



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:42 AM UTC

PDB ID : 9UO1 / pdb_00009uo1
EMDB ID : EMD-64369
Title : Cryo-EM structure of human organic solute transporter Ost-alpha/beta bound with DHEAS
Authors : Yang, X.; Xu, E.
Deposited on : 2025-04-24
Resolution : 2.90 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

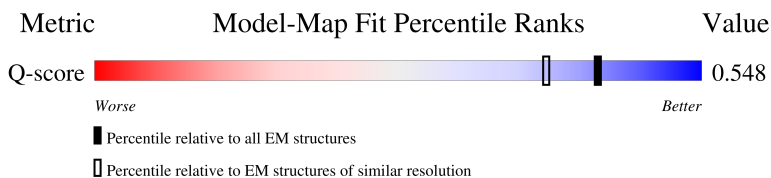
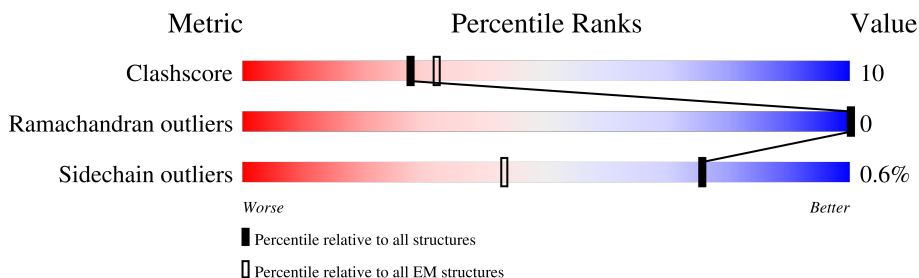
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	351	 76% 17% 7%
1	C	351	 75% 19% 7%
2	B	141	 21% 11% 67%
2	D	141	 20% 13% 67%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7238 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 Organic solute transporter subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	328	Total	C	N	O	S	0	0
			2542	1662	418	438	24		
1	C	328	Total	C	N	O	S	0	0
			2542	1662	418	438	24		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	GLY	-	expression tag	UNP Q86UW1
A	342	GLY	-	expression tag	UNP Q86UW1
A	343	SER	-	expression tag	UNP Q86UW1
A	344	ASP	-	expression tag	UNP Q86UW1
A	345	TYR	-	expression tag	UNP Q86UW1
A	346	LYS	-	expression tag	UNP Q86UW1
A	347	ASP	-	expression tag	UNP Q86UW1
A	348	ASP	-	expression tag	UNP Q86UW1
A	349	ASP	-	expression tag	UNP Q86UW1
A	350	ASP	-	expression tag	UNP Q86UW1
A	351	LYS	-	expression tag	UNP Q86UW1
C	341	GLY	-	expression tag	UNP Q86UW1
C	342	GLY	-	expression tag	UNP Q86UW1
C	343	SER	-	expression tag	UNP Q86UW1
C	344	ASP	-	expression tag	UNP Q86UW1
C	345	TYR	-	expression tag	UNP Q86UW1
C	346	LYS	-	expression tag	UNP Q86UW1
C	347	ASP	-	expression tag	UNP Q86UW1
C	348	ASP	-	expression tag	UNP Q86UW1
C	349	ASP	-	expression tag	UNP Q86UW1
C	350	ASP	-	expression tag	UNP Q86UW1
C	351	LYS	-	expression tag	UNP Q86UW1

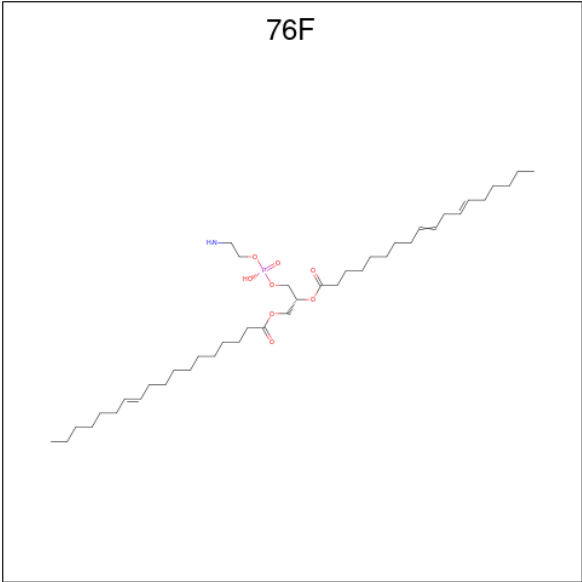
- Molecule 2 is a protein called Organic solute transporter subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	46	Total	C	N	O	S	0	0
			360	237	58	63	2		
2	D	46	Total	C	N	O	S	0	0
			360	237	58	63	2		

There are 26 discrepancies between the modelled and reference sequences:

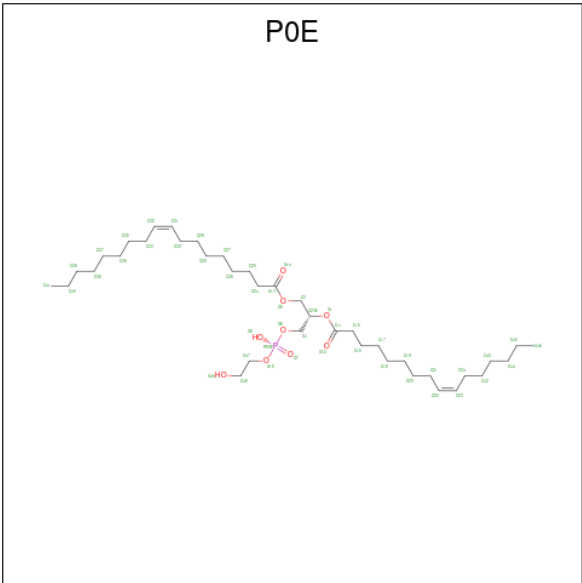
Chain	Residue	Modelled	Actual	Comment	Reference
B	129	GLY	-	expression tag	UNP Q86UW2
B	130	GLY	-	expression tag	UNP Q86UW2
B	131	SER	-	expression tag	UNP Q86UW2
B	132	HIS	-	expression tag	UNP Q86UW2
B	133	HIS	-	expression tag	UNP Q86UW2
B	134	HIS	-	expression tag	UNP Q86UW2
B	135	HIS	-	expression tag	UNP Q86UW2
B	136	HIS	-	expression tag	UNP Q86UW2
B	137	HIS	-	expression tag	UNP Q86UW2
B	138	HIS	-	expression tag	UNP Q86UW2
B	139	HIS	-	expression tag	UNP Q86UW2
B	140	HIS	-	expression tag	UNP Q86UW2
B	141	HIS	-	expression tag	UNP Q86UW2
D	129	GLY	-	expression tag	UNP Q86UW2
D	130	GLY	-	expression tag	UNP Q86UW2
D	131	SER	-	expression tag	UNP Q86UW2
D	132	HIS	-	expression tag	UNP Q86UW2
D	133	HIS	-	expression tag	UNP Q86UW2
D	134	HIS	-	expression tag	UNP Q86UW2
D	135	HIS	-	expression tag	UNP Q86UW2
D	136	HIS	-	expression tag	UNP Q86UW2
D	137	HIS	-	expression tag	UNP Q86UW2
D	138	HIS	-	expression tag	UNP Q86UW2
D	139	HIS	-	expression tag	UNP Q86UW2
D	140	HIS	-	expression tag	UNP Q86UW2
D	141	HIS	-	expression tag	UNP Q86UW2

- Molecule 3 is (7E,21R,24S)-27-amino-24-hydroxy-18,24-dioxo-19,23,25-trioxa-24lambda 5 -phosphaheptacos-7-en-21-yl (9Z,12E)-octadeca-9,12-dienoate (CCD ID: 76F) (formula: C₄₁H₇₆NO₈P) (labeled as "Ligand of Interest" by depositor).



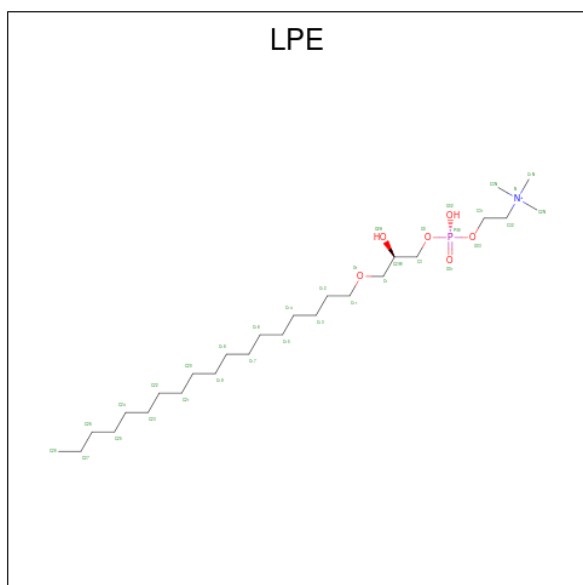
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
3	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
3	C	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 4 is PHOSPHATIDYL ETHANOL (CCD ID: P0E) (formula: C₃₉H₇₃O₉P) (labeled as "Ligand of Interest" by depositor).



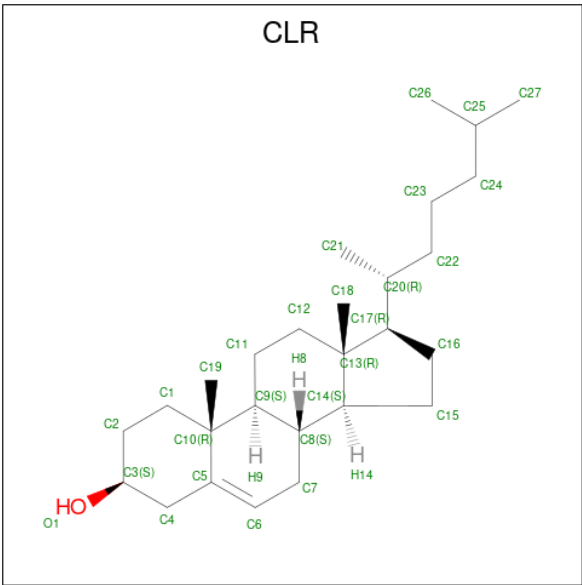
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			49	39	9	1	
4	C	1	Total	C	O	P	0
			49	39	9	1	

- Molecule 5 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: LPE) (formula: $C_{26}H_{57}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			34	26	1	6	1	
5	C	1	Total	C	N	O	P	0
			34	26	1	6	1	

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



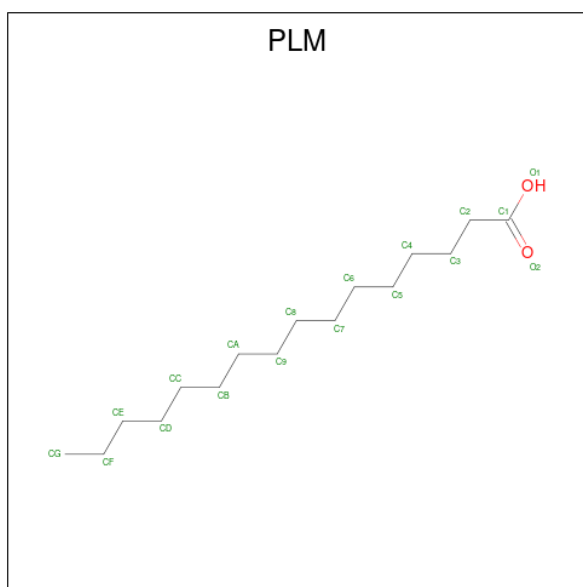
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	

Continued on next page...

Continued from previous page...

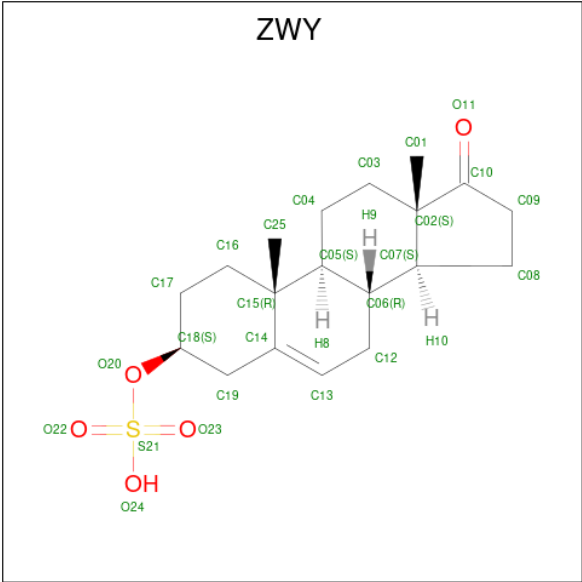
Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	D	1	Total	C	O	0
			28	27	1	
6	D	1	Total	C	O	0
			28	27	1	
6	D	1	Total	C	O	0
			28	27	1	

- Molecule 7 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			6	5	1	
7	A	1	Total	C	O	0
			8	7	1	
7	A	1	Total	C	O	0
			5	4	1	
7	A	1	Total	C	O	0
			7	6	1	
7	A	1	Total	C	O	0
			9	8	1	
7	A	1	Total	C	O	0
			5	4	1	
7	C	1	Total	C	O	0
			6	5	1	
7	C	1	Total	C	O	0
			8	7	1	
7	C	1	Total	C	O	0
			5	4	1	
7	C	1	Total	C	O	0
			7	6	1	
7	C	1	Total	C	O	0
			9	8	1	
7	C	1	Total	C	O	0
			5	4	1	

- Molecule 8 is 17-oxoandrost-5-en-3beta-yl hydrogen sulfate (CCD ID: ZWY) (formula: $C_{19}H_{28}O_5S$) (labeled as "Ligand of Interest" by depositor).

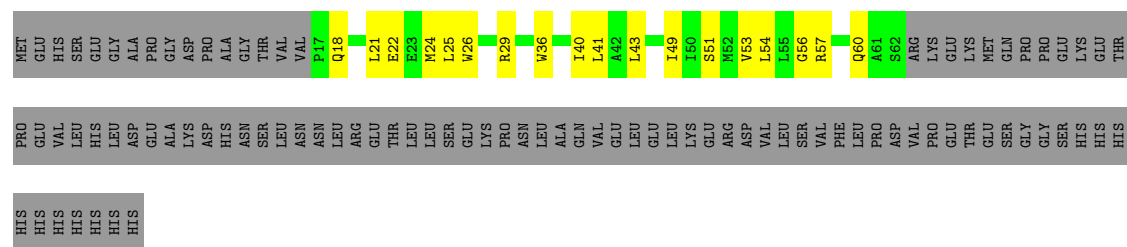


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	O	S	0
			25	19	5	1	
8	A	1	Total	C	O	S	0
			25	19	5	1	
8	C	1	Total	C	O	S	0
			25	19	5	1	
8	C	1	Total	C	O	S	0
			25	19	5	1	

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	O	0
			1	1	
9	C	1	Total	O	0
			1	1	

Chain D: 20% 13% 67%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81957	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.698	Depositor
Minimum map value	-1.843	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.24	Depositor
Map size ($\text{\AA}$)	247.2, 247.2, 247.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.824, 0.824, 0.824	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: CLR, PLM, 76F, ZWY, LPE, P0E

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/2598	0.34	0/3536
1	C	0.26	0/2598	0.44	0/3536
2	B	0.31	0/368	0.44	0/501
2	D	0.23	0/368	0.39	0/501
All	All	0.24	0/5932	0.39	0/8074

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2542	0	2662	52	0
1	C	2542	0	2663	50	0
2	B	360	0	366	16	0
2	D	360	0	366	21	0
3	A	139	0	0	1	0
3	C	51	0	0	0	0
4	A	49	0	72	2	0
4	C	49	0	72	2	0
5	A	34	0	56	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	34	0	56	5	0
6	A	364	0	598	24	0
6	B	84	0	138	3	0
6	C	364	0	598	23	0
6	D	84	0	138	3	0
7	A	40	0	44	2	0
7	C	40	0	44	1	0
8	A	50	0	0	0	0
8	C	50	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
All	All	7238	0	7873	146	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 10.

All (146) 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:C:14:TYR:CD1	2:D:24:MET:HE2	2.18	0.78
6:C:410:CLR:H72	6:C:416:CLR:H152	1.68	0.75
1:A:62:LEU:HD22	6:A:407:CLR:H271	1.70	0.72
1:A:18:LEU:HB3	2:B:24:MET:HE1	1.72	0.72
1:A:149:ARG:HH11	1:A:149:ARG:HB3	1.54	0.71
6:A:409:CLR:H72	6:A:415:CLR:H152	1.72	0.71
1:A:305:GLU:HG2	4:A:403:P0E:H461	1.75	0.69
1:A:201:LEU:HD11	6:A:425:CLR:H72	1.75	0.68
1:A:293:ARG:O	1:A:297:MET:HG3	1.93	0.68
1:C:14:TYR:HD1	2:D:24:MET:HE2	1.59	0.68
1:C:42:LEU:HD22	1:C:109:PRO:HG3	1.76	0.68
1:C:293:ARG:O	1:C:297:MET:HG3	1.93	0.68
1:A:311:VAL:HG21	2:B:51:SER:HB2	1.77	0.67
1:C:62:LEU:HD22	6:C:408:CLR:H271	1.77	0.67
1:C:80:LEU:HD13	1:C:322:HIS:ND1	2.08	0.67
1:C:22:LEU:HD11	2:D:24:MET:HB3	1.77	0.67
1:C:201:LEU:HD11	6:C:403:CLR:H72	1.79	0.65
2:B:36:TRP:NE1	2:B:40:ILE:HD11	2.14	0.63
1:C:305:GLU:HG2	4:C:404:P0E:H461	1.81	0.62
1:A:26:TYR:HE2	2:B:21:LEU:HD11	1.63	0.62
1:A:149:ARG:HB3	1:A:149:ARG:NH1	2.16	0.61
2:D:36:TRP:NE1	2:D:40:ILE:HD11	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HD11	2:B:24:MET:HB3	1.83	0.60
6:A:410:CLR:H152	6:C:403:CLR:H9	1.85	0.59
2:D:49:ILE:O	2:D:53:VAL:HG23	2.03	0.58
1:C:206:ILE:HG21	6:C:403:CLR:H162	1.86	0.57
1:A:94:ALA:HA	1:A:122:PHE:HE2	1.69	0.57
1:A:42:LEU:HD22	1:A:109:PRO:HG3	1.85	0.57
6:A:425:CLR:H9	6:C:411:CLR:H152	1.86	0.56
1:C:220:TRP:HD1	6:C:402:CLR:H71	1.72	0.55
1:C:180:LEU:HD13	1:C:239:ILE:HD11	1.87	0.55
1:A:206:ILE:HG21	6:A:425:CLR:H162	1.88	0.55
5:C:405:LPE:H111	6:C:409:CLR:H41	1.89	0.54
5:A:404:LPE:H111	6:A:408:CLR:H41	1.88	0.54
1:C:261:VAL:HG22	4:C:404:P0E:H372	1.89	0.54
1:C:94:ALA:HA	1:C:122:PHE:HE2	1.72	0.53
2:B:18:GLN:HA	2:B:21:LEU:HB3	1.91	0.52
2:D:26:TRP:O	2:D:29:ARG:HD3	2.08	0.52
1:C:14:TYR:HA	2:D:24:MET:HE1	1.91	0.52
1:C:274:SER:O	1:C:278:ASN:ND2	2.41	0.52
1:A:180:LEU:HD13	1:A:239:ILE:HD11	1.91	0.52
1:A:261:VAL:HG22	4:A:403:P0E:H372	1.90	0.52
1:A:67:ILE:HG13	6:A:406:CLR:H151	1.90	0.52
1:C:80:LEU:HD12	5:C:405:LPE:H3N1	1.92	0.51
1:C:67:ILE:HG13	6:C:407:CLR:H151	1.91	0.51
1:C:141:LYS:NZ	1:C:178:GLN:OE1	2.44	0.51
1:A:76:TYR:HA	1:A:85:ARG:HD2	1.93	0.51
1:A:95:PRO:O	1:A:306:THR:HG21	2.11	0.51
2:D:43:LEU:HD11	6:D:201:CLR:H162	1.93	0.51
1:A:131:MET:HE1	1:A:239:ILE:HG13	1.93	0.50
1:A:38:THR:HB	1:A:41:GLN:HG3	1.92	0.50
1:C:26:TYR:HE2	2:D:21:LEU:HD11	1.77	0.50
1:A:297:MET:HB3	2:B:36:TRP:CZ2	2.47	0.50
1:A:95:PRO:O	1:A:306:THR:CG2	2.60	0.50
1:C:227:VAL:HG13	7:C:421:PLM:H61	1.93	0.49
2:B:43:LEU:HD11	6:B:201:CLR:H162	1.94	0.49
1:A:284:CYS:HB2	2:B:29:ARG:O	2.12	0.49
2:D:41:LEU:HB3	6:D:202:CLR:H213	1.95	0.48
1:A:19:LEU:HB3	1:A:23:LYS:NZ	2.28	0.48
1:A:247:LEU:HB2	1:A:252:MET:HG3	1.96	0.48
1:A:156:HIS:NE2	1:A:169:ARG:NH1	2.61	0.48
1:C:83:ILE:O	1:C:86:ARG:HG3	2.14	0.48
1:A:227:VAL:HG13	7:A:420:PLM:H61	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:TYR:HA	1:C:85:ARG:HD3	1.96	0.48
6:A:412:CLR:H181	6:B:201:CLR:H212	1.96	0.47
2:B:48:VAL:O	2:B:52:MET:HG2	2.15	0.47
1:C:302:LEU:O	1:C:306:THR:OG1	2.21	0.47
6:C:413:CLR:H181	6:D:201:CLR:H212	1.97	0.47
1:C:311:VAL:HG21	2:D:51:SER:HB2	1.97	0.47
1:C:140:GLY:O	1:C:144:VAL:HG23	2.15	0.47
5:C:405:LPE:H132	6:C:409:CLR:H6	1.97	0.46
1:C:19:LEU:C	1:C:23:LYS:HZ2	2.23	0.46
1:A:67:ILE:HG12	6:A:406:CLR:H71	1.97	0.46
1:A:56:ILE:HD13	6:A:414:CLR:H241	1.97	0.46
2:B:36:TRP:CE2	2:B:40:ILE:HD11	2.51	0.46
6:C:413:CLR:H272	6:C:414:CLR:H241	1.99	0.45
5:A:404:LPE:H132	6:A:408:CLR:H6	1.98	0.45
6:A:424:CLR:H222	6:A:424:CLR:H162	1.70	0.45
1:C:87:THR:HG22	1:C:133:VAL:HG23	1.97	0.45
2:D:21:LEU:O	2:D:24:MET:HB2	2.17	0.45
1:C:14:TYR:HA	2:D:24:MET:CE	2.47	0.45
2:D:18:GLN:HA	2:D:21:LEU:HB3	1.99	0.45
1:C:176:LYS:HD3	6:C:412:CLR:H72	1.99	0.45
6:A:412:CLR:H272	6:A:413:CLR:H241	1.99	0.45
2:B:56:GLY:O	2:B:60:GLN:HG2	2.17	0.45
1:C:91:LYS:HG2	1:C:129:LEU:HB3	1.99	0.45
1:C:131:MET:HE1	1:C:239:ILE:HG13	1.98	0.45
6:A:425:CLR:H162	6:A:425:CLR:H222	1.42	0.44
6:C:403:CLR:H162	6:C:403:CLR:H222	1.43	0.44
1:C:70:GLU:HG3	6:C:407:CLR:H41	1.98	0.44
1:A:26:TYR:CE2	2:B:21:LEU:HD11	2.49	0.44
1:A:52:ALA:HA	6:A:415:CLR:H71	1.99	0.44
1:C:269:GLN:HB3	1:C:270:PRO:HD3	2.00	0.44
2:D:36:TRP:CE2	2:D:40:ILE:HD11	2.52	0.44
2:D:54:LEU:HD23	2:D:57:ARG:HH11	1.82	0.44
1:A:191:LYS:HD2	1:A:225:LEU:HD13	2.00	0.44
6:A:414:CLR:H222	6:A:414:CLR:H162	1.82	0.44
1:A:183:GLY:O	1:A:186:GLN:HG3	2.18	0.44
1:A:170:LEU:HD11	1:A:176:LYS:HD3	2.00	0.44
2:B:26:TRP:O	2:B:29:ARG:HG2	2.18	0.43
1:C:67:ILE:HG12	6:C:407:CLR:H71	1.99	0.43
1:C:154:MET:HB2	1:C:156:HIS:CE1	2.53	0.43
6:A:410:CLR:H72	6:C:403:CLR:H122	1.99	0.43
1:C:217:THR:HG23	6:C:402:CLR:H72	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLY:O	1:A:144:VAL:HG23	2.19	0.43
1:C:123:TYR:HE2	1:C:263:LEU:HB2	1.83	0.43
5:C:405:LPE:H311	5:C:405:LPE:H1N2	1.74	0.43
1:A:168:PRO:HG2	6:A:411:CLR:H22	2.00	0.43
1:A:175:LYS:HB2	1:A:175:LYS:HE2	1.66	0.43
5:A:404:LPE:H1N2	5:A:404:LPE:H311	1.72	0.43
1:C:198:GLY:O	1:C:202:VAL:HG23	2.19	0.43
1:A:220:TRP:HD1	6:A:424:CLR:H71	1.84	0.42
1:A:94:ALA:HA	1:A:122:PHE:CE2	2.53	0.42
1:A:86:ARG:HD3	3:A:401:76F:O5	2.19	0.42
1:A:141:LYS:NZ	1:A:178:GLN:OE1	2.47	0.42
2:B:22:GLU:HA	2:B:25:LEU:HD12	2.02	0.42
1:C:56:ILE:HD13	6:C:415:CLR:H241	2.01	0.42
1:C:284:CYS:HB2	2:D:29:ARG:O	2.19	0.42
1:C:271:SER:O	1:C:275:VAL:HG23	2.19	0.42
1:C:283:ALA:HB2	2:D:29:ARG:CZ	2.49	0.42
6:A:425:CLR:H161	6:C:411:CLR:H191	2.02	0.42
1:A:198:GLY:O	1:A:202:VAL:HG23	2.20	0.41
1:A:157:THR:HG22	1:A:241:ARG:HD3	2.02	0.41
6:A:407:CLR:H162	6:A:407:CLR:H222	1.80	0.41
1:A:183:GLY:HA3	1:A:235:THR:HG21	2.01	0.41
1:A:269:GLN:HB3	1:A:270:PRO:HD3	2.03	0.41
1:A:301:LEU:HD22	6:B:201:CLR:H273	2.02	0.41
1:A:19:LEU:HB3	1:A:23:LYS:HZ2	1.85	0.41
6:A:424:CLR:H8	6:A:425:CLR:H183	2.02	0.41
2:D:56:GLY:O	2:D:60:GLN:HG2	2.20	0.41
1:C:19:LEU:C	1:C:23:LYS:NZ	2.79	0.41
5:C:405:LPE:H191	5:C:405:LPE:H162	1.90	0.41
1:C:175:LYS:HB2	1:C:175:LYS:HE2	1.84	0.41
1:C:52:ALA:HA	6:C:416:CLR:H71	2.02	0.41
1:C:247:LEU:HB2	1:C:252:MET:HG3	2.03	0.41
1:C:297:MET:HB3	2:D:36:TRP:CZ2	2.55	0.41
2:D:22:GLU:HA	2:D:25:LEU:HD12	2.03	0.41
1:A:76:TYR:HA	1:A:85:ARG:CD	2.51	0.41
1:A:124:ALA:HB2	1:A:191:LYS:HG2	2.01	0.41
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.93	0.41
7:A:417:PLM:H62	7:A:420:PLM:H22	2.03	0.40
1:A:283:ALA:HB3	2:B:31:GLU:HB2	2.03	0.40
1:A:70:GLU:HG3	6:A:406:CLR:H41	2.04	0.40
1:C:183:GLY:HA3	1:C:235:THR:HG21	2.03	0.40
1:C:235:THR:HG22	6:C:412:CLR:H211	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:408:CLR:H162	6:C:408:CLR:H222	1.80	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	A	326/351 (93%)	320 (98%)	6 (2%)	0	100	100
1	C	326/351 (93%)	323 (99%)	3 (1%)	0	100	100
2	B	44/141 (31%)	44 (100%)	0	0	100	100
2	D	44/141 (31%)	43 (98%)	1 (2%)	0	100	100
All	All	740/984 (75%)	730 (99%)	10 (1%)	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	A	283/306 (92%)	282 (100%)	1 (0%)	84	94
1	C	283/306 (92%)	280 (99%)	3 (1%)	65	88
2	B	39/126 (31%)	39 (100%)	0	100	100
2	D	39/126 (31%)	39 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	644/864 (74%)	640 (99%)	4 (1%)	76	93

