



Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 06:42 PM EST

PDB ID : 7L2R
EMDB ID : EMD-23138
Title : Cryo-EM structure of DkTx-bound minimal TRPV1 at the pre-open state
Authors : Zhang, K.; Julius, D.; Cheng, Y.
Deposited on : 2020-12-17
Resolution : 3.30 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.dev43
Mogul : 1.8.5 (274361), 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) : 2.31.2

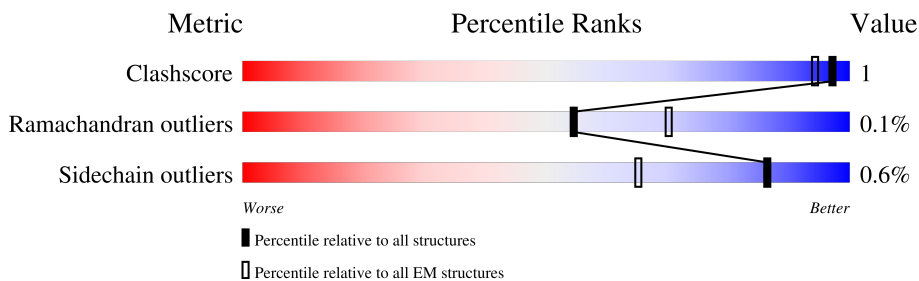
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	637	 95%
1	B	637	 94%
1	C	637	 96%
1	D	637	 93%
2	E	76	 96%
2	F	76	 99%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 21377 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 Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	615	4974	3236	816	894	28	0	0
1	B	614	4963	3230	812	893	28	0	0
1	C	618	5002	3255	819	900	28	0	0
1	D	614	4963	3230	812	893	28	0	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	expression tag	UNP O35433
A	106	ALA	-	expression tag	UNP O35433
A	107	MET	-	expression tag	UNP O35433
A	108	GLY	-	expression tag	UNP O35433
A	109	SER	-	expression tag	UNP O35433
A	?	-	ASN	deletion	UNP O35433
A	?	-	ASN	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
A	?	-	LEU	deletion	UNP O35433
A	?	-	PRO	deletion	UNP O35433
A	?	-	MET	deletion	UNP O35433
A	?	-	GLU	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
A	?	-	THR	deletion	UNP O35433
A	?	-	PRO	deletion	UNP O35433
A	?	-	HIS	deletion	UNP O35433
A	?	-	LYS	deletion	UNP O35433
A	?	-	CYS	deletion	UNP O35433
A	?	-	ARG	deletion	UNP O35433
A	?	-	GLY	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP O35433
A	?	-	CYS	deletion	UNP O35433
A	?	-	LYS	deletion	UNP O35433
A	?	-	PRO	deletion	UNP O35433
A	?	-	GLY	deletion	UNP O35433
A	?	-	ASN	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
B	105	GLY	-	expression tag	UNP O35433
B	106	ALA	-	expression tag	UNP O35433
B	107	MET	-	expression tag	UNP O35433
B	108	GLY	-	expression tag	UNP O35433
B	109	SER	-	expression tag	UNP O35433
B	?	-	ASN	deletion	UNP O35433
B	?	-	ASN	deletion	UNP O35433
B	?	-	SER	deletion	UNP O35433
B	?	-	LEU	deletion	UNP O35433
B	?	-	PRO	deletion	UNP O35433
B	?	-	MET	deletion	UNP O35433
B	?	-	GLU	deletion	UNP O35433
B	?	-	SER	deletion	UNP O35433
B	?	-	THR	deletion	UNP O35433
B	?	-	PRO	deletion	UNP O35433
B	?	-	HIS	deletion	UNP O35433
B	?	-	LYS	deletion	UNP O35433
B	?	-	CYS	deletion	UNP O35433
B	?	-	ARG	deletion	UNP O35433
B	?	-	GLY	deletion	UNP O35433
B	?	-	SER	deletion	UNP O35433
B	?	-	ALA	deletion	UNP O35433
B	?	-	CYS	deletion	UNP O35433
B	?	-	LYS	deletion	UNP O35433
B	?	-	PRO	deletion	UNP O35433
B	?	-	GLY	deletion	UNP O35433
B	?	-	ASN	deletion	UNP O35433
B	?	-	SER	deletion	UNP O35433
C	105	GLY	-	expression tag	UNP O35433
C	106	ALA	-	expression tag	UNP O35433
C	107	MET	-	expression tag	UNP O35433
C	108	GLY	-	expression tag	UNP O35433
C	109	SER	-	expression tag	UNP O35433
C	?	-	ASN	deletion	UNP O35433
C	?	-	ASN	deletion	UNP O35433

