



Full wwPDB EM Validation Report ⓘ

Jun 15, 2026 – 02:57 PM EDT

PDB ID : 9ZKT / pdb_00009zkt
EMDB ID : EMD-74384
Title : The TMD structure of native mouse AMPAR with 2 TARPs 2 CNIHs and PRRT1/SynDIG4
Authors : Fang, C.L.; Gouaux, E.
Deposited on : 2025-12-07
Resolution : 3.04 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
3	E	160	11%69%8%22%
3	F	160	5%74%18%9%
4	G	423	37%.61%
4	H	423	36%.60%
5	M	306	11%.87%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9580 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 Glutamate receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	133	Total	C	N	O	S	0	0
			1028	693	155	173	7		
1	C	150	Total	C	N	O	S	0	0
			1147	766	177	196	8		

- Molecule 2 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	138	Total	C	N	O	S	0	0
			1071	720	166	179	6		
2	D	135	Total	C	N	O	S	0	0
			1038	695	162	175	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	743	ARG	GLY	conflict	UNP C9K0Z0
D	743	ARG	GLY	conflict	UNP C9K0Z0

- Molecule 3 is a protein called Protein cornichon homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	124	Total	C	N	O	S	0	0
			981	677	142	151	11		
3	F	146	Total	C	N	O	S	0	0
			1189	805	183	190	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	40	ASP	ASN	conflict	UNP O35089
F	40	ASP	ASN	conflict	UNP O35089

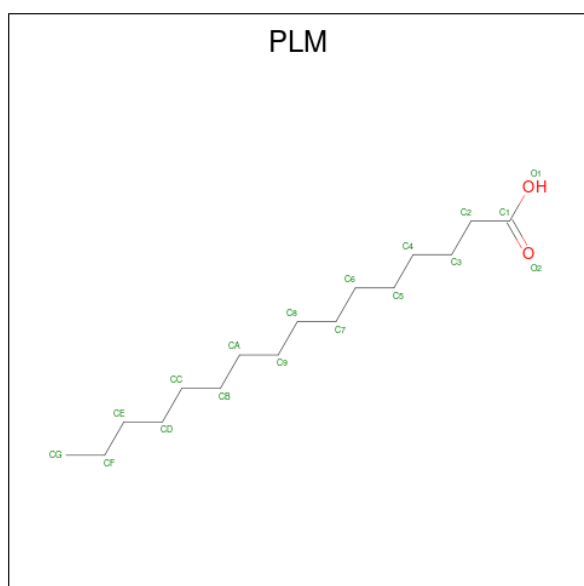
- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	166	Total	C	N	O	S	0	0
			1190	789	192	204	5		
4	H	170	Total	C	N	O	S	0	0
			1218	804	197	211	6		

- Molecule 5 is a protein called Proline-rich transmembrane protein 1.

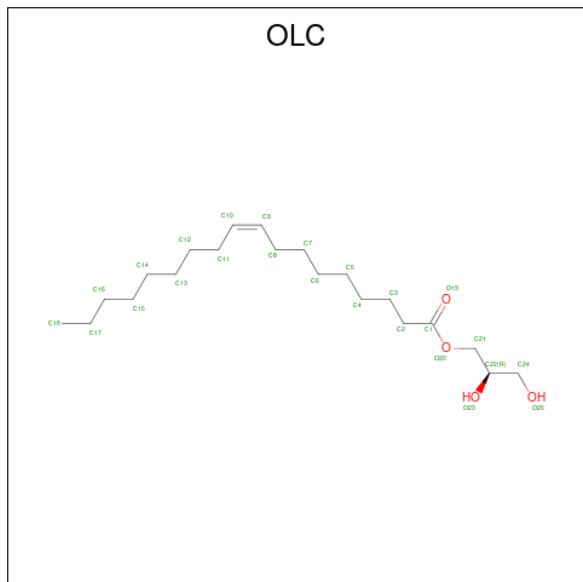
Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	39	Total	C	N	O	S	0	0
			283	183	47	51	2		

- Molecule 6 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



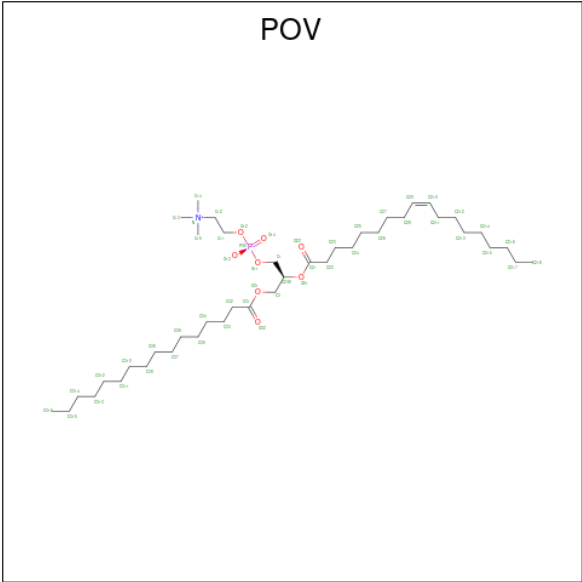
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			18	16	2	
6	A	1	Total	C	O	0
			13	11	2	
6	B	1	Total	C	O	0
			18	16	2	
6	C	1	Total	C	O	0
			18	16	2	
6	D	1	Total	C	O	0
			18	16	2	
6	M	1	Total	C	O	0
			13	11	2	

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).

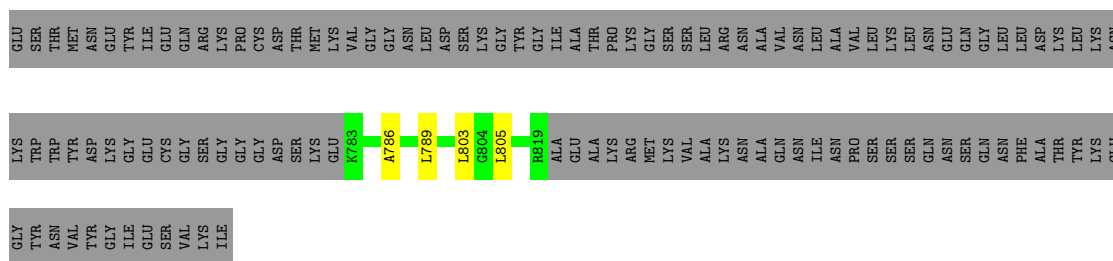


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			25	21	4	
7	A	1	Total	C	O	0
			16	14	2	
7	B	1	Total	C	O	0
			25	21	4	
7	B	1	Total	C	O	0
			14	12	2	
7	C	1	Total	C	O	0
			25	21	4	
7	C	1	Total	C	O	0
			25	21	4	
7	C	1	Total	C	O	0
			16	14	2	
7	D	1	Total	C	O	0
			25	21	4	
7	D	1	Total	C	O	0
			15	13	2	

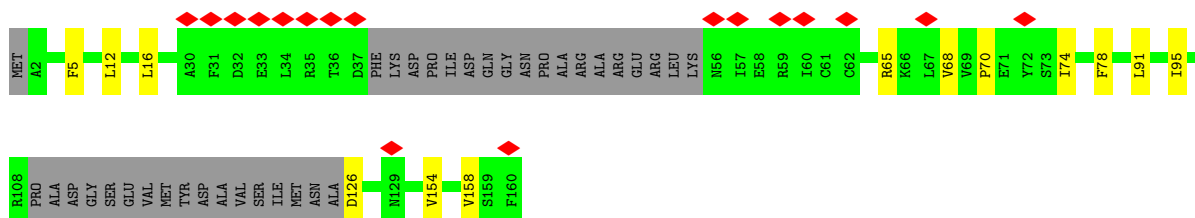
- Molecule 8 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).



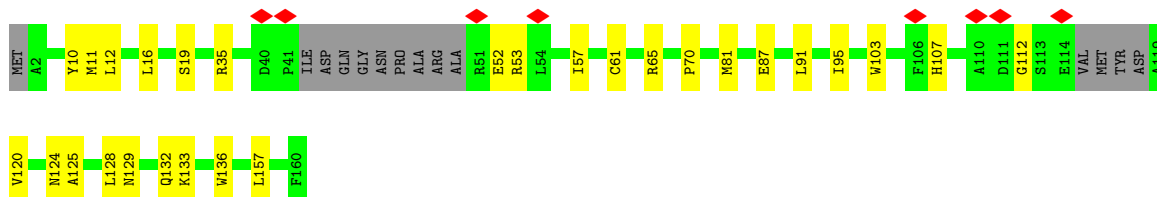
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
8	D	1	Total	C	N	O	P	0
			50	40	1	8	1	
8	G	1	Total	C	N	O	P	0
			50	40	1	8	1	



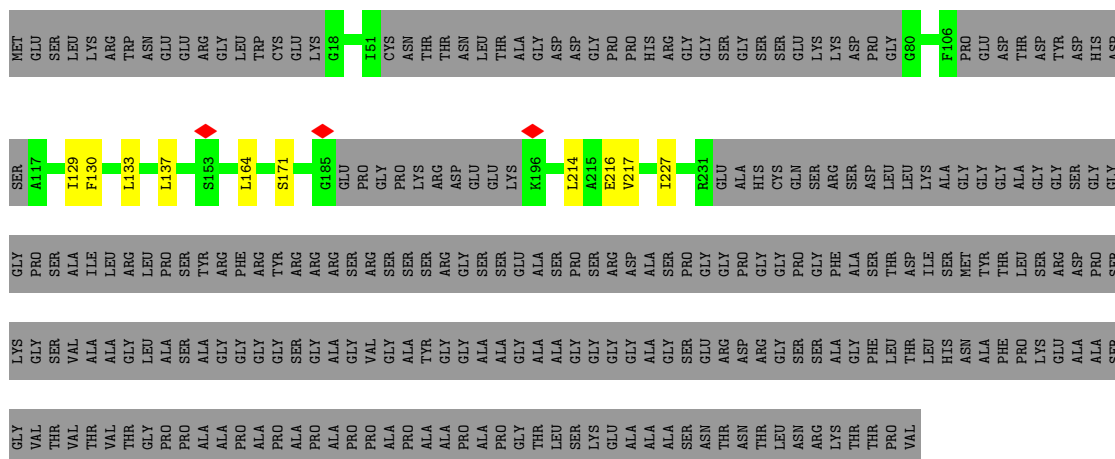
• Molecule 3: Protein cornichon homolog 2



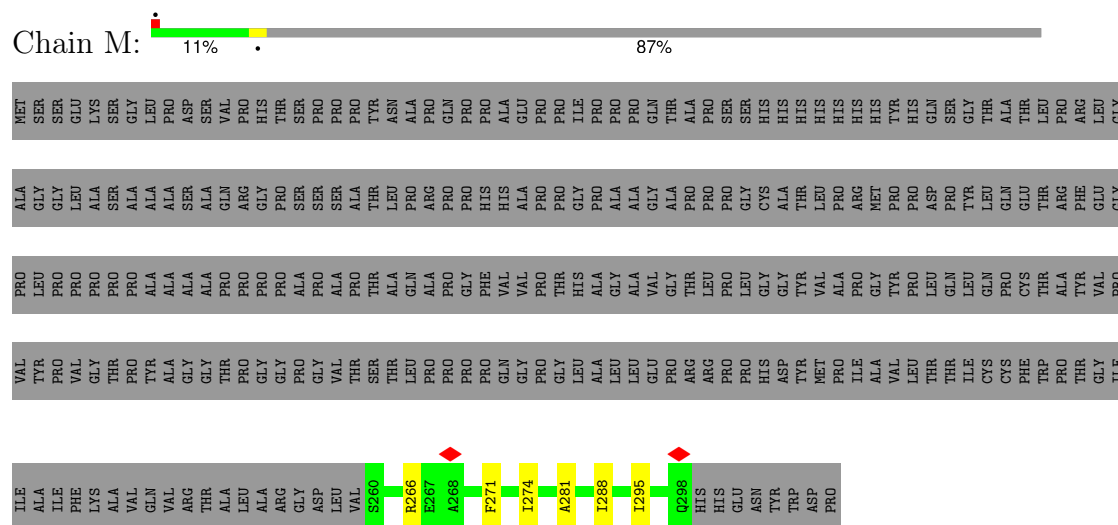
• Molecule 3: Protein cornichon homolog 2



• Molecule 4: Voltage-dependent calcium channel gamma-8 subunit



• Molecule 4: Voltage-dependent calcium channel gamma-8 subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38978	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.239	Depositor
Minimum map value	-0.759	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	323.4, 323.4, 323.4	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, POV, OLC

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	0.15	0/1055	0.35	0/1433
1	C	0.17	0/1176	0.39	0/1594
2	B	0.17	0/1101	0.40	0/1496
2	D	0.15	0/1064	0.36	0/1443
3	E	0.18	0/1013	0.40	0/1382
3	F	0.21	0/1226	0.55	2/1667 (0.1%)
4	G	0.15	0/1212	0.37	0/1651
4	H	0.17	0/1240	0.39	0/1690
5	M	0.23	0/284	0.56	0/385
All	All	0.17	0/9371	0.41	2/12741 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	125	ALA	CA-C-N	5.79	132.59	121.54
3	F	125	ALA	C-N-CA	5.79	132.59	121.54

