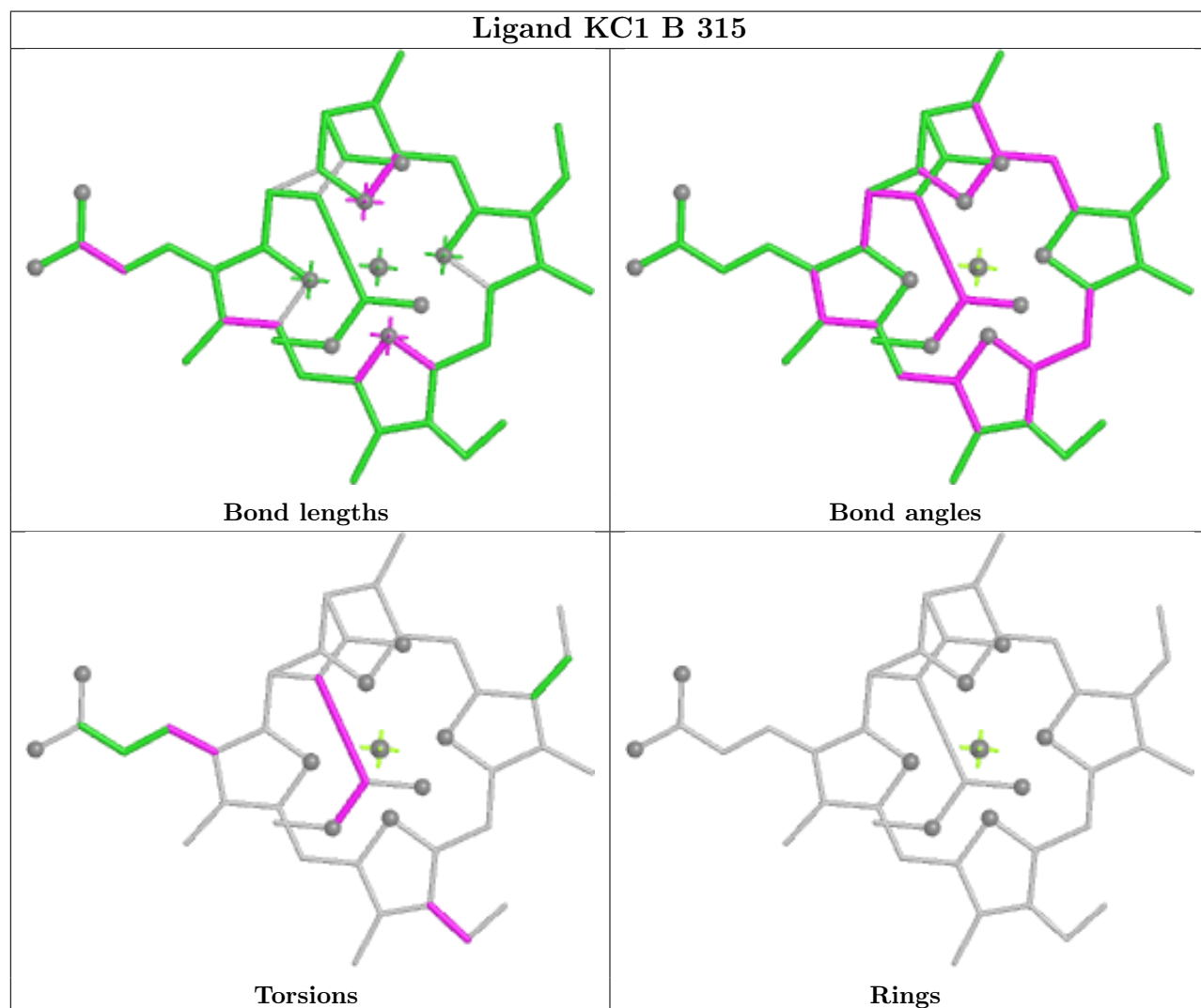
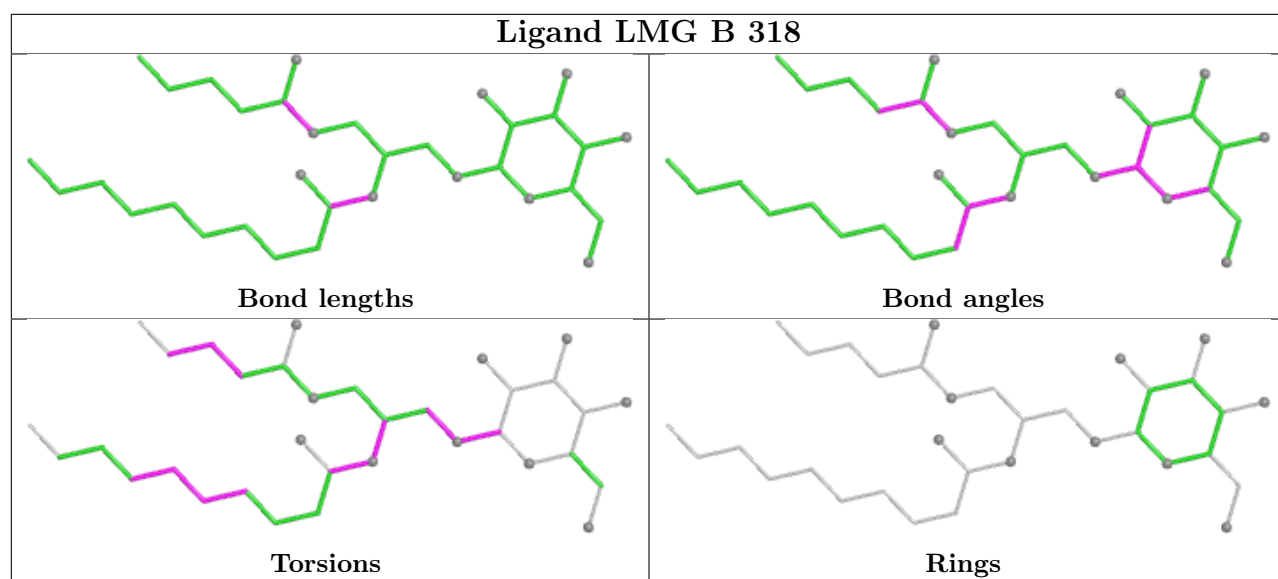