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP O35433
C	?	-	LEU	deletion	UNP O35433
C	?	-	PRO	deletion	UNP O35433
C	?	-	MET	deletion	UNP O35433
C	?	-	GLU	deletion	UNP O35433
C	?	-	SER	deletion	UNP O35433
C	?	-	THR	deletion	UNP O35433
C	?	-	PRO	deletion	UNP O35433
C	?	-	HIS	deletion	UNP O35433
C	?	-	LYS	deletion	UNP O35433
C	?	-	CYS	deletion	UNP O35433
C	?	-	ARG	deletion	UNP O35433
C	?	-	GLY	deletion	UNP O35433
C	?	-	SER	deletion	UNP O35433
C	?	-	ALA	deletion	UNP O35433
C	?	-	CYS	deletion	UNP O35433
C	?	-	LYS	deletion	UNP O35433
C	?	-	PRO	deletion	UNP O35433
C	?	-	GLY	deletion	UNP O35433
C	?	-	ASN	deletion	UNP O35433
C	?	-	SER	deletion	UNP O35433
D	105	GLY	-	expression tag	UNP O35433
D	106	ALA	-	expression tag	UNP O35433
D	107	MET	-	expression tag	UNP O35433
D	108	GLY	-	expression tag	UNP O35433
D	109	SER	-	expression tag	UNP O35433
D	?	-	ASN	deletion	UNP O35433
D	?	-	ASN	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
D	?	-	LEU	deletion	UNP O35433
D	?	-	PRO	deletion	UNP O35433
D	?	-	MET	deletion	UNP O35433
D	?	-	GLU	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
D	?	-	THR	deletion	UNP O35433
D	?	-	PRO	deletion	UNP O35433
D	?	-	HIS	deletion	UNP O35433
D	?	-	LYS	deletion	UNP O35433
D	?	-	CYS	deletion	UNP O35433
D	?	-	ARG	deletion	UNP O35433
D	?	-	GLY	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ALA	deletion	UNP O35433
D	?	-	CYS	deletion	UNP O35433
D	?	-	LYS	deletion	UNP O35433
D	?	-	PRO	deletion	UNP O35433
D	?	-	GLY	deletion	UNP O35433
D	?	-	ASN	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433

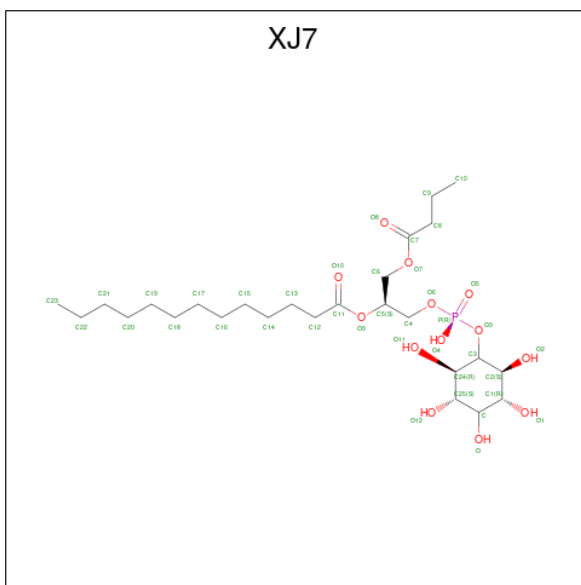
- Molecule 2 is a protein called Tau-theraphotoxin-Hs1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	75	Total	C	N	O	S	0	0
			591	376	95	107	13		
2	E	75	Total	C	N	O	S	0	0
			591	376	95	107	13		

There are 2 discrepancies between the modelled and reference sequences:

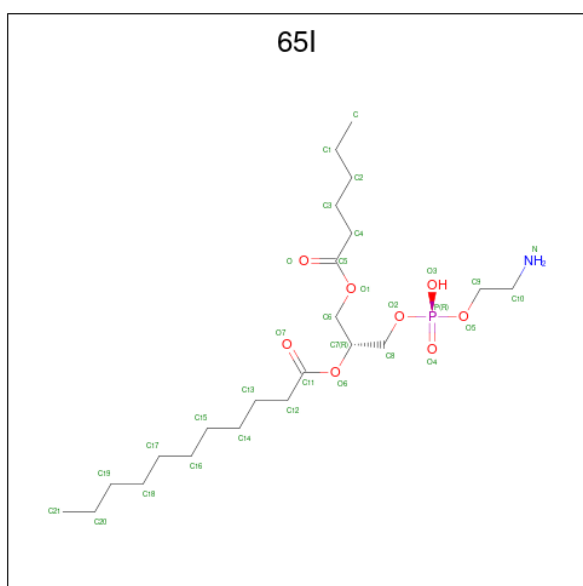
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	initiating methionine	UNP P0CH43
E	0	MET	-	initiating methionine	UNP P0CH43

- Molecule 3 is (2S)-1-(butanoyloxy)-3-[[[(R)-hydroxy{[(1R,2R,3S,4S,5R,6S)-2,3,4,5,6-penta hydroxycyclohexyl]oxy}phosphoryl]oxy}propan-2-yl tridecanoate (three-letter code: XJ7) (formula: C₂₆H₄₉O₁₃P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			40	26	13	1	
3	B	1	Total	C	O	P	0
			40	26	13	1	
3	C	1	Total	C	O	P	0
			40	26	13	1	
3	D	1	Total	C	O	P	0
			40	26	13	1	

- Molecule 4 is (9R,12R)-15-amino-12-hydroxy-6,12-dioxo-7,11,13-trioxa-12lambda 5 -phosphapentadecan-9-yl undecanoate (three-letter code: 65I) (formula: C₂₂H₄₄NO₈P) (labeled as "Ligand of Interest" by depositor).



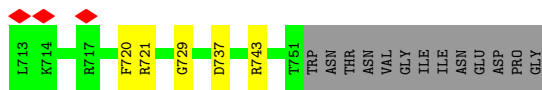
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
4	F	1	Total	C	N	O	P	0
			32	22	1	8	1	
4	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
4	D	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Na	0
			1	1	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total O 1 1	0
6	B	1	Total O 1 1	0
6	C	1	Total O 1 1	0
6	D	1	Total O 1 1	0



- Molecule 2: Tau-theraphotoxin-Hs1a

Chain F:  99%



- Molecule 2: Tau-theraphotoxin-Hs1a

Chain E:  96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39680	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0045	Depositor
Map size (\AA)	271.616, 271.616, 271.616	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8488, 0.8488, 0.8488	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: NA, XJ7, 65I

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	0.42	0/5085	0.60	0/6879
1	B	0.42	0/5074	0.59	0/6865
1	C	0.42	0/5114	0.59	0/6919
1	D	0.43	0/5074	0.59	0/6865
2	E	0.36	0/610	0.64	0/822
2	F	0.36	0/610	0.60	0/822
All	All	0.42	0/21567	0.59	0/29172

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4974	0	5028	6	0
1	B	4963	0	5015	10	0
1	C	5002	0	5052	1	0
1	D	4963	0	5015	7	0
2	E	591	0	549	1	0
2	F	591	0	549	0	0
3	A	40	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	40	0	0	0	0
3	C	40	0	0	0	0
3	D	40	0	0	0	0
4	A	32	0	0	0	0
4	C	32	0	0	0	0
4	D	32	0	0	0	0
4	F	32	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	21377	0	21208	25	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 1.

