



Full wwPDB EM Validation Report ⓘ

Sep 30, 2023 – 07:25 am BST

PDB ID : 8C2H
EMDB ID : EMD-16390
Title : Transmembrane domain of active state homomeric GluA1 AMPA receptor in tandem with TARP gamma 3
Authors : Zhang, D.; Ivica, J.; Krieger, J.M.; Ho, H.; Yamashita, K.; Cais, O.; Greger, I.
Deposited on : 2022-12-22
Resolution : 2.64 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.dev50
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

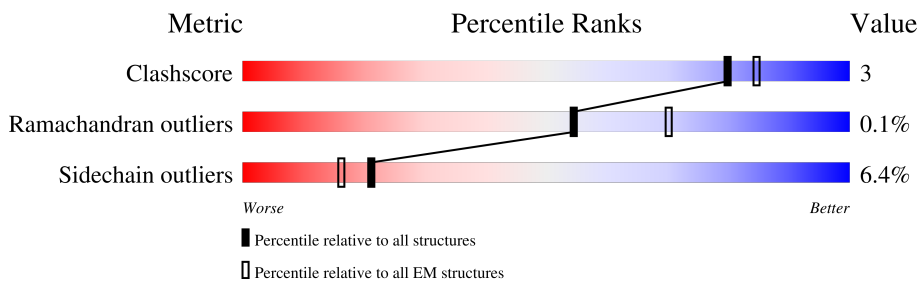
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.64 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	915	
1	B	915	
1	C	915	
1	D	915	
2	E	314	
2	F	314	
2	G	314	
2	H	314	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10071 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 flip isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	133	1037	697	157	176	7	4	0
1	B	134	1071	720	161	183	7	6	0
1	C	134	1043	700	158	178	7	4	0
1	D	141	1120	751	172	189	8	5	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	insertion	UNP P19490
A	-5	TYR	-	insertion	UNP P19490
A	-4	LYS	-	insertion	UNP P19490
A	-3	ASP	-	insertion	UNP P19490
A	-2	ASP	-	insertion	UNP P19490
A	-1	ASP	-	insertion	UNP P19490
A	0	ASP	-	insertion	UNP P19490
A	1	LYS	-	insertion	UNP P19490
B	-6	ASP	-	insertion	UNP P19490
B	-5	TYR	-	insertion	UNP P19490
B	-4	LYS	-	insertion	UNP P19490
B	-3	ASP	-	insertion	UNP P19490
B	-2	ASP	-	insertion	UNP P19490
B	-1	ASP	-	insertion	UNP P19490
B	0	ASP	-	insertion	UNP P19490
B	1	LYS	-	insertion	UNP P19490
C	-6	ASP	-	insertion	UNP P19490
C	-5	TYR	-	insertion	UNP P19490
C	-4	LYS	-	insertion	UNP P19490
C	-3	ASP	-	insertion	UNP P19490
C	-2	ASP	-	insertion	UNP P19490
C	-1	ASP	-	insertion	UNP P19490

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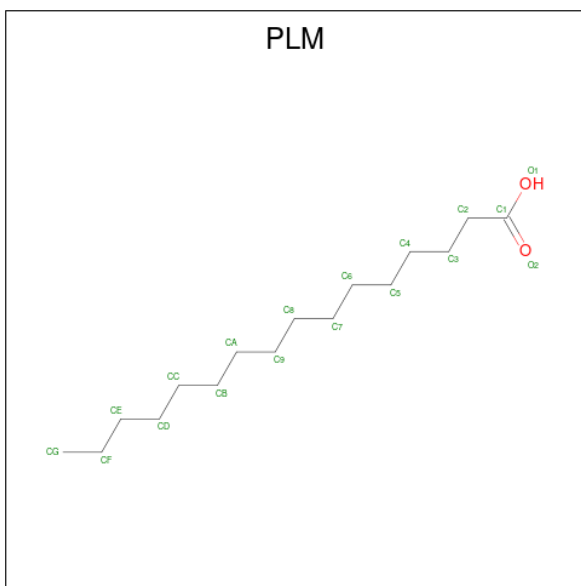
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ASP	-	insertion	UNP P19490
C	1	LYS	-	insertion	UNP P19490
D	-6	ASP	-	insertion	UNP P19490
D	-5	TYR	-	insertion	UNP P19490
D	-4	LYS	-	insertion	UNP P19490
D	-3	ASP	-	insertion	UNP P19490
D	-2	ASP	-	insertion	UNP P19490
D	-1	ASP	-	insertion	UNP P19490
D	0	ASP	-	insertion	UNP P19490
D	1	LYS	-	insertion	UNP P19490

- Molecule 2 is a protein called Voltage-dependent calcium channel gamma-3 subunit.

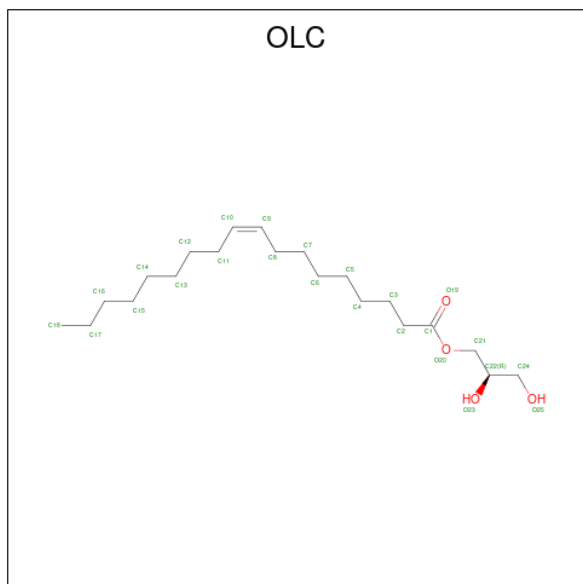
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	174	Total 1354	C 887	N 227	O 232	S 8	0	0
2	F	174	Total 1365	C 896	N 228	O 233	S 8	1	0
2	G	174	Total 1354	C 887	N 227	O 232	S 8	0	0
2	H	174	Total 1365	C 896	N 228	O 233	S 8	1	0

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



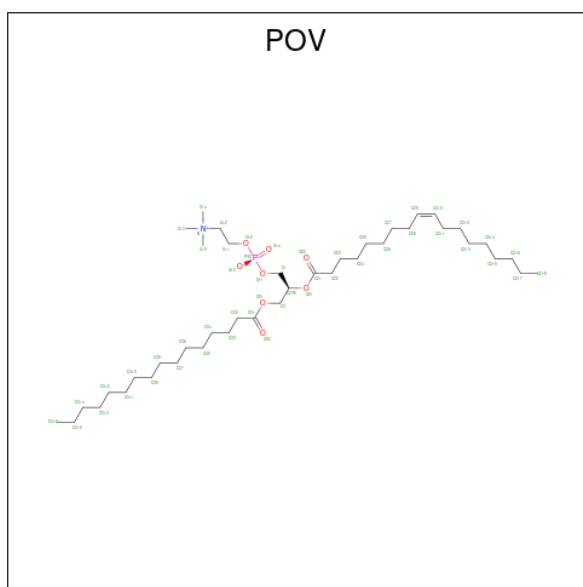
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			13	11	2	
3	B	1	Total	C	O	0
			14	12	2	
3	C	1	Total	C	O	0
			13	11	2	
3	D	1	Total	C	O	0
			14	12	2	
3	F	1	Total	C	O	0
			15	13	2	
3	H	1	Total	C	O	0
			15	13	2	

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			25	21	4	
4	B	1	Total	C	O	0
			25	21	4	
4	C	1	Total	C	O	0
			25	21	4	
4	D	1	Total	C	O	0
			25	21	4	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



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

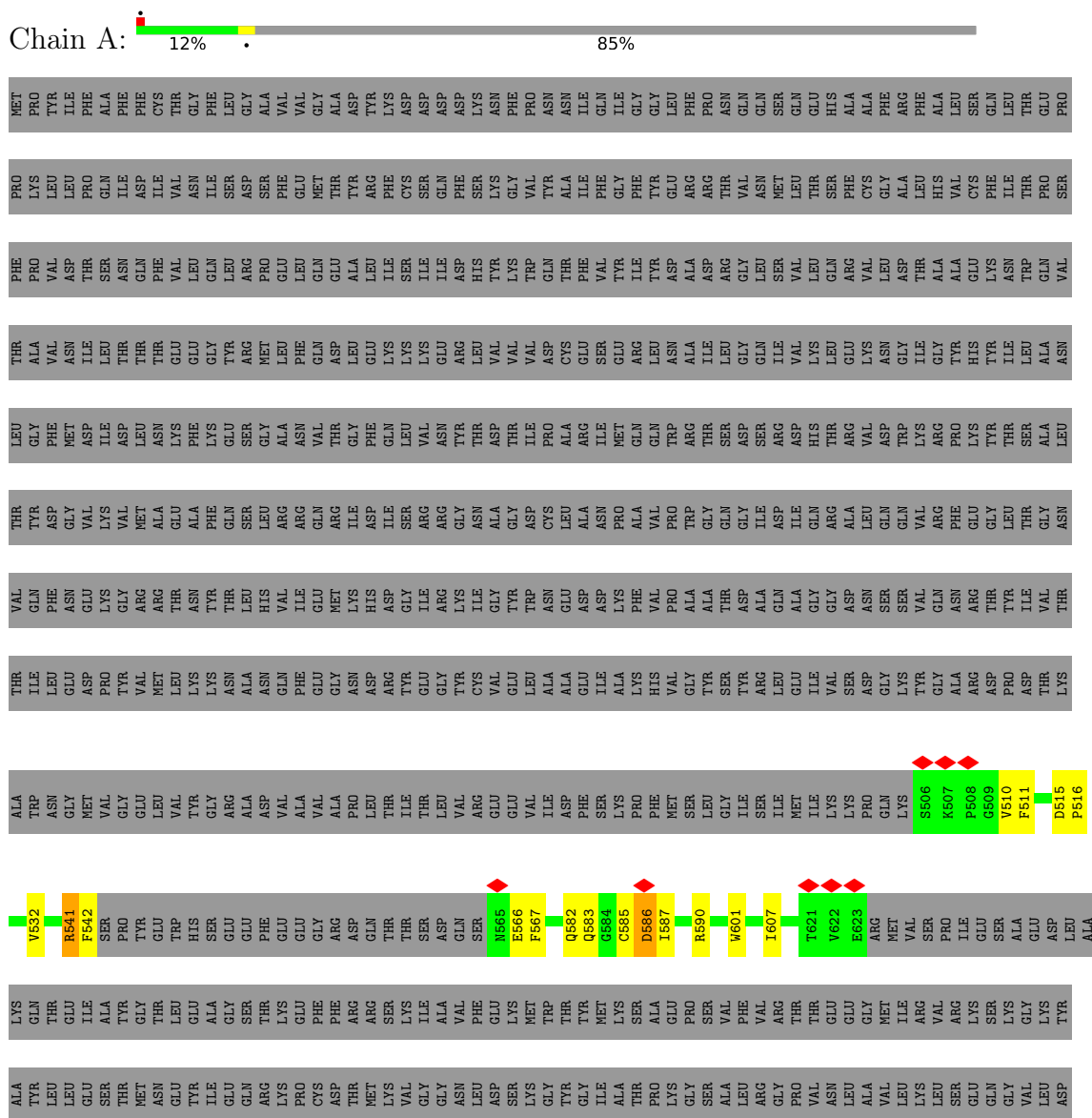
- Molecule 6 is water.

