



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:18 AM UTC

PDB ID : 9LJH / pdb_00009ljh
EMDB ID : EMD-63149
Title : Cryo-EM structure of human organic solute transporter OSTalpha/beta in complex with DHEAS
Authors : Wang, K.; Jiang, D.H.
Deposited on : 2025-01-15
Resolution : 2.73 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

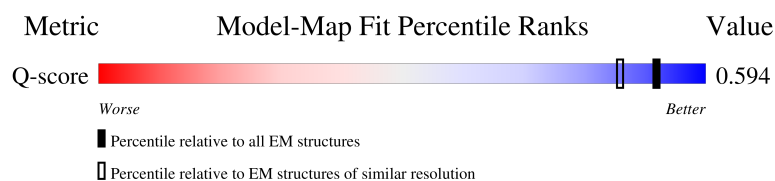
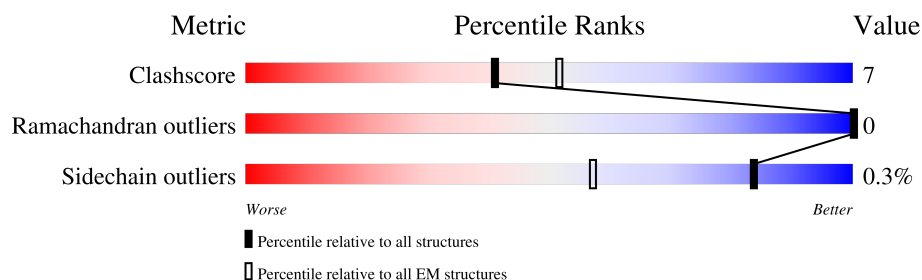
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10432 (2.23 - 3.23)

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

Mol	Chain	Length	Quality of chain
1	A	340	
1	C	340	
2	B	128	
2	D	128	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6415 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.

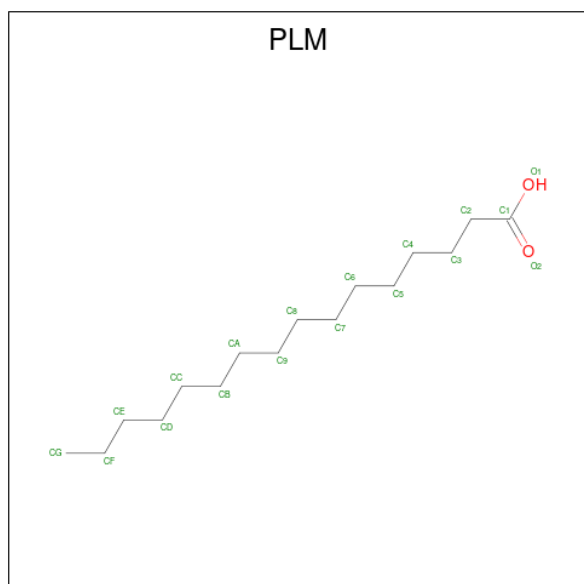
- Molecule 1 is a protein called Organic solute transporter subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	324	Total	C	N	O	S	0	0
			2522	1652	411	435	24		
1	C	324	Total	C	N	O	S	0	0
			2522	1652	411	435	24		

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

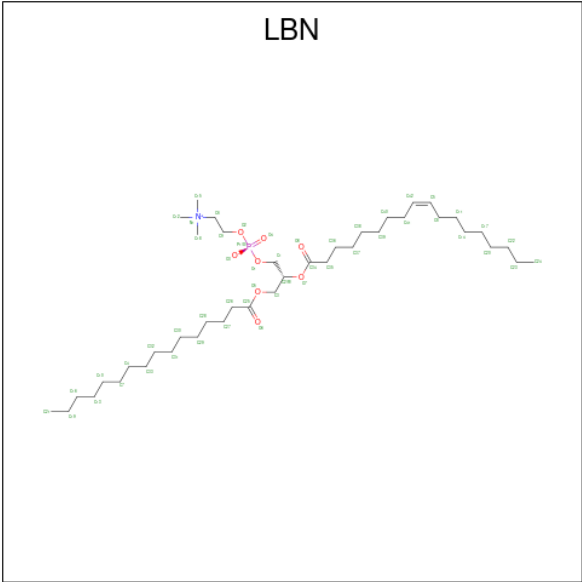
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	48	Total	C	N	O	S	0	0
			382	250	64	66	2		
2	D	49	Total	C	N	O	S	0	0
			391	256	66	67	2		

- Molecule 3 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



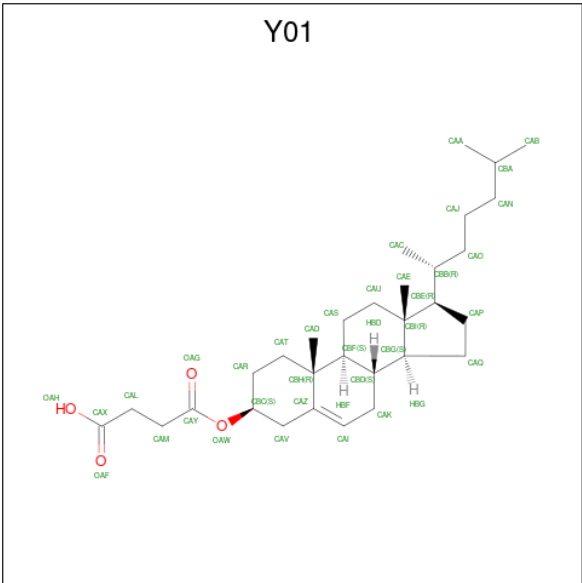
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			8	7	1	
3	A	1	Total	C	O	0
			9	8	1	
3	A	1	Total	C	O	0
			9	8	1	
3	A	1	Total	C	O	0
			8	7	1	
3	A	1	Total	C	O	0
			11	10	1	
3	A	1	Total	C	O	0
			8	7	1	
3	A	1	Total	C	O	0
			11	10	1	
3	C	1	Total	C	O	0
			13	12	1	
3	C	1	Total	C	O	0
			11	10	1	
3	C	1	Total	C	O	0
			9	8	1	
3	C	1	Total	C	O	0
			8	7	1	
3	C	1	Total	C	O	0
			7	6	1	
3	C	1	Total	C	O	0
			7	6	1	
3	C	1	Total	C	O	0
			9	8	1	

- Molecule 4 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



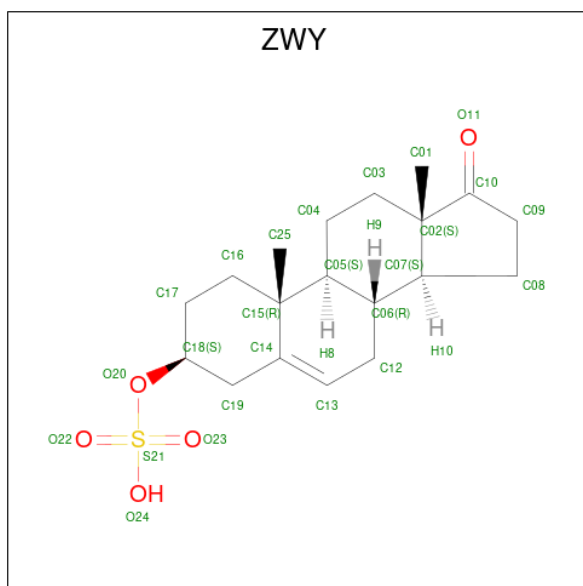
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
4	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
4	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	C	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 5 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			30	28	2	
5	A	1	Total	C	O	0
			30	28	2	
5	A	1	Total	C	O	0
			30	28	2	
5	A	1	Total	C	O	0
			35	31	4	
5	C	1	Total	C	O	0
			30	28	2	
5	C	1	Total	C	O	0
			30	28	2	
5	C	1	Total	C	O	0
			30	28	2	
5	C	1	Total	C	O	0
			35	31	4	

- Molecule 6 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).

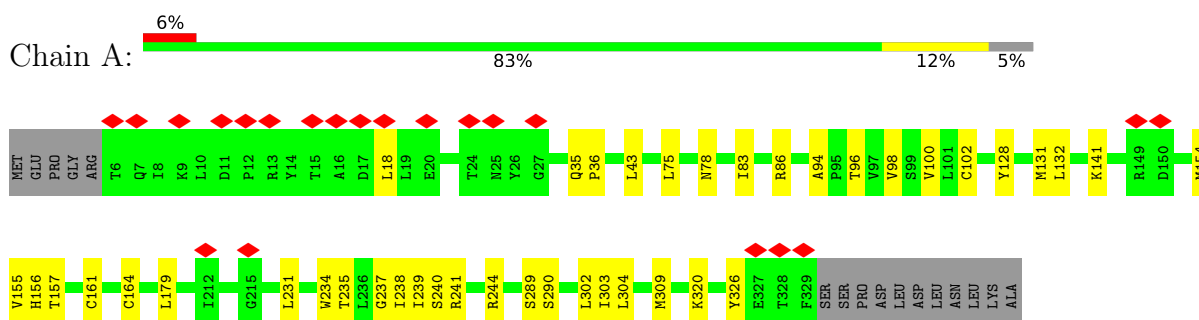


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O	S	0
			25	19	5	1	
6	C	1	Total	C	O	S	0
			25	19	5	1	

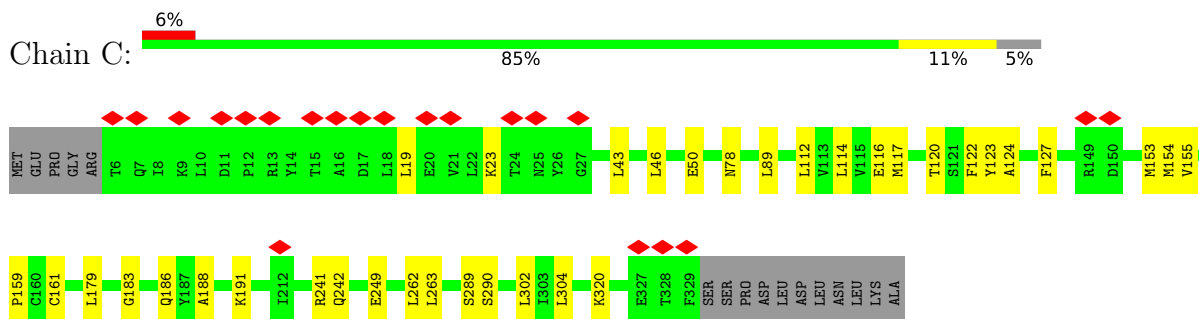
3 Residue-property plots [i](#)

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.

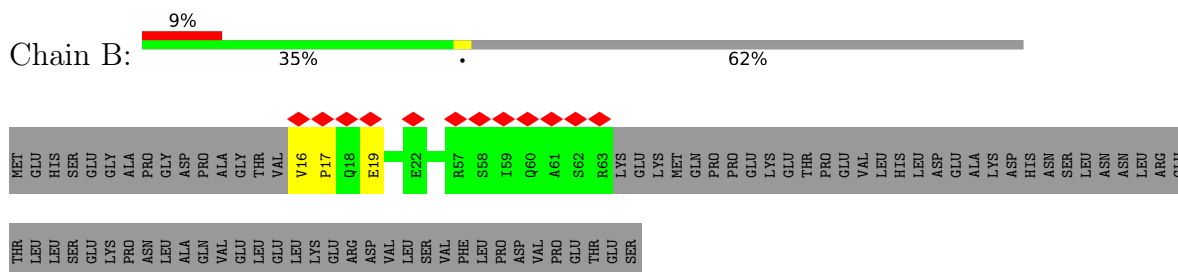
- Molecule 1: Organic solute transporter subunit alpha



- Molecule 1: Organic solute transporter subunit alpha



- Molecule 2: Organic solute transporter subunit beta



- Molecule 2: Organic solute transporter subunit beta





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	189210	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.775	Depositor
Minimum map value	-1.772	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.451	Depositor
Map size (Å)	272.0, 272.0, 272.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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: PLM, LBN, ZWY, Y01

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	0.34	1/2578 (0.0%)	0.49	1/3509 (0.0%)
1	C	0.18	0/2578	0.38	0/3509
2	B	0.12	0/390	0.27	0/531
2	D	0.09	0/399	0.22	0/542
All	All	0.26	1/5945 (0.0%)	0.42	1/8091 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	THR	C-O	5.73	1.30	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	TRP	O-C-N	-5.97	115.92	122.07

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	2522	0	2643	34	0
1	C	2522	0	2643	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	382	0	393	4	0
2	D	391	0	406	1	0
3	A	64	0	86	5	0
3	C	64	0	86	6	0
4	A	46	0	0	8	0
4	C	124	0	0	4	0
5	A	125	0	184	11	0
5	C	125	0	184	8	0
6	A	25	0	0	0	0
6	C	25	0	0	0	0
All	All	6415	0	6625	90	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (90) 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:A:408:LBN:N1	4:C:408:LBN:O4	1.87	1.06
1:A:86:ARG:HH12	4:A:408:LBN:C1	1.71	1.03
1:A:86:ARG:NH1	4:A:408:LBN:C1	2.41	0.83
3:C:404:PLM:H42	3:C:404:PLM:O2	1.84	0.76
1:C:179:LEU:HD13	5:C:412:Y01:HAK1	1.71	0.73
1:A:179:LEU:HD13	5:A:411:Y01:HAK1	1.72	0.70
2:B:17:PRO:HB2	2:B:19:GLU:OE2	1.95	0.66
1:C:154:MET:CE	1:C:241:ARG:HD3	2.27	0.65
1:A:164:CYS:SG	3:A:406:PLM:H32	2.37	0.65
1:A:83:ILE:O	1:A:86:ARG:HG3	1.97	0.64
1:C:154:MET:HE2	1:C:241:ARG:HD3	1.79	0.64
3:A:403:PLM:H61	3:A:405:PLM:H21	1.85	0.57
1:C:78:ASN:HD22	1:C:320:LYS:HZ3	1.53	0.56
1:A:161:CYS:HA	3:A:407:PLM:H21	1.89	0.54
1:A:94:ALA:O	1:A:98:VAL:HG23	2.09	0.53
1:A:237:GLY:O	1:A:241:ARG:HG2	2.10	0.52
1:C:159:PRO:O	3:C:404:PLM:H41	2.10	0.52
4:A:408:LBN:C6	4:C:408:LBN:O4	2.56	0.52
1:C:249:GLU:H	1:C:249:GLU:CD	2.18	0.52
1:A:240:SER:O	1:A:244:ARG:HG3	2.11	0.51
1:C:153:MET:HE3	1:C:242:GLN:HG3	1.93	0.51
1:A:78:ASN:HB3	1:A:320:LYS:HG2	1.93	0.51
1:A:154:MET:HG3	1:A:156:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:SER:OG	1:A:290:SER:N	2.44	0.50
3:C:404:PLM:O2	3:C:404:PLM:C4	2.52	0.50
2:B:16:VAL:HB	2:B:17:PRO:HD2	1.94	0.50
1:A:35:GLN:HB3	1:A:36:PRO:HD2	1.95	0.48
3:C:403:PLM:H31	3:C:404:PLM:H21	1.95	0.48
1:C:112:LEU:O	1:C:116:GLU:HG3	2.13	0.48
1:C:289:SER:OG	1:C:290:SER:N	2.44	0.48
1:C:46:LEU:HG	1:C:50:GLU:HB2	1.96	0.48
1:C:89:LEU:HD13	4:C:408:LBN:C26	2.43	0.48
1:C:78:ASN:ND2	1:C:320:LYS:HZ3	2.12	0.47
1:C:154:MET:CE	1:C:241:ARG:CD	2.93	0.47
5:C:410:Y01:HAE2	5:C:410:Y01:HBB	1.65	0.47
4:A:408:LBN:C14	1:C:122:PHE:CD1	2.97	0.47
1:A:141:LYS:HE3	4:C:408:LBN:C9	2.45	0.46
1:C:114:LEU:HD23	1:C:117:MET:HE3	1.97	0.46
2:B:17:PRO:HB2	2:B:19:GLU:CD	2.41	0.46
1:A:102:CYS:HB3	1:A:303:ILE:HG13	1.98	0.46
5:A:412:Y01:HAE2	5:A:412:Y01:HBB	1.69	0.46
1:A:102:CYS:SG	1:A:302:LEU:HB3	2.55	0.46
1:A:154:MET:HE3	1:A:157:THR:HG22	1.98	0.45
5:A:411:Y01:HAO2	5:A:411:Y01:HAP1	1.48	0.45
1:A:161:CYS:SG	3:A:407:PLM:H31	2.57	0.45
1:A:18:LEU:HD21	2:B:16:VAL:HG11	1.99	0.45
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.86	0.45
5:A:412:Y01:HAO2	5:A:412:Y01:HAP1	1.57	0.45
1:A:83:ILE:HG23	1:A:86:ARG:HH21	1.83	0.44
2:D:20:LEU:O	2:D:24:MET:HG3	2.17	0.44
1:C:78:ASN:HB3	1:C:320:LYS:HG2	1.99	0.44
1:A:96:THR:O	1:A:100:VAL:HG23	2.18	0.44
5:C:413:Y01:HAP1	5:C:413:Y01:HAO2	1.57	0.44
1:A:83:ILE:HD12	1:A:326:TYR:HB2	2.00	0.43
1:A:231:LEU:HD13	5:A:411:Y01:HAC2	2.00	0.43
5:C:412:Y01:HAO2	5:C:412:Y01:HAP1	1.45	0.43
1:C:124:ALA:O	1:C:127:PHE:HB2	2.18	0.43
1:A:132:LEU:CD1	4:A:408:LBN:C1	2.96	0.43
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.92	0.43
5:A:410:Y01:HAE2	5:A:410:Y01:HBB	1.78	0.43
1:C:123:TYR:HE2	1:C:263:LEU:HB2	1.83	0.42
3:C:402:PLM:H41	3:C:407:PLM:H41	2.00	0.42
1:A:131:MET:HE1	1:A:239:ILE:HG13	2.01	0.42
5:C:411:Y01:HAJ1	5:C:411:Y01:HAC3	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:CYS:HA	3:C:402:PLM:H22	2.01	0.42
5:A:409:Y01:HAS2	5:A:409:Y01:HAE1	1.90	0.42
5:A:409:Y01:HAE2	5:A:409:Y01:HBB	1.65	0.42
1:A:309:MET:HE3	1:A:309:MET:HB3	1.95	0.42
1:C:302:LEU:HD12	1:C:302:LEU:HA	1.86	0.41
1:A:128:TYR:HD2	4:A:408:LBN:O8	2.02	0.41
1:A:238:ILE:O	1:A:239:ILE:C	2.62	0.41
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.91	0.41
5:C:413:Y01:HAC2	5:C:413:Y01:HAJ2	1.65	0.41
5:C:411:Y01:HAE2	5:C:411:Y01:HBB	1.77	0.41
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.88	0.41
5:A:411:Y01:HAS2	5:A:411:Y01:HAE1	1.88	0.41
1:C:19:LEU:O	1:C:23:LYS:HG3	2.21	0.41
1:C:124:ALA:HB1	1:C:188:ALA:HA	2.03	0.41
1:A:164:CYS:HB3	3:A:406:PLM:H32	2.03	0.41
1:C:123:TYR:OH	1:C:262:LEU:HB3	2.19	0.41
1:C:304:LEU:HD23	1:C:304:LEU:HA	1.92	0.41
5:A:411:Y01:HAE2	5:A:411:Y01:HBB	1.71	0.41
1:C:183:GLY:O	1:C:186:GLN:HG3	2.20	0.41
1:C:120:THR:HB	1:C:191:LYS:HE2	2.03	0.40
1:A:128:TYR:HE2	4:A:408:LBN:O4	2.04	0.40
1:C:43:LEU:HD23	1:C:43:LEU:HA	1.91	0.40
5:A:410:Y01:HAC3	5:A:410:Y01:HAJ1	1.64	0.40
1:C:46:LEU:HA	1:C:46:LEU:HD12	1.88	0.40
1:C:123:TYR:O	1:C:127:PHE:HD1	2.05	0.40
5:C:412:Y01:HAC2	5:C:412:Y01:HAJ1	1.63	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	322/340 (95%)	320 (99%)	2 (1%)	0	100	100
1	C	322/340 (95%)	319 (99%)	3 (1%)	0	100	100
2	B	46/128 (36%)	46 (100%)	0	0	100	100
2	D	47/128 (37%)	47 (100%)	0	0	100	100
All	All	737/936 (79%)	732 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/297 (95%)	282 (100%)	1 (0%)	84	90
1	C	283/297 (95%)	282 (100%)	1 (0%)	84	90
2	B	42/115 (36%)	42 (100%)	0	100	100
2	D	43/115 (37%)	43 (100%)	0	100	100
All	All	651/824 (79%)	649 (100%)	2 (0%)	84	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	VAL
1	C	155	VAL

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

Mol	Chain	Res	Type
1	A	25	ASN
1	A	222	ASN
1	C	25	ASN
1	C	78	ASN
1	C	246	HIS
1	C	322	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