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

Mol	Chain	Res	Type
1	A	18	LEU
1	C	21	VAL
1	C	151	THR
1	C	266	THR

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

Mol	Chain	Res	Type
1	A	25	ASN
1	A	41	GLN
1	A	242	GLN
1	A	322	HIS
1	C	41	GLN
1	C	78	ASN
1	C	269	GLN
1	C	298	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](#)

56 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	CLR	C	415	-	31,31,31	0.39	0	48,48,48	0.48	0
6	CLR	B	201	-	31,31,31	0.37	0	48,48,48	0.54	0
6	CLR	C	412	-	31,31,31	0.40	0	48,48,48	0.92	3 (6%)
6	CLR	C	411	-	31,31,31	0.39	0	48,48,48	0.56	0
7	PLM	A	418	-	3,4,17	0.57	0	2,3,17	0.78	0
8	ZWY	A	423	-	28,28,28	0.28	0	42,46,46	1.31	7 (16%)
7	PLM	A	419	1	5,6,17	0.48	0	4,5,17	0.59	0
3	76F	A	426	-	43,43,50	1.39	4 (9%)	46,48,55	1.42	7 (15%)
6	CLR	A	415	-	31,31,31	0.38	0	48,48,48	0.50	0
8	ZWY	C	423	-	28,28,28	0.30	0	42,46,46	1.08	4 (9%)
7	PLM	A	417	-	6,7,17	0.44	0	5,6,17	0.52	0
7	PLM	C	421	-	7,8,17	0.40	0	6,7,17	0.48	0
6	CLR	B	202	-	31,31,31	0.37	0	48,48,48	0.55	0
6	CLR	D	201	-	31,31,31	0.37	0	48,48,48	0.55	0
6	CLR	A	408	-	31,31,31	0.38	0	48,48,48	0.60	0
6	CLR	C	408	-	31,31,31	0.39	0	48,48,48	0.49	0
7	PLM	C	418	-	6,7,17	0.44	0	5,6,17	0.52	0
6	CLR	A	407	-	31,31,31	0.39	0	48,48,48	0.49	0
6	CLR	A	425	-	31,31,31	0.42	0	48,48,48	0.56	0
5	LPE	A	404	-	33,33,33	1.06	0	37,39,39	0.84	1 (2%)
7	PLM	A	420	-	7,8,17	0.40	0	6,7,17	0.48	0
6	CLR	C	410	-	31,31,31	0.39	0	48,48,48	0.58	0
6	CLR	A	406	-	31,31,31	0.40	0	48,48,48	0.60	0
8	ZWY	C	424	-	28,28,28	0.28	0	42,46,46	1.30	5 (11%)
7	PLM	C	422	-	3,4,17	0.58	0	2,3,17	0.78	0
6	CLR	D	203	-	31,31,31	0.39	0	48,48,48	0.56	0
4	P0E	C	404	-	48,48,48	0.51	0	51,53,53	0.50	1 (1%)
6	CLR	A	410	-	31,31,31	0.39	0	48,48,48	0.57	0
4	P0E	A	403	-	48,48,48	0.51	0	51,53,53	0.51	1 (1%)
6	CLR	C	407	-	31,31,31	0.40	0	48,48,48	0.57	0
6	CLR	C	416	-	31,31,31	0.37	0	48,48,48	0.52	0
6	CLR	A	409	-	31,31,31	0.38	0	48,48,48	0.54	0
6	CLR	C	409	-	31,31,31	0.38	0	48,48,48	0.60	0
7	PLM	A	416	1	4,5,17	0.52	0	3,4,17	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CLR	A	412	-	31,31,31	0.39	0	48,48,48	0.51	0
6	CLR	A	413	-	31,31,31	0.37	0	48,48,48	0.51	0
6	CLR	A	405	-	31,31,31	0.38	0	48,48,48	0.48	0
7	PLM	C	419	-	3,4,17	0.57	0	2,3,17	0.78	0
6	CLR	A	424	-	31,31,31	0.39	0	48,48,48	0.57	0
5	LPE	C	405	-	33,33,33	1.06	0	37,39,39	0.84	1 (2%)
6	CLR	C	413	-	31,31,31	0.39	0	48,48,48	0.52	0
7	PLM	A	421	1	3,4,17	0.58	0	2,3,17	0.80	0
3	76F	A	402	-	43,43,50	1.39	4 (9%)	46,48,55	1.43	7 (15%)
6	CLR	C	414	-	31,31,31	0.37	0	48,48,48	0.50	0
6	CLR	C	402	-	31,31,31	0.39	0	48,48,48	0.52	0
8	ZWY	A	422	-	28,28,28	0.30	0	42,46,46	1.08	4 (9%)
3	76F	A	401	-	50,50,50	1.62	7 (14%)	53,55,55	1.57	4 (7%)
6	CLR	C	403	-	31,31,31	0.41	0	48,48,48	0.56	0
6	CLR	C	406	-	31,31,31	0.38	0	48,48,48	0.49	0
6	CLR	D	202	-	31,31,31	0.37	0	48,48,48	0.56	0
7	PLM	C	417	1	4,5,17	0.51	0	3,4,17	0.69	0
7	PLM	C	420	1	5,6,17	0.47	0	4,5,17	0.59	0
6	CLR	A	414	-	31,31,31	0.39	0	48,48,48	0.47	0
6	CLR	B	203	-	31,31,31	0.39	0	48,48,48	0.54	0
3	76F	C	401	-	50,50,50	1.62	7 (14%)	53,55,55	1.59	4 (7%)
6	CLR	A	411	-	31,31,31	0.41	0	48,48,48	0.91	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	C	415	-	-	5/10/68/68	0/4/4/4
6	CLR	B	201	-	-	4/10/68/68	0/4/4/4
6	CLR	C	412	-	-	6/10/68/68	0/4/4/4
6	CLR	C	411	-	-	4/10/68/68	0/4/4/4
7	PLM	A	418	-	-	2/2/2/15	-
8	ZWY	A	423	-	-	0/5/63/63	0/4/4/4
7	PLM	A	419	1	-	0/4/4/15	-
3	76F	A	426	-	-	19/47/47/54	-
6	CLR	A	415	-	-	3/10/68/68	0/4/4/4
8	ZWY	C	423	-	-	0/5/63/63	0/4/4/4
7	PLM	A	417	-	-	1/5/5/15	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PLM	C	421	-	-	2/6/6/15	-
6	CLR	B	202	-	-	4/10/68/68	0/4/4/4
6	CLR	D	201	-	-	4/10/68/68	0/4/4/4
6	CLR	A	408	-	-	0/10/68/68	0/4/4/4
6	CLR	C	408	-	-	5/10/68/68	0/4/4/4
7	PLM	C	418	-	-	2/5/5/15	-
6	CLR	A	407	-	-	5/10/68/68	0/4/4/4
6	CLR	A	425	-	-	8/10/68/68	0/4/4/4
5	LPE	A	404	-	-	9/34/34/34	-
7	PLM	A	420	-	-	2/6/6/15	-
6	CLR	C	410	-	-	3/10/68/68	0/4/4/4
6	CLR	A	406	-	-	3/10/68/68	0/4/4/4
8	ZWY	C	424	-	-	0/5/63/63	0/4/4/4
7	PLM	C	422	-	-	1/2/2/15	-
6	CLR	D	203	-	-	0/10/68/68	0/4/4/4
4	P0E	C	404	-	-	14/52/52/52	-
6	CLR	A	410	-	-	4/10/68/68	0/4/4/4
4	P0E	A	403	-	-	15/52/52/52	-
6	CLR	C	407	-	-	3/10/68/68	0/4/4/4
6	CLR	C	416	-	-	3/10/68/68	0/4/4/4
6	CLR	A	409	-	-	3/10/68/68	0/4/4/4
6	CLR	C	409	-	-	0/10/68/68	0/4/4/4
7	PLM	A	416	1	-	0/3/3/15	-
6	CLR	A	412	-	-	0/10/68/68	0/4/4/4
6	CLR	A	413	-	-	0/10/68/68	0/4/4/4
6	CLR	A	405	-	-	4/10/68/68	0/4/4/4
7	PLM	C	419	-	-	2/2/2/15	-
6	CLR	A	424	-	-	4/10/68/68	0/4/4/4
5	LPE	C	405	-	-	9/34/34/34	-
6	CLR	C	413	-	-	0/10/68/68	0/4/4/4
7	PLM	A	421	1	-	1/2/2/15	-
3	76F	A	402	-	-	17/47/47/54	-
6	CLR	C	414	-	-	0/10/68/68	0/4/4/4
6	CLR	C	402	-	-	4/10/68/68	0/4/4/4
8	ZWY	A	422	-	-	0/5/63/63	0/4/4/4
3	76F	A	401	-	-	18/54/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	C	403	-	-	8/10/68/68	0/4/4/4
6	CLR	C	406	-	-	4/10/68/68	0/4/4/4
6	CLR	D	202	-	-	4/10/68/68	0/4/4/4
7	PLM	C	417	1	-	0/3/3/15	-
7	PLM	C	420	1	-	0/4/4/15	-
6	CLR	A	414	-	-	5/10/68/68	0/4/4/4
6	CLR	B	203	-	-	0/10/68/68	0/4/4/4
3	76F	C	401	-	-	19/54/54/54	-
6	CLR	A	411	-	-	6/10/68/68	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	426	76F	P-O3P	4.44	1.76	1.59
3	A	402	76F	P-O3P	4.44	1.76	1.59
3	C	401	76F	C5-N	-4.20	1.13	1.46
3	A	401	76F	C5-N	-4.18	1.13	1.46
3	C	401	76F	C22-C21	4.13	1.55	1.31
3	A	401	76F	C22-C21	4.11	1.55	1.31
3	A	401	76F	C41-C40	4.07	1.54	1.31
3	C	401	76F	C41-C40	4.06	1.54	1.31
3	A	401	76F	C19-C18	3.97	1.54	1.31
3	C	401	76F	C19-C18	3.97	1.54	1.31
3	A	402	76F	P-O4P	3.58	1.73	1.59
3	A	426	76F	P-O4P	3.57	1.73	1.59
3	A	426	76F	C1-C2	3.15	1.60	1.50
3	A	402	76F	C1-C2	3.14	1.60	1.50
3	C	401	76F	O2-C2	-2.95	1.39	1.46
3	A	401	76F	O2-C2	-2.89	1.39	1.46
3	C	401	76F	O2-C10	2.77	1.42	1.34
3	A	401	76F	O2-C10	2.77	1.42	1.34
3	C	401	76F	O3-C30	2.70	1.41	1.33
3	A	401	76F	O3-C30	2.67	1.41	1.33
3	A	402	76F	C3-C2	2.22	1.57	1.50
3	A	426	76F	C3-C2	2.20	1.57	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	76F	C4-C5-N	7.46	179.92	114.11
3	A	401	76F	C4-C5-N	7.22	177.82	114.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	76F	O2-C10-C11	5.95	124.34	111.48
3	A	426	76F	O2-C10-C11	5.93	124.31	111.48
3	C	401	76F	O2-C10-C11	4.03	120.21	111.48
3	A	401	76F	O2-C10-C11	4.02	120.17	111.48
8	C	423	ZWY	C18-C19-C14	3.74	116.97	111.45
8	A	422	ZWY	C18-C19-C14	3.66	116.86	111.45
8	A	423	ZWY	C16-C17-C18	3.60	116.20	110.33
8	C	424	ZWY	C16-C17-C18	3.56	116.14	110.33
6	C	412	CLR	C13-C17-C20	3.47	124.85	119.50
3	A	426	76F	O3-C30-C31	3.45	122.36	111.83
3	A	402	76F	O3-C30-C31	3.44	122.33	111.83
6	A	411	CLR	C13-C17-C20	3.40	124.74	119.50
8	A	423	ZWY	C18-C19-C14	3.30	116.33	111.45
8	C	424	ZWY	C18-C19-C14	3.22	116.20	111.45
3	A	402	76F	O2-C10-O4	-2.97	116.77	123.70
3	A	426	76F	O2-C10-O4	-2.96	116.78	123.70
8	C	423	ZWY	C17-C18-C19	2.95	115.08	110.97
8	A	422	ZWY	C17-C18-C19	2.93	115.05	110.97
3	A	402	76F	O2P-P-O1P	2.90	125.94	112.44
3	A	426	76F	O2P-P-O1P	2.89	125.91	112.44
6	C	412	CLR	C21-C20-C17	2.83	117.13	112.88
8	A	422	ZWY	O23-S21-O22	2.74	122.81	112.24
6	A	411	CLR	C21-C20-C17	2.74	117.00	112.88
8	C	423	ZWY	O23-S21-O22	2.74	122.80	112.24
8	C	424	ZWY	O23-S21-O22	2.72	122.72	112.24
8	A	423	ZWY	O23-S21-O22	2.72	122.71	112.24
3	A	401	76F	O3-C30-C31	2.69	120.05	111.83
8	A	422	ZWY	C16-C17-C18	2.63	114.62	110.33
3	C	401	76F	O3-C30-C31	2.60	119.77	111.83
8	C	423	ZWY	C16-C17-C18	2.60	114.58	110.33
4	C	404	P0E	O9-P8-O7	2.53	124.23	112.44
4	A	403	P0E	O9-P8-O7	2.52	124.17	112.44
3	C	401	76F	O2P-P-O1P	-2.47	100.95	112.44
3	A	401	76F	O2P-P-O1P	-2.47	100.96	112.44
5	C	405	LPE	O32-P-O31	-2.34	101.54	112.44
5	A	404	LPE	O32-P-O31	-2.34	101.57	112.44
3	A	426	76F	C21-C20-C19	2.31	123.38	112.02
3	A	402	76F	C21-C20-C19	2.30	123.36	112.02
3	A	426	76F	O3-C30-O5	-2.29	117.90	123.63
3	A	402	76F	O3-C30-O5	-2.28	117.92	123.63
3	A	402	76F	C2-O2-C10	2.19	123.04	117.80
8	C	424	ZWY	C19-C14-C15	2.18	119.21	116.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	423	ZWY	C19-C14-C15	2.17	119.20	116.42
3	A	426	76F	C2-O2-C10	2.13	122.89	117.80
8	A	423	ZWY	C25-C15-C05	-2.08	109.32	111.66
6	C	412	CLR	C21-C20-C22	-2.06	107.14	110.34
8	A	423	ZWY	C17-C16-C15	2.04	117.12	112.78
8	C	424	ZWY	C25-C15-C05	-2.01	109.40	111.66
8	A	423	ZWY	C12-C06-C05	2.00	112.04	109.72

There are no chirality outliers.

All (239) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	76F	O4-C10-O2-C2
3	A	401	76F	C1-O3P-P-O2P
3	A	401	76F	C1-O3P-P-O4P
3	A	401	76F	C4-O4P-P-O1P
3	A	401	76F	C4-O4P-P-O3P
3	A	402	76F	C11-C10-O2-C2
3	A	402	76F	O4-C10-O2-C2
3	A	426	76F	C11-C10-O2-C2
3	A	426	76F	O4-C10-O2-C2
3	C	401	76F	O4P-C4-C5-N
3	C	401	76F	O4-C10-O2-C2
3	C	401	76F	C1-O3P-P-O1P
3	C	401	76F	C1-O3P-P-O2P
3	C	401	76F	C1-O3P-P-O4P
3	C	401	76F	C4-O4P-P-O1P
4	A	403	P0E	C4-O6-P8-O7
4	A	403	P0E	C4-O6-P8-O9
4	A	403	P0E	C4-O6-P8-O10
4	C	404	P0E	C4-O6-P8-O7
4	C	404	P0E	C4-O6-P8-O9
4	C	404	P0E	C4-O6-P8-O10
5	A	404	LPE	C31-O33-P-O3
5	A	404	LPE	C31-O33-P-O31
5	A	404	LPE	C32-C31-O33-P
5	C	405	LPE	C31-O33-P-O3
5	C	405	LPE	C31-O33-P-O31
5	C	405	LPE	C32-C31-O33-P
6	A	411	CLR	C13-C17-C20-C21
6	A	414	CLR	C13-C17-C20-C21
6	A	414	CLR	C16-C17-C20-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	425	CLR	C13-C17-C20-C21
6	C	403	CLR	C13-C17-C20-C21
6	C	412	CLR	C13-C17-C20-C21
6	C	415	CLR	C13-C17-C20-C21
6	C	415	CLR	C16-C17-C20-C22
7	A	417	PLM	O2-C1-C2-C3
7	A	418	PLM	O2-C1-C2-C3
7	A	421	PLM	O2-C1-C2-C3
7	C	418	PLM	O2-C1-C2-C3
7	C	419	PLM	O2-C1-C2-C3
7	C	422	PLM	O2-C1-C2-C3
4	A	403	P0E	O14-C13-O5-C3
4	C	404	P0E	O14-C13-O5-C3
6	A	414	CLR	C16-C17-C20-C21
6	A	425	CLR	C16-C17-C20-C21
6	C	402	CLR	C16-C17-C20-C21
6	C	403	CLR	C16-C17-C20-C21
6	C	415	CLR	C16-C17-C20-C21
6	C	402	CLR	C13-C17-C20-C21
6	A	425	CLR	C16-C17-C20-C22
6	C	403	CLR	C16-C17-C20-C22
6	A	414	CLR	C13-C17-C20-C22
6	A	424	CLR	C13-C17-C20-C22
6	C	415	CLR	C13-C17-C20-C22
4	A	403	P0E	C24-C13-O5-C3
4	C	404	P0E	C24-C13-O5-C3
3	A	401	76F	C11-C10-O2-C2
3	C	401	76F	C11-C10-O2-C2
6	A	410	CLR	C21-C20-C22-C23
6	A	424	CLR	C16-C17-C20-C21
6	A	424	CLR	C13-C17-C20-C21
6	A	411	CLR	C16-C17-C20-C22
6	C	412	CLR	C16-C17-C20-C22
6	A	425	CLR	C13-C17-C20-C22
6	C	402	CLR	C13-C17-C20-C22
6	C	403	CLR	C13-C17-C20-C22
3	A	402	76F	C20-C21-C22-C23
3	A	426	76F	C20-C21-C22-C23
6	C	411	CLR	C21-C20-C22-C23
6	A	407	CLR	C13-C17-C20-C21
6	C	408	CLR	C13-C17-C20-C21
6	C	402	CLR	C16-C17-C20-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	411	CLR	C17-C20-C22-C23
6	C	408	CLR	C13-C17-C20-C22
6	A	410	CLR	C17-C20-C22-C23
6	C	411	CLR	C17-C20-C22-C23
6	C	412	CLR	C17-C20-C22-C23
6	C	412	CLR	C21-C20-C22-C23
6	C	408	CLR	C16-C17-C20-C21
6	A	407	CLR	C13-C17-C20-C22
6	A	411	CLR	C21-C20-C22-C23
6	C	412	CLR	C13-C17-C20-C22
6	A	410	CLR	C22-C23-C24-C25
6	C	411	CLR	C22-C23-C24-C25
6	A	407	CLR	C16-C17-C20-C21
3	A	402	76F	C31-C32-C33-C34
3	A	426	76F	C31-C32-C33-C34
6	A	424	CLR	C16-C17-C20-C22
6	C	415	CLR	C22-C23-C24-C25
6	A	414	CLR	C22-C23-C24-C25
6	C	412	CLR	C16-C17-C20-C21
6	A	411	CLR	C13-C17-C20-C22
6	C	410	CLR	C20-C22-C23-C24
6	A	409	CLR	C20-C22-C23-C24
3	A	402	76F	C31-C30-O3-C3
6	C	403	CLR	C20-C22-C23-C24
6	B	201	CLR	C13-C17-C20-C22
6	A	425	CLR	C20-C22-C23-C24
3	A	426	76F	C31-C30-O3-C3
6	A	411	CLR	C16-C17-C20-C21
3	A	402	76F	C35-C36-C37-C38
3	A	402	76F	O5-C30-O3-C3
3	A	426	76F	C2-C1-O3P-P
3	A	426	76F	C35-C36-C37-C38
3	A	426	76F	O5-C30-O3-C3
6	D	201	CLR	C13-C17-C20-C22
6	B	201	CLR	C13-C17-C20-C21
4	A	403	P0E	C15-C11-O1-C2
4	C	404	P0E	C15-C11-O1-C2
4	A	403	P0E	O12-C11-O1-C2
4	C	404	P0E	O12-C11-O1-C2
6	C	408	CLR	C16-C17-C20-C22
3	A	401	76F	O2-C2-C3-O3
3	C	401	76F	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	402	76F	C2-C1-O3P-P
7	A	420	PLM	C2-C3-C4-C5
6	A	407	CLR	C16-C17-C20-C22
7	C	421	PLM	C2-C3-C4-C5
6	D	201	CLR	C13-C17-C20-C21
7	A	418	PLM	C1-C2-C3-C4
7	C	419	PLM	C1-C2-C3-C4
6	B	201	CLR	C16-C17-C20-C21
3	A	401	76F	C20-C21-C22-C23
3	C	401	76F	C20-C21-C22-C23
6	D	201	CLR	C16-C17-C20-C21
3	A	402	76F	C1-C2-O2-C10
3	A	426	76F	C1-C2-O2-C10
3	A	402	76F	C17-C18-C19-C20
3	A	401	76F	O3-C30-C31-C32
6	B	201	CLR	C16-C17-C20-C22
3	C	401	76F	O3-C30-C31-C32
6	D	201	CLR	C16-C17-C20-C22
5	A	404	LPE	C2-C3-O3-P
5	C	405	LPE	C2-C3-O3-P
6	C	403	CLR	C23-C24-C25-C26
6	C	407	CLR	C22-C23-C24-C25
6	A	406	CLR	C23-C24-C25-C27
6	A	425	CLR	C23-C24-C25-C26
6	A	406	CLR	C22-C23-C24-C25
6	B	202	CLR	C13-C17-C20-C22
3	A	402	76F	C34-C35-C36-C37
6	C	406	CLR	C13-C17-C20-C21
3	A	426	76F	C34-C35-C36-C37
6	C	407	CLR	C23-C24-C25-C27
6	B	202	CLR	C13-C17-C20-C21
6	D	202	CLR	C13-C17-C20-C22
3	C	401	76F	C1-C2-C3-O3
6	A	409	CLR	C23-C24-C25-C26
6	C	410	CLR	C23-C24-C25-C26
5	A	404	LPE	C14-C15-C16-C17
3	A	426	76F	C16-C17-C18-C19
3	A	426	76F	C5-C4-O4P-P
3	A	426	76F	C17-C18-C19-C20
3	A	402	76F	O2-C2-C3-O3
3	A	426	76F	O2-C2-C3-O3
6	A	405	CLR	C13-C17-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	425	CLR	C23-C24-C25-C27
6	C	403	CLR	C23-C24-C25-C27
6	D	202	CLR	C13-C17-C20-C21
6	C	407	CLR	C23-C24-C25-C26
6	A	425	CLR	C22-C23-C24-C25
6	C	403	CLR	C22-C23-C24-C25
3	A	402	76F	C16-C17-C18-C19
4	A	403	P0E	C22-C23-C34-C42
6	C	408	CLR	C23-C24-C25-C26
5	C	405	LPE	C14-C15-C16-C17
3	A	401	76F	C2-C1-O3P-P
6	B	202	CLR	C16-C17-C20-C22
6	C	406	CLR	C13-C17-C20-C22
3	A	401	76F	C1-C2-C3-O3
3	A	402	76F	C1-C2-C3-O3
3	A	426	76F	C1-C2-C3-O3
6	A	405	CLR	C13-C17-C20-C22
3	A	401	76F	C1-O3P-P-O1P
3	A	402	76F	C4-O4P-P-O1P
3	A	426	76F	C4-O4P-P-O1P
6	D	202	CLR	C16-C17-C20-C22
3	C	401	76F	C2-C1-O3P-P
3	A	401	76F	C24-C25-C26-C27
4	C	404	P0E	C15-C16-C17-C18
3	C	401	76F	C24-C25-C26-C27
5	A	404	LPE	C2-C1-O1-C11
6	C	406	CLR	C16-C17-C20-C22
6	A	406	CLR	C23-C24-C25-C26
5	C	405	LPE	C2-C1-O1-C11
6	C	406	CLR	C16-C17-C20-C21
6	B	202	CLR	C16-C17-C20-C21
6	A	405	CLR	C16-C17-C20-C22
3	C	401	76F	C10-C11-C12-C13
5	A	404	LPE	O2H-C2-C3-O3
4	A	403	P0E	C15-C16-C17-C18
3	A	401	76F	C16-C17-C18-C19
4	A	403	P0E	C20-C21-C22-C23
3	A	401	76F	C10-C11-C12-C13
3	A	402	76F	C36-C37-C38-C39
6	A	405	CLR	C16-C17-C20-C21
4	C	404	P0E	C2-C4-O6-P8
7	A	420	PLM	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	409	CLR	C23-C24-C25-C27
5	C	405	LPE	O2H-C2-C3-O3
4	C	404	P0E	C22-C23-C34-C42
4	C	404	P0E	C17-C18-C19-C20
4	A	403	P0E	C4-C2-O1-C11
4	C	404	P0E	C4-C2-O1-C11
7	C	421	PLM	C4-C5-C6-C7
6	D	202	CLR	C16-C17-C20-C21
3	A	401	76F	O5-C30-C31-C32
4	A	403	P0E	C2-C4-O6-P8
6	C	416	CLR	C13-C17-C20-C21
3	A	401	76F	C30-C31-C32-C33
3	C	401	76F	C16-C17-C18-C19
4	C	404	P0E	C20-C21-C22-C23
6	A	415	CLR	C13-C17-C20-C21
6	C	411	CLR	C20-C22-C23-C24
6	A	407	CLR	C23-C24-C25-C26
4	A	403	P0E	C17-C18-C19-C20
6	C	410	CLR	C23-C24-C25-C27
3	C	401	76F	O5-C30-C31-C32
5	A	404	LPE	C1-C2-C3-O3
5	C	405	LPE	C1-C2-C3-O3
6	A	410	CLR	C20-C22-C23-C24
3	A	402	76F	C5-C4-O4P-P
3	A	426	76F	C32-C33-C34-C35
3	C	401	76F	C40-C41-C42-C43
3	A	426	76F	C36-C37-C38-C39
3	A	426	76F	C11-C12-C13-C14
3	A	401	76F	C40-C41-C42-C43
5	C	405	LPE	C12-C11-O1-C1
4	A	403	P0E	C34-C42-C43-C44
5	A	404	LPE	C12-C11-O1-C1
4	A	403	P0E	C3-C2-O1-C11
4	C	404	P0E	C3-C2-O1-C11
6	A	415	CLR	C16-C17-C20-C22
6	C	416	CLR	C13-C17-C20-C22
6	C	416	CLR	C16-C17-C20-C22
3	C	401	76F	C31-C30-O3-C3
6	A	415	CLR	C13-C17-C20-C22
3	C	401	76F	O5-C30-O3-C3
7	C	418	PLM	C4-C5-C6-C7

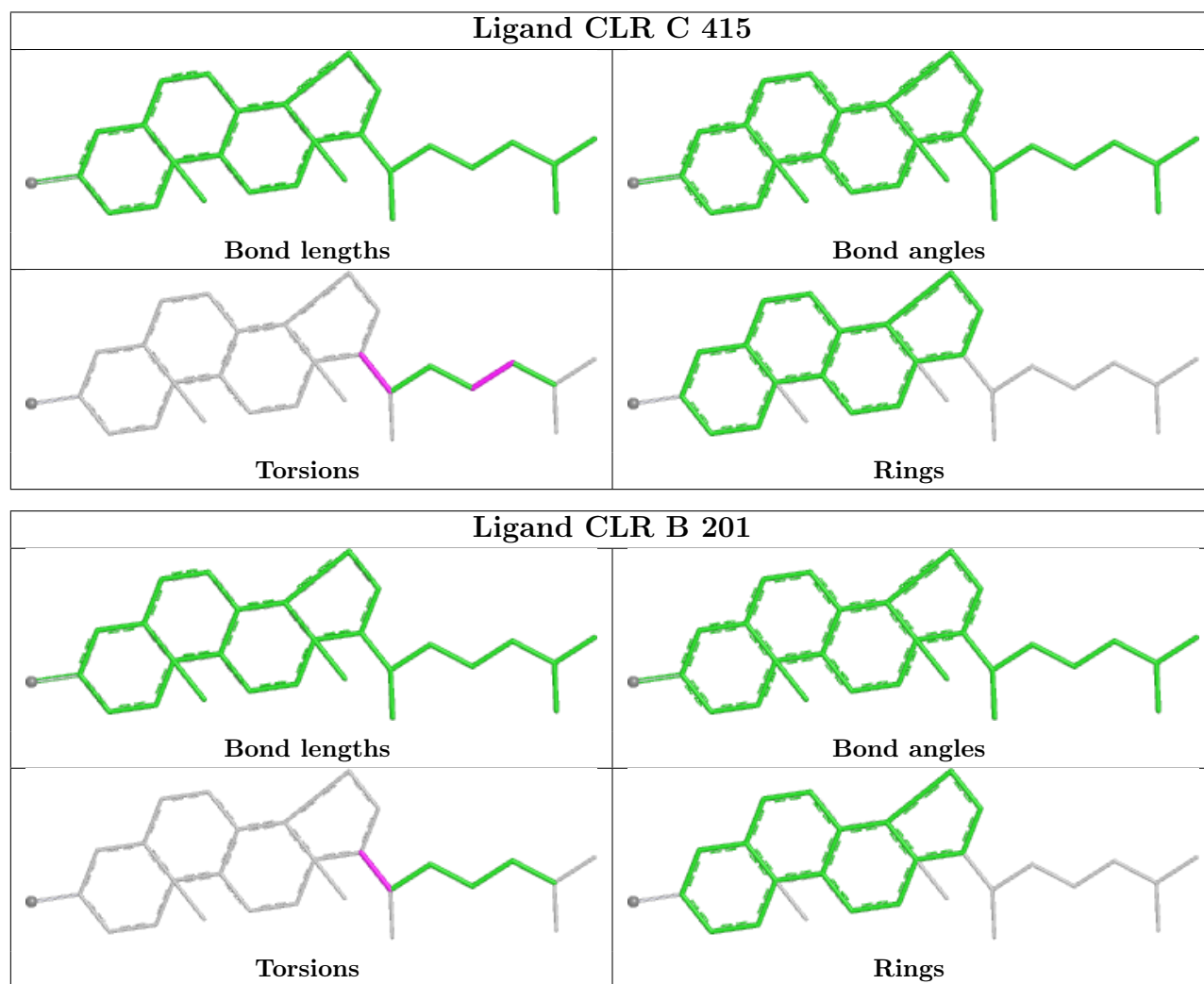
There are no ring outliers.