All (25) 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:B:536:GLU:N	1:B:536:GLU:OE1	2.37	0.58
1:A:536:GLU:N	1:A:536:GLU:OE1	2.38	0.56
2:E:18:LEU:HA	2:E:21:PHE:HD2	1.70	0.56
1:D:672:ILE:O	1:D:676:ASN:ND2	2.40	0.54
1:A:509:ASP:OD1	1:A:510:SER:N	2.42	0.53
1:D:390:CYS:SG	1:D:393:ASN:N	2.82	0.50
1:A:184:ASP:N	1:A:184:ASP:OD1	2.47	0.47
1:D:509:ASP:OD1	1:D:510:SER:N	2.47	0.47
1:B:504:LYS:O	1:B:508:VAL:HG22	2.15	0.47
1:B:722:SER:OG	1:B:741:CYS:O	2.16	0.47
1:A:601:ASP:OD1	1:A:602:GLY:N	2.48	0.46
1:D:514:ILE:O	1:D:518:VAL:HG23	2.16	0.45
1:A:127:GLN:OE1	1:A:127:GLN:N	2.46	0.45
1:D:371:GLU:OE1	1:D:743:ARG:NH1	2.47	0.45
1:B:122:ALA:O	1:B:164:ASN:ND2	2.49	0.45
1:B:474:ARG:NH1	1:B:478:GLU:OE2	2.52	0.43
1:A:672:ILE:O	1:A:676:ASN:ND2	2.52	0.43
1:D:383:ASP:OD1	1:D:384:LEU:N	2.52	0.43
1:B:393:ASN:N	1:B:393:ASN:OD1	2.51	0.42
1:B:672:ILE:O	1:B:676:ASN:ND2	2.51	0.42
1:C:748:ASN:OD1	1:C:749:TRP:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:ASP:OD1	1:B:510:SER:N	2.51	0.42
1:B:388:ASP:OD2	1:B:721:ARG:NE	2.53	0.41
1:B:737:ASP:N	1:B:737:ASP:OD1	2.53	0.41
1:D:729:GLY:N	1:D:737:ASP:OD1	2.52	0.41

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	613/637 (96%)	572 (93%)	40 (6%)	1 (0%)	47 77
1	B	612/637 (96%)	576 (94%)	36 (6%)	0	100 100
1	C	616/637 (97%)	573 (93%)	43 (7%)	0	100 100
1	D	612/637 (96%)	574 (94%)	37 (6%)	1 (0%)	47 77
2	E	73/76 (96%)	66 (90%)	7 (10%)	0	100 100
2	F	73/76 (96%)	64 (88%)	9 (12%)	0	100 100
All	All	2599/2700 (96%)	2425 (93%)	172 (7%)	2 (0%)	54 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	712	PHE
1	D	712	PHE

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	545/562 (97%)	543 (100%)	2 (0%)	91	95
1	B	544/562 (97%)	542 (100%)	2 (0%)	91	95
1	C	548/562 (98%)	545 (100%)	3 (0%)	88	93
1	D	544/562 (97%)	539 (99%)	5 (1%)	78	87
2	E	66/67 (98%)	65 (98%)	1 (2%)	65	81
2	F	66/67 (98%)	66 (100%)	0	100	100
All	All	2313/2382 (97%)	2300 (99%)	13 (1%)	86	91

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ARG
1	A	390	CYS
2	E	21	PHE
1	B	304	PHE
1	B	721	ARG
1	C	210	GLU
1	C	304	PHE
1	C	390	CYS
1	D	210	GLU
1	D	304	PHE
1	D	390	CYS
1	D	720	PHE
1	D	721	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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
3	XJ7	B	801	-	40,40,40	1.10	4 (10%)	50,52,52	1.51	7 (14%)
4	65I	D	802	-	31,31,31	1.16	5 (16%)	34,36,36	1.24	3 (8%)
3	XJ7	C	902	-	40,40,40	1.13	4 (10%)	50,52,52	1.40	5 (10%)
3	XJ7	D	801	-	40,40,40	1.13	4 (10%)	50,52,52	1.50	8 (16%)
3	XJ7	A	801	-	40,40,40	1.14	4 (10%)	50,52,52	1.35	4 (8%)
4	65I	C	901	-	31,31,31	1.14	5 (16%)	34,36,36	1.17	3 (8%)
4	65I	A	802	-	31,31,31	1.15	4 (12%)	34,36,36	1.09	3 (8%)
4	65I	F	901	-	31,31,31	1.14	5 (16%)	34,36,36	1.26	3 (8%)

