



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:14 PM UTC

PDB ID : 8W4P / pdb_00008w4p
EMDB ID : EMD-37268
Title : Structure of PSII-FCPII-I/J/K complex in the PSII-FCPII supercomplex from *Cyclotella meneghiniana*
Authors : Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2023-08-24
Resolution : 3.48 Å(reported)

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

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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:

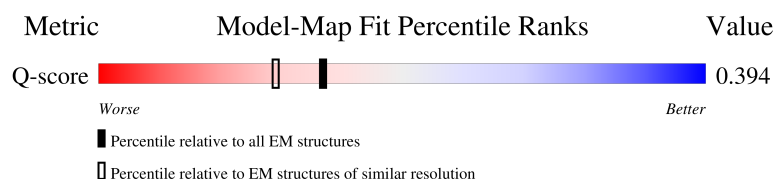
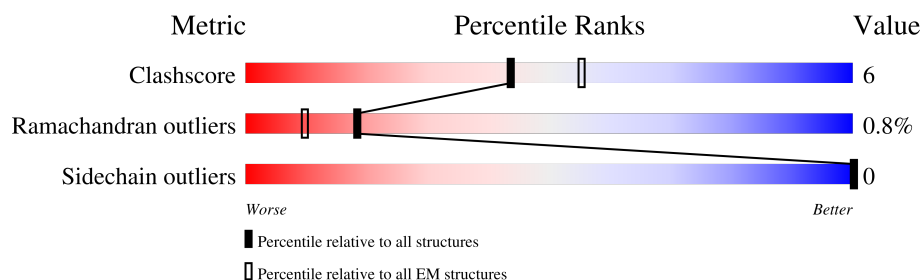
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.48 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	13672 (2.98 - 3.98)

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	p	214	39% 87% 13%
2	4	153	42% 96% .
3	3	163	23% 86% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CLA	3	304	X	-	-	-
4	CLA	3	305	X	-	-	-
4	CLA	3	306	X	-	-	-
4	CLA	3	307	X	-	-	-
4	CLA	3	308	X	-	-	-
4	CLA	3	309	X	-	-	-
4	CLA	3	310	X	-	-	-
4	CLA	3	311	X	-	-	-
4	CLA	3	312	X	-	-	-
4	CLA	3	313	X	-	-	-
4	CLA	3	314	X	-	-	-
4	CLA	4	204	X	-	-	-
4	CLA	4	205	X	-	-	-
4	CLA	4	206	X	-	-	-
4	CLA	4	207	X	-	-	-
4	CLA	4	208	X	-	-	-
4	CLA	4	209	X	-	-	-
4	CLA	4	210	X	-	-	-
4	CLA	4	211	X	-	-	-
4	CLA	4	212	X	-	-	-
4	CLA	4	213	X	-	-	-
4	CLA	p	601	X	-	-	-
4	CLA	p	602	X	-	-	-
4	CLA	p	603	X	-	-	-
4	CLA	p	604	X	-	-	-
4	CLA	p	605	X	-	-	-
4	CLA	p	606	X	-	-	-
4	CLA	p	607	X	-	-	-
4	CLA	p	608	X	-	-	-
4	CLA	p	609	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4531 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 FCPII-I, Fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	p	214	Total	C	N	O	S	0	0
			1271	795	230	245	1		

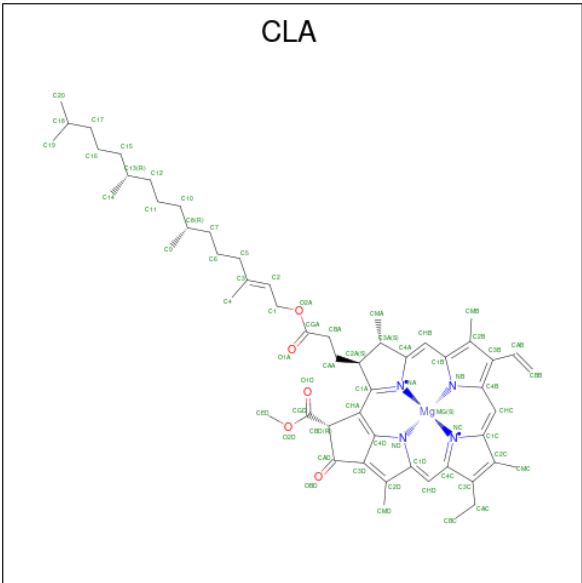
- Molecule 2 is a protein called FCPII-K, Fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	4	153	Total	C	N	O	0	0
			765	459	153	153		

- Molecule 3 is a protein called FCPII-J, Fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	163	Total	C	N	O	0	0
			992	616	192	184		

- Molecule 4 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



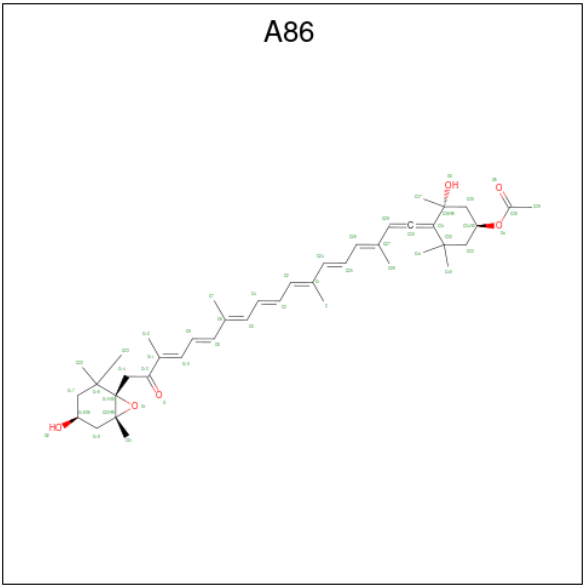
Mol	Chain	Residues	Atoms					AltConf
4	p	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
4	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
4	p	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
4	p	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
4	p	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
4	p	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
4	p	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
4	p	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
4	p	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
4	4	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
4	4	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
4	4	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
4	4	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
4	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
4	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
4	4	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
4	4	1	Total	C	Mg	N	O	0
			34	28	1	4	1	
4	4	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
4	4	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
4	3	1	Total	C	Mg	N	O	0
			34	28	1	4	1	
4	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
4	3	1	Total	C	Mg	N	O	0
			33	27	1	4	1	

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Mol	Chain	Residues	Atoms					AltConf
4	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
4	3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
4	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
4	3	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
4	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
4	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
4	3	1	Total	C	Mg	N	O	0
			39	33	1	4	1	
4	3	1	Total	C	Mg	N	O	0
			35	29	1	4	1	

- Molecule 5 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).



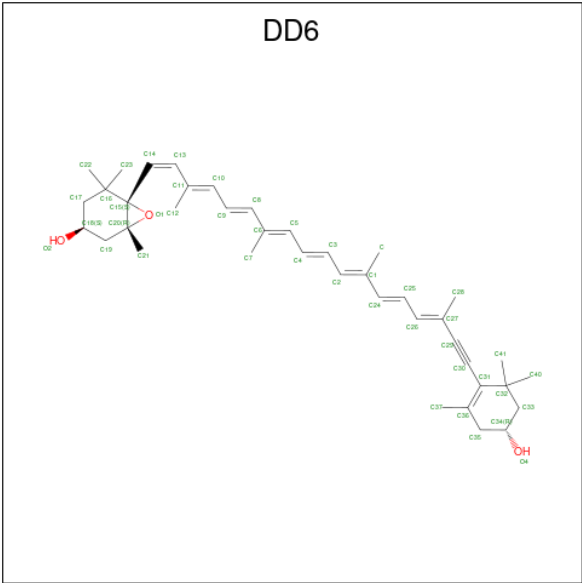
Mol	Chain	Residues	Atoms			AltConf
5	p	1	Total	C	O	0
			48	42	6	
5	4	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
5	4	1	Total	C	O	0
			48	42	6	
5	4	1	Total	C	O	0
			48	42	6	
5	3	1	Total	C	O	0
			48	42	6	
5	3	1	Total	C	O	0
			48	42	6	

- Molecule 6 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).

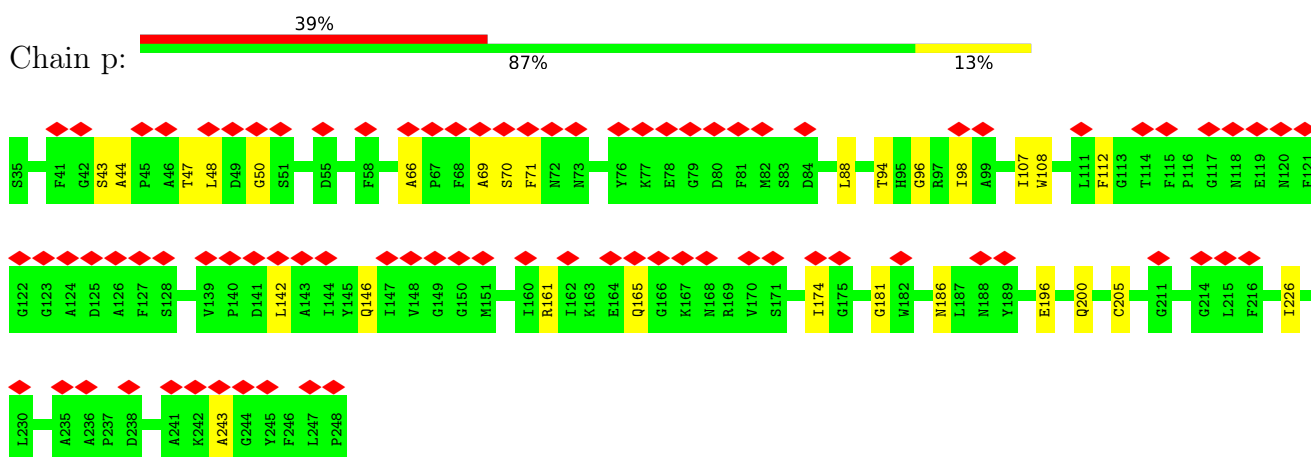


Mol	Chain	Residues	Atoms			AltConf
6	p	1	Total	C	O	0
			43	40	3	
6	3	1	Total	C	O	0
			43	40	3	

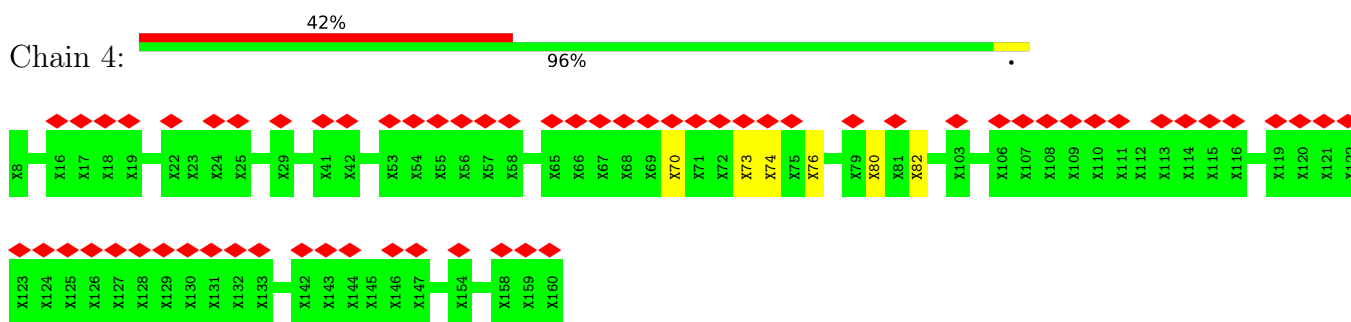
3 Residue-property plots

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.

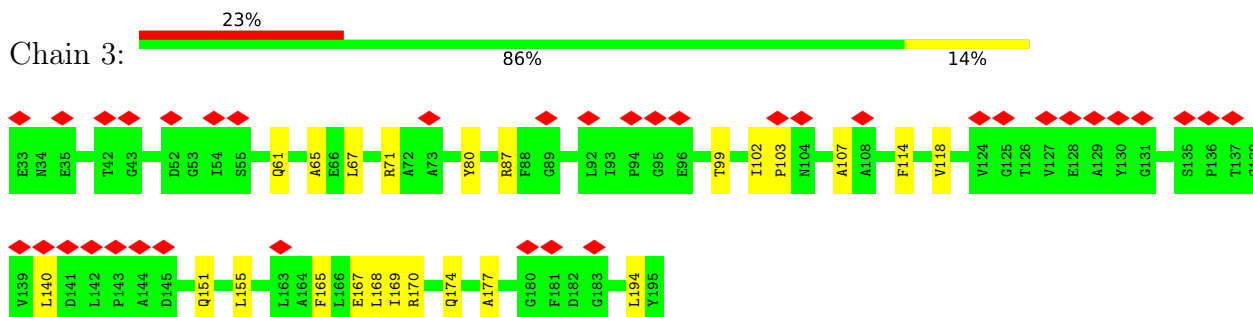
- Molecule 1: FCPH-I, Fucoxanthin chlorophyll a/c binding protein



- Molecule 2: FCPH-K, Fucoxanthin chlorophyll a/c binding protein



- Molecule 3: FCPH-J, Fucoxanthin chlorophyll a/c binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	314409	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.683	Depositor
Minimum map value	-0.377	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.178	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: DD6, A86, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	p	0.33	0/1294	0.69	1/1787 (0.1%)
3	3	0.40	0/1003	0.64	0/1373
All	All	0.36	0/2297	0.67	1/3160 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	p	243	ALA	CB-CA-C	-5.34	110.40	116.54

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	p	1271	0	953	17	0
2	4	765	0	161	3	0
3	3	992	0	778	17	0
4	3	416	0	257	6	0
4	4	372	0	234	1	0
4	p	341	0	213	10	0
5	3	96	0	0	0	0
5	4	144	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	p	48	0	0	0	0
6	3	43	0	0	1	0
6	p	43	0	0	7	0
All	All	4531	0	2596	46	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 (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:p:604:CLA:C2B	6:p:611:DD6:C37	2.31	1.08
4:p:604:CLA:CMB	6:p:611:DD6:C37	2.35	1.04
4:p:604:CLA:HMB1	6:p:611:DD6:C37	2.10	0.82
1:p:107:ILE:CD1	1:p:226:ILE:HG21	2.18	0.73
3:3:80:TYR:HD2	3:3:168:LEU:HD13	1.55	0.70
3:3:67:LEU:HD11	3:3:71:ARG:CZ	2.23	0.69
1:p:96:GLY:HA3	1:p:205:CYS:HB3	1.77	0.66
1:p:88:LEU:HG	4:p:602:CLA:HHB	1.79	0.63
1:p:107:ILE:HD13	1:p:226:ILE:HG21	1.80	0.61
1:p:44:ALA:HB3	1:p:47:THR:HB	1.84	0.60
4:p:603:CLA:HMC1	6:p:611:DD6:C	2.31	0.60
4:3:310:CLA:HBB1	4:3:310:CLA:HHC	1.84	0.60
4:p:604:CLA:C3B	6:p:611:DD6:C37	2.80	0.60
1:p:200:GLN:NE2	4:p:607:CLA:OBD	2.37	0.58
1:p:181:GLY:HA3	1:p:186:ASN:HA	1.87	0.56
3:3:165:PHE:O	3:3:169:ILE:HG22	2.06	0.56
2:4:70:UNK:O	2:4:73:UNK:N	2.40	0.55
3:3:80:TYR:CD2	3:3:168:LEU:HD13	2.39	0.54
3:3:99:THR:HA	3:3:102:ILE:HD13	1.91	0.53
3:3:170:ARG:O	3:3:174:GLN:HG2	2.10	0.52
1:p:48:LEU:HG	1:p:50:GLY:H	1.76	0.50
3:3:65:ALA:HA	4:3:308:CLA:OBD	2.12	0.50
1:p:88:LEU:HD23	4:p:602:CLA:H3A	1.95	0.48
6:3:303:DD6:C9	4:3:305:CLA:HMC2	2.44	0.48
3:3:87:ARG:NH1	3:3:99:THR:O	2.47	0.48
3:3:114:PHE:O	3:3:118:VAL:HG23	2.14	0.47
1:p:66:ALA:HA	3:3:140:LEU:HA	1.95	0.47
4:p:604:CLA:HMB3	6:p:611:DD6:C37	2.37	0.46
1:p:69:ALA:O	1:p:71:PHE:N	2.43	0.45
3:3:61:GLN:OE1	3:3:61:GLN:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:167:GLU:HB2	4:3:311:CLA:C4B	2.47	0.45
1:p:161:ARG:O	1:p:165:GLN:N	2.34	0.44
1:p:196:GLU:O	1:p:200:GLN:HG2	2.17	0.44
3:3:151:GLN:O	3:3:155:LEU:HG	2.18	0.44
2:4:74:UNK:O	2:4:76:UNK:N	2.51	0.43
1:p:43:SER:HB3	1:p:47:THR:HG21	2.01	0.43
3:3:169:ILE:HG13	4:3:312:CLA:HAC1	2.00	0.43
1:p:142:LEU:O	1:p:146:GLN:HG2	2.19	0.43
3:3:167:GLU:CD	3:3:170:ARG:HH21	2.27	0.43
3:3:103:PRO:HB2	3:3:107:ALA:HB3	2.01	0.43
3:3:194:LEU:HD21	4:3:314:CLA:HMD2	2.00	0.43
1:p:108:TRP:HA	1:p:112:PHE:H	1.86	0.41
4:p:603:CLA:CMC	6:p:611:DD6:C	2.97	0.40
2:4:80:UNK:C	2:4:82:UNK:N	2.84	0.40
4:4:209:CLA:HED2	4:4:209:CLA:HBD	1.93	0.40
1:p:94:THR:O	1:p:98:ILE:HG12	2.21	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	p	212/214 (99%)	173 (82%)	37 (18%)	2 (1%)	14	47
3	3	161/163 (99%)	140 (87%)	20 (12%)	1 (1%)	21	53
All	All	373/377 (99%)	313 (84%)	57 (15%)	3 (1%)	18	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	177	ALA
1	p	174	ILE

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Mol	Chain	Res	Type
1	p	70	SER

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	p	71/166 (43%)	71 (100%)	0	100	100
3	3	54/128 (42%)	54 (100%)	0	100	100
All	All	125/294 (42%)	125 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	p	200	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

38 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	CLA	p	605	-	39,45,73	1.46	10 (25%)	51,79,113	1.65	5 (9%)
4	CLA	3	313	-	41,47,73	1.43	10 (24%)	51,81,113	1.47	4 (7%)
6	DD6	3	303	-	40,45,45	1.61	3 (7%)	51,67,67	2.83	16 (31%)
4	CLA	3	314	-	39,43,73	1.61	10 (25%)	50,76,113	1.53	7 (14%)
5	A86	4	201	-	47,50,50	1.69	6 (12%)	51,76,76	3.95	23 (45%)
4	CLA	4	213	-	37,43,73	1.66	10 (27%)	49,76,113	1.69	11 (22%)
4	CLA	4	211	-	37,42,73	1.64	10 (27%)	47,74,113	1.50	5 (10%)
4	CLA	3	304	-	39,42,73	1.66	12 (30%)	49,74,113	1.62	7 (14%)
4	CLA	4	212	-	40,44,73	1.59	10 (25%)	51,77,113	1.53	6 (11%)
4	CLA	3	306	-	35,41,73	1.74	10 (28%)	47,72,113	1.65	8 (17%)
4	CLA	4	205	-	38,43,73	1.62	12 (31%)	48,75,113	1.47	5 (10%)
4	CLA	3	309	-	43,48,73	1.40	8 (18%)	51,83,113	1.70	6 (11%)
4	CLA	3	308	-	40,43,73	1.57	11 (27%)	46,73,113	2.00	6 (13%)
5	A86	4	202	-	47,50,50	1.85	7 (14%)	51,76,76	3.72	28 (54%)
4	CLA	p	609	-	42,47,73	1.58	10 (23%)	49,81,113	1.54	5 (10%)
5	A86	3	302	-	47,50,50	1.82	7 (14%)	51,76,76	3.04	24 (47%)
4	CLA	p	607	-	38,44,73	1.61	10 (26%)	50,77,113	1.49	7 (14%)
4	CLA	3	307	-	46,50,73	1.37	10 (21%)	55,84,113	1.44	5 (9%)
5	A86	4	203	-	47,50,50	1.82	6 (12%)	51,76,76	3.65	22 (43%)
5	A86	3	301	-	47,50,50	1.77	9 (19%)	51,76,76	4.95	22 (43%)
4	CLA	4	207	-	40,46,73	1.44	8 (20%)	52,80,113	1.59	6 (11%)
4	CLA	p	604	-	43,48,73	1.40	9 (20%)	51,83,113	1.58	7 (13%)
4	CLA	3	310	-	40,43,73	1.58	10 (25%)	48,75,113	1.61	5 (10%)
4	CLA	3	311	-	43,48,73	1.43	9 (20%)	51,83,113	1.57	6 (11%)
4	CLA	4	208	-	43,48,73	1.45	10 (23%)	51,83,113	1.60	8 (15%)
4	CLA	p	601	-	39,44,73	1.51	8 (20%)	50,77,113	1.69	7 (14%)
4	CLA	3	305	-	44,49,73	1.40	10 (22%)	50,84,113	1.54	5 (10%)
4	CLA	3	312	-	44,49,73	1.40	8 (18%)	50,84,113	1.43	4 (8%)
5	A86	p	610	-	47,50,50	1.60	7 (14%)	51,76,76	3.91	24 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CLA	4	206	-	39,45,73	1.48	9 (23%)	49,78,113	1.49	5 (10%)
4	CLA	p	606	-	39,45,73	1.50	10 (25%)	49,78,113	1.51	6 (12%)
4	CLA	4	204	-	40,46,73	1.46	9 (22%)	52,80,113	1.52	5 (9%)
6	DD6	p	611	-	40,45,45	1.54	2 (5%)	51,67,67	1.87	14 (27%)
4	CLA	p	602	-	45,49,73	1.39	9 (20%)	54,84,113	1.59	9 (16%)
4	CLA	4	209	-	45,49,73	1.38	9 (20%)	54,84,113	1.56	5 (9%)
4	CLA	p	603	-	39,45,73	1.48	9 (23%)	51,79,113	1.65	7 (13%)
4	CLA	4	210	-	40,46,73	1.44	9 (22%)	52,80,113	1.58	7 (13%)
4	CLA	p	608	-	41,46,73	1.56	10 (24%)	49,80,113	1.53	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLA	p	605	-	1/1/9/20	2/2/78/115	-
4	CLA	3	313	-	1/1/9/20	3/6/82/115	-
6	DD6	3	303	-	-	2/26/80/80	0/3/3/3
4	CLA	3	314	-	1/1/8/20	-	-
5	A86	4	201	-	-	7/34/90/90	1/3/3/3
4	CLA	4	213	-	1/1/8/20	-	-
4	CLA	4	211	-	1/1/7/20	-	-
4	CLA	3	304	-	1/1/8/20	-	-
4	CLA	4	212	-	1/1/8/20	0/2/74/115	-
4	CLA	3	306	-	1/1/7/20	-	-
4	CLA	4	205	-	1/1/7/20	0/2/70/115	-
4	CLA	3	309	-	1/1/10/20	3/8/84/115	-
4	CLA	3	308	-	1/1/6/20	4/6/66/115	-
5	A86	4	202	-	-	7/34/90/90	0/3/3/3
4	CLA	p	609	-	1/1/9/20	0/4/82/115	-
5	A86	3	302	-	-	6/34/90/90	0/3/3/3
4	CLA	p	607	-	1/1/8/20	0/2/74/115	-
4	CLA	3	307	-	1/1/9/20	2/11/83/115	-
5	A86	4	203	-	-	6/34/90/90	0/3/3/3
5	A86	3	301	-	-	12/34/90/90	0/3/3/3
4	CLA	4	207	-	1/1/9/20	2/4/80/115	-
4	CLA	p	604	-	1/1/10/20	2/8/84/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLA	3	310	-	1/1/8/20	0/2/74/115	-
4	CLA	3	311	-	1/1/10/20	2/8/84/115	-
4	CLA	4	208	-	1/1/10/20	2/8/84/115	-
4	CLA	p	601	-	1/1/9/20	2/2/78/115	-
4	CLA	3	305	-	1/1/10/20	3/10/86/115	-
4	CLA	3	312	-	1/1/10/20	4/10/86/115	-
5	A86	p	610	-	-	9/34/90/90	0/3/3/3
4	CLA	4	206	-	1/1/8/20	2/4/76/115	-
4	CLA	p	606	-	1/1/8/20	2/4/76/115	-
4	CLA	4	204	-	1/1/9/20	2/4/80/115	-
6	DD6	p	611	-	-	5/26/80/80	0/3/3/3
4	CLA	p	602	-	1/1/10/20	2/10/86/115	-
4	CLA	4	209	-	1/1/10/20	4/10/86/115	-
4	CLA	p	603	-	1/1/9/20	0/2/78/115	-
4	CLA	4	210	-	1/1/9/20	0/4/80/115	-
4	CLA	p	608	-	1/1/9/20	2/6/78/115	-

