



## Full wwPDB EM Validation Report ⓘ

Jun 4, 2026 – 04:17 PM JST

PDB ID : 9WQR / pdb\_00009wqr  
EMDB ID : EMD-66180  
Title : cryo-EM structure of human organic solute transporter in complex with fidaxomicin  
Authors : Sun, X.; Yao, D.; Xue, J.  
Deposited on : 2025-09-11  
Resolution : 2.79 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](mailto: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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

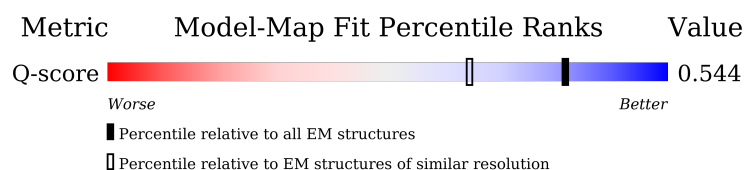
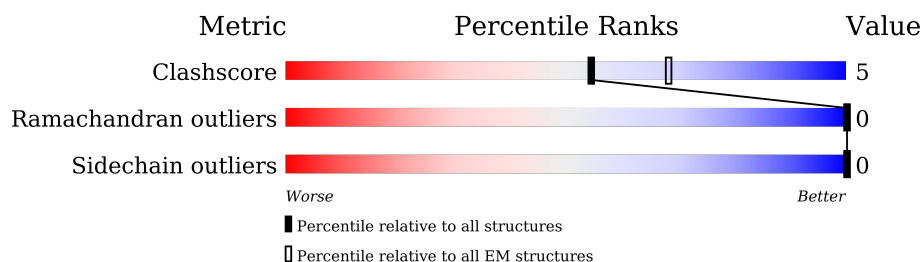
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.79 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	10811 ( 2.29 - 3.29 )

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  $\geq 3$ , 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	B	128	
1	D	128	
2	A	340	
2	C	340	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6930 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.

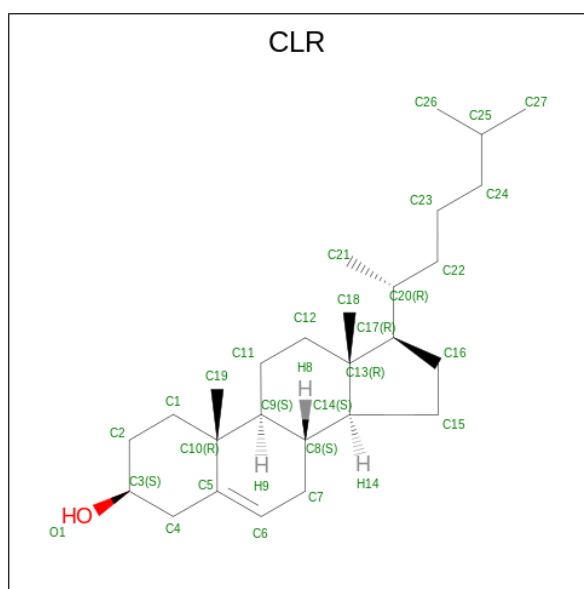
- Molecule 1 is a protein called Organic solute transporter subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	53	Total	C	N	O	S	0	0
			426	277	72	74	3		
1	D	53	Total	C	N	O	S	0	0
			426	277	72	74	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	327	Total	C	N	O	S	0	0
			2542	1661	417	440	24		
2	C	327	Total	C	N	O	S	0	0
			2542	1661	417	440	24		

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula:  $C_{27}H_{46}O$ ).



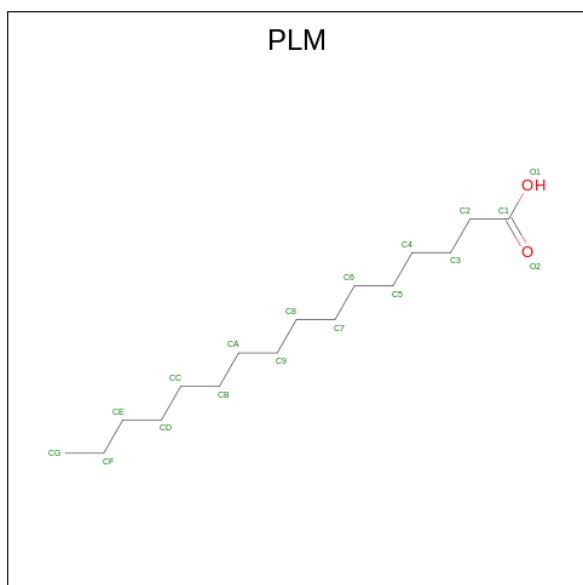
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	

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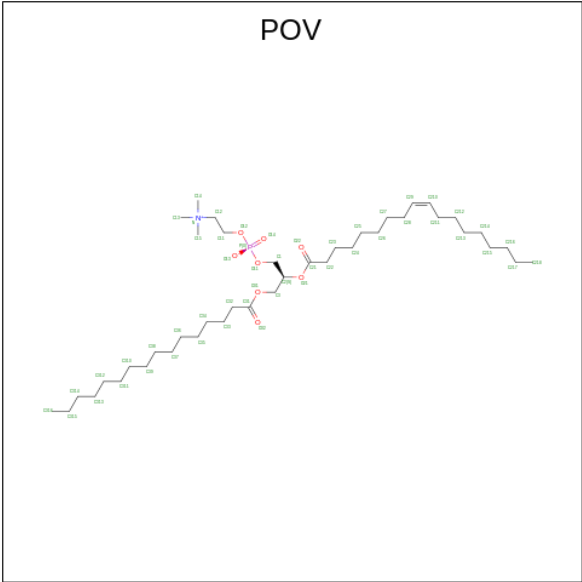
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	C	1	Total	C	O	0
			28	27	1	
3	C	1	Total	C	O	0
			28	27	1	
3	C	1	Total	C	O	0
			28	27	1	
3	C	1	Total	C	O	0
			28	27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

- Molecule 4 is PALMITIC ACID (CCD ID: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



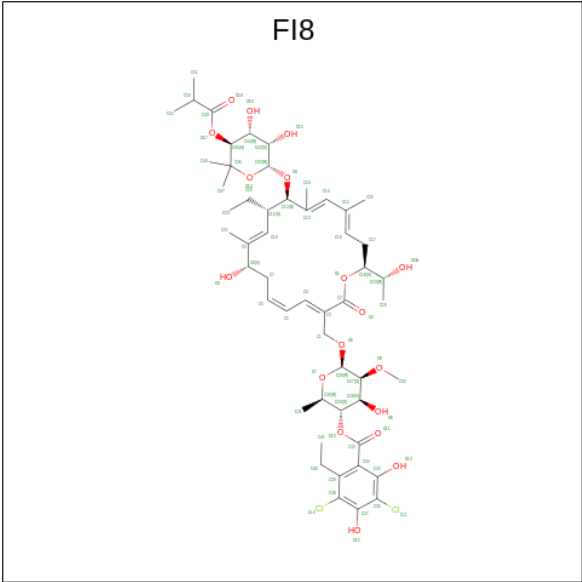
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			17	16	1	
4	A	1	Total	C	O	0
			17	16	1	
4	A	1	Total	C	O	0
			17	16	1	
4	A	1	Total	C	O	0
			17	16	1	
4	A	1	Total	C	O	0
			17	16	1	
4	A	1	Total	C	O	0
			17	16	1	
4	C	1	Total	C	O	0
			17	16	1	
4	C	1	Total	C	O	0
			17	16	1	
4	C	1	Total	C	O	0
			17	16	1	
4	C	1	Total	C	O	0
			17	16	1	
4	C	1	Total	C	O	0
			17	16	1	
4	C	1	Total	C	O	0
			17	16	1	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			46	37	8	1	
5	A	1	Total	C	O	P	0
			46	37	8	1	
5	A	1	Total	C	O	P	0
			46	37	8	1	
5	A	1	Total	C	O	P	0
			46	37	8	1	
5	C	1	Total	C	O	P	0
			46	37	8	1	
5	C	1	Total	C	O	P	0
			46	37	8	1	

- Molecule 6 is Fidaxomicin (CCD ID: FI8) (formula: C<sub>52</sub>H<sub>74</sub>Cl<sub>2</sub>O<sub>18</sub>) (labeled as "Ligand of Interest" by depositor).

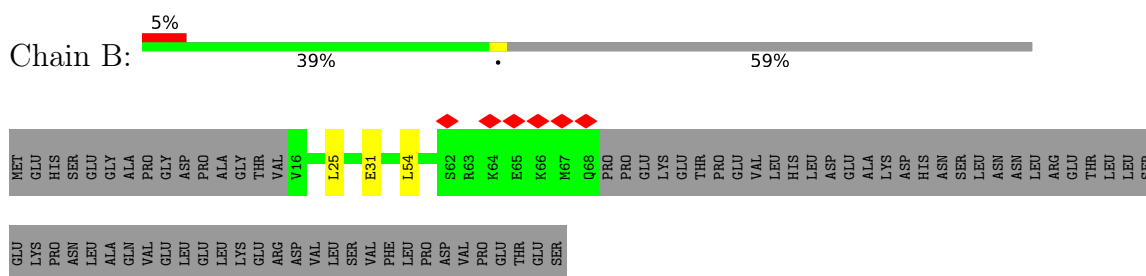


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	Cl	O	0
			72	52	2	18	
6	C	1	Total	C	Cl	O	0
			72	52	2	18	

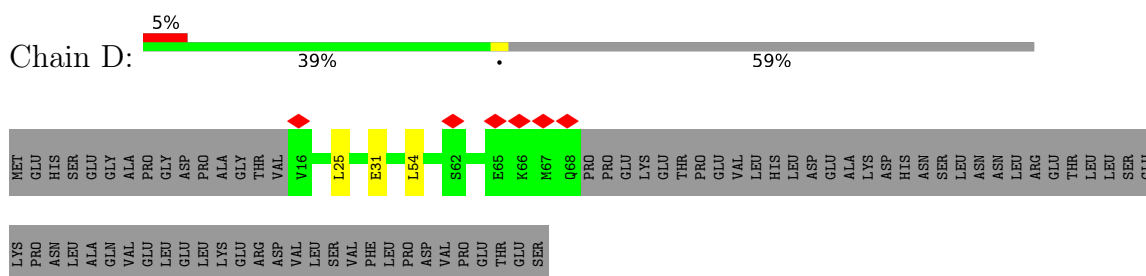
### 3 Residue-property plots [i](#)

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.

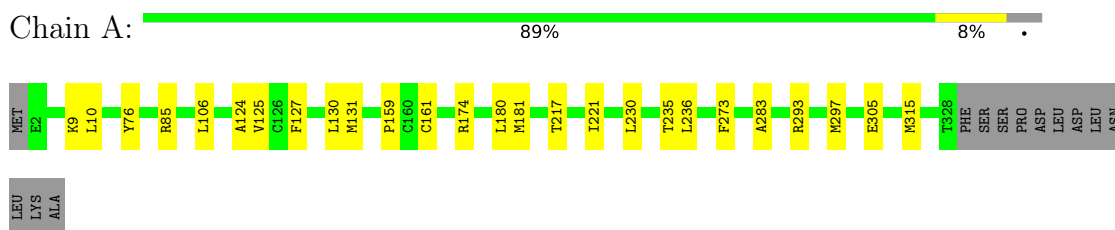
- Molecule 1: Organic solute transporter subunit beta



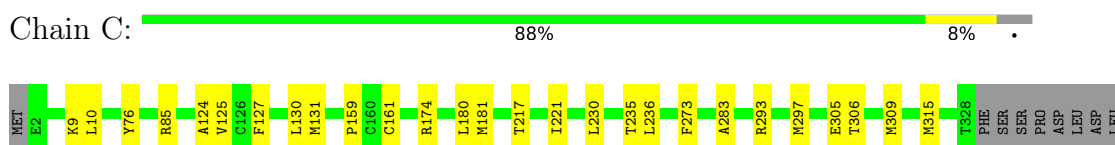
- Molecule 1: Organic solute transporter subunit beta



- Molecule 2: Organic solute transporter subunit alpha



- Molecule 2: Organic solute transporter subunit alpha





ASN  
LEU  
LYS  
ALA

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	689213	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.135	Depositor
Minimum map value	-1.919	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.2	Depositor
Map size ( $\text{\AA}$ )	220.0, 220.0, 220.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	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, POV, FI8

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	B	0.21	0/434	0.36	0/587
1	D	0.22	0/434	0.36	0/587
2	A	0.19	0/2598	0.42	0/3536
2	C	0.19	0/2598	0.42	0/3536
All	All	0.19	0/6064	0.41	0/8246

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	B	426	0	442	3	0
1	D	426	0	442	3	0
2	A	2542	0	2663	21	0
2	C	2542	0	2663	21	0
3	A	168	0	276	10	0
3	C	168	0	276	9	0
4	A	119	0	217	14	0
4	C	119	0	217	12	0
5	A	184	0	276	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	92	0	138	3	0
6	A	72	0	0	0	0
6	C	72	0	0	0	0
All	All	6930	0	7610	74	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 5.