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	XJ7	B	801	-	-	19/35/59/59	0/1/1/1
4	65I	D	802	-	-	12/35/35/35	-
3	XJ7	C	902	-	-	14/35/59/59	0/1/1/1
3	XJ7	D	801	-	-	16/35/59/59	0/1/1/1
3	XJ7	A	801	-	-	12/35/59/59	0/1/1/1
4	65I	C	901	-	-	10/35/35/35	-
4	65I	A	802	-	-	12/35/35/35	-
4	65I	F	901	-	-	11/35/35/35	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	XJ7	O9-C5	-2.72	1.39	1.46
3	D	801	XJ7	O9-C5	-2.65	1.40	1.46
4	A	802	65I	O6-C7	-2.57	1.40	1.46
3	A	801	XJ7	O9-C5	-2.56	1.40	1.46
4	C	901	65I	O6-C7	-2.52	1.40	1.46
3	B	801	XJ7	O9-C5	-2.52	1.40	1.46
4	F	901	65I	O6-C7	-2.48	1.40	1.46
3	D	801	XJ7	O7-C6	-2.45	1.39	1.45
4	D	802	65I	O1-C5	2.40	1.40	1.33
3	A	801	XJ7	O7-C6	-2.39	1.39	1.45
4	D	802	65I	O6-C7	-2.37	1.40	1.46
4	F	901	65I	O1-C5	2.34	1.40	1.33
4	A	802	65I	O1-C5	2.29	1.40	1.33
3	C	902	XJ7	O7-C7	2.25	1.39	1.33
4	C	901	65I	O1-C6	-2.24	1.40	1.45
4	D	802	65I	O6-C11	2.23	1.40	1.34
3	B	801	XJ7	O7-C7	2.23	1.39	1.33
3	B	801	XJ7	O7-C6	-2.23	1.40	1.45
4	A	802	65I	O6-C11	2.22	1.40	1.34
4	F	901	65I	O6-C11	2.19	1.40	1.34
3	A	801	XJ7	P-O4	-2.19	1.45	1.55
4	C	901	65I	O6-C11	2.19	1.40	1.34
4	C	901	65I	O1-C5	2.19	1.39	1.33
3	B	801	XJ7	P-O4	-2.15	1.45	1.55
3	A	801	XJ7	O7-C7	2.15	1.39	1.33
3	C	902	XJ7	P-O4	-2.14	1.45	1.55
4	D	802	65I	P-O3	-2.12	1.45	1.55
3	D	801	XJ7	O9-C11	2.11	1.40	1.34
3	D	801	XJ7	P-O4	-2.11	1.45	1.55
4	D	802	65I	O1-C6	-2.11	1.40	1.45
4	A	802	65I	O1-C6	-2.08	1.40	1.45
4	C	901	65I	P-O3	-2.06	1.45	1.55
3	C	902	XJ7	O7-C6	-2.06	1.40	1.45
4	F	901	65I	O1-C6	-2.04	1.40	1.45
4	F	901	65I	P-O3	-2.02	1.45	1.55

