



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:24 AM UTC

PDB ID : 8WCK / pdb_00008wck
EMDB ID : EMD-37441
Title : FCP tetramer in Chaetoceros gracilis
Authors : Feng, Y.; Li, Z.; Zhou, C.; Shen, J.-R.; Liu, C.; Wang, W.
Deposited on : 2023-09-12
Resolution : 2.71 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

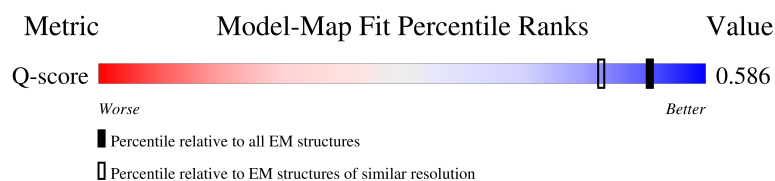
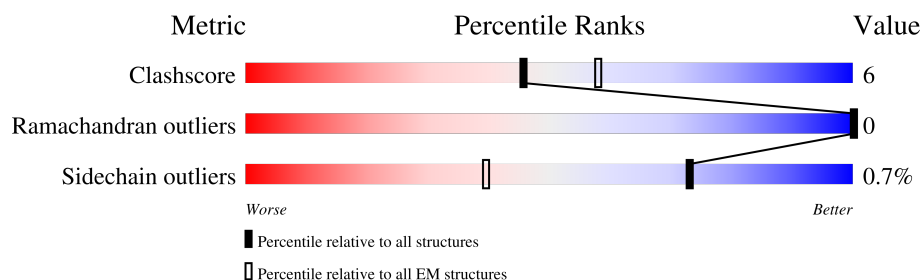
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.71 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	10297 (2.21 - 3.21)

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

Mol	Chain	Length	Quality of chain
1	1	207	
1	2	207	
1	3	207	
1	4	207	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CLA	1	307	X	-	-	-
3	CLA	1	309	X	-	-	-
3	CLA	1	312	X	-	-	-
3	CLA	1	314	X	-	-	-
3	CLA	1	315	X	-	-	-
3	CLA	1	318	X	-	-	-
3	CLA	2	401	X	-	-	-
3	CLA	2	408	X	-	-	-
3	CLA	2	409	X	-	-	-
3	CLA	2	411	X	-	-	-
3	CLA	2	414	X	-	-	-
3	CLA	2	416	X	-	-	-
3	CLA	2	417	X	-	-	-
3	CLA	3	307	X	-	-	-
3	CLA	3	308	X	-	-	-
3	CLA	3	310	X	-	-	-
3	CLA	3	313	X	-	-	-
3	CLA	3	315	X	-	-	-
3	CLA	3	316	X	-	-	-
3	CLA	4	307	X	-	-	-
3	CLA	4	309	X	-	-	-
3	CLA	4	312	X	-	-	-
3	CLA	4	314	X	-	-	-
3	CLA	4	315	X	-	-	-

2 Entry composition [i](#)

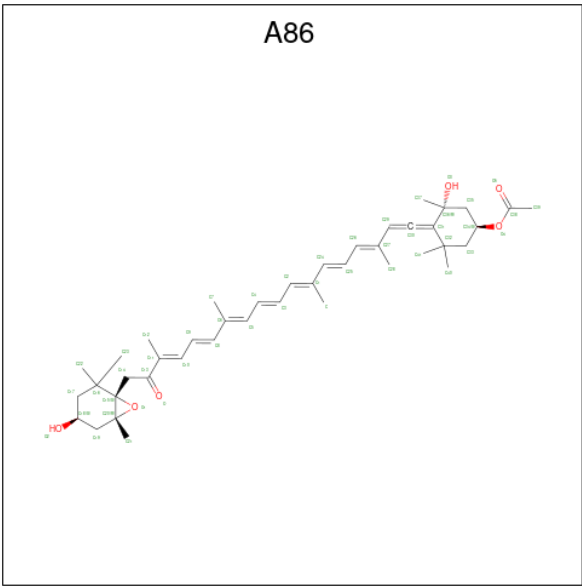
There are 6 unique types of molecules in this entry. The entry contains 8612 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	170	Total	C	N	O	S	0	0
			1307	832	221	247	7		
1	2	170	Total	C	N	O	S	0	0
			1307	832	221	247	7		
1	3	170	Total	C	N	O	S	0	0
			1307	832	221	247	7		
1	4	170	Total	C	N	O	S	0	0
			1307	832	221	247	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	1	1	Total	C	O	0
			48	42	6	
2	1	1	Total	C	O	0
			48	42	6	

Continued on next page...

Continued from previous page...

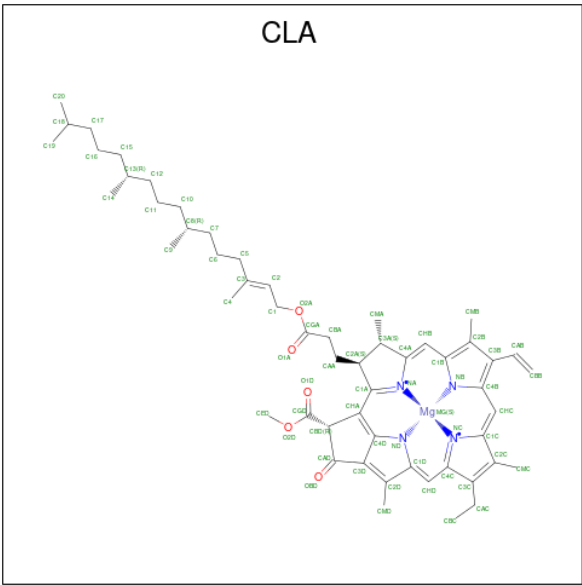
Mol	Chain	Residues	Atoms			AltConf
2	1	1	Total	C	O	0
			48	42	6	
2	1	1	Total	C	O	0
			48	42	6	
2	1	1	Total	C	O	0
			48	42	6	
2	1	1	Total	C	O	0
			48	42	6	
2	2	1	Total	C	O	0
			48	42	6	
2	2	1	Total	C	O	0
			48	42	6	
2	2	1	Total	C	O	0
			48	42	6	
2	2	1	Total	C	O	0
			48	42	6	
2	2	1	Total	C	O	0
			48	42	6	
2	2	1	Total	C	O	0
			48	42	6	
2	3	1	Total	C	O	0
			48	42	6	
2	3	1	Total	C	O	0
			48	42	6	
2	3	1	Total	C	O	0
			48	42	6	
2	3	1	Total	C	O	0
			48	42	6	
2	3	1	Total	C	O	0
			48	42	6	
2	3	1	Total	C	O	0
			48	42	6	
2	4	1	Total	C	O	0
			48	42	6	
2	4	1	Total	C	O	0
			48	42	6	
2	4	1	Total	C	O	0
			48	42	6	
2	4	1	Total	C	O	0
			48	42	6	
2	4	1	Total	C	O	0
			48	42	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
2	4	1	Total	C	O	0
			48	42	6	

- Molecule 3 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
3	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	1	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
3	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	2	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
3	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

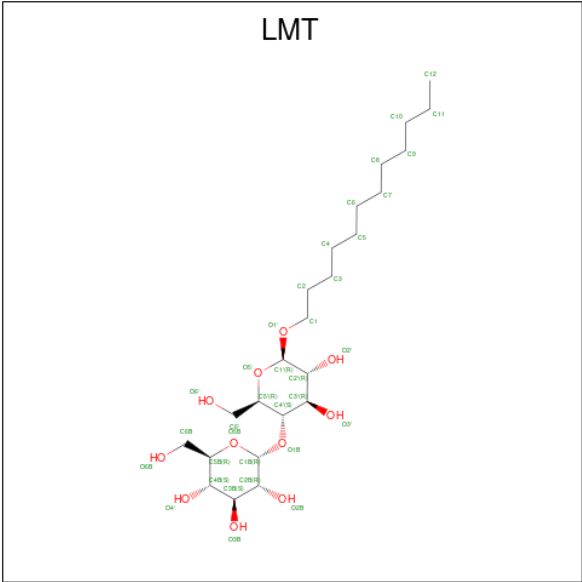
Mol	Chain	Residues	Atoms					AltConf
3	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
3	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	3	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
3	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
3	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	4	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
3	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
3	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 4 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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



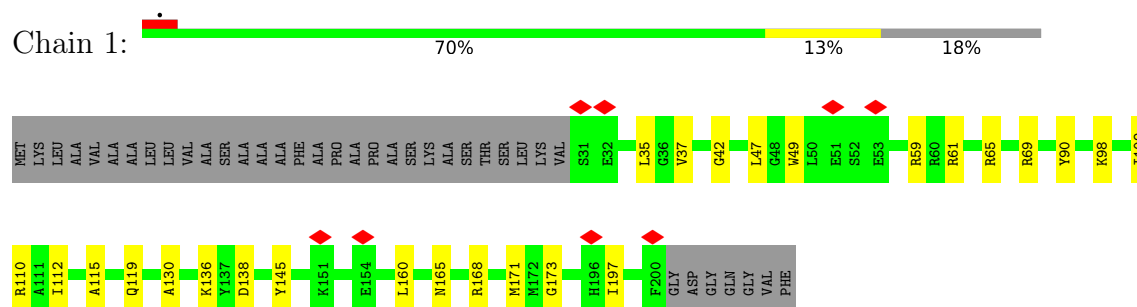


Mol	Chain	Residues	Atoms			AltConf
6	1	1	Total	C	O	0
			28	17	11	
6	1	1	Total	C	O	0
			32	21	11	
6	2	1	Total	C	O	0
			28	17	11	
6	2	1	Total	C	O	0
			32	21	11	
6	3	1	Total	C	O	0
			28	17	11	
6	3	1	Total	C	O	0
			32	21	11	
6	4	1	Total	C	O	0
			28	17	11	
6	4	1	Total	C	O	0
			32	21	11	

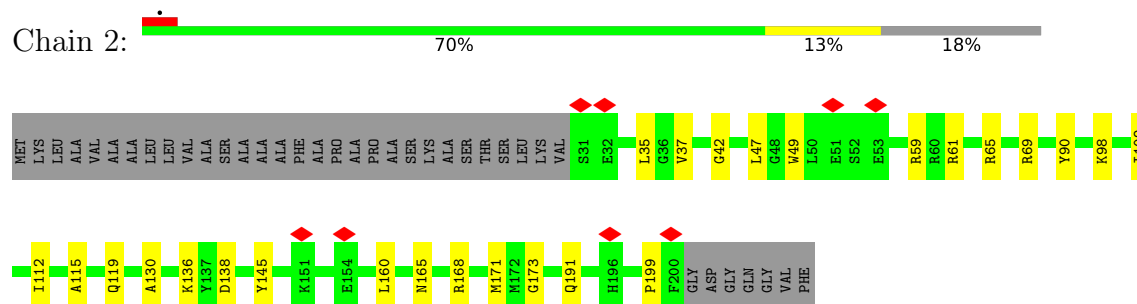
3 Residue-property plots

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

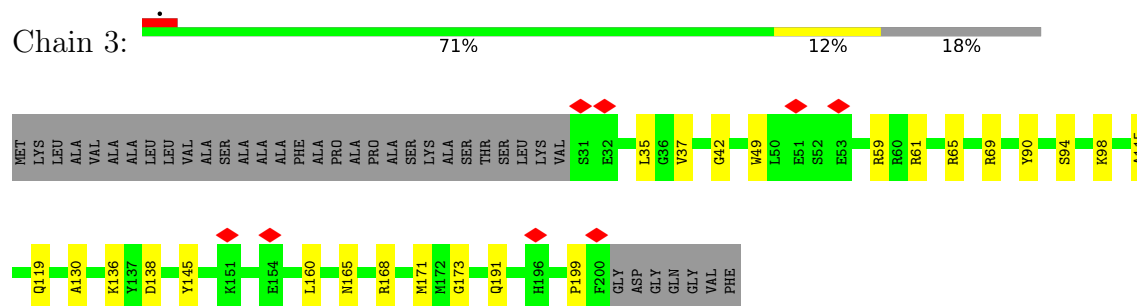
• Molecule 1: Chlorophyll a/b-binding protein



• Molecule 1: Chlorophyll a/b-binding protein

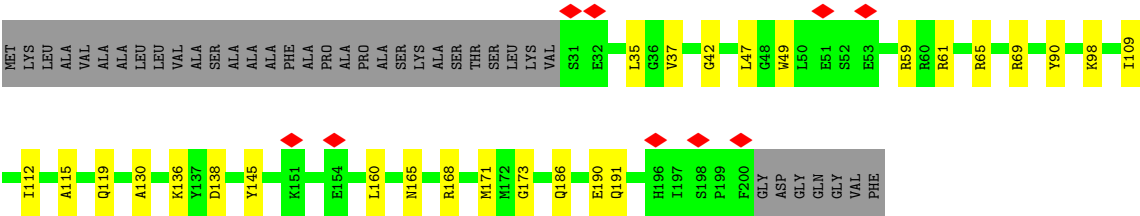


• Molecule 1: Chlorophyll a/b-binding protein



• Molecule 1: Chlorophyll a/b-binding protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	946436	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	1.174	Depositor
Minimum map value	-0.373	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, CLA, KC2, KC1, A86

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.20	0/1337	0.30	0/1813
1	2	0.20	0/1337	0.29	0/1813
1	3	0.20	0/1337	0.30	0/1813
1	4	0.20	0/1337	0.29	0/1813
All	All	0.20	0/5348	0.29	0/7252

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	1	1307	0	1276	20	0
1	2	1307	0	1276	22	0
1	3	1307	0	1276	19	0
1	4	1307	0	1276	21	0
2	1	288	0	0	2	0
2	2	288	0	0	3	0
2	3	288	0	0	2	0
2	4	288	0	0	1	0
3	1	318	0	280	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	383	0	352	16	0
3	3	318	0	280	11	0
3	4	253	0	208	8	0
4	1	90	0	0	1	0
4	2	90	0	0	1	0
4	3	90	0	0	2	0
4	4	90	0	0	1	0
5	1	90	0	0	1	0
5	2	90	0	0	1	0
5	3	90	0	0	0	0
5	4	90	0	0	1	0
6	1	60	0	64	2	0
6	2	60	0	64	1	0
6	3	60	0	64	2	0
6	4	60	0	64	1	0
All	All	8612	0	6480	94	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 6.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:165:ASN:ND2	3:2:401:CLA:O1D	2.34	0.61
3:1:318:CLA:O1D	1:4:165:ASN:ND2	2.34	0.60
1:2:165:ASN:ND2	3:2:408:CLA:O1D	2.34	0.60
1:3:165:ASN:ND2	3:3:307:CLA:O1D	2.34	0.58
2:2:405:A86:C24	3:2:414:CLA:HAB	2.34	0.58
2:3:304:A86:C24	3:3:313:CLA:HAB	2.34	0.58
2:4:304:A86:C24	3:4:312:CLA:HAB	2.34	0.58
2:1:304:A86:C24	3:1:312:CLA:HAB	2.34	0.57
1:1:110:ARG:NH2	3:1:315:CLA:O1D	2.38	0.56
1:1:168:ARG:HA	1:1:171:MET:HE3	1.89	0.55
1:2:168:ARG:HA	1:2:171:MET:HE3	1.89	0.55
1:3:168:ARG:HA	1:3:171:MET:HE3	1.89	0.54
1:4:168:ARG:HA	1:4:171:MET:HE3	1.89	0.53
1:2:145:TYR:HB2	3:2:414:CLA:HAA1	1.91	0.53
1:1:145:TYR:HB2	3:1:312:CLA:HAA1	1.91	0.52
1:3:145:TYR:HB2	3:3:313:CLA:H3A	1.92	0.52
1:4:115:ALA:O	1:4:119:GLN:HG3	2.10	0.51
1:3:115:ALA:O	1:3:119:GLN:HG3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:112:ILE:HD11	3:2:411:CLA:H3A	1.93	0.51
1:3:145:TYR:HB2	3:3:313:CLA:HAA1	1.91	0.51
1:1:115:ALA:O	1:1:119:GLN:HG3	2.10	0.51
1:1:112:ILE:HD11	3:1:309:CLA:H3A	1.93	0.50
1:2:115:ALA:O	1:2:119:GLN:HG3	2.11	0.50
1:4:145:TYR:HB2	3:4:312:CLA:HAA1	1.93	0.50
1:1:145:TYR:HB2	3:1:312:CLA:H3A	1.93	0.49
1:2:145:TYR:HB2	3:2:414:CLA:H3A	1.95	0.49
1:4:112:ILE:HD11	3:4:309:CLA:H3A	1.94	0.49
1:1:109:ILE:HD12	1:1:112:ILE:HD12	1.96	0.47
1:4:90:TYR:HA	1:4:98:LYS:HA	1.97	0.47
1:2:90:TYR:HA	1:2:98:LYS:HA	1.98	0.46
1:3:59:ARG:NH1	4:3:309:KC2:O2A	2.48	0.46
1:1:173:GLY:HA2	3:1:314:CLA:HBB1	1.97	0.46
6:3:318:LMT:O6B	6:3:318:LMT:O4'	2.31	0.46
1:2:173:GLY:HA2	3:2:416:CLA:HBB1	1.98	0.46
1:3:173:GLY:HA2	3:3:315:CLA:HBB1	1.98	0.46
1:1:59:ARG:NH1	4:1:308:KC2:O2A	2.48	0.46
1:4:173:GLY:HA2	3:4:314:CLA:HBB1	1.98	0.45
3:1:318:CLA:H93	3:1:318:CLA:H111	1.72	0.45
1:2:59:ARG:NH1	4:2:410:KC2:O2A	2.49	0.45
1:4:191:GLN:NE2	3:4:314:CLA:O1D	2.50	0.45
1:1:90:TYR:HA	1:1:98:LYS:HA	1.99	0.45
1:2:145:TYR:OH	5:2:415:KC1:O1A	2.31	0.44
1:4:59:ARG:NH1	4:4:308:KC2:O2A	2.49	0.44
1:3:35:LEU:HD11	1:3:160:LEU:HD13	1.99	0.44
1:1:136:LYS:HG2	1:1:138:ASP:OD1	2.18	0.44
6:1:317:LMT:O6B	6:1:317:LMT:O4'	2.31	0.44
1:4:61:ARG:NH2	3:4:307:CLA:O1D	2.51	0.44
1:2:109:ILE:HD12	1:2:112:ILE:HD12	1.99	0.44
1:3:90:TYR:HA	1:3:98:LYS:HA	2.00	0.44
1:4:109:ILE:HD12	1:4:112:ILE:HD12	1.99	0.44
1:1:61:ARG:NH2	3:1:307:CLA:O1D	2.51	0.43
1:1:35:LEU:HD11	1:1:160:LEU:HD13	2.00	0.43
1:1:145:TYR:OH	5:1:313:KC1:O1A	2.28	0.43
1:4:35:LEU:HD11	1:4:160:LEU:HD13	1.99	0.43
1:2:35:LEU:HD11	1:2:160:LEU:HD13	1.99	0.43
1:4:65:ARG:HD3	1:4:69:ARG:NH2	2.34	0.43
1:2:136:LYS:HG2	1:2:138:ASP:OD1	2.19	0.43
1:3:65:ARG:HD3	1:3:69:ARG:NH2	2.33	0.43
1:1:65:ARG:HD3	1:1:69:ARG:NH2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:136:LYS:HG2	1:3:138:ASP:OD1	2.19	0.43
3:2:408:CLA:H93	3:2:408:CLA:H111	1.72	0.43
1:2:37:VAL:HG13	1:2:42:GLY:C	2.44	0.42
1:2:61:ARG:NH2	3:2:409:CLA:O1D	2.51	0.42
1:2:65:ARG:HD3	1:2:69:ARG:NH2	2.33	0.42
1:1:49:TRP:HZ3	3:1:307:CLA:H42	1.84	0.42
1:3:49:TRP:HZ3	3:3:308:CLA:H42	1.84	0.42
1:3:37:VAL:HG13	1:3:42:GLY:C	2.45	0.42
2:1:305:A86:O	3:1:315:CLA:HAA2	2.19	0.42
1:4:49:TRP:HZ3	3:4:307:CLA:H42	1.84	0.42
1:4:136:LYS:HG2	1:4:138:ASP:OD1	2.19	0.42
1:4:145:TYR:OH	5:4:313:KC1:O1A	2.31	0.42
1:2:49:TRP:HZ3	3:2:409:CLA:H42	1.84	0.42
1:4:37:VAL:HG13	1:4:42:GLY:C	2.45	0.42
1:3:61:ARG:NH2	3:3:308:CLA:O1D	2.53	0.41
1:1:59:ARG:HD2	6:1:317:LMT:H3B	2.02	0.41
1:3:94:SER:OG	4:3:311:KC2:O2A	2.29	0.41
3:2:408:CLA:C2B	1:3:130:ALA:HB1	2.50	0.41
2:3:305:A86:O	3:3:316:CLA:HAA2	2.20	0.41
1:4:186:GLN:HB3	1:4:190:GLU:HB2	2.02	0.41
1:2:130:ALA:HB1	3:2:401:CLA:C2B	2.51	0.41
1:1:130:ALA:HB1	3:1:318:CLA:C2B	2.50	0.41
1:2:90:TYR:O	2:2:403:A86:O3	2.37	0.41
1:3:199:PRO:HD3	3:3:315:CLA:HAA1	2.01	0.41
1:2:199:PRO:HD3	3:2:416:CLA:HAA1	2.02	0.41
1:3:191:GLN:NE2	3:3:315:CLA:O1D	2.51	0.41
1:2:59:ARG:HD2	6:2:419:LMT:H3B	2.02	0.41
3:2:401:CLA:H93	3:2:401:CLA:H111	1.72	0.41
1:2:191:GLN:NE2	3:2:416:CLA:O1D	2.51	0.40
1:4:59:ARG:HD2	6:4:317:LMT:H3B	2.02	0.40
1:4:168:ARG:HB3	3:4:307:CLA:CAC	2.52	0.40
2:2:402:A86:O	3:2:408:CLA:HAC2	2.22	0.40
1:3:59:ARG:HD2	6:3:318:LMT:H3B	2.02	0.40
3:3:307:CLA:C2B	1:4:130:ALA:HB1	2.51	0.40
1:1:37:VAL:HG13	1:1:42:GLY:C	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	168/207 (81%)	165 (98%)	3 (2%)	0	100	100
1	2	168/207 (81%)	165 (98%)	3 (2%)	0	100	100
1	3	168/207 (81%)	165 (98%)	3 (2%)	0	100	100
1	4	168/207 (81%)	165 (98%)	3 (2%)	0	100	100
All	All	672/828 (81%)	660 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	135/158 (85%)	133 (98%)	2 (2%)	57	79
1	2	135/158 (85%)	134 (99%)	1 (1%)	76	89
1	3	135/158 (85%)	135 (100%)	0	100	100
1	4	135/158 (85%)	134 (99%)	1 (1%)	76	89
All	All	540/632 (85%)	536 (99%)	4 (1%)	73	89

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

Mol	Chain	Res	Type
1	1	47	LEU
1	1	197	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	47	LEU
1	4	47	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	166	ASN
1	2	95	ASN
1	3	166	ASN
1	4	166	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

72 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A86	2	407	-	47,50,50	1.56	6 (12%)	51,76,76	3.44	17 (33%)
3	CLA	1	314	-	50,54,73	1.33	8 (16%)	59,90,113	1.38	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLA	4	312	1	51,55,73	1.34	9 (17%)	60,91,113	1.45	6 (10%)
2	A86	4	305	-	47,50,50	1.47	5 (10%)	51,76,76	3.49	15 (29%)
3	CLA	1	318	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	6 (7%)
3	CLA	1	312	1	51,55,73	1.34	8 (15%)	60,91,113	1.44	6 (10%)
2	A86	3	304	-	47,50,50	1.45	6 (12%)	51,76,76	5.04	19 (37%)
2	A86	4	306	-	47,50,50	1.55	6 (12%)	51,76,76	3.30	16 (31%)
4	KC2	2	410	-	49,53,53	1.75	12 (24%)	60,89,89	1.93	16 (26%)
6	LMT	1	316	-	29,29,36	1.27	5 (17%)	40,40,47	1.07	3 (7%)
2	A86	1	306	-	47,50,50	1.59	6 (12%)	51,76,76	3.12	18 (35%)
2	A86	2	402	-	47,50,50	1.46	6 (12%)	51,76,76	3.66	17 (33%)
2	A86	1	304	-	47,50,50	1.45	6 (12%)	51,76,76	5.05	19 (37%)
2	A86	4	302	-	47,50,50	1.48	7 (14%)	51,76,76	4.30	16 (31%)
4	KC2	4	310	-	49,53,53	1.76	10 (20%)	60,89,89	1.90	15 (25%)
5	KC1	2	415	1	49,53,53	1.40	6 (12%)	61,89,89	1.73	12 (19%)
5	KC1	3	312	1	49,53,53	1.43	7 (14%)	61,89,89	1.74	13 (21%)
6	LMT	4	317	-	33,33,36	1.19	5 (15%)	44,44,47	1.00	2 (4%)
2	A86	1	303	-	47,50,50	1.51	6 (12%)	51,76,76	4.94	16 (31%)
4	KC2	4	308	-	49,53,53	1.75	11 (22%)	60,89,89	1.93	16 (26%)
5	KC1	4	311	1	49,53,53	1.42	7 (14%)	61,89,89	1.74	13 (21%)
3	CLA	4	307	1	63,67,73	1.20	9 (14%)	74,105,113	1.34	7 (9%)
5	KC1	1	311	1	49,53,53	1.42	7 (14%)	61,89,89	1.75	13 (21%)
6	LMT	2	418	-	29,29,36	1.28	5 (17%)	40,40,47	1.06	3 (7%)
3	CLA	1	307	1	63,67,73	1.20	9 (14%)	74,105,113	1.35	7 (9%)
3	CLA	3	307	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	6 (7%)
2	A86	4	303	-	47,50,50	1.50	6 (12%)	51,76,76	4.93	17 (33%)
3	CLA	2	414	1	51,55,73	1.35	9 (17%)	60,91,113	1.45	6 (10%)
2	A86	2	406	-	47,50,50	1.47	5 (10%)	51,76,76	3.49	15 (29%)
6	LMT	3	318	-	33,33,36	1.19	5 (15%)	44,44,47	1.00	2 (4%)
3	CLA	3	308	1	63,67,73	1.20	9 (14%)	74,105,113	1.35	7 (9%)
6	LMT	4	316	-	29,29,36	1.29	5 (17%)	40,40,47	1.07	3 (7%)
6	LMT	1	317	-	33,33,36	1.19	5 (15%)	44,44,47	1.01	2 (4%)
6	LMT	2	419	-	33,33,36	1.20	5 (15%)	44,44,47	1.00	2 (4%)
2	A86	3	301	-	47,50,50	1.46	6 (12%)	51,76,76	3.67	17 (33%)
3	CLA	3	313	1	51,55,73	1.34	8 (15%)	60,91,113	1.44	6 (10%)
5	KC1	3	314	-	49,53,53	1.40	6 (12%)	61,89,89	1.72	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A86	2	403	-	47,50,50	1.47	7 (14%)	51,76,76	4.21	16 (31%)
3	CLA	4	309	-	59,63,73	1.25	9 (15%)	70,101,113	1.35	6 (8%)
3	CLA	2	416	-	50,54,73	1.34	8 (16%)	59,90,113	1.39	4 (6%)
3	CLA	2	401	-	69,73,73	1.15	8 (11%)	82,113,113	1.32	6 (7%)
3	CLA	4	315	-	50,54,73	1.37	8 (16%)	59,90,113	1.36	4 (6%)
2	A86	1	305	-	47,50,50	1.46	5 (10%)	51,76,76	3.37	15 (29%)
2	A86	4	301	-	47,50,50	1.46	6 (12%)	51,76,76	3.66	17 (33%)
3	CLA	1	315	-	50,54,73	1.37	7 (14%)	59,90,113	1.36	4 (6%)
2	A86	4	304	-	47,50,50	1.45	6 (12%)	51,76,76	5.05	19 (37%)
3	CLA	3	316	-	50,54,73	1.37	8 (16%)	59,90,113	1.36	4 (6%)
3	CLA	1	309	-	59,63,73	1.25	9 (15%)	70,101,113	1.34	6 (8%)
3	CLA	4	314	-	50,54,73	1.34	8 (16%)	59,90,113	1.38	4 (6%)
2	A86	3	306	-	47,50,50	1.56	6 (12%)	51,76,76	3.78	17 (33%)
4	KC2	1	310	-	49,53,53	1.76	10 (20%)	60,89,89	1.90	15 (25%)
2	A86	1	301	-	47,50,50	1.46	6 (12%)	51,76,76	3.67	17 (33%)
2	A86	2	404	-	47,50,50	1.51	6 (12%)	51,76,76	4.88	16 (31%)
4	KC2	3	311	-	49,53,53	1.76	10 (20%)	60,89,89	1.89	15 (25%)
3	CLA	2	411	-	59,63,73	1.25	9 (15%)	70,101,113	1.34	6 (8%)
2	A86	3	302	-	47,50,50	1.48	7 (14%)	51,76,76	4.31	16 (31%)
2	A86	1	302	-	47,50,50	1.49	7 (14%)	51,76,76	4.30	16 (31%)
4	KC2	1	308	-	49,53,53	1.75	11 (22%)	60,89,89	1.93	16 (26%)
2	A86	2	405	-	47,50,50	1.45	6 (12%)	51,76,76	5.05	19 (37%)
3	CLA	3	315	-	50,54,73	1.34	9 (18%)	59,90,113	1.39	4 (6%)
3	CLA	2	409	1	63,67,73	1.20	9 (14%)	74,105,113	1.34	7 (9%)
4	KC2	3	309	-	49,53,53	1.75	11 (22%)	60,89,89	1.93	16 (26%)
2	A86	3	303	-	47,50,50	1.51	6 (12%)	51,76,76	5.08	16 (31%)
3	CLA	2	417	-	50,54,73	1.37	8 (16%)	59,90,113	1.37	4 (6%)
5	KC1	4	313	-	49,53,53	1.40	6 (12%)	61,89,89	1.72	12 (19%)
3	CLA	2	408	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
4	KC2	2	412	-	49,53,53	1.76	10 (20%)	60,89,89	1.90	16 (26%)
6	LMT	3	317	-	29,29,36	1.28	5 (17%)	40,40,47	1.06	3 (7%)
5	KC1	1	313	-	49,53,53	1.40	6 (12%)	61,89,89	1.72	12 (19%)
3	CLA	3	310	-	59,63,73	1.25	9 (15%)	70,101,113	1.35	6 (8%)
2	A86	3	305	-	47,50,50	1.46	5 (10%)	51,76,76	3.37	15 (29%)
5	KC1	2	413	1	49,53,53	1.42	7 (14%)	61,89,89	1.75	13 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A86	2	407	-	-	10/34/90/90	0/3/3/3
3	CLA	1	314	-	1/1/11/20	7/17/93/115	-
3	CLA	4	312	1	1/1/11/20	8/18/94/115	-
3	CLA	1	318	-	1/1/15/20	8/39/115/115	-
2	A86	4	305	-	-	15/34/90/90	0/3/3/3
3	CLA	1	312	1	1/1/11/20	9/18/94/115	-
2	A86	3	304	-	-	8/34/90/90	0/3/3/3
2	A86	4	306	-	-	10/34/90/90	0/3/3/3
4	KC2	2	410	-	-	10/15/71/71	-
6	LMT	1	316	-	-	6/14/54/61	0/2/2/2
2	A86	1	306	-	-	8/34/90/90	0/3/3/3
2	A86	2	402	-	-	9/34/90/90	0/3/3/3
2	A86	1	304	-	-	8/34/90/90	0/3/3/3
2	A86	4	302	-	-	11/34/90/90	0/3/3/3
4	KC2	4	310	-	-	8/15/71/71	-
5	KC1	2	415	1	-	6/15/71/71	-
5	KC1	3	312	1	-	3/15/71/71	-
6	LMT	4	317	-	-	9/18/58/61	0/2/2/2
2	A86	1	303	-	-	9/34/90/90	0/3/3/3
4	KC2	4	308	-	-	10/15/71/71	-
5	KC1	4	311	1	-	3/15/71/71	-
3	CLA	4	307	1	1/1/13/20	6/32/108/115	-
5	KC1	1	311	1	-	3/15/71/71	-
6	LMT	2	418	-	-	6/14/54/61	0/2/2/2
3	CLA	1	307	1	1/1/13/20	6/32/108/115	-
3	CLA	3	307	-	1/1/15/20	8/39/115/115	-
2	A86	4	303	-	-	9/34/90/90	0/3/3/3
3	CLA	2	414	1	1/1/11/20	8/18/94/115	-
2	A86	2	406	-	-	15/34/90/90	0/3/3/3
6	LMT	3	318	-	-	9/18/58/61	0/2/2/2
3	CLA	3	308	1	1/1/13/20	6/32/108/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LMT	4	316	-	-	6/14/54/61	0/2/2/2
6	LMT	1	317	-	-	9/18/58/61	0/2/2/2
6	LMT	2	419	-	-	9/18/58/61	0/2/2/2
2	A86	3	301	-	-	9/34/90/90	0/3/3/3
2	A86	3	305	-	-	15/34/90/90	0/3/3/3
3	CLA	3	313	1	1/1/11/20	8/18/94/115	-
5	KC1	3	314	-	-	6/15/71/71	-
2	A86	2	403	-	-	11/34/90/90	0/3/3/3
3	CLA	4	309	-	1/1/13/20	10/27/103/115	-
3	CLA	2	416	-	1/1/11/20	6/17/93/115	-
3	CLA	2	401	-	1/1/15/20	8/39/115/115	-
3	CLA	4	315	-	1/1/11/20	7/17/93/115	-
2	A86	1	305	-	-	15/34/90/90	0/3/3/3
3	CLA	1	315	-	1/1/11/20	6/17/93/115	-
3	CLA	3	316	-	1/1/11/20	6/17/93/115	-
2	A86	4	301	-	-	9/34/90/90	0/3/3/3
3	CLA	4	314	-	1/1/11/20	7/17/93/115	-
2	A86	4	304	-	-	8/34/90/90	0/3/3/3
4	KC2	1	310	-	-	7/15/71/71	-
2	A86	3	306	-	-	10/34/90/90	0/3/3/3
4	KC2	3	311	-	-	8/15/71/71	-
2	A86	1	301	-	-	9/34/90/90	0/3/3/3
2	A86	2	404	-	-	9/34/90/90	0/3/3/3
3	CLA	2	411	-	1/1/13/20	10/27/103/115	-
2	A86	3	302	-	-	11/34/90/90	0/3/3/3
2	A86	1	302	-	-	11/34/90/90	0/3/3/3
4	KC2	1	308	-	-	11/15/71/71	-
3	CLA	3	315	-	1/1/11/20	6/17/93/115	-
2	A86	2	405	-	-	8/34/90/90	0/3/3/3
3	CLA	2	409	1	1/1/13/20	6/32/108/115	-
4	KC2	3	309	-	-	10/15/71/71	-
2	A86	3	303	-	-	9/34/90/90	0/3/3/3
3	CLA	2	417	-	1/1/11/20	4/17/93/115	-
5	KC1	4	313	-	-	7/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	2	408	-	1/1/15/20	8/39/115/115	-
4	KC2	2	412	-	-	9/15/71/71	-
6	LMT	3	317	-	-	5/14/54/61	0/2/2/2
5	KC1	1	313	-	-	7/15/71/71	-
3	CLA	3	310	-	1/1/13/20	10/27/103/115	-
3	CLA	1	309	-	1/1/13/20	10/27/103/115	-
5	KC1	2	413	1	-	3/15/71/71	-