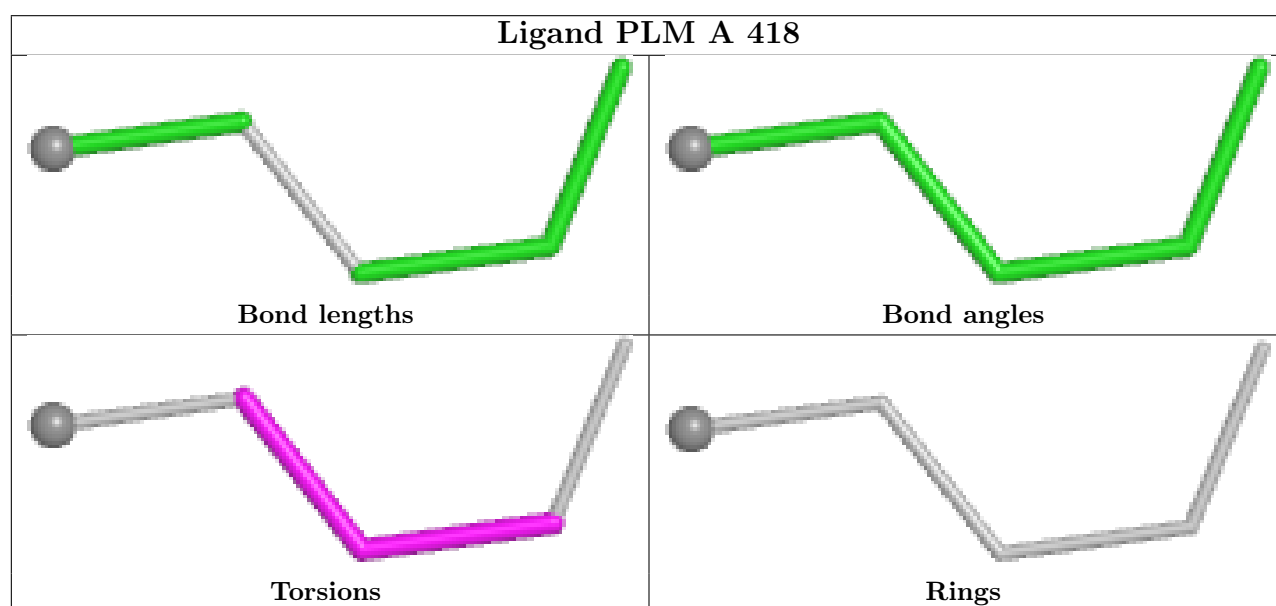
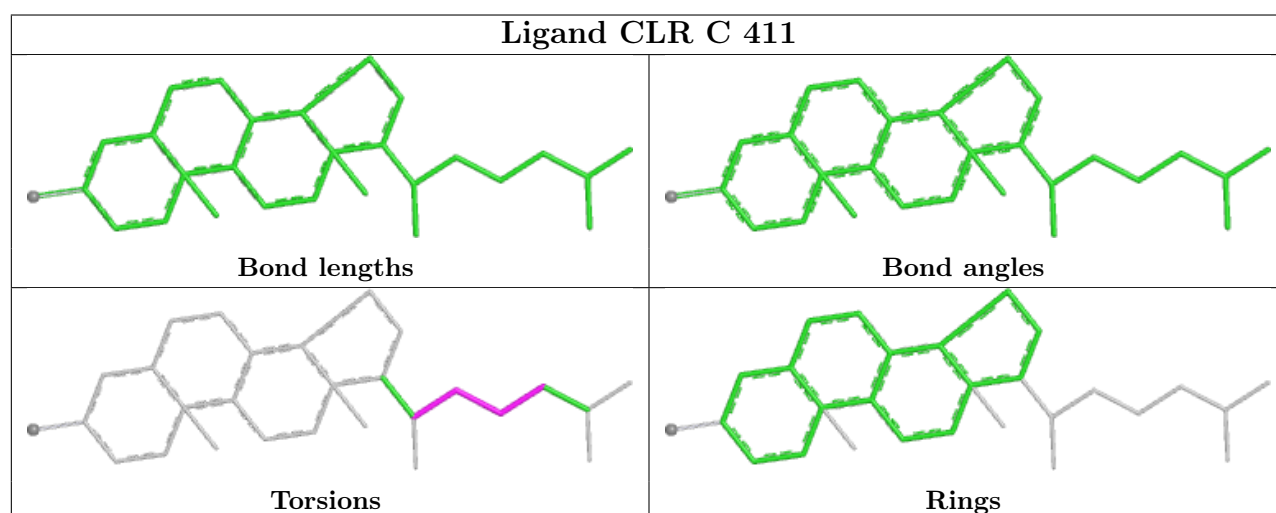
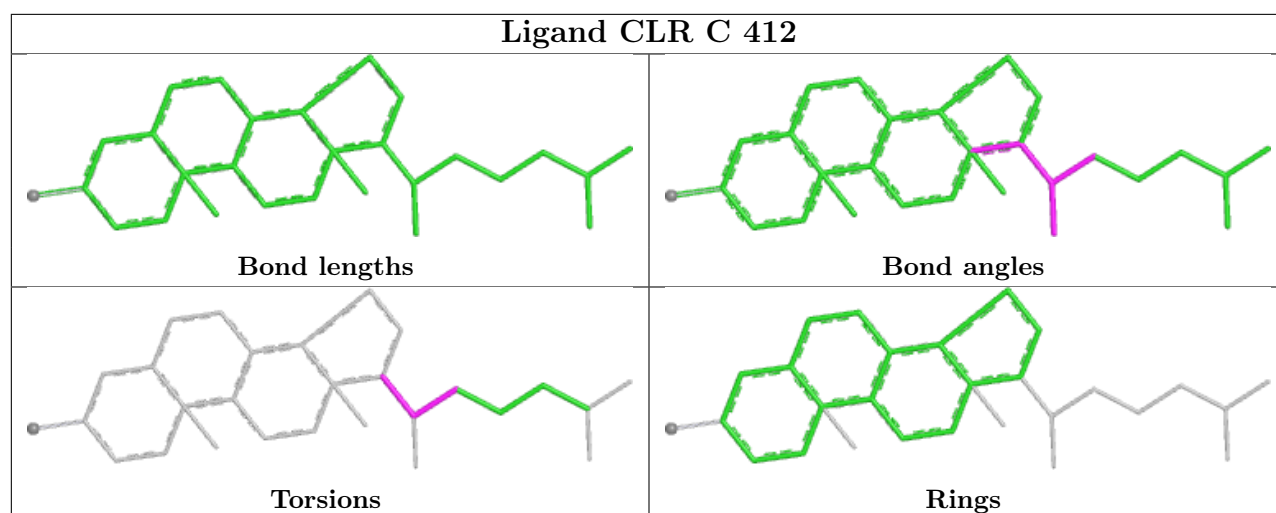
35 monomers are involved in 59 short contacts:

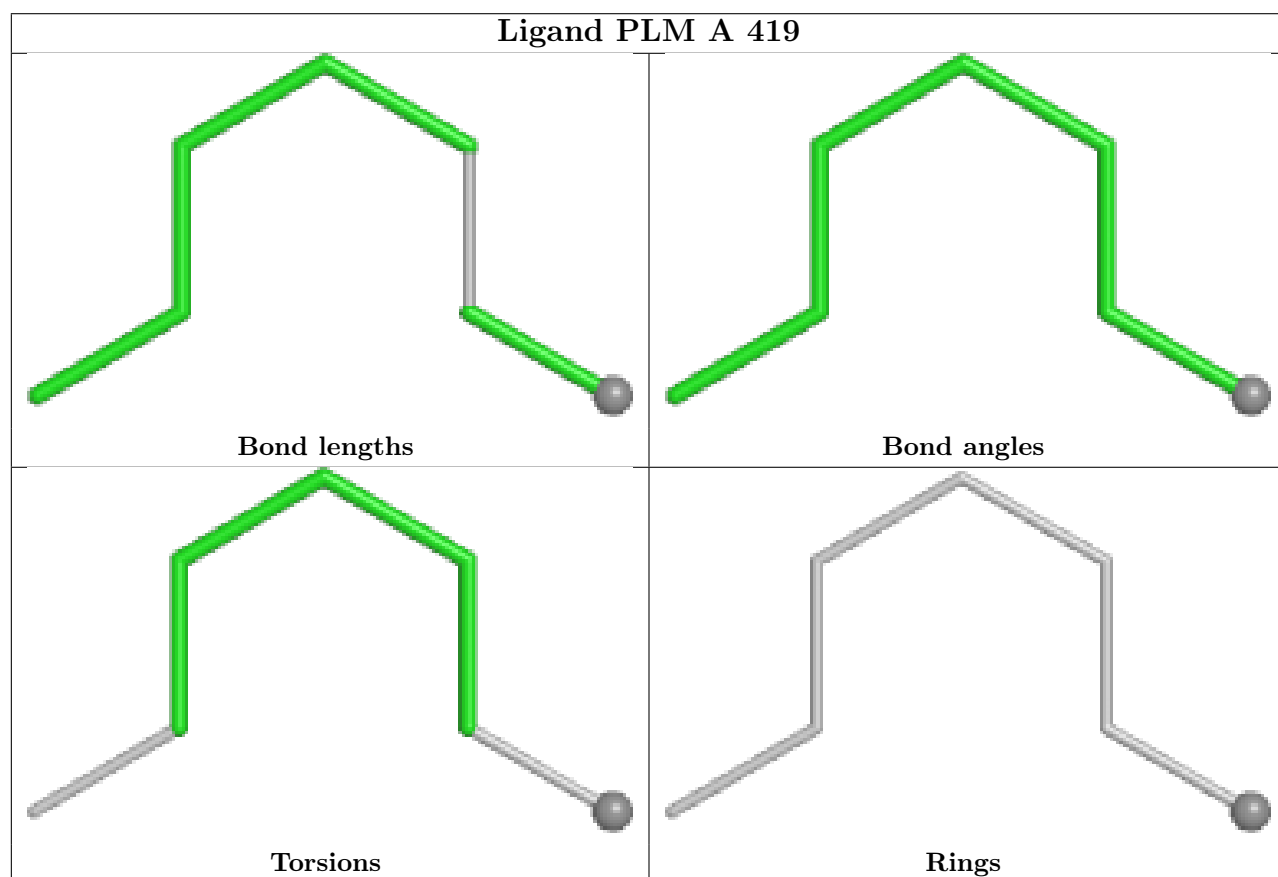
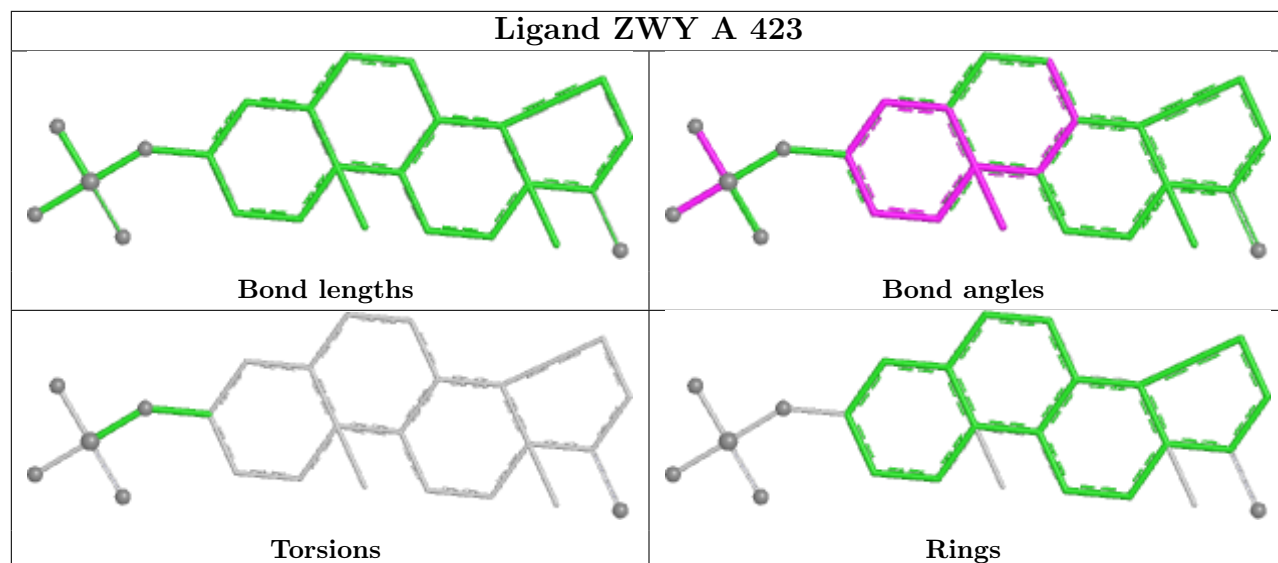
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	415	CLR	1	0
6	B	201	CLR	3	0
6	C	412	CLR	2	0
6	C	411	CLR	2	0
6	A	415	CLR	2	0
7	A	417	PLM	1	0
7	C	421	PLM	1	0
6	D	201	CLR	2	0
6	A	408	CLR	2	0
6	C	408	CLR	2	0
6	A	407	CLR	2	0
6	A	425	CLR	6	0
5	A	404	LPE	3	0
7	A	420	PLM	2	0
6	C	410	CLR	1	0
6	A	406	CLR	3	0
4	C	404	P0E	2	0
6	A	410	CLR	2	0
4	A	403	P0E	2	0
6	C	407	CLR	3	0
6	C	416	CLR	2	0
6	A	409	CLR	1	0
6	C	409	CLR	2	0
6	A	412	CLR	2	0
6	A	413	CLR	1	0
6	A	424	CLR	3	0
5	C	405	LPE	5	0
6	C	413	CLR	2	0
6	C	414	CLR	1	0
6	C	402	CLR	2	0
3	A	401	76F	1	0
6	C	403	CLR	5	0
6	D	202	CLR	1	0
6	A	414	CLR	2	0
6	A	411	CLR	1	0

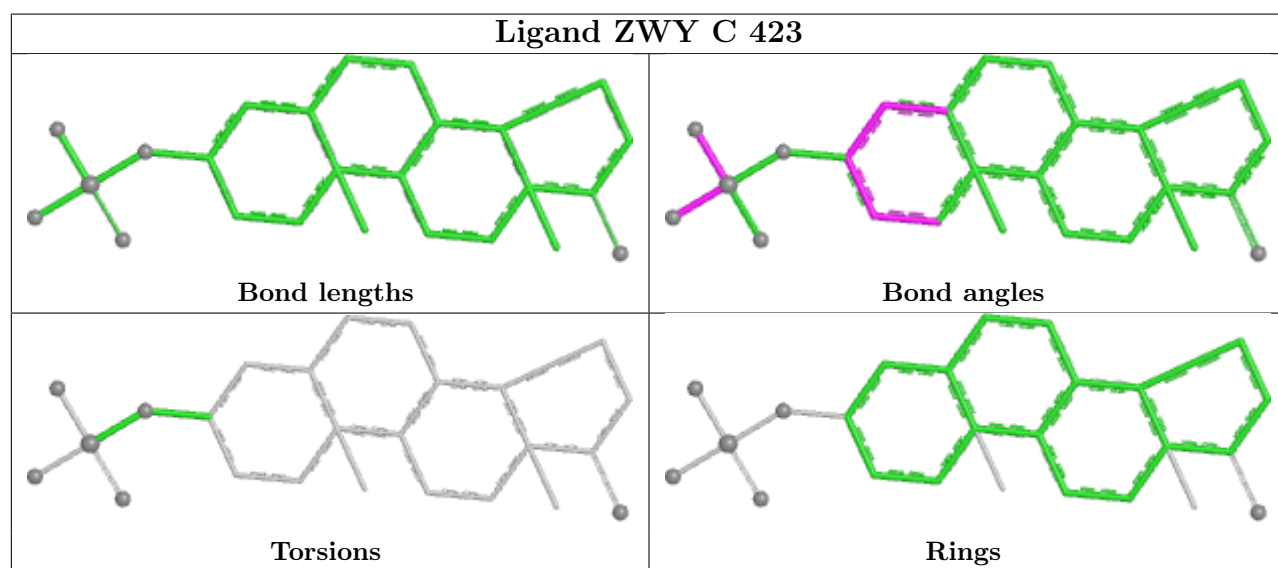
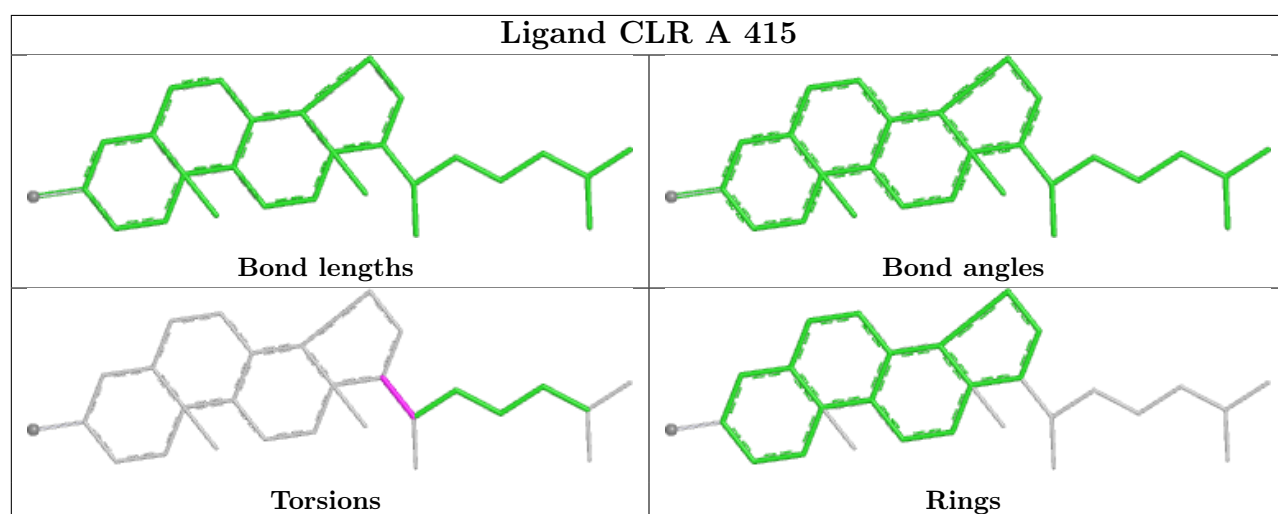
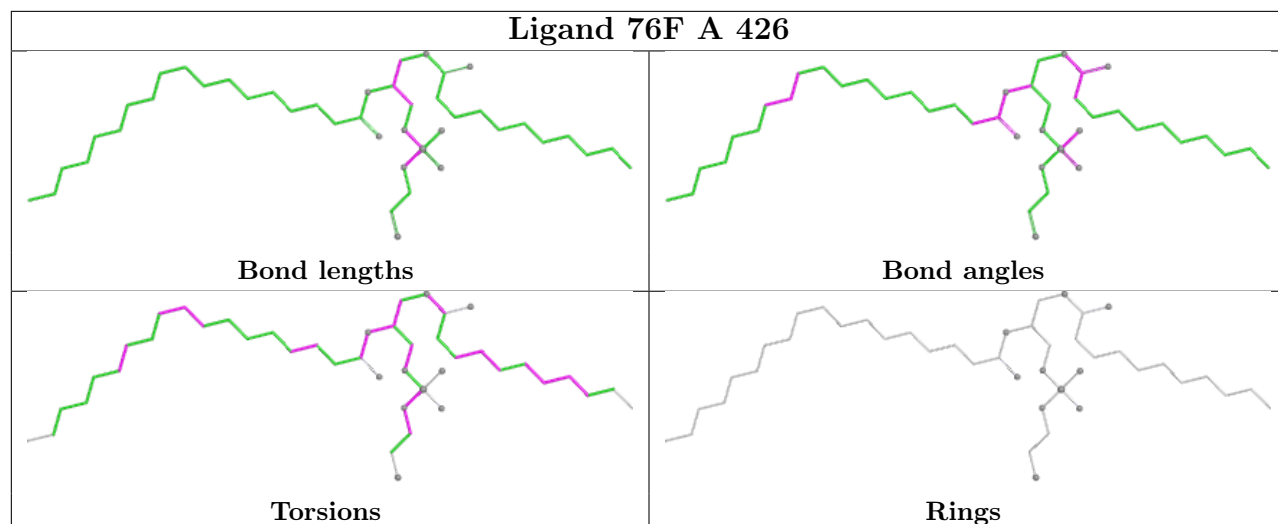
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

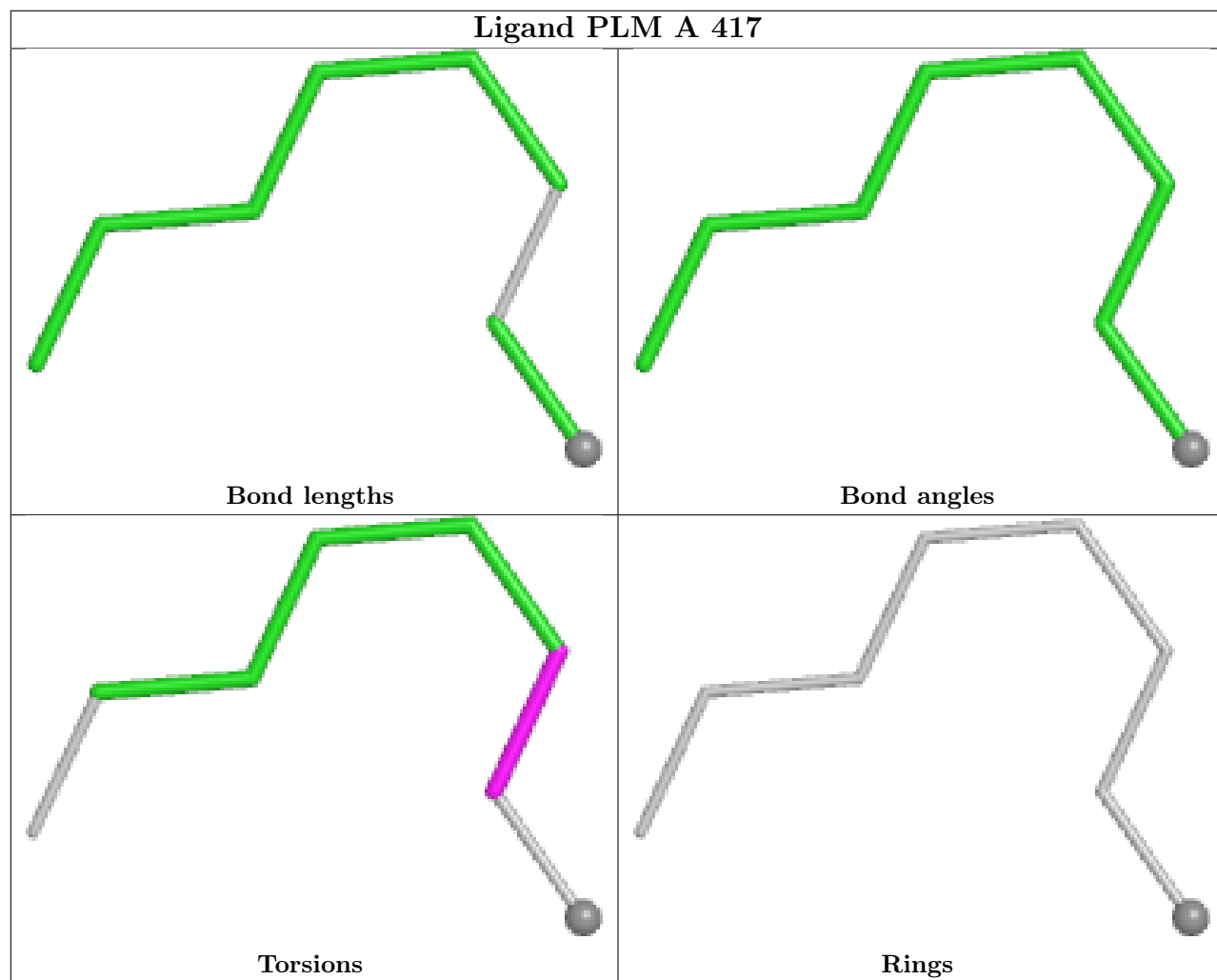
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