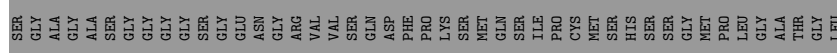
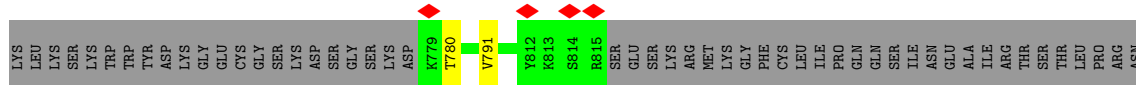
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
6	A	10	10	10	0
6	B	20	20	20	0
6	C	14	14	14	0
6	D	21	21	21	0
6	E	4	4	4	0
6	F	6	6	6	0
6	G	4	4	4	0
6	H	7	7	7	0

3 Residue-property plots i

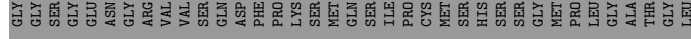
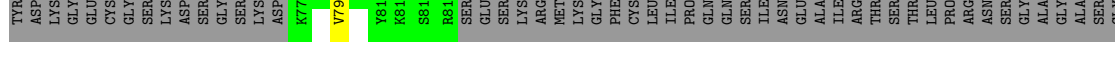
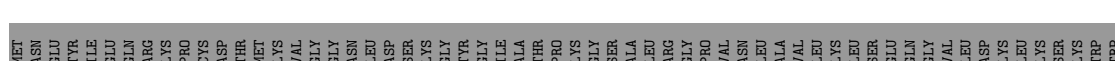
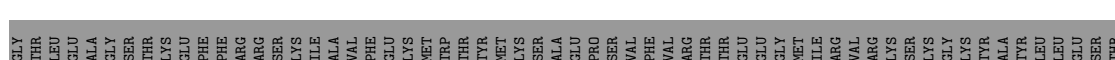
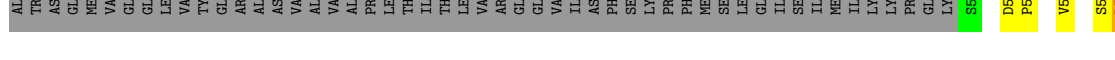
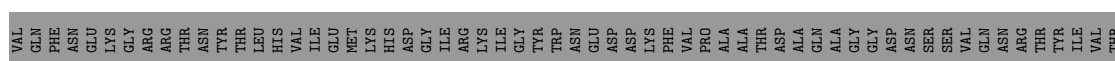
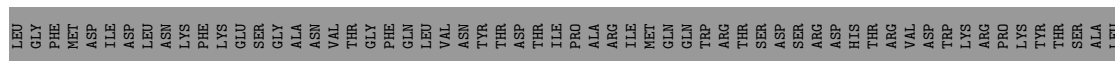
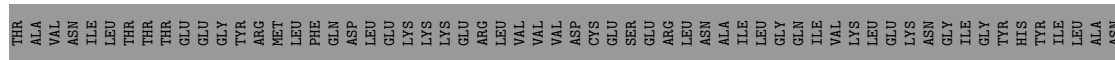
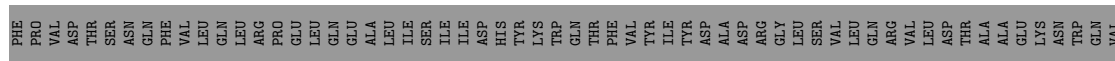
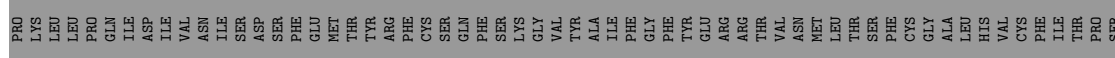
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Glutamate receptor 1 flip isoform





• Molecule 1: Glutamate receptor 1 flip isoform



• Molecule 1: Glutamate receptor 1 flip isoform

Chain C: 12% 85%

MET PRO TYR ILE PHE PHE PHE CYS THR GLY PHE LEU GLY ALA SER ASP VAL VAL VAL ALA ASP THR TYR

PRO LYS LEU LEU PRO GLN PHE ASP

PHE PRO VAL ASP THR SER ASN GLN PHE VAL VAL VAL LEU GLY LEU ARG PRO SER VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL

THR ALA VAL ASN ILE LEU THR THR THR LEU THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR

LEU PHE MET ASP ILE ASP LEU ASN ASN PHE PHE LEU SER GLY GLY THR ARG LEU ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP

THR TYR ASP GLY VAL LYS VAL

VAL GLN PHE ASN GLU ASP VAL THR

THR ILE LEU GLU ASP VAL TYR VAL MET TYR VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL

ALA TRP ASN GLY MET VAL GLU LEU VAL THR TYR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR THR

V532 S540 R541 F542 S543 V532 S540 R541 F542 S543 V532 S540 R541 F542 S543 V532 S540 R541 F542 S543 V532 S540 R541 F542 S543

ALA LYS THR

TYR ALA TYR LEU

ASP LYS LEU SER TRP TYR ASP GLY CYS GLY SER ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP

ASN SER GLY ALA

• Molecule 1: Glutamate receptor 1 flip isoform

Chain D: 13% 85%

MET PRO TYR ILE PHE PHE PHE CYS THR GLY PHE LEU GLY ALA SER ASP VAL VAL VAL ALA ASP THR TYR

PRO LYS LEU LEU PRO GLN PHE ASP

PHE PRO VAL ASP THR SER ASN GLN PHE VAL VAL VAL LEU GLY LEU ARG PRO SER VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	247485	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)	1400	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.078	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	252.756, 252.756, 252.756	wwPDB
Map dimensions	306, 306, 306	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	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: OLC, POV, PLM

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	0.45	0/1064	0.72	0/1448
1	B	0.46	0/1099	0.68	0/1493
1	C	0.45	0/1070	0.69	0/1456
1	D	0.44	0/1149	0.75	2/1558 (0.1%)
2	E	0.37	0/1386	0.68	0/1874
2	F	0.38	0/1398	0.70	0/1890
2	G	0.37	0/1386	0.68	0/1874
2	H	0.39	0/1398	0.68	0/1890
All	All	0.41	0/9950	0.70	2/13483 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	624	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	624	ARG	NE-CZ-NH1	5.35	122.97	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1037	0	1011	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1071	0	1053	12	0
1	C	1043	0	1016	12	0
1	D	1120	0	1110	11	0
2	E	1354	0	1346	6	0
2	F	1365	0	1354	3	0
2	G	1354	0	1346	3	0
2	H	1365	0	1354	6	0
3	A	13	0	18	0	0
3	B	14	0	20	0	0
3	C	13	0	18	0	0
3	D	14	0	20	0	0
3	F	15	0	22	0	0
3	H	15	0	22	0	0
4	A	25	0	40	0	0
4	B	25	0	40	0	0
4	C	25	0	40	0	0
4	D	25	0	40	0	0
5	E	46	0	69	0	0
5	G	46	0	69	0	0
6	A	10	0	0	0	0
6	B	20	0	0	2	0
6	C	14	0	0	1	0
6	D	21	0	0	0	0
6	E	4	0	0	0	0
6	F	6	0	0	0	0
6	G	4	0	0	0	0
6	H	7	0	0	1	0
All	All	10071	0	10008	54	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 3.

All (54) 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:541:ARG:NH1	1:A:566:GLU:HB2	2.13	0.64
2:G:30:THR:HG21	2:G:177:TRP:CH2	2.35	0.61
2:E:30:THR:HG21	2:E:177:TRP:CH2	2.36	0.61
2:F:60:HIS:HD2	2:F:69:LEU:HD13	1.67	0.60
1:B:586[A]:ASP:O	1:B:587[A]:ILE:HG23	2.02	0.60
1:B:541:ARG:NH1	1:B:566:GLU:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82:HIS:ND1	6:H:1701:HOH:O	2.32	0.59
2:H:30:THR:HG21	2:H:177:TRP:HH2	1.67	0.59
1:A:586[B]:ASP:OD2	1:A:586[B]:ASP:N	2.35	0.59
1:D:541:ARG:NH1	1:D:566:GLU:OE1	2.35	0.59
2:F:30:THR:HG21	2:F:177:TRP:HH2	1.68	0.58
2:F:68:CYS:SG	2:F:73:PHE:O	2.62	0.57
2:H:68:CYS:SG	2:H:73:PHE:O	2.63	0.56
1:D:541:ARG:HG2	2:E:201:ILE:HD11	1.89	0.55
1:C:510:VAL:HG13	1:C:511:PHE:CD1	2.42	0.54
1:A:541:ARG:HH11	1:A:566:GLU:HB2	1.72	0.54
1:D:584[B]:GLY:O	1:D:585[B]:CYS:HB3	2.08	0.54
1:A:510:VAL:HG13	1:A:511:PHE:CD1	2.43	0.53
1:A:607:ILE:HG21	1:B:791:VAL:HG21	1.90	0.53
1:B:618:ALA:N	6:B:1501:HOH:O	2.42	0.51
1:C:607:ILE:HG21	1:D:791:VAL:HG21	1.92	0.50
1:B:602:TRP:CG	1:C:583[B]:GLN:HG3	2.47	0.50
2:H:66:THR:HG23	2:H:78:LYS:HG3	1.94	0.49
1:A:583[B]:GLN:HG3	1:D:602:TRP:CG	2.48	0.49
1:D:532:VAL:HG21	1:D:601:TRP:CE3	2.48	0.49
1:A:532:VAL:HG21	1:A:601:TRP:CE3	2.48	0.48
1:C:541:ARG:NH1	1:C:566:GLU:OE2	2.46	0.48
1:B:540:SER:C	1:B:542:PHE:H	2.15	0.48
1:C:532:VAL:HG21	1:C:601:TRP:CE3	2.48	0.48
1:B:532:VAL:HG21	1:B:601:TRP:CE3	2.49	0.47
2:G:30:THR:HG21	2:G:177:TRP:CZ2	2.51	0.46
2:G:30:THR:HG22	2:G:31:ASP:H	1.81	0.46
1:A:585[B]:CYS:HB2	1:A:587:ILE:O	2.15	0.46
1:C:541:ARG:NH2	6:C:1502:HOH:O	2.49	0.46
1:D:542:PHE:O	1:D:543:SER:HB2	2.17	0.45
2:E:30:THR:HG22	2:E:31:ASP:H	1.81	0.45
2:E:30:THR:HG21	2:E:177:TRP:CZ2	2.50	0.45
1:A:515:ASP:N	1:A:516:PRO:CD	2.81	0.44
1:A:541:ARG:HH11	1:A:567:PHE:H	1.64	0.44
1:B:541:ARG:NH2	6:B:1502:HOH:O	2.50	0.44
1:B:602:TRP:CD1	1:C:583[B]:GLN:HG3	2.53	0.43
1:C:542:PHE:HE2	2:H:136:LEU:HD11	1.83	0.43
1:C:540:SER:C	1:C:542:PHE:H	2.22	0.43
1:C:585[B]:CYS:HB2	1:C:587:ILE:O	2.18	0.43
1:D:515:ASP:N	1:D:516:PRO:CD	2.81	0.43
1:D:538:LEU:HD11	2:E:140:ILE:CD1	2.48	0.43
1:B:515:ASP:N	1:B:516:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:ARG:HD2	1:C:570:PHE:CZ	2.55	0.42
1:C:515:ASP:N	1:C:516:PRO:CD	2.83	0.42
1:D:584[B]:GLY:O	1:D:585[B]:CYS:CB	2.65	0.41
2:H:40:CYS:HA	2:H:78:LYS:HG2	2.01	0.41
2:E:65:ARG:HB3	2:E:77:CYS:SG	2.61	0.40
1:A:583[B]:GLN:HG3	1:D:602:TRP:CD1	2.56	0.40
1:B:585[A]:CYS:SG	1:B:587[A]:ILE:HG13	2.61	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	131/915 (14%)	125 (95%)	6 (5%)	0	100	100
1	B	134/915 (15%)	126 (94%)	8 (6%)	0	100	100
1	C	132/915 (14%)	125 (95%)	7 (5%)	0	100	100
1	D	140/915 (15%)	131 (94%)	7 (5%)	2 (1%)	11	15
2	E	166/314 (53%)	165 (99%)	1 (1%)	0	100	100
2	F	167/314 (53%)	166 (99%)	1 (1%)	0	100	100
2	G	166/314 (53%)	165 (99%)	1 (1%)	0	100	100
2	H	167/314 (53%)	166 (99%)	1 (1%)	0	100	100
All	All	1203/4916 (24%)	1169 (97%)	32 (3%)	2 (0%)	54	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	585[A]	CYS
1	D	585[B]	CYS

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	106/778 (14%)	98 (92%)	8 (8%)	13	20
1	B	112/778 (14%)	106 (95%)	6 (5%)	22	35
1	C	107/778 (14%)	100 (94%)	7 (6%)	17	26
1	D	117/778 (15%)	109 (93%)	8 (7%)	16	24
2	E	141/273 (52%)	133 (94%)	8 (6%)	20	31
2	F	142/273 (52%)	132 (93%)	10 (7%)	15	23
2	G	141/273 (52%)	133 (94%)	8 (6%)	20	31
2	H	142/273 (52%)	131 (92%)	11 (8%)	13	19
All	All	1008/4204 (24%)	942 (94%)	66 (6%)	21	26