All (74) 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:405:PLM:H21	4:A:407:PLM:H71	1.77	0.66
4:C:407:PLM:H21	4:C:409:PLM:H71	1.77	0.65
2:A:161:CYS:HA	4:A:409:PLM:H22	1.80	0.63
2:C:161:CYS:HA	4:C:411:PLM:H22	1.80	0.63
2:A:124:ALA:O	2:A:127:PHE:HB2	1.99	0.62
2:C:124:ALA:O	2:C:127:PHE:HB2	1.99	0.62
4:C:408:PLM:H52	4:C:409:PLM:H22	1.83	0.60
4:A:406:PLM:H52	4:A:407:PLM:H22	1.83	0.60
2:A:230:LEU:HB3	4:A:408:PLM:H42	1.84	0.60
2:A:305:GLU:HG2	5:A:413:POV:H21D	1.83	0.59
4:C:410:PLM:H72	4:C:411:PLM:H81	1.85	0.59
2:C:230:LEU:HB3	4:C:410:PLM:H42	1.84	0.59
4:A:405:PLM:HB1	3:A:414:CLR:H271	1.85	0.58
2:C:305:GLU:HG2	5:C:414:POV:H21D	1.83	0.58
4:C:407:PLM:HB1	3:C:415:CLR:H271	1.86	0.58
2:A:159:PRO:HA	3:A:414:CLR:H193	1.86	0.58
2:C:159:PRO:HA	3:C:415:CLR:H193	1.86	0.58
4:A:408:PLM:H72	4:A:409:PLM:H81	1.85	0.57
4:A:406:PLM:H61	4:A:407:PLM:H42	1.88	0.56
4:C:408:PLM:H61	4:C:409:PLM:H42	1.88	0.55
2:C:293:ARG:O	2:C:297:MET:HG3	2.07	0.55
2:C:315:MET:HE1	1:D:54:LEU:HD22	1.88	0.55
2:A:293:ARG:O	2:A:297:MET:HG3	2.07	0.54
2:A:217:THR:HG23	3:A:402:CLR:H112	1.90	0.53
2:C:217:THR:HG23	3:C:404:CLR:H112	1.90	0.53
1:B:54:LEU:HD22	2:A:315:MET:HE1	1.92	0.51
2:C:297:MET:HE1	3:C:405:CLR:H193	1.93	0.51
1:B:31:GLU:HG2	2:A:283:ALA:HB3	1.93	0.50
2:A:297:MET:HE1	3:A:403:CLR:H193	1.93	0.50
2:C:283:ALA:HB3	1:D:31:GLU:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:405:PLM:H32	4:A:406:PLM:HC1	1.95	0.49
2:A:273:PHE:HE1	2:A:297:MET:HE2	1.79	0.48
4:C:407:PLM:H32	4:C:408:PLM:HC1	1.95	0.48
2:C:76:TYR:HA	2:C:85:ARG:HD2	1.96	0.48
2:A:76:TYR:HA	2:A:85:ARG:HD2	1.96	0.47
2:C:273:PHE:HE1	2:C:297:MET:HE2	1.79	0.47
3:A:401:CLR:H191	3:A:402:CLR:H12	1.97	0.46
2:C:221:ILE:HG12	3:C:404:CLR:H212	1.97	0.46
4:A:406:PLM:H62	4:A:406:PLM:H31	1.74	0.46
3:C:403:CLR:H152	3:C:404:CLR:H14	1.97	0.46
2:A:125:VAL:HG11	5:C:402:POV:H35A	1.98	0.46
5:A:417:POV:H35A	2:C:125:VAL:HG11	1.98	0.45
3:C:403:CLR:H191	3:C:404:CLR:H12	1.97	0.45
2:A:221:ILE:HG12	3:A:402:CLR:H212	1.97	0.45
5:C:402:POV:H21D	5:C:402:POV:H21A	1.73	0.45
4:A:405:PLM:H92	3:A:414:CLR:H261	1.98	0.45
4:C:407:PLM:H92	3:C:415:CLR:H261	1.98	0.45
3:A:401:CLR:H152	3:A:402:CLR:H14	1.97	0.45
5:A:417:POV:H21D	5:A:417:POV:H21A	1.73	0.44
4:A:406:PLM:HE2	4:A:407:PLM:HA2	2.00	0.44
4:C:408:PLM:HE2	4:C:409:PLM:HA2	2.00	0.44
2:C:180:LEU:O	2:C:235:THR:HG21	2.18	0.44
2:C:174:ARG:HB3	2:C:174:ARG:NH1	2.33	0.43
2:A:9:LYS:HA	2:A:9:LYS:HD2	1.68	0.43
2:A:174:ARG:HB3	2:A:174:ARG:NH1	2.34	0.43
2:A:10:LEU:HD23	2:A:10:LEU:HA	1.85	0.43
2:A:180:LEU:O	2:A:235:THR:HG21	2.18	0.43
2:A:131:MET:HG2	2:A:181:MET:HG3	2.01	0.42
5:A:412:POV:H22	5:A:412:POV:H25A	1.90	0.42
2:C:131:MET:HG2	2:C:181:MET:HG3	2.01	0.42
2:C:10:LEU:HD23	2:C:10:LEU:HA	1.85	0.42
1:B:25:LEU:HD23	1:B:25:LEU:HA	1.84	0.42
2:C:306:THR:HA	2:C:309:MET:HB2	2.02	0.42
1:D:25:LEU:HD23	1:D:25:LEU:HA	1.84	0.41
4:A:406:PLM:HC2	3:A:414:CLR:H231	2.02	0.41
2:A:106:LEU:HD23	2:A:106:LEU:HA	1.93	0.41
4:C:408:PLM:HC2	3:C:415:CLR:H231	2.02	0.41
4:A:409:PLM:H21	4:A:410:PLM:C2	2.51	0.41
3:A:416:CLR:H211	3:A:416:CLR:H232	1.88	0.41
2:C:9:LYS:HA	2:C:9:LYS:HD2	1.68	0.40
2:C:130:LEU:HD23	2:C:236:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:411:PLM:H21	4:C:412:PLM:C2	2.51	0.40
2:A:130:LEU:HD23	2:A:236:LEU:HD22	2.03	0.40
4:A:410:PLM:H91	4:A:410:PLM:HD2	2.04	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	B	51/128 (40%)	51 (100%)	0	0	100	100
1	D	51/128 (40%)	51 (100%)	0	0	100	100
2	A	325/340 (96%)	322 (99%)	3 (1%)	0	100	100
2	C	325/340 (96%)	322 (99%)	3 (1%)	0	100	100
All	All	752/936 (80%)	746 (99%)	6 (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	B	47/115 (41%)	47 (100%)	0	100	100
1	D	47/115 (41%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	285/297 (96%)	285 (100%)	0	100	100
2	C	285/297 (96%)	285 (100%)	0	100	100
All	All	664/824 (81%)	664 (100%)	0	100	100

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

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

Mol	Chain	Res	Type
2	A	78	ASN
2	A	242	GLN
2	A	246	HIS
2	A	281	GLN
2	C	78	ASN
2	C	242	GLN
2	C	246	HIS
2	C	281	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

34 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PLM	C	408	-	16,16,17	0.37	0	15,15,17	0.41	0
4	PLM	C	411	-	16,16,17	0.37	0	15,15,17	0.44	0
3	CLR	C	405	-	31,31,31	0.37	0	48,48,48	0.62	0
5	POV	A	413	-	45,45,51	0.62	1 (2%)	49,50,59	0.77	2 (4%)
4	PLM	A	408	-	16,16,17	0.38	0	15,15,17	0.50	0
3	CLR	C	404	-	31,31,31	0.37	0	48,48,48	0.64	0
3	CLR	C	403	-	31,31,31	0.36	0	48,48,48	0.66	0
4	PLM	C	409	-	16,16,17	0.37	0	15,15,17	0.45	0
3	CLR	A	403	-	31,31,31	0.37	0	48,48,48	0.62	0
3	CLR	A	404	-	31,31,31	0.36	0	48,48,48	0.55	0
3	CLR	A	416	-	31,31,31	0.38	0	48,48,48	0.73	2 (4%)
5	POV	C	414	-	45,45,51	0.62	1 (2%)	49,50,59	0.77	2 (4%)
4	PLM	A	409	-	16,16,17	0.37	0	15,15,17	0.44	0
4	PLM	A	411	-	16,16,17	0.36	0	15,15,17	0.42	0
4	PLM	A	405	-	16,16,17	0.37	0	15,15,17	0.44	0
3	CLR	A	402	-	31,31,31	0.37	0	48,48,48	0.64	0
6	FI8	A	415	-	74,75,75	0.79	1 (1%)	88,109,109	1.09	4 (4%)
5	POV	A	418	-	45,45,51	0.62	1 (2%)	49,50,59	0.77	2 (4%)
3	CLR	C	406	-	31,31,31	0.37	0	48,48,48	0.55	0
3	CLR	A	401	-	31,31,31	0.36	0	48,48,48	0.65	0
4	PLM	C	412	-	16,16,17	0.36	0	15,15,17	0.41	0
4	PLM	C	410	-	16,16,17	0.37	0	15,15,17	0.50	0
5	POV	A	417	-	45,45,51	0.63	1 (2%)	49,50,59	0.78	2 (4%)
5	POV	C	402	-	45,45,51	0.63	1 (2%)	49,50,59	0.78	2 (4%)
4	PLM	A	410	-	16,16,17	0.36	0	15,15,17	0.41	0
3	CLR	A	414	-	31,31,31	0.37	0	48,48,48	0.64	0
4	PLM	A	406	-	16,16,17	0.36	0	15,15,17	0.40	0
3	CLR	C	401	-	31,31,31	0.37	0	48,48,48	0.73	2 (4%)
4	PLM	C	407	-	16,16,17	0.38	0	15,15,17	0.44	0
6	FI8	C	416	-	74,75,75	0.79	1 (1%)	88,109,109	1.09	4 (4%)
4	PLM	C	413	-	16,16,17	0.36	0	15,15,17	0.42	0
5	POV	A	412	-	45,45,51	0.62	1 (2%)	49,50,59	0.77	2 (4%)
3	CLR	C	415	-	31,31,31	0.37	0	48,48,48	0.65	0
4	PLM	A	407	-	16,16,17	0.37	0	15,15,17	0.45	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
4	PLM	C	408	-	-	5/13/14/15	-
4	PLM	C	411	-	-	3/13/14/15	-
3	CLR	C	405	-	-	4/10/68/68	0/4/4/4
5	POV	A	413	-	-	9/47/47/55	-
4	PLM	A	408	-	-	2/13/14/15	-
3	CLR	C	404	-	-	2/10/68/68	0/4/4/4
3	CLR	C	403	-	-	4/10/68/68	0/4/4/4
4	PLM	C	409	-	-	3/13/14/15	-
3	CLR	A	403	-	-	4/10/68/68	0/4/4/4
3	CLR	A	404	-	-	3/10/68/68	0/4/4/4
3	CLR	A	416	-	-	1/10/68/68	0/4/4/4
5	POV	C	414	-	-	9/47/47/55	-
4	PLM	A	409	-	-	3/13/14/15	-
4	PLM	A	411	-	-	0/13/14/15	-
4	PLM	A	405	-	-	1/13/14/15	-
3	CLR	A	402	-	-	2/10/68/68	0/4/4/4
6	FI8	A	415	-	-	14/75/118/118	0/3/4/4
5	POV	A	418	-	-	15/47/47/55	-
3	CLR	C	406	-	-	3/10/68/68	0/4/4/4
3	CLR	A	401	-	-	4/10/68/68	0/4/4/4
4	PLM	C	412	-	-	2/13/14/15	-
4	PLM	C	410	-	-	2/13/14/15	-
5	POV	A	417	-	-	14/47/47/55	-
5	POV	C	402	-	-	14/47/47/55	-
4	PLM	A	410	-	-	2/13/14/15	-
3	CLR	A	414	-	-	0/10/68/68	0/4/4/4
4	PLM	A	406	-	-	5/13/14/15	-
3	CLR	C	401	-	-	1/10/68/68	0/4/4/4
4	PLM	C	407	-	-	1/13/14/15	-
6	FI8	C	416	-	-	14/75/118/118	0/3/4/4
4	PLM	C	413	-	-	0/13/14/15	-
5	POV	A	412	-	-	15/47/47/55	-
3	CLR	C	415	-	-	0/10/68/68	0/4/4/4
4	PLM	A	407	-	-	3/13/14/15	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	412	POV	P-O12	2.94	1.66	1.54
5	A	413	POV	P-O12	2.93	1.66	1.54
5	A	418	POV	P-O12	2.92	1.66	1.54
5	C	414	POV	P-O12	2.92	1.66	1.54
5	C	402	POV	P-O12	2.91	1.66	1.54
5	A	417	POV	P-O12	2.91	1.66	1.54
6	A	415	FI8	O14-C46	-2.81	1.42	1.45
6	C	416	FI8	O14-C46	-2.80	1.42	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	415	FI8	C40-C39-C34	3.49	124.46	120.99
6	C	416	FI8	C40-C39-C34	3.49	124.46	120.99
5	A	412	POV	O12-P-O11	-3.45	97.56	106.73
5	A	418	POV	O12-P-O11	-3.44	97.58	106.73
5	C	414	POV	O12-P-O11	-3.35	97.83	106.73
5	A	413	POV	O12-P-O11	-3.34	97.84	106.73
5	A	417	POV	O12-P-O11	-3.34	97.84	106.73
5	C	402	POV	O12-P-O11	-3.34	97.86	106.73
6	A	415	FI8	C29-O10-C33	3.20	122.34	117.21
6	C	416	FI8	C29-O10-C33	3.20	122.34	117.21
5	C	414	POV	O13-P-O14	2.70	121.26	110.68
5	A	413	POV	O13-P-O14	2.70	121.24	110.68
5	A	412	POV	O13-P-O14	2.67	121.13	110.68
5	A	418	POV	O13-P-O14	2.66	121.11	110.68
5	A	417	POV	O13-P-O14	2.65	121.04	110.68
5	C	402	POV	O13-P-O14	2.64	121.03	110.68
6	C	416	FI8	C45-O17-C49	2.42	121.57	117.92
6	A	415	FI8	C45-O17-C49	2.41	121.55	117.92
6	A	415	FI8	C35-C34-C33	-2.09	113.76	117.47
6	C	416	FI8	C35-C34-C33	-2.09	113.77	117.47
3	C	401	CLR	C21-C20-C17	2.06	116.07	112.92
3	C	401	CLR	C13-C17-C20	2.06	122.70	119.49
3	A	416	CLR	C13-C17-C20	2.05	122.70	119.49
3	A	416	CLR	C21-C20-C17	2.04	116.05	112.92

There are no chirality outliers.

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	412	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
5	A	413	POV	C1-O11-P-O12
5	A	413	POV	C1-O11-P-O13
5	A	417	POV	C1-O11-P-O12
5	A	417	POV	C1-O11-P-O13
5	A	417	POV	C1-O11-P-O14
5	A	418	POV	C1-O11-P-O13
5	C	402	POV	C1-O11-P-O12
5	C	402	POV	C1-O11-P-O13
5	C	402	POV	C1-O11-P-O14
5	C	414	POV	C1-O11-P-O12
5	C	414	POV	C1-O11-P-O13
6	A	415	FI8	C3-C1-O6-C26
6	A	415	FI8	C13-C12-O4-C42
6	A	415	FI8	O1-C2-C3-C1
6	A	415	FI8	O2-C2-C3-C1
6	A	415	FI8	O2-C2-C3-C4
6	A	415	FI8	C3-C4-C5-C6
6	A	415	FI8	C7-C8-C9-C10
6	A	415	FI8	C7-C8-C9-C21
6	A	415	FI8	O3-C8-C9-C21
6	C	416	FI8	C3-C1-O6-C26
6	C	416	FI8	C13-C12-O4-C42
6	C	416	FI8	O1-C2-C3-C1
6	C	416	FI8	O2-C2-C3-C1
6	C	416	FI8	O2-C2-C3-C4
6	C	416	FI8	C3-C4-C5-C6
6	C	416	FI8	C7-C8-C9-C10
6	C	416	FI8	C7-C8-C9-C21
6	C	416	FI8	O3-C8-C9-C21
3	A	404	CLR	C20-C22-C23-C24
3	C	406	CLR	C20-C22-C23-C24
3	A	404	CLR	C22-C23-C24-C25
3	C	406	CLR	C22-C23-C24-C25
4	A	410	PLM	C9-CA-CB-CC
4	C	412	PLM	C9-CA-CB-CC
5	A	417	POV	C22-C21-O21-C2
5	C	402	POV	C22-C21-O21-C2
5	A	413	POV	C25-C26-C27-C28
5	C	414	POV	C25-C26-C27-C28
3	A	402	CLR	C23-C24-C25-C27
3	C	404	CLR	C23-C24-C25-C27
4	A	406	PLM	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	C	408	PLM	C2-C3-C4-C5
4	C	409	PLM	C9-CA-CB-CC
5	A	417	POV	O22-C21-O21-C2
5	C	402	POV	O22-C21-O21-C2
4	A	407	PLM	C9-CA-CB-CC
4	A	408	PLM	C6-C7-C8-C9
4	C	410	PLM	C6-C7-C8-C9
4	C	408	PLM	C3-C4-C5-C6
4	A	406	PLM	C3-C4-C5-C6
5	A	417	POV	C212-C213-C214-C215
5	C	402	POV	C212-C213-C214-C215
3	C	404	CLR	C23-C24-C25-C26
3	A	402	CLR	C23-C24-C25-C26
3	C	406	CLR	C17-C20-C22-C23
3	A	404	CLR	C17-C20-C22-C23
6	A	415	FI8	O1-C2-C3-C4
6	C	416	FI8	O1-C2-C3-C4
5	A	413	POV	C36-C37-C38-C39
5	C	414	POV	C36-C37-C38-C39
6	A	415	FI8	O3-C8-C9-C10
6	C	416	FI8	O3-C8-C9-C10
5	A	412	POV	O11-C1-C2-C3
5	A	418	POV	O11-C1-C2-C3
4	A	409	PLM	C3-C4-C5-C6
4	C	411	PLM	C3-C4-C5-C6
6	A	415	FI8	O1-C18-C19-C20
6	C	416	FI8	O1-C18-C19-C20
4	A	406	PLM	CA-CB-CC-CD
4	C	408	PLM	CA-CB-CC-CD
5	A	412	POV	C312-C313-C314-C315
5	A	418	POV	C312-C313-C314-C315
5	A	417	POV	C25-C26-C27-C28
5	C	402	POV	C25-C26-C27-C28
5	A	413	POV	C33-C34-C35-C36
5	C	414	POV	C33-C34-C35-C36
5	A	413	POV	C311-C310-C39-C38
5	C	414	POV	C311-C310-C39-C38
5	A	412	POV	O11-C1-C2-O21
5	A	418	POV	O11-C1-C2-O21
5	A	412	POV	C25-C26-C27-C28
5	A	418	POV	C25-C26-C27-C28
5	A	417	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	C	402	POV	O11-C1-C2-C3
5	A	418	POV	C211-C212-C213-C214
5	A	412	POV	C211-C212-C213-C214
5	A	417	POV	O11-C1-C2-O21
5	C	402	POV	O11-C1-C2-O21
3	A	401	CLR	C13-C17-C20-C21
3	C	403	CLR	C13-C17-C20-C21
6	A	415	FI8	O11-C33-C34-C35
6	C	416	FI8	O11-C33-C34-C35
3	A	401	CLR	C13-C17-C20-C22
3	C	403	CLR	C13-C17-C20-C22
5	A	412	POV	C37-C38-C39-C310
5	A	418	POV	C37-C38-C39-C310
5	A	417	POV	C211-C212-C213-C214
5	C	402	POV	C211-C212-C213-C214
5	A	417	POV	C311-C312-C313-C314
5	C	402	POV	C311-C312-C313-C314
3	A	401	CLR	C16-C17-C20-C21
3	C	403	CLR	C16-C17-C20-C21
4	A	410	PLM	C1-C2-C3-C4
4	C	412	PLM	C1-C2-C3-C4
3	A	401	CLR	C16-C17-C20-C22
3	C	403	CLR	C16-C17-C20-C22
4	A	409	PLM	C8-C9-CA-CB
4	C	411	PLM	C8-C9-CA-CB
4	A	407	PLM	C4-C5-C6-C7
4	C	409	PLM	C4-C5-C6-C7
5	A	412	POV	C35-C36-C37-C38
5	A	418	POV	C35-C36-C37-C38
3	A	403	CLR	C23-C24-C25-C26
3	C	405	CLR	C23-C24-C25-C26
6	A	415	FI8	O10-C33-C34-C35
6	C	416	FI8	O10-C33-C34-C35
4	A	407	PLM	C5-C6-C7-C8
4	C	409	PLM	C5-C6-C7-C8
3	A	416	CLR	C20-C22-C23-C24
3	C	401	CLR	C20-C22-C23-C24
5	A	412	POV	O22-C21-O21-C2
5	A	418	POV	O22-C21-O21-C2
5	A	413	POV	C214-C215-C216-C217
5	C	414	POV	C214-C215-C216-C217
4	C	411	PLM	C5-C6-C7-C8