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	XJ7	O9-C11-C12	5.28	122.88	111.50
3	B	801	XJ7	O9-C11-C12	4.91	122.08	111.50
4	F	901	65I	O6-C11-C12	4.66	121.54	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	801	XJ7	O9-C11-C12	4.50	121.20	111.50
3	C	902	XJ7	O9-C11-C12	4.50	121.19	111.50
3	B	801	XJ7	O7-C7-C8	4.19	125.05	111.91
4	D	802	65I	O6-C11-C12	4.17	120.49	111.50
4	C	901	65I	O6-C11-C12	3.95	120.02	111.50
4	A	802	65I	O6-C11-C12	3.70	119.48	111.50
3	B	801	XJ7	O7-C7-O8	-3.61	114.48	123.59
3	D	801	XJ7	O7-C7-C8	3.42	122.64	111.91
3	C	902	XJ7	C24-C3-C2	-3.18	106.26	110.85
3	A	801	XJ7	O7-C7-C8	3.12	121.71	111.91
3	D	801	XJ7	C1-C-C25	3.09	116.21	110.82
3	C	902	XJ7	O7-C7-C8	3.05	121.47	111.91
3	C	902	XJ7	C2-C1-C	3.04	116.12	110.82
3	D	801	XJ7	C24-C3-C2	-3.00	106.53	110.85
3	B	801	XJ7	C24-C3-C2	-2.94	106.62	110.85
4	F	901	65I	O1-C5-C4	2.72	120.44	111.91
4	D	802	65I	O1-C5-C4	2.67	120.28	111.91
3	D	801	XJ7	O7-C7-O8	-2.59	117.05	123.59
3	D	801	XJ7	C2-C1-C	2.48	115.16	110.82
3	A	801	XJ7	O4-P-O5	-2.46	100.07	112.24
3	A	801	XJ7	C24-C3-C2	-2.46	107.31	110.85
4	A	802	65I	O1-C5-C4	2.46	119.62	111.91
3	B	801	XJ7	O4-P-O5	-2.43	100.22	112.24
4	C	901	65I	O1-C5-C4	2.38	119.39	111.91
3	C	902	XJ7	O4-P-O5	-2.38	100.47	112.24
4	A	802	65I	O3-P-O4	-2.34	100.69	112.24
3	D	801	XJ7	O4-P-O5	-2.32	100.76	112.24
4	F	901	65I	O3-P-O4	-2.32	100.77	112.24
3	B	801	XJ7	O7-C6-C5	2.31	115.16	108.43
4	D	802	65I	O3-P-O4	-2.31	100.83	112.24
3	B	801	XJ7	O9-C11-O10	-2.22	118.33	123.70
4	C	901	65I	O3-P-O4	-2.22	101.24	112.24
3	D	801	XJ7	O2-C2-C1	-2.10	105.49	110.35

There are no chirality outliers.

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	XJ7	C3-O3-P-O4
3	A	801	XJ7	C4-O6-P-O4
3	A	801	XJ7	C4-O6-P-O5
3	B	801	XJ7	C12-C11-O9-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	801	XJ7	C3-O3-P-O4
3	B	801	XJ7	C4-O6-P-O4
3	B	801	XJ7	C4-O6-P-O5
3	C	902	XJ7	C3-O3-P-O4
3	D	801	XJ7	C3-O3-P-O4
3	D	801	XJ7	C4-O6-P-O4
3	D	801	XJ7	C4-O6-P-O5
4	A	802	65I	C9-O5-P-O4
4	F	901	65I	N-C10-C9-O5
4	C	901	65I	N-C10-C9-O5
4	C	901	65I	C9-O5-P-O4
4	D	802	65I	O-C5-O1-C6
3	B	801	XJ7	O10-C11-O9-C5
3	D	801	XJ7	O10-C11-O9-C5
4	F	901	65I	C4-C5-O1-C6
3	D	801	XJ7	C12-C11-O9-C5
4	A	802	65I	C4-C5-O1-C6
4	C	901	65I	C4-C5-O1-C6
4	D	802	65I	C4-C5-O1-C6
4	A	802	65I	O-C5-O1-C6
4	F	901	65I	O-C5-O1-C6
4	C	901	65I	O-C5-O1-C6
3	A	801	XJ7	C8-C7-O7-C6
3	A	801	XJ7	O8-C7-O7-C6
3	D	801	XJ7	C8-C7-O7-C6
3	D	801	XJ7	O8-C7-O7-C6
3	B	801	XJ7	C8-C7-O7-C6
3	C	902	XJ7	C8-C7-O7-C6
3	B	801	XJ7	C3-O3-P-O6
3	B	801	XJ7	C11-C12-C13-C14
3	C	902	XJ7	C11-C12-C13-C14
3	B	801	XJ7	O8-C7-O7-C6
3	C	902	XJ7	O8-C7-O7-C6
3	A	801	XJ7	C11-C12-C13-C14
3	A	801	XJ7	C4-O6-P-O3
3	B	801	XJ7	C4-O6-P-O3
3	D	801	XJ7	C4-O6-P-O3
4	A	802	65I	C9-O5-P-O2
4	C	901	65I	C9-O5-P-O2
4	A	802	65I	C11-C12-C13-C14
3	A	801	XJ7	C3-O3-P-O6
3	C	902	XJ7	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	801	XJ7	C3-O3-P-O6
4	F	901	65I	C1-C2-C3-C4
4	C	901	65I	C1-C2-C3-C4
4	D	802	65I	C13-C14-C15-C16
4	D	802	65I	C11-C12-C13-C14
3	B	801	XJ7	C19-C20-C21-C22
4	A	802	65I	C1-C2-C3-C4
3	C	902	XJ7	O10-C11-O9-C5
3	A	801	XJ7	C12-C11-O9-C5
3	C	902	XJ7	C12-C11-O9-C5
4	A	802	65I	C13-C14-C15-C16
4	A	802	65I	N-C10-C9-O5
3	A	801	XJ7	O10-C11-O9-C5
3	D	801	XJ7	C11-C12-C13-C14
3	B	801	XJ7	C4-C5-C6-O7
4	D	802	65I	C-C1-C2-C3
3	D	801	XJ7	C16-C17-C18-C19
4	D	802	65I	C17-C18-C19-C20
3	C	902	XJ7	O9-C5-C6-O7
3	D	801	XJ7	C24-C3-O3-P
4	C	901	65I	C17-C18-C19-C20
3	C	902	XJ7	C4-C5-C6-O7
3	A	801	XJ7	C3-O3-P-O5
3	C	902	XJ7	C3-O3-P-O5
3	D	801	XJ7	C3-O3-P-O5
4	D	802	65I	C1-C2-C3-C4
3	B	801	XJ7	C20-C21-C22-C23
4	F	901	65I	C17-C18-C19-C20
3	B	801	XJ7	C13-C14-C15-C16
3	B	801	XJ7	O9-C5-C6-O7
4	D	802	65I	O1-C6-C7-O6
4	A	802	65I	C17-C18-C19-C20
4	F	901	65I	C13-C14-C15-C16
3	C	902	XJ7	C4-O6-P-O5
4	F	901	65I	C11-C12-C13-C14
4	C	901	65I	C13-C14-C15-C16
4	F	901	65I	C9-O5-P-O2
3	D	801	XJ7	C2-C3-O3-P
4	A	802	65I	C-C1-C2-C3
4	D	802	65I	O7-C11-O6-C7
4	F	901	65I	O6-C11-C12-C13
3	B	801	XJ7	C3-O3-P-O5