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	1028	0	1023	16	0
1	C	1147	0	1133	16	0
2	B	1071	0	1064	14	0
2	D	1038	0	1038	17	0
3	E	981	0	930	8	0
3	F	1189	0	1168	19	0
4	G	1190	0	1171	7	0
4	H	1218	0	1194	10	0
5	M	283	0	306	6	0
6	A	31	0	49	0	0
6	B	18	0	31	2	0
6	C	18	0	31	1	0
6	D	18	0	31	3	0
6	M	13	0	18	0	0
7	A	41	0	62	2	0
7	B	39	0	58	2	0
7	C	66	0	102	3	0
7	D	40	0	60	2	0
8	A	51	0	77	3	0
8	D	50	0	75	2	0
8	G	50	0	75	4	0
All	All	9580	0	9696	97	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 (97) 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)
2:B:619:ASN:HD22	1:C:783:LEU:HG	1.62	0.65
2:B:514:VAL:HG21	8:G:501:POV:H2	1.79	0.64
1:C:796:ILE:HD12	3:F:11:MET:HE3	1.80	0.63
1:A:624:ARG:NH1	2:D:626:VAL:O	2.32	0.62
2:D:520:PRO:O	2:D:619:ASN:ND2	2.33	0.62
3:F:65:ARG:HH22	3:F:120:VAL:HG22	1.65	0.61
1:A:600:VAL:HG11	2:B:802:GLY:HA3	1.82	0.61
3:F:124:ASN:H	3:F:128:LEU:HD13	1.66	0.59
6:C:902:PLM:H32	7:C:903:OLC:H21	1.84	0.58
3:E:70:PRO:O	3:E:74:ILE:HG12	2.03	0.58
6:B:1001:PLM:HC2	7:B:1003:OLC:H10	1.85	0.58
3:E:91:LEU:O	3:E:95:ILE:HG12	2.05	0.57
6:D:1001:PLM:H81	7:D:1002:OLC:H2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:91:LEU:O	3:F:95:ILE:HG12	2.06	0.56
1:C:516:PRO:O	1:C:615:ASN:ND2	2.37	0.56
1:A:794:ILE:HA	8:A:1003:POV:H38	1.89	0.55
2:B:526:TRP:HB3	6:B:1001:PLM:H82	1.89	0.55
8:A:1003:POV:H28	8:A:1003:POV:H36	1.87	0.54
2:B:545:ARG:HH12	3:F:70:PRO:HG2	1.72	0.54
2:B:798:ILE:HA	8:G:501:POV:H38	1.88	0.54
1:A:599:GLY:HA3	7:B:1002:OLC:H13A	1.90	0.54
3:F:52:GLU:HG2	3:F:53:ARG:HD3	1.90	0.53
5:M:271:PHE:HA	5:M:274:ILE:HG22	1.91	0.53
1:C:822:LYS:O	5:M:266:ARG:NH1	2.41	0.53
3:F:10:TYR:OH	3:F:87:GLU:OE1	2.23	0.53
1:A:791:VAL:HG21	2:D:611:ILE:HG21	1.92	0.52
2:B:619:ASN:ND2	1:C:783:LEU:HG	2.25	0.52
3:F:65:ARG:HH12	3:F:112:GLY:HA3	1.75	0.51
1:A:516:PRO:O	1:A:615:ASN:ND2	2.44	0.51
2:D:526:TRP:HB3	6:D:1001:PLM:H92	1.91	0.51
4:G:129:ILE:O	4:G:133:LEU:HB2	2.11	0.50
3:E:65:ARG:HA	3:E:68:VAL:HG12	1.93	0.50
3:F:157:LEU:HB3	5:M:295:ILE:HD11	1.93	0.50
2:B:626:VAL:O	1:C:624:ARG:NH2	2.36	0.50
1:C:537:PHE:O	1:C:541:ARG:HB2	2.12	0.49
4:G:137:LEU:HD22	4:G:164:LEU:HD22	1.94	0.49
3:F:53:ARG:O	3:F:57:ILE:HG12	2.13	0.49
3:F:132:GLN:O	3:F:136:TRP:HD1	1.95	0.49
4:H:214:LEU:HA	4:H:217:VAL:HG22	1.93	0.49
1:C:804:LEU:HD23	5:M:281:ALA:HB1	1.96	0.48
8:G:501:POV:H32A	8:G:501:POV:H3	1.63	0.47
3:F:129:ASN:O	3:F:133:LYS:HG2	2.14	0.47
1:A:592:LEU:O	1:A:596:ILE:HG13	2.15	0.47
4:H:221:LEU:O	4:H:225:ILE:HG12	2.14	0.47
4:G:214:LEU:HA	4:G:217:VAL:HG22	1.97	0.46
3:E:126:ASP:N	3:E:126:ASP:OD1	2.48	0.46
4:H:122:ARG:HA	4:H:122:ARG:HD3	1.78	0.46
1:C:615:ASN:HD21	2:D:786:ALA:HA	1.80	0.46
3:F:12:LEU:HD23	3:F:81:MET:HE1	1.96	0.46
4:H:172:ASN:ND2	4:H:212:PHE:HB2	2.29	0.46
6:D:1001:PLM:H71	7:D:1004:OLC:H6A	1.98	0.46
4:H:217:VAL:O	4:H:221:LEU:HD23	2.17	0.45
1:C:602:TRP:CD2	2:D:587:GLN:HG3	2.51	0.45
1:C:796:ILE:HD13	3:F:11:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:51:ILE:HD12	4:H:89:ILE:HD13	1.99	0.45
1:A:799:LEU:HD22	2:D:539:VAL:HG11	1.98	0.45
1:C:819:LYS:HE3	1:C:819:LYS:HB3	1.80	0.45
8:D:1003:POV:H3	8:D:1003:POV:H32A	1.52	0.45
1:A:534:VAL:HG21	4:G:216:GLU:HB3	1.99	0.44
7:A:1002:OLC:H12	8:A:1003:POV:H31D	2.00	0.44
2:B:520:PRO:HB3	2:B:619:ASN:HB3	2.00	0.44
1:C:532:VAL:HG22	2:D:803:LEU:HD21	1.99	0.44
2:D:805:LEU:HD13	8:D:1003:POV:H31B	1.99	0.44
2:D:520:PRO:HB3	2:D:619:ASN:HB3	1.99	0.44
3:E:154:VAL:O	3:E:158:VAL:HG12	2.17	0.43
4:H:83:HIS:CE1	4:H:90:CYS:HB3	2.53	0.43
1:A:607:ILE:HG21	2:B:795:VAL:HG21	2.00	0.43
2:B:801:GLY:HA2	8:G:501:POV:H21C	2.01	0.42
2:D:524:GLU:N	2:D:524:GLU:OE1	2.52	0.42
4:G:130:PHE:O	4:G:171:SER:OG	2.37	0.42
4:H:159:LEU:HD12	4:H:226:TYR:CE2	2.53	0.42
1:A:516:PRO:HG2	1:A:612:TYR:CE1	2.54	0.42
2:B:525:ILE:HD11	1:C:785:LEU:HA	2.02	0.42
3:F:61:CYS:O	3:F:65:ARG:HG3	2.20	0.42
3:E:12:LEU:HD23	3:E:12:LEU:HA	1.87	0.42
1:C:811:CYS:SG	5:M:274:ILE:HD11	2.58	0.42
3:E:16:LEU:HB2	3:E:78:PHE:CE1	2.55	0.42
1:C:794:ILE:HD13	7:C:903:OLC:H4A	2.02	0.42
2:B:600:ILE:HA	7:C:903:OLC:H14	2.01	0.42
1:A:541:ARG:HB3	4:G:227:ILE:HD11	2.01	0.42
3:F:35:ARG:HH11	3:F:128:LEU:HB3	1.86	0.41
1:A:602:TRP:HA	1:A:605:THR:HG22	2.03	0.41
1:A:625:MET:HG2	2:D:626:VAL:HG21	2.02	0.41
4:G:133:LEU:HD12	4:G:133:LEU:HA	1.91	0.41
5:M:288:ILE:HD13	5:M:288:ILE:HA	1.93	0.41
2:B:605:TRP:O	2:B:609:THR:HG23	2.21	0.41
4:H:163:ILE:HA	4:H:166:VAL:HG22	2.03	0.41
2:D:612:ILE:HD13	2:D:612:ILE:HA	1.95	0.41
2:D:789:LEU:HD12	2:D:789:LEU:HA	1.93	0.41
3:F:16:LEU:O	3:F:19:SER:OG	2.29	0.41
2:D:586:ARG:HD3	2:D:613:ILE:HG13	2.02	0.41
3:F:65:ARG:NH1	3:F:112:GLY:HA3	2.36	0.40
1:A:577:LEU:HD22	7:A:1002:OLC:H15	2.03	0.40
1:A:791:VAL:HG12	2:D:608:PHE:HD1	1.86	0.40
2:D:527:MET:HB3	3:E:5:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:103:TRP:O	3:F:107:HIS:HB2	2.22	0.40
4:H:106:PHE:HE1	4:H:122:ARG:HB3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	127/500 (25%)	123 (97%)	4 (3%)	0	100	100
1	C	144/500 (29%)	142 (99%)	2 (1%)	0	100	100
2	B	132/467 (28%)	128 (97%)	4 (3%)	0	100	100
2	D	129/467 (28%)	128 (99%)	1 (1%)	0	100	100
3	E	118/160 (74%)	117 (99%)	1 (1%)	0	100	100
3	F	140/160 (88%)	133 (95%)	7 (5%)	0	100	100
4	G	158/423 (37%)	154 (98%)	4 (2%)	0	100	100
4	H	162/423 (38%)	158 (98%)	4 (2%)	0	100	100
5	M	37/306 (12%)	37 (100%)	0	0	100	100
All	All	1147/3406 (34%)	1120 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	108/420 (26%)	108 (100%)	0	100	100
1	C	120/420 (29%)	120 (100%)	0	100	100
2	B	112/394 (28%)	112 (100%)	0	100	100
2	D	109/394 (28%)	109 (100%)	0	100	100
3	E	96/143 (67%)	96 (100%)	0	100	100
3	F	124/143 (87%)	124 (100%)	0	100	100
4	G	113/310 (36%)	113 (100%)	0	100	100
4	H	117/310 (38%)	117 (100%)	0	100	100
5	M	30/236 (13%)	30 (100%)	0	100	100
All	All	929/2770 (34%)	929 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	565	ASN
1	A	582	GLN
2	B	619	ASN
3	E	94	ASN
3	F	27	HIS
4	G	224	ASN
5	M	298	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

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PLM	D	1001	-	17,17,17	0.53	0	17,17,17	0.50	0
7	OLC	A	1002	-	24,24,24	0.23	0	25,25,25	0.33	0
7	OLC	B	1003	-	13,13,24	0.34	0	13,13,25	0.32	0
6	PLM	M	401	-	12,12,17	0.64	0	12,12,17	0.60	0
8	POV	D	1003	-	49,49,51	0.29	0	55,57,59	0.35	0
8	POV	G	501	-	49,49,51	0.29	0	55,57,59	0.43	0
7	OLC	C	901	-	24,24,24	0.24	0	25,25,25	0.22	0
7	OLC	B	1002	-	24,24,24	0.24	0	25,25,25	0.23	0
6	PLM	B	1001	-	17,17,17	0.54	0	17,17,17	0.50	0
7	OLC	C	904	-	15,15,24	0.34	0	15,15,25	0.32	0
6	PLM	A	1001	-	17,17,17	0.54	0	17,17,17	0.51	0
7	OLC	C	903	-	24,24,24	0.24	0	25,25,25	0.32	0
6	PLM	C	902	-	17,17,17	0.54	0	17,17,17	0.50	0
7	OLC	A	1004	-	15,15,24	0.34	0	15,15,25	0.30	0
7	OLC	D	1002	-	24,24,24	0.24	0	25,25,25	0.28	0
6	PLM	A	1005	-	12,12,17	0.63	0	12,12,17	0.64	0
7	OLC	D	1004	-	14,14,24	0.34	0	14,14,25	0.33	0
8	POV	A	1003	-	50,50,51	0.29	0	56,58,59	0.30	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
6	PLM	D	1001	-	-	4/15/15/15	-
7	OLC	A	1002	-	-	2/24/24/24	-
7	OLC	B	1003	-	-	1/11/11/24	-
6	PLM	M	401	-	-	2/10/10/15	-
8	POV	D	1003	-	-	9/53/53/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	POV	G	501	-	-	11/53/53/55	-
7	OLC	C	901	-	-	1/24/24/24	-
7	OLC	B	1002	-	-	0/24/24/24	-
6	PLM	B	1001	-	-	3/15/15/15	-
7	OLC	C	904	-	-	4/13/13/24	-
6	PLM	A	1001	-	-	2/15/15/15	-
7	OLC	C	903	-	-	2/24/24/24	-
6	PLM	C	902	-	-	4/15/15/15	-
7	OLC	A	1004	-	-	1/13/13/24	-
7	OLC	D	1002	-	-	2/24/24/24	-
6	PLM	A	1005	-	-	5/10/10/15	-
7	OLC	D	1004	-	-	3/12/12/24	-
8	POV	A	1003	-	-	6/54/54/55	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1003	POV	C11-O12-P-O14
8	A	1003	POV	C32-C31-O31-C3
8	A	1003	POV	O32-C31-O31-C3
8	D	1003	POV	C32-C31-O31-C3
8	D	1003	POV	O32-C31-O31-C3
8	G	501	POV	C1-O11-P-O12
8	G	501	POV	C32-C31-O31-C3
8	G	501	POV	O32-C31-O31-C3
8	A	1003	POV	C22-C23-C24-C25
6	A	1001	PLM	CB-CC-CD-CE
8	G	501	POV	O11-C1-C2-C3
6	C	902	PLM	C6-C7-C8-C9
6	A	1005	PLM	C2-C3-C4-C5
7	D	1004	OLC	C5-C6-C7-C8
8	G	501	POV	C2-C1-O11-P
8	A	1003	POV	O12-C11-C12-N
8	G	501	POV	C24-C25-C26-C27
6	D	1001	PLM	C2-C3-C4-C5
8	D	1003	POV	C29-C210-C211-C212