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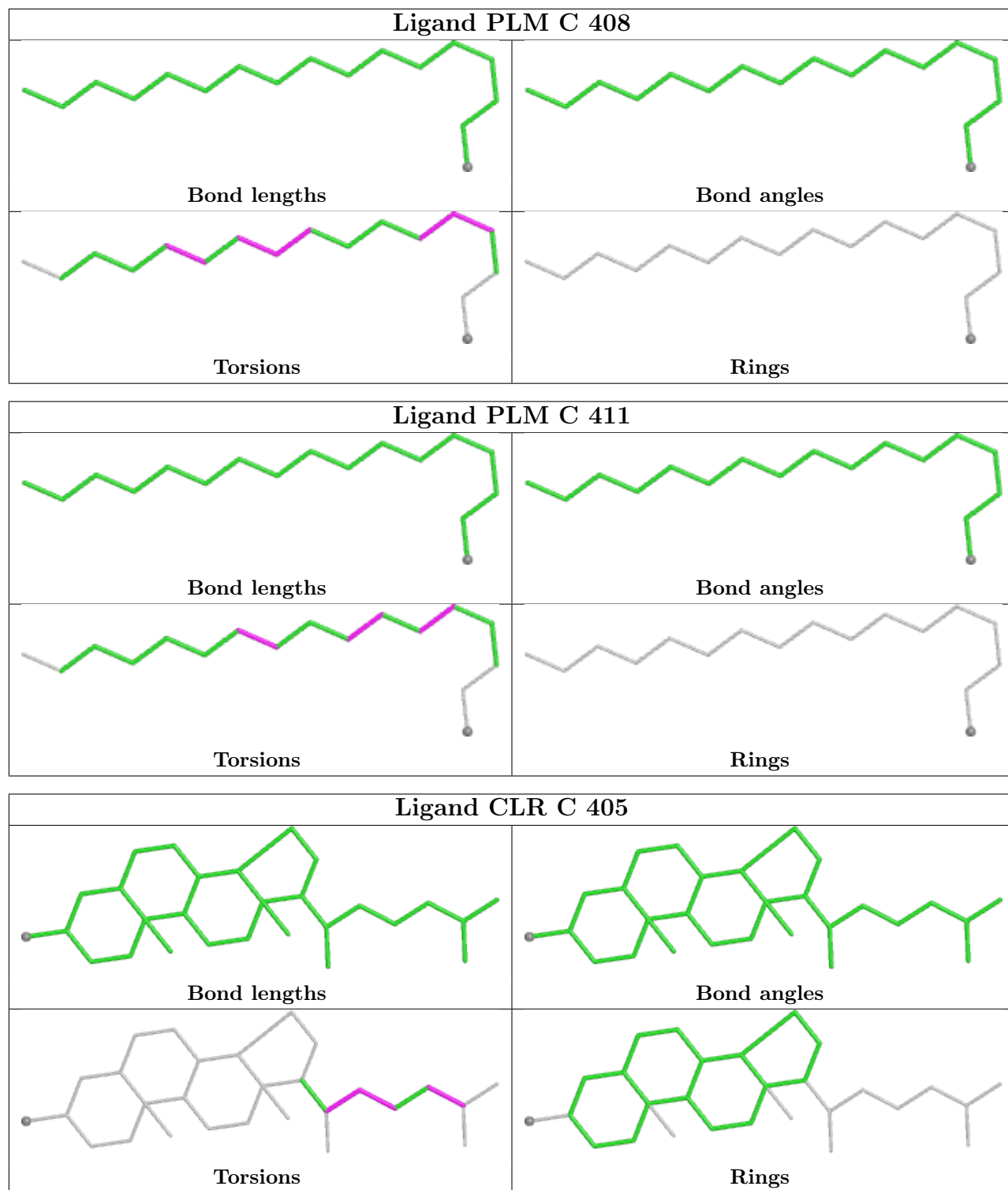
Mol	Chain	Res	Type	Atoms
4	A	409	PLM	C5-C6-C7-C8
5	C	414	POV	C22-C23-C24-C25
5	A	413	POV	C22-C23-C24-C25
5	A	412	POV	C31-C32-C33-C34
5	A	418	POV	C31-C32-C33-C34
4	A	408	PLM	C2-C3-C4-C5
4	C	410	PLM	C2-C3-C4-C5
5	A	412	POV	C22-C21-O21-C2
5	A	418	POV	C22-C21-O21-C2
3	A	403	CLR	C23-C24-C25-C27
3	C	405	CLR	C23-C24-C25-C27
5	A	412	POV	C213-C214-C215-C216
5	A	418	POV	C213-C214-C215-C216
5	A	412	POV	O31-C31-C32-C33
5	A	417	POV	C27-C28-C29-C210
5	C	402	POV	C27-C28-C29-C210
5	A	418	POV	O31-C31-C32-C33
5	A	417	POV	O31-C31-C32-C33
5	C	402	POV	O31-C31-C32-C33
3	A	403	CLR	C21-C20-C22-C23
3	C	405	CLR	C21-C20-C22-C23
4	A	406	PLM	C7-C8-C9-CA
4	C	408	PLM	C7-C8-C9-CA
5	A	412	POV	O32-C31-C32-C33
5	A	418	POV	O32-C31-C32-C33
5	C	402	POV	O32-C31-C32-C33
5	A	417	POV	O32-C31-C32-C33
4	A	405	PLM	C9-CA-CB-CC
3	A	403	CLR	C20-C22-C23-C24
3	C	405	CLR	C20-C22-C23-C24
4	C	407	PLM	C9-CA-CB-CC
4	A	406	PLM	C8-C9-CA-CB
5	A	412	POV	C212-C213-C214-C215
4	C	408	PLM	C8-C9-CA-CB
5	A	418	POV	C212-C213-C214-C215
5	A	413	POV	C35-C36-C37-C38
5	C	414	POV	C35-C36-C37-C38

There are no ring outliers.

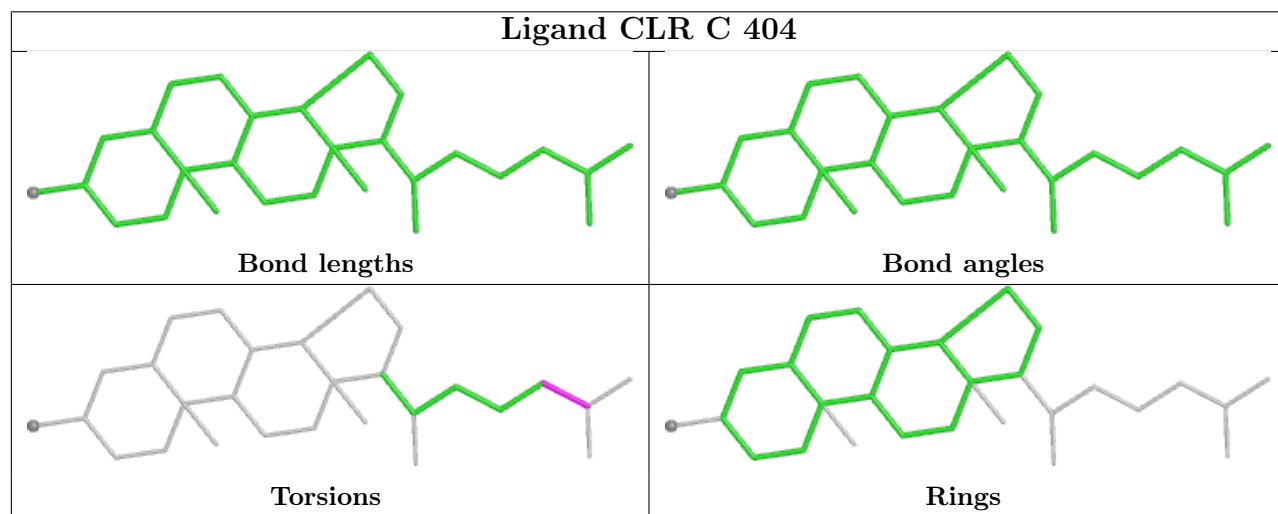
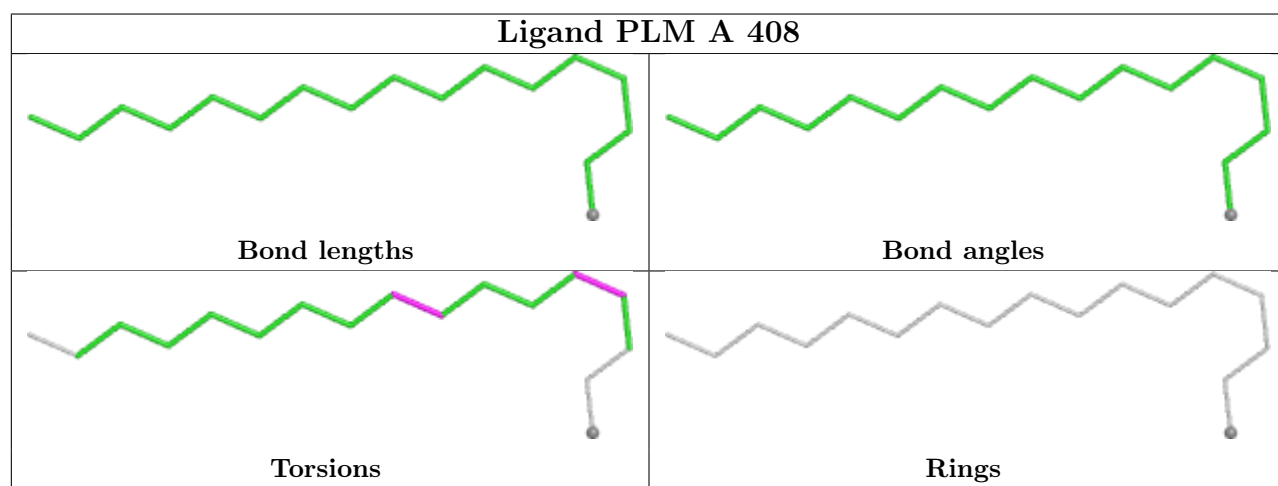
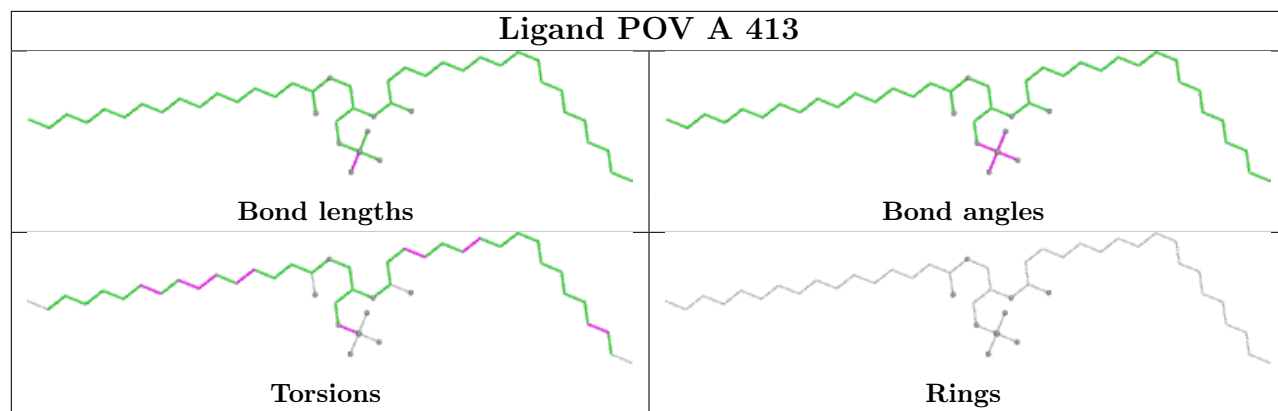
26 monomers are involved in 46 short contacts:

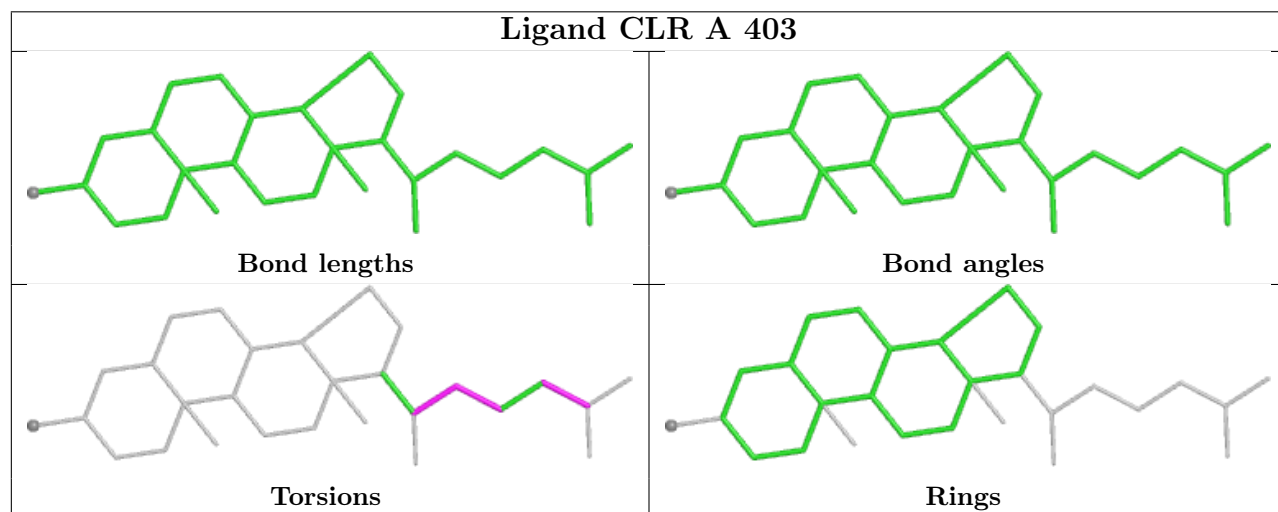
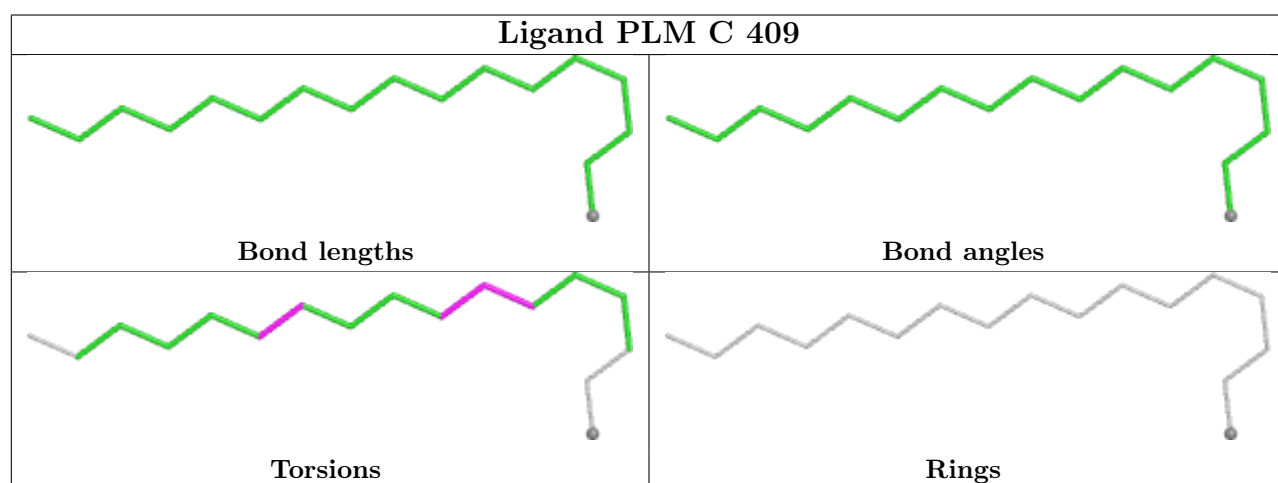
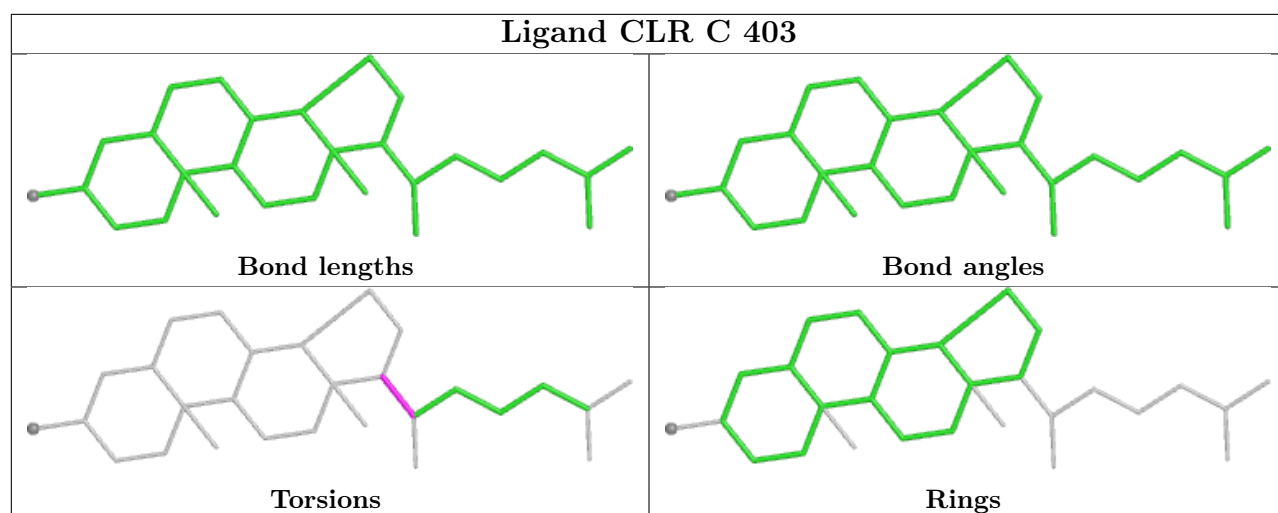
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	408	PLM	5	0
4	C	411	PLM	3	0
3	C	405	CLR	1	0
5	A	413	POV	1	0
4	A	408	PLM	2	0
3	C	404	CLR	4	0
3	C	403	CLR	2	0
4	C	409	PLM	4	0
3	A	403	CLR	1	0
3	A	416	CLR	1	0
5	C	414	POV	1	0
4	A	409	PLM	3	0
4	A	405	PLM	4	0
3	A	402	CLR	4	0
3	A	401	CLR	2	0
4	C	412	PLM	1	0
4	C	410	PLM	2	0
5	A	417	POV	2	0
5	C	402	POV	2	0
4	A	410	PLM	2	0
3	A	414	CLR	4	0
4	A	406	PLM	6	0
4	C	407	PLM	4	0
5	A	412	POV	1	0
3	C	415	CLR	4	0
4	A	407	PLM	4	0

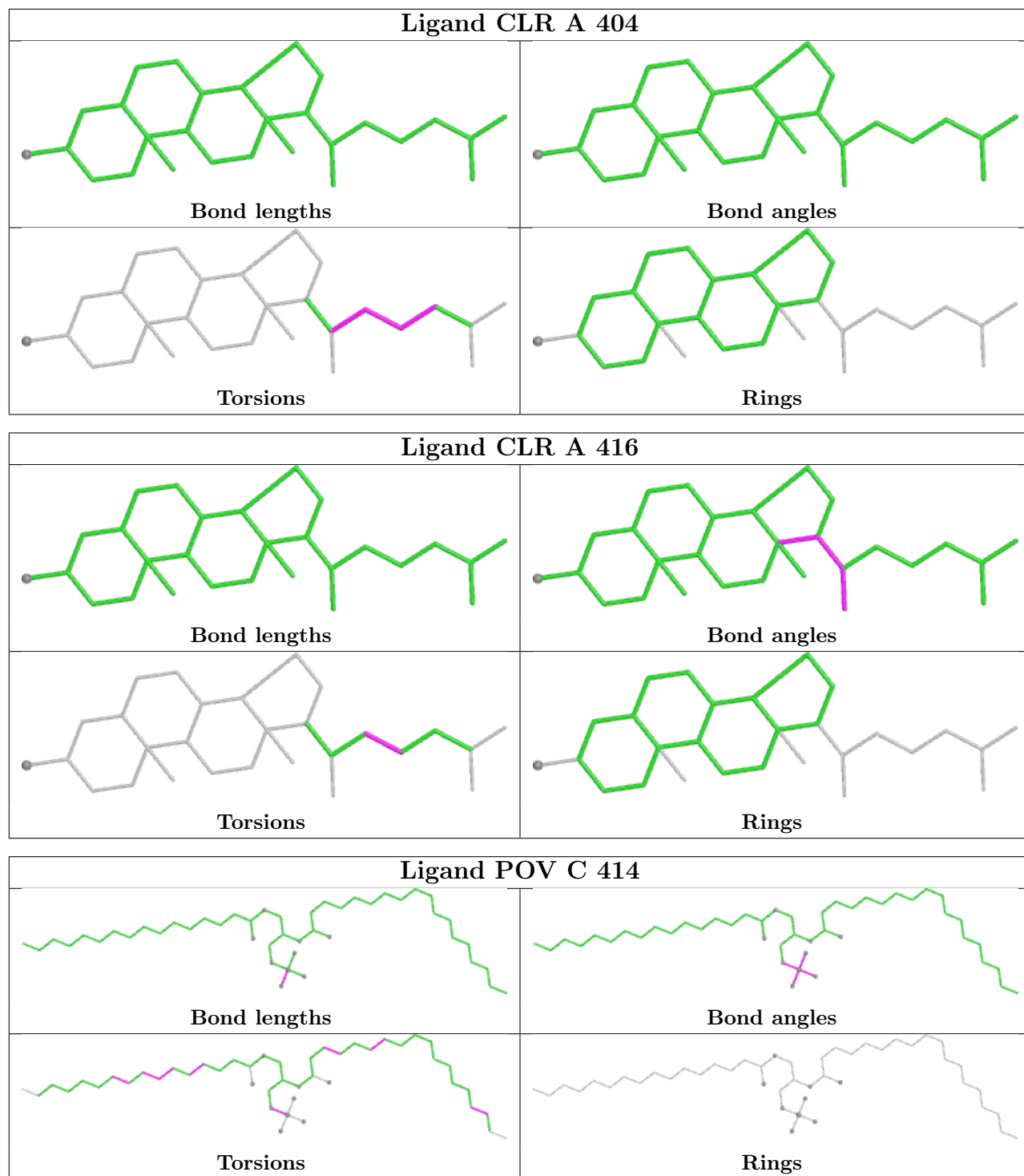
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