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	541	ARG
1	A	542	PHE
1	A	582	GLN
1	A	586[A]	ASP
1	A	586[B]	ASP
1	A	590	ARG
1	A	780	THR
1	A	791	VAL
1	B	541	ARG
1	B	543	SER
1	B	566	GLU
1	B	587[A]	ILE
1	B	587[B]	ILE
1	B	590	ARG
1	C	542	PHE
1	C	582	GLN
1	C	586[A]	ASP
1	C	586[B]	ASP
1	C	590	ARG

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Mol	Chain	Res	Type
1	C	780	THR
1	C	791	VAL
1	D	504	GLN
1	D	505	LYS
1	D	541	ARG
1	D	542	PHE
1	D	566	GLU
1	D	590	ARG
1	D	624	ARG
1	D	780	THR
2	E	5	ASP
2	E	30	THR
2	E	31	ASP
2	E	37	ARG
2	E	41	ARG
2	E	58	MET
2	E	120	LEU
2	E	203	LYS
2	F	68	CYS
2	F	74	ARG
2	F	78	LYS
2	F	120	LEU
2	F	128	HIS
2	F	174	SER
2	F	203	LYS
2	F	206	GLN
2	F	207	LEU
2	F	208	ARG
2	G	5	ASP
2	G	30	THR
2	G	31	ASP
2	G	37	ARG
2	G	41	ARG
2	G	58	MET
2	G	120	LEU
2	G	203	LYS
2	H	66	THR
2	H	68	CYS
2	H	74	ARG
2	H	79	LYS
2	H	99	ARG
2	H	120	LEU

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Mol	Chain	Res	Type
2	H	132	HIS
2	H	174	SER
2	H	206	GLN
2	H	207	LEU
2	H	208	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	160	ASN
2	F	204	HIS
2	F	206	GLN
2	G	160	ASN
2	H	132	HIS
2	H	204	HIS
2	H	206	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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
3	PLM	A	1401	-	12,12,17	0.62	0	12,12,17	0.79	0
3	PLM	C	1401	-	12,12,17	0.64	0	12,12,17	0.66	0
3	PLM	B	1401	-	13,13,17	0.60	0	13,13,17	0.66	0
4	OLC	B	1402	-	24,24,24	0.31	0	25,25,25	0.67	0
3	PLM	D	1401	-	13,13,17	0.59	0	13,13,17	0.64	0
4	OLC	C	1402	-	24,24,24	0.26	0	25,25,25	0.39	0
5	POV	G	401	-	45,45,51	0.41	0	49,50,59	0.65	1 (2%)
4	OLC	A	1402	-	24,24,24	0.25	0	25,25,25	0.40	0
3	PLM	F	1601	-	14,14,17	0.49	0	14,14,17	0.65	0
5	POV	E	401	-	45,45,51	0.41	0	49,50,59	0.63	1 (2%)
3	PLM	H	1601	-	14,14,17	0.53	0	14,14,17	0.65	0
4	OLC	D	1402	-	24,24,24	0.37	0	25,25,25	0.70	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLM	A	1401	-	-	6/10/10/15	-
3	PLM	C	1401	-	-	5/10/10/15	-
3	PLM	B	1401	-	-	9/11/11/15	-
4	OLC	B	1402	-	-	14/24/24/24	-
3	PLM	D	1401	-	-	10/11/11/15	-
4	OLC	C	1402	-	-	6/24/24/24	-
5	POV	G	401	-	-	14/47/47/55	-
4	OLC	A	1402	-	-	8/24/24/24	-
3	PLM	F	1601	-	-	6/12/12/15	-
5	POV	E	401	-	-	14/47/47/55	-
3	PLM	H	1601	-	-	7/12/12/15	-
4	OLC	D	1402	-	-	14/24/24/24	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	401	POV	O13-P-O14	2.38	119.99	110.68
5	G	401	POV	O13-P-O14	2.33	119.81	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1402	OLC	O20-C1-C2	2.10	118.48	111.91

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1402	OLC	O20-C21-C22-O23
4	B	1402	OLC	C2-C1-O20-C21
4	B	1402	OLC	O19-C1-O20-C21
4	D	1402	OLC	O20-C21-C22-O23
4	D	1402	OLC	C2-C1-O20-C21
4	D	1402	OLC	O19-C1-O20-C21
5	E	401	POV	C1-O11-P-O14
5	G	401	POV	C1-O11-P-O14
5	G	401	POV	C21-C22-C23-C24
3	B	1401	PLM	C4-C5-C6-C7
4	A	1402	OLC	C11-C12-C13-C14
4	C	1402	OLC	C11-C12-C13-C14
4	B	1402	OLC	O20-C21-C22-C24
4	D	1402	OLC	O20-C21-C22-C24
5	E	401	POV	C311-C312-C313-C314
3	F	1601	PLM	C5-C6-C7-C8
3	D	1401	PLM	C4-C5-C6-C7
4	A	1402	OLC	C5-C6-C7-C8
3	H	1601	PLM	C5-C6-C7-C8
5	E	401	POV	C21-C22-C23-C24
5	E	401	POV	C31-C32-C33-C34
3	F	1601	PLM	C4-C5-C6-C7
3	H	1601	PLM	C4-C5-C6-C7
5	E	401	POV	C310-C311-C312-C313
4	D	1402	OLC	C11-C12-C13-C14
5	G	401	POV	C310-C311-C312-C313
5	G	401	POV	C311-C312-C313-C314
3	D	1401	PLM	C3-C4-C5-C6
4	D	1402	OLC	C2-C3-C4-C5
3	B	1401	PLM	C3-C4-C5-C6
4	B	1402	OLC	C11-C12-C13-C14
5	G	401	POV	C31-C32-C33-C34
5	G	401	POV	C212-C213-C214-C215
3	A	1401	PLM	C6-C7-C8-C9
3	D	1401	PLM	C7-C8-C9-CA
4	C	1402	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
4	B	1402	OLC	C3-C4-C5-C6
4	A	1402	OLC	C14-C15-C16-C17
3	B	1401	PLM	C7-C8-C9-CA
3	C	1401	PLM	C3-C4-C5-C6
4	D	1402	OLC	C12-C13-C14-C15
5	G	401	POV	C35-C36-C37-C38
4	B	1402	OLC	C2-C3-C4-C5
3	D	1401	PLM	C2-C3-C4-C5
4	A	1402	OLC	C10-C11-C12-C13
3	A	1401	PLM	C3-C4-C5-C6
5	E	401	POV	C212-C213-C214-C215
4	C	1402	OLC	C9-C10-C11-C12
5	E	401	POV	C23-C24-C25-C26
3	B	1401	PLM	C2-C3-C4-C5
5	G	401	POV	C33-C34-C35-C36
4	B	1402	OLC	C12-C13-C14-C15
3	H	1601	PLM	C8-C9-CA-CB
5	G	401	POV	C23-C24-C25-C26
3	F	1601	PLM	CA-CB-CC-CD
4	A	1402	OLC	C6-C7-C8-C9
3	F	1601	PLM	C1-C2-C3-C4
3	D	1401	PLM	C6-C7-C8-C9
4	A	1402	OLC	C9-C10-C11-C12
3	B	1401	PLM	C6-C7-C8-C9
4	B	1402	OLC	C15-C16-C17-C18
5	E	401	POV	C35-C36-C37-C38
3	A	1401	PLM	C1-C2-C3-C4
3	H	1601	PLM	C1-C2-C3-C4
4	D	1402	OLC	C15-C16-C17-C18
3	C	1401	PLM	C4-C5-C6-C7
4	B	1402	OLC	C6-C7-C8-C9
3	C	1401	PLM	C6-C7-C8-C9
5	E	401	POV	C33-C34-C35-C36
4	C	1402	OLC	C5-C6-C7-C8
4	D	1402	OLC	C3-C4-C5-C6
4	C	1402	OLC	C14-C15-C16-C17
3	F	1601	PLM	C9-CA-CB-CC
5	G	401	POV	C211-C212-C213-C214
5	E	401	POV	C211-C212-C213-C214
3	H	1601	PLM	CA-CB-CC-CD
4	D	1402	OLC	C6-C7-C8-C9
3	B	1401	PLM	C1-C2-C3-C4

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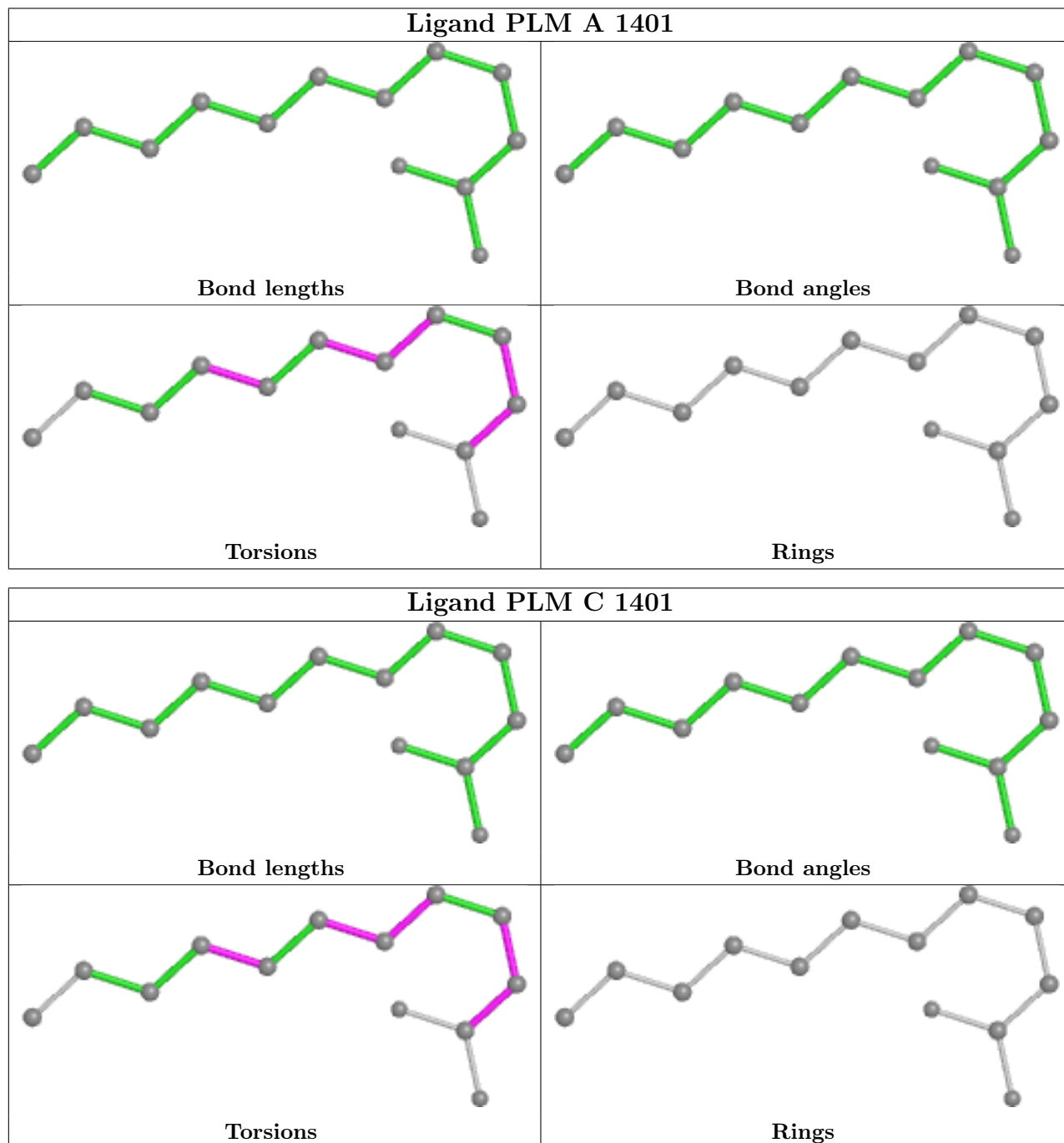
Mol	Chain	Res	Type	Atoms
4	D	1402	OLC	C4-C5-C6-C7
4	A	1402	OLC	C15-C16-C17-C18
4	B	1402	OLC	C4-C5-C6-C7
4	D	1402	OLC	C5-C6-C7-C8
3	B	1401	PLM	C5-C6-C7-C8
3	C	1401	PLM	C1-C2-C3-C4
3	H	1601	PLM	C9-CA-CB-CC
3	F	1601	PLM	C8-C9-CA-CB
4	C	1402	OLC	C15-C16-C17-C18
3	D	1401	PLM	C5-C6-C7-C8
5	G	401	POV	C22-C23-C24-C25
5	E	401	POV	C22-C23-C24-C25
5	E	401	POV	C313-C314-C315-C316
4	B	1402	OLC	C7-C8-C9-C10
3	D	1401	PLM	O1-C1-C2-C3
3	B	1401	PLM	O2-C1-C2-C3
3	D	1401	PLM	O2-C1-C2-C3
3	B	1401	PLM	O1-C1-C2-C3
5	G	401	POV	C313-C314-C315-C316
4	D	1402	OLC	C9-C10-C11-C12
5	G	401	POV	C29-C210-C211-C212
3	H	1601	PLM	C3-C4-C5-C6
4	B	1402	OLC	C9-C10-C11-C12
5	E	401	POV	C29-C210-C211-C212
5	G	401	POV	O11-C1-C2-O21
4	B	1402	OLC	C5-C6-C7-C8
3	D	1401	PLM	C1-C2-C3-C4
4	A	1402	OLC	C7-C8-C9-C10
4	D	1402	OLC	C7-C8-C9-C10
3	A	1401	PLM	C4-C5-C6-C7
3	D	1401	PLM	C8-C9-CA-CB
3	A	1401	PLM	O1-C1-C2-C3
3	C	1401	PLM	O1-C1-C2-C3
5	E	401	POV	O11-C1-C2-O21
3	A	1401	PLM	O2-C1-C2-C3