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Mol	Chain	Res	Type	Atoms
8	D	1003	POV	C11-O12-P-O14
8	G	501	POV	C1-O11-P-O14
8	G	501	POV	C11-O12-P-O14
7	A	1002	OLC	C7-C8-C9-C10
7	C	904	OLC	C7-C8-C9-C10
8	G	501	POV	O11-C1-C2-O21
7	A	1002	OLC	C5-C6-C7-C8
8	D	1003	POV	O21-C21-C22-C23
7	A	1004	OLC	C9-C10-C11-C12
7	B	1003	OLC	C7-C8-C9-C10
8	G	501	POV	C29-C210-C211-C212
7	C	903	OLC	C9-C10-C11-C12
7	D	1004	OLC	C9-C10-C11-C12
8	D	1003	POV	C27-C28-C29-C210
7	C	901	OLC	C7-C8-C9-C10
7	C	903	OLC	C7-C8-C9-C10
8	D	1003	POV	C2-C1-O11-P
7	D	1002	OLC	C7-C8-C9-C10
6	A	1005	PLM	O1-C1-C2-C3
6	M	401	PLM	O2-C1-C2-C3
8	D	1003	POV	C25-C26-C27-C28
6	A	1001	PLM	C5-C6-C7-C8
6	A	1005	PLM	O2-C1-C2-C3
8	G	501	POV	C27-C28-C29-C210
6	M	401	PLM	O1-C1-C2-C3
7	C	904	OLC	O20-C1-C2-C3
7	D	1002	OLC	C9-C10-C11-C12
6	C	902	PLM	O1-C1-C2-C3
6	B	1001	PLM	O1-C1-C2-C3
6	D	1001	PLM	O1-C1-C2-C3
6	B	1001	PLM	O2-C1-C2-C3
7	D	1004	OLC	C7-C8-C9-C10
7	C	904	OLC	O19-C1-C2-C3
6	A	1005	PLM	C3-C4-C5-C6
6	D	1001	PLM	C4-C5-C6-C7
6	C	902	PLM	O2-C1-C2-C3
6	D	1001	PLM	O2-C1-C2-C3
8	A	1003	POV	C12-C11-O12-P
6	C	902	PLM	C5-C6-C7-C8
7	C	904	OLC	C9-C10-C11-C12
8	D	1003	POV	C22-C23-C24-C25
6	B	1001	PLM	C5-C6-C7-C8

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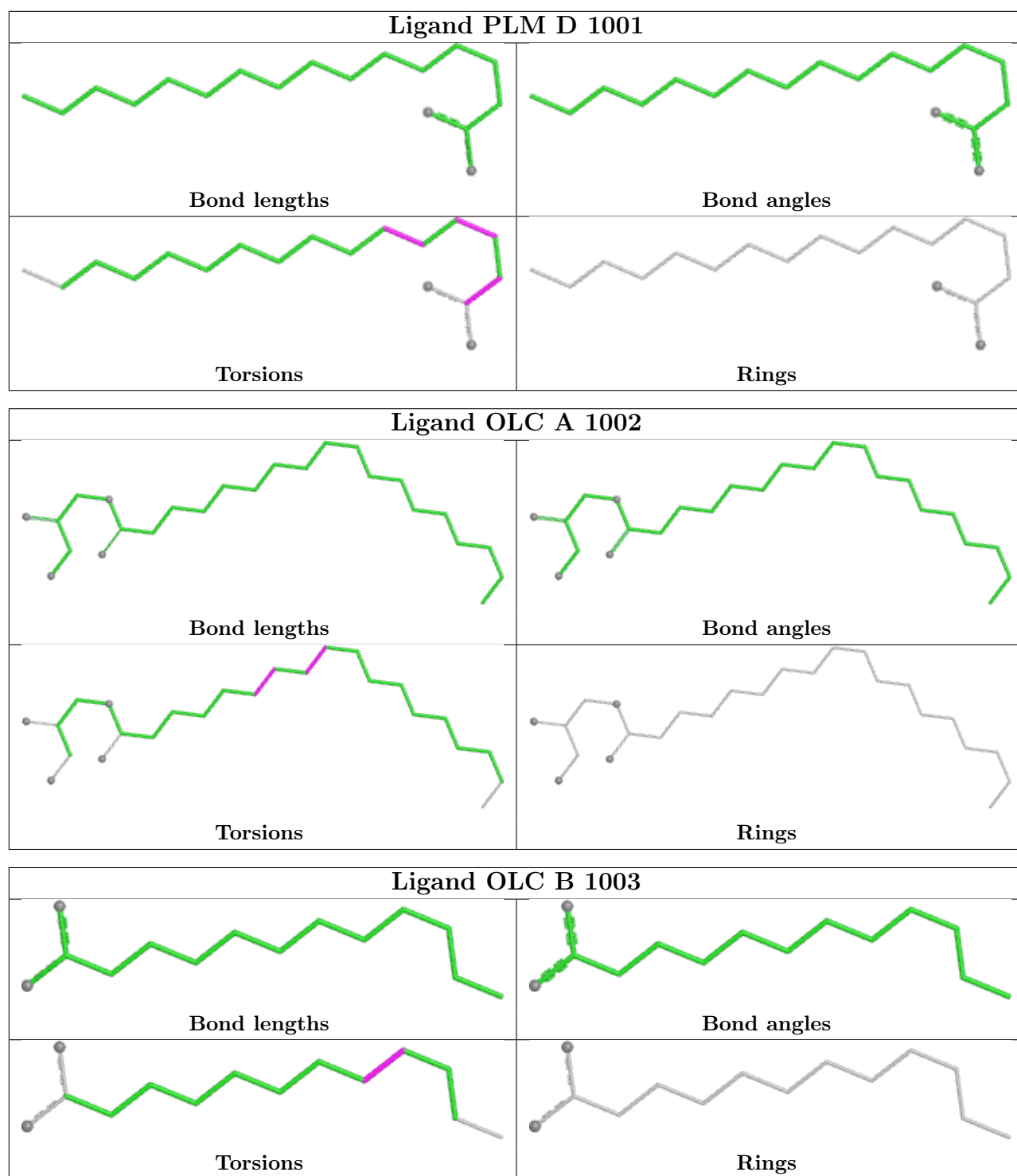
Mol	Chain	Res	Type	Atoms
6	A	1005	PLM	C5-C6-C7-C8

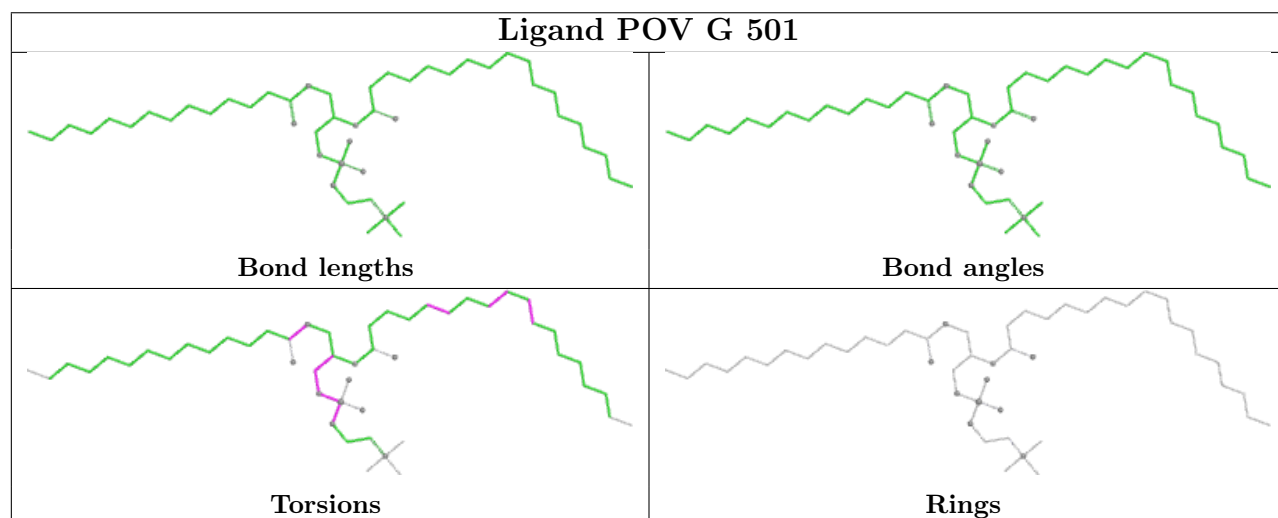
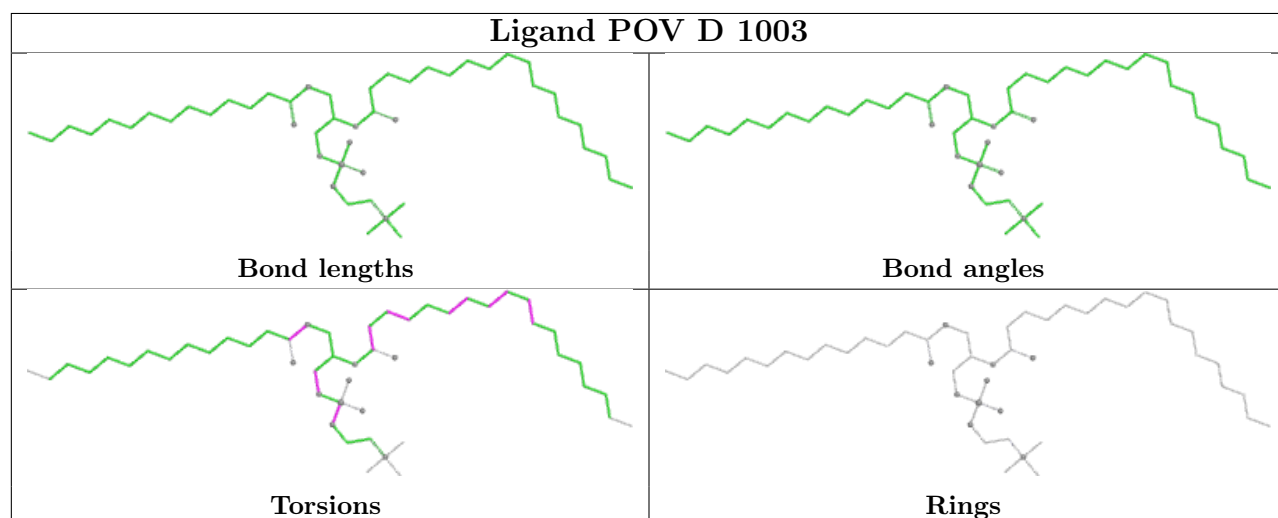
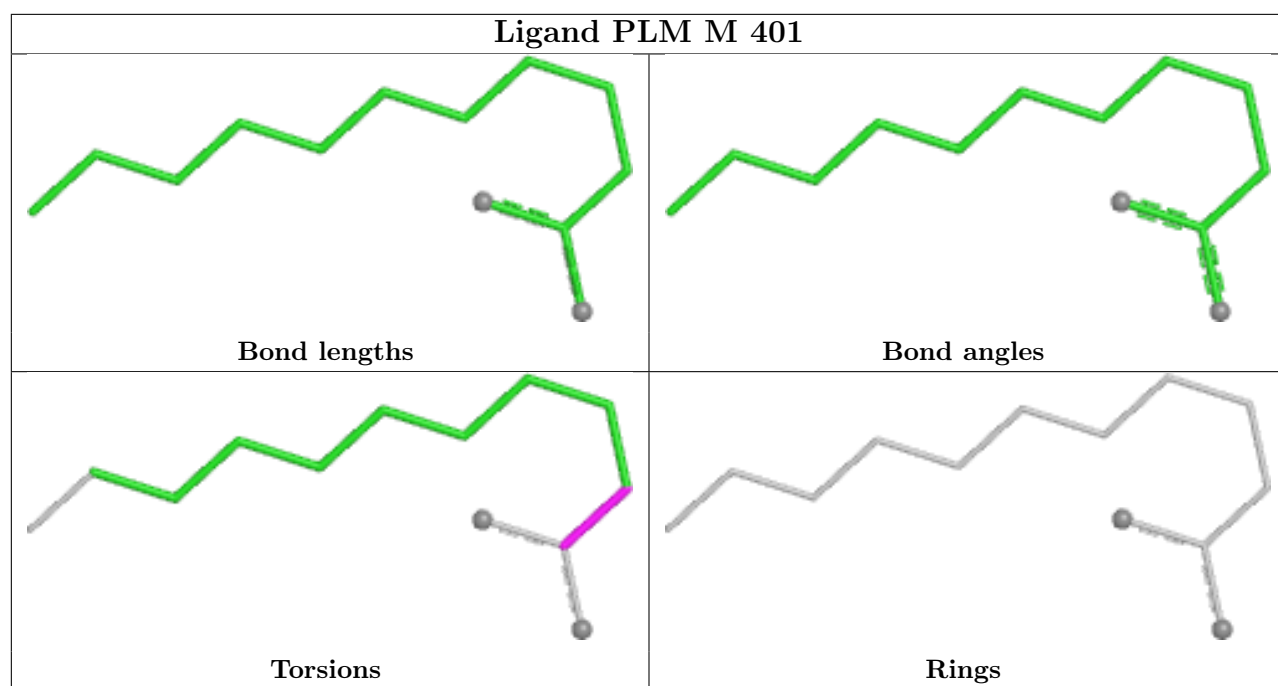
There are no ring outliers.