All (524) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	306	A86	C20-C15	5.49	1.55	1.48
2	2	407	A86	C20-C15	5.38	1.55	1.48
2	3	306	A86	C20-C15	5.36	1.55	1.48
2	4	306	A86	C20-C15	5.36	1.55	1.48
5	1	311	KC1	MG-ND	-5.20	1.95	2.05
5	2	413	KC1	MG-ND	-5.19	1.95	2.05
5	3	312	KC1	MG-ND	-5.19	1.95	2.05
5	4	311	KC1	MG-ND	-5.18	1.95	2.05
4	4	308	KC2	CHD-C4C	5.18	1.48	1.38
4	2	412	KC2	CHD-C4C	5.17	1.48	1.38
4	3	311	KC2	CHD-C4C	5.15	1.48	1.38
4	1	310	KC2	CHD-C4C	5.15	1.48	1.38
4	1	308	KC2	CHD-C4C	5.14	1.48	1.38
4	2	410	KC2	CHD-C4C	5.13	1.48	1.38
4	4	310	KC2	CHD-C4C	5.12	1.48	1.38
4	3	309	KC2	CHD-C4C	5.12	1.48	1.38
5	3	314	KC1	MG-ND	-5.08	1.95	2.05
5	1	313	KC1	MG-ND	-5.08	1.95	2.05
5	2	415	KC1	MG-ND	-5.06	1.95	2.05
5	4	313	KC1	MG-ND	-5.02	1.95	2.05
2	2	402	A86	O4-C38	4.87	1.46	1.35
5	4	311	KC1	MG-NB	-4.86	1.96	2.05
2	4	301	A86	O4-C38	4.86	1.45	1.35
2	4	305	A86	O4-C38	4.85	1.45	1.35
5	4	313	KC1	MG-NB	-4.85	1.96	2.05
2	3	305	A86	O4-C38	4.85	1.45	1.35
2	1	301	A86	O4-C38	4.84	1.45	1.35
2	1	305	A86	O4-C38	4.83	1.45	1.35
5	3	314	KC1	MG-NB	-4.83	1.96	2.05
5	2	415	KC1	MG-NB	-4.82	1.96	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	311	KC1	MG-NB	-4.82	1.96	2.05
5	1	313	KC1	MG-NB	-4.82	1.96	2.05
5	3	312	KC1	MG-NB	-4.81	1.96	2.05
2	2	406	A86	O4-C38	4.81	1.45	1.35
2	3	301	A86	O4-C38	4.80	1.45	1.35
5	2	413	KC1	MG-NB	-4.79	1.96	2.05
2	2	407	A86	O4-C38	4.75	1.45	1.35
2	1	303	A86	O4-C38	4.74	1.45	1.35
2	2	404	A86	O4-C38	4.73	1.45	1.35
2	3	303	A86	O4-C38	4.73	1.45	1.35
2	1	304	A86	O4-C38	4.73	1.45	1.35
2	4	303	A86	O4-C38	4.71	1.45	1.35
2	1	306	A86	O4-C38	4.71	1.45	1.35
2	4	306	A86	O4-C38	4.70	1.45	1.35
2	4	304	A86	O4-C38	4.69	1.45	1.35
2	3	304	A86	O4-C38	4.69	1.45	1.35
2	2	405	A86	O4-C38	4.68	1.45	1.35
2	1	302	A86	O4-C38	4.67	1.45	1.35
2	3	302	A86	O4-C38	4.66	1.45	1.35
2	2	403	A86	O4-C38	4.66	1.45	1.35
2	3	306	A86	O4-C38	4.65	1.45	1.35
2	4	302	A86	O4-C38	4.62	1.45	1.35
4	1	310	KC2	MG-ND	-4.53	1.96	2.05
4	3	311	KC2	MG-ND	-4.52	1.96	2.05
4	2	412	KC2	MG-ND	-4.52	1.96	2.05
4	4	310	KC2	MG-ND	-4.50	1.96	2.05
4	4	308	KC2	MG-ND	-4.41	1.97	2.05
4	2	410	KC2	MG-ND	-4.40	1.97	2.05
4	3	309	KC2	MG-ND	-4.40	1.97	2.05
4	1	308	KC2	MG-ND	-4.38	1.97	2.05
4	3	309	KC2	MG-NB	-4.23	1.97	2.05
4	1	308	KC2	MG-NB	-4.22	1.97	2.05
4	4	308	KC2	MG-NB	-4.21	1.97	2.05
2	2	404	A86	C20-C15	4.19	1.53	1.48
4	2	410	KC2	MG-NB	-4.18	1.97	2.05
2	1	303	A86	C20-C15	4.16	1.53	1.48
2	3	303	A86	C20-C15	4.16	1.53	1.48
2	4	303	A86	C20-C15	4.14	1.53	1.48
4	2	412	KC2	MG-NB	-4.14	1.97	2.05
2	4	305	A86	C20-C15	4.13	1.53	1.48
4	4	310	KC2	MG-NB	-4.13	1.97	2.05
4	1	310	KC2	MG-NB	-4.13	1.97	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	311	KC2	MG-NB	-4.11	1.97	2.05
2	2	406	A86	C20-C15	4.11	1.53	1.48
2	4	302	A86	C30-C31	-4.10	1.25	1.30
4	4	310	KC2	CHC-C1C	4.08	1.48	1.39
2	1	302	A86	C30-C31	-4.08	1.25	1.30
4	2	412	KC2	CHC-C1C	4.08	1.48	1.39
4	3	311	KC2	CHC-C1C	4.05	1.48	1.39
2	3	302	A86	C30-C31	-4.05	1.25	1.30
2	2	403	A86	C30-C31	-4.05	1.25	1.30
4	2	410	KC2	CHC-C1C	4.03	1.48	1.39
4	4	308	KC2	CHC-C1C	4.03	1.48	1.39
2	3	305	A86	C20-C15	4.02	1.53	1.48
4	1	308	KC2	CHC-C1C	4.01	1.48	1.39
4	1	310	KC2	CHC-C1C	4.01	1.48	1.39
4	3	309	KC2	CHC-C1C	3.99	1.48	1.39
2	2	405	A86	C20-C15	3.97	1.53	1.48
2	1	306	A86	C30-C31	-3.97	1.26	1.30
2	3	304	A86	C20-C15	3.96	1.53	1.48
2	1	304	A86	C20-C15	3.95	1.53	1.48
2	1	305	A86	C20-C15	3.93	1.53	1.48
2	4	304	A86	C20-C15	3.92	1.53	1.48
4	3	311	KC2	CHC-C4B	3.91	1.46	1.38
2	3	303	A86	C30-C31	-3.91	1.26	1.30
2	1	303	A86	C30-C31	-3.91	1.26	1.30
4	4	310	KC2	CHC-C4B	3.89	1.46	1.38
4	1	310	KC2	CHC-C4B	3.89	1.46	1.38
2	3	306	A86	C30-C31	-3.88	1.26	1.30
2	2	404	A86	C30-C31	-3.88	1.26	1.30
2	4	303	A86	C30-C31	-3.87	1.26	1.30
2	2	407	A86	C30-C31	-3.86	1.26	1.30
4	2	412	KC2	CHC-C4B	3.86	1.45	1.38
4	1	308	KC2	CHC-C4B	3.84	1.45	1.38
2	1	301	A86	C20-C15	3.81	1.53	1.48
4	2	410	KC2	CHC-C4B	3.80	1.45	1.38
4	3	309	KC2	CHC-C4B	3.80	1.45	1.38
4	4	308	KC2	CHC-C4B	3.79	1.45	1.38
2	1	301	A86	C30-C31	-3.78	1.26	1.30
2	3	301	A86	C30-C31	-3.78	1.26	1.30
2	4	306	A86	C30-C31	-3.77	1.26	1.30
2	1	305	A86	C30-C31	-3.77	1.26	1.30
2	4	301	A86	C20-C15	3.76	1.53	1.48
2	4	301	A86	C30-C31	-3.75	1.26	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	402	A86	C20-C15	3.75	1.53	1.48
2	3	302	A86	C30-C29	-3.74	1.25	1.31
2	3	301	A86	C20-C15	3.74	1.53	1.48
2	4	305	A86	C30-C31	-3.73	1.26	1.30
2	1	306	A86	C30-C29	-3.73	1.25	1.31
2	2	402	A86	C30-C31	-3.72	1.26	1.30
2	3	305	A86	C30-C31	-3.72	1.26	1.30
2	4	302	A86	C30-C29	-3.71	1.25	1.31
2	2	406	A86	C30-C31	-3.71	1.26	1.30
2	1	302	A86	C30-C29	-3.70	1.25	1.31
2	3	304	A86	C30-C31	-3.69	1.26	1.30
2	2	405	A86	C30-C31	-3.68	1.26	1.30
2	2	403	A86	C30-C29	-3.67	1.25	1.31
2	2	404	A86	C30-C29	-3.67	1.25	1.31
2	1	304	A86	C30-C31	-3.67	1.26	1.30
2	1	303	A86	C30-C29	-3.66	1.25	1.31
2	3	303	A86	C30-C29	-3.65	1.26	1.31
2	4	304	A86	C30-C31	-3.64	1.26	1.30
2	4	306	A86	C30-C29	-3.62	1.26	1.31
2	2	407	A86	C30-C29	-3.61	1.26	1.31
2	4	303	A86	C30-C29	-3.61	1.26	1.31
2	3	306	A86	C30-C29	-3.61	1.26	1.31
2	3	301	A86	C30-C29	-3.55	1.26	1.31
2	1	301	A86	C30-C29	-3.55	1.26	1.31
2	2	402	A86	C30-C29	-3.54	1.26	1.31
2	4	301	A86	C30-C29	-3.54	1.26	1.31
3	1	315	CLA	C1D-ND	3.52	1.42	1.37
3	3	316	CLA	C1D-ND	3.52	1.42	1.37
2	3	305	A86	C30-C29	-3.52	1.26	1.31
3	2	417	CLA	C1D-ND	3.50	1.42	1.37
2	2	406	A86	C30-C29	-3.48	1.26	1.31
3	4	315	CLA	C1D-ND	3.48	1.42	1.37
2	1	302	A86	C20-C15	3.48	1.52	1.48
3	1	318	CLA	C1D-ND	3.47	1.42	1.37
2	4	304	A86	C30-C29	-3.47	1.26	1.31
2	4	305	A86	C30-C29	-3.47	1.26	1.31
2	4	302	A86	C20-C15	3.47	1.52	1.48
2	1	305	A86	C30-C29	-3.47	1.26	1.31
2	2	403	A86	C20-C15	3.45	1.52	1.48
3	3	307	CLA	C1D-ND	3.44	1.42	1.37
2	3	302	A86	C20-C15	3.43	1.52	1.48
2	1	304	A86	C30-C29	-3.43	1.26	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	405	A86	C30-C29	-3.43	1.26	1.31
3	1	312	CLA	C1D-ND	3.42	1.42	1.37
3	2	408	CLA	C1D-ND	3.41	1.42	1.37
2	3	304	A86	C30-C29	-3.40	1.26	1.31
3	3	313	CLA	C1D-ND	3.40	1.42	1.37
3	2	401	CLA	C1D-ND	3.39	1.42	1.37
3	2	416	CLA	C1D-ND	3.38	1.42	1.37
3	4	312	CLA	C1D-ND	3.36	1.42	1.37
3	2	414	CLA	C1D-ND	3.36	1.42	1.37
3	1	314	CLA	C1D-ND	3.35	1.42	1.37
3	4	314	CLA	C1D-ND	3.35	1.42	1.37
4	2	412	KC2	CHD-C1D	3.35	1.46	1.39
3	3	315	CLA	C1D-ND	3.34	1.42	1.37
4	4	310	KC2	CHD-C1D	3.31	1.46	1.39
4	1	310	KC2	CHD-C1D	3.31	1.46	1.39
4	3	311	KC2	CHD-C1D	3.30	1.46	1.39
3	3	310	CLA	C1D-ND	3.28	1.42	1.37
3	4	309	CLA	C1D-ND	3.23	1.42	1.37
3	3	316	CLA	C4B-NB	3.22	1.42	1.37
3	4	315	CLA	C4B-NB	3.22	1.42	1.37
4	3	309	KC2	CHD-C1D	3.20	1.46	1.39
3	2	411	CLA	C1D-ND	3.20	1.42	1.37
4	2	410	KC2	CHD-C1D	3.19	1.46	1.39
4	1	308	KC2	CHD-C1D	3.17	1.46	1.39
3	1	309	CLA	C1D-ND	3.17	1.42	1.37
4	4	308	KC2	CHD-C1D	3.17	1.46	1.39
3	3	308	CLA	C1D-ND	3.17	1.42	1.37
3	1	307	CLA	C1D-ND	3.16	1.42	1.37
3	4	307	CLA	C1D-ND	3.16	1.42	1.37
3	1	315	CLA	C4B-NB	3.15	1.42	1.37
3	2	417	CLA	C4B-NB	3.14	1.42	1.37
3	2	409	CLA	C1D-ND	3.14	1.42	1.37
2	3	303	A86	O1-C20	-3.13	1.42	1.46
2	2	404	A86	O1-C20	-3.13	1.42	1.46
2	4	303	A86	O1-C20	-3.09	1.42	1.46
2	1	303	A86	O1-C20	-3.07	1.42	1.46
5	2	415	KC1	C4B-NB	-3.00	1.33	1.37
5	1	311	KC1	C4B-NB	-2.97	1.34	1.37
5	2	413	KC1	C4B-NB	-2.97	1.34	1.37
5	1	313	KC1	C4B-NB	-2.96	1.34	1.37
5	3	312	KC1	C4B-NB	-2.95	1.34	1.37
5	3	314	KC1	C4B-NB	-2.93	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	313	KC1	C4B-NB	-2.93	1.34	1.37
3	3	310	CLA	C4B-NB	2.93	1.41	1.37
5	4	311	KC1	C4B-NB	-2.92	1.34	1.37
3	1	309	CLA	C4B-NB	2.90	1.41	1.37
3	2	411	CLA	C4B-NB	2.90	1.41	1.37
3	2	414	CLA	C4B-NB	2.89	1.41	1.37
2	1	306	A86	O1-C20	-2.88	1.42	1.46
3	4	309	CLA	C4B-NB	2.84	1.41	1.37
3	1	312	CLA	C4B-NB	2.82	1.41	1.37
3	3	313	CLA	C4B-NB	2.82	1.41	1.37
3	4	312	CLA	C4B-NB	2.79	1.41	1.37
5	3	312	KC1	CBA-CGA	-2.79	1.41	1.48
5	1	311	KC1	CBA-CGA	-2.77	1.41	1.48
2	1	304	A86	O1-C20	-2.77	1.42	1.46
5	2	413	KC1	CBA-CGA	-2.76	1.41	1.48
2	1	305	A86	O1-C20	-2.75	1.42	1.46
3	4	314	CLA	C4B-NB	2.75	1.41	1.37
3	2	401	CLA	C4B-NB	2.74	1.41	1.37
2	2	405	A86	O1-C20	-2.73	1.42	1.46
3	3	315	CLA	C4B-NB	2.73	1.41	1.37
2	3	304	A86	O1-C20	-2.73	1.42	1.46
3	2	416	CLA	C4B-NB	2.72	1.41	1.37
5	4	311	KC1	CBA-CGA	-2.72	1.41	1.48
3	2	417	CLA	C1B-C2B	2.72	1.49	1.43
3	1	314	CLA	C4B-NB	2.71	1.41	1.37
3	1	315	CLA	C1B-C2B	2.71	1.49	1.43
2	4	304	A86	O1-C20	-2.71	1.42	1.46
3	3	307	CLA	C4B-NB	2.70	1.41	1.37
3	4	315	CLA	C1B-C2B	2.70	1.49	1.43
4	3	311	KC2	CBA-CGA	-2.70	1.41	1.48
3	3	316	CLA	C1B-C2B	2.69	1.49	1.43
5	1	313	KC1	CBA-CGA	-2.69	1.41	1.48
4	2	412	KC2	CBA-CGA	-2.68	1.41	1.48
3	4	307	CLA	C4B-NB	2.68	1.41	1.37
3	1	318	CLA	C4B-NB	2.68	1.41	1.37
3	2	408	CLA	C4B-NB	2.68	1.41	1.37
3	1	307	CLA	C4B-NB	2.67	1.41	1.37
4	1	308	KC2	CBA-CGA	-2.67	1.41	1.48
5	2	415	KC1	CBA-CGA	-2.66	1.41	1.48
5	4	313	KC1	CBA-CGA	-2.66	1.41	1.48
3	1	318	CLA	C1B-C2B	2.66	1.49	1.43
2	3	305	A86	O1-C20	-2.66	1.42	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	410	KC2	CBA-CGA	-2.64	1.41	1.48
4	4	308	KC2	CBA-CGA	-2.64	1.41	1.48
3	3	307	CLA	C1B-C2B	2.64	1.49	1.43
6	2	419	LMT	O3'-C3'	-2.64	1.36	1.43
3	2	401	CLA	C1B-C2B	2.63	1.49	1.43
4	4	310	KC2	CBA-CGA	-2.63	1.41	1.48
4	3	309	KC2	CBA-CGA	-2.63	1.41	1.48
5	3	314	KC1	CBA-CGA	-2.63	1.41	1.48
3	2	408	CLA	C1B-C2B	2.63	1.49	1.43
3	2	409	CLA	C4B-NB	2.62	1.41	1.37
4	1	310	KC2	CBA-CGA	-2.62	1.41	1.48
6	1	317	LMT	O3'-C3'	-2.61	1.36	1.43
6	4	317	LMT	O3'-C3'	-2.61	1.36	1.43
3	3	308	CLA	C4B-NB	2.61	1.41	1.37
6	3	318	LMT	O3'-C3'	-2.61	1.36	1.43
3	4	307	CLA	C1B-C2B	2.58	1.49	1.43
3	2	416	CLA	C1B-C2B	2.58	1.49	1.43
2	4	302	A86	O1-C20	-2.56	1.42	1.46
3	2	409	CLA	C1B-C2B	2.56	1.49	1.43
2	1	302	A86	O1-C20	-2.56	1.42	1.46
2	2	403	A86	O1-C20	-2.56	1.42	1.46
3	1	307	CLA	C1B-C2B	2.55	1.49	1.43
3	4	314	CLA	C1B-C2B	2.55	1.49	1.43
2	3	306	A86	O1-C20	-2.55	1.42	1.46
3	4	309	CLA	C1B-C2B	2.55	1.49	1.43
4	1	308	KC2	C4B-NB	-2.54	1.34	1.37
4	3	309	KC2	C4B-NB	-2.54	1.34	1.37
3	3	308	CLA	C1B-C2B	2.54	1.49	1.43
4	4	310	KC2	C4B-NB	-2.54	1.34	1.37
6	2	418	LMT	O3'-C3'	-2.54	1.36	1.43
2	2	407	A86	O1-C20	-2.53	1.42	1.46
6	1	316	LMT	O3'-C3'	-2.53	1.36	1.43
3	1	309	CLA	C1B-C2B	2.53	1.49	1.43
6	4	316	LMT	O3'-C3'	-2.53	1.36	1.43
2	3	302	A86	O1-C20	-2.53	1.43	1.46
3	1	314	CLA	C1B-C2B	2.52	1.49	1.43
3	3	310	CLA	C1B-C2B	2.52	1.49	1.43
6	3	317	LMT	O3'-C3'	-2.52	1.36	1.43
3	3	315	CLA	C1B-C2B	2.51	1.49	1.43
3	2	411	CLA	C1B-C2B	2.51	1.49	1.43
2	3	301	A86	O1-C20	-2.51	1.43	1.46
2	4	301	A86	O1-C20	-2.51	1.43	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	414	CLA	C1B-C2B	2.51	1.49	1.43
4	2	412	KC2	C4B-NB	-2.50	1.34	1.37
4	3	311	KC2	C4B-NB	-2.50	1.34	1.37
4	2	410	KC2	C4B-NB	-2.50	1.34	1.37
2	4	306	A86	O1-C20	-2.50	1.43	1.46
5	1	311	KC1	C1B-NB	-2.50	1.34	1.37
2	1	301	A86	O1-C20	-2.50	1.43	1.46
4	1	310	KC2	C4B-NB	-2.48	1.34	1.37
3	1	312	CLA	C1B-C2B	2.48	1.48	1.43
4	4	308	KC2	C4B-NB	-2.47	1.34	1.37
5	3	312	KC1	C1B-NB	-2.47	1.34	1.37
3	4	312	CLA	C1B-C2B	2.47	1.48	1.43
2	2	402	A86	O1-C20	-2.47	1.43	1.46
3	3	313	CLA	C1B-C2B	2.46	1.48	1.43
5	4	311	KC1	C1B-NB	-2.46	1.34	1.37
5	2	413	KC1	C1B-NB	-2.45	1.34	1.37
5	2	415	KC1	C1B-NB	-2.45	1.34	1.37
5	4	313	KC1	C1B-NB	-2.45	1.34	1.37
5	1	313	KC1	C1B-NB	-2.45	1.34	1.37
5	3	314	KC1	C1B-NB	-2.45	1.34	1.37
3	1	315	CLA	C3B-C4B	2.42	1.49	1.42
2	4	305	A86	O1-C20	-2.41	1.43	1.46
2	2	406	A86	O1-C20	-2.40	1.43	1.46
3	3	316	CLA	C3B-C4B	2.39	1.49	1.42
3	4	315	CLA	C3B-C4B	2.39	1.49	1.42
2	3	301	A86	C13-C11	-2.37	1.45	1.49
3	2	417	CLA	C3B-C4B	2.37	1.49	1.42
3	4	314	CLA	C3B-C4B	2.37	1.49	1.42
3	3	315	CLA	C3B-C4B	2.37	1.49	1.42
2	4	301	A86	C13-C11	-2.36	1.45	1.49
3	2	416	CLA	C3B-C4B	2.36	1.49	1.42
3	1	314	CLA	C3B-C4B	2.33	1.49	1.42
2	2	402	A86	C13-C11	-2.33	1.45	1.49
5	3	312	KC1	C4A-C3A	-2.32	1.39	1.44
3	1	309	CLA	C3B-C4B	2.32	1.49	1.42
3	4	309	CLA	C3B-C4B	2.32	1.49	1.42
4	4	308	KC2	C4A-C3A	-2.31	1.39	1.44
2	1	301	A86	C13-C11	-2.31	1.45	1.49
5	2	413	KC1	C4A-C3A	-2.30	1.39	1.44
3	1	315	CLA	CHC-C1C	2.30	1.43	1.38
4	2	410	KC2	C4A-C3A	-2.29	1.39	1.44
4	1	308	KC2	C4A-C3A	-2.29	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	309	KC2	C4A-C3A	-2.29	1.39	1.44
3	2	411	CLA	C3B-C4B	2.29	1.49	1.42
3	3	316	CLA	CHC-C1C	2.28	1.43	1.38
3	3	310	CLA	C3B-C4B	2.28	1.49	1.42
6	3	317	LMT	O2'-C2'	-2.28	1.37	1.43
3	2	417	CLA	CHC-C1C	2.27	1.43	1.38
3	4	315	CLA	CHC-C1C	2.27	1.43	1.38
3	1	307	CLA	MG-NB	-2.27	2.01	2.05
6	3	318	LMT	O2'-C2'	-2.26	1.37	1.43
3	3	308	CLA	MG-NB	-2.26	2.01	2.05
3	4	312	CLA	C3B-C4B	2.26	1.49	1.42
5	1	311	KC1	C4A-C3A	-2.26	1.39	1.44
5	4	311	KC1	C4A-C3A	-2.26	1.39	1.44
3	3	313	CLA	C3B-C4B	2.26	1.49	1.42
6	1	316	LMT	O3B-C3B	-2.25	1.37	1.43
3	1	312	CLA	C3B-C4B	2.25	1.49	1.42
3	2	414	CLA	C3B-C4B	2.25	1.49	1.42
2	1	302	A86	C32-C31	-2.25	1.50	1.54
6	4	316	LMT	O3B-C3B	-2.25	1.37	1.43
3	2	409	CLA	MG-NB	-2.25	2.01	2.05
3	4	307	CLA	MG-NB	-2.25	2.01	2.05
6	2	419	LMT	O2'-C2'	-2.25	1.37	1.43
3	3	315	CLA	CMD-C2D	-2.25	1.46	1.50
6	1	317	LMT	O2'-C2'	-2.24	1.37	1.43
6	4	317	LMT	O2'-C2'	-2.24	1.37	1.43
6	1	317	LMT	O2B-C2B	-2.24	1.37	1.43
6	3	317	LMT	O3B-C3B	-2.24	1.37	1.43
6	4	317	LMT	O2B-C2B	-2.24	1.37	1.43
6	2	418	LMT	O3B-C3B	-2.24	1.37	1.43
2	2	403	A86	C32-C31	-2.23	1.50	1.54
2	3	302	A86	C32-C31	-2.23	1.50	1.54
3	3	315	CLA	MG-NB	-2.23	2.01	2.05
6	2	419	LMT	O2B-C2B	-2.23	1.37	1.43
4	2	412	KC2	C4A-C3A	-2.23	1.40	1.44
3	2	416	CLA	CMD-C2D	-2.23	1.46	1.50
3	1	314	CLA	CMD-C2D	-2.23	1.46	1.50
4	1	310	KC2	C4A-C3A	-2.22	1.40	1.44
3	4	307	CLA	C3B-C4B	2.22	1.49	1.42
3	2	411	CLA	MG-NB	-2.22	2.01	2.05
6	4	317	LMT	O3B-C3B	-2.22	1.37	1.43
3	1	309	CLA	CHC-C1C	2.22	1.42	1.38
6	3	318	LMT	O2B-C2B	-2.22	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	313	CLA	MG-NB	-2.22	2.01	2.05
3	1	314	CLA	MG-NB	-2.22	2.01	2.05
4	4	310	KC2	C4A-C3A	-2.22	1.40	1.44
3	1	307	CLA	CHC-C1C	2.21	1.42	1.38
3	2	409	CLA	C3B-C4B	2.21	1.49	1.42
3	3	308	CLA	C3B-C4B	2.21	1.49	1.42
6	4	316	LMT	O2'-C2'	-2.21	1.37	1.43
3	2	409	CLA	CHC-C1C	2.21	1.42	1.38
3	1	312	CLA	MG-NB	-2.21	2.01	2.05
3	2	414	CLA	MG-NB	-2.21	2.01	2.05
4	3	311	KC2	C4A-C3A	-2.21	1.40	1.44
6	3	318	LMT	O3B-C3B	-2.21	1.37	1.43
3	2	411	CLA	CHC-C1C	2.21	1.42	1.38
6	2	419	LMT	O3B-C3B	-2.21	1.37	1.43
3	4	314	CLA	MG-NB	-2.21	2.01	2.05
3	1	307	CLA	C3B-C4B	2.21	1.49	1.42
2	1	302	A86	C13-C11	-2.20	1.45	1.49
6	1	316	LMT	O2'-C2'	-2.20	1.37	1.43
6	2	418	LMT	O2'-C2'	-2.20	1.37	1.43
6	2	418	LMT	O2B-C2B	-2.20	1.37	1.43
3	4	314	CLA	CMD-C2D	-2.20	1.46	1.50
3	3	308	CLA	CHC-C1C	2.20	1.42	1.38
3	4	312	CLA	MG-NB	-2.20	2.01	2.05
2	4	302	A86	C32-C31	-2.20	1.50	1.54
3	3	307	CLA	CMD-C2D	-2.19	1.46	1.50
3	4	309	CLA	MG-NB	-2.19	2.01	2.05
3	4	309	CLA	CHC-C1C	2.19	1.42	1.38
6	1	316	LMT	O2B-C2B	-2.19	1.37	1.43
6	4	316	LMT	O2B-C2B	-2.19	1.37	1.43
3	3	307	CLA	MG-NB	-2.19	2.01	2.05
3	3	310	CLA	MG-NB	-2.19	2.01	2.05
6	1	317	LMT	O3B-C3B	-2.19	1.37	1.43
3	3	310	CLA	CHC-C1C	2.19	1.42	1.38
6	3	317	LMT	O2B-C2B	-2.19	1.37	1.43
3	1	309	CLA	MG-NB	-2.18	2.01	2.05
5	3	314	KC1	C1D-ND	-2.18	1.35	1.37
3	2	414	CLA	CMB-C2B	-2.18	1.46	1.50
3	2	408	CLA	CMD-C2D	-2.18	1.46	1.50
3	2	409	CLA	CMD-C2D	-2.18	1.46	1.50
3	4	307	CLA	CMD-C2D	-2.18	1.46	1.50
3	1	318	CLA	CMD-C2D	-2.18	1.46	1.50
3	2	401	CLA	CMD-C2D	-2.18	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	408	CLA	MG-NB	-2.18	2.01	2.05
3	1	312	CLA	CMB-C2B	-2.17	1.46	1.50
3	3	313	CLA	CMB-C2B	-2.17	1.46	1.50
3	4	312	CLA	CMB-C2B	-2.17	1.46	1.50
3	1	307	CLA	CMD-C2D	-2.17	1.46	1.50
3	4	314	CLA	CMB-C2B	-2.17	1.46	1.50
3	3	313	CLA	CMD-C2D	-2.16	1.46	1.50
3	4	312	CLA	CHC-C1C	2.16	1.42	1.38
3	2	416	CLA	MG-NB	-2.16	2.01	2.05
3	4	307	CLA	CHC-C1C	2.16	1.42	1.38
3	3	310	CLA	CMD-C2D	-2.16	1.46	1.50
3	1	312	CLA	CMD-C2D	-2.16	1.46	1.50
3	4	312	CLA	CMD-C2D	-2.16	1.46	1.50
2	3	302	A86	C13-C11	-2.15	1.45	1.49
2	4	302	A86	C13-C11	-2.15	1.45	1.49
3	2	414	CLA	CMD-C2D	-2.15	1.46	1.50
3	2	408	CLA	C3B-C4B	2.15	1.49	1.42
3	1	318	CLA	MG-NB	-2.15	2.01	2.05
5	4	313	KC1	C1D-ND	-2.15	1.35	1.37
5	1	313	KC1	C1D-ND	-2.15	1.35	1.37
3	3	310	CLA	CMB-C2B	-2.15	1.46	1.50
3	2	411	CLA	CMD-C2D	-2.14	1.46	1.50
3	3	308	CLA	CMD-C2D	-2.14	1.46	1.50
5	2	415	KC1	C1D-ND	-2.14	1.35	1.37
3	3	307	CLA	C3B-C4B	2.14	1.49	1.42
3	1	309	CLA	CMB-C2B	-2.14	1.46	1.50
5	2	413	KC1	C1D-ND	-2.13	1.35	1.37
3	2	411	CLA	CMB-C2B	-2.13	1.46	1.50
3	4	309	CLA	CMB-C2B	-2.13	1.46	1.50
3	2	401	CLA	MG-NB	-2.13	2.01	2.05
3	1	309	CLA	CMD-C2D	-2.13	1.46	1.50
3	2	409	CLA	CMC-C2C	-2.13	1.46	1.50
5	3	312	KC1	C1D-ND	-2.13	1.35	1.37
3	1	318	CLA	C3B-C4B	2.12	1.48	1.42
3	2	401	CLA	C3B-C4B	2.12	1.48	1.42
3	3	313	CLA	CHC-C1C	2.12	1.42	1.38
2	1	306	A86	C13-C11	-2.12	1.45	1.49
3	3	307	CLA	CMB-C2B	-2.11	1.46	1.50
3	3	315	CLA	CMB-C2B	-2.11	1.46	1.50
3	1	312	CLA	CHC-C1C	2.11	1.42	1.38
3	2	414	CLA	CHC-C1C	2.11	1.42	1.38
3	1	314	CLA	CMB-C2B	-2.11	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	309	CLA	CMD-C2D	-2.11	1.46	1.50
2	2	403	A86	C13-C11	-2.11	1.45	1.49
3	4	307	CLA	CMB-C2B	-2.11	1.46	1.50
3	2	416	CLA	CMB-C2B	-2.10	1.46	1.50
3	4	307	CLA	CMC-C2C	-2.10	1.46	1.50
2	2	404	A86	C13-C11	-2.09	1.45	1.49
4	4	308	KC2	C1C-C2C	-2.09	1.40	1.44
2	4	303	A86	C13-C11	-2.09	1.45	1.49
5	1	311	KC1	C1D-ND	-2.09	1.35	1.37
3	3	308	CLA	CMC-C2C	-2.09	1.46	1.50
4	4	310	KC2	C1C-C2C	-2.08	1.40	1.44
3	1	307	CLA	CMC-C2C	-2.08	1.46	1.50
6	2	418	LMT	O1'-C1'	-2.08	1.36	1.40
6	3	317	LMT	O1'-C1'	-2.08	1.36	1.40
3	2	409	CLA	CMB-C2B	-2.08	1.46	1.50
3	3	316	CLA	CMB-C2B	-2.08	1.46	1.50
4	1	308	KC2	C1C-C2C	-2.08	1.40	1.44
4	3	309	KC2	C1C-C2C	-2.08	1.40	1.44
4	2	410	KC2	C1C-C2C	-2.07	1.40	1.44
3	2	417	CLA	CMB-C2B	-2.07	1.46	1.50
3	3	308	CLA	CMB-C2B	-2.07	1.46	1.50
5	4	311	KC1	C1D-ND	-2.07	1.35	1.37
3	2	401	CLA	CMB-C2B	-2.07	1.46	1.50
3	2	408	CLA	CMB-C2B	-2.07	1.46	1.50
3	4	315	CLA	CMD-C2D	-2.07	1.46	1.50
6	4	316	LMT	O1'-C1'	-2.07	1.36	1.40
3	1	318	CLA	CMB-C2B	-2.06	1.46	1.50
3	4	315	CLA	MG-NB	-2.06	2.01	2.05
3	1	315	CLA	CMB-C2B	-2.06	1.46	1.50
6	3	318	LMT	O4'-C4B	-2.06	1.37	1.43
3	3	316	CLA	CMD-C2D	-2.06	1.46	1.50
3	1	318	CLA	CMC-C2C	-2.06	1.46	1.50
3	2	417	CLA	CMD-C2D	-2.06	1.46	1.50
3	1	307	CLA	CMB-C2B	-2.05	1.46	1.50
3	4	309	CLA	CMC-C2C	-2.05	1.46	1.50
3	2	401	CLA	CMC-C2C	-2.05	1.46	1.50
4	2	412	KC2	C1C-C2C	-2.04	1.40	1.44
6	2	419	LMT	O4'-C4B	-2.04	1.37	1.43
6	4	317	LMT	O4'-C4B	-2.04	1.37	1.43
3	3	310	CLA	CMC-C2C	-2.04	1.46	1.50
2	1	303	A86	C13-C11	-2.04	1.45	1.49
3	3	307	CLA	CMC-C2C	-2.04	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	314	CLA	CMC-C2C	-2.04	1.46	1.50
3	3	315	CLA	CMC-C2C	-2.04	1.46	1.50
2	3	303	A86	C13-C11	-2.04	1.45	1.49
6	1	316	LMT	O1'-C1'	-2.03	1.36	1.40
4	1	310	KC2	C1C-C2C	-2.03	1.40	1.44
3	4	315	CLA	CMB-C2B	-2.03	1.46	1.50
3	2	416	CLA	CMC-C2C	-2.03	1.46	1.50
4	3	309	KC2	C1B-NB	-2.03	1.35	1.37
2	1	304	A86	C13-C11	-2.03	1.45	1.49
4	4	308	KC2	C1B-NB	-2.03	1.35	1.37
6	1	317	LMT	O4'-C4B	-2.03	1.37	1.43
3	3	316	CLA	MG-NB	-2.03	2.01	2.05
2	4	304	A86	C13-C11	-2.03	1.45	1.49
3	2	408	CLA	CHC-C1C	2.03	1.42	1.38
4	1	308	KC2	C1B-NB	-2.03	1.35	1.37
3	1	314	CLA	CMC-C2C	-2.03	1.46	1.50
2	2	407	A86	C13-C11	-2.03	1.45	1.49
4	2	410	KC2	C1B-NB	-2.03	1.35	1.37
2	2	405	A86	C13-C11	-2.02	1.45	1.49
2	4	306	A86	C13-C11	-2.02	1.45	1.49
3	3	315	CLA	CHC-C1C	2.02	1.42	1.38
3	2	408	CLA	CMC-C2C	-2.02	1.46	1.50
3	1	309	CLA	CMC-C2C	-2.02	1.46	1.50
3	1	315	CLA	CMD-C2D	-2.02	1.46	1.50
4	3	311	KC2	C1C-C2C	-2.02	1.40	1.44
4	2	410	KC2	C1D-ND	-2.02	1.35	1.37
3	2	414	CLA	CMC-C2C	-2.01	1.46	1.50
3	4	312	CLA	CMC-C2C	-2.01	1.46	1.50
2	3	304	A86	C13-C11	-2.01	1.45	1.49
3	2	411	CLA	CMC-C2C	-2.01	1.46	1.50
3	2	417	CLA	MG-NB	-2.00	2.01	2.05
2	3	306	A86	C13-C11	-2.00	1.46	1.49

All (778) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	303	A86	C34-O4-C38	31.21	172.97	117.85
2	1	303	A86	C34-O4-C38	30.09	171.00	117.85
2	4	303	A86	C34-O4-C38	30.03	170.88	117.85
2	2	404	A86	C34-O4-C38	29.60	170.12	117.85
2	4	304	A86	C29-C30-C31	-29.00	143.44	177.66
2	3	304	A86	C29-C30-C31	-28.91	143.55	177.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	304	A86	C29-C30-C31	-28.87	143.59	177.66
2	2	405	A86	C29-C30-C31	-28.83	143.64	177.66
2	3	302	A86	C29-C30-C31	-25.61	147.45	177.66
2	4	302	A86	C29-C30-C31	-25.48	147.59	177.66
2	1	302	A86	C29-C30-C31	-25.48	147.60	177.66
2	2	403	A86	C29-C30-C31	-24.75	148.46	177.66
2	4	301	A86	C34-O4-C38	18.25	150.07	117.85
2	3	301	A86	C34-O4-C38	18.19	149.97	117.85
2	1	301	A86	C34-O4-C38	18.19	149.97	117.85
2	2	402	A86	C34-O4-C38	18.16	149.92	117.85
2	2	406	A86	C34-O4-C38	17.78	149.26	117.85
2	4	305	A86	C34-O4-C38	17.68	149.07	117.85
2	3	306	A86	C34-O4-C38	17.47	148.70	117.85
2	3	305	A86	C34-O4-C38	16.95	147.77	117.85
2	1	305	A86	C34-O4-C38	16.94	147.76	117.85
2	2	407	A86	C34-O4-C38	13.06	140.92	117.85
2	2	405	A86	C34-O4-C38	12.42	139.78	117.85
2	1	304	A86	C34-O4-C38	12.32	139.60	117.85
2	3	304	A86	C34-O4-C38	12.09	139.20	117.85
2	4	304	A86	C34-O4-C38	12.07	139.16	117.85
2	4	306	A86	C34-O4-C38	11.44	138.05	117.85
2	1	306	A86	C34-O4-C38	11.25	137.71	117.85
2	2	407	A86	C20-O1-C15	10.76	65.65	61.03
2	3	306	A86	C20-O1-C15	10.75	65.65	61.03
2	1	306	A86	C20-O1-C15	10.73	65.64	61.03
2	4	306	A86	C20-O1-C15	10.66	65.61	61.03
2	2	404	A86	C20-O1-C15	9.45	65.09	61.03
2	3	303	A86	C20-O1-C15	9.41	65.07	61.03
2	1	303	A86	C20-O1-C15	9.39	65.06	61.03
2	4	303	A86	C20-O1-C15	9.34	65.04	61.03
2	4	305	A86	C20-O1-C15	8.85	64.83	61.03
2	1	304	A86	C20-O1-C15	8.83	64.82	61.03
2	2	405	A86	C20-O1-C15	8.82	64.82	61.03
2	3	304	A86	C20-O1-C15	8.77	64.80	61.03
2	2	406	A86	C20-O1-C15	8.74	64.79	61.03
2	4	304	A86	C20-O1-C15	8.74	64.78	61.03
2	3	305	A86	C20-O1-C15	8.69	64.76	61.03
2	1	305	A86	C20-O1-C15	8.69	64.76	61.03
2	2	407	A86	C23-C16-C22	-8.65	94.81	107.37
2	1	301	A86	C20-O1-C15	8.63	64.74	61.03
2	3	306	A86	C23-C16-C22	-8.63	94.84	107.37
2	4	306	A86	C23-C16-C22	-8.63	94.84	107.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	301	A86	C20-O1-C15	8.59	64.72	61.03
2	4	301	A86	C20-O1-C15	8.59	64.72	61.03
2	2	402	A86	C20-O1-C15	8.51	64.69	61.03
2	1	302	A86	C20-O1-C15	8.11	64.51	61.03
2	2	403	A86	C20-O1-C15	8.06	64.49	61.03
2	4	302	A86	C20-O1-C15	8.05	64.49	61.03
2	3	302	A86	C20-O1-C15	7.99	64.46	61.03
2	4	305	A86	C29-C30-C31	-7.38	168.95	177.66
2	2	406	A86	C29-C30-C31	-7.29	169.06	177.66
3	2	401	CLA	C4A-NA-C1A	6.91	109.83	106.68
3	3	307	CLA	C4A-NA-C1A	6.87	109.81	106.68
2	2	402	A86	C4-C5-C6	-6.85	117.67	127.28
2	4	301	A86	C4-C5-C6	-6.85	117.68	127.28
2	3	301	A86	C4-C5-C6	-6.84	117.68	127.28
3	2	408	CLA	C4A-NA-C1A	6.84	109.80	106.68
2	1	303	A86	O1-C20-C21	-6.81	107.44	115.05
3	1	318	CLA	C4A-NA-C1A	6.81	109.79	106.68
2	3	303	A86	O1-C20-C21	-6.80	107.44	115.05
2	1	301	A86	C4-C5-C6	-6.80	117.74	127.28
2	4	303	A86	O1-C20-C21	-6.80	107.45	115.05
2	2	404	A86	O1-C20-C21	-6.77	107.48	115.05
2	3	305	A86	C29-C30-C31	-6.77	169.67	177.66
3	3	308	CLA	C4A-NA-C1A	6.71	109.74	106.68
2	1	305	A86	C29-C30-C31	-6.68	169.78	177.66
3	1	307	CLA	C4A-NA-C1A	6.66	109.72	106.68
3	4	307	CLA	C4A-NA-C1A	6.66	109.72	106.68
3	2	409	CLA	C4A-NA-C1A	6.64	109.71	106.68
3	4	312	CLA	C4A-NA-C1A	6.59	109.69	106.68
3	1	314	CLA	C4A-NA-C1A	6.57	109.67	106.68
3	2	414	CLA	C4A-NA-C1A	6.56	109.67	106.68
3	1	312	CLA	C4A-NA-C1A	6.55	109.67	106.68
3	2	417	CLA	C4A-NA-C1A	6.54	109.66	106.68
3	2	416	CLA	C4A-NA-C1A	6.47	109.63	106.68
2	3	303	A86	C29-C30-C31	-6.45	170.05	177.66
3	3	313	CLA	C4A-NA-C1A	6.45	109.62	106.68
3	3	316	CLA	C4A-NA-C1A	6.44	109.62	106.68
3	3	315	CLA	C4A-NA-C1A	6.43	109.61	106.68
2	1	304	A86	C33-C32-C31	-6.43	102.96	109.21
2	3	304	A86	C33-C32-C31	-6.43	102.96	109.21
3	1	315	CLA	C4A-NA-C1A	6.43	109.61	106.68
3	4	315	CLA	C4A-NA-C1A	6.42	109.61	106.68
2	4	304	A86	C33-C32-C31	-6.41	102.98	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	405	A86	C33-C32-C31	-6.39	103.00	109.21
3	4	314	CLA	C4A-NA-C1A	6.35	109.58	106.68
2	4	303	A86	C29-C30-C31	-6.25	170.28	177.66
3	4	309	CLA	C4A-NA-C1A	6.24	109.53	106.68
3	3	310	CLA	C4A-NA-C1A	6.24	109.53	106.68
3	2	411	CLA	C4A-NA-C1A	6.23	109.52	106.68
3	1	309	CLA	C4A-NA-C1A	6.16	109.49	106.68
2	2	404	A86	C29-C30-C31	-6.06	170.50	177.66
2	1	303	A86	C29-C30-C31	-6.04	170.54	177.66
2	2	402	A86	O1-C20-C21	-5.70	108.68	115.05
2	1	301	A86	O1-C20-C21	-5.69	108.69	115.05
2	3	301	A86	O1-C20-C21	-5.67	108.71	115.05
2	4	301	A86	O1-C20-C21	-5.64	108.74	115.05
2	1	305	A86	C3-C2-C1	-5.62	119.40	127.28
2	3	305	A86	C3-C2-C1	-5.54	119.51	127.28
5	2	413	KC1	C1D-ND-C4D	5.44	110.13	106.31
5	1	311	KC1	C1D-ND-C4D	5.36	110.07	106.31
5	4	311	KC1	C1D-ND-C4D	5.34	110.06	106.31
5	3	312	KC1	C1D-ND-C4D	5.33	110.06	106.31
2	1	304	A86	C25-C26-C27	-5.33	119.80	127.28
2	4	304	A86	C25-C26-C27	-5.33	119.81	127.28
2	3	304	A86	C25-C26-C27	-5.32	119.81	127.28
2	2	405	A86	C25-C26-C27	-5.32	119.81	127.28
4	3	309	KC2	O2D-CGD-CBD	5.24	120.38	111.23
2	2	406	A86	C3-C2-C1	-5.23	119.94	127.28
4	1	308	KC2	O2D-CGD-CBD	5.22	120.36	111.23
2	4	305	A86	C3-C2-C1	-5.22	119.95	127.28
4	4	308	KC2	O2D-CGD-CBD	5.20	120.32	111.23
4	2	410	KC2	O2D-CGD-CBD	5.16	120.24	111.23
2	3	301	A86	C25-C26-C27	-5.14	120.07	127.28
2	2	403	A86	O4-C38-C39	5.14	120.25	111.09
2	2	407	A86	O4-C38-C39	5.14	120.25	111.09
2	3	305	A86	O1-C20-C21	-5.13	109.31	115.05
2	2	402	A86	C25-C26-C27	-5.13	120.08	127.28
2	4	301	A86	C25-C26-C27	-5.12	120.09	127.28
2	1	301	A86	C25-C26-C27	-5.11	120.11	127.28
2	1	305	A86	O1-C20-C21	-5.09	109.36	115.05
2	3	306	A86	O1-C20-C21	-5.08	109.37	115.05
2	4	306	A86	O1-C20-C21	-5.08	109.38	115.05
5	1	313	KC1	O2D-CGD-CBD	5.07	120.10	111.23
2	4	306	A86	O4-C38-C39	5.07	120.12	111.09
5	2	415	KC1	O2D-CGD-CBD	5.03	120.03	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	407	A86	O1-C20-C21	-5.03	109.43	115.05
5	4	313	KC1	O2D-CGD-CBD	5.03	120.02	111.23
5	3	314	KC1	O2D-CGD-CBD	5.01	119.99	111.23
2	1	306	A86	O4-C38-C39	4.99	119.99	111.09
2	3	302	A86	O4-C38-C39	4.95	119.91	111.09
2	1	302	A86	O4-C38-C39	4.95	119.91	111.09
2	1	304	A86	O1-C20-C21	-4.94	109.53	115.05
2	3	304	A86	O1-C20-C21	-4.93	109.53	115.05
2	4	302	A86	O4-C38-C39	4.93	119.88	111.09
2	4	304	A86	O1-C20-C21	-4.92	109.55	115.05
2	2	405	A86	O1-C20-C21	-4.91	109.56	115.05
2	2	407	A86	O1-C20-C15	-4.91	57.26	59.23
2	3	306	A86	O1-C20-C15	-4.90	57.26	59.23
2	2	406	A86	O1-C20-C21	-4.87	109.61	115.05
2	2	402	A86	O1-C20-C19	-4.86	108.94	113.49
2	1	306	A86	C3-C2-C1	-4.85	120.47	127.28
2	3	301	A86	O1-C20-C19	-4.85	108.95	113.49
2	4	306	A86	O1-C20-C15	-4.83	57.29	59.23
2	3	302	A86	C25-C26-C27	-4.82	120.52	127.28
2	4	302	A86	C25-C26-C27	-4.82	120.52	127.28
2	4	305	A86	O1-C20-C21	-4.82	109.66	115.05
5	3	314	KC1	C1D-ND-C4D	4.80	109.68	106.31
2	1	303	A86	O4-C38-C39	4.80	119.64	111.09
2	4	301	A86	O1-C20-C19	-4.79	109.00	113.49
2	3	303	A86	O4-C38-C39	4.79	119.63	111.09
5	1	313	KC1	C1D-ND-C4D	4.79	109.67	106.31
2	4	303	A86	O4-C38-C39	4.78	119.61	111.09
5	4	313	KC1	C1D-ND-C4D	4.77	109.66	106.31
2	1	301	A86	O1-C20-C19	-4.77	109.02	113.49
2	1	302	A86	C25-C26-C27	-4.77	120.59	127.28
2	2	404	A86	O4-C38-C39	4.76	119.58	111.09
2	2	403	A86	C25-C26-C27	-4.74	120.63	127.28
5	2	415	KC1	C1D-ND-C4D	4.74	109.64	106.31
2	2	406	A86	O4-C38-C39	4.73	119.53	111.09
2	1	305	A86	O4-C38-C39	4.73	119.53	111.09
2	3	305	A86	O4-C38-C39	4.73	119.53	111.09
2	3	301	A86	O4-C38-C39	4.72	119.51	111.09
2	1	301	A86	O4-C38-C39	4.72	119.50	111.09
2	3	306	A86	C3-C2-C1	-4.72	120.67	127.28
2	2	402	A86	O4-C38-C39	4.71	119.49	111.09
2	4	305	A86	O4-C38-C39	4.71	119.49	111.09
2	4	301	A86	O4-C38-C39	4.69	119.46	111.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	310	KC2	O2D-CGD-CBD	4.67	119.40	111.23
2	1	303	A86	C3-C2-C1	-4.67	120.73	127.28
2	1	302	A86	C40-C32-C31	-4.67	106.30	110.47
2	2	403	A86	C40-C32-C31	-4.67	106.30	110.47
2	2	407	A86	C3-C2-C1	-4.66	120.74	127.28
2	4	306	A86	C3-C2-C1	-4.66	120.75	127.28
2	2	404	A86	C3-C2-C1	-4.65	120.76	127.28
2	4	303	A86	C3-C2-C1	-4.65	120.76	127.28
2	3	303	A86	C3-C2-C1	-4.64	120.77	127.28
4	4	310	KC2	O2D-CGD-CBD	4.64	119.33	111.23
4	2	412	KC2	O2D-CGD-CBD	4.60	119.27	111.23
2	1	302	A86	C4-C5-C6	-4.60	120.83	127.28
2	4	304	A86	O4-C38-C39	4.60	119.29	111.09
2	2	405	A86	O4-C38-C39	4.59	119.28	111.09
2	4	302	A86	C40-C32-C31	-4.59	106.36	110.47
2	3	302	A86	C40-C32-C31	-4.59	106.37	110.47
4	3	311	KC2	O2D-CGD-CBD	4.58	119.24	111.23
2	1	304	A86	O4-C38-C39	4.58	119.25	111.09
2	4	302	A86	C4-C5-C6	-4.58	120.86	127.28
2	3	304	A86	O4-C38-C39	4.57	119.24	111.09
2	3	306	A86	O4-C38-C39	4.57	119.24	111.09
2	3	302	A86	C4-C5-C6	-4.56	120.88	127.28
2	1	301	A86	C3-C2-C1	-4.54	120.91	127.28
2	2	403	A86	O1-C20-C21	-4.54	109.98	115.05
2	2	403	A86	C4-C5-C6	-4.54	120.92	127.28
2	4	302	A86	O1-C20-C21	-4.52	110.00	115.05
2	1	302	A86	O1-C20-C21	-4.50	110.02	115.05
2	3	302	A86	O1-C20-C21	-4.50	110.02	115.05
2	1	306	A86	C25-C26-C27	-4.50	120.97	127.28
2	4	301	A86	C3-C2-C1	-4.46	121.02	127.28
2	3	301	A86	C3-C2-C1	-4.45	121.04	127.28
4	1	310	KC2	CHB-C1B-NB	4.44	131.06	124.80
2	2	402	A86	C3-C2-C1	-4.44	121.05	127.28
4	2	412	KC2	CHB-C1B-NB	4.39	130.99	124.80
4	2	410	KC2	CHB-C1B-NB	4.39	130.98	124.80
4	4	308	KC2	CHB-C1B-NB	4.39	130.98	124.80
4	4	310	KC2	CHB-C1B-NB	4.39	130.97	124.80
4	1	308	KC2	CHB-C1B-NB	4.38	130.97	124.80
4	3	309	KC2	CHB-C1B-NB	4.37	130.96	124.80
4	3	311	KC2	CHB-C1B-NB	4.37	130.96	124.80
5	1	311	KC1	O2D-CGD-CBD	4.33	118.81	111.23
5	3	312	KC1	O2D-CGD-CBD	4.30	118.74	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	413	KC1	O2D-CGD-CBD	4.29	118.74	111.23
5	4	311	KC1	O2D-CGD-CBD	4.29	118.72	111.23
2	3	306	A86	C25-C26-C27	-4.27	121.28	127.28
2	1	306	A86	C4-C5-C6	-4.27	121.29	127.28
2	2	407	A86	C25-C26-C27	-4.26	121.30	127.28
2	4	306	A86	C25-C26-C27	-4.25	121.32	127.28
5	1	313	KC1	CHC-C4B-NB	4.20	130.71	124.80
5	2	415	KC1	CHC-C4B-NB	4.19	130.70	124.80
5	1	311	KC1	CHC-C4B-NB	4.18	130.69	124.80
5	2	413	KC1	CHC-C4B-NB	4.18	130.69	124.80
2	2	407	A86	C4-C5-C6	-4.17	121.42	127.28
5	3	314	KC1	CHC-C4B-NB	4.17	130.67	124.80
5	4	311	KC1	CHC-C4B-NB	4.17	130.67	124.80
2	4	306	A86	C4-C5-C6	-4.16	121.44	127.28
5	4	313	KC1	CHC-C4B-NB	4.16	130.66	124.80
2	3	306	A86	C4-C5-C6	-4.16	121.45	127.28
2	2	406	A86	C4-C5-C6	-4.14	121.47	127.28
5	3	312	KC1	CHC-C4B-NB	4.13	130.62	124.80
4	1	308	KC2	CHC-C4B-NB	4.10	130.57	124.80
4	2	410	KC2	C4B-CHC-C1C	-4.10	117.31	126.02
4	2	410	KC2	CHC-C4B-NB	4.10	130.57	124.80
4	1	308	KC2	C4B-CHC-C1C	-4.09	117.32	126.02
2	4	305	A86	C4-C5-C6	-4.09	121.54	127.28
4	3	309	KC2	C4B-CHC-C1C	-4.09	117.33	126.02
4	4	308	KC2	C4B-CHC-C1C	-4.09	117.33	126.02
4	3	309	KC2	CHC-C4B-NB	4.09	130.55	124.80
2	1	306	A86	O1-C20-C21	-4.08	110.48	115.05
4	4	308	KC2	CHC-C4B-NB	4.08	130.54	124.80
2	4	304	A86	C3-C2-C1	-4.04	121.61	127.28
2	3	301	A86	O1-C20-C15	-4.04	57.61	59.23
2	1	304	A86	C3-C2-C1	-4.03	121.62	127.28
2	2	405	A86	C3-C2-C1	-4.03	121.63	127.28
2	1	301	A86	O1-C20-C15	-4.01	57.61	59.23
2	1	306	A86	C29-C30-C31	-4.01	172.94	177.66
2	1	303	A86	C4-C5-C6	-4.00	121.67	127.28
2	4	301	A86	O1-C20-C15	-3.98	57.63	59.23
2	3	304	A86	C3-C2-C1	-3.98	121.69	127.28
4	4	310	KC2	CHC-C4B-NB	3.98	130.40	124.80
2	4	305	A86	O1-C20-C15	-3.98	57.63	59.23
4	2	412	KC2	CHC-C4B-NB	3.98	130.40	124.80
2	1	306	A86	O1-C20-C15	-3.97	57.63	59.23
2	2	404	A86	C4-C5-C6	-3.97	121.71	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	311	KC2	CHC-C4B-NB	3.97	130.39	124.80
4	1	310	KC2	CHC-C4B-NB	3.97	130.38	124.80
2	4	303	A86	C4-C5-C6	-3.96	121.73	127.28
2	2	402	A86	O1-C20-C15	-3.94	57.64	59.23
4	2	412	KC2	C4B-CHC-C1C	-3.94	117.66	126.02
2	3	303	A86	C4-C5-C6	-3.93	121.77	127.28
4	3	311	KC2	C4B-CHC-C1C	-3.92	117.68	126.02
4	4	310	KC2	C4B-CHC-C1C	-3.92	117.69	126.02
4	1	310	KC2	C4B-CHC-C1C	-3.91	117.71	126.02
5	3	314	KC1	CHB-C1B-NB	3.90	130.29	124.80
5	2	415	KC1	CHB-C1B-NB	3.90	130.29	124.80
5	1	313	KC1	CHB-C1B-NB	3.86	130.23	124.80
5	4	313	KC1	CHB-C1B-NB	3.86	130.23	124.80
2	2	406	A86	O1-C20-C15	-3.84	57.68	59.23
2	3	302	A86	C3-C2-C1	-3.84	121.89	127.28
2	1	302	A86	C3-C2-C1	-3.82	121.92	127.28
2	4	302	A86	C3-C2-C1	-3.81	121.94	127.28
2	2	403	A86	C3-C2-C1	-3.80	121.94	127.28
4	2	412	KC2	C1D-CHD-C4C	-3.77	117.39	126.25
4	1	308	KC2	C1D-CHD-C4C	-3.75	117.43	126.25
4	1	310	KC2	C1D-CHD-C4C	-3.74	117.44	126.25
4	4	310	KC2	C1D-CHD-C4C	-3.74	117.44	126.25
4	3	309	KC2	C1D-CHD-C4C	-3.74	117.46	126.25
4	2	410	KC2	C1D-CHD-C4C	-3.73	117.47	126.25
4	3	311	KC2	C1D-CHD-C4C	-3.73	117.48	126.25
4	4	308	KC2	C1D-CHD-C4C	-3.73	117.48	126.25
2	4	306	A86	O1-C20-C19	-3.70	110.02	113.49
2	2	407	A86	O1-C20-C19	-3.69	110.03	113.49
5	1	311	KC1	CHB-C1B-NB	3.68	129.98	124.80
5	4	311	KC1	CHB-C1B-NB	3.66	129.95	124.80
2	3	306	A86	O1-C20-C19	-3.65	110.07	113.49
2	2	402	A86	C12-C11-C13	3.65	121.91	116.00
5	3	312	KC1	CHB-C1B-NB	3.65	129.94	124.80
5	2	413	KC1	CHB-C1B-NB	3.64	129.93	124.80
2	4	305	A86	O1-C20-C19	-3.64	110.08	113.49
2	1	301	A86	C12-C11-C13	3.63	121.89	116.00
2	3	301	A86	C12-C11-C13	3.62	121.88	116.00
2	4	301	A86	C12-C11-C13	3.61	121.85	116.00
5	2	413	KC1	CHD-C1D-ND	3.60	129.45	124.05
4	1	308	KC2	CHC-C4B-C3B	-3.59	119.16	125.21
5	3	312	KC1	CHD-C1D-ND	3.58	129.42	124.05
4	3	309	KC2	CHC-C4B-C3B	-3.58	119.17	125.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	405	A86	C4-C5-C6	-3.57	122.27	127.28
5	1	311	KC1	CHD-C1D-ND	3.57	129.40	124.05
2	1	306	A86	C33-C32-C31	-3.56	105.75	109.21
2	2	407	A86	C33-C32-C31	-3.56	105.75	109.21
5	4	311	KC1	CHD-C1D-ND	3.56	129.39	124.05
2	1	304	A86	O1-C20-C15	-3.56	57.80	59.23
2	1	303	A86	O1-C20-C15	-3.56	57.80	59.23
2	4	304	A86	O1-C20-C15	-3.56	57.80	59.23
2	2	405	A86	O1-C20-C15	-3.55	57.80	59.23
2	3	304	A86	C4-C5-C6	-3.55	122.30	127.28
2	3	305	A86	C4-C5-C6	-3.55	122.30	127.28
2	4	304	A86	C4-C5-C6	-3.54	122.31	127.28
2	1	305	A86	C4-C5-C6	-3.54	122.32	127.28
4	4	308	KC2	CHC-C4B-C3B	-3.54	119.25	125.21
4	2	410	KC2	CHC-C4B-C3B	-3.53	119.25	125.21
2	1	302	A86	O1-C20-C15	-3.53	57.81	59.23
2	1	304	A86	C4-C5-C6	-3.52	122.34	127.28
2	2	404	A86	O1-C20-C15	-3.51	57.82	59.23
2	4	303	A86	C25-C26-C27	-3.51	122.36	127.28
2	2	403	A86	O1-C20-C15	-3.51	57.82	59.23
2	3	304	A86	O1-C20-C15	-3.51	57.82	59.23
2	3	303	A86	C25-C26-C27	-3.50	122.37	127.28
2	4	303	A86	O1-C20-C15	-3.49	57.82	59.23
2	2	404	A86	C25-C26-C27	-3.49	122.38	127.28
2	1	303	A86	C25-C26-C27	-3.49	122.38	127.28
2	3	303	A86	O1-C20-C15	-3.48	57.83	59.23
2	3	302	A86	O1-C20-C19	-3.48	110.23	113.49
2	3	306	A86	C33-C32-C31	-3.47	105.84	109.21
2	2	403	A86	O1-C20-C19	-3.47	110.24	113.49
2	4	302	A86	O1-C20-C19	-3.47	110.24	113.49
5	2	415	KC1	CHD-C1D-ND	3.46	129.25	124.05
4	1	308	KC2	CHD-C1D-ND	3.46	129.24	124.05
2	1	302	A86	O1-C20-C19	-3.46	110.25	113.49
2	1	301	A86	C9-C8-C6	-3.45	116.89	126.36
2	3	302	A86	O1-C20-C15	-3.45	57.84	59.23
4	1	310	KC2	CHB-C1B-C2B	-3.45	118.31	125.49
5	4	313	KC1	CHD-C1D-ND	3.44	129.22	124.05
5	3	314	KC1	CHD-C1D-ND	3.44	129.21	124.05
4	4	308	KC2	CHD-C1D-ND	3.43	129.20	124.05
4	1	310	KC2	CHD-C1D-ND	3.43	129.19	124.05
5	1	313	KC1	CHD-C1D-ND	3.43	129.19	124.05
4	2	412	KC2	CHD-C1D-ND	3.43	129.19	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	310	KC2	CHC-C4B-C3B	-3.42	119.44	125.21
2	4	302	A86	O1-C20-C15	-3.42	57.85	59.23
2	4	301	A86	C9-C8-C6	-3.42	116.99	126.36
4	2	410	KC2	CHD-C1D-ND	3.42	129.17	124.05
4	3	309	KC2	CHB-C1B-C2B	-3.42	118.38	125.49
2	2	402	A86	C9-C8-C6	-3.41	117.01	126.36
2	3	301	A86	C9-C8-C6	-3.41	117.02	126.36
4	4	308	KC2	CHB-C1B-C2B	-3.40	118.41	125.49
4	4	310	KC2	CHD-C1D-ND	3.40	129.15	124.05
4	1	310	KC2	CHC-C4B-C3B	-3.40	119.48	125.21
4	2	412	KC2	C1D-ND-C4D	3.40	108.70	106.31
4	3	311	KC2	CHB-C1B-C2B	-3.39	118.43	125.49
4	1	308	KC2	CHB-C1B-C2B	-3.39	118.43	125.49
4	4	310	KC2	CHB-C1B-C2B	-3.39	118.44	125.49
4	2	410	KC2	CHB-C1B-C2B	-3.39	118.44	125.49
4	2	412	KC2	CHB-C1B-C2B	-3.39	118.44	125.49
4	3	311	KC2	CHD-C1D-ND	3.38	129.13	124.05
4	3	309	KC2	CHD-C1D-ND	3.38	129.12	124.05
4	2	412	KC2	CHC-C4B-C3B	-3.38	119.51	125.21
2	3	305	A86	O1-C20-C15	-3.38	57.87	59.23
4	3	311	KC2	CHC-C4B-C3B	-3.38	119.51	125.21
2	1	305	A86	O1-C20-C15	-3.35	57.88	59.23
2	1	306	A86	C22-C16-C17	3.34	114.84	108.97
4	3	311	KC2	C1D-ND-C4D	3.30	108.63	106.31
4	1	310	KC2	C1D-ND-C4D	3.29	108.62	106.31
2	4	304	A86	C12-C11-C13	3.28	121.31	116.00
2	3	304	A86	C12-C11-C13	3.27	121.30	116.00
2	1	304	A86	C12-C11-C13	3.27	121.30	116.00
5	3	314	KC1	CHC-C4B-C3B	-3.27	119.70	125.21
5	2	415	KC1	CHC-C4B-C3B	-3.26	119.71	125.21
2	2	405	A86	C12-C11-C13	3.26	121.29	116.00
5	1	313	KC1	CHC-C4B-C3B	-3.26	119.71	125.21
4	4	310	KC2	C1D-ND-C4D	3.25	108.59	106.31
2	4	306	A86	C33-C32-C31	-3.25	106.05	109.21
5	4	313	KC1	CHC-C4B-C3B	-3.23	119.76	125.21
5	1	311	KC1	CHC-C4B-C3B	-3.22	119.78	125.21
5	4	311	KC1	CHC-C4B-C3B	-3.21	119.80	125.21
2	1	306	A86	O1-C15-C20	-3.21	56.73	59.45
5	2	413	KC1	CHC-C4B-C3B	-3.21	119.80	125.21
5	3	312	KC1	CHC-C4B-C3B	-3.20	119.81	125.21
3	1	309	CLA	C3B-C4B-NB	-3.17	107.70	110.53
2	2	406	A86	O1-C20-C19	-3.16	110.53	113.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	309	CLA	C3B-C4B-NB	-3.15	107.72	110.53
2	1	306	A86	C23-C16-C22	3.15	111.95	107.37
4	2	410	KC2	C1D-ND-C4D	3.14	108.52	106.31
3	2	411	CLA	C3B-C4B-NB	-3.14	107.73	110.53
4	1	308	KC2	C1D-ND-C4D	3.13	108.51	106.31
2	2	406	A86	C40-C32-C31	-3.13	107.67	110.47
4	4	308	KC2	C1D-ND-C4D	3.12	108.50	106.31
3	3	310	CLA	C3B-C4B-NB	-3.12	107.75	110.53
2	4	305	A86	C40-C32-C31	-3.09	107.70	110.47
3	1	309	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
3	2	411	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
3	3	310	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
4	3	309	KC2	C1D-ND-C4D	3.03	108.44	106.31
3	4	309	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
3	2	416	CLA	C3B-C4B-NB	-3.02	107.83	110.53
3	2	414	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
6	4	316	LMT	C3'-C4'-C5'	-2.99	104.30	110.93
2	1	301	A86	C40-C32-C31	-2.99	107.80	110.47
3	4	312	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
3	4	314	CLA	C3B-C4B-NB	-2.97	107.88	110.53
3	3	313	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
3	3	315	CLA	C3B-C4B-NB	-2.97	107.88	110.53
6	1	316	LMT	C3'-C4'-C5'	-2.97	104.35	110.93
6	2	418	LMT	C3'-C4'-C5'	-2.97	104.35	110.93
5	1	311	KC1	O1D-CGD-CBD	-2.97	118.67	124.52
3	1	312	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
3	4	314	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
3	2	401	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
3	2	408	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
3	1	318	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
3	3	307	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
5	3	312	KC1	O1D-CGD-CBD	-2.95	118.71	124.52
5	4	311	KC1	O1D-CGD-CBD	-2.93	118.73	124.52
3	3	308	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
3	2	416	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
2	1	302	A86	C12-C11-C13	2.92	120.74	116.00
2	3	301	A86	C40-C32-C31	-2.92	107.86	110.47
3	3	315	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
5	1	311	KC1	C2D-C1D-ND	-2.92	107.30	110.33
3	1	314	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
5	2	413	KC1	O1D-CGD-CBD	-2.91	118.78	124.52
2	3	302	A86	C12-C11-C13	2.91	120.71	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	302	A86	C12-C11-C13	2.91	120.71	116.00
2	2	402	A86	C40-C32-C31	-2.90	107.87	110.47
5	2	413	KC1	C2D-C1D-ND	-2.90	107.32	110.33
3	1	307	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
3	4	307	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
3	1	315	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
3	2	409	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
5	4	311	KC1	C2D-C1D-ND	-2.88	107.34	110.33
5	3	312	KC1	C2D-C1D-ND	-2.87	107.35	110.33
3	4	315	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
2	4	301	A86	C40-C32-C31	-2.87	107.91	110.47
2	2	403	A86	C12-C11-C13	2.86	120.64	116.00
3	3	316	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
3	2	417	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
3	1	314	CLA	C3B-C4B-NB	-2.83	108.00	110.53
5	4	313	KC1	C2D-C1D-ND	-2.83	107.39	110.33
3	1	307	CLA	C3B-C4B-NB	-2.82	108.01	110.53
3	4	312	CLA	C3B-C4B-NB	-2.82	108.02	110.53
3	2	414	CLA	C3B-C4B-NB	-2.81	108.02	110.53
5	2	415	KC1	C2D-C1D-ND	-2.81	107.41	110.33
6	1	317	LMT	C1'-O5'-C5'	-2.81	108.23	113.72
6	4	317	LMT	C1'-O5'-C5'	-2.81	108.24	113.72
3	4	307	CLA	C3B-C4B-NB	-2.81	108.02	110.53
6	3	318	LMT	C1'-O5'-C5'	-2.80	108.25	113.72
3	3	313	CLA	C3B-C4B-NB	-2.79	108.04	110.53
5	3	314	KC1	C2D-C1D-ND	-2.79	107.44	110.33
3	3	308	CLA	C3B-C4B-NB	-2.79	108.04	110.53
6	2	419	LMT	C1'-O5'-C5'	-2.79	108.28	113.72
2	2	407	A86	O1-C15-C20	-2.78	57.09	59.45
3	3	316	CLA	C3B-C4B-NB	-2.78	108.05	110.53
6	3	317	LMT	C3'-C4'-C5'	-2.78	104.76	110.93
2	3	306	A86	O1-C15-C20	-2.78	57.09	59.45
3	1	315	CLA	C3B-C4B-NB	-2.78	108.05	110.53
2	2	404	A86	O1-C15-C20	-2.78	57.09	59.45
2	3	303	A86	O1-C15-C20	-2.77	57.10	59.45
5	1	313	KC1	C2D-C1D-ND	-2.77	107.46	110.33
2	4	306	A86	O1-C15-C20	-2.77	57.10	59.45
3	2	409	CLA	C3B-C4B-NB	-2.77	108.06	110.53
2	3	302	A86	C4-C3-C2	-2.76	117.87	123.52
2	1	305	A86	C40-C32-C31	-2.75	108.01	110.47
3	1	312	CLA	C3B-C4B-NB	-2.75	108.08	110.53
2	1	302	A86	C4-C3-C2	-2.74	117.92	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	303	A86	O1-C15-C20	-2.73	57.13	59.45
2	2	403	A86	O4-C38-O5	-2.73	117.72	122.99
2	1	303	A86	O1-C15-C20	-2.73	57.14	59.45
2	3	301	A86	C4-C3-C2	-2.72	117.95	123.52
3	2	417	CLA	C3B-C4B-NB	-2.72	108.10	110.53
2	4	302	A86	C4-C3-C2	-2.72	117.95	123.52
4	1	310	KC2	C1A-NA-C4A	-2.71	105.44	106.68
4	3	311	KC2	C1A-NA-C4A	-2.71	105.44	106.68
2	2	402	A86	C4-C3-C2	-2.71	117.97	123.52
2	1	306	A86	C12-C11-C13	2.71	120.39	116.00
2	4	301	A86	C4-C3-C2	-2.71	117.98	123.52
4	4	310	KC2	C1A-NA-C4A	-2.70	105.45	106.68
2	3	305	A86	C40-C32-C31	-2.70	108.06	110.47
2	2	403	A86	C4-C3-C2	-2.68	118.03	123.52
3	4	315	CLA	C3B-C4B-NB	-2.67	108.14	110.53
5	2	415	KC1	CHB-C1B-C2B	-2.66	119.95	125.49
5	2	413	KC1	O2D-CGD-O1D	-2.66	118.67	123.85
5	3	314	KC1	CHB-C1B-C2B	-2.65	119.97	125.49
5	2	415	KC1	C1D-CHD-C4C	-2.65	120.02	126.25
2	1	302	A86	O4-C38-O5	-2.65	117.88	122.99
3	2	401	CLA	CHB-C4A-NA	2.65	128.22	124.40
3	2	408	CLA	CHB-C4A-NA	2.64	128.22	124.40
5	4	313	KC1	C1D-CHD-C4C	-2.64	120.03	126.25
5	4	313	KC1	CHB-C1B-C2B	-2.64	120.00	125.49
2	3	302	A86	O4-C38-O5	-2.63	117.91	122.99
2	1	301	A86	C4-C3-C2	-2.63	118.14	123.52
2	2	407	A86	O4-C38-O5	-2.63	117.92	122.99
5	1	313	KC1	CHB-C1B-C2B	-2.62	120.03	125.49
3	1	318	CLA	CHB-C4A-NA	2.62	128.18	124.40
3	1	312	CLA	CHB-C4A-NA	2.62	128.18	124.40
5	3	312	KC1	O2D-CGD-O1D	-2.62	118.75	123.85
3	4	312	CLA	CHB-C4A-NA	2.62	128.18	124.40
5	3	314	KC1	C1D-CHD-C4C	-2.61	120.10	126.25
5	4	311	KC1	O2D-CGD-O1D	-2.61	118.76	123.85
5	4	311	KC1	C4B-CHC-C1C	-2.61	120.47	126.02
3	3	307	CLA	CHB-C4A-NA	2.61	128.17	124.40
5	1	313	KC1	C1D-CHD-C4C	-2.61	120.11	126.25
2	4	302	A86	O4-C38-O5	-2.61	117.95	122.99
5	1	311	KC1	C4B-CHC-C1C	-2.61	120.47	126.02
5	3	312	KC1	C1D-CHD-C4C	-2.61	120.11	126.25
6	3	317	LMT	C1'-O5'-C5'	-2.61	108.63	113.72
5	1	311	KC1	C1D-CHD-C4C	-2.61	120.12	126.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	311	KC1	O2D-CGD-O1D	-2.61	118.78	123.85
3	2	414	CLA	CHB-C4A-NA	2.60	128.16	124.40
4	4	310	KC2	O1D-CGD-CBD	-2.60	119.39	124.52
5	2	413	KC1	C1D-CHD-C4C	-2.59	120.15	126.25
3	3	310	CLA	CHB-C4A-NA	2.59	128.14	124.40
5	4	311	KC1	C1D-CHD-C4C	-2.59	120.16	126.25
5	2	413	KC1	C4B-CHC-C1C	-2.59	120.52	126.02
5	3	312	KC1	C4B-CHC-C1C	-2.58	120.53	126.02
3	3	313	CLA	CHB-C4A-NA	2.58	128.12	124.40
5	3	314	KC1	C4B-CHC-C1C	-2.57	120.55	126.02
5	1	311	KC1	CHB-C1B-C2B	-2.57	120.14	125.49
2	2	407	A86	C12-C11-C13	2.57	120.17	116.00
5	2	415	KC1	C4B-CHC-C1C	-2.57	120.56	126.02
2	4	306	A86	O4-C38-O5	-2.57	118.03	122.99
2	3	306	A86	C12-C11-C13	2.57	120.16	116.00
5	1	313	KC1	C4B-CHC-C1C	-2.56	120.57	126.02
4	2	412	KC2	O1D-CGD-CBD	-2.56	119.46	124.52
2	1	304	A86	C10-C9-C8	-2.56	115.78	123.20
3	4	309	CLA	CHB-C4A-NA	2.56	128.09	124.40
5	4	311	KC1	CHB-C1B-C2B	-2.56	120.17	125.49
2	4	304	A86	C10-C9-C8	-2.56	115.79	123.20
2	2	405	A86	C10-C9-C8	-2.56	115.79	123.20
6	4	316	LMT	C1'-O5'-C5'	-2.56	108.72	113.72
4	3	311	KC2	O1D-CGD-CBD	-2.56	119.47	124.52
4	2	412	KC2	C1A-NA-C4A	-2.54	105.52	106.68
3	1	309	CLA	CHB-C4A-NA	2.54	128.07	124.40
2	3	304	A86	C10-C9-C8	-2.54	115.83	123.20
3	2	411	CLA	CHB-C4A-NA	2.54	128.07	124.40
5	4	313	KC1	C4B-CHC-C1C	-2.54	120.63	126.02
2	1	303	A86	O4-C38-O5	-2.54	118.09	122.99
2	1	306	A86	O4-C38-O5	-2.53	118.10	122.99
4	1	310	KC2	O1D-CGD-CBD	-2.53	119.53	124.52
5	2	413	KC1	CHB-C1B-C2B	-2.53	120.23	125.49
2	4	306	A86	C12-C11-C13	2.53	120.10	116.00
5	3	312	KC1	CHB-C1B-C2B	-2.53	120.23	125.49
3	3	315	CLA	CHB-C4A-NA	2.52	128.04	124.40
4	3	309	KC2	CHD-C4C-NC	2.51	128.10	124.31
2	4	303	A86	O4-C38-O5	-2.51	118.14	122.99
3	4	314	CLA	CHB-C4A-NA	2.51	128.03	124.40
2	1	305	A86	C9-C8-C6	-2.51	119.47	126.36
2	3	304	A86	C3-C4-C5	-2.51	118.38	123.52
2	1	304	A86	C3-C4-C5	-2.50	118.40	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	307	CLA	CHB-C4A-NA	2.50	128.01	124.40
3	4	307	CLA	CHB-C4A-NA	2.50	128.01	124.40
3	1	314	CLA	CHB-C4A-NA	2.50	128.00	124.40
2	2	405	A86	C3-C4-C5	-2.49	118.41	123.52
3	1	309	CLA	C1-C2-C3	-2.49	122.11	126.20
3	2	416	CLA	CHB-C4A-NA	2.49	128.00	124.40
6	1	316	LMT	C1'-O5'-C5'	-2.49	108.86	113.72
2	3	303	A86	O4-C38-O5	-2.49	118.19	122.99
2	1	306	A86	O1-C20-C19	2.49	115.82	113.49
2	3	305	A86	C9-C8-C6	-2.49	119.54	126.36
3	4	309	CLA	C1-C2-C3	-2.49	122.12	126.20
3	2	409	CLA	CHB-C4A-NA	2.48	127.99	124.40
2	4	304	A86	C3-C4-C5	-2.48	118.44	123.52
3	3	308	CLA	CHB-C4A-NA	2.48	127.98	124.40
4	2	410	KC2	CHD-C4C-NC	2.48	128.05	124.31
2	1	303	A86	C3-C4-C5	-2.48	118.45	123.52
3	2	411	CLA	C1-C2-C3	-2.48	122.14	126.20
2	2	404	A86	O4-C38-O5	-2.47	118.22	122.99
2	3	305	A86	C3-C4-C5	-2.47	118.46	123.52
4	1	308	KC2	CHD-C4C-NC	2.47	128.03	124.31
2	1	305	A86	O1-C15-C20	-2.47	57.36	59.45
2	4	303	A86	C3-C4-C5	-2.47	118.47	123.52
4	2	410	KC2	O1D-CGD-CBD	-2.47	119.65	124.52
3	2	417	CLA	CHB-C4A-NA	2.46	127.95	124.40
3	1	315	CLA	CHB-C4A-NA	2.46	127.95	124.40
2	2	402	A86	O4-C38-O5	-2.46	118.25	122.99
2	2	405	A86	O1-C20-C19	-2.46	111.19	113.49
3	3	316	CLA	CHB-C4A-NA	2.46	127.95	124.40
2	3	305	A86	O1-C15-C20	-2.46	57.37	59.45
2	3	306	A86	O4-C38-O5	-2.46	118.25	122.99
2	2	404	A86	C3-C4-C5	-2.45	118.50	123.52
3	3	310	CLA	C1-C2-C3	-2.45	122.18	126.20
2	3	305	A86	C25-C24-C1	-2.45	119.64	126.36
2	4	305	A86	O4-C38-O5	-2.45	118.26	122.99
2	1	305	A86	C3-C4-C5	-2.45	118.50	123.52
2	2	406	A86	O4-C38-O5	-2.45	118.26	122.99
2	1	304	A86	O1-C20-C19	-2.45	111.20	113.49
2	3	303	A86	C3-C4-C5	-2.45	118.51	123.52
2	1	306	A86	C3-C4-C5	-2.45	118.52	123.52
4	4	308	KC2	CHD-C4C-NC	2.44	127.99	124.31
2	1	304	A86	O1-C15-C20	-2.44	57.38	59.45
2	2	405	A86	O1-C15-C20	-2.44	57.38	59.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	301	A86	O4-C38-O5	-2.44	118.28	122.99
2	3	304	A86	O1-C15-C20	-2.44	57.38	59.45
2	3	301	A86	O4-C38-O5	-2.44	118.29	122.99
3	4	315	CLA	CHB-C4A-NA	2.44	127.92	124.40
2	4	301	A86	O4-C38-O5	-2.44	118.29	122.99
2	1	305	A86	C25-C24-C1	-2.43	119.69	126.36
2	3	304	A86	O1-C20-C19	-2.43	111.21	113.49
2	1	305	A86	O4-C38-O5	-2.43	118.30	122.99
4	4	308	KC2	O1D-CGD-CBD	-2.43	119.72	124.52
2	3	305	A86	O4-C38-O5	-2.43	118.30	122.99
2	4	304	A86	O1-C20-C19	-2.43	111.22	113.49
3	2	409	CLA	C1-C2-C3	-2.41	122.25	126.20
6	2	418	LMT	C1'-O5'-C5'	-2.40	109.03	113.72
4	1	308	KC2	O1D-CGD-CBD	-2.40	119.78	124.52
2	4	304	A86	O1-C15-C20	-2.40	57.42	59.45
3	4	307	CLA	C1-C2-C3	-2.39	122.28	126.20
3	1	307	CLA	C1-C2-C3	-2.39	122.29	126.20
2	3	306	A86	C3-C4-C5	-2.38	118.64	123.52
4	3	309	KC2	O1D-CGD-CBD	-2.38	119.82	124.52
5	3	314	KC1	O1D-CGD-CBD	-2.37	119.84	124.52
3	2	401	CLA	C3B-C4B-NB	-2.37	108.41	110.53
4	3	311	KC2	O2D-CGD-O1D	-2.36	119.25	123.85
4	4	310	KC2	CHD-C4C-NC	2.35	127.85	124.31
4	1	310	KC2	CHB-C4A-C3A	-2.34	121.33	125.03
5	2	415	KC1	O1D-CGD-CBD	-2.34	119.90	124.52
5	4	313	KC1	O1D-CGD-CBD	-2.34	119.91	124.52
4	1	310	KC2	CHD-C4C-NC	2.34	127.83	124.31
4	2	412	KC2	CHD-C4C-NC	2.34	127.83	124.31
3	1	318	CLA	C3B-C4B-NB	-2.33	108.45	110.53
3	3	308	CLA	C1-C2-C3	-2.33	122.38	126.20
2	2	406	A86	C3-C4-C5	-2.33	118.75	123.52
4	4	310	KC2	O2D-CGD-O1D	-2.33	119.31	123.85
4	2	412	KC2	O2D-CGD-O1D	-2.33	119.32	123.85
5	1	313	KC1	O1D-CGD-CBD	-2.33	119.93	124.52
2	4	304	A86	O4-C38-O5	-2.32	118.50	122.99
2	4	305	A86	C3-C4-C5	-2.32	118.76	123.52
3	2	408	CLA	C3B-C4B-NB	-2.32	108.46	110.53
4	3	311	KC2	CHD-C4C-NC	2.32	127.81	124.31
2	1	304	A86	O4-C38-O5	-2.32	118.51	122.99
2	4	305	A86	C25-C24-C1	-2.32	120.01	126.36
2	2	405	A86	O4-C38-O5	-2.31	118.53	122.99
2	3	304	A86	O4-C38-O5	-2.31	118.54	122.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	307	CLA	C3B-C4B-NB	-2.30	108.47	110.53
4	4	310	KC2	CHB-C4A-C3A	-2.30	121.39	125.03
4	1	310	KC2	O2D-CGD-O1D	-2.30	119.37	123.85
2	3	305	A86	C12-C11-C13	2.29	119.71	116.00
4	2	412	KC2	CHB-C4A-C3A	-2.29	121.42	125.03
4	3	311	KC2	CHB-C4A-C3A	-2.28	121.42	125.03
2	1	305	A86	C12-C11-C13	2.27	119.69	116.00
2	3	303	A86	C26-C25-C24	-2.27	116.62	123.20
4	2	410	KC2	CHB-C4A-C3A	-2.27	121.45	125.03
2	2	406	A86	C25-C24-C1	-2.27	120.15	126.36
2	2	406	A86	O1-C15-C20	-2.27	57.53	59.45
2	3	301	A86	C25-C24-C1	-2.27	120.15	126.36
4	2	410	KC2	O2D-CGD-O1D	-2.26	119.44	123.85
2	2	402	A86	C25-C24-C1	-2.26	120.16	126.36
2	4	306	A86	C3-C4-C5	-2.26	118.90	123.52
2	2	407	A86	C3-C4-C5	-2.26	118.90	123.52
2	4	305	A86	O1-C15-C20	-2.25	57.54	59.45
2	4	303	A86	C26-C25-C24	-2.25	116.67	123.20
4	2	412	KC2	C1B-CHB-C4A	-2.25	121.23	126.02
4	1	310	KC2	C1B-CHB-C4A	-2.25	121.24	126.02
2	1	301	A86	C25-C24-C1	-2.25	120.20	126.36
2	2	404	A86	C26-C25-C24	-2.25	116.69	123.20
2	4	301	A86	C25-C24-C1	-2.25	120.20	126.36
2	1	303	A86	C26-C25-C24	-2.25	116.69	123.20
4	4	308	KC2	C1A-NA-C4A	-2.24	105.66	106.68
4	3	309	KC2	O2D-CGD-O1D	-2.24	119.49	123.85
4	4	308	KC2	O2D-CGD-O1D	-2.24	119.49	123.85
3	2	409	CLA	CMB-C2B-C1B	-2.24	122.02	125.42
6	3	318	LMT	C3'-C4'-C5'	-2.23	106.00	110.93
6	1	317	LMT	C3'-C4'-C5'	-2.22	106.00	110.93
4	1	308	KC2	O2A-CGA-O1A	-2.22	118.18	122.70
4	4	310	KC2	C1B-CHB-C4A	-2.22	121.30	126.02
4	3	309	KC2	CHB-C4A-C3A	-2.22	121.52	125.03
6	2	419	LMT	C3'-C4'-C5'	-2.22	106.01	110.93
3	3	308	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
4	4	308	KC2	CHB-C4A-C3A	-2.21	121.53	125.03
4	1	308	KC2	O2D-CGD-O1D	-2.21	119.54	123.85
4	3	311	KC2	C1B-CHB-C4A	-2.21	121.32	126.02
4	1	308	KC2	CHB-C4A-C3A	-2.21	121.54	125.03
6	4	317	LMT	C3'-C4'-C5'	-2.21	106.04	110.93
3	1	307	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
3	4	307	CLA	CMB-C2B-C1B	-2.20	122.07	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	410	KC2	O2A-CGA-O1A	-2.20	118.22	122.70
2	1	306	A86	C10-C9-C8	-2.19	116.85	123.20
4	3	309	KC2	O2A-CGA-O1A	-2.19	118.24	122.70
2	2	404	A86	C10-C9-C8	-2.19	116.85	123.20
2	1	303	A86	C10-C9-C8	-2.19	116.85	123.20
4	4	308	KC2	O2A-CGA-O1A	-2.19	118.25	122.70
4	1	308	KC2	C1A-NA-C4A	-2.18	105.68	106.68
4	3	309	KC2	C1A-NA-C4A	-2.18	105.68	106.68
2	1	302	A86	C10-C9-C8	-2.18	116.88	123.20
2	3	302	A86	C10-C9-C8	-2.18	116.88	123.20
2	4	303	A86	C10-C9-C8	-2.17	116.90	123.20
2	3	303	A86	C10-C9-C8	-2.17	116.91	123.20
2	4	302	A86	C10-C9-C8	-2.17	116.92	123.20
2	1	301	A86	C8-C6-C5	2.16	122.41	119.01
4	4	308	KC2	C1B-CHB-C4A	-2.16	121.44	126.02
4	2	410	KC2	C1B-CHB-C4A	-2.15	121.44	126.02
4	3	309	KC2	C1B-CHB-C4A	-2.15	121.44	126.02
2	2	406	A86	C9-C8-C6	-2.15	120.46	126.36
3	1	318	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
3	2	401	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
3	2	408	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
5	1	311	KC1	C2A-C3A-C4A	2.14	108.02	106.41
5	2	413	KC1	C2A-C3A-C4A	2.14	108.02	106.41
5	2	415	KC1	O2D-CGD-O1D	-2.14	119.68	123.85
3	1	312	CLA	C2A-C1A-CHA	2.14	127.58	123.87
3	3	307	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
4	1	308	KC2	C1B-CHB-C4A	-2.14	121.48	126.02
5	3	314	KC1	O2D-CGD-O1D	-2.13	119.69	123.85
3	3	313	CLA	C2A-C1A-CHA	2.13	127.57	123.87
4	2	410	KC2	C1A-NA-C4A	-2.13	105.71	106.68
2	1	301	A86	O1-C15-C20	-2.13	57.65	59.45
3	4	312	CLA	C2A-C1A-CHA	2.12	127.55	123.87
2	1	303	A86	C12-C11-C13	2.12	119.44	116.00
2	2	403	A86	C10-C9-C8	-2.12	117.05	123.20
2	2	404	A86	C12-C11-C13	2.12	119.43	116.00
2	4	301	A86	O1-C15-C20	-2.12	57.66	59.45
5	4	313	KC1	O2D-CGD-O1D	-2.12	119.73	123.85
2	4	302	A86	O1-C15-C20	-2.11	57.66	59.45
5	3	312	KC1	C2A-C3A-C4A	2.11	107.99	106.41
3	2	414	CLA	C2A-C1A-CHA	2.11	127.52	123.87
5	1	313	KC1	O2D-CGD-O1D	-2.11	119.75	123.85
2	4	303	A86	C12-C11-C13	2.10	119.41	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	303	A86	C12-C11-C13	2.10	119.41	116.00
2	2	402	A86	O1-C15-C20	-2.10	57.67	59.45
2	3	301	A86	O1-C15-C20	-2.10	57.67	59.45
2	2	407	A86	C21-C20-C15	2.10	130.12	123.35
2	1	302	A86	O1-C15-C20	-2.09	57.68	59.45
5	4	311	KC1	C2A-C3A-C4A	2.09	107.98	106.41
2	4	304	A86	C41-C32-C31	2.09	112.34	110.47
2	2	405	A86	C25-C24-C1	-2.09	120.64	126.36
2	4	306	A86	C21-C20-C15	2.08	130.08	123.35
2	2	403	A86	O1-C15-C20	-2.08	57.69	59.45
2	3	306	A86	C29-C30-C31	-2.08	175.21	177.66
3	3	310	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
2	1	304	A86	C41-C32-C31	2.07	112.33	110.47
2	3	306	A86	C21-C20-C15	2.07	130.04	123.35
2	3	304	A86	C41-C32-C31	2.07	112.33	110.47
2	3	302	A86	C21-C20-C15	2.07	130.03	123.35
2	4	305	A86	C9-C8-C6	-2.07	120.69	126.36
2	3	302	A86	O1-C15-C20	-2.07	57.70	59.45
2	1	304	A86	C25-C24-C1	-2.06	120.71	126.36
3	4	309	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
2	2	407	A86	C29-C30-C31	-2.06	175.23	177.66
6	4	316	LMT	O5B-C5B-C4B	2.06	113.41	109.70
2	3	301	A86	C8-C6-C5	2.06	122.25	119.01
2	4	304	A86	C25-C24-C1	-2.06	120.72	126.36
2	4	302	A86	C21-C20-C15	2.05	129.98	123.35
2	2	402	A86	C8-C6-C5	2.05	122.24	119.01
2	4	303	A86	C33-C32-C31	-2.05	107.22	109.21
2	3	304	A86	C25-C24-C1	-2.05	120.74	126.36
3	2	411	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
2	4	303	A86	C21-C20-C15	2.05	129.96	123.35
2	2	403	A86	C21-C20-C15	2.05	129.96	123.35
2	2	405	A86	C4-C3-C2	-2.05	119.33	123.52
2	1	302	A86	C21-C20-C15	2.04	129.95	123.35
6	3	317	LMT	O5B-C5B-C4B	2.04	113.38	109.70
2	2	404	A86	C21-C20-C15	2.04	129.94	123.35
2	2	405	A86	C41-C32-C31	2.04	112.30	110.47
3	4	307	CLA	CMB-C2B-C3B	2.04	131.35	126.55
3	3	307	CLA	C1-C2-C3	-2.04	122.86	126.20
2	4	304	A86	C4-C3-C2	-2.04	119.35	123.52
2	3	304	A86	C4-C3-C2	-2.04	119.35	123.52
2	1	303	A86	C21-C20-C15	2.04	129.93	123.35
3	1	309	CLA	O2A-CGA-O1A	-2.04	118.53	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	303	A86	C21-C20-C15	2.04	129.92	123.35
3	2	409	CLA	CMB-C2B-C3B	2.03	131.33	126.55
3	2	414	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
2	1	304	A86	C4-C3-C2	-2.03	119.36	123.52
3	3	313	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
3	1	307	CLA	CMB-C2B-C3B	2.03	131.32	126.55
2	4	301	A86	C8-C6-C5	2.02	122.19	119.01
3	3	308	CLA	CMB-C2B-C3B	2.02	131.30	126.55
3	4	312	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
6	1	316	LMT	O5B-C5B-C4B	2.01	113.33	109.70
6	2	418	LMT	O5B-C5B-C4B	2.01	113.33	109.70
3	1	312	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
4	2	412	KC2	C2D-C1D-ND	-2.00	108.25	110.33
3	1	318	CLA	C1-C2-C3	-2.00	122.92	126.20
3	2	401	CLA	C1-C2-C3	-2.00	122.92	126.20
3	2	408	CLA	C1-C2-C3	-2.00	122.92	126.20

