



## Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 07:50 PM JST

PDB ID : 9LW3 / pdb\_00009lw3  
EMDB ID : EMD-63427  
Title : TMEM164-substrate  
Authors : Zhang, M.F.  
Deposited on : 2025-02-13  
Resolution : 3.00 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:

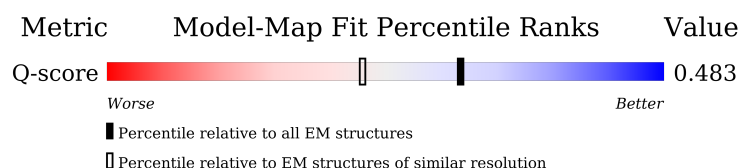
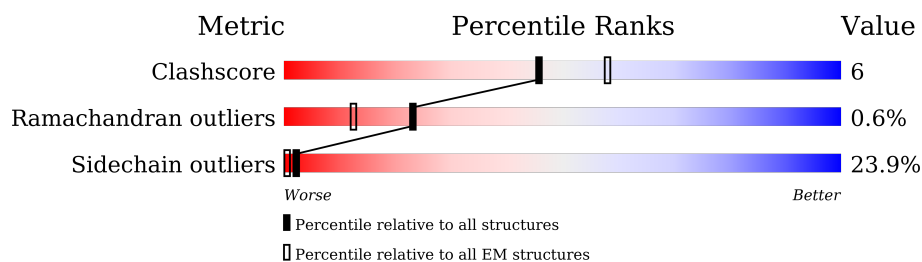
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.00 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	14081 ( 2.50 - 3.50 )

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	A	297	<div> <div style="width: 62%; background-color: green;"></div> <div style="width: 21%; background-color: yellow;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 4%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>62% 21% • 13%</div>
1	B	297	<div> <div style="width: 61%; background-color: green;"></div> <div style="width: 23%; background-color: yellow;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 4%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>61% 23% • 13%</div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEE	A	303	X	-	-	-
4	PEE	B	304	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4650 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.

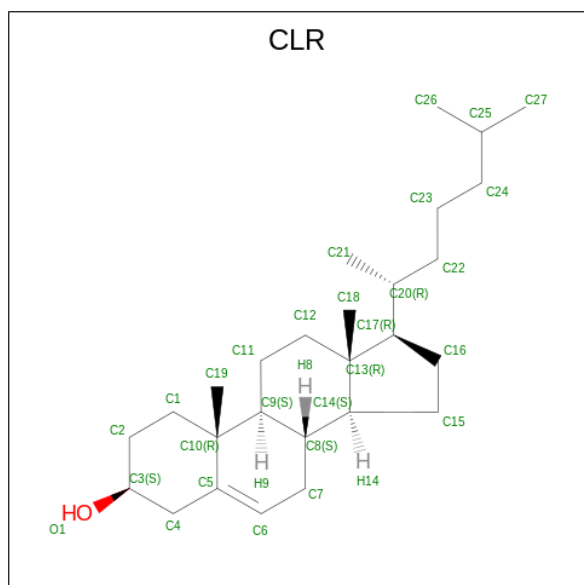
- Molecule 1 is a protein called Transmembrane protein 164.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	258	Total	C	N	O	S	0	0
			2052	1369	327	340	16		
1	B	258	Total	C	N	O	S	0	0
			2052	1369	327	340	16		

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

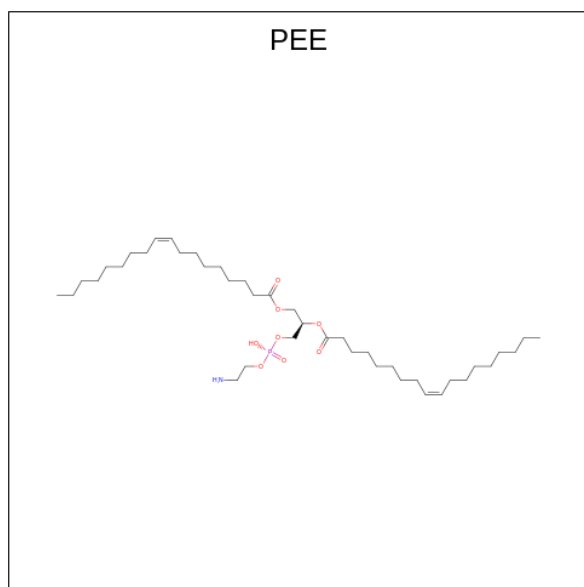
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O) (labeled as "Ligand of Interest" by depositor).



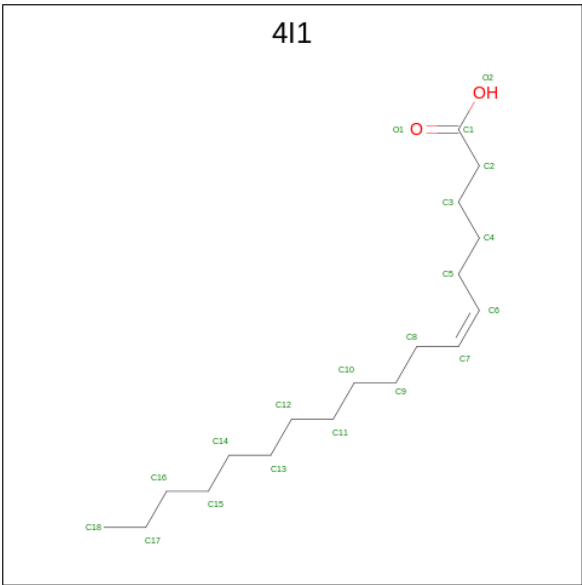
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	

- Molecule 4 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 5 is Petroselinic acid (CCD ID: 4I1) (formula:  $C_{18}H_{34}O_2$ ).



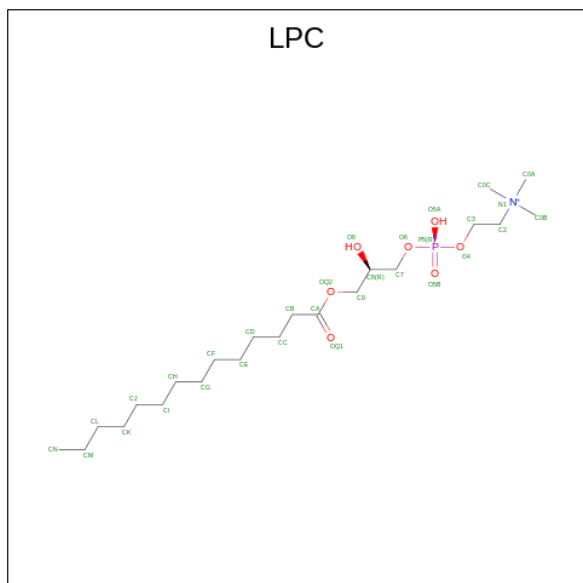
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			20	18	2	
5	A	1	Total	C	O	0
			20	18	2	
5	A	1	Total	C	O	0
			20	18	2	
5	A	1	Total	C	O	0
			20	18	2	
5	A	1	Total	C	O	0
			20	18	2	
5	A	1	Total	C	O	0
			20	18	2	
5	A	1	Total	C	O	0
			20	18	2	
5	B	1	Total	C	O	0
			20	18	2	
5	B	1	Total	C	O	0
			20	18	2	
5	B	1	Total	C	O	0
			20	18	2	
5	B	1	Total	C	O	0
			20	18	2	

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Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			20	18	2	
5	B	1	Total	C	O	0
			20	18	2	

- Molecule 6 is [1-MYRISTOYL-GLYCEROL-3-YL]PHOSPHONYLCHOLINE (CCD ID: LPC) (formula:  $C_{22}H_{47}NO_7P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	22	1	7	1	
6	B	1	Total	C	N	O	P	0
			31	22	1	7	1	

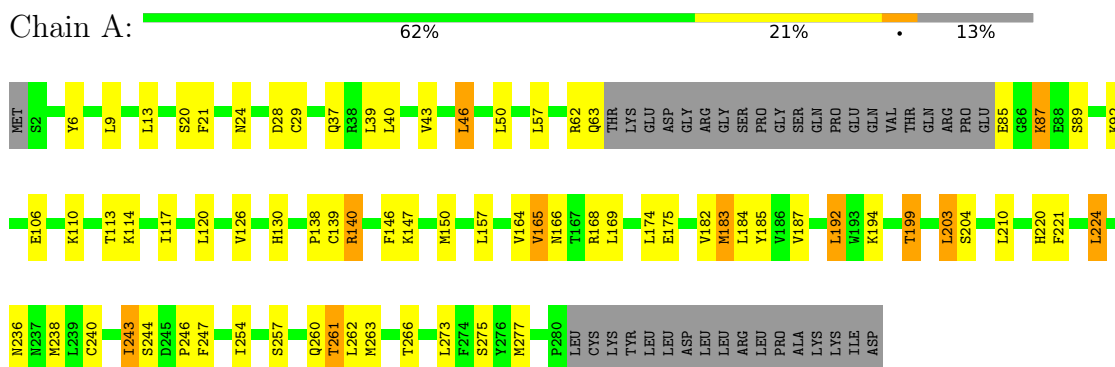
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	O	0
			2	2	
7	B	2	Total	O	0
			2	2	

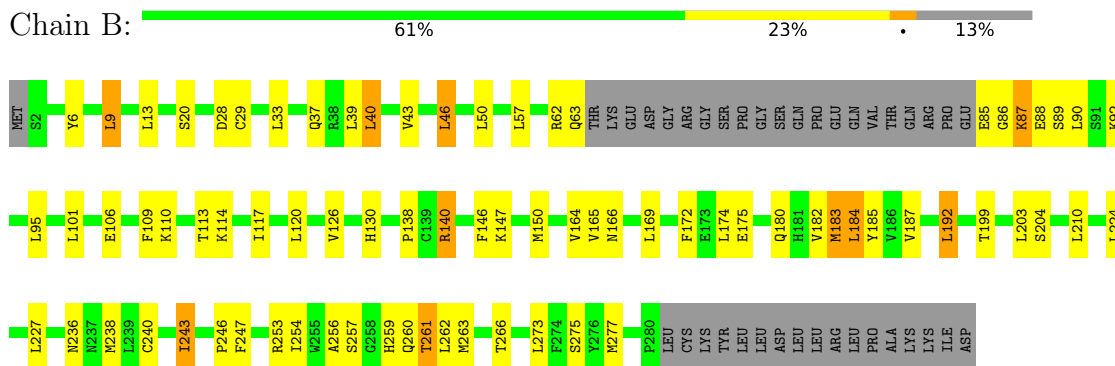
### 3 Residue-property plots

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

#### • Molecule 1: Transmembrane protein 164



#### • Molecule 1: Transmembrane protein 164





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.522	Depositor
Minimum map value	-0.289	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	291.84, 291.84, 291.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.57, 0.57, 0.57	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, 4I1, LPC, PEE, ZN

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	0.73	1/2112 (0.0%)	0.93	11/2879 (0.4%)
1	B	0.73	0/2112	0.91	11/2879 (0.4%)
All	All	0.73	1/4224 (0.0%)	0.92	22/5758 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	CYS	CA-C	-5.56	1.50	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	LEU	N-CA-C	-9.70	99.06	113.61
1	A	184	LEU	N-CA-C	-9.65	99.13	113.61
1	B	261	THR	N-CA-C	-9.48	100.03	111.69
1	A	261	THR	N-CA-C	-8.66	101.92	111.36
1	A	182	VAL	N-CA-C	-7.62	103.51	111.58
1	B	140	ARG	N-CA-C	-7.28	105.01	114.04
1	A	140	ARG	N-CA-C	-7.05	105.29	114.04
1	B	247	PHE	N-CA-C	-6.60	104.45	113.30
1	B	182	VAL	N-CA-C	-6.37	103.37	112.35
1	A	185	TYR	N-CA-C	-6.36	105.42	113.43
1	A	120	LEU	N-CA-C	-6.32	105.61	113.38
1	B	120	LEU	N-CA-C	-6.11	105.86	113.38
1	A	240	CYS	CA-C-N	-5.96	114.41	120.85
1	A	240	CYS	C-N-CA	-5.96	114.41	120.85
1	B	185	TYR	N-CA-C	-5.83	106.08	113.43
1	A	247	PHE	N-CA-C	-5.73	104.87	112.94
1	B	257	SER	N-CA-C	-5.69	105.16	111.36
1	B	240	CYS	CA-C-N	-5.65	114.78	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	CYS	C-N-CA	-5.65	114.78	120.31
1	A	199	THR	N-CA-C	-5.34	102.26	110.32
1	A	266	THR	N-CA-C	5.25	118.15	111.69
1	B	266	THR	N-CA-C	5.15	118.02	111.69

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	2052	0	2101	26	0
1	B	2052	0	2101	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	46	4	0
3	B	28	0	46	3	0
4	A	51	0	82	2	0
4	B	51	0	82	2	0
5	A	180	0	0	0	0
5	B	140	0	0	0	0
6	A	31	0	46	9	0
6	B	31	0	46	7	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
All	All	4650	0	4550	57	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (57) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLU:HG3	1:B:87:LYS:HA	1.59	0.85
1:A:246:PRO:HD3	6:A:312:LPC:HI1	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:VAL:HG12	1:A:168:ARG:HD2	1.65	0.78
1:B:109:PHE:CE2	1:B:172:PHE:O	2.36	0.77
1:B:260:GLN:HB2	6:B:301:LPC:H0A2	1.77	0.66
1:B:175:GLU:HA	4:B:304:PEE:H49	1.78	0.64
1:A:175:GLU:HA	4:A:303:PEE:H49	1.81	0.62
1:A:87:LYS:HA	1:B:85:GLU:HG3	1.83	0.60
1:B:246:PRO:HD3	6:B:301:LPC:HG1	1.86	0.58
1:A:221:PHE:HE1	6:A:312:LPC:H32	1.70	0.57
1:B:109:PHE:CZ	1:B:172:PHE:O	2.59	0.55
1:A:165:VAL:HG12	1:A:168:ARG:CD	2.35	0.53
1:B:256:ALA:HA	1:B:259:HIS:CD2	2.43	0.53
1:B:109:PHE:HE2	1:B:172:PHE:O	1.89	0.50
1:A:21:PHE:HB3	1:A:24:ASN:HB2	1.94	0.49
1:A:246:PRO:HD3	6:A:312:LPC:CI	2.40	0.49
6:B:301:LPC:HJ2	6:B:301:LPC:HM2	1.60	0.48
1:A:260:GLN:HB2	6:A:312:LPC:H0A1	1.96	0.47
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.64	0.47
1:A:243:ILE:H	1:A:243:ILE:HG13	1.24	0.47
6:A:312:LPC:HF2	6:A:312:LPC:HI2	1.48	0.47
1:A:130:HIS:HB3	1:A:187:VAL:HG11	1.97	0.46
1:A:165:VAL:HG12	1:A:168:ARG:CG	2.46	0.46
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.78	0.46
1:B:243:ILE:H	1:B:243:ILE:HG13	1.27	0.46
6:B:301:LPC:H0C3	6:B:301:LPC:H32	1.43	0.46
1:B:46:LEU:HD23	1:B:46:LEU:HA	1.78	0.45
1:A:221:PHE:CE1	6:A:312:LPC:H32	2.51	0.45
1:A:87:LYS:HB3	1:A:87:LYS:HE3	1.34	0.45
3:A:302:CLR:H183	3:A:302:CLR:H20	1.63	0.45
1:A:183:MET:HE3	1:A:183:MET:HB3	1.76	0.45
4:B:304:PEE:H65	4:B:304:PEE:H71	1.57	0.45
1:B:130:HIS:HB3	1:B:187:VAL:HG11	1.98	0.45
6:B:301:LPC:HD2	6:B:301:LPC:HG2	1.64	0.45
3:A:302:CLR:H21	3:A:302:CLR:H193	1.66	0.45
1:B:146:PHE:HZ	1:B:192:LEU:HG	1.81	0.44
6:B:301:LPC:HK1	6:B:301:LPC:HH1	1.60	0.44
1:B:57:LEU:HD23	1:B:57:LEU:HA	1.58	0.44
1:A:165:VAL:HA	1:A:168:ARG:HG3	2.00	0.44
1:B:9:LEU:HD12	1:B:9:LEU:HA	1.81	0.43
6:B:301:LPC:HI2	6:B:301:LPC:HF1	1.71	0.43
3:B:303:CLR:H21	3:B:303:CLR:H193	1.66	0.42
1:A:57:LEU:HD23	1:A:57:LEU:HA	1.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:MET:HB3	1:B:183:MET:HE3	1.71	0.42
1:A:257:SER:HA	6:A:312:LPC:H21	2.02	0.42
3:B:303:CLR:H231	3:B:303:CLR:H211	1.71	0.42
1:B:40:LEU:HD13	1:B:40:LEU:HA	1.84	0.42
1:A:165:VAL:HG12	1:A:168:ARG:HG3	2.02	0.42
3:B:303:CLR:H8	3:B:303:CLR:H182	1.81	0.41
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.82	0.41
3:A:302:CLR:H231	3:A:302:CLR:H211	1.71	0.41
1:A:146:PHE:HZ	1:A:192:LEU:HG	1.85	0.41
1:A:220:HIS:HA	1:A:224:LEU:HB2	2.03	0.41
4:A:303:PEE:H71	4:A:303:PEE:H65	1.57	0.40
6:A:312:LPC:HD2	6:A:312:LPC:HG1	1.49	0.40
1:A:260:GLN:CB	6:A:312:LPC:H0A1	2.52	0.40
3:A:302:CLR:H8	3:A:302:CLR:H182	1.81	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	254/297 (86%)	228 (90%)	25 (10%)	1 (0%)	30	65
1	B	254/297 (86%)	229 (90%)	23 (9%)	2 (1%)	16	50
All	All	508/594 (86%)	457 (90%)	48 (9%)	3 (1%)	23	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	PRO
1	B	86	GLY
1	B	138	PRO