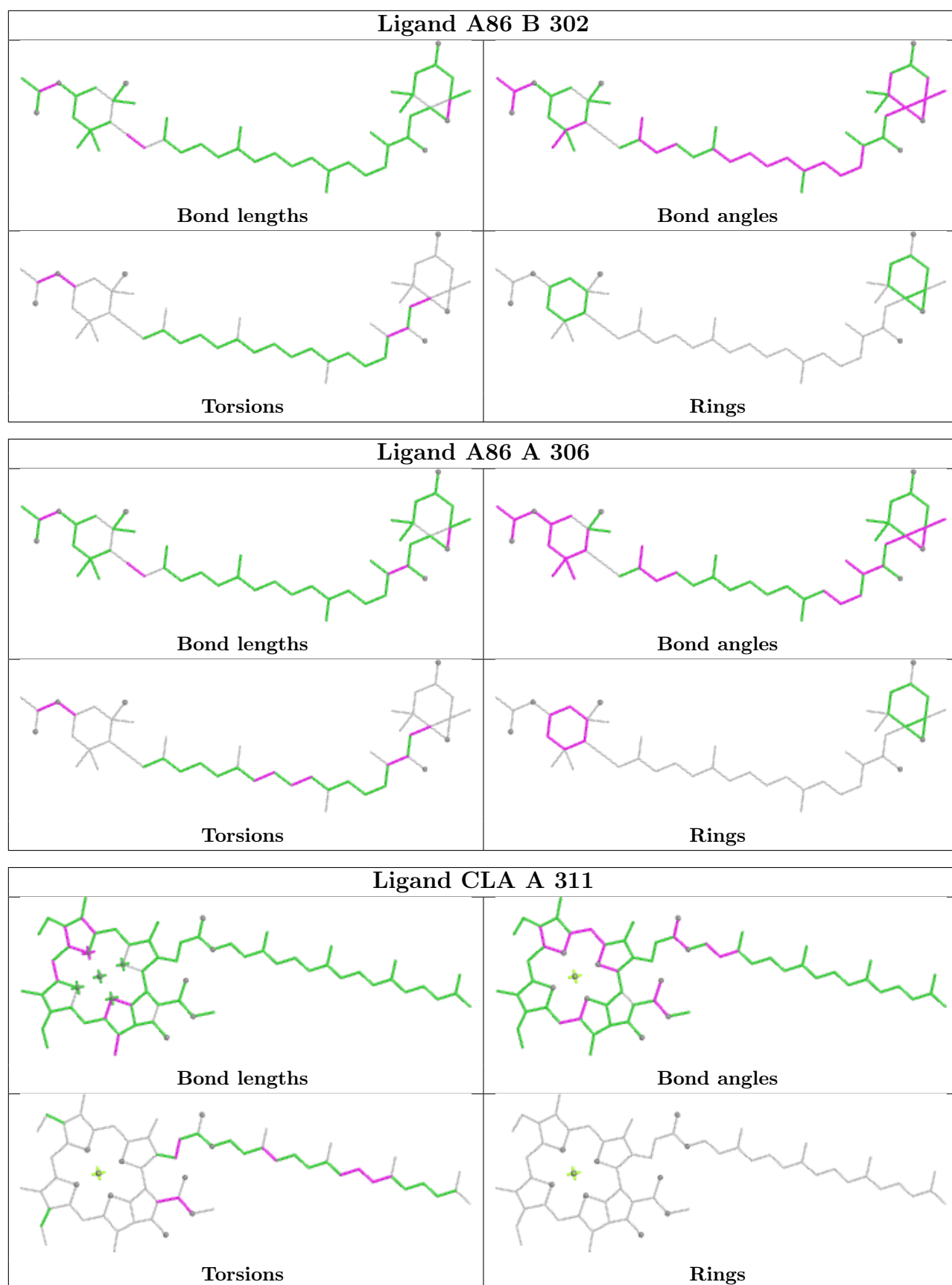
Rings

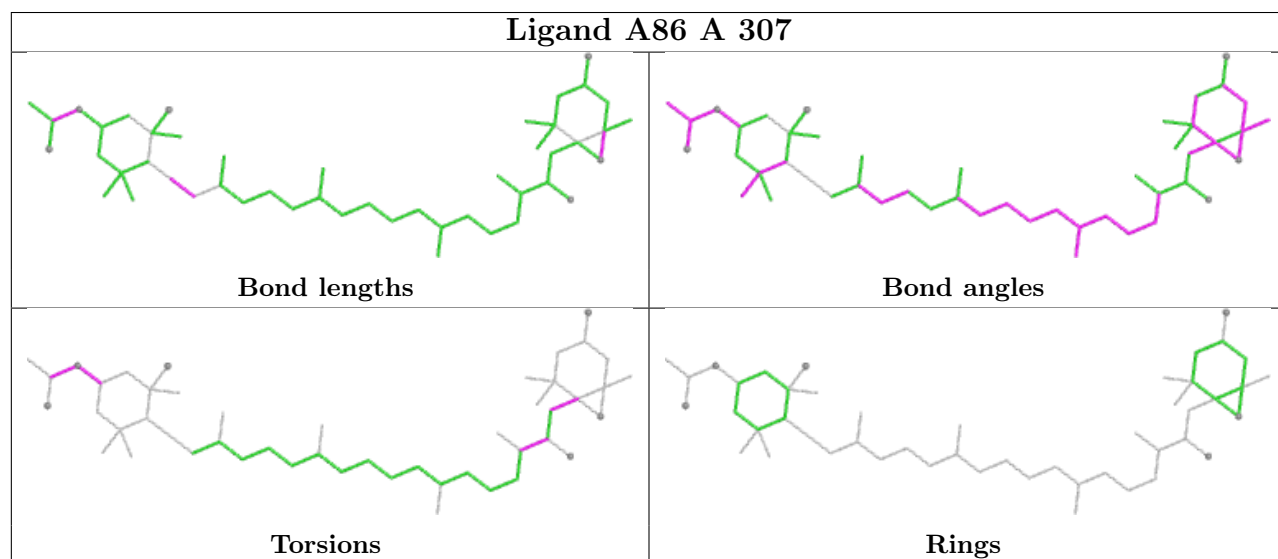
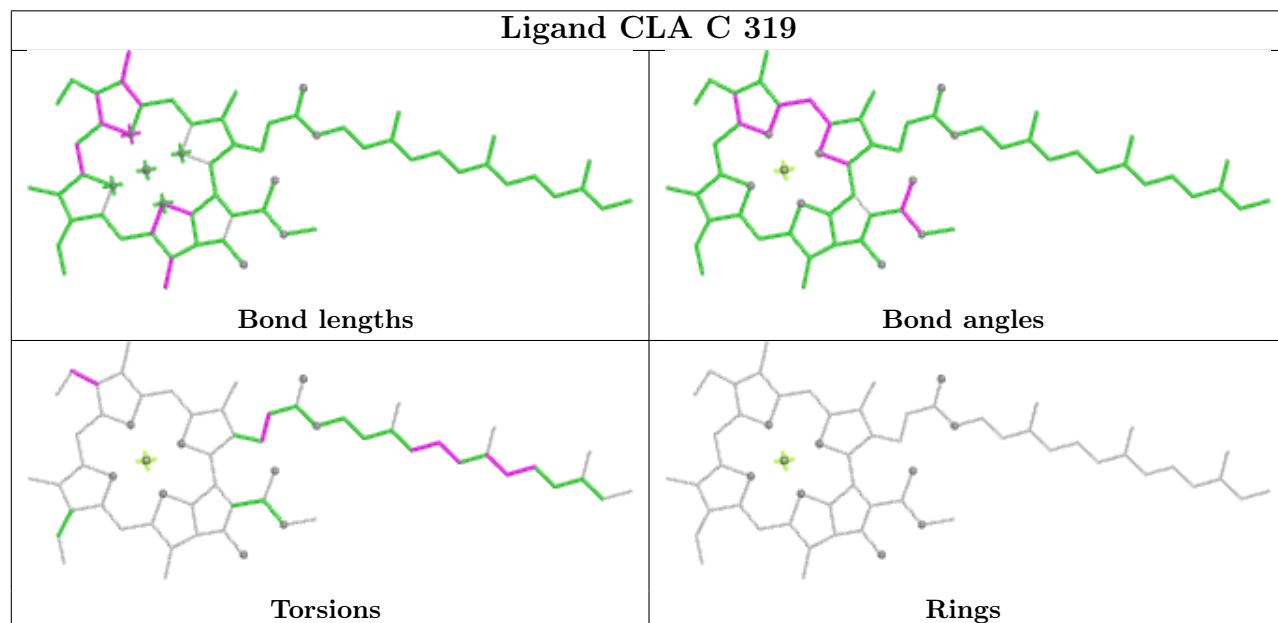
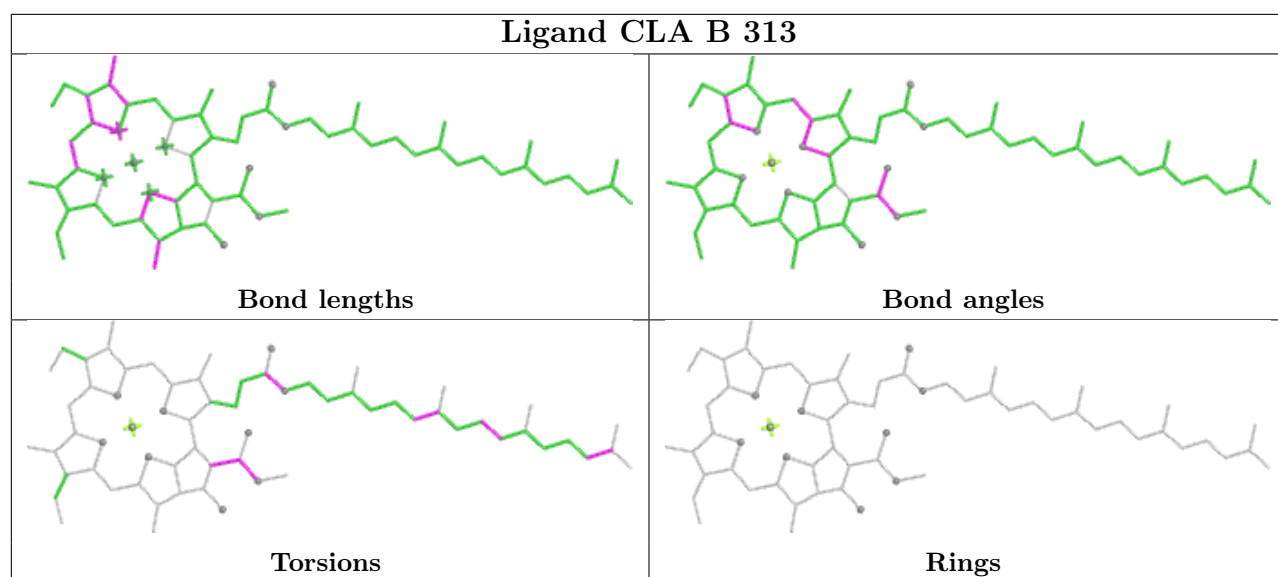