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	1	307	CLA	ND
3	1	309	CLA	ND
3	1	312	CLA	ND
3	1	314	CLA	ND
3	1	315	CLA	ND
3	1	318	CLA	ND
3	2	401	CLA	ND
3	2	408	CLA	ND
3	2	409	CLA	ND
3	2	411	CLA	ND
3	2	414	CLA	ND
3	2	416	CLA	ND
3	2	417	CLA	ND
3	3	307	CLA	ND
3	3	308	CLA	ND
3	3	310	CLA	ND
3	3	313	CLA	ND
3	3	315	CLA	ND
3	3	316	CLA	ND
3	4	307	CLA	ND
3	4	309	CLA	ND
3	4	312	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	4	314	CLA	ND
3	4	315	CLA	ND

All (594) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1	301	A86	C13-C14-C15-O1
2	1	302	A86	C10-C11-C13-O
2	1	302	A86	C12-C11-C13-O
2	1	302	A86	C13-C14-C15-O1
2	1	305	A86	C-C1-C24-C25
2	1	305	A86	C2-C1-C24-C25
2	1	305	A86	C11-C10-C9-C8
2	1	305	A86	C24-C25-C26-C27
2	1	306	A86	C10-C11-C13-O
2	1	306	A86	C12-C11-C13-O
2	1	306	A86	C39-C38-O4-C34
2	2	402	A86	C13-C14-C15-O1
2	2	403	A86	C10-C11-C13-O
2	2	403	A86	C12-C11-C13-O
2	2	403	A86	C13-C14-C15-O1
2	2	406	A86	C11-C10-C9-C8
2	2	406	A86	C10-C11-C13-C14
2	2	406	A86	C12-C11-C13-O
2	2	406	A86	C12-C11-C13-C14
2	2	406	A86	C13-C14-C15-O1
2	2	406	A86	C24-C25-C26-C27
2	2	407	A86	C12-C11-C13-O
2	2	407	A86	C13-C14-C15-O1
2	3	301	A86	C13-C14-C15-O1
2	3	302	A86	C10-C11-C13-O
2	3	302	A86	C12-C11-C13-O
2	3	302	A86	C13-C14-C15-O1
2	3	305	A86	C-C1-C24-C25
2	3	305	A86	C2-C1-C24-C25
2	3	305	A86	C11-C10-C9-C8
2	3	305	A86	C24-C25-C26-C27
2	3	306	A86	C12-C11-C13-O
2	3	306	A86	C13-C14-C15-O1
2	4	301	A86	C13-C14-C15-O1
2	4	302	A86	C10-C11-C13-O
2	4	302	A86	C12-C11-C13-O

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	4	302	A86	C13-C14-C15-O1
2	4	305	A86	C11-C10-C9-C8
2	4	305	A86	C10-C11-C13-C14
2	4	305	A86	C12-C11-C13-O
2	4	305	A86	C12-C11-C13-C14
2	4	305	A86	C13-C14-C15-O1
2	4	305	A86	C24-C25-C26-C27
2	4	306	A86	C12-C11-C13-O
2	4	306	A86	C13-C14-C15-O1
3	1	314	CLA	C1A-C2A-CAA-CBA
3	1	315	CLA	CBA-CGA-O2A-C1
3	2	417	CLA	CBA-CGA-O2A-C1
3	2	417	CLA	O1A-CGA-O2A-C1
3	3	316	CLA	CBA-CGA-O2A-C1
3	4	315	CLA	CBA-CGA-O2A-C1
3	4	315	CLA	O1A-CGA-O2A-C1
4	1	308	KC2	C3A-C2A-CAA-CBA
4	1	308	KC2	C2B-C3B-CAB-CBB
4	1	308	KC2	CHA-CBD-CGD-O1D
4	1	308	KC2	CHA-CBD-CGD-O2D
4	1	310	KC2	C2B-C3B-CAB-CBB
4	1	310	KC2	C4B-C3B-CAB-CBB
4	1	310	KC2	C2C-C3C-CAC-CBC
4	2	410	KC2	C3A-C2A-CAA-CBA
4	2	410	KC2	C2B-C3B-CAB-CBB
4	2	410	KC2	C4B-C3B-CAB-CBB
4	2	410	KC2	CHA-CBD-CGD-O1D
4	2	410	KC2	CHA-CBD-CGD-O2D
4	2	412	KC2	C2B-C3B-CAB-CBB
4	2	412	KC2	C4B-C3B-CAB-CBB
4	2	412	KC2	C2C-C3C-CAC-CBC
4	2	412	KC2	C2A-CAA-CBA-CGA
4	3	309	KC2	C3A-C2A-CAA-CBA
4	3	309	KC2	C2B-C3B-CAB-CBB
4	3	309	KC2	CHA-CBD-CGD-O1D
4	3	309	KC2	CHA-CBD-CGD-O2D
4	3	311	KC2	C2B-C3B-CAB-CBB
4	3	311	KC2	C4B-C3B-CAB-CBB
4	3	311	KC2	C2A-CAA-CBA-CGA
4	4	308	KC2	C3A-C2A-CAA-CBA
4	4	308	KC2	C2B-C3B-CAB-CBB
4	4	308	KC2	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	4	308	KC2	CHA-CBD-CGD-O1D
4	4	308	KC2	CHA-CBD-CGD-O2D
4	4	310	KC2	C2B-C3B-CAB-CBB
4	4	310	KC2	C4B-C3B-CAB-CBB
4	4	310	KC2	C2A-CAA-CBA-CGA
5	1	311	KC1	C2B-C3B-CAB-CBB
5	1	313	KC1	C2B-C3B-CAB-CBB
5	2	413	KC1	C2B-C3B-CAB-CBB
5	2	415	KC1	C2B-C3B-CAB-CBB
5	2	415	KC1	CHA-CBD-CGD-O1D
5	3	312	KC1	C2B-C3B-CAB-CBB
5	3	314	KC1	C2B-C3B-CAB-CBB
5	3	314	KC1	CHA-CBD-CGD-O1D
5	4	311	KC1	C2B-C3B-CAB-CBB
5	4	313	KC1	C2B-C3B-CAB-CBB
5	4	313	KC1	CHA-CBD-CGD-O1D
6	1	317	LMT	O5'-C1'-O1'-C1
6	2	419	LMT	O5'-C1'-O1'-C1
6	3	318	LMT	O5'-C1'-O1'-C1
6	4	317	LMT	O5'-C1'-O1'-C1
3	1	314	CLA	O1D-CGD-O2D-CED
2	1	302	A86	C39-C38-O4-C34
2	1	303	A86	C39-C38-O4-C34
2	1	304	A86	C39-C38-O4-C34
2	2	403	A86	C39-C38-O4-C34
2	2	404	A86	C39-C38-O4-C34
2	2	405	A86	C39-C38-O4-C34
2	2	407	A86	C39-C38-O4-C34
2	3	302	A86	C39-C38-O4-C34
2	3	303	A86	C39-C38-O4-C34
2	3	304	A86	C39-C38-O4-C34
2	3	306	A86	C39-C38-O4-C34
2	4	302	A86	C39-C38-O4-C34
2	4	303	A86	C39-C38-O4-C34
2	4	304	A86	C39-C38-O4-C34
2	4	306	A86	C39-C38-O4-C34
3	1	314	CLA	CBD-CGD-O2D-CED
3	2	416	CLA	CBD-CGD-O2D-CED
3	3	315	CLA	CBD-CGD-O2D-CED
3	4	314	CLA	CBD-CGD-O2D-CED
3	1	315	CLA	O1A-CGA-O2A-C1
3	3	316	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	1	316	LMT	O5B-C1B-O1B-C4'
6	2	418	LMT	O5B-C1B-O1B-C4'
6	3	317	LMT	O5B-C1B-O1B-C4'
6	4	316	LMT	O5B-C1B-O1B-C4'
3	2	416	CLA	O1D-CGD-O2D-CED
3	3	315	CLA	O1D-CGD-O2D-CED
3	4	314	CLA	O1D-CGD-O2D-CED
3	1	312	CLA	O1A-CGA-O2A-C1
3	2	414	CLA	O1A-CGA-O2A-C1
3	3	313	CLA	O1A-CGA-O2A-C1
3	4	312	CLA	O1A-CGA-O2A-C1
6	1	316	LMT	C2B-C1B-O1B-C4'
6	2	418	LMT	C2B-C1B-O1B-C4'
6	3	317	LMT	C2B-C1B-O1B-C4'
6	4	316	LMT	C2B-C1B-O1B-C4'
2	1	302	A86	O5-C38-O4-C34
2	1	303	A86	O5-C38-O4-C34
2	1	304	A86	O5-C38-O4-C34
2	1	306	A86	O5-C38-O4-C34
2	2	403	A86	O5-C38-O4-C34
2	2	404	A86	O5-C38-O4-C34
2	2	405	A86	O5-C38-O4-C34
2	2	407	A86	O5-C38-O4-C34
2	3	302	A86	O5-C38-O4-C34
2	3	303	A86	O5-C38-O4-C34
2	3	304	A86	O5-C38-O4-C34
2	3	306	A86	O5-C38-O4-C34
2	4	302	A86	O5-C38-O4-C34
2	4	303	A86	O5-C38-O4-C34
2	4	304	A86	O5-C38-O4-C34
2	4	306	A86	O5-C38-O4-C34
2	1	306	A86	C35-C34-O4-C38
2	2	407	A86	C35-C34-O4-C38
2	4	306	A86	C35-C34-O4-C38
3	4	314	CLA	CBA-CGA-O2A-C1
3	1	309	CLA	CBD-CGD-O2D-CED
3	2	411	CLA	CBD-CGD-O2D-CED
3	3	310	CLA	CBD-CGD-O2D-CED
3	4	309	CLA	CBD-CGD-O2D-CED
3	2	416	CLA	O1A-CGA-O2A-C1
3	3	315	CLA	O1A-CGA-O2A-C1
5	1	313	KC1	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	2	415	KC1	CAA-CBA-CGA-O2A
5	3	314	KC1	CAA-CBA-CGA-O2A
5	4	313	KC1	CAA-CBA-CGA-O2A
3	1	314	CLA	CBA-CGA-O2A-C1
3	2	416	CLA	CBA-CGA-O2A-C1
3	3	315	CLA	CBA-CGA-O2A-C1
3	1	315	CLA	CBD-CGD-O2D-CED
3	1	314	CLA	C2A-CAA-CBA-CGA
3	1	312	CLA	CBA-CGA-O2A-C1
3	2	414	CLA	CBA-CGA-O2A-C1
3	3	313	CLA	CBA-CGA-O2A-C1
3	4	312	CLA	CBA-CGA-O2A-C1
3	4	314	CLA	O1A-CGA-O2A-C1
2	1	301	A86	C39-C38-O4-C34
2	1	305	A86	C39-C38-O4-C34
2	2	402	A86	C39-C38-O4-C34
2	2	406	A86	C39-C38-O4-C34
2	3	301	A86	C39-C38-O4-C34
2	3	305	A86	C39-C38-O4-C34
2	4	301	A86	C39-C38-O4-C34
2	4	305	A86	C39-C38-O4-C34
2	1	301	A86	O5-C38-O4-C34
2	1	305	A86	O5-C38-O4-C34
2	2	402	A86	O5-C38-O4-C34
2	2	406	A86	O5-C38-O4-C34
2	3	301	A86	O5-C38-O4-C34
2	3	305	A86	O5-C38-O4-C34
2	4	301	A86	O5-C38-O4-C34
2	4	305	A86	O5-C38-O4-C34
3	4	315	CLA	CBD-CGD-O2D-CED
5	1	313	KC1	CAA-CBA-CGA-O1A
5	2	415	KC1	CAA-CBA-CGA-O1A
5	4	313	KC1	CAA-CBA-CGA-O1A
3	1	314	CLA	O1A-CGA-O2A-C1
2	1	303	A86	C35-C34-O4-C38
2	2	404	A86	C35-C34-O4-C38
2	3	303	A86	C35-C34-O4-C38
2	4	303	A86	C35-C34-O4-C38
3	3	307	CLA	C11-C12-C13-C14
6	1	317	LMT	C2'-C1'-O1'-C1
6	2	419	LMT	C2'-C1'-O1'-C1
6	3	318	LMT	C2'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	4	317	LMT	C2'-C1'-O1'-C1
2	1	304	A86	C35-C34-O4-C38
2	2	405	A86	C35-C34-O4-C38
2	3	304	A86	C35-C34-O4-C38
2	4	304	A86	C35-C34-O4-C38
2	2	406	A86	C-C1-C24-C25
2	2	406	A86	C7-C6-C8-C9
2	4	305	A86	C-C1-C24-C25
2	4	305	A86	C7-C6-C8-C9
3	2	416	CLA	C2A-CAA-CBA-CGA
3	3	315	CLA	C2A-CAA-CBA-CGA
3	3	310	CLA	O1D-CGD-O2D-CED
2	3	301	A86	C35-C34-O4-C38
2	3	306	A86	C35-C34-O4-C38
6	2	419	LMT	O5B-C5B-C6B-O6B
6	3	318	LMT	O5B-C5B-C6B-O6B
6	4	317	LMT	O5B-C5B-C6B-O6B
3	1	309	CLA	O1D-CGD-O2D-CED
3	2	411	CLA	O1D-CGD-O2D-CED
2	1	301	A86	C35-C34-O4-C38
2	1	305	A86	C35-C34-O4-C38
2	2	402	A86	C35-C34-O4-C38
2	3	305	A86	C35-C34-O4-C38
2	4	301	A86	C35-C34-O4-C38
6	1	317	LMT	O5B-C5B-C6B-O6B
3	4	309	CLA	O1D-CGD-O2D-CED
3	4	314	CLA	C2A-CAA-CBA-CGA
2	2	403	A86	C33-C34-O4-C38
2	2	406	A86	C35-C34-O4-C38
2	4	305	A86	C35-C34-O4-C38
3	1	315	CLA	O1D-CGD-O2D-CED
3	3	307	CLA	C8-C10-C11-C12
4	3	311	KC2	CBD-CGD-O2D-CED
4	1	310	KC2	C2A-CAA-CBA-CGA
4	1	308	KC2	CAA-CBA-CGA-O2A
4	2	410	KC2	CAA-CBA-CGA-O2A
4	3	309	KC2	CAA-CBA-CGA-O2A
4	4	308	KC2	CAA-CBA-CGA-O2A
2	1	302	A86	C35-C34-O4-C38
2	3	302	A86	C35-C34-O4-C38
2	4	302	A86	C35-C34-O4-C38
3	1	318	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	2	408	CLA	C10-C11-C12-C13
3	4	315	CLA	O1D-CGD-O2D-CED
3	2	401	CLA	C10-C11-C12-C13
2	2	403	A86	C35-C34-O4-C38
2	4	302	A86	C33-C34-O4-C38
4	2	412	KC2	CBD-CGD-O2D-CED
6	3	317	LMT	C2'-C1'-O1'-C1
2	1	302	A86	C33-C34-O4-C38
2	3	302	A86	C33-C34-O4-C38
6	1	316	LMT	O5'-C5'-C6'-O6'
6	3	317	LMT	O5'-C5'-C6'-O6'
6	4	316	LMT	O5'-C5'-C6'-O6'
2	2	406	A86	C2-C1-C24-C25
2	2	406	A86	C5-C6-C8-C9
2	4	305	A86	C2-C1-C24-C25
2	4	305	A86	C5-C6-C8-C9
6	3	317	LMT	O5'-C1'-O1'-C1
6	2	418	LMT	O5'-C5'-C6'-O6'
5	3	314	KC1	CAA-CBA-CGA-O1A
2	2	402	A86	C33-C34-O4-C38
2	4	301	A86	C33-C34-O4-C38
3	1	312	CLA	C3A-C2A-CAA-CBA
3	2	414	CLA	C3A-C2A-CAA-CBA
3	3	313	CLA	C3A-C2A-CAA-CBA
3	4	312	CLA	C3A-C2A-CAA-CBA
2	1	301	A86	C33-C34-O4-C38
2	3	301	A86	C33-C34-O4-C38
2	1	303	A86	C33-C34-O4-C38
4	4	310	KC2	CBD-CGD-O2D-CED
2	3	303	A86	C33-C34-O4-C38
6	4	316	LMT	O5'-C1'-O1'-C1
3	2	401	CLA	C8-C10-C11-C12
2	1	305	A86	C33-C34-O4-C38
2	2	406	A86	C33-C34-O4-C38
2	4	305	A86	C33-C34-O4-C38
3	1	318	CLA	C8-C10-C11-C12
3	2	408	CLA	C8-C10-C11-C12
2	1	305	A86	C7-C6-C8-C9
2	3	305	A86	C7-C6-C8-C9
2	1	305	A86	C5-C6-C8-C9
2	3	305	A86	C5-C6-C8-C9
4	1	308	KC2	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	2	410	KC2	C2C-C3C-CAC-CBC
4	3	309	KC2	C2C-C3C-CAC-CBC
4	3	311	KC2	C2C-C3C-CAC-CBC
4	4	308	KC2	C2C-C3C-CAC-CBC
4	4	310	KC2	C2C-C3C-CAC-CBC
2	2	404	A86	C33-C34-O4-C38
2	3	305	A86	C33-C34-O4-C38
2	4	303	A86	C33-C34-O4-C38
3	1	318	CLA	C5-C6-C7-C8
3	2	408	CLA	C5-C6-C7-C8
4	1	308	KC2	C4B-C3B-CAB-CBB
4	3	309	KC2	C4B-C3B-CAB-CBB
5	1	311	KC1	C4B-C3B-CAB-CBB
5	1	313	KC1	C4B-C3B-CAB-CBB
5	2	413	KC1	C4B-C3B-CAB-CBB
5	2	415	KC1	C4B-C3B-CAB-CBB
5	3	312	KC1	C4B-C3B-CAB-CBB
5	3	314	KC1	C4B-C3B-CAB-CBB
5	4	311	KC1	C4B-C3B-CAB-CBB
5	4	313	KC1	C4B-C3B-CAB-CBB
3	2	401	CLA	C5-C6-C7-C8
2	3	306	A86	C33-C34-O4-C38
4	1	310	KC2	CBD-CGD-O2D-CED
3	3	307	CLA	C10-C11-C12-C13
3	1	312	CLA	C1A-C2A-CAA-CBA
3	2	414	CLA	C1A-C2A-CAA-CBA
3	3	313	CLA	C1A-C2A-CAA-CBA
3	4	312	CLA	C1A-C2A-CAA-CBA
3	1	318	CLA	C6-C7-C8-C10
3	2	401	CLA	C6-C7-C8-C10
3	2	408	CLA	C6-C7-C8-C10
4	1	310	KC2	CAA-CBA-CGA-O2A
4	2	412	KC2	CAA-CBA-CGA-O2A
4	4	310	KC2	CAA-CBA-CGA-O2A
3	2	401	CLA	C6-C7-C8-C9
3	2	408	CLA	C6-C7-C8-C9
3	3	307	CLA	C14-C13-C15-C16
2	2	405	A86	C33-C34-O4-C38
2	4	304	A86	C33-C34-O4-C38
2	1	304	A86	C33-C34-O4-C38
2	3	304	A86	C33-C34-O4-C38
5	1	311	KC1	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	2	413	KC1	CAA-CBA-CGA-O2A
5	4	311	KC1	CAA-CBA-CGA-O2A
3	3	316	CLA	CBD-CGD-O2D-CED
5	3	312	KC1	CAA-CBA-CGA-O2A
6	4	316	LMT	C2-C1-O1'-C1'
3	1	318	CLA	C6-C7-C8-C9
3	2	417	CLA	C4B-C3B-CAB-CBB
6	4	316	LMT	C2'-C1'-O1'-C1
3	3	307	CLA	C12-C13-C15-C16
3	1	314	CLA	C3A-C2A-CAA-CBA
3	1	307	CLA	C5-C6-C7-C8
3	2	409	CLA	C5-C6-C7-C8
2	1	301	A86	C12-C11-C13-O
2	1	303	A86	C12-C11-C13-O
2	1	304	A86	C12-C11-C13-O
2	1	305	A86	C12-C11-C13-O
2	2	402	A86	C12-C11-C13-O
2	2	404	A86	C12-C11-C13-O
2	2	405	A86	C12-C11-C13-O
2	3	301	A86	C12-C11-C13-O
2	3	303	A86	C12-C11-C13-O
2	3	304	A86	C12-C11-C13-O
2	3	305	A86	C12-C11-C13-O
2	4	301	A86	C12-C11-C13-O
2	4	303	A86	C12-C11-C13-O
2	4	304	A86	C12-C11-C13-O
2	1	301	A86	C10-C11-C13-O
2	1	303	A86	C10-C11-C13-O
2	1	304	A86	C10-C11-C13-O
2	1	305	A86	C10-C11-C13-O
2	2	402	A86	C10-C11-C13-O
2	2	404	A86	C10-C11-C13-O
2	2	405	A86	C10-C11-C13-O
2	2	406	A86	C10-C11-C13-O
2	2	407	A86	C10-C11-C13-O
2	3	301	A86	C10-C11-C13-O
2	3	303	A86	C10-C11-C13-O
2	3	304	A86	C10-C11-C13-O
2	3	305	A86	C10-C11-C13-O
2	3	306	A86	C10-C11-C13-O
2	4	301	A86	C10-C11-C13-O
2	4	303	A86	C10-C11-C13-O