### 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	224/259 (86%)	174 (78%)	50 (22%)	1	5
1	B	224/259 (86%)	167 (75%)	57 (25%)	0	3
All	All	448/518 (86%)	341 (76%)	107 (24%)	2	4

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	9	LEU
1	A	13	LEU
1	A	20	SER
1	A	28	ASP
1	A	29	CYS
1	A	37	GLN
1	A	39	LEU
1	A	40	LEU
1	A	43	VAL
1	A	46	LEU
1	A	50	LEU
1	A	62	ARG
1	A	63	GLN
1	A	87	LYS
1	A	89	SER
1	A	92	LYS
1	A	106	GLU
1	A	110	LYS
1	A	113	THR
1	A	114	LYS
1	A	117	ILE
1	A	126	VAL
1	A	140	ARG
1	A	147	LYS
1	A	150	MET
1	A	164	VAL

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Mol	Chain	Res	Type
1	A	165	VAL
1	A	166	ASN
1	A	169	LEU
1	A	174	LEU
1	A	183	MET
1	A	192	LEU
1	A	194	LYS
1	A	199	THR
1	A	203	LEU
1	A	204	SER
1	A	210	LEU
1	A	224	LEU
1	A	236	ASN
1	A	238	MET
1	A	243	ILE
1	A	244	SER
1	A	254	ILE
1	A	261	THR
1	A	262	LEU
1	A	263	MET
1	A	273	LEU
1	A	275	SER
1	A	277	MET
1	B	6	TYR
1	B	9	LEU
1	B	13	LEU
1	B	20	SER
1	B	28	ASP
1	B	29	CYS
1	B	33	LEU
1	B	37	GLN
1	B	39	LEU
1	B	40	LEU
1	B	43	VAL
1	B	46	LEU
1	B	50	LEU
1	B	62	ARG
1	B	63	GLN
1	B	87	LYS
1	B	88	GLU
1	B	89	SER
1	B	90	LEU

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Mol	Chain	Res	Type
1	B	92	LYS
1	B	95	LEU
1	B	101	LEU
1	B	106	GLU
1	B	110	LYS
1	B	113	THR
1	B	114	LYS
1	B	117	ILE
1	B	126	VAL
1	B	140	ARG
1	B	147	LYS
1	B	150	MET
1	B	164	VAL
1	B	165	VAL
1	B	166	ASN
1	B	169	LEU
1	B	174	LEU
1	B	180	GLN
1	B	183	MET
1	B	184	LEU
1	B	192	LEU
1	B	199	THR
1	B	203	LEU
1	B	204	SER
1	B	210	LEU
1	B	224	LEU
1	B	227	LEU
1	B	236	ASN
1	B	238	MET
1	B	243	ILE
1	B	253	ARG
1	B	254	ILE
1	B	261	THR
1	B	262	LEU
1	B	263	MET
1	B	273	LEU
1	B	275	SER
1	B	277	MET

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



Mol	Chain	Res	Type
1	A	7	GLN
1	A	124	HIS
1	B	7	GLN
1	B	154	ASN
1	B	225	GLN
1	B	236	ASN
1	B	259	HIS
1	B	260	GLN

### 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 ⓘ

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 for Mogul analysis.

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	4I1	A	304	-	19,19,19	1.32	2 (10%)	19,19,19	1.12	2 (10%)
5	4I1	A	313	-	19,19,19	1.33	2 (10%)	19,19,19	1.13	1 (5%)
3	CLR	B	303	-	31,31,31	0.74	0	48,48,48	5.33	16 (33%)
5	4I1	B	307	-	19,19,19	1.33	2 (10%)	19,19,19	1.06	0
3	CLR	A	302	-	31,31,31	0.74	0	48,48,48	5.33	16 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	4I1	A	306	-	19,19,19	1.33	2 (10%)	19,19,19	1.06	0
5	4I1	B	308	-	19,19,19	1.33	2 (10%)	19,19,19	5.47	4 (21%)
5	4I1	A	311	-	19,19,19	1.34	2 (10%)	19,19,19	1.12	1 (5%)
5	4I1	B	309	-	19,19,19	1.34	2 (10%)	19,19,19	1.21	2 (10%)
4	PEE	A	303	-	50,50,50	1.16	4 (8%)	53,55,55	1.14	3 (5%)
5	4I1	A	309	-	19,19,19	1.34	2 (10%)	19,19,19	1.21	2 (10%)
5	4I1	A	308	-	19,19,19	1.33	2 (10%)	19,19,19	5.47	4 (21%)
6	LPC	A	312	-	30,30,30	0.92	1 (3%)	35,37,37	0.81	1 (2%)
4	PEE	B	304	-	50,50,50	1.16	4 (8%)	53,55,55	1.14	3 (5%)
5	4I1	B	306	-	19,19,19	1.33	2 (10%)	19,19,19	1.05	0
5	4I1	A	307	-	19,19,19	1.33	2 (10%)	19,19,19	1.13	1 (5%)
5	4I1	B	305	-	19,19,19	1.32	2 (10%)	19,19,19	1.12	2 (10%)
5	4I1	B	311	-	19,19,19	1.34	2 (10%)	19,19,19	1.12	1 (5%)
5	4I1	B	310	-	19,19,19	1.33	2 (10%)	19,19,19	1.09	0
5	4I1	A	305	-	19,19,19	1.33	2 (10%)	19,19,19	1.05	0
6	LPC	B	301	-	30,30,30	0.94	1 (3%)	35,37,37	0.85	2 (5%)
5	4I1	A	310	-	19,19,19	1.33	2 (10%)	19,19,19	1.09	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	4I1	A	304	-	-	15/17/17/17	-
5	4I1	A	313	-	-	11/17/17/17	-
3	CLR	B	303	-	-	9/10/68/68	0/4/4/4
5	4I1	B	307	-	-	13/17/17/17	-
3	CLR	A	302	-	-	9/10/68/68	0/4/4/4
5	4I1	A	306	-	-	13/17/17/17	-
5	4I1	B	308	-	-	10/17/17/17	-
5	4I1	A	311	-	-	9/17/17/17	-
5	4I1	B	309	-	-	7/17/17/17	-
4	PEE	A	303	-	1/1/4/8	34/54/54/54	-
5	4I1	A	309	-	-	7/17/17/17	-
5	4I1	A	308	-	-	10/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LPC	A	312	-	-	25/32/32/32	-
4	PEE	B	304	-	1/1/4/8	34/54/54/54	-
5	4I1	B	306	-	-	11/17/17/17	-
5	4I1	A	307	-	-	11/17/17/17	-
5	4I1	B	305	-	-	15/17/17/17	-
5	4I1	B	311	-	-	9/17/17/17	-
5	4I1	B	310	-	-	11/17/17/17	-
5	4I1	A	305	-	-	11/17/17/17	-
6	LPC	B	301	-	-	20/32/32/32	-
5	4I1	A	310	-	-	11/17/17/17	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	311	4I1	O2-C1	4.51	1.45	1.30
5	B	311	4I1	O2-C1	4.51	1.45	1.30
5	A	309	4I1	O2-C1	4.50	1.45	1.30
5	B	309	4I1	O2-C1	4.50	1.45	1.30
5	A	307	4I1	O2-C1	4.48	1.45	1.30
5	A	313	4I1	O2-C1	4.48	1.45	1.30
5	A	305	4I1	O2-C1	4.45	1.45	1.30
5	B	306	4I1	O2-C1	4.45	1.45	1.30
5	A	310	4I1	O2-C1	4.45	1.45	1.30
5	B	310	4I1	O2-C1	4.45	1.45	1.30
5	A	308	4I1	O2-C1	4.45	1.45	1.30
5	B	308	4I1	O2-C1	4.45	1.45	1.30
5	A	306	4I1	O2-C1	4.44	1.45	1.30
5	B	307	4I1	O2-C1	4.44	1.45	1.30
5	A	304	4I1	O2-C1	4.42	1.45	1.30
5	B	305	4I1	O2-C1	4.42	1.45	1.30
6	B	301	LPC	OQ2-CA	4.28	1.45	1.33
6	A	312	LPC	OQ2-CA	4.19	1.45	1.33
4	A	303	PEE	O2-C10	4.12	1.45	1.34
4	B	304	PEE	O2-C10	4.12	1.45	1.34
4	A	303	PEE	O3-C30	4.10	1.45	1.33
4	B	304	PEE	O3-C30	4.10	1.45	1.33
5	A	309	4I1	C7-C6	3.63	1.52	1.31
5	B	309	4I1	C7-C6	3.63	1.52	1.31
5	A	311	4I1	C7-C6	3.62	1.52	1.31
5	B	311	4I1	C7-C6	3.62	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	306	4I1	C7-C6	3.61	1.52	1.31
5	B	307	4I1	C7-C6	3.61	1.52	1.31
5	A	308	4I1	C7-C6	3.60	1.52	1.31
5	B	308	4I1	C7-C6	3.60	1.52	1.31
5	A	305	4I1	C7-C6	3.59	1.52	1.31
5	B	306	4I1	C7-C6	3.59	1.52	1.31
4	A	303	PEE	C18-C19	3.59	1.52	1.31
4	B	304	PEE	C18-C19	3.59	1.52	1.31
5	A	307	4I1	C7-C6	3.59	1.52	1.31
5	A	313	4I1	C7-C6	3.59	1.52	1.31
4	A	303	PEE	C39-C38	3.59	1.52	1.31
4	B	304	PEE	C39-C38	3.59	1.52	1.31
5	A	304	4I1	C7-C6	3.58	1.52	1.31
5	B	305	4I1	C7-C6	3.58	1.52	1.31
5	A	310	4I1	C7-C6	3.58	1.52	1.31
5	B	310	4I1	C7-C6	3.58	1.52	1.31

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	CLR	C19-C10-C9	-24.50	82.47	111.68
3	B	303	CLR	C19-C10-C9	-24.50	82.47	111.68
5	A	308	4I1	O2-C1-O1	-17.66	79.29	123.30
5	B	308	4I1	O2-C1-O1	-17.66	79.29	123.30
3	A	302	CLR	C19-C10-C1	-17.28	82.13	109.43
3	B	303	CLR	C19-C10-C1	-17.28	82.13	109.43
3	A	302	CLR	C19-C10-C5	-11.89	89.10	108.34
3	B	303	CLR	C19-C10-C5	-11.89	89.10	108.34
5	A	308	4I1	O1-C1-C2	11.41	159.75	123.08
5	B	308	4I1	O1-C1-C2	11.41	159.75	123.08
3	A	302	CLR	C1-C10-C9	11.18	124.34	108.73
3	B	303	CLR	C1-C10-C9	11.18	124.34	108.73
5	A	308	4I1	O2-C1-C2	-10.45	80.46	114.03
5	B	308	4I1	O2-C1-C2	-10.45	80.46	114.03
3	A	302	CLR	C7-C8-C9	6.27	117.31	109.71
3	B	303	CLR	C7-C8-C9	6.27	117.31	109.71
3	A	302	CLR	C1-C10-C5	4.72	117.39	108.75
3	B	303	CLR	C1-C10-C5	4.72	117.39	108.75
3	A	302	CLR	C14-C8-C9	-4.54	103.01	109.09
3	B	303	CLR	C14-C8-C9	-4.54	103.01	109.09
4	A	303	PEE	O2-C10-C11	3.86	119.82	111.50
4	B	304	PEE	O2-C10-C11	3.86	119.82	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	CLR	C9-C10-C5	3.71	115.46	109.65
3	B	303	CLR	C9-C10-C5	3.71	115.46	109.65
3	A	302	CLR	C13-C17-C20	-3.60	113.86	119.49
3	B	303	CLR	C13-C17-C20	-3.60	113.86	119.49
3	A	302	CLR	C4-C5-C10	3.57	121.17	116.42
3	B	303	CLR	C4-C5-C10	3.57	121.17	116.42
3	A	302	CLR	C13-C14-C8	-3.56	109.11	114.38
3	B	303	CLR	C13-C14-C8	-3.56	109.11	114.38
3	A	302	CLR	C10-C5-C6	-3.18	118.03	122.90
3	B	303	CLR	C10-C5-C6	-3.18	118.03	122.90
3	A	302	CLR	C18-C13-C17	-3.05	106.02	111.71
3	B	303	CLR	C18-C13-C17	-3.05	106.02	111.71
3	A	302	CLR	C17-C13-C14	3.05	103.69	100.07
3	B	303	CLR	C17-C13-C14	3.05	103.69	100.07
5	A	309	4I1	C3-C2-C1	-2.92	107.10	114.47
5	B	309	4I1	C3-C2-C1	-2.92	107.10	114.47
4	A	303	PEE	O3-C30-C31	2.70	120.39	111.91
4	B	304	PEE	O3-C30-C31	2.70	120.39	111.91
3	A	302	CLR	C1-C2-C3	2.64	113.86	110.47
3	B	303	CLR	C1-C2-C3	2.64	113.86	110.47
6	B	301	LPC	OQ2-CA-CB	2.51	119.78	111.91
5	A	307	4I1	C3-C2-C1	-2.34	108.58	114.47
5	A	313	4I1	C3-C2-C1	-2.34	108.58	114.47
4	A	303	PEE	C2-O2-C10	-2.25	112.25	117.79
4	B	304	PEE	C2-O2-C10	-2.25	112.25	117.79
6	A	312	LPC	OQ2-CA-CB	2.19	118.79	111.91
5	A	308	4I1	C3-C2-C1	-2.17	109.01	114.47
5	B	308	4I1	C3-C2-C1	-2.17	109.01	114.47
5	A	311	4I1	O2-C1-C2	2.10	120.79	114.03
5	B	311	4I1	O2-C1-C2	2.10	120.79	114.03
5	A	304	4I1	C3-C2-C1	-2.10	109.17	114.47
5	B	305	4I1	C3-C2-C1	-2.10	109.17	114.47
5	A	309	4I1	C5-C6-C7	-2.07	108.87	124.73
5	B	309	4I1	C5-C6-C7	-2.07	108.87	124.73
3	A	302	CLR	C11-C9-C8	-2.05	108.80	111.75
3	B	303	CLR	C11-C9-C8	-2.05	108.80	111.75
6	B	301	LPC	OQ2-CA-OQ1	-2.04	118.45	123.59
5	A	304	4I1	O2-C1-C2	2.02	120.53	114.03
5	B	305	4I1	O2-C1-C2	2.02	120.53	114.03