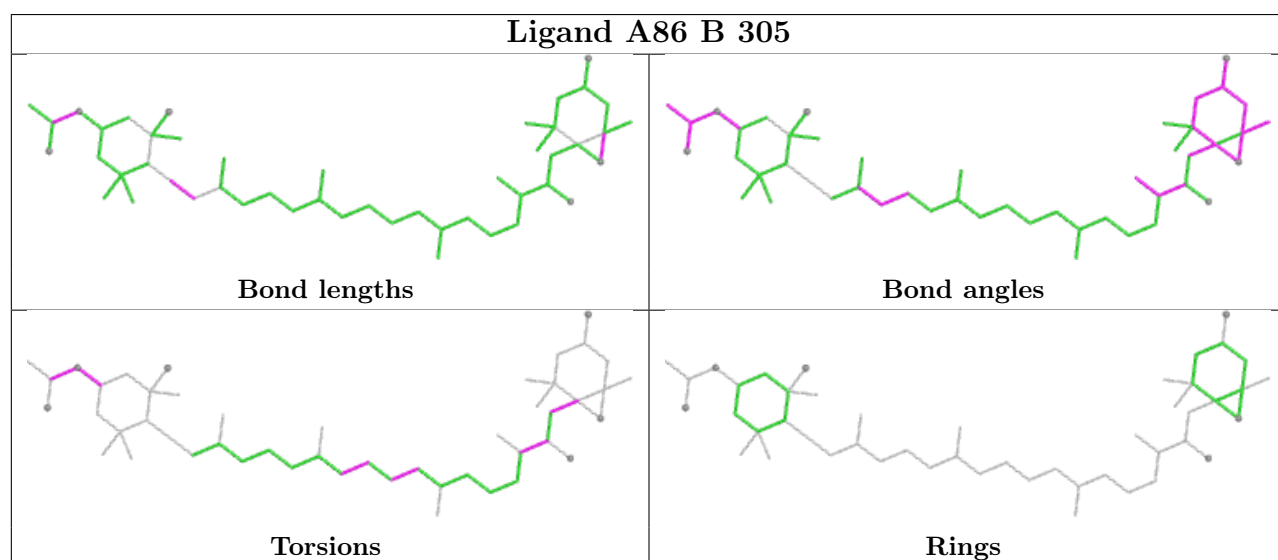
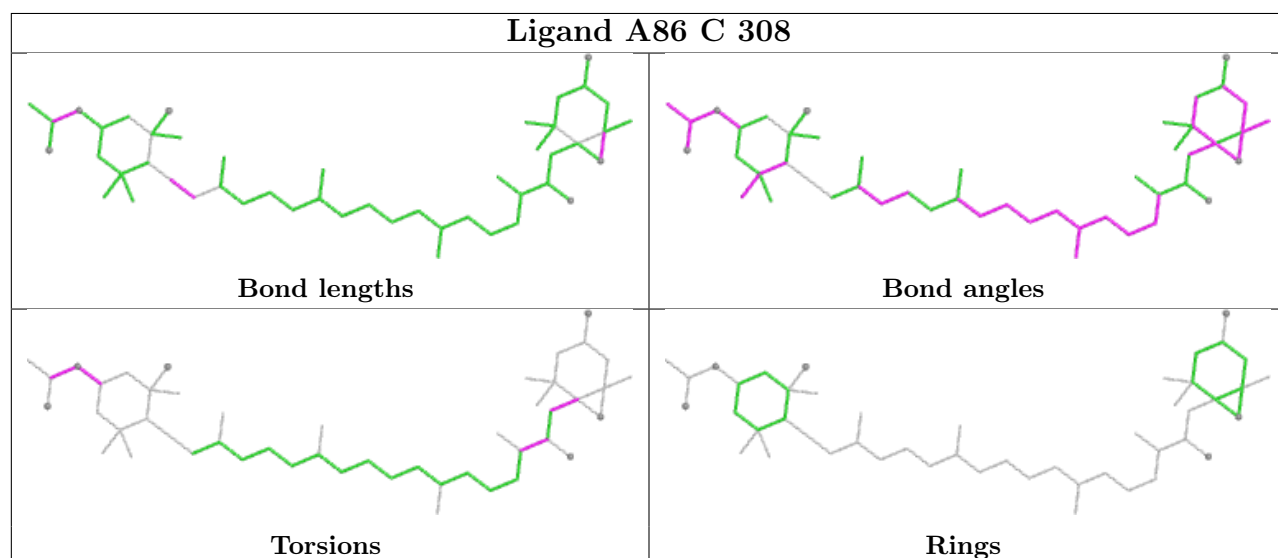
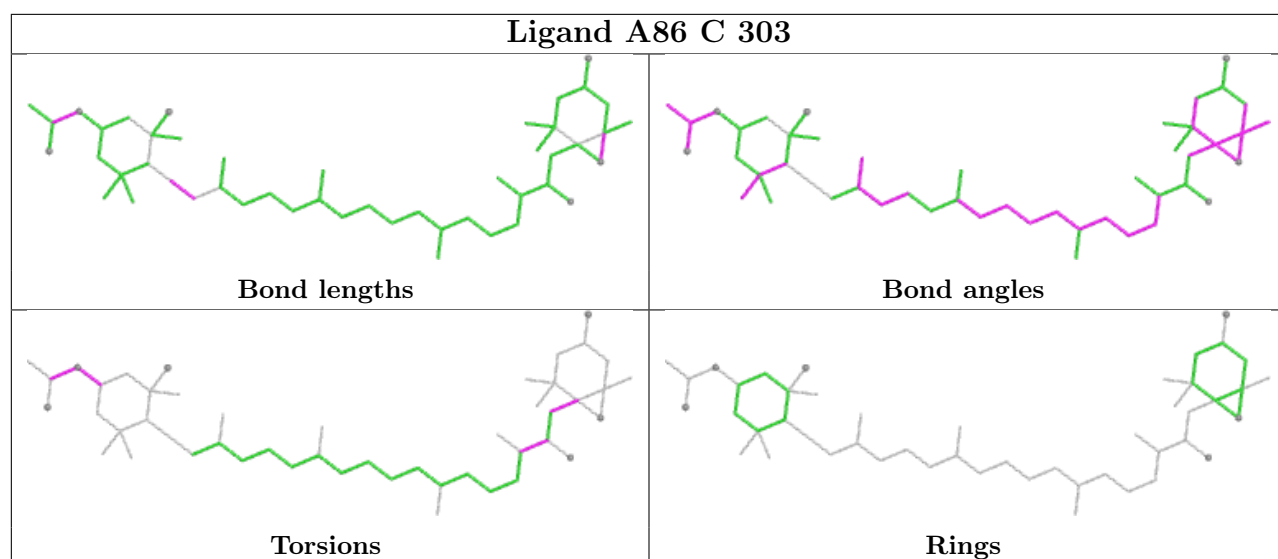