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	4	304	A86	C10-C11-C13-O
2	4	305	A86	C10-C11-C13-O
2	4	306	A86	C10-C11-C13-O
3	3	310	CLA	C4-C3-C5-C6
3	3	310	CLA	C2-C3-C5-C6
3	4	307	CLA	C5-C6-C7-C8
3	3	307	CLA	CBA-CGA-O2A-C1
3	1	318	CLA	C12-C13-C15-C16
3	2	401	CLA	C12-C13-C15-C16
3	2	408	CLA	C12-C13-C15-C16
3	2	409	CLA	CBA-CGA-O2A-C1
3	1	309	CLA	C6-C7-C8-C10
3	2	411	CLA	C6-C7-C8-C10
3	4	309	CLA	C6-C7-C8-C10
3	3	310	CLA	C6-C7-C8-C10
4	1	310	KC2	C4C-C3C-CAC-CBC
4	2	412	KC2	C4C-C3C-CAC-CBC
4	4	310	KC2	C4C-C3C-CAC-CBC
3	1	318	CLA	C14-C13-C15-C16
3	2	401	CLA	C14-C13-C15-C16
3	2	408	CLA	C14-C13-C15-C16
3	1	309	CLA	C6-C7-C8-C9
3	4	309	CLA	C6-C7-C8-C9
3	3	307	CLA	O1A-CGA-O2A-C1
6	1	317	LMT	O5'-C5'-C6'-O6'
3	1	307	CLA	CBA-CGA-O2A-C1
6	2	419	LMT	O5'-C5'-C6'-O6'
6	3	318	LMT	O5'-C5'-C6'-O6'
3	3	310	CLA	C6-C7-C8-C9
3	3	308	CLA	C5-C6-C7-C8
6	4	317	LMT	O5'-C5'-C6'-O6'
3	2	411	CLA	C6-C7-C8-C9
3	1	309	CLA	C4B-C3B-CAB-CBB
3	1	315	CLA	C4B-C3B-CAB-CBB
3	2	411	CLA	C4B-C3B-CAB-CBB
3	3	310	CLA	C4B-C3B-CAB-CBB
3	3	316	CLA	C4B-C3B-CAB-CBB
3	4	309	CLA	C4B-C3B-CAB-CBB
3	4	315	CLA	C4B-C3B-CAB-CBB
3	2	411	CLA	C4-C3-C5-C6
3	2	409	CLA	O1A-CGA-O2A-C1
3	3	316	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	4	307	CLA	CBA-CGA-O2A-C1
3	1	307	CLA	O1A-CGA-O2A-C1
3	4	309	CLA	C4-C3-C5-C6
3	4	314	CLA	C3A-C2A-CAA-CBA
4	1	308	KC2	C1A-C2A-CAA-CBA
4	2	410	KC2	C1A-C2A-CAA-CBA
4	3	309	KC2	C1A-C2A-CAA-CBA
4	4	308	KC2	C1A-C2A-CAA-CBA
3	1	309	CLA	C4-C3-C5-C6
2	1	302	A86	C13-C14-C15-C20
2	1	303	A86	C13-C14-C15-C20
2	1	305	A86	C13-C14-C15-C20
2	2	403	A86	C13-C14-C15-C20
2	2	404	A86	C13-C14-C15-C20
2	3	302	A86	C13-C14-C15-C20
2	3	303	A86	C13-C14-C15-C20
2	3	305	A86	C13-C14-C15-C20
2	4	302	A86	C13-C14-C15-C20
2	4	303	A86	C13-C14-C15-C20
6	1	316	LMT	O5'-C1'-O1'-C1
3	1	309	CLA	C2A-CAA-CBA-CGA
3	2	411	CLA	C2A-CAA-CBA-CGA
3	4	309	CLA	C2A-CAA-CBA-CGA
3	4	307	CLA	O1A-CGA-O2A-C1
2	1	301	A86	C10-C11-C13-C14
2	1	302	A86	C10-C11-C13-C14
2	1	303	A86	C10-C11-C13-C14
2	1	304	A86	C10-C11-C13-C14
2	1	305	A86	C10-C11-C13-C14
2	1	306	A86	C10-C11-C13-C14
2	2	402	A86	C10-C11-C13-C14
2	2	403	A86	C10-C11-C13-C14
2	2	404	A86	C10-C11-C13-C14
2	2	405	A86	C10-C11-C13-C14
2	2	407	A86	C10-C11-C13-C14
2	3	301	A86	C10-C11-C13-C14
2	3	302	A86	C10-C11-C13-C14
2	3	303	A86	C10-C11-C13-C14
2	3	304	A86	C10-C11-C13-C14
2	3	305	A86	C10-C11-C13-C14
2	3	306	A86	C10-C11-C13-C14
2	4	301	A86	C10-C11-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	4	302	A86	C10-C11-C13-C14
2	4	303	A86	C10-C11-C13-C14
2	4	304	A86	C10-C11-C13-C14
2	4	306	A86	C10-C11-C13-C14
3	1	312	CLA	CHA-CBD-CGD-O1D
3	1	312	CLA	CHA-CBD-CGD-O2D
3	2	414	CLA	CHA-CBD-CGD-O1D
3	2	414	CLA	CHA-CBD-CGD-O2D
3	3	313	CLA	CHA-CBD-CGD-O1D
3	3	313	CLA	CHA-CBD-CGD-O2D
3	4	312	CLA	CHA-CBD-CGD-O1D
3	4	312	CLA	CHA-CBD-CGD-O2D
4	2	412	KC2	CHA-CBD-CGD-O1D
5	1	313	KC1	CHA-CBD-CGD-O1D
5	1	313	KC1	CHA-CBD-CGD-O2D
5	2	415	KC1	CHA-CBD-CGD-O2D
5	3	314	KC1	CHA-CBD-CGD-O2D
5	4	313	KC1	CHA-CBD-CGD-O2D
3	1	315	CLA	C2B-C3B-CAB-CBB
3	2	417	CLA	C2B-C3B-CAB-CBB
3	3	316	CLA	C2B-C3B-CAB-CBB
3	4	315	CLA	C2B-C3B-CAB-CBB
2	1	301	A86	C12-C11-C13-C14
2	1	302	A86	C12-C11-C13-C14
2	1	303	A86	C12-C11-C13-C14
2	1	304	A86	C12-C11-C13-C14
2	1	305	A86	C12-C11-C13-C14
2	1	306	A86	C12-C11-C13-C14
2	2	402	A86	C12-C11-C13-C14
2	2	403	A86	C12-C11-C13-C14
2	2	404	A86	C12-C11-C13-C14
2	2	405	A86	C12-C11-C13-C14
2	2	407	A86	C12-C11-C13-C14
2	3	301	A86	C12-C11-C13-C14
2	3	302	A86	C12-C11-C13-C14
2	3	303	A86	C12-C11-C13-C14
2	3	304	A86	C12-C11-C13-C14
2	3	305	A86	C12-C11-C13-C14
2	3	306	A86	C12-C11-C13-C14
2	4	301	A86	C12-C11-C13-C14
2	4	302	A86	C12-C11-C13-C14
2	4	303	A86	C12-C11-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	4	304	A86	C12-C11-C13-C14
2	4	306	A86	C12-C11-C13-C14
3	2	411	CLA	C2-C3-C5-C6
3	3	310	CLA	C2A-CAA-CBA-CGA
3	4	309	CLA	C2-C3-C5-C6
6	2	418	LMT	O5'-C1'-O1'-C1
2	1	302	A86	C13-C14-C15-C16
2	2	403	A86	C13-C14-C15-C16
2	2	407	A86	C13-C14-C15-C16
2	3	302	A86	C13-C14-C15-C16
2	3	306	A86	C13-C14-C15-C16
2	4	302	A86	C13-C14-C15-C16
2	4	306	A86	C13-C14-C15-C16
6	1	316	LMT	C2-C1-O1'-C1'
6	1	317	LMT	C4'-C5'-C6'-O6'
3	1	309	CLA	C2-C3-C5-C6
6	3	318	LMT	C4B-C5B-C6B-O6B
4	1	308	KC2	C4C-C3C-CAC-CBC
4	2	410	KC2	C4C-C3C-CAC-CBC
4	3	309	KC2	C4C-C3C-CAC-CBC
4	3	311	KC2	C4C-C3C-CAC-CBC
4	4	308	KC2	C4C-C3C-CAC-CBC
3	3	308	CLA	C11-C10-C8-C7
6	3	318	LMT	C4'-C5'-C6'-O6'
6	4	317	LMT	C4B-C5B-C6B-O6B
6	2	419	LMT	C4B-C5B-C6B-O6B
6	2	419	LMT	C4'-C5'-C6'-O6'
6	4	317	LMT	C4'-C5'-C6'-O6'
3	1	307	CLA	C11-C10-C8-C9
3	1	318	CLA	C11-C10-C8-C9
3	2	401	CLA	C11-C10-C8-C9
3	2	408	CLA	C11-C10-C8-C9
3	3	308	CLA	C11-C10-C8-C9
3	4	307	CLA	C11-C10-C8-C9
6	1	317	LMT	C4B-C5B-C6B-O6B
4	1	308	KC2	CAA-CBA-CGA-O1A
4	3	309	KC2	CAA-CBA-CGA-O1A
3	4	314	CLA	C1A-C2A-CAA-CBA
3	1	309	CLA	C2B-C3B-CAB-CBB
3	2	411	CLA	C2B-C3B-CAB-CBB
3	3	310	CLA	C2B-C3B-CAB-CBB
3	4	309	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	1	307	CLA	C11-C10-C8-C7
3	2	409	CLA	C11-C10-C8-C7
3	3	307	CLA	C11-C12-C13-C15
3	4	307	CLA	C11-C10-C8-C7
3	1	307	CLA	C2A-CAA-CBA-CGA
3	2	409	CLA	C2A-CAA-CBA-CGA
6	2	419	LMT	C3-C4-C5-C6
6	1	317	LMT	C3-C4-C5-C6
6	4	317	LMT	C3-C4-C5-C6
3	4	307	CLA	C2A-CAA-CBA-CGA
3	2	409	CLA	C11-C10-C8-C9
6	3	318	LMT	C3-C4-C5-C6
2	1	306	A86	C33-C34-O4-C38
2	2	407	A86	C33-C34-O4-C38
3	3	310	CLA	C3-C5-C6-C7
6	2	419	LMT	C2-C1-O1'-C1'
6	3	318	LMT	C2-C1-O1'-C1'
6	4	317	LMT	C2-C1-O1'-C1'
2	4	306	A86	C33-C34-O4-C38
4	4	308	KC2	CAA-CBA-CGA-O1A
6	1	317	LMT	O1'-C1-C2-C3
3	3	308	CLA	C2A-CAA-CBA-CGA
4	2	410	KC2	CAA-CBA-CGA-O1A
6	2	419	LMT	O1'-C1-C2-C3
3	2	416	CLA	C3A-C2A-CAA-CBA
3	3	315	CLA	C3A-C2A-CAA-CBA
6	3	318	LMT	O1'-C1-C2-C3
6	1	316	LMT	C2'-C1'-O1'-C1
6	4	317	LMT	O1'-C1-C2-C3
3	3	308	CLA	O1A-CGA-O2A-C1
3	1	312	CLA	C2B-C3B-CAB-CBB
3	3	308	CLA	CBA-CGA-O2A-C1
3	2	411	CLA	C3-C5-C6-C7
3	3	313	CLA	CAA-CBA-CGA-O2A
3	1	312	CLA	CAA-CBA-CGA-O2A
3	2	414	CLA	CAA-CBA-CGA-O2A
3	4	312	CLA	CAA-CBA-CGA-O2A
4	3	311	KC2	CAA-CBA-CGA-O2A
6	1	317	LMT	C2-C1-O1'-C1'
6	2	418	LMT	C2-C1-O1'-C1'
3	4	309	CLA	C3-C5-C6-C7
3	1	309	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	2	418	LMT	C2'-C1'-O1'-C1
3	1	312	CLA	CAA-CBA-CGA-O1A
3	2	414	CLA	CAA-CBA-CGA-O1A
3	3	313	CLA	CAA-CBA-CGA-O1A
3	4	312	CLA	CAA-CBA-CGA-O1A
5	1	313	KC1	C1A-C2A-CAA-CBA
5	4	313	KC1	C1A-C2A-CAA-CBA
4	2	412	KC2	CAD-CBD-CGD-O2D
4	3	311	KC2	CAD-CBD-CGD-O2D
4	4	310	KC2	CAD-CBD-CGD-O2D
3	4	315	CLA	CAA-CBA-CGA-O2A
4	1	308	KC2	O1D-CGD-O2D-CED

There are no ring outliers.

41 monomers are involved in 62 short contacts:

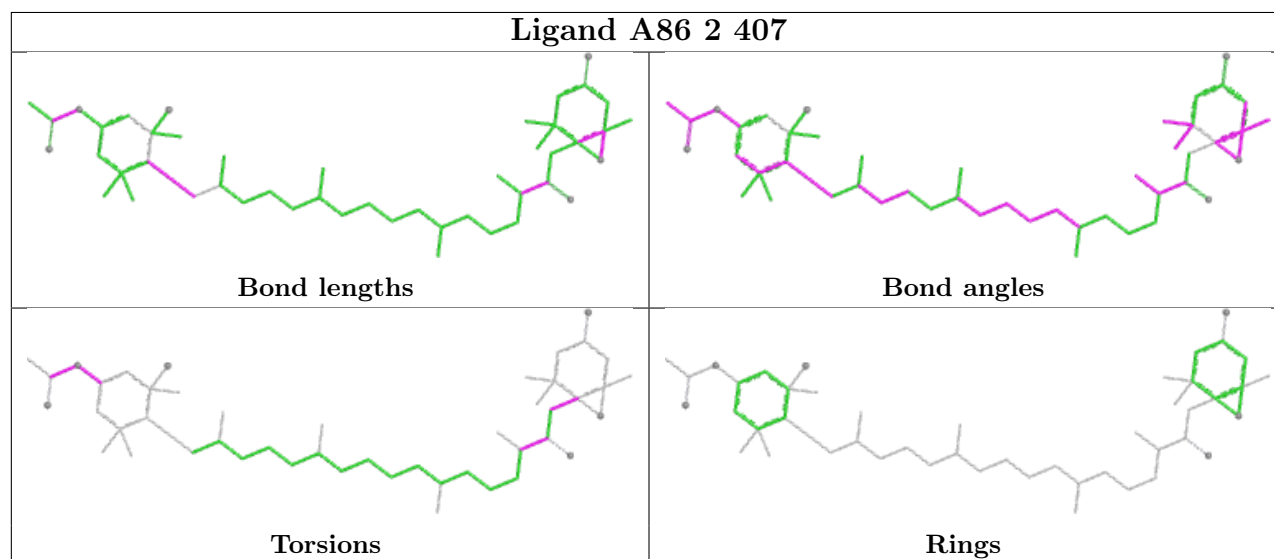
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1	314	CLA	1	0
3	4	312	CLA	2	0
3	1	318	CLA	3	0
3	1	312	CLA	3	0
2	3	304	A86	1	0
4	2	410	KC2	1	0
2	2	402	A86	1	0
2	1	304	A86	1	0
5	2	415	KC1	1	0
6	4	317	LMT	1	0
4	4	308	KC2	1	0
3	4	307	CLA	3	0
3	1	307	CLA	2	0
3	3	307	CLA	2	0
3	2	414	CLA	3	0
6	3	318	LMT	2	0
3	3	308	CLA	2	0
6	1	317	LMT	2	0
6	2	419	LMT	1	0
3	3	313	CLA	3	0
2	2	403	A86	1	0
3	4	309	CLA	1	0
3	2	416	CLA	3	0
3	2	401	CLA	3	0
2	1	305	A86	1	0

Continued on next page...

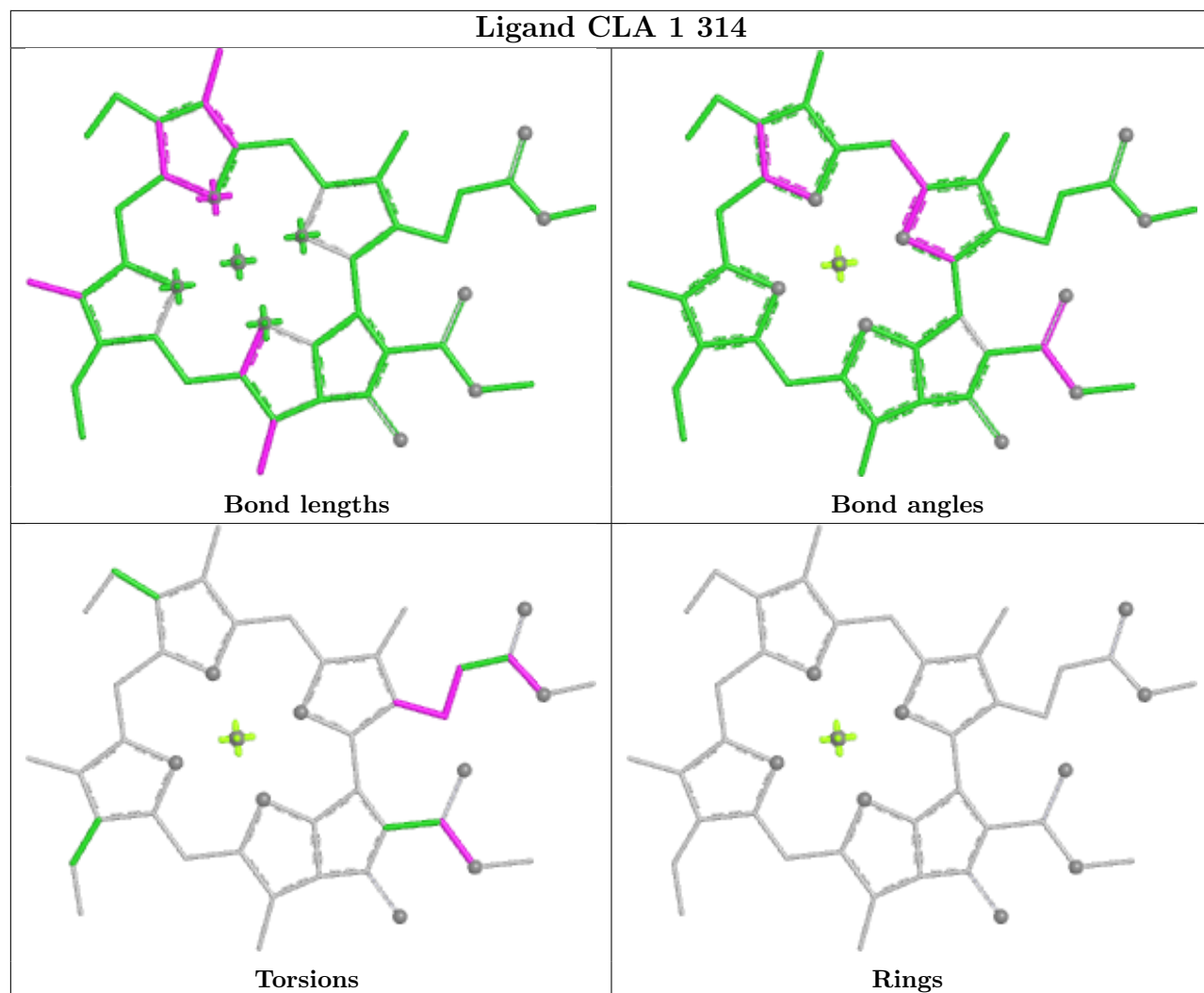
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1	315	CLA	2	0
2	4	304	A86	1	0
3	3	316	CLA	1	0
3	1	309	CLA	1	0
3	4	314	CLA	2	0
4	3	311	KC2	1	0
3	2	411	CLA	1	0
4	1	308	KC2	1	0
2	2	405	A86	1	0
3	3	315	CLA	3	0
3	2	409	CLA	2	0
4	3	309	KC2	1	0
5	4	313	KC1	1	0
3	2	408	CLA	4	0
5	1	313	KC1	1	0
2	3	305	A86	1	0

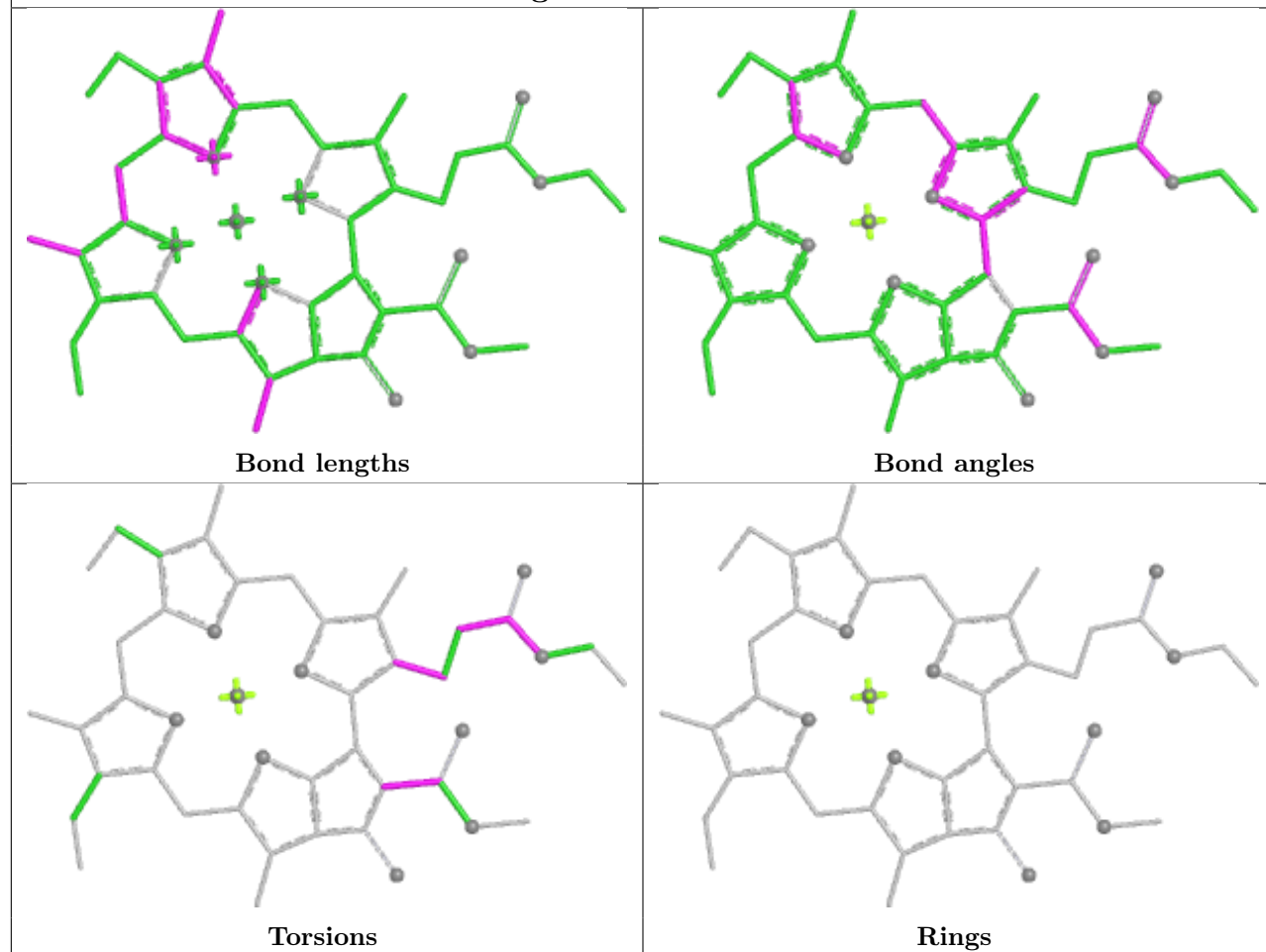
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



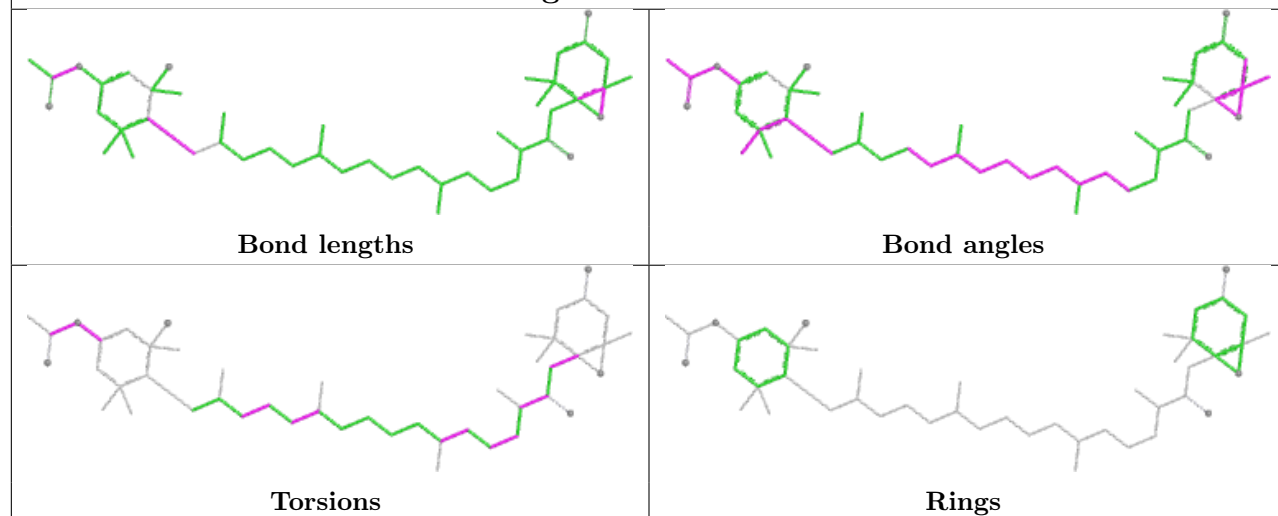
Ligand CLA 1 314



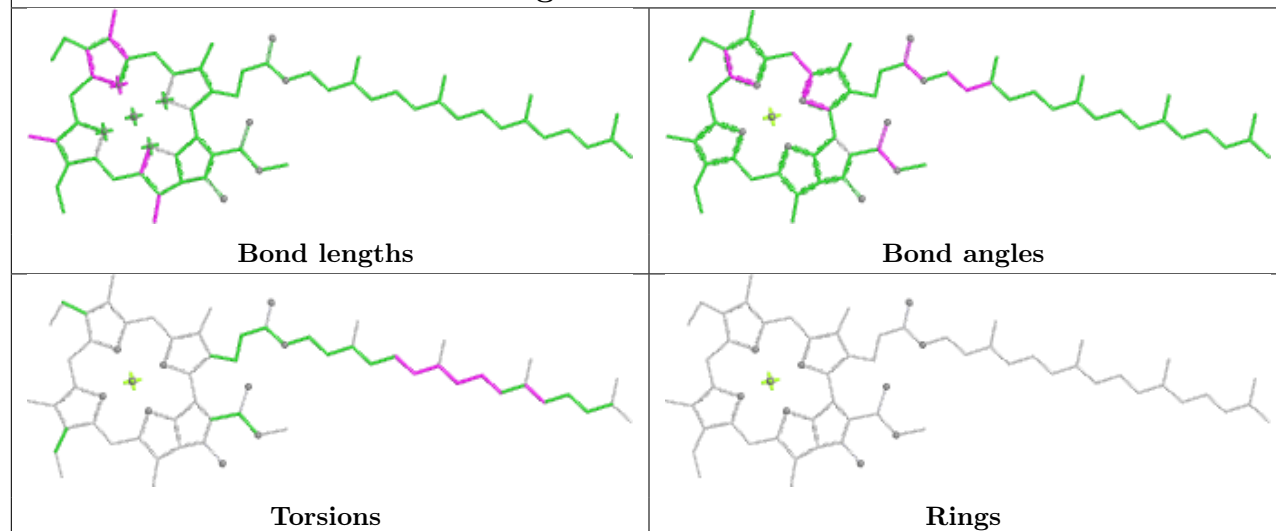
Ligand CLA 4 312



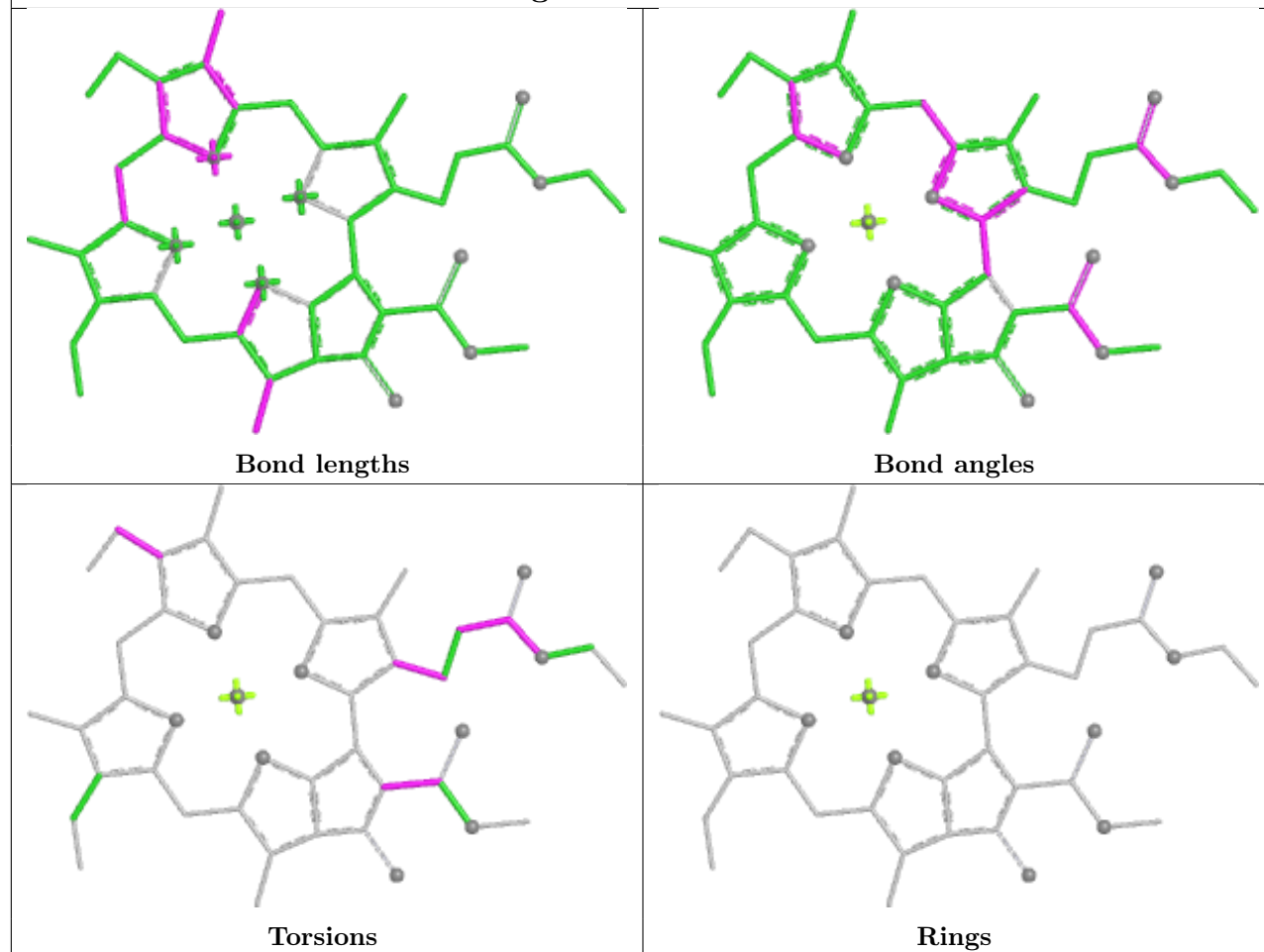
Ligand A86 4 305

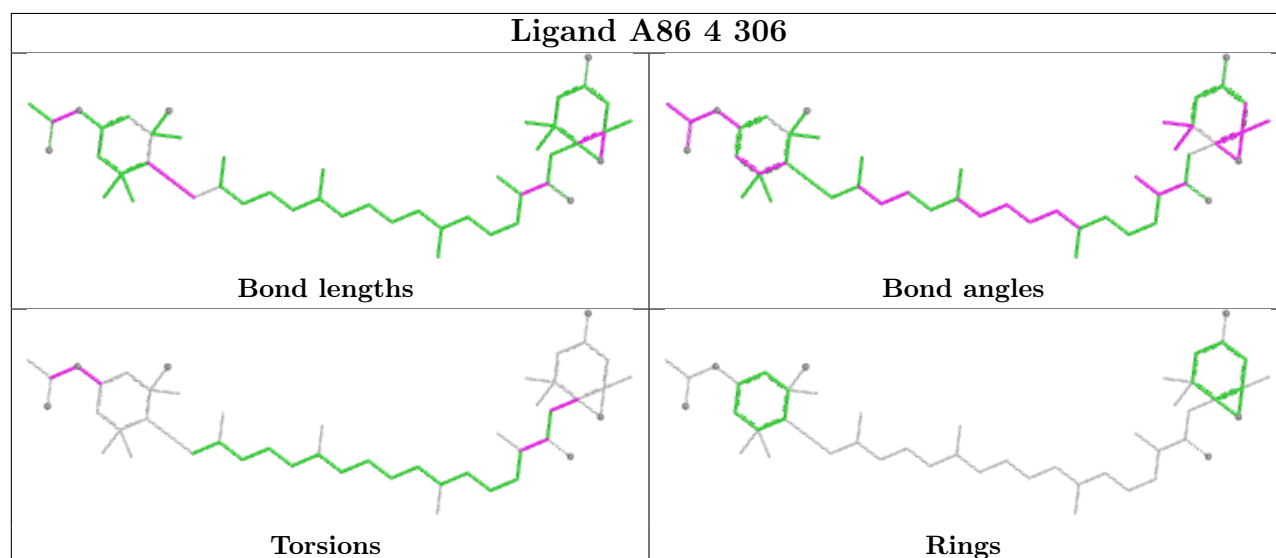
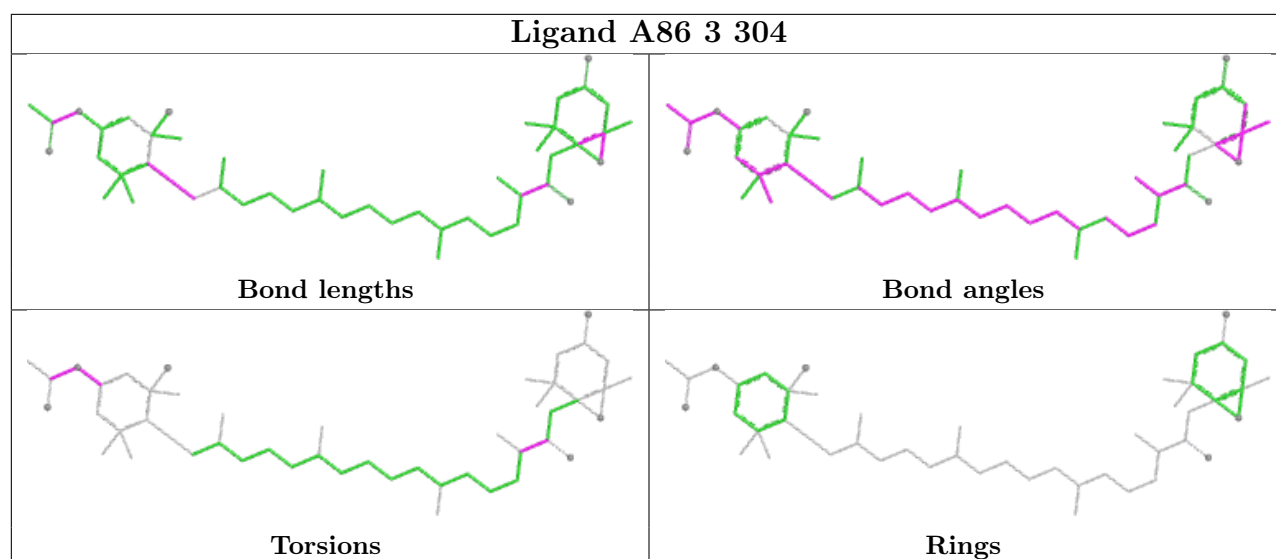


Ligand CLA 1 318

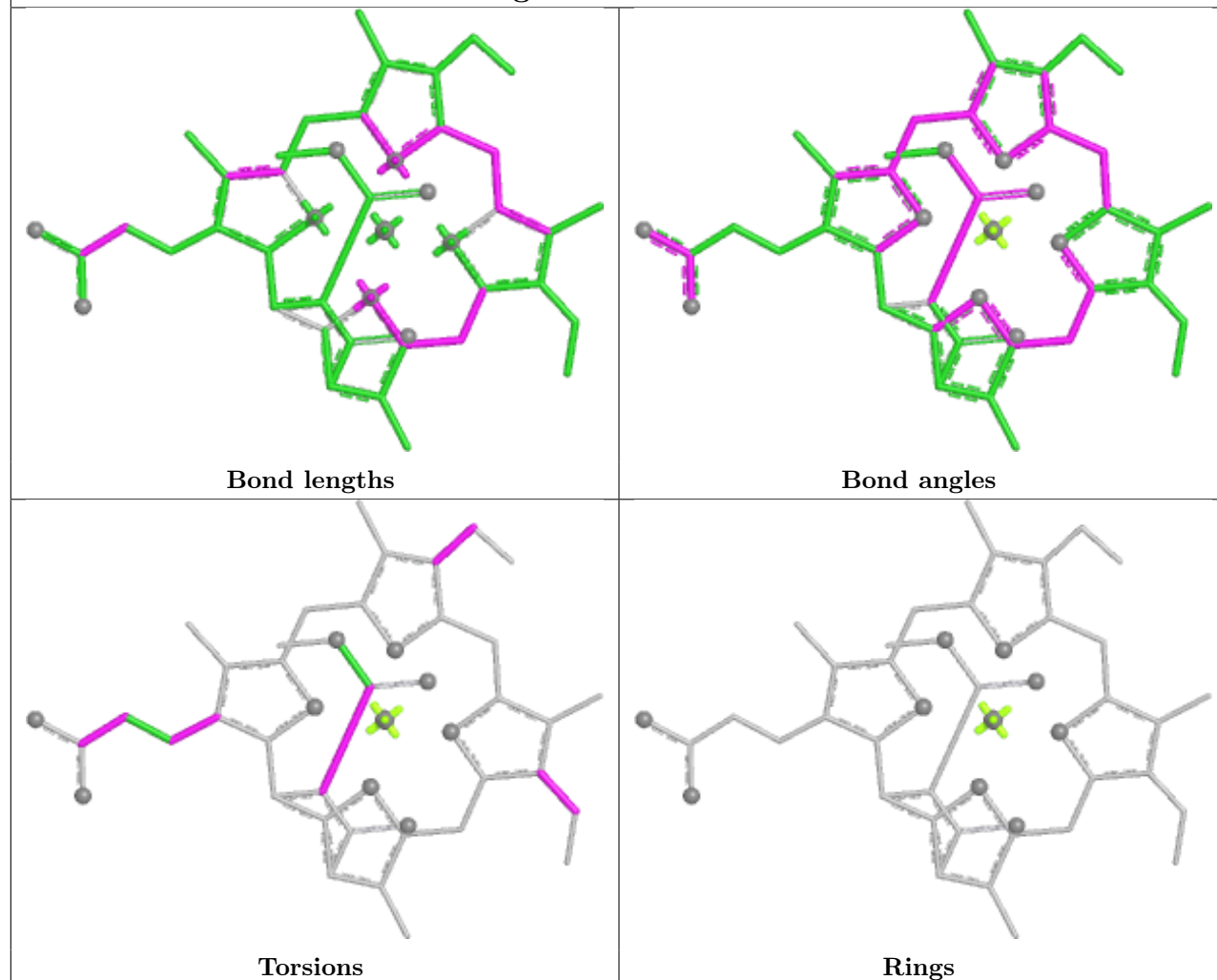


Ligand CLA 1 312

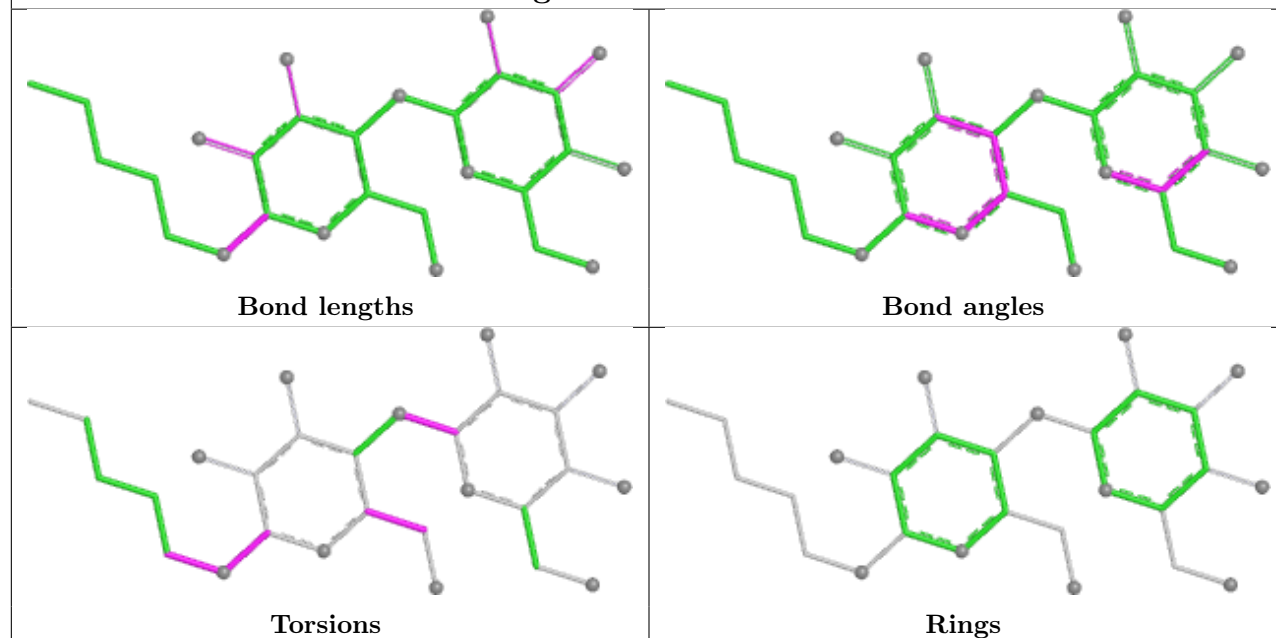


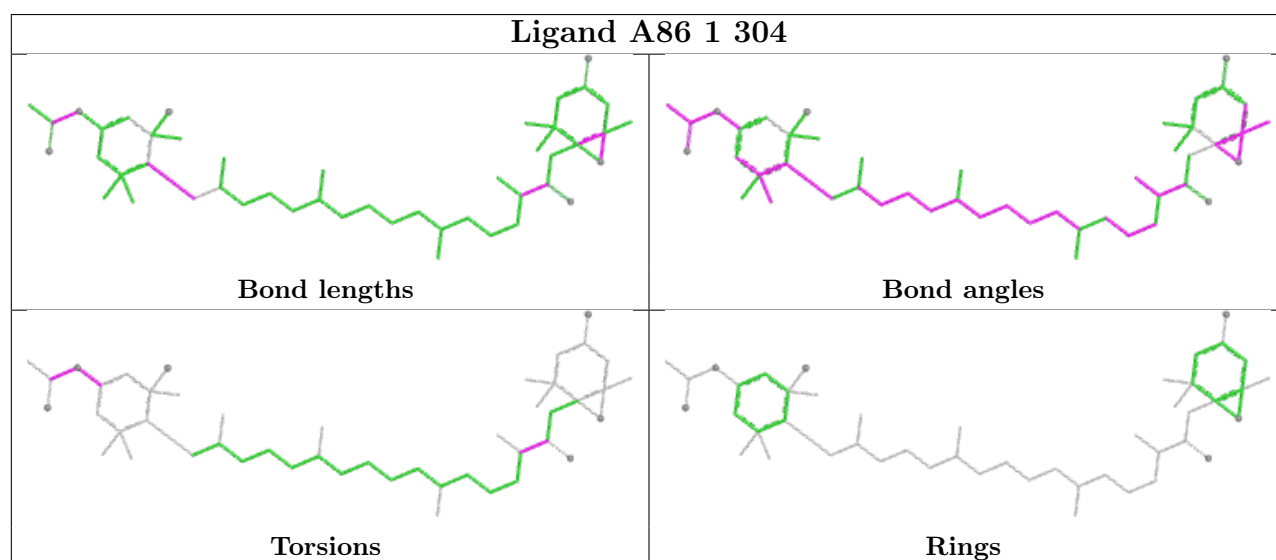
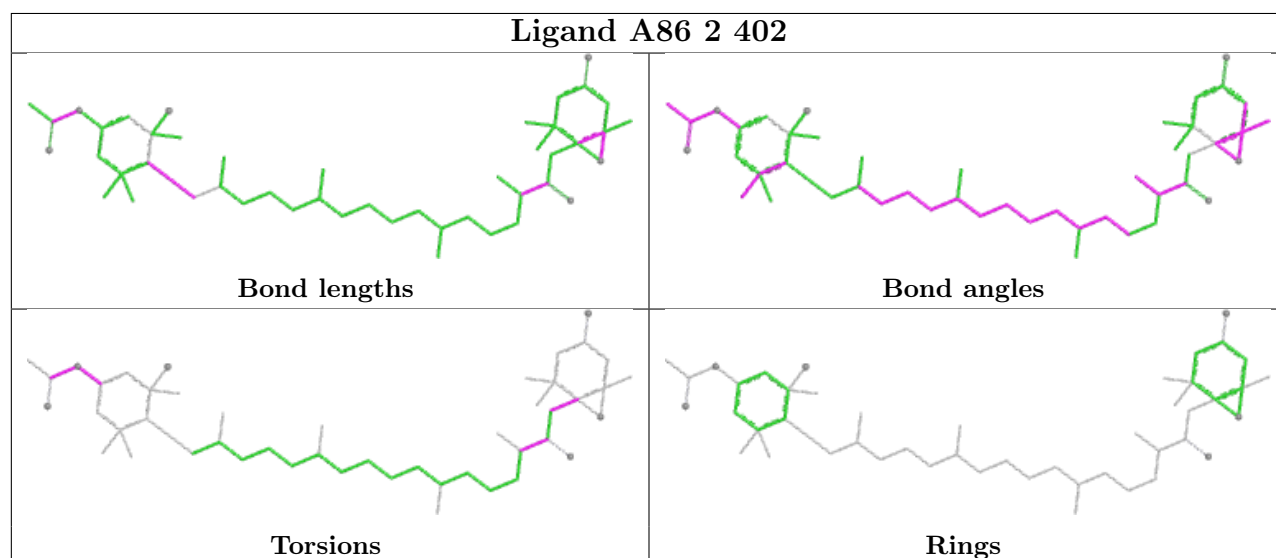
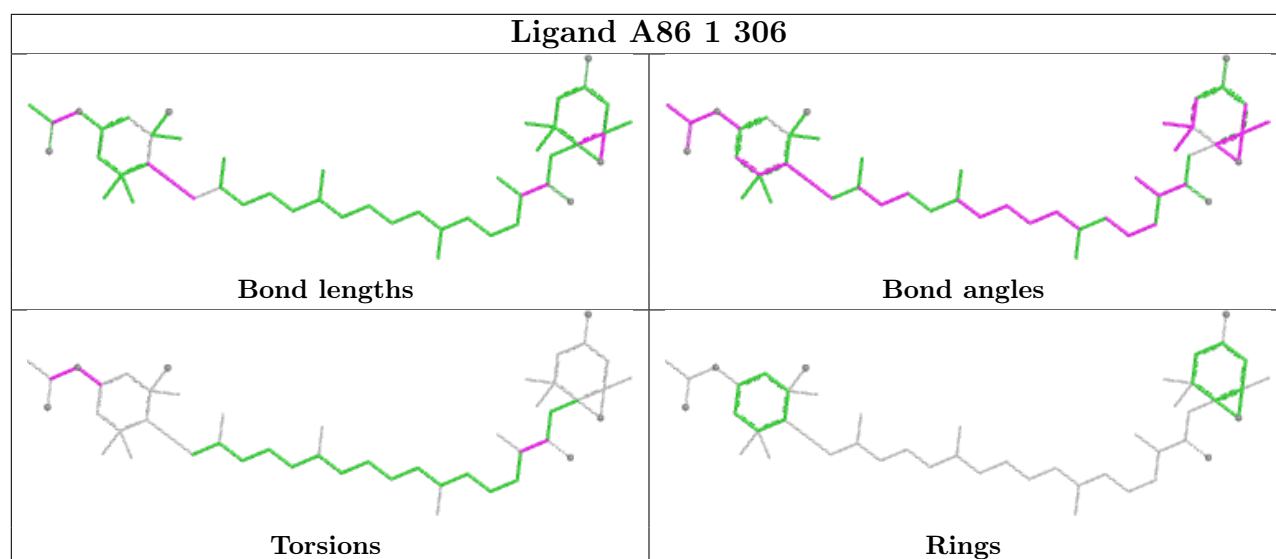


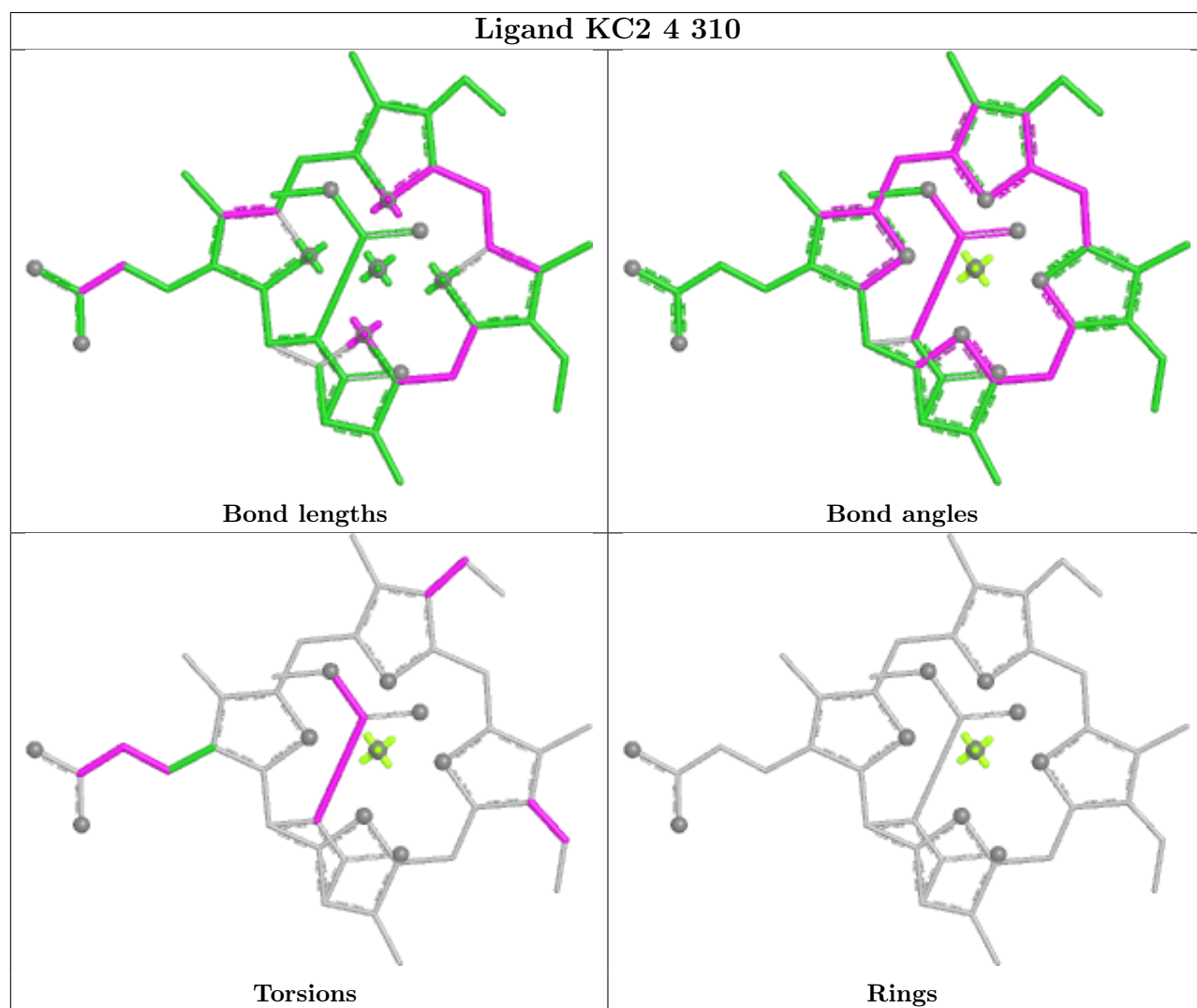
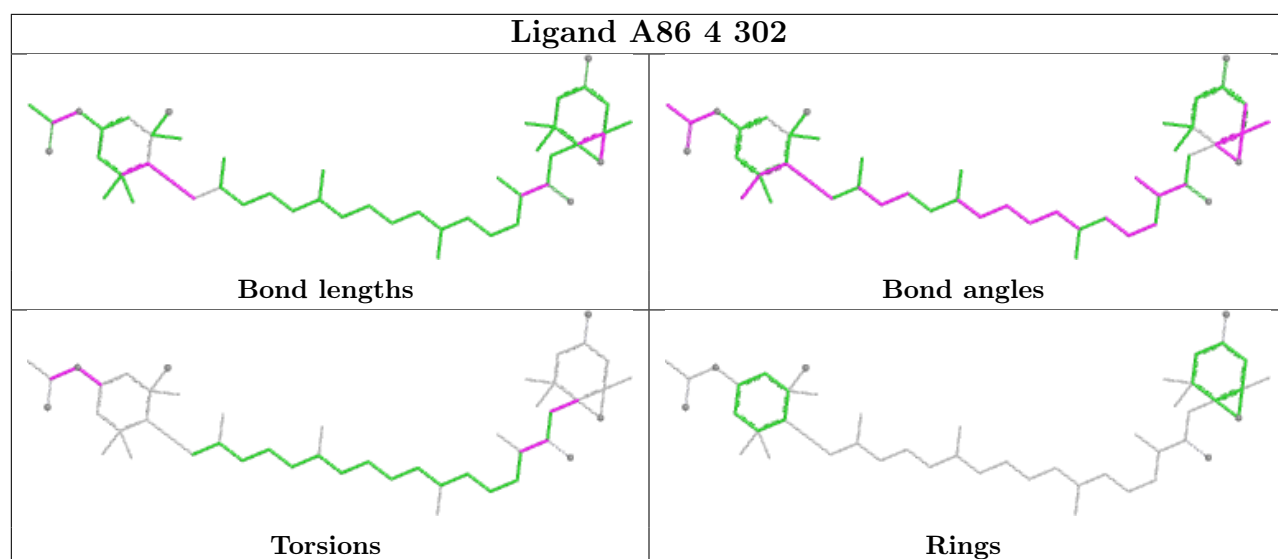
Ligand KC2 2 410