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	303	PEE	C2
4	B	304	PEE	C2

All (305) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	PEE	C1-O3P-P-O1P
4	A	303	PEE	C4-O4P-P-O3P
4	A	303	PEE	C4-O4P-P-O2P
4	A	303	PEE	C4-O4P-P-O1P
4	A	303	PEE	O4P-C4-C5-N
4	B	304	PEE	C1-O3P-P-O1P
4	B	304	PEE	C4-O4P-P-O3P
4	B	304	PEE	C4-O4P-P-O2P
4	B	304	PEE	C4-O4P-P-O1P
4	B	304	PEE	O4P-C4-C5-N
5	A	308	4I1	C3-C4-C5-C6
5	A	308	4I1	C7-C8-C9-C10
5	B	308	4I1	C3-C4-C5-C6
5	B	308	4I1	C7-C8-C9-C10
6	A	312	LPC	N1-C2-C3-O4
6	A	312	LPC	C3-O4-P5-O5B
6	A	312	LPC	C7-O6-P5-O5B
6	A	312	LPC	OQ1-CA-OQ2-C9
6	A	312	LPC	CB-CA-OQ2-C9
6	B	301	LPC	N1-C2-C3-O4
6	B	301	LPC	C3-O4-P5-O5A
6	B	301	LPC	O6-C7-C8-O8
6	B	301	LPC	O6-C7-C8-C9
3	A	302	CLR	C16-C17-C20-C21
3	B	303	CLR	C16-C17-C20-C21
3	A	302	CLR	C13-C17-C20-C21
3	B	303	CLR	C13-C17-C20-C21
4	A	303	PEE	C31-C30-O3-C3
4	B	304	PEE	C31-C30-O3-C3
6	B	301	LPC	CB-CA-OQ2-C9
3	A	302	CLR	C13-C17-C20-C22
3	B	303	CLR	C13-C17-C20-C22
4	A	303	PEE	C37-C38-C39-C40
4	B	304	PEE	C37-C38-C39-C40
4	A	303	PEE	O5-C30-O3-C3
4	B	304	PEE	O5-C30-O3-C3
3	A	302	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
3	B	303	CLR	C16-C17-C20-C22
4	A	303	PEE	C43-C44-C45-C46
4	B	304	PEE	C43-C44-C45-C46
5	A	309	4I1	C11-C12-C13-C14
5	B	309	4I1	C11-C12-C13-C14
5	A	306	4I1	C7-C8-C9-C10
5	B	307	4I1	C7-C8-C9-C10
5	A	310	4I1	C2-C3-C4-C5
5	B	310	4I1	C2-C3-C4-C5
6	B	301	LPC	CB-CC-CD-CE
5	A	308	4I1	C9-C10-C11-C12
5	B	308	4I1	C9-C10-C11-C12
6	B	301	LPC	CF-CG-CH-CI
6	A	312	LPC	O6-C7-C8-C9
6	B	301	LPC	CA-CB-CC-CD
6	B	301	LPC	OQ1-CA-OQ2-C9
4	A	303	PEE	C23-C24-C25-C26
4	A	303	PEE	C41-C42-C43-C44
4	B	304	PEE	C23-C24-C25-C26
4	B	304	PEE	C41-C42-C43-C44
4	A	303	PEE	O2-C2-C3-O3
4	B	304	PEE	O2-C2-C3-O3
5	A	307	4I1	C11-C10-C9-C8
5	A	313	4I1	C11-C10-C9-C8
6	B	301	LPC	CD-CE-CF-CG
5	A	307	4I1	C1-C2-C3-C4
5	A	313	4I1	C1-C2-C3-C4
6	A	312	LPC	CF-CG-CH-CI
4	A	303	PEE	C17-C18-C19-C20
4	B	304	PEE	C17-C18-C19-C20
5	A	310	4I1	C1-C2-C3-C4
5	B	310	4I1	C1-C2-C3-C4
6	A	312	LPC	CA-CB-CC-CD
5	A	305	4I1	C12-C13-C14-C15
5	B	306	4I1	C12-C13-C14-C15
5	A	309	4I1	C9-C10-C11-C12
5	B	309	4I1	C9-C10-C11-C12
6	A	312	LPC	C3-C2-N1-C0B
5	A	306	4I1	C12-C13-C14-C15
5	B	307	4I1	C12-C13-C14-C15
6	B	301	LPC	CJ-CK-CL-CM
6	B	301	LPC	CH-CI-CJ-CK

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Mol	Chain	Res	Type	Atoms
5	A	304	4I1	C5-C6-C7-C8
5	B	305	4I1	C5-C6-C7-C8
6	A	312	LPC	C7-O6-P5-O4
6	B	301	LPC	C3-O4-P5-O6
6	A	312	LPC	CD-CE-CF-CG
5	A	306	4I1	C1-C2-C3-C4
5	B	307	4I1	C1-C2-C3-C4
3	A	302	CLR	C21-C20-C22-C23
3	B	303	CLR	C21-C20-C22-C23
4	A	303	PEE	C34-C35-C36-C37
4	B	304	PEE	C34-C35-C36-C37
5	A	305	4I1	C13-C14-C15-C16
5	B	306	4I1	C13-C14-C15-C16
6	A	312	LPC	CH-CI-CJ-CK
5	A	304	4I1	C11-C10-C9-C8
5	A	306	4I1	C9-C10-C11-C12
5	B	305	4I1	C11-C10-C9-C8
5	B	307	4I1	C9-C10-C11-C12
6	A	312	LPC	CI-CJ-CK-CL
5	A	305	4I1	C5-C6-C7-C8
5	B	306	4I1	C5-C6-C7-C8
6	A	312	LPC	O6-C7-C8-O8
5	A	304	4I1	C12-C13-C14-C15
5	B	305	4I1	C12-C13-C14-C15
5	A	304	4I1	C2-C3-C4-C5
5	A	306	4I1	C10-C11-C12-C13
5	A	306	4I1	C14-C15-C16-C17
5	A	309	4I1	C2-C3-C4-C5
5	B	305	4I1	C2-C3-C4-C5
5	B	307	4I1	C10-C11-C12-C13
5	B	307	4I1	C14-C15-C16-C17
5	B	309	4I1	C2-C3-C4-C5
5	A	311	4I1	C9-C10-C11-C12
5	B	311	4I1	C9-C10-C11-C12
6	A	312	LPC	CG-CH-CI-CJ
4	A	303	PEE	C15-C16-C17-C18
4	A	303	PEE	C39-C40-C41-C42
4	B	304	PEE	C15-C16-C17-C18
4	B	304	PEE	C39-C40-C41-C42
5	A	307	4I1	C2-C3-C4-C5
5	A	311	4I1	C11-C12-C13-C14
5	A	313	4I1	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	B	311	4I1	C11-C12-C13-C14
6	B	301	LPC	CI-CJ-CK-CL
6	A	312	LPC	C3-C2-N1-C0C
5	A	311	4I1	C14-C15-C16-C17
5	B	311	4I1	C14-C15-C16-C17
5	A	310	4I1	C9-C10-C11-C12
5	B	310	4I1	C9-C10-C11-C12
5	A	311	4I1	C5-C6-C7-C8
5	B	311	4I1	C5-C6-C7-C8
4	A	303	PEE	C32-C33-C34-C35
4	B	304	PEE	C32-C33-C34-C35
5	A	309	4I1	C13-C14-C15-C16
5	B	309	4I1	C13-C14-C15-C16
5	A	310	4I1	C14-C15-C16-C17
5	B	310	4I1	C14-C15-C16-C17
4	A	303	PEE	C31-C32-C33-C34
4	B	304	PEE	C31-C32-C33-C34
5	A	307	4I1	C11-C12-C13-C14
5	A	313	4I1	C11-C12-C13-C14
5	A	307	4I1	C10-C11-C12-C13
5	A	313	4I1	C10-C11-C12-C13
5	A	305	4I1	C10-C11-C12-C13
5	B	306	4I1	C10-C11-C12-C13
6	A	312	LPC	C3-C2-N1-C0A
5	A	310	4I1	C11-C12-C13-C14
5	B	310	4I1	C11-C12-C13-C14
5	A	305	4I1	C9-C10-C11-C12
5	A	308	4I1	C12-C13-C14-C15
5	B	306	4I1	C9-C10-C11-C12
5	B	308	4I1	C12-C13-C14-C15
4	A	303	PEE	C1-O3P-P-O4P
4	B	304	PEE	C1-O3P-P-O4P
6	A	312	LPC	C3-O4-P5-O6
4	A	303	PEE	C33-C34-C35-C36
4	B	304	PEE	C33-C34-C35-C36
5	A	308	4I1	C1-C2-C3-C4
5	B	308	4I1	C1-C2-C3-C4
4	A	303	PEE	C14-C15-C16-C17
4	B	304	PEE	C14-C15-C16-C17
6	A	312	LPC	CJ-CK-CL-CM
5	A	306	4I1	C3-C4-C5-C6
5	A	311	4I1	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	B	307	4I1	C3-C4-C5-C6
5	B	311	4I1	C3-C4-C5-C6
4	A	303	PEE	C13-C14-C15-C16
4	B	304	PEE	C13-C14-C15-C16
5	A	304	4I1	C11-C12-C13-C14
5	A	308	4I1	C14-C15-C16-C17
5	B	305	4I1	C11-C12-C13-C14
5	B	308	4I1	C14-C15-C16-C17
3	A	302	CLR	C23-C24-C25-C27
3	B	303	CLR	C23-C24-C25-C27
4	A	303	PEE	C1-C2-C3-O3
4	B	304	PEE	C1-C2-C3-O3
5	A	310	4I1	C12-C13-C14-C15
5	B	310	4I1	C12-C13-C14-C15
5	A	304	4I1	C15-C16-C17-C18
5	B	305	4I1	C15-C16-C17-C18
5	A	307	4I1	C6-C7-C8-C9
5	A	313	4I1	C6-C7-C8-C9
5	A	306	4I1	C11-C10-C9-C8
5	A	311	4I1	C13-C14-C15-C16
5	B	307	4I1	C11-C10-C9-C8
5	B	311	4I1	C13-C14-C15-C16
5	A	306	4I1	C5-C6-C7-C8
5	B	307	4I1	C5-C6-C7-C8
6	B	301	LPC	C3-C2-N1-C0C
5	A	304	4I1	C6-C7-C8-C9
5	B	305	4I1	C6-C7-C8-C9
4	A	303	PEE	C11-C10-O2-C2
4	B	304	PEE	C11-C10-O2-C2
6	B	301	LPC	CC-CD-CE-CF
5	A	307	4I1	C9-C10-C11-C12
5	A	313	4I1	C9-C10-C11-C12
4	A	303	PEE	C21-C22-C23-C24
4	B	304	PEE	C21-C22-C23-C24
6	A	312	LPC	CK-CL-CM-CN
4	A	303	PEE	C19-C20-C21-C22
4	B	304	PEE	C19-C20-C21-C22
5	A	310	4I1	C11-C10-C9-C8
5	B	310	4I1	C11-C10-C9-C8
4	A	303	PEE	O4-C10-O2-C2
4	B	304	PEE	O4-C10-O2-C2
3	A	302	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	B	303	CLR	C20-C22-C23-C24
5	A	310	4I1	C13-C14-C15-C16
5	B	310	4I1	C13-C14-C15-C16
6	B	301	LPC	C3-C2-N1-C0B
3	A	302	CLR	C23-C24-C25-C26
3	B	303	CLR	C23-C24-C25-C26
4	A	303	PEE	C44-C45-C46-C47
4	B	304	PEE	C44-C45-C46-C47
5	A	308	4I1	C11-C12-C13-C14
5	B	308	4I1	C11-C12-C13-C14
5	A	311	4I1	C6-C7-C8-C9
5	B	311	4I1	C6-C7-C8-C9
5	A	304	4I1	C9-C10-C11-C12
5	B	305	4I1	C9-C10-C11-C12
6	A	312	LPC	CB-CC-CD-CE
5	A	305	4I1	C3-C4-C5-C6
5	B	306	4I1	C3-C4-C5-C6
5	A	305	4I1	C6-C7-C8-C9
5	B	306	4I1	C6-C7-C8-C9
5	A	307	4I1	C14-C15-C16-C17
5	A	313	4I1	C14-C15-C16-C17
4	A	303	PEE	C1-O3P-P-O2P
4	B	304	PEE	C1-O3P-P-O2P
6	A	312	LPC	C3-O4-P5-O5A
6	A	312	LPC	C7-O6-P5-O5A
6	B	301	LPC	C3-O4-P5-O5B
5	A	307	4I1	C13-C14-C15-C16
5	A	313	4I1	C13-C14-C15-C16
5	A	309	4I1	C15-C16-C17-C18
5	B	309	4I1	C15-C16-C17-C18
4	A	303	PEE	C11-C12-C13-C14
4	B	304	PEE	C11-C12-C13-C14
4	A	303	PEE	O2-C10-C11-C12
4	B	304	PEE	O2-C10-C11-C12
5	A	311	4I1	C12-C13-C14-C15
5	B	311	4I1	C12-C13-C14-C15
6	B	301	LPC	C3-C2-N1-C0A
5	A	304	4I1	C10-C11-C12-C13
5	B	305	4I1	C10-C11-C12-C13
5	A	308	4I1	C13-C14-C15-C16
5	B	308	4I1	C13-C14-C15-C16
5	A	304	4I1	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	B	305	4I1	C4-C5-C6-C7
5	A	305	4I1	O1-C1-C2-C3
5	B	306	4I1	O1-C1-C2-C3
5	A	307	4I1	C15-C16-C17-C18
5	A	313	4I1	C15-C16-C17-C18
5	A	306	4I1	C2-C3-C4-C5
5	B	307	4I1	C2-C3-C4-C5
5	A	306	4I1	C15-C16-C17-C18
5	B	307	4I1	C15-C16-C17-C18
4	A	303	PEE	O3P-C1-C2-C3
4	B	304	PEE	O3P-C1-C2-C3
3	A	302	CLR	C22-C23-C24-C25
3	B	303	CLR	C22-C23-C24-C25
5	A	305	4I1	O2-C1-C2-C3
5	B	306	4I1	O2-C1-C2-C3
5	A	304	4I1	C14-C15-C16-C17
5	B	305	4I1	C14-C15-C16-C17
5	A	304	4I1	C13-C14-C15-C16
5	B	305	4I1	C13-C14-C15-C16
4	A	303	PEE	C20-C21-C22-C23
4	B	304	PEE	C20-C21-C22-C23
5	A	311	4I1	C1-C2-C3-C4
5	B	311	4I1	C1-C2-C3-C4
5	A	308	4I1	C4-C5-C6-C7
5	B	308	4I1	C4-C5-C6-C7
5	A	304	4I1	O2-C1-C2-C3
5	B	305	4I1	O2-C1-C2-C3
5	A	310	4I1	C15-C16-C17-C18
5	B	310	4I1	C15-C16-C17-C18
5	A	308	4I1	C6-C7-C8-C9
5	B	308	4I1	C6-C7-C8-C9
5	A	304	4I1	O1-C1-C2-C3
5	B	305	4I1	O1-C1-C2-C3
5	A	304	4I1	C7-C8-C9-C10
5	B	305	4I1	C7-C8-C9-C10
6	A	312	LPC	CE-CF-CG-CH
5	A	305	4I1	C1-C2-C3-C4
5	B	306	4I1	C1-C2-C3-C4
5	A	307	4I1	C4-C5-C6-C7
5	A	313	4I1	C4-C5-C6-C7
6	A	312	LPC	CC-CD-CE-CF
5	A	305	4I1	C2-C3-C4-C5