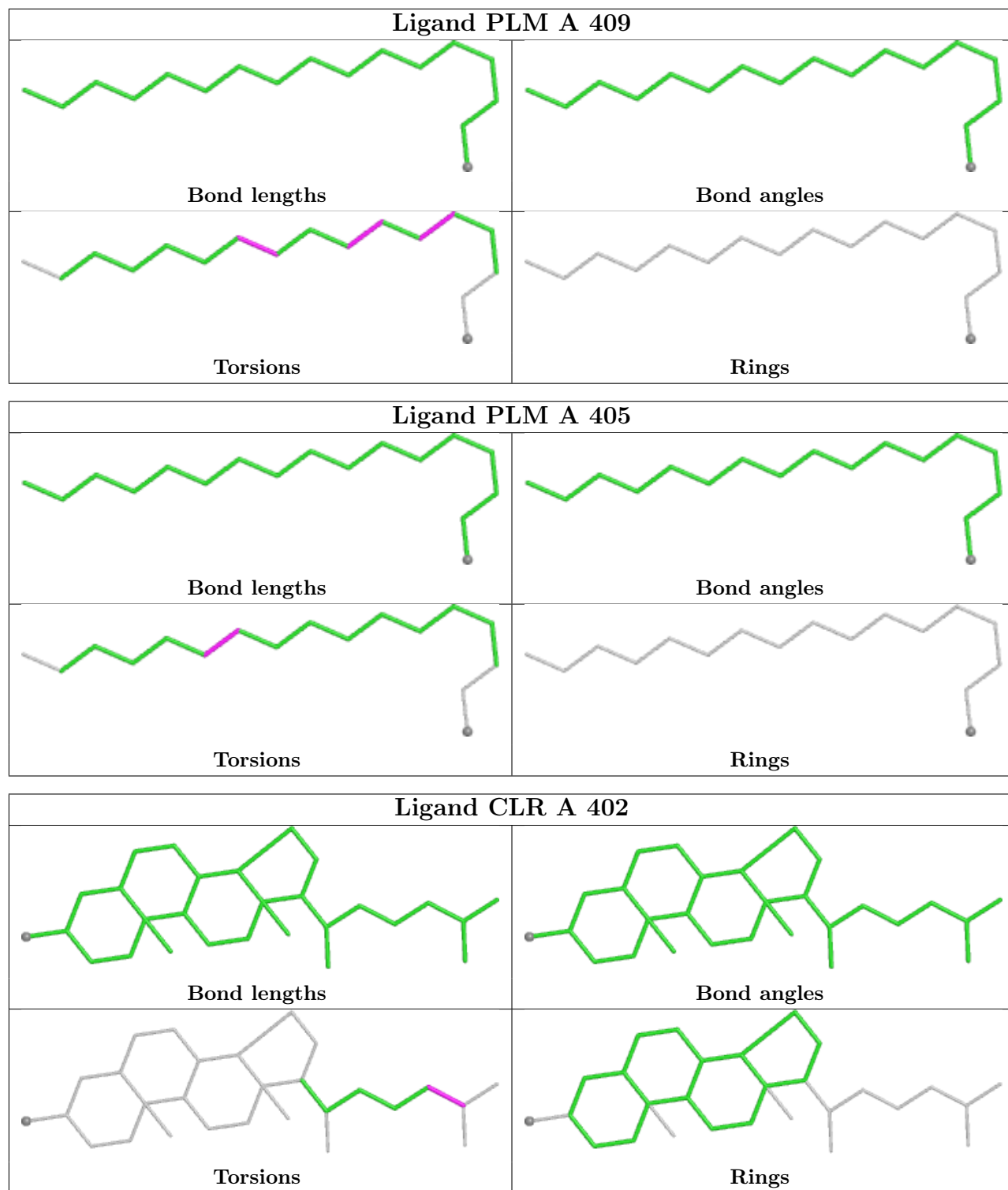


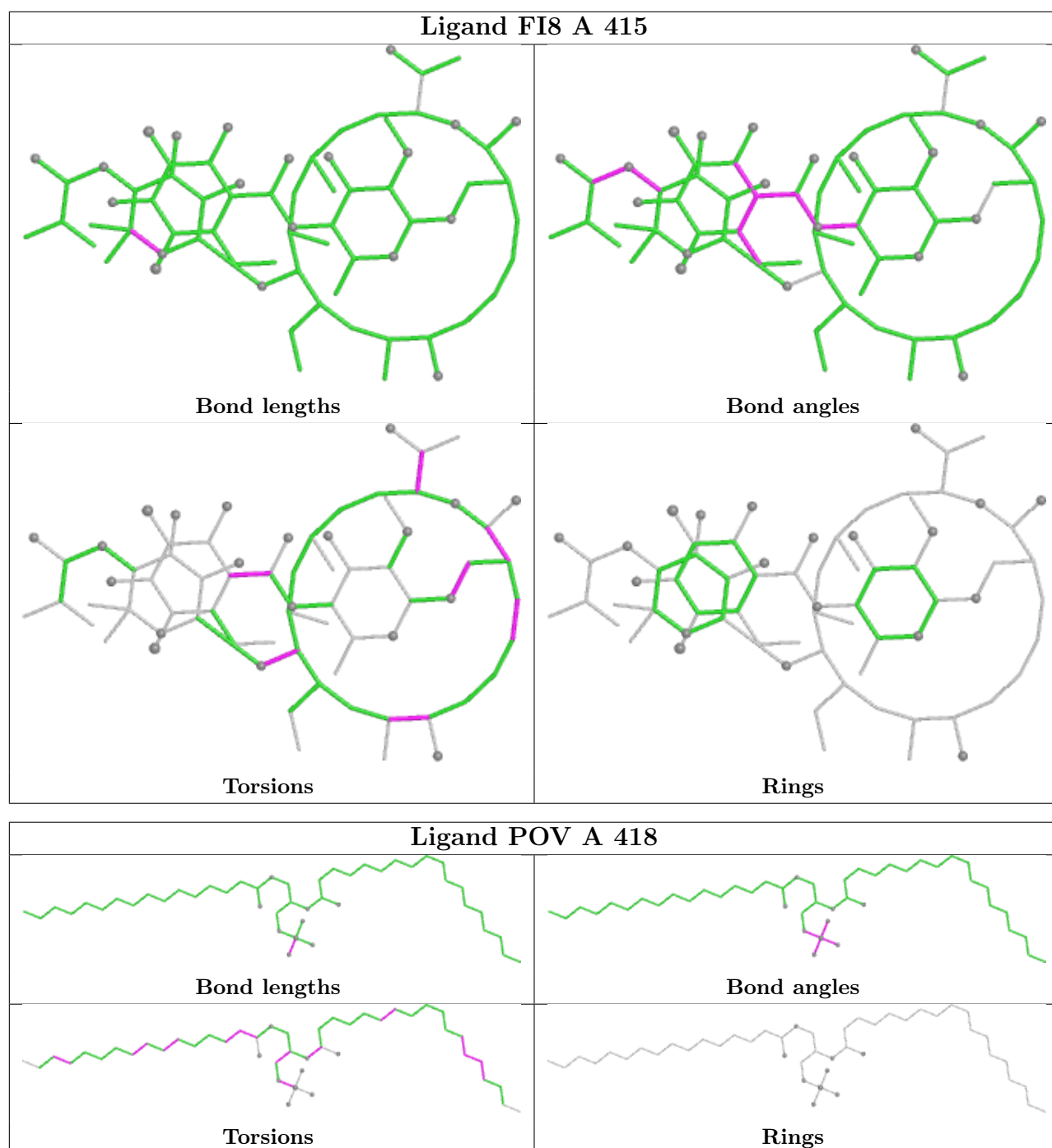


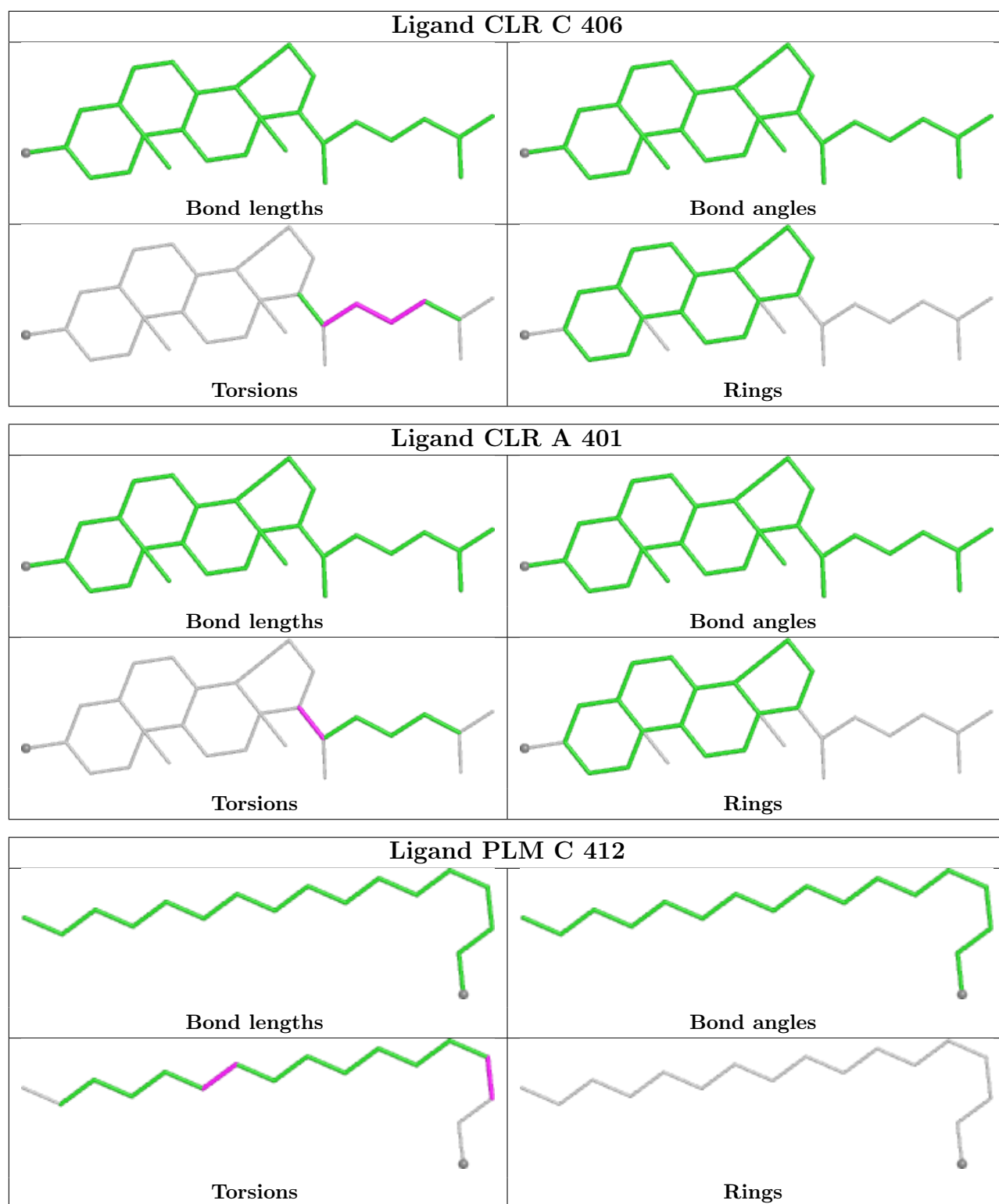


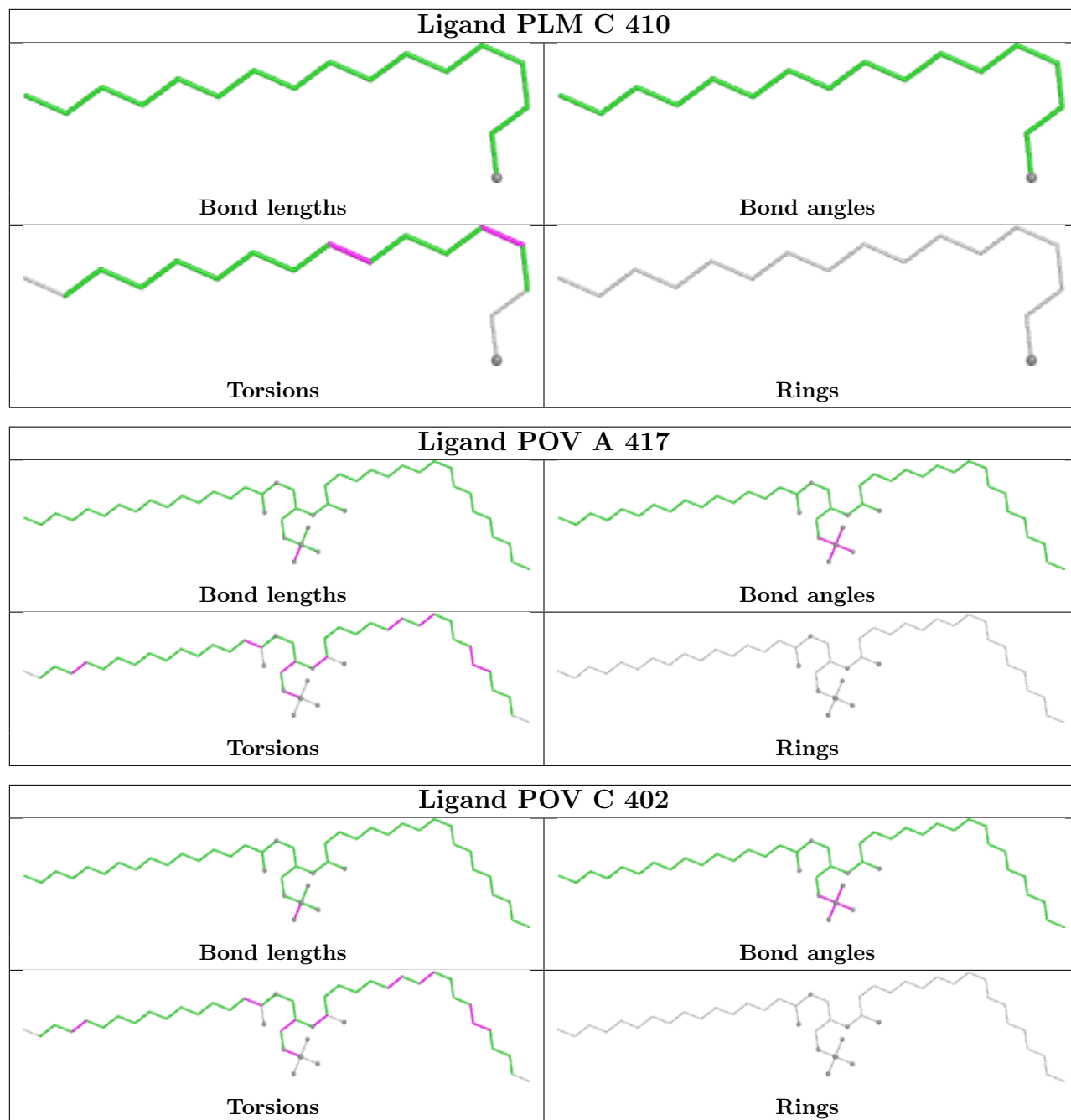


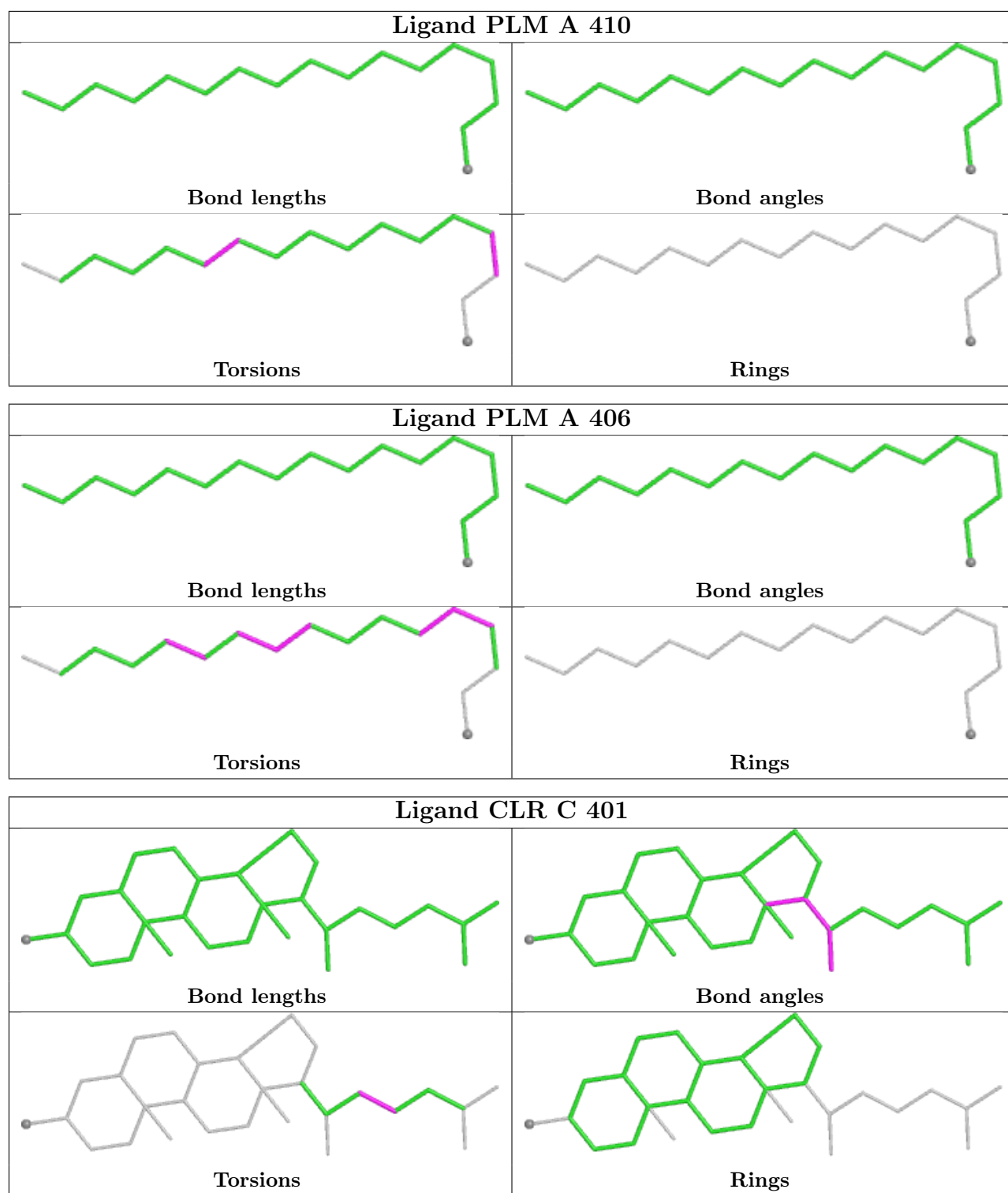




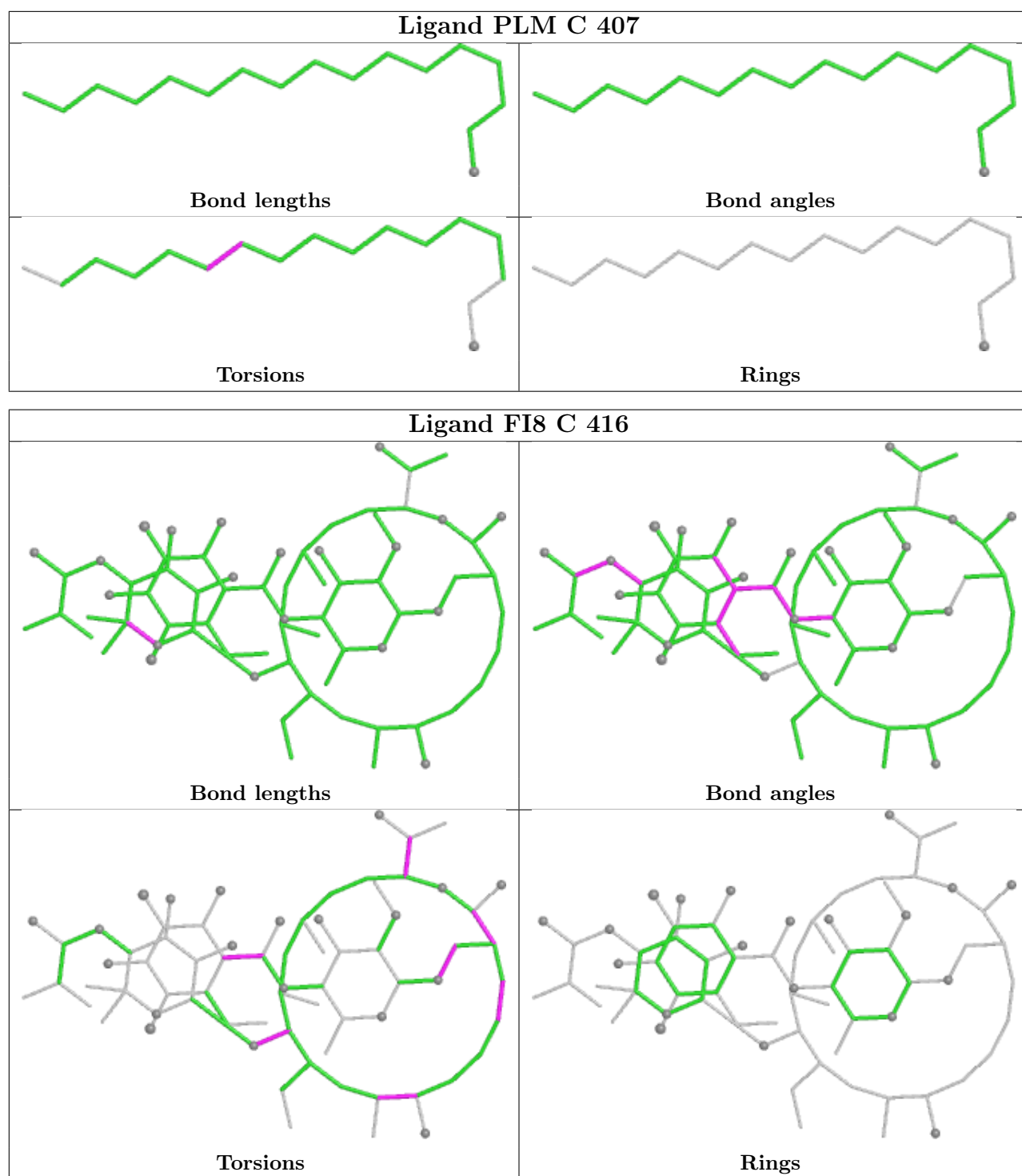


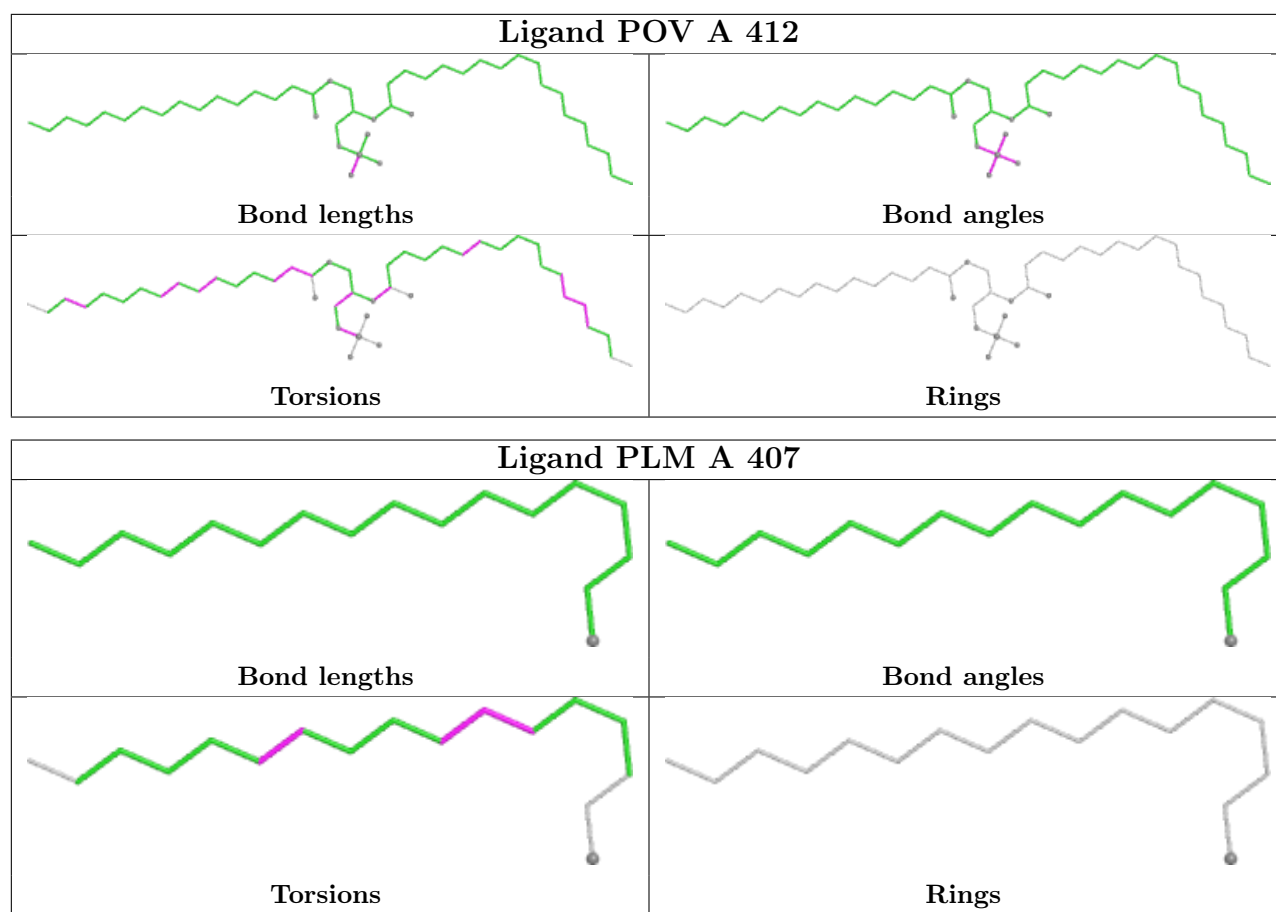












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

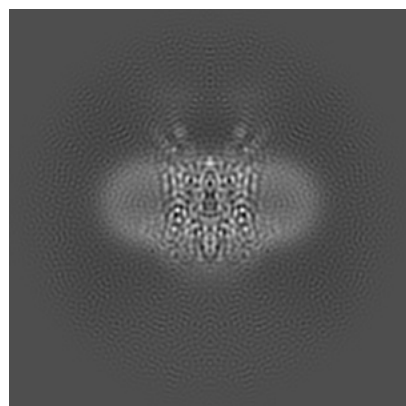
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66180. These allow visual inspection of the internal detail of the map and identification of artifacts.

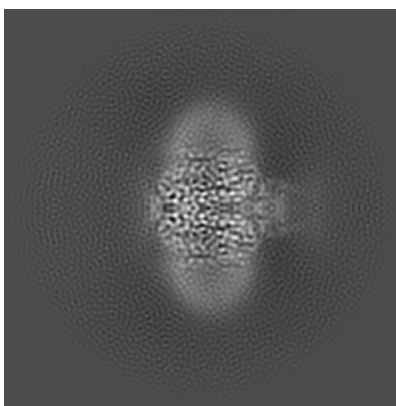
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

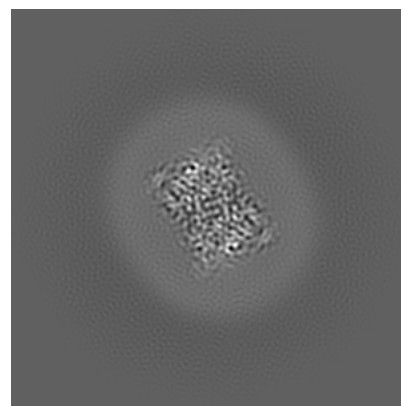
#### 6.1.1 Primary map



X

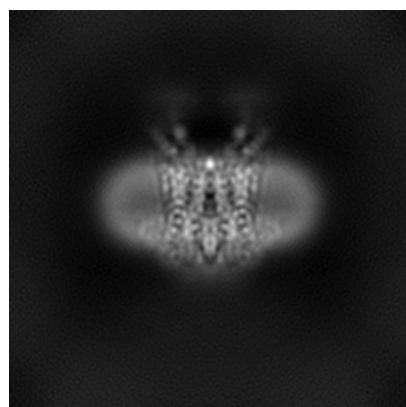


Y

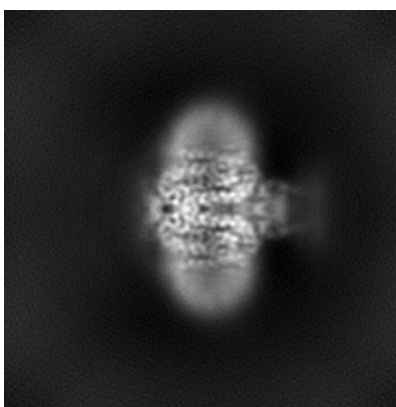


Z

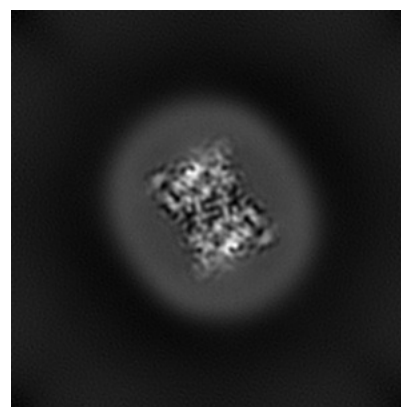
#### 6.1.2 Raw map



X



Y

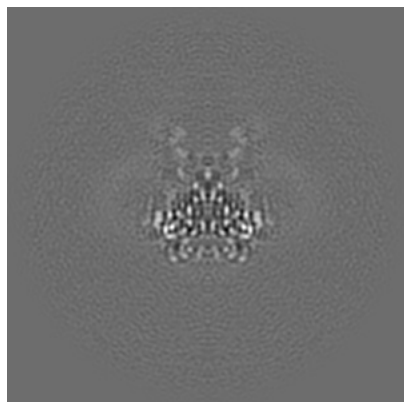


Z

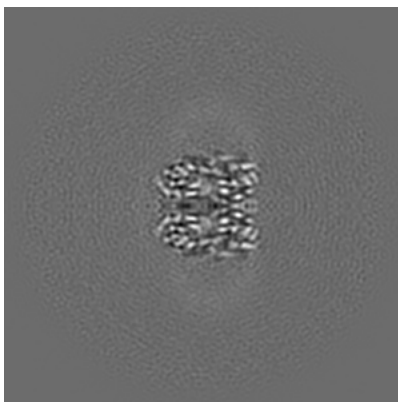