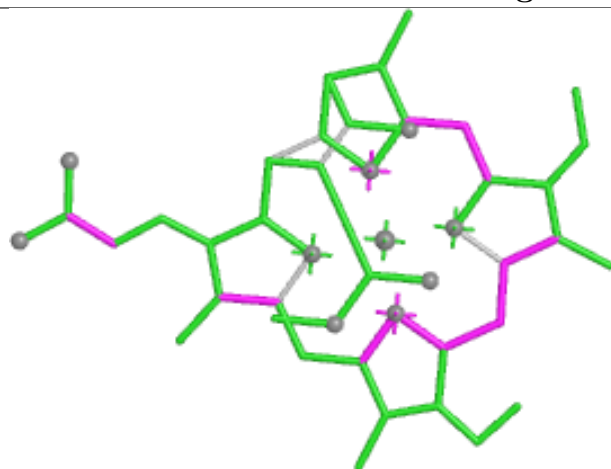




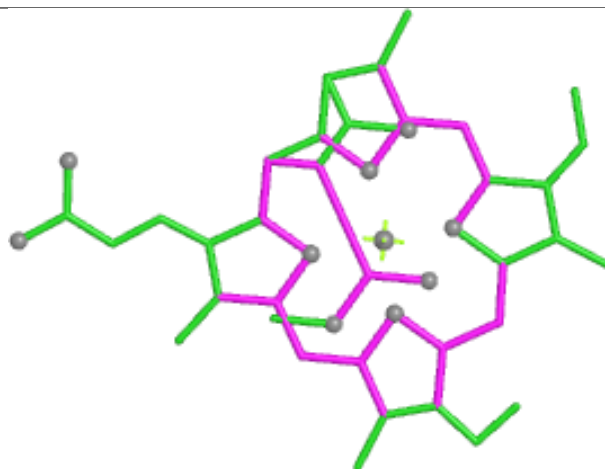




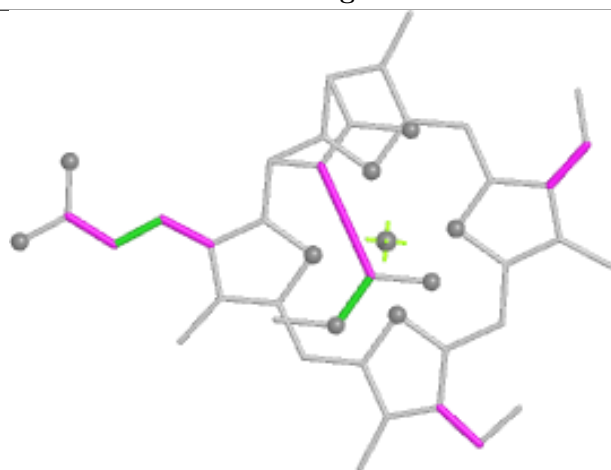
Ligand KC2 C 311



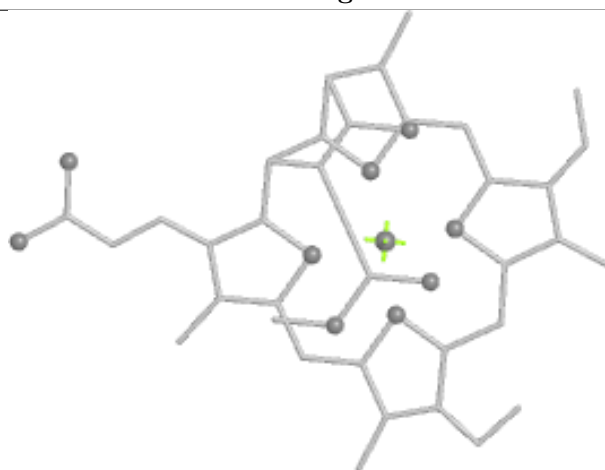
Bond lengths



Bond angles



Torsions

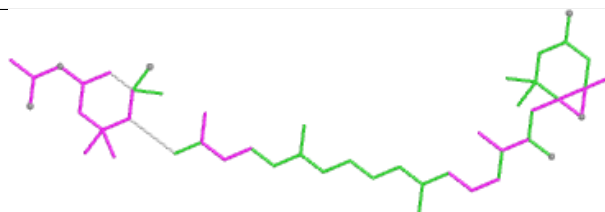


Rings

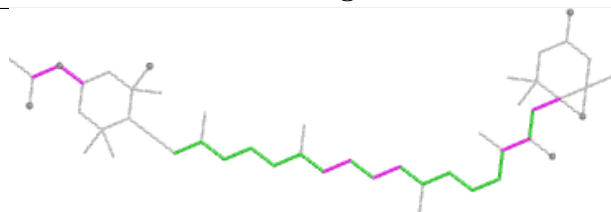
Ligand A86 C 307



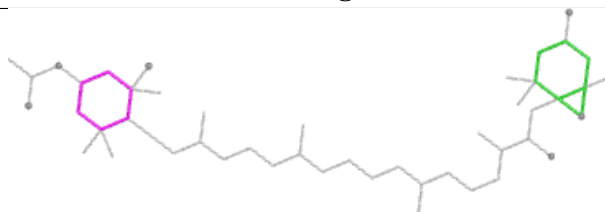
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

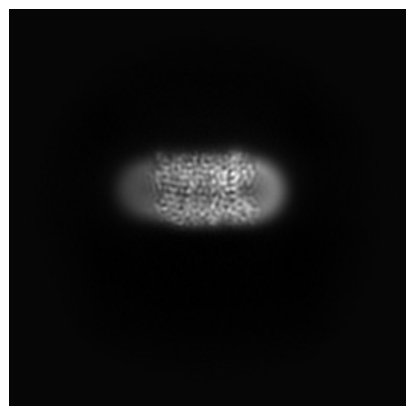
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36466. These allow visual inspection of the internal detail of the map and identification of artifacts.

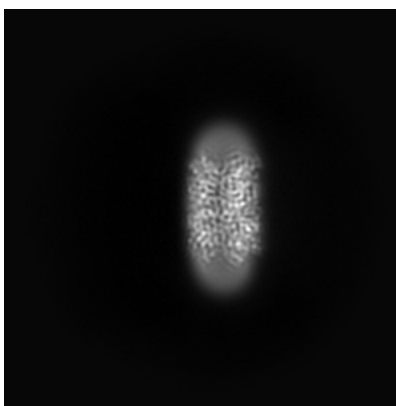
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

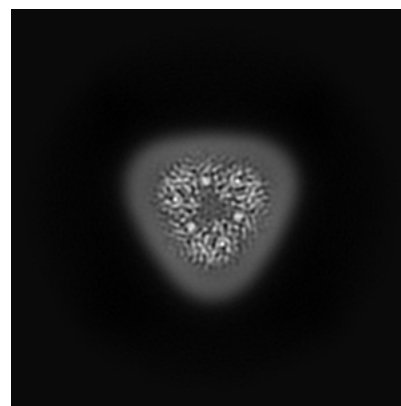
6.1.1 Primary map



X

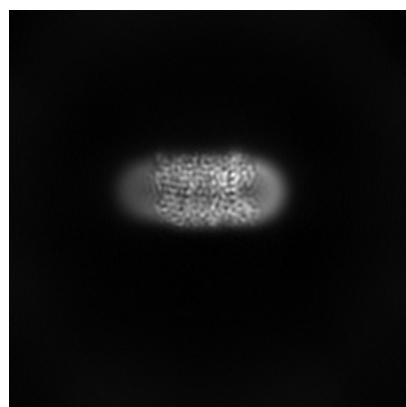


Y

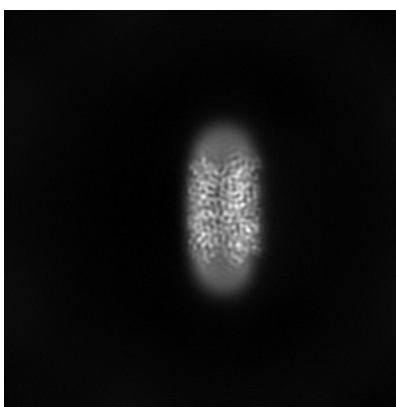


Z

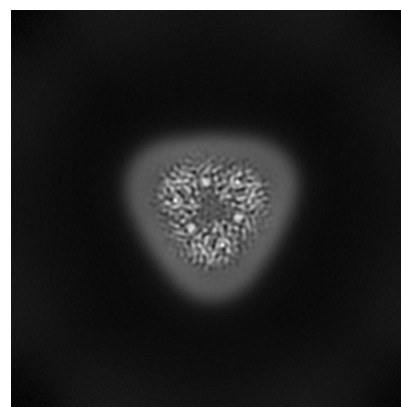
6.1.2 Raw map



X



Y

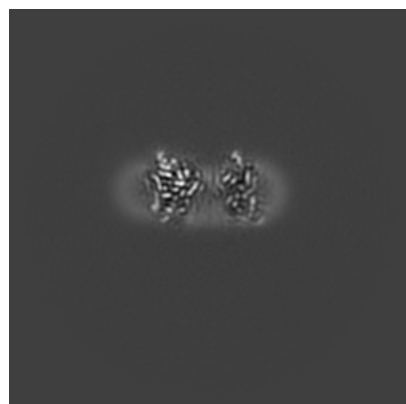


Z

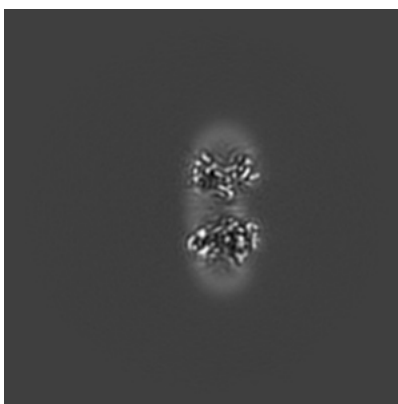
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