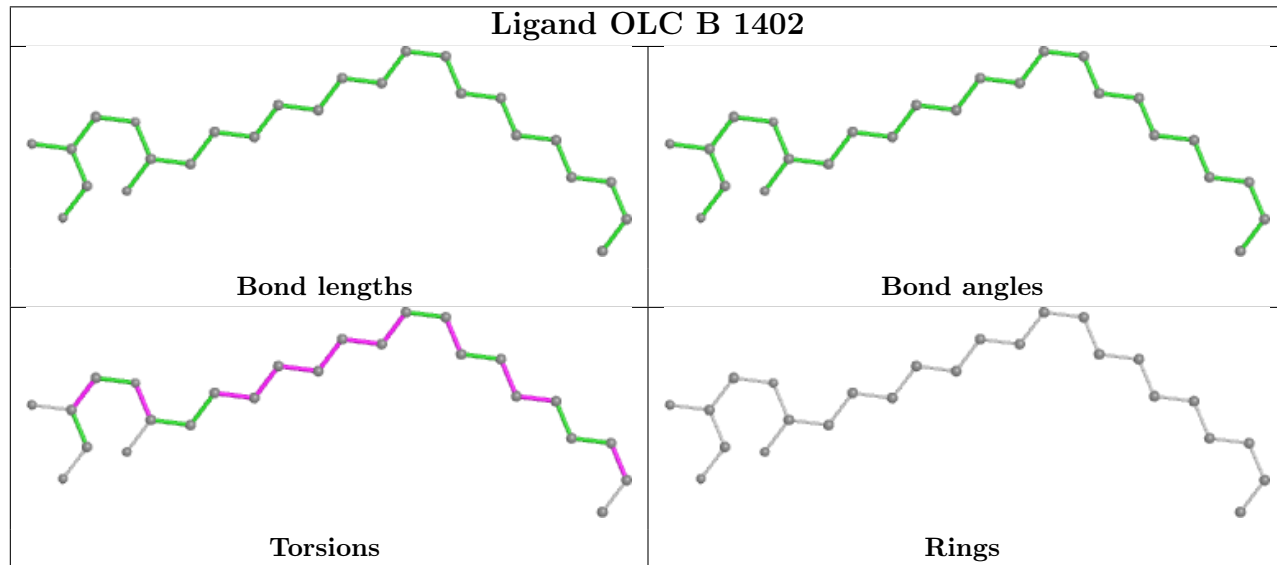
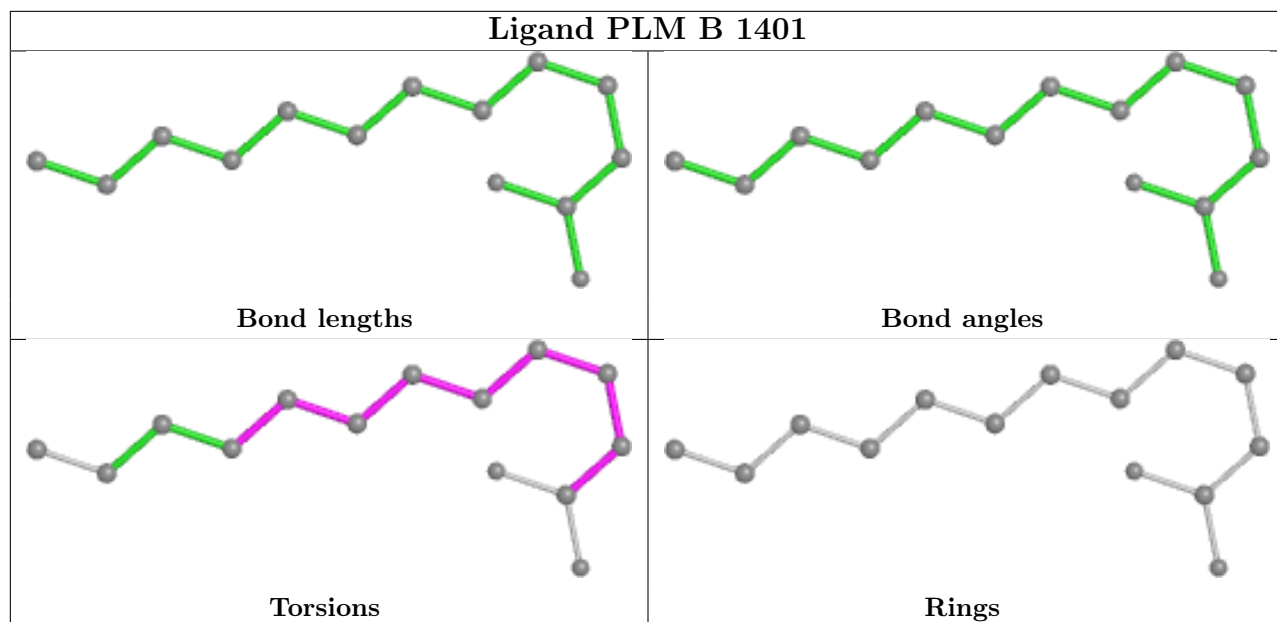
There are no ring outliers.

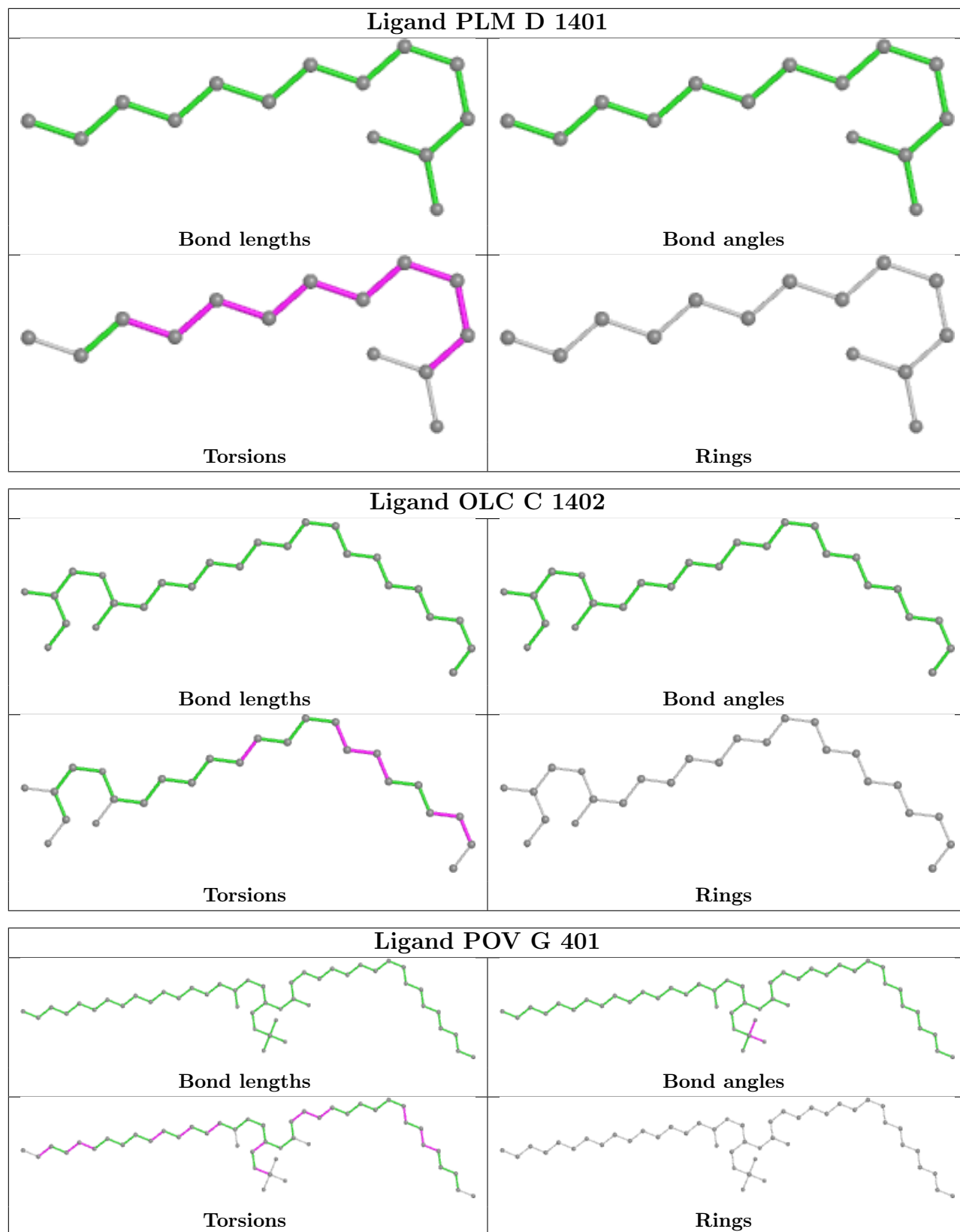
No monomer is involved in short contacts.

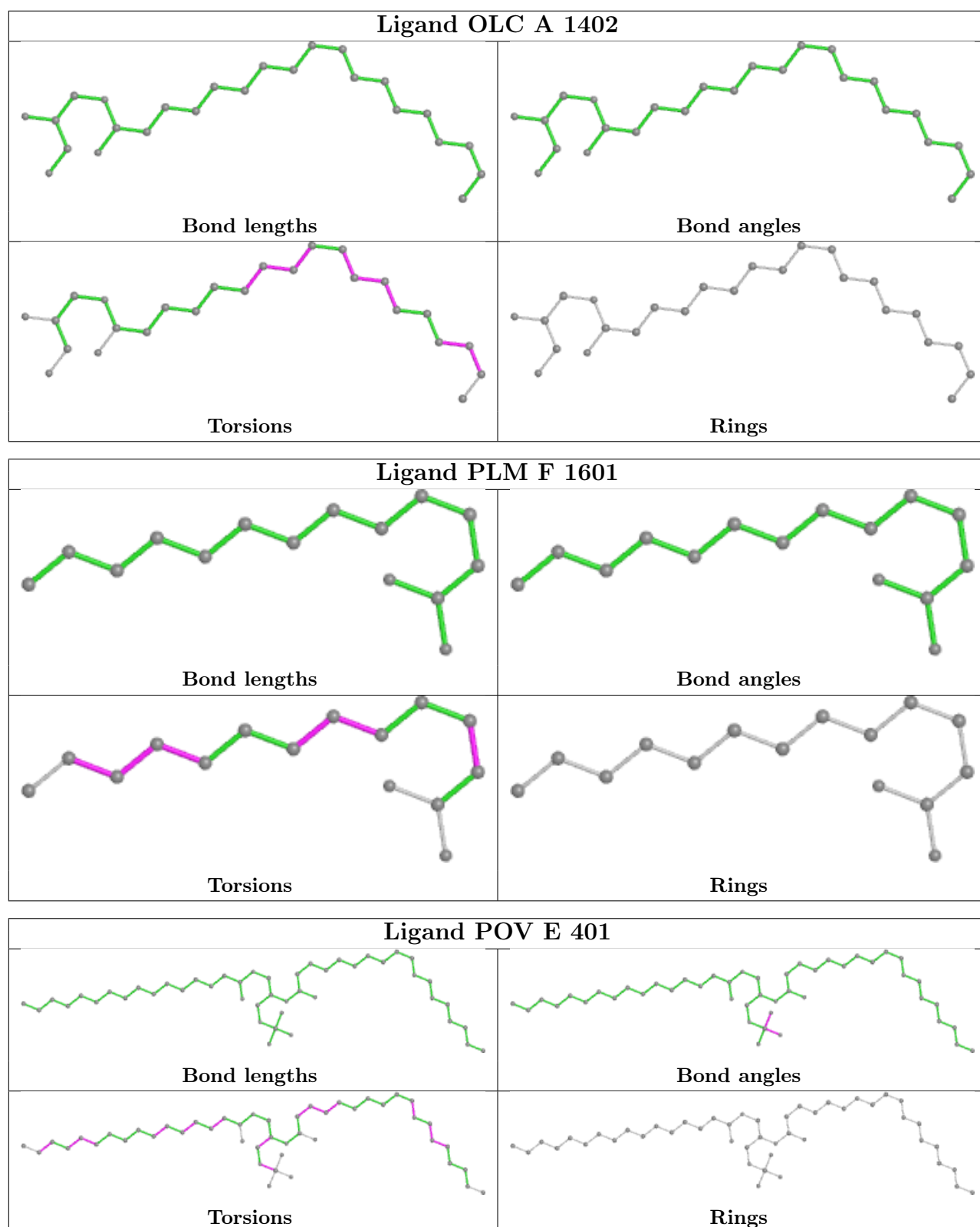
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