28 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	$\# Z > 2$
5	Y01	A	409	-	33,33,38	4.95	14 (42%)	49,50,57	2.06	15 (30%)
3	PLM	C	406	1	5,6,17	0.60	0	4,5,17	0.63	0
5	Y01	A	410	-	33,33,38	4.96	14 (42%)	49,50,57	2.15	16 (32%)
3	PLM	A	403	1	7,8,17	0.51	0	6,7,17	0.96	0
5	Y01	C	412	-	33,33,38	4.95	14 (42%)	49,50,57	2.19	17 (34%)
3	PLM	A	405	1	9,10,17	0.52	0	8,9,17	0.43	0
5	Y01	C	413	-	38,38,38	4.56	14 (36%)	57,57,57	1.99	15 (26%)
3	PLM	A	401	1	6,7,17	0.56	0	5,6,17	0.57	0
5	Y01	C	411	-	33,33,38	4.96	14 (42%)	49,50,57	2.11	16 (32%)
3	PLM	C	404	1	6,7,17	0.49	0	5,6,17	0.69	0
3	PLM	C	401	1	11,12,17	0.36	0	10,11,17	0.85	0
4	LBN	C	408	-	39,39,51	0.33	0	42,44,59	0.32	0
3	PLM	A	402	1	7,8,17	0.56	0	6,7,17	0.50	0
3	PLM	A	406	1	6,7,17	0.44	0	5,6,17	0.57	0
6	ZWY	A	413	-	28,28,28	5.51	12 (42%)	42,46,46	2.25	15 (35%)
3	PLM	C	405	1	5,6,17	0.48	0	4,5,17	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLM	C	407	1	7,8,17	0.49	0	6,7,17	0.72	0
3	PLM	A	407	1	9,10,17	0.40	0	8,9,17	0.84	0
3	PLM	A	404	1	6,7,17	0.50	0	5,6,17	0.94	0
5	Y01	A	412	-	38,38,38	4.57	14 (36%)	57,57,57	1.99	14 (24%)
5	Y01	A	411	-	33,33,38	4.94	14 (42%)	49,50,57	2.20	16 (32%)
3	PLM	C	402	1	9,10,17	0.36	0	8,9,17	0.88	0
4	LBN	A	408	-	45,45,51	0.31	0	48,50,59	0.33	0
6	ZWY	C	415	-	28,28,28	5.51	12 (42%)	42,46,46	2.17	15 (35%)
4	LBN	C	409	-	38,38,51	0.34	0	41,43,59	0.35	0
4	LBN	C	414	-	44,44,51	1.34	4 (9%)	47,49,59	1.28	3 (6%)
5	Y01	C	410	-	33,33,38	4.94	14 (42%)	49,50,57	2.06	15 (30%)
3	PLM	C	403	1	7,8,17	0.54	0	6,7,17	0.52	0

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
5	Y01	A	409	-	-	11/13/71/77	0/4/4/4
3	PLM	C	406	1	-	0/4/4/15	-
5	Y01	A	410	-	-	9/13/71/77	0/4/4/4
3	PLM	A	403	1	-	4/6/6/15	-
5	Y01	C	412	-	-	10/13/71/77	0/4/4/4
3	PLM	A	405	1	-	5/8/8/15	-
5	Y01	C	413	-	-	15/19/77/77	0/4/4/4
3	PLM	A	401	1	-	1/5/5/15	-
5	Y01	C	411	-	-	9/13/71/77	0/4/4/4
3	PLM	C	404	1	-	0/5/5/15	-
3	PLM	C	401	1	-	4/10/10/15	-
4	LBN	C	408	-	-	7/43/43/55	-
3	PLM	A	402	1	-	2/6/6/15	-
3	PLM	A	406	1	-	0/5/5/15	-
6	ZWY	A	413	-	-	3/5/63/63	0/4/4/4
3	PLM	C	405	1	-	0/4/4/15	-
3	PLM	C	407	1	-	1/6/6/15	-
3	PLM	A	407	1	-	2/8/8/15	-
3	PLM	A	404	1	-	0/5/5/15	-
5	Y01	A	412	-	-	14/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	Y01	A	411	-	-	9/13/71/77	0/4/4/4
3	PLM	C	402	1	-	0/8/8/15	-
4	LBN	A	408	-	-	8/49/49/55	-
6	ZWY	C	415	-	-	3/5/63/63	0/4/4/4
4	LBN	C	409	-	-	4/42/42/55	-
4	LBN	C	414	-	-	24/48/48/55	-
5	Y01	C	410	-	-	11/13/71/77	0/4/4/4
3	PLM	C	403	1	-	0/6/6/15	-

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	409	Y01	CAI-CAZ	17.59	1.69	1.33
5	C	410	Y01	CAI-CAZ	17.58	1.69	1.33
5	C	411	Y01	CAI-CAZ	17.55	1.69	1.33
5	A	412	Y01	CAI-CAZ	17.55	1.69	1.33
5	A	410	Y01	CAI-CAZ	17.53	1.69	1.33
5	C	413	Y01	CAI-CAZ	17.51	1.69	1.33
5	C	412	Y01	CAI-CAZ	17.50	1.69	1.33
5	A	411	Y01	CAI-CAZ	17.48	1.69	1.33
6	A	413	ZWY	C13-C14	17.41	1.68	1.33
6	C	415	ZWY	C13-C14	17.37	1.68	1.33
6	A	413	ZWY	C02-C10	12.92	1.69	1.52
6	C	415	ZWY	C02-C10	12.85	1.69	1.52
5	C	411	Y01	CBB-CBE	-10.34	1.36	1.54
5	A	410	Y01	CBB-CBE	-10.34	1.36	1.54
5	A	409	Y01	CBB-CBE	-10.29	1.36	1.54
6	C	415	ZWY	C09-C10	10.29	1.68	1.51
5	C	412	Y01	CBB-CBE	-10.26	1.36	1.54
5	C	410	Y01	CBB-CBE	-10.26	1.36	1.54
5	A	411	Y01	CBB-CBE	-10.24	1.36	1.54
5	A	412	Y01	CBB-CBE	-10.24	1.36	1.54
5	C	413	Y01	CBB-CBE	-10.23	1.36	1.54
6	A	413	ZWY	C09-C10	10.22	1.68	1.51
5	A	409	Y01	CBH-CBF	8.93	1.70	1.56
5	C	411	Y01	CBH-CBF	8.89	1.70	1.56
5	C	410	Y01	CBH-CBF	8.89	1.70	1.56
5	A	410	Y01	CBH-CBF	8.85	1.70	1.56
5	C	413	Y01	CBH-CBF	8.69	1.69	1.56
5	A	412	Y01	CBH-CBF	8.69	1.69	1.56
5	A	411	Y01	CBH-CBF	8.68	1.69	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	412	Y01	CBH-CBF	8.64	1.69	1.56
6	A	413	ZWY	C03-C02	-7.39	1.40	1.54
6	C	415	ZWY	C03-C02	-7.37	1.40	1.54
5	A	410	Y01	CAP-CBE	7.32	1.69	1.54
5	A	409	Y01	CAP-CBE	7.32	1.69	1.54
5	C	412	Y01	CAP-CBE	7.32	1.69	1.54
5	A	411	Y01	CAP-CBE	7.32	1.69	1.54
5	C	410	Y01	CAP-CBE	7.32	1.69	1.54
5	C	413	Y01	CAP-CBE	7.30	1.69	1.54
5	C	411	Y01	CAP-CBE	7.28	1.69	1.54
5	A	412	Y01	CAP-CBE	7.28	1.69	1.54
6	A	413	ZWY	C12-C06	7.01	1.64	1.53
5	A	410	Y01	CAU-CAS	6.98	1.67	1.53
5	C	411	Y01	CAU-CAS	6.93	1.67	1.53
6	C	415	ZWY	C12-C06	6.93	1.64	1.53
5	C	412	Y01	CAU-CAS	6.87	1.67	1.53
5	A	409	Y01	CAU-CAS	6.85	1.67	1.53
5	C	410	Y01	CAU-CBI	-6.85	1.42	1.54
5	C	410	Y01	CAU-CAS	6.84	1.67	1.53
5	A	411	Y01	CAU-CAS	6.83	1.67	1.53
5	A	409	Y01	CAU-CBI	-6.82	1.42	1.54
5	A	410	Y01	CAU-CBI	-6.78	1.42	1.54
5	C	411	Y01	CAU-CBI	-6.77	1.42	1.54
5	C	412	Y01	CAU-CBI	-6.75	1.42	1.54
5	A	412	Y01	CAU-CBI	-6.75	1.42	1.54
5	C	413	Y01	CAU-CBI	-6.75	1.42	1.54
5	C	413	Y01	CAU-CAS	6.74	1.66	1.53
5	C	412	Y01	CAK-CBD	6.72	1.64	1.53
5	A	411	Y01	CAU-CBI	-6.71	1.42	1.54
5	A	412	Y01	CAU-CAS	6.71	1.66	1.53
5	A	411	Y01	CAK-CBD	6.70	1.63	1.53
6	C	415	ZWY	C15-C05	6.55	1.66	1.56
5	A	410	Y01	CAK-CBD	6.49	1.63	1.53
6	A	413	ZWY	C15-C05	6.46	1.66	1.56
5	A	412	Y01	CAK-CBD	6.45	1.63	1.53
5	C	411	Y01	CAK-CBD	6.43	1.63	1.53
5	C	413	Y01	CAK-CBD	6.43	1.63	1.53
5	A	409	Y01	CAK-CBD	6.33	1.63	1.53
5	C	410	Y01	CAK-CBD	6.31	1.63	1.53
6	C	415	ZWY	C03-C04	6.22	1.65	1.53
6	A	413	ZWY	C03-C04	6.14	1.65	1.53
6	A	413	ZWY	C08-C07	6.09	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	415	ZWY	C08-C07	6.03	1.66	1.54
5	C	411	Y01	CBI-CBE	5.83	1.65	1.55
5	A	410	Y01	CBI-CBE	5.80	1.65	1.55
5	C	411	Y01	OAW-CAY	5.73	1.45	1.33
5	C	412	Y01	CBI-CBE	5.71	1.65	1.55
5	A	411	Y01	CBI-CBE	5.71	1.65	1.55
5	A	409	Y01	OAW-CAY	5.68	1.45	1.33
5	A	410	Y01	OAW-CAY	5.68	1.45	1.33
5	C	410	Y01	OAW-CAY	5.67	1.45	1.33
5	C	412	Y01	OAW-CAY	5.67	1.45	1.33
5	A	411	Y01	OAW-CAY	5.66	1.45	1.33
5	C	413	Y01	CBI-CBE	5.62	1.65	1.55
5	A	412	Y01	CBI-CBE	5.58	1.65	1.55
5	A	409	Y01	CBI-CBE	5.54	1.65	1.55
5	C	410	Y01	CBI-CBE	5.54	1.65	1.55
6	A	413	ZWY	C08-C09	4.74	1.63	1.53
6	C	415	ZWY	C08-C09	4.73	1.63	1.53
4	C	414	LBN	C42-C5	4.27	1.55	1.31
5	A	412	Y01	OAW-CAY	3.97	1.45	1.34
5	C	413	Y01	OAW-CAY	3.95	1.45	1.34
5	C	412	Y01	CAC-CBB	3.71	1.62	1.53
5	C	410	Y01	CAC-CBB	3.70	1.62	1.53
5	A	411	Y01	CAC-CBB	3.69	1.62	1.53
5	C	411	Y01	CAC-CBB	3.68	1.62	1.53
5	A	412	Y01	CAC-CBB	3.68	1.62	1.53
5	A	410	Y01	CAC-CBB	3.68	1.62	1.53
5	A	409	Y01	CAC-CBB	3.67	1.62	1.53
5	C	413	Y01	CAC-CBB	3.67	1.62	1.53
5	A	412	Y01	CAQ-CBG	3.25	1.61	1.54
5	A	411	Y01	CAQ-CBG	3.23	1.61	1.54
5	C	412	Y01	CAQ-CBG	3.23	1.61	1.54
5	A	409	Y01	CAQ-CBG	3.22	1.61	1.54
5	C	413	Y01	CAQ-CBG	3.21	1.60	1.54
5	C	410	Y01	CAQ-CBG	3.17	1.60	1.54
5	C	411	Y01	CAQ-CBG	3.17	1.60	1.54
5	A	410	Y01	CAQ-CBG	3.16	1.60	1.54
4	C	414	LBN	O5-C25	2.91	1.41	1.33
6	A	413	ZWY	O20-S21	2.79	1.65	1.57
5	A	411	Y01	CBH-CAZ	-2.78	1.47	1.52
5	A	412	Y01	CAV-CAZ	2.78	1.57	1.51
5	C	413	Y01	CAV-CAZ	2.76	1.57	1.51
5	C	412	Y01	CBH-CAZ	-2.76	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	415	ZWY	O20-S21	2.75	1.65	1.57
5	C	410	Y01	CAV-CAZ	2.74	1.57	1.51
5	A	409	Y01	CAV-CAZ	2.74	1.57	1.51
5	C	411	Y01	CAV-CAZ	2.71	1.57	1.51
4	C	414	LBN	O7-C2	-2.68	1.40	1.46
6	C	415	ZWY	O20-C18	-2.67	1.42	1.48
6	A	413	ZWY	O20-C18	-2.66	1.42	1.48
5	A	411	Y01	CAV-CAZ	2.64	1.57	1.51
4	C	414	LBN	O7-C34	2.63	1.41	1.34
5	A	410	Y01	CAV-CAZ	2.62	1.56	1.51
5	C	412	Y01	CAV-CAZ	2.61	1.56	1.51
5	A	410	Y01	CBH-CAZ	-2.60	1.47	1.52
5	A	412	Y01	CBH-CAZ	-2.54	1.48	1.52
5	C	411	Y01	CBH-CAZ	-2.53	1.48	1.52
5	C	413	Y01	CBH-CAZ	-2.52	1.48	1.52
5	C	410	Y01	CBH-CAZ	-2.40	1.48	1.52
5	A	409	Y01	CBH-CAZ	-2.33	1.48	1.52
5	C	412	Y01	CAK-CAI	2.26	1.54	1.50
5	A	411	Y01	CAK-CAI	2.23	1.54	1.50
5	A	412	Y01	CAK-CAI	2.09	1.54	1.50
5	C	413	Y01	CAK-CAI	2.09	1.54	1.50
5	C	410	Y01	CAK-CAI	2.07	1.54	1.50
6	C	415	ZWY	C02-C07	2.06	1.58	1.54
6	A	413	ZWY	C02-C07	2.05	1.58	1.54
5	A	409	Y01	CAK-CAI	2.05	1.54	1.50
5	A	410	Y01	CAK-CAI	2.05	1.54	1.50
5	C	411	Y01	CAK-CAI	2.04	1.54	1.50

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	411	Y01	CAK-CAI-CAZ	-5.92	115.02	125.02
5	C	412	Y01	CAK-CAI-CAZ	-5.84	115.17	125.02
5	A	410	Y01	CAK-CAI-CAZ	-5.78	115.27	125.02
4	C	414	LBN	C13-C10-C7	-5.73	85.39	114.37
5	C	411	Y01	CAK-CAI-CAZ	-5.41	115.88	125.02
6	A	413	ZWY	C12-C13-C14	-5.24	116.17	125.02
6	A	413	ZWY	C01-C02-C03	-5.20	105.16	111.10
6	A	413	ZWY	C01-C02-C07	-5.17	105.56	112.99
5	C	413	Y01	CAK-CAI-CAZ	-5.02	116.53	125.02
5	A	412	Y01	CAK-CAI-CAZ	-5.02	116.54	125.02
6	C	415	ZWY	C01-C02-C07	-4.89	105.98	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	410	Y01	CAK-CAI-CAZ	-4.88	116.77	125.02
6	C	415	ZWY	C12-C13-C14	-4.87	116.80	125.02
5	A	409	Y01	CAK-CAI-CAZ	-4.82	116.87	125.02
6	C	415	ZWY	C01-C02-C03	-4.77	105.65	111.10
5	C	412	Y01	OAW-CAY-OAG	-4.53	119.89	125.70
5	A	411	Y01	OAW-CAY-OAG	-4.51	119.91	125.70
5	A	410	Y01	OAW-CAY-OAG	-4.49	119.93	125.70
5	C	411	Y01	OAW-CAY-OAG	-4.48	119.95	125.70
5	C	410	Y01	OAW-CAY-OAG	-4.40	120.05	125.70
5	A	409	Y01	OAW-CAY-OAG	-4.37	120.09	125.70
5	A	409	Y01	CBI-CBE-CBB	-4.36	112.76	119.50
5	C	410	Y01	CBI-CBE-CBB	-4.35	112.78	119.50
5	C	413	Y01	OAW-CAY-CAM	4.35	120.89	111.48
5	A	412	Y01	OAW-CAY-CAM	4.31	120.81	111.48
5	C	412	Y01	CBI-CBE-CBB	-4.25	112.93	119.50
5	A	411	Y01	CBI-CBE-CBB	-4.13	113.12	119.50
5	A	411	Y01	CAU-CBI-CBE	4.13	122.68	116.60
5	A	411	Y01	CAE-CBI-CAU	-4.10	104.56	110.61
5	C	413	Y01	CBI-CBE-CBB	-4.10	113.16	119.50
5	C	412	Y01	CAE-CBI-CAU	-4.07	104.61	110.61
5	C	412	Y01	CBH-CAZ-CAI	-4.06	116.99	122.93
5	A	412	Y01	CBI-CBE-CBB	-4.03	113.27	119.50
5	C	412	Y01	CAU-CBI-CBE	4.03	122.53	116.60
5	C	411	Y01	CAE-CBI-CAU	-4.00	104.71	110.61
5	A	410	Y01	CAE-CBI-CAU	-4.00	104.72	110.61
6	C	415	ZWY	C25-C15-C05	-3.98	107.19	111.66
5	C	413	Y01	CAU-CBI-CBG	3.95	113.15	107.25
5	C	410	Y01	CAE-CBI-CAU	-3.94	104.79	110.61
4	C	414	LBN	O7-C34-C35	3.94	120.00	111.48
5	A	412	Y01	CAU-CBI-CBG	3.93	113.13	107.25
5	A	409	Y01	CAE-CBI-CAU	-3.92	104.82	110.61
5	C	411	Y01	CBI-CBE-CBB	-3.88	113.51	119.50
5	C	413	Y01	CAU-CBI-CBE	3.86	122.28	116.60
5	C	411	Y01	CBG-CBI-CBE	3.84	104.50	100.10
5	A	410	Y01	CBI-CBE-CBB	-3.83	113.59	119.50
5	A	412	Y01	CAU-CBI-CBE	3.82	122.23	116.60
5	A	410	Y01	CBG-CBI-CBE	3.80	104.46	100.10
5	C	413	Y01	CAE-CBI-CAU	-3.78	105.03	110.61
5	A	412	Y01	CAE-CBI-CAU	-3.78	105.03	110.61
5	A	410	Y01	CAU-CBI-CBE	3.78	122.17	116.60
5	C	411	Y01	CAU-CBI-CBE	3.77	122.15	116.60
6	A	413	ZWY	C12-C06-C05	3.71	114.01	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	413	ZWY	C15-C14-C13	-3.71	117.52	122.93
5	C	410	Y01	CAU-CBI-CBE	3.70	122.06	116.60
5	A	409	Y01	CAU-CBI-CBE	3.70	122.05	116.60
5	A	410	Y01	CAE-CBI-CBG	-3.69	104.99	111.68
5	C	413	Y01	CAD-CBH-CBF	-3.67	107.54	111.66
5	A	411	Y01	CBH-CAZ-CAI	-3.66	117.58	122.93
5	A	412	Y01	CAD-CBH-CBF	-3.64	107.58	111.66
5	C	411	Y01	CAE-CBI-CBG	-3.63	105.09	111.68
5	A	409	Y01	CBG-CBI-CBE	3.58	104.21	100.10
5	C	412	Y01	CAU-CBI-CBG	3.56	112.58	107.25
6	A	413	ZWY	C03-C02-C10	3.55	121.74	116.71
5	A	412	Y01	CAE-CBI-CBG	-3.54	105.25	111.68
5	C	412	Y01	CAE-CBI-CBG	-3.54	105.26	111.68
5	A	411	Y01	CAE-CBI-CBG	-3.53	105.28	111.68
6	C	415	ZWY	C15-C14-C13	-3.53	117.78	122.93
6	C	415	ZWY	C03-C02-C10	3.52	121.70	116.71
5	C	410	Y01	CBG-CBI-CBE	3.52	104.14	100.10
5	C	410	Y01	CAU-CBI-CBG	3.52	112.51	107.25
5	A	412	Y01	CBH-CAZ-CAI	-3.51	117.80	122.93
5	A	411	Y01	CAU-CBI-CBG	3.51	112.50	107.25
6	A	413	ZWY	C25-C15-C05	-3.50	107.74	111.66
5	C	413	Y01	CAE-CBI-CBG	-3.49	105.34	111.68
5	C	413	Y01	CBH-CAZ-CAI	-3.49	117.84	122.93
5	A	409	Y01	CAU-CBI-CBG	3.44	112.39	107.25
5	A	409	Y01	CAD-CBH-CBF	-3.43	107.81	111.66
5	C	410	Y01	CAE-CBI-CBG	-3.41	105.49	111.68
5	C	411	Y01	CAD-CBH-CBF	-3.40	107.84	111.66
6	A	413	ZWY	C03-C02-C07	3.40	114.16	108.88
5	A	409	Y01	CAE-CBI-CBG	-3.40	105.51	111.68
5	A	411	Y01	CAD-CBH-CBF	-3.40	107.84	111.66
5	C	410	Y01	CAD-CBH-CBF	-3.38	107.87	111.66
5	C	412	Y01	CBG-CBI-CBE	3.37	103.97	100.10
5	A	411	Y01	CBG-CBI-CBE	3.36	103.95	100.10
5	C	411	Y01	CBF-CBH-CAZ	3.30	114.48	109.65
5	C	412	Y01	CAD-CBH-CBF	-3.26	108.00	111.66
6	C	415	ZWY	C03-C02-C07	3.25	113.92	108.88
5	A	410	Y01	CAD-CBH-CBF	-3.24	108.03	111.66
5	C	410	Y01	CBF-CBH-CAZ	3.13	114.24	109.65
5	A	409	Y01	CBF-CBH-CAZ	3.10	114.19	109.65
5	A	411	Y01	CAT-CAR-CBC	3.09	115.38	110.33
6	C	415	ZWY	C12-C06-C05	3.08	113.28	109.72
5	A	410	Y01	CAK-CBD-CBF	3.01	113.20	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	410	Y01	CAU-CBI-CBG	3.00	111.74	107.25
5	C	411	Y01	CAU-CBI-CBG	2.99	111.71	107.25
6	C	415	ZWY	C04-C05-C15	-2.98	109.41	113.08
5	C	412	Y01	CAT-CAR-CBC	2.94	115.12	110.33
5	A	410	Y01	CBF-CBH-CAZ	2.93	113.95	109.65
5	A	412	Y01	CBG-CBI-CBE	2.91	103.44	100.10
5	C	413	Y01	CAE-CBI-CBE	-2.87	106.47	111.68
5	A	412	Y01	CAV-CAZ-CBH	-2.87	112.75	116.42
5	C	413	Y01	CAV-CAZ-CBH	-2.86	112.75	116.42
5	A	412	Y01	CAE-CBI-CBE	-2.85	106.51	111.68
6	C	415	ZWY	O23-S21-O22	-2.84	101.27	112.24
6	A	413	ZWY	O23-S21-O22	-2.84	101.28	112.24
5	A	409	Y01	CBF-CBD-CBG	2.82	112.77	109.09
6	A	413	ZWY	C04-C05-C15	-2.82	109.61	113.08
5	A	411	Y01	CAE-CBI-CBE	-2.81	106.59	111.68
5	C	413	Y01	CBG-CBI-CBE	2.80	103.32	100.10
5	C	412	Y01	CAE-CBI-CBE	-2.79	106.61	111.68
5	A	410	Y01	CAT-CAR-CBC	2.78	114.87	110.33
5	C	410	Y01	CAE-CBI-CBE	-2.75	106.68	111.68
5	A	409	Y01	CAE-CBI-CBE	-2.75	106.69	111.68
5	C	410	Y01	CBF-CBD-CBG	2.75	112.67	109.09
6	C	415	ZWY	C07-C02-C10	2.72	103.81	100.61
5	A	410	Y01	CAV-CAZ-CAI	2.72	124.25	120.57
6	A	413	ZWY	C07-C02-C10	2.72	103.80	100.61
5	C	412	Y01	CAV-CAZ-CBH	-2.68	112.98	116.42
6	A	413	ZWY	C19-C14-C15	-2.63	113.05	116.42
4	C	414	LBN	O5-C25-C26	2.63	119.84	111.83
6	C	415	ZWY	C19-C14-C15	-2.62	113.06	116.42
5	A	411	Y01	CBF-CBD-CBG	2.61	112.50	109.09
5	A	412	Y01	CAK-CBD-CBF	2.61	112.74	109.72
5	C	411	Y01	CAK-CBD-CBF	2.59	112.72	109.72
5	C	413	Y01	CAK-CBD-CBF	2.59	112.72	109.72
5	A	411	Y01	CAV-CAZ-CBH	-2.59	113.11	116.42
5	C	412	Y01	CAK-CBD-CBF	2.51	112.62	109.72
5	C	411	Y01	CAT-CAR-CBC	2.49	114.39	110.33
5	C	411	Y01	CAV-CAZ-CAI	2.47	123.92	120.57
6	A	413	ZWY	C09-C10-C02	-2.46	106.11	108.56
5	C	410	Y01	CAC-CBB-CBE	-2.43	109.24	112.88
5	C	411	Y01	CAC-CBB-CBE	-2.43	109.24	112.88
5	A	409	Y01	CAC-CBB-CBE	-2.43	109.24	112.88
6	C	415	ZWY	C08-C07-C06	2.40	122.92	119.10
5	A	410	Y01	CAC-CBB-CBE	-2.40	109.29	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	413	ZWY	C05-C15-C14	2.36	113.11	109.65
6	C	415	ZWY	C09-C10-C02	-2.36	106.21	108.56
5	A	409	Y01	CAT-CAR-CBC	2.34	114.15	110.33
6	A	413	ZWY	C08-C07-C06	2.33	122.81	119.10
5	C	411	Y01	CAE-CBI-CBE	-2.32	107.48	111.68
5	C	410	Y01	CAT-CAR-CBC	2.31	114.10	110.33
5	A	411	Y01	CAK-CBD-CBF	2.30	112.38	109.72
5	A	410	Y01	CAE-CBI-CBE	-2.27	107.56	111.68
5	C	412	Y01	CBF-CBD-CBG	2.25	112.03	109.09
5	A	409	Y01	CAS-CBF-CBH	-2.25	110.31	113.08
5	C	411	Y01	CAS-CBF-CBH	-2.24	110.33	113.08
6	C	415	ZWY	C05-C15-C14	2.23	112.91	109.65
5	C	410	Y01	CAS-CBF-CBH	-2.21	110.36	113.08
5	A	410	Y01	CAS-CBF-CBH	-2.13	110.46	113.08
5	C	412	Y01	CAT-CBH-CAZ	2.06	112.30	108.74
5	C	412	Y01	CAC-CBB-CBE	-2.06	109.80	112.88
5	A	411	Y01	CAT-CBH-CAZ	2.05	112.28	108.74
5	C	413	Y01	CBF-CBD-CBG	2.05	111.77	109.09
5	A	412	Y01	CAS-CBF-CBH	-2.05	110.56	113.08
5	C	413	Y01	CAS-CBF-CBH	-2.01	110.60	113.08