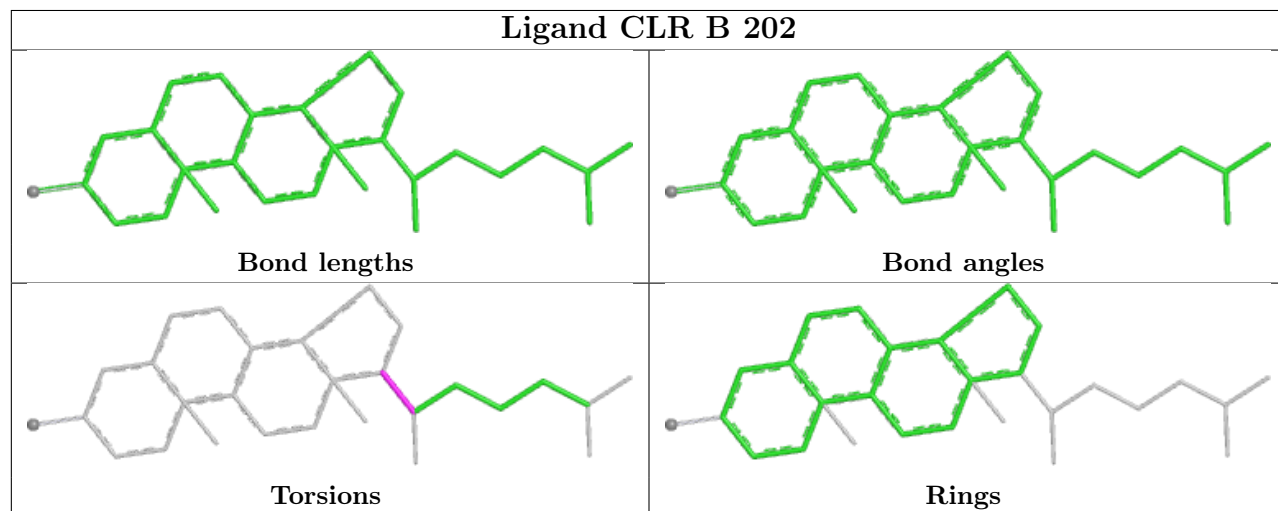
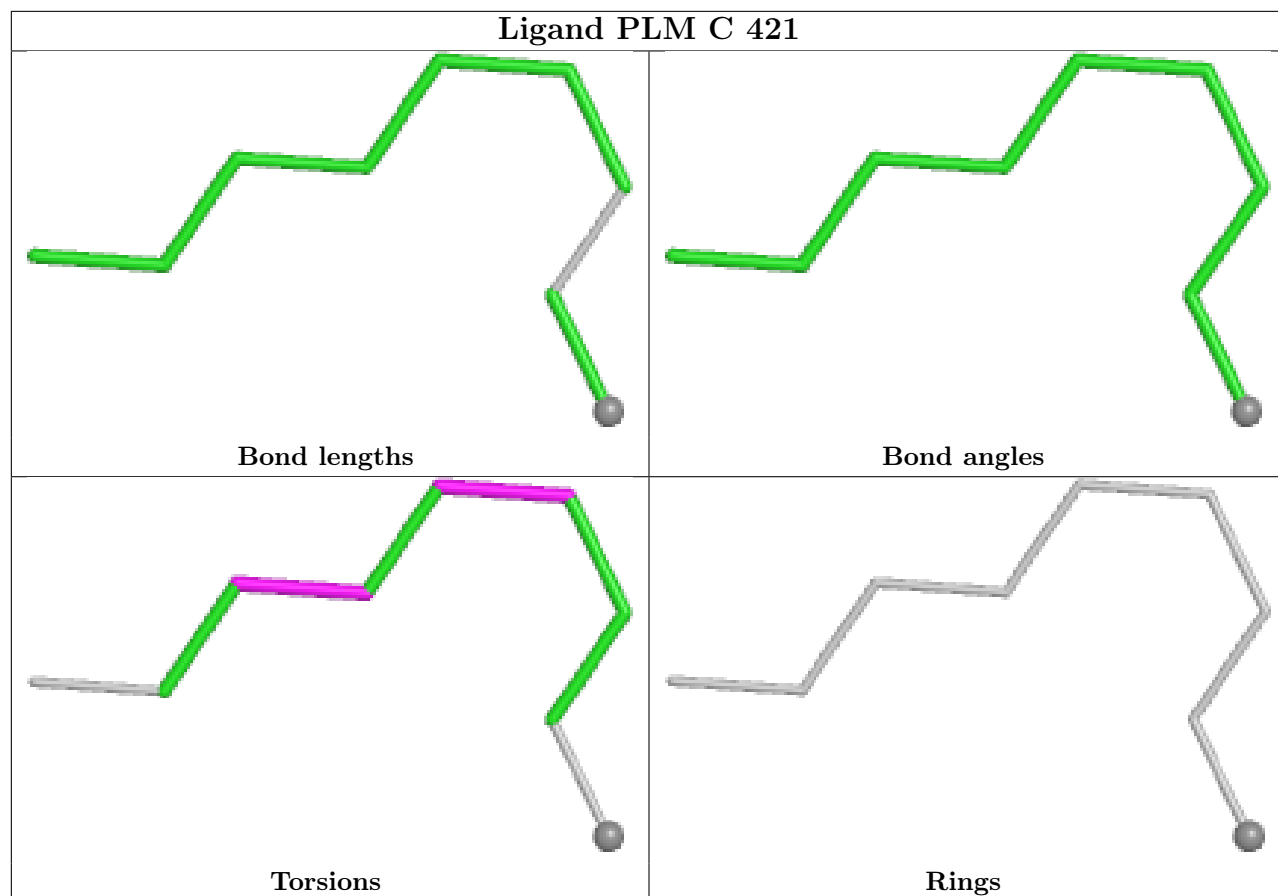


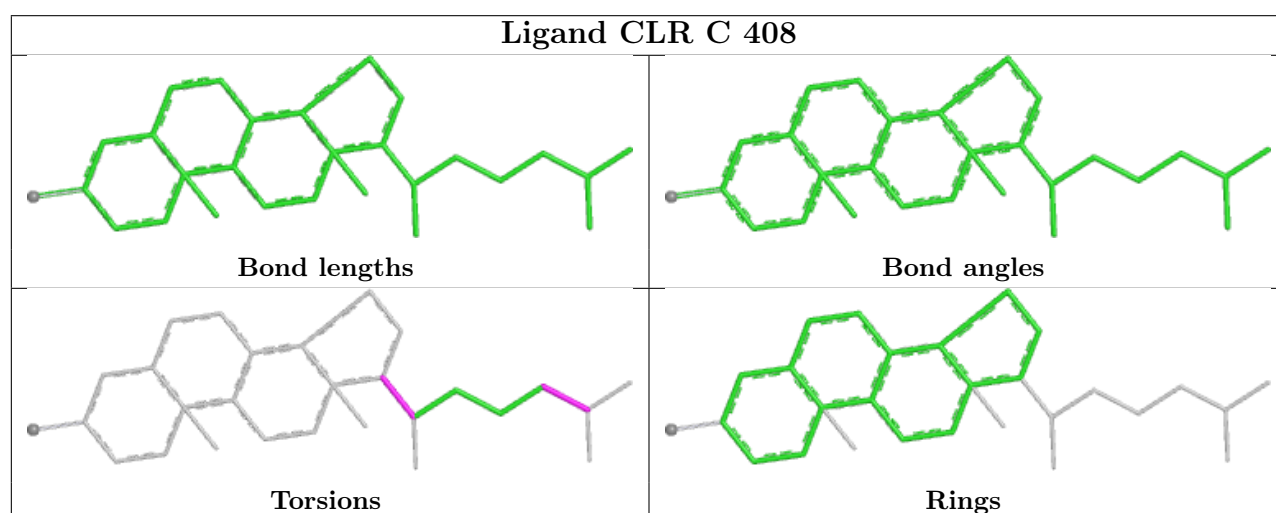
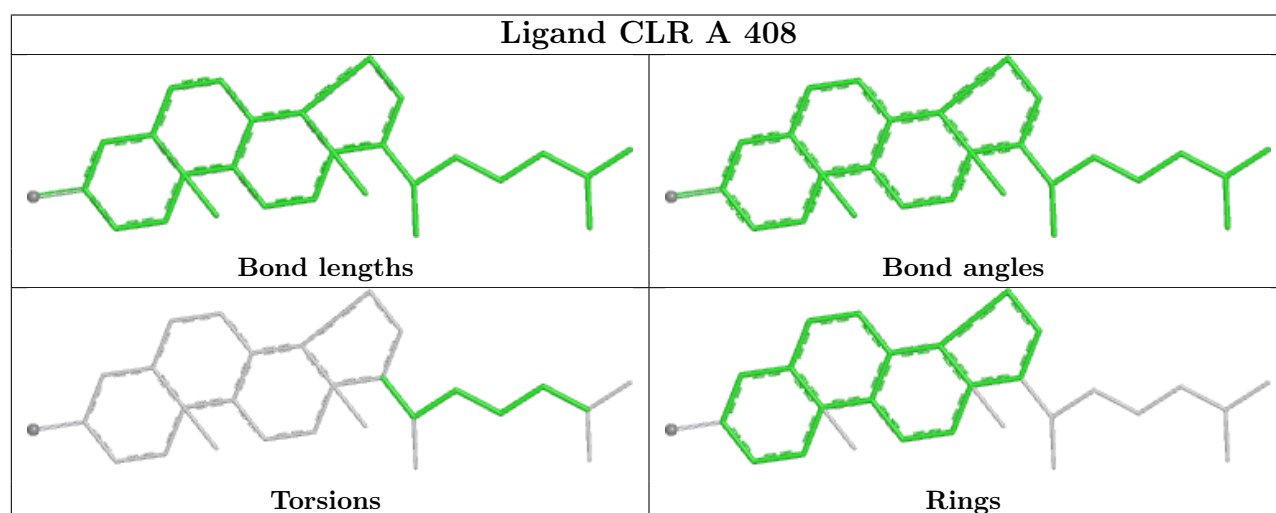
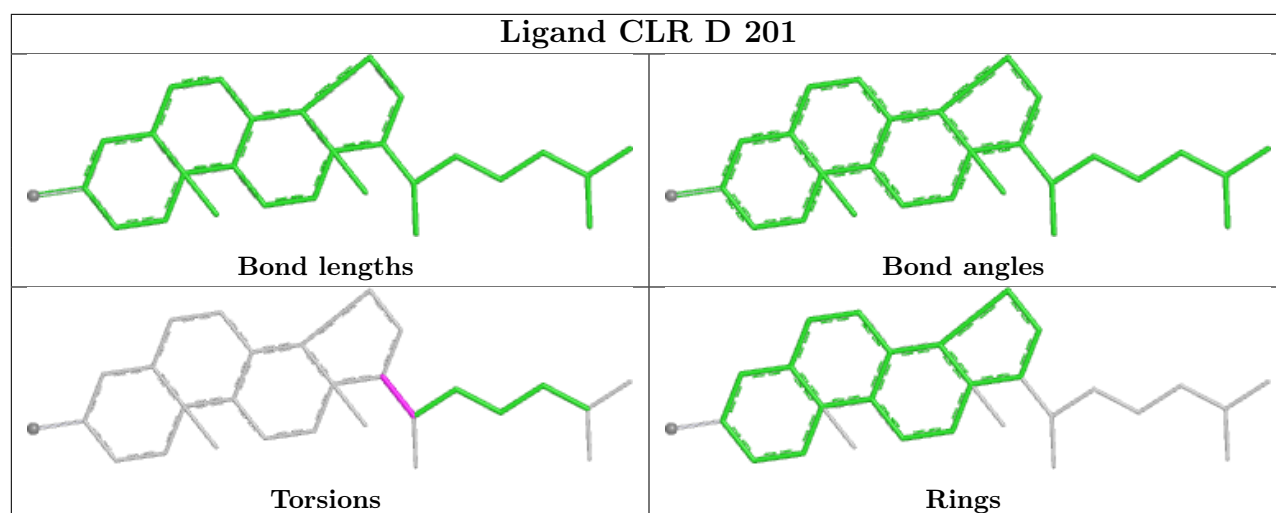


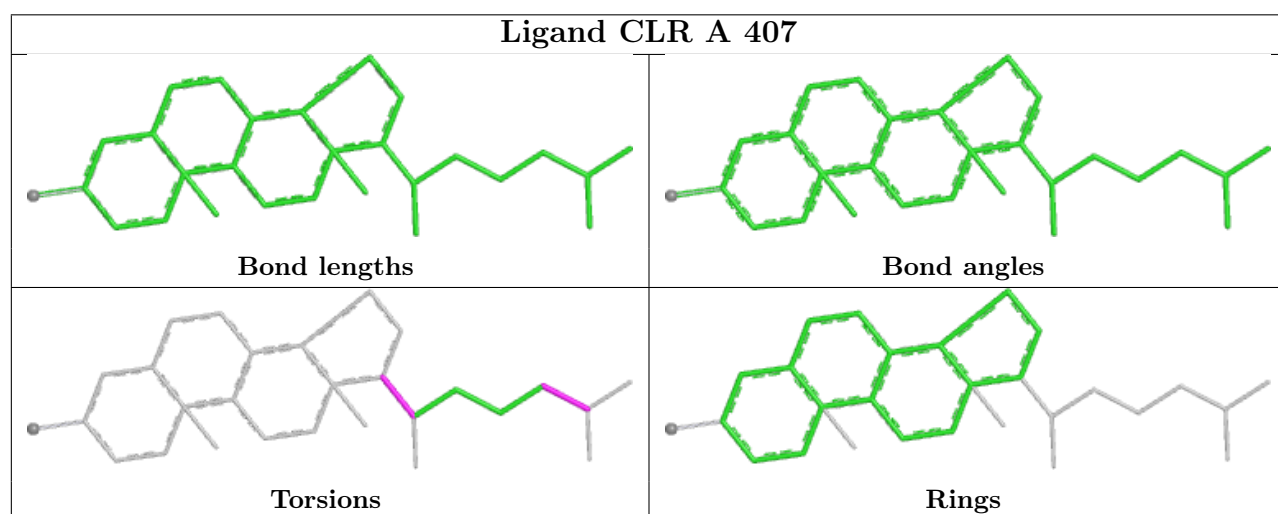
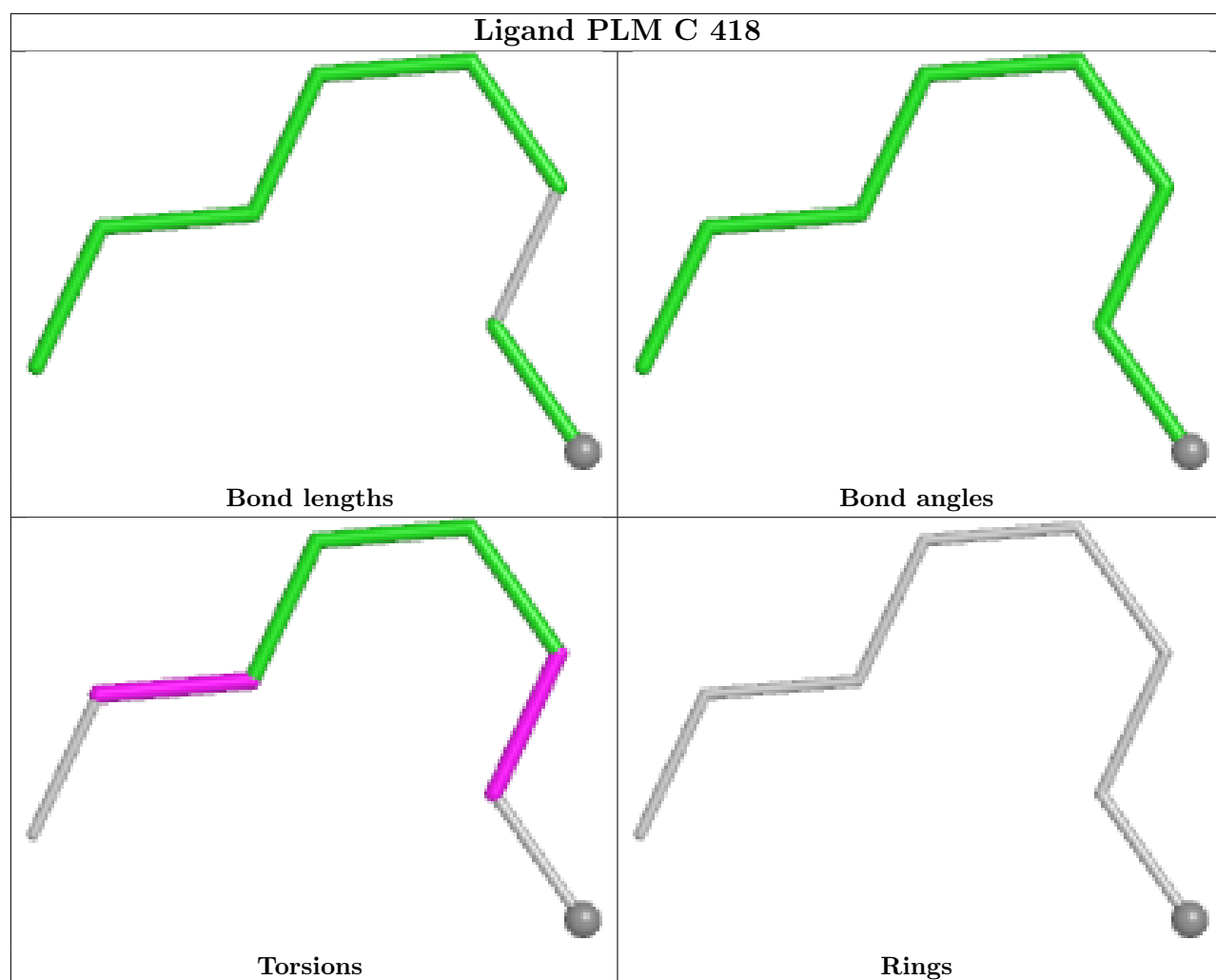


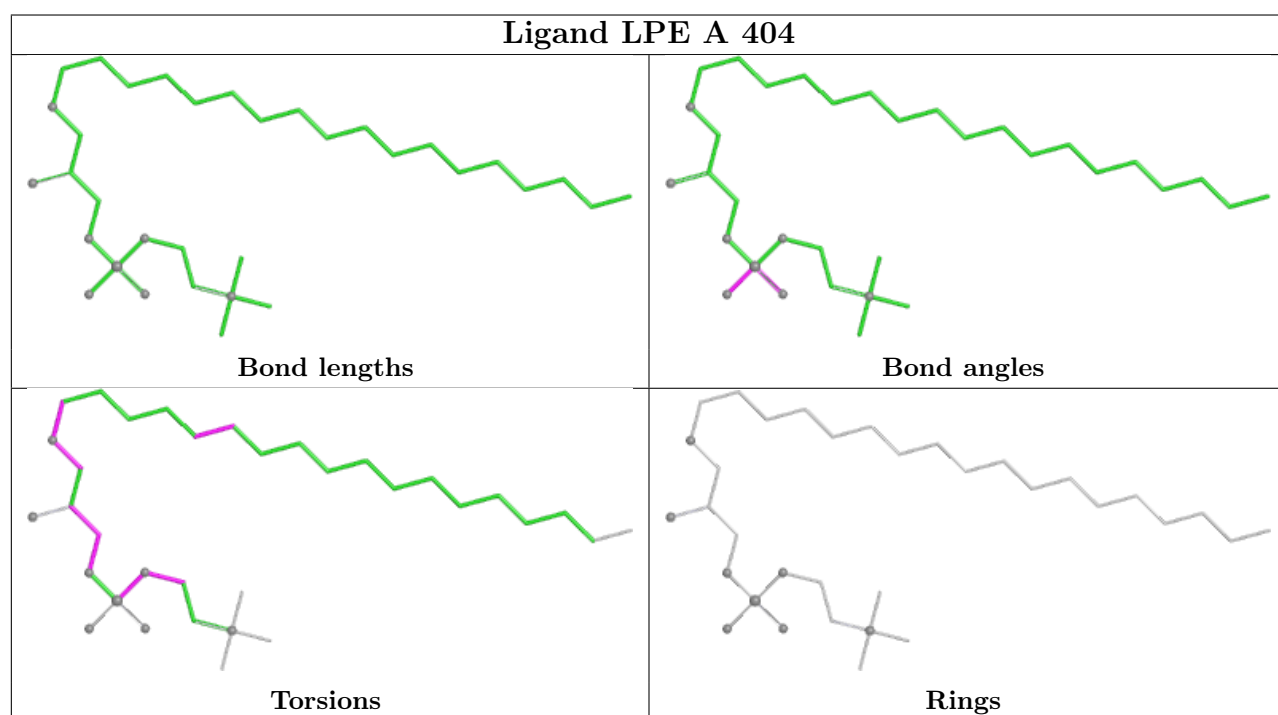
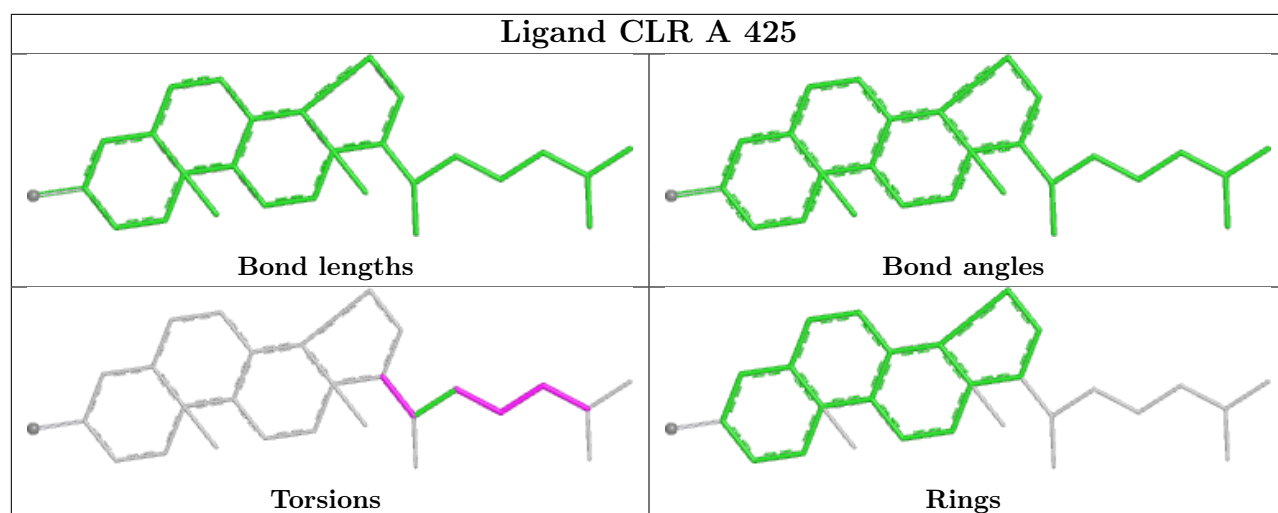


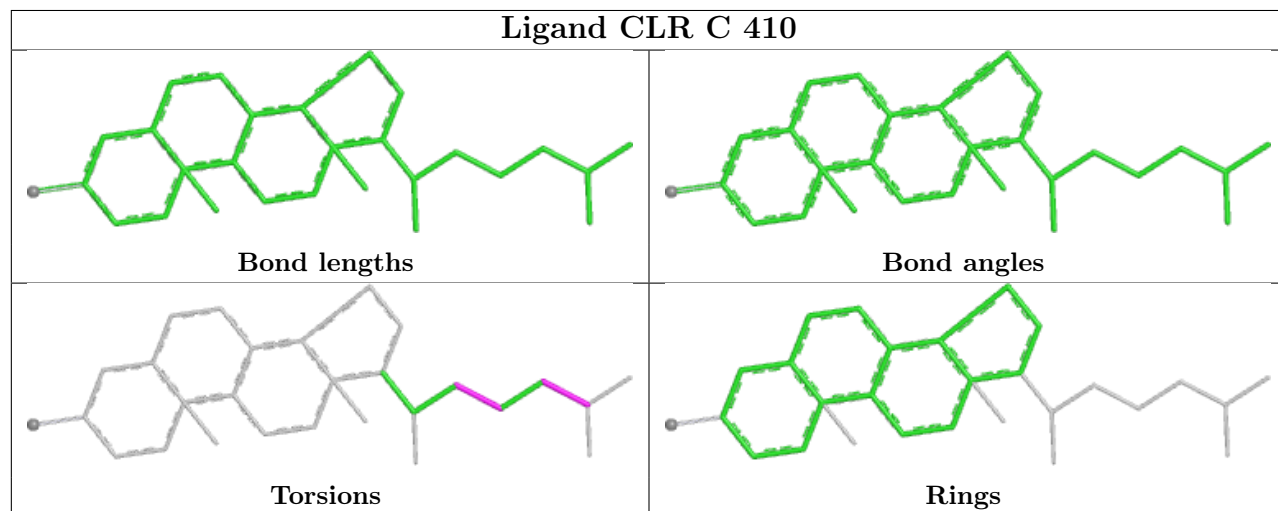
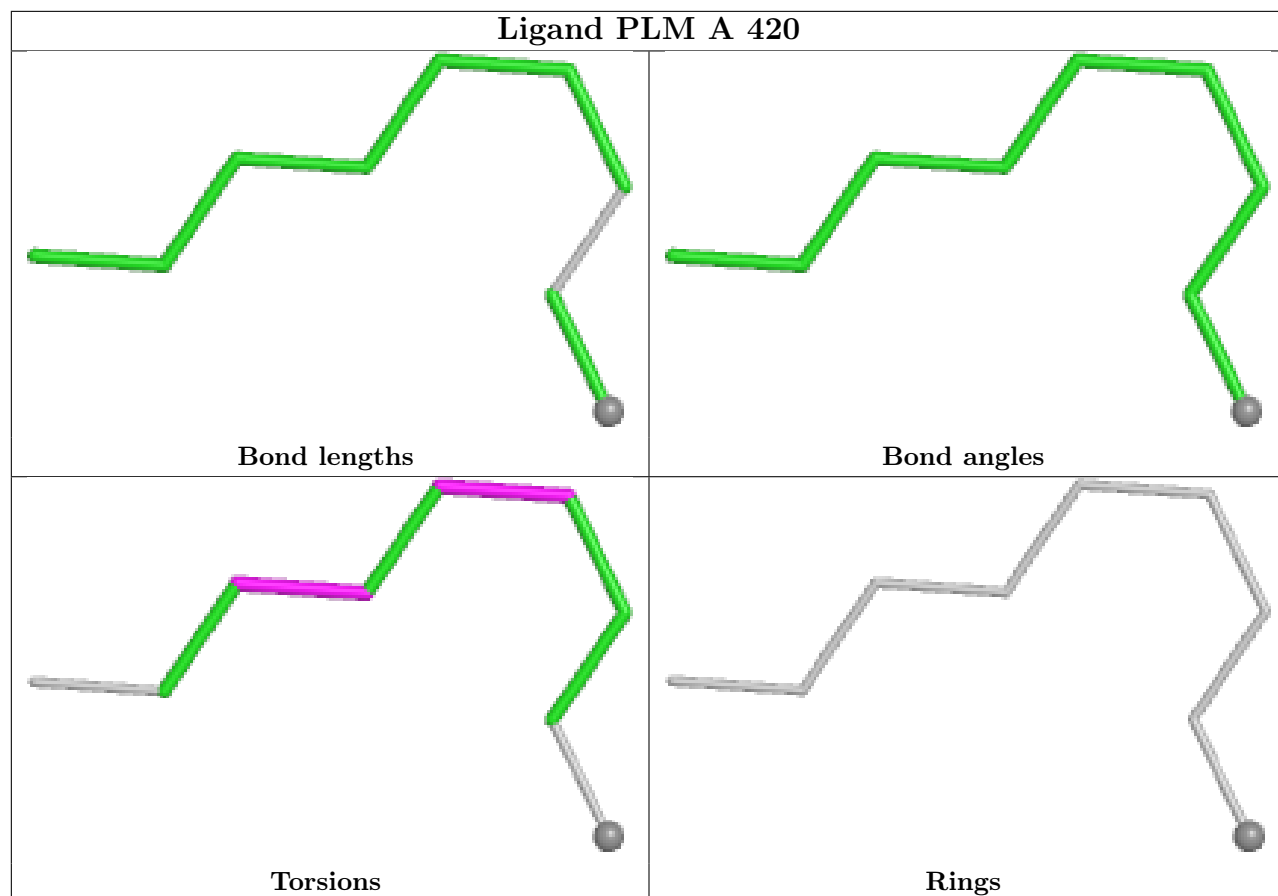