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

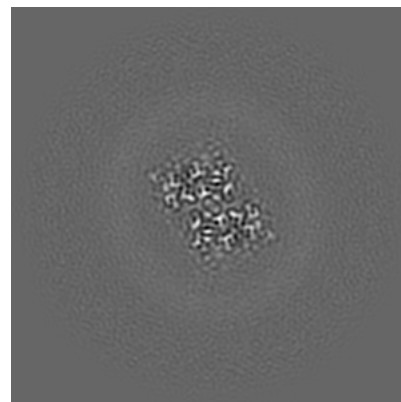
### 6.2.1 Primary map



X Index: 100

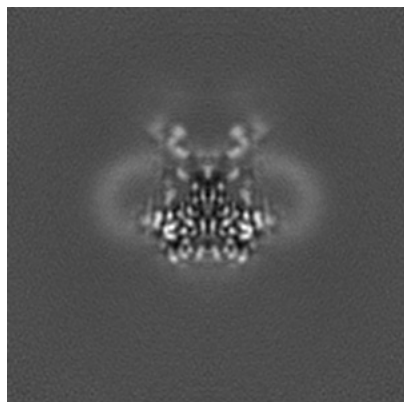


Y Index: 100

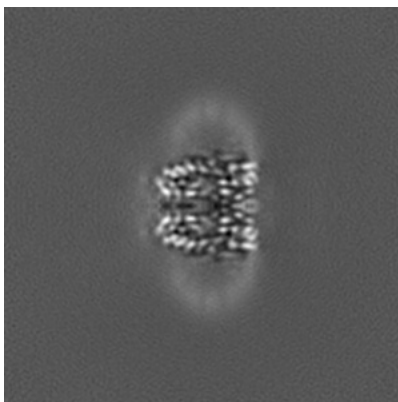


Z Index: 100

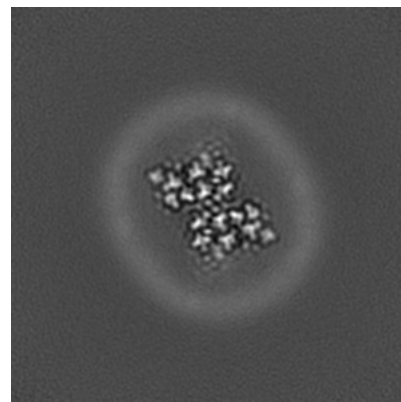
### 6.2.2 Raw map



X Index: 100



Y Index: 100

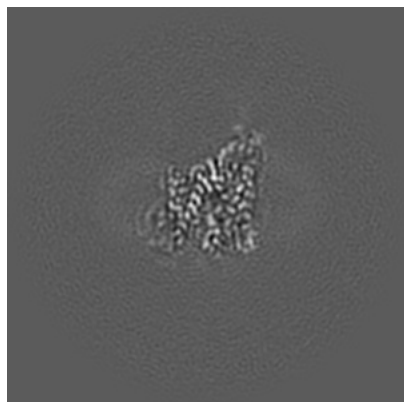


Z Index: 100

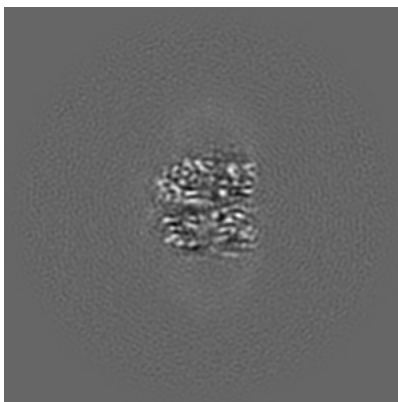
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

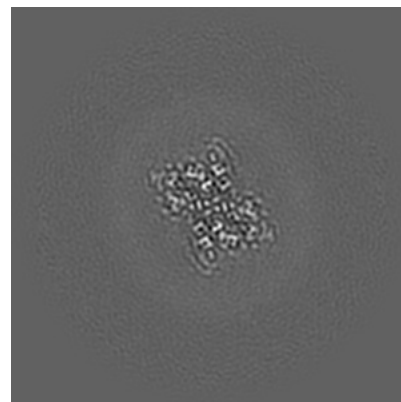
### 6.3.1 Primary map



X Index: 93

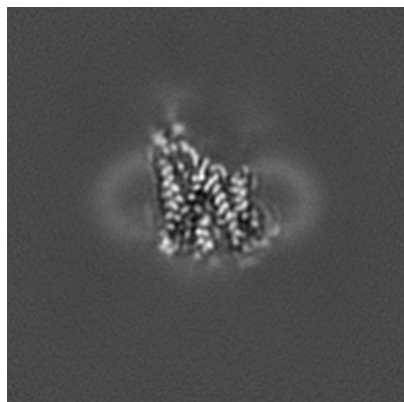


Y Index: 99

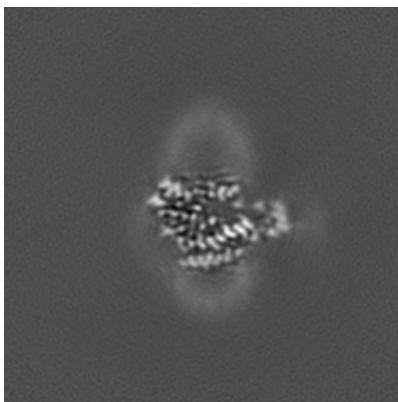


Z Index: 94

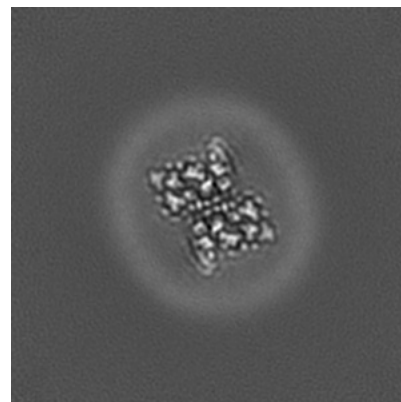
### 6.3.2 Raw map



X Index: 107



Y Index: 114

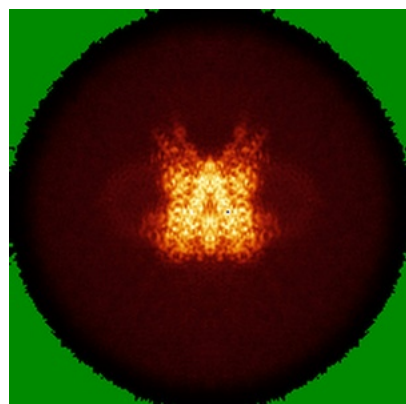


Z Index: 94

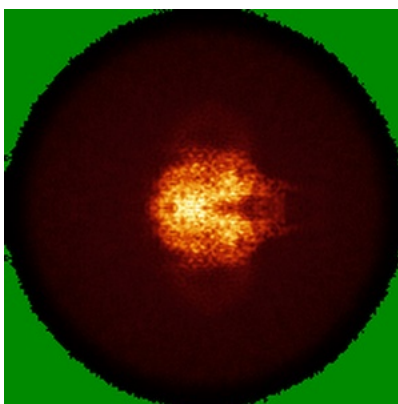
The images above show the largest variance slices of the map in three orthogonal directions.