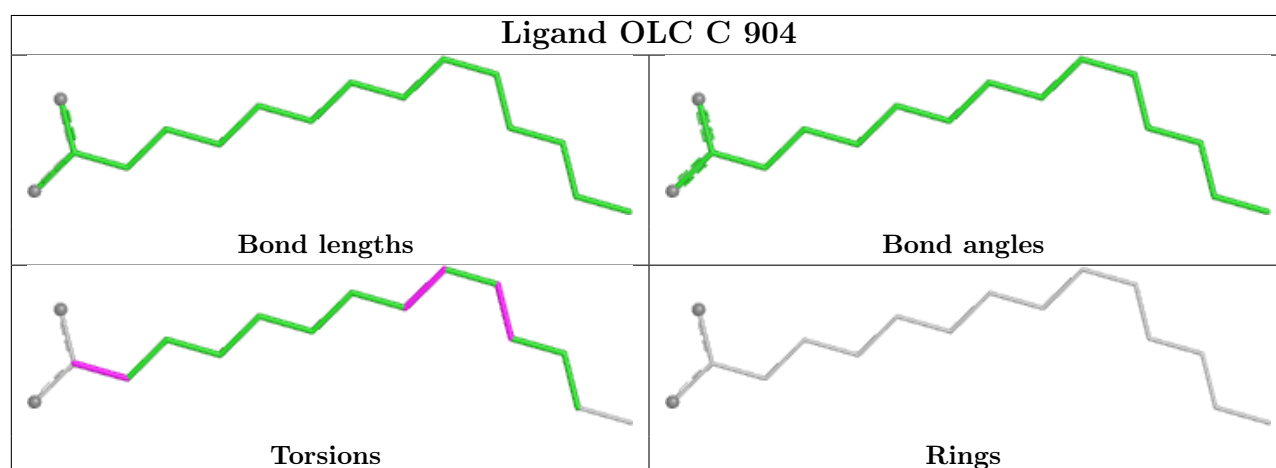
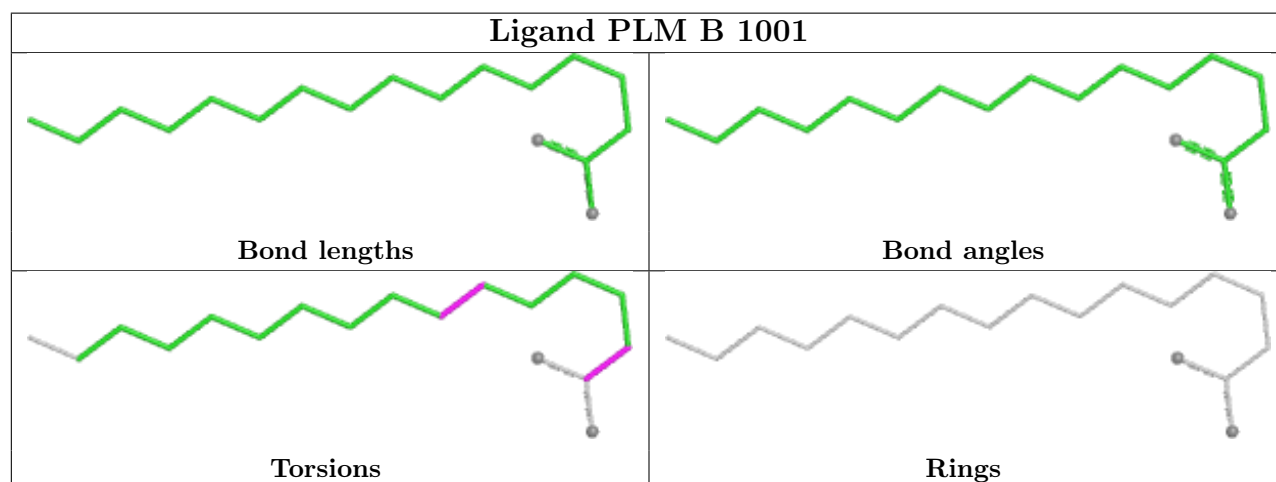
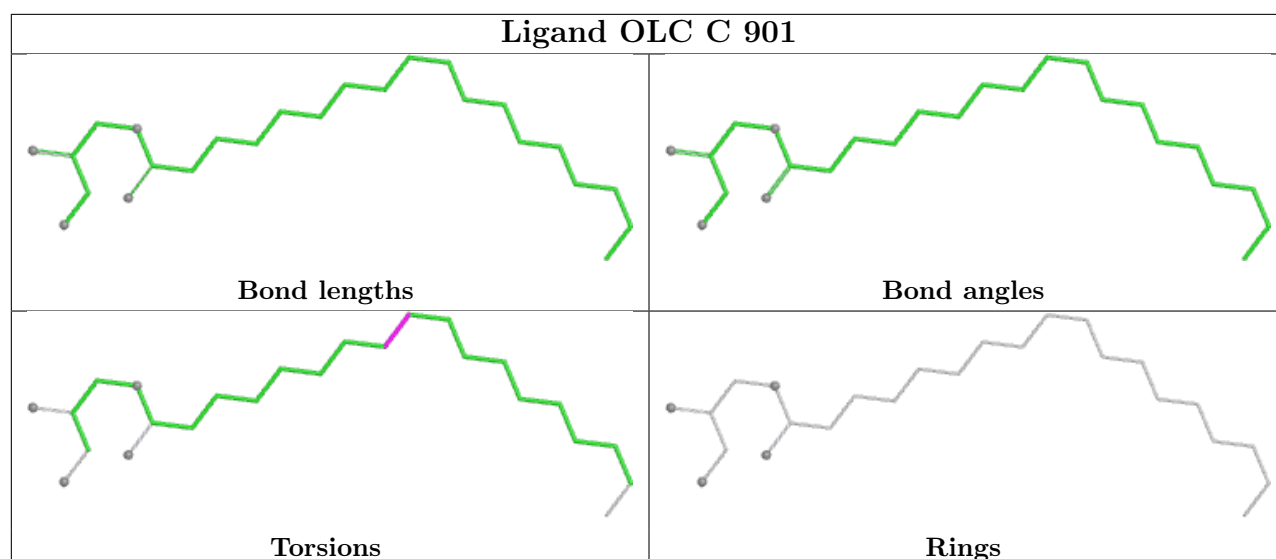
12 monomers are involved in 19 short contacts:

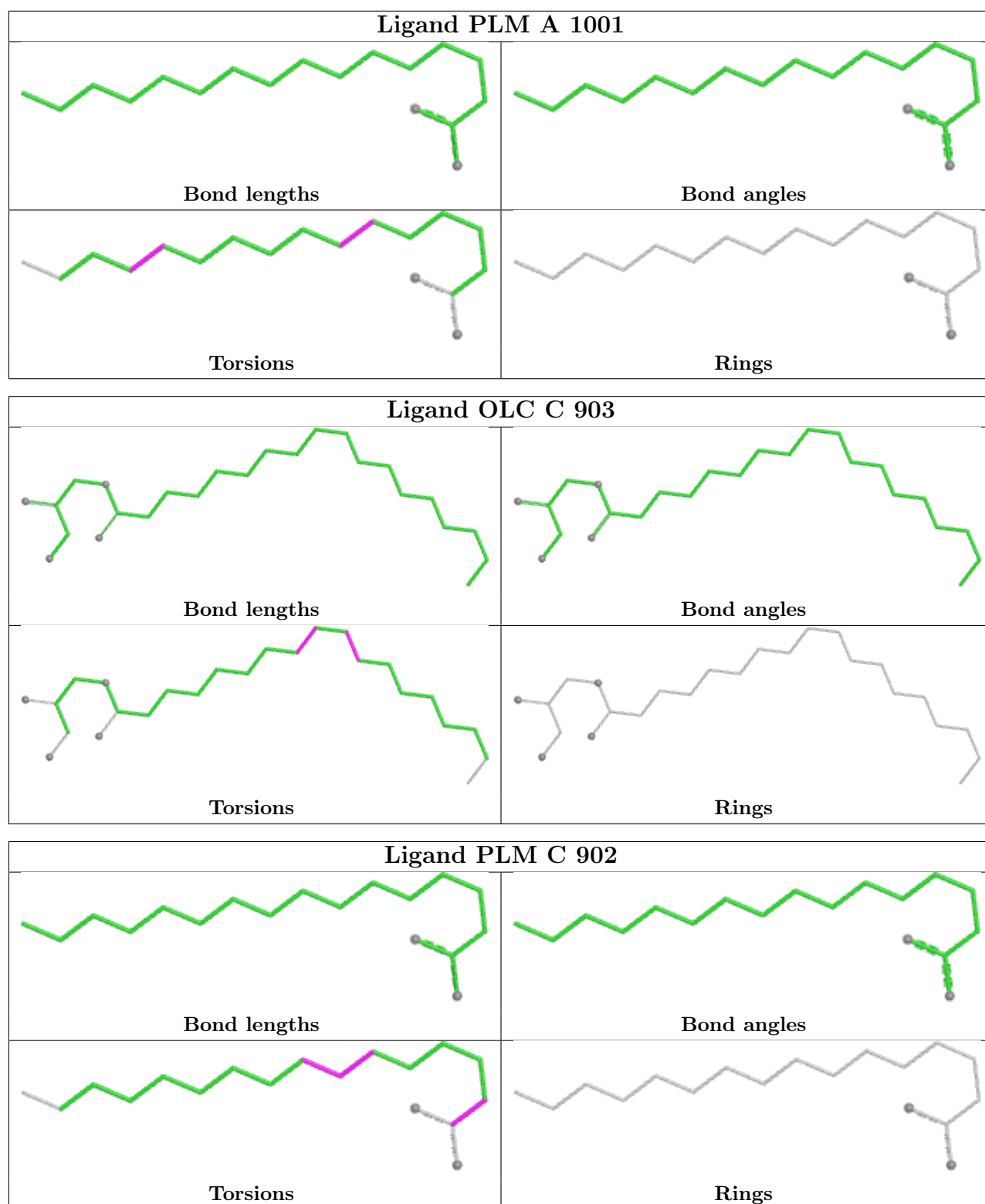
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1001	PLM	3	0
7	A	1002	OLC	2	0
7	B	1003	OLC	1	0
8	D	1003	POV	2	0
8	G	501	POV	4	0
7	B	1002	OLC	1	0
6	B	1001	PLM	2	0
7	C	903	OLC	3	0
6	C	902	PLM	1	0
7	D	1002	OLC	1	0
7	D	1004	OLC	1	0
8	A	1003	POV	3	0