All (336) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	p	611	DD6	C30-C31	-8.34	1.26	1.42
6	3	303	DD6	C30-C31	-8.19	1.26	1.42
5	4	202	A86	C20-C15	7.04	1.57	1.48
5	4	203	A86	C20-C15	6.80	1.56	1.48
5	3	302	A86	C20-C15	5.72	1.55	1.48
5	4	201	A86	C20-C15	5.66	1.55	1.48
5	4	202	A86	O4-C38	5.30	1.46	1.35
5	4	203	A86	O4-C38	5.23	1.46	1.35
5	3	302	A86	C30-C31	-4.96	1.24	1.30
5	3	302	A86	O4-C38	4.94	1.46	1.35
5	p	610	A86	C20-C15	4.90	1.54	1.48
5	3	301	A86	C20-C15	4.73	1.54	1.48
5	3	301	A86	O4-C38	4.72	1.45	1.35
5	4	201	A86	O4-C38	4.56	1.45	1.35
5	p	610	A86	O4-C38	4.44	1.45	1.35
4	p	609	CLA	O1D-CGD	4.44	1.36	1.20
5	3	302	A86	C30-C29	-4.25	1.25	1.31
5	4	203	A86	O1-C20	-4.23	1.40	1.46
5	3	301	A86	C30-C31	-4.20	1.25	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	201	A86	O1-C20	-4.13	1.40	1.46
5	4	202	A86	O1-C20	-4.09	1.40	1.46
5	p	610	A86	O1-C20	-3.99	1.41	1.46
5	3	301	A86	C21-C20	3.97	1.57	1.51
5	4	203	A86	C30-C31	-3.93	1.26	1.30
5	3	301	A86	O1-C20	-3.91	1.41	1.46
5	3	302	A86	O1-C20	-3.77	1.41	1.46
5	3	301	A86	C30-C29	-3.68	1.25	1.31
4	3	308	CLA	C4D-ND	-3.66	1.33	1.37
5	4	202	A86	C30-C31	-3.63	1.26	1.30
5	4	201	A86	C30-C31	-3.62	1.26	1.30
4	4	212	CLA	C1D-ND	3.58	1.42	1.37
4	3	310	CLA	C1D-ND	3.51	1.42	1.37
5	4	202	A86	C30-C29	-3.46	1.26	1.31
5	4	203	A86	C30-C29	-3.42	1.26	1.31
5	4	201	A86	C30-C29	-3.37	1.26	1.31
4	p	607	CLA	C1D-ND	3.36	1.42	1.37
4	3	314	CLA	CAB-C3B	-3.33	1.43	1.50
4	3	310	CLA	C4B-NB	3.31	1.42	1.37
4	3	307	CLA	C1D-ND	3.30	1.42	1.37
4	p	607	CLA	CAB-C3B	-3.28	1.44	1.50
4	4	211	CLA	CAB-C3B	-3.28	1.44	1.50
4	p	604	CLA	C1D-ND	3.27	1.42	1.37
4	3	306	CLA	CAB-C3B	-3.27	1.44	1.50
4	3	304	CLA	CAB-C3B	-3.26	1.44	1.50
4	3	308	CLA	C1D-ND	3.26	1.42	1.37
4	p	609	CLA	C1D-ND	3.25	1.42	1.37
4	p	603	CLA	C1D-ND	3.24	1.42	1.37
4	4	205	CLA	CAB-C3B	-3.24	1.44	1.50
4	4	211	CLA	C1D-ND	3.24	1.42	1.37
4	4	207	CLA	C1D-ND	3.23	1.42	1.37
4	4	208	CLA	C1D-ND	3.22	1.42	1.37
4	4	204	CLA	C1D-ND	3.21	1.42	1.37
4	4	213	CLA	CAB-C3B	-3.20	1.44	1.50
4	p	608	CLA	CAB-C3B	-3.20	1.44	1.50
4	4	210	CLA	C1D-ND	3.19	1.42	1.37
4	4	212	CLA	CAB-C3B	-3.19	1.44	1.50
4	3	304	CLA	C1D-ND	3.18	1.42	1.37
4	3	311	CLA	C1D-ND	3.17	1.42	1.37
4	3	314	CLA	C1D-ND	3.16	1.42	1.37
4	3	306	CLA	C1D-ND	3.14	1.42	1.37
4	4	205	CLA	C1D-ND	3.14	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	p	602	CLA	C1D-ND	3.12	1.42	1.37
4	4	211	CLA	C4B-NB	3.09	1.41	1.37
4	3	313	CLA	C1D-ND	3.06	1.41	1.37
4	p	606	CLA	C1D-ND	3.06	1.41	1.37
4	3	305	CLA	C1D-ND	3.05	1.41	1.37
4	4	206	CLA	C4B-NB	3.04	1.41	1.37
4	3	312	CLA	C1D-ND	3.04	1.41	1.37
4	4	212	CLA	C4B-NB	3.02	1.41	1.37
4	4	213	CLA	C1D-ND	3.02	1.41	1.37
4	p	601	CLA	C4B-NB	3.02	1.41	1.37
4	4	213	CLA	C4B-NB	3.02	1.41	1.37
4	4	209	CLA	C1D-ND	3.00	1.41	1.37
4	3	309	CLA	C1B-C2B	2.99	1.50	1.43
4	3	304	CLA	C4B-NB	2.99	1.41	1.37
4	4	206	CLA	C1D-ND	2.98	1.41	1.37
5	p	610	A86	C19-C18	-2.96	1.48	1.52
4	p	608	CLA	C1D-ND	2.92	1.41	1.37
4	p	606	CLA	MG-NB	-2.92	2.00	2.05
4	4	204	CLA	C4B-NB	2.91	1.41	1.37
4	p	605	CLA	C1D-ND	2.90	1.41	1.37
4	3	306	CLA	C4B-NB	2.90	1.41	1.37
4	3	308	CLA	C4B-NB	2.88	1.41	1.37
4	3	310	CLA	C3C-C4C	2.88	1.46	1.40
6	3	303	DD6	O1-C20	-2.88	1.42	1.46
4	3	314	CLA	C4B-NB	2.87	1.41	1.37
4	3	306	CLA	C3C-C4C	2.85	1.46	1.40
4	p	605	CLA	MG-NB	-2.84	2.00	2.05
4	p	608	CLA	C4B-NB	2.83	1.41	1.37
4	4	205	CLA	C1B-C2B	2.83	1.49	1.43
4	3	304	CLA	C3C-C4C	2.83	1.46	1.40
4	p	601	CLA	C3C-C4C	2.81	1.46	1.40
4	3	304	CLA	C1B-C2B	2.81	1.49	1.43
4	4	210	CLA	C4B-NB	2.81	1.41	1.37
4	p	606	CLA	C4B-NB	2.80	1.41	1.37
4	p	609	CLA	C4B-NB	2.80	1.41	1.37
4	p	603	CLA	C4B-NB	2.80	1.41	1.37
6	3	303	DD6	C28-C27	-2.77	1.49	1.50
4	p	601	CLA	C1D-ND	2.77	1.41	1.37
4	4	213	CLA	MG-NB	-2.76	2.00	2.05
4	4	207	CLA	C4B-NB	2.75	1.41	1.37
4	3	309	CLA	C1D-ND	2.75	1.41	1.37
4	4	205	CLA	C4B-NB	2.74	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	310	CLA	C3B-C4B	2.73	1.50	1.42
4	3	313	CLA	C4B-NB	2.70	1.41	1.37
4	3	311	CLA	C4B-NB	2.70	1.41	1.37
5	p	610	A86	C32-C31	-2.69	1.50	1.54
4	p	601	CLA	C1B-C2B	2.68	1.49	1.43
4	4	204	CLA	C1B-C2B	2.68	1.49	1.43
4	4	212	CLA	C4B-C3B	2.68	1.49	1.43
4	p	602	CLA	C4B-NB	2.67	1.41	1.37
4	4	209	CLA	C4B-NB	2.65	1.41	1.37
4	p	608	CLA	C1B-C2B	2.65	1.49	1.43
4	p	609	CLA	C1B-C2B	2.64	1.49	1.43
4	3	309	CLA	C4B-NB	2.64	1.41	1.37
4	3	312	CLA	C4B-NB	2.64	1.41	1.37
4	4	208	CLA	C4B-NB	2.63	1.41	1.37
4	3	314	CLA	C4B-C3B	2.62	1.49	1.43
4	3	314	CLA	C1B-C2B	2.62	1.49	1.43
4	3	311	CLA	C1B-C2B	2.61	1.49	1.43
4	4	211	CLA	C1B-C2B	2.61	1.49	1.43
4	p	602	CLA	C1B-C2B	2.61	1.49	1.43
4	p	607	CLA	C4B-NB	2.58	1.41	1.37
4	4	212	CLA	C1B-C2B	2.57	1.49	1.43
4	p	604	CLA	C4B-NB	2.57	1.41	1.37
4	p	608	CLA	C4B-C3B	2.57	1.49	1.43
4	3	307	CLA	C4B-NB	2.57	1.41	1.37
4	4	208	CLA	MG-NB	-2.56	2.00	2.05
4	p	604	CLA	C1B-C2B	2.56	1.49	1.43
4	3	306	CLA	C1B-C2B	2.55	1.49	1.43
4	3	306	CLA	C4B-C3B	2.55	1.49	1.43
4	4	205	CLA	C4B-C3B	2.55	1.49	1.43
4	4	209	CLA	MG-NB	-2.55	2.00	2.05
4	3	305	CLA	C4B-NB	2.54	1.41	1.37
4	3	311	CLA	MG-NB	-2.54	2.00	2.05
4	p	607	CLA	C1B-C2B	2.53	1.49	1.43
4	3	308	CLA	MG-NB	-2.53	2.00	2.05
4	4	207	CLA	C1B-C2B	2.53	1.49	1.43
4	4	205	CLA	MG-NB	-2.52	2.00	2.05
4	4	213	CLA	C1B-C2B	2.52	1.49	1.43
4	3	305	CLA	C1B-C2B	2.51	1.49	1.43
4	p	607	CLA	C4B-C3B	2.50	1.49	1.43
4	4	209	CLA	C1B-C2B	2.49	1.49	1.43
4	p	607	CLA	MG-NB	-2.49	2.00	2.05
4	3	312	CLA	MG-NB	-2.48	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	208	CLA	C1B-C2B	2.48	1.49	1.43
4	3	307	CLA	MG-NB	-2.48	2.00	2.05
4	3	313	CLA	C1B-C2B	2.47	1.48	1.43
4	4	211	CLA	C4B-C3B	2.46	1.48	1.43
4	p	603	CLA	C1B-C2B	2.46	1.48	1.43
5	3	301	A86	C19-C18	2.46	1.55	1.52
4	p	605	CLA	C4B-NB	2.44	1.41	1.37
4	4	206	CLA	C1B-C2B	2.44	1.48	1.43
4	4	207	CLA	MG-NB	-2.43	2.01	2.05
4	4	206	CLA	MG-NB	-2.43	2.01	2.05
4	p	605	CLA	MG-ND	-2.43	2.01	2.05
4	3	305	CLA	MG-NB	-2.43	2.01	2.05
4	3	307	CLA	C1B-C2B	2.42	1.48	1.43
5	p	610	A86	C13-C11	-2.42	1.45	1.49
5	p	610	A86	C19-C20	-2.41	1.48	1.52
4	3	308	CLA	C1B-C2B	2.41	1.48	1.43
4	3	306	CLA	MG-NB	-2.41	2.01	2.05
4	4	210	CLA	MG-NB	-2.41	2.01	2.05
4	3	304	CLA	C4B-C3B	2.39	1.48	1.43
4	4	213	CLA	CMB-C2B	-2.39	1.45	1.50
5	3	301	A86	C13-C11	-2.39	1.45	1.49
4	3	313	CLA	MG-NB	-2.39	2.01	2.05
4	4	205	CLA	CHC-C1C	2.38	1.43	1.38
4	p	606	CLA	MG-ND	-2.38	2.01	2.05
4	3	309	CLA	MG-NB	-2.37	2.01	2.05
4	4	210	CLA	C1B-C2B	2.37	1.48	1.43
4	p	606	CLA	C1B-C2B	2.37	1.48	1.43
5	4	201	A86	C19-C18	-2.36	1.49	1.52
4	p	603	CLA	MG-NB	-2.35	2.01	2.05
4	3	308	CLA	C3B-C4B	2.35	1.49	1.42
4	4	210	CLA	C3B-C4B	2.35	1.49	1.42
5	3	301	A86	C32-C31	-2.35	1.50	1.54
4	3	310	CLA	C1B-C2B	2.34	1.48	1.43
4	4	206	CLA	C3B-C4B	2.33	1.49	1.42
4	3	312	CLA	C1B-C2B	2.33	1.48	1.43
4	3	308	CLA	CHA-C4D	2.33	1.42	1.38
4	4	213	CLA	C4B-C3B	2.33	1.48	1.43
4	p	605	CLA	CMD-C2D	-2.33	1.46	1.50
4	3	314	CLA	MG-NB	-2.32	2.01	2.05
5	3	302	A86	C19-C18	-2.32	1.49	1.52
4	p	601	CLA	MG-NB	-2.32	2.01	2.05
4	3	310	CLA	CHC-C1C	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	p	603	CLA	C3B-C4B	2.31	1.49	1.42
4	3	304	CLA	MG-NB	-2.31	2.01	2.05
4	p	602	CLA	MG-NB	-2.29	2.01	2.05
4	p	601	CLA	C3B-C4B	2.29	1.49	1.42
4	p	608	CLA	MG-NB	-2.29	2.01	2.05
5	4	202	A86	C19-C18	-2.28	1.49	1.52
4	p	604	CLA	MG-NB	-2.28	2.01	2.05
4	4	208	CLA	MG-ND	-2.28	2.01	2.05
4	3	311	CLA	CMB-C2B	-2.28	1.46	1.50
4	4	204	CLA	MG-NB	-2.28	2.01	2.05
5	3	302	A86	C13-C11	-2.27	1.45	1.49
4	3	312	CLA	CMB-C2B	-2.27	1.46	1.50
4	p	605	CLA	C1B-C2B	2.27	1.48	1.43
4	p	608	CLA	CHC-C1C	2.27	1.43	1.38
4	p	606	CLA	CMB-C2B	-2.26	1.46	1.50
4	3	305	CLA	C3B-C4B	2.25	1.49	1.42
4	4	212	CLA	CBD-CAD	2.25	1.56	1.51
4	p	602	CLA	CMC-C2C	-2.25	1.46	1.50
6	p	611	DD6	O1-C20	-2.25	1.43	1.46
4	4	211	CLA	MG-NB	-2.24	2.01	2.05
4	p	604	CLA	C3B-C4B	2.24	1.49	1.42
4	4	204	CLA	C3B-C4B	2.23	1.49	1.42
4	3	307	CLA	CMD-C2D	-2.23	1.46	1.50
4	3	305	CLA	CMC-C2C	-2.23	1.46	1.50
4	3	304	CLA	CMB-C2B	-2.23	1.46	1.50
4	4	212	CLA	CHC-C1C	2.23	1.42	1.38
4	p	602	CLA	C3B-C4B	2.23	1.49	1.42
4	p	603	CLA	CHC-C1C	2.22	1.42	1.38
4	3	306	CLA	CMD-C2D	-2.22	1.46	1.50
4	3	313	CLA	C3B-C4B	2.22	1.49	1.42
4	p	609	CLA	CMD-C2D	-2.21	1.46	1.50
4	4	208	CLA	C3B-C4B	2.21	1.49	1.42
4	p	609	CLA	MG-NB	-2.21	2.01	2.05
4	p	602	CLA	CHC-C1C	2.21	1.42	1.38
4	4	206	CLA	CMB-C2B	-2.21	1.46	1.50
4	3	307	CLA	C3B-C4B	2.21	1.49	1.42
4	3	313	CLA	CMB-C2B	-2.21	1.46	1.50
4	p	601	CLA	CMD-C2D	-2.20	1.46	1.50
4	4	207	CLA	CMB-C2B	-2.20	1.46	1.50
4	3	313	CLA	CMD-C2D	-2.19	1.46	1.50
4	4	206	CLA	CMD-C2D	-2.19	1.46	1.50
4	3	311	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	304	CLA	CMD-C2D	-2.19	1.46	1.50
4	3	314	CLA	CMD-C2D	-2.19	1.46	1.50
4	p	606	CLA	CMD-C2D	-2.18	1.46	1.50
4	3	310	CLA	CMB-C2B	-2.18	1.46	1.50
4	3	310	CLA	CMD-C2D	-2.18	1.46	1.50
4	p	609	CLA	C3B-C4B	2.18	1.49	1.42
4	3	309	CLA	CMC-C2C	-2.18	1.46	1.50
4	4	208	CLA	CMD-C2D	-2.18	1.46	1.50
4	3	307	CLA	CMB-C2B	-2.17	1.46	1.50
4	p	603	CLA	CMD-C2D	-2.17	1.46	1.50
4	3	314	CLA	CHC-C1C	2.17	1.42	1.38
4	4	204	CLA	CMD-C2D	-2.17	1.46	1.50
4	4	208	CLA	CMB-C2B	-2.17	1.46	1.50
4	p	602	CLA	CMD-C2D	-2.17	1.46	1.50
4	3	312	CLA	CMD-C2D	-2.16	1.46	1.50
4	3	308	CLA	CHC-C1C	2.16	1.42	1.38
4	4	206	CLA	CHC-C1C	2.16	1.42	1.38
4	4	213	CLA	CMD-C2D	-2.16	1.46	1.50
4	4	212	CLA	MG-NB	-2.16	2.01	2.05
4	4	209	CLA	CMD-C2D	-2.16	1.46	1.50
4	4	205	CLA	CMB-C2B	-2.15	1.46	1.50
4	3	305	CLA	CMB-C2B	-2.15	1.46	1.50
4	p	604	CLA	CHC-C1C	2.15	1.42	1.38
4	4	210	CLA	CHC-C1C	2.15	1.42	1.38
4	4	210	CLA	CMB-C2B	-2.15	1.46	1.50
4	p	608	CLA	CMD-C2D	-2.15	1.46	1.50
4	3	314	CLA	CMB-C2B	-2.15	1.46	1.50
4	3	308	CLA	CMB-C2B	-2.15	1.46	1.50
4	3	304	CLA	CHC-C1C	2.14	1.42	1.38
4	3	307	CLA	MG-ND	-2.14	2.01	2.05
4	4	205	CLA	CMD-C2D	-2.14	1.46	1.50
4	p	609	CLA	CMB-C2B	-2.14	1.46	1.50
4	4	209	CLA	CMB-C2B	-2.14	1.46	1.50
4	3	305	CLA	CMD-C2D	-2.14	1.46	1.50
4	p	604	CLA	CMC-C2C	-2.13	1.46	1.50
4	3	306	CLA	CHC-C1C	2.13	1.42	1.38
4	p	607	CLA	CMD-C2D	-2.13	1.46	1.50
4	p	606	CLA	C3B-C4B	2.13	1.49	1.42
4	3	308	CLA	CMC-C2C	-2.13	1.46	1.50
4	p	607	CLA	CMB-C2B	-2.13	1.46	1.50
4	3	306	CLA	CMB-C2B	-2.13	1.46	1.50
4	4	204	CLA	CHC-C1C	2.13	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	309	CLA	CMB-C2B	-2.13	1.46	1.50
4	p	601	CLA	CMB-C2B	-2.12	1.46	1.50
4	3	304	CLA	MG-ND	-2.12	2.01	2.05
4	4	211	CLA	CBD-CAD	2.12	1.56	1.51
4	p	606	CLA	CMC-C2C	-2.12	1.46	1.50
4	p	604	CLA	CMD-C2D	-2.12	1.46	1.50
4	p	602	CLA	CMB-C2B	-2.11	1.46	1.50
4	p	609	CLA	CMC-C2C	-2.11	1.46	1.50
4	3	307	CLA	CMC-C2C	-2.11	1.46	1.50
4	4	207	CLA	CMD-C2D	-2.11	1.46	1.50
4	p	605	CLA	CMB-C2B	-2.10	1.46	1.50
4	4	206	CLA	CMC-C2C	-2.10	1.46	1.50
4	p	608	CLA	CMB-C2B	-2.10	1.46	1.50
4	3	312	CLA	C3B-C4B	2.10	1.48	1.42
4	3	307	CLA	CHC-C1C	2.10	1.42	1.38
4	3	314	CLA	CBD-CAD	2.10	1.56	1.51
4	4	207	CLA	CMC-C2C	-2.09	1.46	1.50
4	3	313	CLA	CHC-C1C	2.09	1.42	1.38
4	4	213	CLA	CMC-C2C	-2.09	1.46	1.50
4	3	310	CLA	CBD-CAD	2.09	1.56	1.51
4	p	604	CLA	CMB-C2B	-2.09	1.46	1.50
4	4	208	CLA	CMC-C2C	-2.09	1.46	1.50
4	4	205	CLA	CBD-CAD	2.09	1.56	1.51
4	4	204	CLA	CMB-C2B	-2.09	1.46	1.50
4	4	209	CLA	CMC-C2C	-2.09	1.46	1.50
4	3	304	CLA	CBD-CAD	2.08	1.56	1.51
4	p	603	CLA	CMC-C2C	-2.08	1.46	1.50
4	3	308	CLA	CMD-C2D	-2.08	1.46	1.50
4	3	305	CLA	CHC-C1C	2.08	1.42	1.38
4	p	606	CLA	CHC-C1C	2.08	1.42	1.38
4	p	605	CLA	CMC-C2C	-2.08	1.46	1.50
4	4	209	CLA	C3B-C4B	2.08	1.48	1.42
4	4	205	CLA	MG-ND	-2.07	2.01	2.05
5	4	203	A86	C13-C11	-2.07	1.45	1.49
4	p	603	CLA	CMB-C2B	-2.07	1.46	1.50
4	4	211	CLA	CMB-C2B	-2.07	1.46	1.50
4	3	309	CLA	CMD-C2D	-2.07	1.46	1.50
4	p	607	CLA	CHC-C1C	2.06	1.42	1.38
4	p	607	CLA	CMC-C2C	-2.06	1.46	1.50
4	p	605	CLA	C3B-C4B	2.06	1.48	1.42
5	4	202	A86	C13-C11	-2.06	1.45	1.49
4	4	211	CLA	CHC-C1C	2.06	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	p	605	CLA	CHC-C1C	2.06	1.42	1.38
4	p	608	CLA	CMC-C2C	-2.05	1.46	1.50
4	4	212	CLA	CMB-C2B	-2.05	1.46	1.50
4	4	213	CLA	CAC-C3C	-2.05	1.46	1.50
4	3	311	CLA	MG-ND	-2.05	2.01	2.05
4	3	313	CLA	CMC-C2C	-2.05	1.46	1.50
4	3	305	CLA	MG-ND	-2.05	2.01	2.05
4	4	211	CLA	CMD-C2D	-2.03	1.46	1.50
4	4	204	CLA	CMC-C2C	-2.03	1.46	1.50
4	4	209	CLA	MG-ND	-2.03	2.01	2.05
4	4	210	CLA	CMD-C2D	-2.03	1.46	1.50
4	p	609	CLA	CHC-C1C	2.03	1.42	1.38
4	3	311	CLA	CMC-C2C	-2.03	1.46	1.50
4	3	313	CLA	MG-ND	-2.03	2.01	2.05
4	4	207	CLA	C3B-C4B	2.03	1.48	1.42
4	4	212	CLA	CMD-C2D	-2.03	1.46	1.50
4	4	210	CLA	CMC-C2C	-2.02	1.46	1.50
4	3	310	CLA	MG-NB	-2.02	2.01	2.05
4	3	312	CLA	CMC-C2C	-2.02	1.46	1.50
4	4	208	CLA	C1B-NB	-2.01	1.35	1.37
4	4	205	CLA	CMC-C2C	-2.01	1.46	1.50
4	3	311	CLA	C3B-C4B	2.00	1.48	1.42
4	3	309	CLA	C3B-C4B	2.00	1.48	1.42

All (360) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	3	301	A86	C40-C32-C31	-17.37	94.92	110.47
5	3	301	A86	O1-C20-C19	-16.74	97.80	113.49
5	4	202	A86	C20-O1-C15	14.52	67.27	61.03
5	4	203	A86	C20-O1-C15	13.91	67.01	61.03
5	4	201	A86	C41-C32-C31	13.01	122.11	110.47
5	4	201	A86	C20-O1-C15	12.64	66.46	61.03
5	3	302	A86	C20-O1-C15	12.09	66.23	61.03
5	p	610	A86	C20-O1-C15	11.26	65.87	61.03
5	p	610	A86	C29-C30-C31	-10.91	164.79	177.66
5	3	301	A86	C35-C34-C33	-10.16	91.63	109.89
6	3	303	DD6	C10-C9-C8	9.93	151.98	123.20
5	4	203	A86	O1-C20-C21	-9.76	104.14	115.05
5	3	301	A86	C23-C16-C22	-9.74	93.22	107.37
5	3	301	A86	C20-O1-C15	9.07	64.92	61.03
5	p	610	A86	C41-C32-C31	-9.06	102.36	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	202	A86	O4-C38-C39	8.71	126.63	111.09
6	3	303	DD6	C9-C10-C11	8.57	139.30	127.28
5	3	301	A86	O1-C20-C21	-8.45	105.61	115.05
5	4	201	A86	C33-C32-C31	-8.27	101.17	109.21
4	3	309	CLA	C4A-NA-C1A	8.23	110.44	106.68
6	3	303	DD6	C9-C8-C6	7.88	147.96	126.36
5	4	201	A86	O4-C34-C35	-7.82	87.62	107.64
5	3	301	A86	C21-C20-C19	-7.47	105.84	114.24
5	4	202	A86	C34-O4-C38	7.38	130.88	117.85
4	3	308	CLA	CHA-C4D-ND	7.31	135.09	124.80
5	4	203	A86	O4-C38-C39	7.22	123.97	111.09
4	3	308	CLA	CHA-C4D-C3D	-7.22	113.04	125.21
5	p	610	A86	C33-C32-C31	7.21	116.22	109.21
4	3	304	CLA	C4A-NA-C1A	7.11	109.92	106.68
5	4	203	A86	O1-C20-C19	7.07	120.12	113.49
5	p	610	A86	O1-C20-C19	6.85	119.91	113.49
4	4	207	CLA	C4A-NA-C1A	6.79	109.78	106.68
4	p	603	CLA	C4A-NA-C1A	6.78	109.77	106.68
5	p	610	A86	C4-C5-C6	-6.67	117.93	127.28
4	3	305	CLA	C4A-NA-C1A	6.66	109.72	106.68
4	p	601	CLA	C4A-NA-C1A	6.66	109.72	106.68
4	3	311	CLA	C4A-NA-C1A	6.65	109.71	106.68
4	3	313	CLA	C4A-NA-C1A	6.62	109.70	106.68
4	p	609	CLA	C4A-NA-C1A	6.61	109.69	106.68
4	4	209	CLA	C4A-NA-C1A	6.56	109.67	106.68
5	4	203	A86	C29-C30-C31	-6.55	169.93	177.66
5	3	301	A86	C29-C30-C31	-6.54	169.95	177.66
4	p	604	CLA	C4A-NA-C1A	6.52	109.65	106.68
5	4	201	A86	C21-C20-C19	6.52	121.56	114.24
4	3	307	CLA	C4A-NA-C1A	6.46	109.62	106.68
4	4	204	CLA	C4A-NA-C1A	6.44	109.62	106.68
4	3	314	CLA	C4A-NA-C1A	6.38	109.59	106.68
4	3	310	CLA	C4A-NA-C1A	6.36	109.58	106.68
5	4	201	A86	O4-C34-C33	6.35	123.88	107.64
5	p	610	A86	C21-C20-C19	6.24	121.25	114.24
4	4	205	CLA	C4A-NA-C1A	6.23	109.52	106.68
5	p	610	A86	O4-C38-C39	6.21	122.16	111.09
5	3	302	A86	O1-C20-C19	6.20	119.30	113.49
4	p	605	CLA	C4A-NA-C1A	6.17	109.50	106.68
4	4	212	CLA	C4A-NA-C1A	6.15	109.49	106.68
4	4	213	CLA	C4A-NA-C1A	6.08	109.45	106.68
4	4	210	CLA	C4A-NA-C1A	6.08	109.45	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	312	CLA	C4A-NA-C1A	6.08	109.45	106.68
4	p	608	CLA	C4A-NA-C1A	6.05	109.44	106.68
5	3	301	A86	O4-C38-C39	6.04	121.86	111.09
4	3	306	CLA	C4A-NA-C1A	5.97	109.40	106.68
5	4	202	A86	C29-C30-C31	-5.94	170.65	177.66
4	4	211	CLA	C4A-NA-C1A	5.90	109.37	106.68
4	4	206	CLA	C4A-NA-C1A	5.88	109.36	106.68
5	3	302	A86	O4-C38-C39	5.84	121.50	111.09
5	3	301	A86	C41-C32-C31	5.79	115.66	110.47
4	4	208	CLA	C4A-NA-C1A	5.72	109.29	106.68
4	p	602	CLA	C4A-NA-C1A	5.68	109.27	106.68
5	3	302	A86	O1-C20-C21	-5.59	108.81	115.05
5	4	202	A86	O1-C20-C15	-5.54	57.00	59.23
5	4	202	A86	C3-C2-C1	-5.42	119.68	127.28
6	p	611	DD6	C4-C5-C6	-5.09	120.14	127.28
5	3	302	A86	C25-C26-C27	-5.07	120.17	127.28
4	p	606	CLA	C4A-NA-C1A	5.02	108.97	106.68
6	p	611	DD6	C21-C20-C19	4.94	119.79	114.24
5	4	202	A86	O4-C38-O5	-4.93	113.47	122.99
6	3	303	DD6	C4-C5-C6	-4.92	120.38	127.28
5	4	201	A86	C4-C5-C6	-4.91	120.39	127.28
4	p	607	CLA	C4A-NA-C1A	4.81	108.87	106.68
4	3	308	CLA	C4A-NA-C1A	4.70	108.83	106.68
6	3	303	DD6	C21-C20-C19	4.70	119.52	114.24
6	p	611	DD6	C3-C2-C1	-4.67	120.72	127.28
5	4	203	A86	C4-C5-C6	-4.62	120.80	127.28
5	4	203	A86	O1-C20-C15	-4.60	57.38	59.23
5	4	201	A86	O1-C20-C15	-4.60	57.38	59.23
5	4	203	A86	C3-C2-C1	-4.58	120.85	127.28
5	4	201	A86	C29-C30-C31	-4.53	172.31	177.66
5	4	203	A86	O1-C15-C20	-4.52	55.62	59.45
5	4	202	A86	C41-C32-C31	4.44	114.45	110.47
5	4	203	A86	C35-C34-C33	-4.41	101.96	109.89
5	4	202	A86	O1-C15-C20	-4.39	55.73	59.45
5	p	610	A86	C36-C31-C32	-4.35	115.38	119.70
5	p	610	A86	C35-C34-C33	-4.34	102.09	109.89
5	p	610	A86	C34-O4-C38	-4.33	110.19	117.85
5	3	302	A86	C4-C5-C6	-4.32	121.22	127.28
5	4	201	A86	O1-C20-C21	-4.30	110.24	115.05
5	p	610	A86	O4-C38-O5	-4.24	114.80	122.99
5	4	202	A86	C25-C26-C27	-4.22	121.36	127.28
5	3	302	A86	O1-C20-C15	-4.22	57.53	59.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	p	602	CLA	CMA-C3A-C2A	-4.17	106.68	116.23
4	p	605	CLA	C3B-C4B-NB	-4.15	106.83	110.53
5	3	301	A86	O1-C15-C20	-4.12	55.96	59.45
5	4	203	A86	C23-C16-C17	-4.09	101.78	108.97
5	4	201	A86	O1-C20-C19	4.08	117.32	113.49
5	4	201	A86	C3-C2-C1	-4.04	121.61	127.28
5	3	302	A86	C3-C2-C1	-4.04	121.61	127.28
4	4	209	CLA	CAA-C2A-C3A	-3.97	107.13	116.23
5	4	202	A86	O1-C20-C19	3.97	117.21	113.49
5	3	301	A86	C34-O4-C38	-3.97	110.84	117.85
5	4	201	A86	C40-C32-C31	-3.93	106.96	110.47
4	p	601	CLA	CAA-C2A-C3A	-3.91	107.25	116.23
4	p	605	CLA	CAA-C2A-C3A	-3.91	107.28	116.23
5	4	202	A86	C28-C27-C26	-3.89	116.52	122.82
5	4	201	A86	O1-C15-C20	-3.88	56.16	59.45
5	4	201	A86	O4-C38-C39	3.87	117.99	111.09
6	3	303	DD6	C14-C13-C11	-3.83	119.58	125.53
5	3	301	A86	C25-C26-C27	-3.82	121.92	127.28
5	p	610	A86	C9-C8-C6	-3.82	115.90	126.36
4	4	208	CLA	CAA-C2A-C1A	3.81	121.21	111.81
5	4	203	A86	O4-C38-O5	-3.79	115.68	122.99
5	3	302	A86	O1-C15-C20	-3.78	56.24	59.45
5	4	203	A86	C23-C16-C22	-3.78	101.88	107.37
6	p	611	DD6	C9-C10-C11	-3.78	121.98	127.28
5	p	610	A86	O1-C20-C15	-3.75	57.72	59.23
5	p	610	A86	C21-C20-C15	-3.74	111.27	123.35
5	4	202	A86	C23-C16-C22	-3.74	101.94	107.37
4	4	207	CLA	CAA-C2A-C3A	-3.74	107.66	116.23
4	p	603	CLA	CAA-C2A-C3A	-3.71	107.72	116.23
5	4	202	A86	O1-C20-C21	-3.68	110.93	115.05
6	3	303	DD6	C37-C36-C35	3.68	121.20	114.42
5	4	201	A86	C25-C26-C27	-3.65	122.16	127.28
4	4	210	CLA	CAA-C2A-C3A	-3.64	107.89	116.23
5	p	610	A86	C25-C26-C27	-3.61	122.22	127.28
5	p	610	A86	O1-C15-C20	-3.58	56.41	59.45
5	3	302	A86	C21-C20-C19	3.58	118.27	114.24
6	3	303	DD6	C37-C36-C31	-3.58	117.47	124.16
4	3	314	CLA	CAA-C2A-C3A	-3.56	108.06	116.23
4	3	310	CLA	CAA-C2A-C3A	-3.56	108.08	116.23
5	3	301	A86	O4-C38-O5	-3.55	116.13	122.99
4	3	309	CLA	CAA-C2A-C3A	-3.54	108.11	116.23
5	p	610	A86	C3-C2-C1	-3.53	122.33	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	p	601	CLA	CBD-CHA-C1A	3.51	132.67	127.38
4	3	304	CLA	CAA-C2A-C3A	-3.50	108.21	116.23
5	4	202	A86	C3-C4-C5	-3.46	116.44	123.52
6	3	303	DD6	O1-C15-C14	-3.44	107.03	116.88
5	4	203	A86	C10-C9-C8	-3.42	113.29	123.20
5	3	301	A86	C9-C10-C11	-3.41	117.00	126.64
4	p	604	CLA	CAA-C2A-C3A	-3.40	108.42	116.23
4	p	605	CLA	CBD-CHA-C1A	3.40	132.51	127.38
4	4	212	CLA	CAA-C2A-C3A	-3.40	108.43	116.23
4	p	606	CLA	C3A-C2A-C1A	-3.39	102.83	106.30
4	p	607	CLA	C3A-C2A-C1A	-3.36	102.87	106.30
4	4	204	CLA	CAA-C2A-C3A	-3.29	108.68	116.23
4	p	602	CLA	CAA-C2A-C3A	-3.29	108.69	116.23
5	4	202	A86	C4-C5-C6	-3.28	122.67	127.28
5	4	203	A86	C25-C26-C27	-3.27	122.69	127.28
4	4	206	CLA	CBD-CHA-C1A	3.25	131.47	128.03
4	4	213	CLA	C3A-C2A-C1A	-3.24	102.99	106.30
4	3	306	CLA	CBD-CHA-C1A	3.23	131.46	128.03
4	p	602	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
4	4	205	CLA	C3A-C2A-C1A	-3.20	103.03	106.30
4	p	603	CLA	CBD-CHA-C1A	3.16	132.15	127.38
4	3	308	CLA	C3B-C4B-NB	-3.15	107.71	110.53
4	p	606	CLA	C3B-C4B-NB	-3.15	107.72	110.53
5	p	610	A86	C28-C27-C26	-3.15	117.72	122.82
4	4	207	CLA	CBD-CHA-C1A	3.10	132.06	127.38
4	4	206	CLA	C3A-C2A-C1A	-3.10	103.13	106.30
4	3	311	CLA	CAA-C2A-C3A	-3.10	109.12	116.23
4	3	313	CLA	C3B-C4B-NB	-3.08	107.78	110.53
5	3	302	A86	C23-C16-C22	-3.08	102.90	107.37
4	3	310	CLA	C3B-C4B-NB	-3.07	107.79	110.53
4	3	313	CLA	CBD-CHA-C1A	3.06	132.00	127.38
4	4	204	CLA	C3B-C4B-NB	-3.06	107.80	110.53
6	3	303	DD6	C4-C3-C2	-3.04	117.30	123.52
5	3	302	A86	C4-C3-C2	-3.02	117.33	123.52
5	4	203	A86	C12-C11-C13	3.02	120.90	116.00
4	p	603	CLA	CMB-C2B-C1B	-3.02	120.82	125.42
6	p	611	DD6	C21-C20-C15	-3.02	117.34	122.30
4	4	211	CLA	C3A-C2A-C1A	-2.97	103.26	106.30
4	3	306	CLA	C3A-C4A-CHB	-2.97	120.28	123.91
4	4	206	CLA	C3B-C4B-NB	-2.96	107.89	110.53
5	3	302	A86	C28-C27-C26	-2.95	118.04	122.82
5	4	202	A86	C21-C20-C19	2.95	117.55	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	201	A86	C41-C32-C40	-2.94	100.20	108.63
4	p	608	CLA	C3A-C2A-C1A	-2.92	103.31	106.30
4	4	208	CLA	C3B-C4B-NB	-2.92	107.92	110.53
4	3	305	CLA	CAC-C3C-C4C	2.92	128.59	124.79
4	3	310	CLA	CHC-C1C-C2C	-2.91	123.57	129.94
5	3	302	A86	O4-C38-O5	-2.91	117.37	122.99
4	p	609	CLA	CAA-C2A-C3A	-2.91	109.56	116.23
4	4	210	CLA	C3B-C4B-NB	-2.89	107.95	110.53
4	3	305	CLA	C3B-C4B-NB	-2.88	107.96	110.53
5	4	202	A86	C9-C10-C11	-2.87	118.51	126.64
4	p	604	CLA	CMB-C2B-C1B	-2.87	121.05	125.42
4	4	209	CLA	C3B-C4B-NB	-2.87	107.97	110.53
4	p	609	CLA	CHB-C4A-NA	2.87	128.54	124.40
4	p	601	CLA	CHC-C1C-C2C	-2.84	123.72	129.94
4	3	307	CLA	CMB-C2B-C1B	-2.82	121.12	125.42
4	4	208	CLA	C2A-C1A-CHA	2.82	128.75	123.86
4	3	312	CLA	C3B-C4B-NB	-2.82	108.01	110.53
5	3	301	A86	C19-C18-C17	2.81	116.04	110.79
4	4	208	CLA	O2D-CGD-O1D	-2.80	117.72	124.08
5	p	610	A86	C23-C16-C17	-2.80	104.05	108.97
4	p	606	CLA	C4D-C3D-CAD	-2.79	105.07	108.11
4	3	306	CLA	CHC-C1C-C2C	-2.79	123.83	129.94
4	4	207	CLA	C3B-C4B-NB	-2.78	108.05	110.53
4	3	309	CLA	CMA-C3A-C2A	-2.76	109.91	116.23
4	p	601	CLA	CHB-C4A-NA	2.76	128.38	124.40
6	p	611	DD6	C15-C14-C13	-2.75	120.18	125.99
4	3	304	CLA	CHC-C1C-C2C	-2.75	123.92	129.94
5	4	202	A86	C35-C34-C33	-2.75	104.95	109.89
5	p	610	A86	C4-C3-C2	-2.74	117.92	123.52
4	4	205	CLA	C3B-C4B-NB	-2.73	107.49	110.33
4	3	304	CLA	CHB-C4A-NA	2.72	128.32	124.40
4	3	310	CLA	CHB-C4A-NA	2.71	128.32	124.40
4	4	207	CLA	CHB-C4A-NA	2.71	128.31	124.40
4	4	210	CLA	CBD-CHA-C1A	2.71	131.46	127.38
4	3	307	CLA	C3B-C4B-NB	-2.70	108.12	110.53
5	4	203	A86	C21-C20-C19	2.68	117.25	114.24
4	3	309	CLA	CHB-C4A-NA	2.68	128.26	124.40
5	4	202	A86	O4-C34-C35	2.67	114.46	107.64
5	4	202	A86	C9-C8-C6	-2.66	119.06	126.36
4	4	213	CLA	CAB-C3B-C2B	2.66	130.60	123.53
4	3	311	CLA	CHB-C4A-NA	2.66	128.23	124.40
4	p	603	CLA	CHB-C4A-NA	2.65	128.23	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	p	603	CLA	C3B-C4B-NB	-2.65	108.16	110.53
4	3	307	CLA	CHB-C4A-NA	2.65	128.23	124.40
4	4	211	CLA	CAB-C3B-C2B	2.65	130.56	123.53
4	4	209	CLA	CHB-C4A-NA	2.64	128.22	124.40
5	3	301	A86	O-C13-C11	-2.64	115.35	121.04
5	4	202	A86	O4-C34-C33	-2.64	100.88	107.64
4	p	605	CLA	CHB-C4A-NA	2.64	128.21	124.40
4	4	204	CLA	CBD-CHA-C1A	2.63	131.35	127.38
6	3	303	DD6	O1-C20-C21	-2.61	112.13	115.05
5	p	610	A86	C41-C32-C40	2.61	116.10	108.63
4	3	311	CLA	CMA-C3A-C2A	-2.60	110.26	116.23
4	p	602	CLA	C3B-C4B-NB	-2.60	108.20	110.53
6	p	611	DD6	C37-C36-C35	2.60	119.21	114.42
5	3	301	A86	C8-C6-C5	2.60	123.10	119.01
4	p	608	CLA	CAB-C3B-C2B	2.59	130.42	123.53
4	p	601	CLA	C3B-C4B-NB	-2.58	108.22	110.53
4	4	209	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
5	4	203	A86	C26-C25-C24	-2.58	115.74	123.20
4	3	312	CLA	O2D-CGD-O1D	-2.56	118.26	124.08
6	3	303	DD6	C26-C25-C24	-2.56	115.78	123.20
4	4	210	CLA	CHB-C4A-NA	2.56	128.09	124.40
4	4	212	CLA	CMB-C2B-C3B	2.56	130.33	123.53
4	p	603	CLA	CMB-C2B-C3B	2.55	132.55	126.55
5	4	203	A86	C28-C27-C26	-2.55	118.68	122.82
4	4	210	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
4	p	604	CLA	CHB-C4A-NA	2.54	128.07	124.40
4	3	305	CLA	O2D-CGD-O1D	-2.53	118.33	124.08
4	p	602	CLA	O2D-CGD-CBD	2.53	115.65	111.23
4	3	305	CLA	CHB-C4A-NA	2.53	128.05	124.40
5	3	302	A86	C3-C4-C5	-2.53	118.35	123.52
4	3	306	CLA	CAB-C3B-C2B	2.53	130.25	123.53
4	3	313	CLA	CHB-C4A-NA	2.52	128.04	124.40
6	p	611	DD6	C25-C24-C1	-2.52	119.46	126.36
4	4	211	CLA	CMB-C2B-C3B	2.52	130.22	123.53
5	3	302	A86	C26-C25-C24	-2.52	115.91	123.20
6	3	303	DD6	C3-C2-C1	-2.52	123.75	127.28
4	3	311	CLA	C3B-C4B-NB	-2.52	108.28	110.53
4	3	314	CLA	CHB-C4A-NA	2.51	128.03	124.40
4	4	212	CLA	CAB-C3B-C2B	2.51	130.19	123.53
4	p	604	CLA	CMB-C2B-C3B	2.48	132.38	126.55
4	4	212	CLA	CHB-C4A-NA	2.48	127.98	124.40
5	3	302	A86	C10-C9-C8	-2.47	116.03	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	201	A86	C12-C11-C13	2.47	120.01	116.00
4	4	208	CLA	CHA-C1A-NA	-2.47	120.79	126.39
4	4	204	CLA	CHB-C4A-NA	2.47	127.97	124.40
5	4	201	A86	C35-C34-C33	-2.46	105.46	109.89
4	3	312	CLA	CHB-C4A-NA	2.46	127.96	124.40
4	p	604	CLA	C3B-C4B-NB	-2.46	108.33	110.53
4	p	607	CLA	CMB-C2B-C3B	2.46	130.07	123.53
4	3	311	CLA	O2D-CGD-O1D	-2.45	118.52	124.08
4	3	306	CLA	CMB-C2B-C3B	2.45	130.05	123.53
4	3	309	CLA	C3B-C4B-NB	-2.45	108.34	110.53
4	p	602	CLA	CHB-C4A-NA	2.42	127.89	124.40
5	p	610	A86	O-C13-C11	-2.42	115.83	121.04
4	p	607	CLA	C3B-C4B-NB	-2.41	107.83	110.33
4	3	314	CLA	C3B-C4B-NB	-2.41	107.83	110.33
4	p	607	CLA	CAB-C3B-C2B	2.41	129.93	123.53
4	p	608	CLA	CHB-C4A-NA	2.40	127.87	124.40
5	4	201	A86	C41-C32-C33	2.40	120.42	109.06
4	4	208	CLA	CHB-C4A-NA	2.40	127.86	124.40
4	p	604	CLA	O2D-CGD-O1D	-2.39	118.65	124.08
4	3	307	CLA	CMB-C2B-C3B	2.39	132.17	126.55
4	p	609	CLA	C3B-C4B-NB	-2.39	108.40	110.53
4	p	602	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
4	p	608	CLA	O2D-CGD-O1D	-2.38	118.68	124.08
4	4	213	CLA	CMB-C2B-C3B	2.37	129.84	123.53
4	p	608	CLA	CMB-C2B-C3B	2.37	129.83	123.53
4	3	304	CLA	C3B-C4B-NB	-2.35	107.89	110.33
4	3	314	CLA	CAB-C3B-C2B	2.34	129.76	123.53
5	4	203	A86	O-C13-C11	-2.33	116.02	121.04
4	3	304	CLA	CAB-C3B-C2B	2.32	129.69	123.53
5	4	202	A86	C23-C16-C17	-2.28	104.96	108.97
4	3	306	CLA	C3B-C4B-NB	-2.28	107.96	110.33
4	3	314	CLA	CMA-C3A-C2A	-2.27	111.03	116.23
6	p	611	DD6	C28-C27-C26	-2.27	119.78	124.18
5	3	302	A86	C36-C31-C32	-2.26	117.45	119.70
4	4	205	CLA	CAB-C3B-C2B	2.26	129.53	123.53
5	3	301	A86	C26-C25-C24	-2.24	116.70	123.20
5	3	301	A86	C4-C3-C2	-2.24	118.93	123.52
4	4	213	CLA	C3B-C4B-NB	-2.24	108.00	110.33
5	4	202	A86	O-C13-C11	-2.24	116.22	121.04
4	p	606	CLA	CHB-C1B-NB	2.23	127.40	124.05
5	3	301	A86	C9-C8-C6	-2.23	120.25	126.36
5	3	301	A86	C41-C32-C40	2.23	115.01	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	203	A86	C3-C4-C5	-2.23	118.97	123.52
6	3	303	DD6	C21-C20-C15	-2.22	118.64	122.30
4	3	309	CLA	O2D-CGD-O1D	-2.22	119.04	124.08
5	3	302	A86	C40-C32-C31	2.21	112.45	110.47
4	4	208	CLA	CAA-C2A-C3A	-2.21	111.15	116.23
4	4	213	CLA	CHB-C1B-NB	2.21	127.37	124.05
5	4	202	A86	C19-C18-C17	-2.21	106.65	110.79
4	4	210	CLA	CMB-C2B-C3B	2.21	131.75	126.55
4	3	306	CLA	CHB-C4A-NA	2.20	127.56	124.43
4	3	314	CLA	CMB-C2B-C3B	2.20	129.37	123.53
4	p	608	CLA	CAC-C3C-C4C	2.19	127.64	124.79
5	4	202	A86	C33-C32-C31	-2.19	107.09	109.21
6	3	303	DD6	C28-C27-C26	-2.18	119.94	124.18
4	4	212	CLA	C3B-C4B-NB	-2.18	108.07	110.33
4	3	308	CLA	CHB-C1B-NB	2.17	127.31	124.05
5	3	302	A86	O-C13-C11	-2.16	116.38	121.04
5	3	302	A86	C-C1-C24	2.16	121.39	118.09
4	4	213	CLA	CBD-CHA-C1A	2.15	130.31	128.03
4	p	608	CLA	C3B-C4B-NB	-2.15	108.10	110.33
6	3	303	DD6	C12-C11-C10	-2.14	119.35	122.82
6	p	611	DD6	C37-C36-C31	-2.14	120.16	124.16
5	3	302	A86	C23-C16-C17	-2.14	105.21	108.97
4	4	206	CLA	CHB-C4A-NA	2.14	127.48	124.40
6	p	611	DD6	C7-C6-C5	-2.14	119.36	122.82
5	4	201	A86	C4-C3-C2	-2.13	119.16	123.52
5	4	202	A86	C26-C25-C24	-2.13	117.04	123.20
4	4	213	CLA	CMB-C2B-C1B	-2.12	122.18	125.42
4	p	601	CLA	CMA-C3A-C2A	-2.12	111.38	116.23
4	p	602	CLA	CMB-C2B-C3B	2.10	131.49	126.55
6	p	611	DD6	C-C1-C2	-2.10	119.42	122.82
4	4	213	CLA	CHD-C4C-NC	2.08	127.46	124.23
4	4	211	CLA	CHB-C4A-NA	2.08	127.39	124.40
4	4	205	CLA	CHB-C4A-NA	2.07	127.39	124.40
5	p	610	A86	C41-C32-C33	-2.07	99.25	109.06
5	4	201	A86	C9-C8-C6	-2.07	120.69	126.36
6	p	611	DD6	C32-C33-C34	-2.07	109.06	113.59
4	p	607	CLA	C4D-CHA-C1A	2.07	123.71	121.24
5	3	302	A86	C12-C11-C13	2.06	119.34	116.00
4	4	213	CLA	CHD-C1D-ND	-2.06	121.90	124.80
5	3	302	A86	C9-C10-C11	-2.06	120.81	126.64
5	4	202	A86	C12-C11-C13	2.04	119.31	116.00
6	p	611	DD6	C9-C8-C6	-2.03	120.79	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	308	CLA	C2A-C1A-CHA	2.03	124.83	122.46
5	4	203	A86	C34-O4-C38	2.03	121.44	117.85
4	p	606	CLA	CHB-C4A-NA	2.03	127.33	124.40
4	p	609	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
4	3	304	CLA	CMA-C3A-C2A	-2.03	111.58	116.23
4	4	213	CLA	C4D-CHA-C1A	2.03	123.66	121.24
4	4	207	CLA	CMA-C3A-C2A	-2.01	111.61	116.23
5	4	201	A86	C9-C10-C11	-2.01	120.97	126.64
4	p	607	CLA	CHB-C1B-NB	2.00	127.05	124.05