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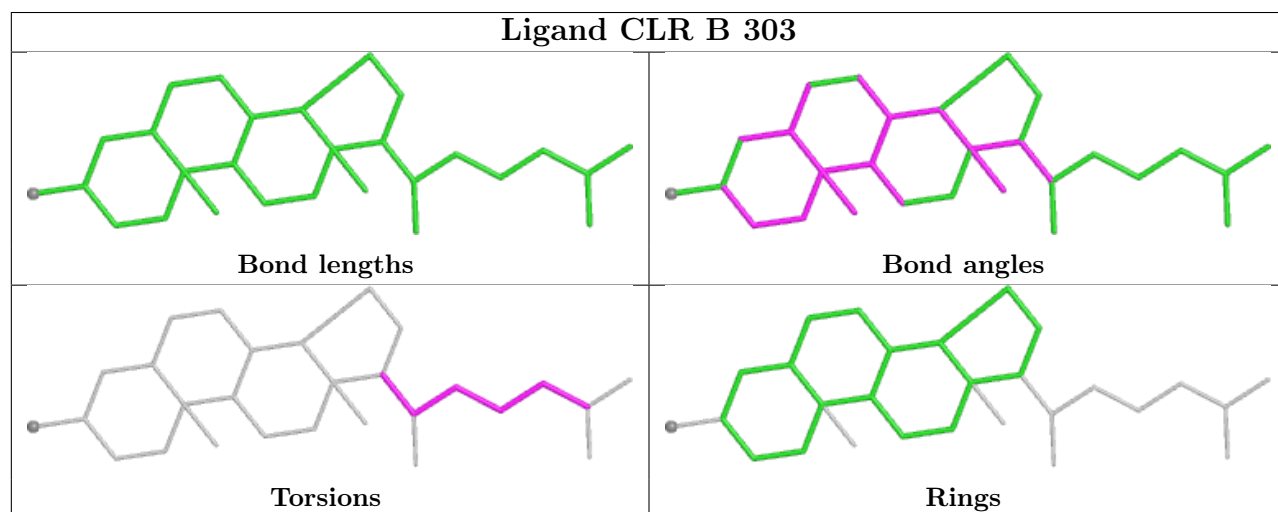
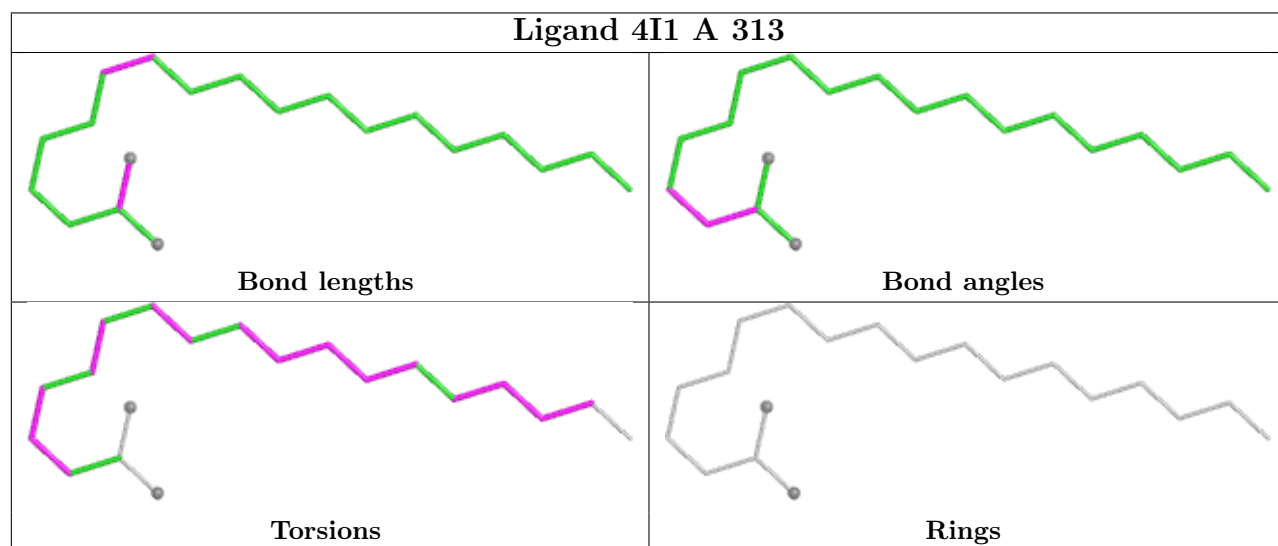
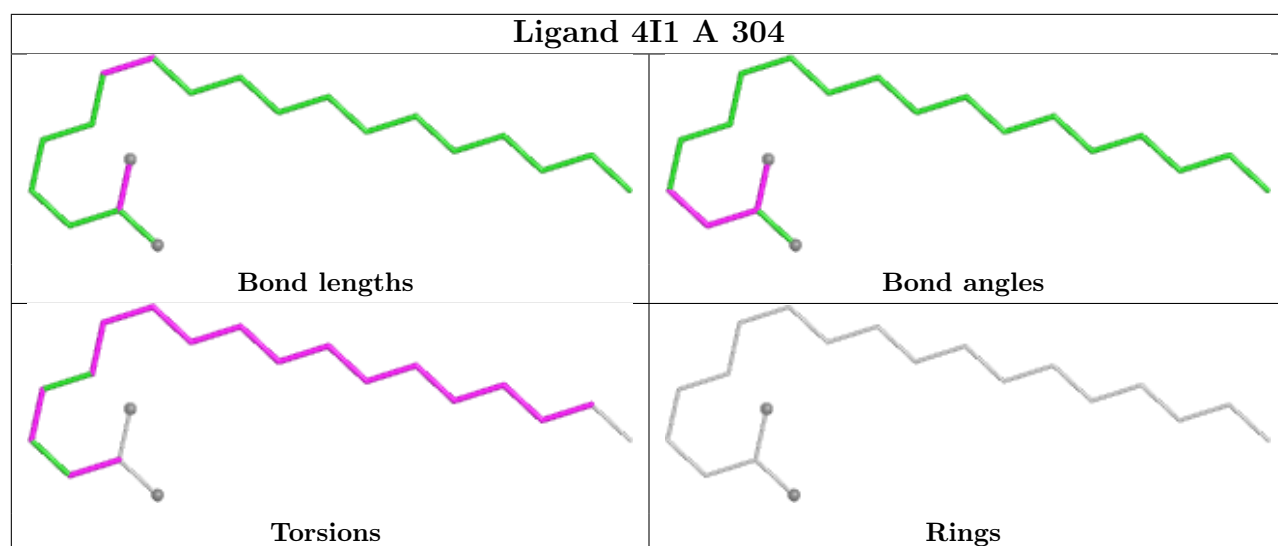
Mol	Chain	Res	Type	Atoms
5	B	306	4I1	C2-C3-C4-C5
5	A	309	4I1	O2-C1-C2-C3
5	B	309	4I1	O2-C1-C2-C3
5	A	310	4I1	O2-C1-C2-C3
5	B	310	4I1	O2-C1-C2-C3
6	B	301	LPC	C2-C3-O4-P5
4	A	303	PEE	C10-C11-C12-C13
4	B	304	PEE	C10-C11-C12-C13
5	A	310	4I1	O1-C1-C2-C3
5	B	310	4I1	O1-C1-C2-C3
5	A	306	4I1	O2-C1-C2-C3
5	B	307	4I1	O2-C1-C2-C3
5	A	306	4I1	C4-C5-C6-C7
5	B	307	4I1	C4-C5-C6-C7
5	A	309	4I1	O1-C1-C2-C3
5	B	309	4I1	O1-C1-C2-C3

There are no ring outliers.

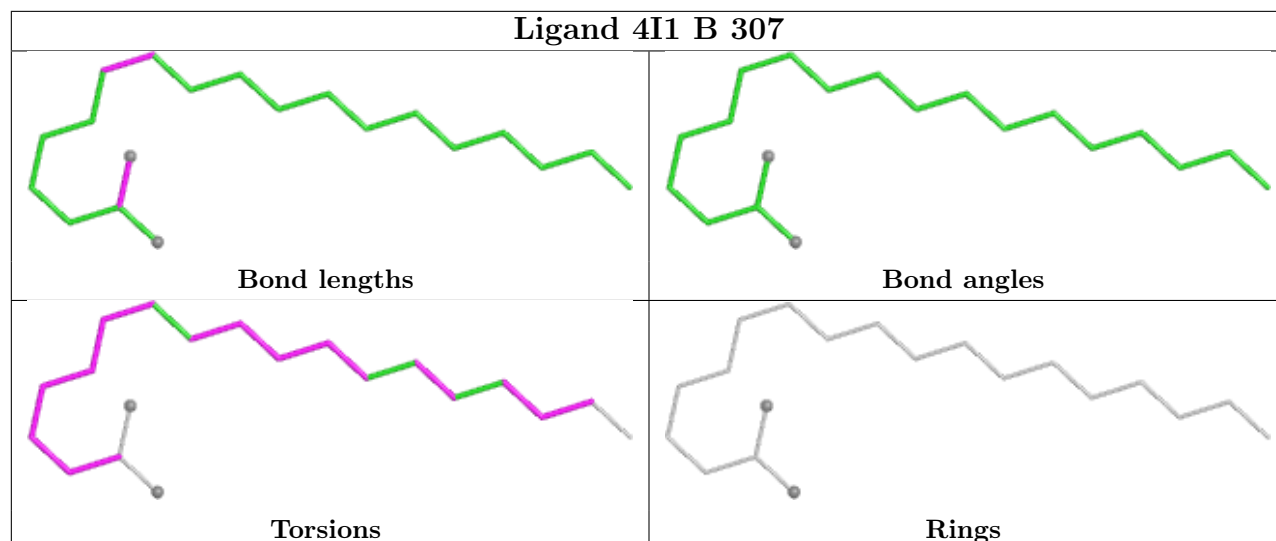
6 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	CLR	3	0
3	A	302	CLR	4	0
4	A	303	PEE	2	0
6	A	312	LPC	9	0
4	B	304	PEE	2	0
6	B	301	LPC	7	0

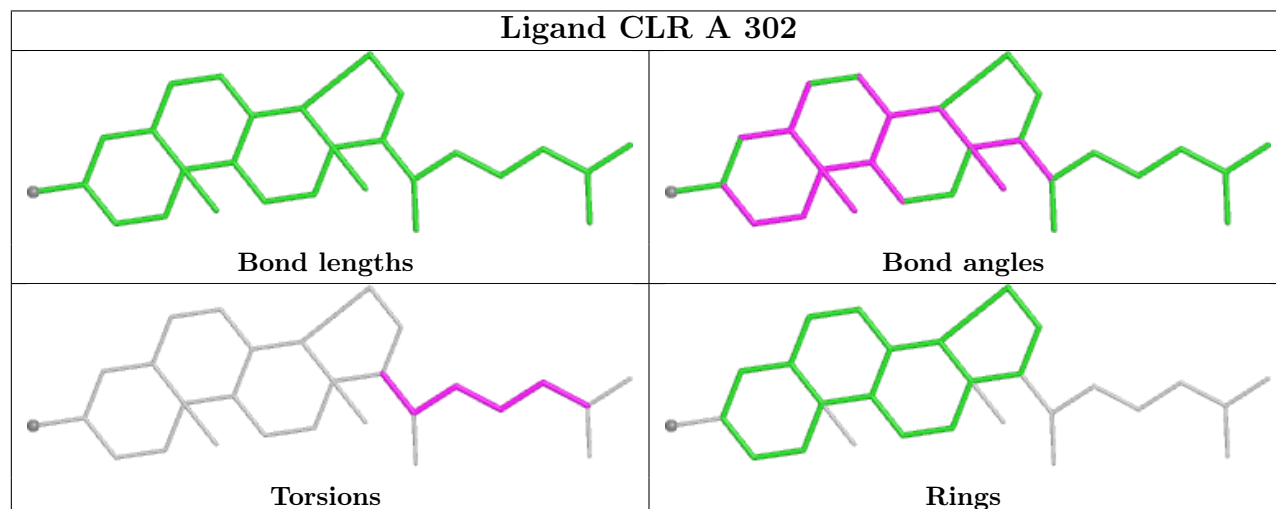
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



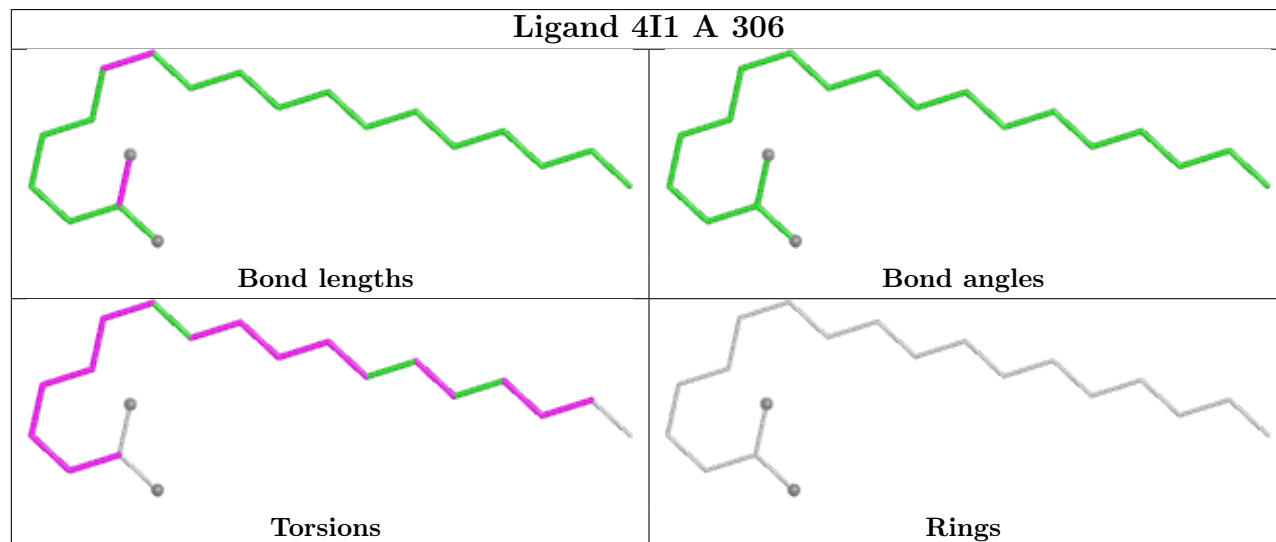
## Ligand 4I1 B 307

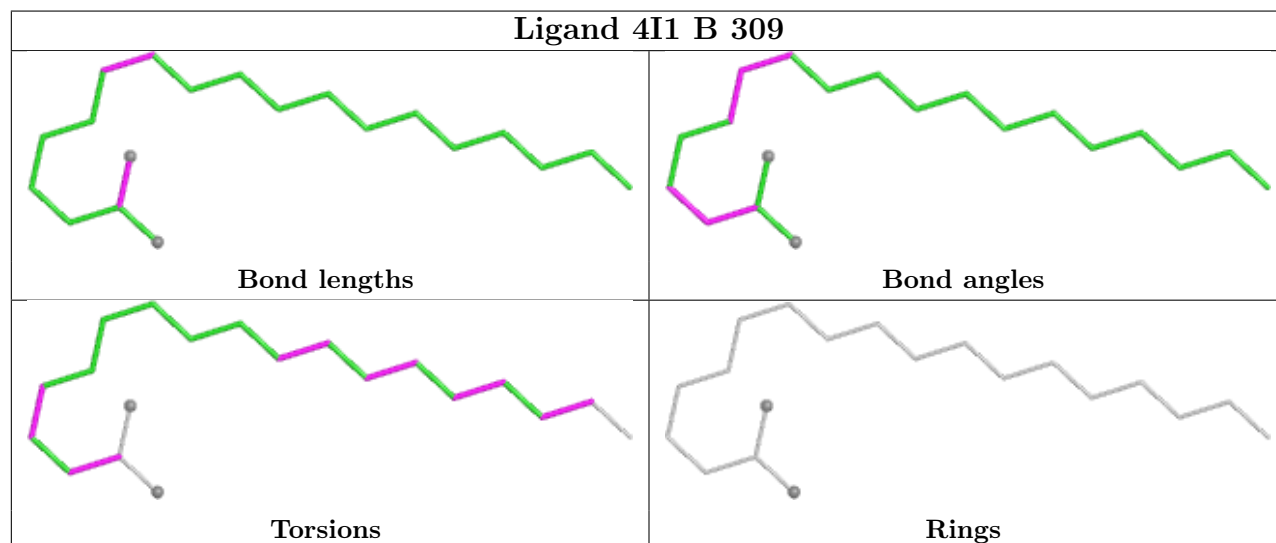
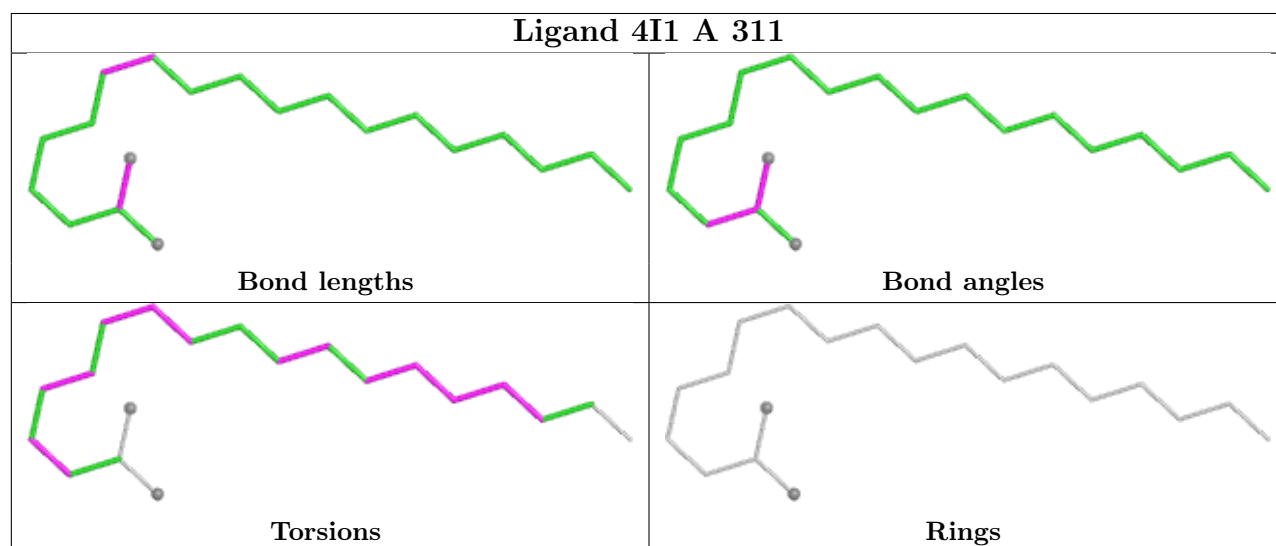
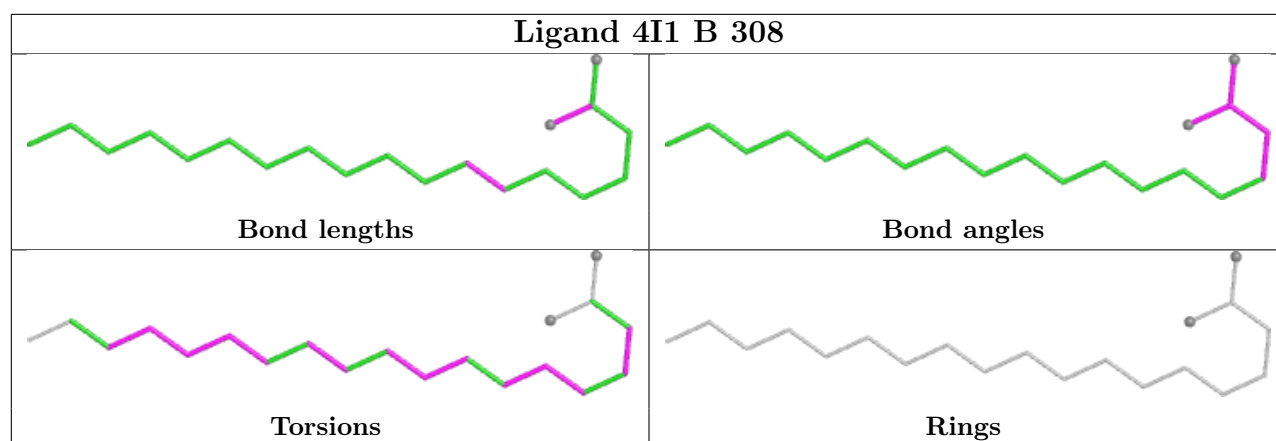