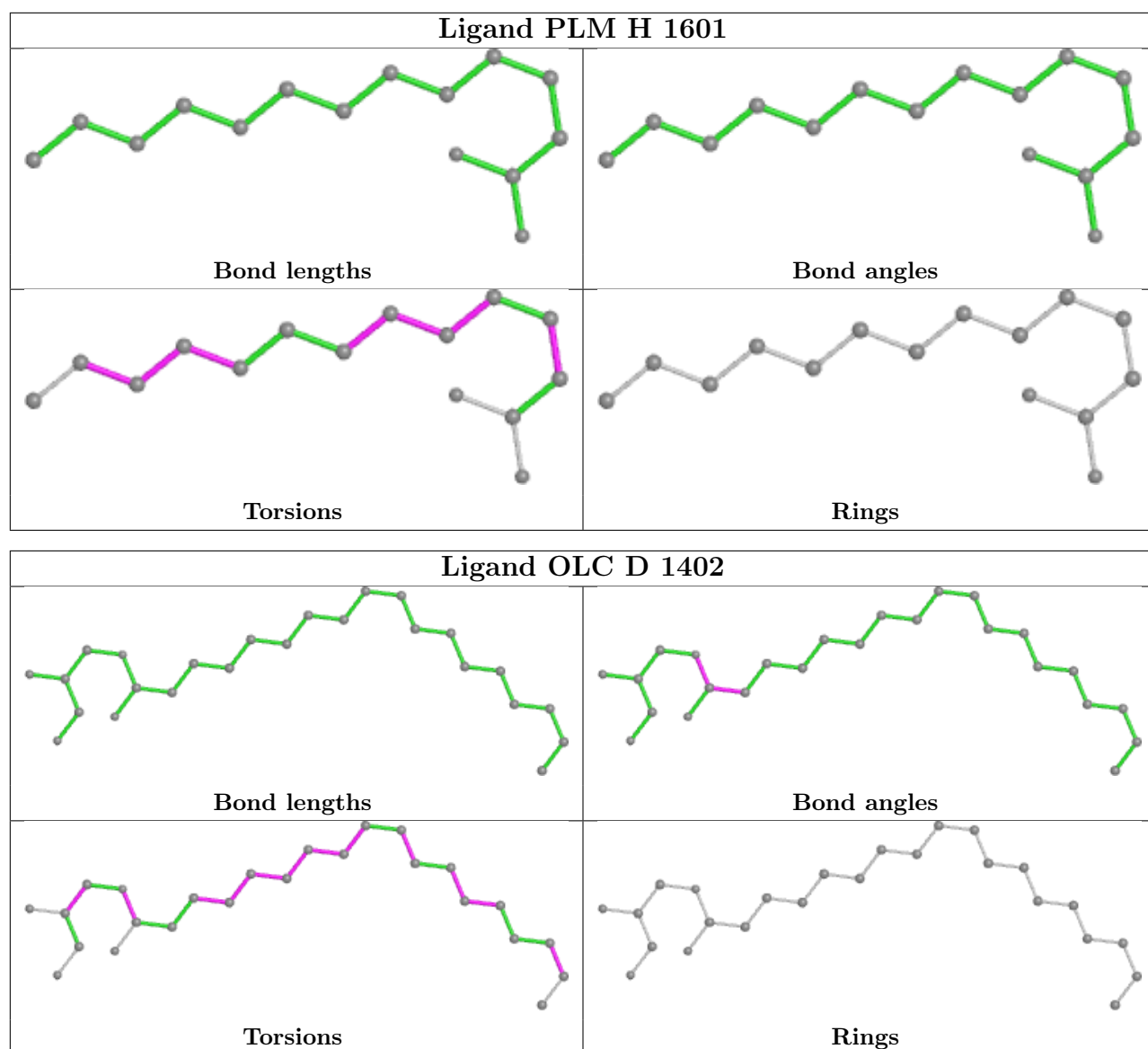
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

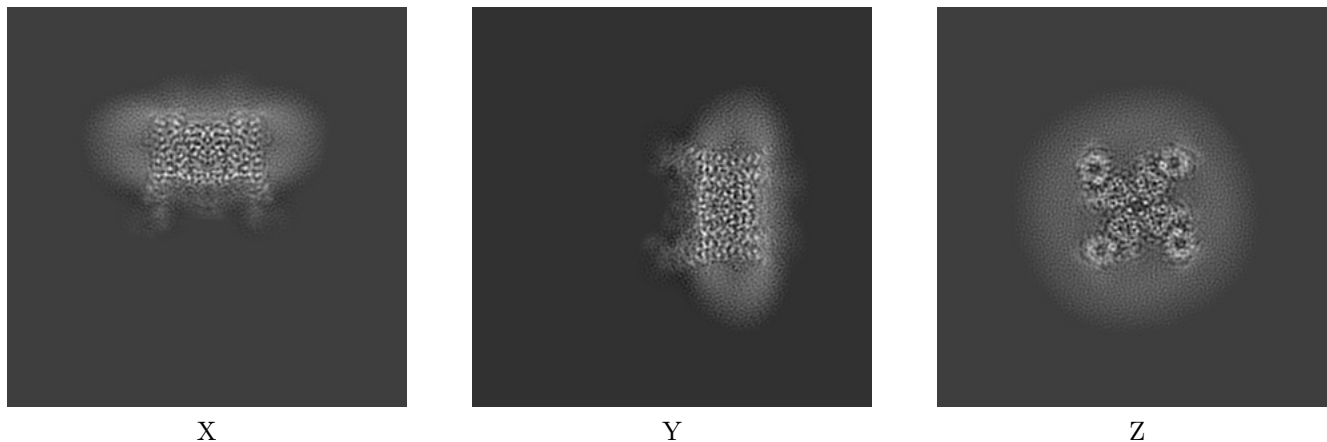
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16390. These allow visual inspection of the internal detail of the map and identification of artifacts.

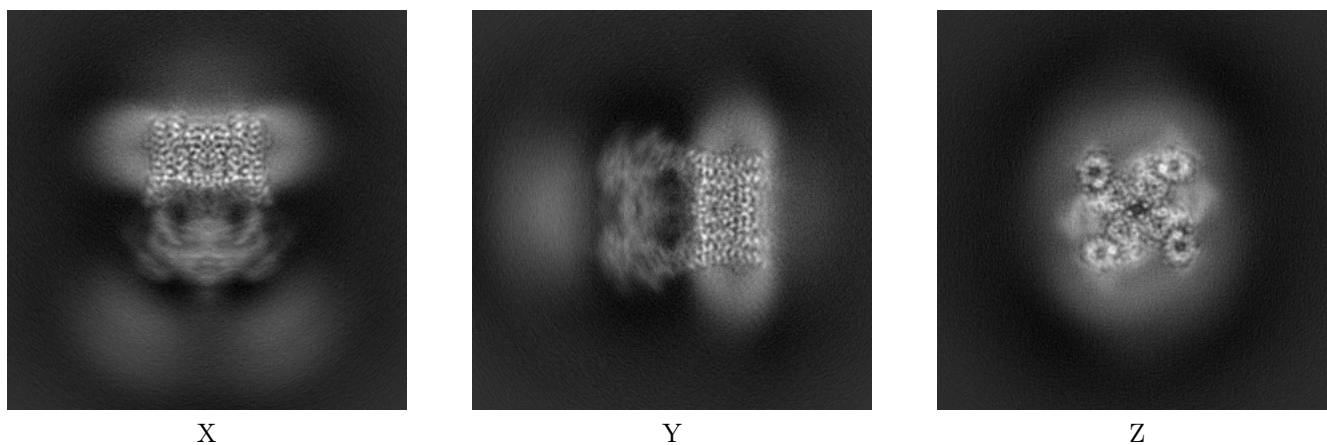
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



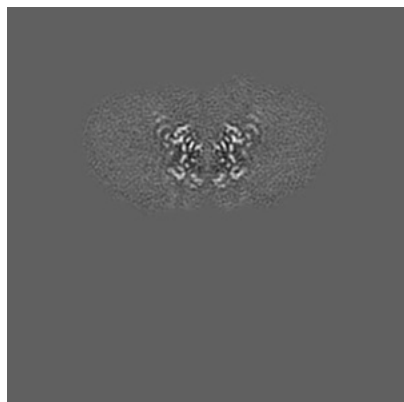
6.1.2 Raw map



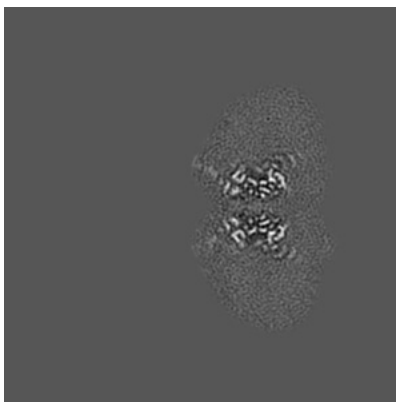
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

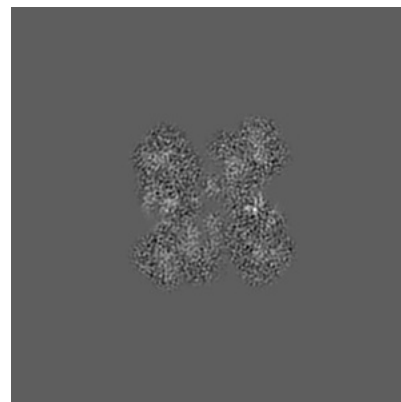
6.2.1 Primary map



X Index: 153

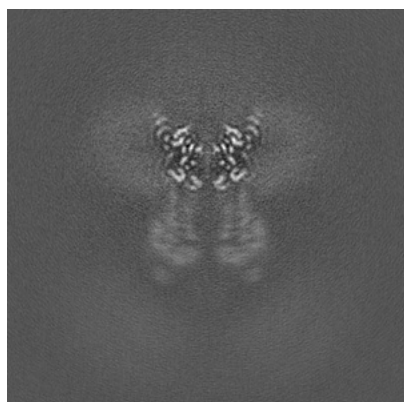


Y Index: 153

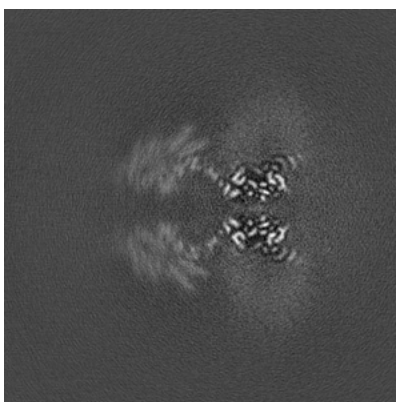


Z Index: 153

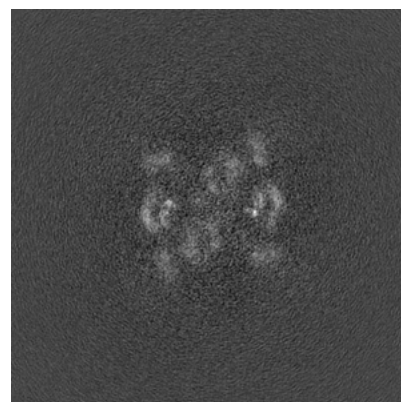
6.2.2 Raw map



X Index: 153



Y Index: 153

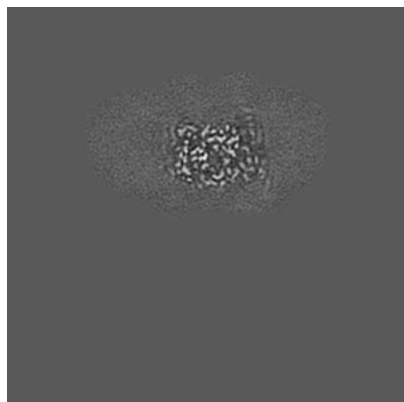


Z Index: 153

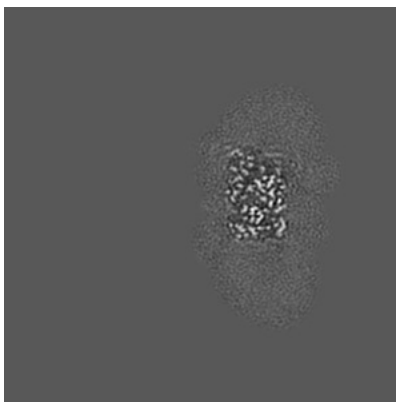
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