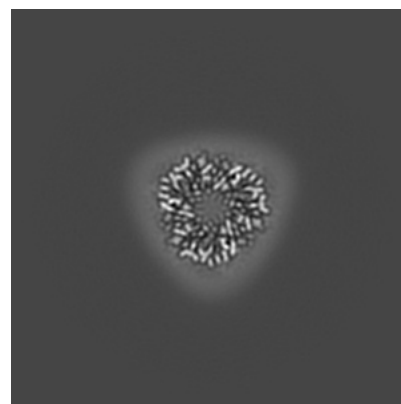
6.2.1 Primary map



X Index: 128

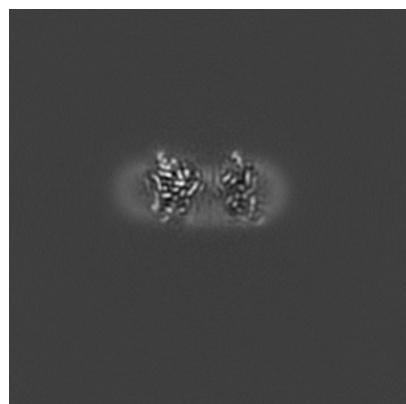


Y Index: 128

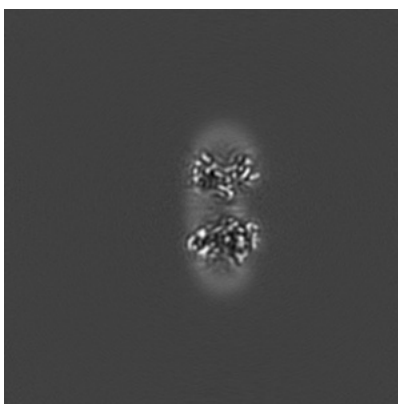


Z Index: 128

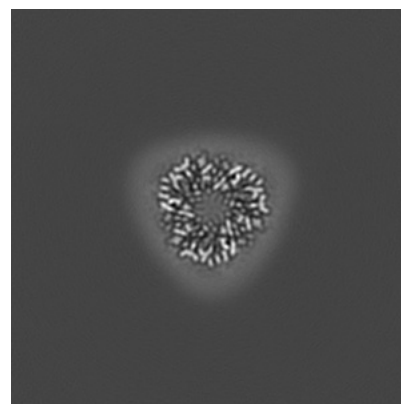
6.2.2 Raw map



X Index: 128



Y Index: 128

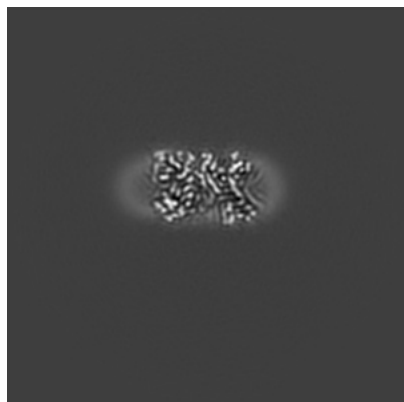


Z Index: 128

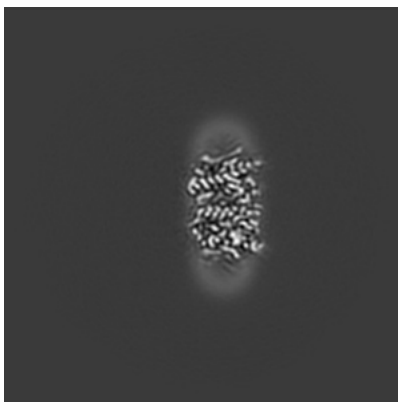
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

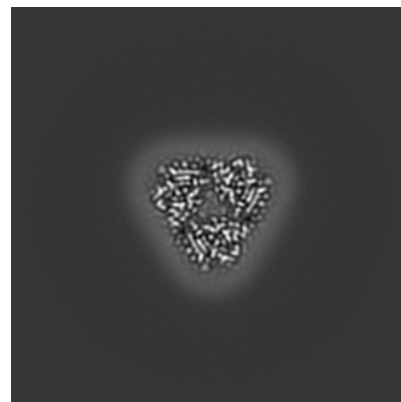
6.3.1 Primary map



X Index: 117

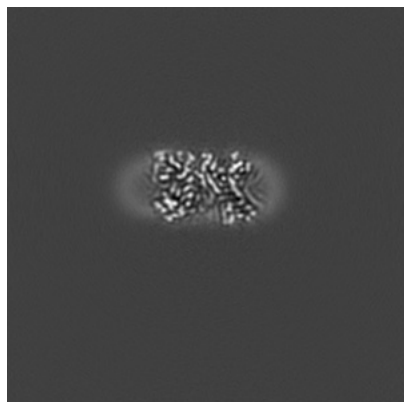


Y Index: 145

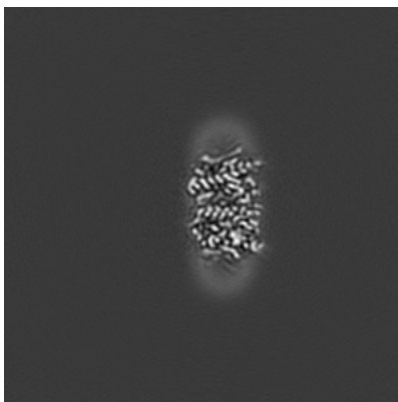


Z Index: 151

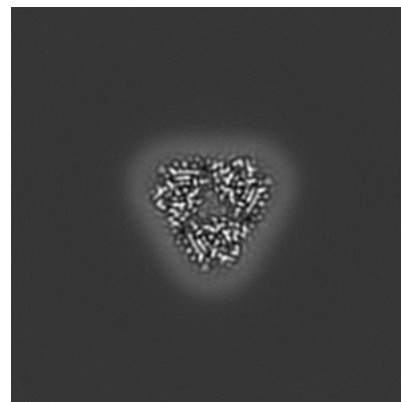
6.3.2 Raw map



X Index: 117



Y Index: 145

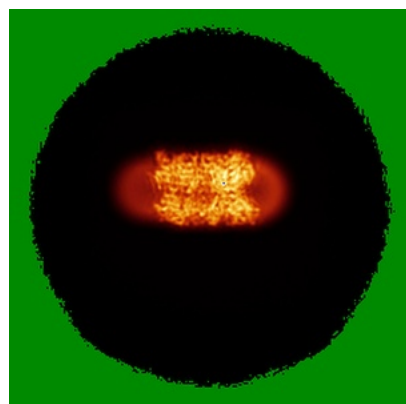


Z Index: 151

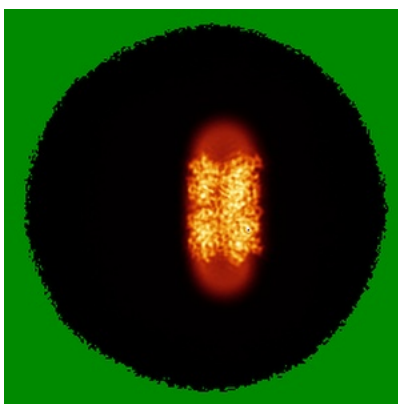
The images above show the largest variance slices of the map in three orthogonal directions.