## Ligand CLR A 302

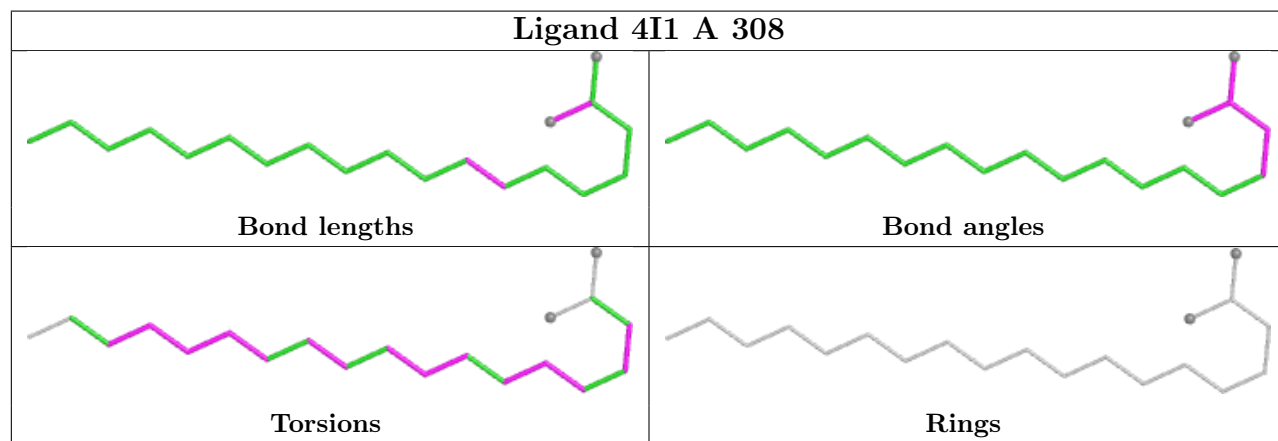
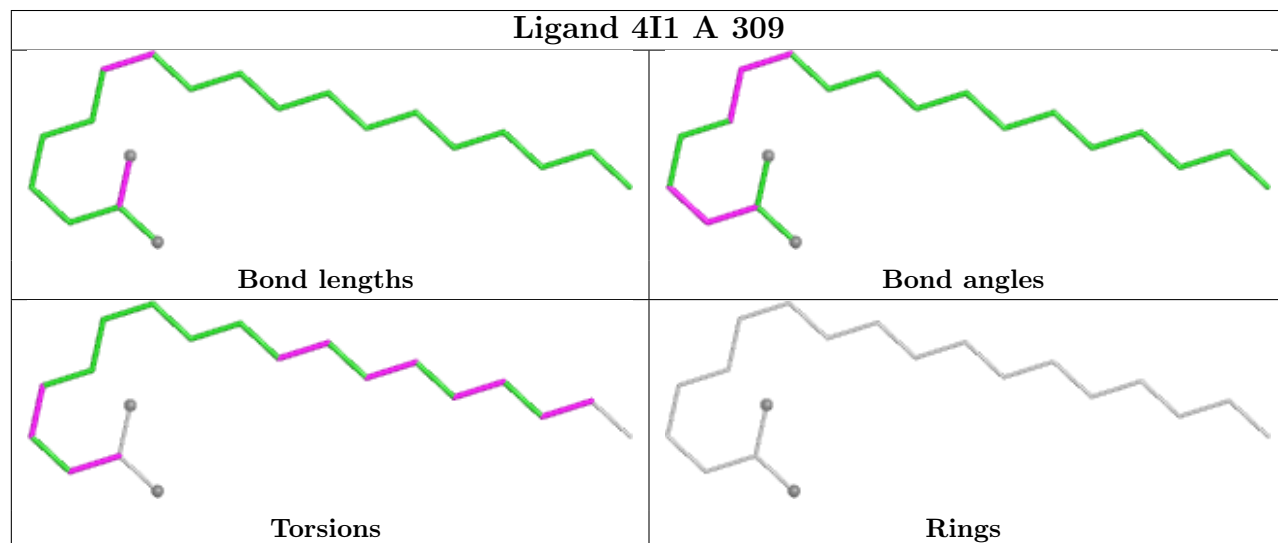
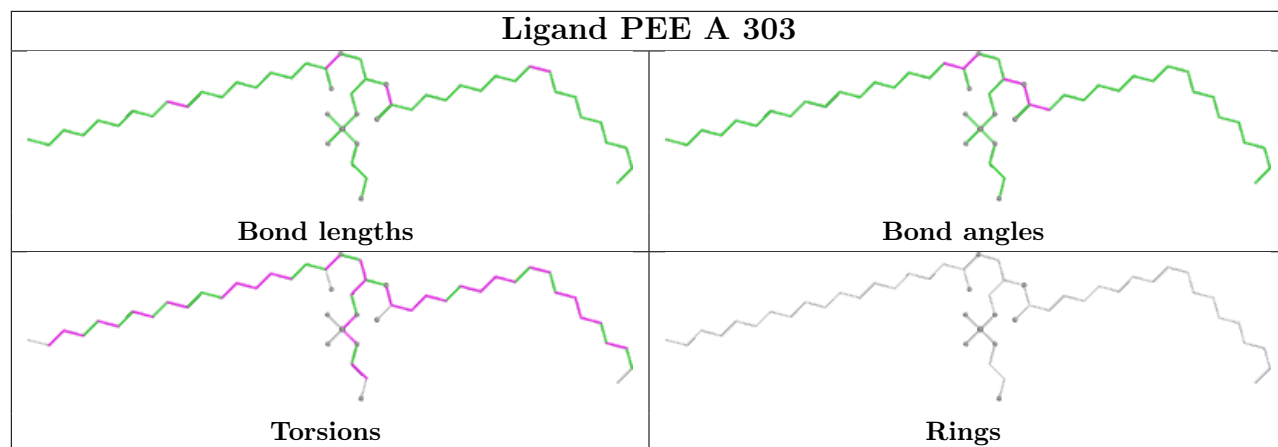


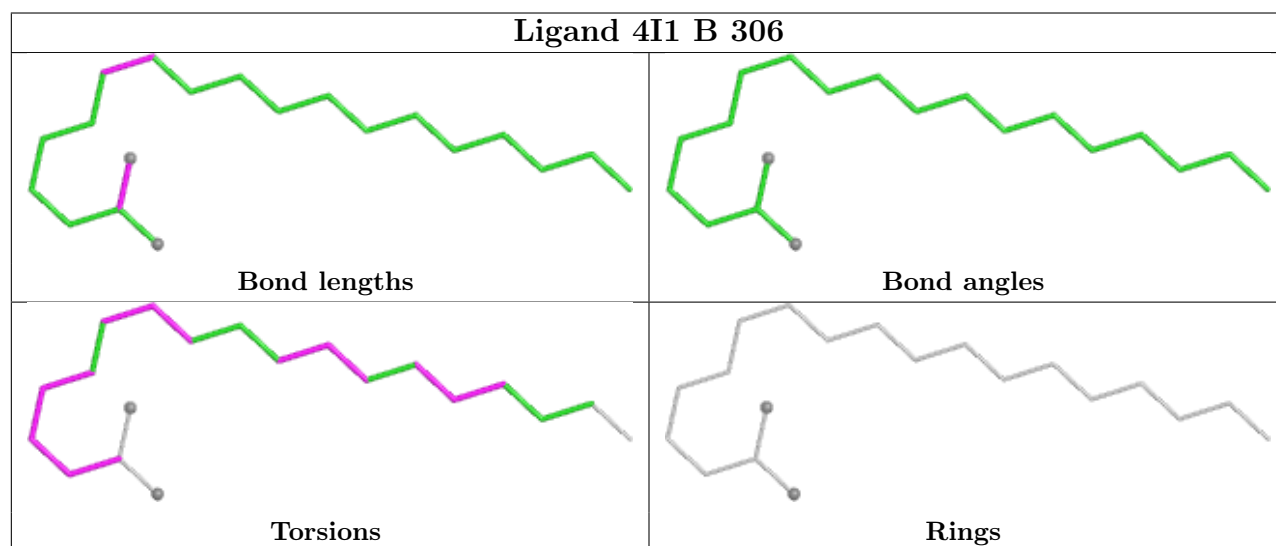
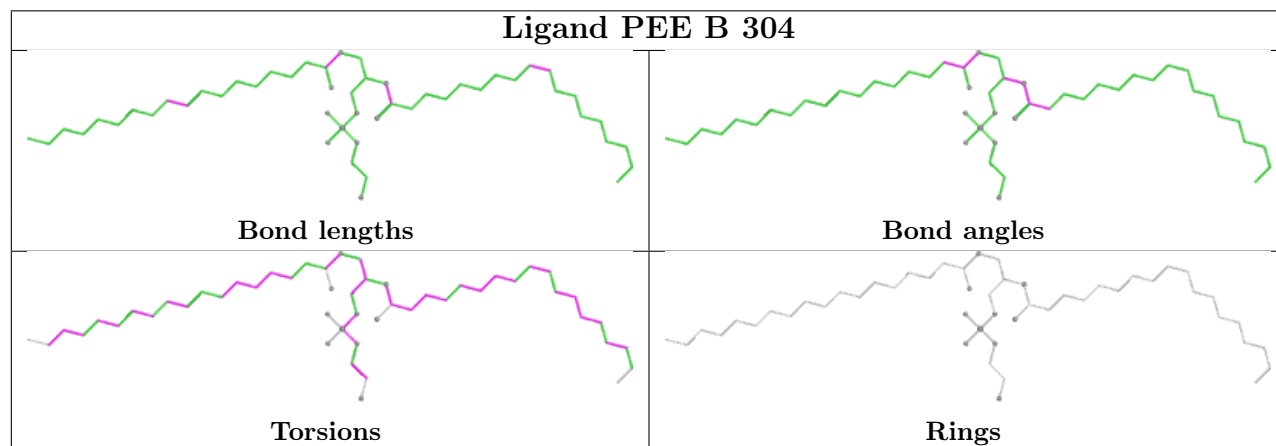
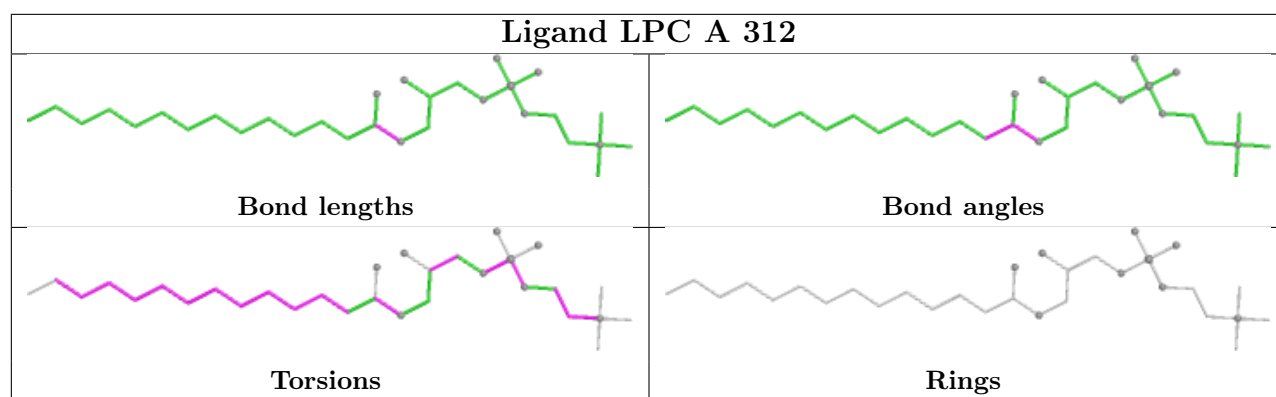
## Ligand 4I1 A 306