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	PLM	O2-C1-C2-C3
3	A	405	PLM	O2-C1-C2-C3
4	A	408	LBN	C1-O1-P1-O2
4	A	408	LBN	C1-O1-P1-O4
4	A	408	LBN	N1-C6-C9-O2
4	C	408	LBN	C9-O2-P1-O1
4	C	408	LBN	O7-C2-C3-O5
4	C	408	LBN	N1-C6-C9-O2
4	C	409	LBN	C9-O2-P1-O1
4	C	409	LBN	N1-C6-C9-O2
4	C	414	LBN	C1-O1-P1-O2
4	C	414	LBN	C1-O1-P1-O3
4	C	414	LBN	C1-O1-P1-O4
4	C	414	LBN	C9-O2-P1-O4
5	A	409	Y01	CAV-CBC-OAW-CAY
5	A	409	Y01	CAR-CBC-OAW-CAY
5	A	409	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
5	A	410	Y01	OAG-CAY-OAW-CBC
5	A	411	Y01	OAG-CAY-OAW-CBC
5	A	412	Y01	OAG-CAY-OAW-CBC
5	A	412	Y01	CAM-CAY-OAW-CBC
5	C	410	Y01	CAV-CBC-OAW-CAY
5	C	410	Y01	CAR-CBC-OAW-CAY
5	C	410	Y01	OAG-CAY-OAW-CBC
5	C	411	Y01	OAG-CAY-OAW-CBC
5	C	412	Y01	OAG-CAY-OAW-CBC
5	C	413	Y01	OAG-CAY-OAW-CBC
5	C	413	Y01	CAM-CAY-OAW-CBC
6	A	413	ZWY	C17-C18-O20-S21
6	A	413	ZWY	C19-C18-O20-S21
5	C	410	Y01	CAJ-CAO-CBB-CAC
5	A	409	Y01	CAC-CBB-CBE-CBI
5	C	410	Y01	CAC-CBB-CBE-CBI
5	A	409	Y01	CAO-CBB-CBE-CBI
5	C	410	Y01	CAO-CBB-CBE-CBI
5	A	409	Y01	CAJ-CAO-CBB-CAC
5	C	411	Y01	CAJ-CAO-CBB-CAC
5	A	410	Y01	CAJ-CAO-CBB-CAC
5	A	410	Y01	CAC-CBB-CBE-CBI
5	C	411	Y01	CAC-CBB-CBE-CBI
5	C	412	Y01	CAJ-CAO-CBB-CBE
5	A	411	Y01	CAJ-CAO-CBB-CBE
5	A	412	Y01	CAJ-CAO-CBB-CBE
5	C	413	Y01	CAJ-CAO-CBB-CBE
5	C	412	Y01	CAJ-CAO-CBB-CAC
5	C	412	Y01	CAN-CAJ-CAO-CBB
4	C	414	LBN	C25-C26-C27-C28
5	A	409	Y01	CAC-CBB-CBE-CAP
5	A	410	Y01	CAN-CAJ-CAO-CBB
5	A	412	Y01	CAO-CAJ-CAN-CBA
5	A	411	Y01	CAN-CAJ-CAO-CBB
5	C	411	Y01	CAN-CAJ-CAO-CBB
5	C	410	Y01	CAC-CBB-CBE-CAP
5	C	413	Y01	CAO-CAJ-CAN-CBA
5	C	411	Y01	CAO-CBB-CBE-CBI
4	C	414	LBN	C26-C25-O5-C3
5	A	410	Y01	CAO-CBB-CBE-CBI
5	C	412	Y01	CAC-CBB-CBE-CBI
5	A	412	Y01	CAJ-CAN-CBA-CAA

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Mol	Chain	Res	Type	Atoms
5	C	413	Y01	CAJ-CAN-CBA-CAA
5	C	413	Y01	CAC-CBB-CBE-CBI
5	A	412	Y01	CAJ-CAO-CBB-CAC
5	C	413	Y01	CAJ-CAO-CBB-CAC
6	C	415	ZWY	C17-C18-O20-S21
6	C	415	ZWY	C19-C18-O20-S21
5	A	412	Y01	CAJ-CAN-CBA-CAB
5	C	413	Y01	CAJ-CAN-CBA-CAB
3	C	401	PLM	C6-C7-C8-C9
5	A	411	Y01	CAJ-CAO-CBB-CAC
4	C	414	LBN	O6-C25-O5-C3
3	A	405	PLM	C6-C7-C8-C9
3	A	407	PLM	C2-C3-C4-C5
5	A	411	Y01	CAC-CBB-CBE-CBI
5	A	412	Y01	CAC-CBB-CBE-CBI
5	C	412	Y01	CAO-CBB-CBE-CBI
3	C	401	PLM	C7-C8-C9-CA
5	A	410	Y01	CAC-CBB-CBE-CAP
5	C	411	Y01	CAC-CBB-CBE-CAP
4	C	414	LBN	C35-C34-O7-C2
5	C	410	Y01	CAJ-CAN-CBA-CAA
5	C	413	Y01	CAO-CBB-CBE-CBI
3	A	405	PLM	C2-C3-C4-C5
3	C	401	PLM	C2-C3-C4-C5
3	A	403	PLM	C3-C4-C5-C6
5	C	413	Y01	CAN-CAJ-CAO-CBB
5	A	409	Y01	CAJ-CAN-CBA-CAA
4	C	414	LBN	O8-C34-O7-C2
5	A	412	Y01	CAN-CAJ-CAO-CBB
5	A	412	Y01	CAO-CBB-CBE-CBI
4	C	414	LBN	C26-C27-C28-C29
4	C	408	LBN	C1-C2-C3-O5
5	A	411	Y01	CAO-CBB-CBE-CBI
5	C	412	Y01	CAC-CBB-CBE-CAP
5	C	413	Y01	CAC-CBB-CBE-CAP
5	A	409	Y01	CAO-CBB-CBE-CAP
5	C	410	Y01	CAO-CBB-CBE-CAP
5	C	410	Y01	CAJ-CAO-CBB-CBE
5	A	411	Y01	CAC-CBB-CBE-CAP
4	C	414	LBN	O1-C1-C2-O7
5	A	412	Y01	CAC-CBB-CBE-CAP
3	C	401	PLM	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	A	408	LBN	C1-C2-C3-O5
5	A	409	Y01	CAJ-CAO-CBB-CBE
5	A	409	Y01	CAJ-CAN-CBA-CAB
5	A	410	Y01	CAO-CBB-CBE-CAP
5	C	411	Y01	CAO-CBB-CBE-CAP
5	C	410	Y01	CAJ-CAN-CBA-CAB
3	A	403	PLM	C2-C3-C4-C5
5	C	411	Y01	CAJ-CAO-CBB-CBE
6	A	413	ZWY	C18-O20-S21-O23
6	C	415	ZWY	C18-O20-S21-O23
5	C	412	Y01	CAO-CBB-CBE-CAP
4	C	414	LBN	C1-C2-C3-O5
4	C	414	LBN	O7-C2-C3-O5
4	C	414	LBN	C36-C37-C38-C39
3	A	405	PLM	C3-C4-C5-C6
3	A	401	PLM	C1-C2-C3-C4
3	A	403	PLM	C1-C2-C3-C4
3	A	405	PLM	C1-C2-C3-C4
5	A	410	Y01	CAJ-CAO-CBB-CBE
4	C	414	LBN	O1-C1-C2-C3
5	C	412	Y01	CAJ-CAN-CBA-CAA
4	A	408	LBN	C40-C41-C42-C5
4	A	408	LBN	O7-C2-C3-O5
5	C	413	Y01	CAO-CBB-CBE-CAP
3	A	402	PLM	C5-C6-C7-C8
4	C	414	LBN	C8-C11-C14-C17
4	A	408	LBN	C1-O1-P1-O3
4	C	408	LBN	C1-O1-P1-O4
4	C	408	LBN	C9-O2-P1-O4
4	C	409	LBN	C9-O2-P1-O4
4	C	414	LBN	N1-C6-C9-O2
5	A	411	Y01	CAO-CBB-CBE-CAP
5	A	412	Y01	CAO-CBB-CBE-CAP
4	C	414	LBN	C2-C1-O1-P1
4	C	414	LBN	C31-C32-C33-C4
5	A	411	Y01	CAJ-CAN-CBA-CAA
5	C	412	Y01	CAJ-CAN-CBA-CAB
4	A	408	LBN	C2-C1-O1-P1
5	C	413	Y01	CAM-CAL-CAX-OAH
4	C	414	LBN	C32-C33-C4-C7
5	C	413	Y01	CAM-CAL-CAX-OAF
5	A	412	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
5	A	412	Y01	CAM-CAL-CAX-OAF
3	A	403	PLM	C5-C6-C7-C8
4	C	414	LBN	C13-C16-C19-C21
4	C	414	LBN	C40-C41-C42-C5
5	C	411	Y01	CAJ-CAN-CBA-CAB
4	C	414	LBN	C39-C40-C41-C42
4	C	414	LBN	C37-C38-C39-C40
4	C	409	LBN	O7-C34-C35-C36
5	A	410	Y01	CAJ-CAN-CBA-CAB
3	A	407	PLM	C5-C6-C7-C8
4	C	408	LBN	O5-C25-C26-C27
3	C	407	PLM	C5-C6-C7-C8
5	C	413	Y01	CAL-CAM-CAY-OAW

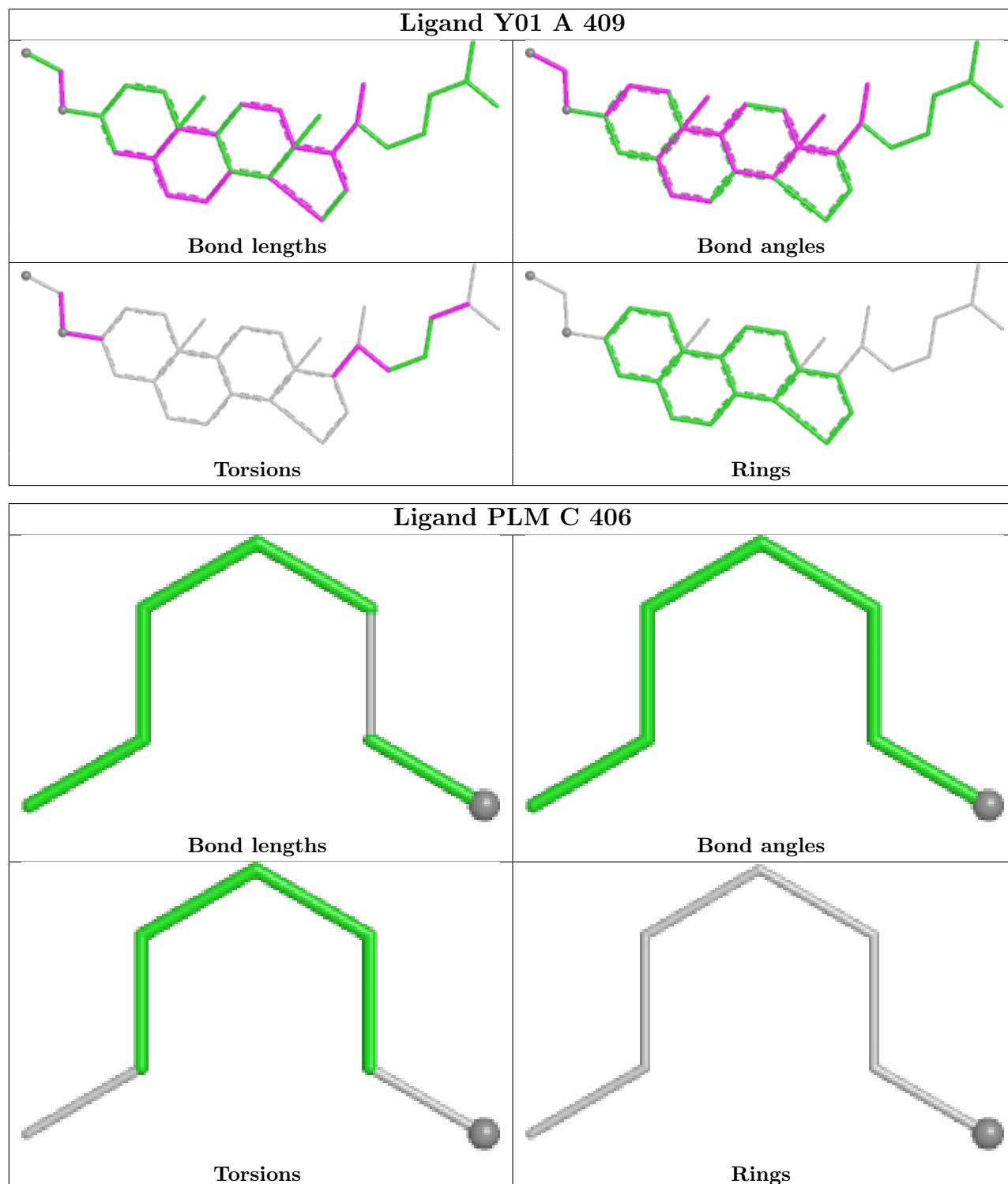
There are no ring outliers.

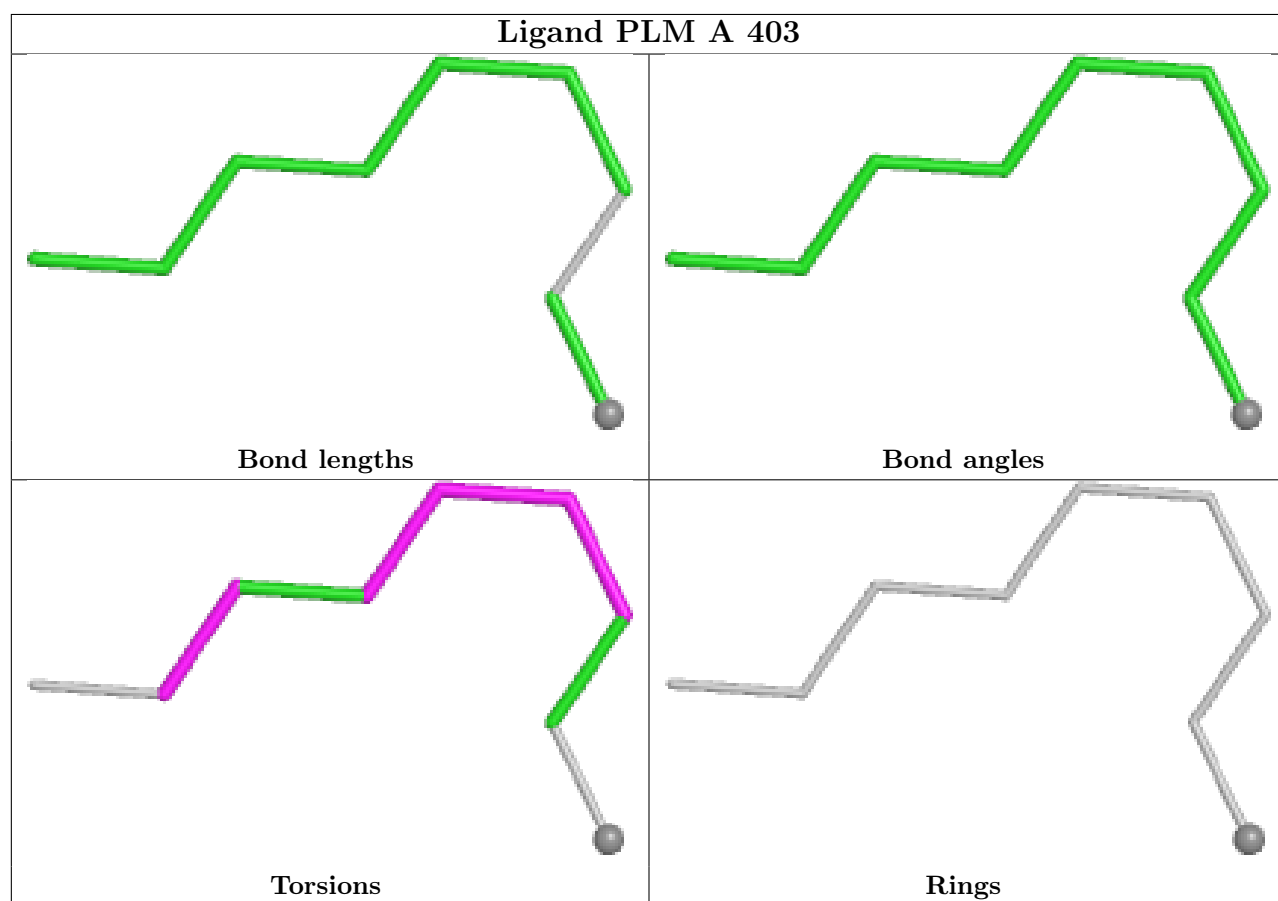
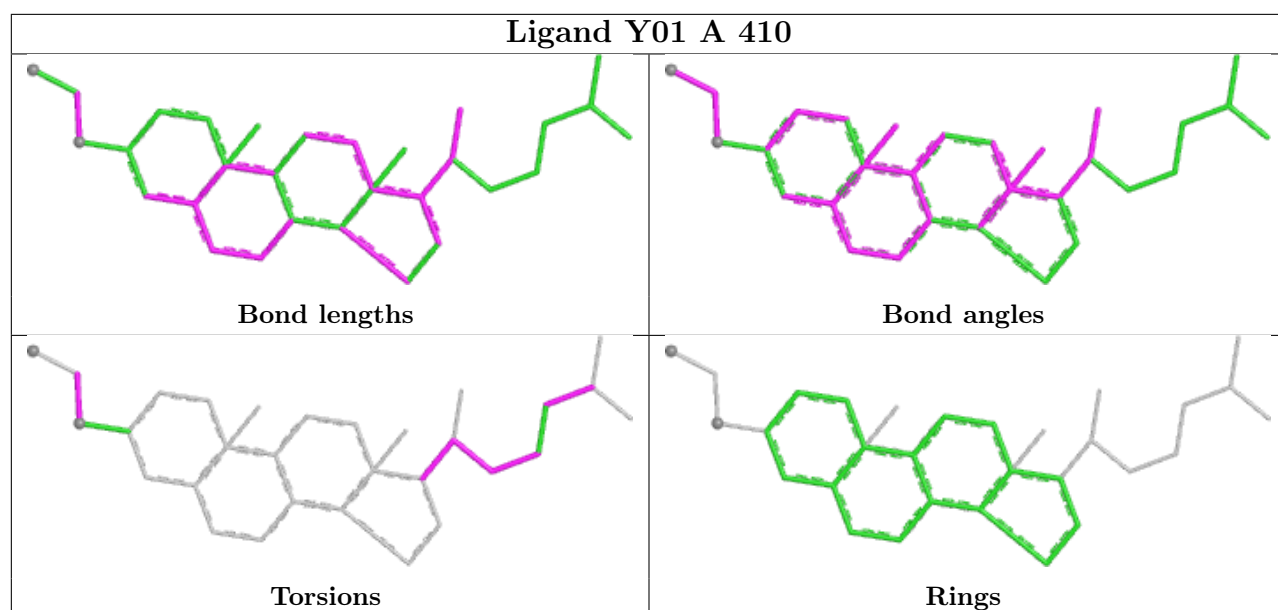
18 monomers are involved in 40 short contacts:

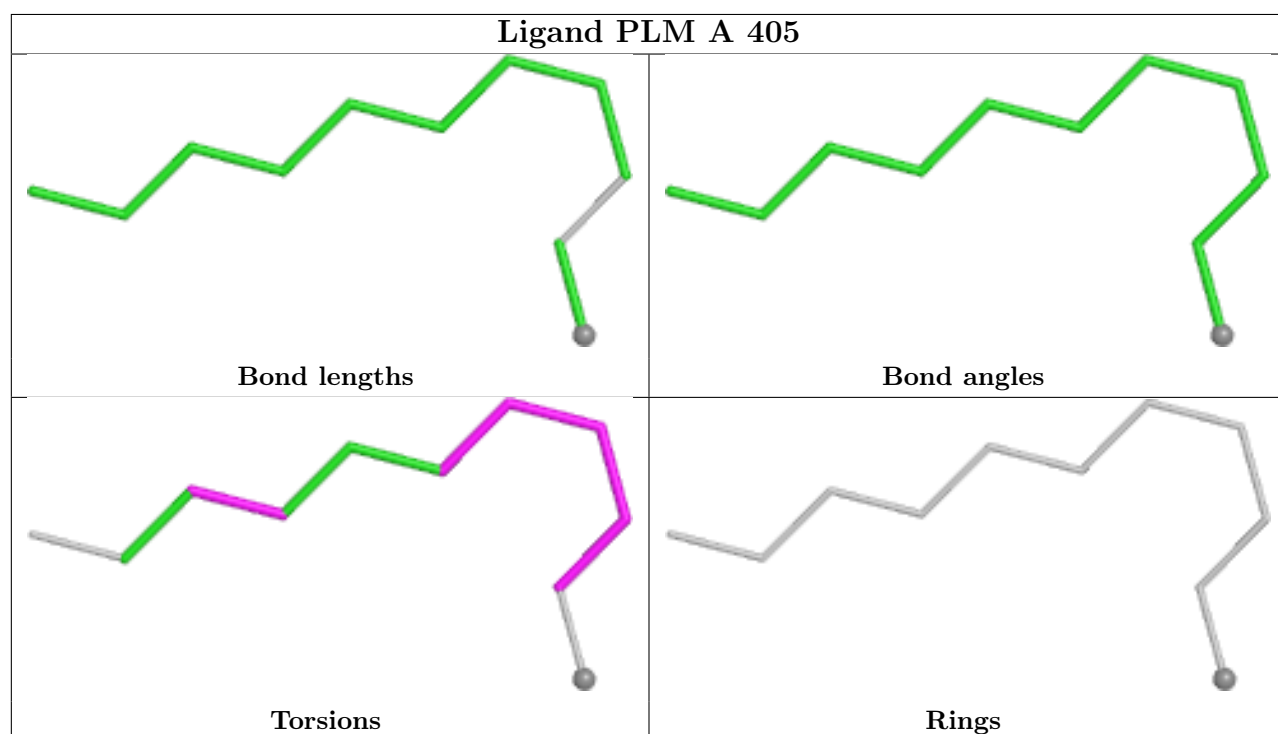
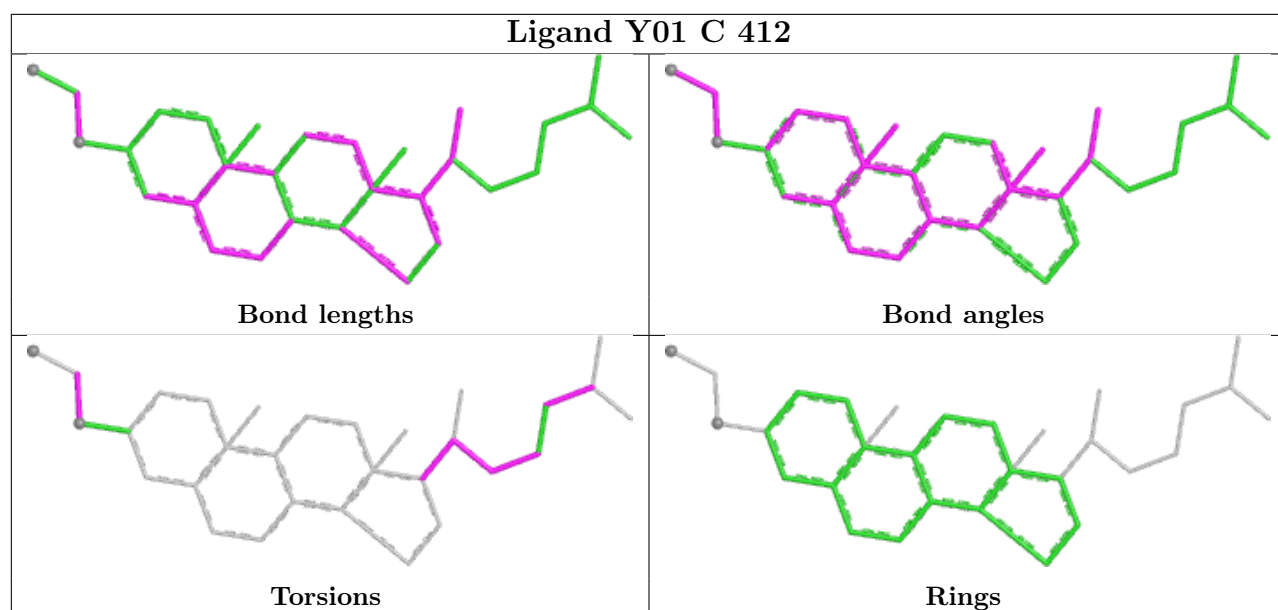
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	409	Y01	2	0
5	A	410	Y01	2	0
3	A	403	PLM	1	0
5	C	412	Y01	3	0
3	A	405	PLM	1	0
5	C	413	Y01	2	0
5	C	411	Y01	2	0
3	C	404	PLM	4	0
4	C	408	LBN	4	0
3	A	406	PLM	2	0
3	C	407	PLM	1	0
3	A	407	PLM	2	0
5	A	412	Y01	2	0
5	A	411	Y01	5	0
3	C	402	PLM	2	0
4	A	408	LBN	8	0
5	C	410	Y01	1	0
3	C	403	PLM	1	0

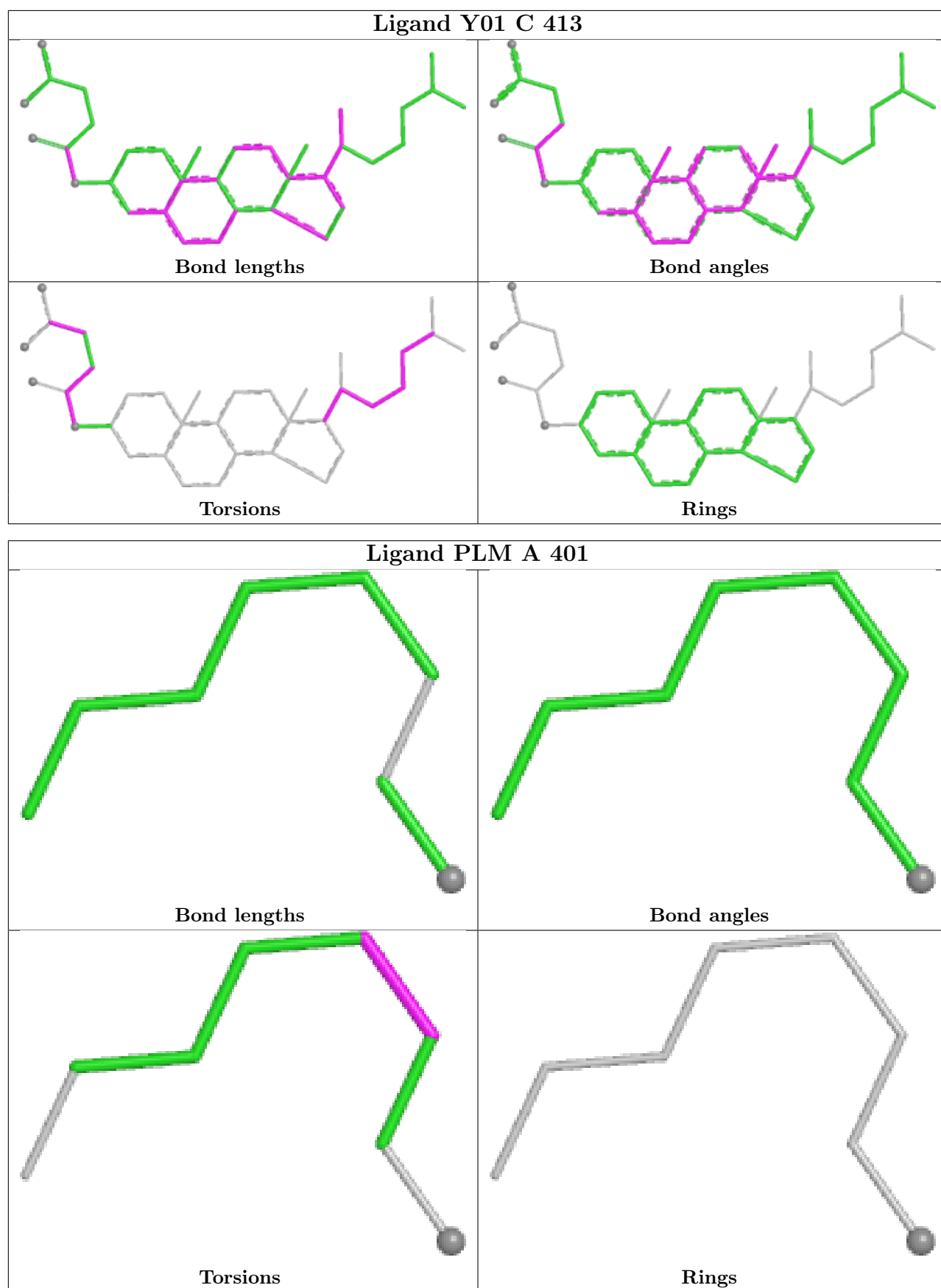
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

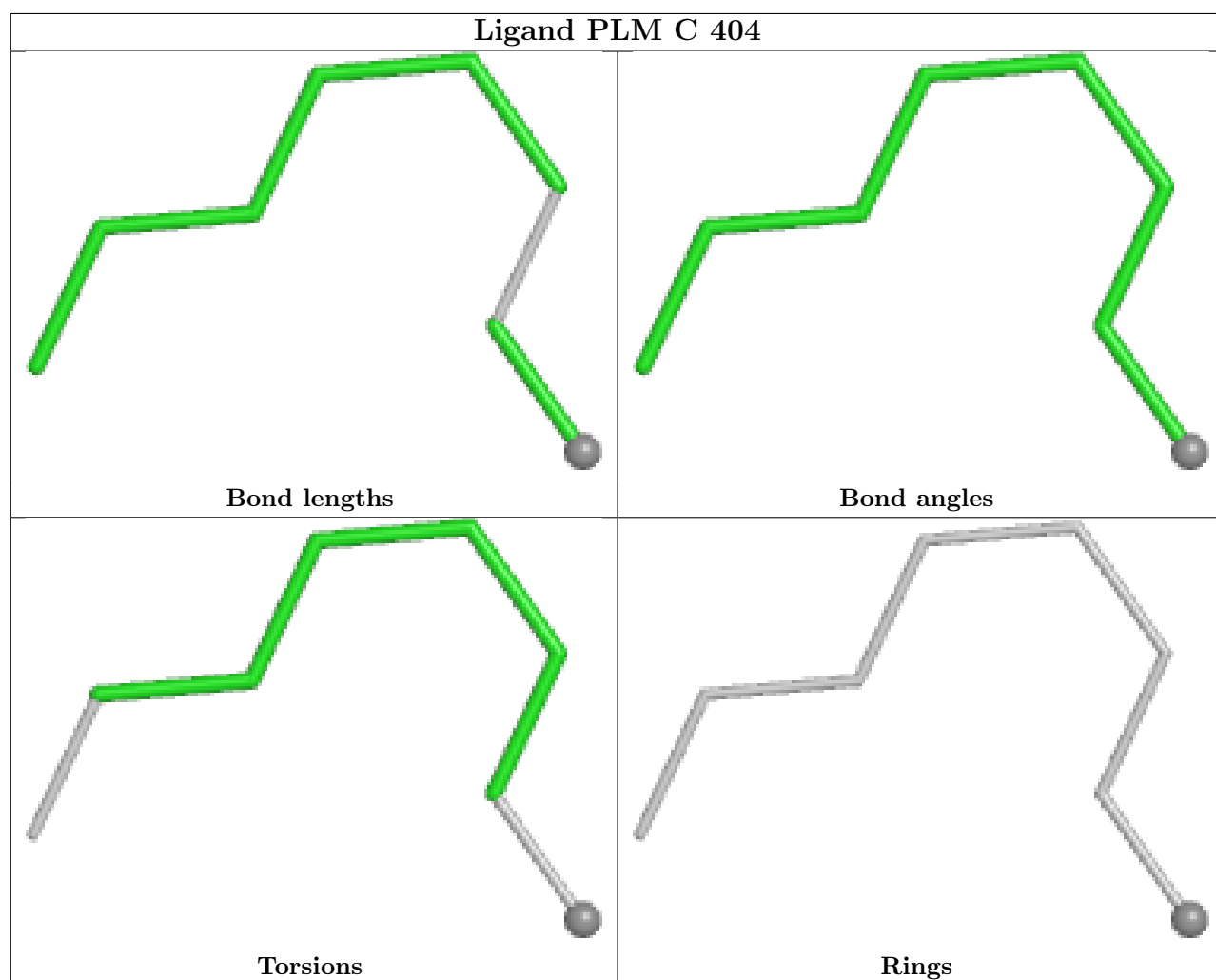
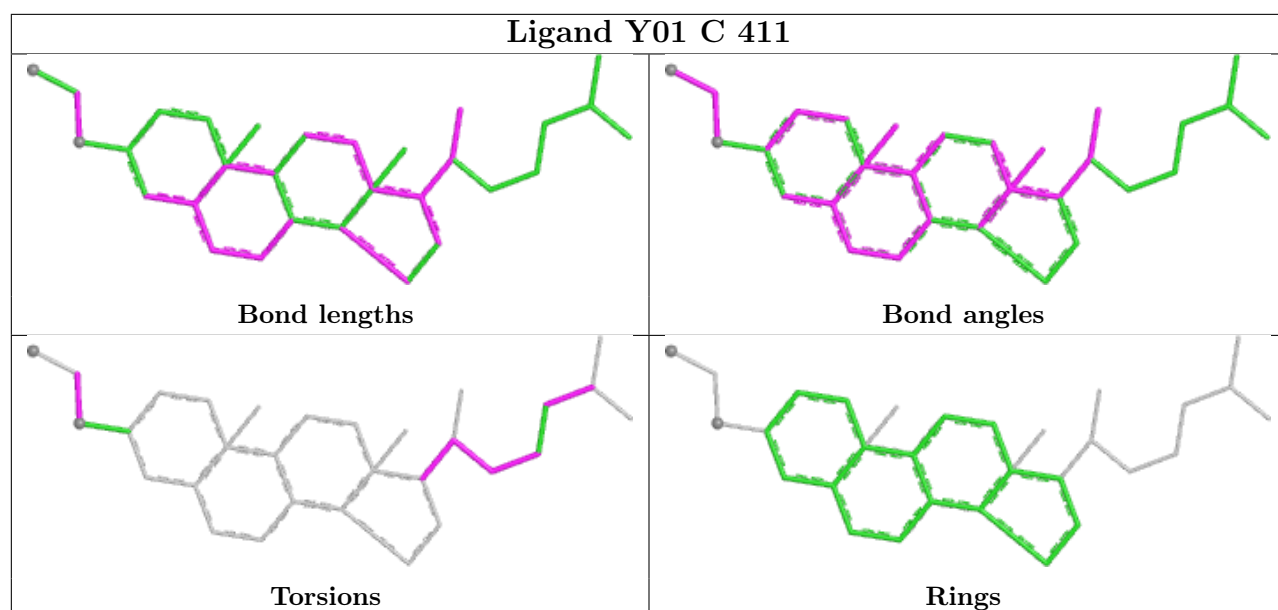
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

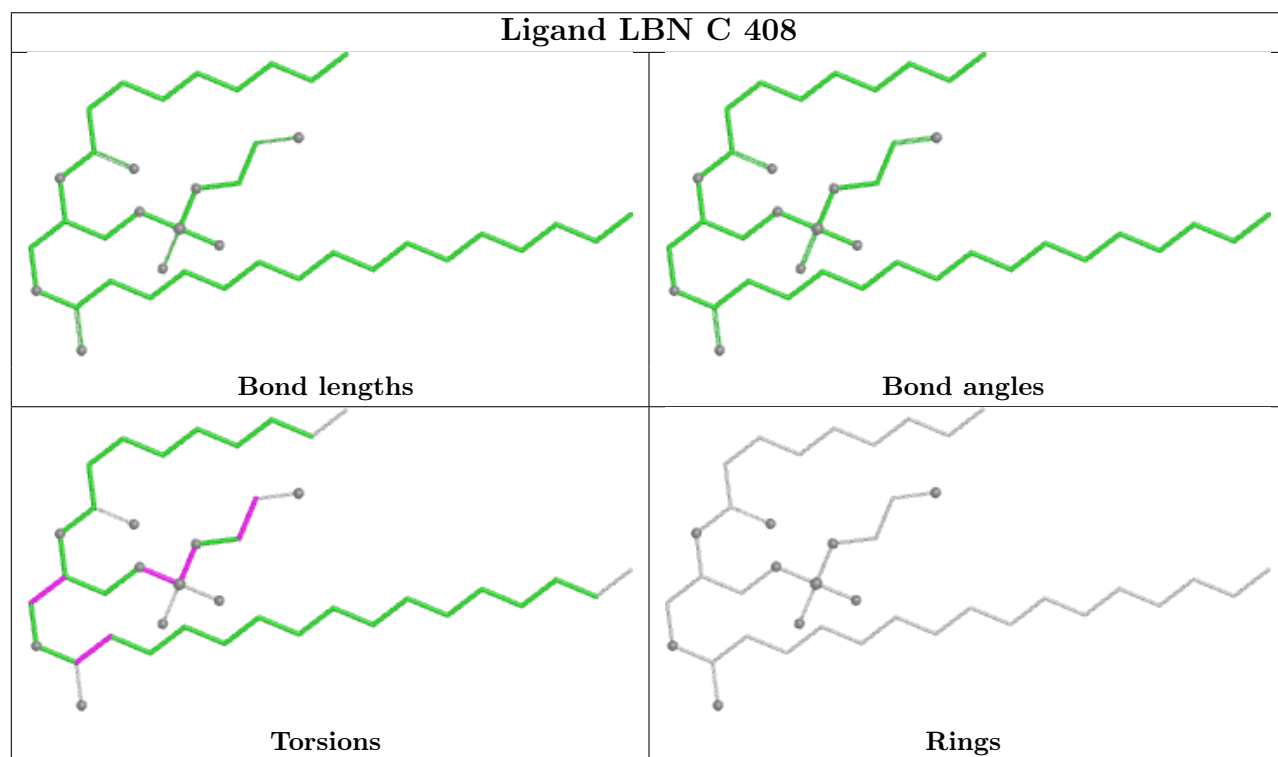
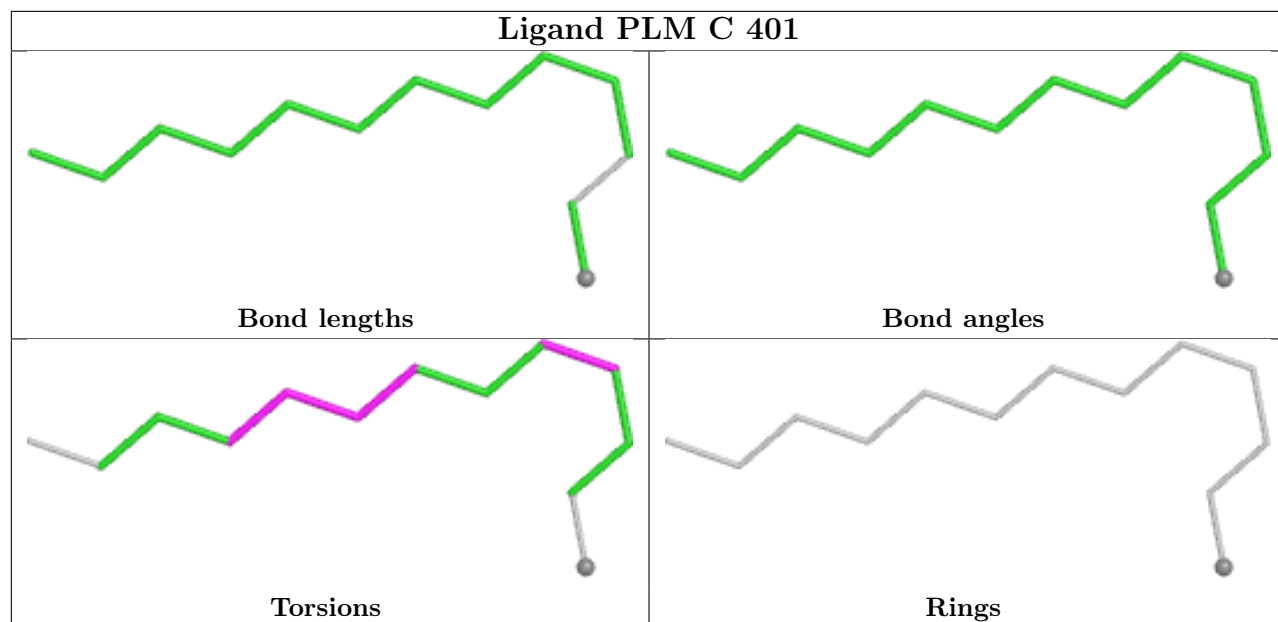