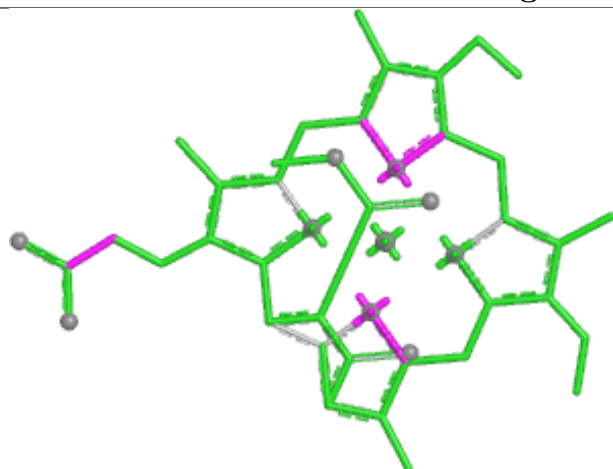
Ligand LMT 1 316



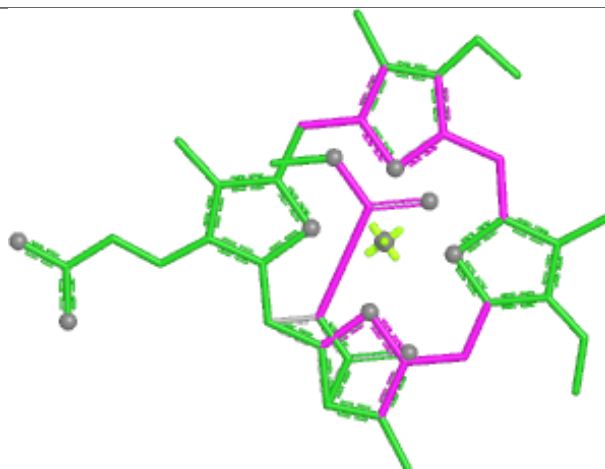




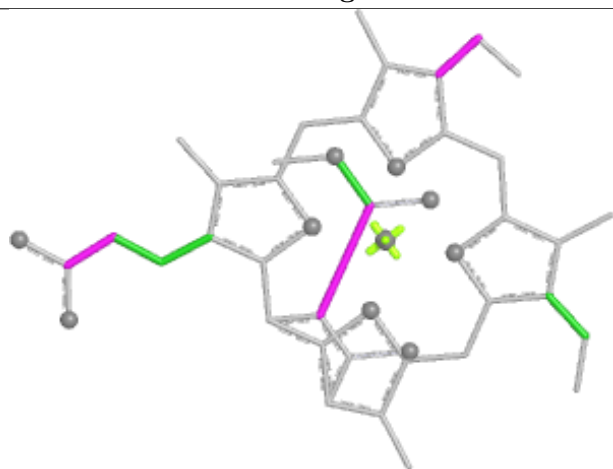
Ligand KC1 2 415



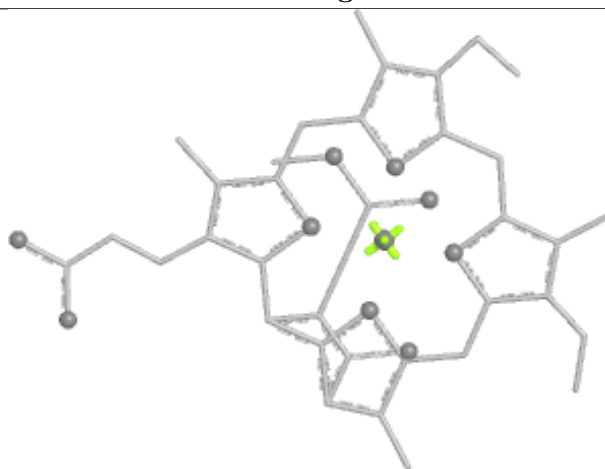
Bond lengths



Bond angles

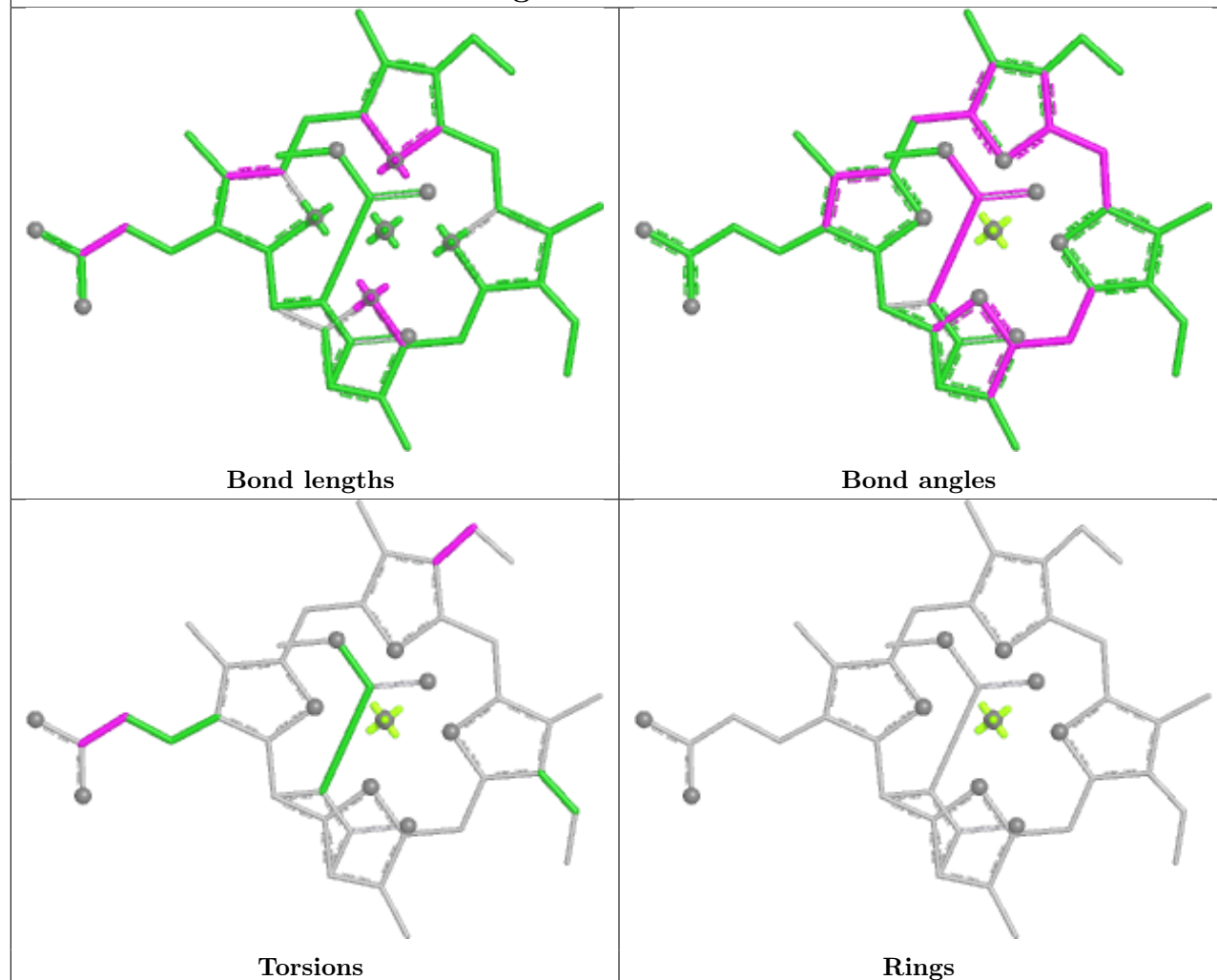


Torsions

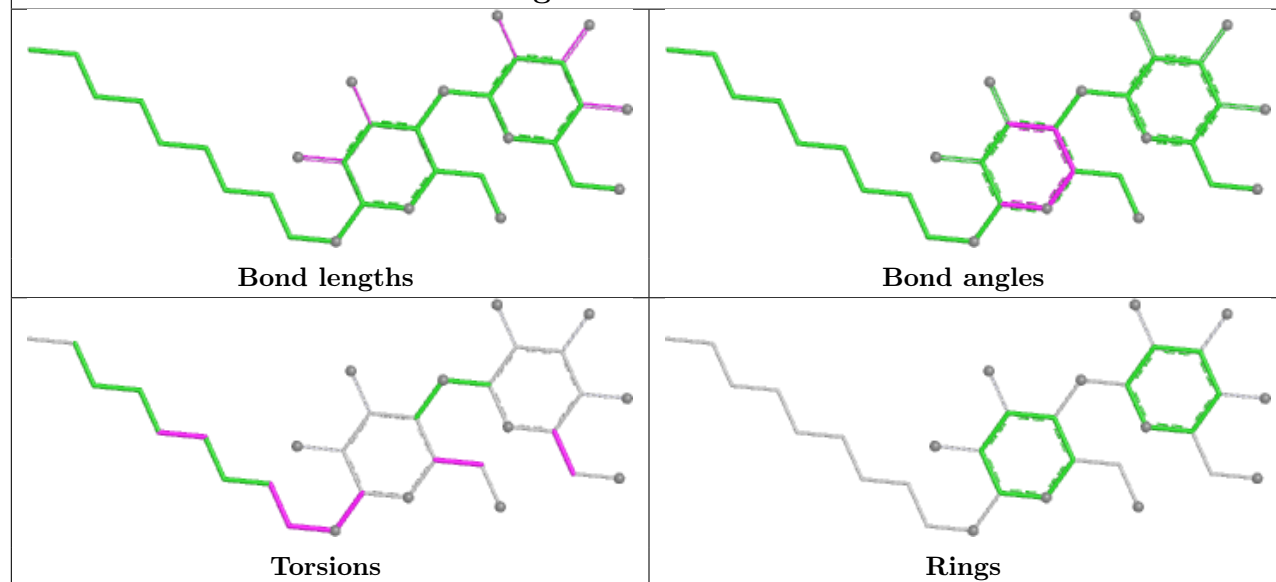


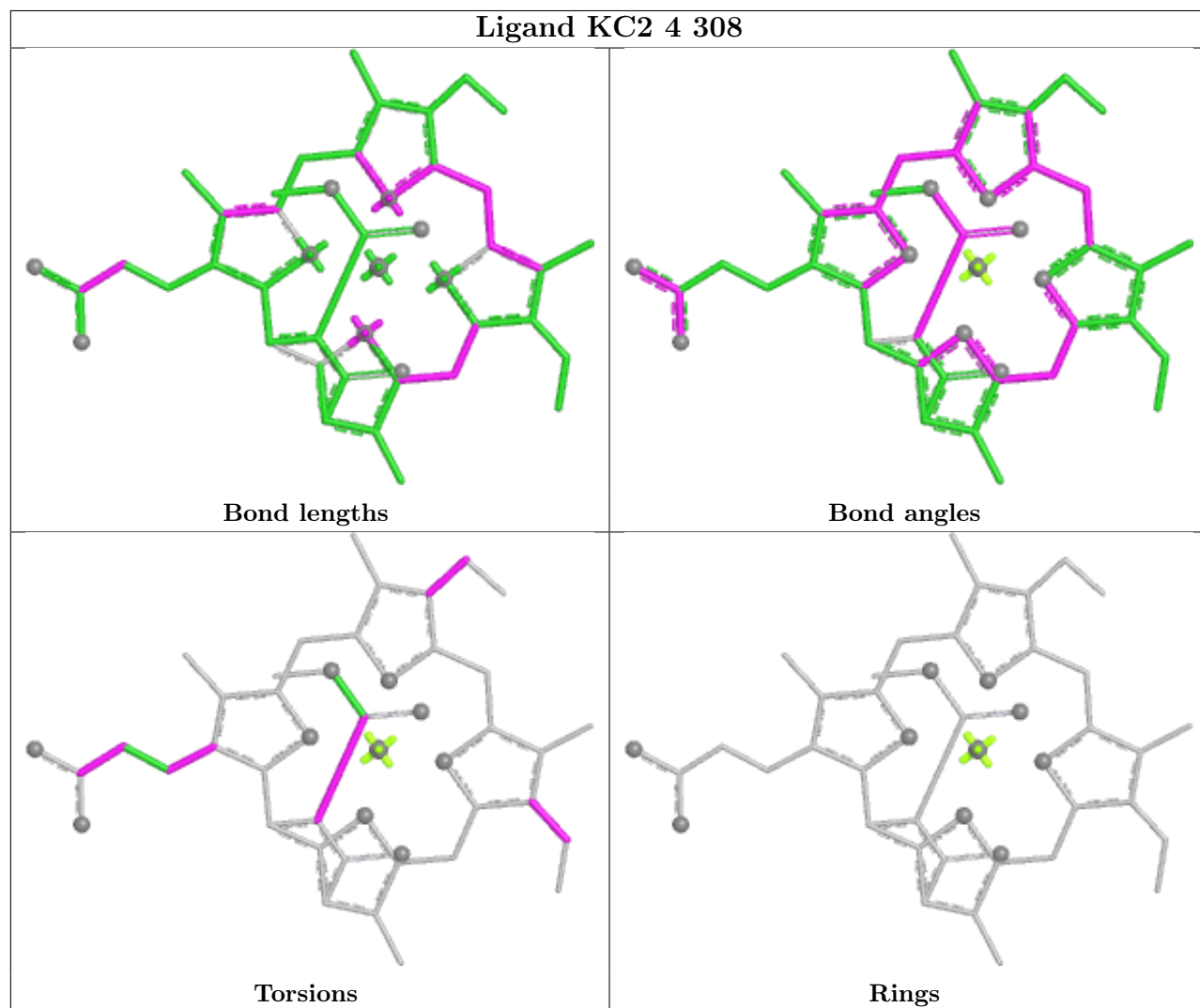
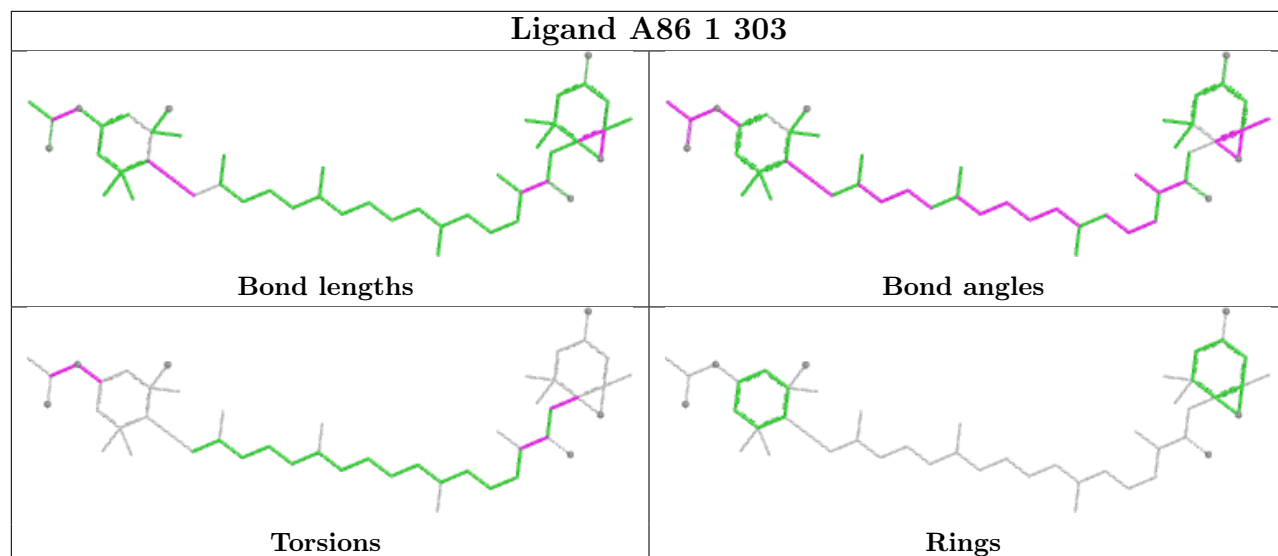
Rings

Ligand KC1 3 312

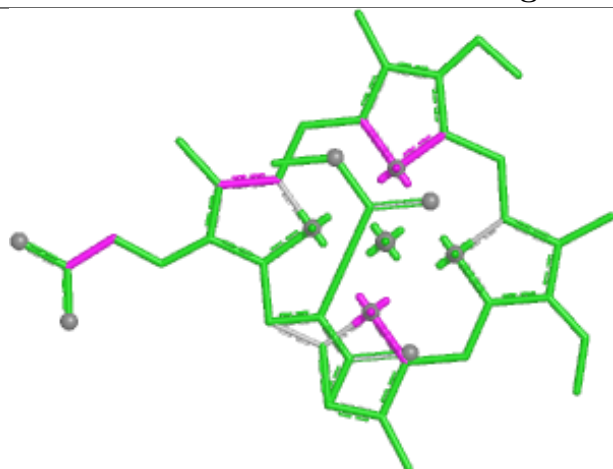


Ligand LMT 4 317

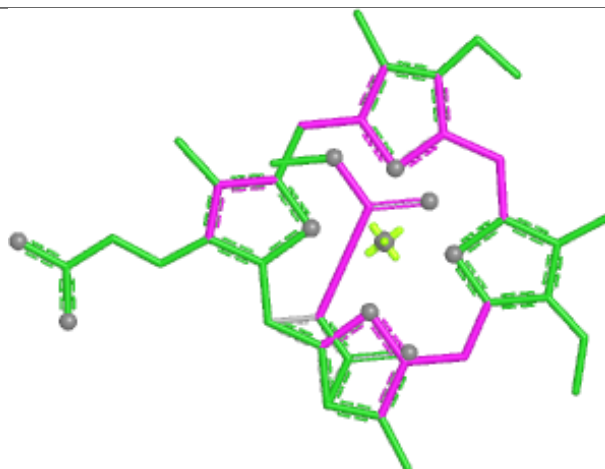




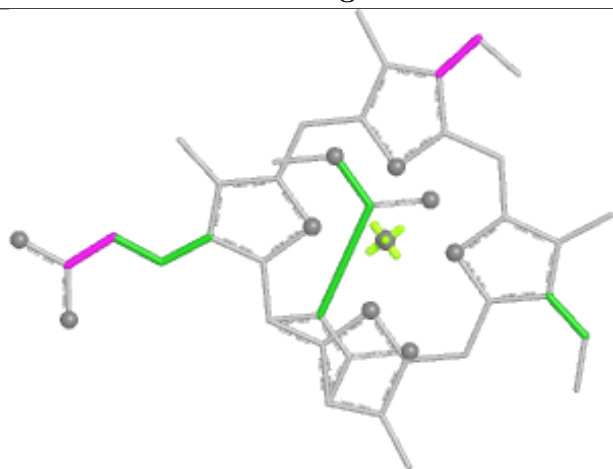
Ligand KC1 4 311



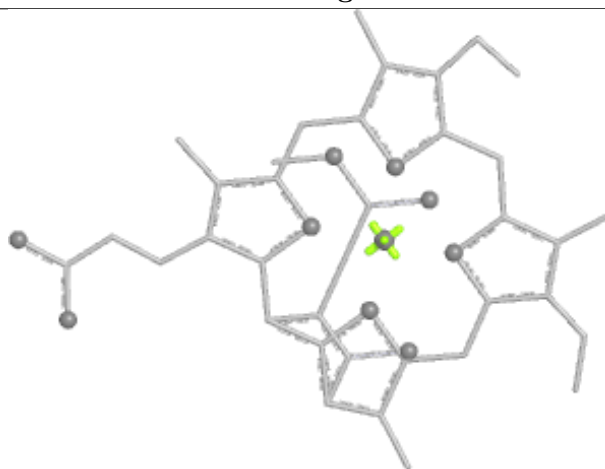
Bond lengths



Bond angles

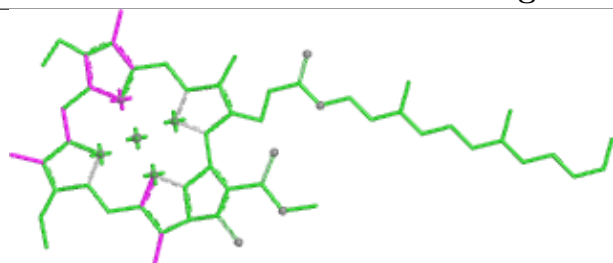


Torsions

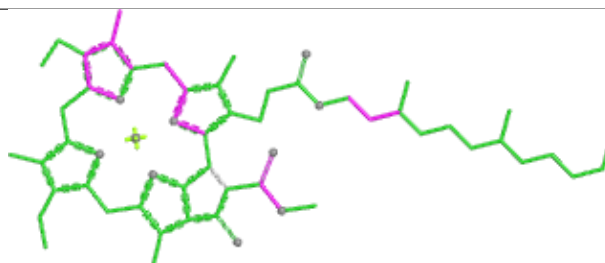


Rings

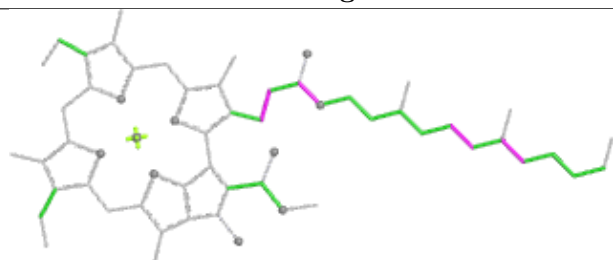
Ligand CLA 4 307



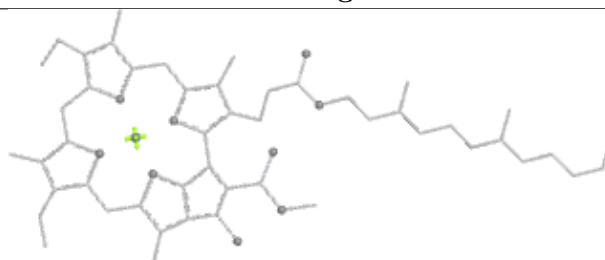
Bond lengths



Bond angles

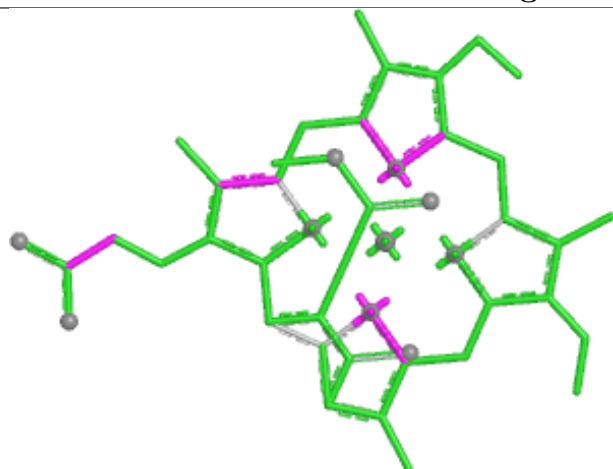


Torsions

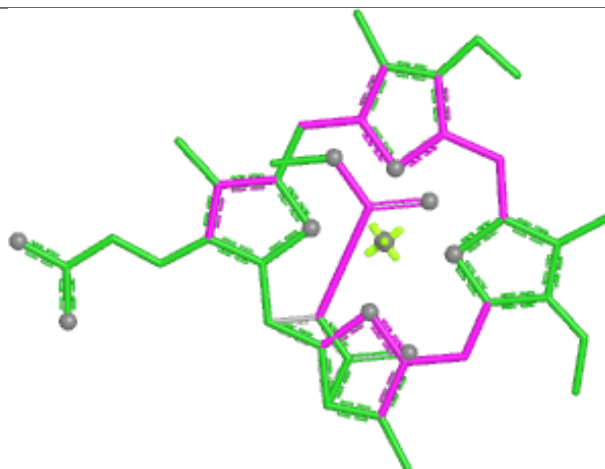


Rings

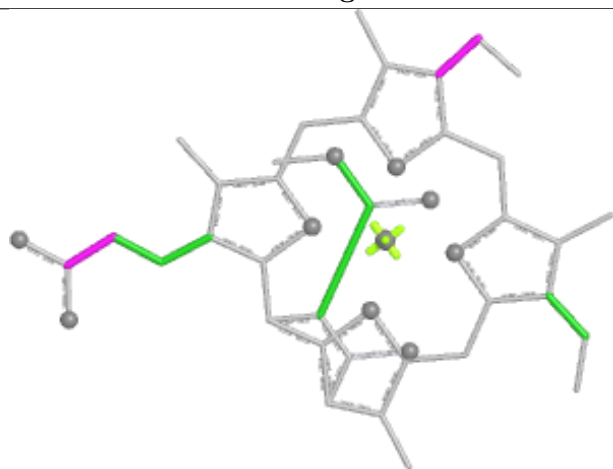
Ligand KC1 1 311



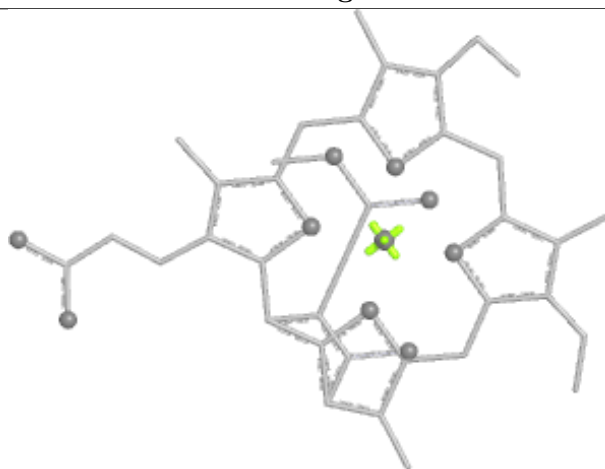
Bond lengths



Bond angles

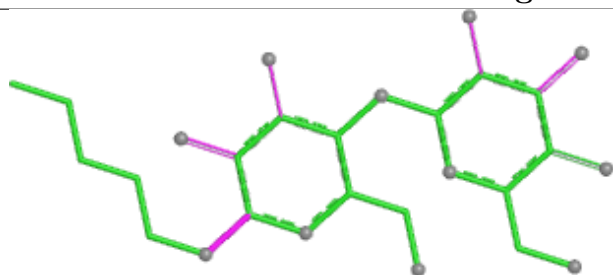


Torsions

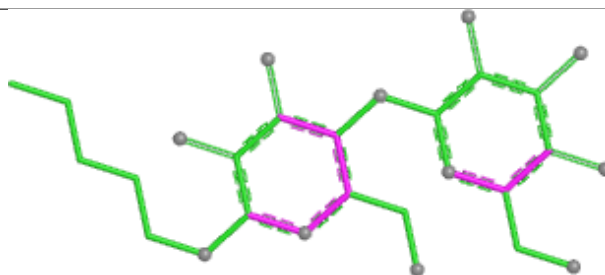


Rings

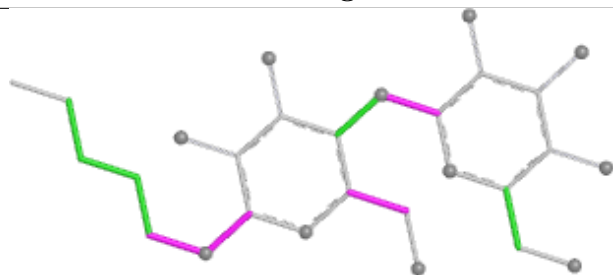
Ligand LMT 2 418



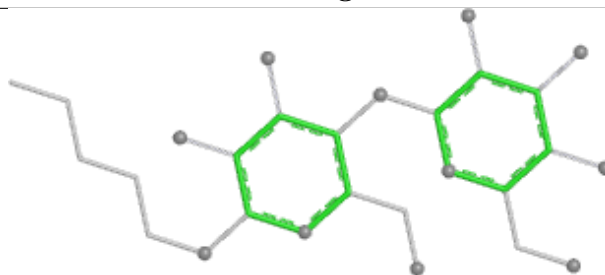
Bond lengths



Bond angles

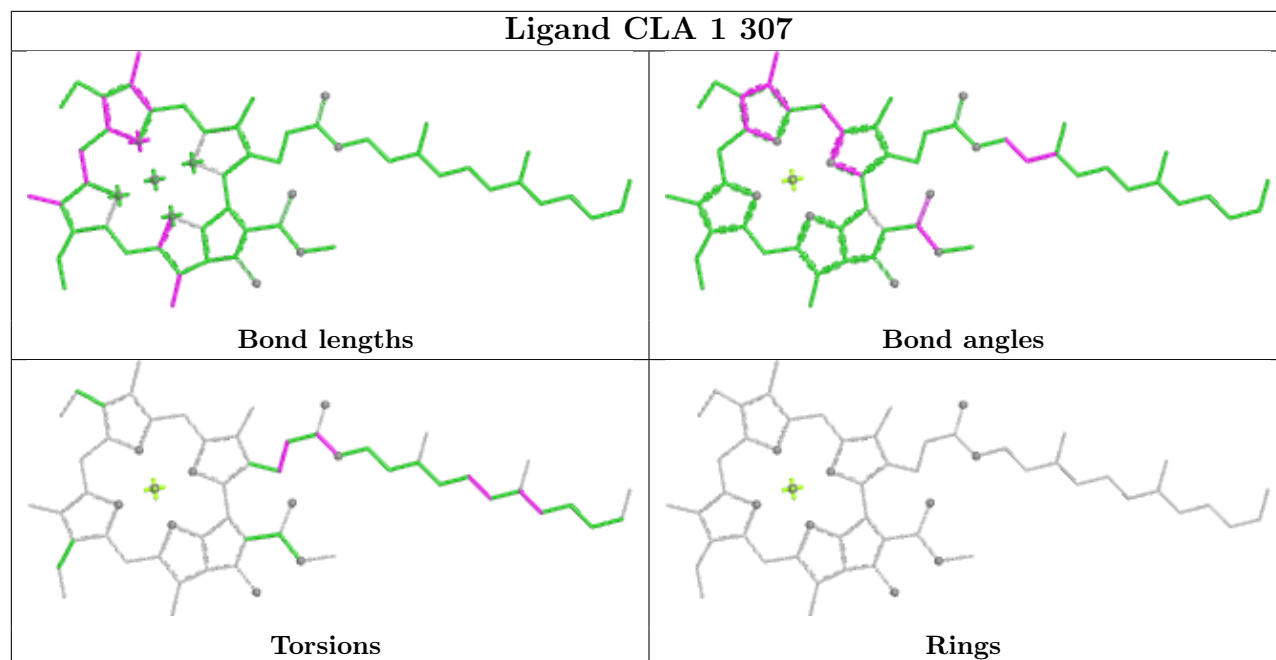


Torsions

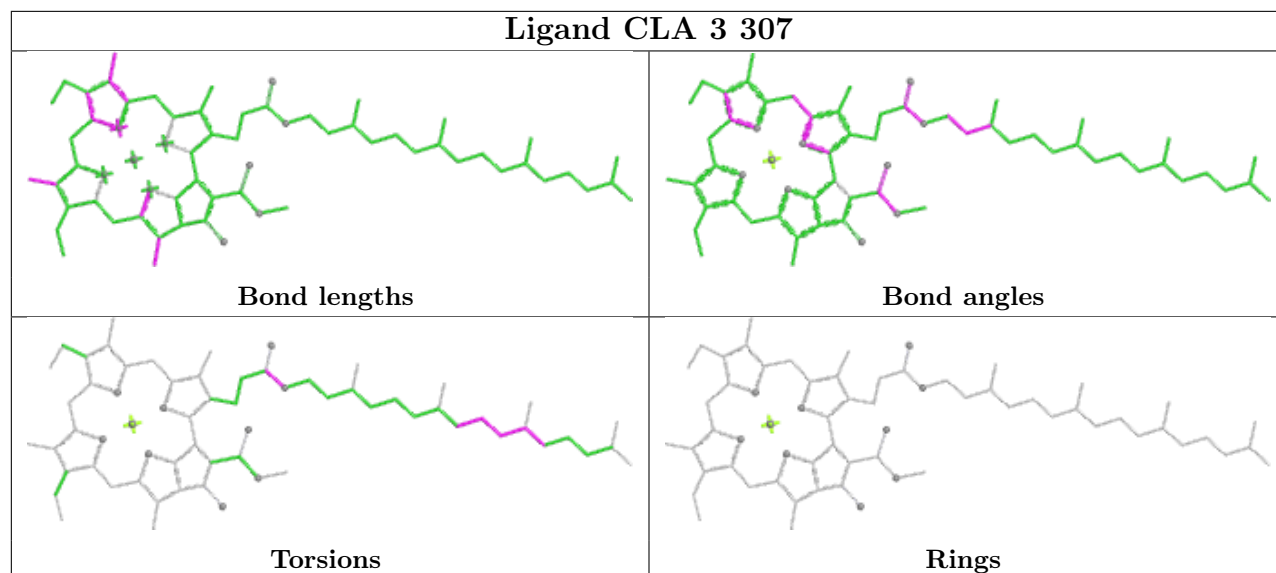


Rings

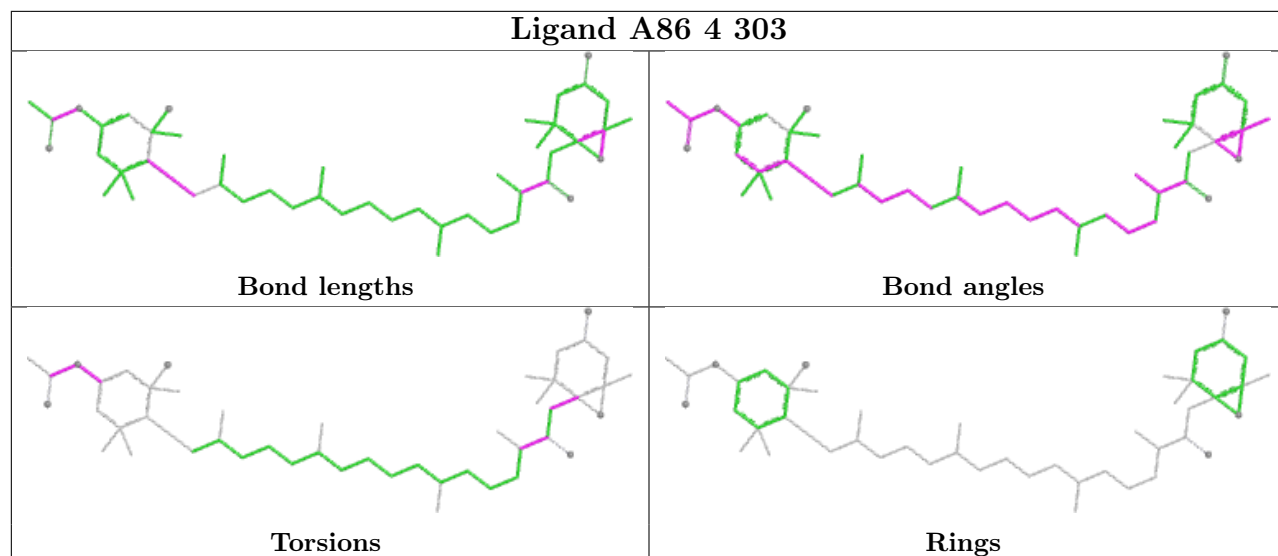
Ligand CLA 1 307



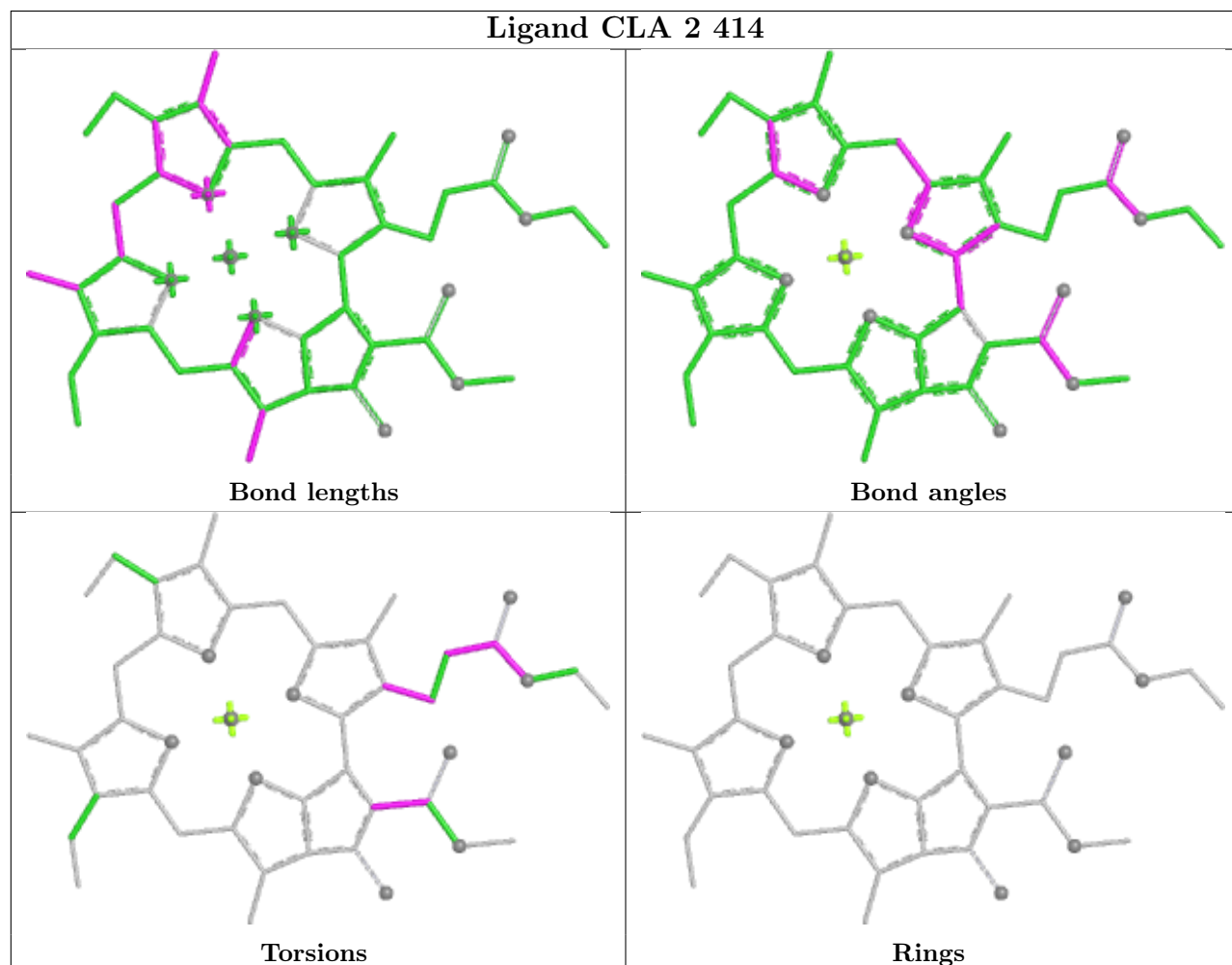
Ligand CLA 3 307

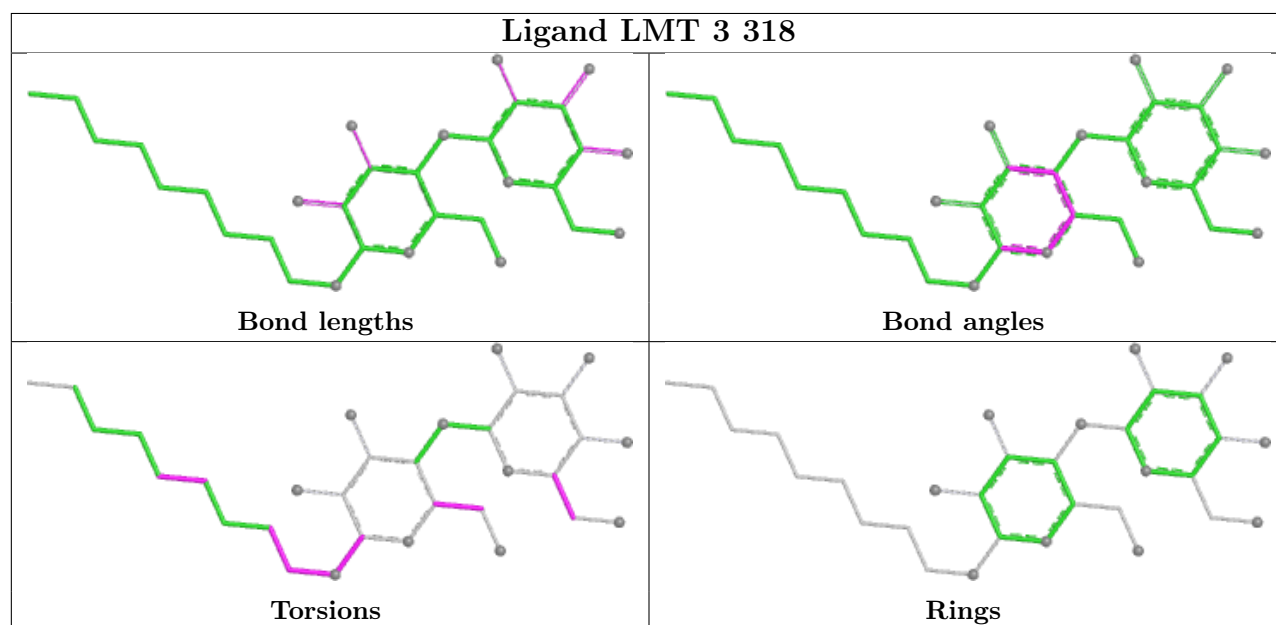
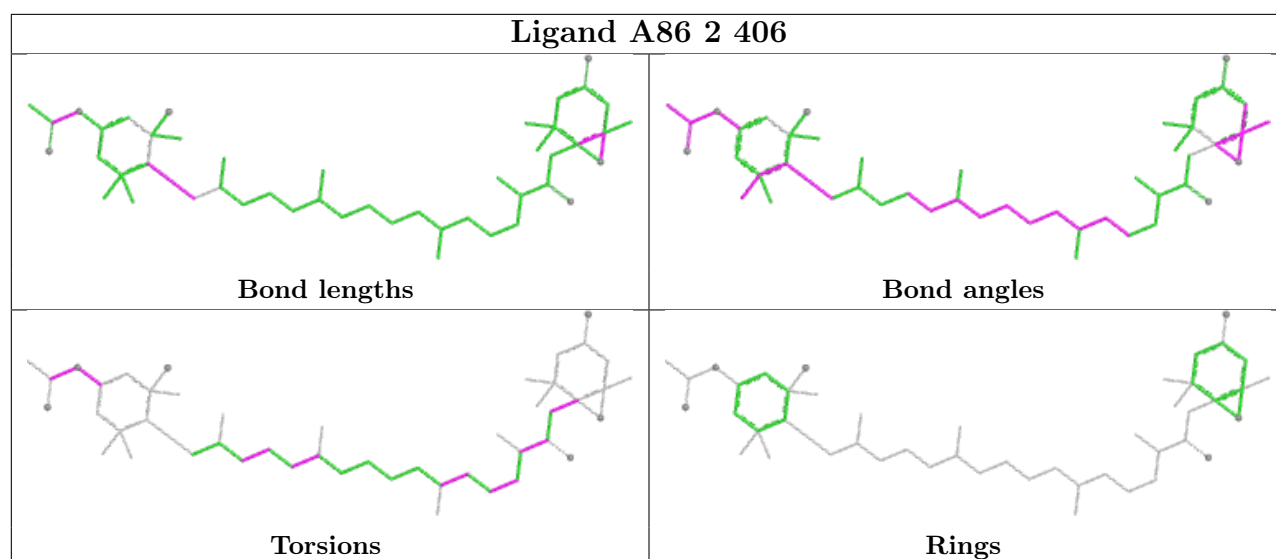


Ligand A86 4 303

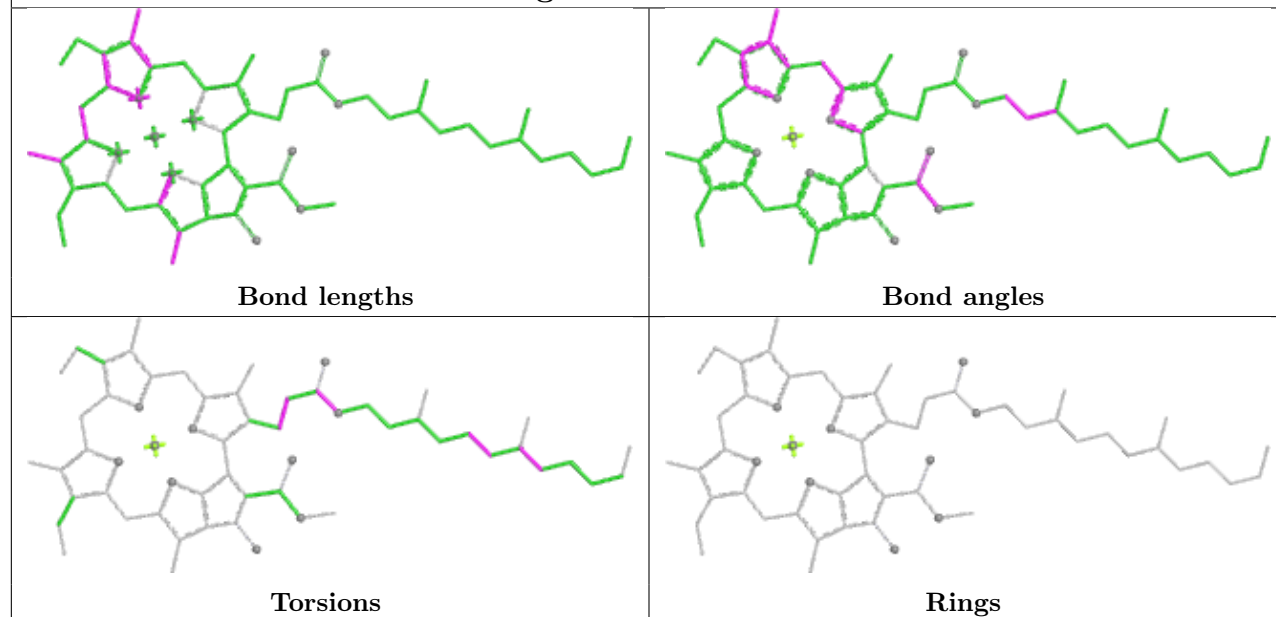


Ligand CLA 2 414

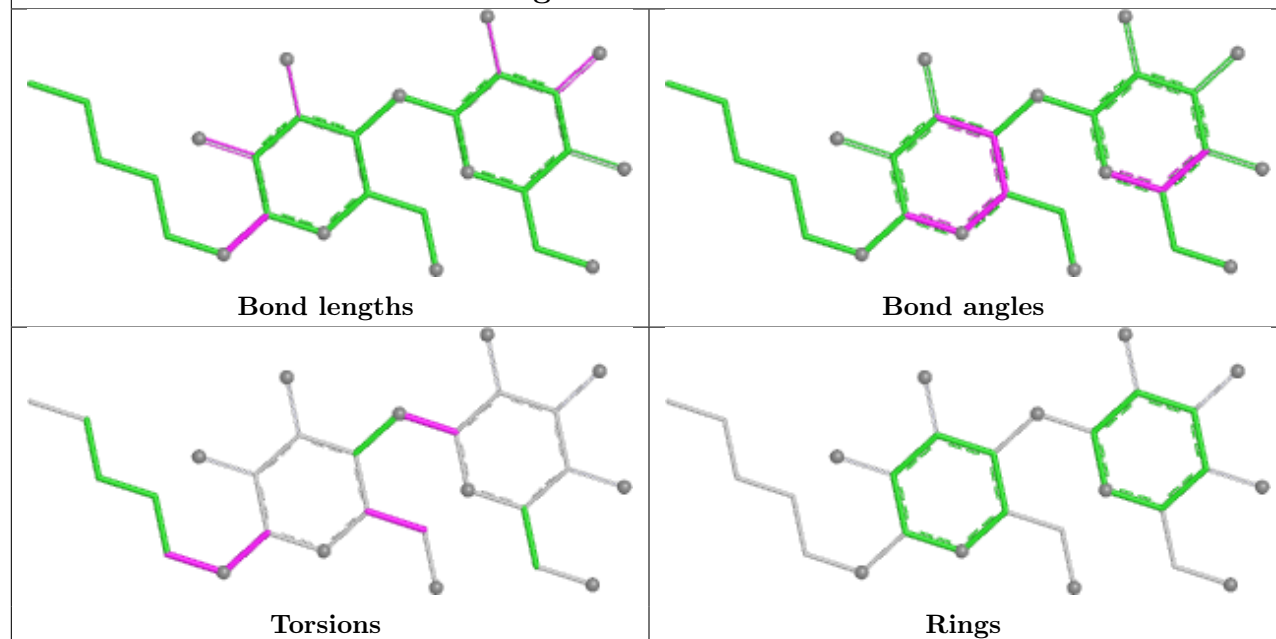


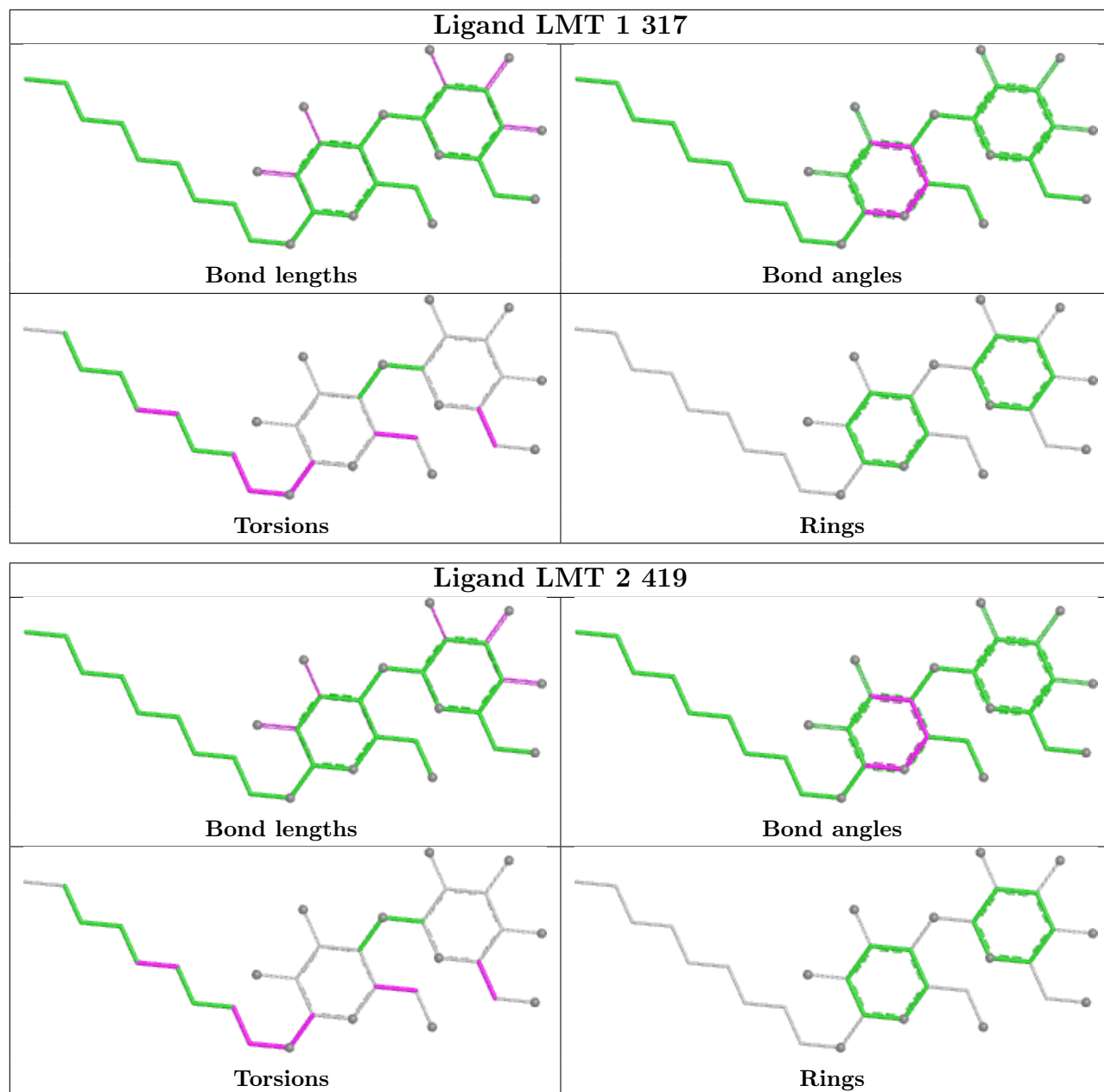


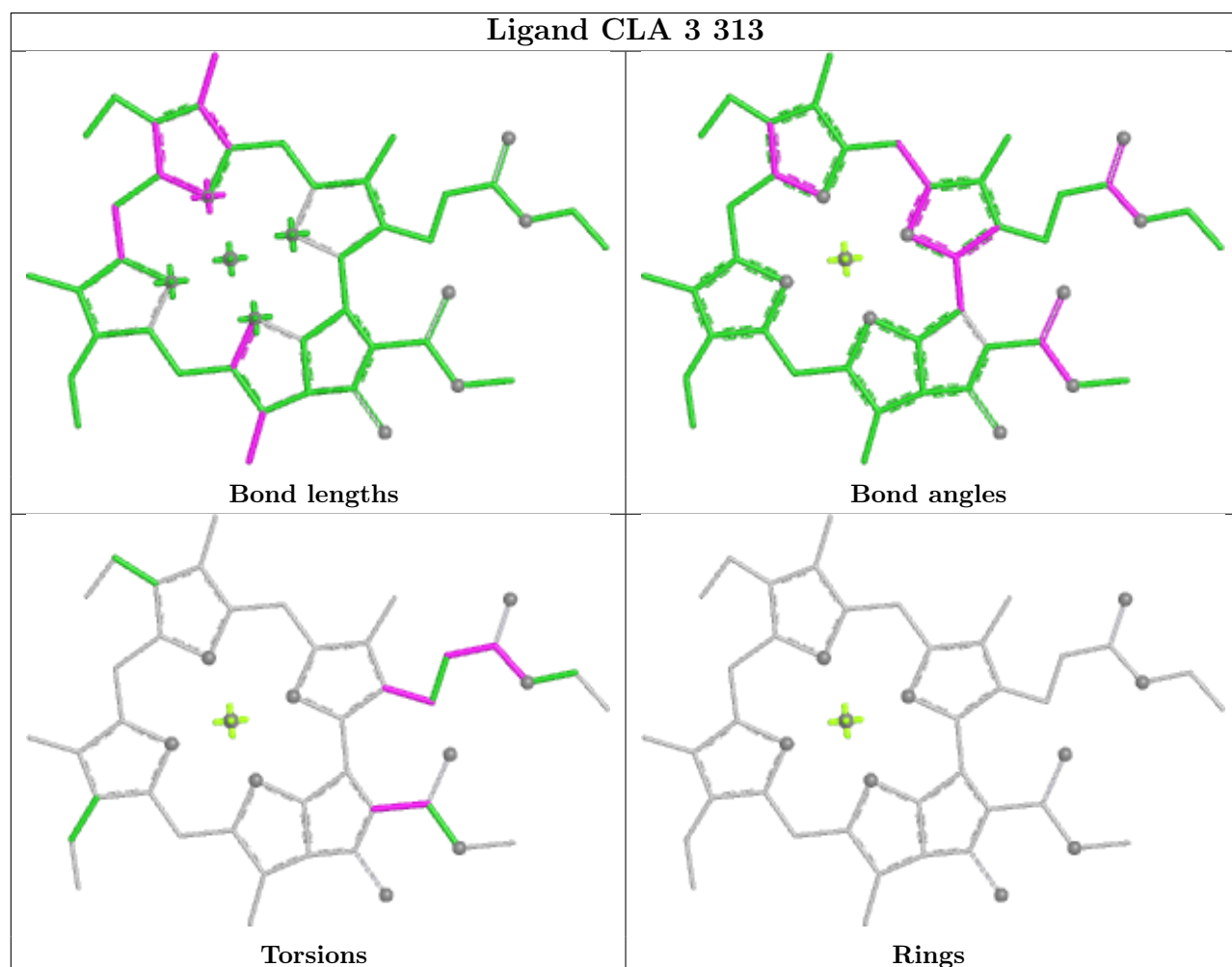
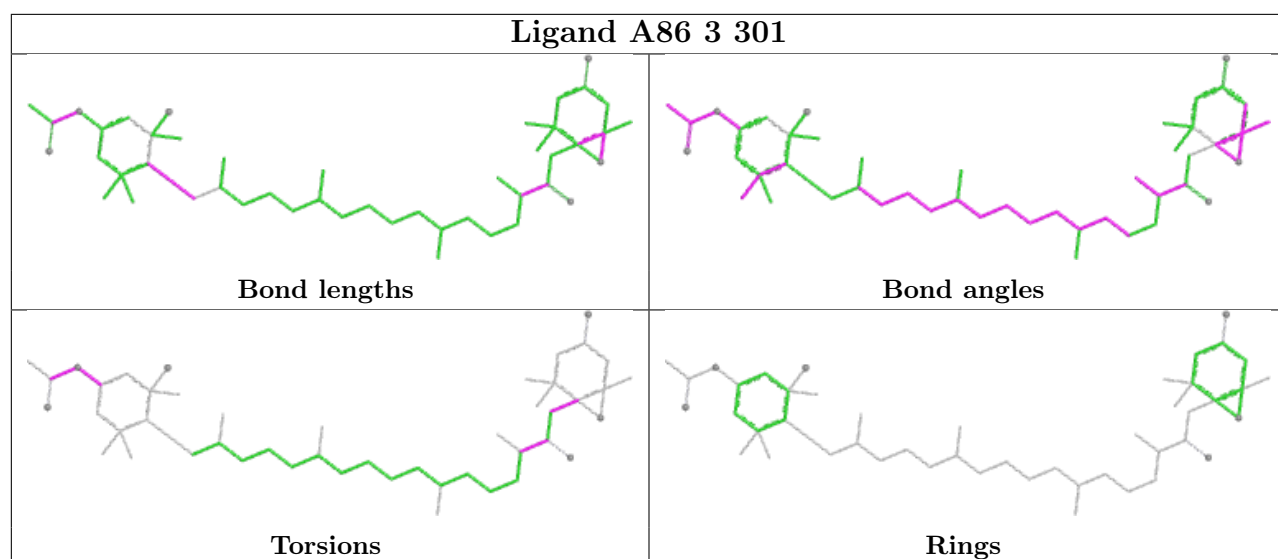
Ligand CLA 3 308