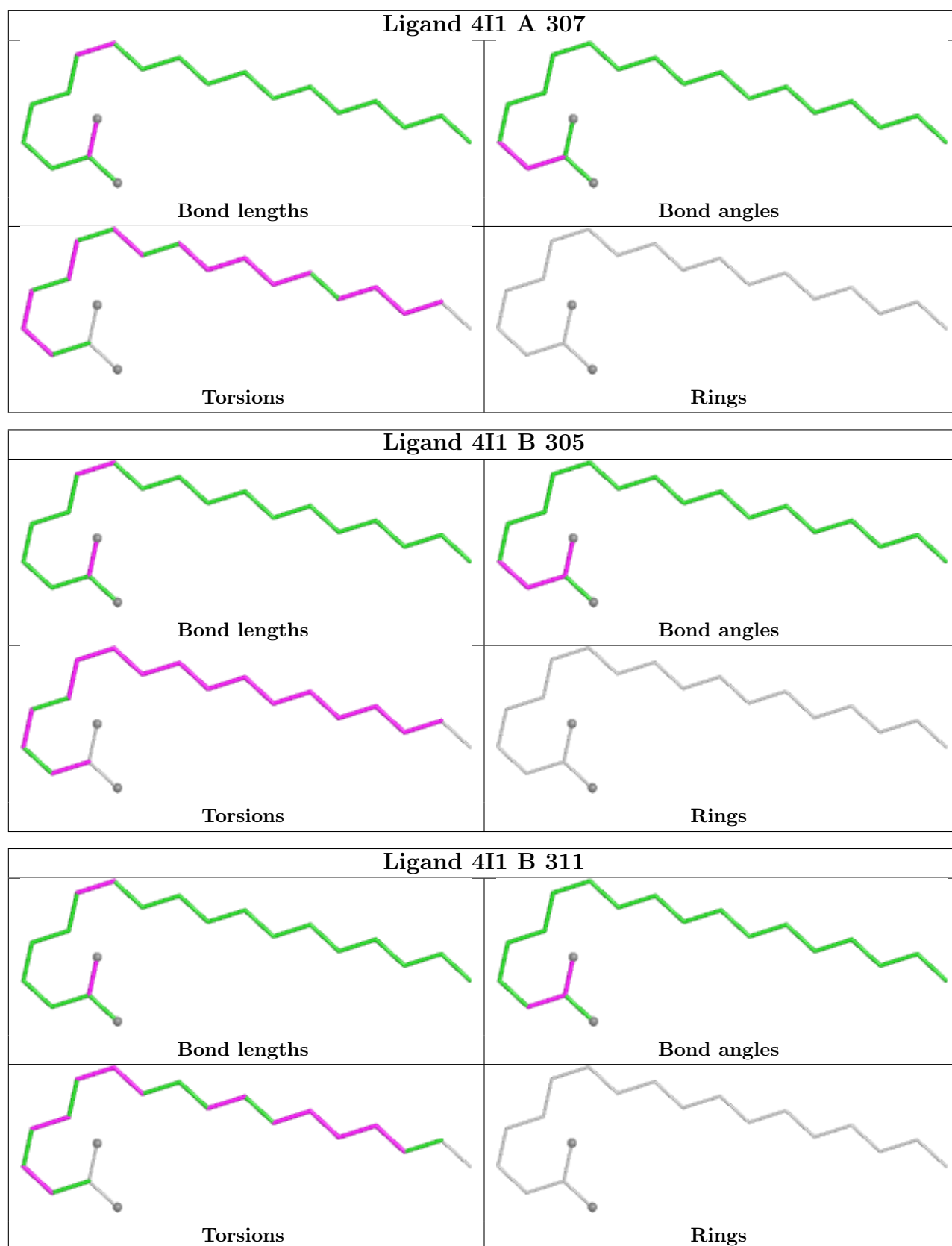


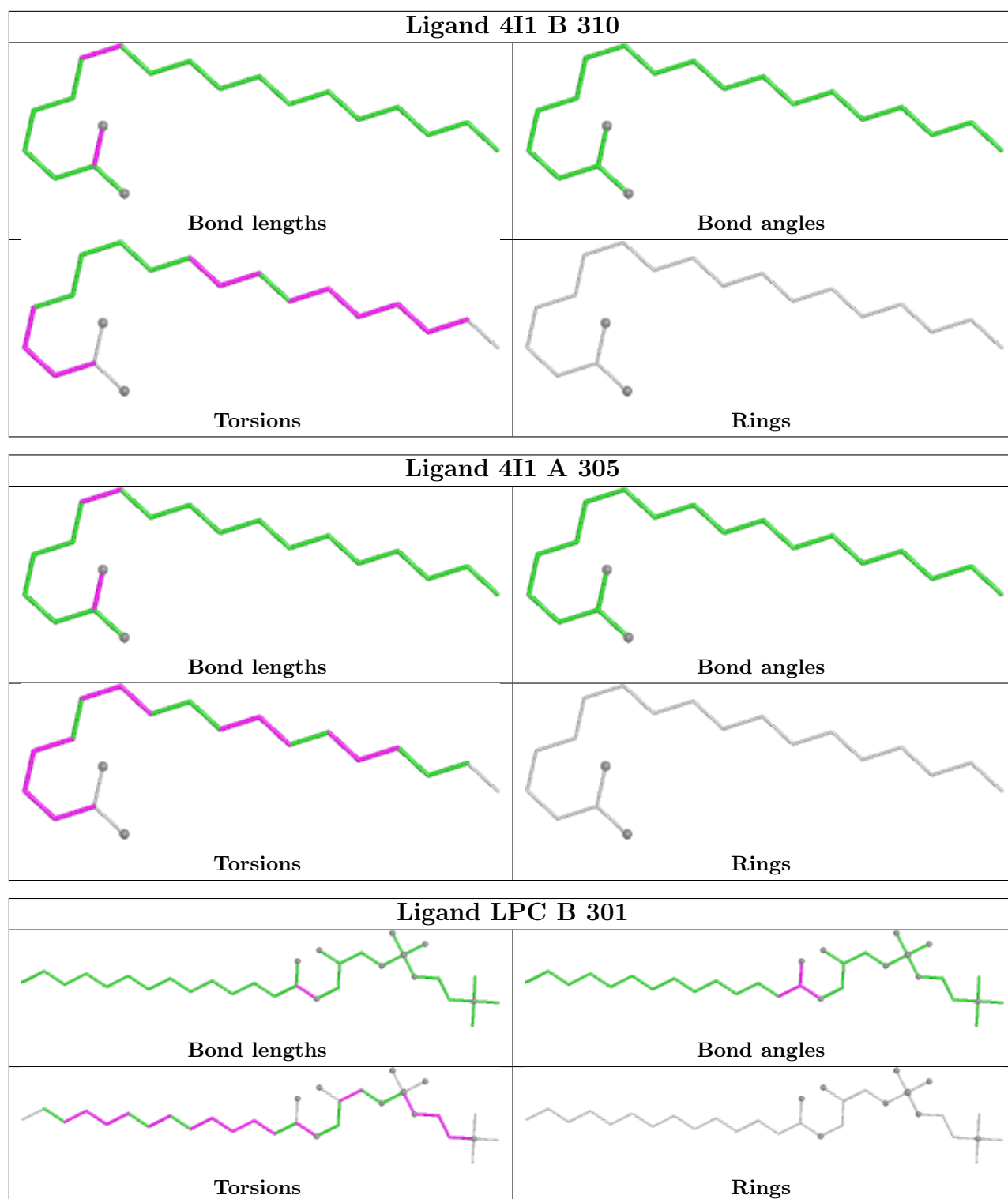


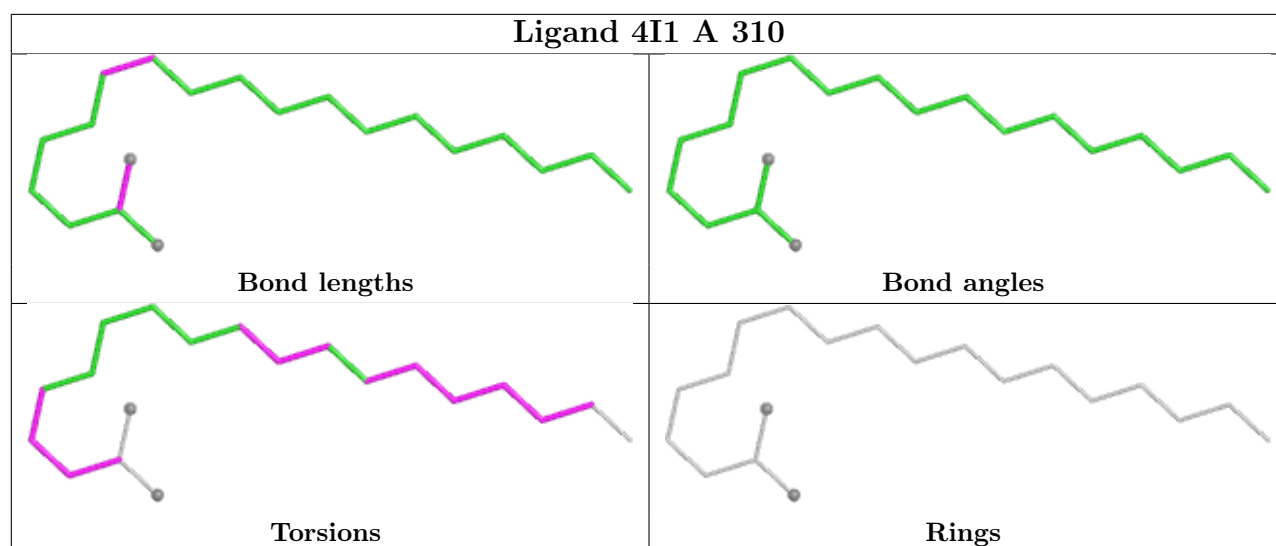












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

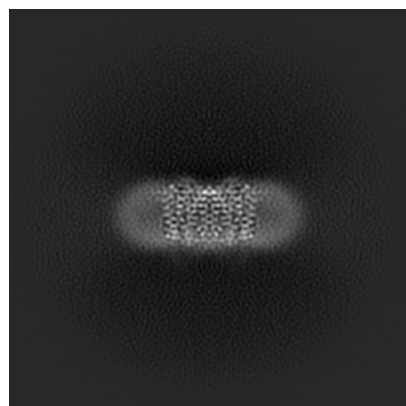
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63427. These allow visual inspection of the internal detail of the map and identification of artifacts.

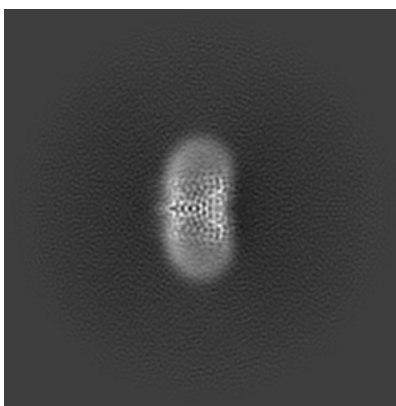
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

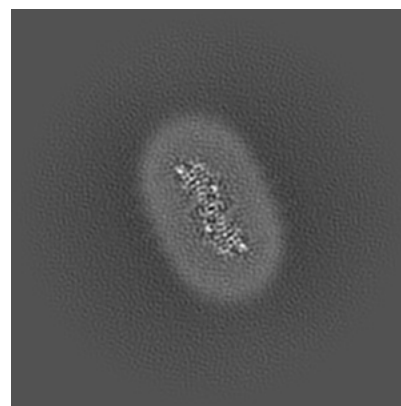
#### 6.1.1 Primary map



X

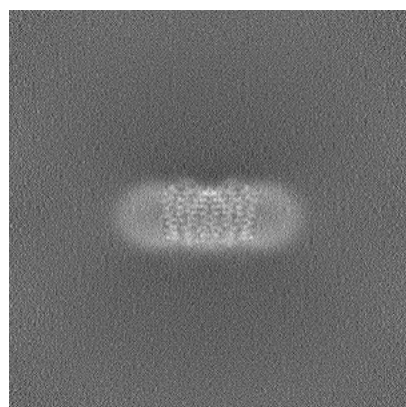


Y

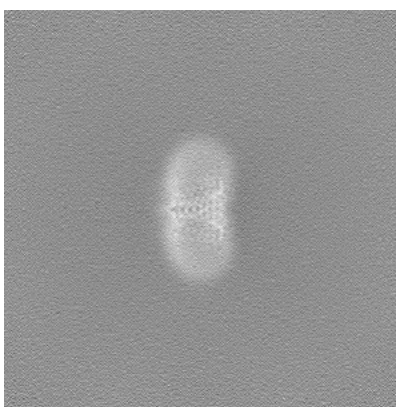


Z

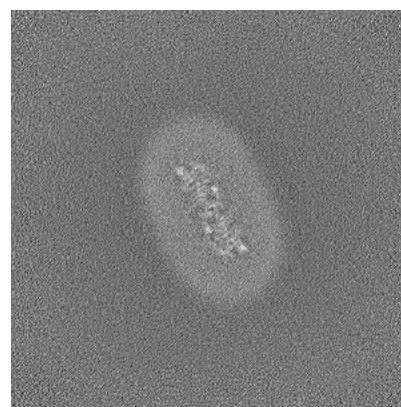
#### 6.1.2 Raw map



X



Y

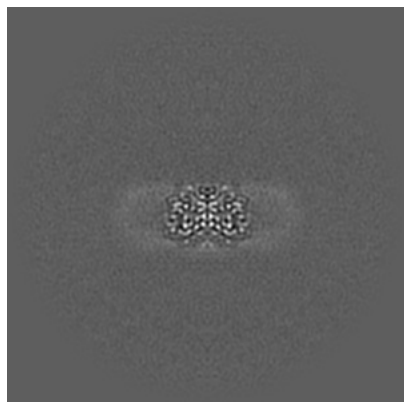


Z

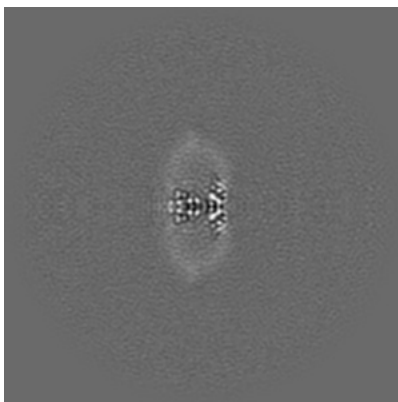
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