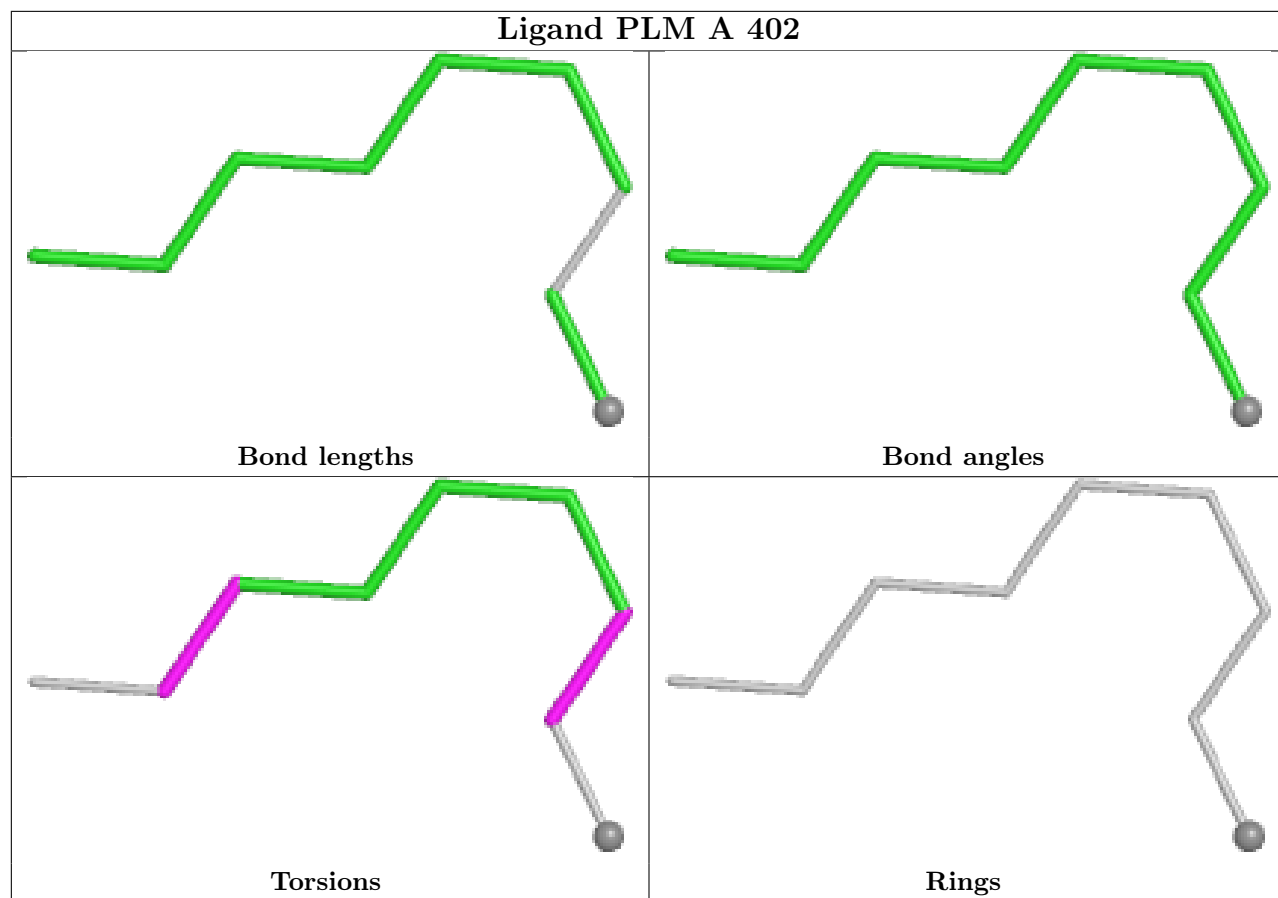


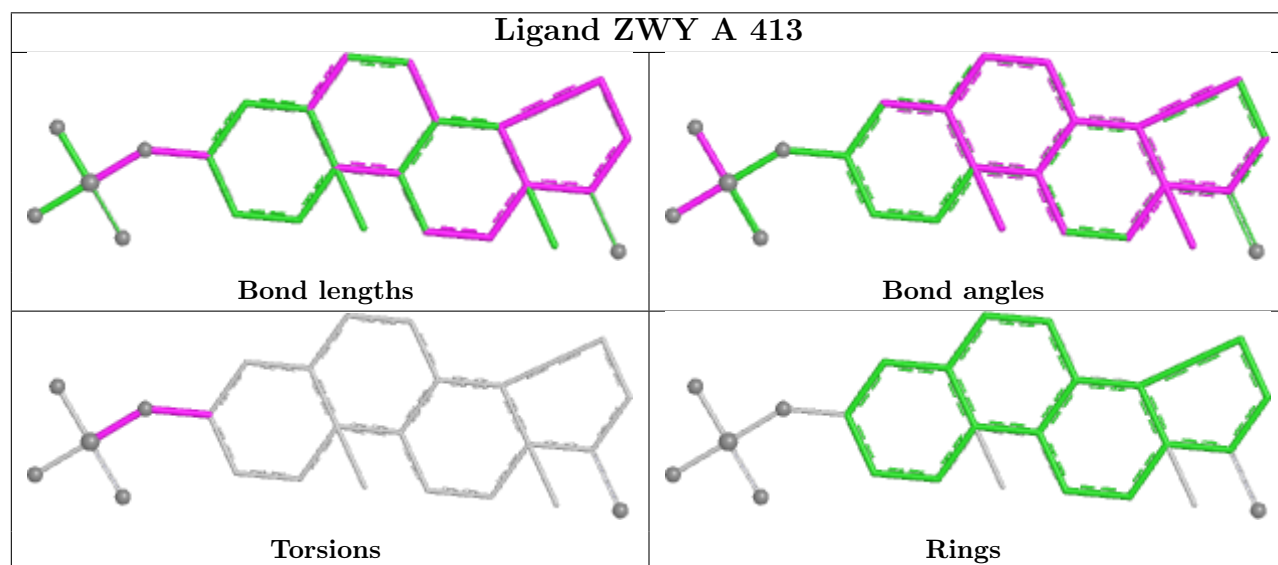
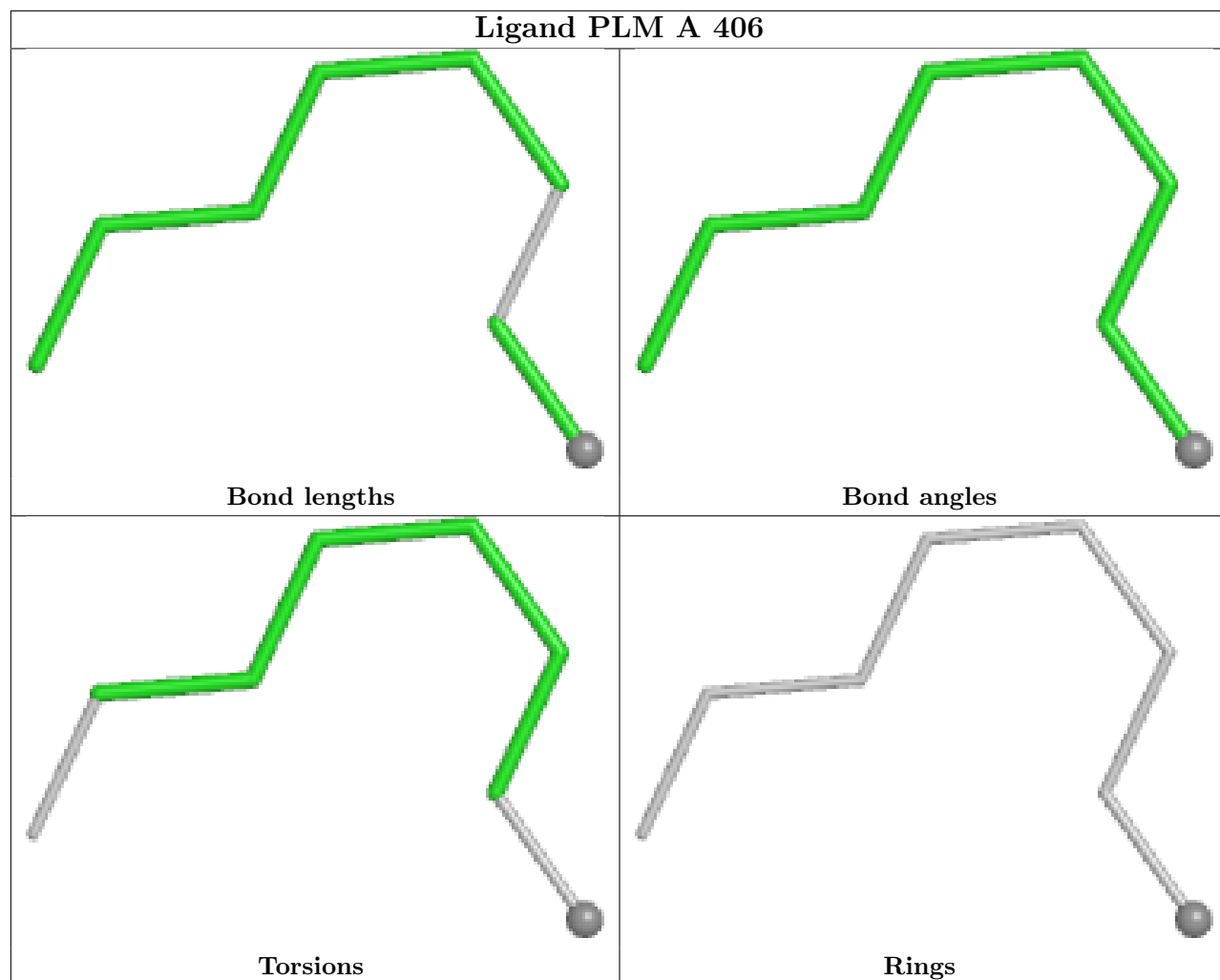


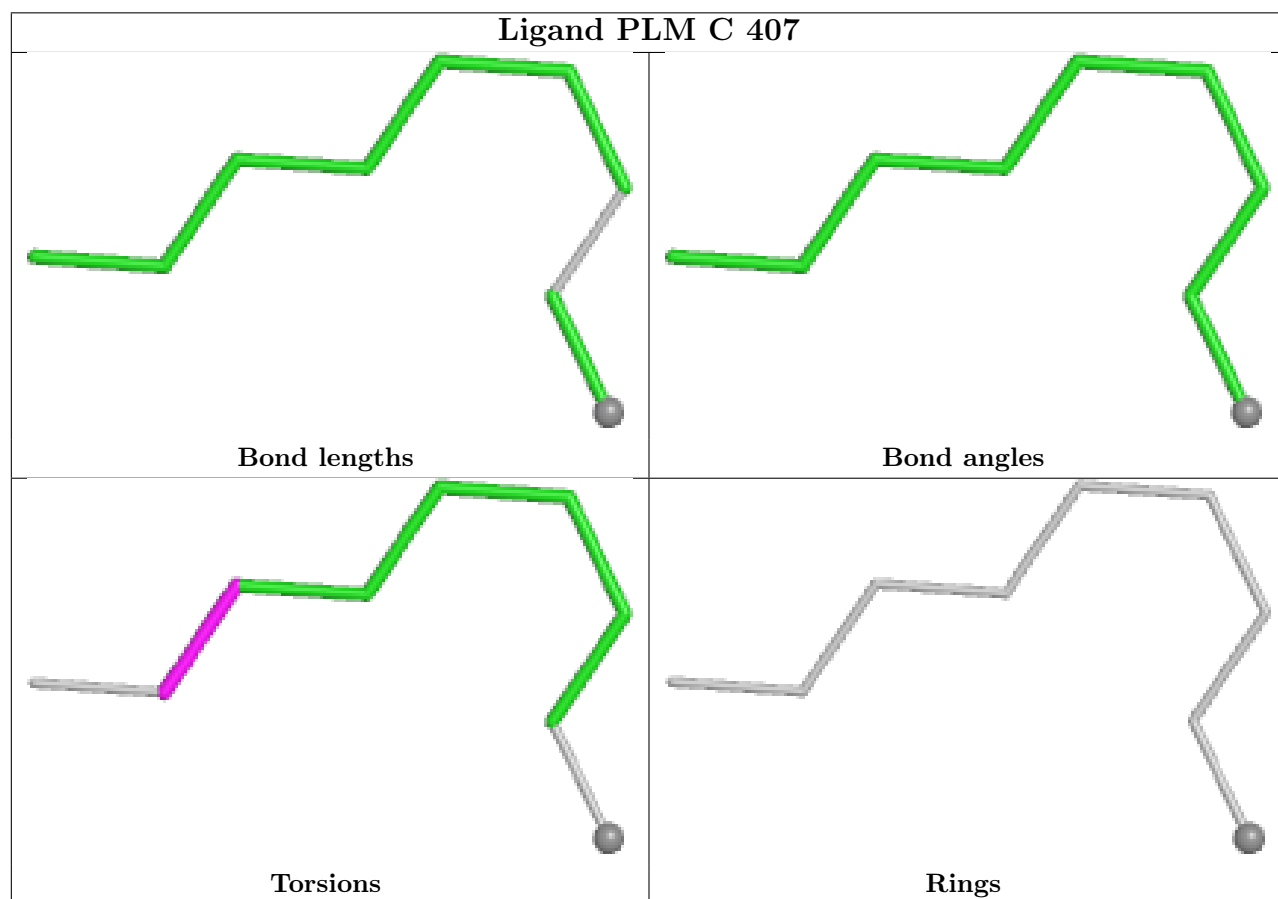
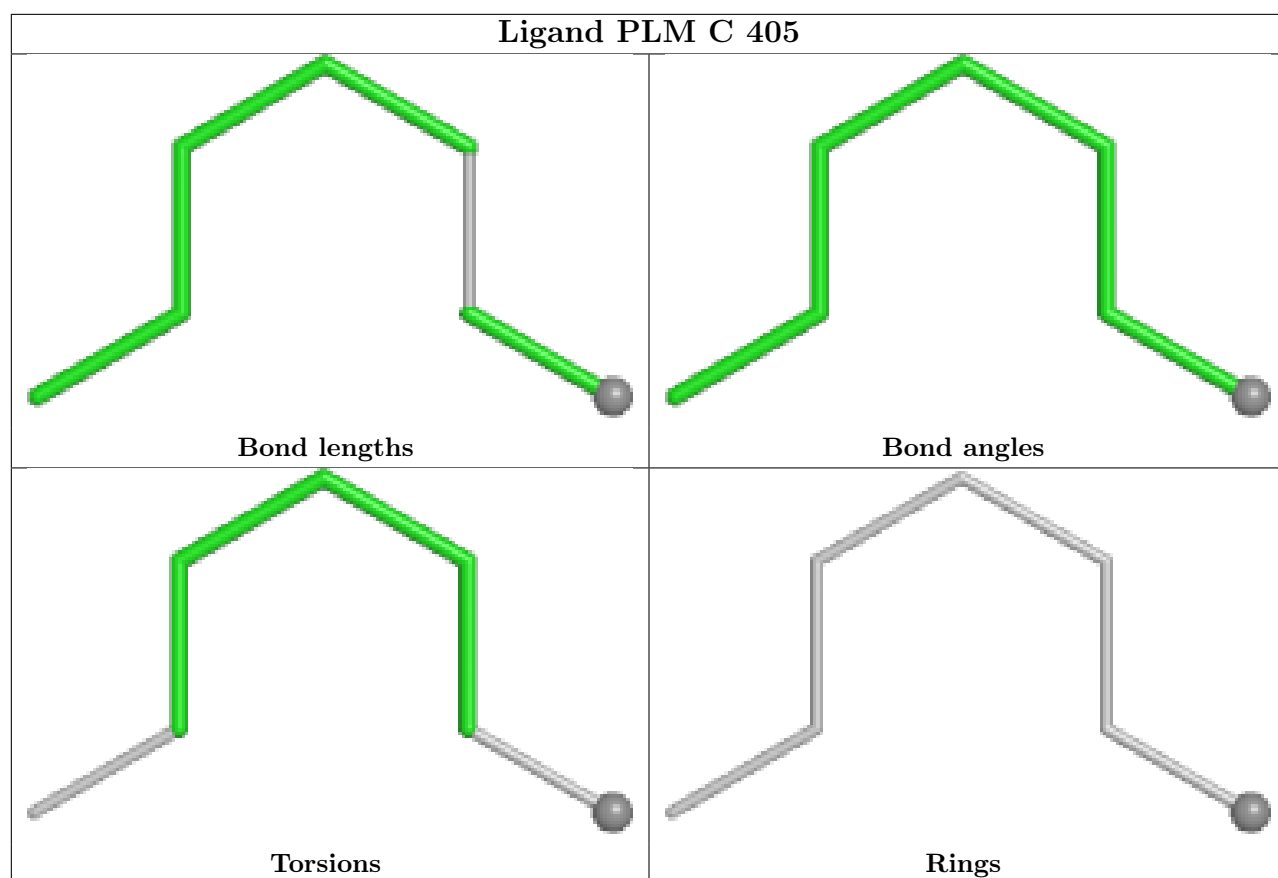


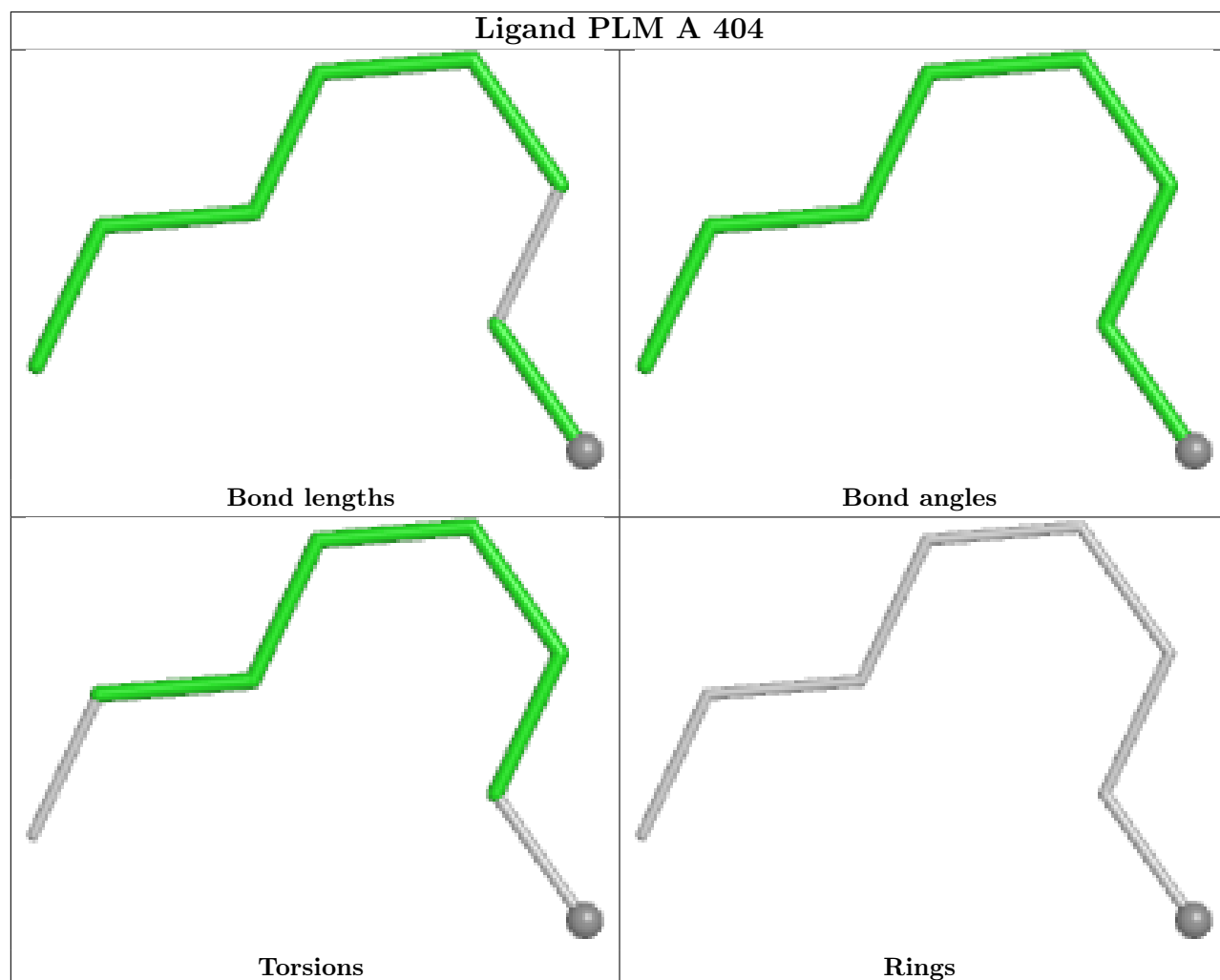
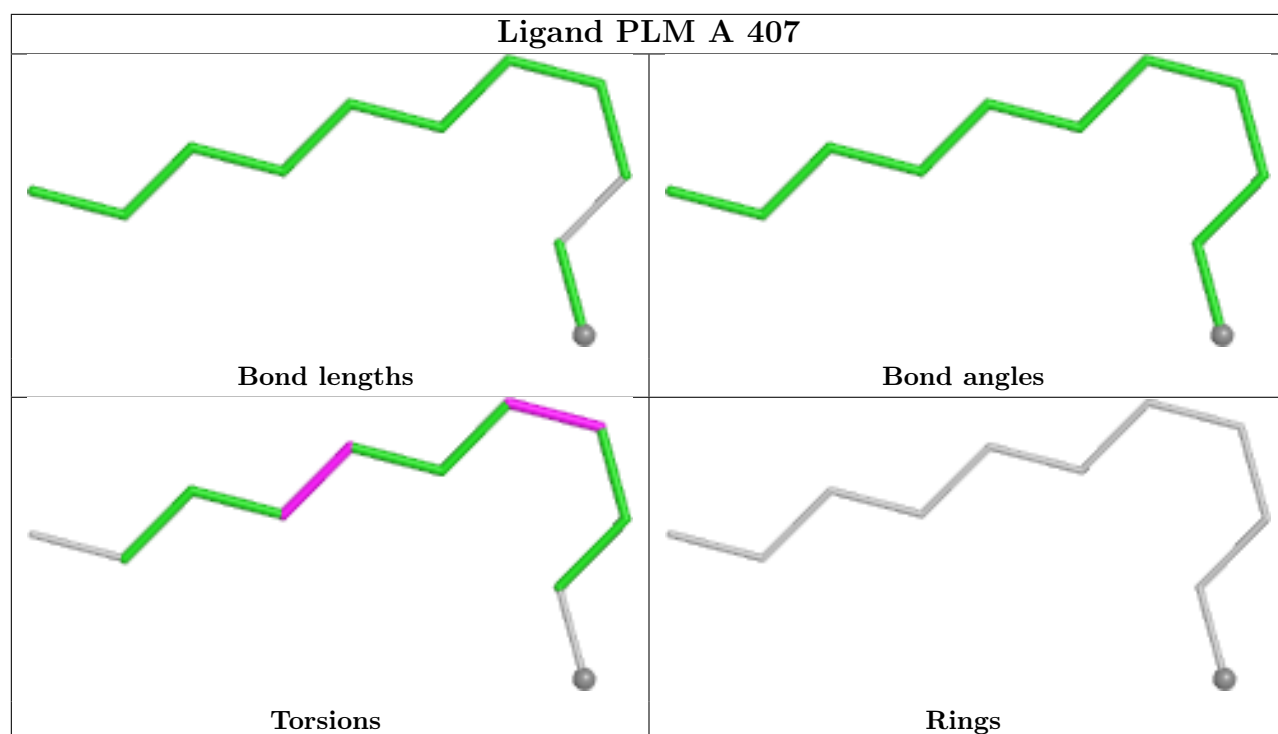