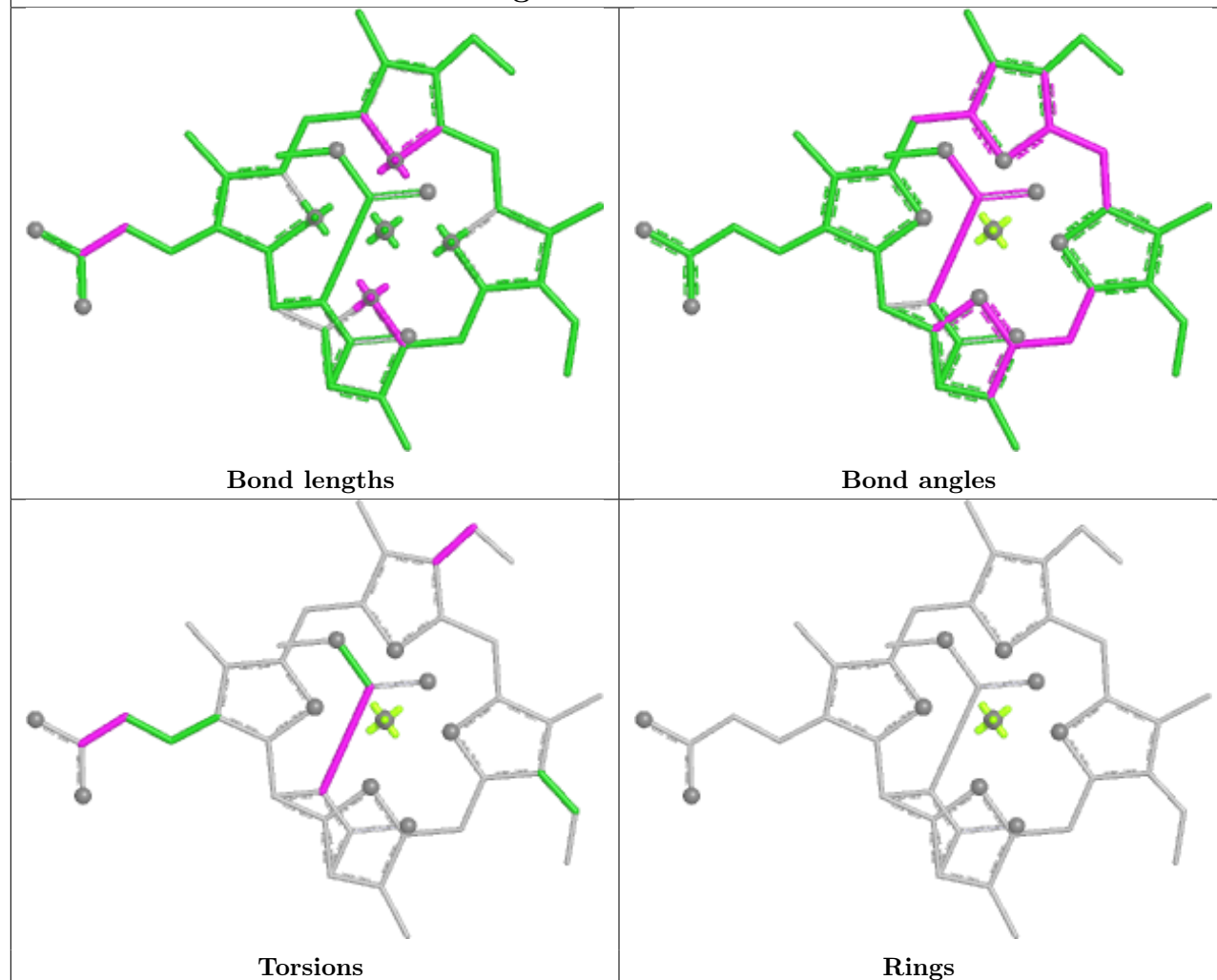
Ligand LMT 4 316



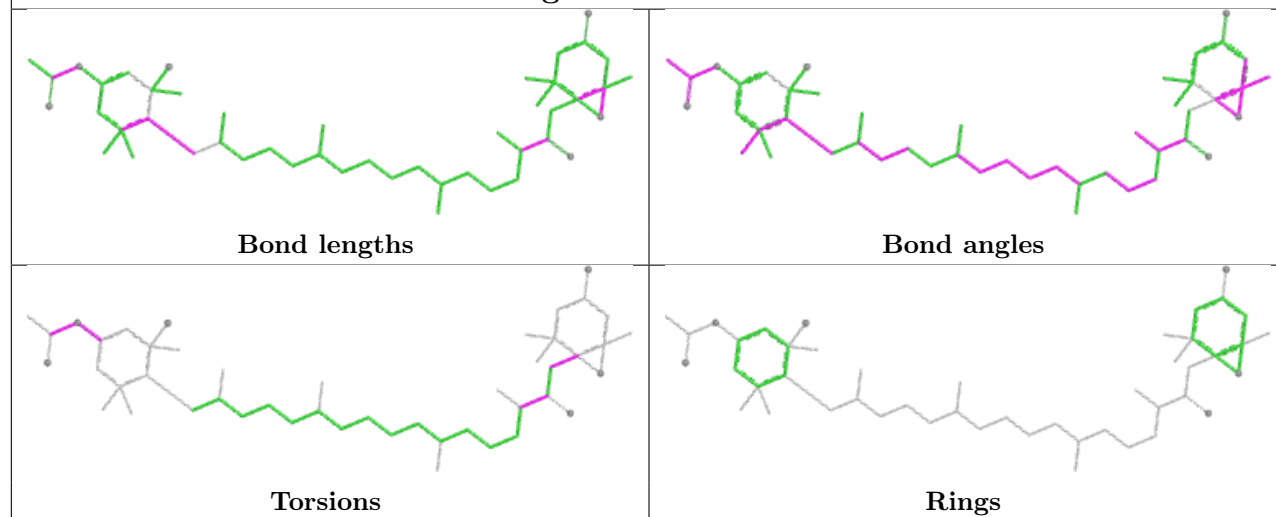


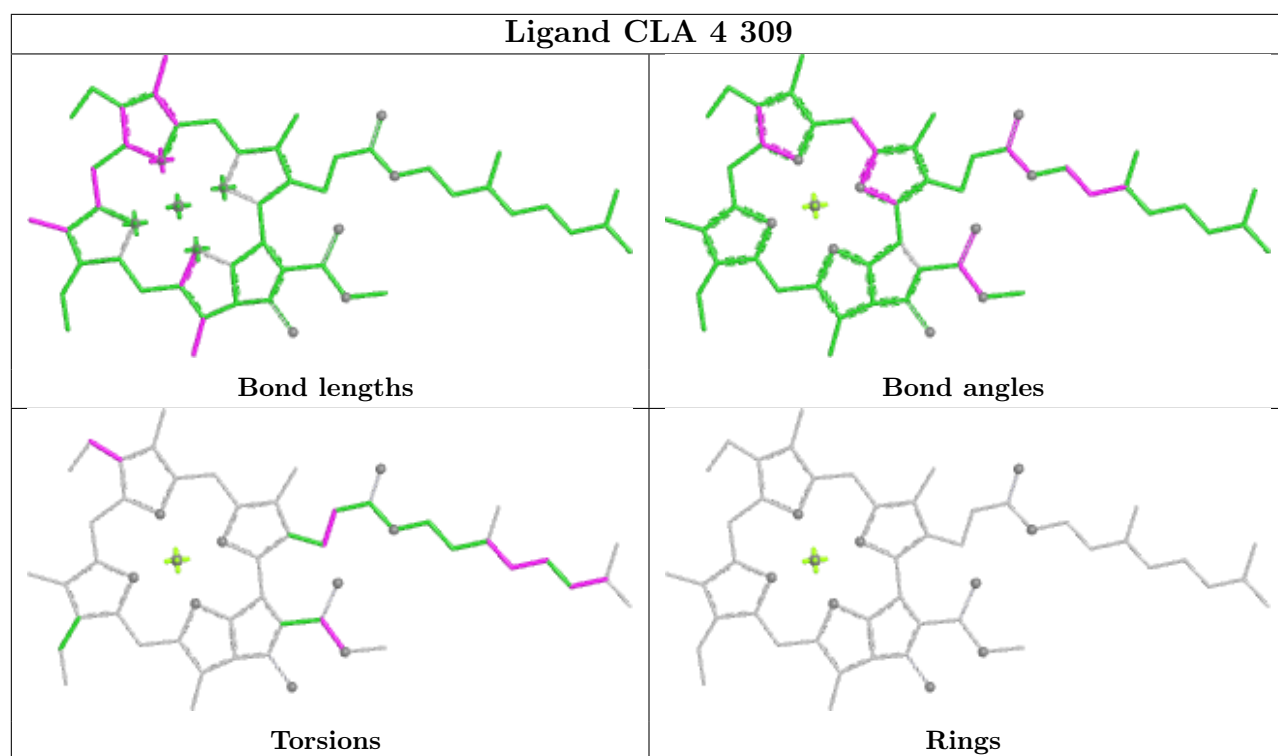


Ligand KC1 3 314

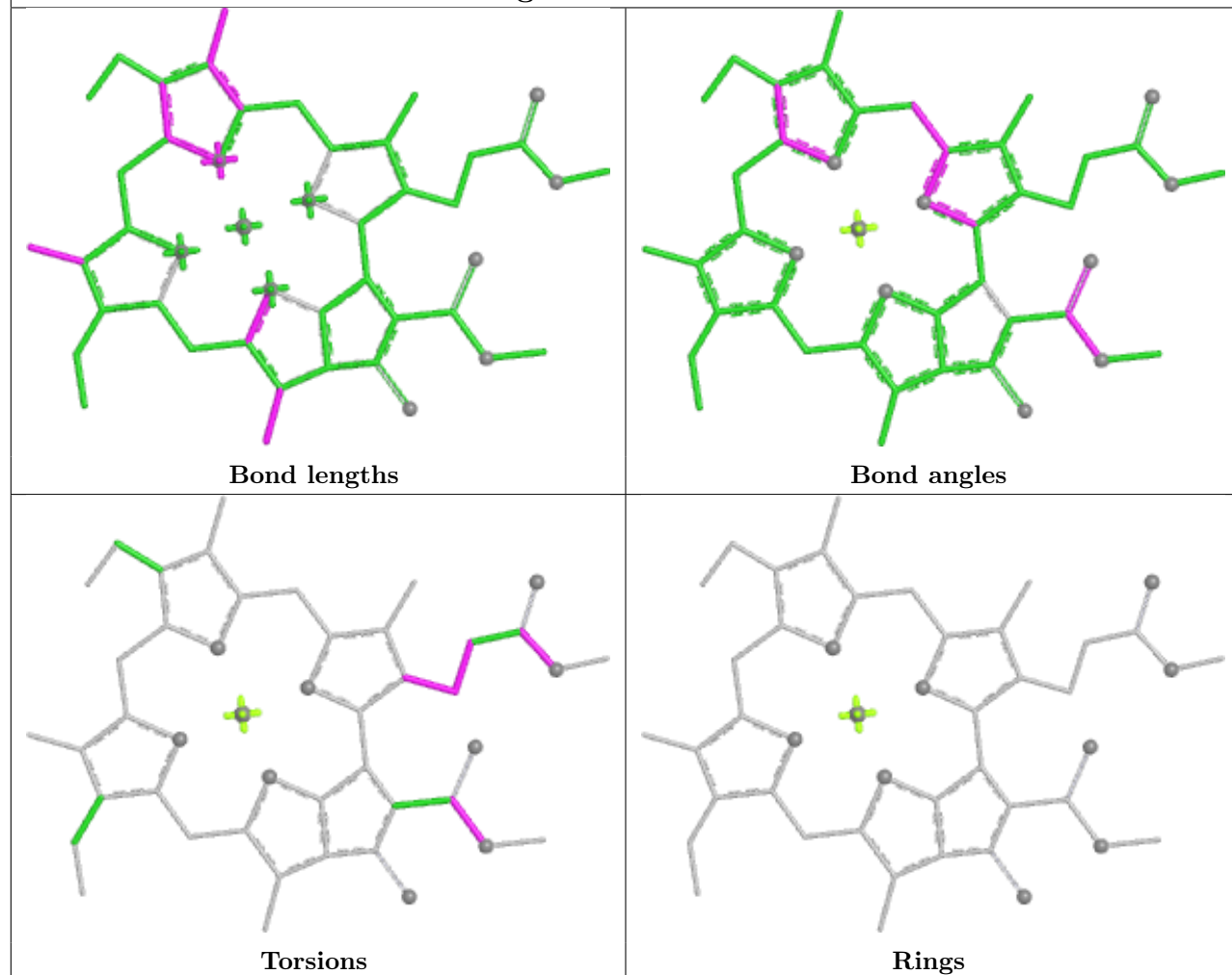


Ligand A86 2 403

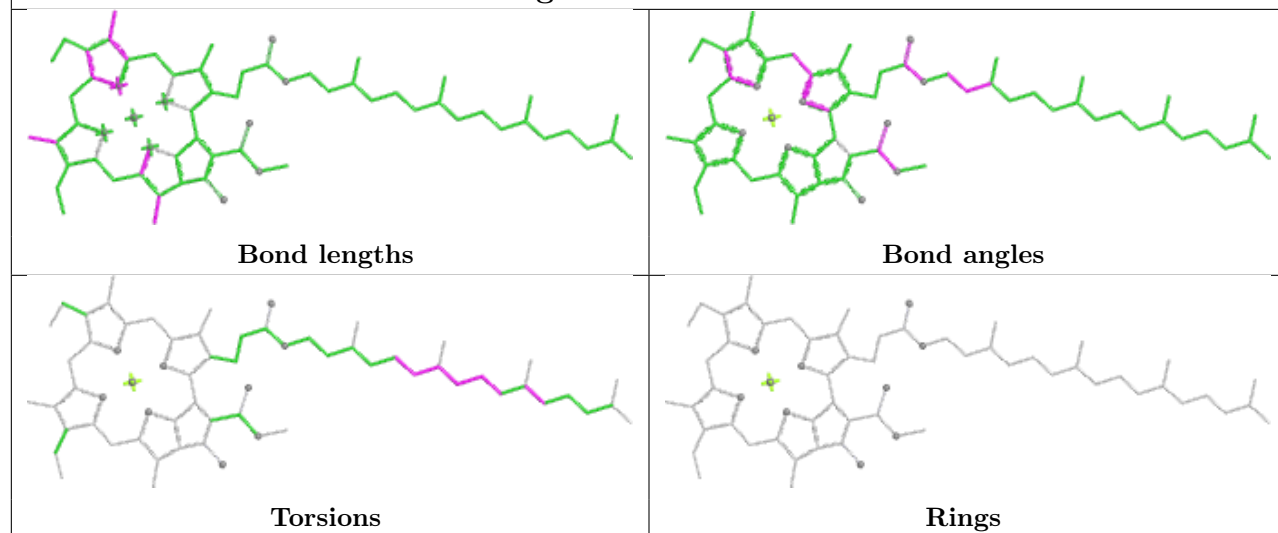




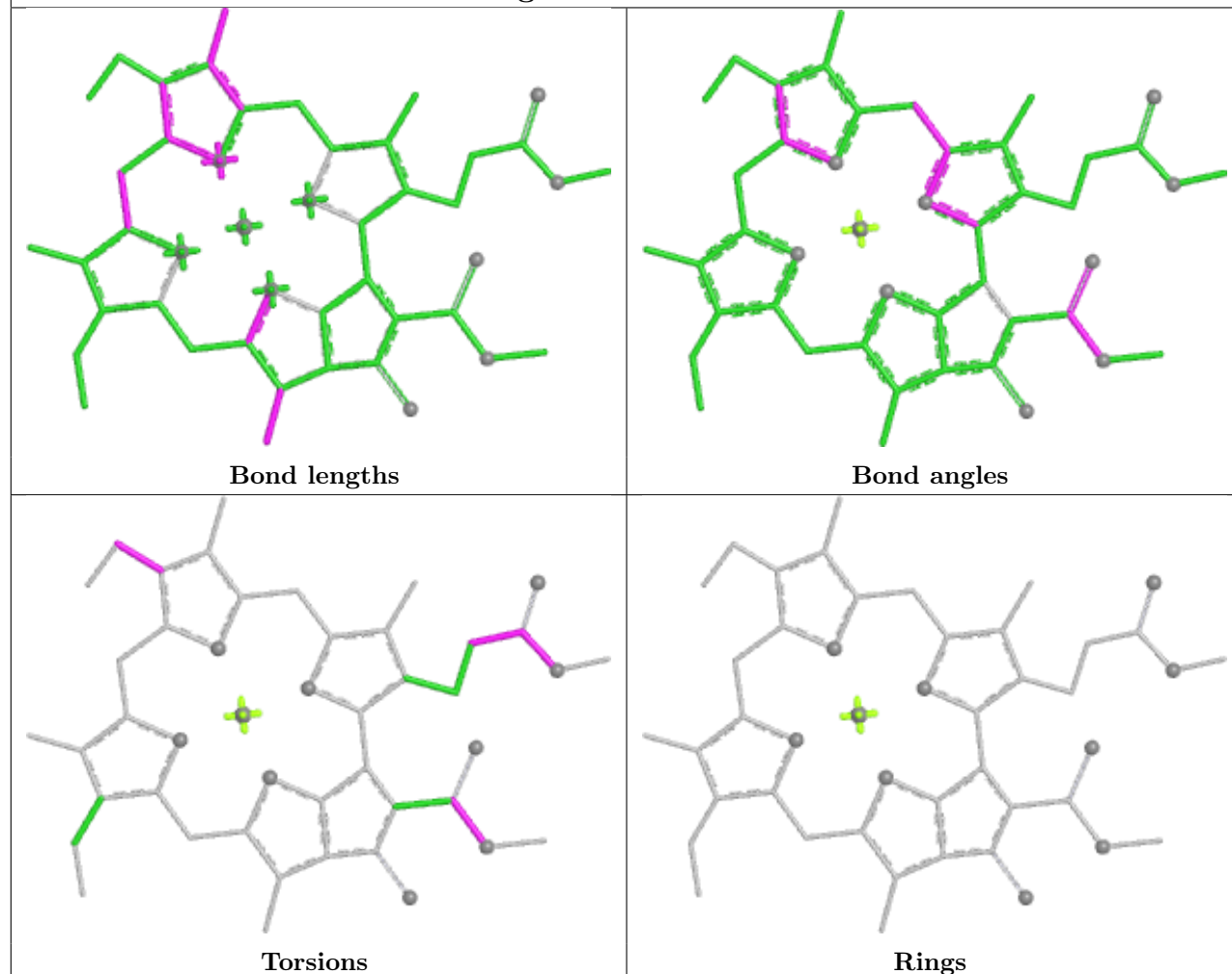
Ligand CLA 2 416



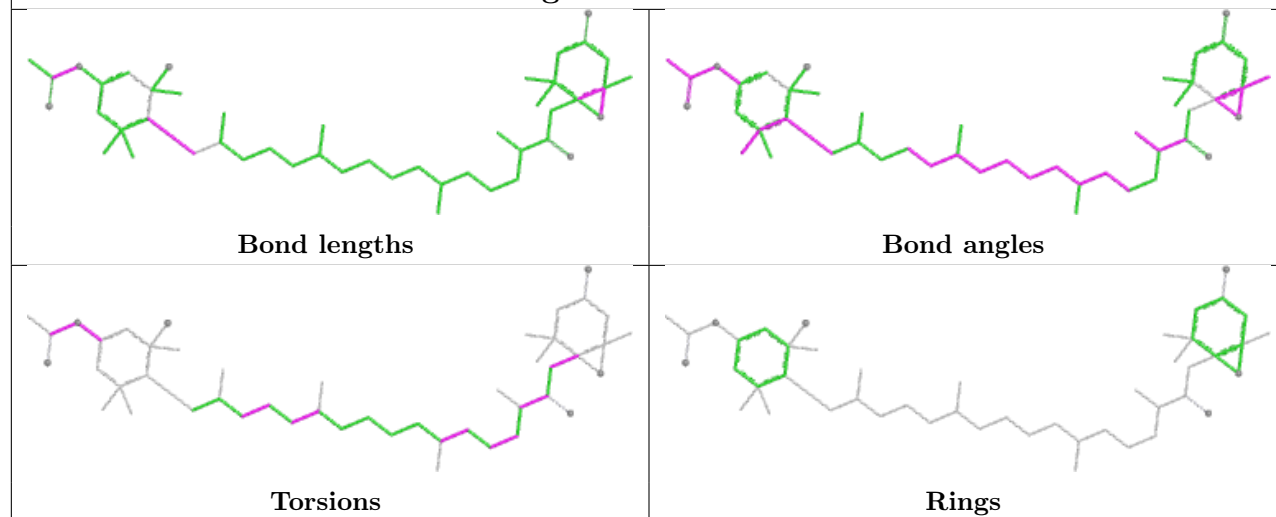
Ligand CLA 2 401

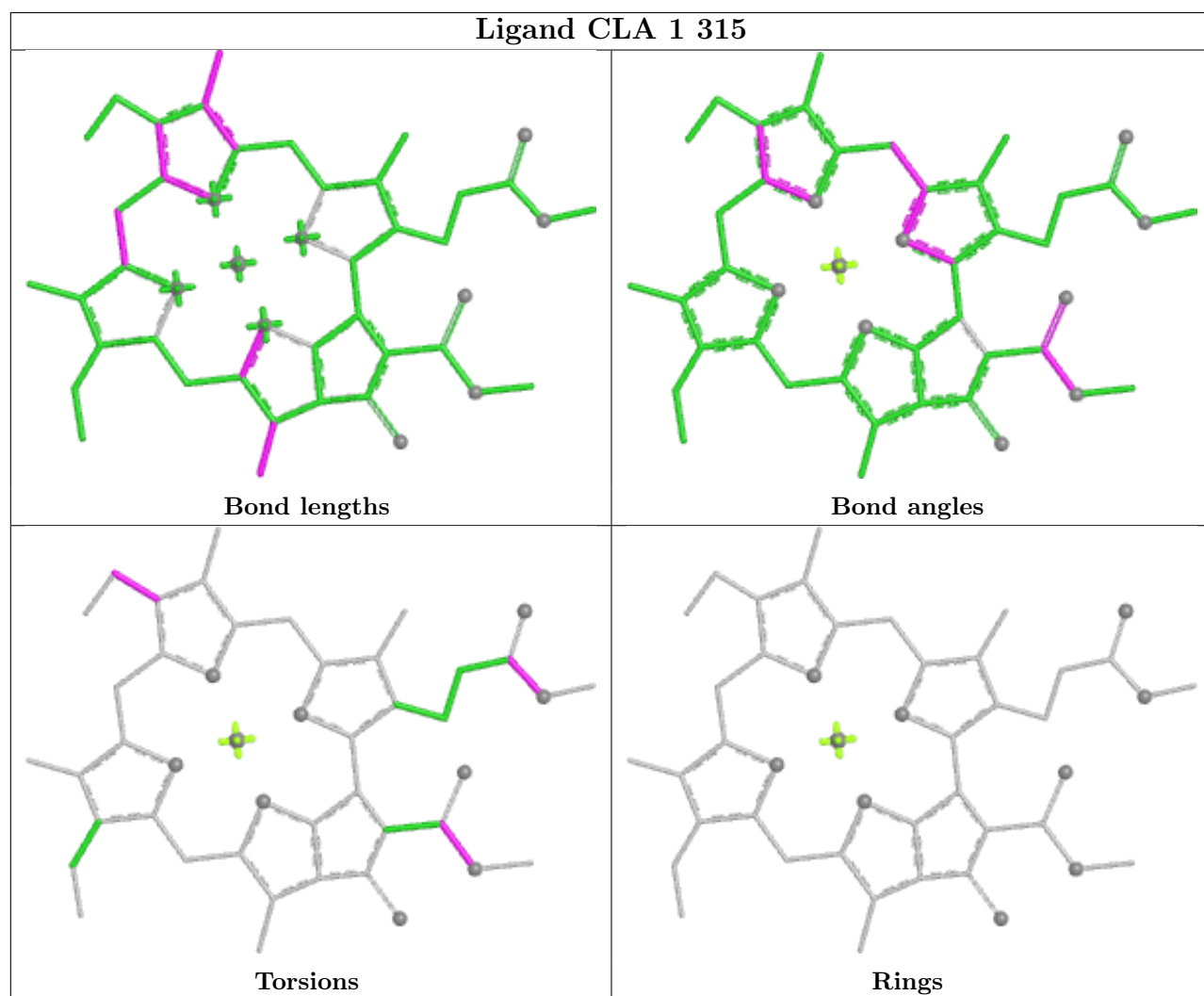
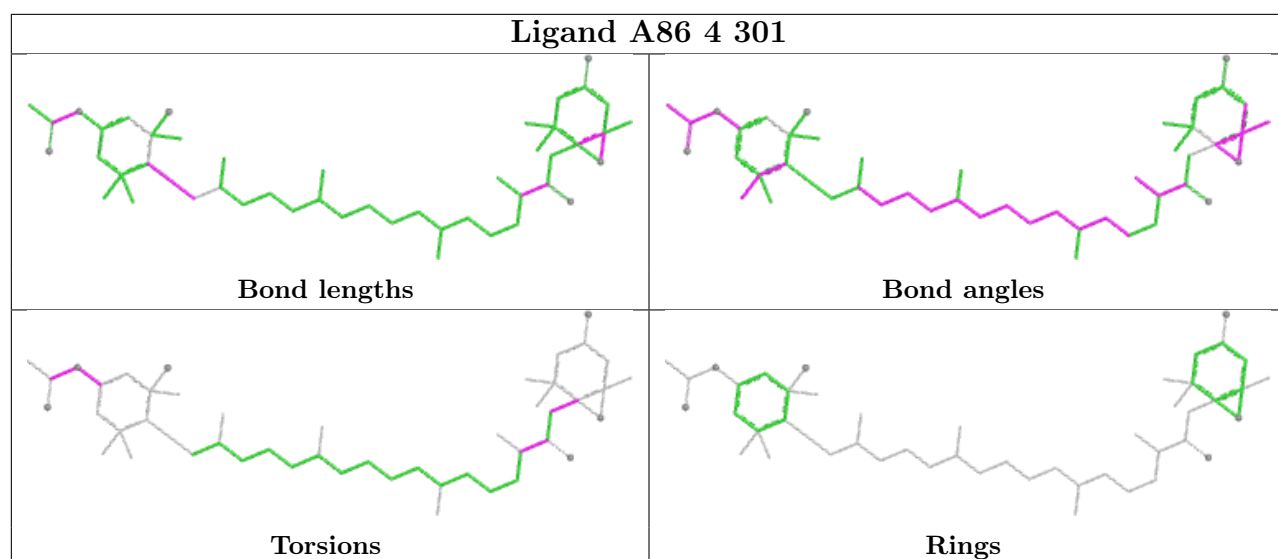


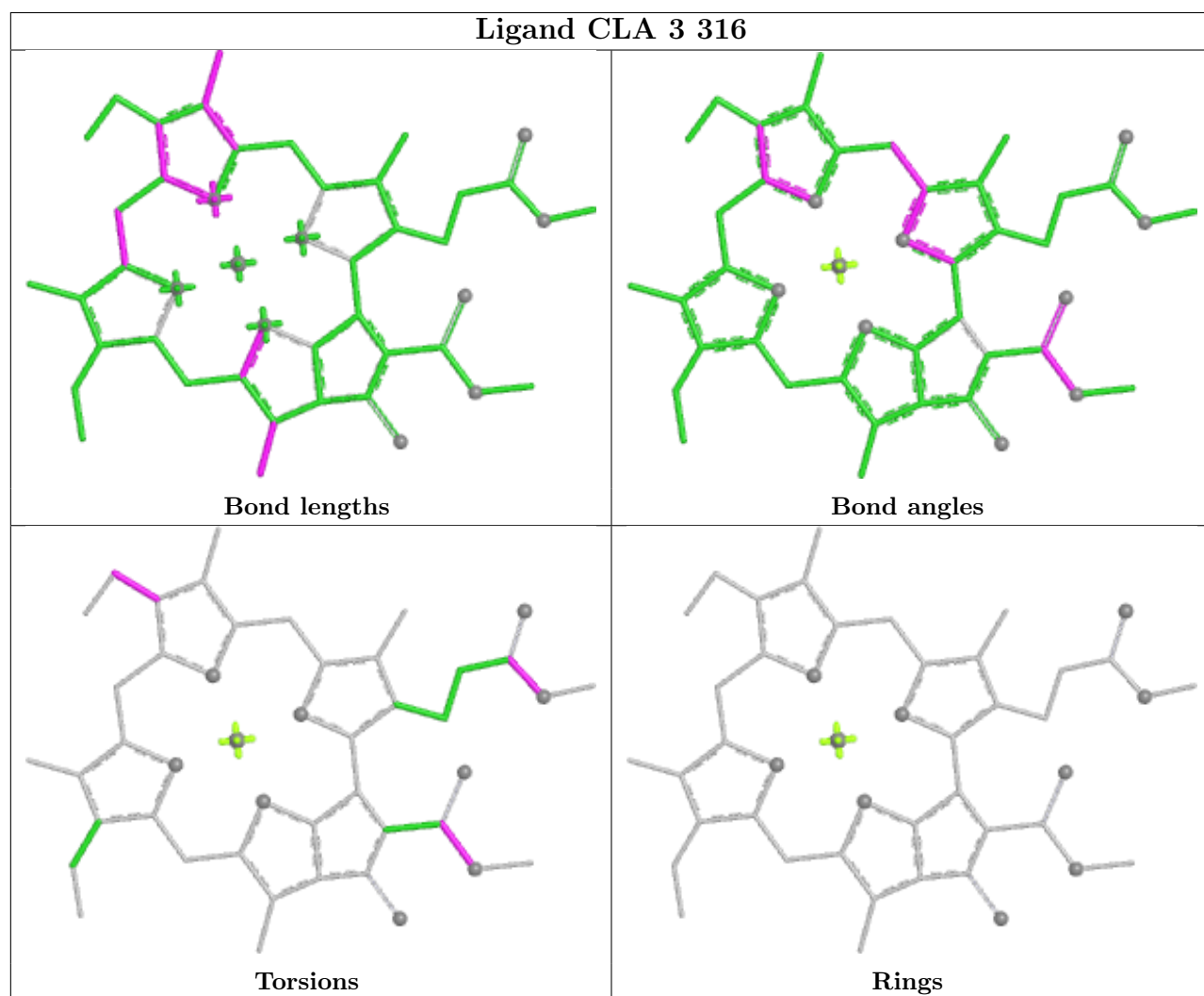
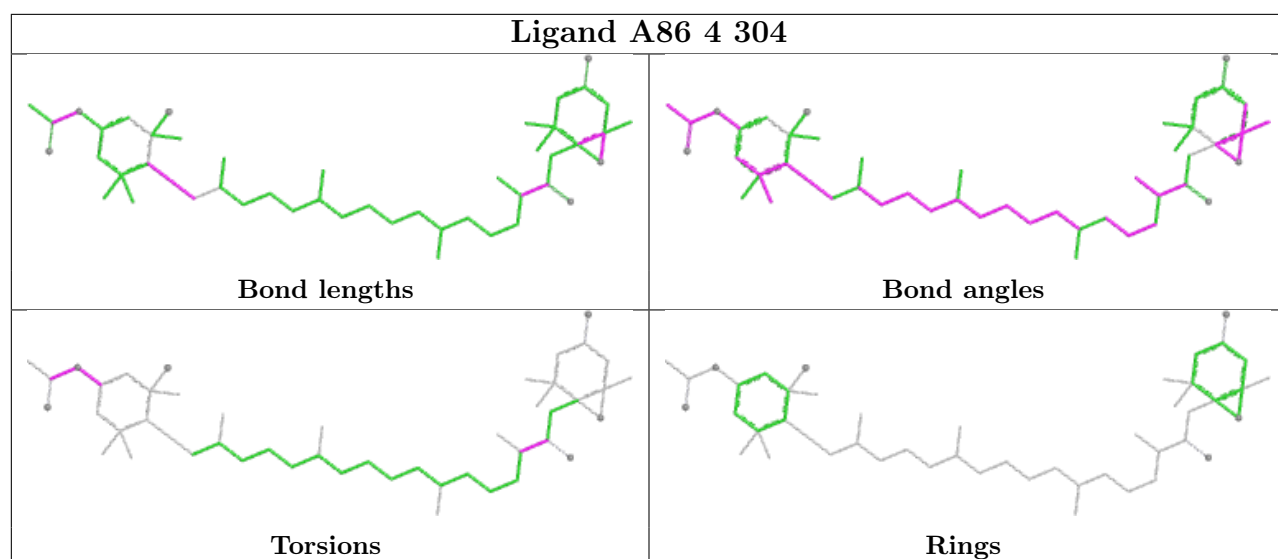
Ligand CLA 4 315