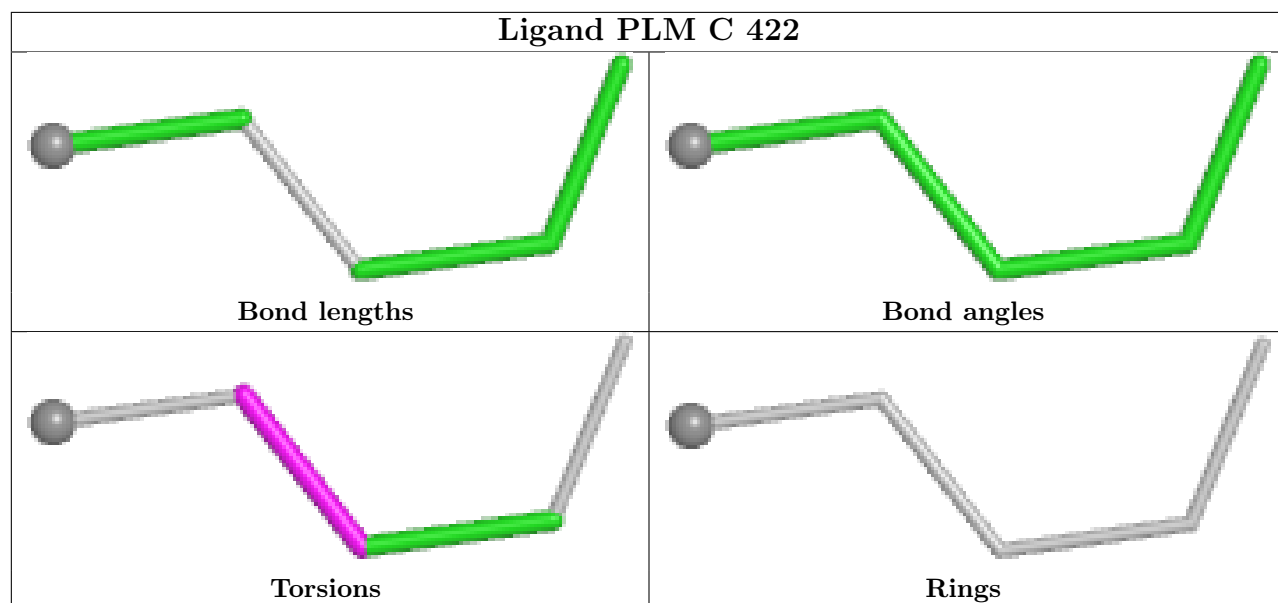
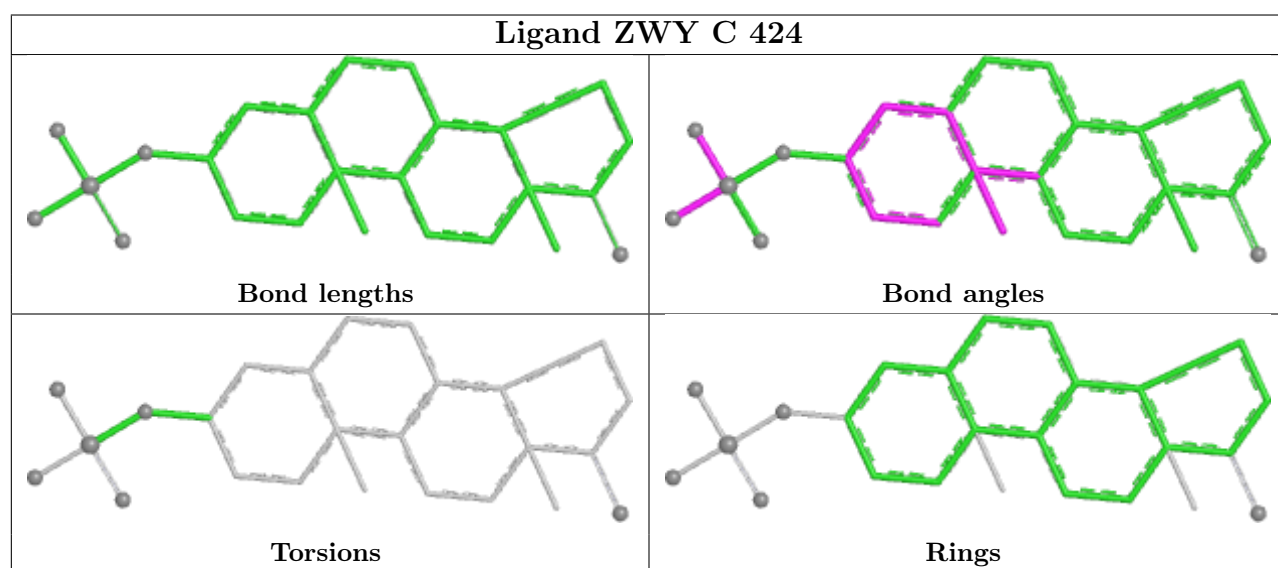
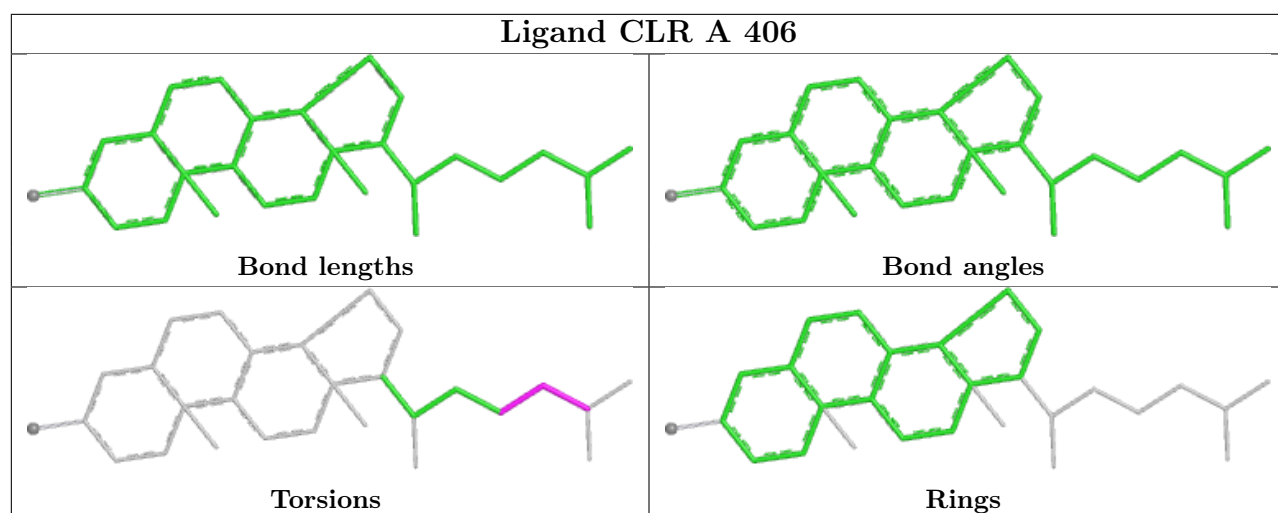


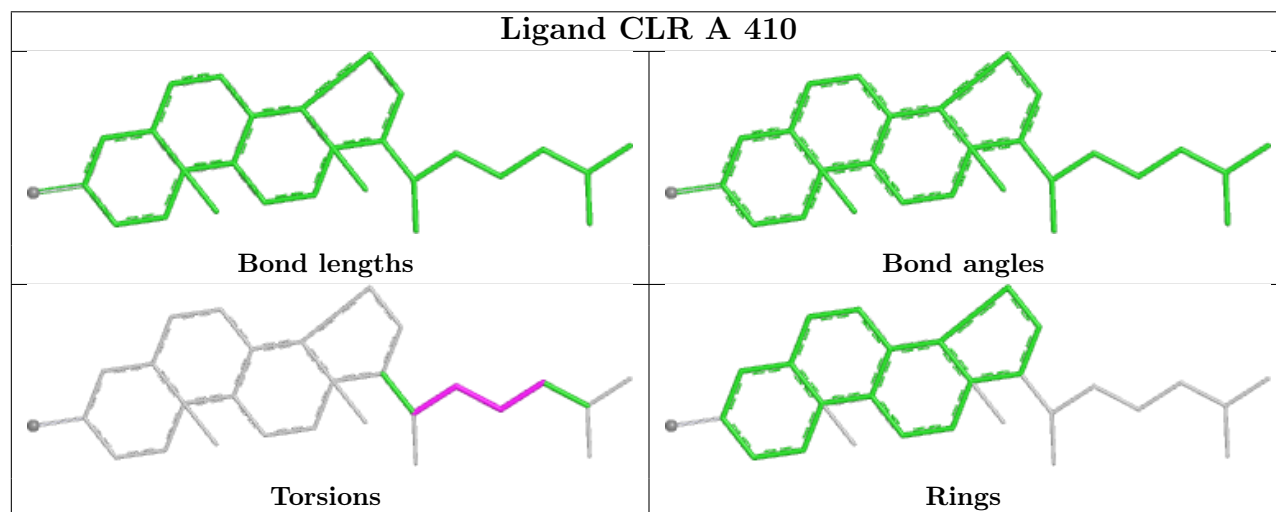
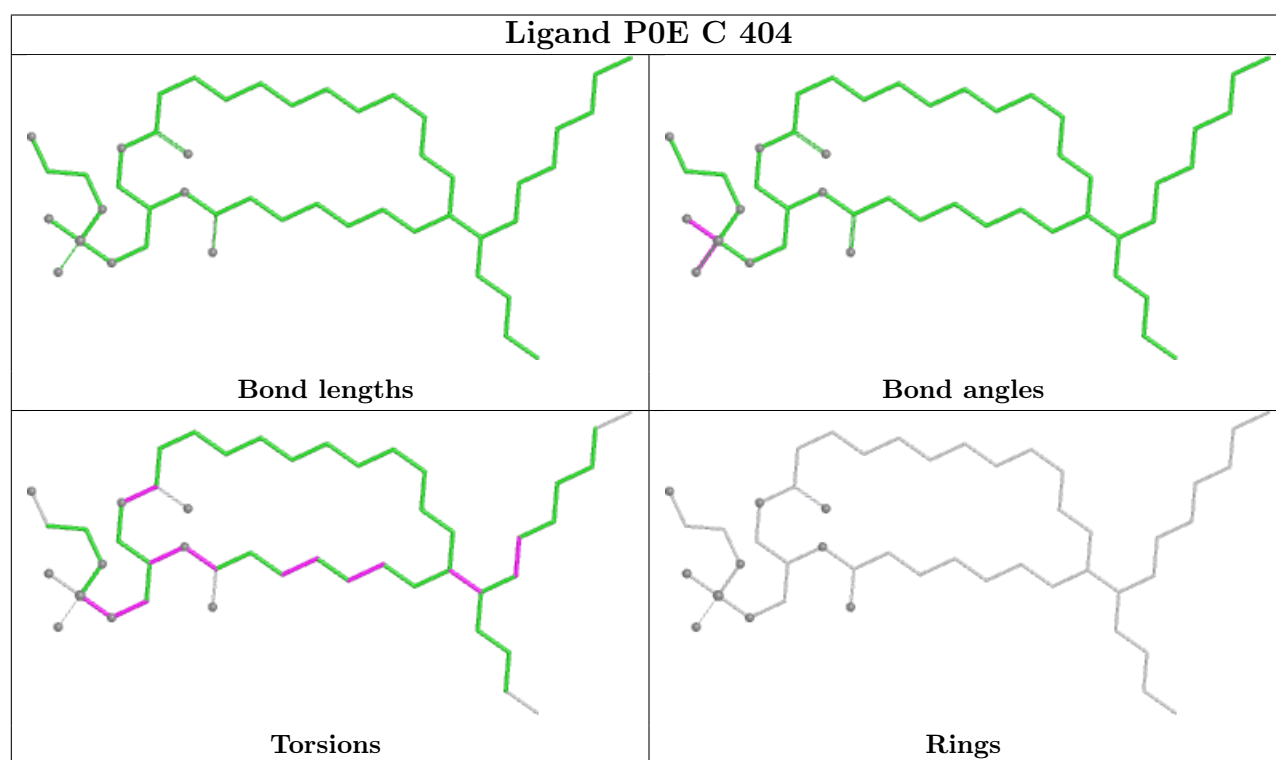
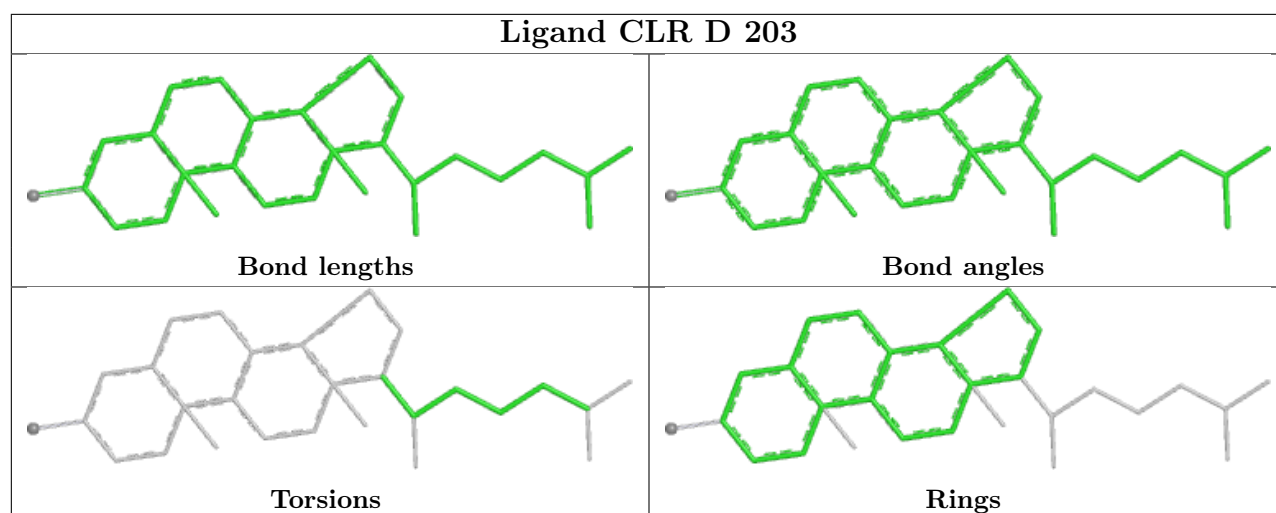


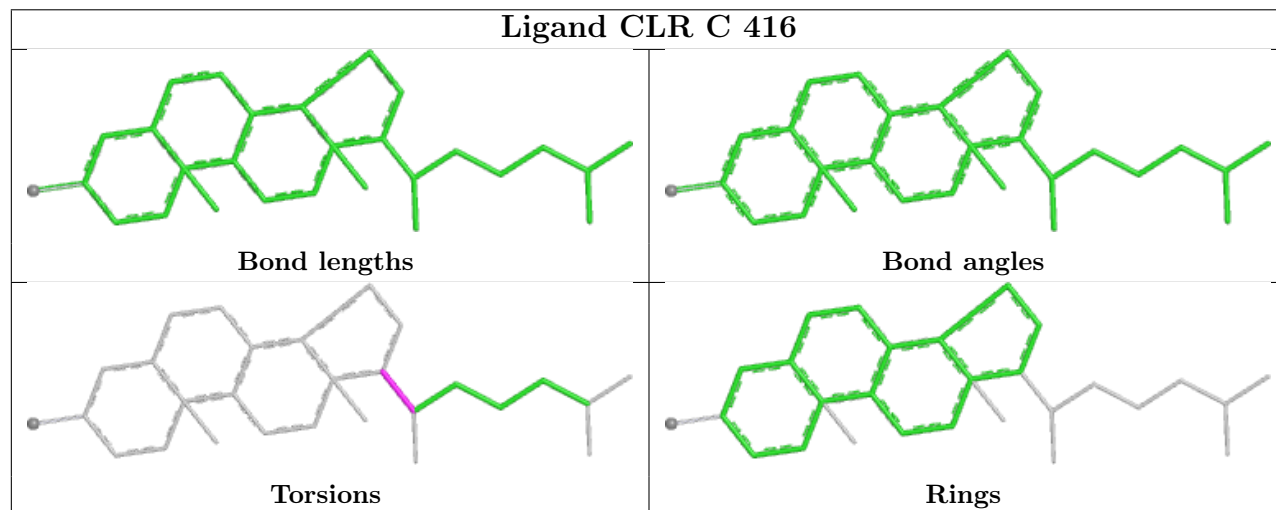
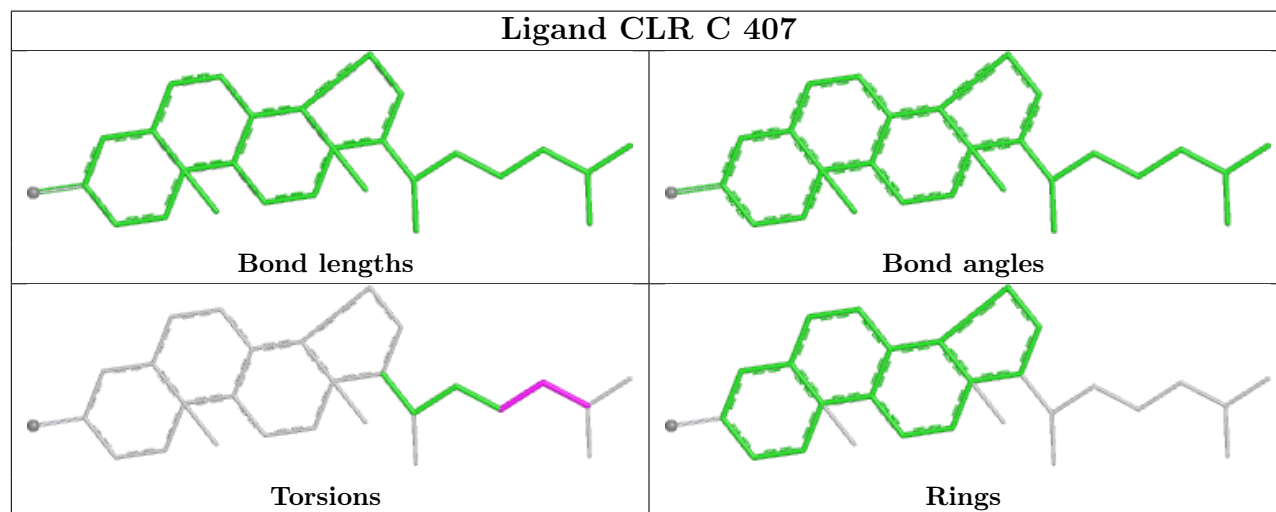
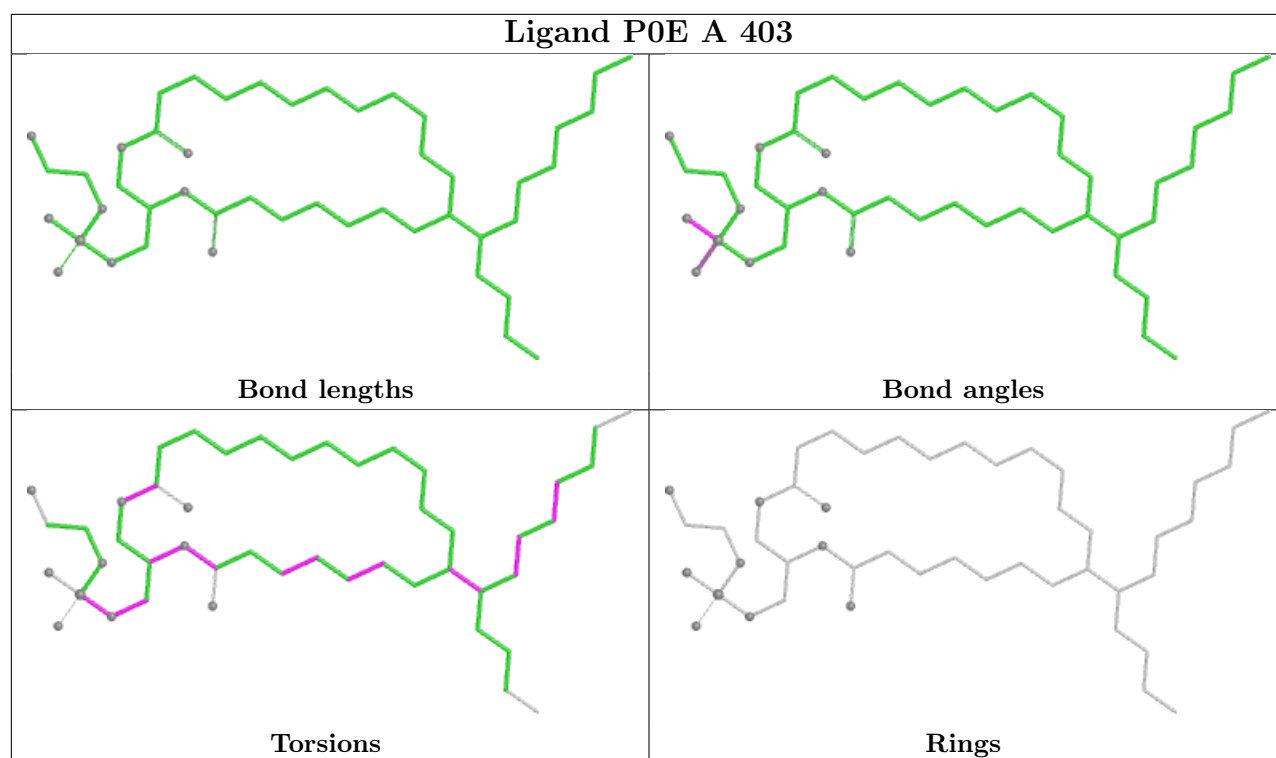


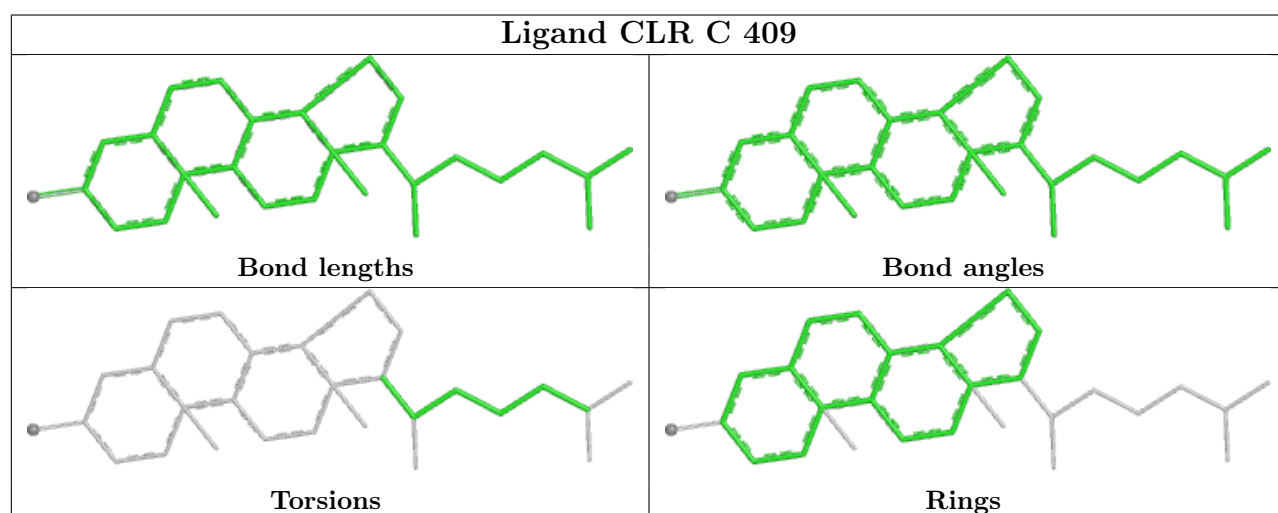
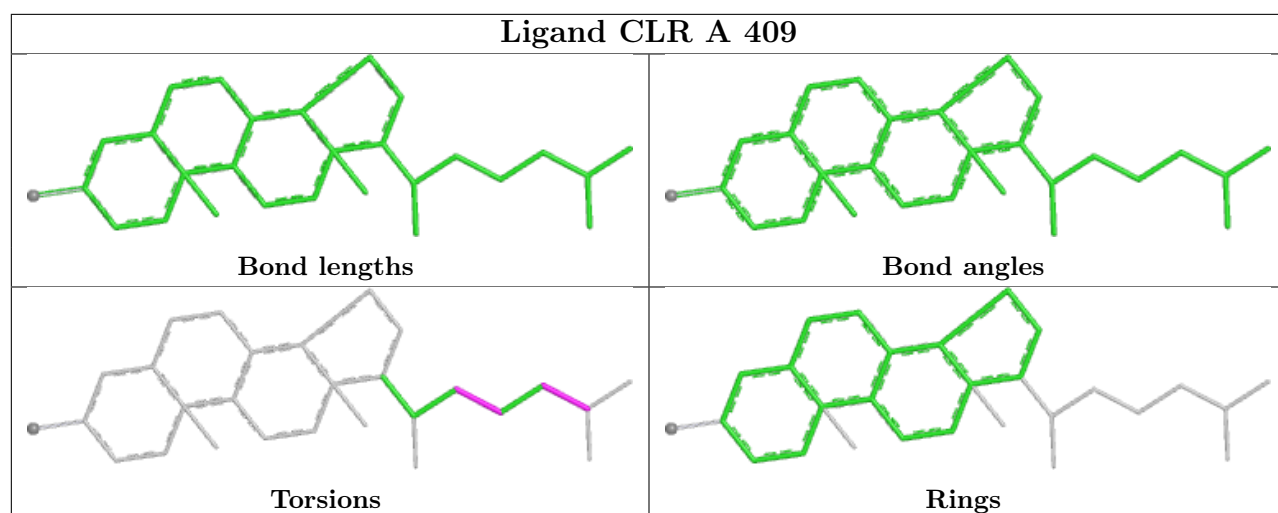


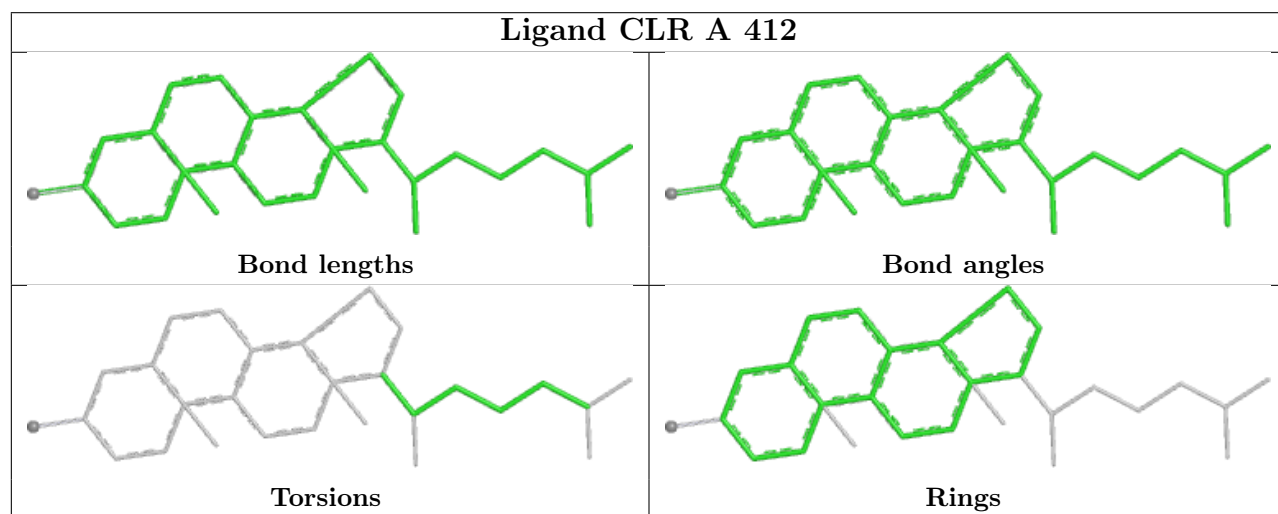
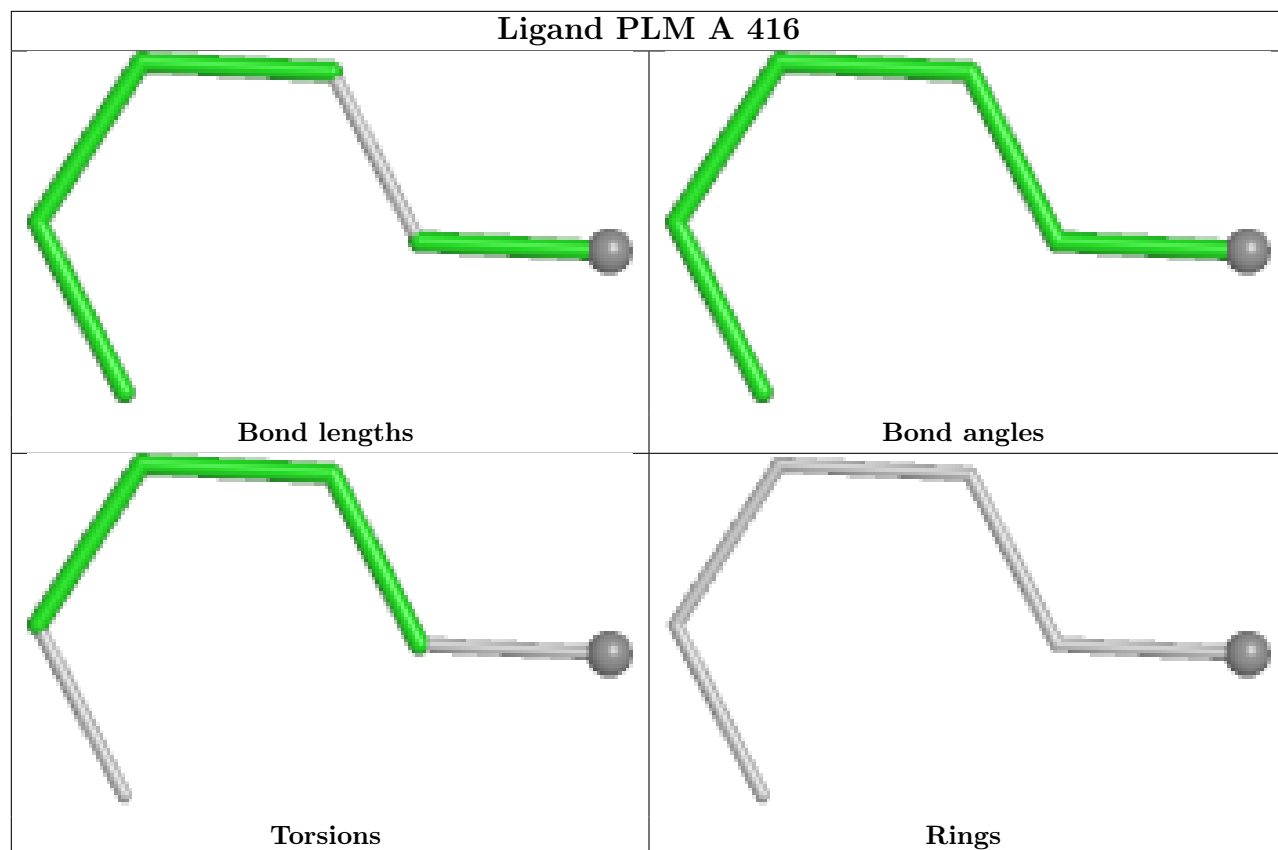