All (30) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	p	601	CLA	ND
4	p	602	CLA	ND
4	p	603	CLA	ND
4	p	604	CLA	ND
4	p	605	CLA	ND
4	p	606	CLA	ND
4	p	607	CLA	ND
4	p	608	CLA	ND
4	p	609	CLA	ND
4	4	204	CLA	ND
4	4	205	CLA	ND
4	4	206	CLA	ND
4	4	207	CLA	ND
4	4	208	CLA	ND
4	4	209	CLA	ND
4	4	210	CLA	ND
4	4	211	CLA	ND
4	4	212	CLA	ND
4	4	213	CLA	ND
4	3	304	CLA	ND
4	3	305	CLA	ND
4	3	306	CLA	ND
4	3	307	CLA	ND
4	3	308	CLA	ND
4	3	309	CLA	ND
4	3	310	CLA	ND
4	3	311	CLA	ND
4	3	312	CLA	ND
4	3	313	CLA	ND

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Mol	Chain	Res	Type	Atom
4	3	314	CLA	ND

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	p	604	CLA	CAD-CBD-CGD-O2D
4	p	605	CLA	C2B-C3B-CAB-CBB
4	p	605	CLA	C4B-C3B-CAB-CBB
4	4	204	CLA	C2B-C3B-CAB-CBB
4	4	204	CLA	C4B-C3B-CAB-CBB
4	4	207	CLA	C4B-C3B-CAB-CBB
4	4	209	CLA	CBD-CGD-O2D-CED
4	4	209	CLA	O1D-CGD-O2D-CED
4	3	308	CLA	C2D-C3D-CAD-OB
4	3	308	CLA	C4D-C3D-CAD-OB
4	3	312	CLA	C1A-C2A-CAA-CBA
4	3	312	CLA	C2B-C3B-CAB-CBB
4	3	312	CLA	C4B-C3B-CAB-CBB
4	3	312	CLA	CAD-CBD-CGD-O2D
5	p	610	A86	C5-C6-C8-C9
5	p	610	A86	C7-C6-C8-C9
5	4	201	A86	C12-C11-C13-O
5	4	202	A86	C10-C11-C13-C14
5	4	202	A86	C12-C11-C13-C14
5	3	301	A86	C13-C14-C15-C16
5	3	301	A86	C13-C14-C15-O1
5	3	301	A86	C3-C4-C5-C6
5	3	301	A86	C5-C6-C8-C9
5	3	301	A86	C7-C6-C8-C9
6	p	611	DD6	C10-C11-C13-C14
6	p	611	DD6	C12-C11-C13-C14
5	p	610	A86	C39-C38-O4-C34
5	4	201	A86	C39-C38-O4-C34
5	3	301	A86	C39-C38-O4-C34
5	3	302	A86	C39-C38-O4-C34
5	p	610	A86	O5-C38-O4-C34
5	4	201	A86	O5-C38-O4-C34
5	3	301	A86	O5-C38-O4-C34
4	p	602	CLA	CBD-CGD-O2D-CED
5	p	610	A86	C11-C10-C9-C8
5	4	202	A86	C39-C38-O4-C34
5	3	302	A86	O5-C38-O4-C34

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Mol	Chain	Res	Type	Atoms
5	4	202	A86	O5-C38-O4-C34
5	4	203	A86	C39-C38-O4-C34
5	4	203	A86	O5-C38-O4-C34
5	4	202	A86	C35-C34-O4-C38
6	3	303	DD6	C12-C11-C13-C14
4	p	602	CLA	O1D-CGD-O2D-CED
5	4	201	A86	C35-C34-O4-C38
5	p	610	A86	C33-C34-O4-C38
4	p	601	CLA	C4B-C3B-CAB-CBB
4	4	208	CLA	C4B-C3B-CAB-CBB
4	3	308	CLA	C4B-C3B-CAB-CBB
4	3	311	CLA	C4B-C3B-CAB-CBB
4	p	601	CLA	C2B-C3B-CAB-CBB
4	4	207	CLA	C2B-C3B-CAB-CBB
4	4	208	CLA	C2B-C3B-CAB-CBB
4	3	308	CLA	C2B-C3B-CAB-CBB
6	3	303	DD6	C10-C11-C13-C14
4	p	606	CLA	C4B-C3B-CAB-CBB
4	3	313	CLA	C4B-C3B-CAB-CBB
4	3	307	CLA	C3A-C2A-CAA-CBA
5	4	202	A86	C12-C11-C13-O
5	3	302	A86	C12-C11-C13-O
5	p	610	A86	C10-C11-C13-O
5	4	201	A86	C10-C11-C13-O
5	4	202	A86	C10-C11-C13-O
5	3	302	A86	C10-C11-C13-O
4	3	305	CLA	C1A-C2A-CAA-CBA
4	3	313	CLA	C1A-C2A-CAA-CBA
6	p	611	DD6	C-C1-C24-C25
4	4	206	CLA	C4B-C3B-CAB-CBB
4	3	305	CLA	C4B-C3B-CAB-CBB
4	3	307	CLA	C1A-C2A-CAA-CBA
6	p	611	DD6	C2-C1-C24-C25
5	4	203	A86	C35-C34-O4-C38
4	p	604	CLA	CAD-CBD-CGD-O1D
5	p	610	A86	C13-C14-C15-C20
5	4	203	A86	C13-C14-C15-C20
4	3	309	CLA	CHA-CBD-CGD-O2D
5	4	201	A86	C10-C11-C13-C14
5	3	302	A86	C10-C11-C13-C14
4	p	606	CLA	C2B-C3B-CAB-CBB
4	3	311	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
4	3	313	CLA	C2B-C3B-CAB-CBB
5	4	201	A86	C12-C11-C13-C14
5	3	301	A86	C12-C11-C13-C14
4	3	309	CLA	C4B-C3B-CAB-CBB
5	3	301	A86	C35-C34-O4-C38
5	p	610	A86	C12-C11-C13-O
5	3	301	A86	C12-C11-C13-O
5	4	203	A86	C10-C11-C13-O
5	3	301	A86	C10-C11-C13-O
4	4	206	CLA	C2B-C3B-CAB-CBB
4	3	305	CLA	C2B-C3B-CAB-CBB
4	3	309	CLA	C2B-C3B-CAB-CBB
4	4	209	CLA	C4B-C3B-CAB-CBB
6	p	611	DD6	C13-C14-C15-O1
4	p	608	CLA	C2C-C3C-CAC-CBC
4	4	209	CLA	C2B-C3B-CAB-CBB
4	p	608	CLA	CHA-CBD-CGD-O1D
5	4	203	A86	C12-C11-C13-O
5	3	301	A86	C13-C14-C15-C20
5	3	302	A86	C13-C14-C15-C20

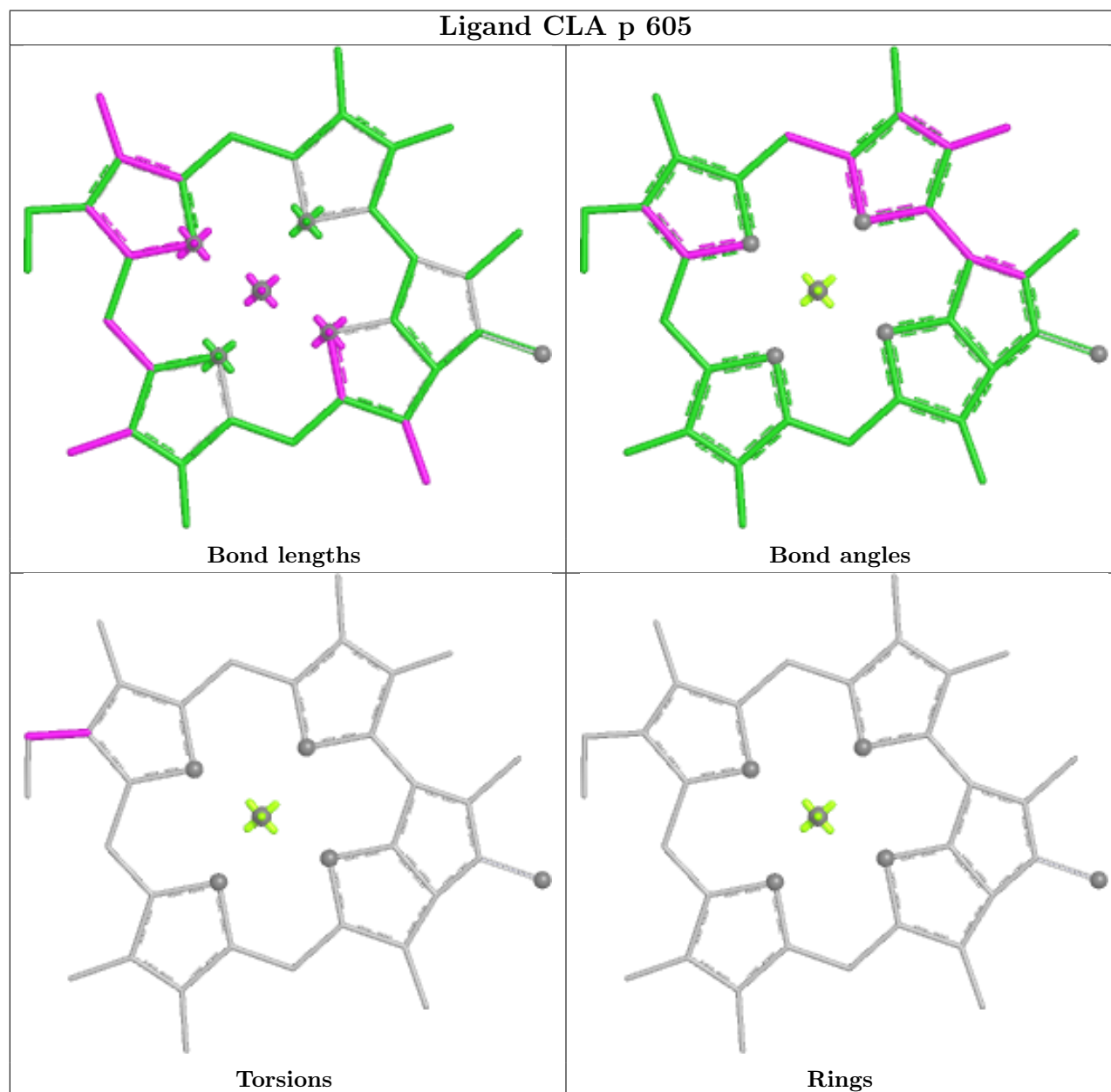
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	4	201	A86	C31-C32-C33-C34-C35-C36

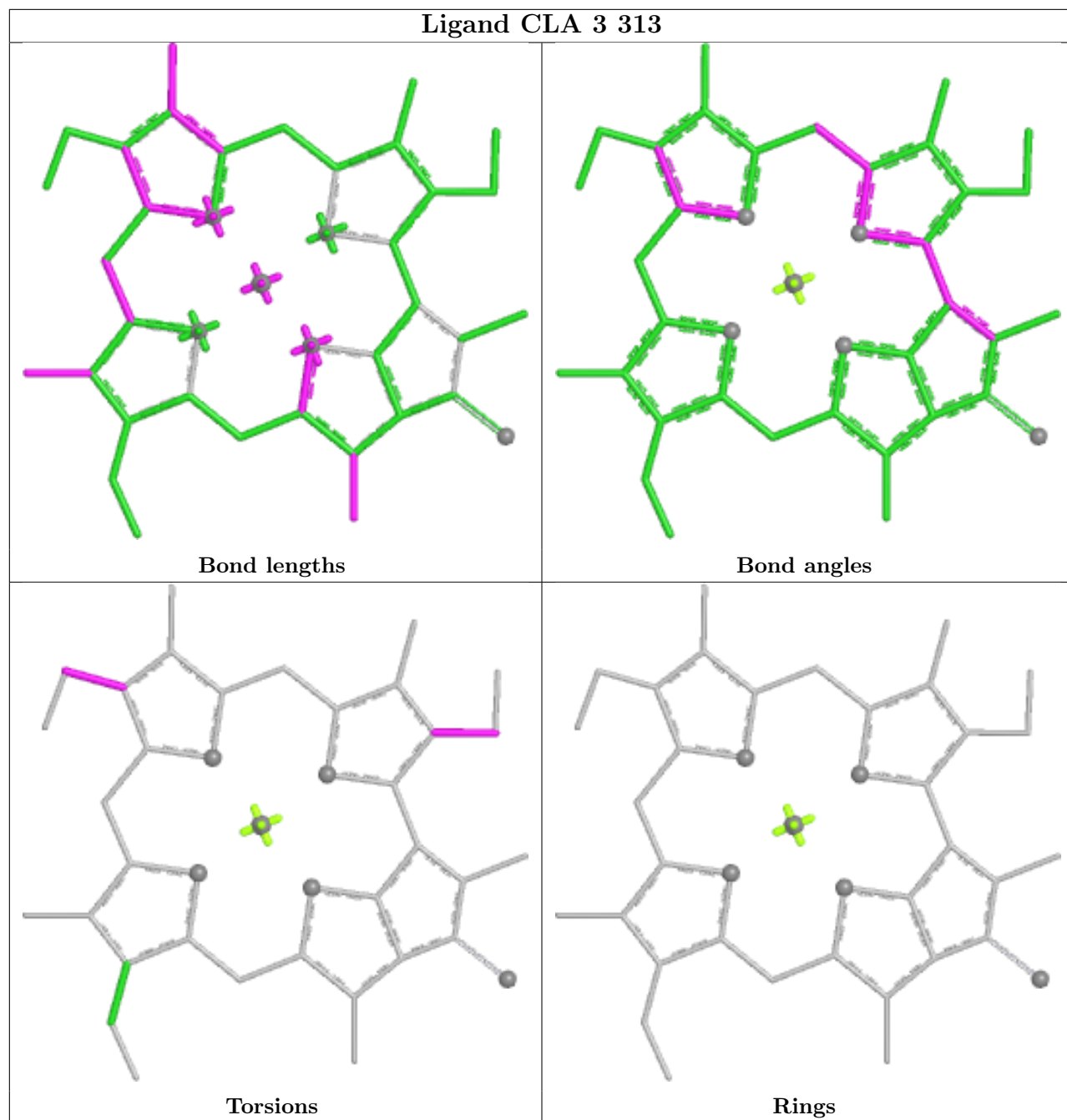
13 monomers are involved in 17 short contacts:

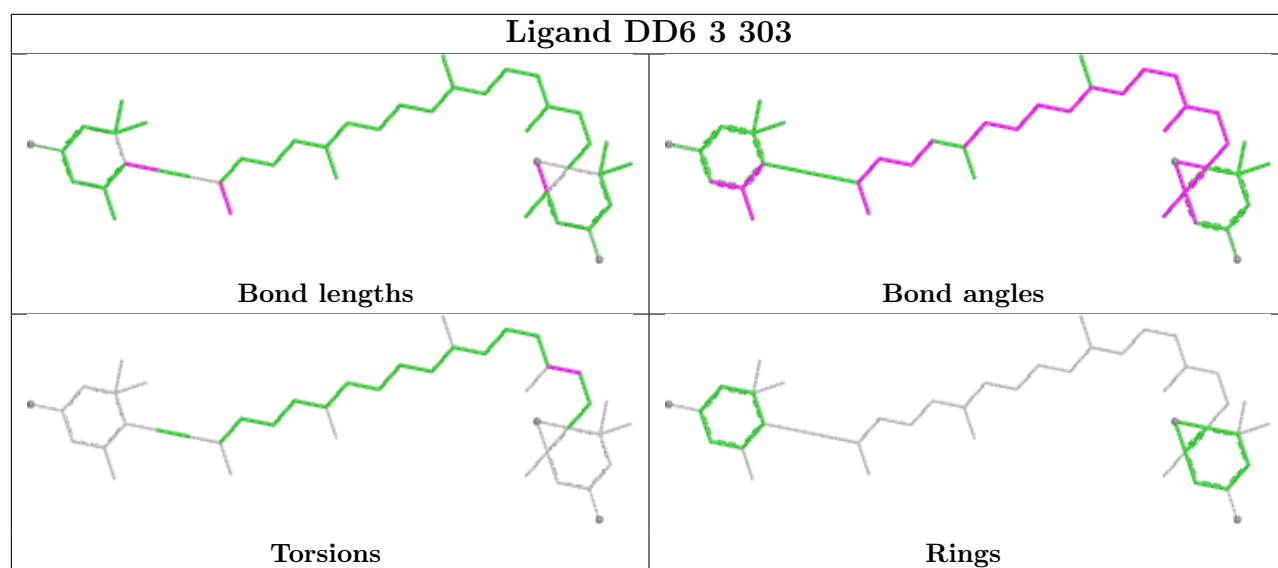
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	3	303	DD6	1	0
4	3	314	CLA	1	0
4	3	308	CLA	1	0
4	p	607	CLA	1	0
4	p	604	CLA	5	0
4	3	310	CLA	1	0
4	3	311	CLA	1	0
4	3	305	CLA	1	0
4	3	312	CLA	1	0
6	p	611	DD6	7	0
4	p	602	CLA	2	0
4	4	209	CLA	1	0
4	p	603	CLA	2	0

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.