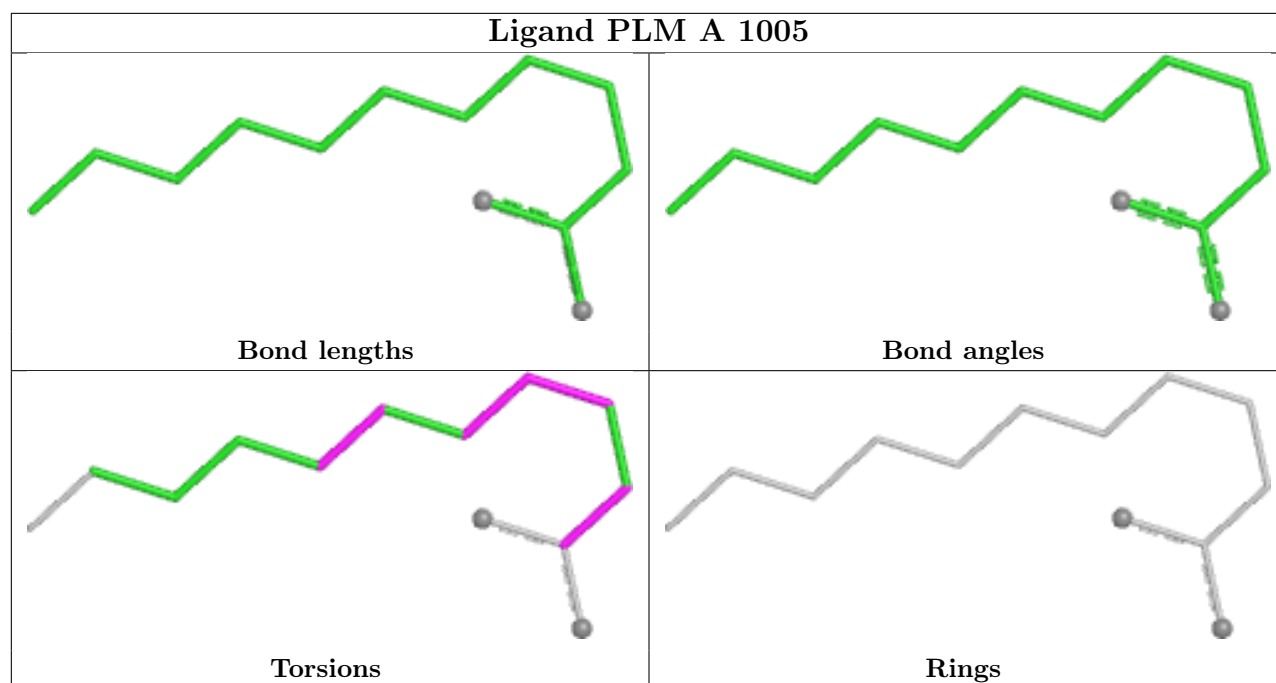
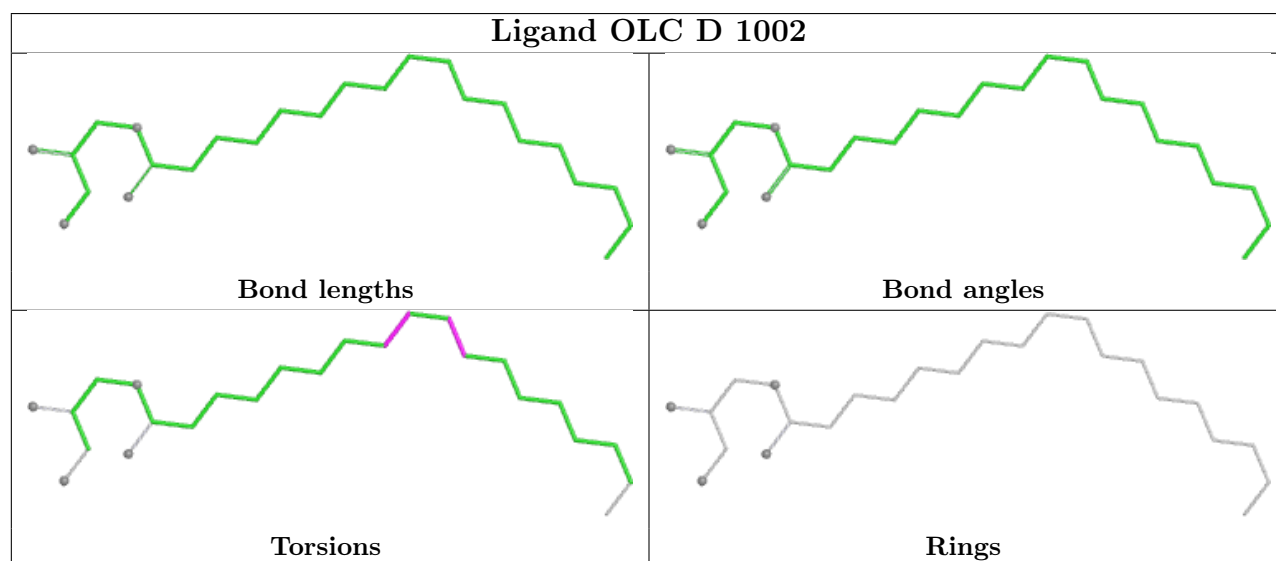
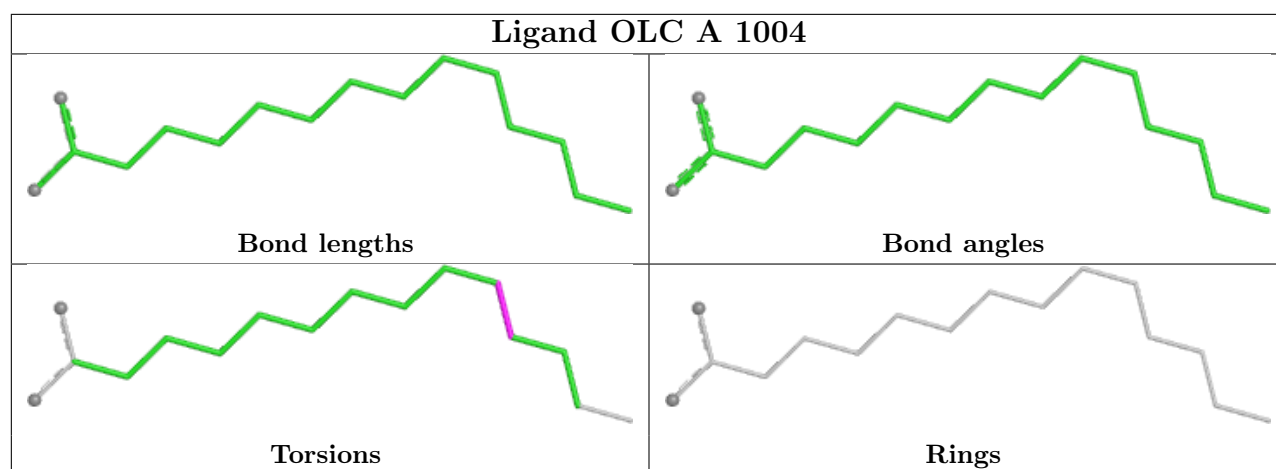
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

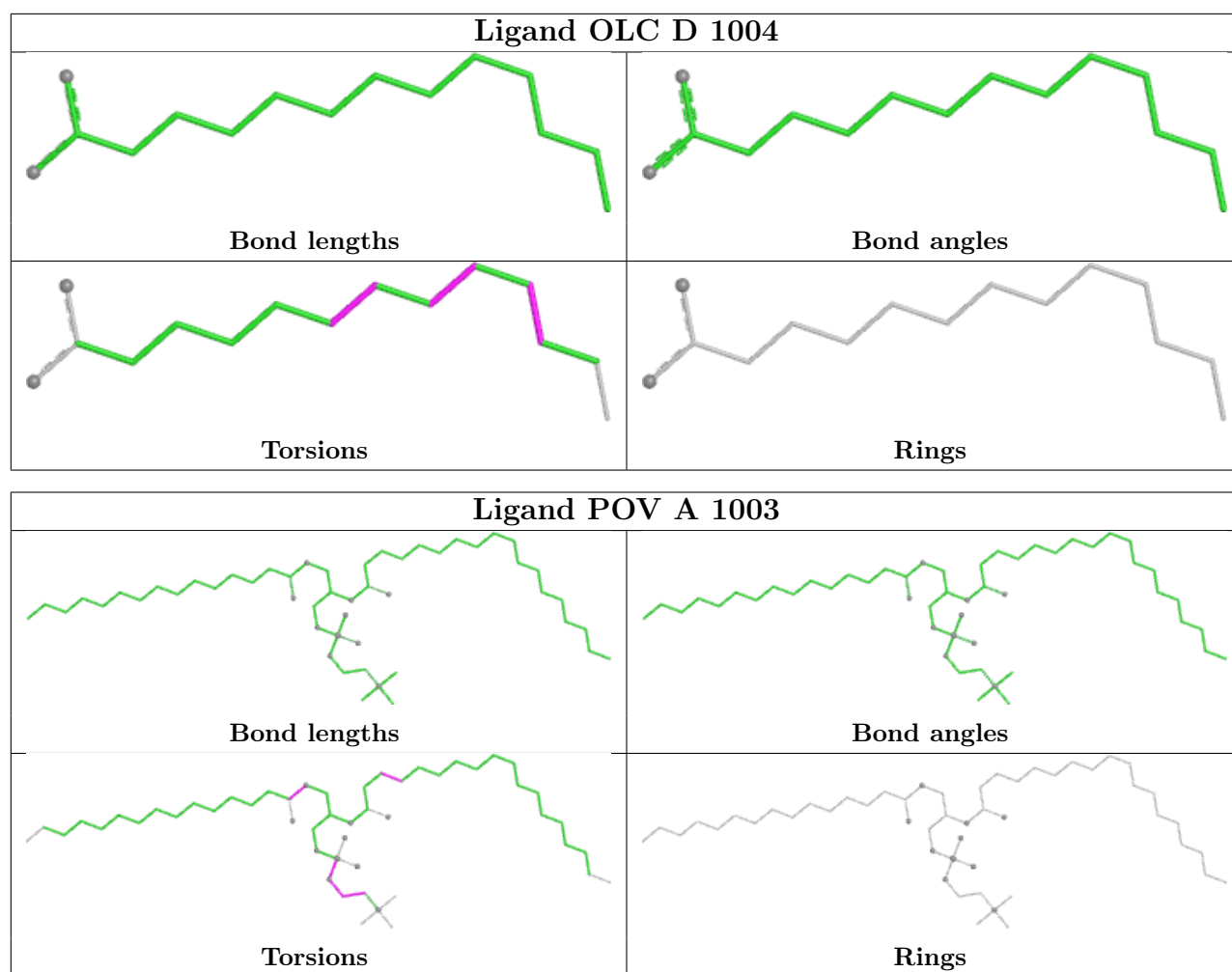












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

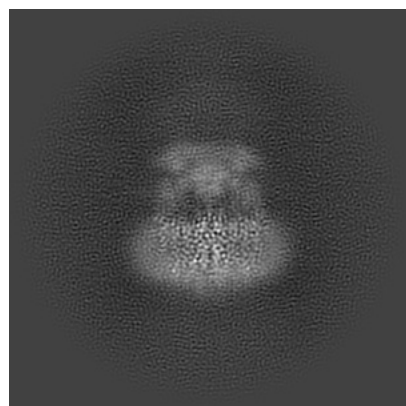
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74384. These allow visual inspection of the internal detail of the map and identification of artifacts.

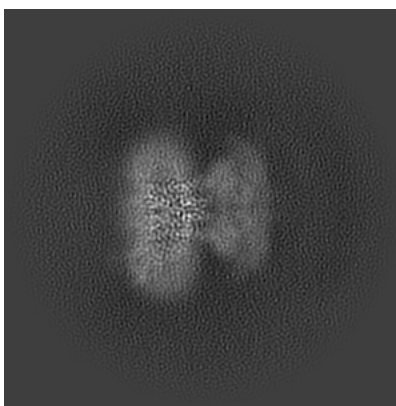
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

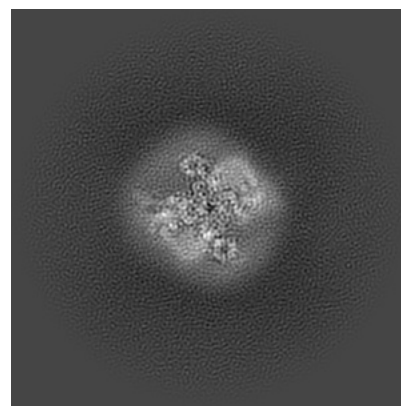
6.1.1 Primary map



X

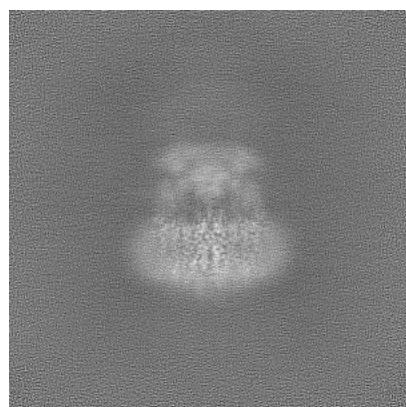


Y

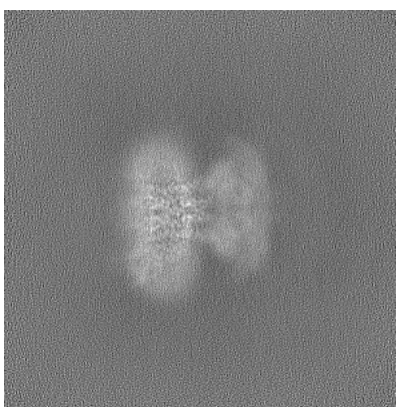


Z

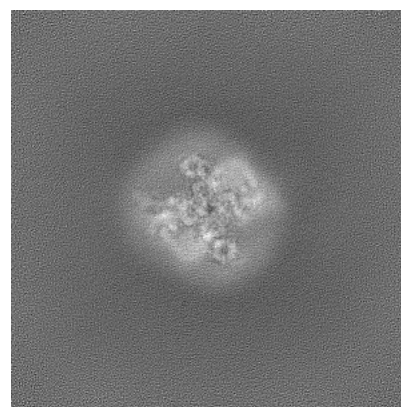
6.1.2 Raw map



X



Y

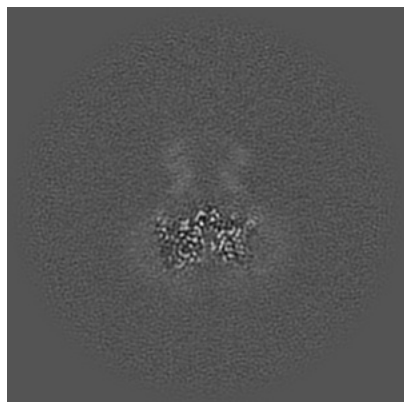


Z

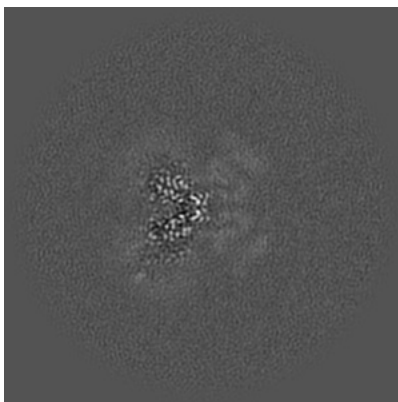
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