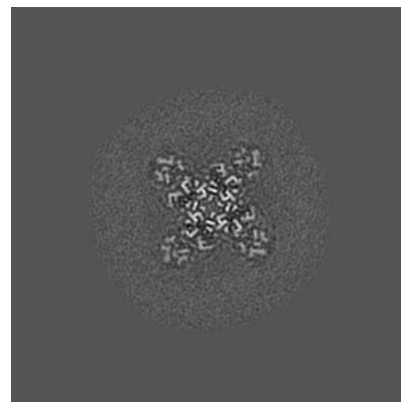
6.3.1 Primary map



X Index: 169

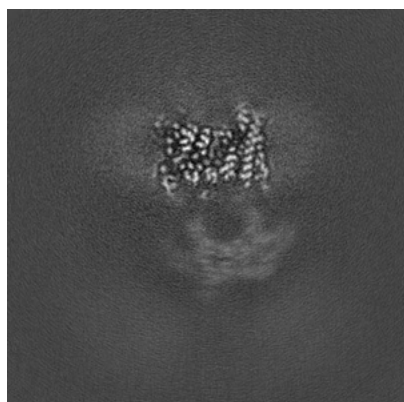


Y Index: 137

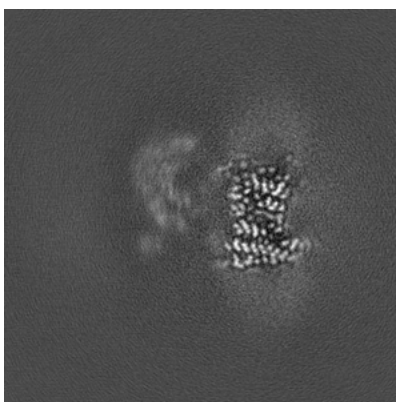


Z Index: 199

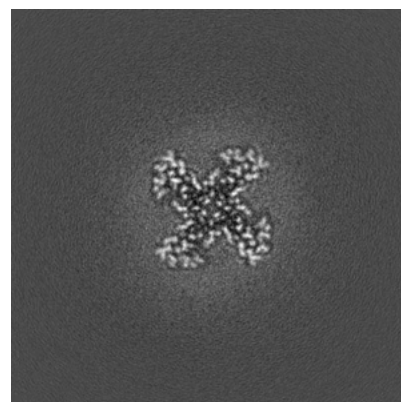
6.3.2 Raw map



X Index: 174



Y Index: 174

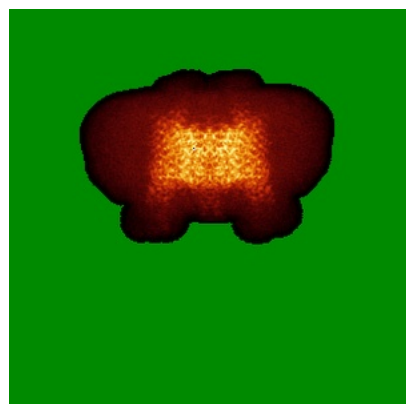


Z Index: 177

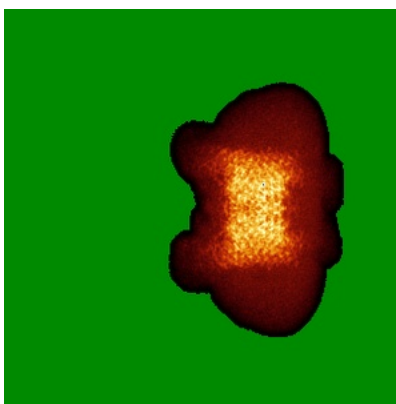
The images above show the largest variance slices of the map in three orthogonal directions.

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

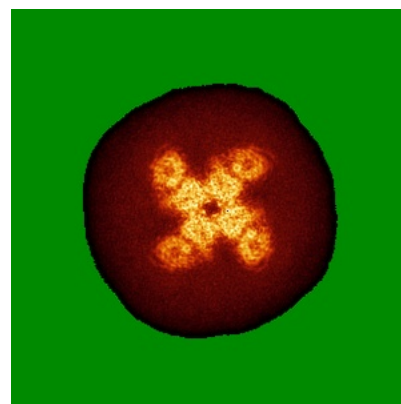
6.4.1 Primary map



X

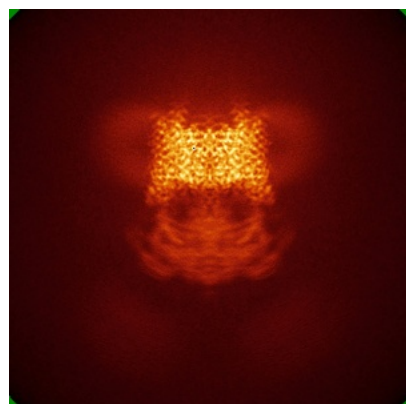


Y

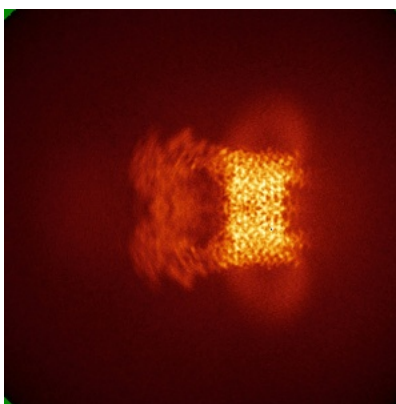


Z

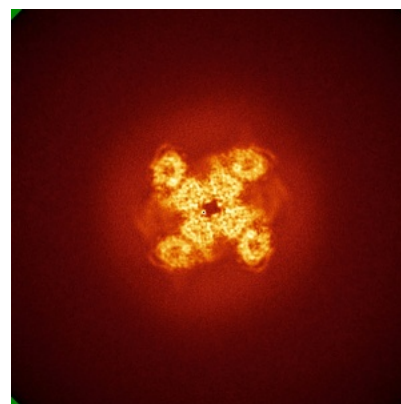
6.4.2 Raw map



X



Y

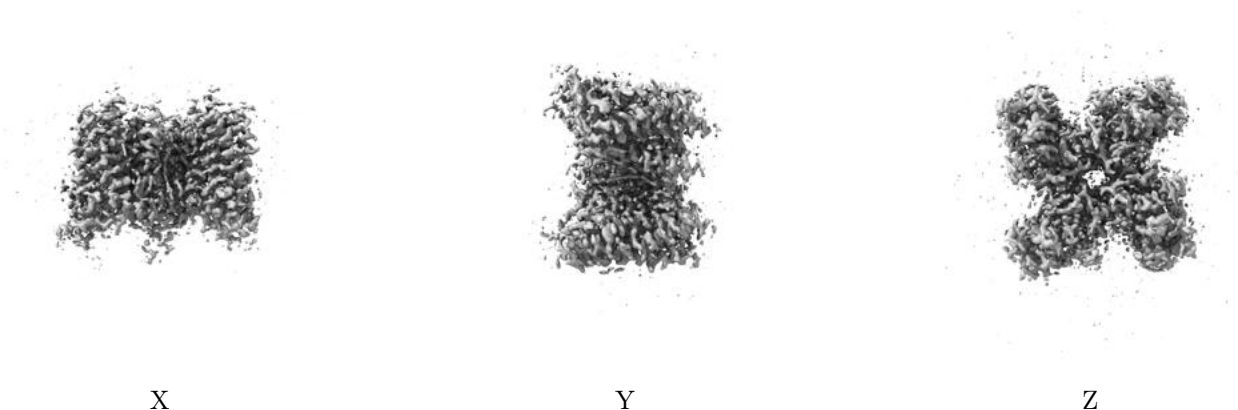


Z

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.

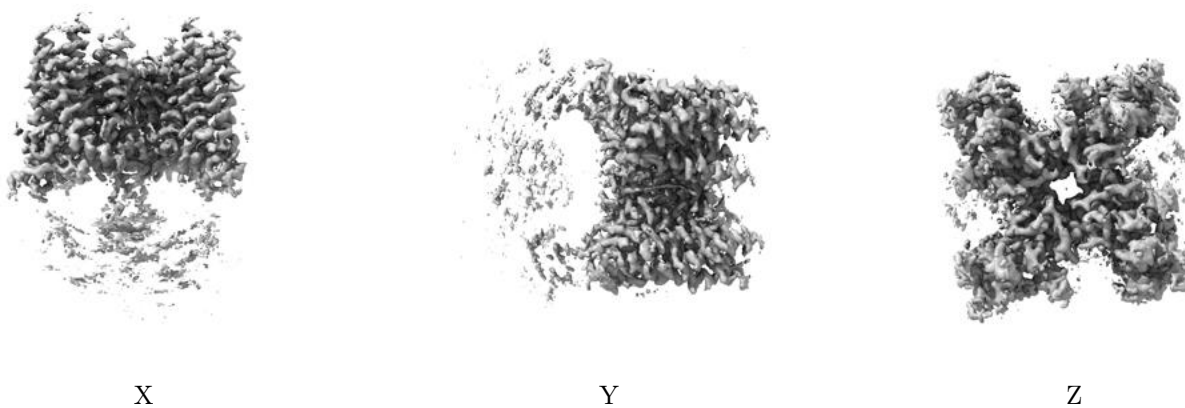
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

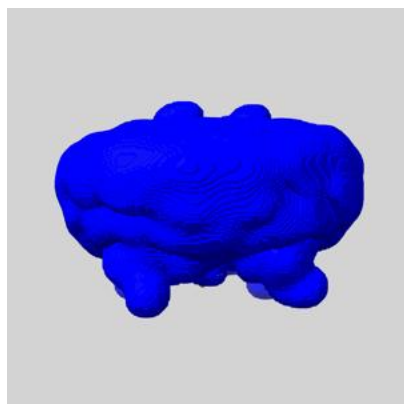
6.6 Mask visualisation [i](#)

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

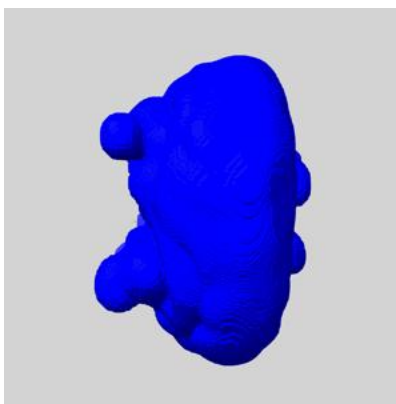
A mask typically either:

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

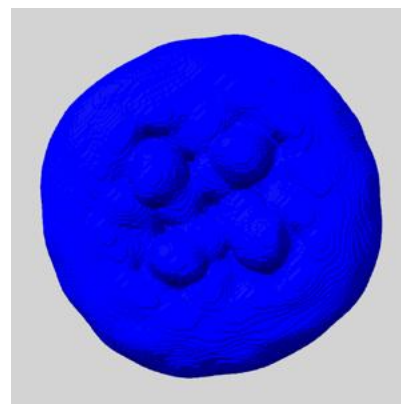
6.6.1 emd_16390_msk_1.map [i](#)