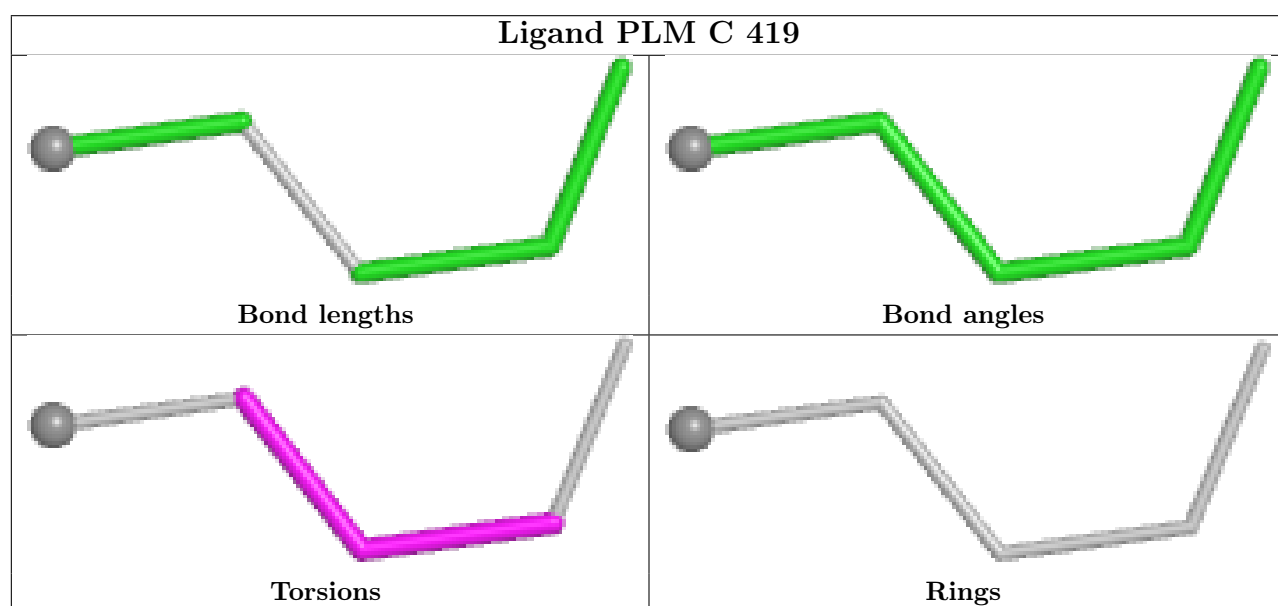
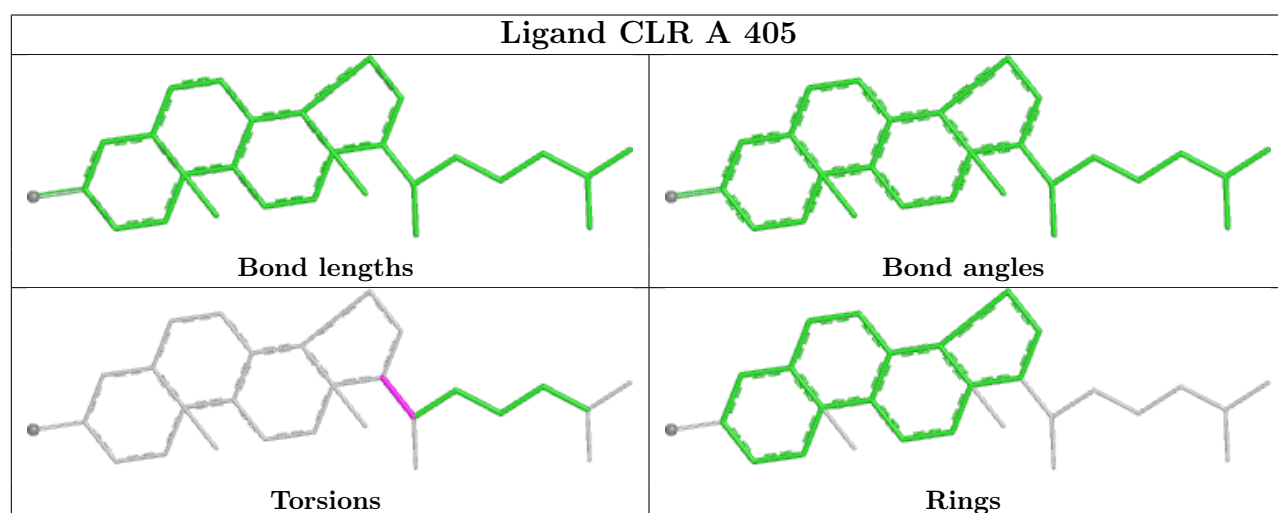
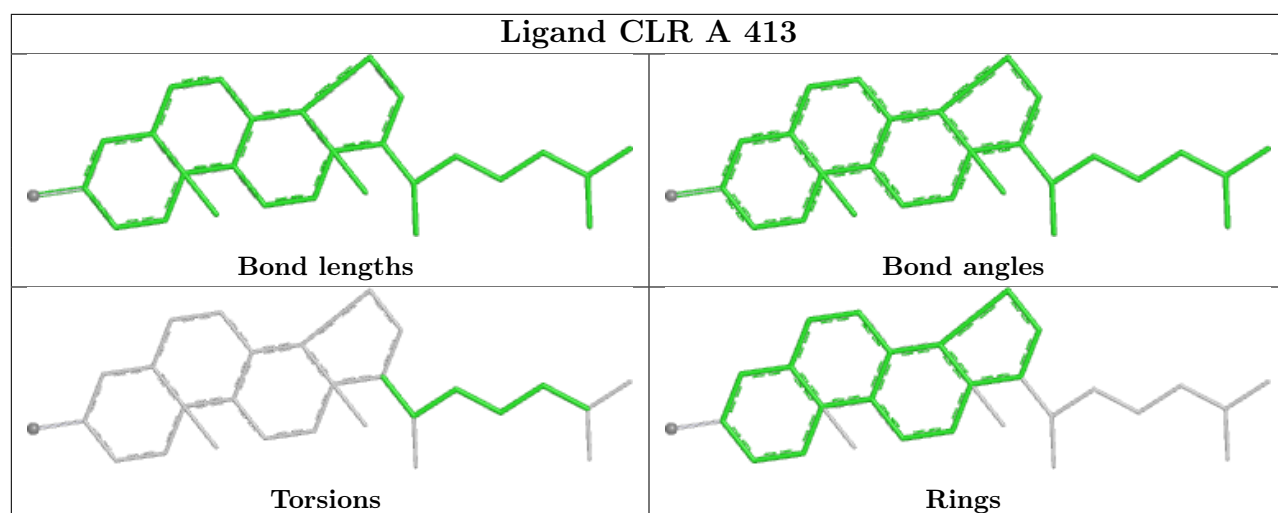


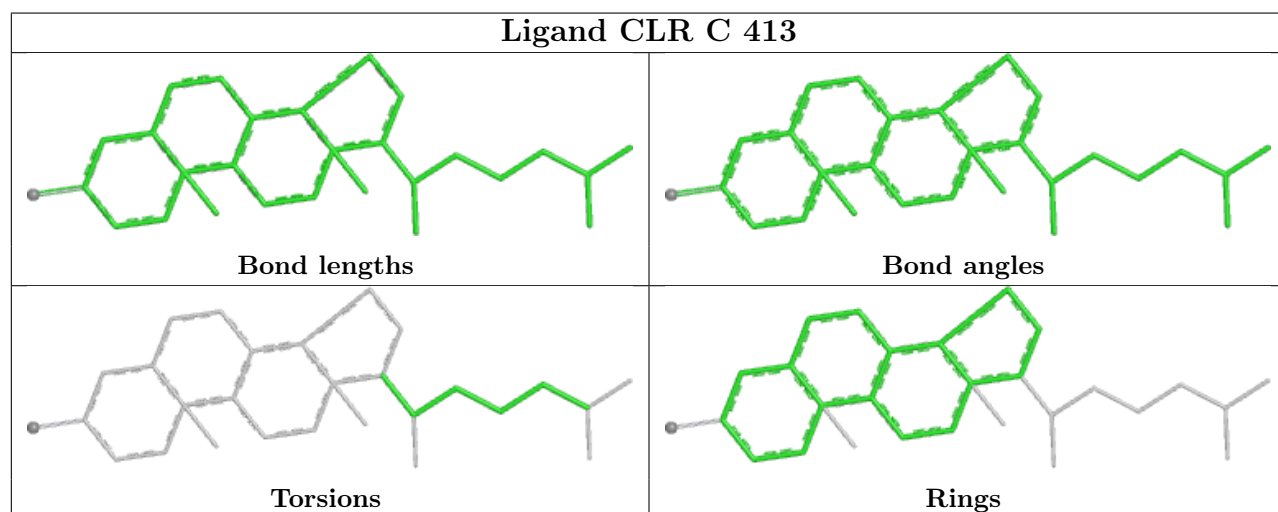
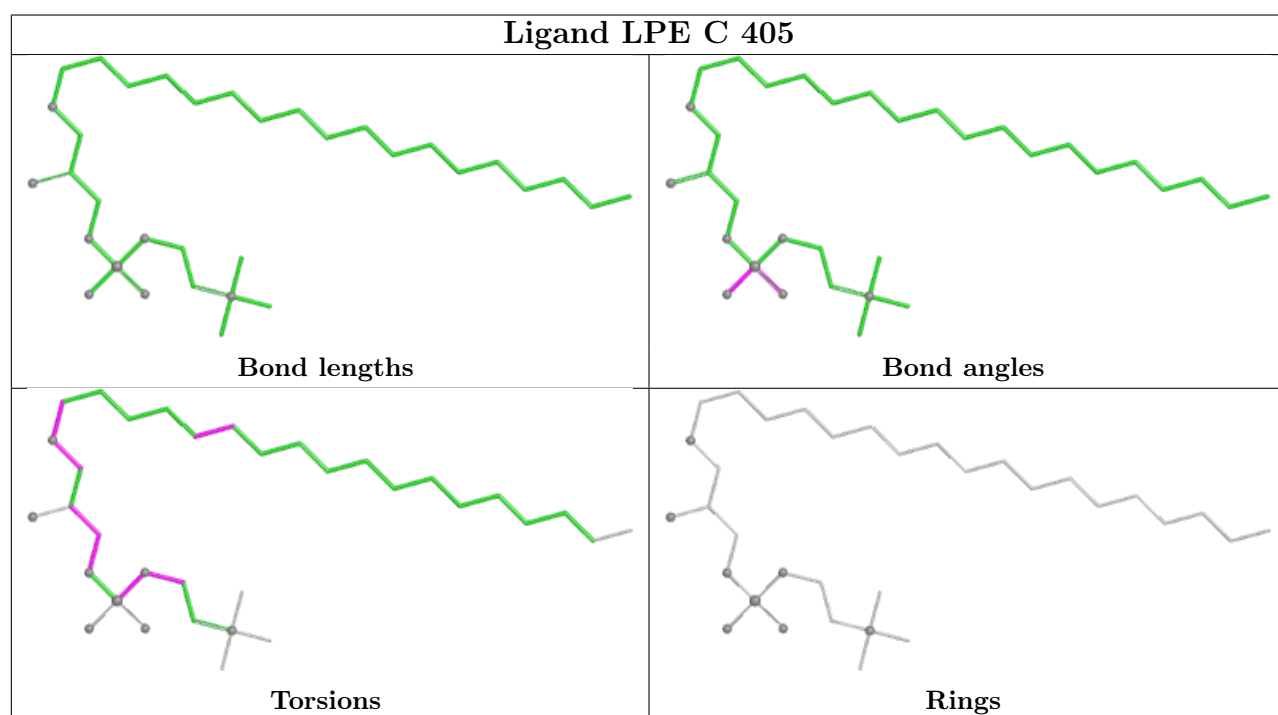
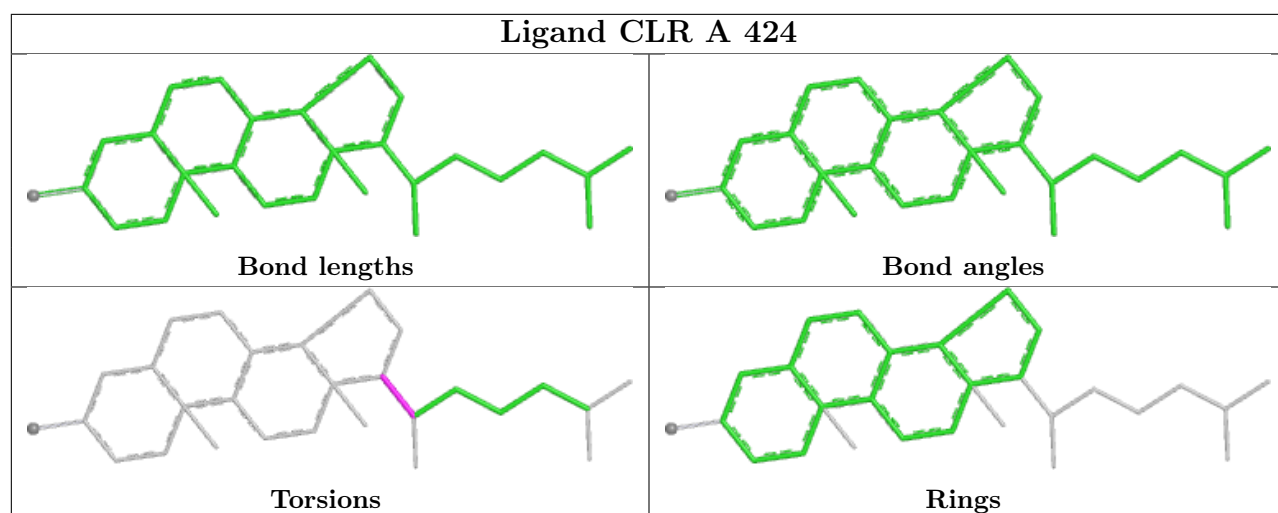


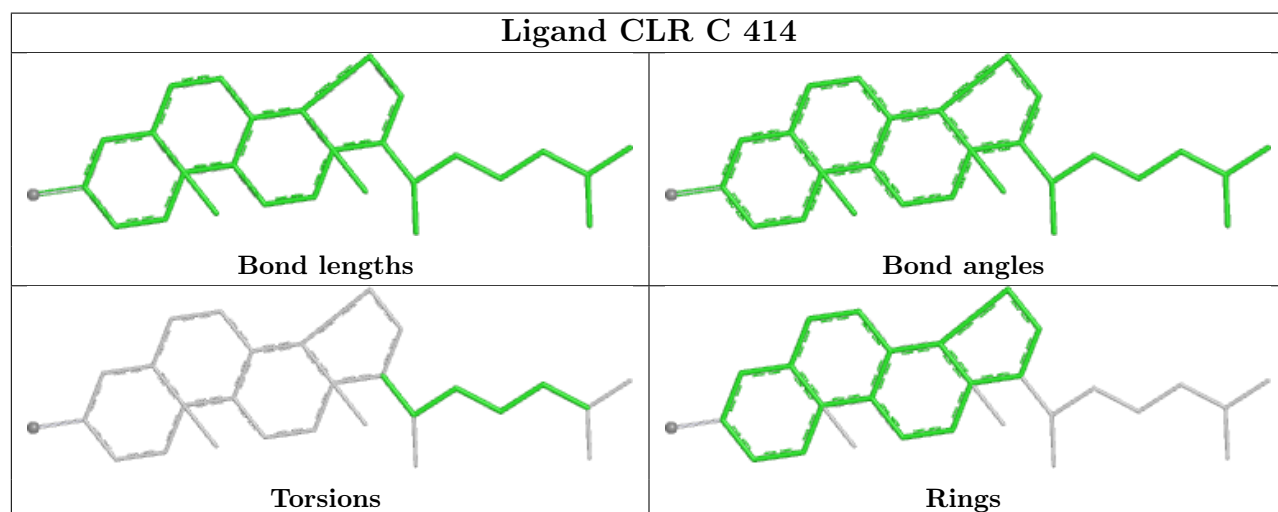
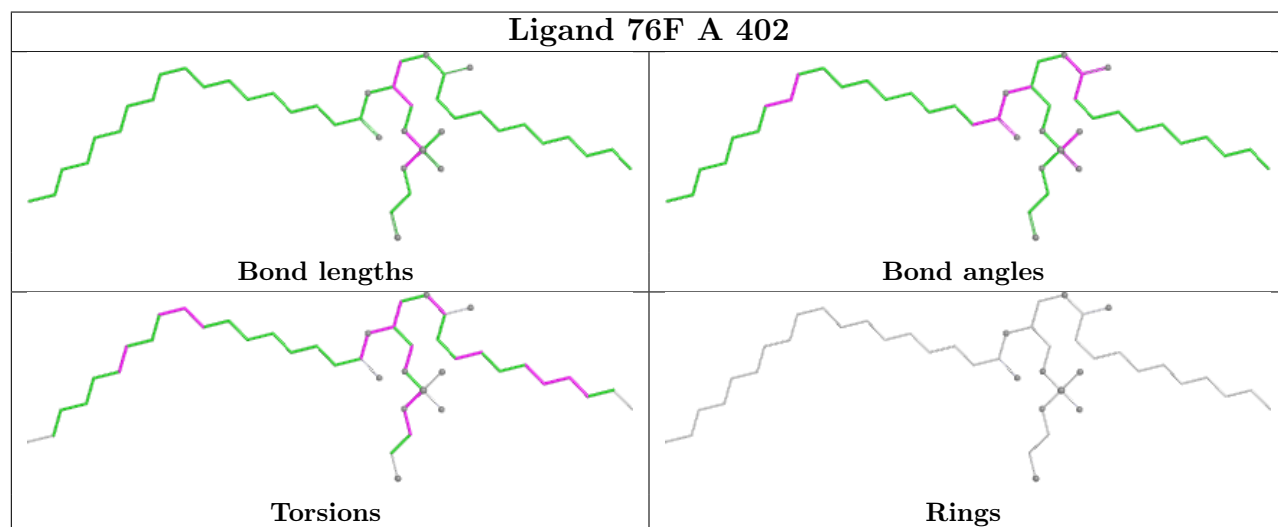
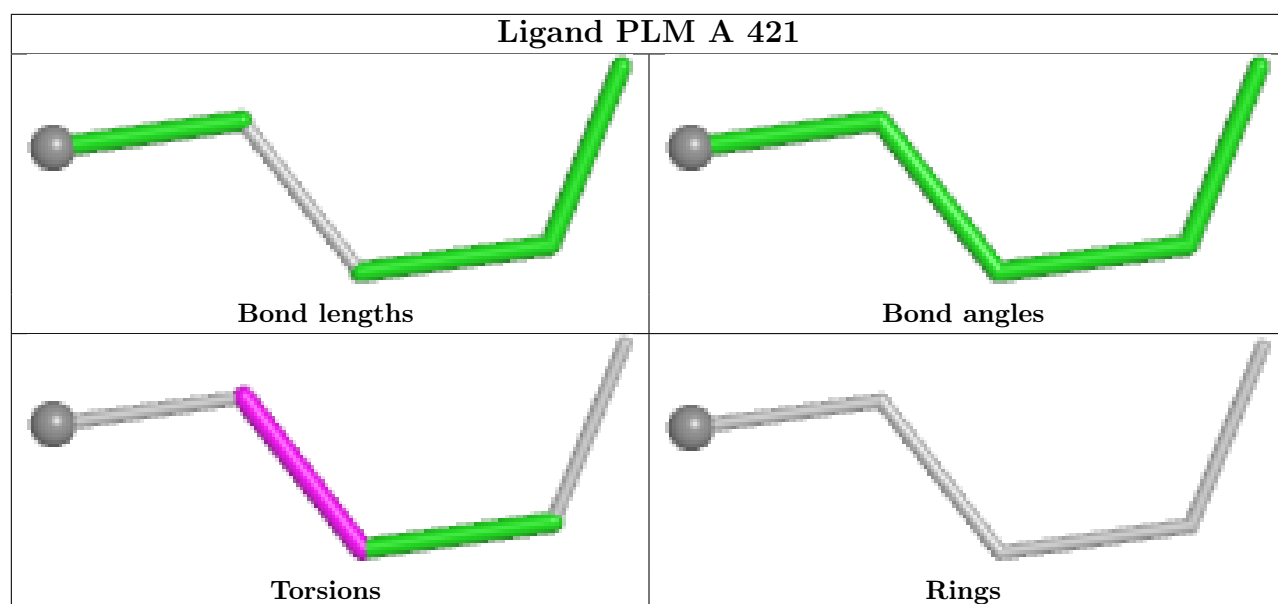


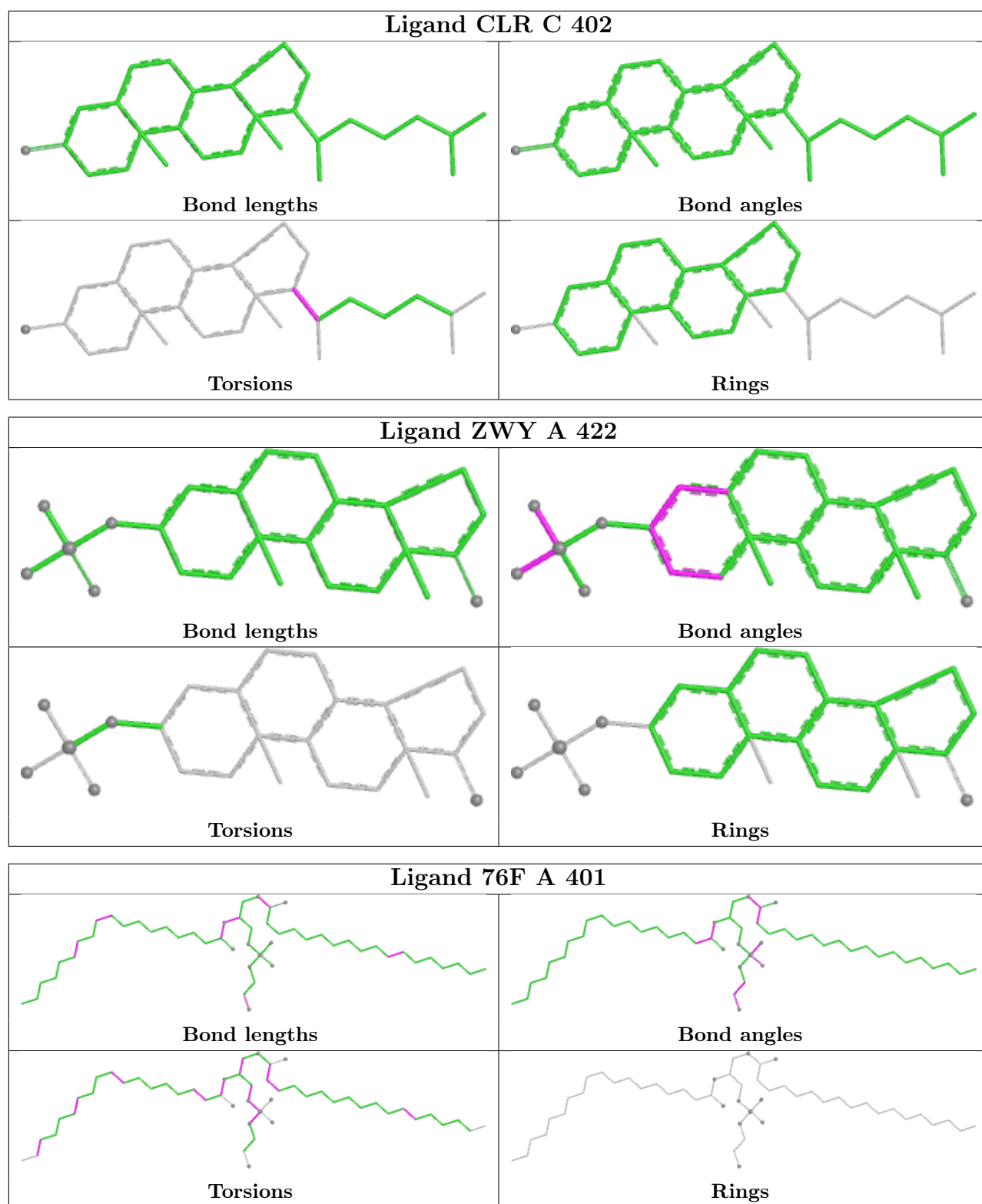


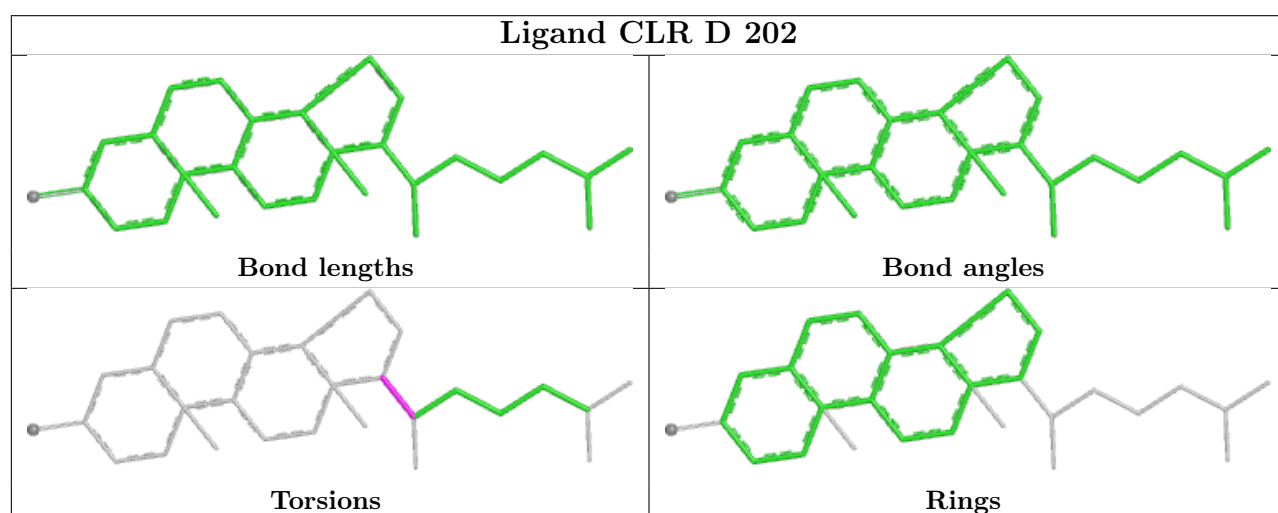
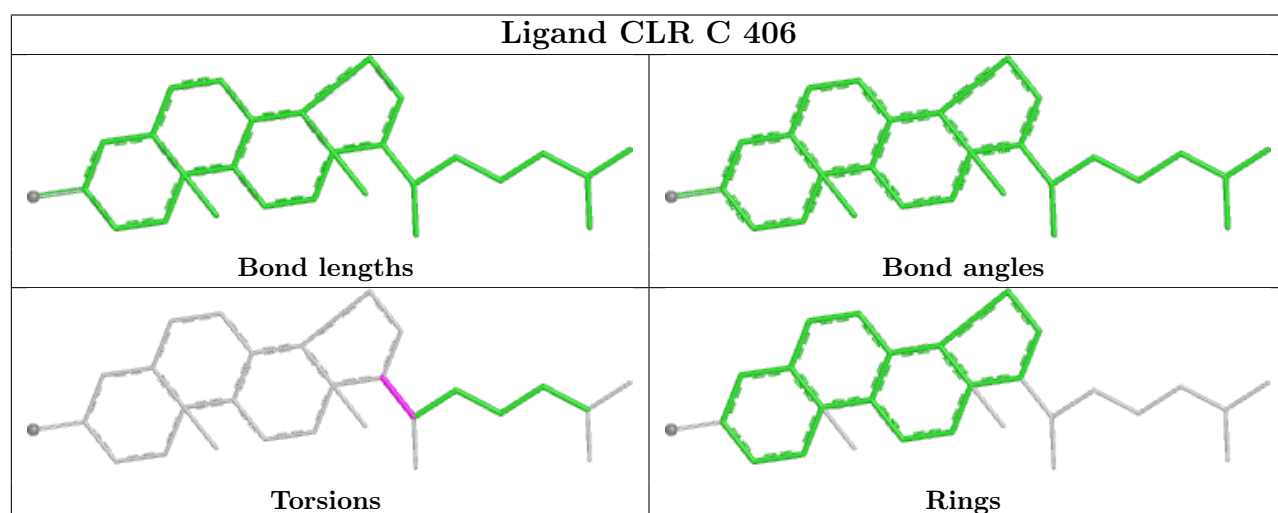
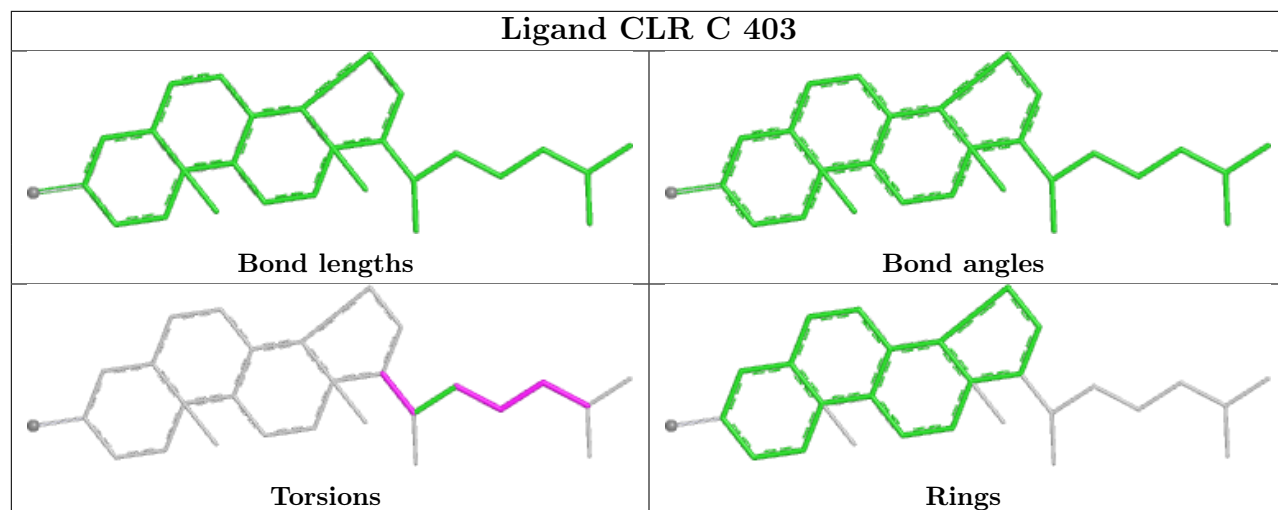