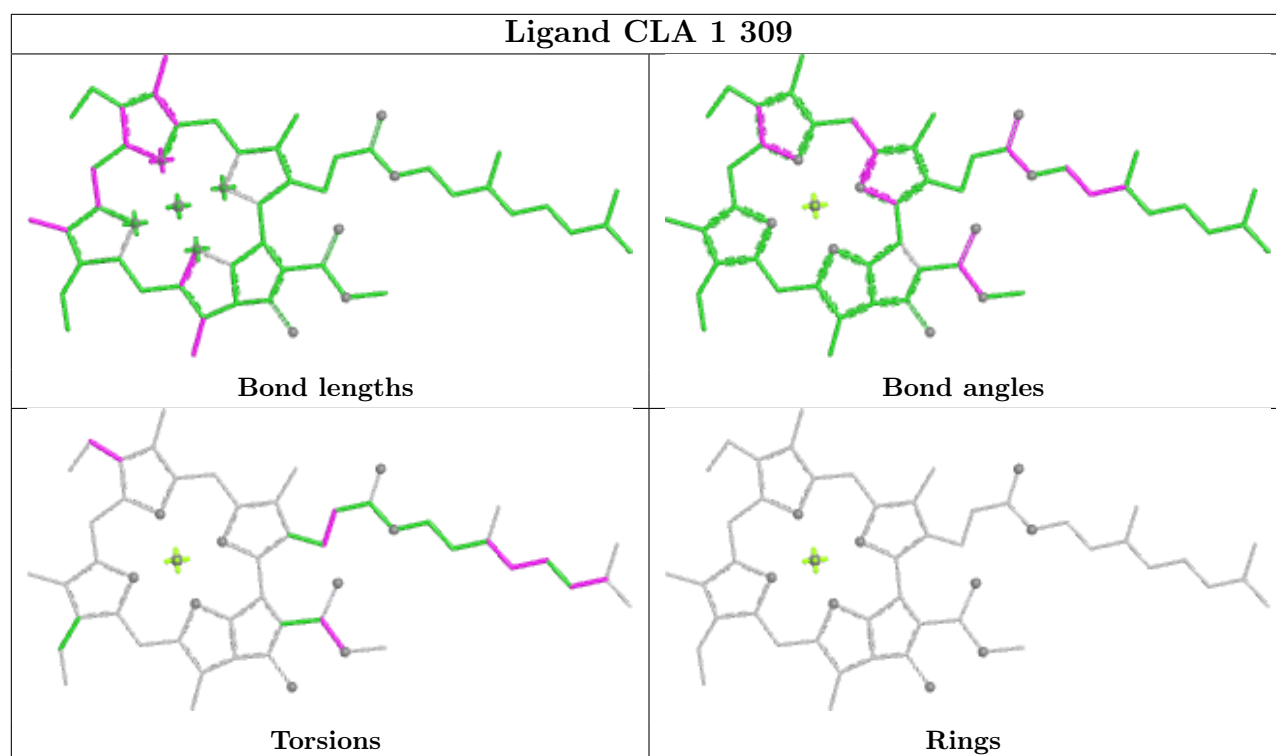


Ligand A86 1 305

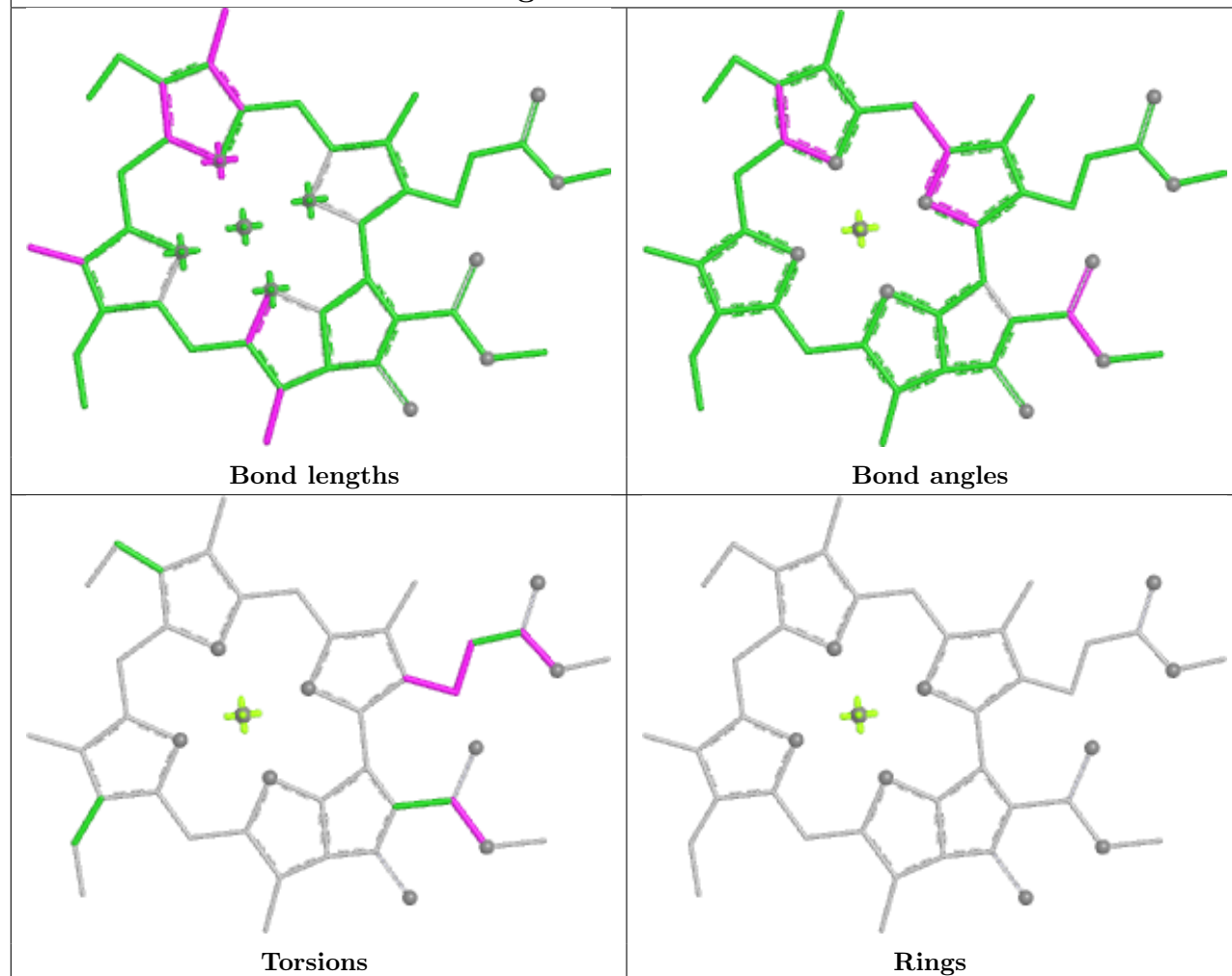




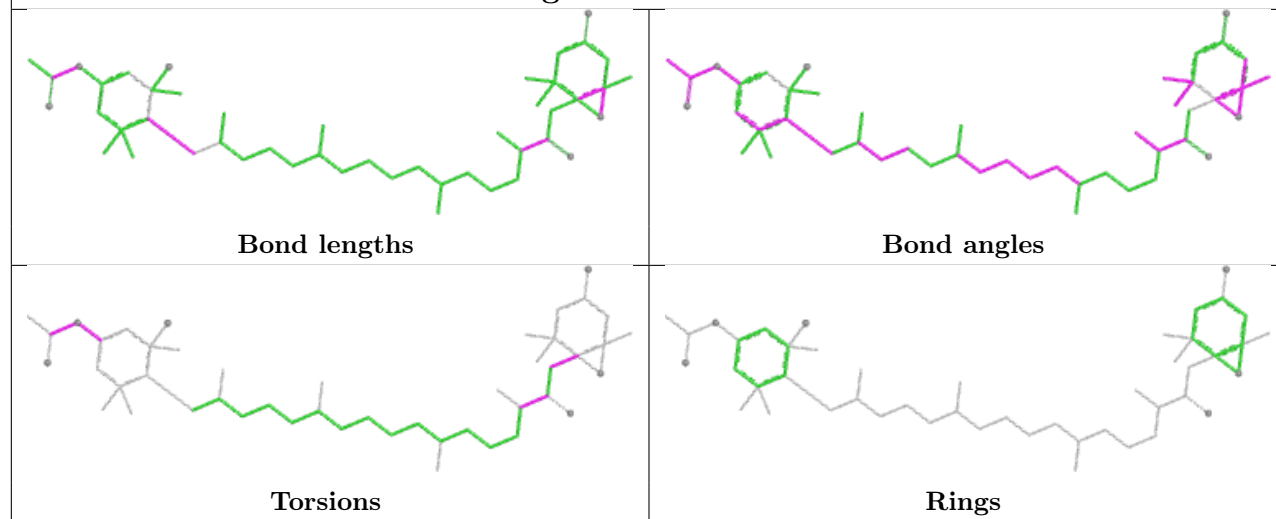




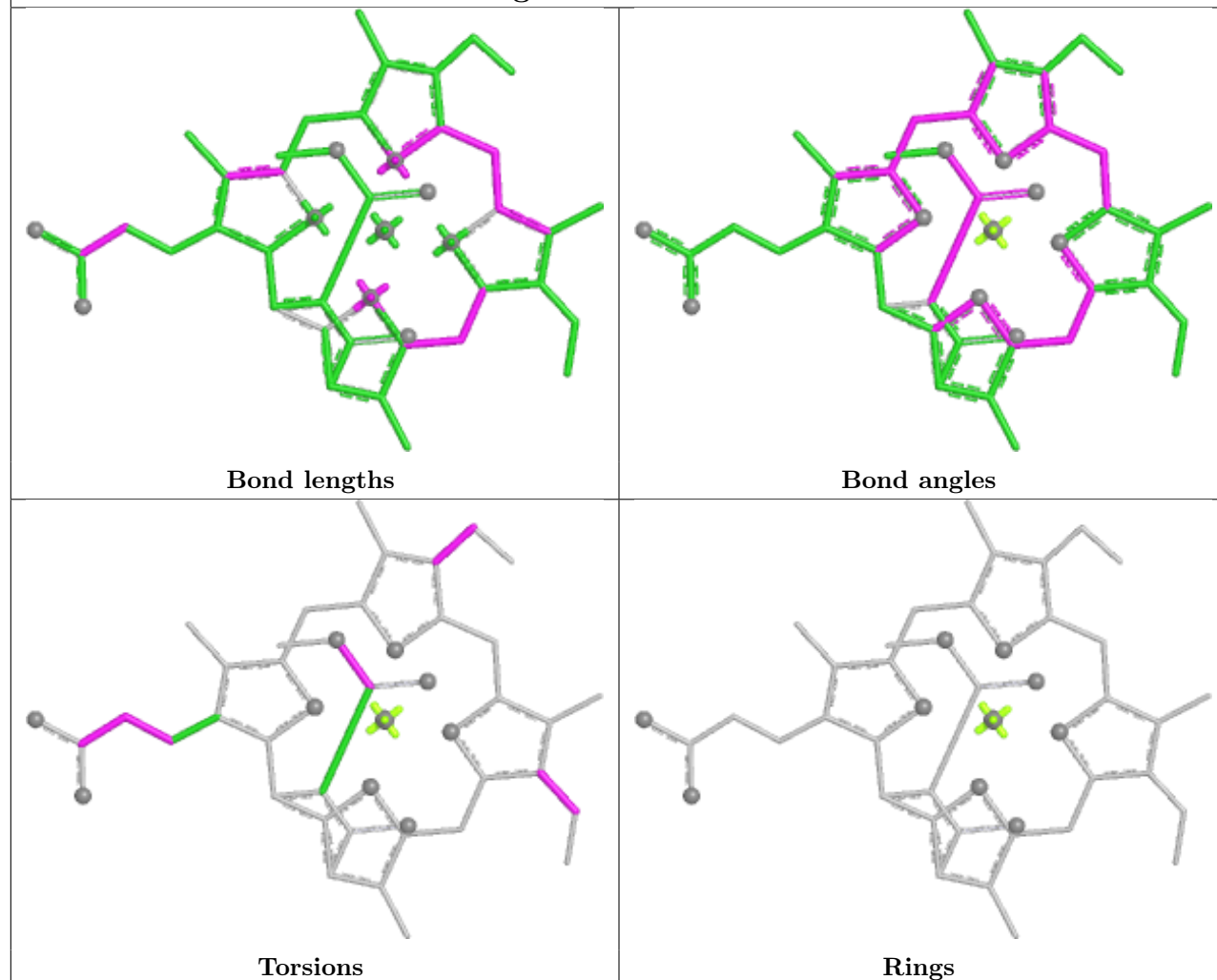
Ligand CLA 4 314



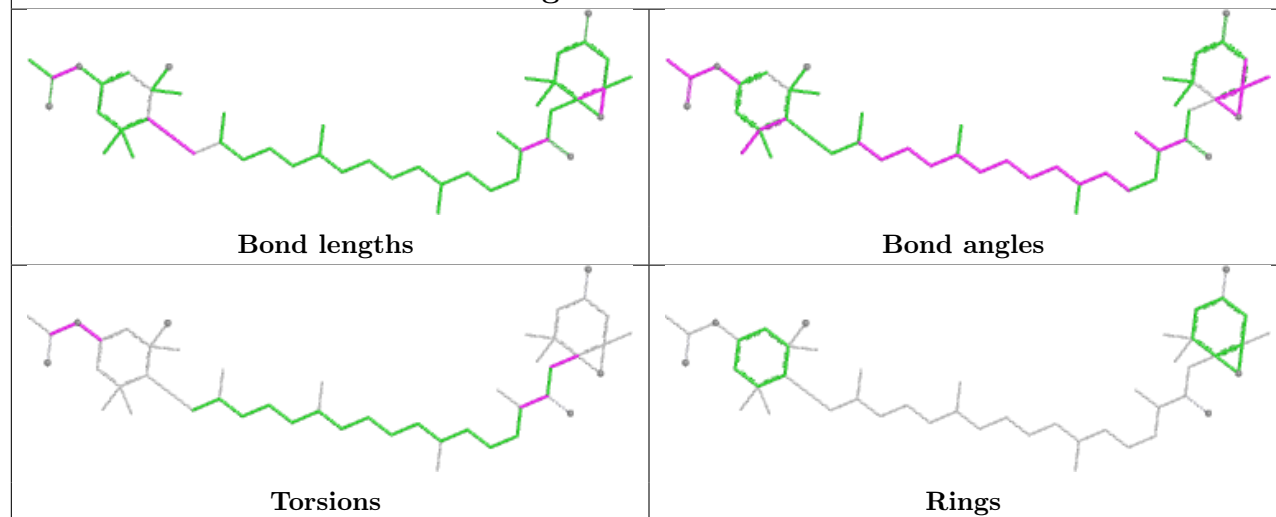
Ligand A86 3 306

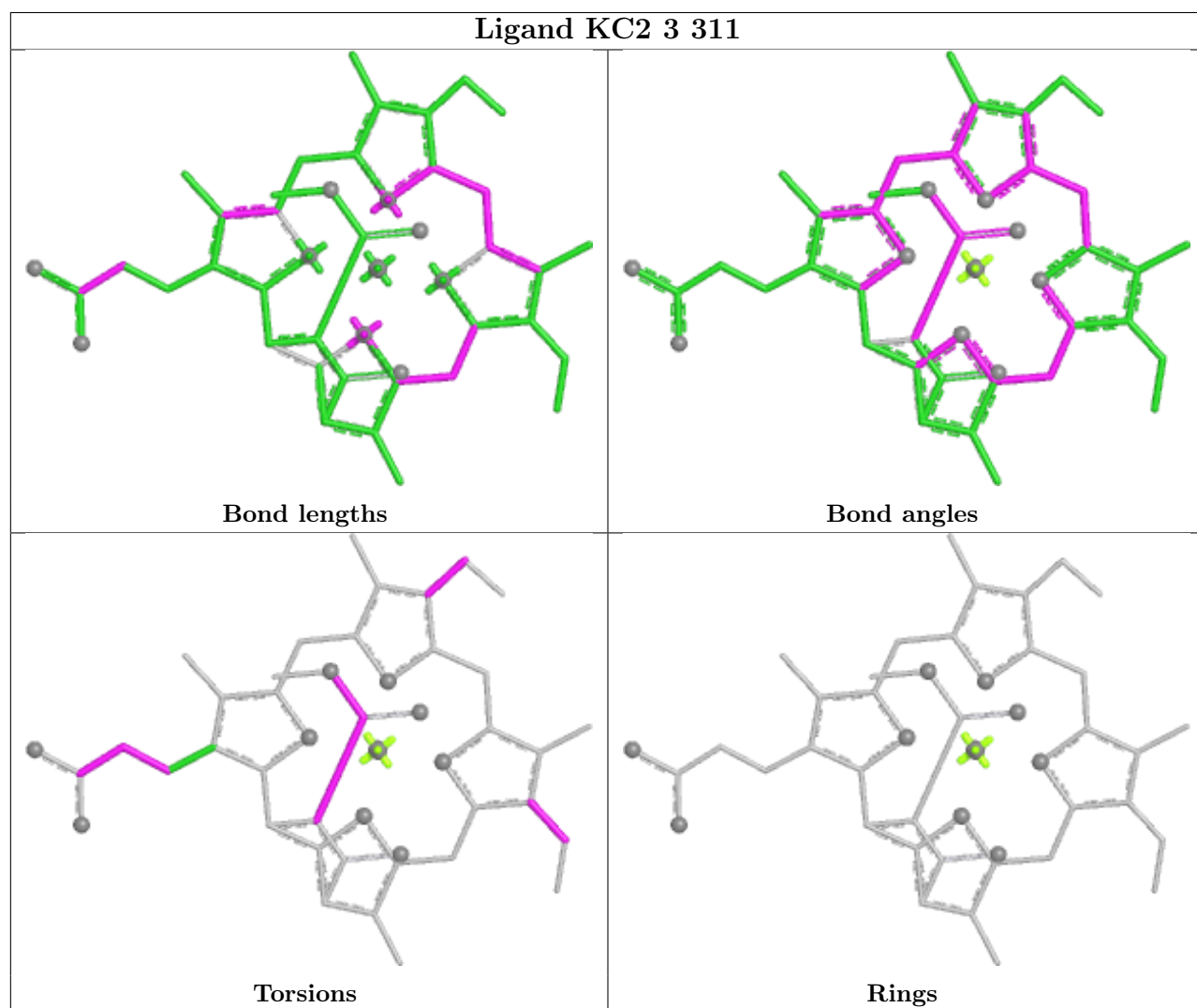
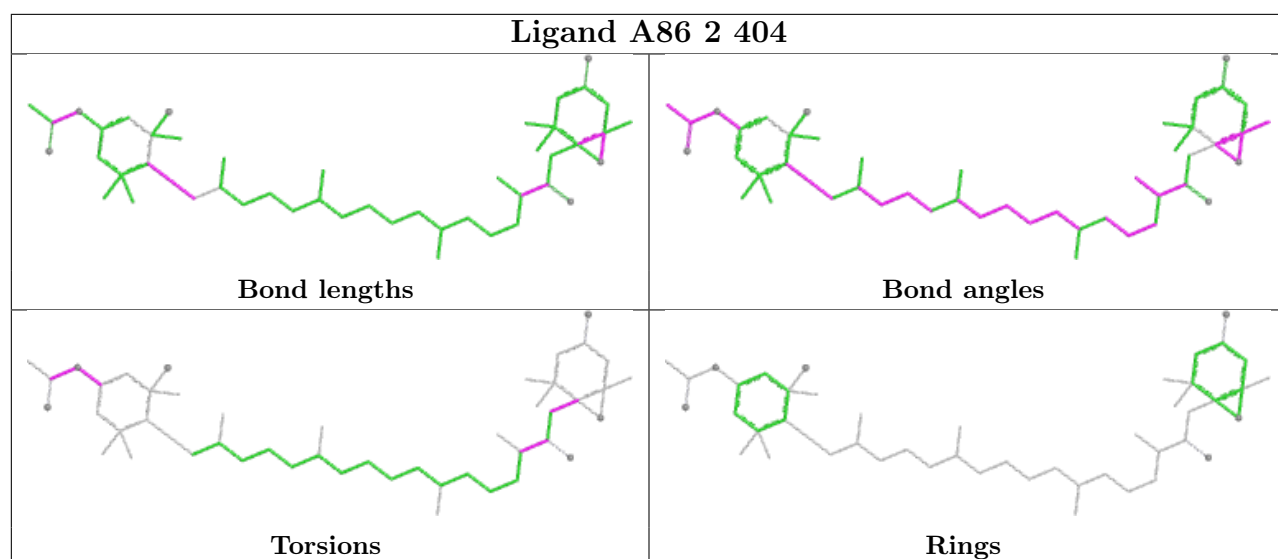


Ligand KC2 1 310

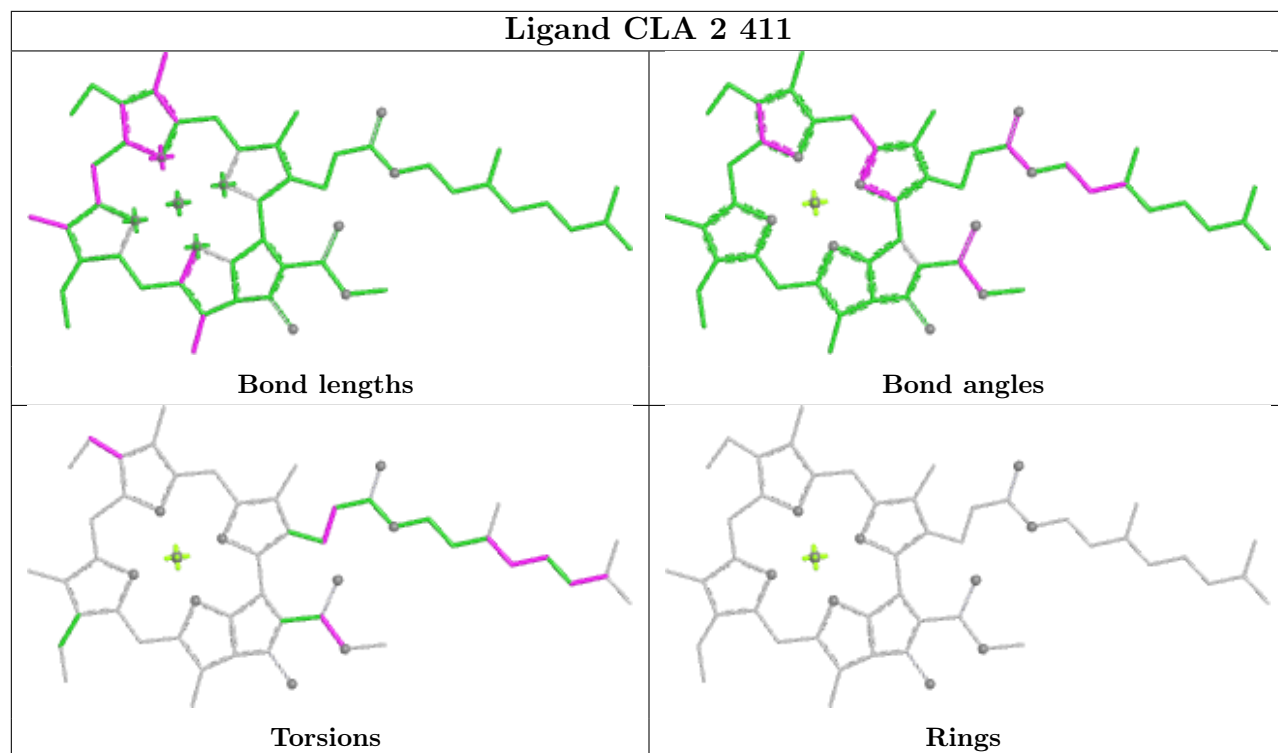


Ligand A86 1 301

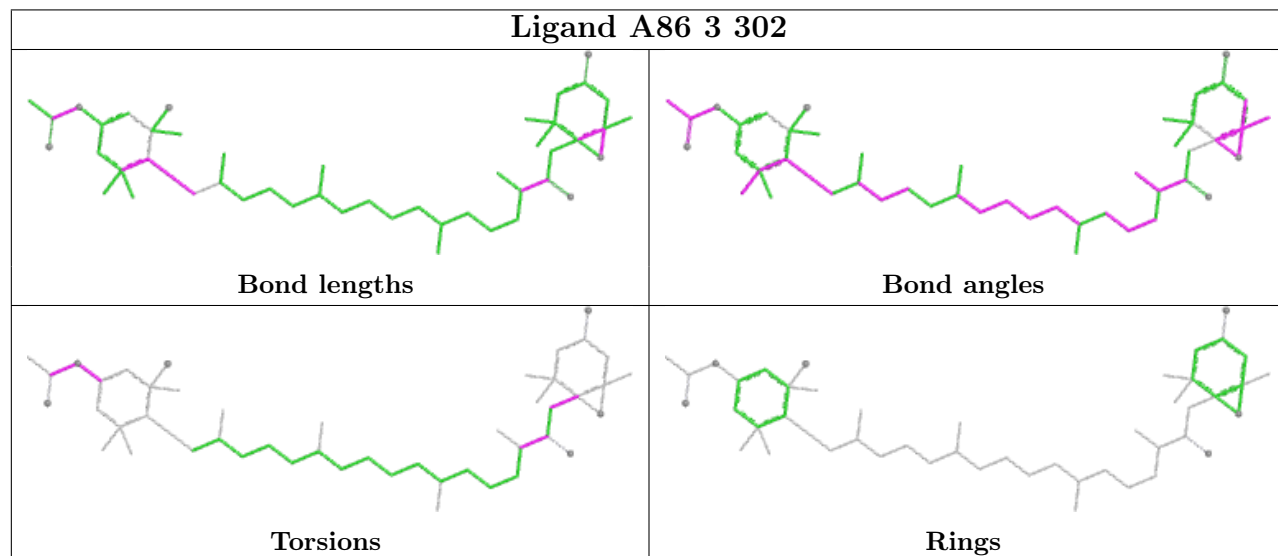


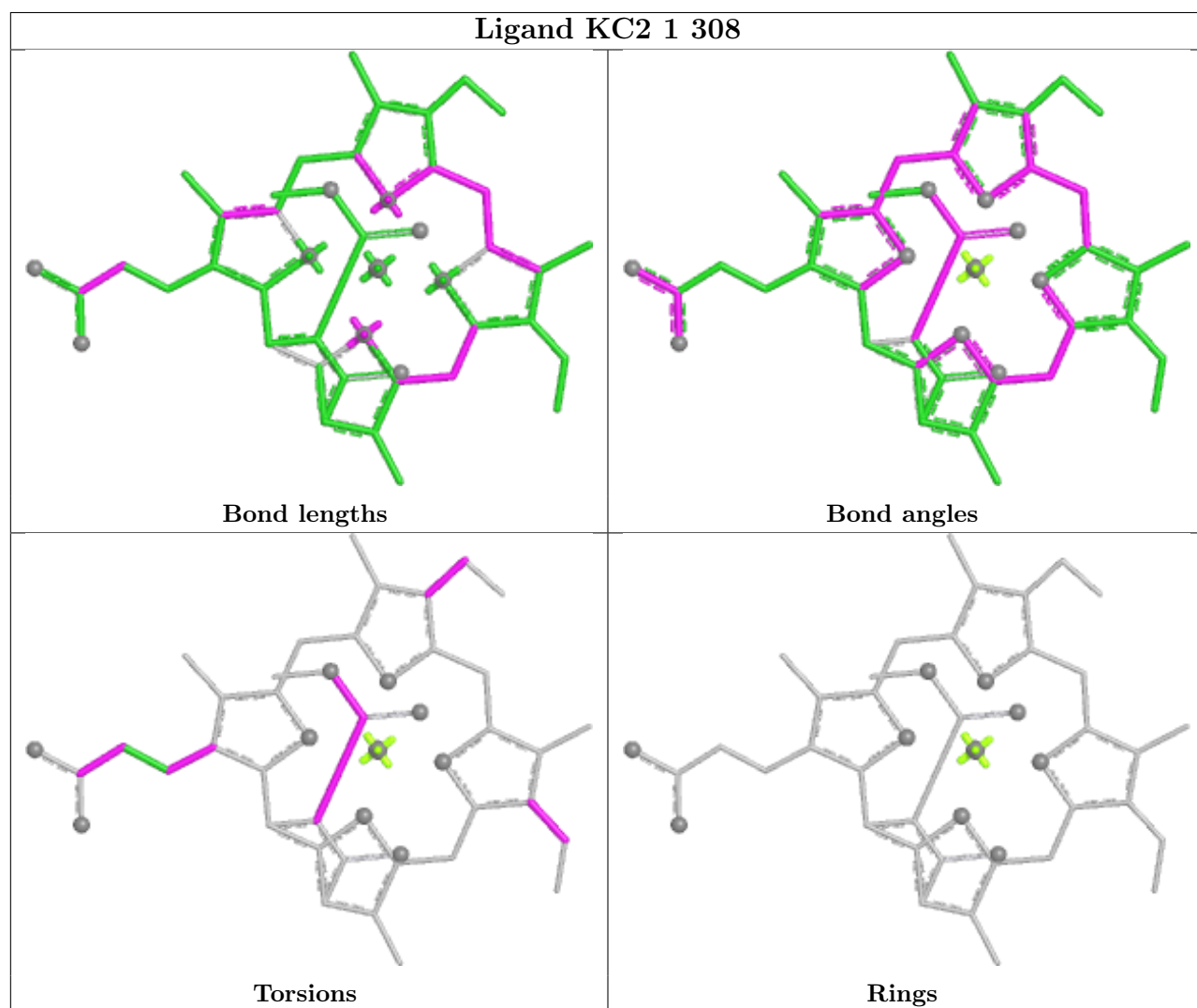
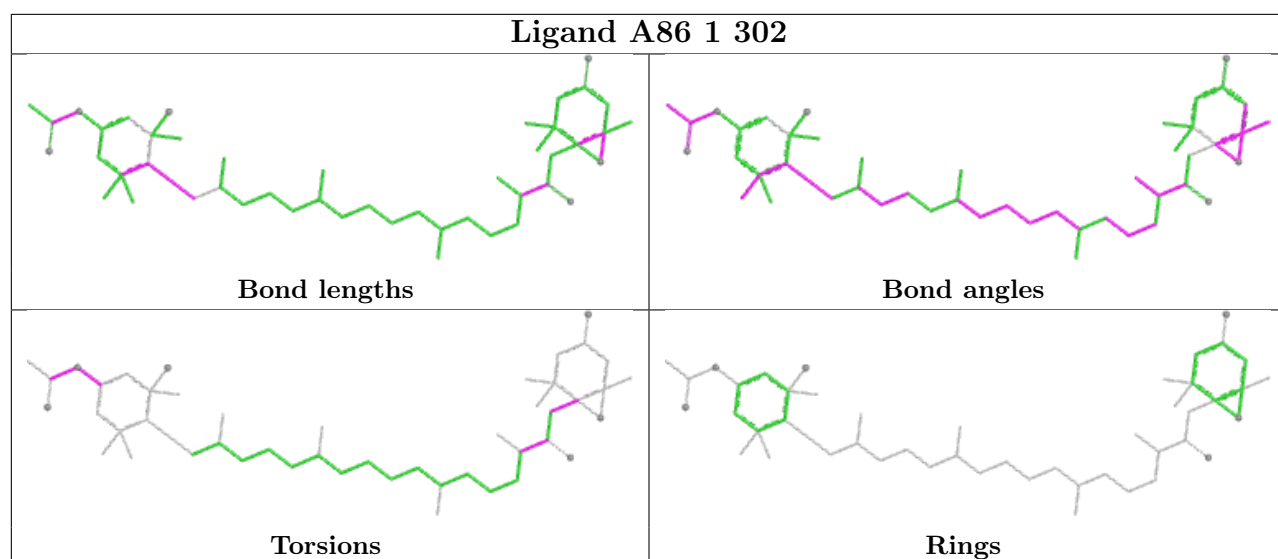


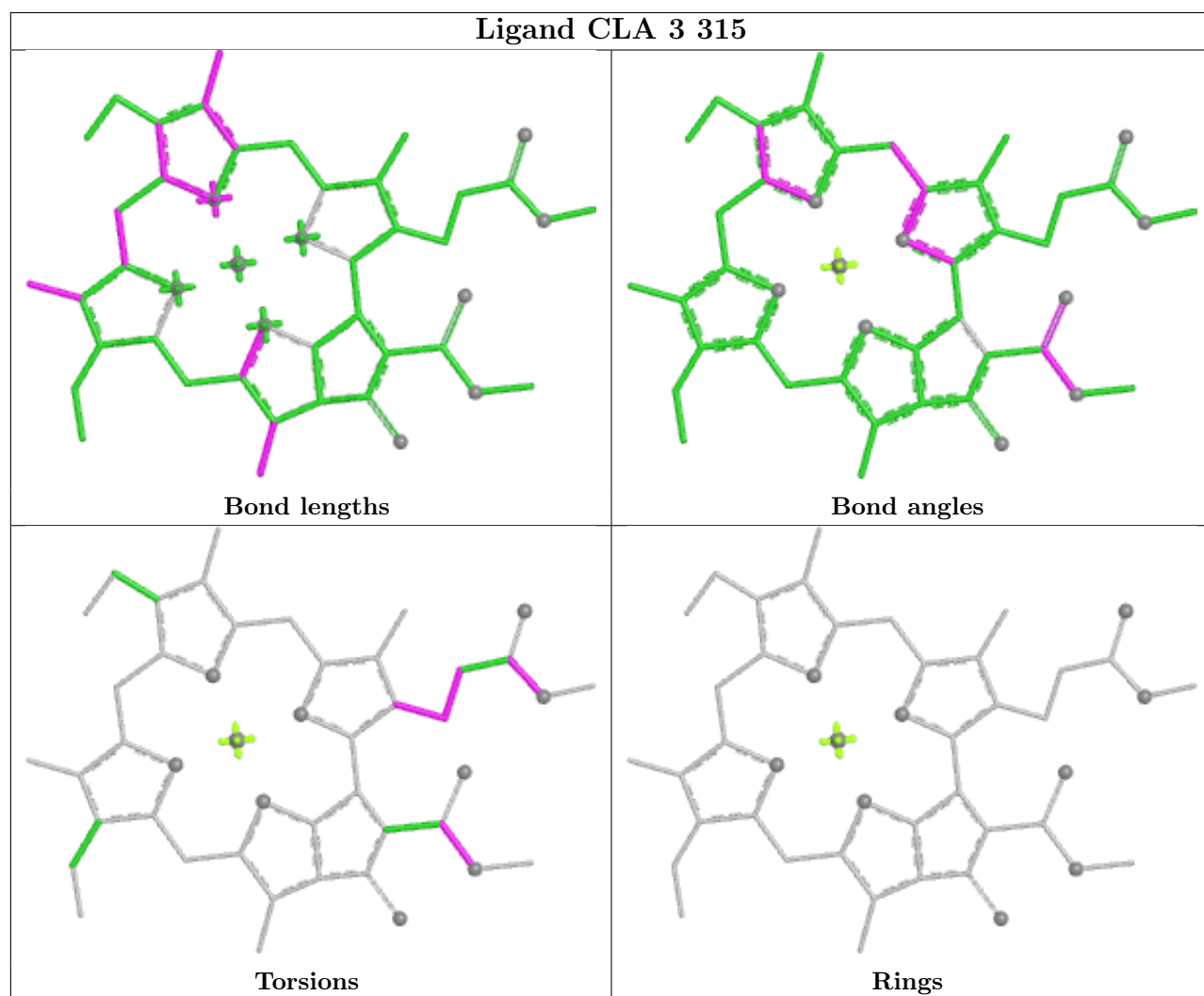
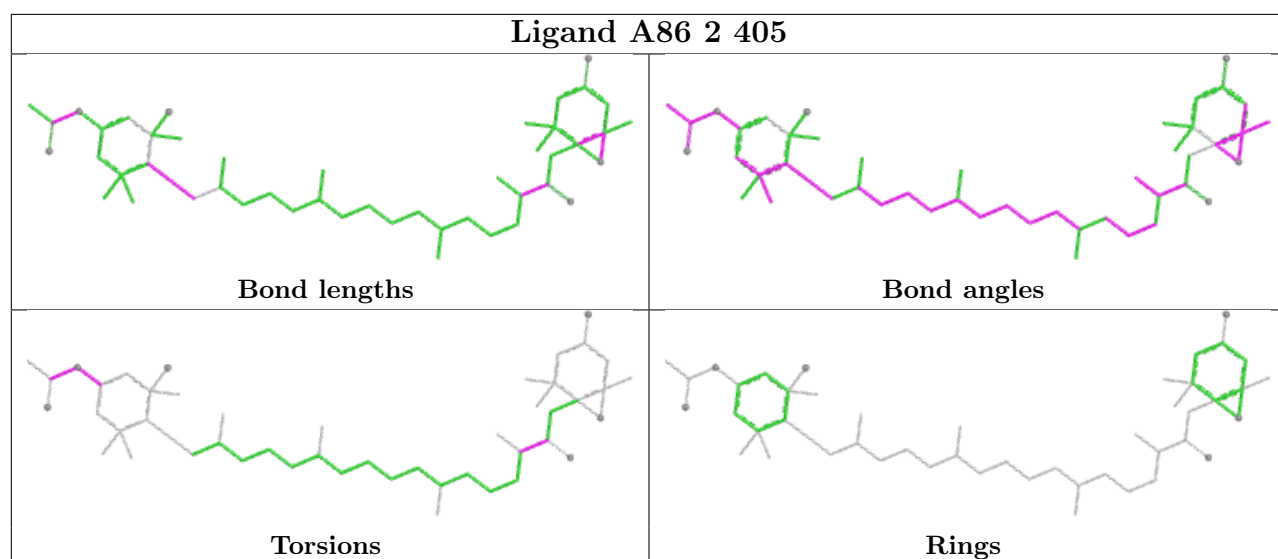
Ligand CLA 2 411



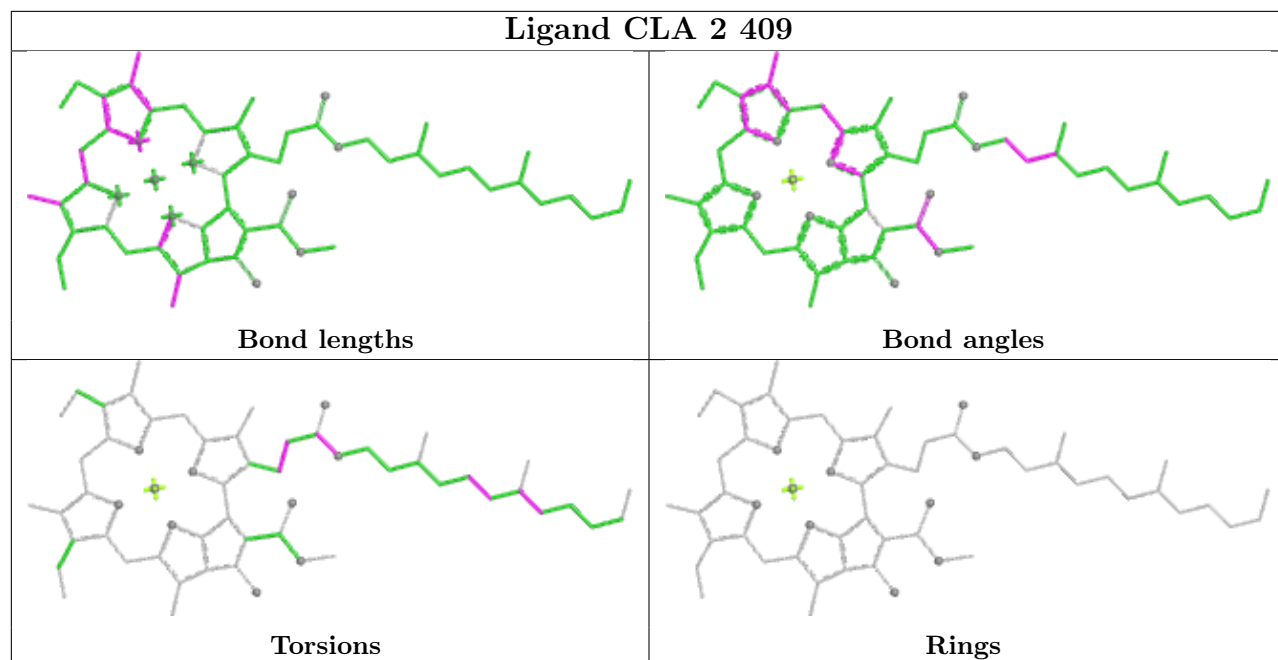
Ligand A86 3 302



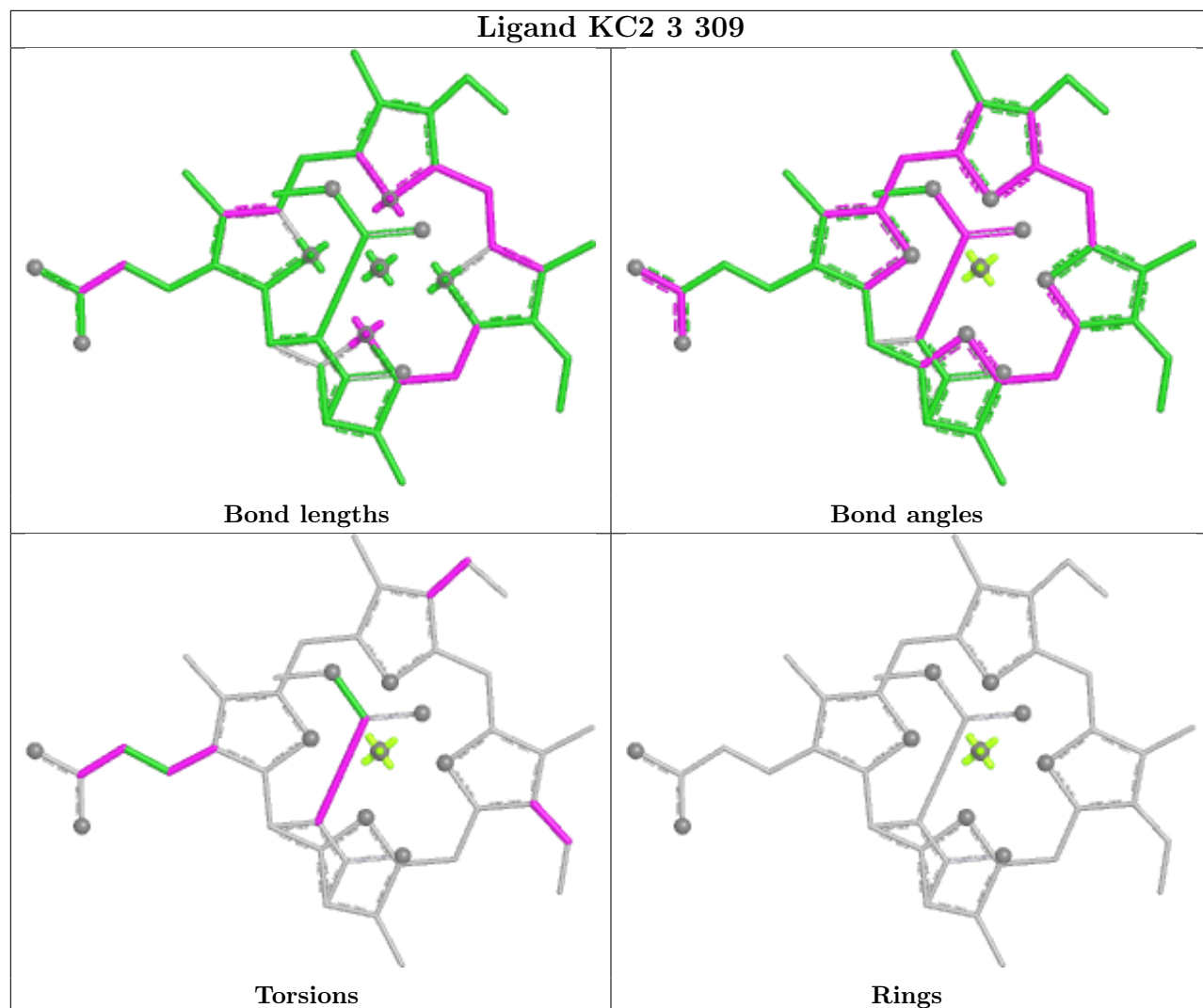


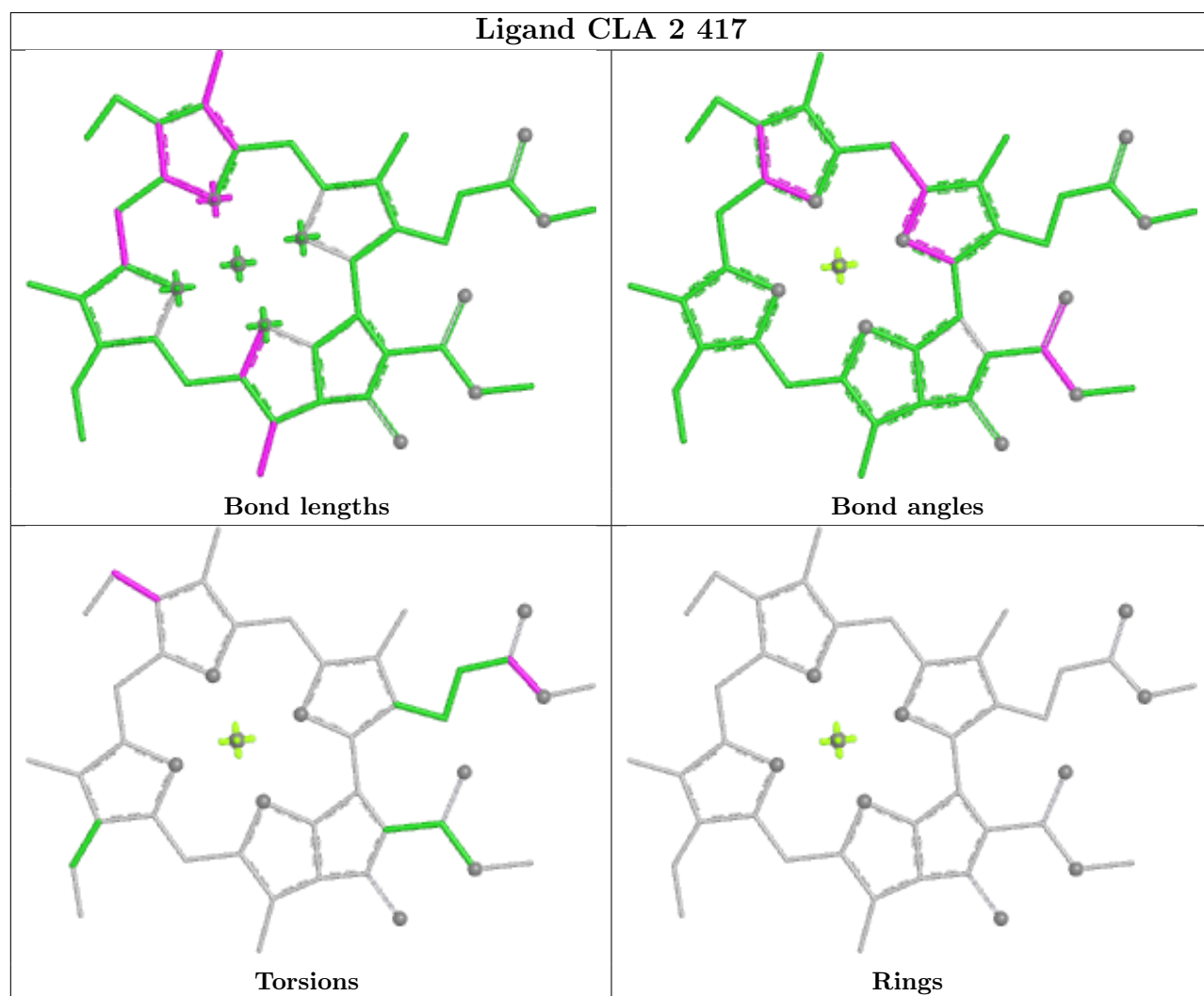
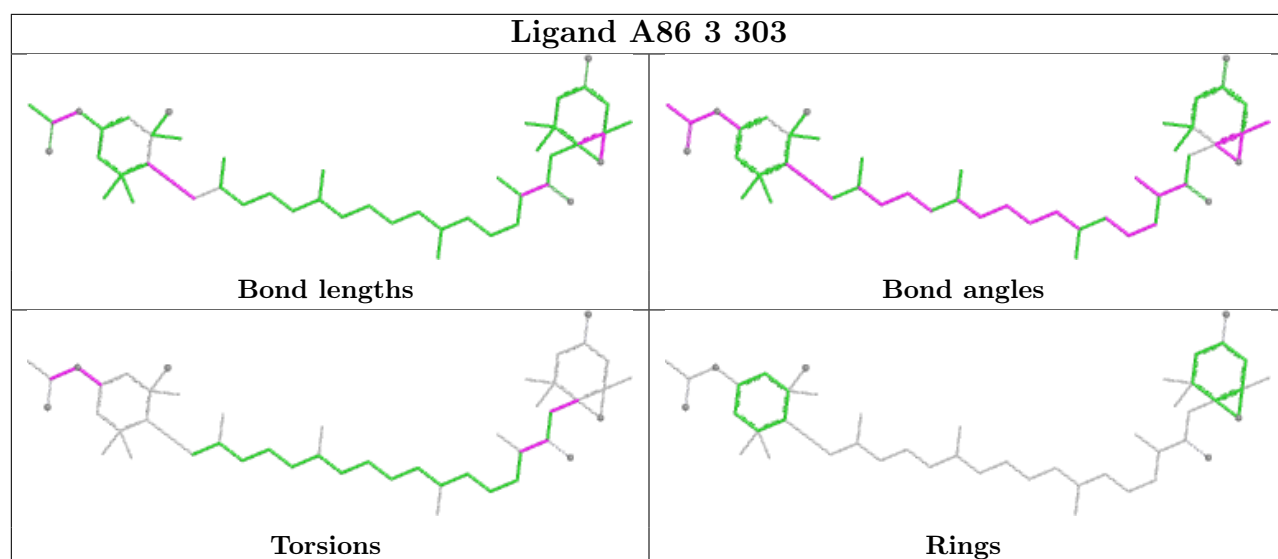