X



Y

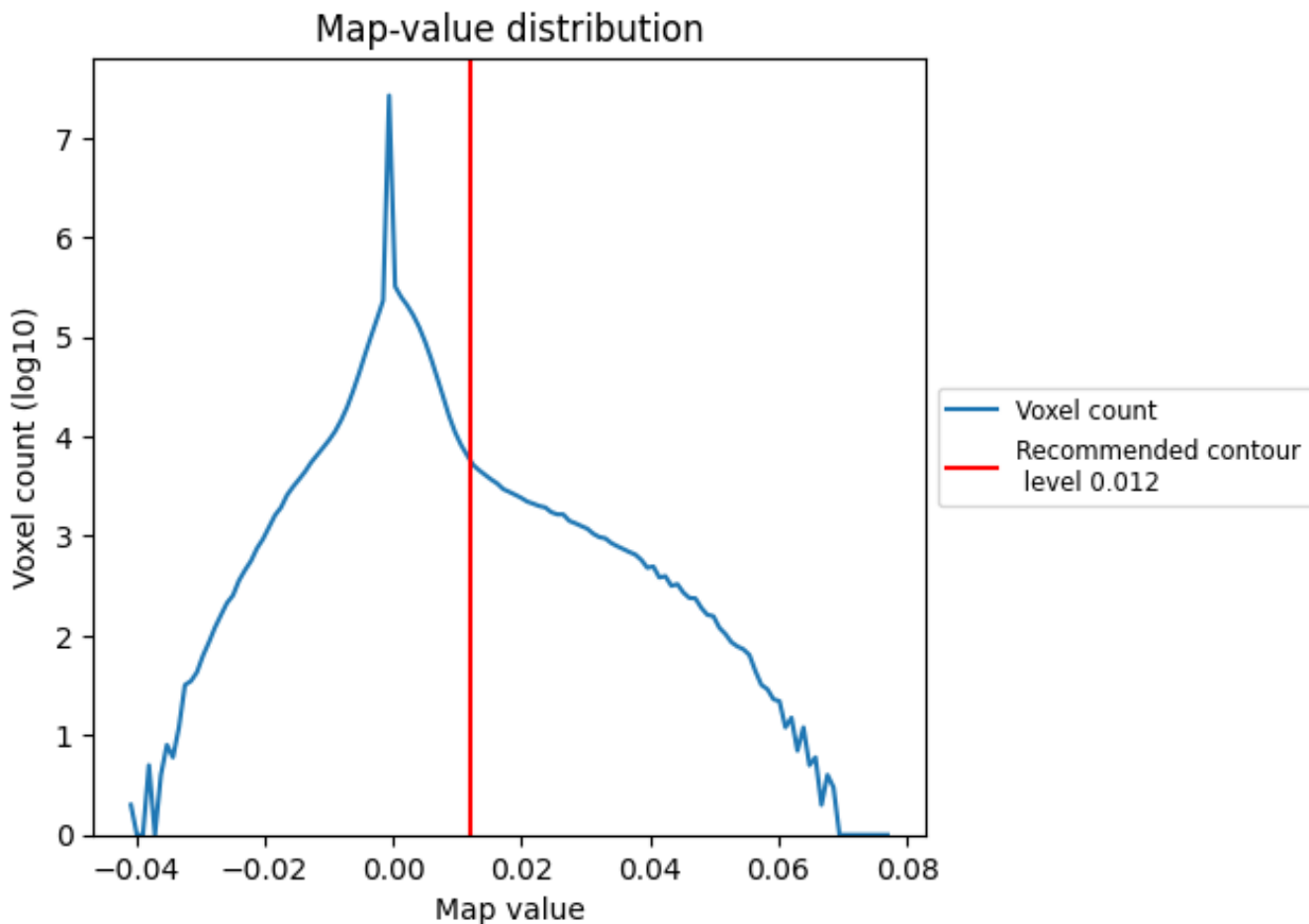


Z

7 Map analysis [i](#)

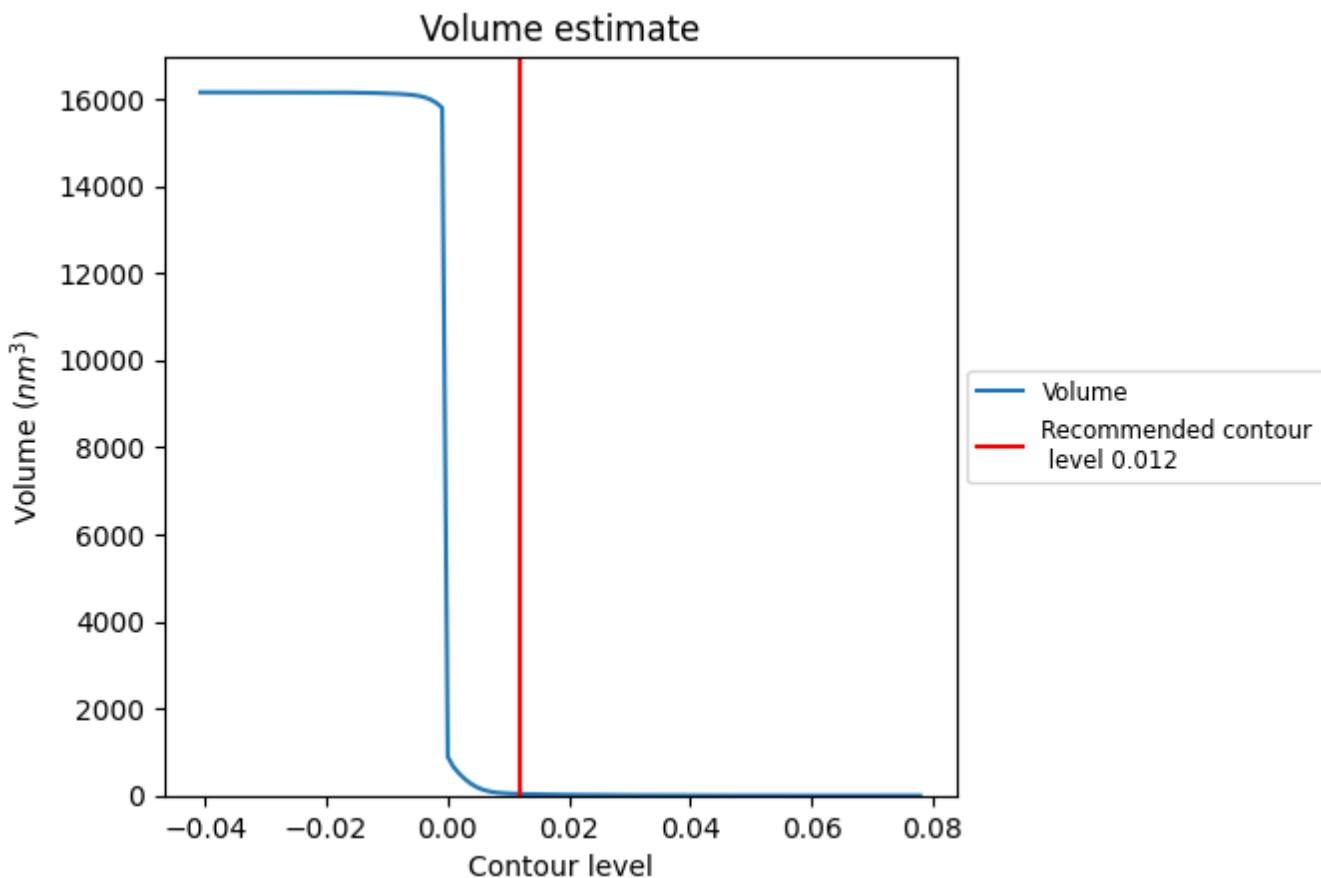
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

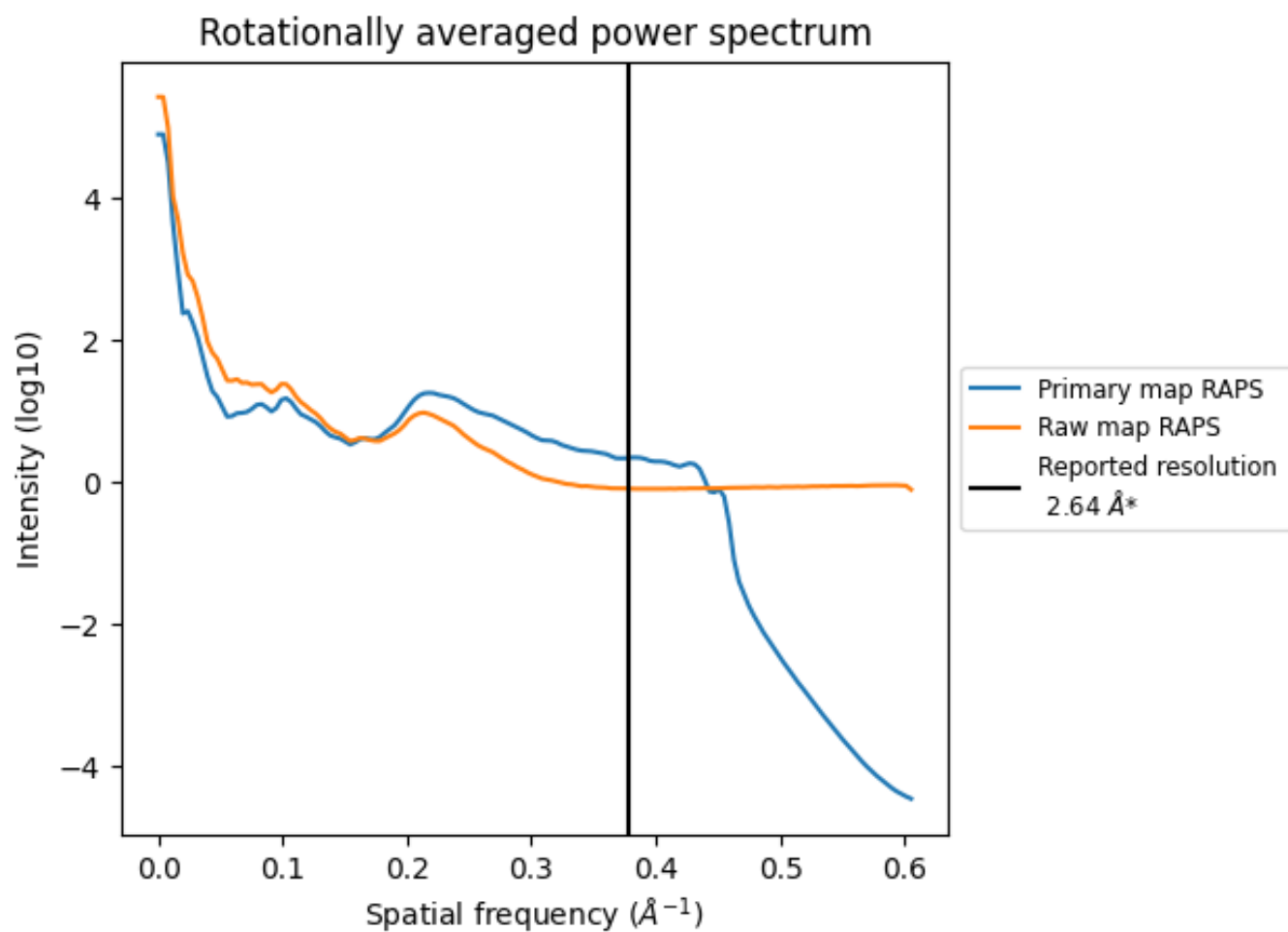
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 37 nm^3 ; this corresponds to an approximate mass of 33 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 i