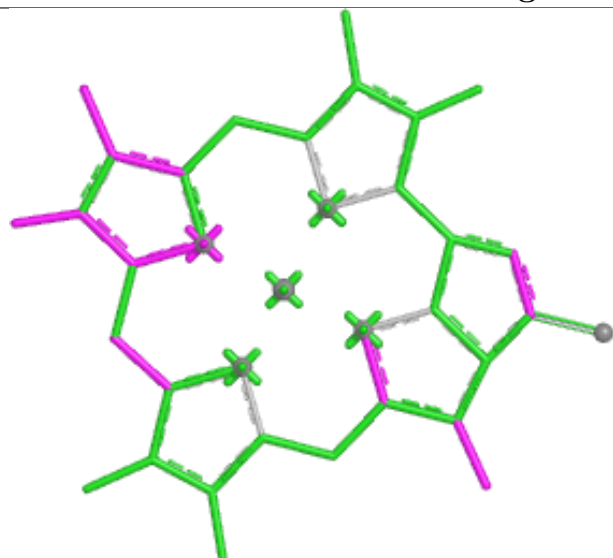


Ligand CLA 3 313

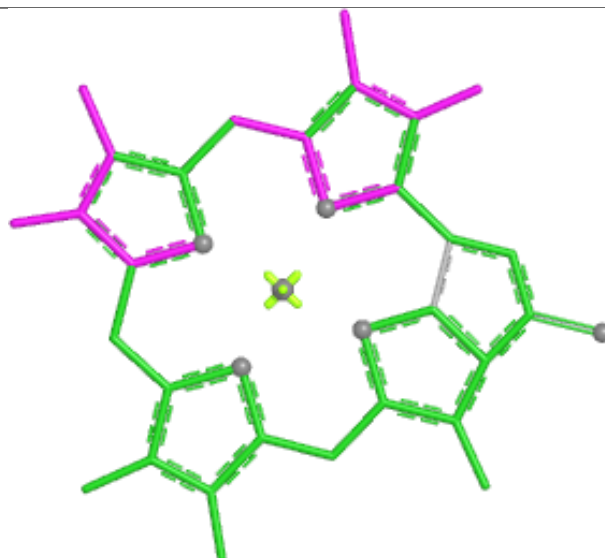




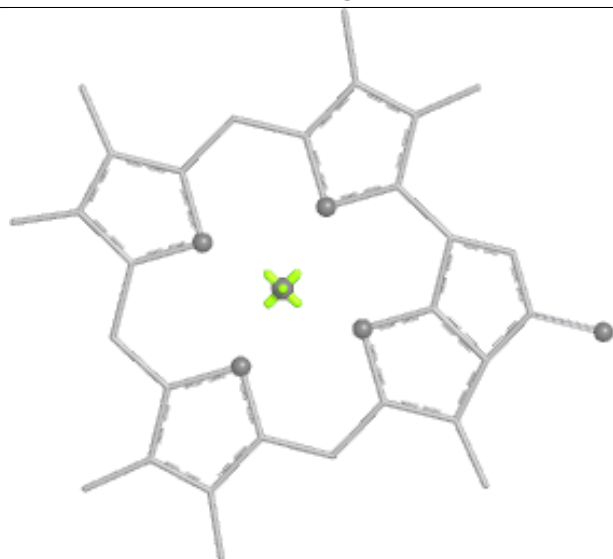
Ligand CLA 3 314



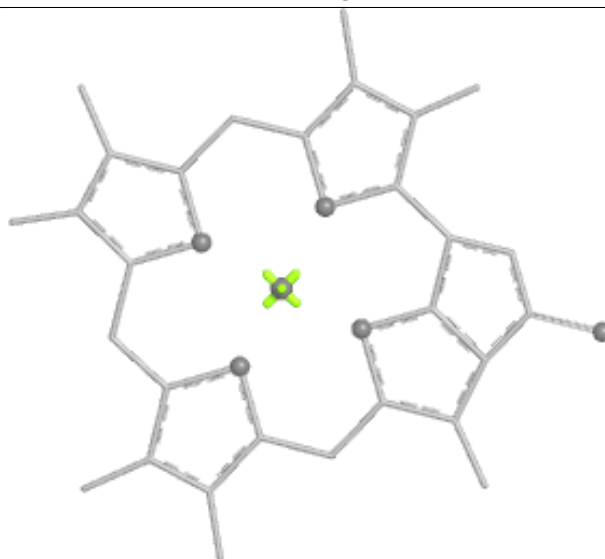
Bond lengths



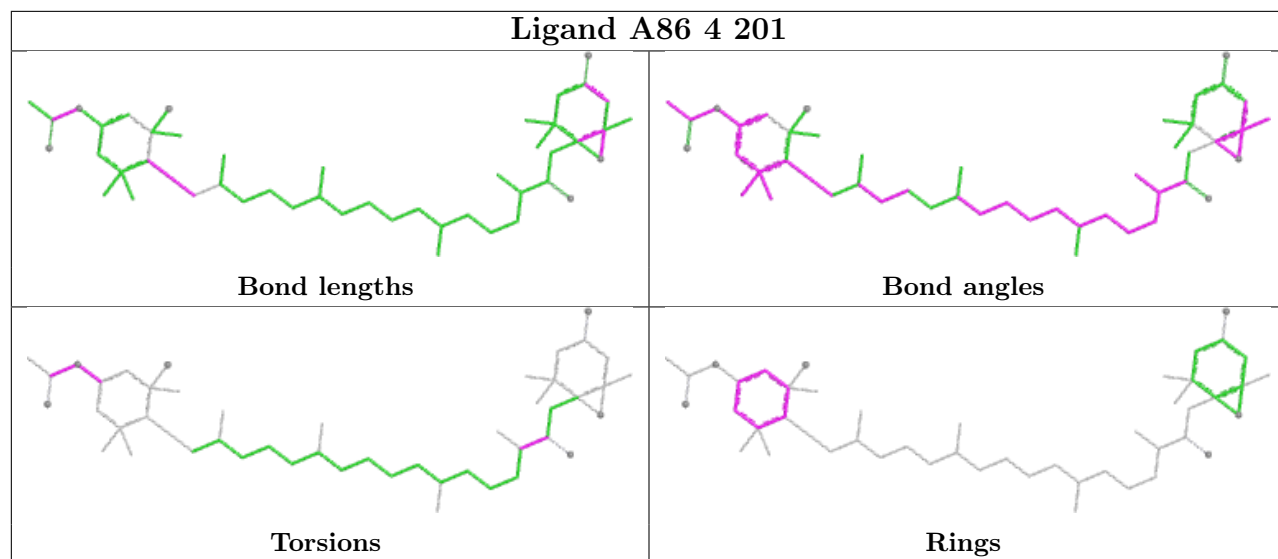
Bond angles



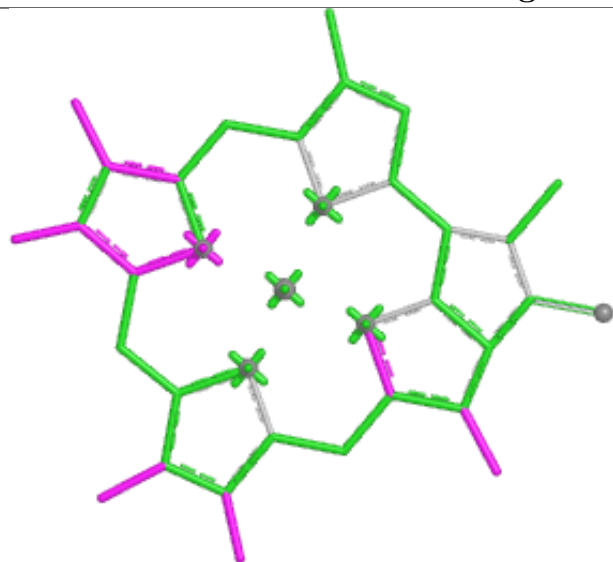
Torsions



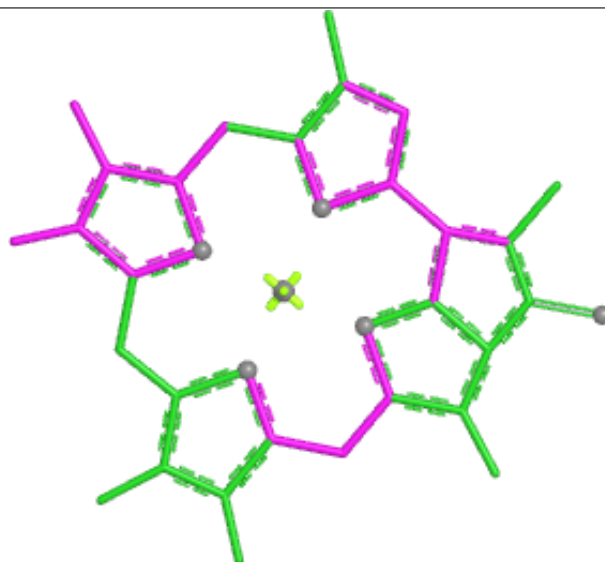
Rings



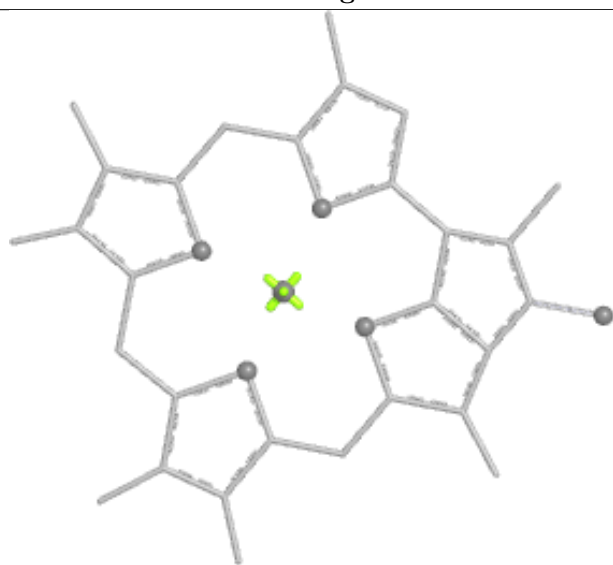
Ligand CLA 4 213



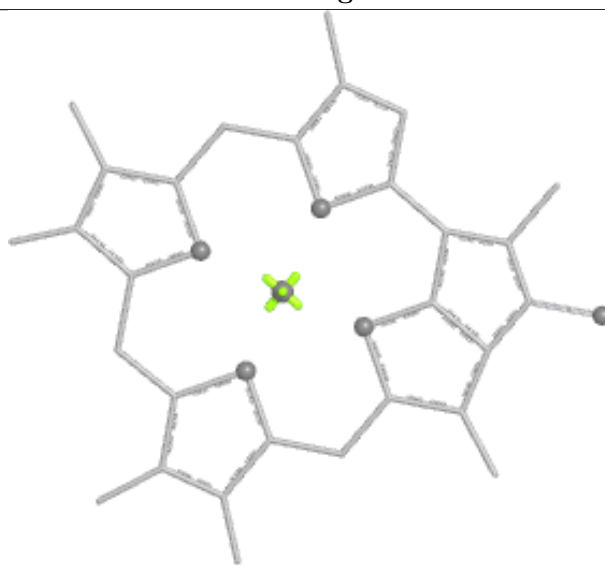
Bond lengths



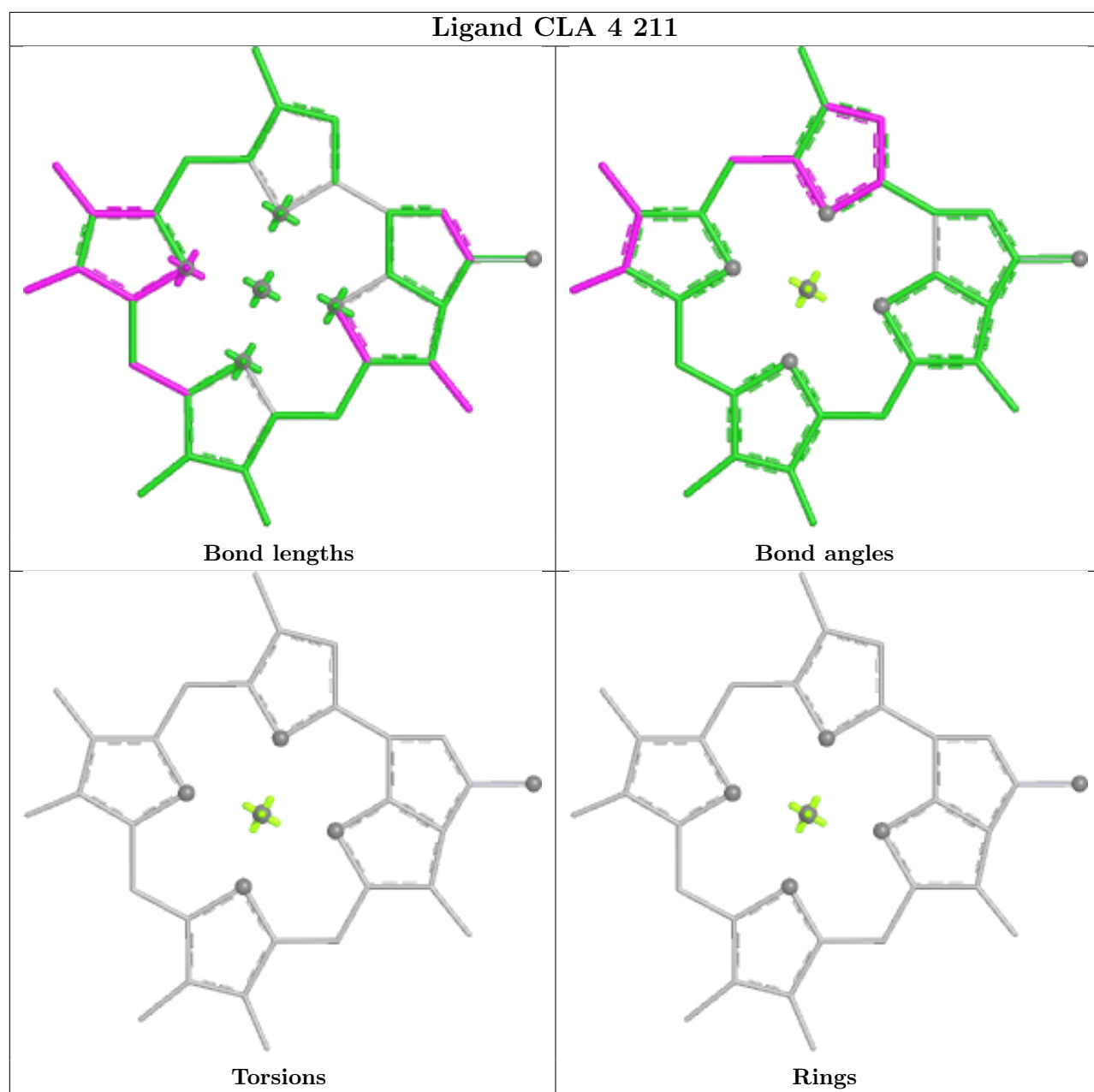
Bond angles



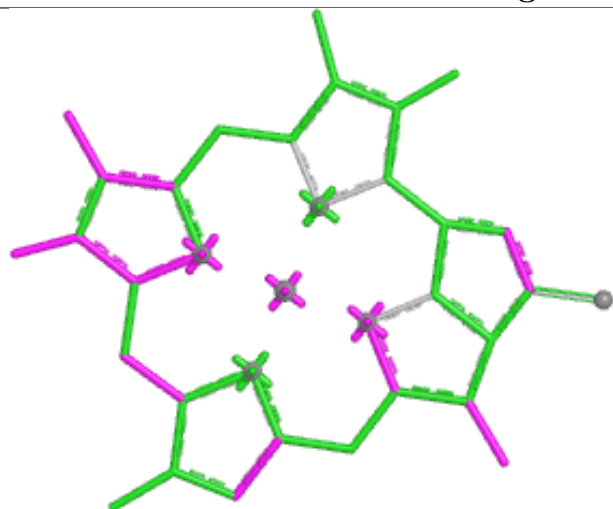
Torsions



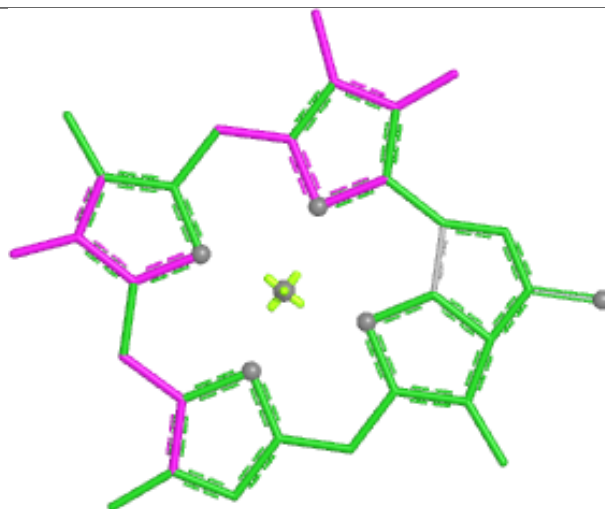
Rings



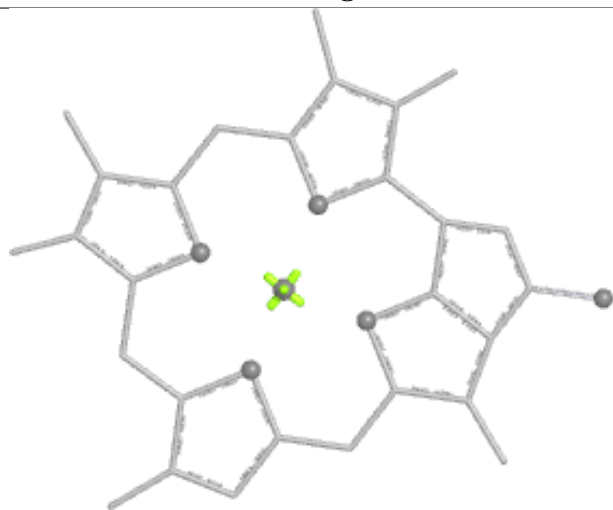
Ligand CLA 3 304



Bond lengths



Bond angles

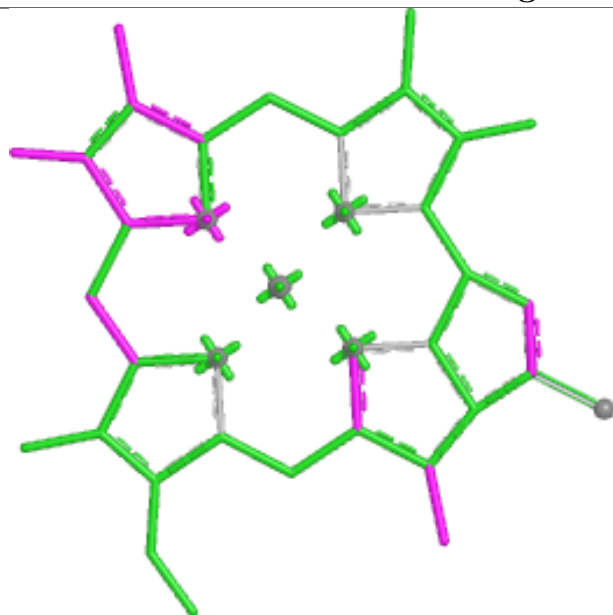


Torsions

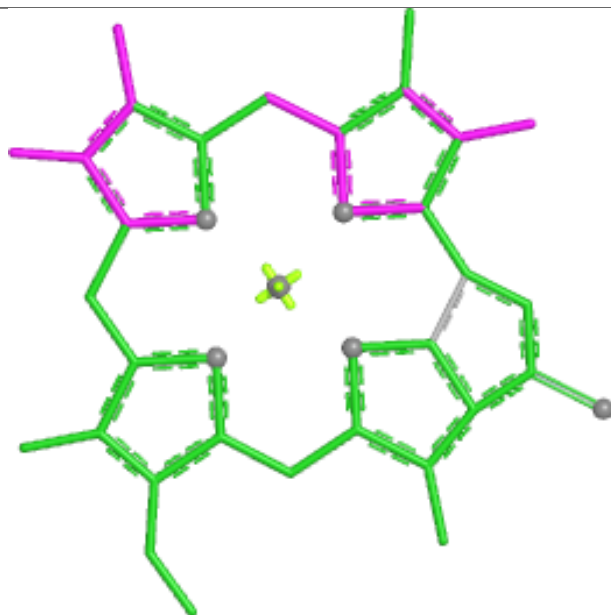


Rings

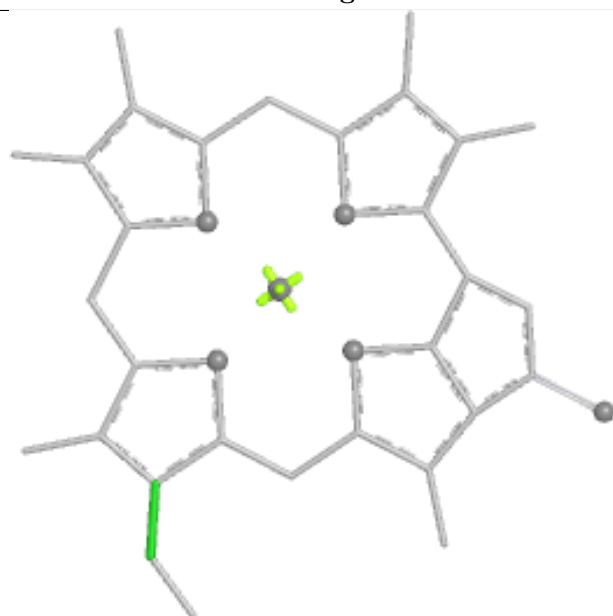
Ligand CLA 4 212



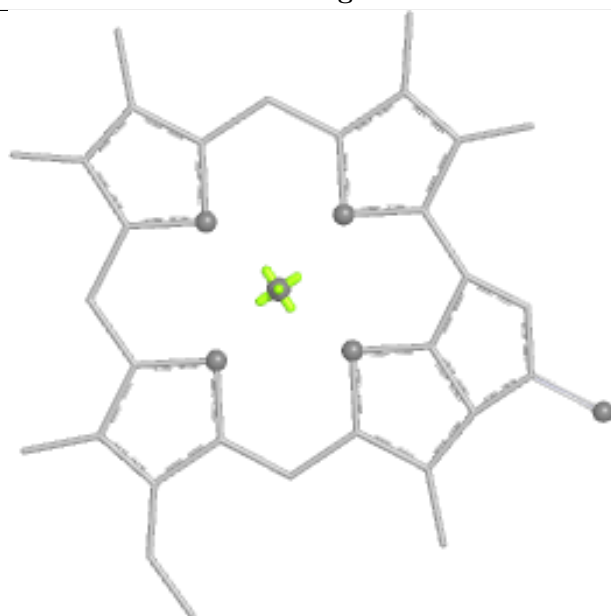
Bond lengths



Bond angles

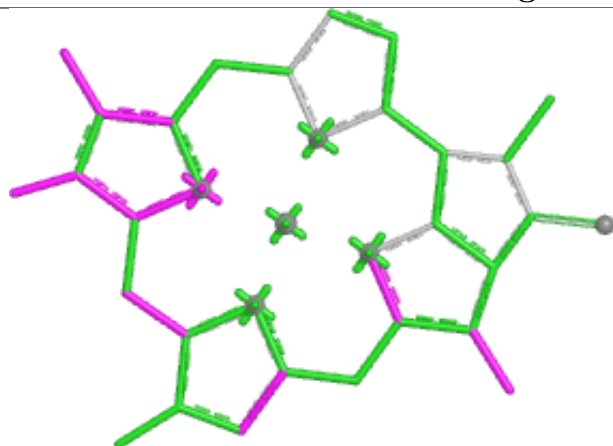


Torsions

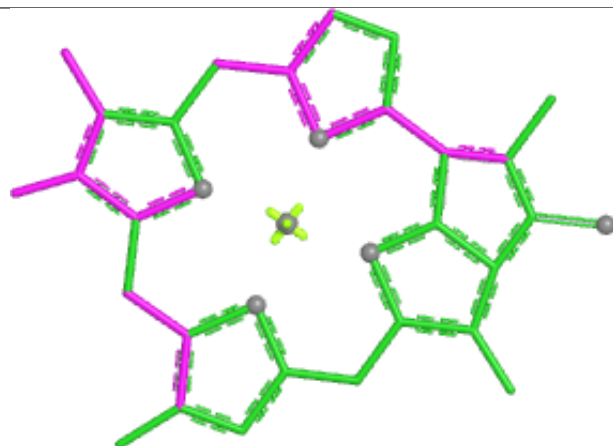


Rings

Ligand CLA 3 306



Bond lengths



Bond angles

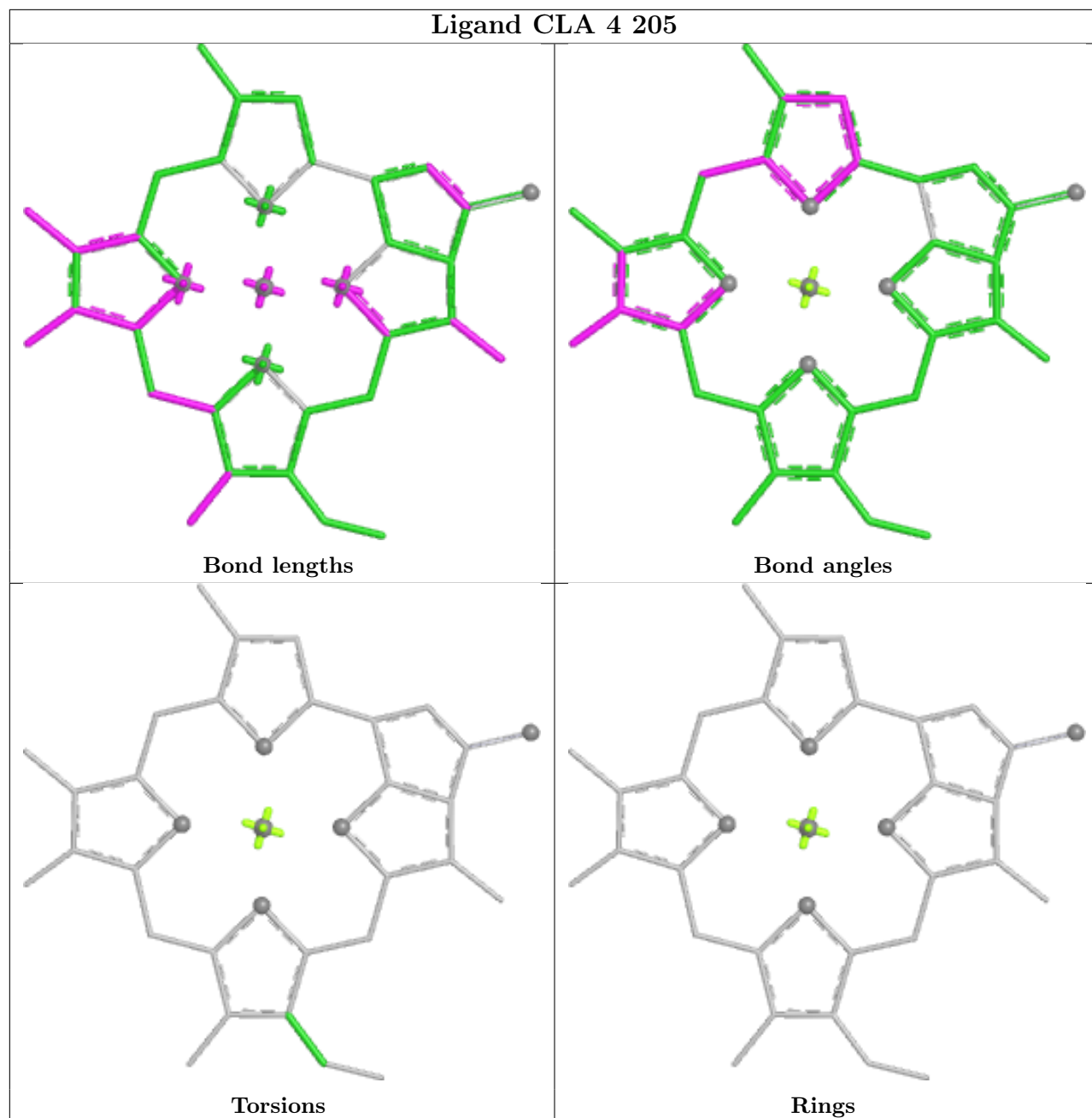


Torsions

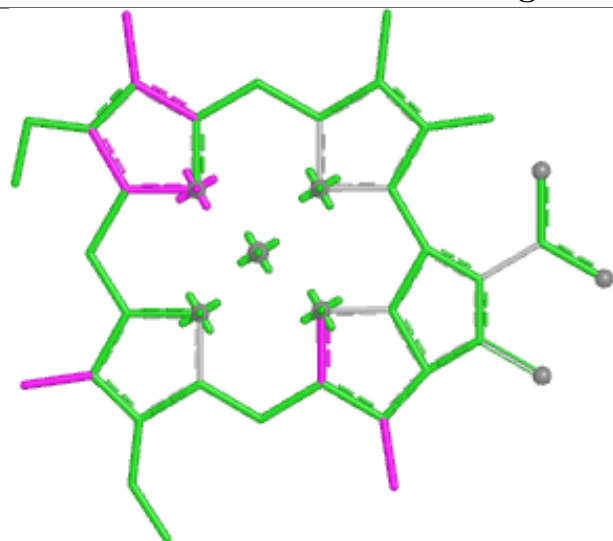


Rings

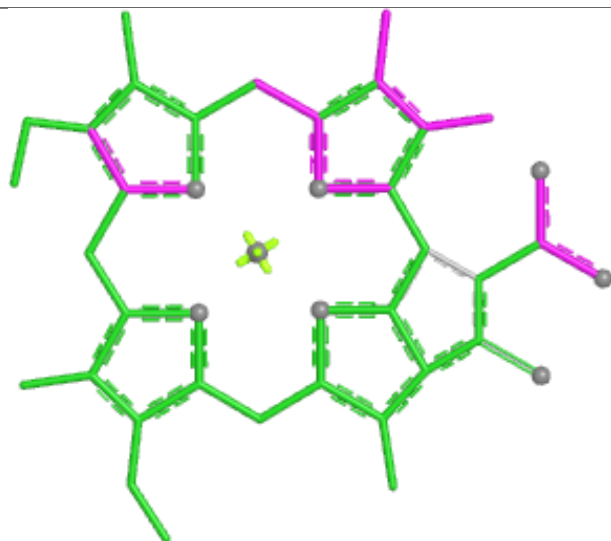
Ligand CLA 4 205



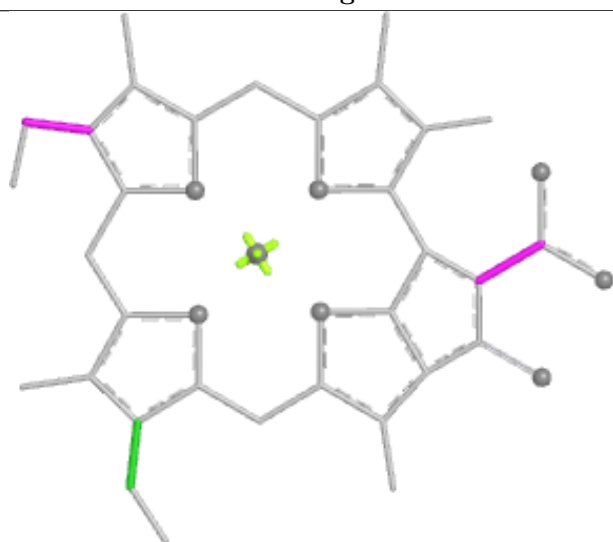
Ligand CLA 3 309



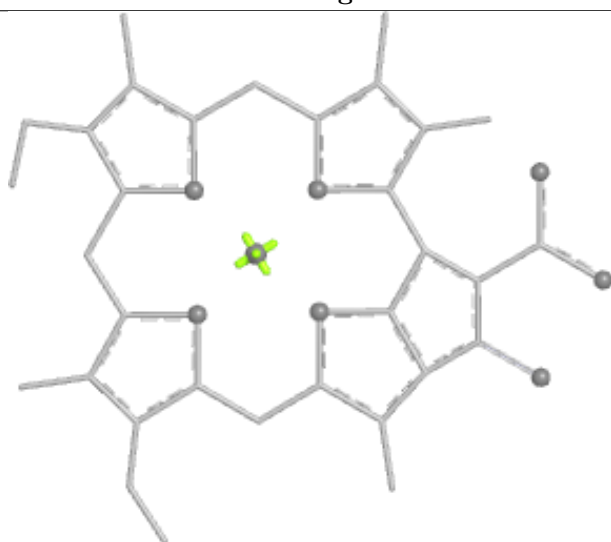
Bond lengths



Bond angles

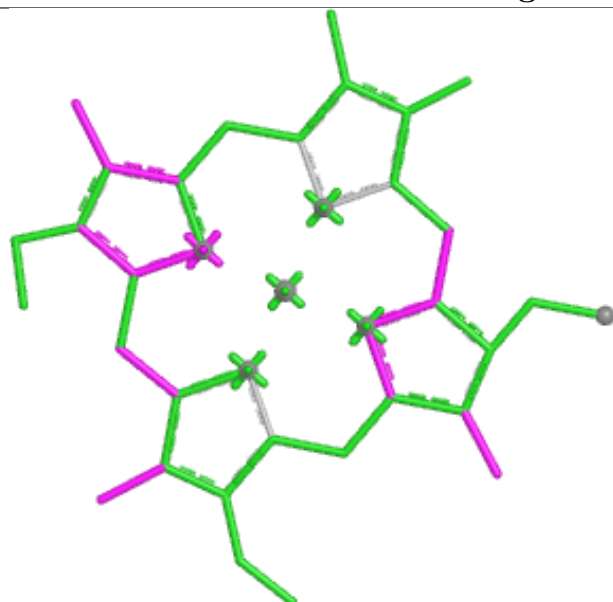


Torsions

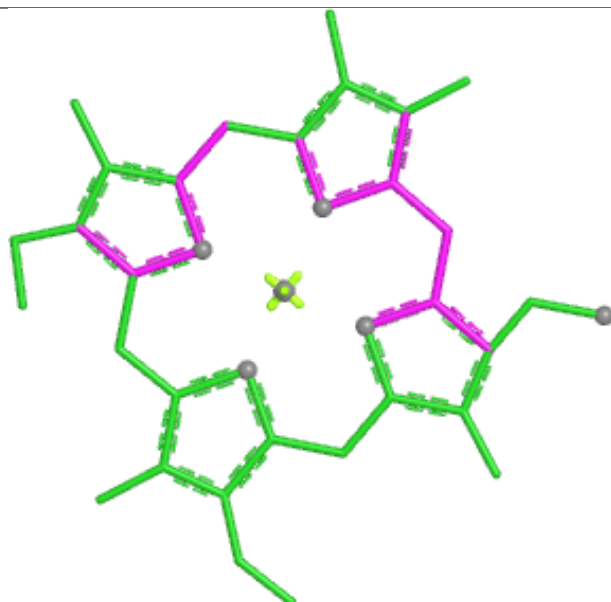


Rings