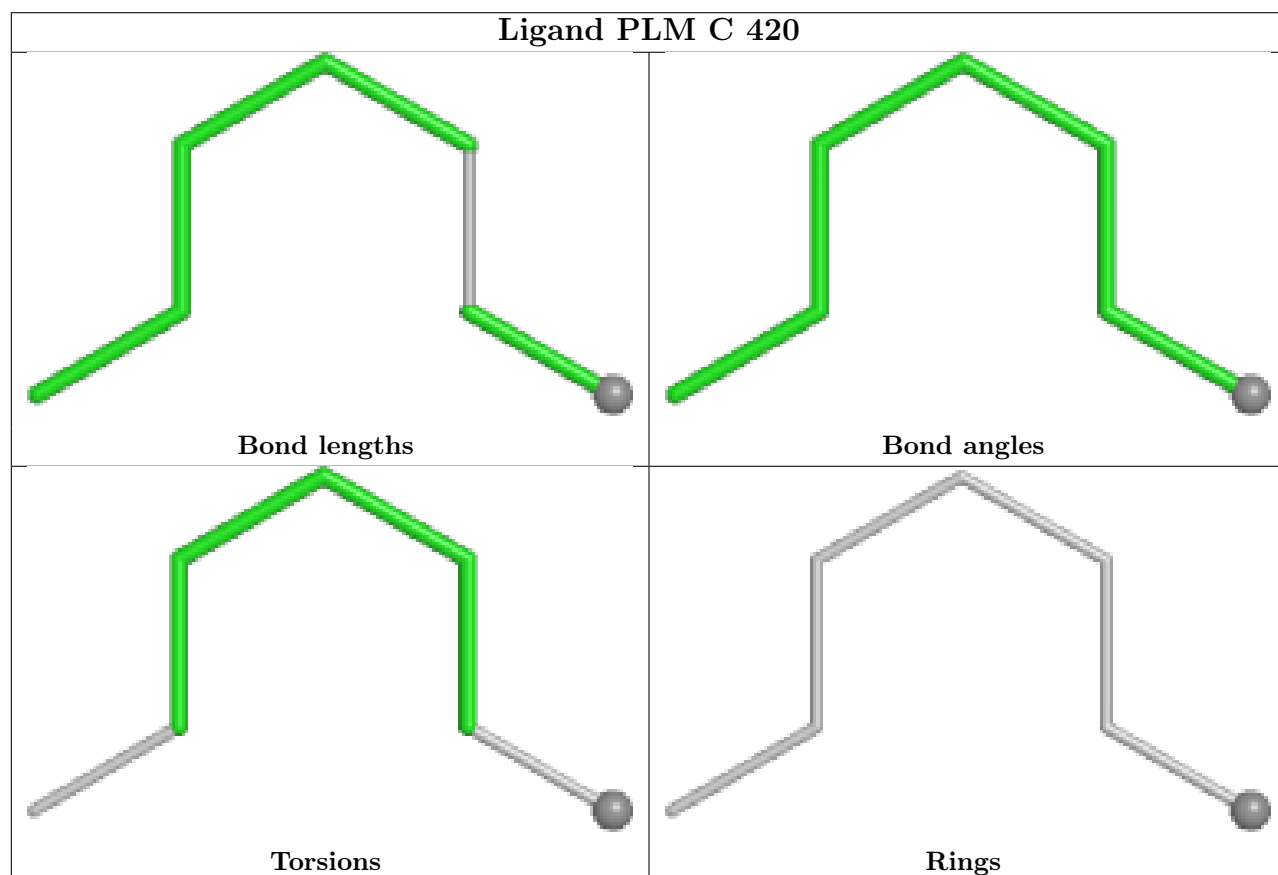
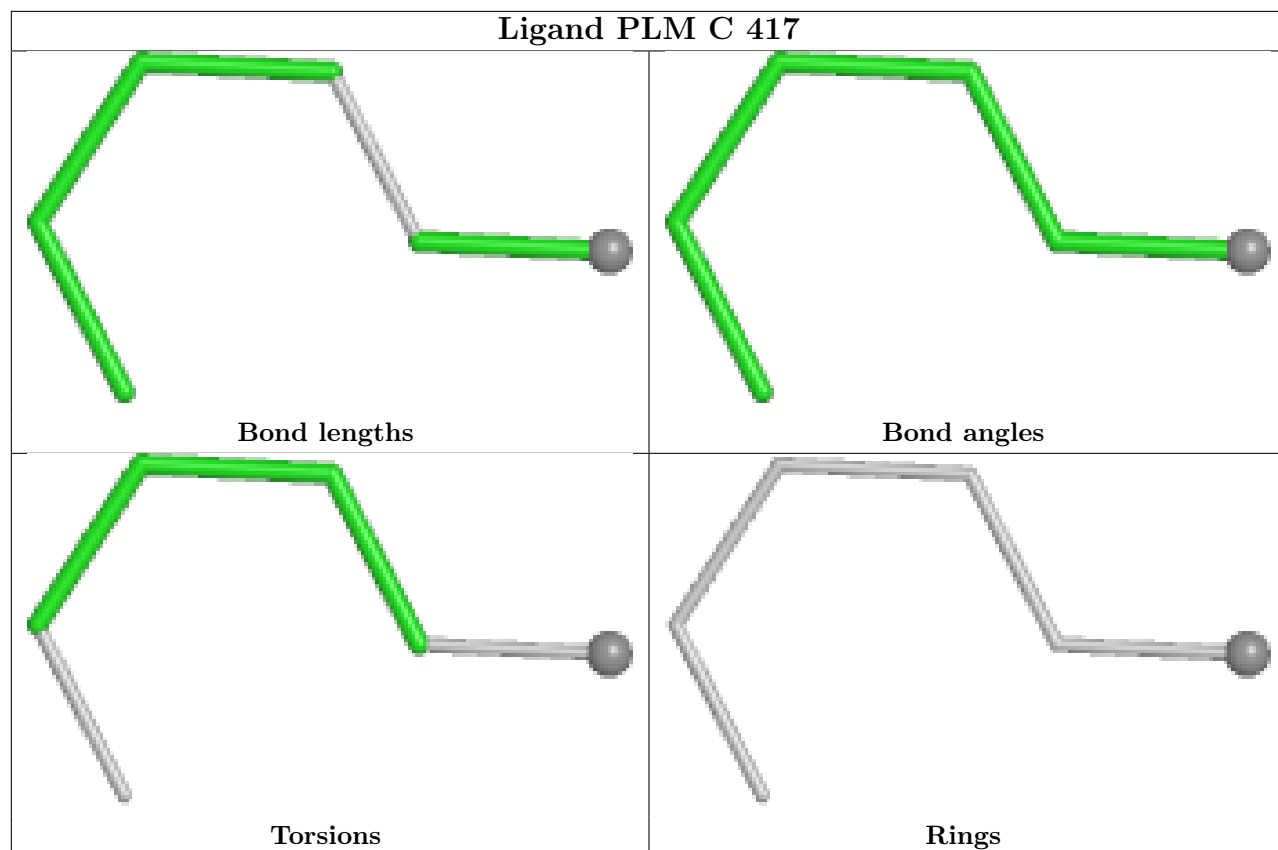


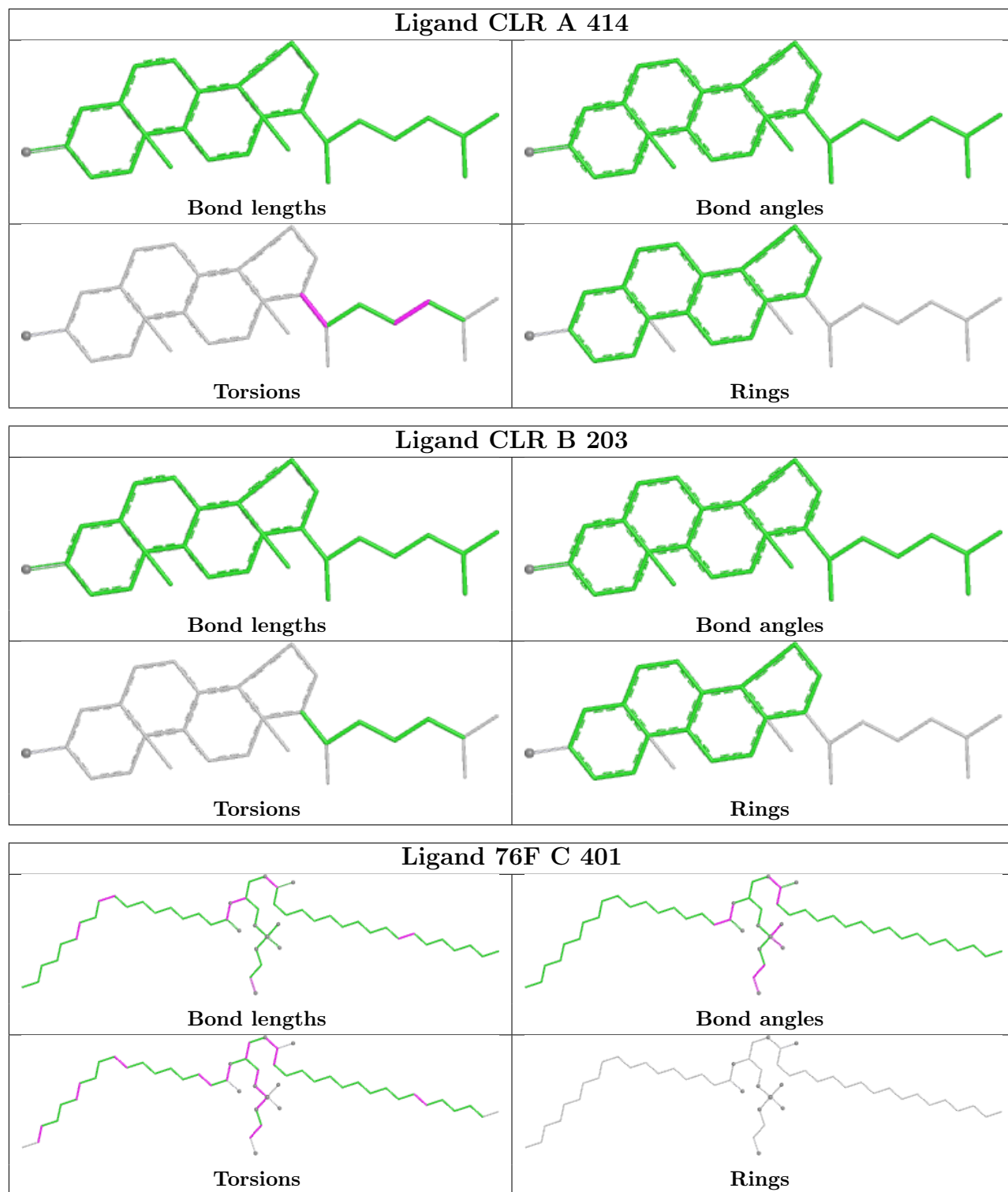


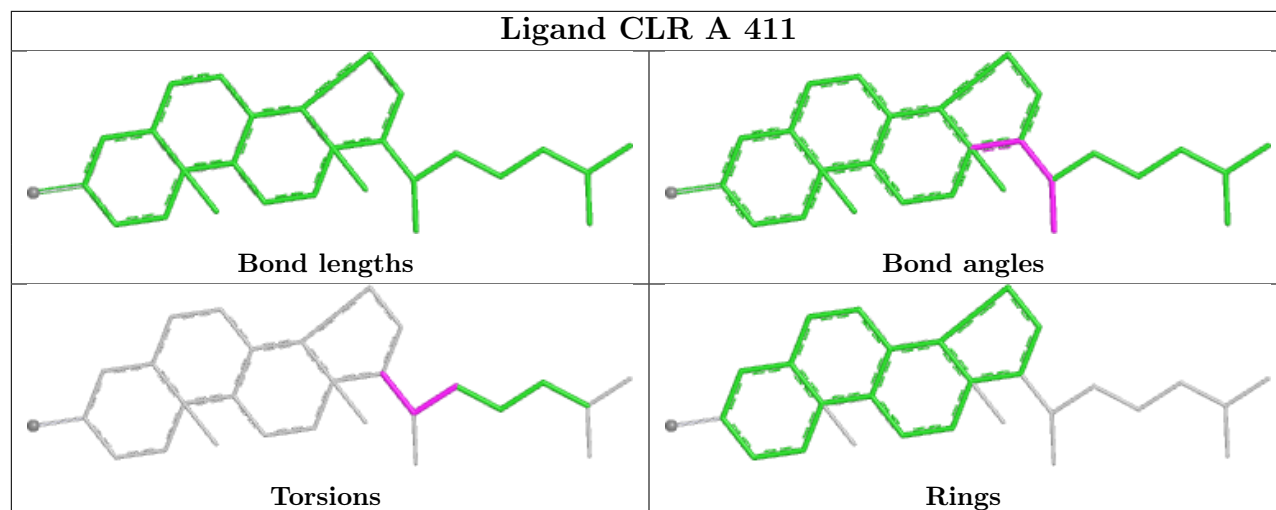












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

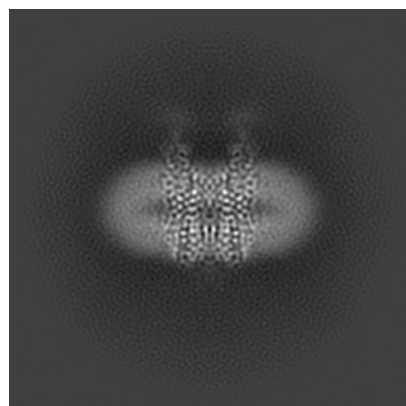
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64369. These allow visual inspection of the internal detail of the map and identification of artifacts.

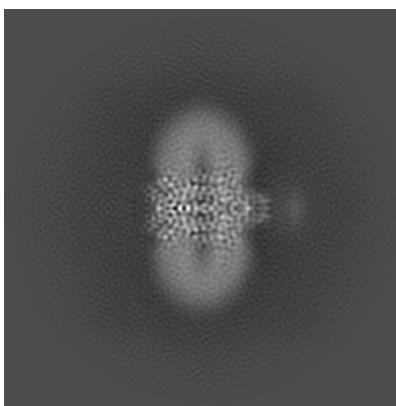
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

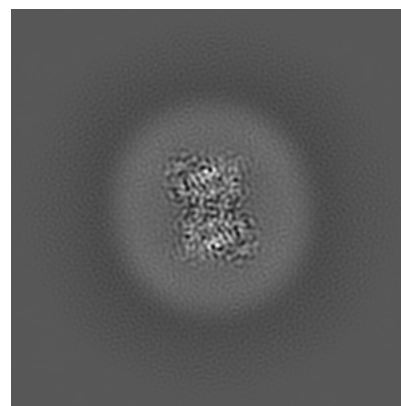
6.1.1 Primary map



X

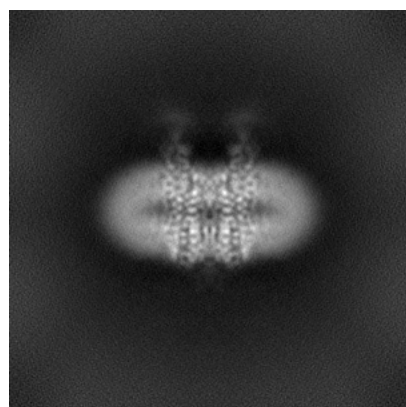


Y

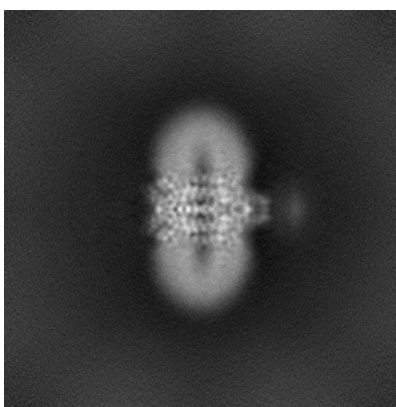


Z

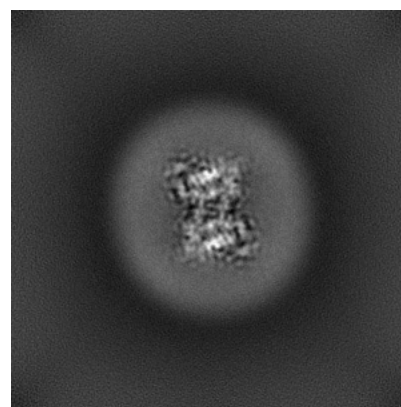
6.1.2 Raw map



X



Y

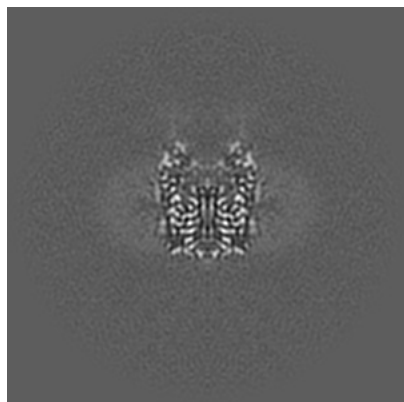


Z

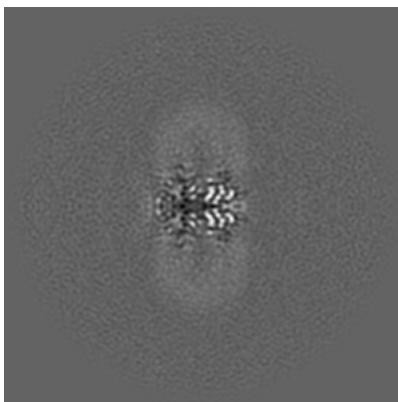
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

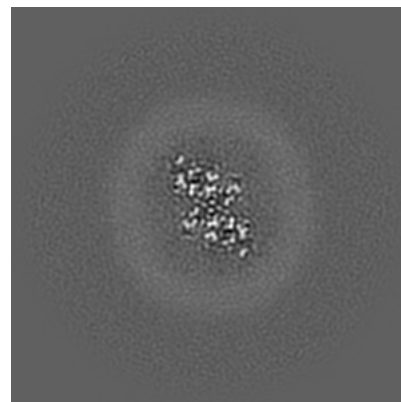
6.2.1 Primary map



X Index: 150

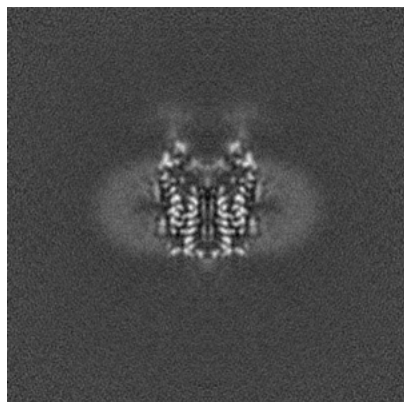


Y Index: 150

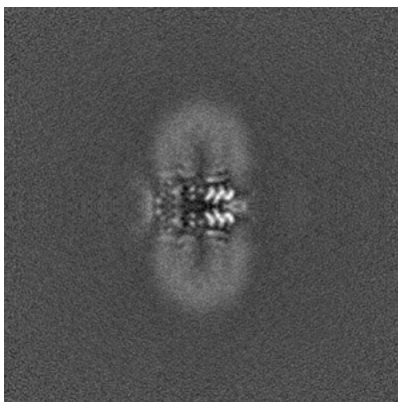


Z Index: 150

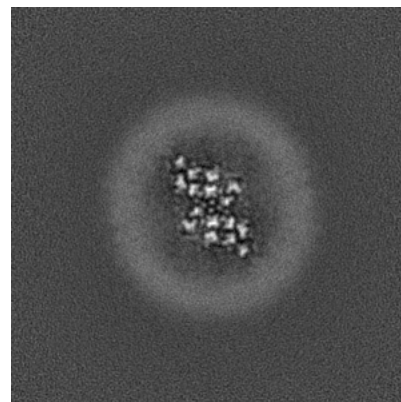
6.2.2 Raw map



X Index: 150



Y Index: 150

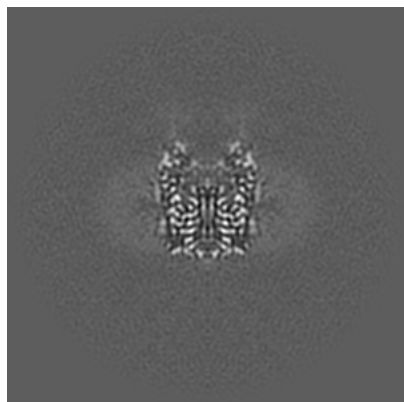


Z Index: 150

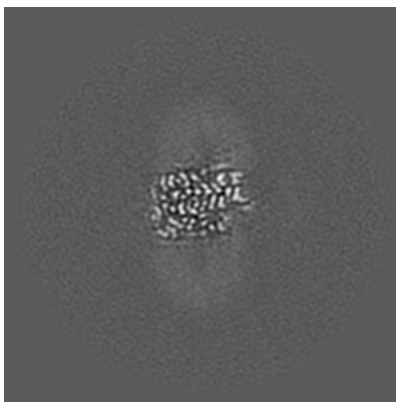
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

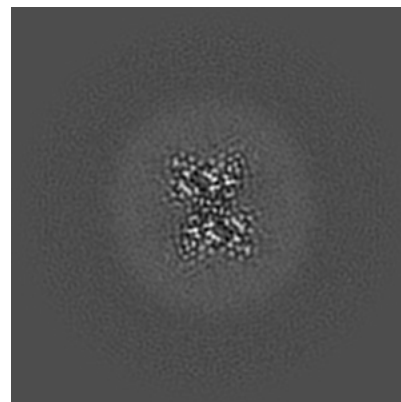
6.3.1 Primary map



X Index: 150

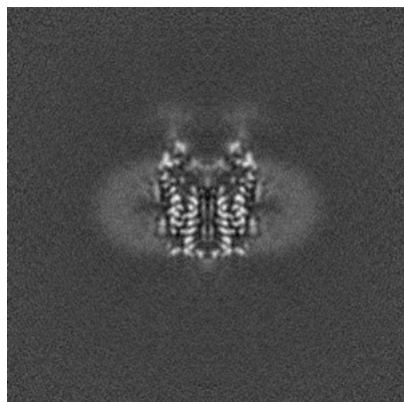


Y Index: 139

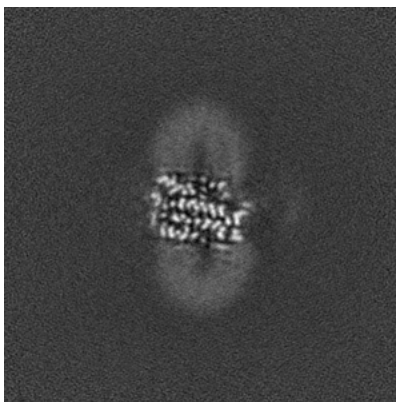


Z Index: 137

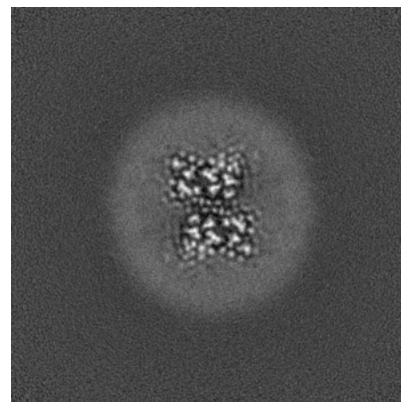
6.3.2 Raw map



X Index: 150



Y Index: 161

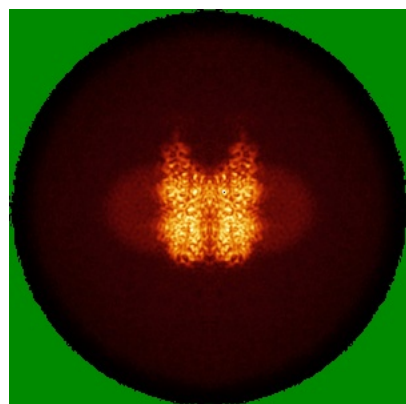


Z Index: 137

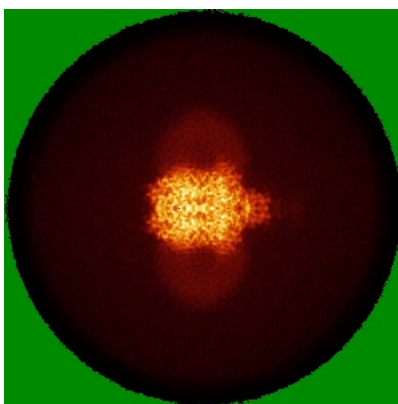
The images above show the largest variance slices of the map in three orthogonal directions.