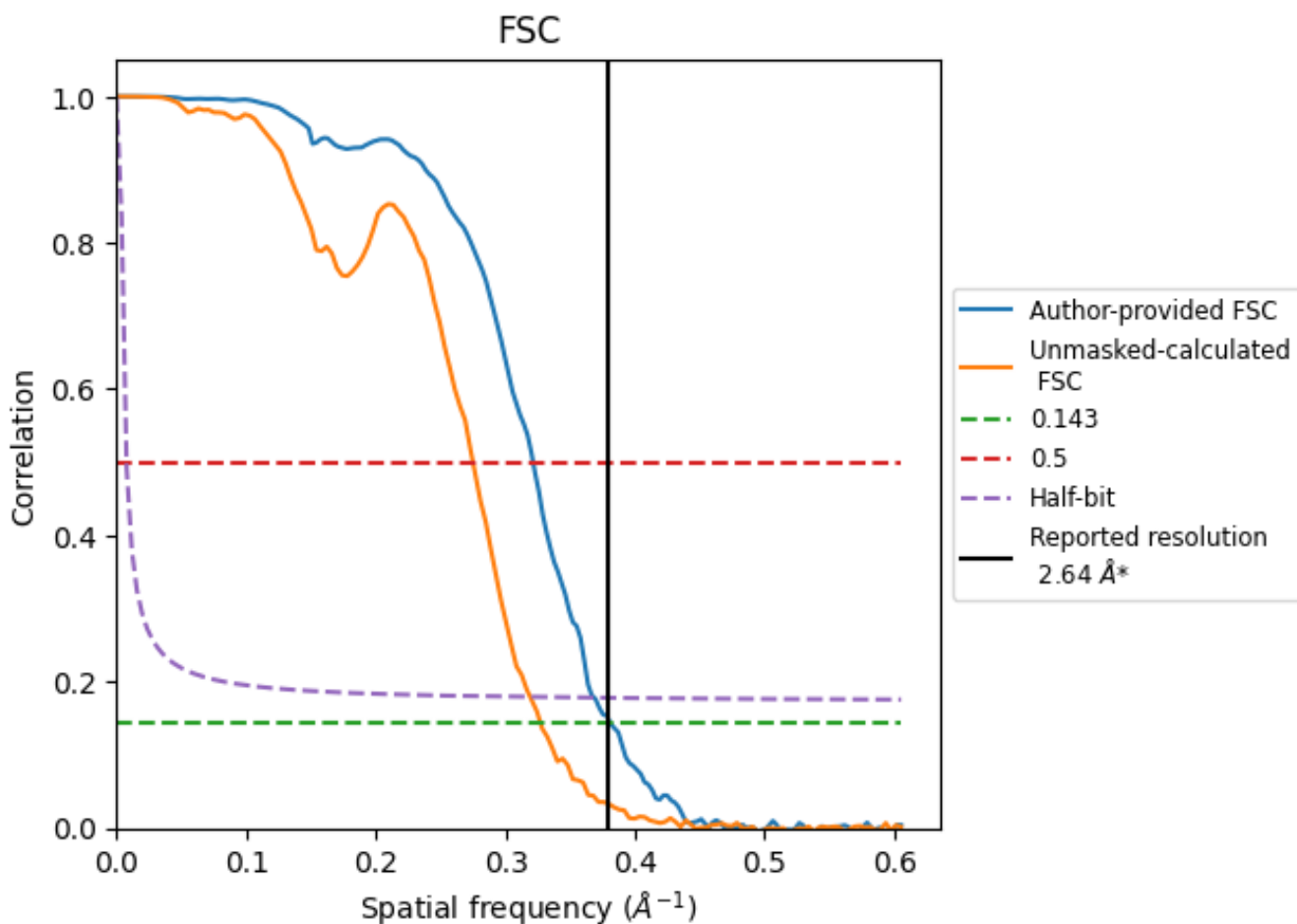


*Reported resolution corresponds to spatial frequency of 0.379 Å⁻¹

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 0.379 Å⁻¹

8.2 Resolution estimates

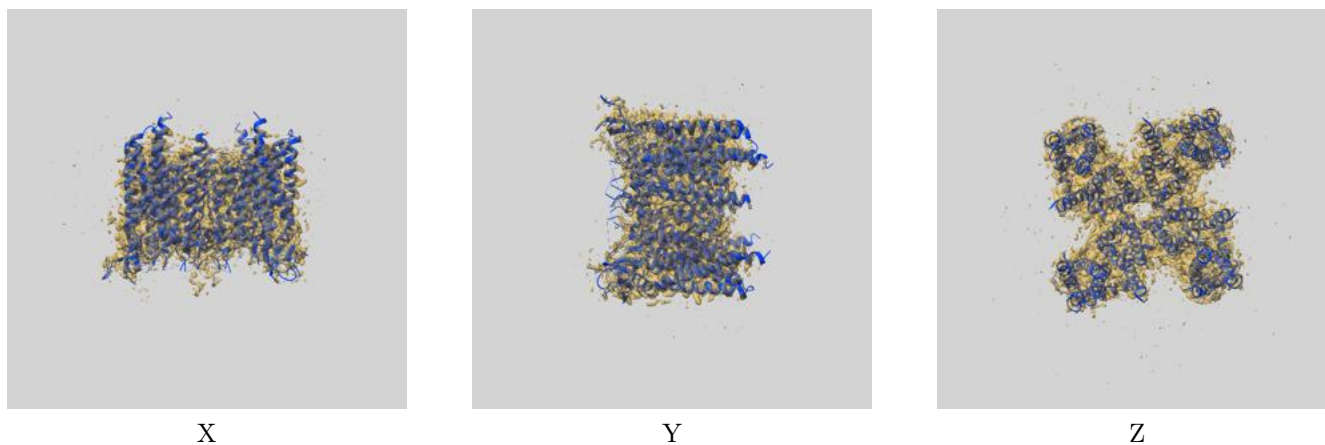
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	2.62	3.11	2.71
Unmasked-calculated*	3.06	3.64	3.13

*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 3.06 differs from the reported value 2.64 by more than 10 %

9 Map-model fit [i](#)

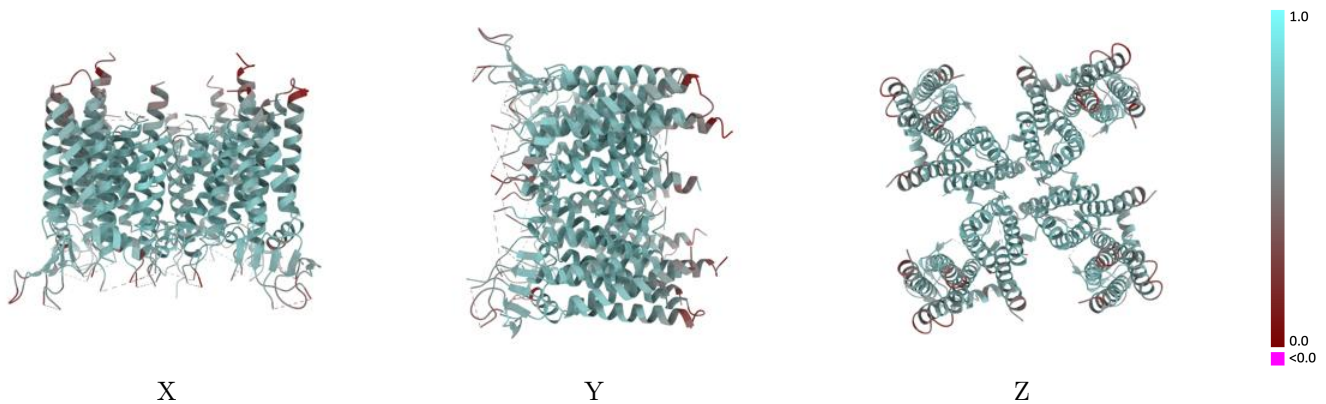
This section contains information regarding the fit between EMDB map EMD-16390 and PDB model 8C2H. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



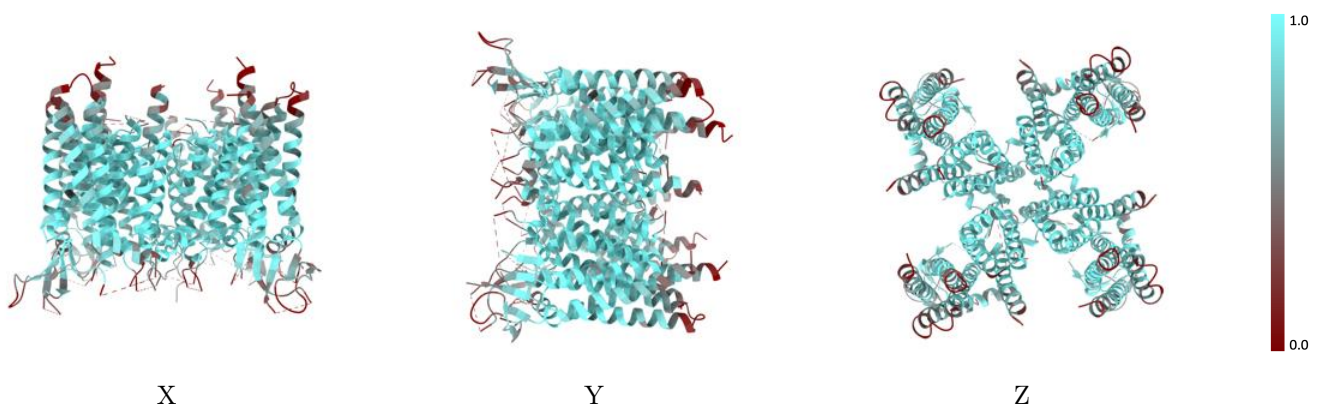
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



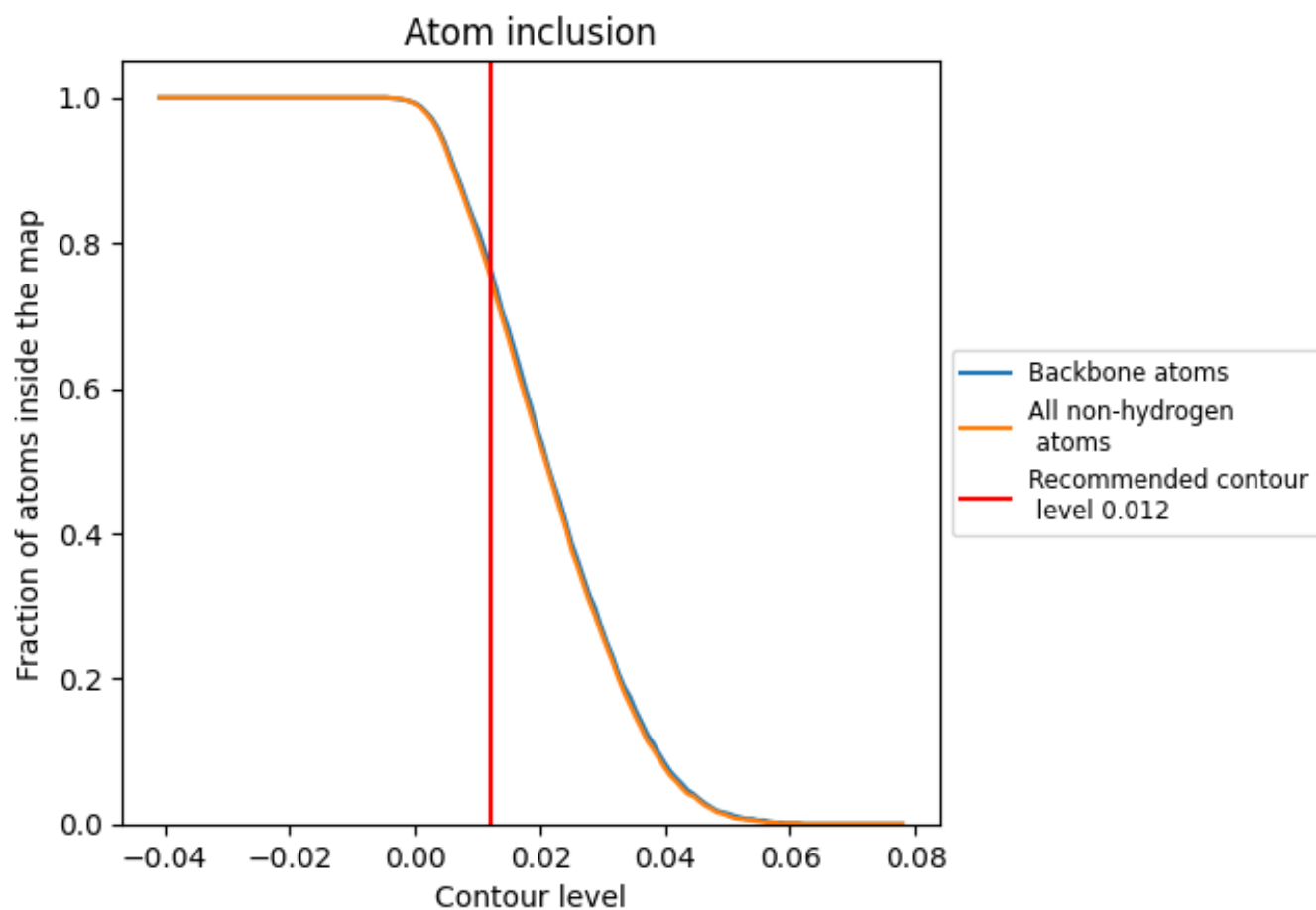
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7560	 0.6190
A	 0.8730	 0.6650
B	 0.8820	 0.6710
C	 0.8730	 0.6680
D	 0.8480	 0.6650
E	 0.6290	 0.5740
F	 0.7190	 0.5890
G	 0.6580	 0.5740
H	 0.7190	 0.5920