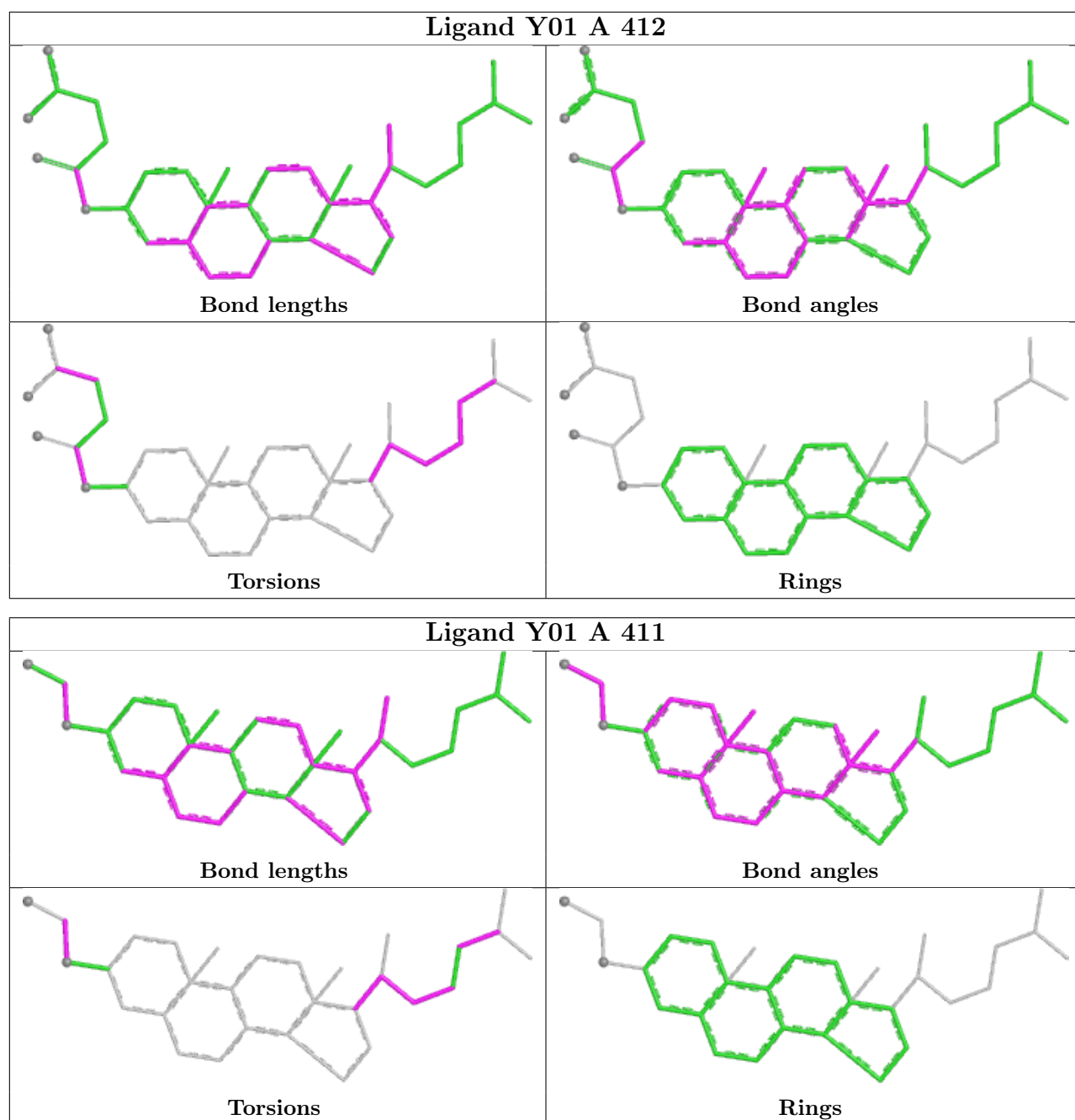


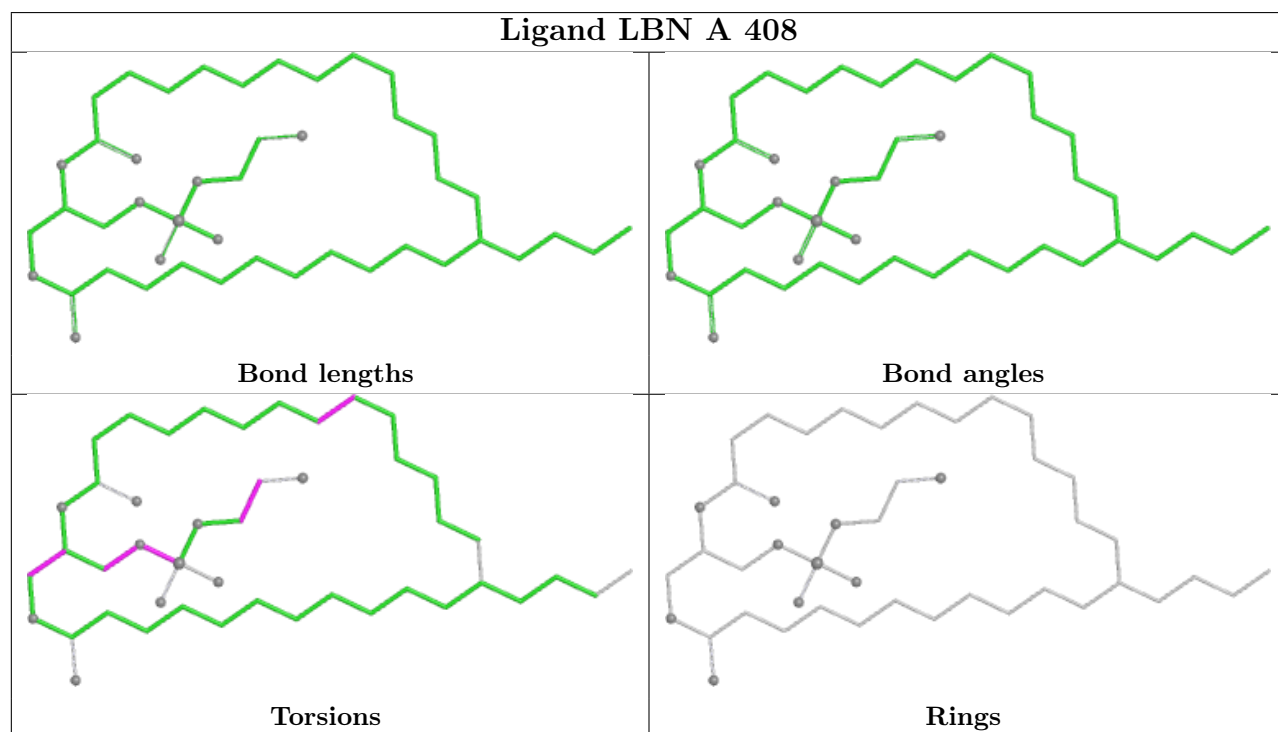
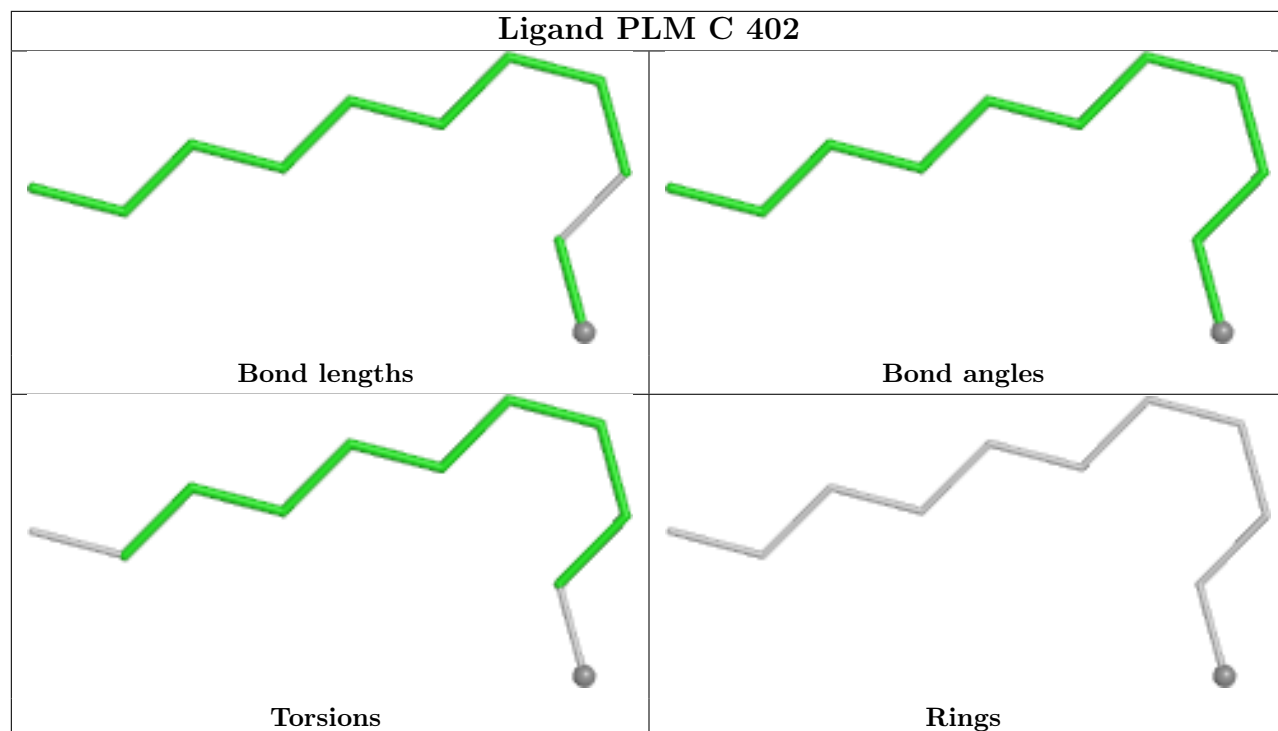


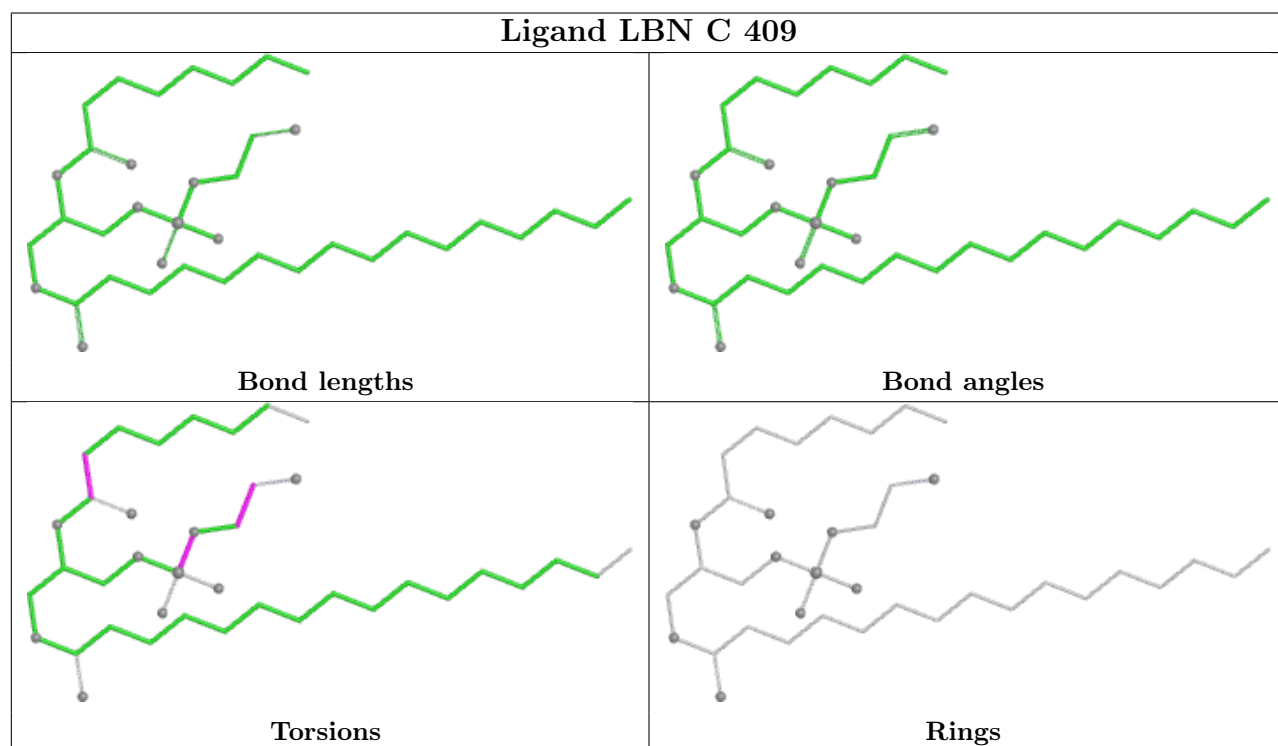
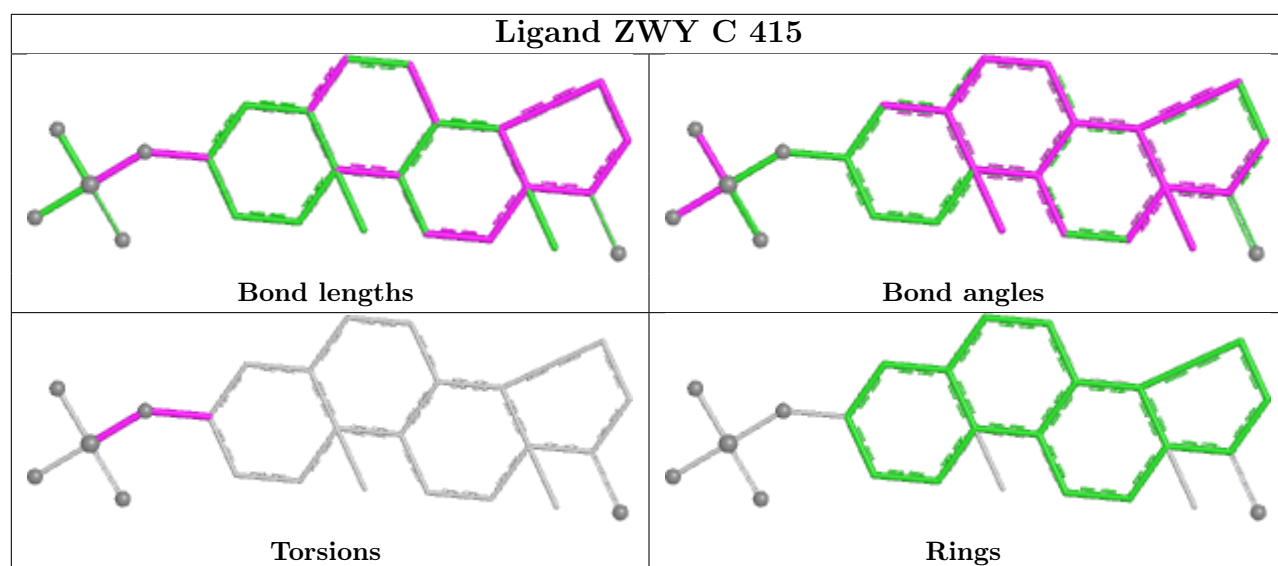


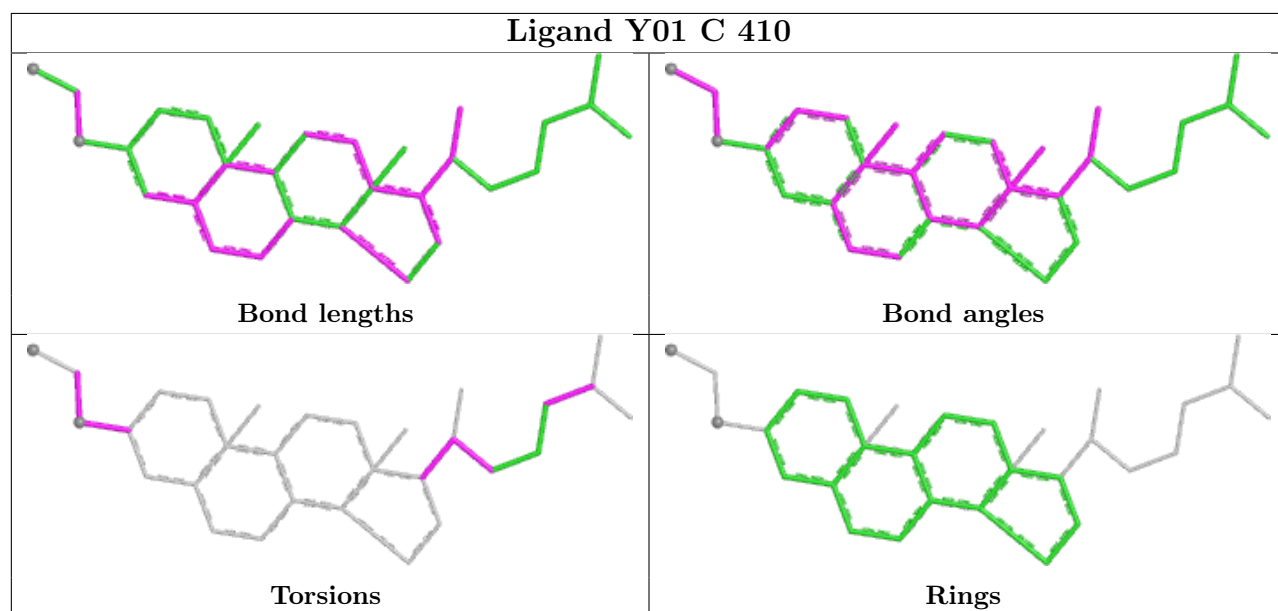
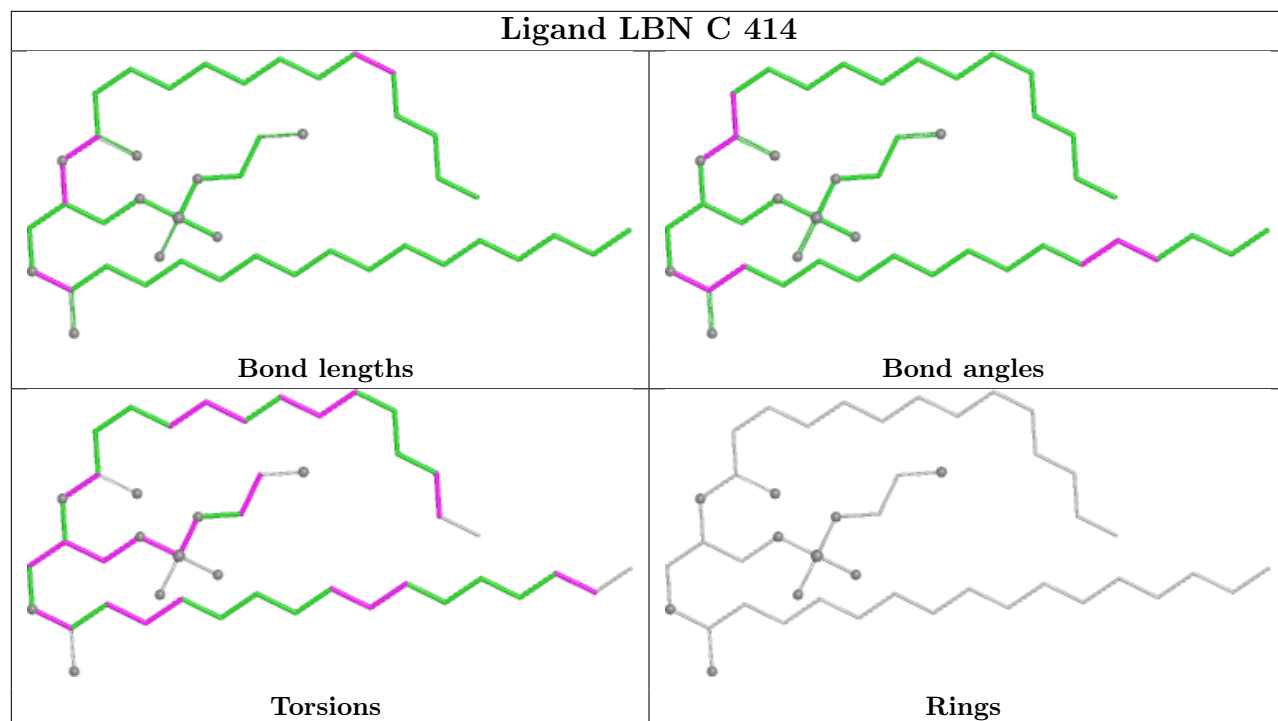