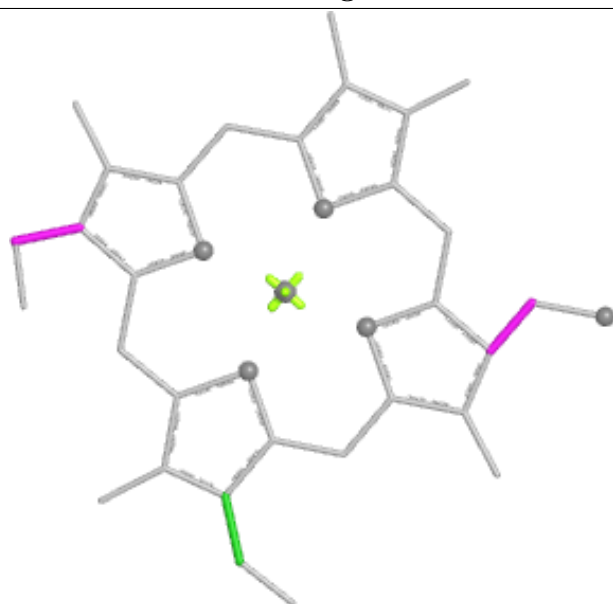
Ligand CLA 3 308



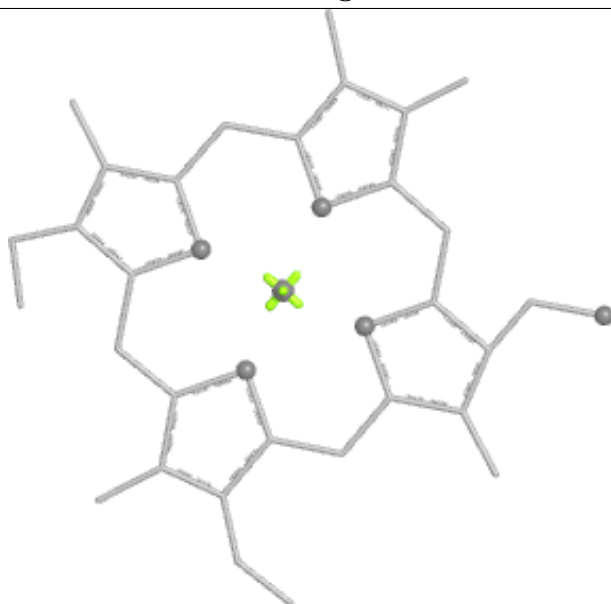
Bond lengths



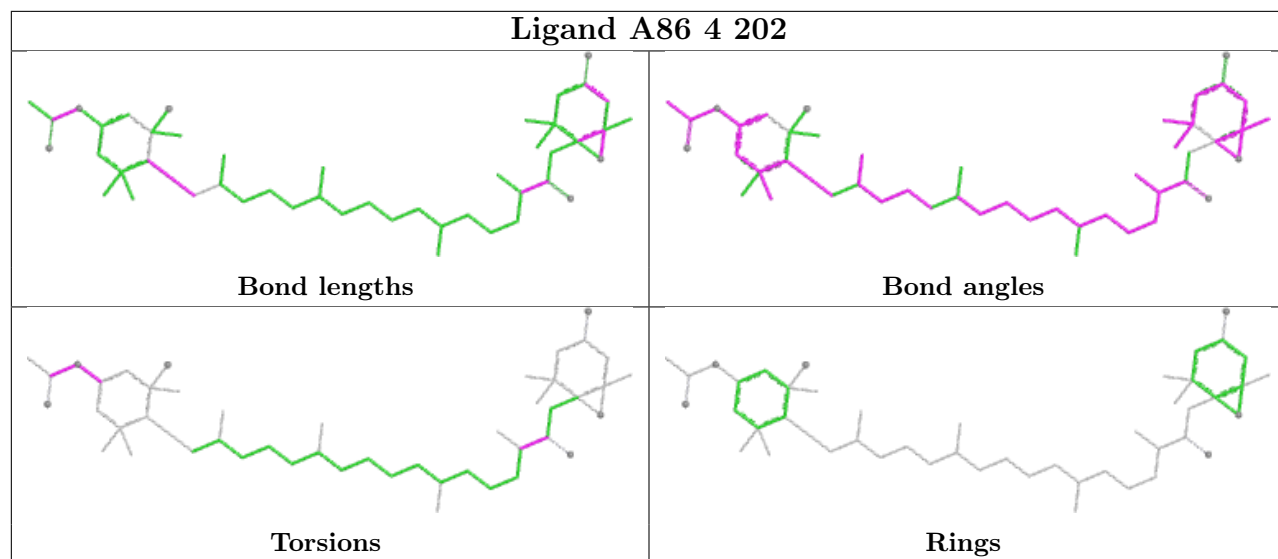
Bond angles



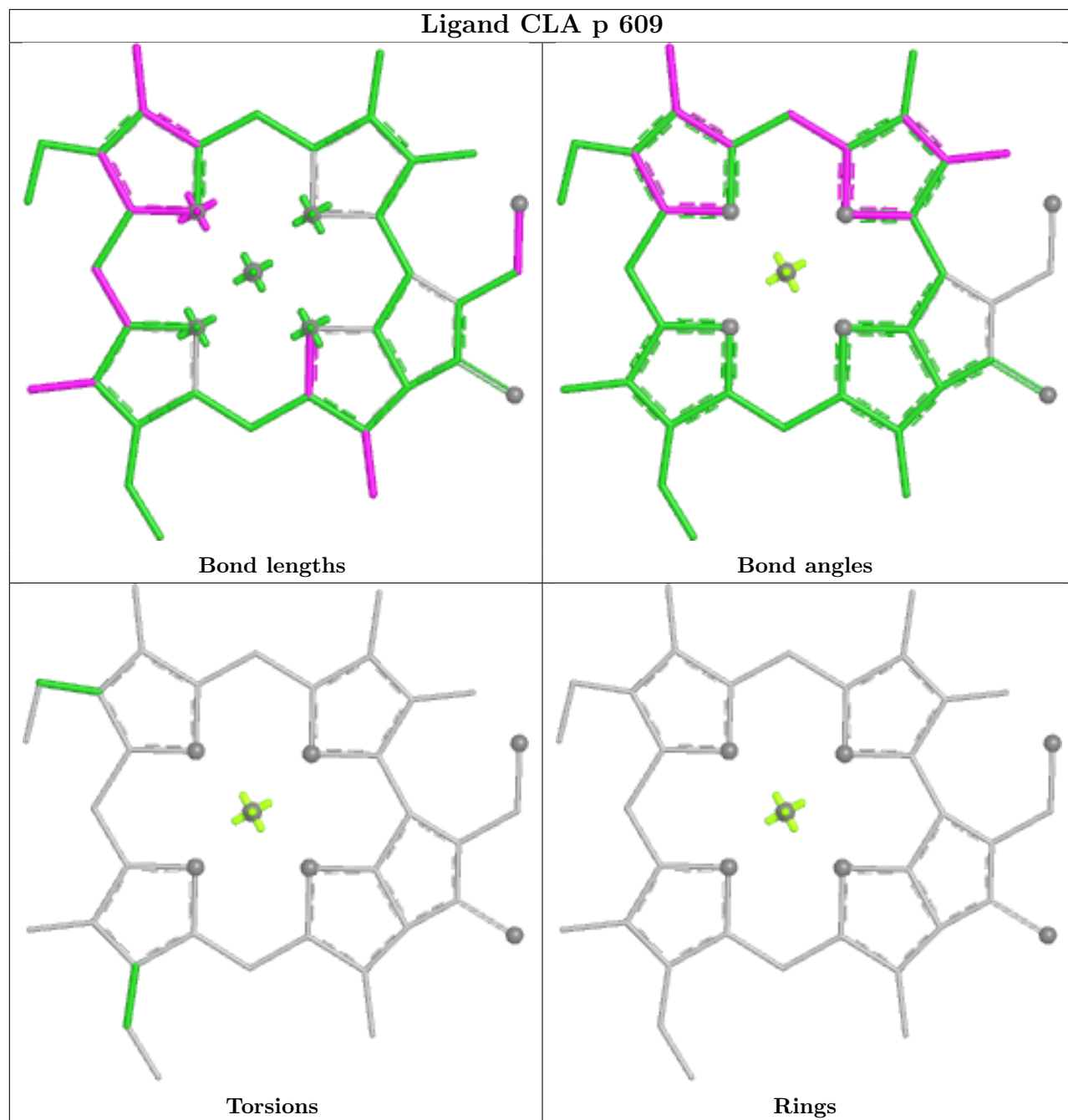
Torsions

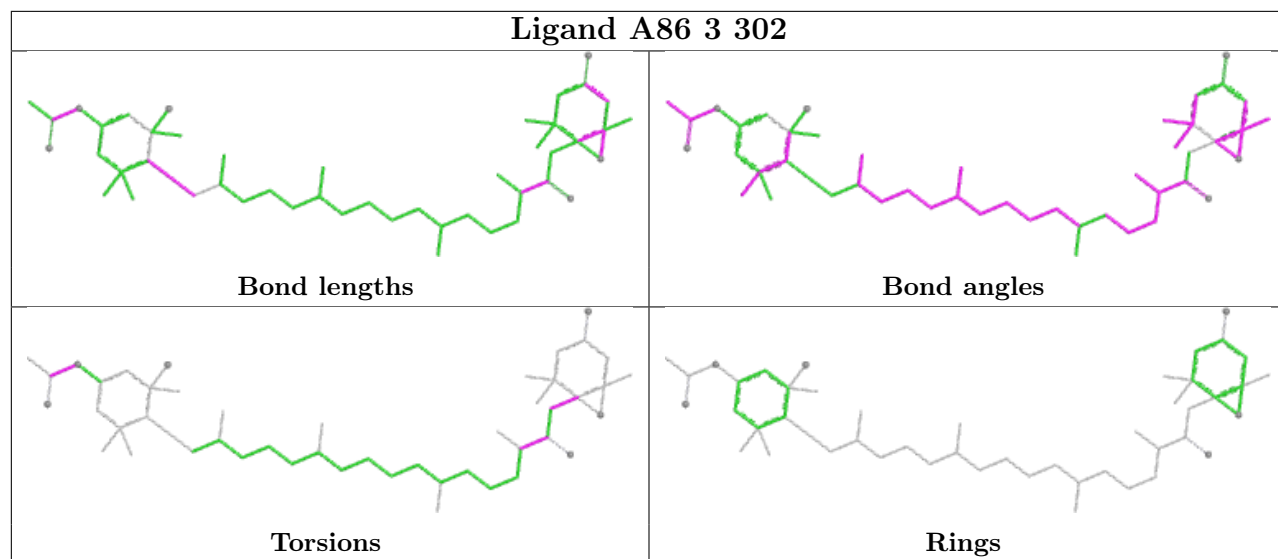


Rings

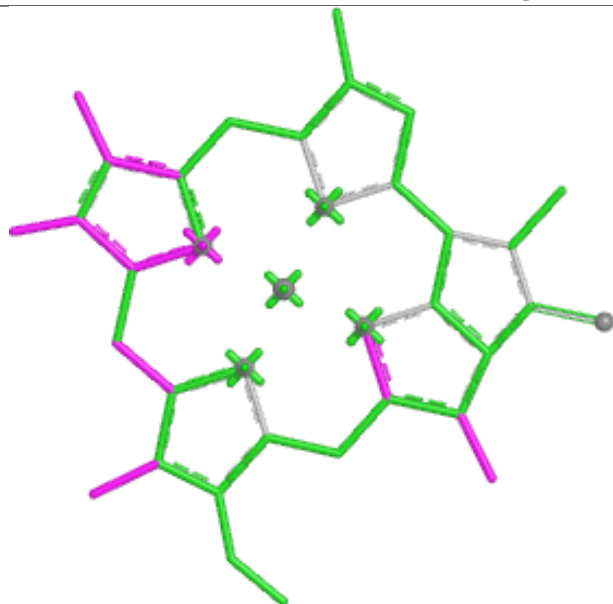


Ligand CLA p 609

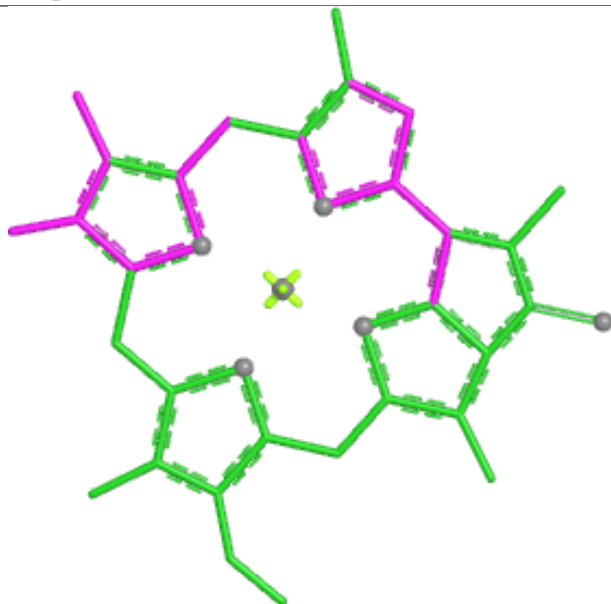




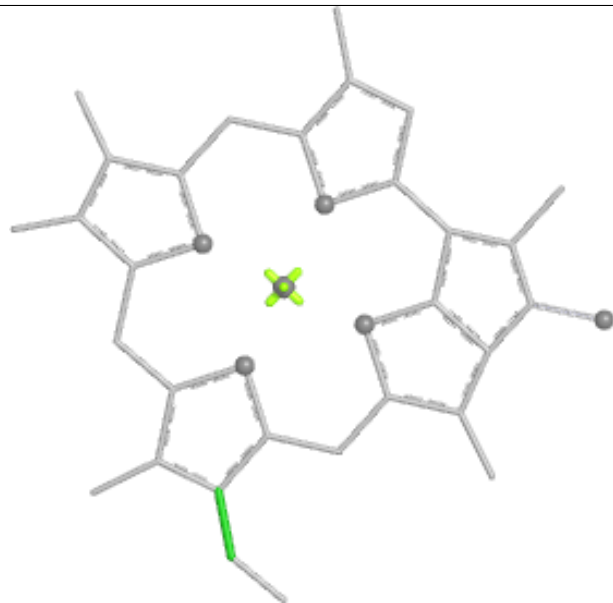
Ligand CLA p 607



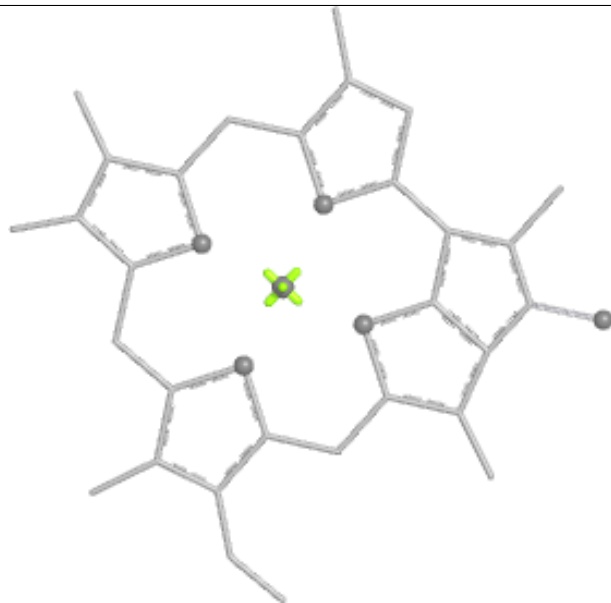
Bond lengths



Bond angles

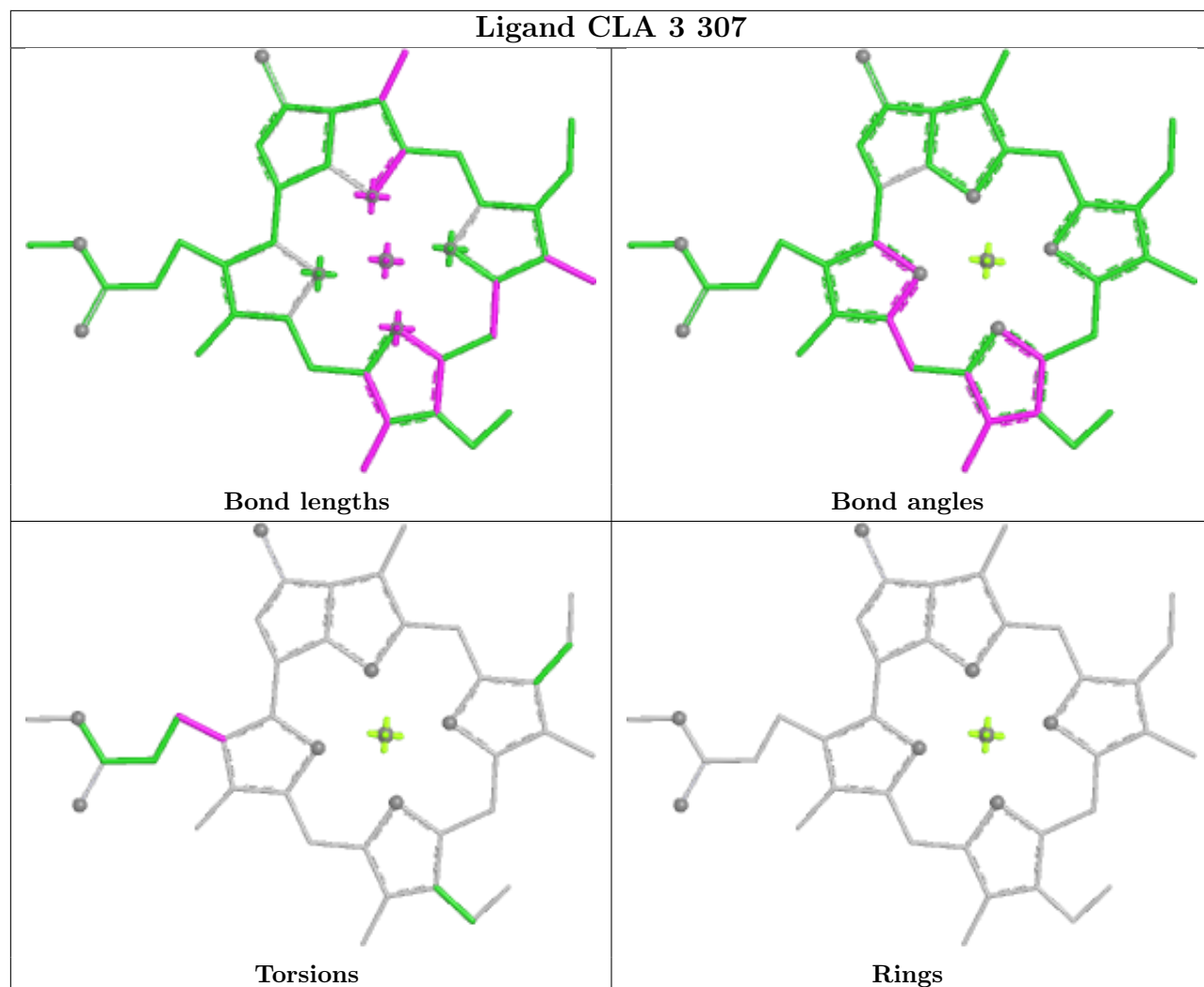


Torsions

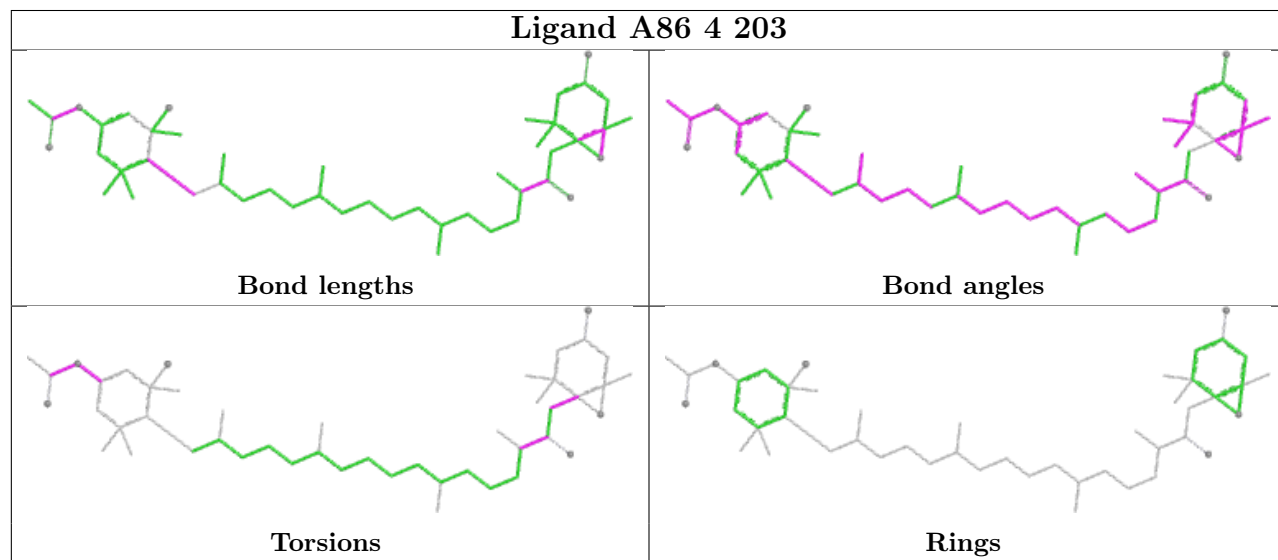


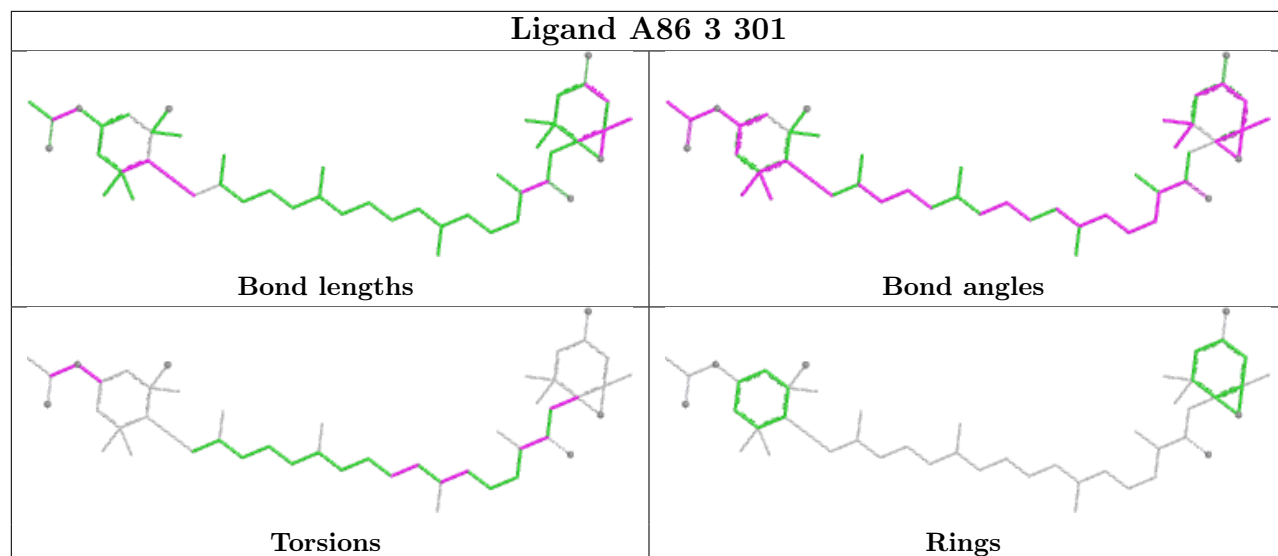
Rings

Ligand CLA 3 307

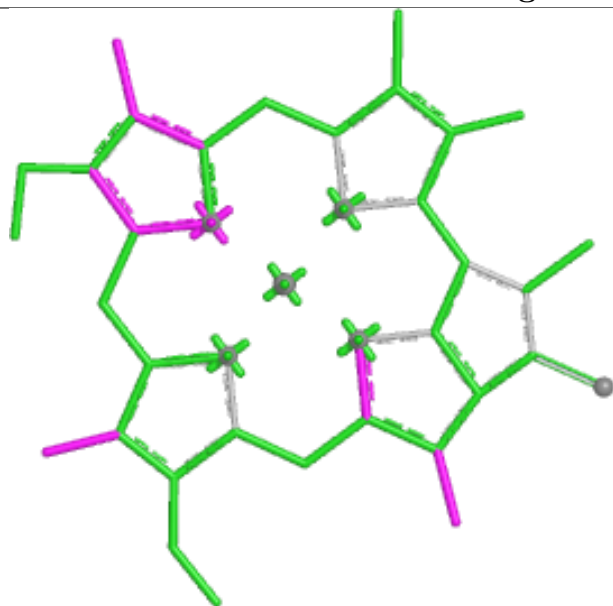


Ligand A86 4 203

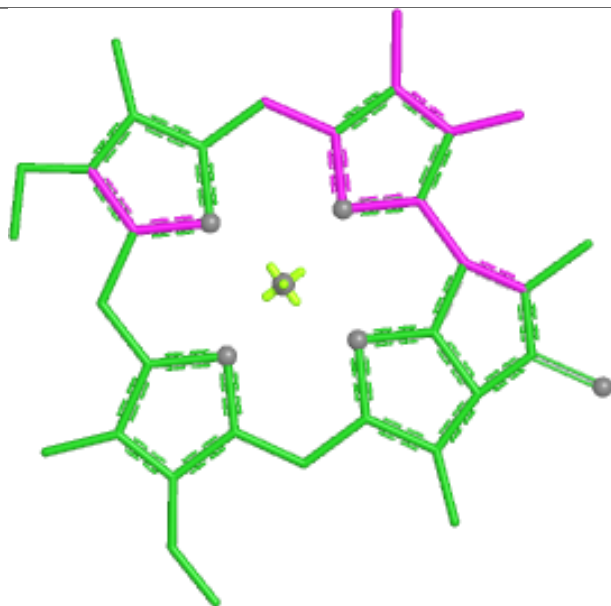




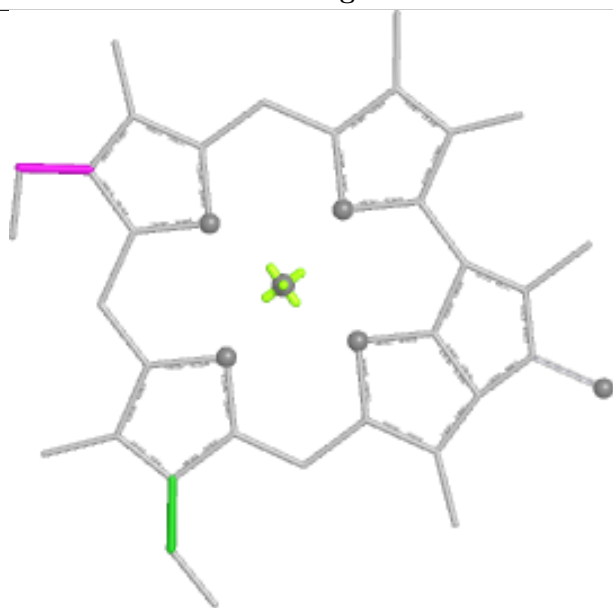
Ligand CLA 4 207



Bond lengths



Bond angles

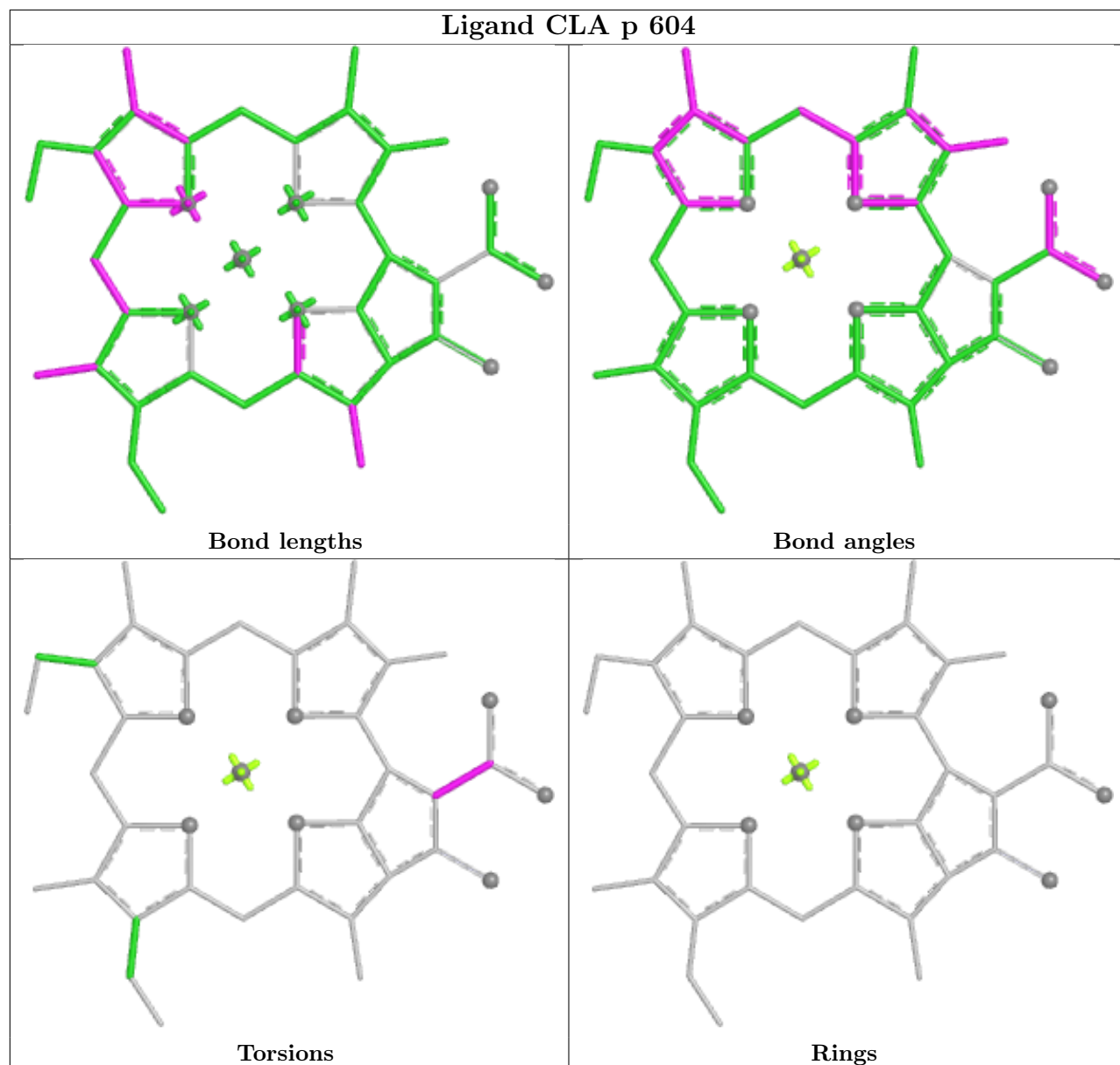


Torsions

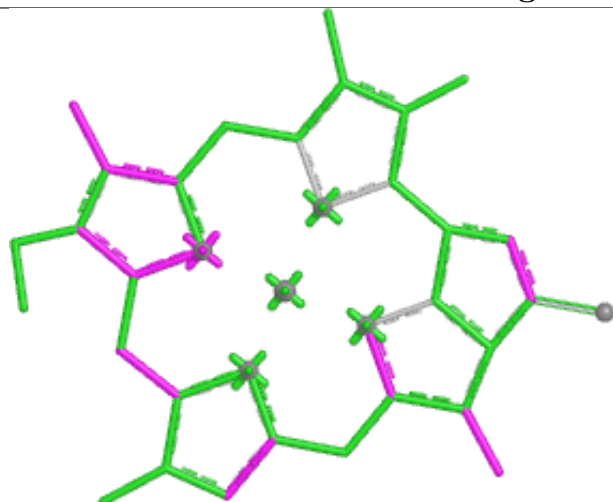


Rings

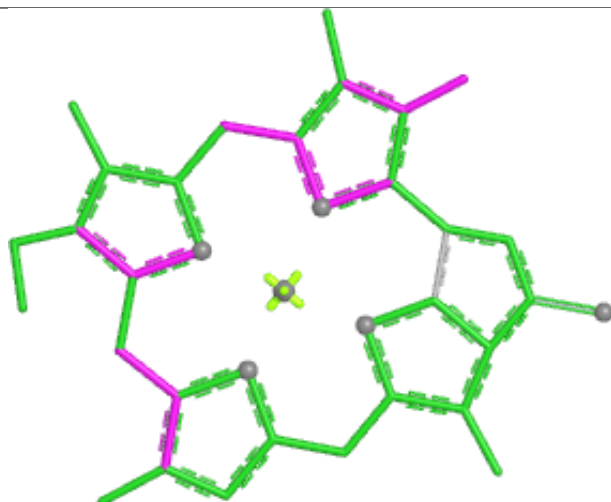
Ligand CLA p 604



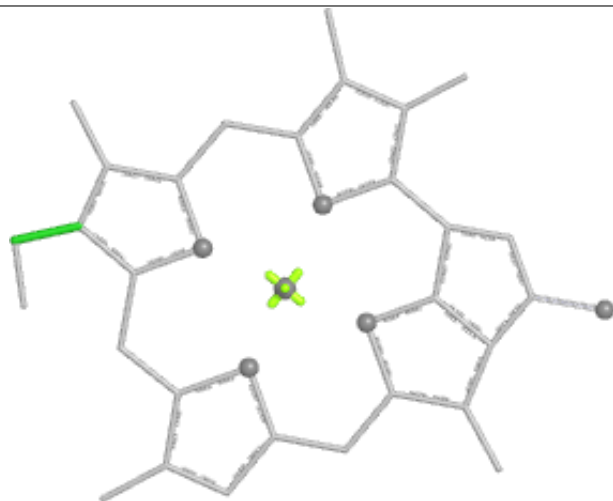
Ligand CLA 3 310



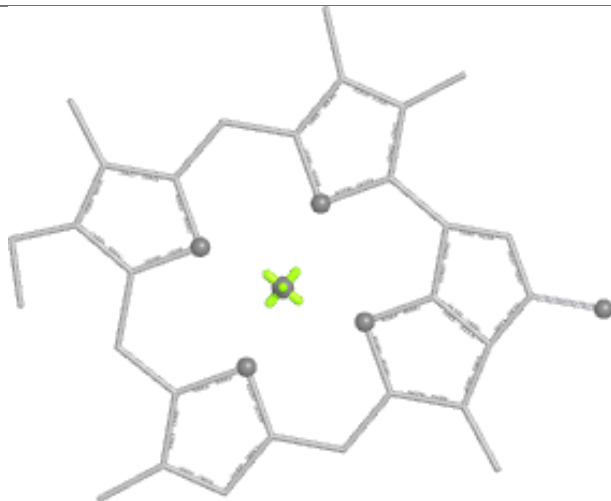
Bond lengths



Bond angles

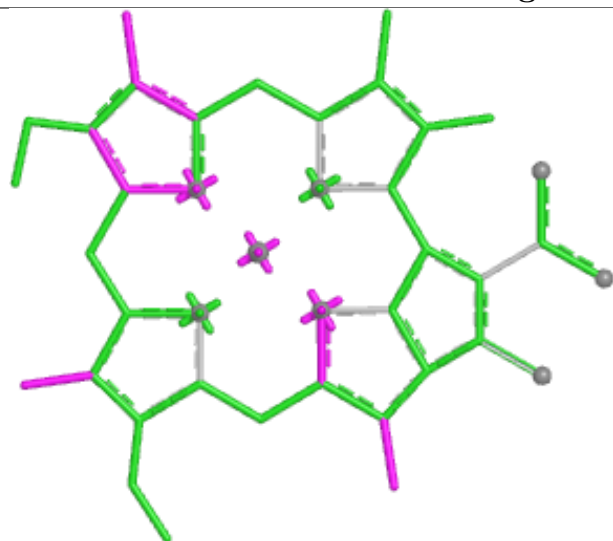


Torsions

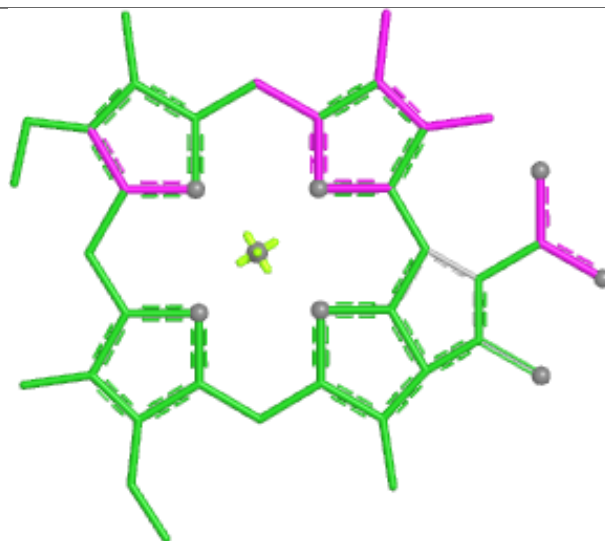


Rings

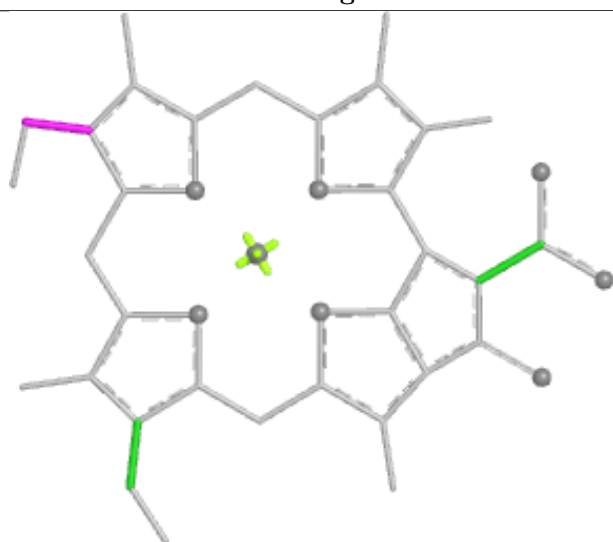
Ligand CLA 3 311



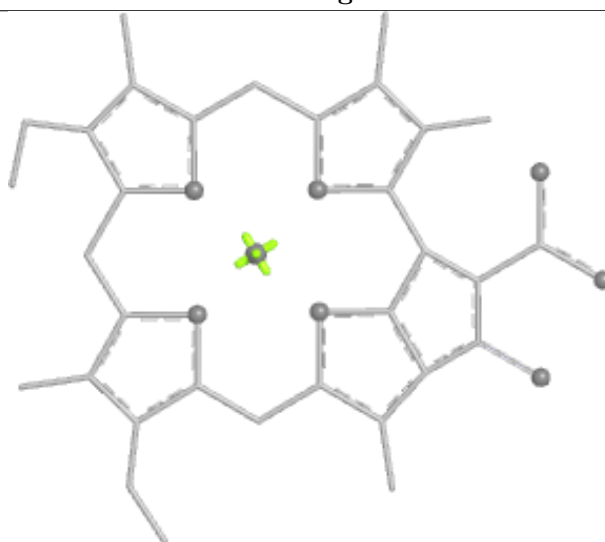
Bond lengths



Bond angles

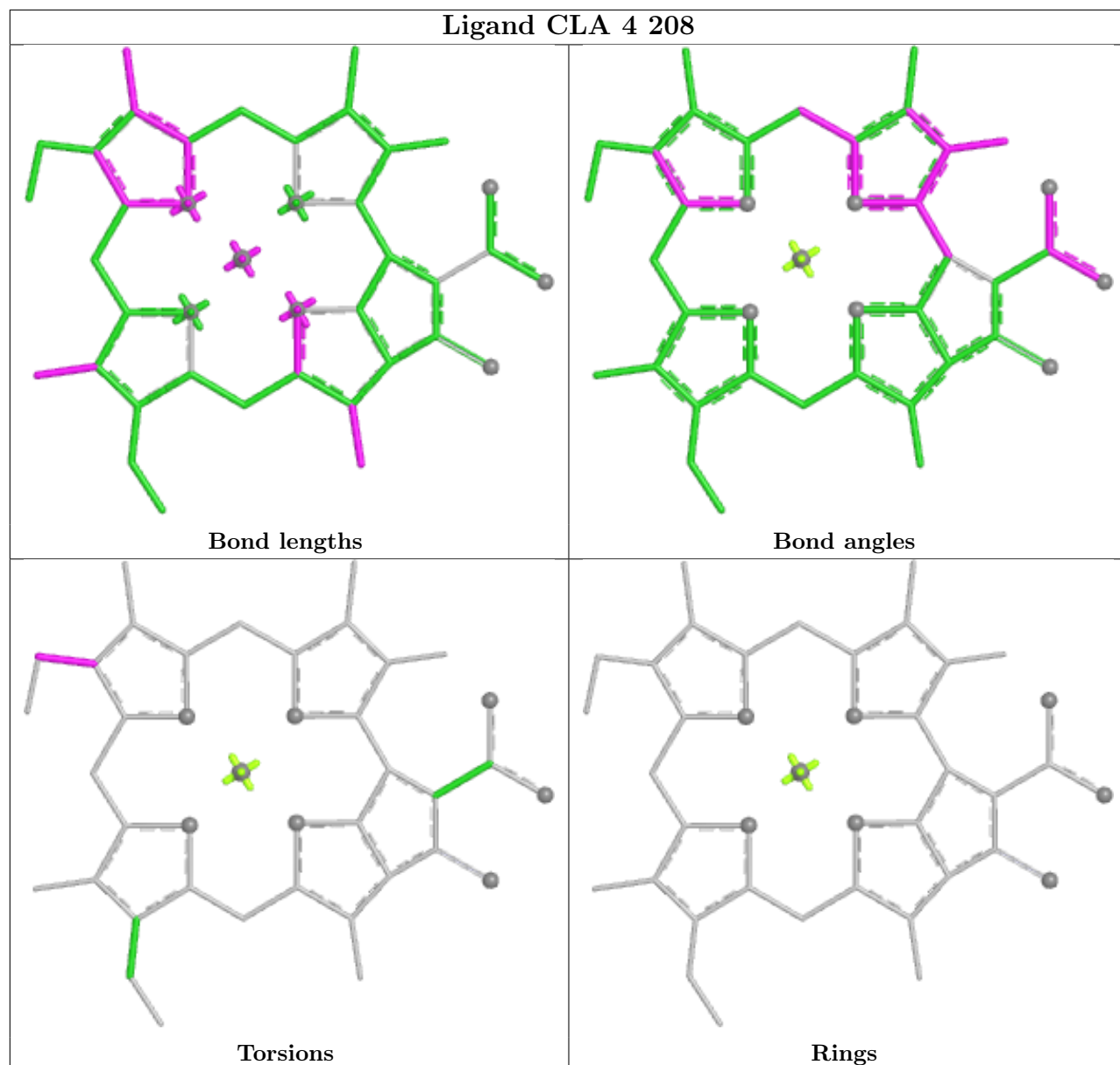


Torsions

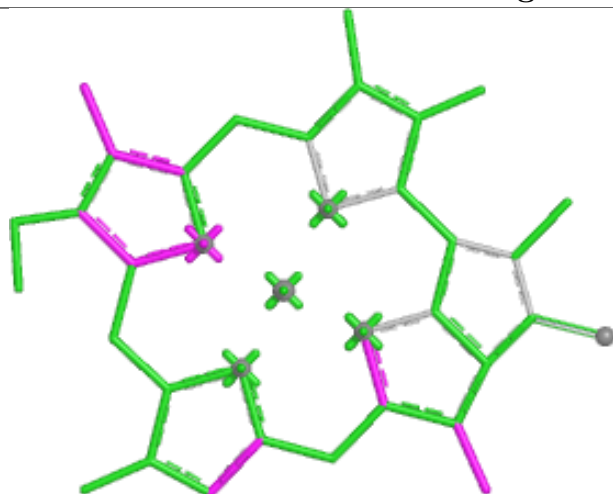


Rings

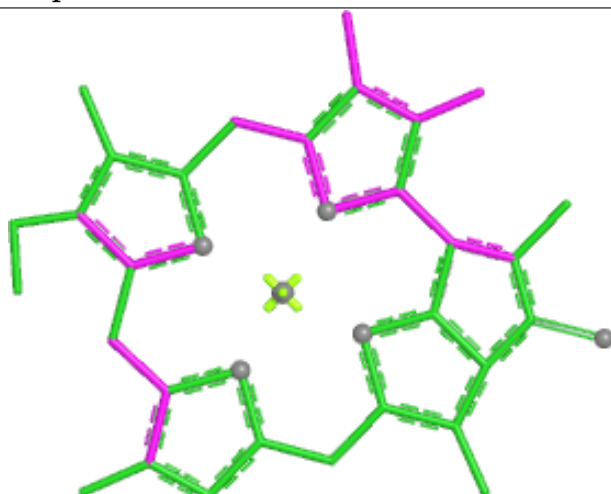