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

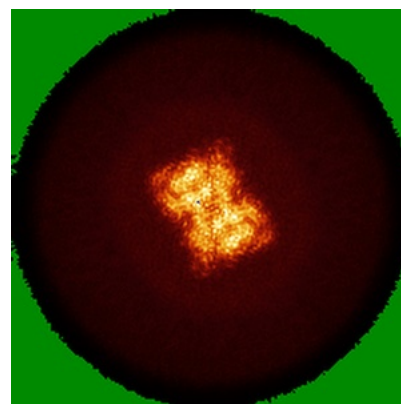
### 6.4.1 Primary map



X

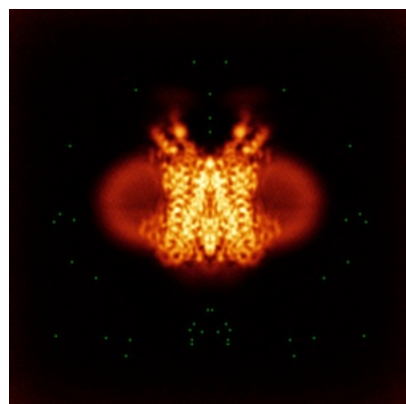


Y

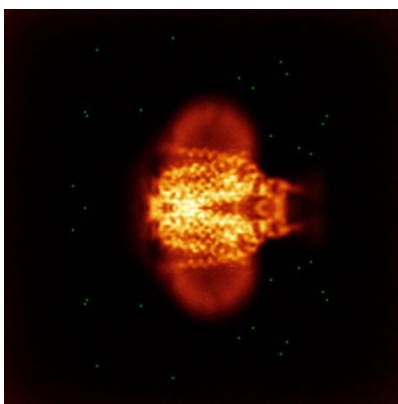


Z

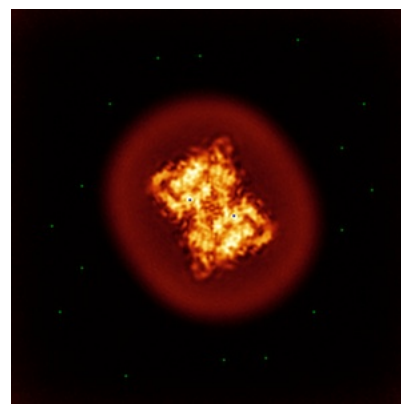
### 6.4.2 Raw map



X



Y



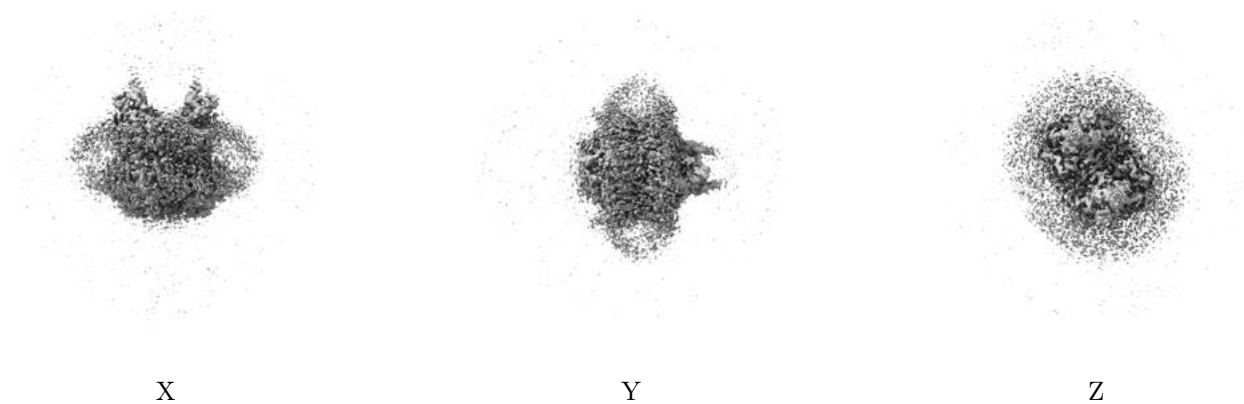
Z

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.



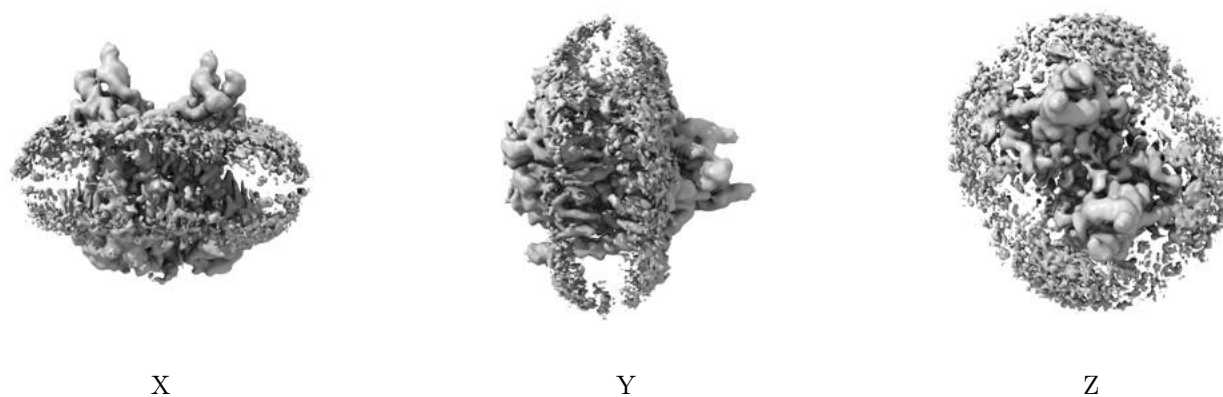
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

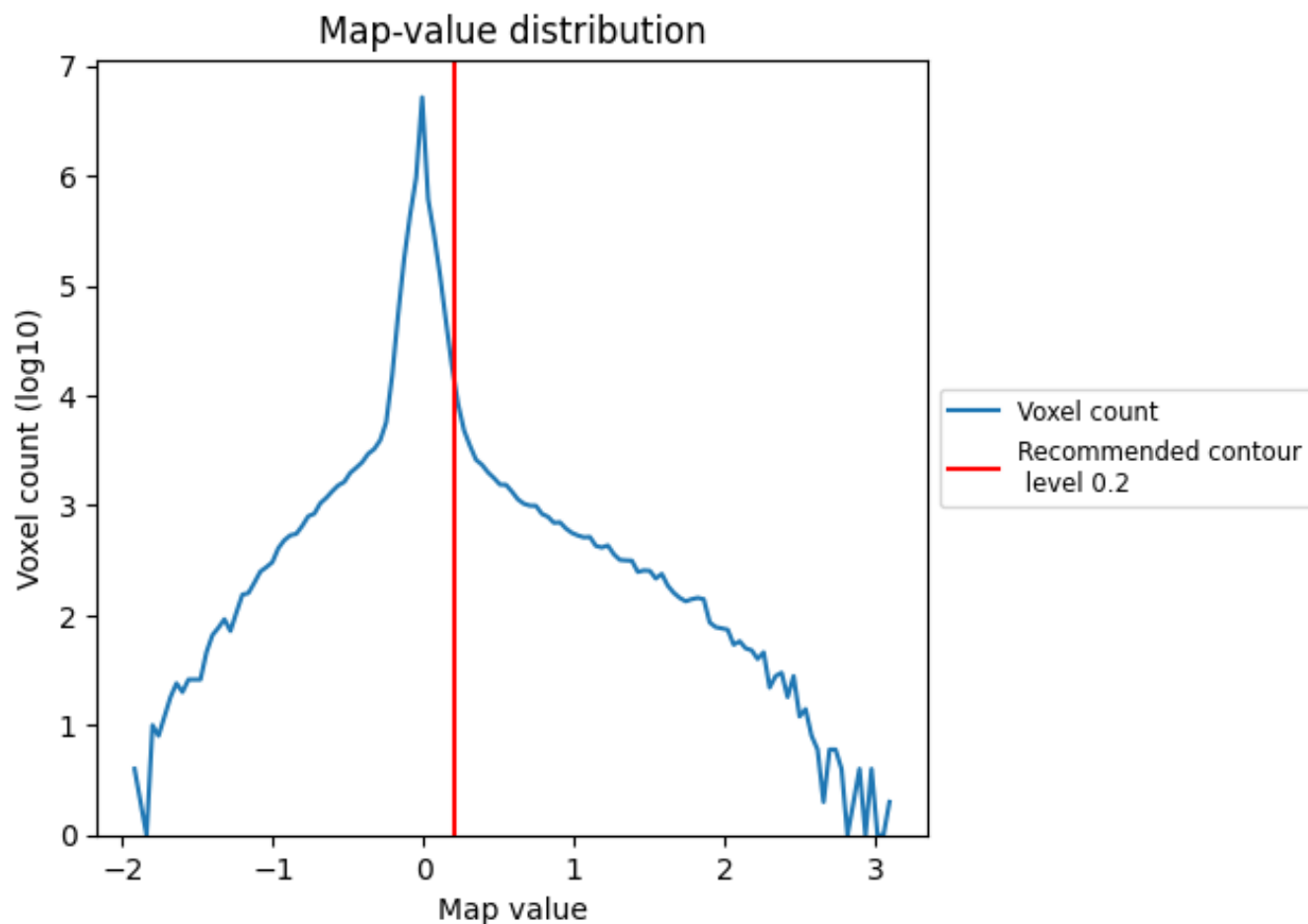
## 6.6 Mask visualisation [i](#)

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.

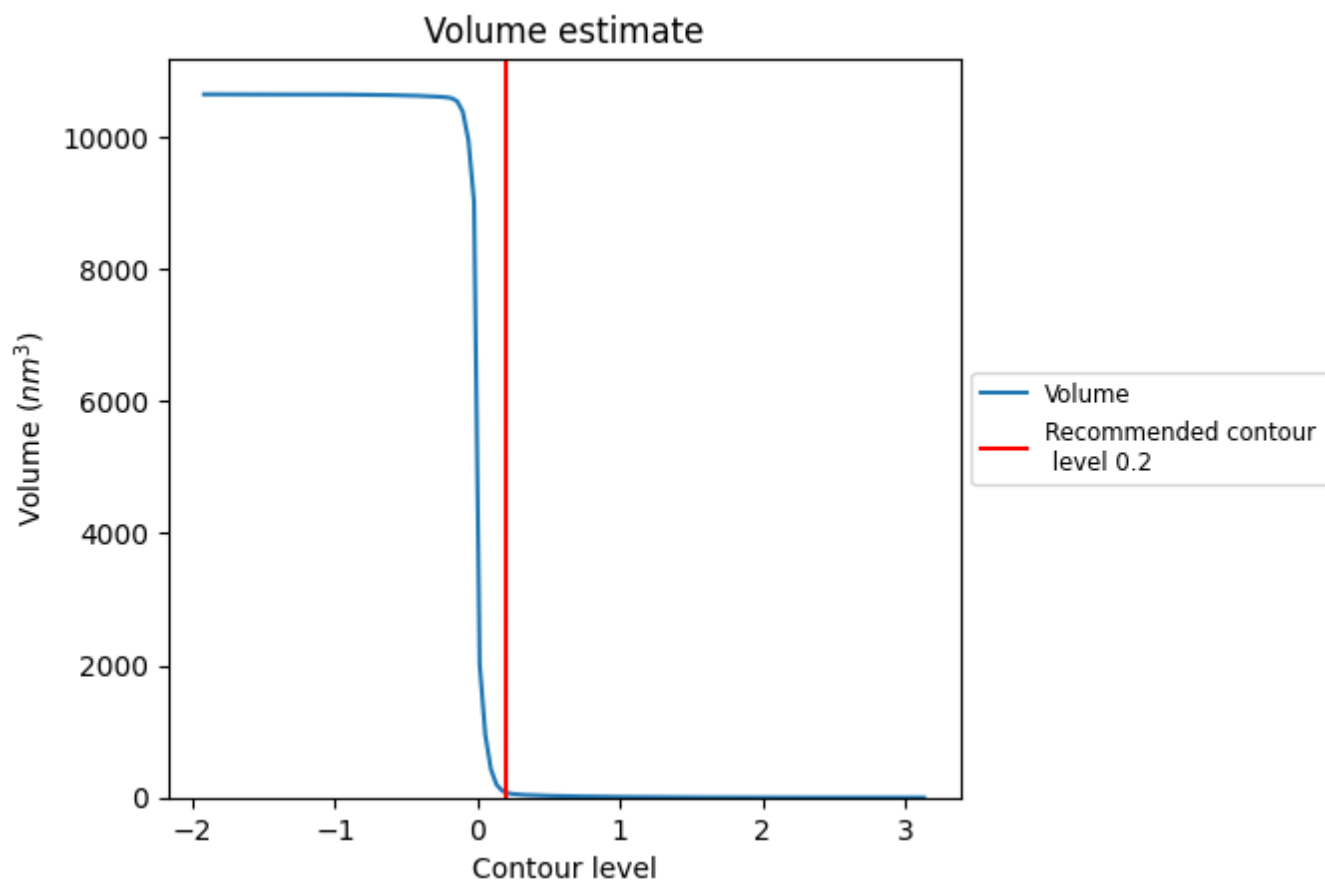
### 7.1 Map-value distribution [i](#)



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.