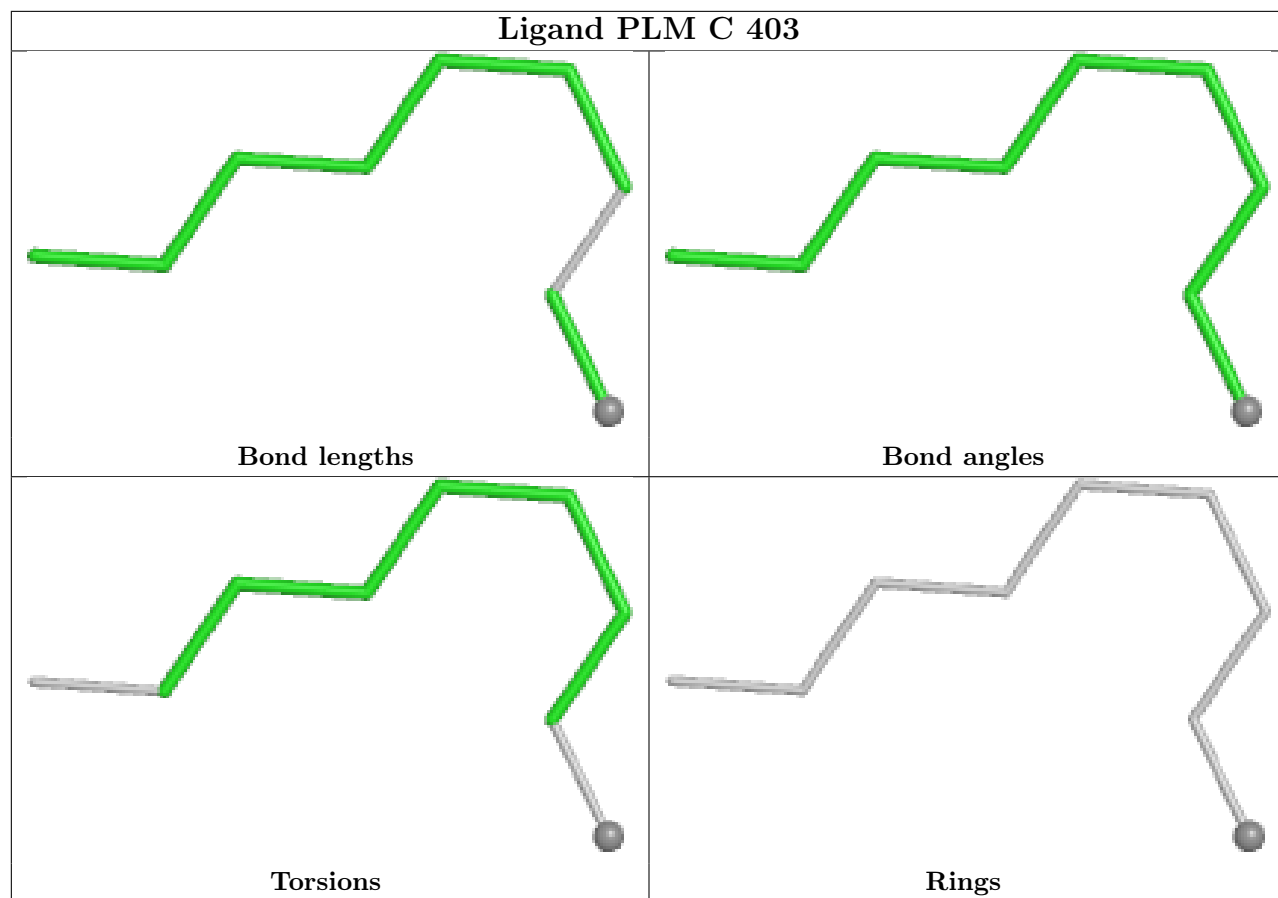












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

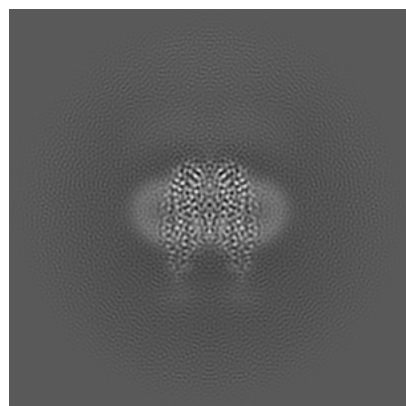
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63149. These allow visual inspection of the internal detail of the map and identification of artifacts.

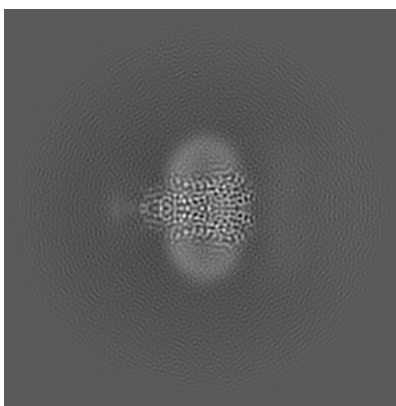
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

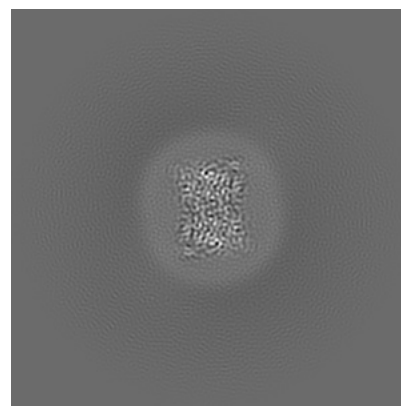
6.1.1 Primary map



X

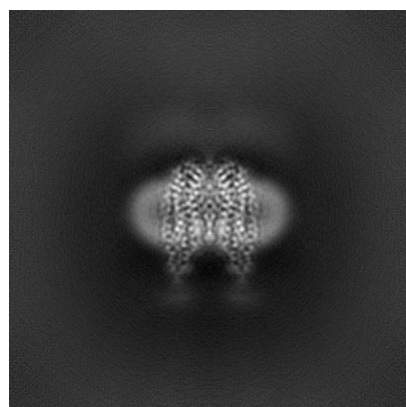


Y

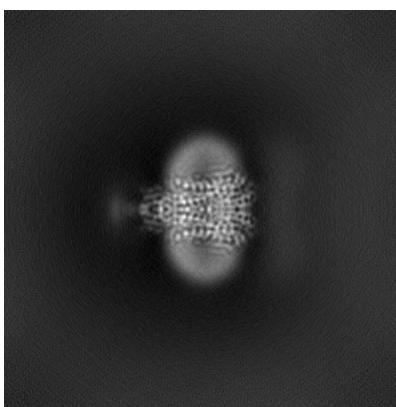


Z

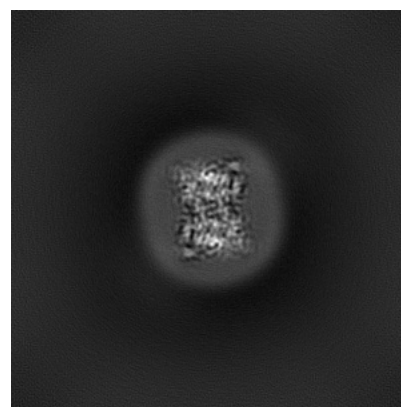
6.1.2 Raw map



X



Y

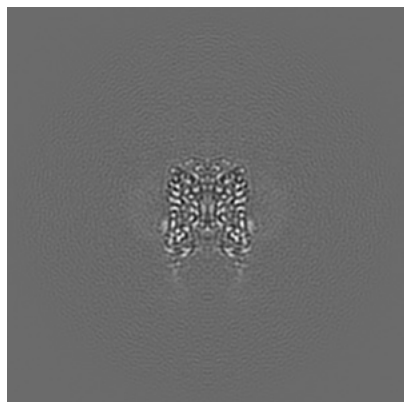


Z

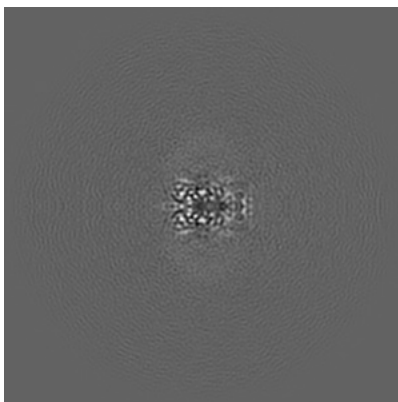
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

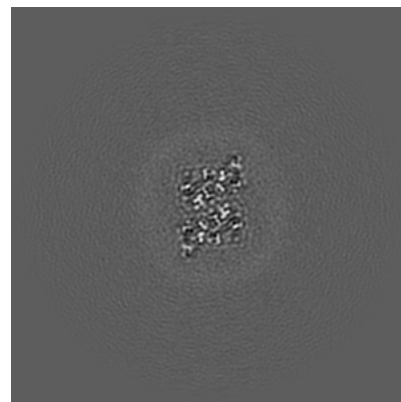
6.2.1 Primary map



X Index: 160

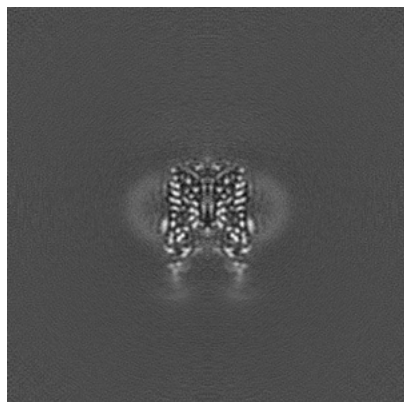


Y Index: 160

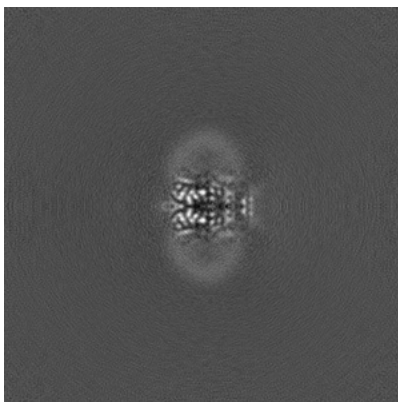


Z Index: 160

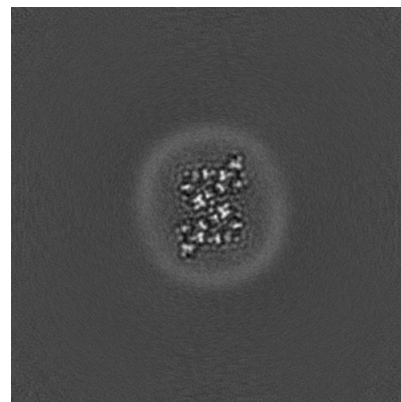
6.2.2 Raw map



X Index: 160



Y Index: 160

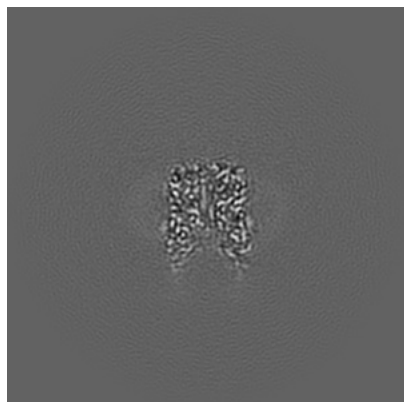


Z Index: 160

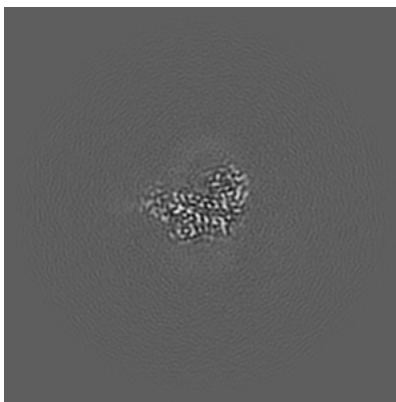
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

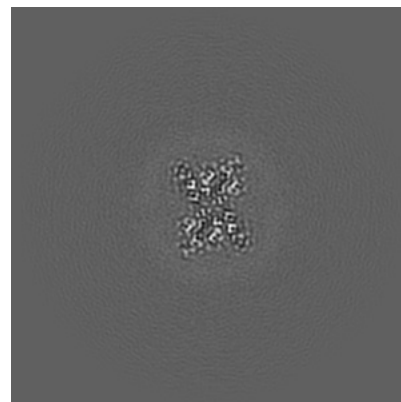
6.3.1 Primary map



X Index: 159

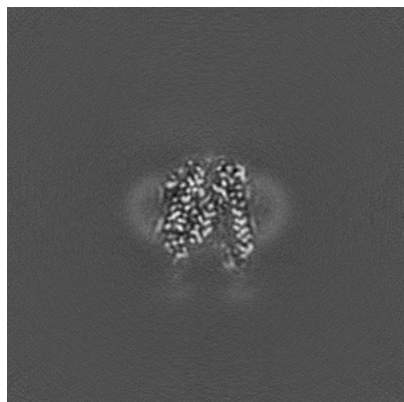


Y Index: 136

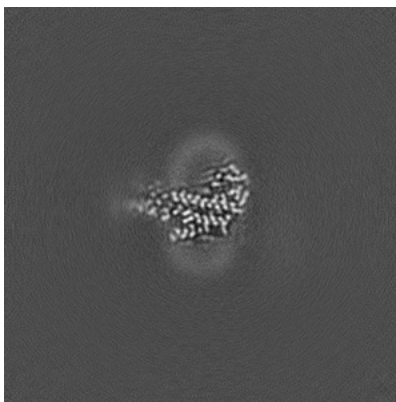


Z Index: 170

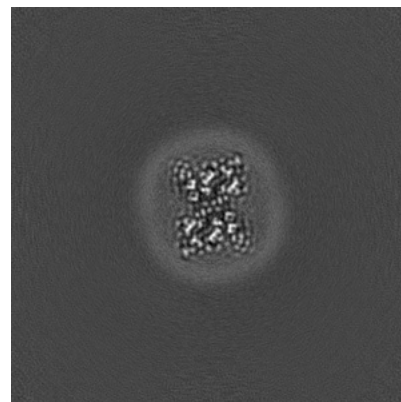
6.3.2 Raw map



X Index: 153



Y Index: 135

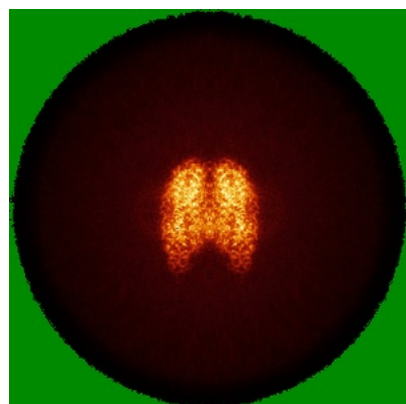


Z Index: 170

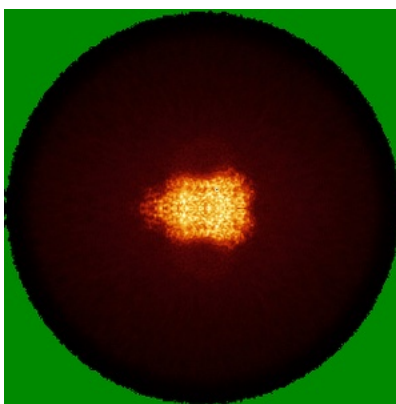
The images above show the largest variance slices of the map in three orthogonal directions.

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

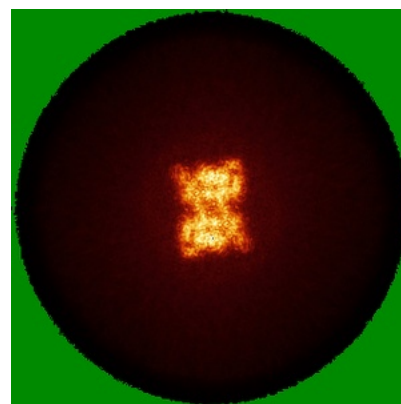
6.4.1 Primary map



X

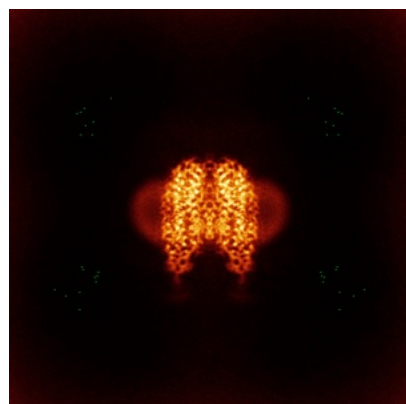


Y

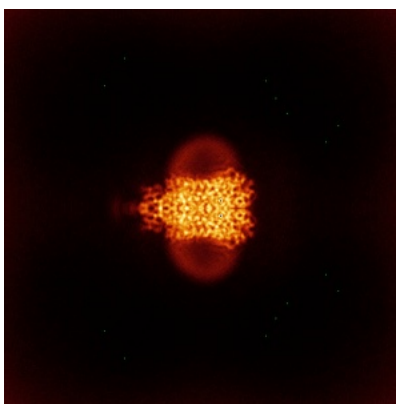


Z

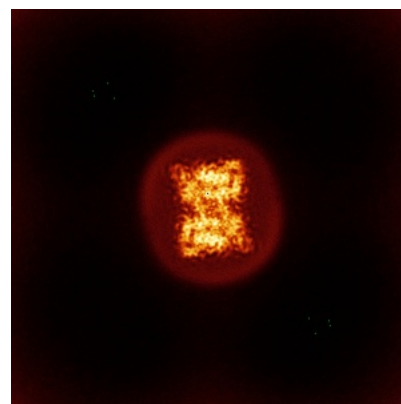
6.4.2 Raw map



X



Y

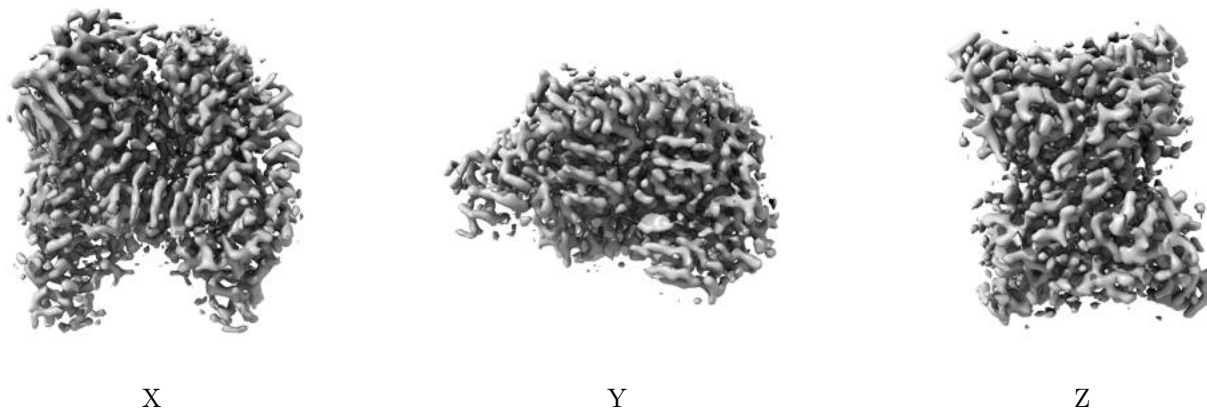


Z

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

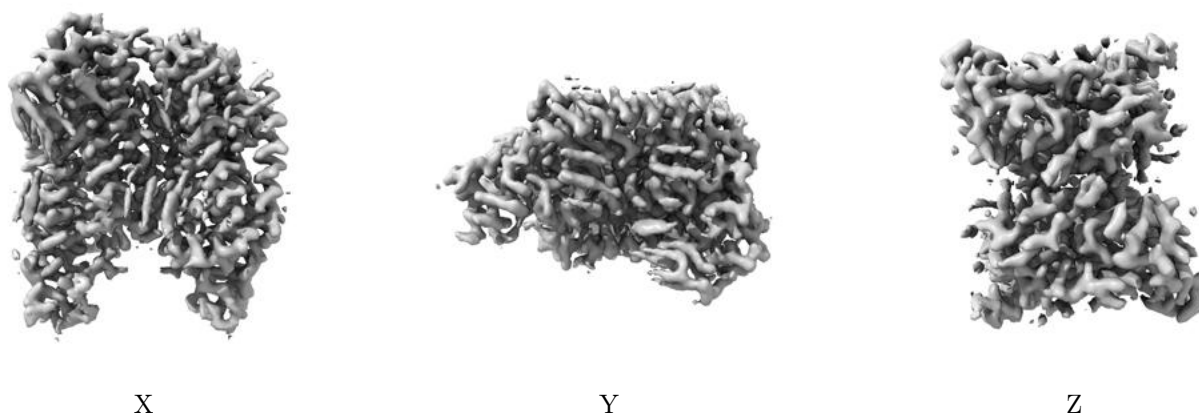
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.451. 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.