Ligand CLA 2 409

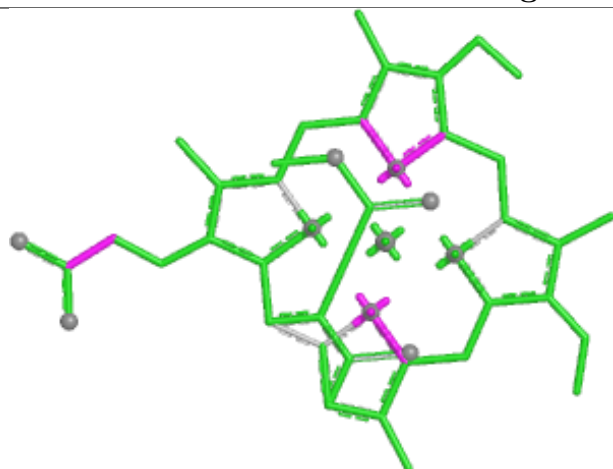


Ligand KC2 3 309

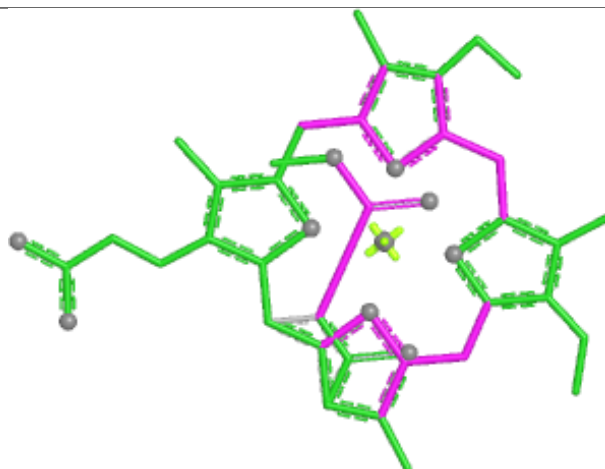




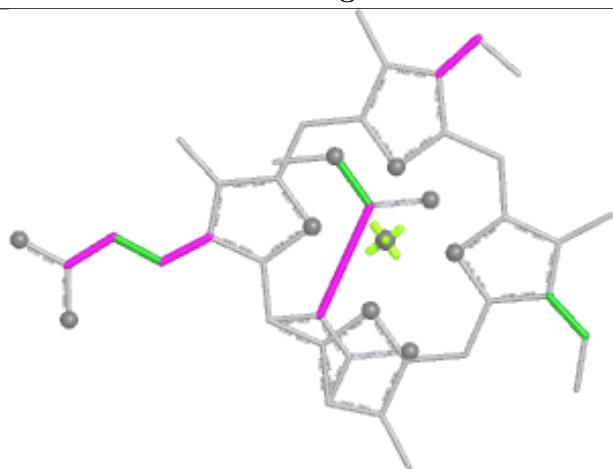
Ligand KC1 4 313



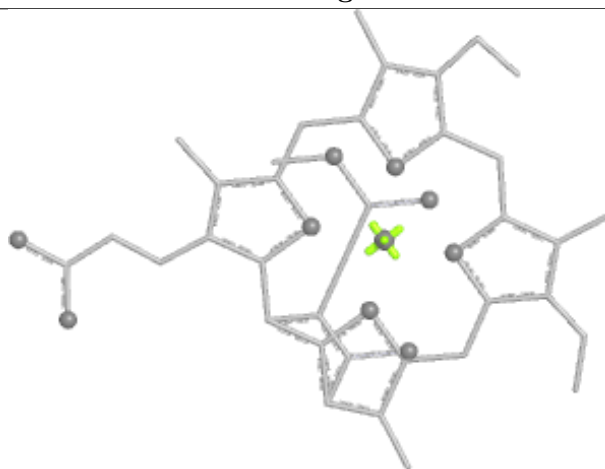
Bond lengths



Bond angles

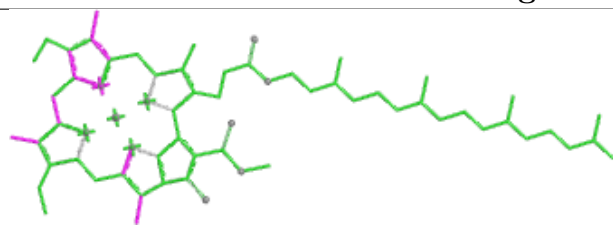


Torsions

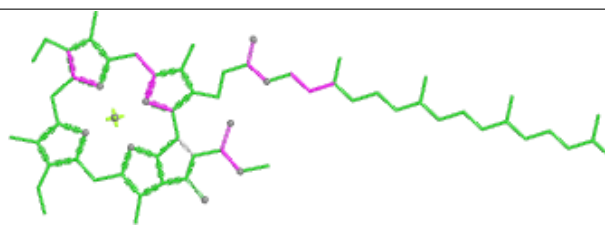


Rings

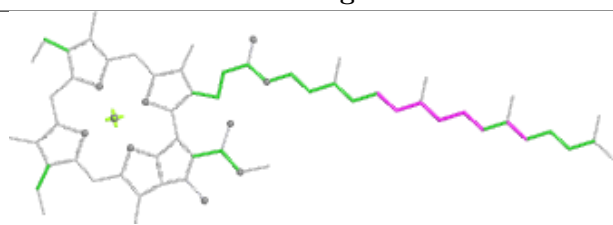
Ligand CLA 2 408



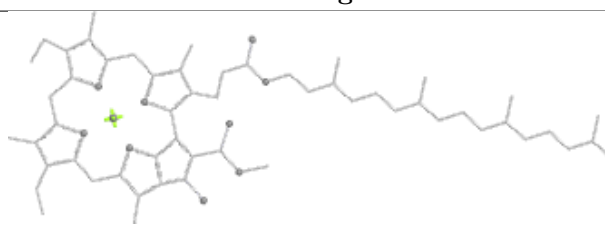
Bond lengths



Bond angles

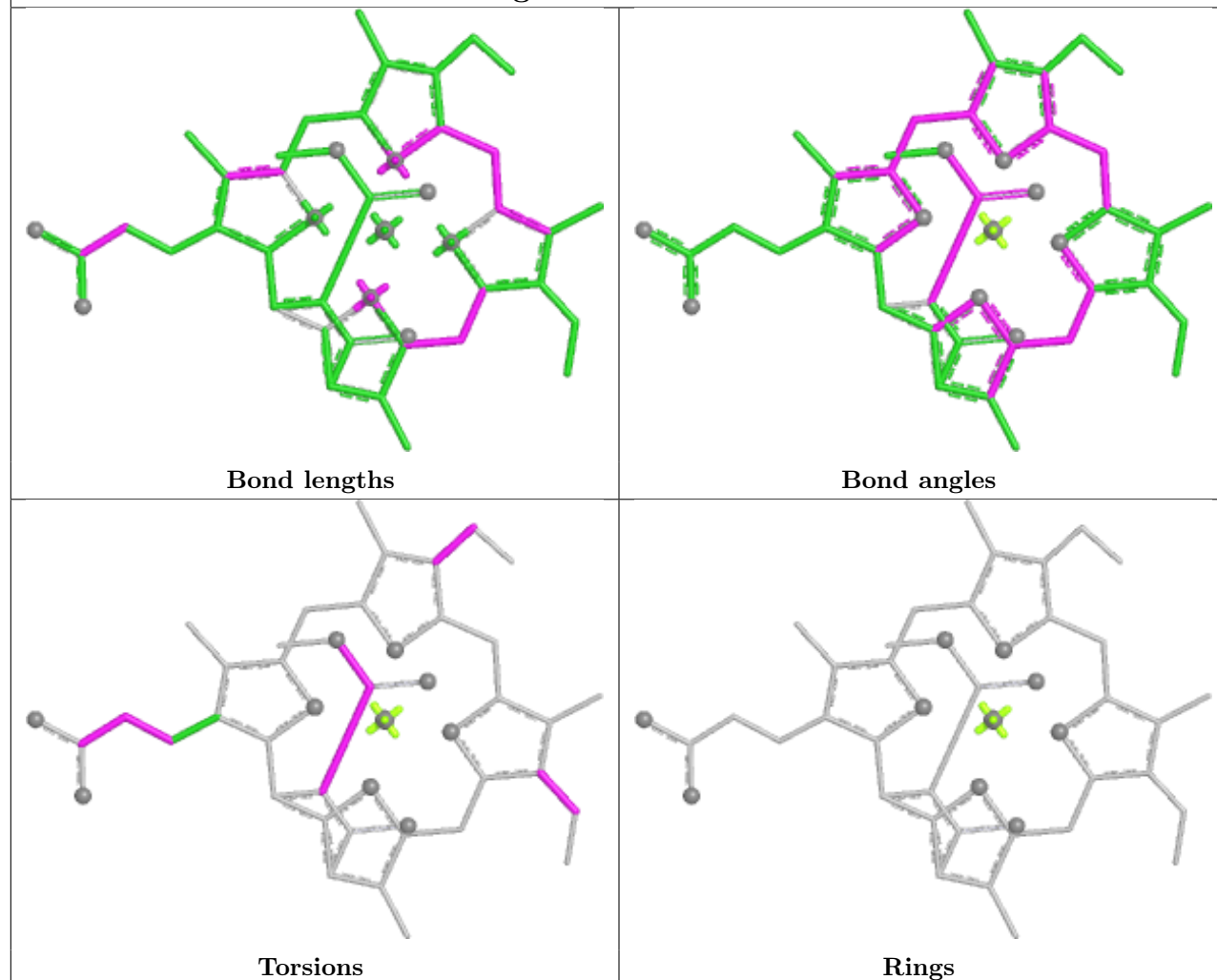


Torsions

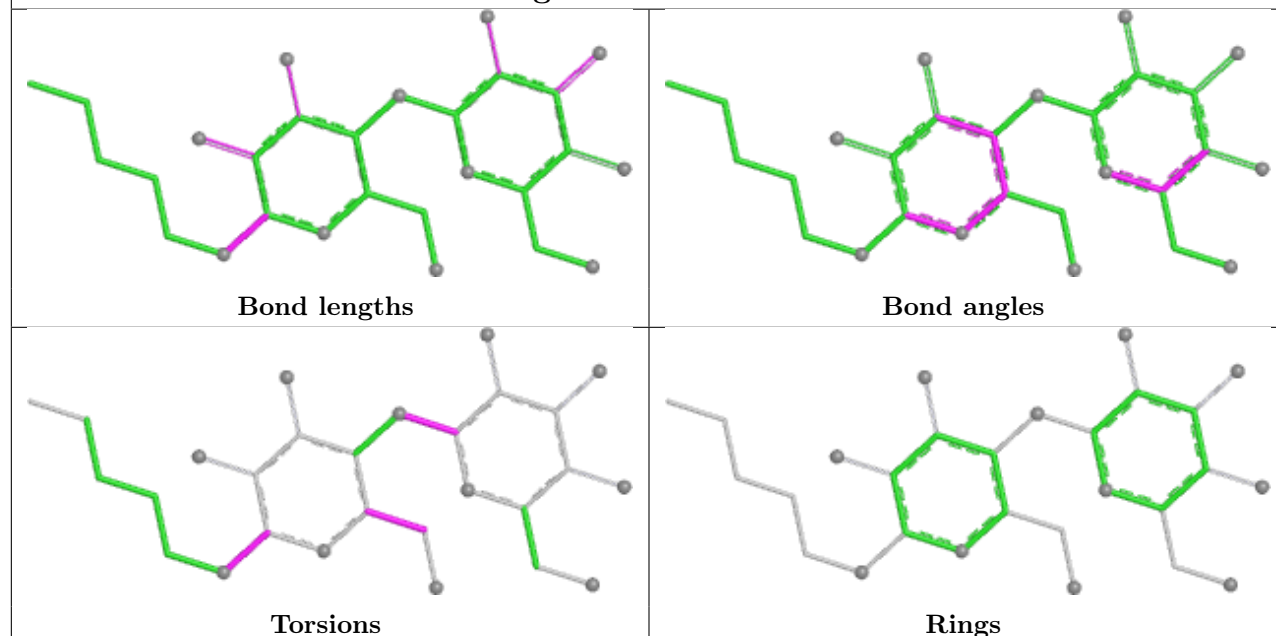


Rings

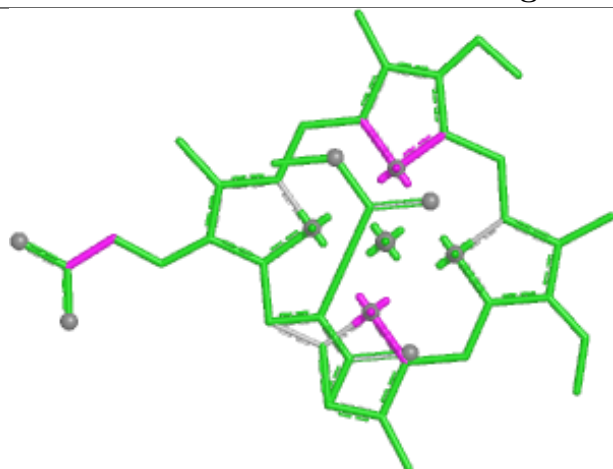
Ligand KC2 2 412



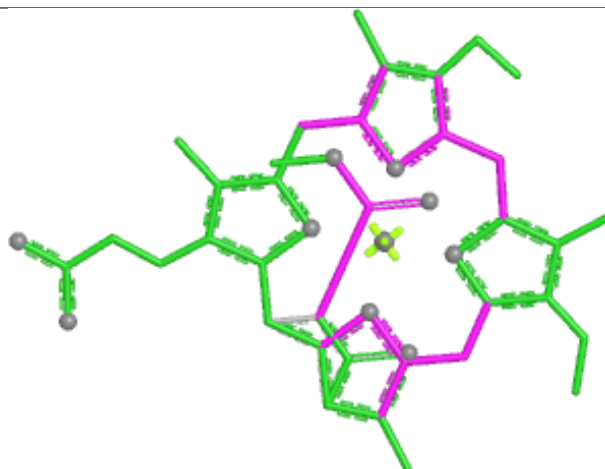
Ligand LMT 3 317



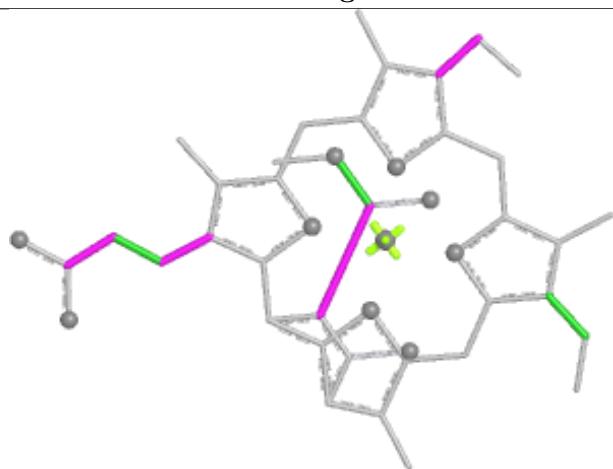
Ligand KC1 1 313



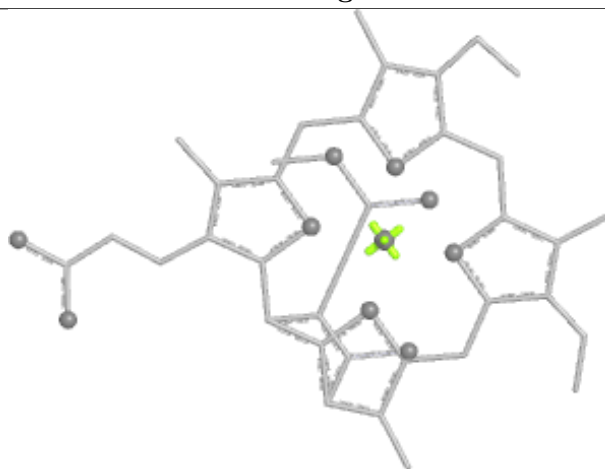
Bond lengths



Bond angles

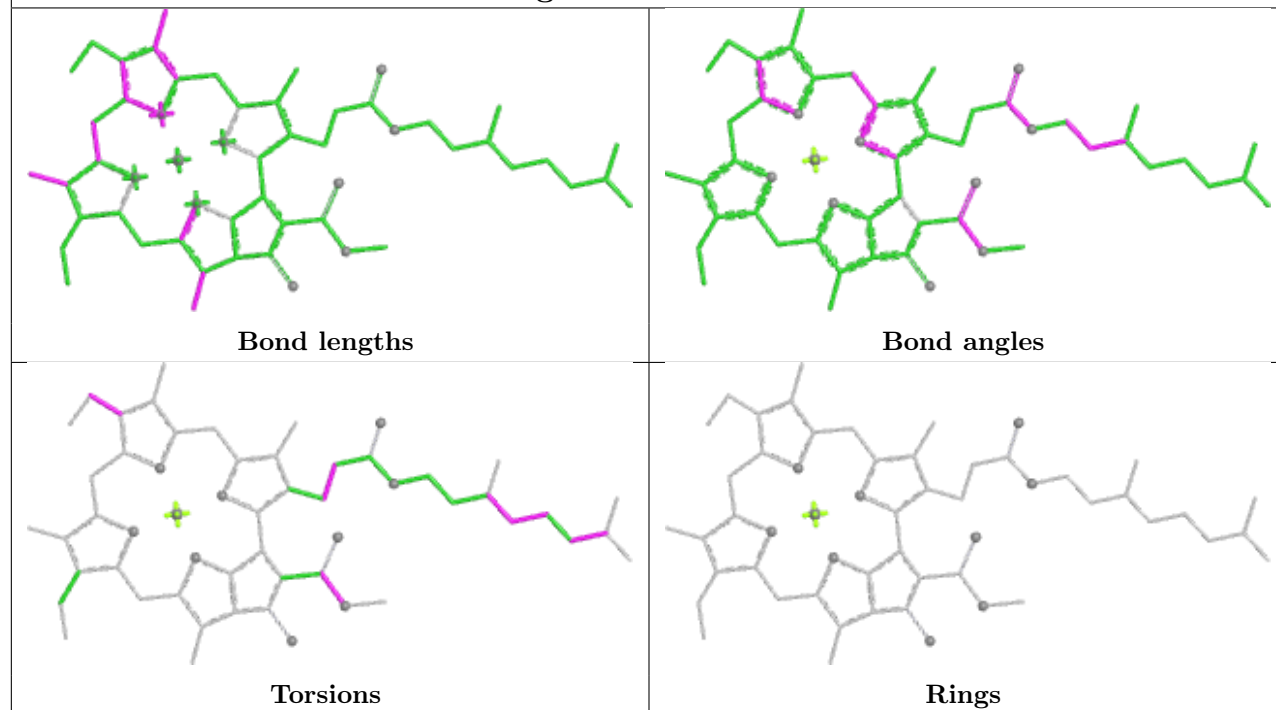


Torsions

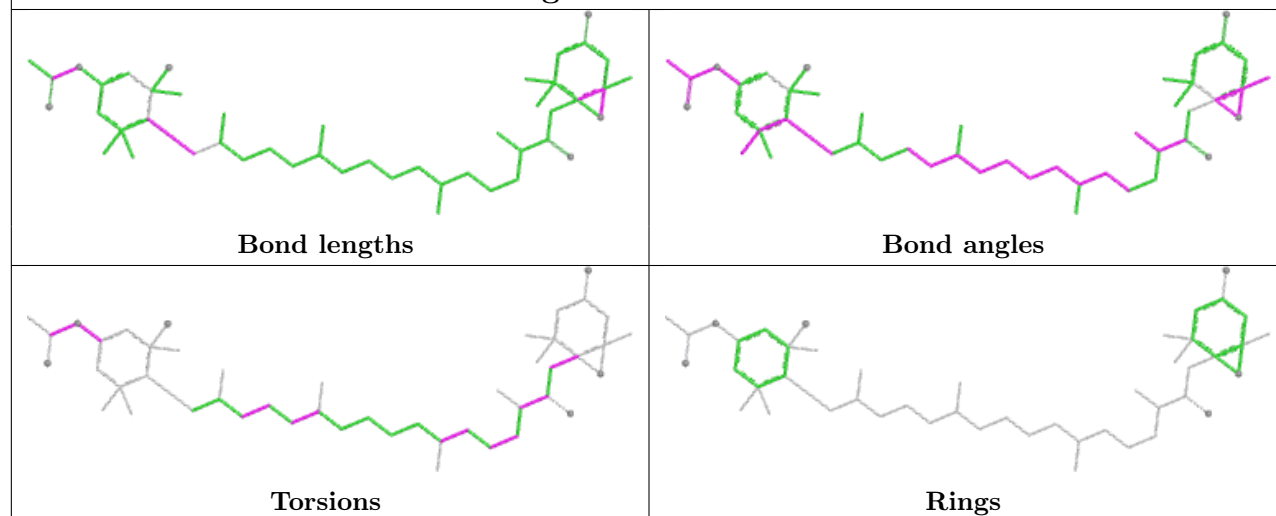


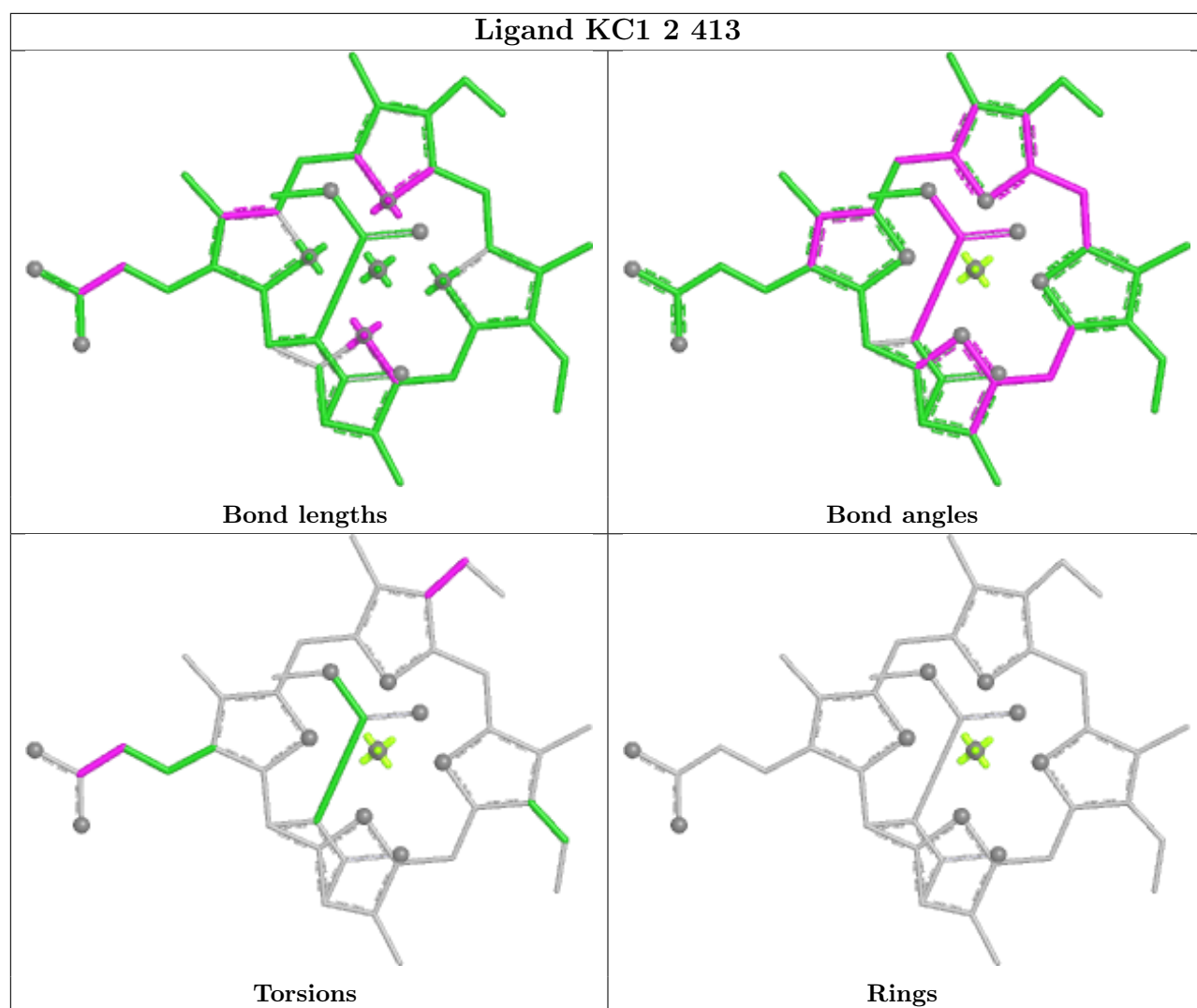
Rings

Ligand CLA 3 310



Ligand A86 3 305





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

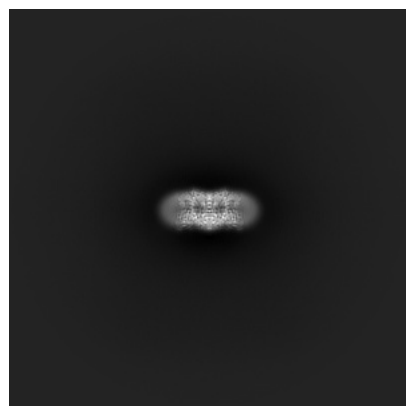
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37441. These allow visual inspection of the internal detail of the map and identification of artifacts.

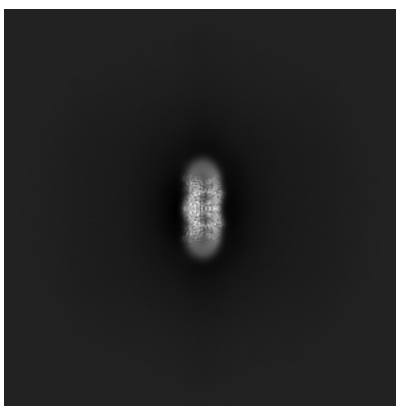
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

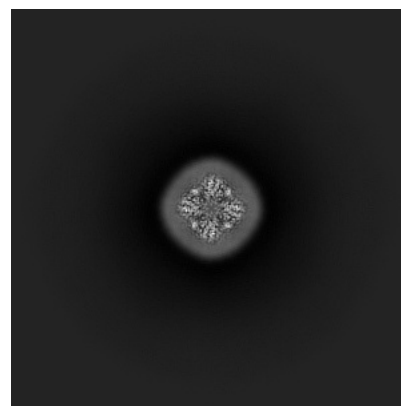
6.1.1 Primary map



X

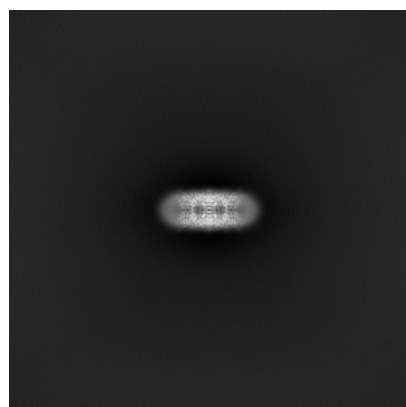


Y

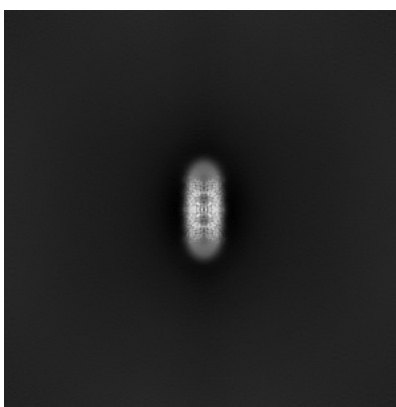


Z

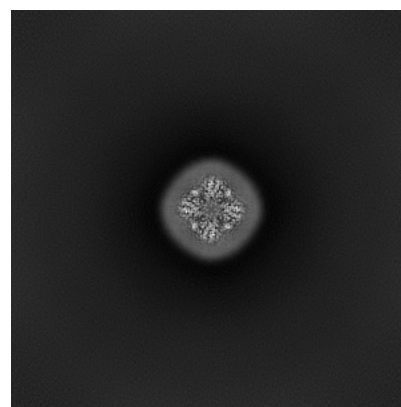
6.1.2 Raw map



X



Y

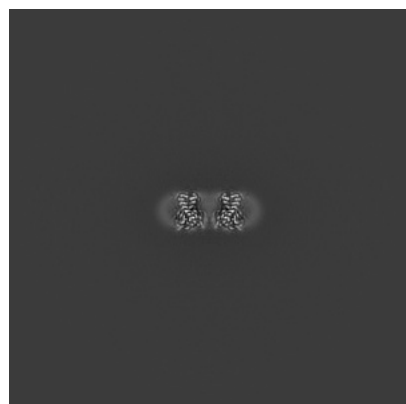


Z

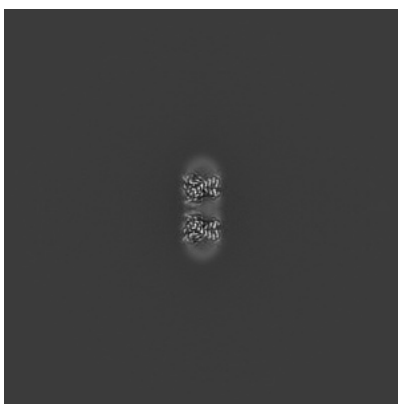
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

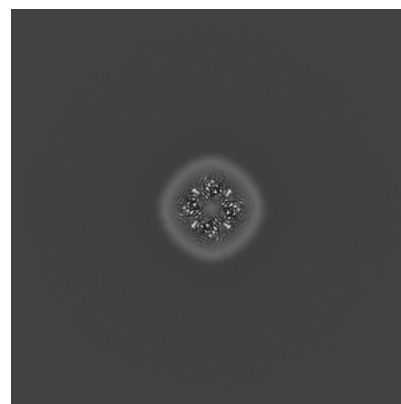
6.2.1 Primary map



X Index: 240

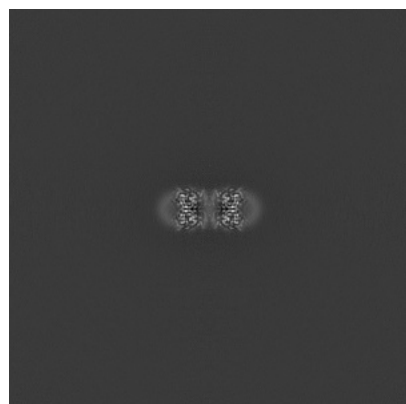


Y Index: 240

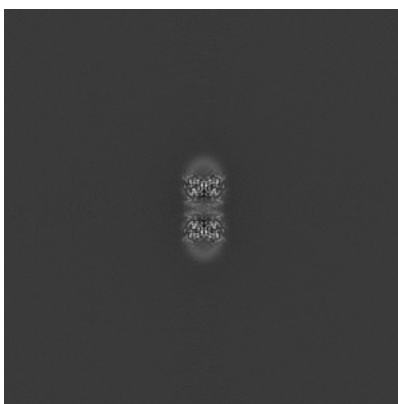


Z Index: 240

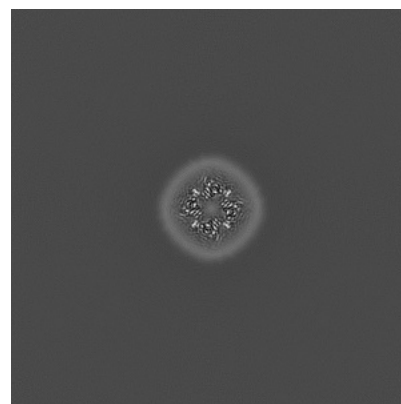
6.2.2 Raw map



X Index: 240



Y Index: 240

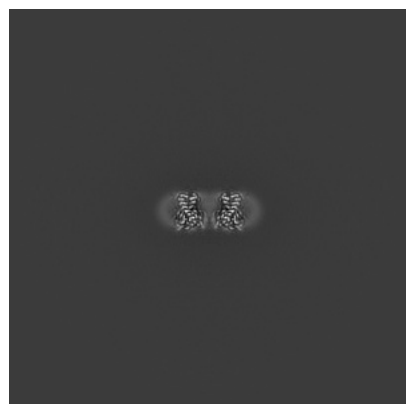


Z Index: 240

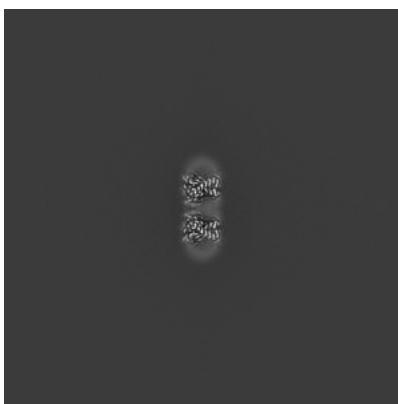
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

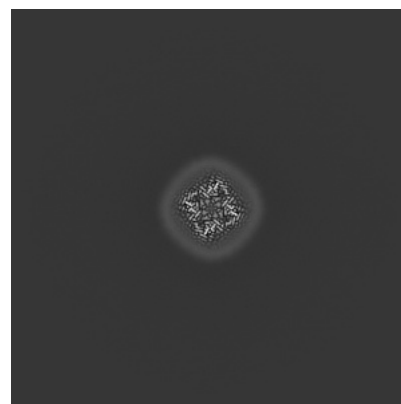
6.3.1 Primary map



X Index: 240

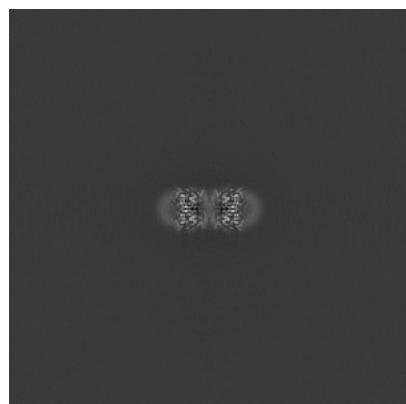


Y Index: 240

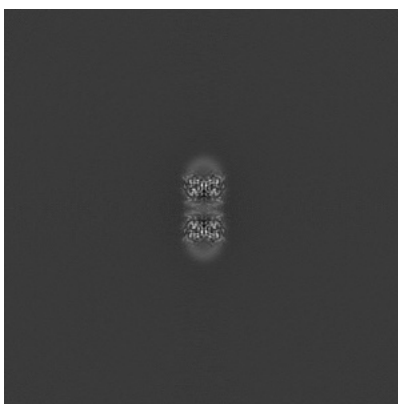


Z Index: 233

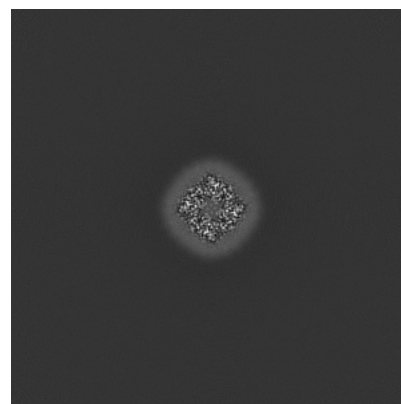
6.3.2 Raw map



X Index: 240



Y Index: 240

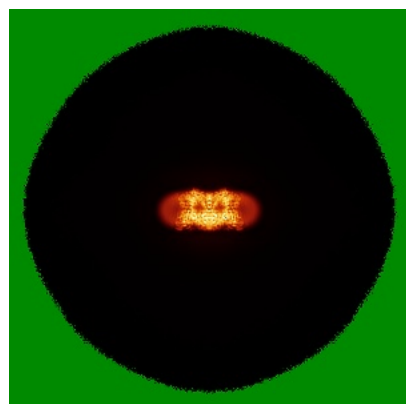


Z Index: 251

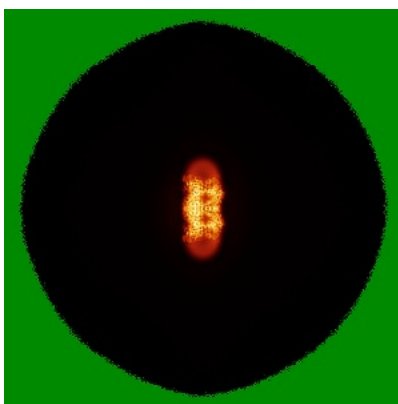
The images above show the largest variance slices of the map in three orthogonal directions.

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

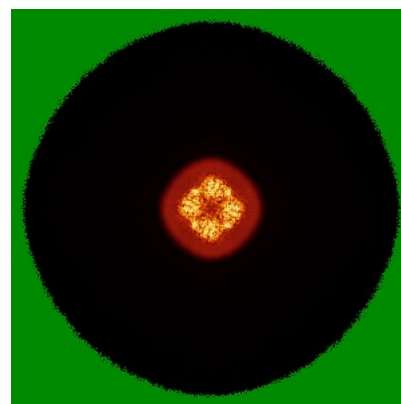
6.4.1 Primary map



X

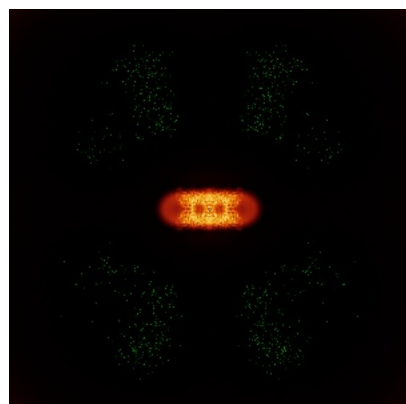


Y

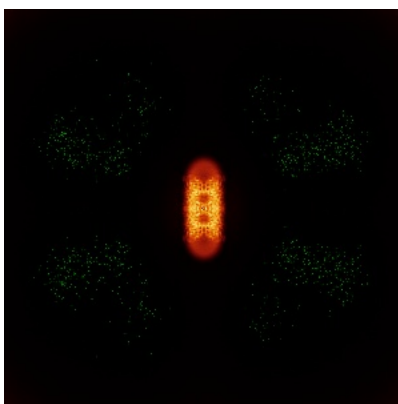


Z

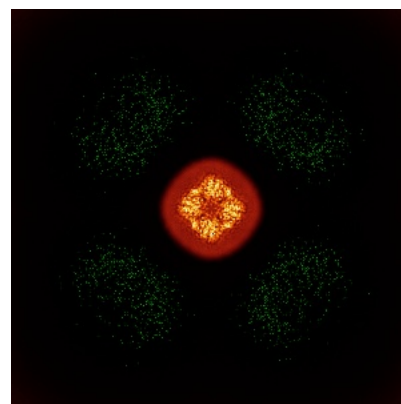
6.4.2 Raw map



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.

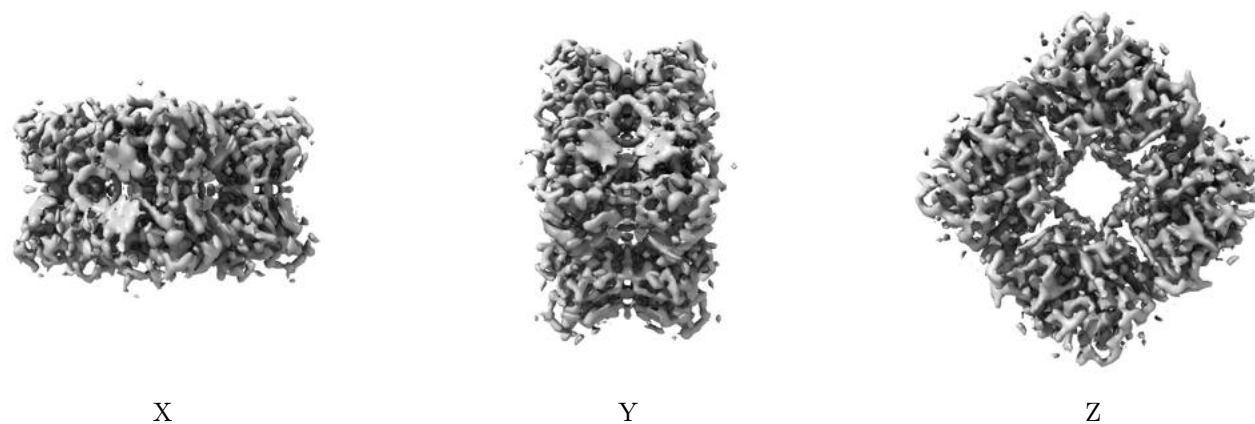
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.28. 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.

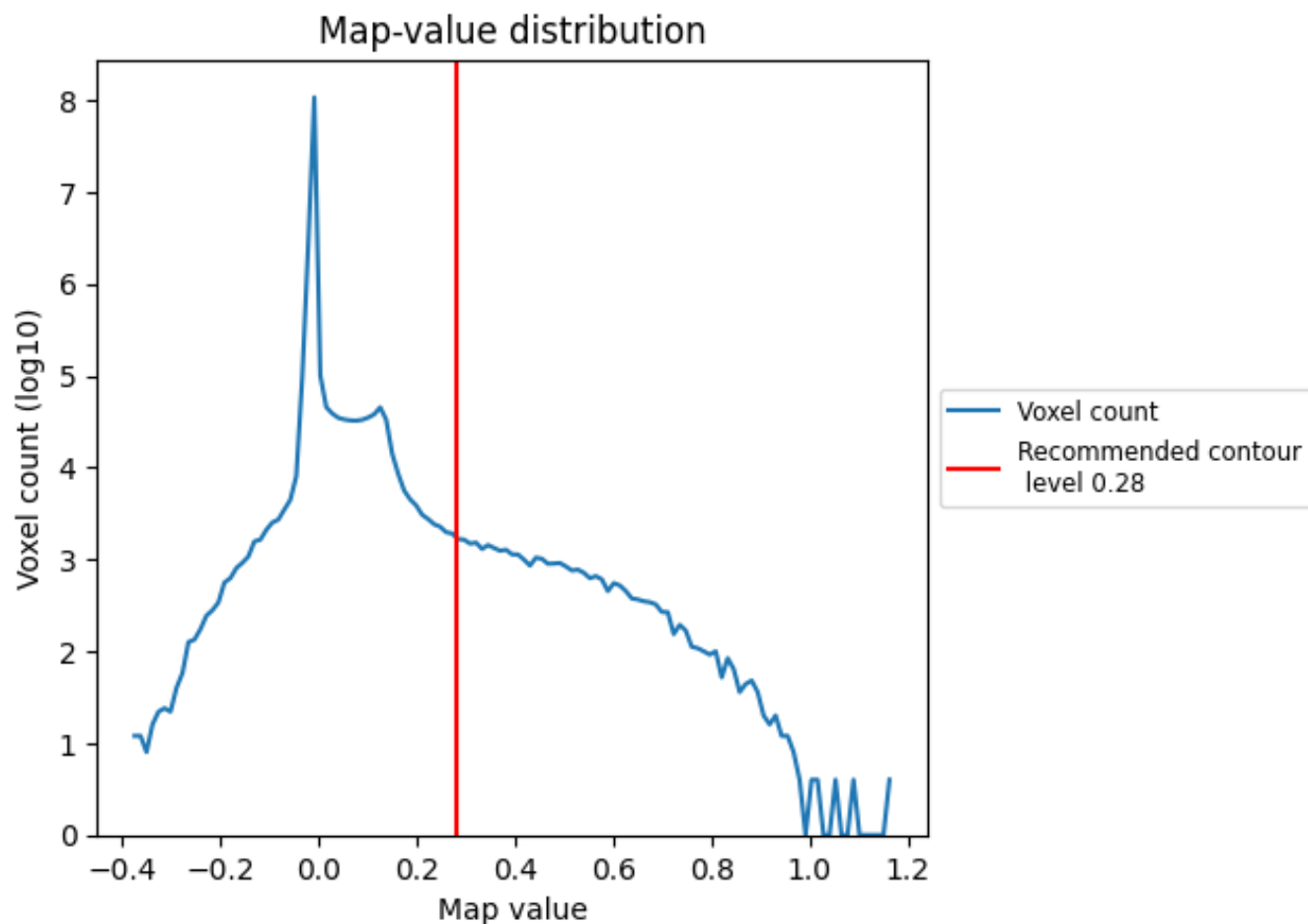
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

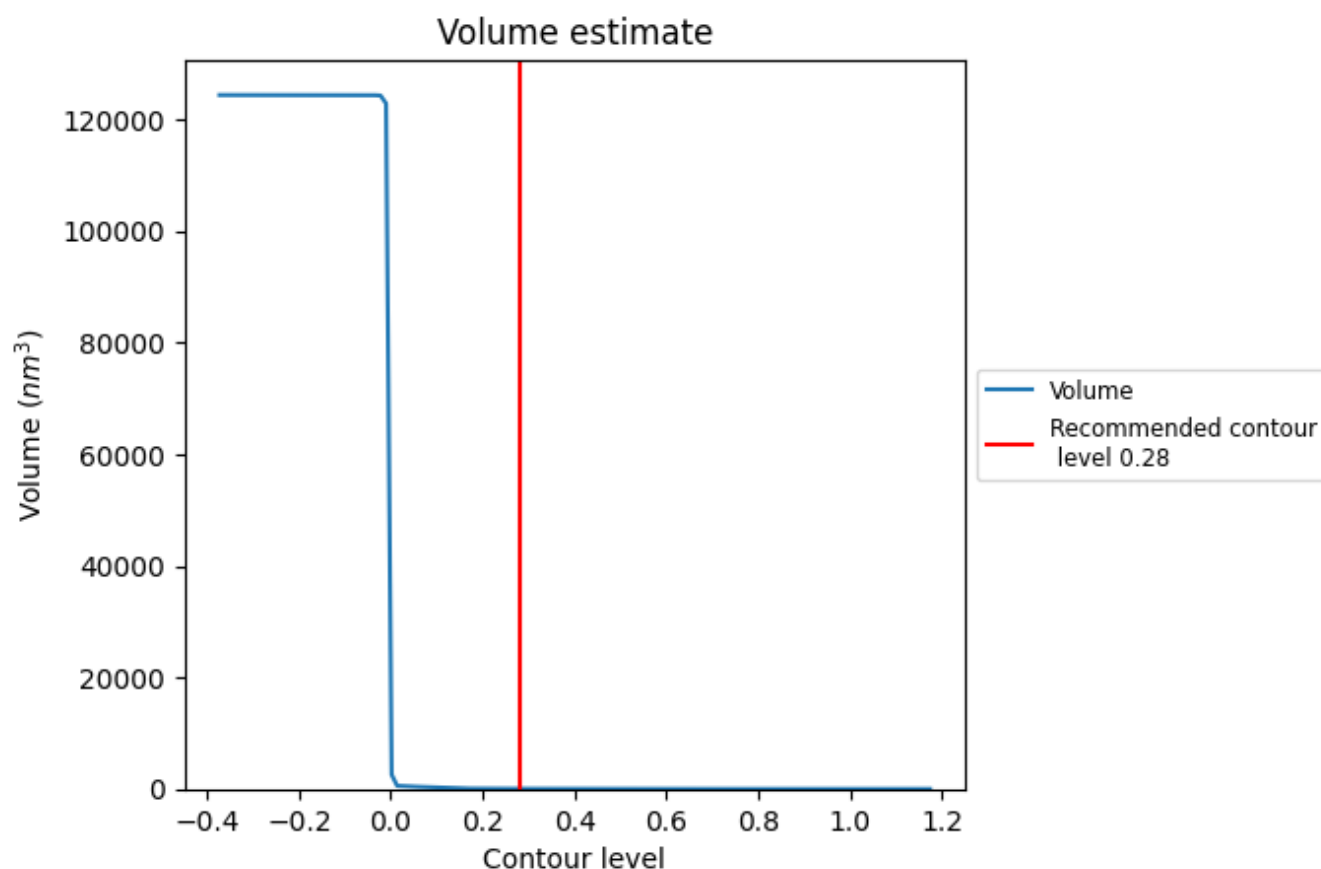
This section contains the results of statistical analysis of the map.

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.

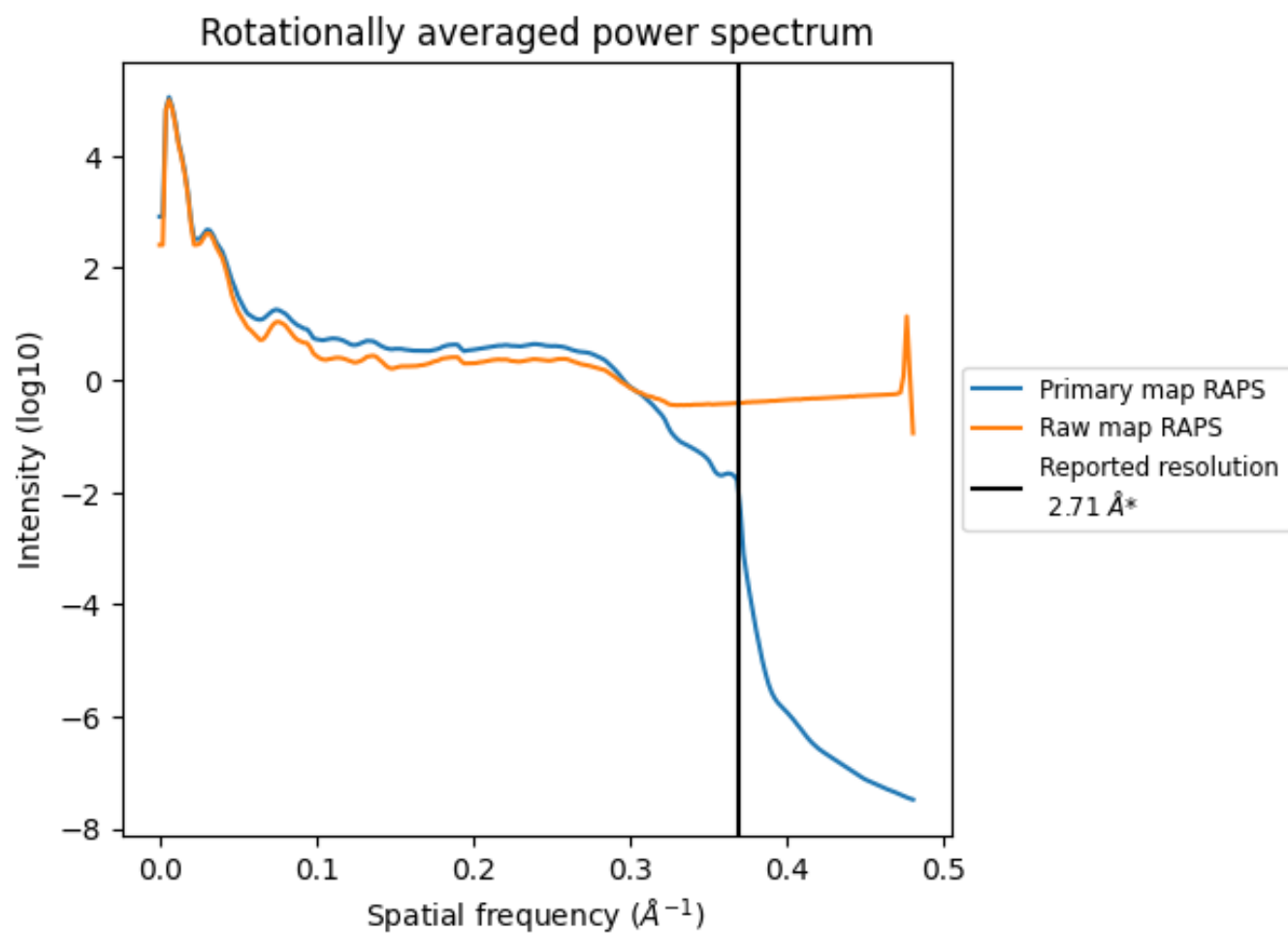
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38 nm^3 ; this corresponds to an approximate mass of 34 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 ⓘ

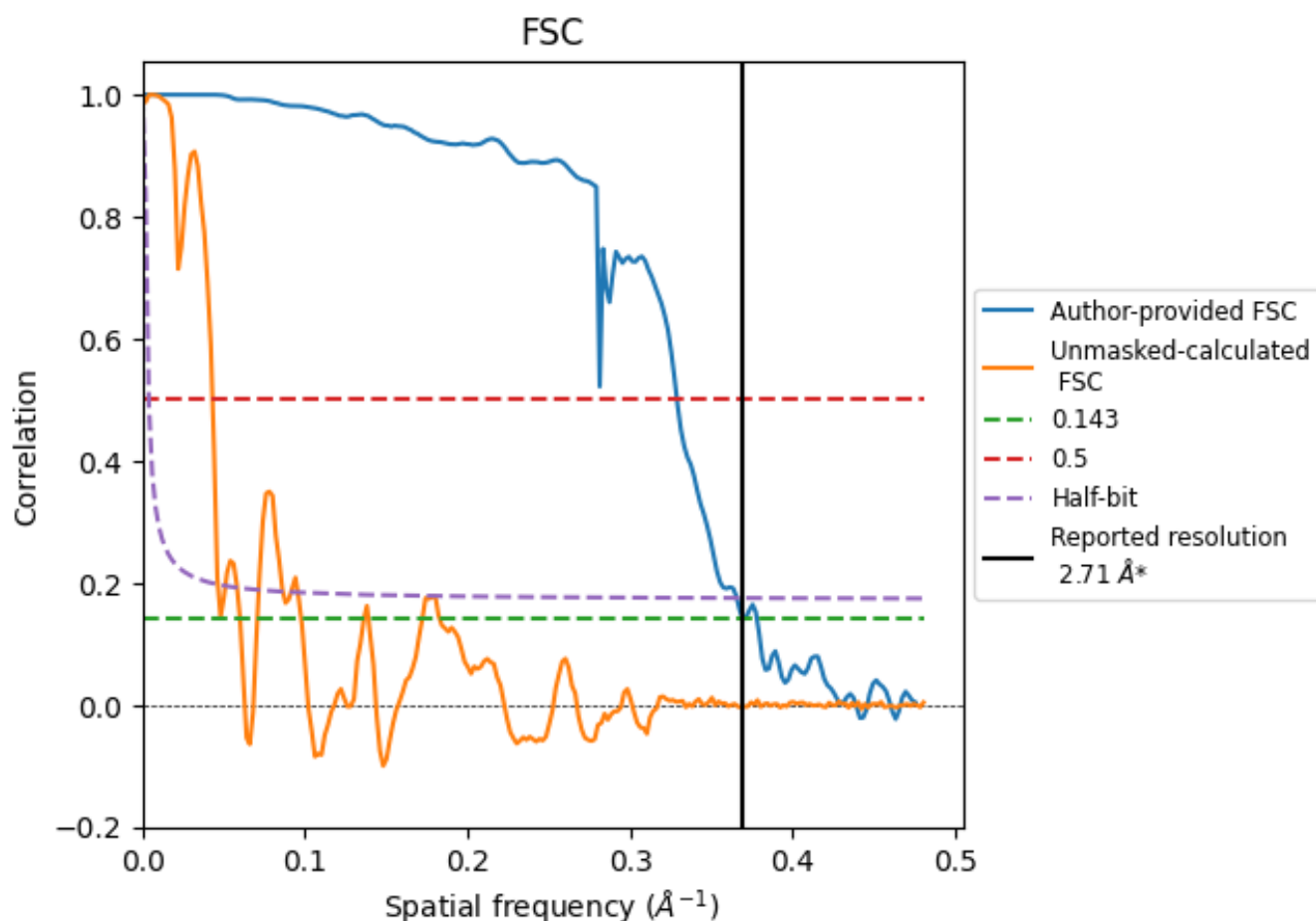


*Reported resolution corresponds to spatial frequency of 0.369 $\text{\AA}^{-1}$

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 0.369 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

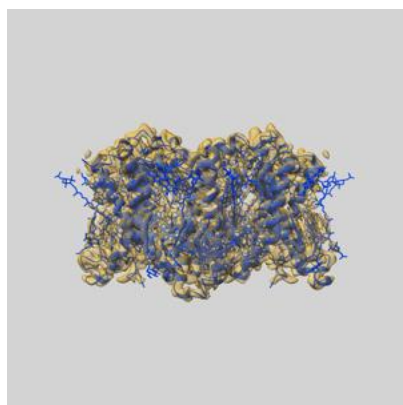
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	2.71	3.04	2.73
Unmasked-calculated*	16.67	23.20	21.55

*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 16.67 differs from the reported value 2.71 by more than 10 %

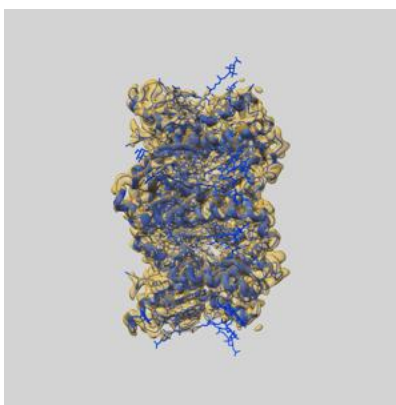
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37441 and PDB model 8WCK. Per-residue inclusion information can be found in section [3](#) on page [11](#).

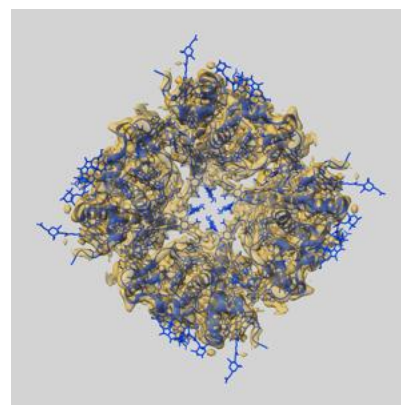
9.1 Map-model overlay [i](#)



X



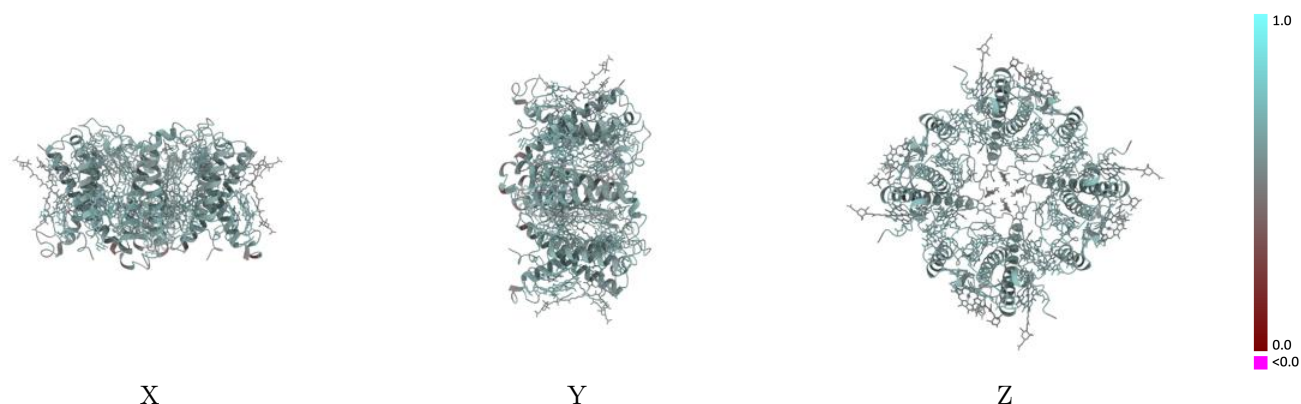
Y



Z

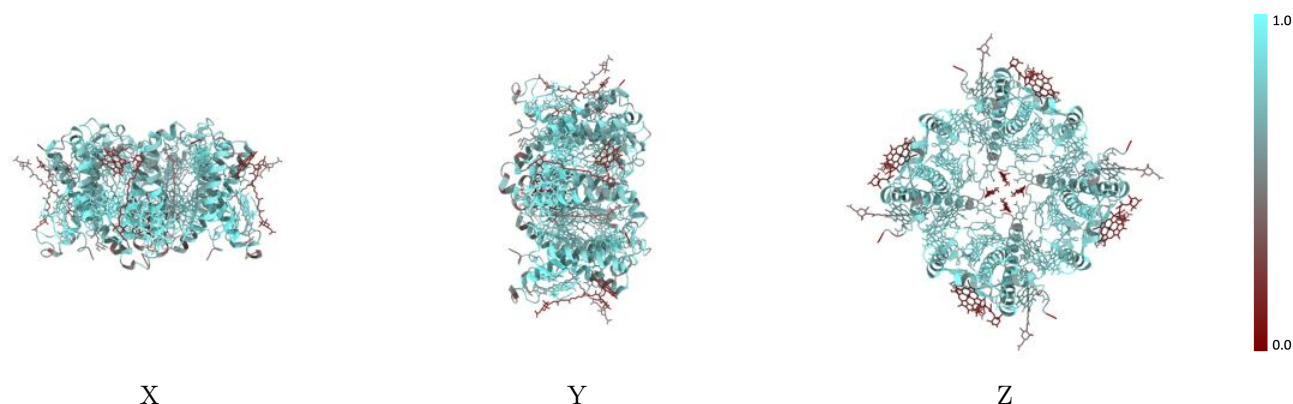
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



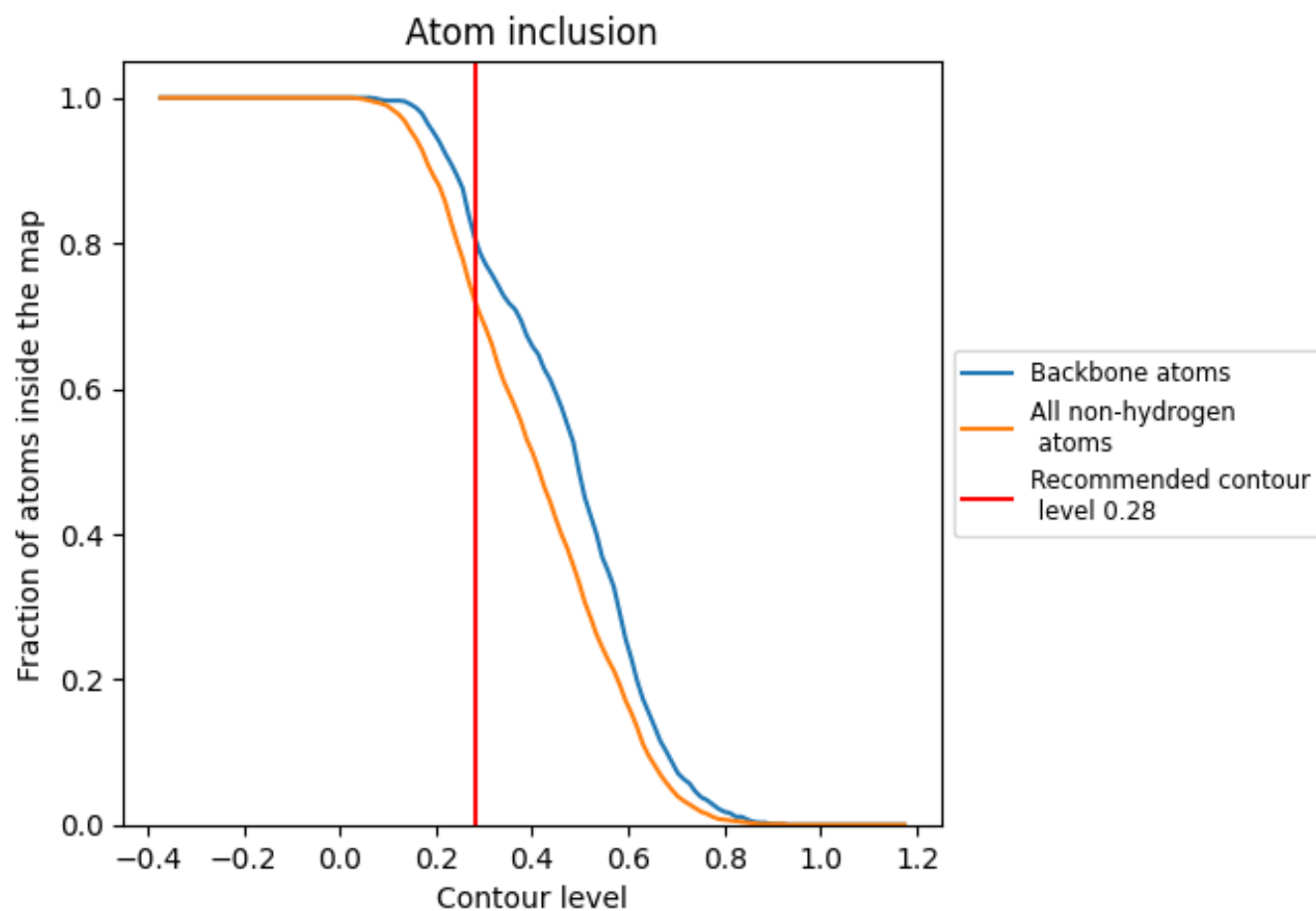
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.28).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 72% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7220	0.5860
1	0.7230	0.5840
2	0.7240	0.5860
3	0.7210	0.5860
4	0.7210	0.5860