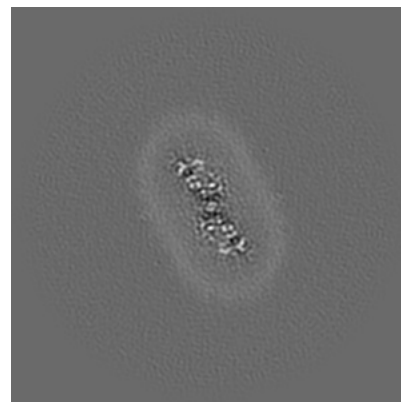
### 6.2.1 Primary map



X Index: 256

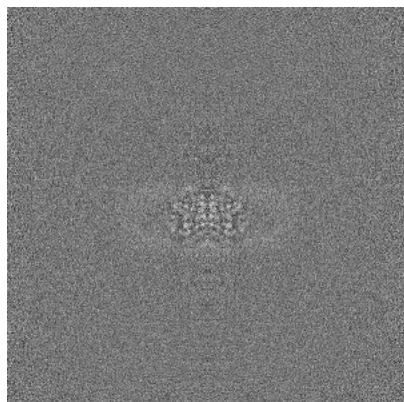


Y Index: 256

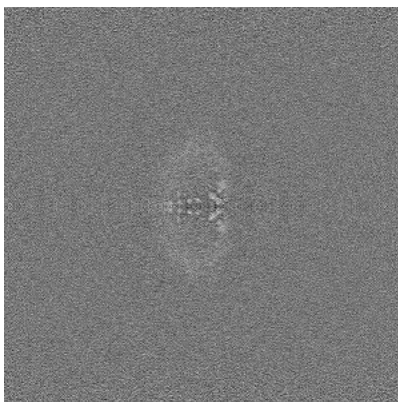


Z Index: 256

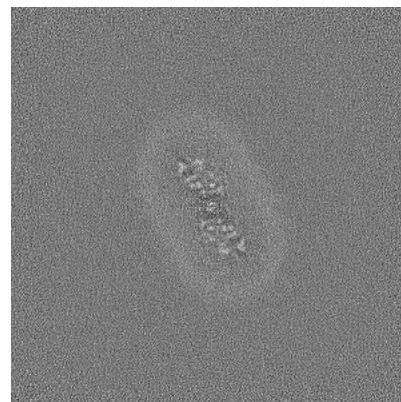
### 6.2.2 Raw map



X Index: 256



Y Index: 256



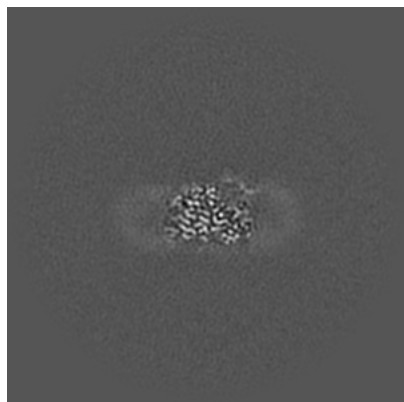
Z Index: 256

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

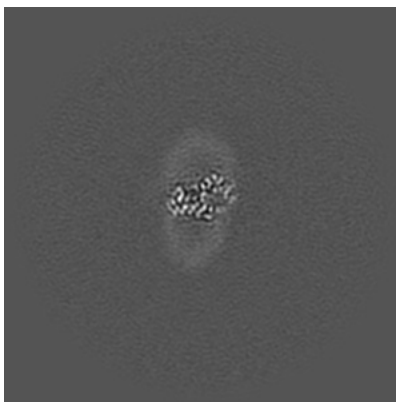


## 6.3 Largest variance slices [i](#)

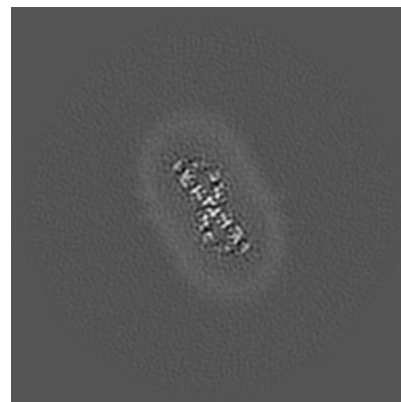
### 6.3.1 Primary map



X Index: 249

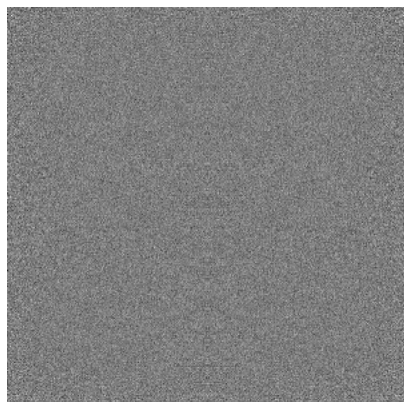


Y Index: 228

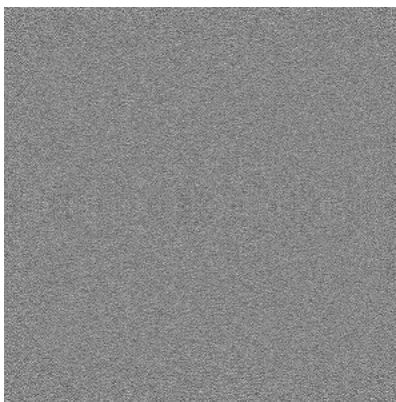


Z Index: 260

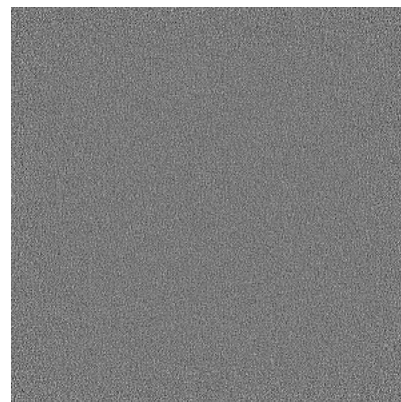
### 6.3.2 Raw map



X Index: 0



Y Index: 0



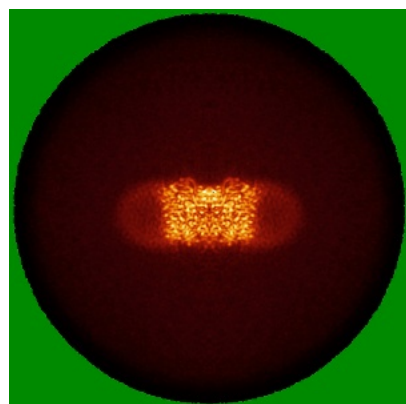
Z Index: 0

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

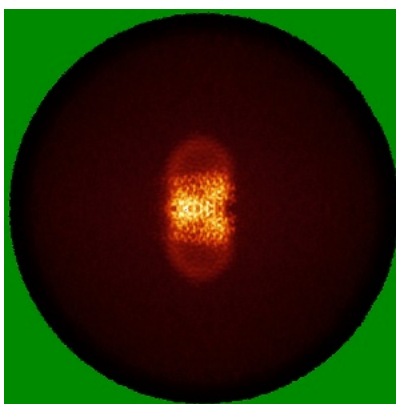


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

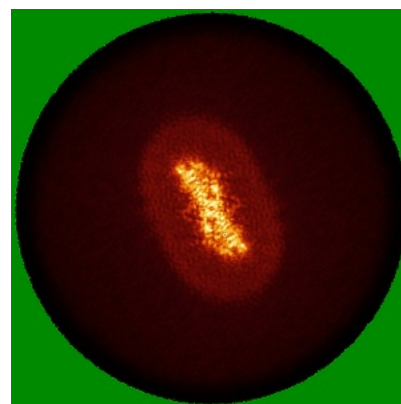
### 6.4.1 Primary map



X

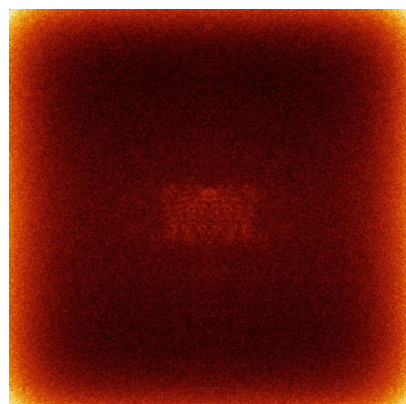


Y

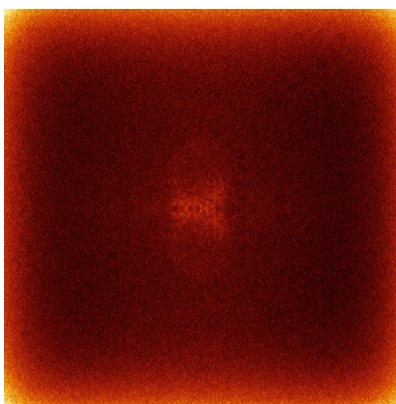


Z

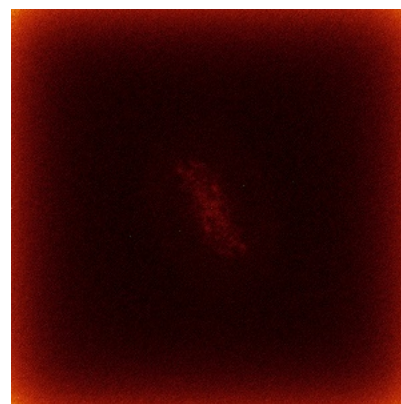
### 6.4.2 Raw map



X



Y

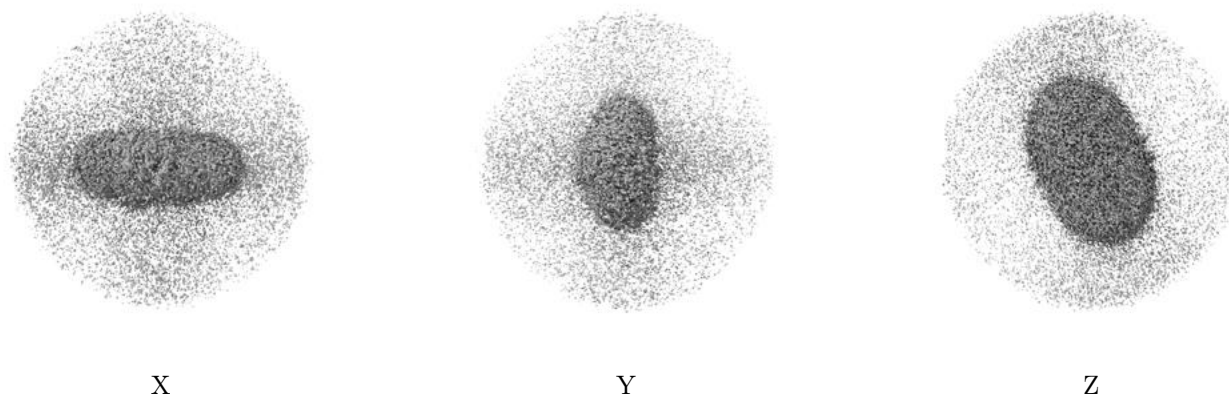


Z

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.

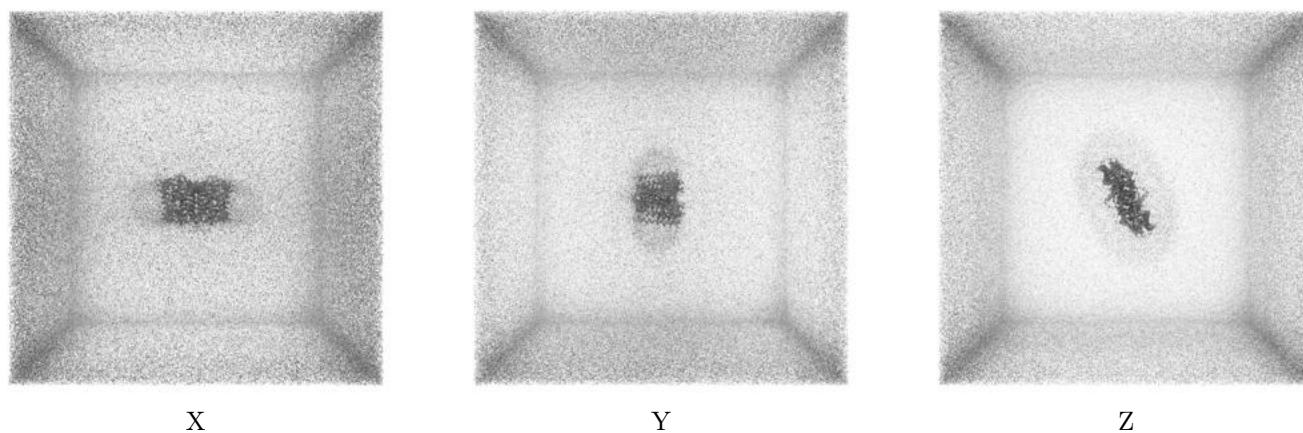
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

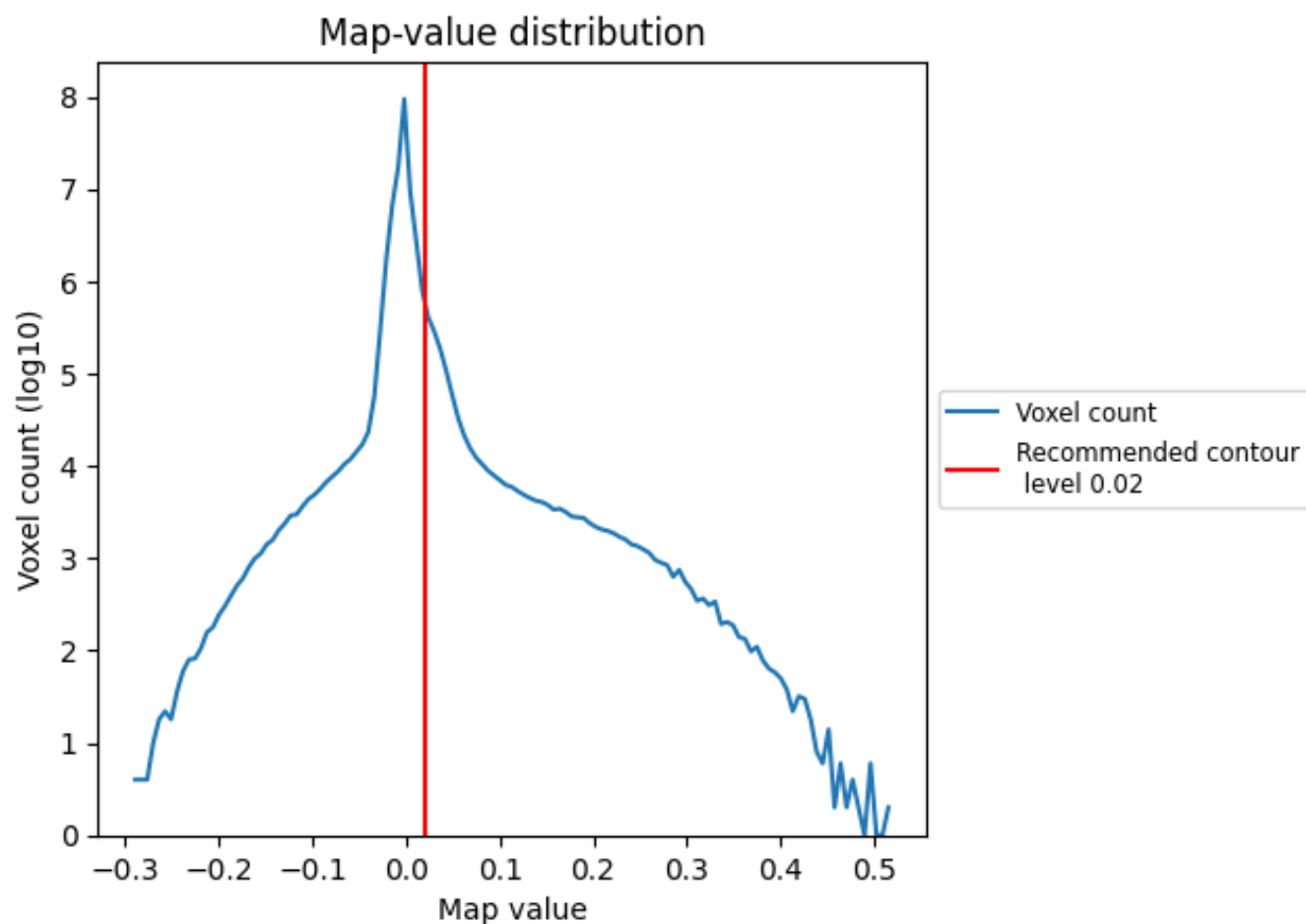
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

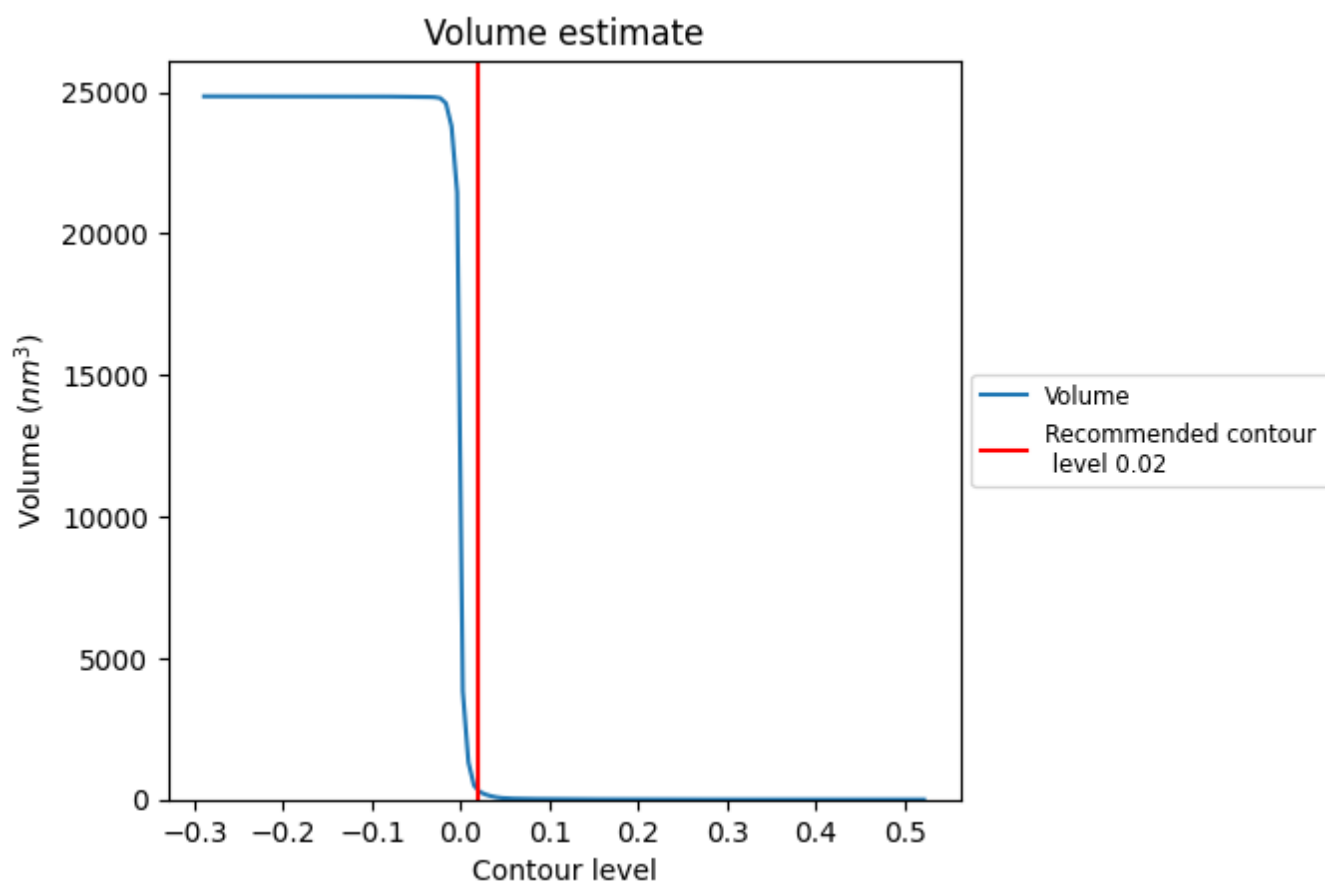
This section contains the results of statistical analysis of the map.