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

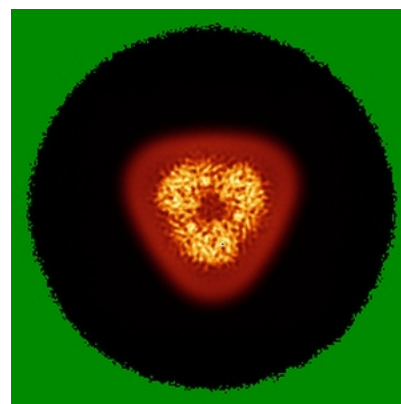
6.4.1 Primary map



X

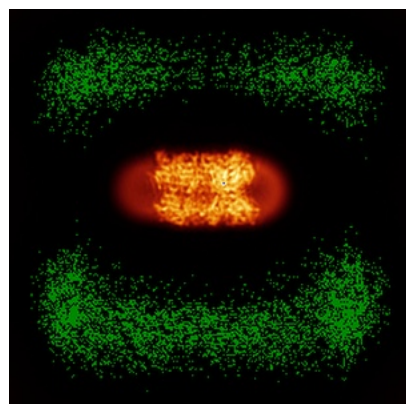


Y

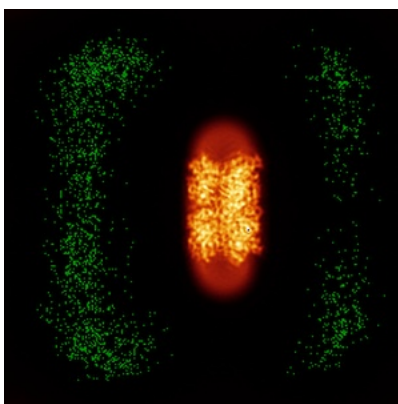


Z

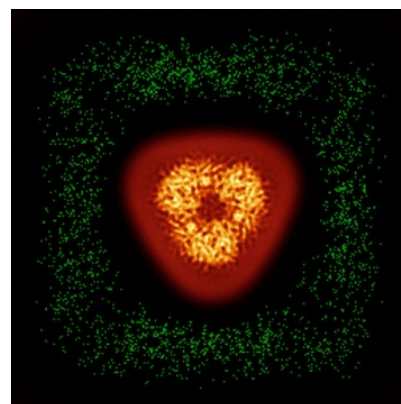
6.4.2 Raw map



X



Y

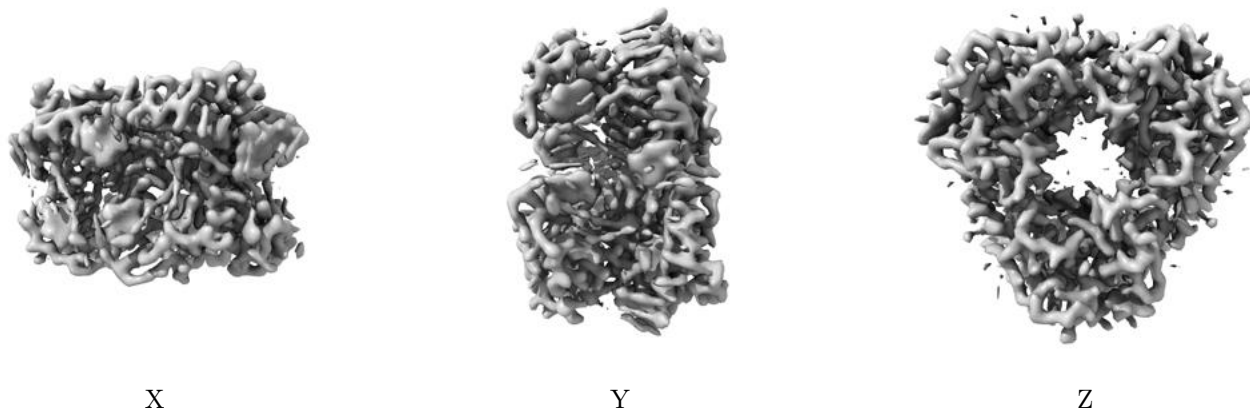


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

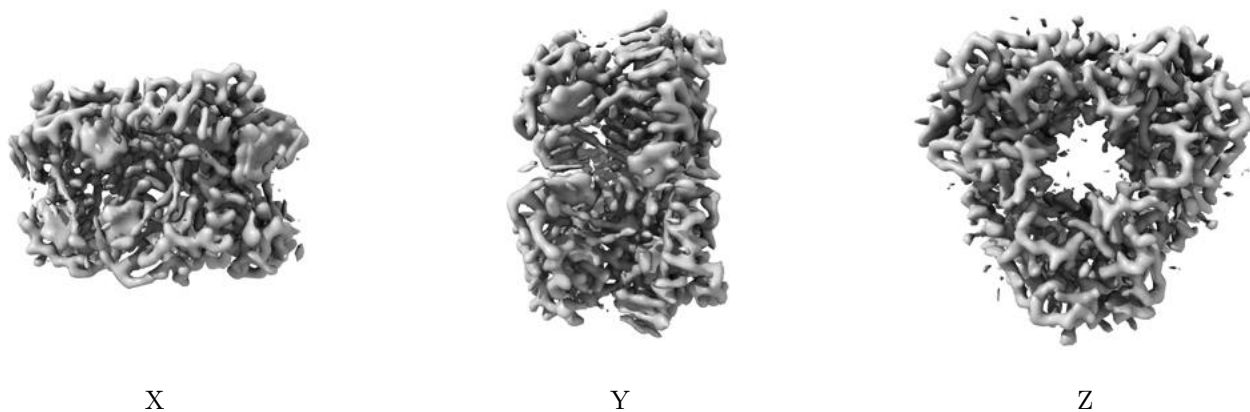
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.253. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

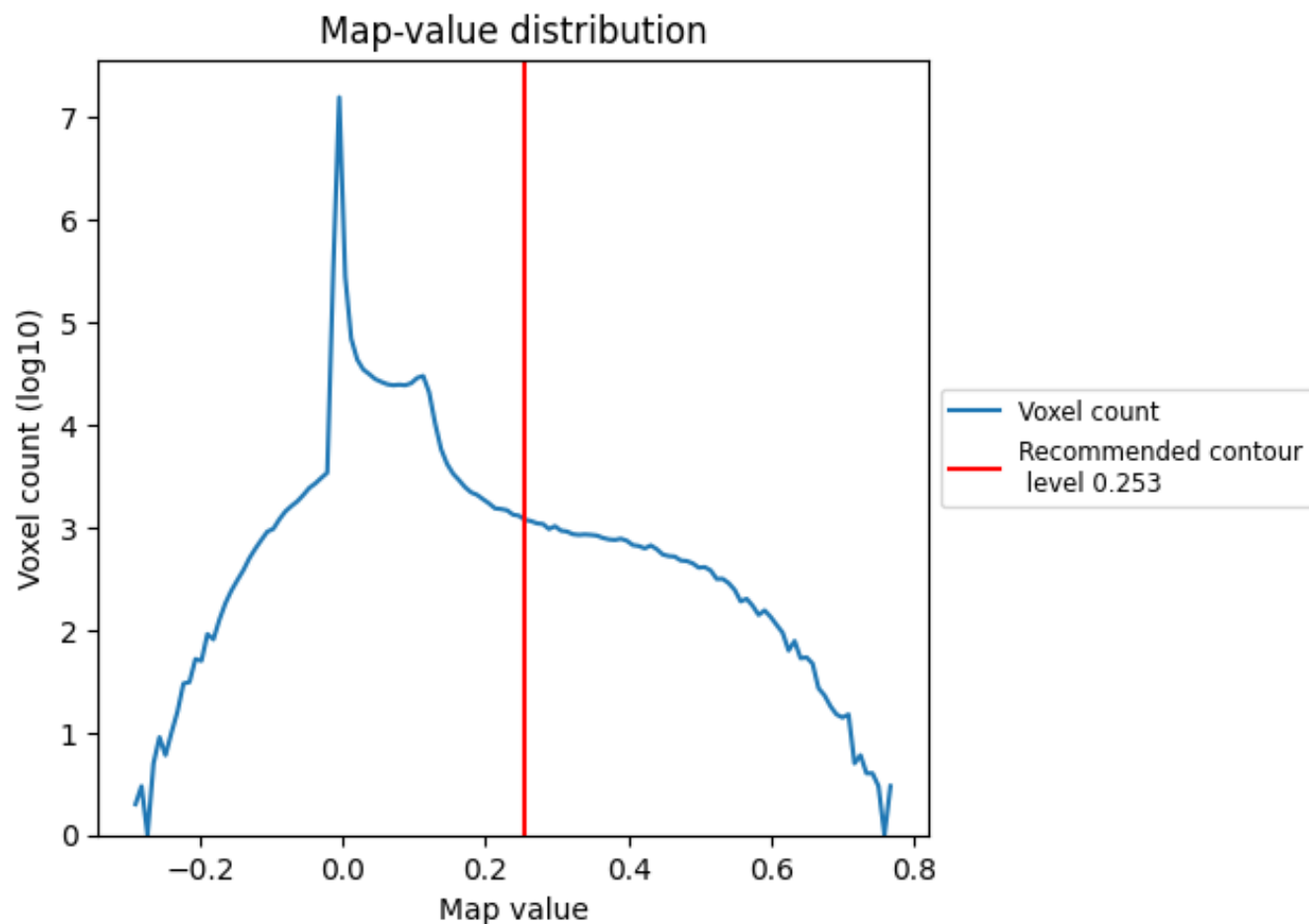
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

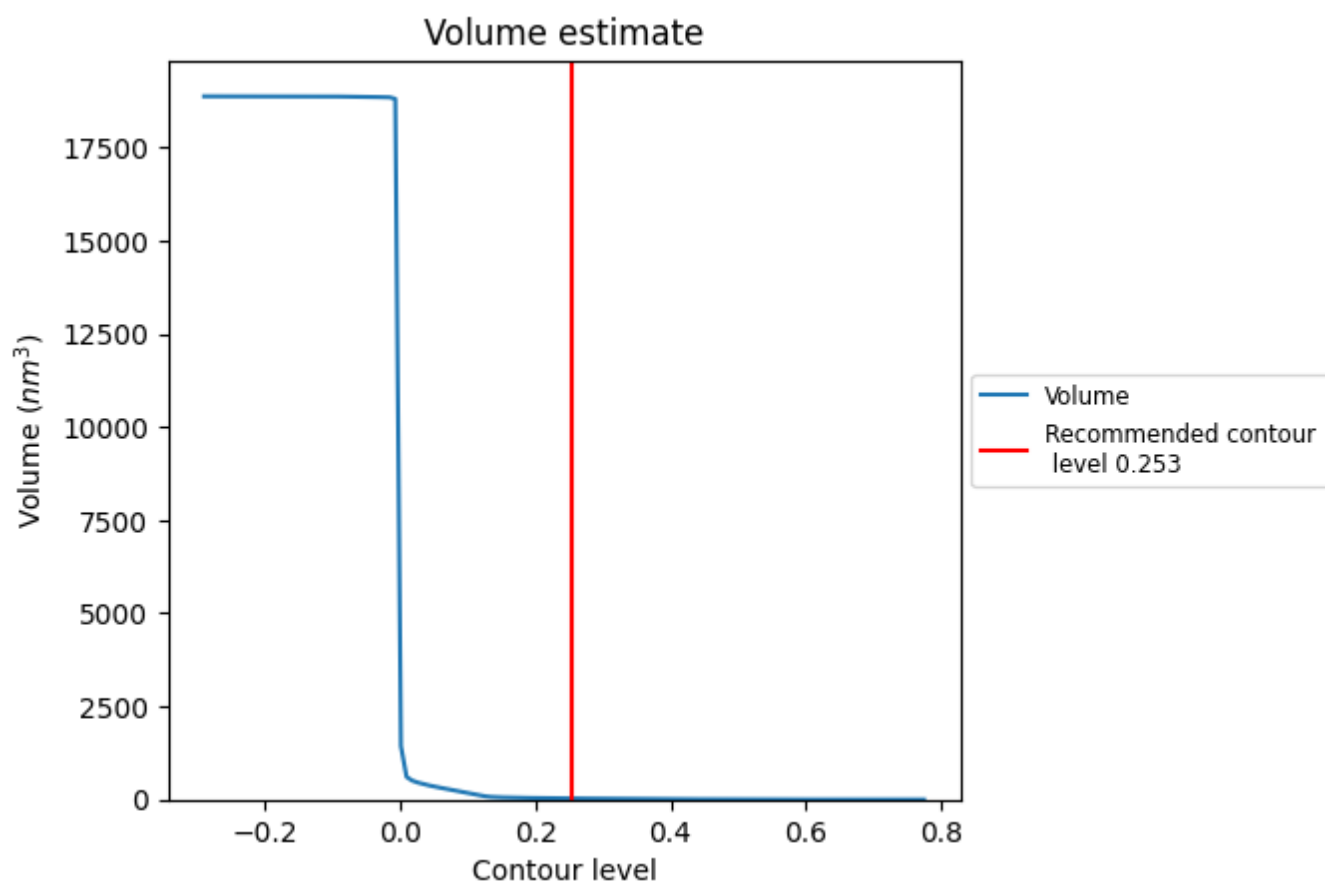
This section contains the results of statistical analysis of the map.