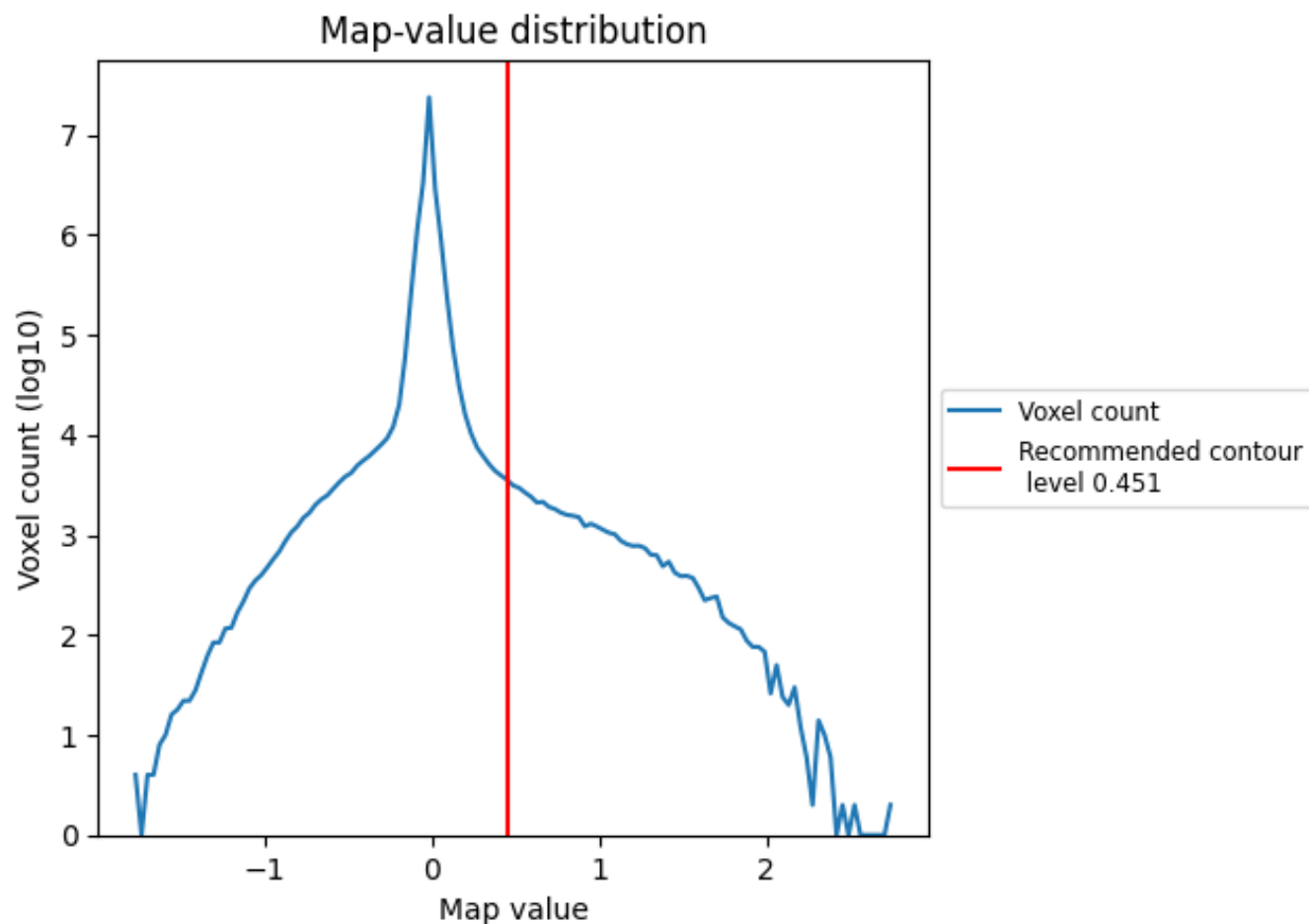
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

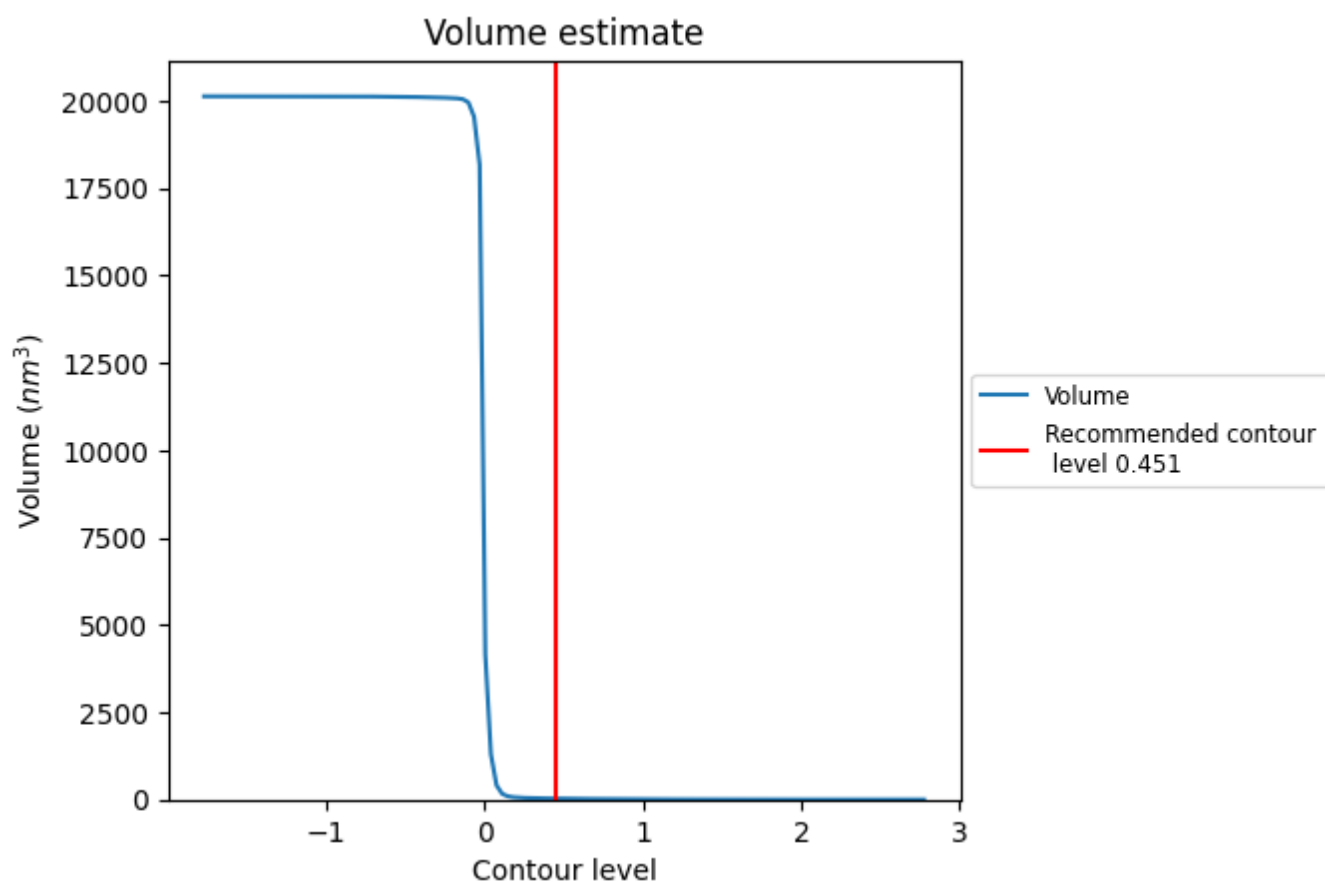
This section contains the results of statistical analysis of the map.

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.

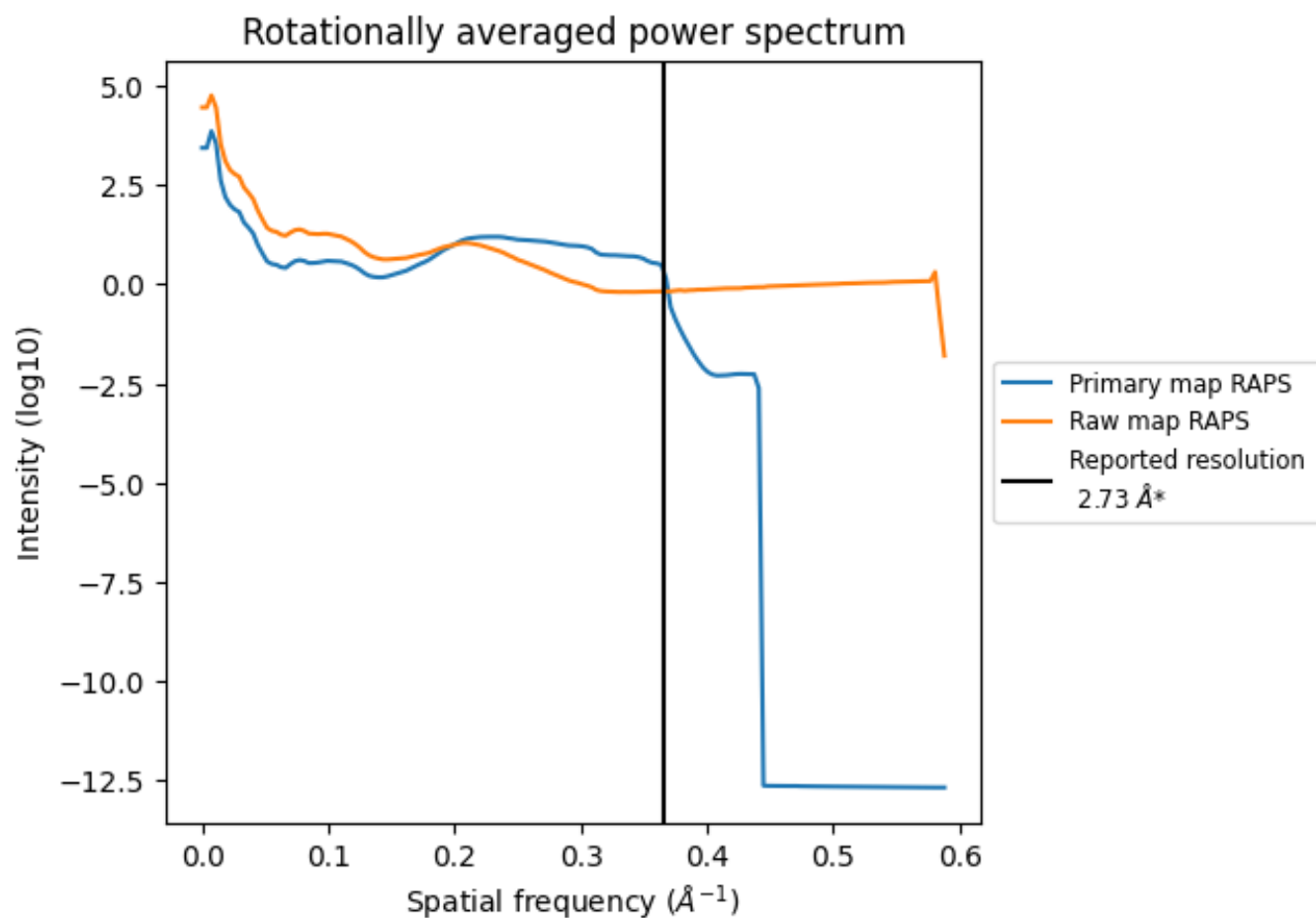
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 28 nm³; this corresponds to an approximate mass of 25 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

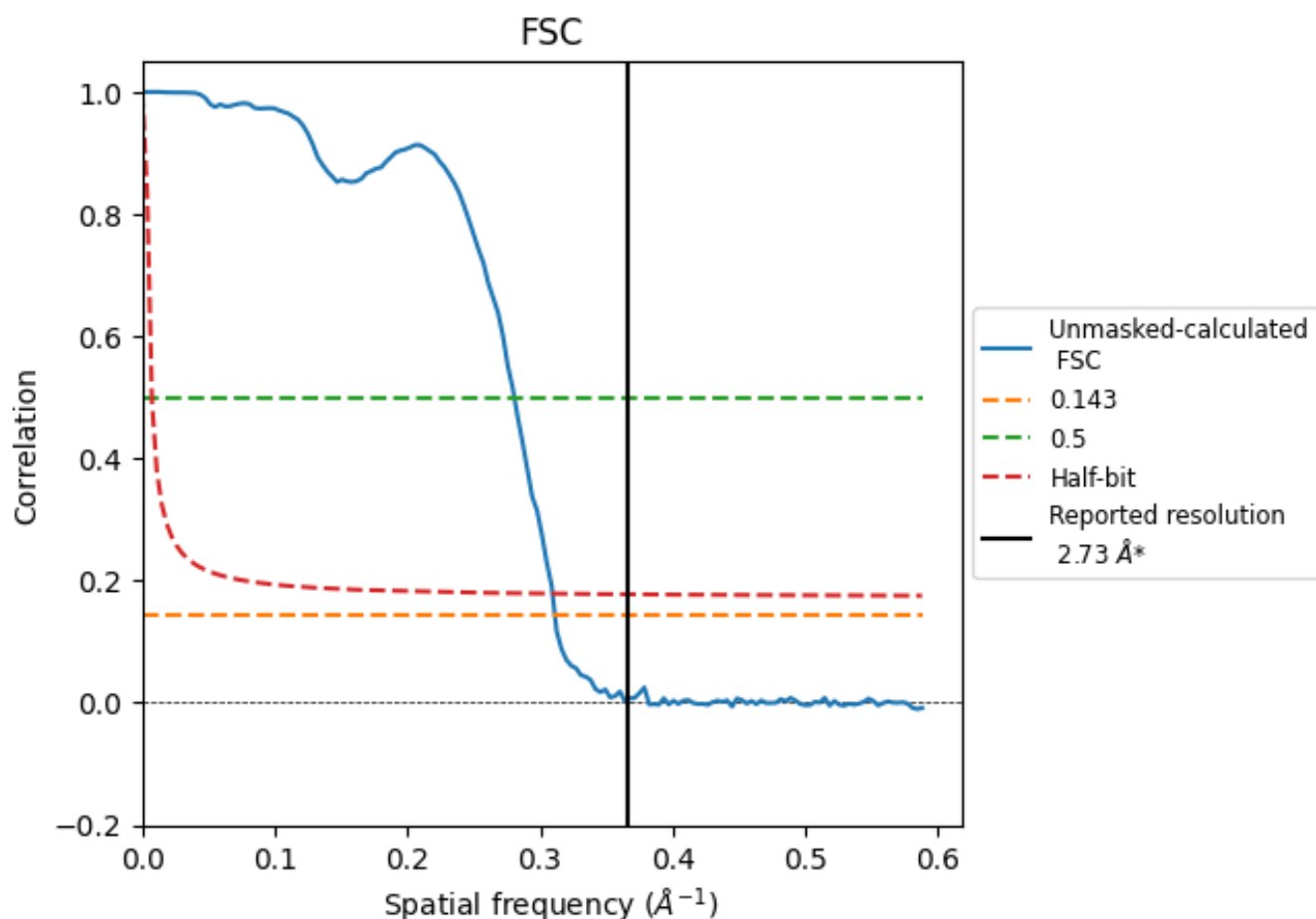


*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

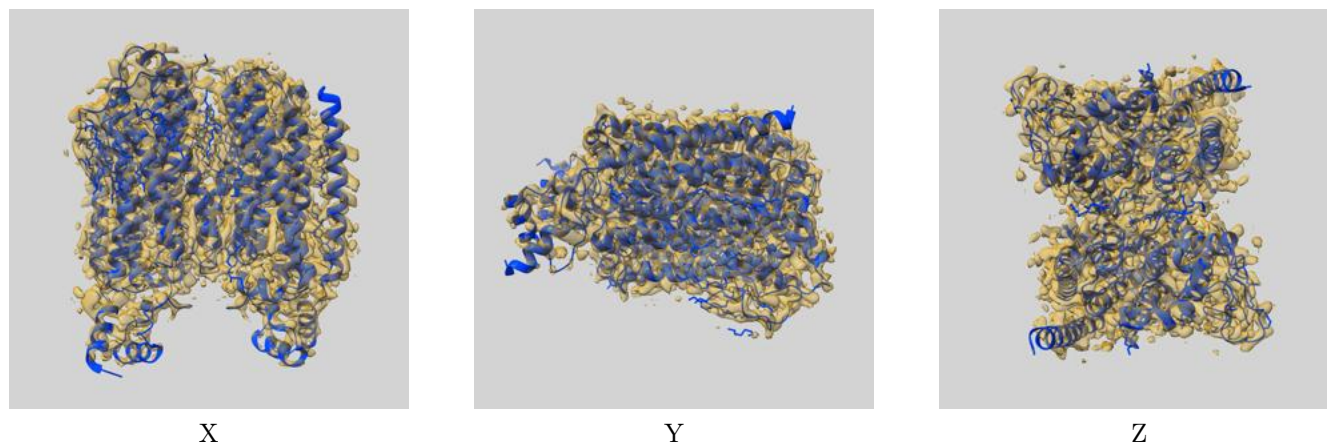
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.21	3.56	3.23

*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 3.21 differs from the reported value 2.73 by more than 10 %

9 Map-model fit [i](#)

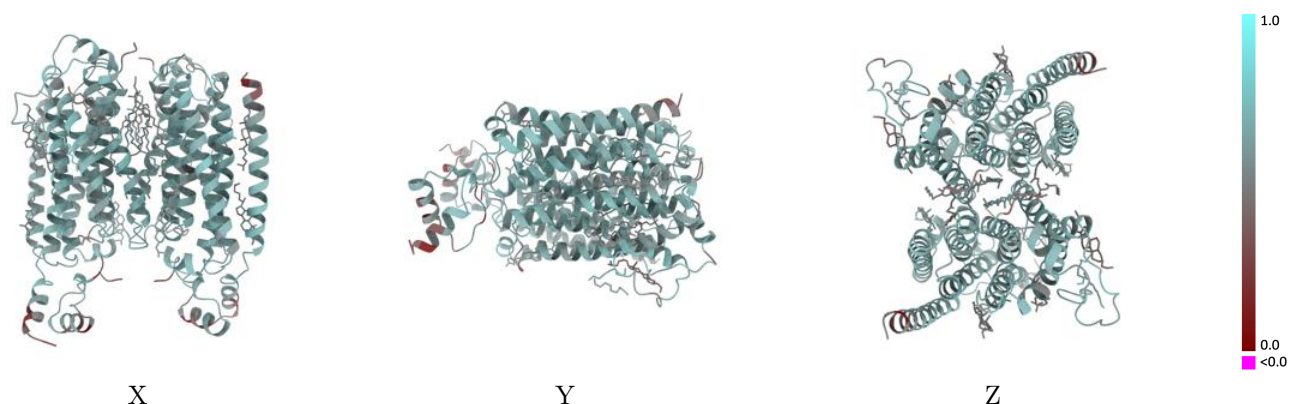
This section contains information regarding the fit between EMDB map EMD-63149 and PDB model 9LJH. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.451 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](#)

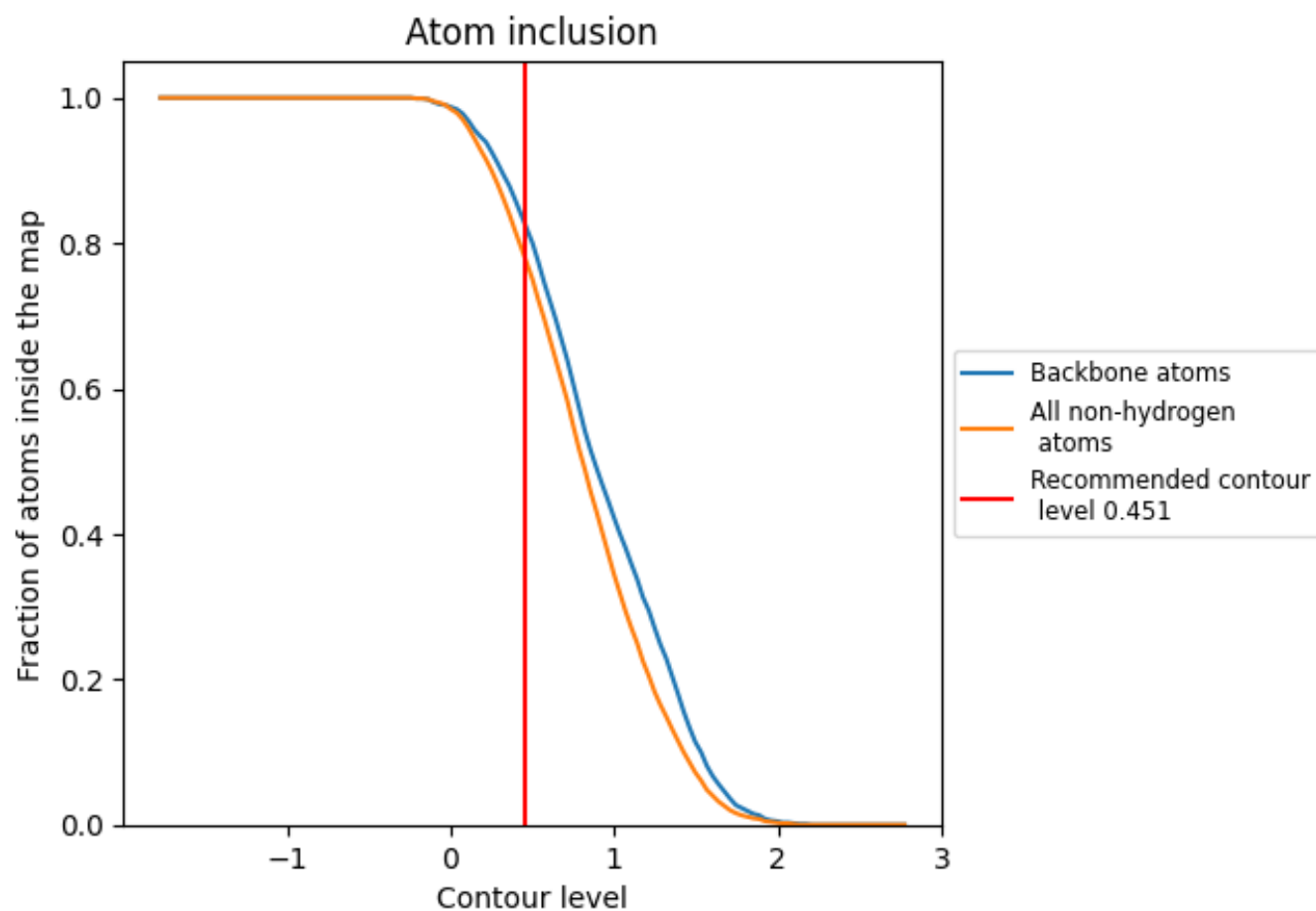


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 78% 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 (0.451) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7830	0.5940
A	0.8060	0.6000
B	0.6420	0.5540
C	0.8010	0.5990
D	0.6290	0.5490