### 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.

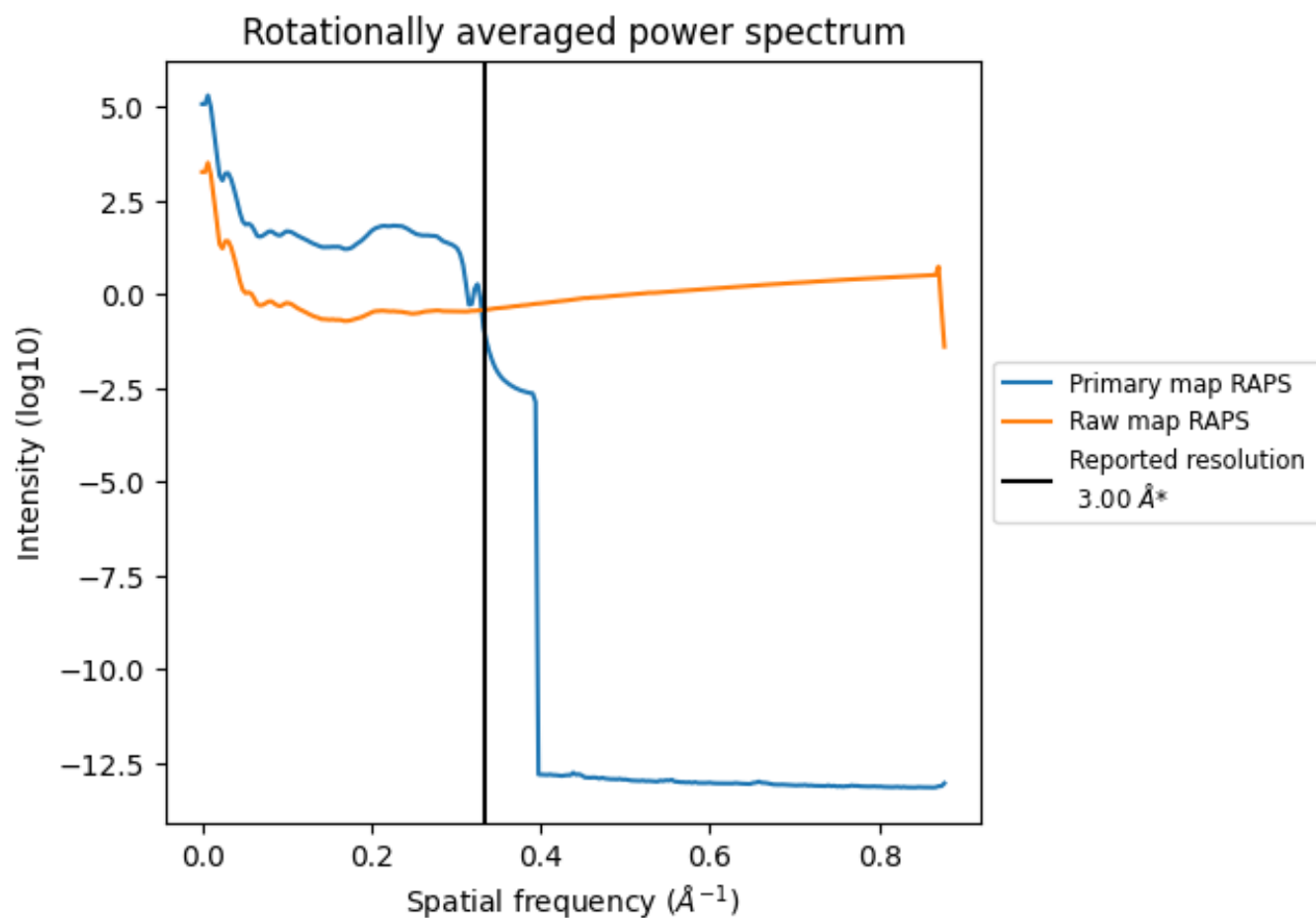
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 318  $\text{nm}^3$ ; this corresponds to an approximate mass of 288 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 ⓘ

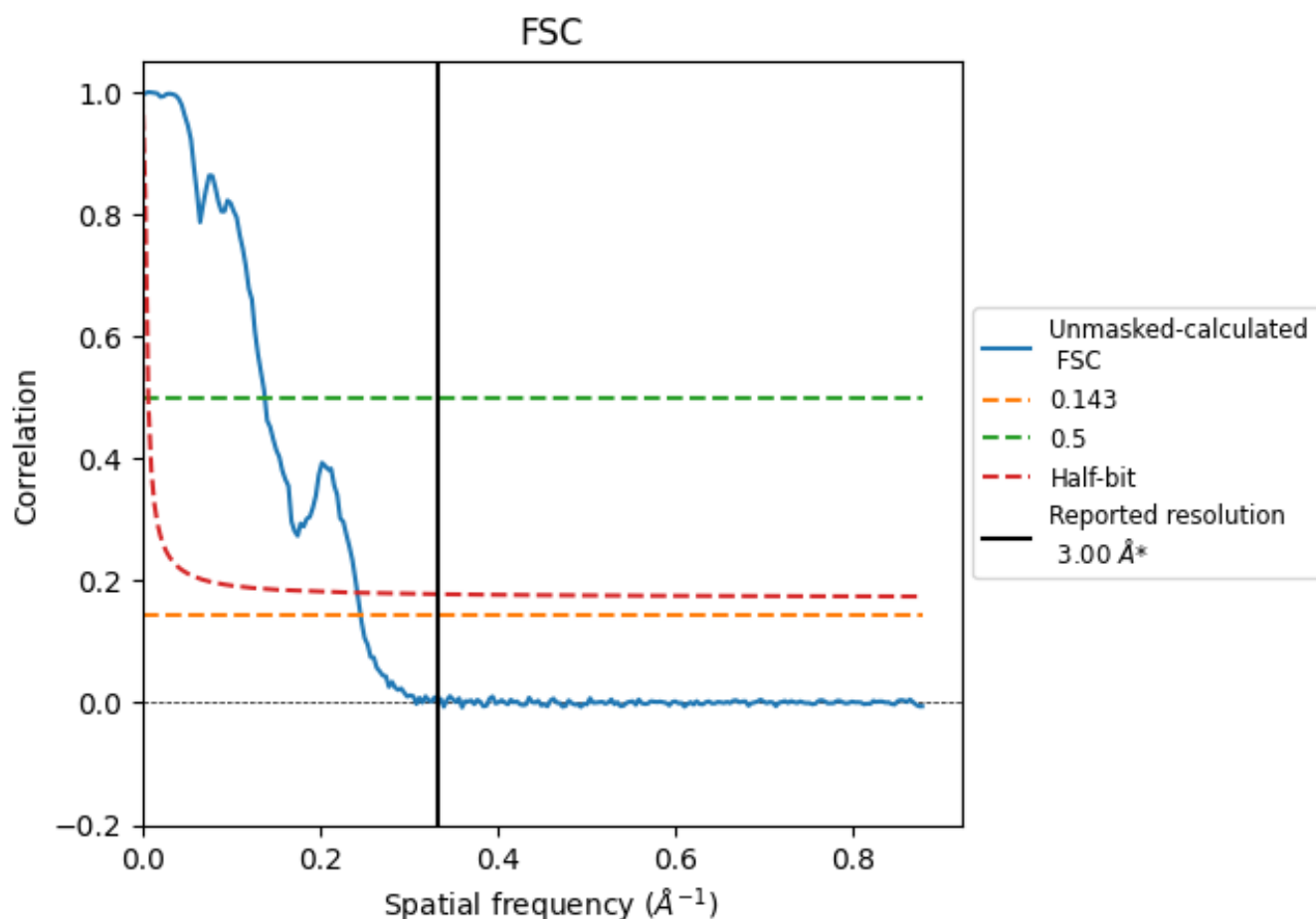


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 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 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

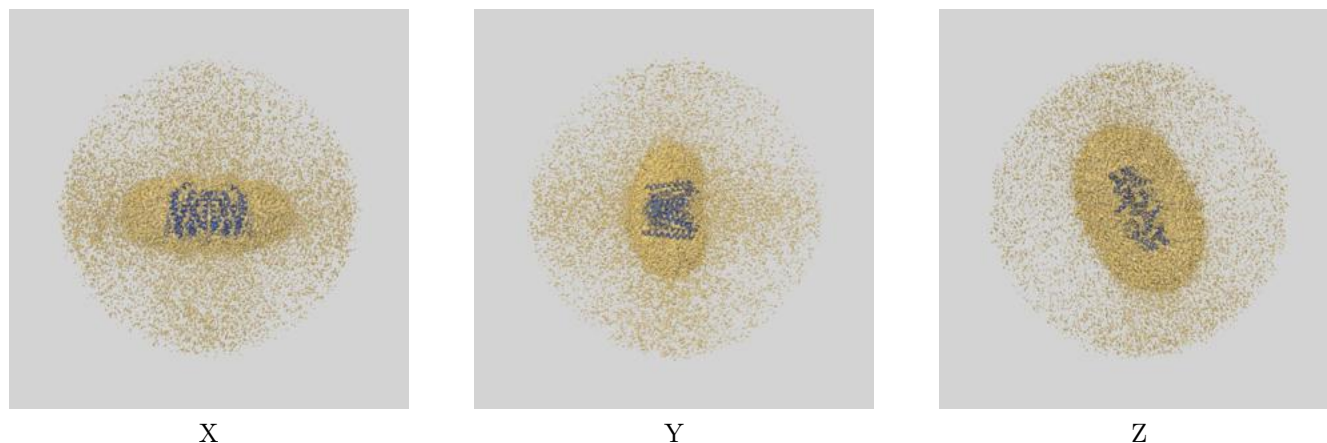
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.07	7.26	4.13

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.0 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-63427 and PDB model 9LW3. Per-residue inclusion information can be found in section [3](#) on page [8](#).

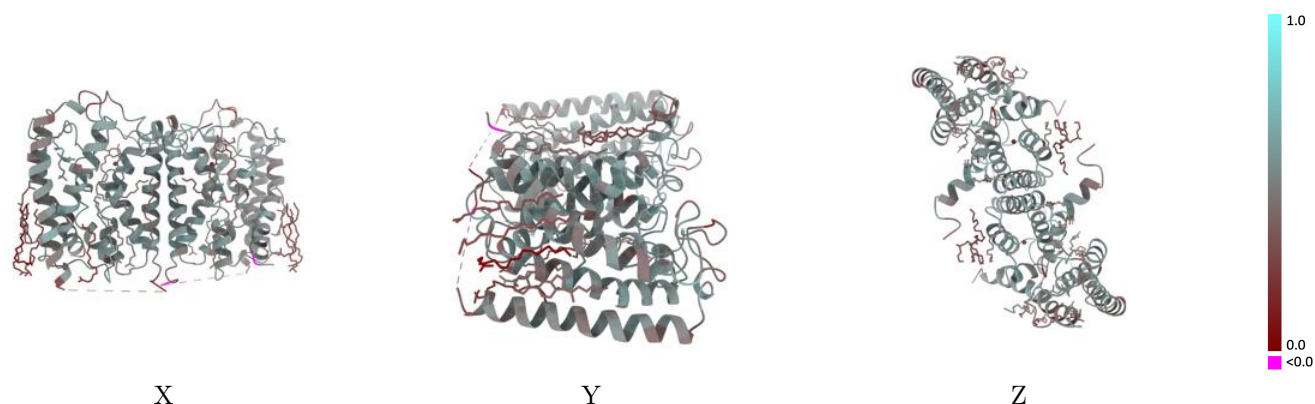
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

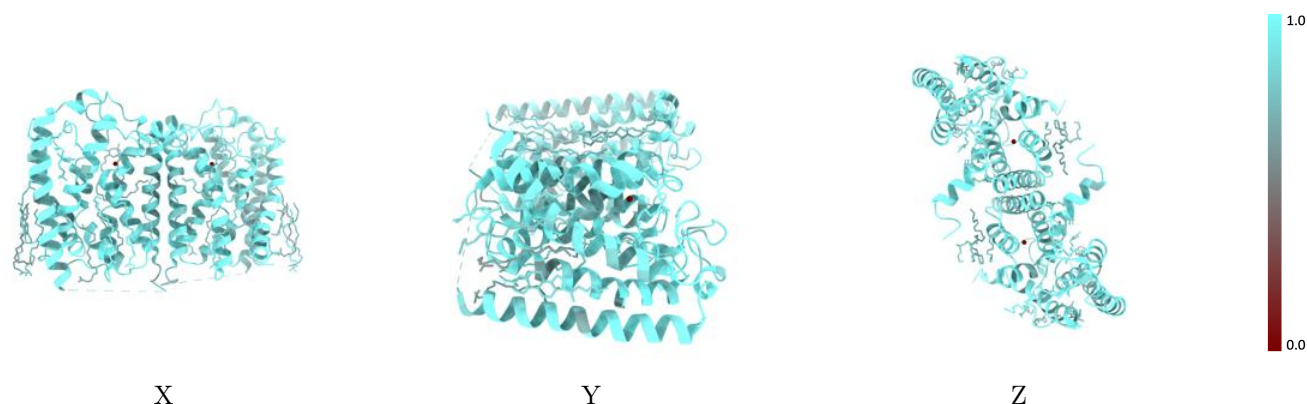


## 9.2 Q-score mapped to coordinate model [i](#)



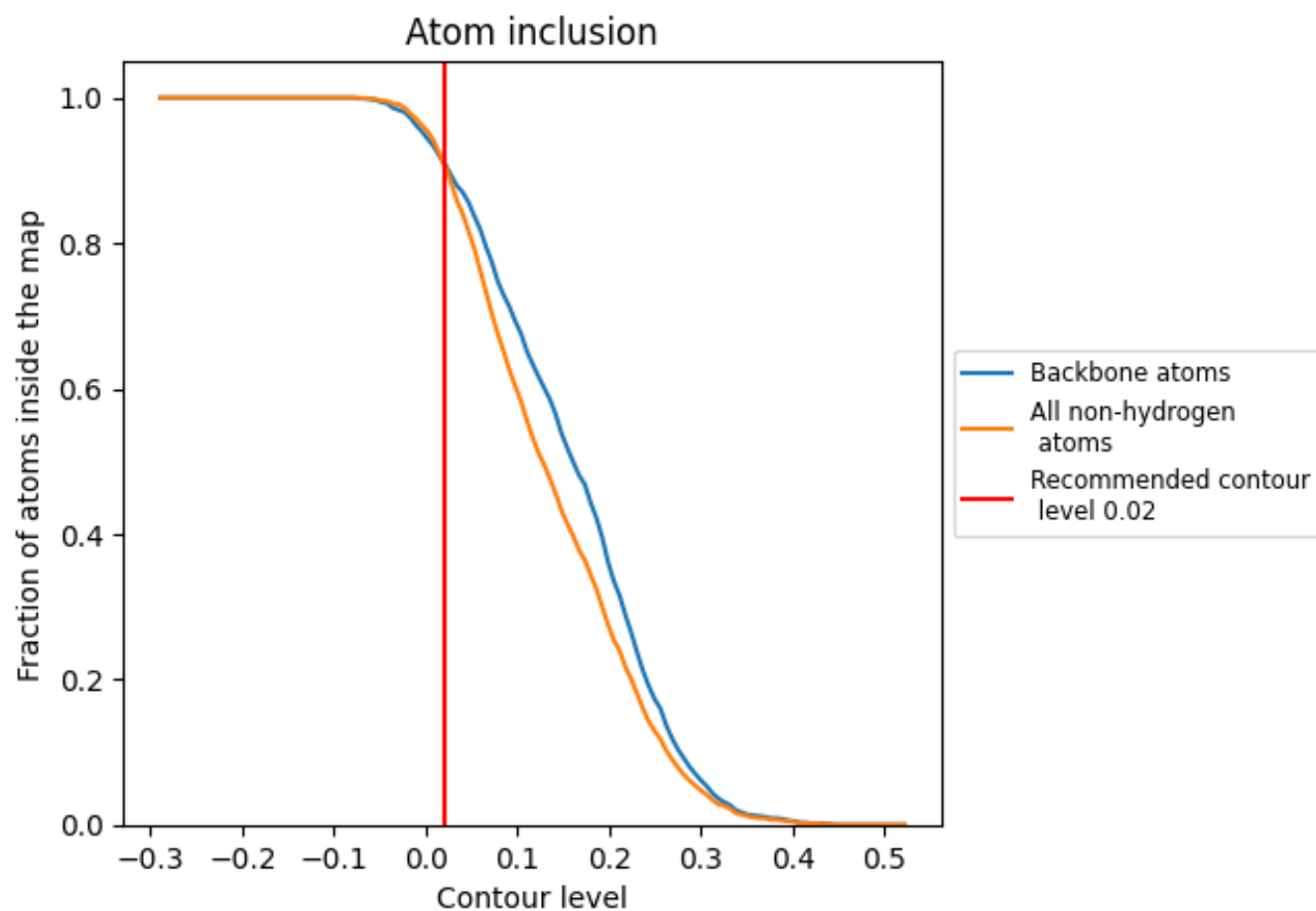
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9080	<div></div> 0.4830
A	<div></div> 0.9100	<div></div> 0.4830
B	<div></div> 0.9100	<div></div> 0.4830