Ligand CLA 4 208



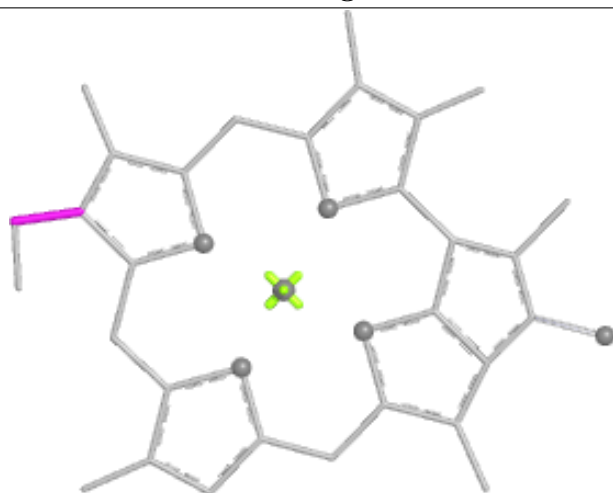
Ligand CLA p 601



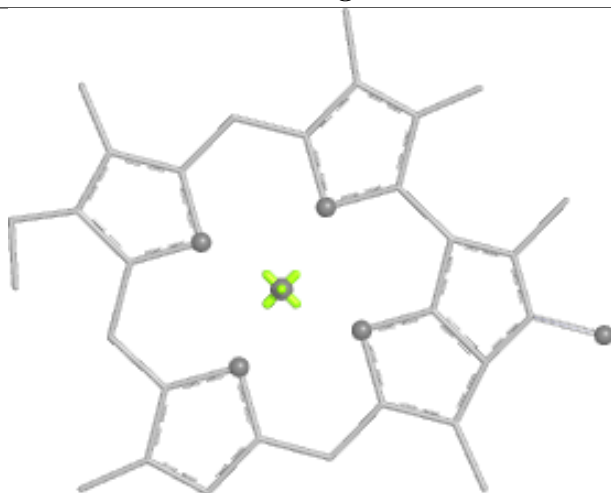
Bond lengths



Bond angles

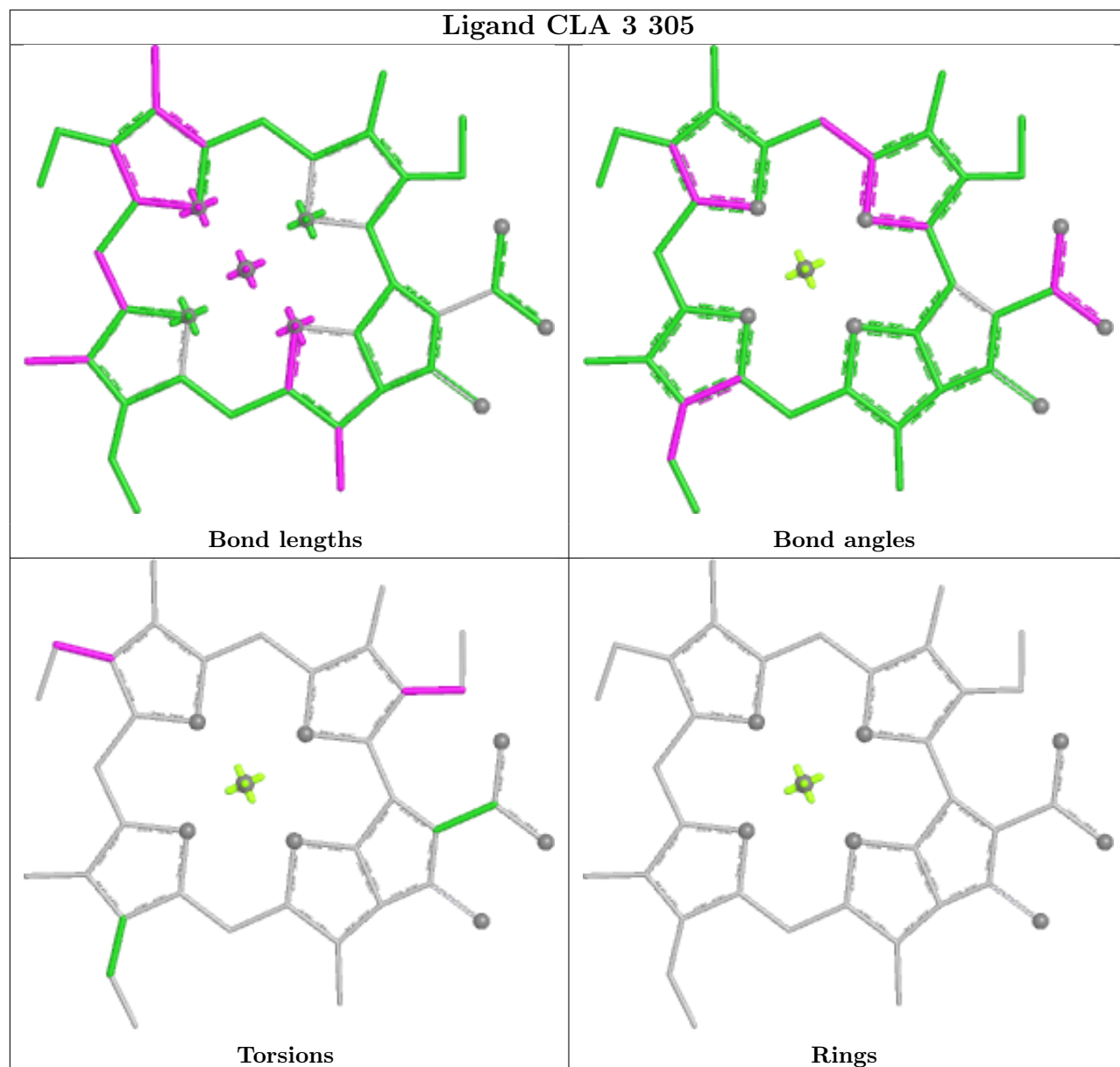


Torsions

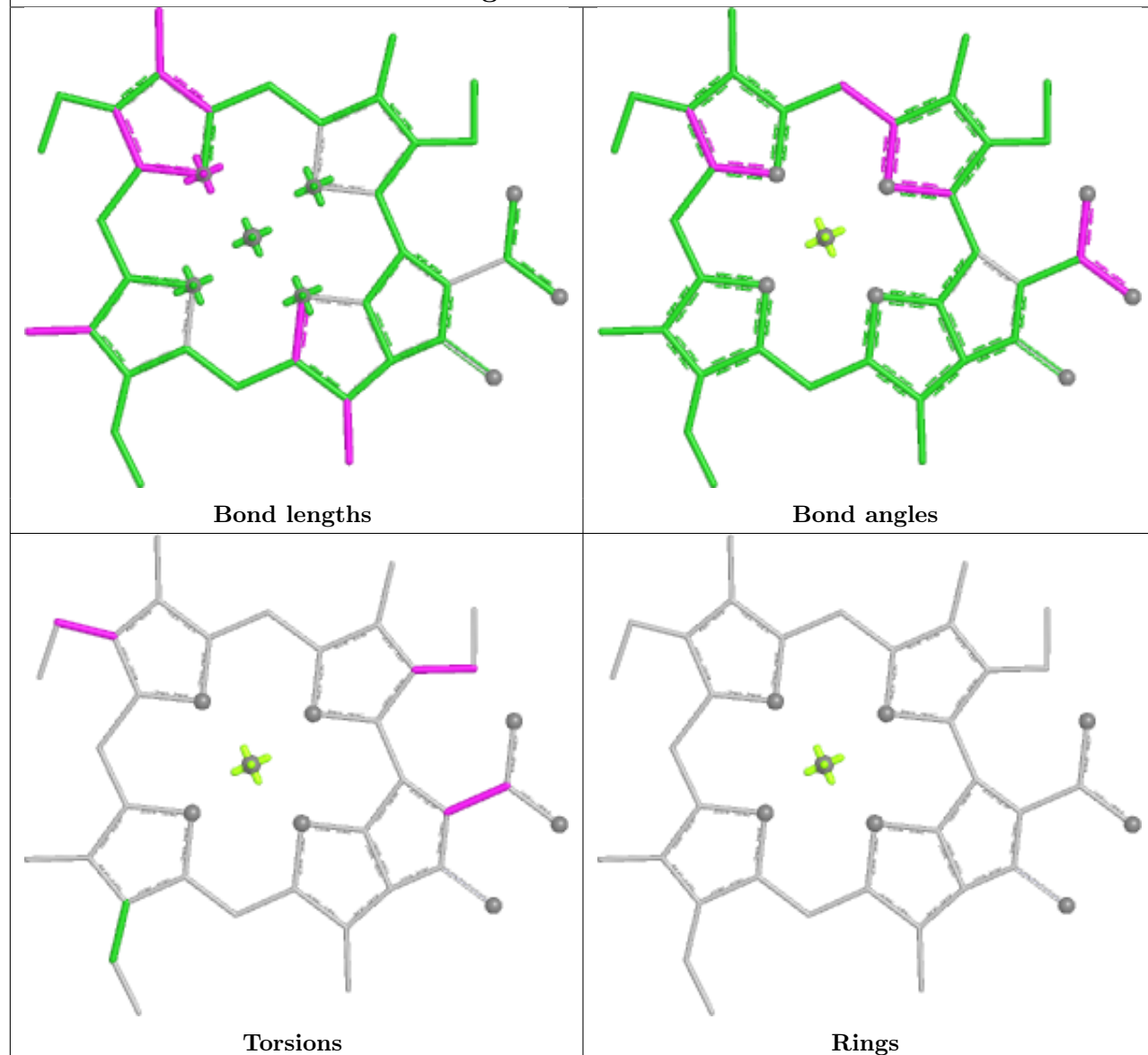


Rings

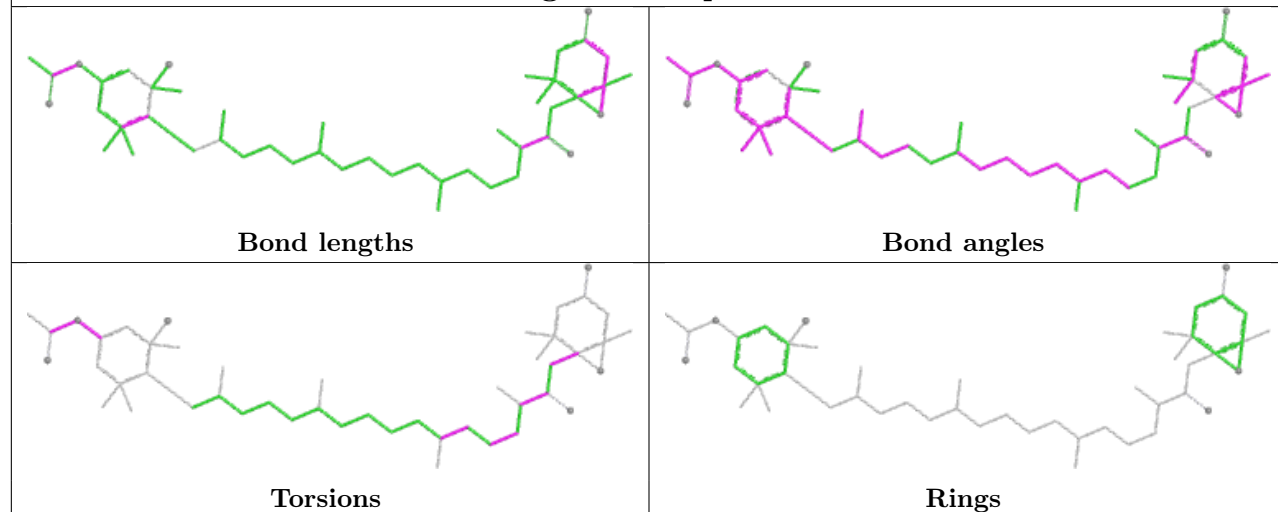
Ligand CLA 3 305



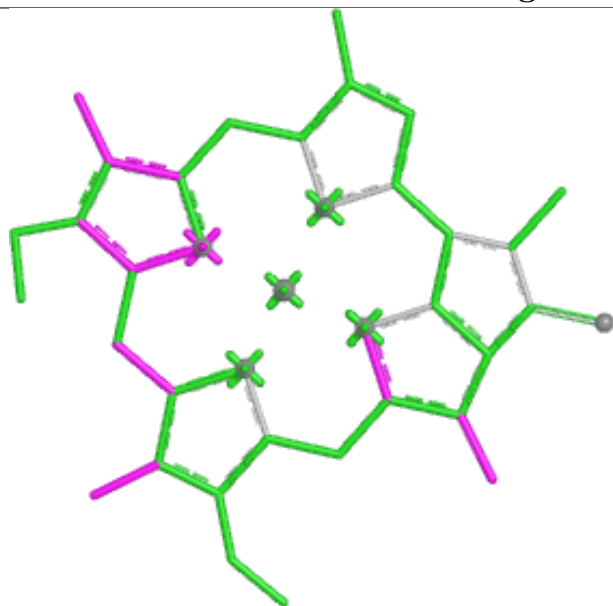
Ligand CLA 3 312



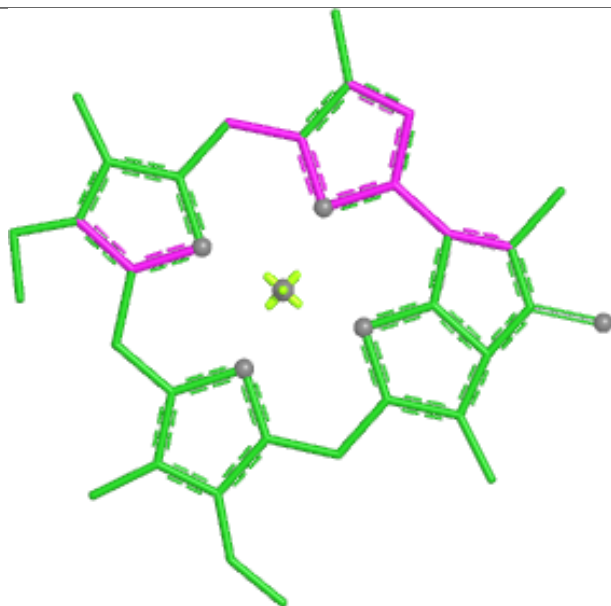
Ligand A86 p 610



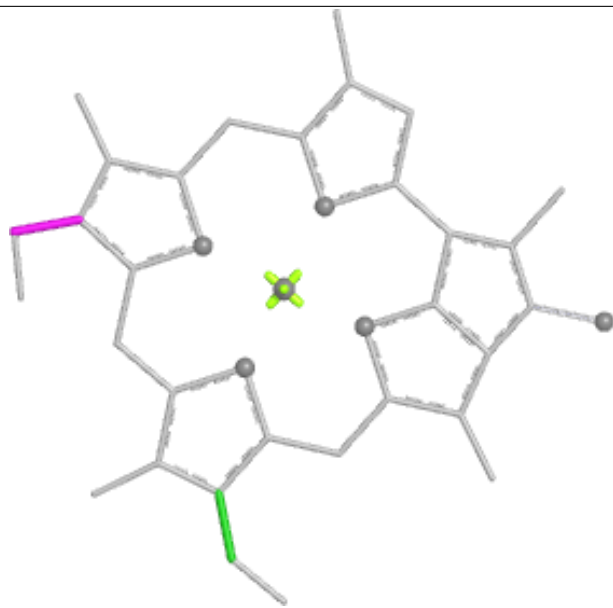
Ligand CLA 4 206



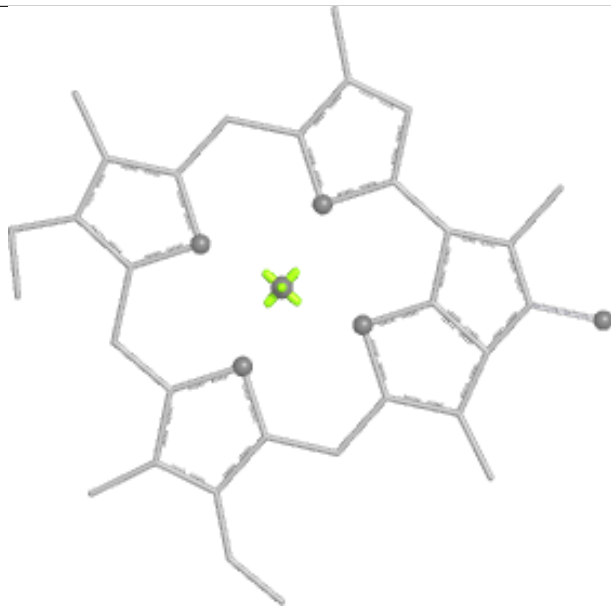
Bond lengths



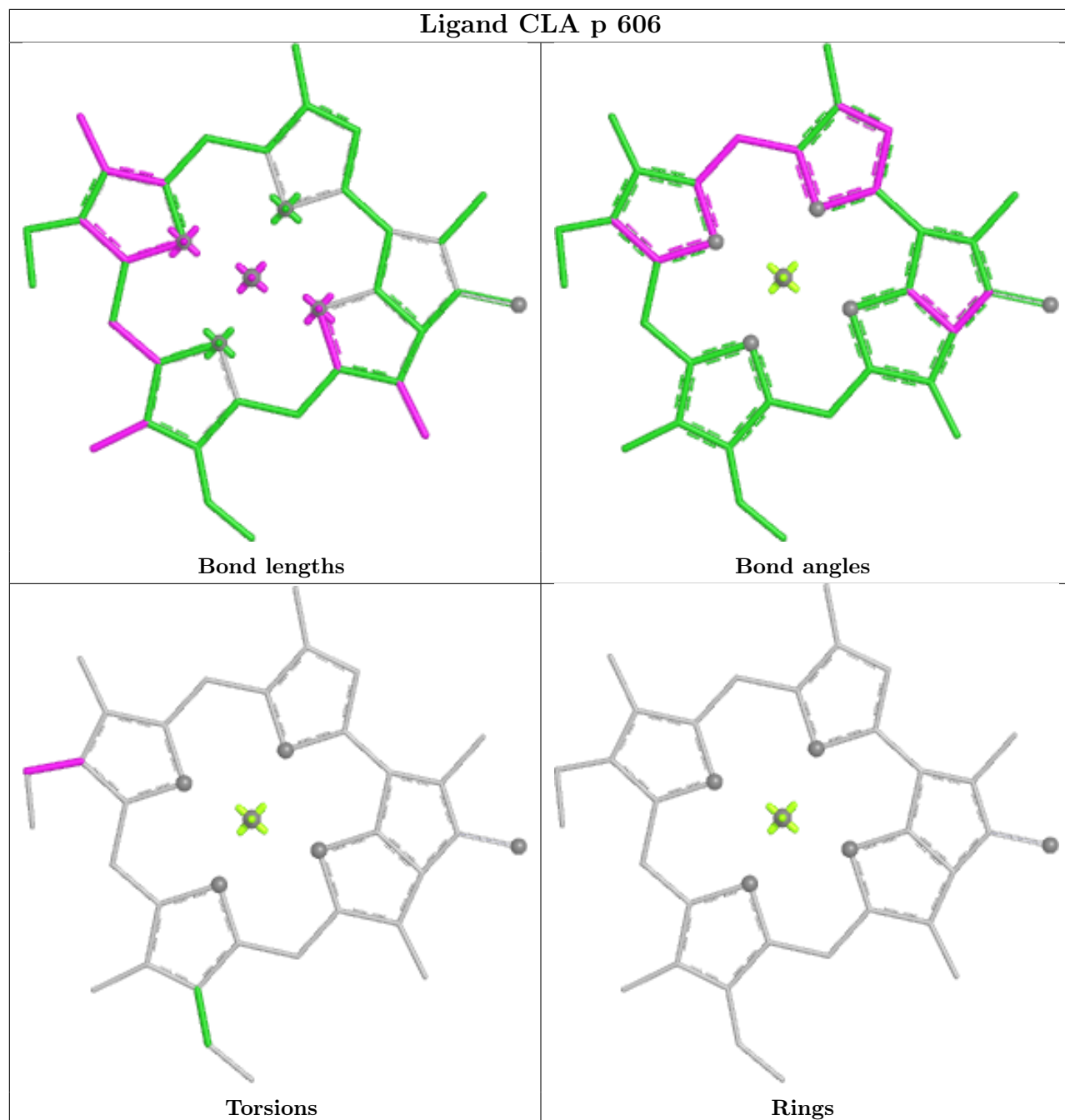
Bond angles



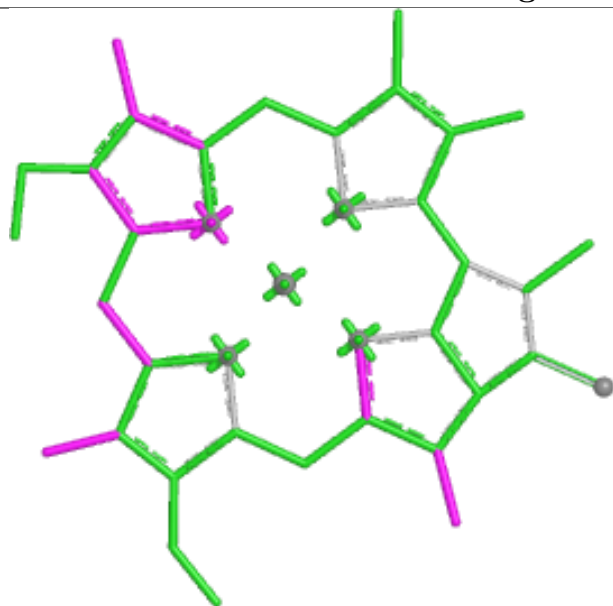
Torsions



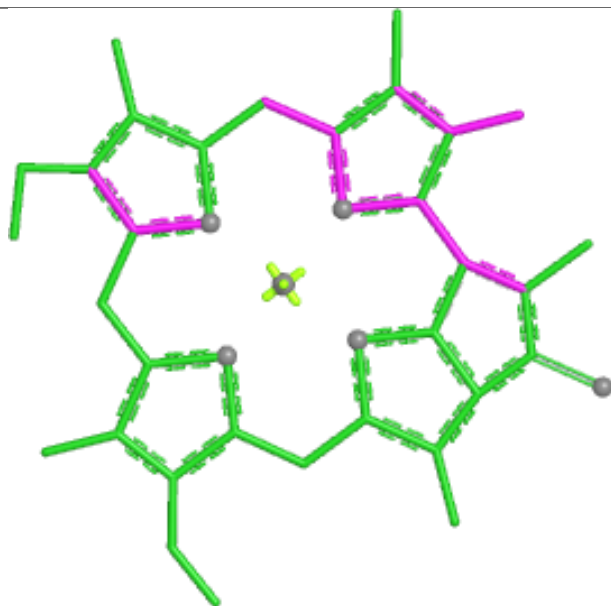
Rings



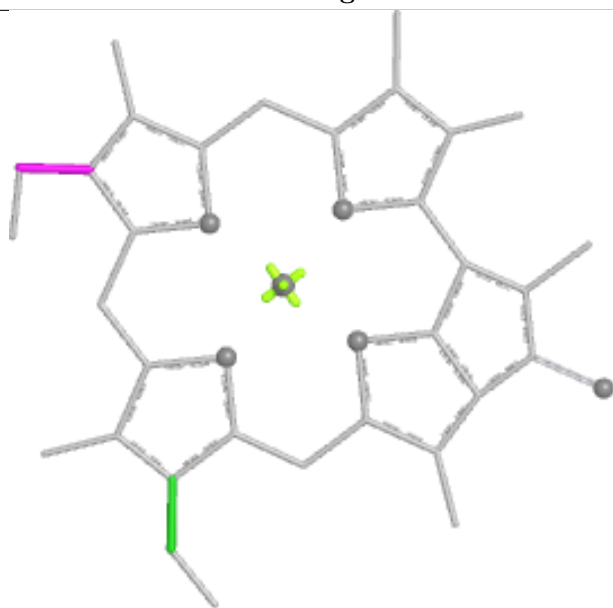
Ligand CLA 4 204



Bond lengths



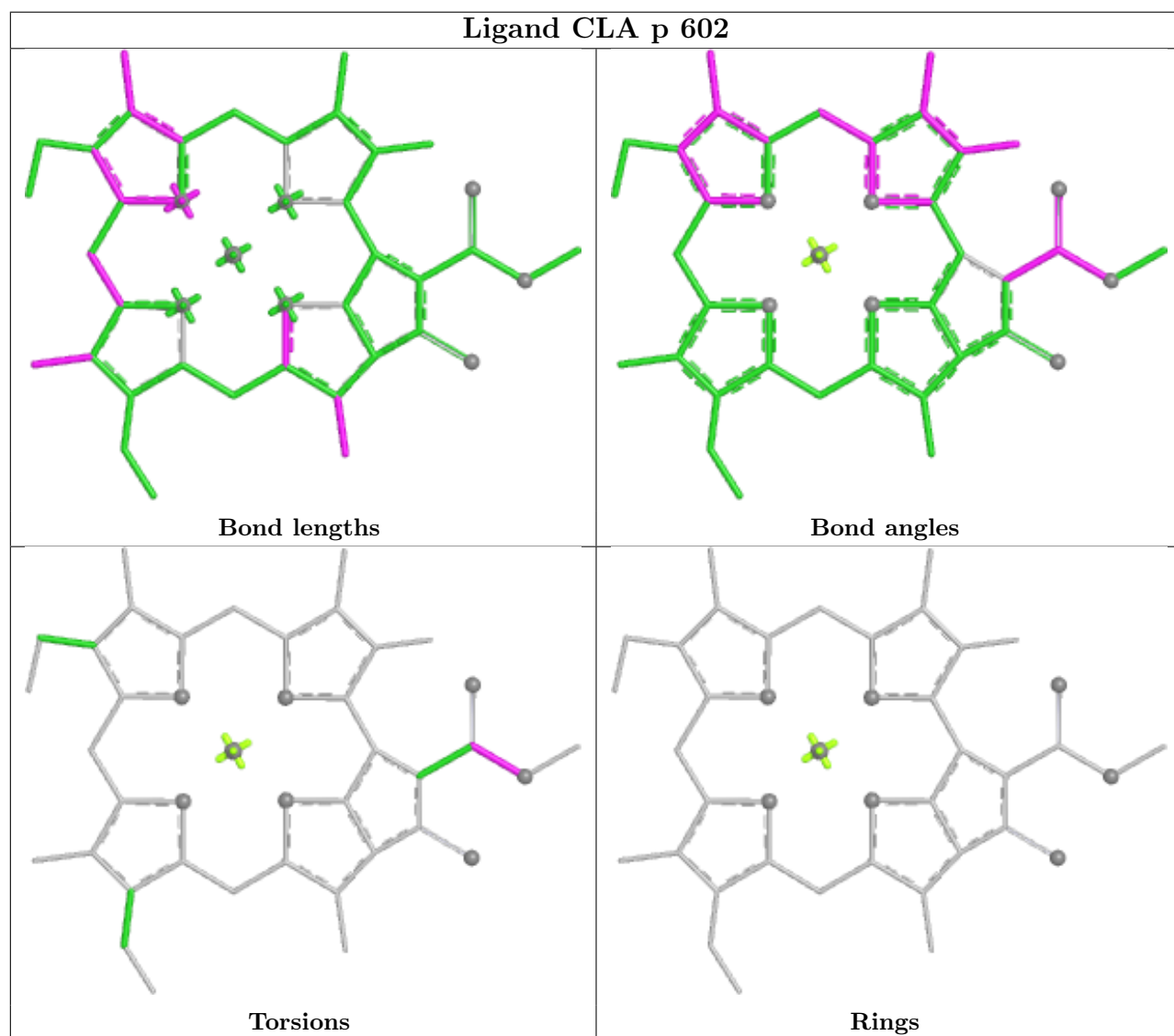
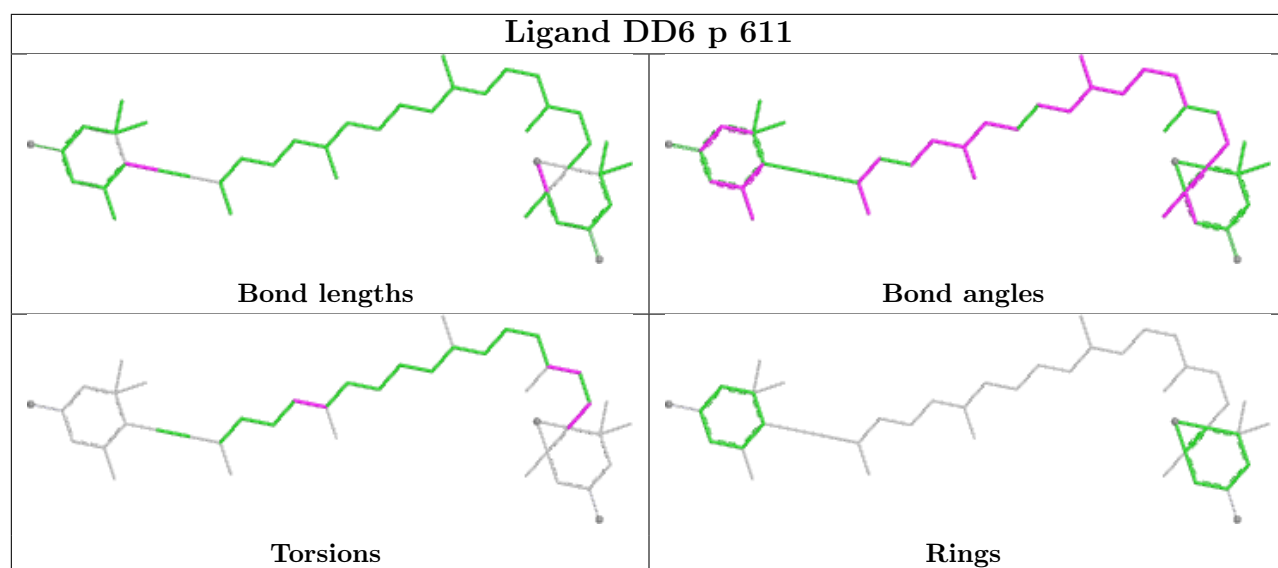
Bond angles



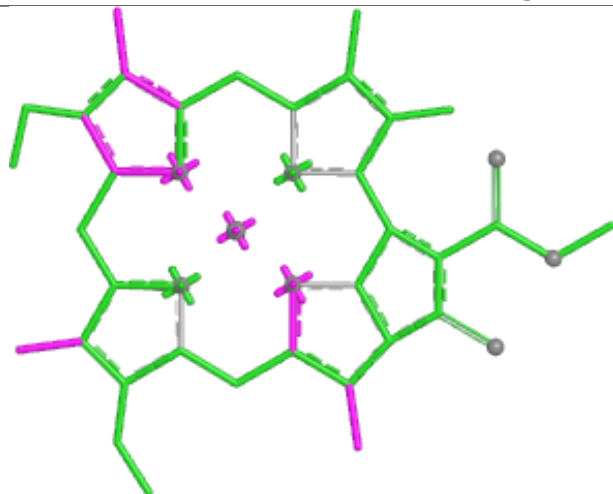
Torsions



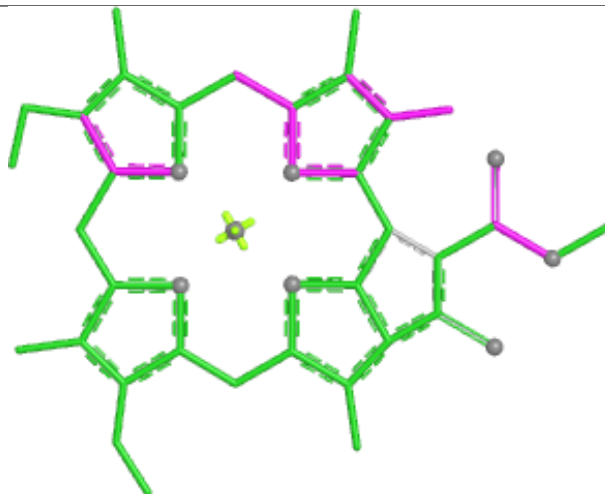
Rings



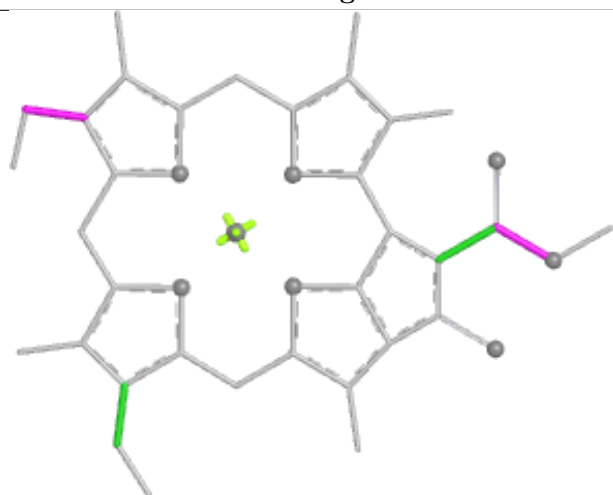
Ligand CLA 4 209



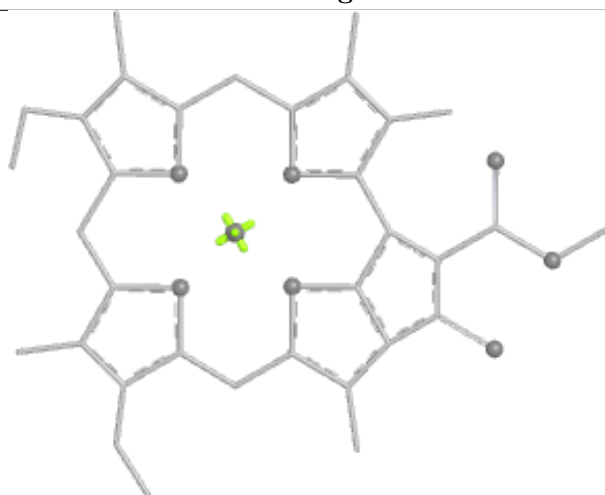
Bond lengths



Bond angles

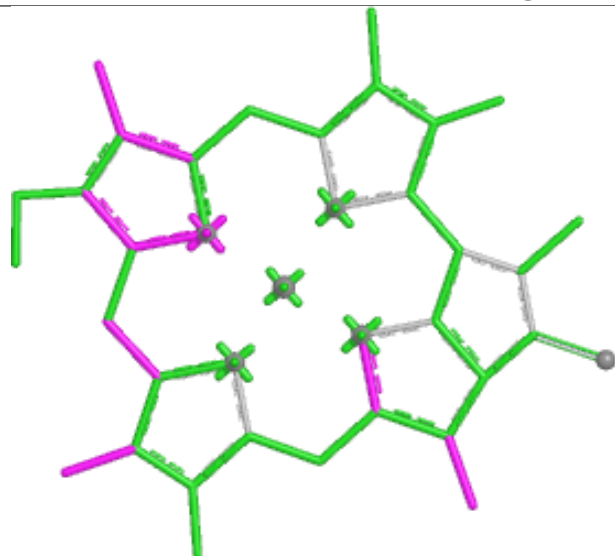


Torsions

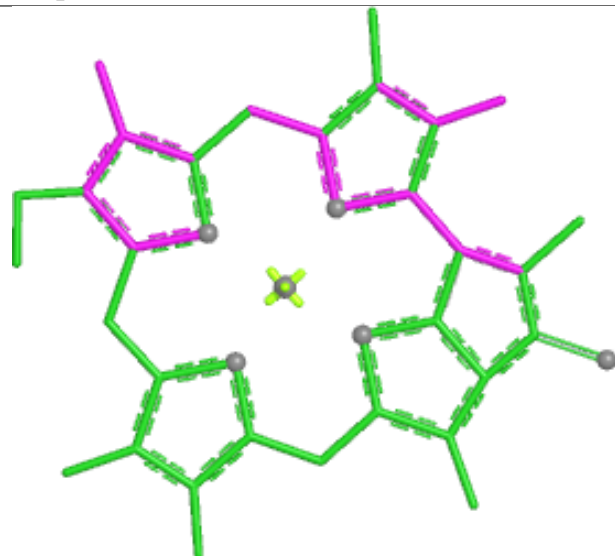


Rings

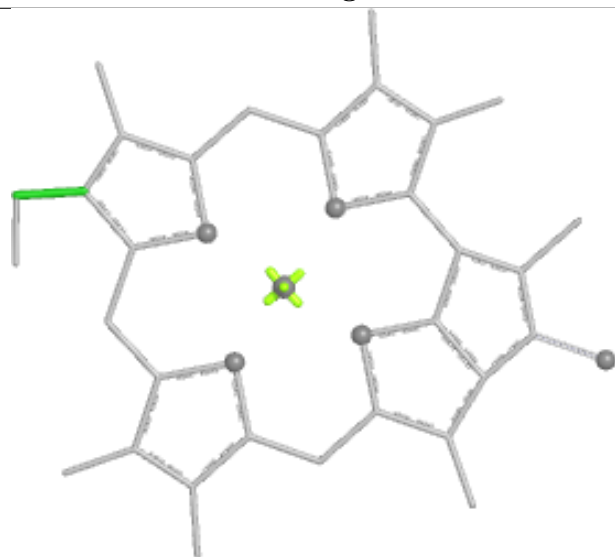
Ligand CLA p 603



Bond lengths



Bond angles

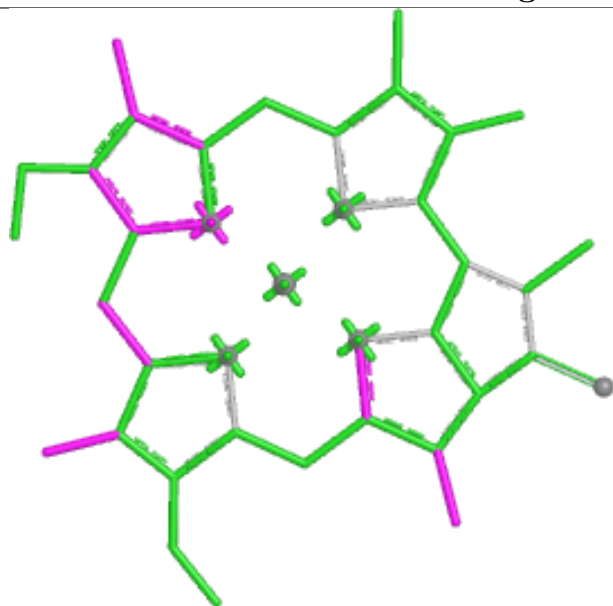


Torsions

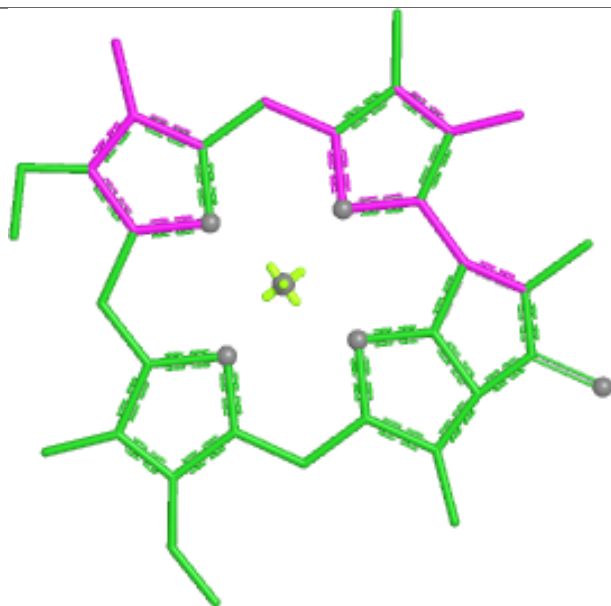


Rings

Ligand CLA 4 210



Bond lengths



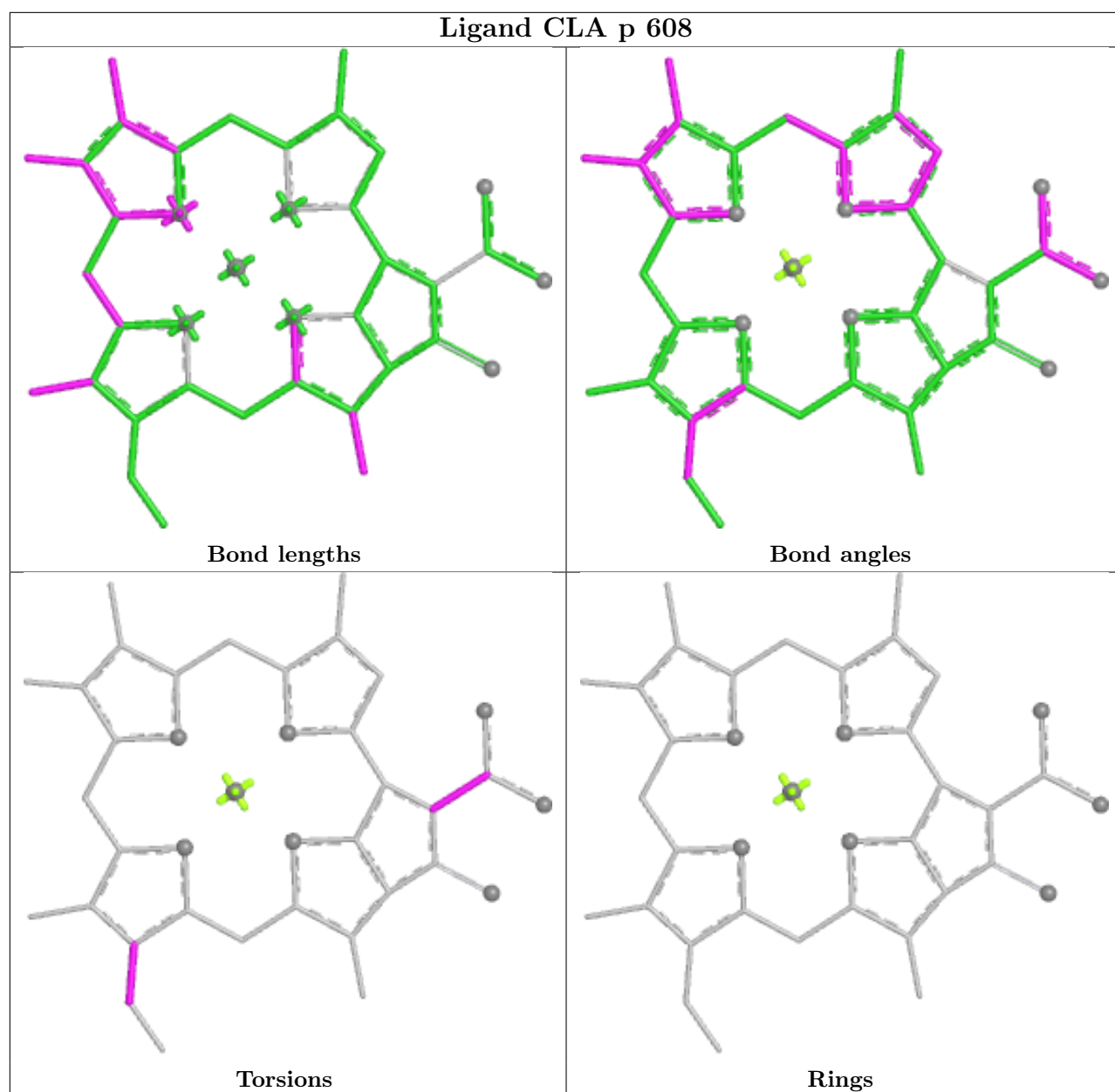
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