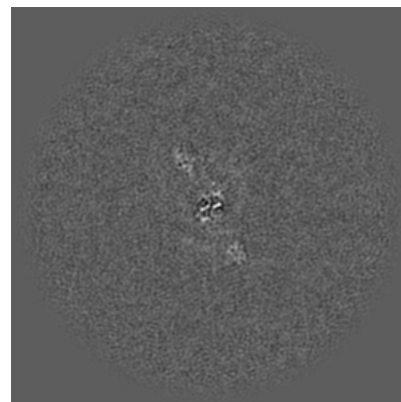
6.2.1 Primary map



X Index: 196

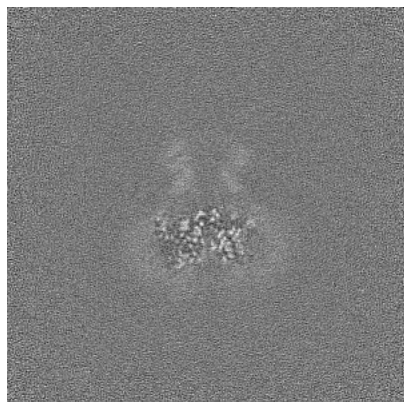


Y Index: 196

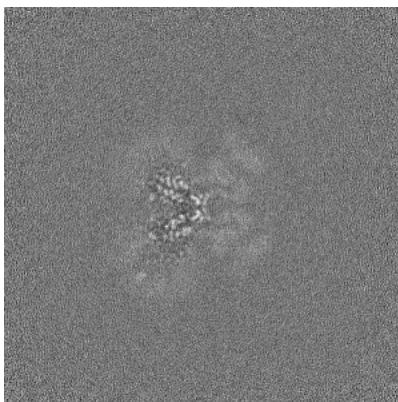


Z Index: 196

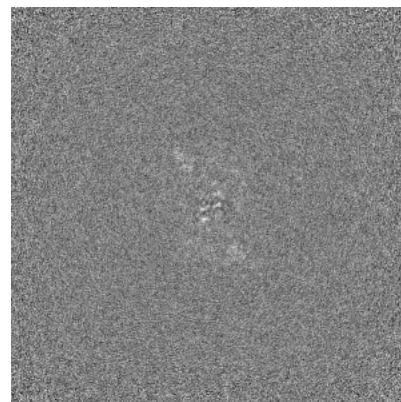
6.2.2 Raw map



X Index: 196



Y Index: 196

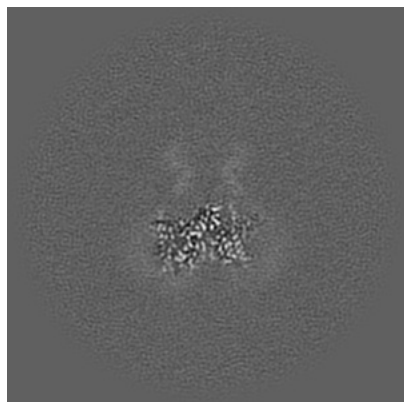


Z Index: 196

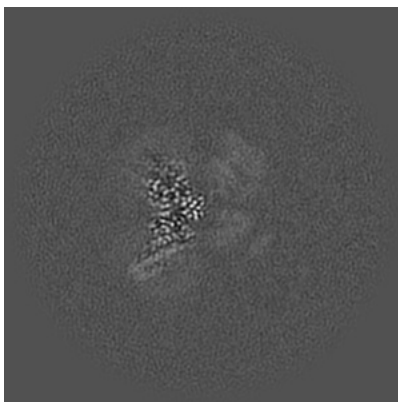
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

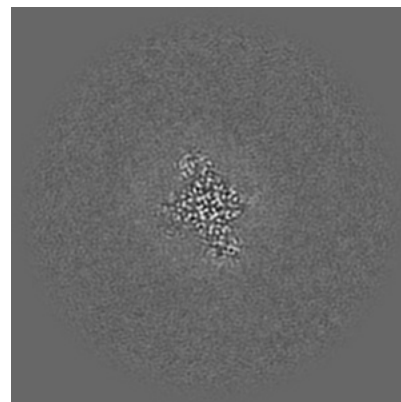
6.3.1 Primary map



X Index: 198

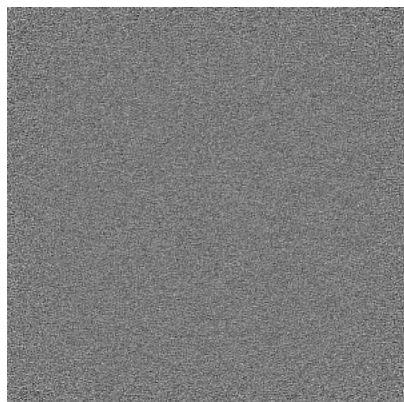


Y Index: 201

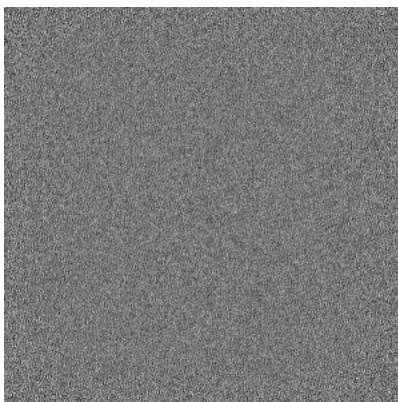


Z Index: 175

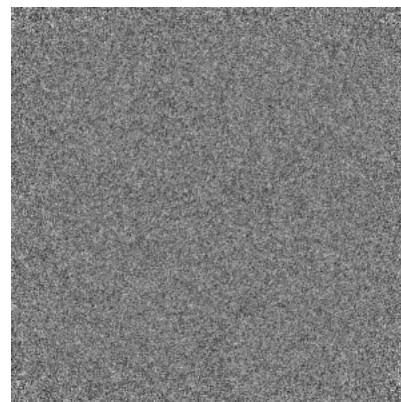
6.3.2 Raw map



X Index: 0



Y Index: 0

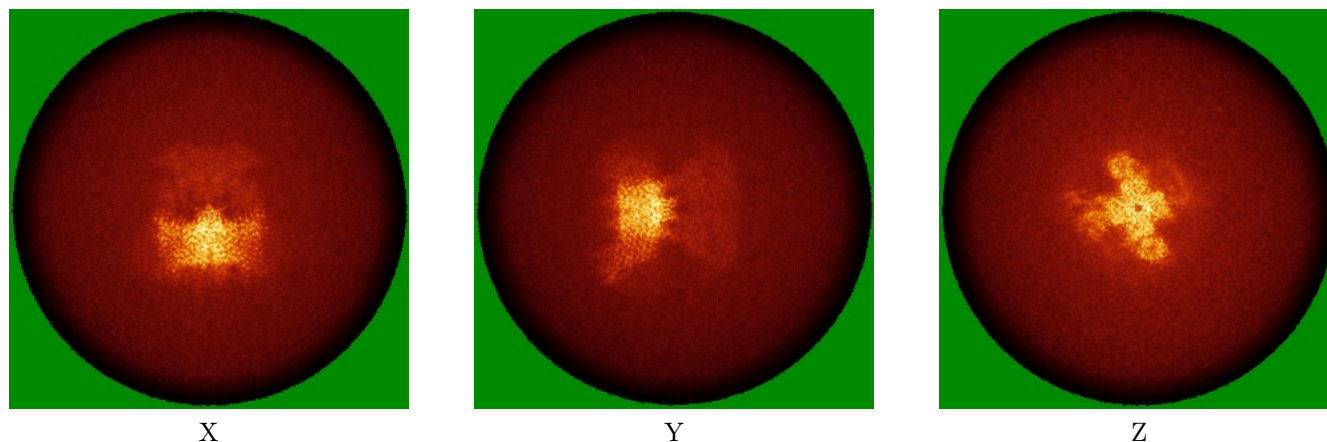


Z Index: 0

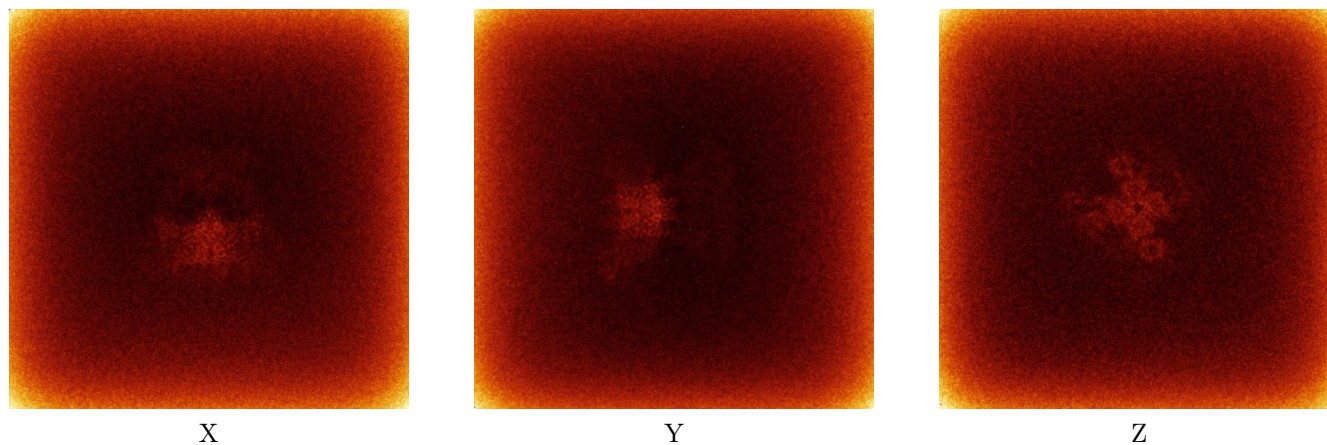
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



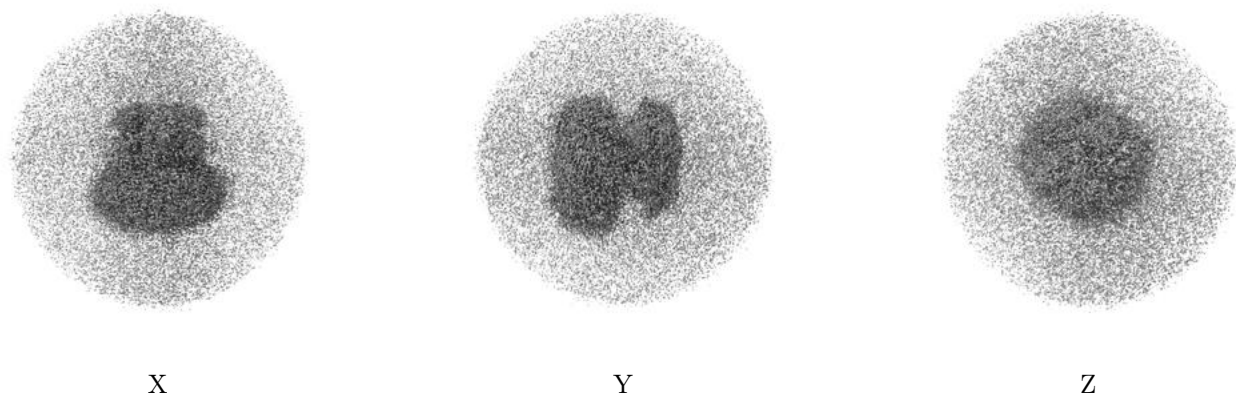
6.4.2 Raw map



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.