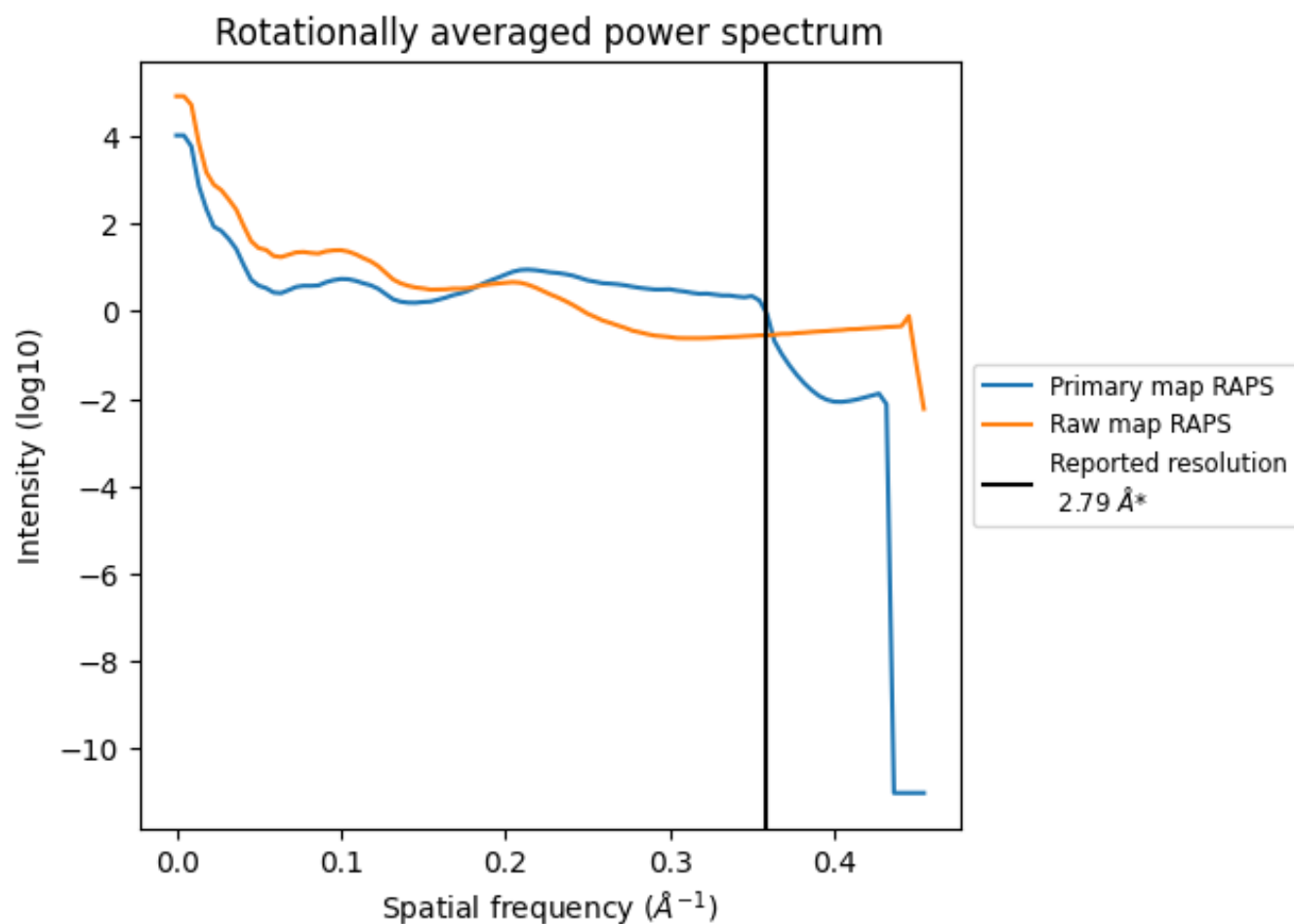
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80  $\text{nm}^3$ ; this corresponds to an approximate mass of 72 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 ⓘ

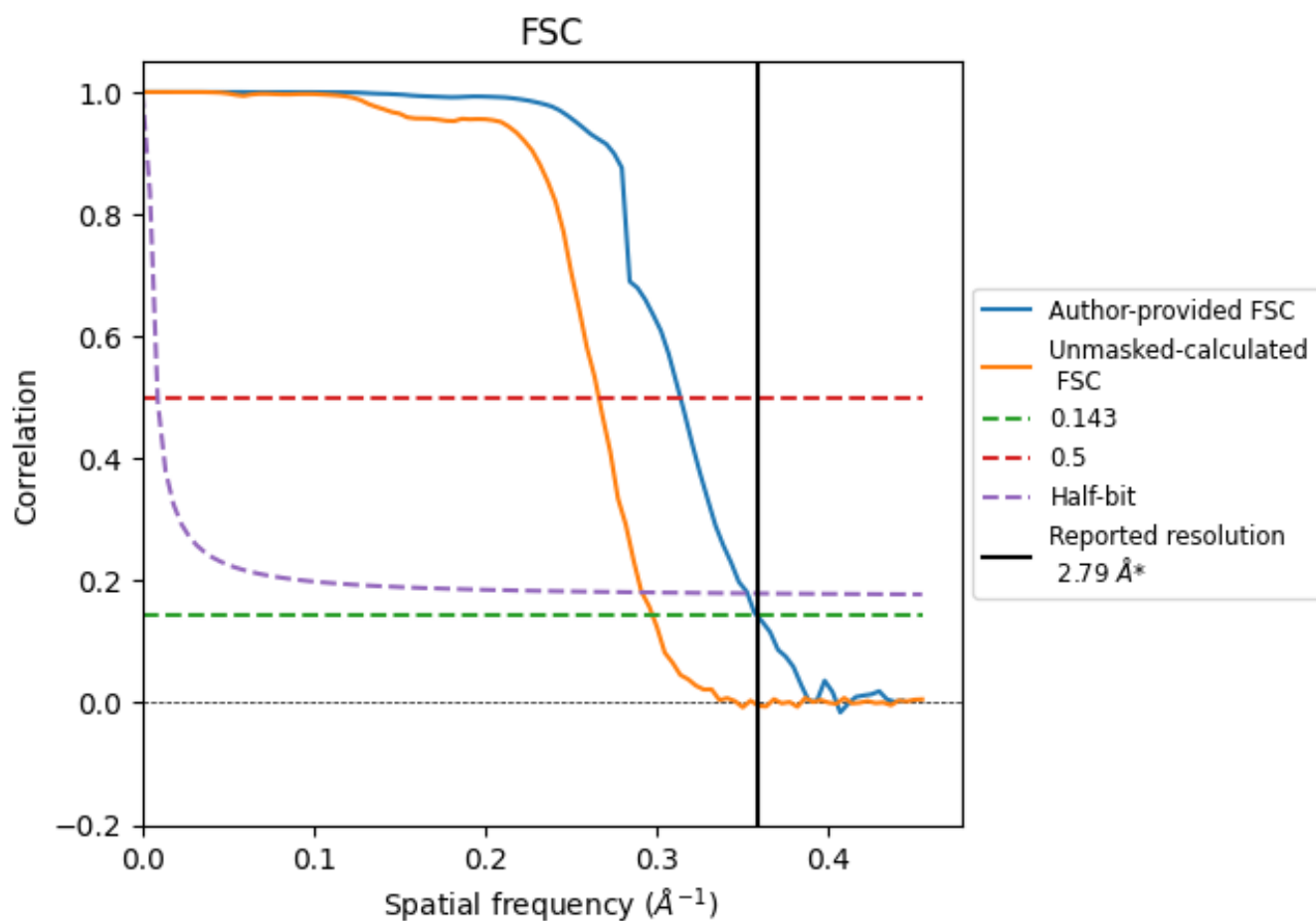


\*Reported resolution corresponds to spatial frequency of 0.358 Å<sup>-1</sup>

## 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  $0.358 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

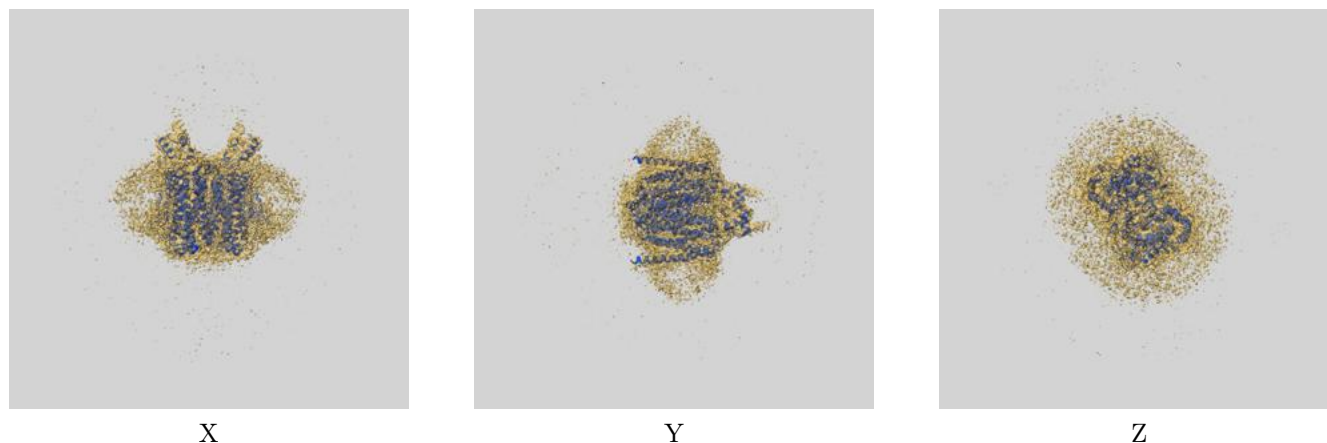
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.19	2.84
Unmasked-calculated*	3.36	3.76	3.44

\*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 3.36 differs from the reported value 2.79 by more than 10 %

## 9 Map-model fit [i](#)

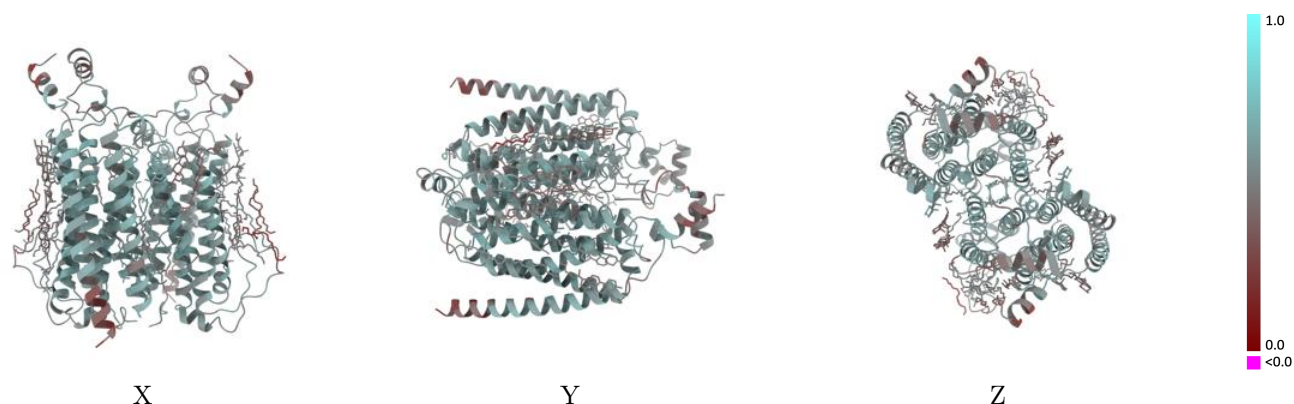
This section contains information regarding the fit between EMDB map EMD-66180 and PDB model 9WQR. Per-residue inclusion information can be found in section [3](#) on page [8](#).

### 9.1 Map-model overlay [i](#)



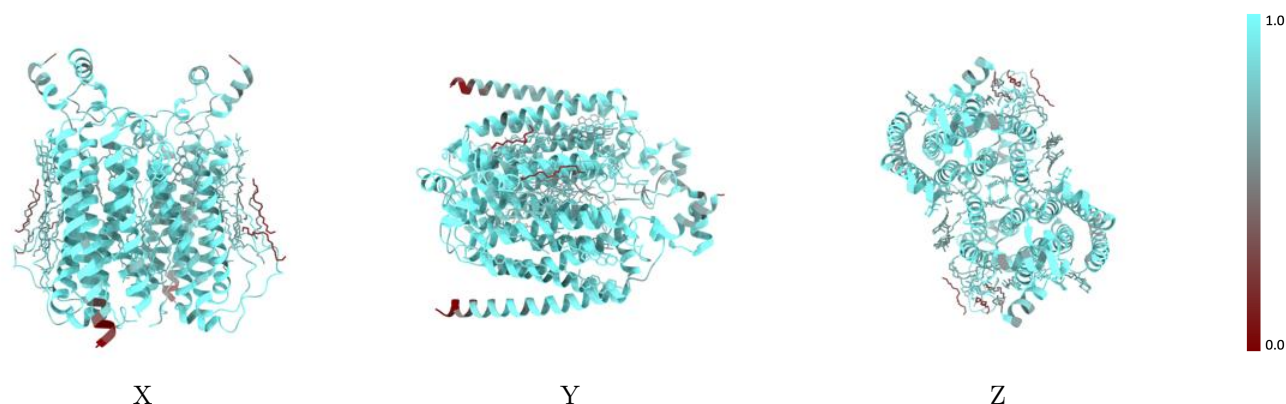
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



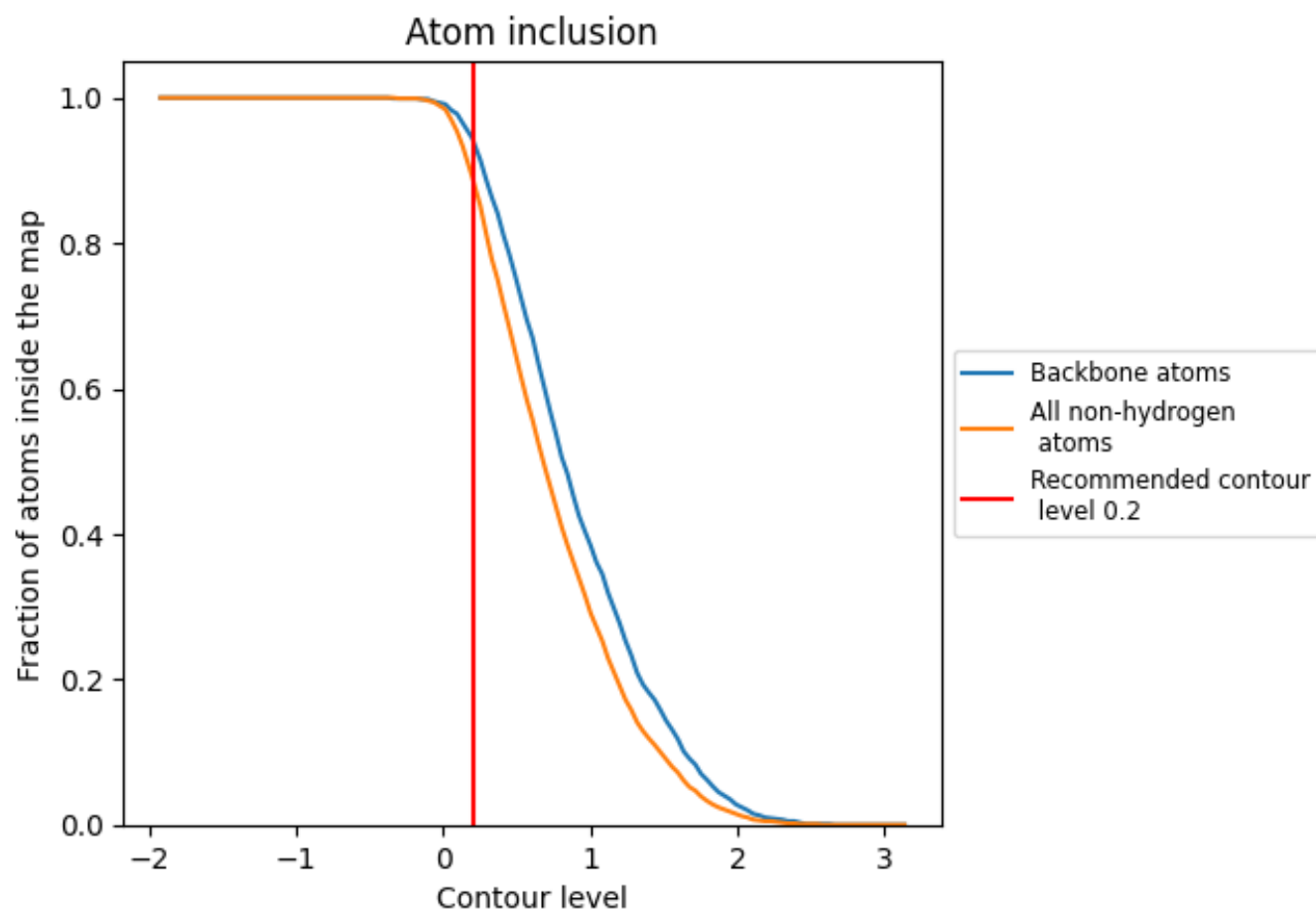
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8900	<div></div> 0.5440
A	<div></div> 0.9080	<div></div> 0.5510
B	<div></div> 0.7580	<div></div> 0.4880
C	<div></div> 0.9090	<div></div> 0.5530
D	<div></div> 0.7510	<div></div> 0.4850