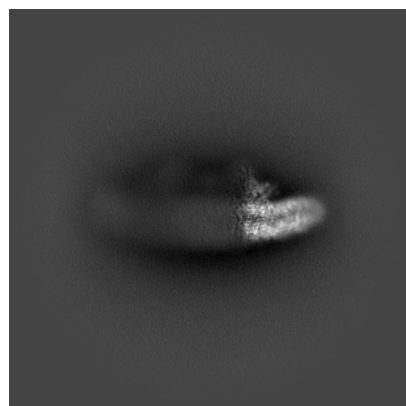
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37268. These allow visual inspection of the internal detail of the map and identification of artifacts.

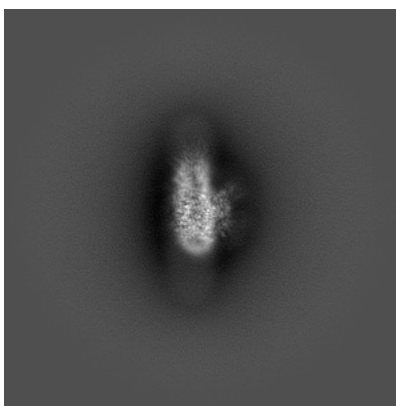
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

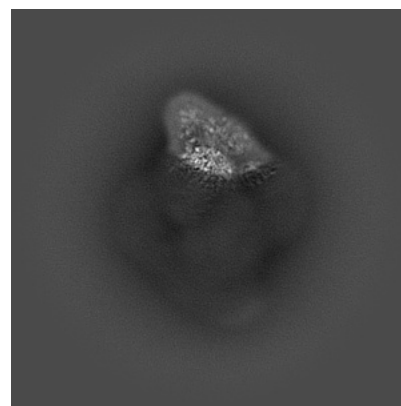
6.1.1 Primary map



X

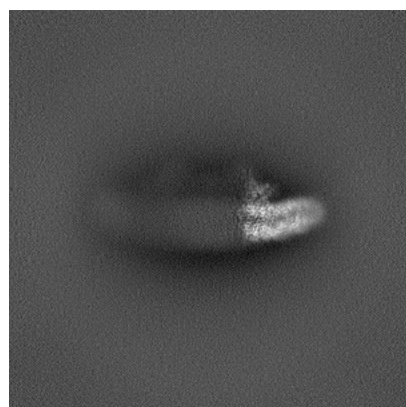


Y

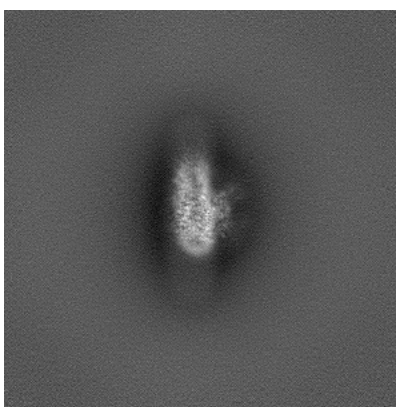


Z

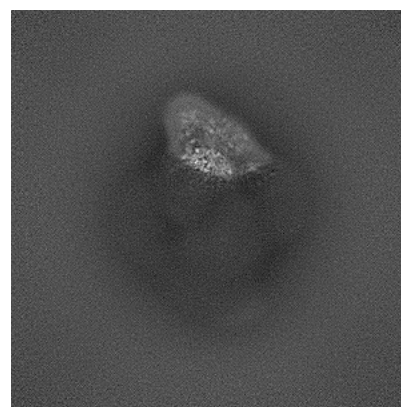
6.1.2 Raw map



X



Y

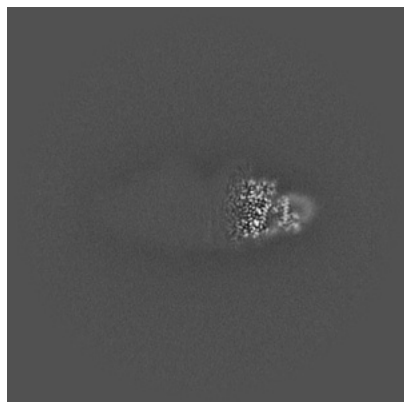


Z

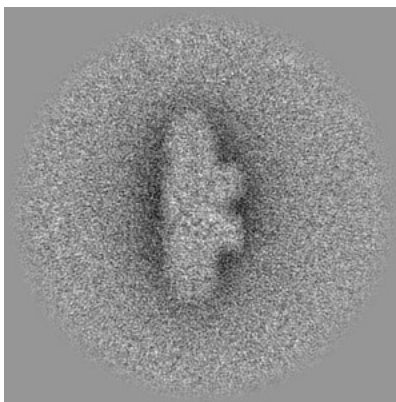
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

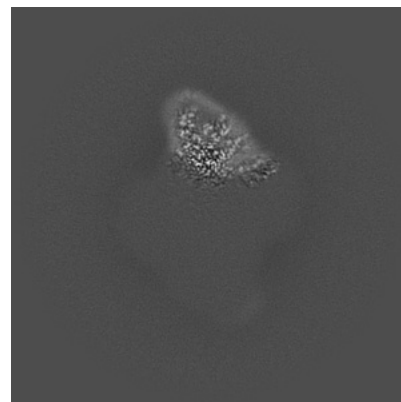
6.2.1 Primary map



X Index: 256



Y Index: 256

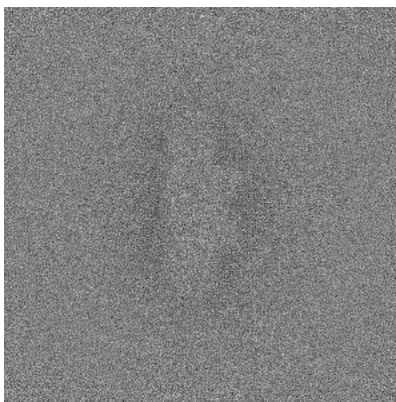


Z Index: 256

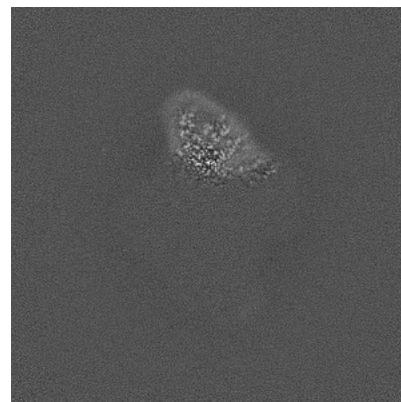
6.2.2 Raw map



X Index: 256



Y Index: 256

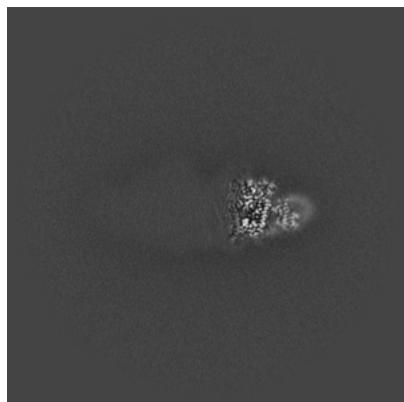


Z Index: 256

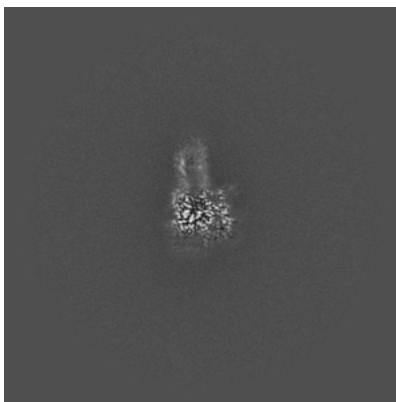
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

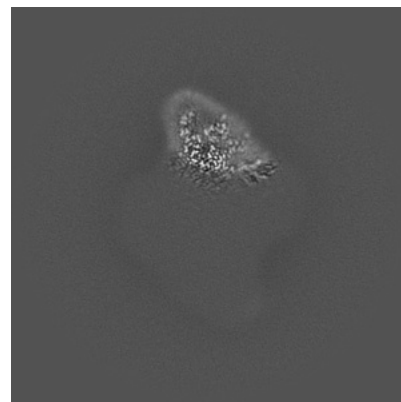
6.3.1 Primary map



X Index: 258

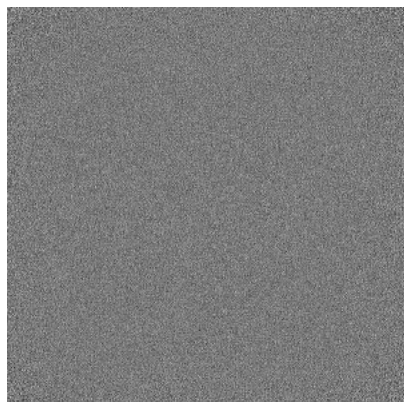


Y Index: 317

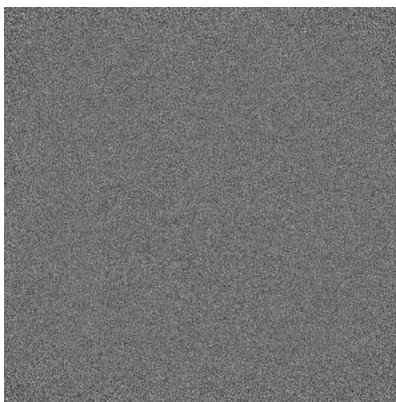


Z Index: 254

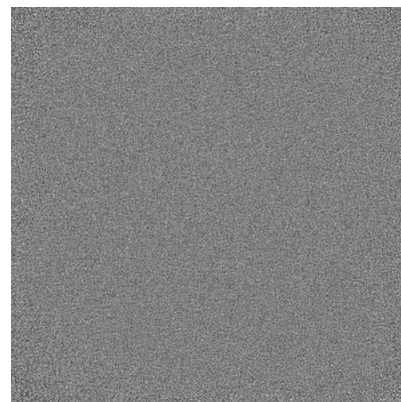
6.3.2 Raw map



X Index: 0



Y Index: 0

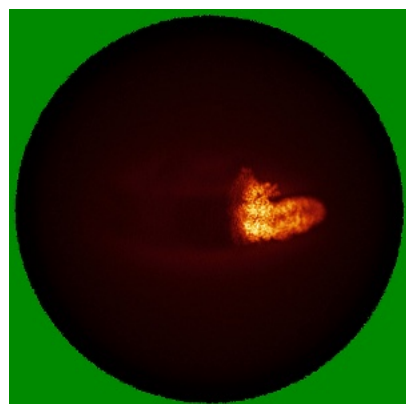


Z Index: 511

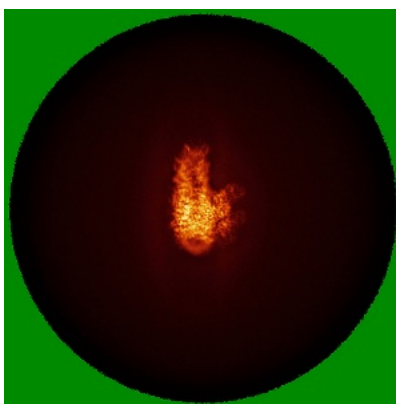
The images above show the largest variance slices of the map in three orthogonal directions.