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

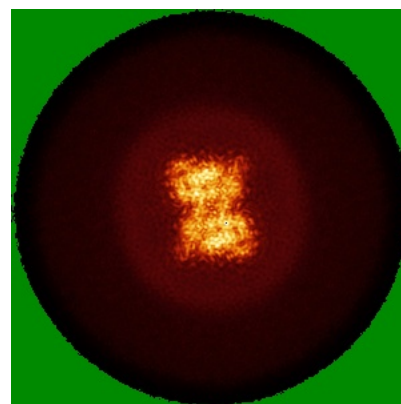
6.4.1 Primary map



X

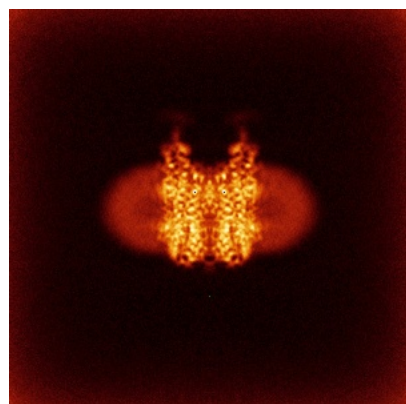


Y

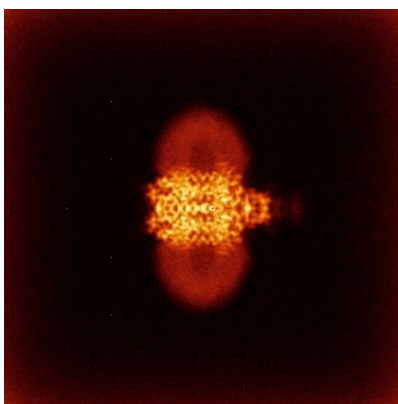


Z

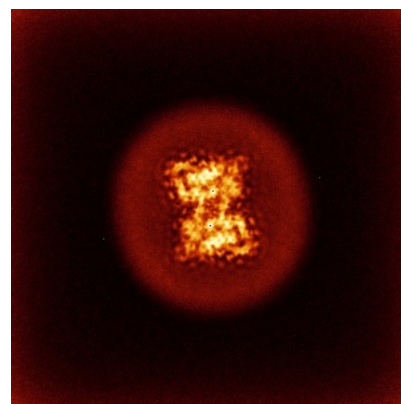
6.4.2 Raw map



X



Y

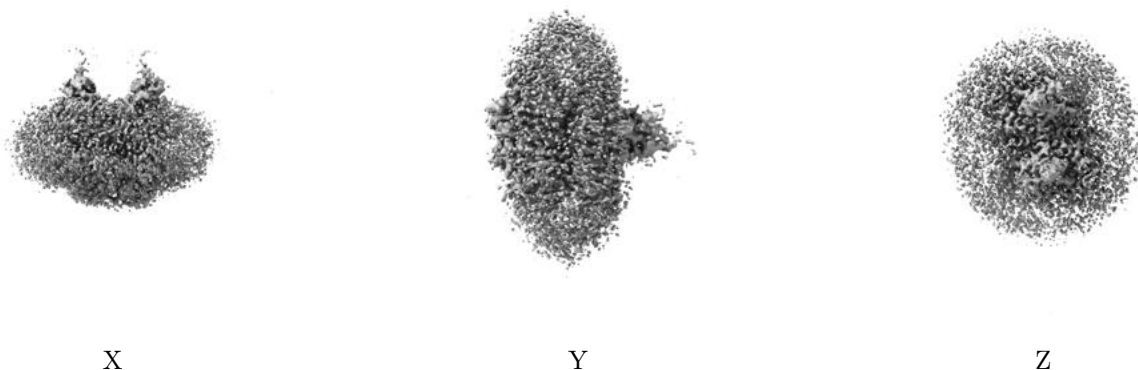


Z

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.

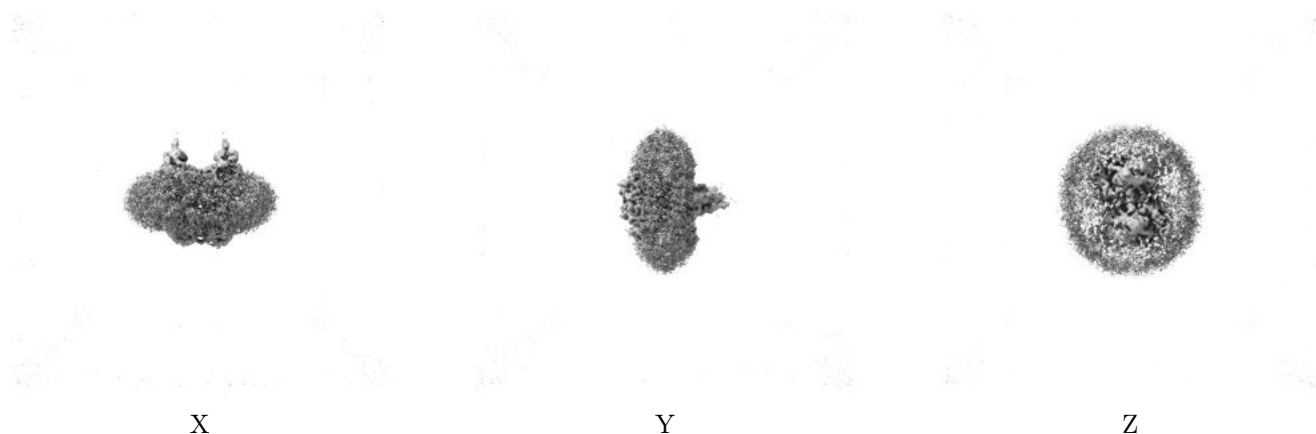
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.24. 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.

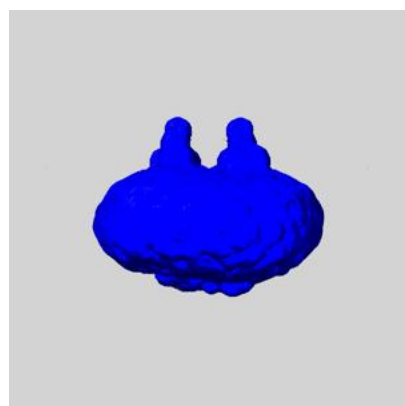
6.6 Mask visualisation [i](#)

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

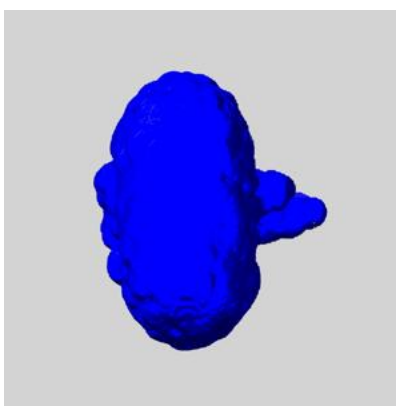
A mask typically either:

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

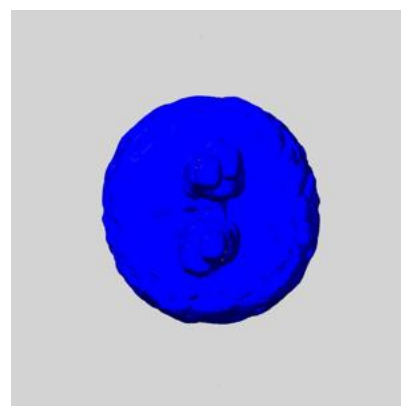
6.6.1 emd_64369_msk_1.map [i](#)



X



Y

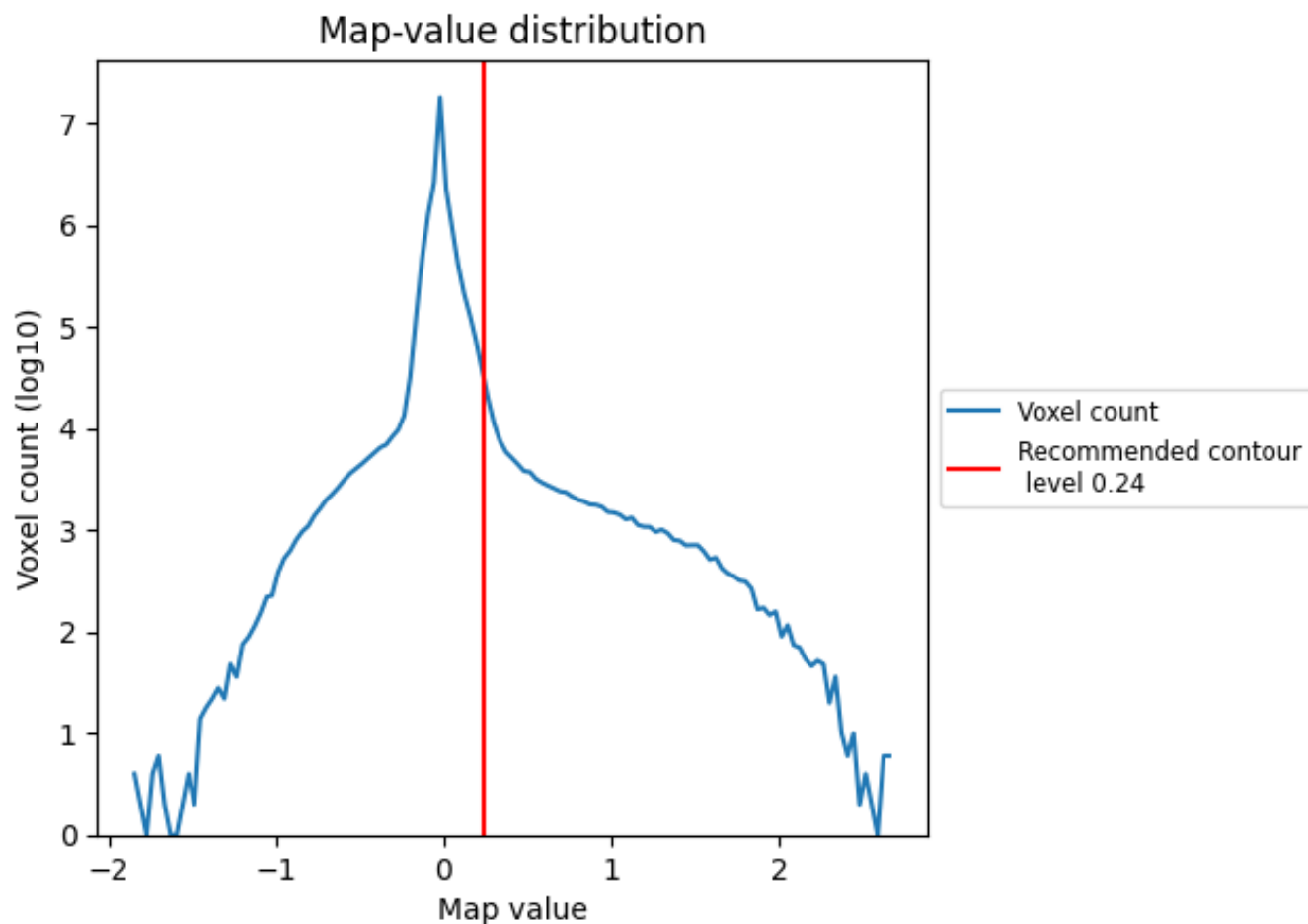


Z

7 Map analysis [i](#)

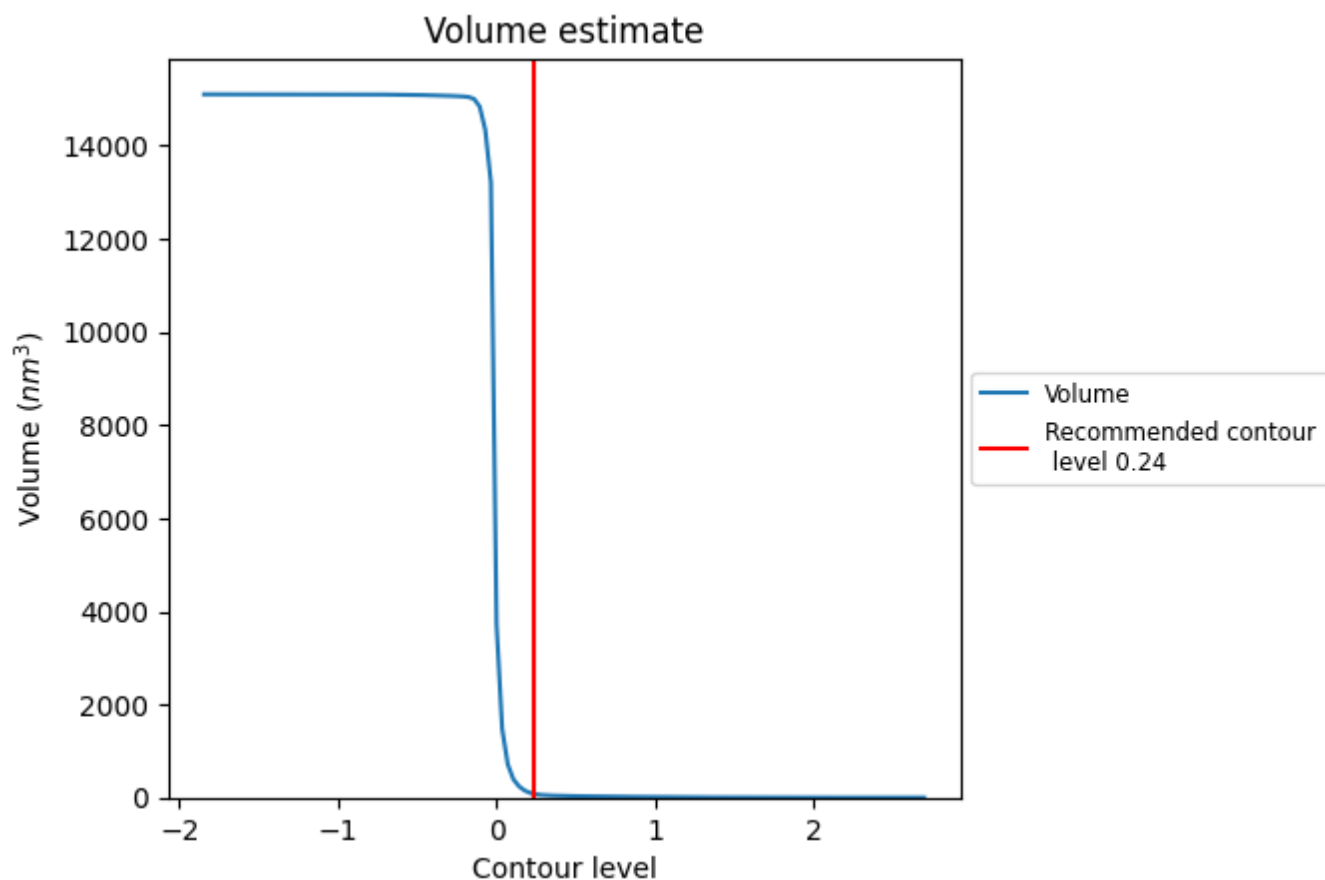
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

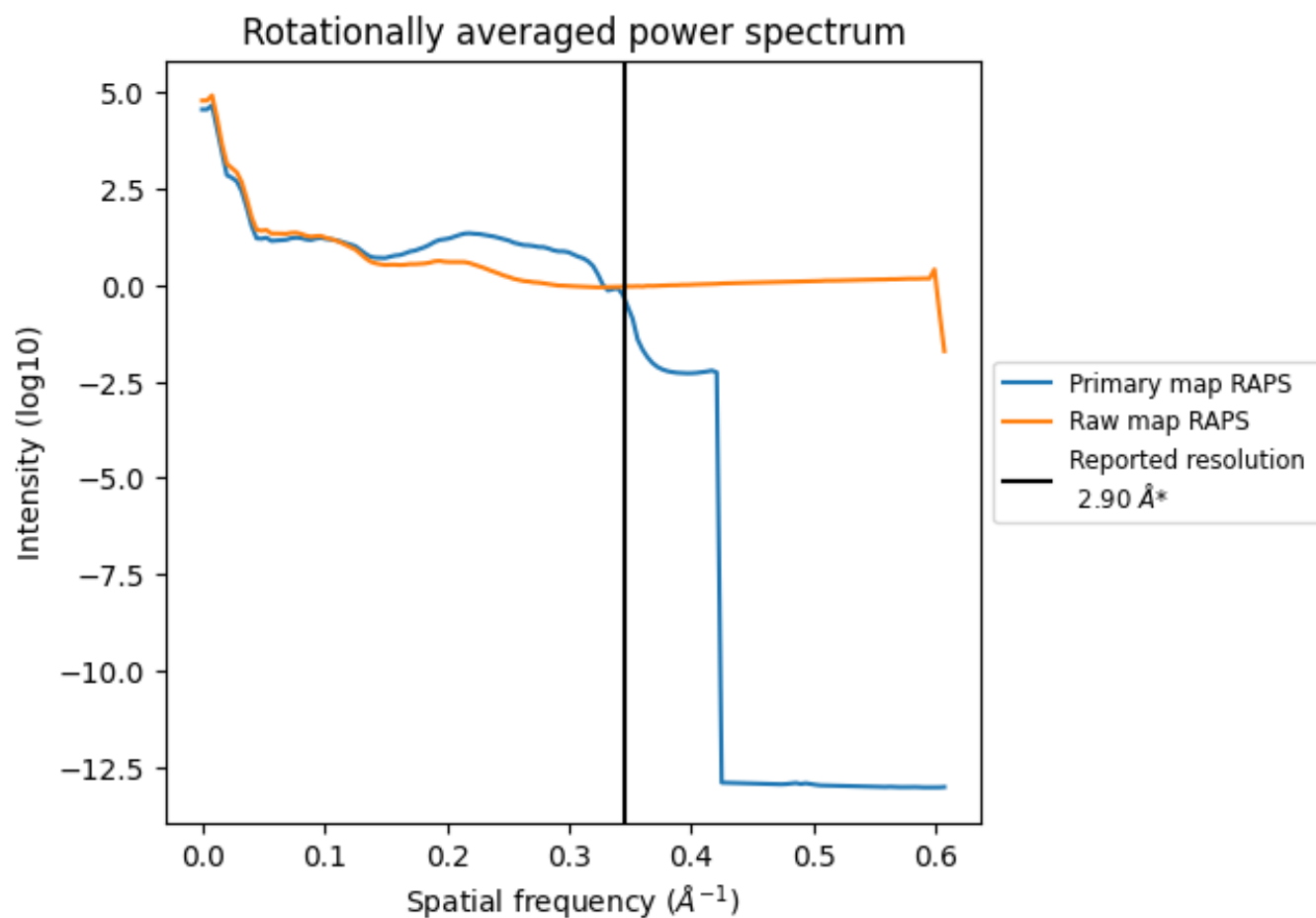
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 78 nm³; this corresponds to an approximate mass of 70 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 ⓘ

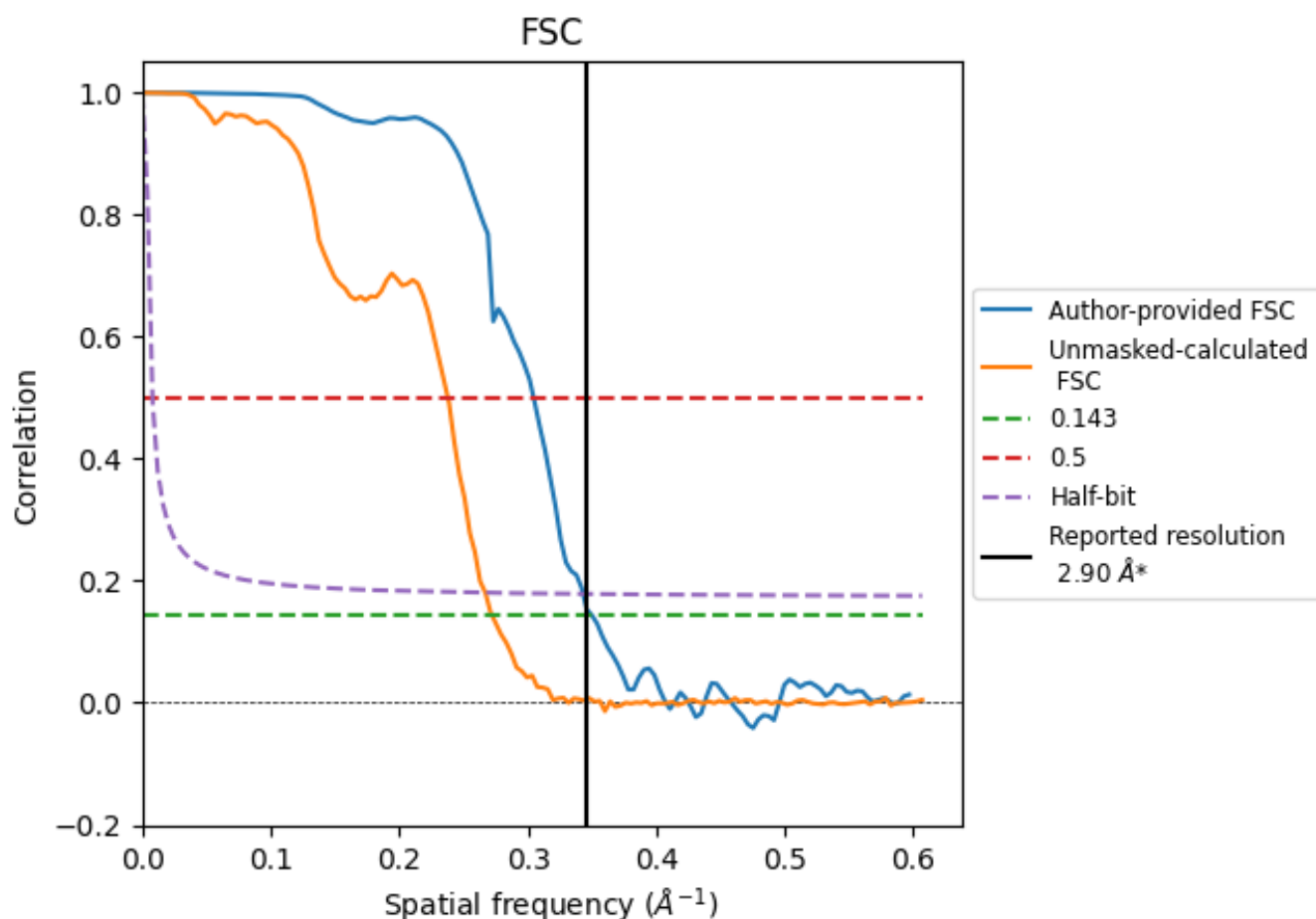


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.86	3.28	2.92
Unmasked-calculated*	3.67	4.21	3.75

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 2.9 by more than 10 %

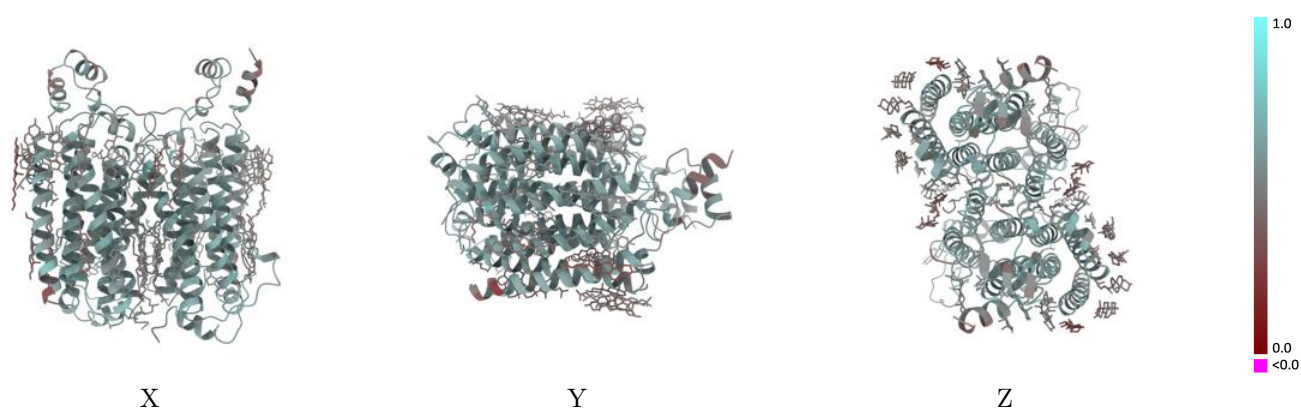
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-64369 and PDB model 9UO1. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

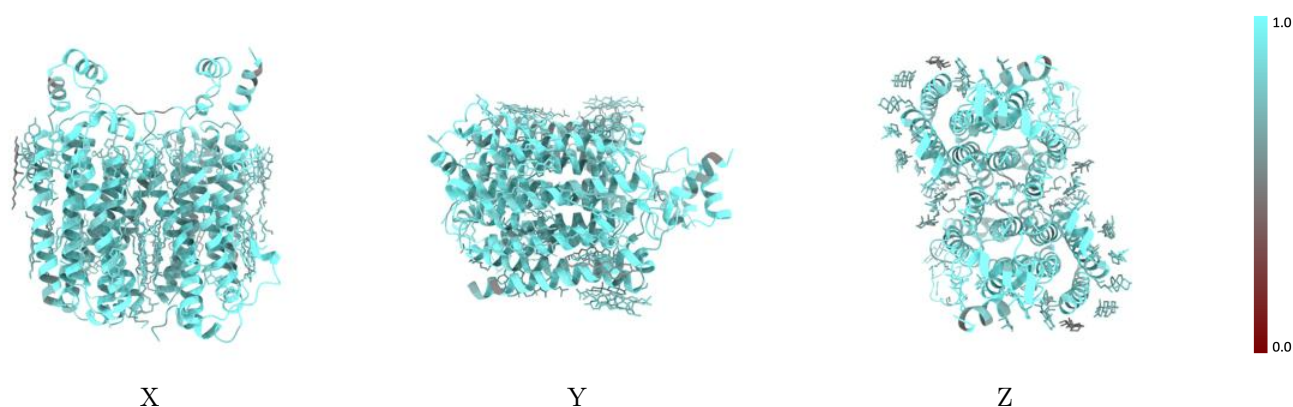
This section was not generated.

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



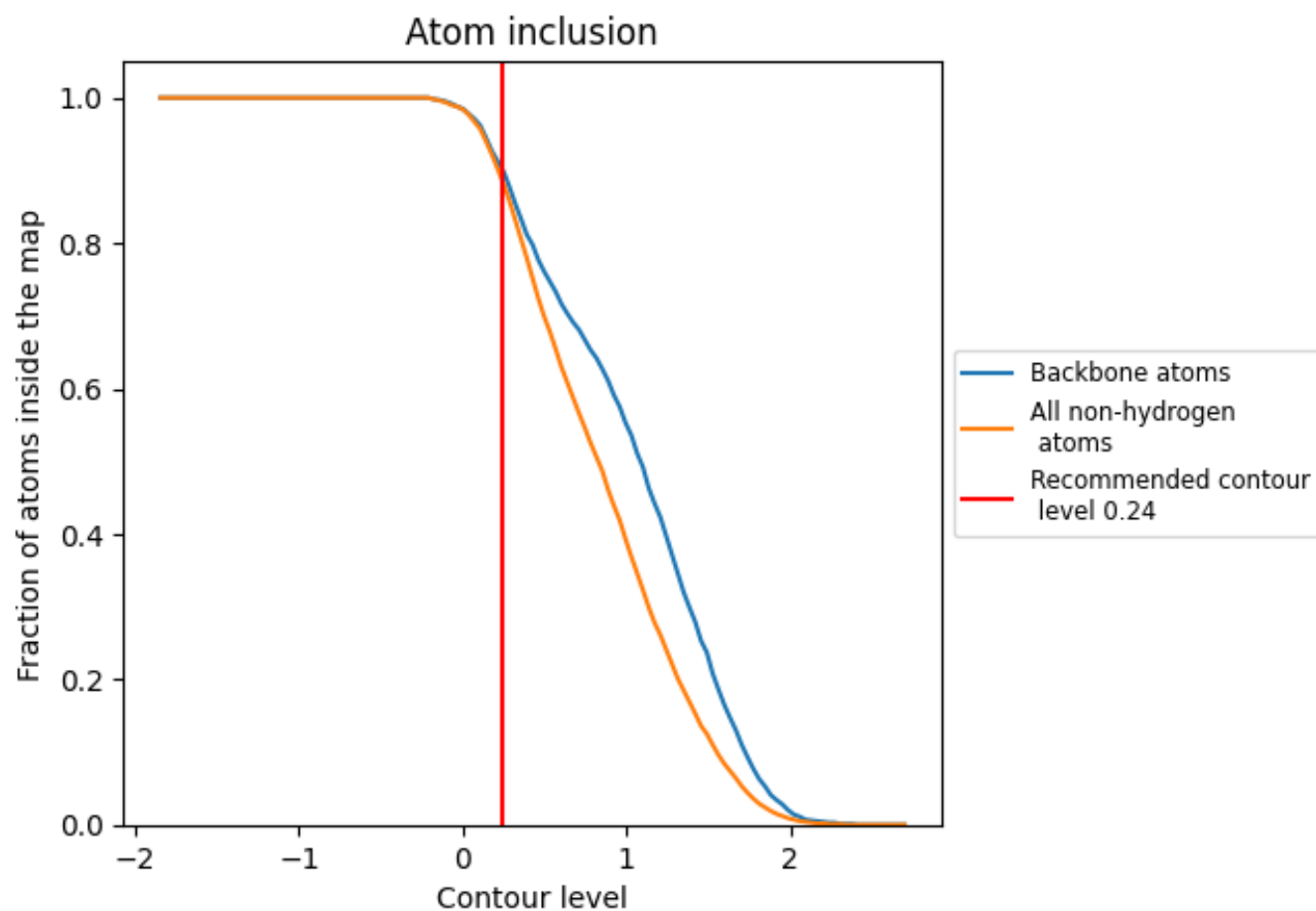
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.24).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8870	0.5480
A	0.8980	0.5540
B	0.8040	0.5060
C	0.9030	0.5560
D	0.8100	0.4900