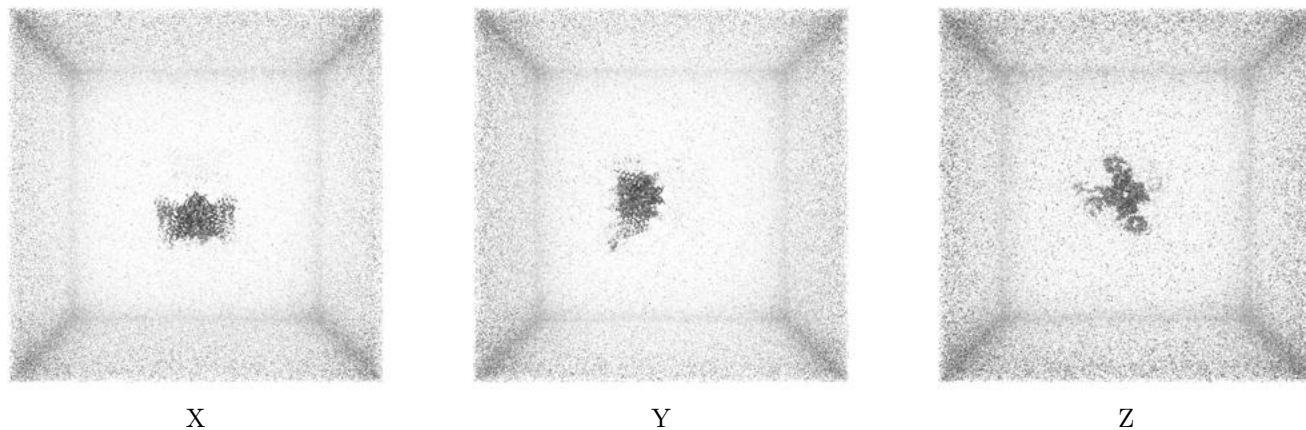
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

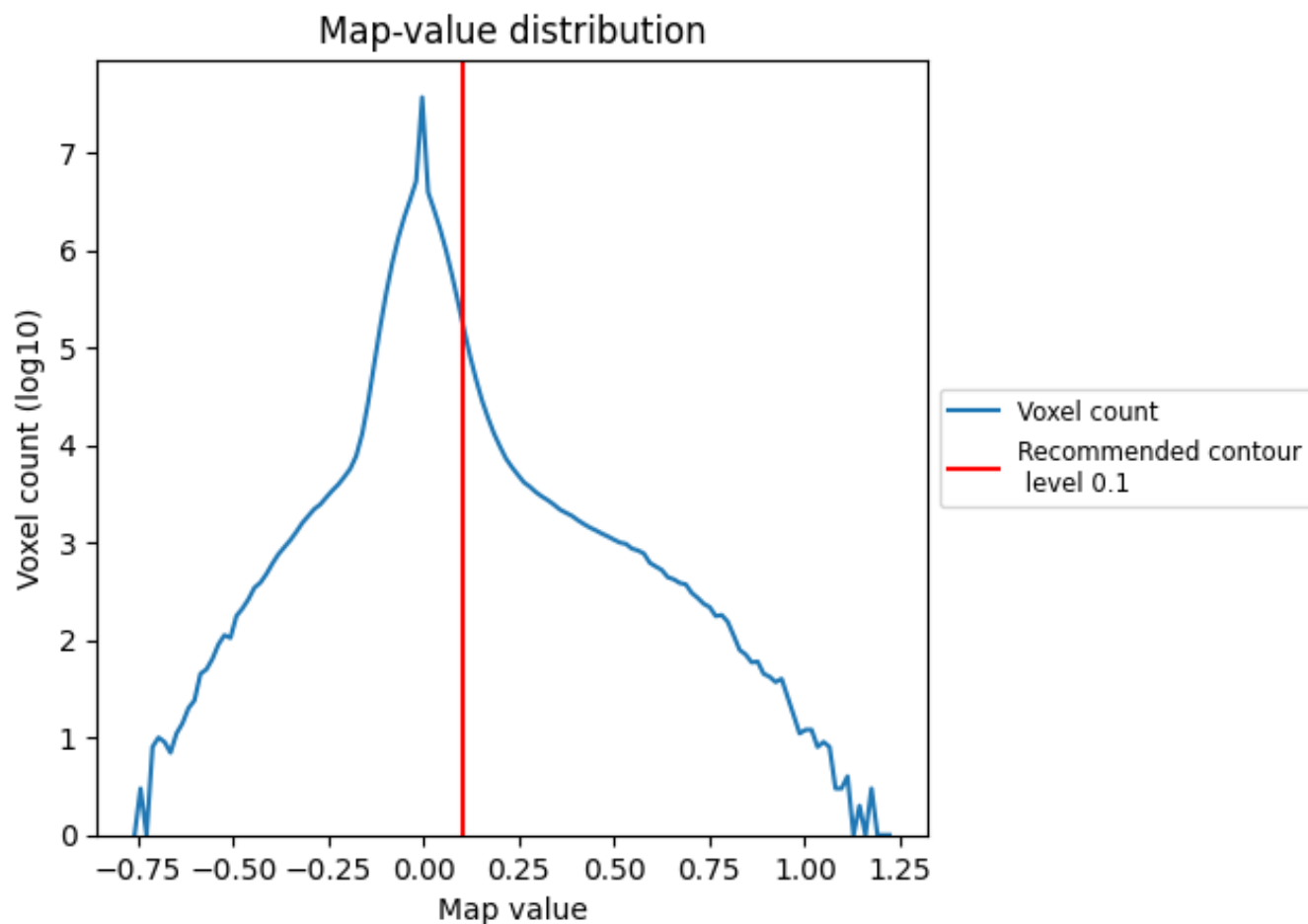
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

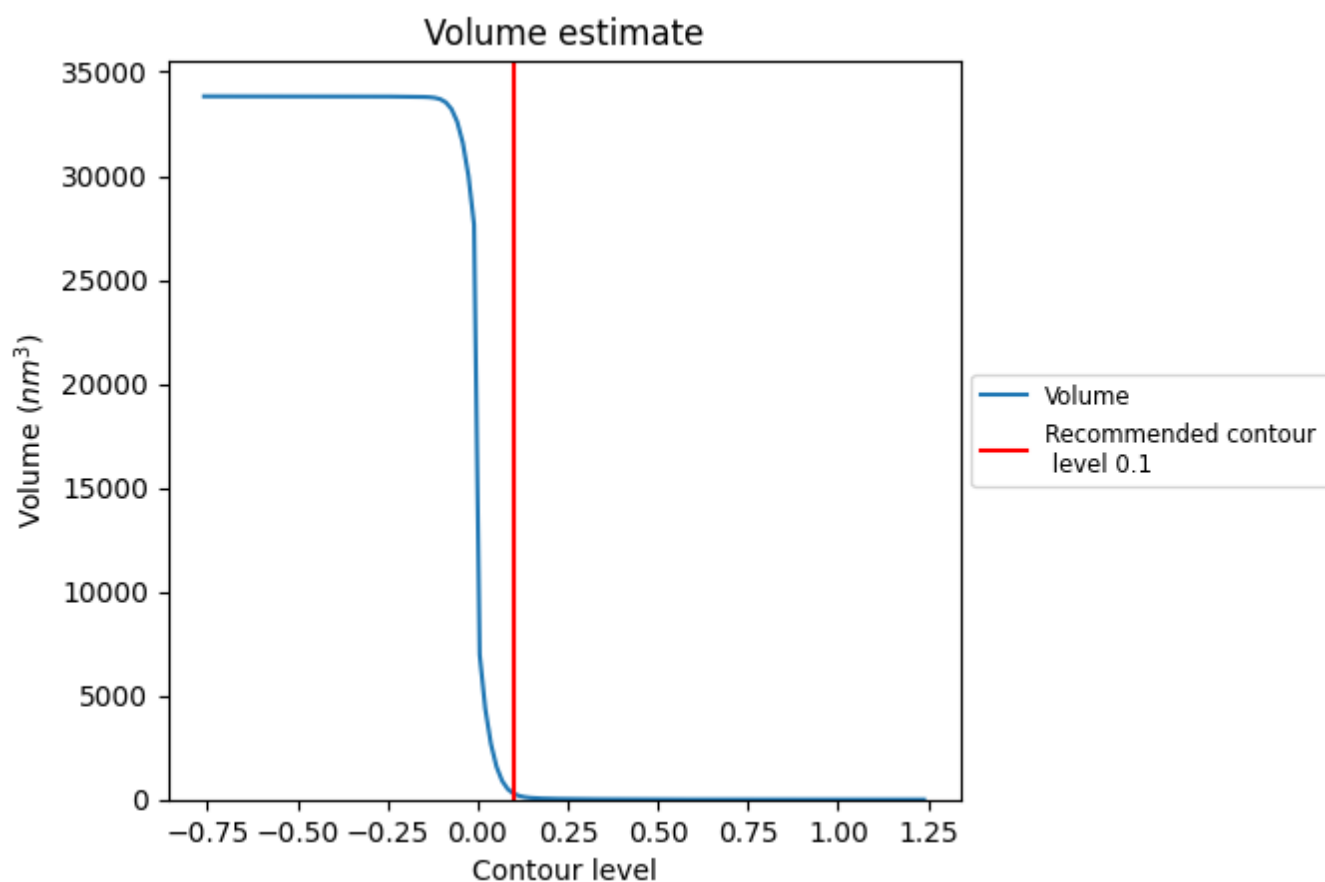
This section contains the results of statistical analysis of the map.

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.

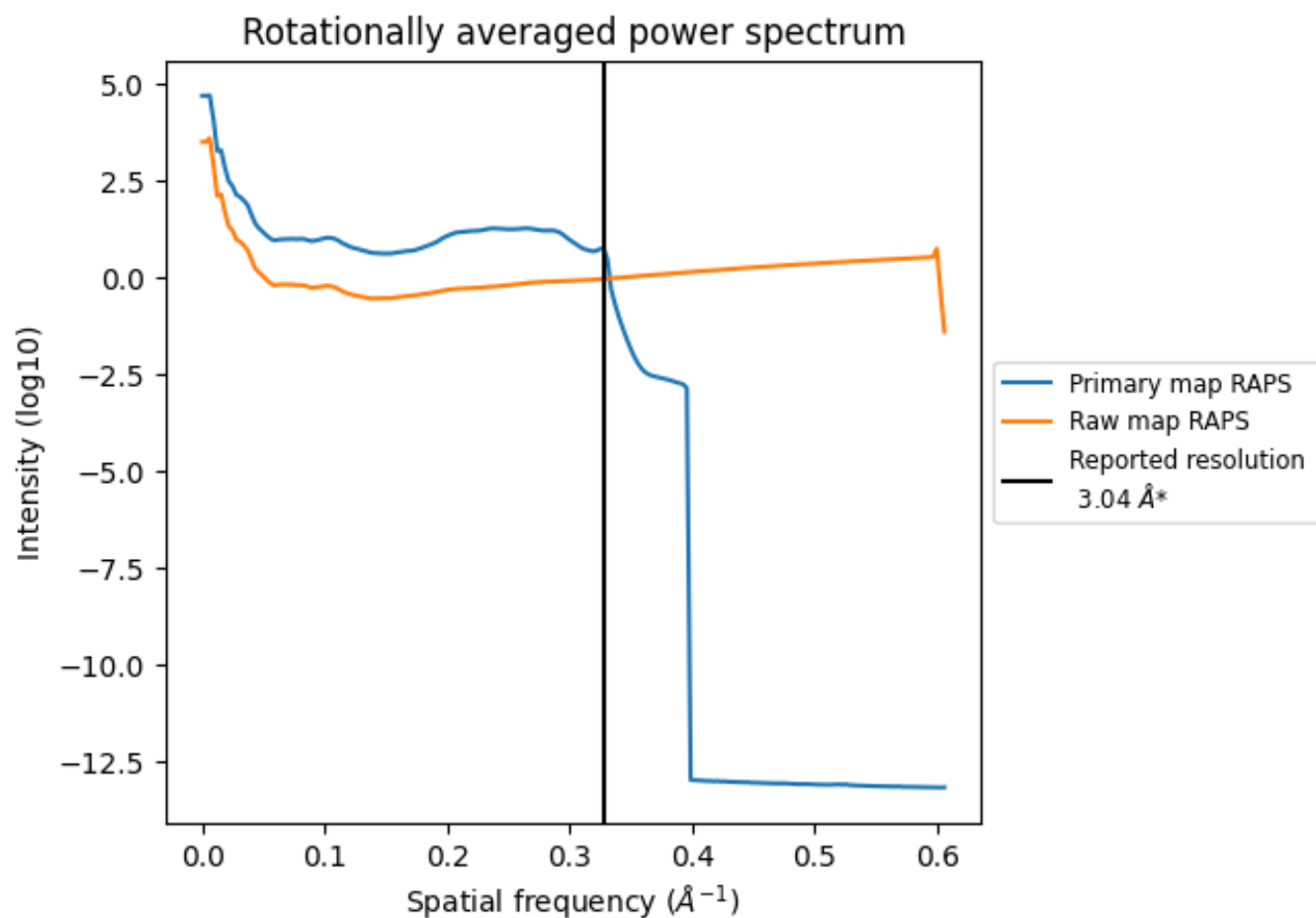
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 284 nm³; this corresponds to an approximate mass of 256 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 ⓘ