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.

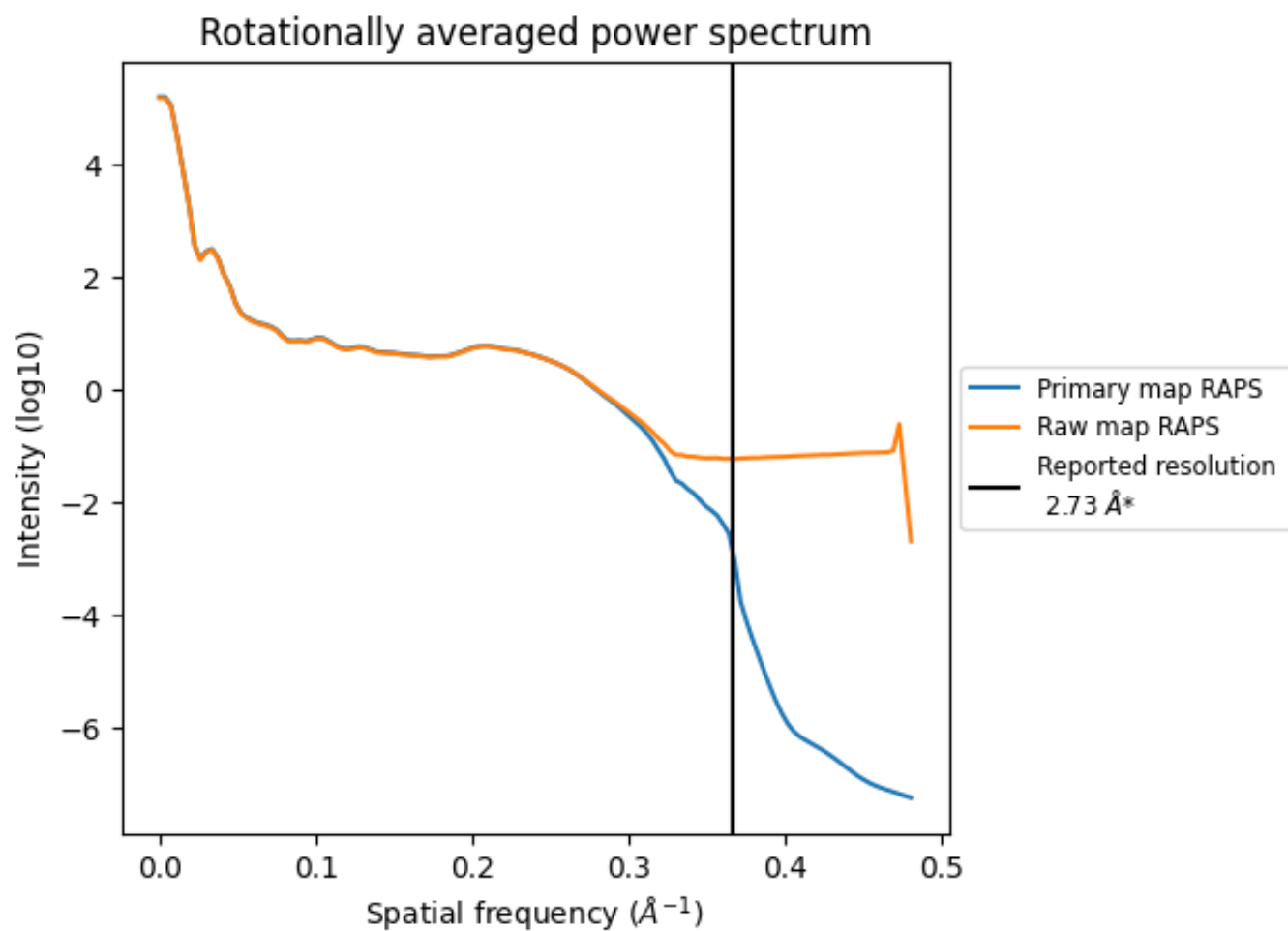
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 30 nm³; this corresponds to an approximate mass of 27 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 ⓘ

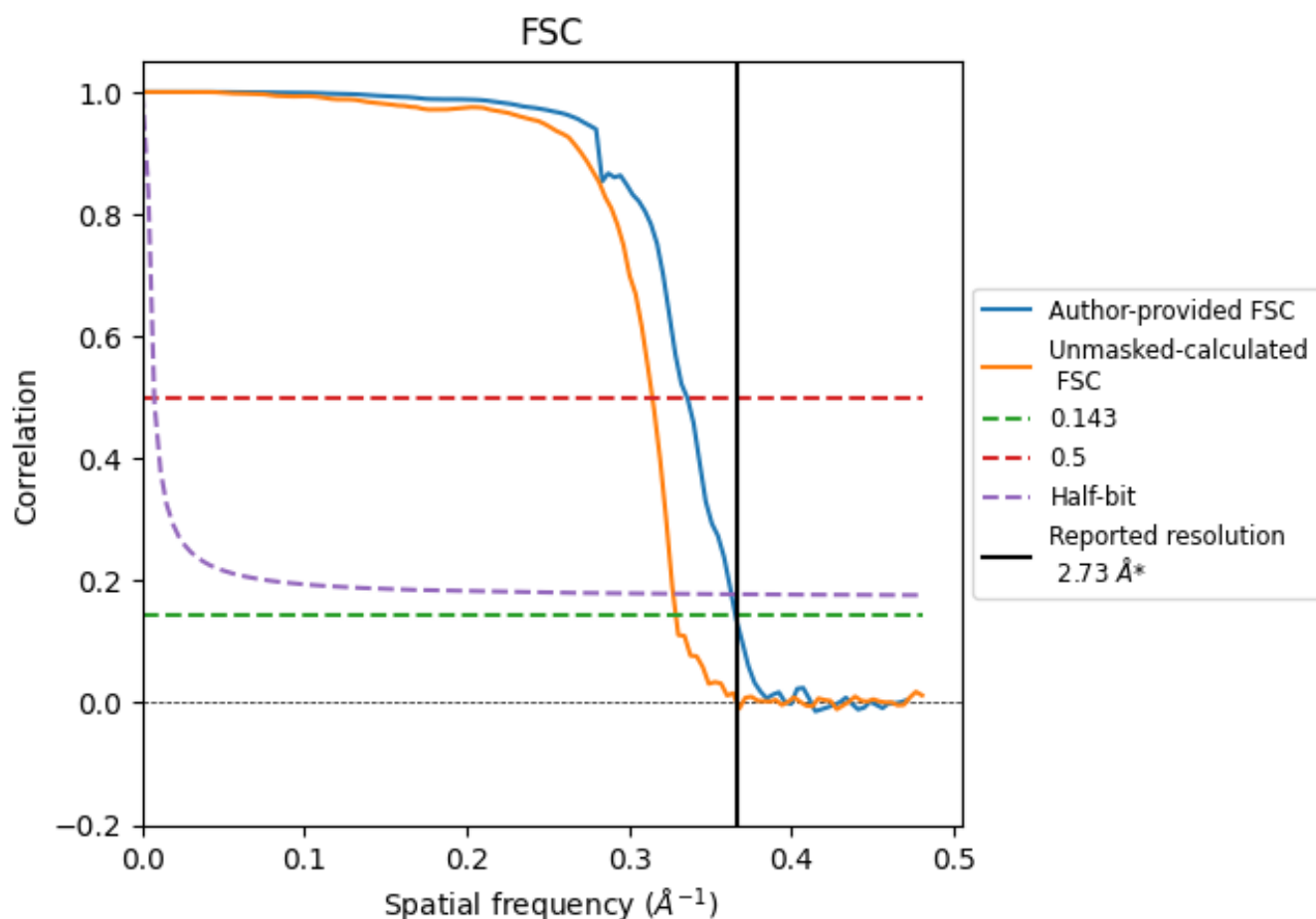


*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.366 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

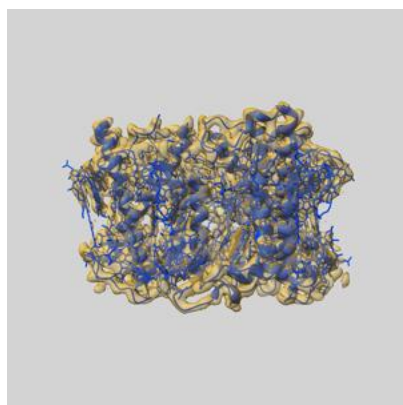
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	2.98	2.75
Unmasked-calculated*	3.04	3.18	3.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.04 differs from the reported value 2.73 by more than 10 %

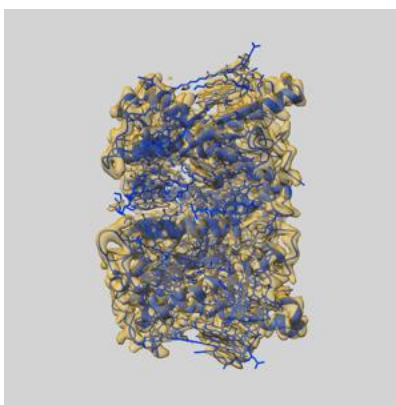
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36466 and PDB model 8JP3. Per-residue inclusion information can be found in section [3](#) on page [9](#).