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

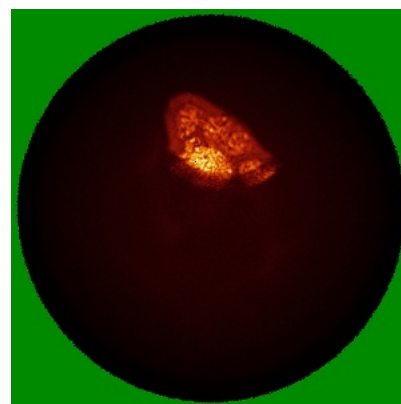
6.4.1 Primary map



X

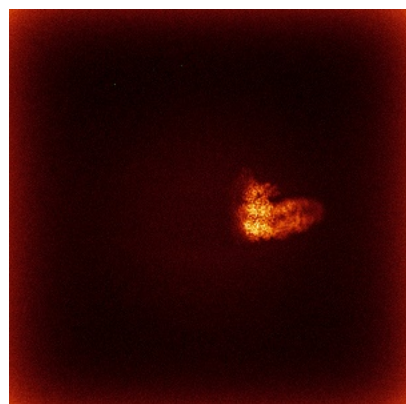


Y

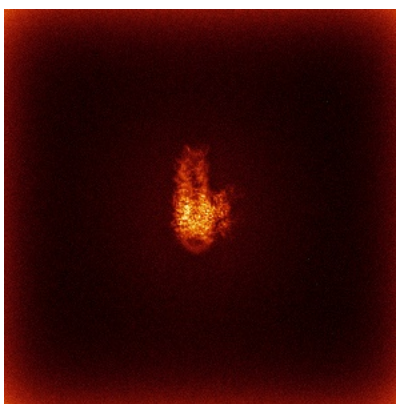


Z

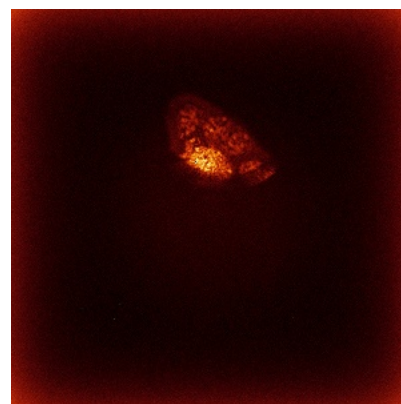
6.4.2 Raw map



X



Y

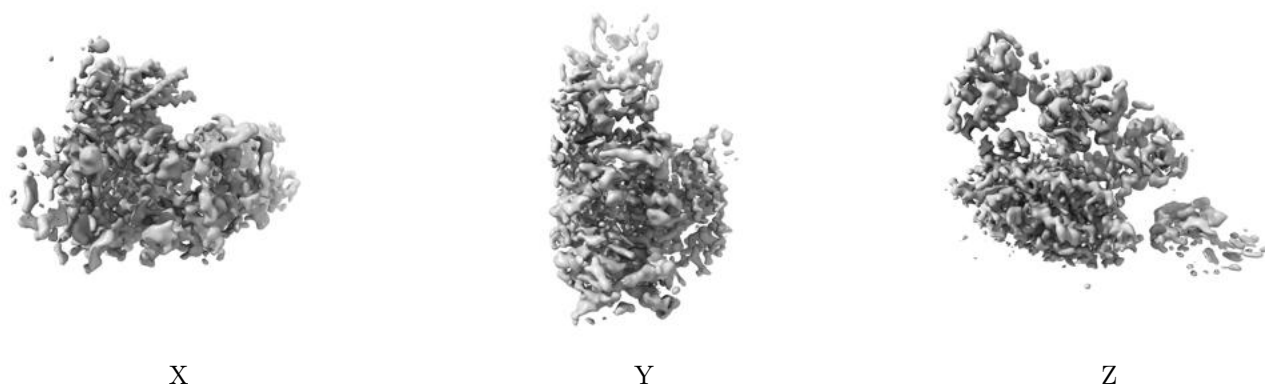


Z

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

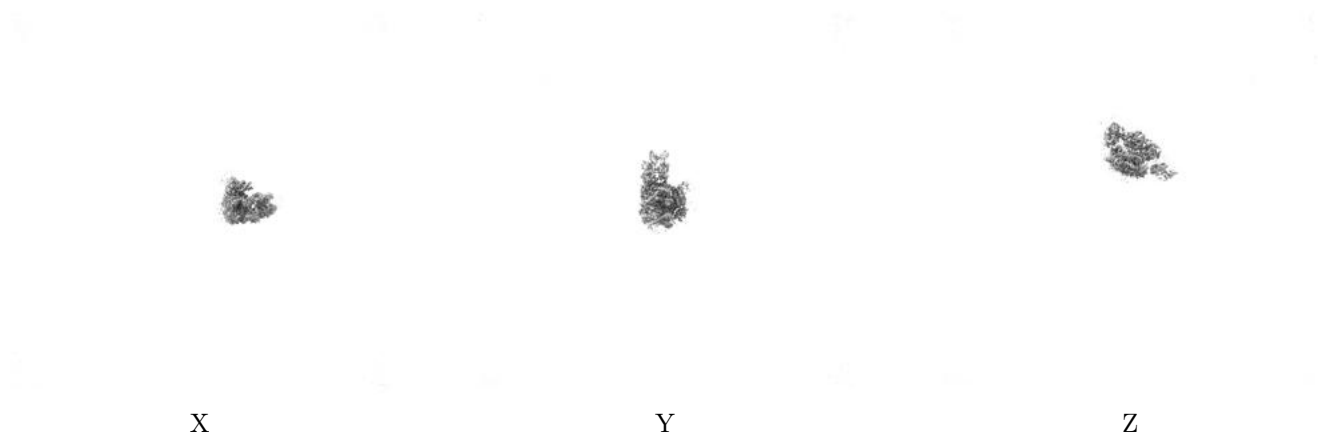
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.178. 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.

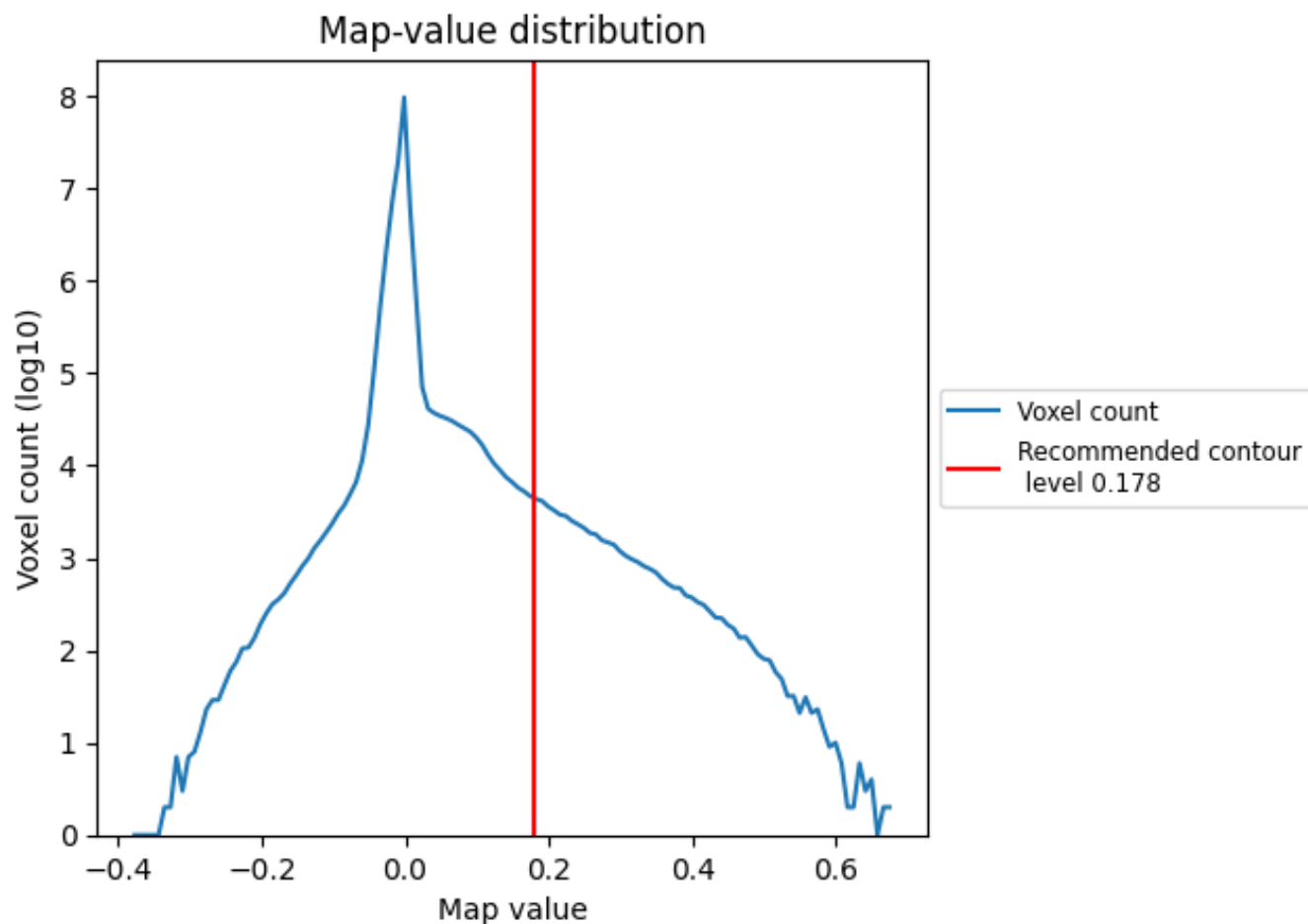
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

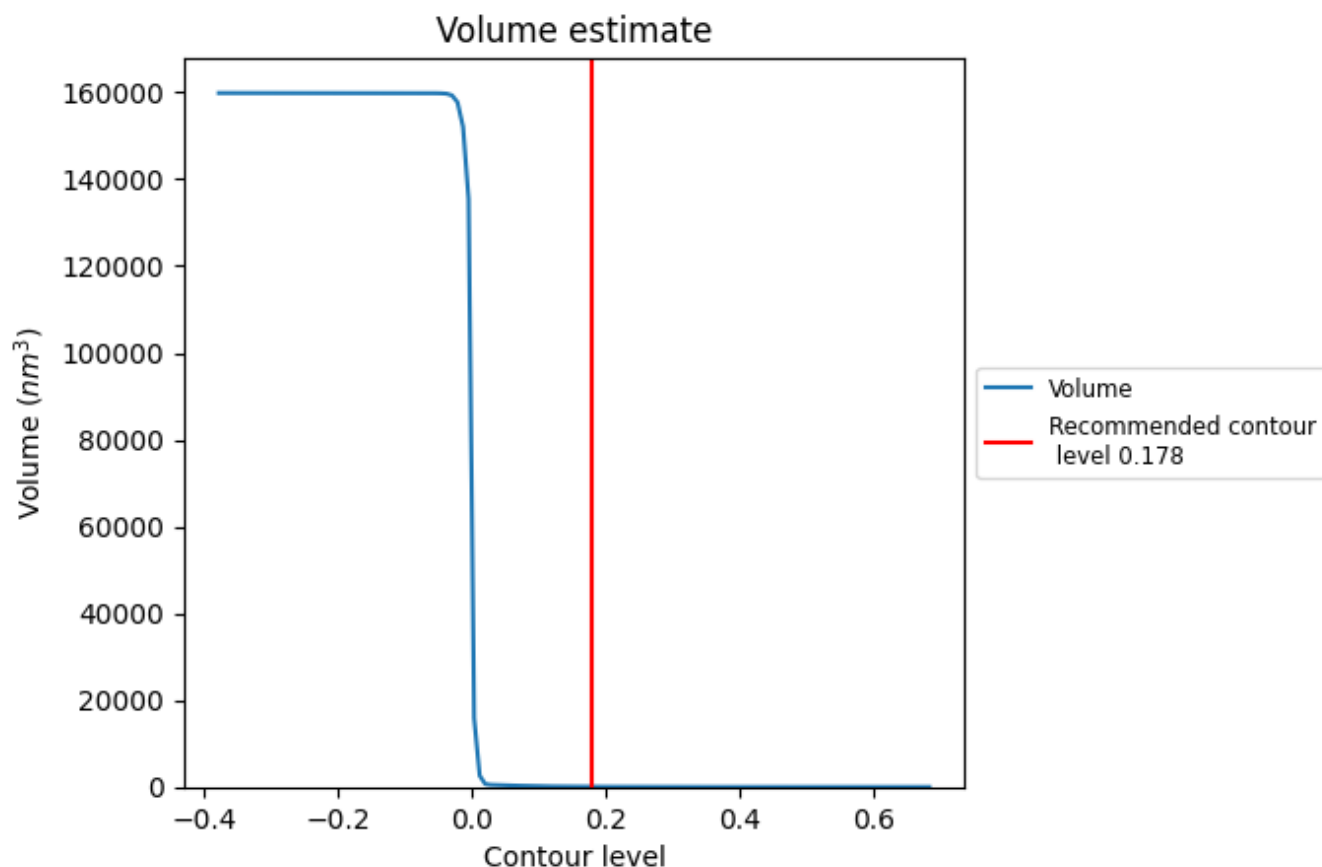
This section contains the results of statistical analysis of the map.

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.

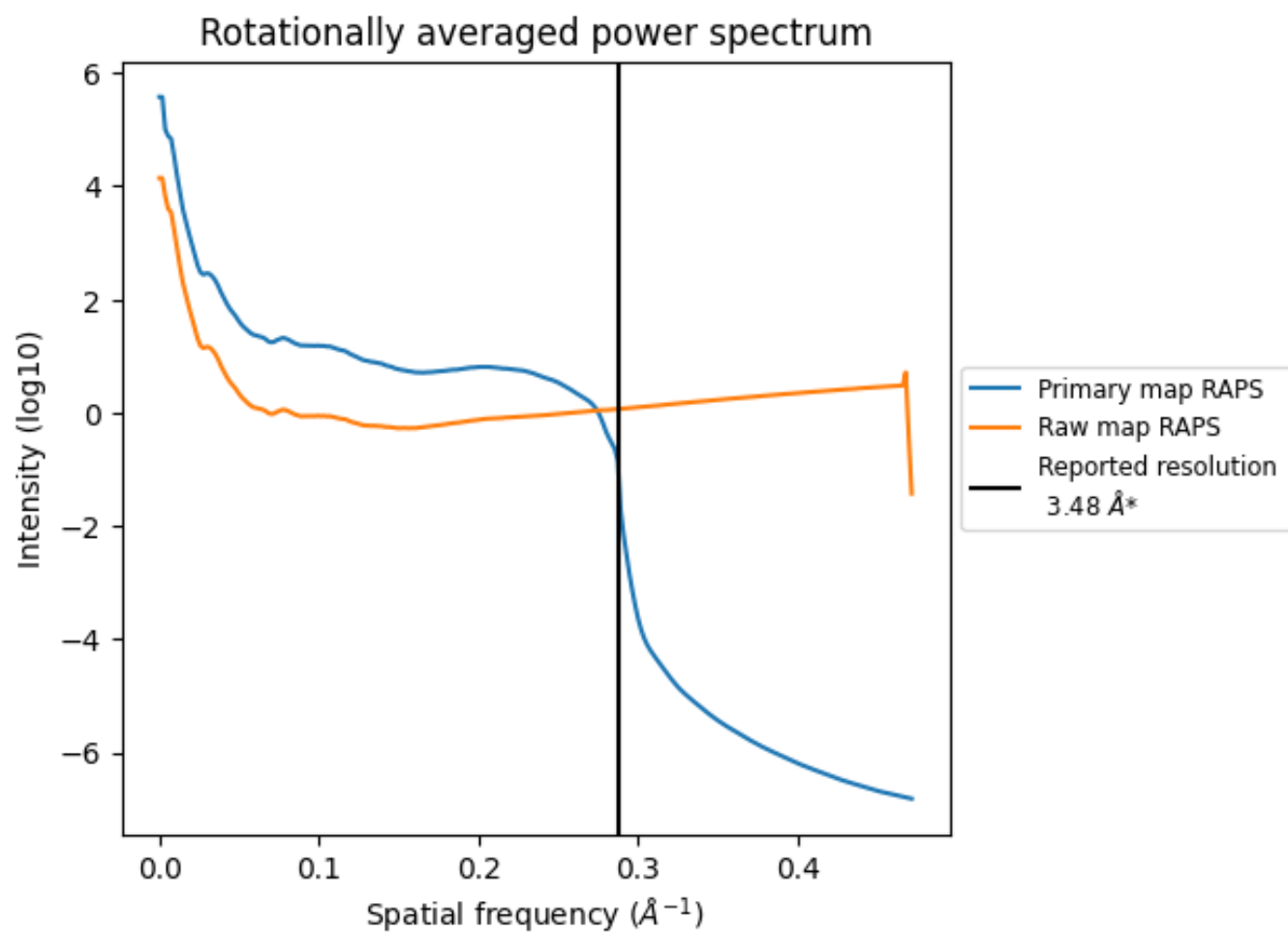
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm^3 ; this corresponds to an approximate mass of 54 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 ⓘ

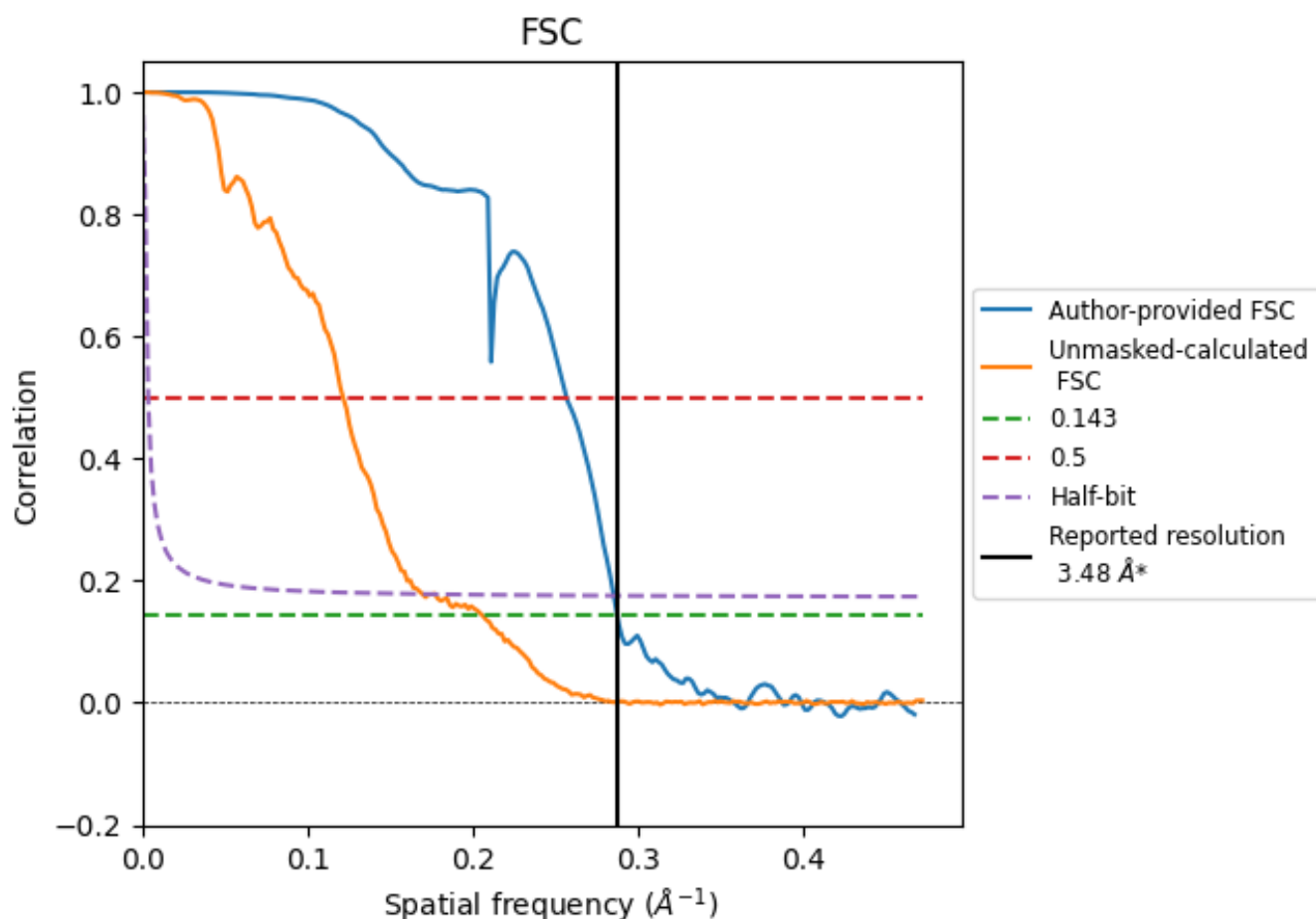


*Reported resolution corresponds to spatial frequency of 0.287 $\text{\AA}^{-1}$

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 0.287 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

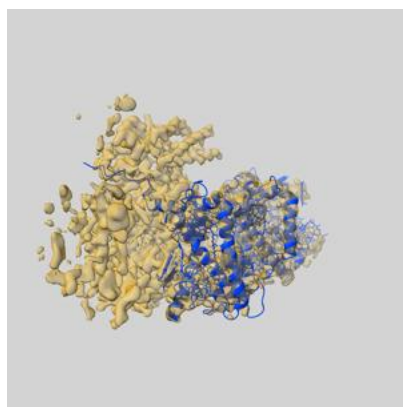
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	3.48	3.90	3.51
Unmasked-calculated*	4.86	8.23	5.90

*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 4.86 differs from the reported value 3.48 by more than 10 %

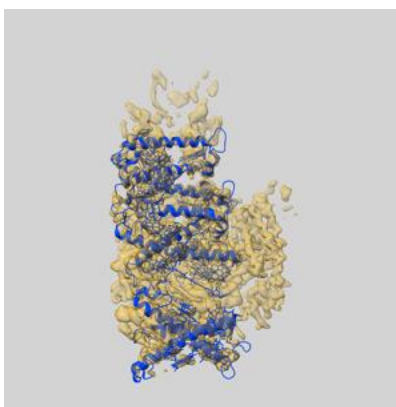
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37268 and PDB model 8W4P. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

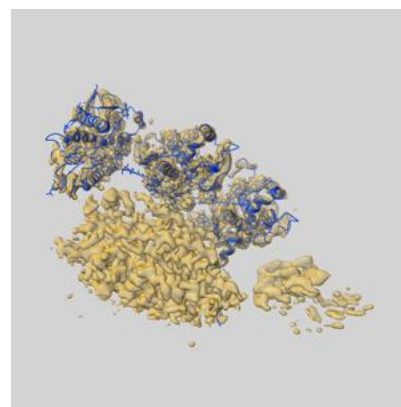
9.1 Map-model overlay [i](#)



X



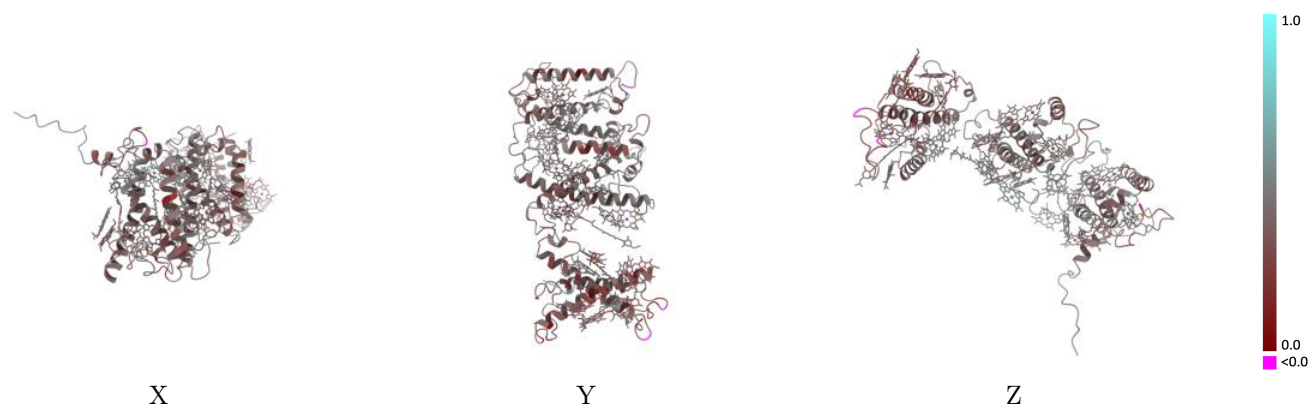
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.178 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

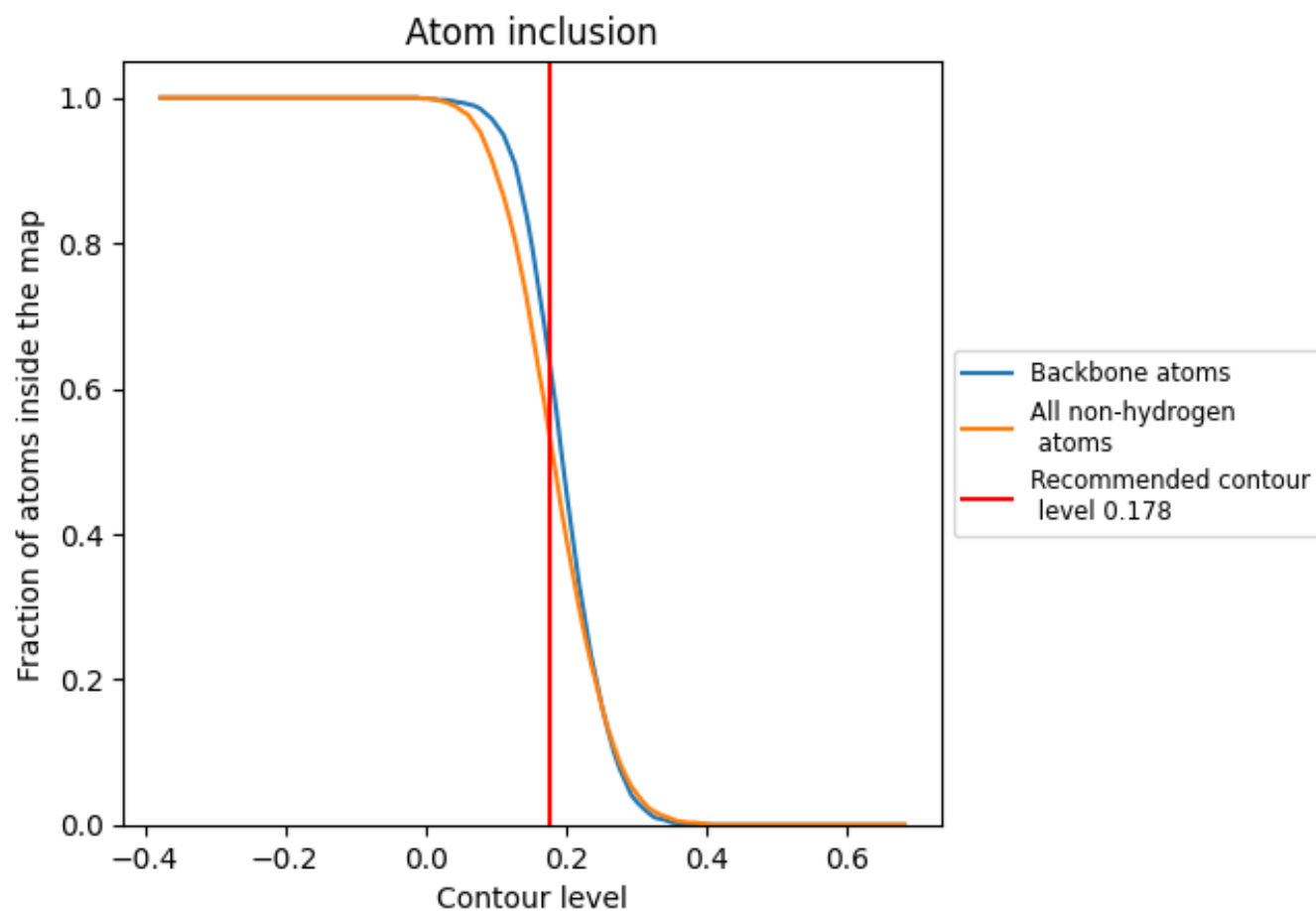


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 53% 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 (0.178) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5300	0.3940
3	0.5870	0.4130
4	0.5040	0.3580
p	0.4980	0.4030