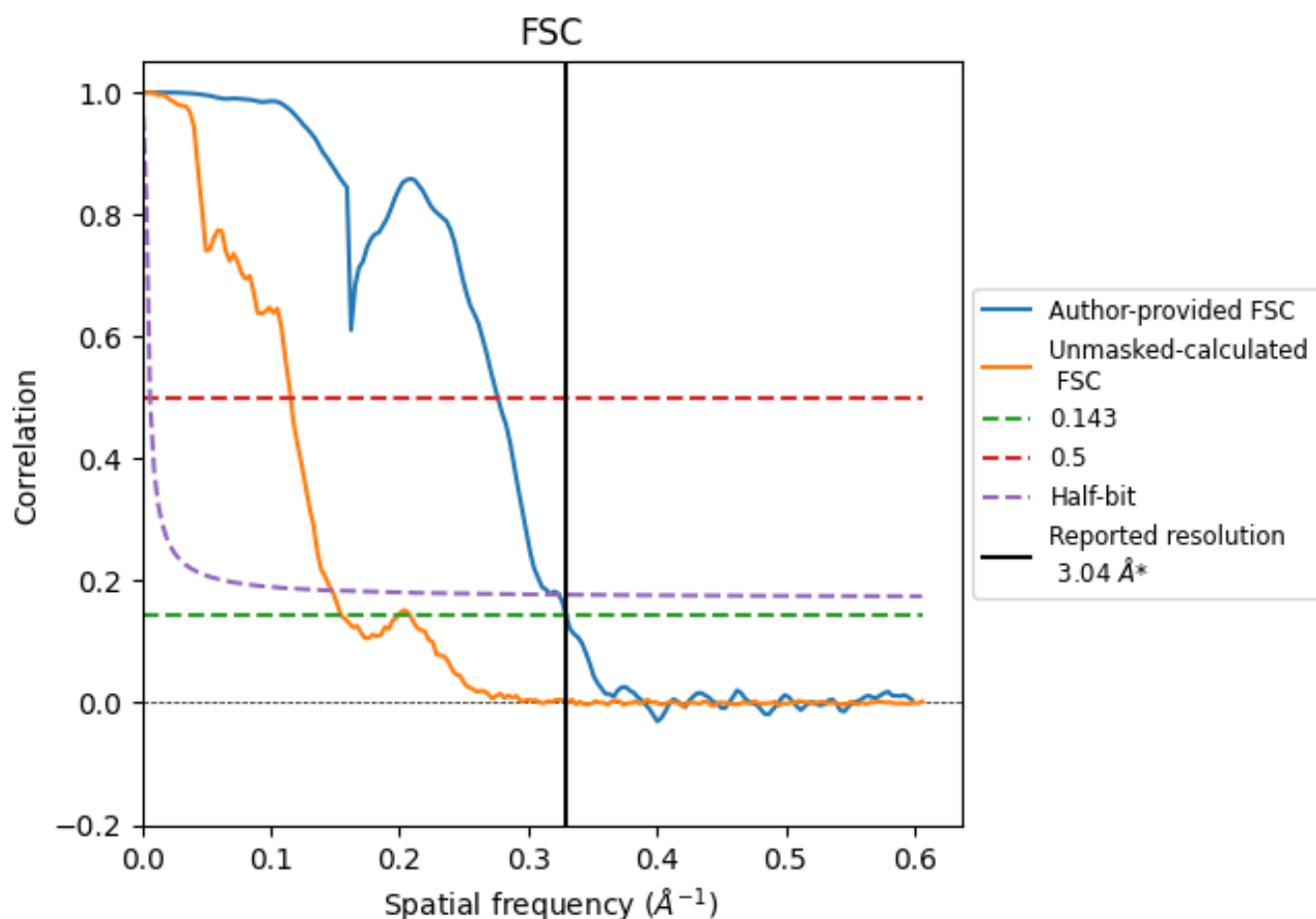


*Reported resolution corresponds to spatial frequency of 0.329 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.329 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

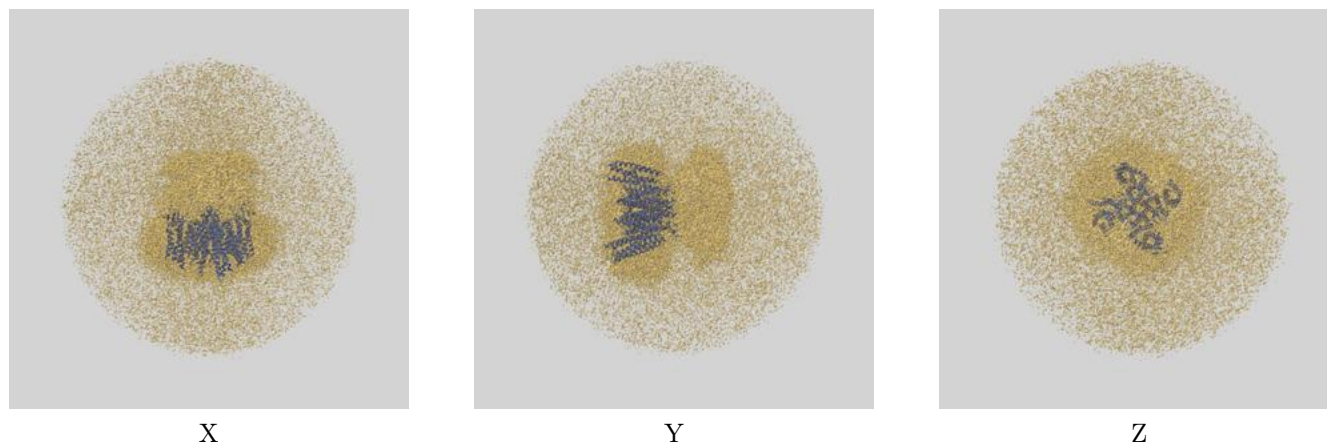
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.62	3.09
Unmasked-calculated*	6.47	8.67	6.78

*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 6.47 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

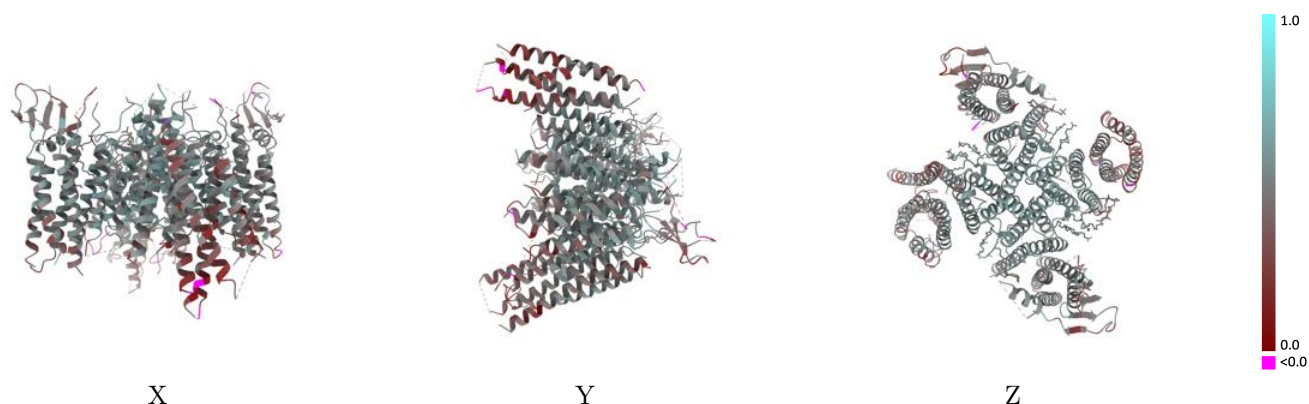
This section contains information regarding the fit between EMDB map EMD-74384 and PDB model 9ZKT. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



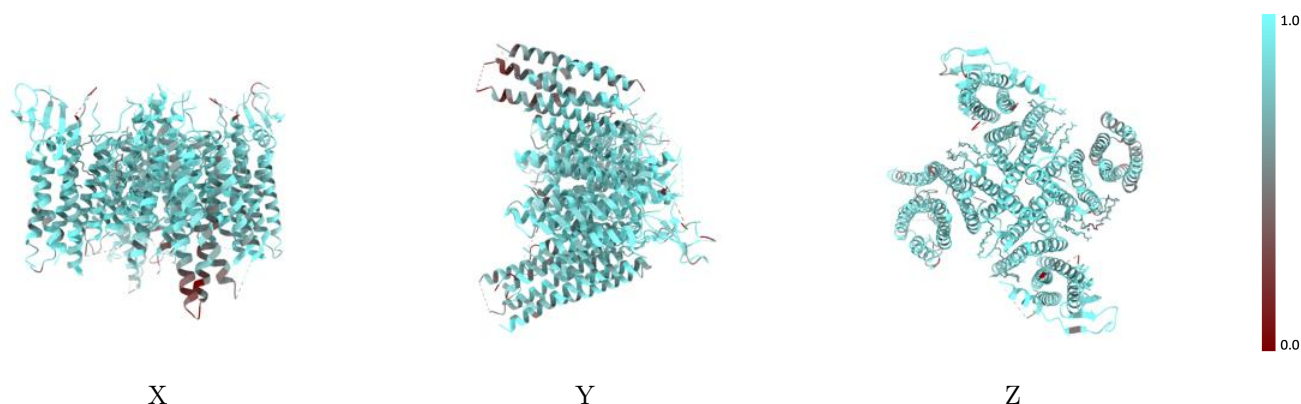
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



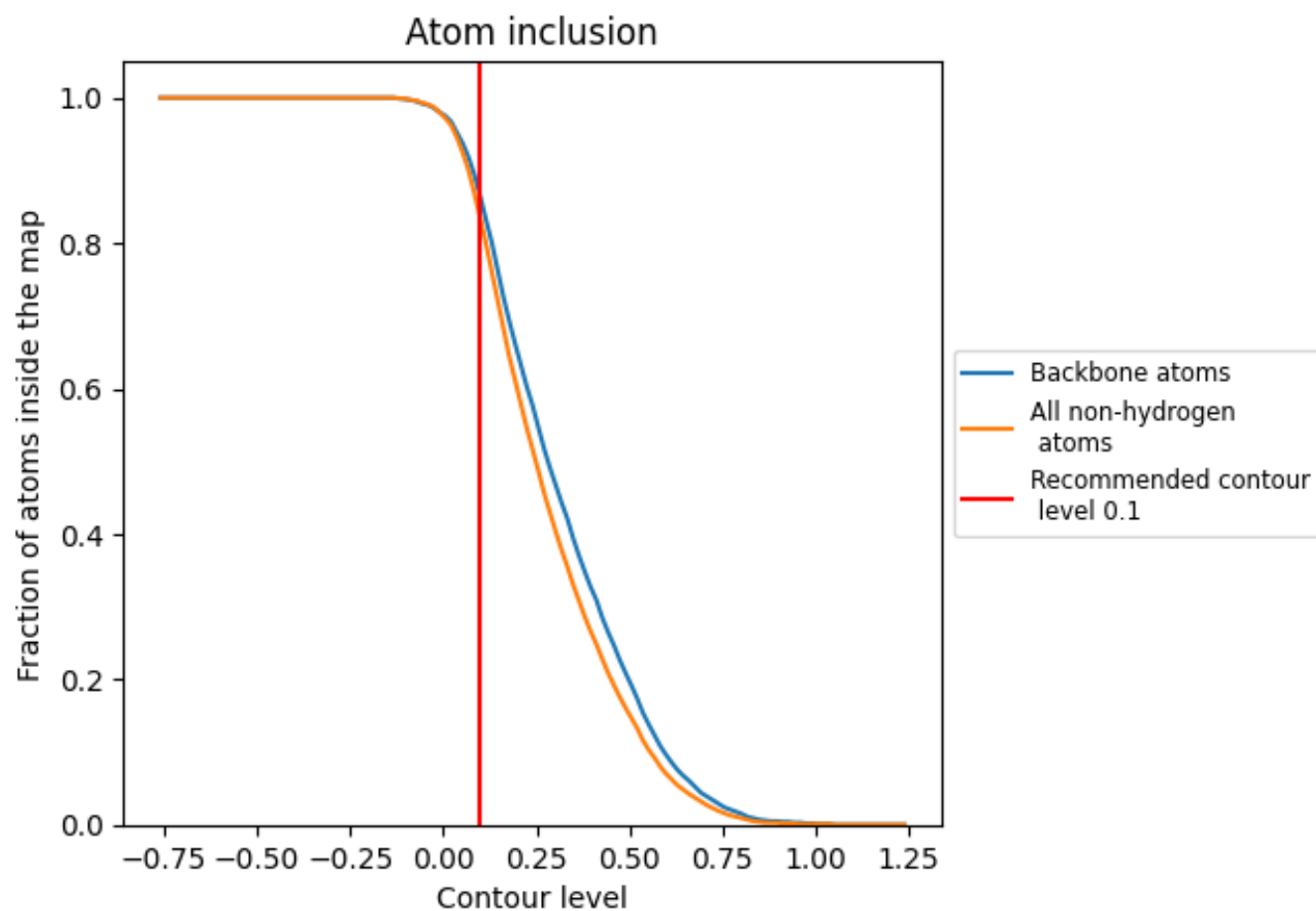
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 83% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8330	0.4720
A	0.8760	0.5280
B	0.8820	0.5170
C	0.8610	0.5080
D	0.8780	0.5240
E	0.6840	0.3550
F	0.8020	0.4300
G	0.8400	0.4670
H	0.8360	0.4550
M	0.7770	0.3650