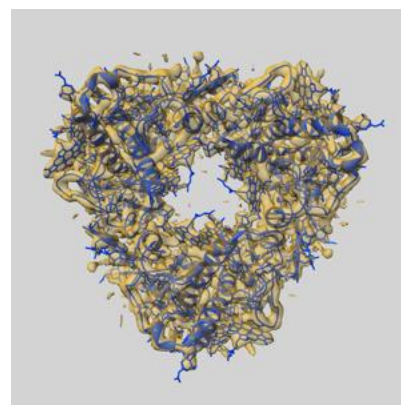
9.1 Map-model overlay [i](#)



X



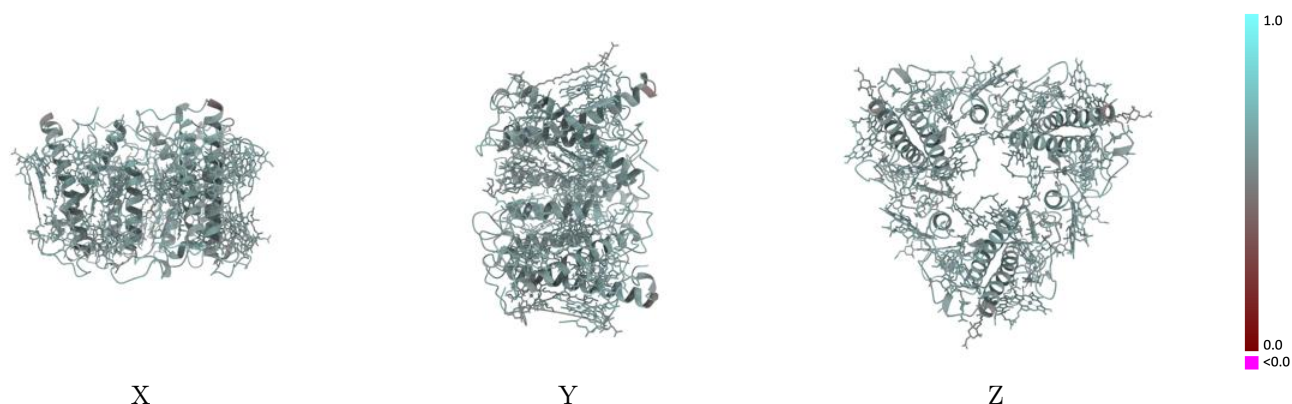
Y



Z

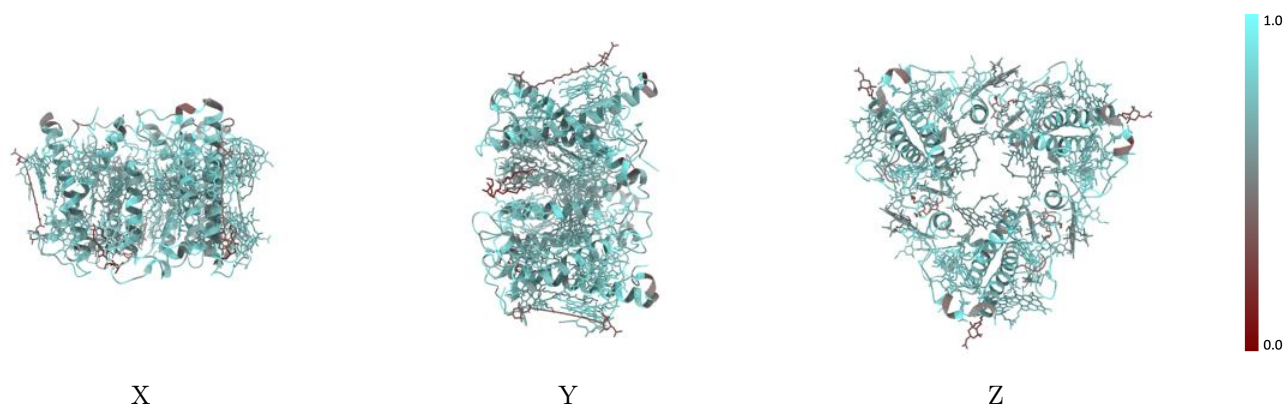
The images above show the 3D surface view of the map at the recommended contour level 0.253 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



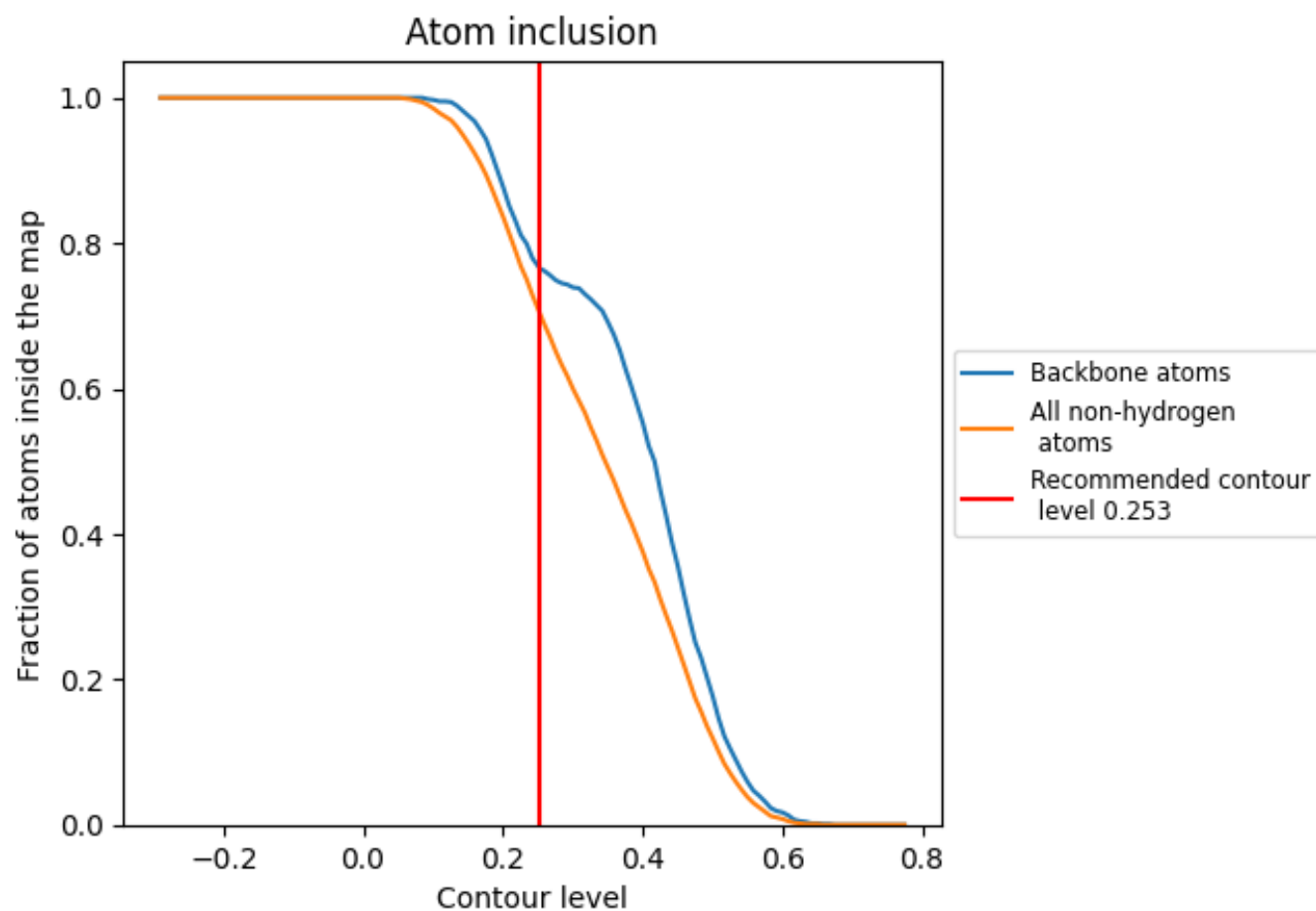
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.253).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.253) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7030	0.5750
A	0.7040	0.5750
B	0.7080	0.5760
C	0.6990	0.5750