Continued on next page...

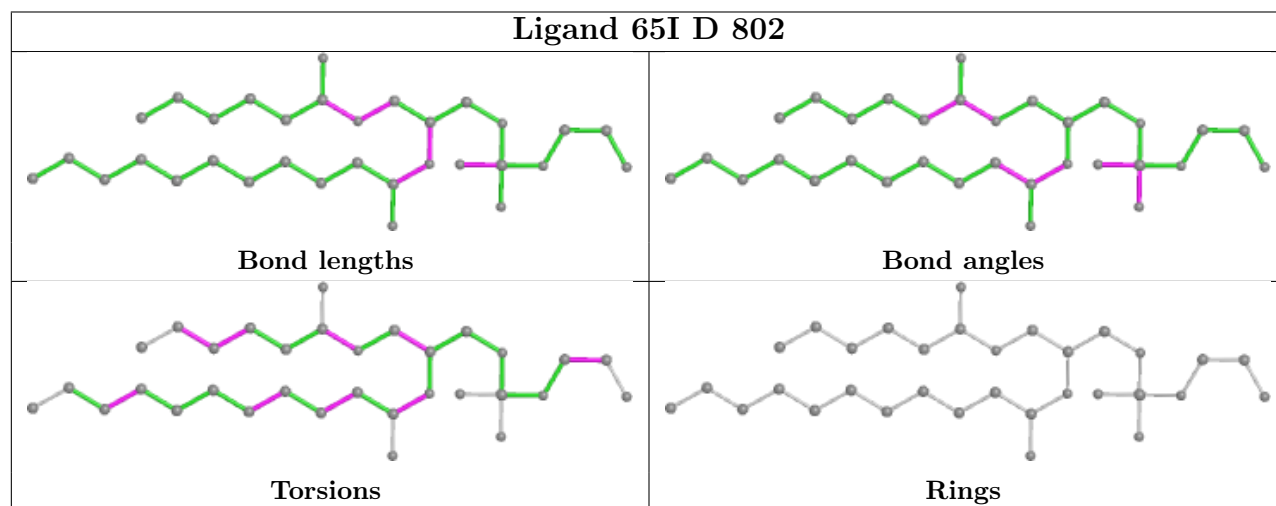
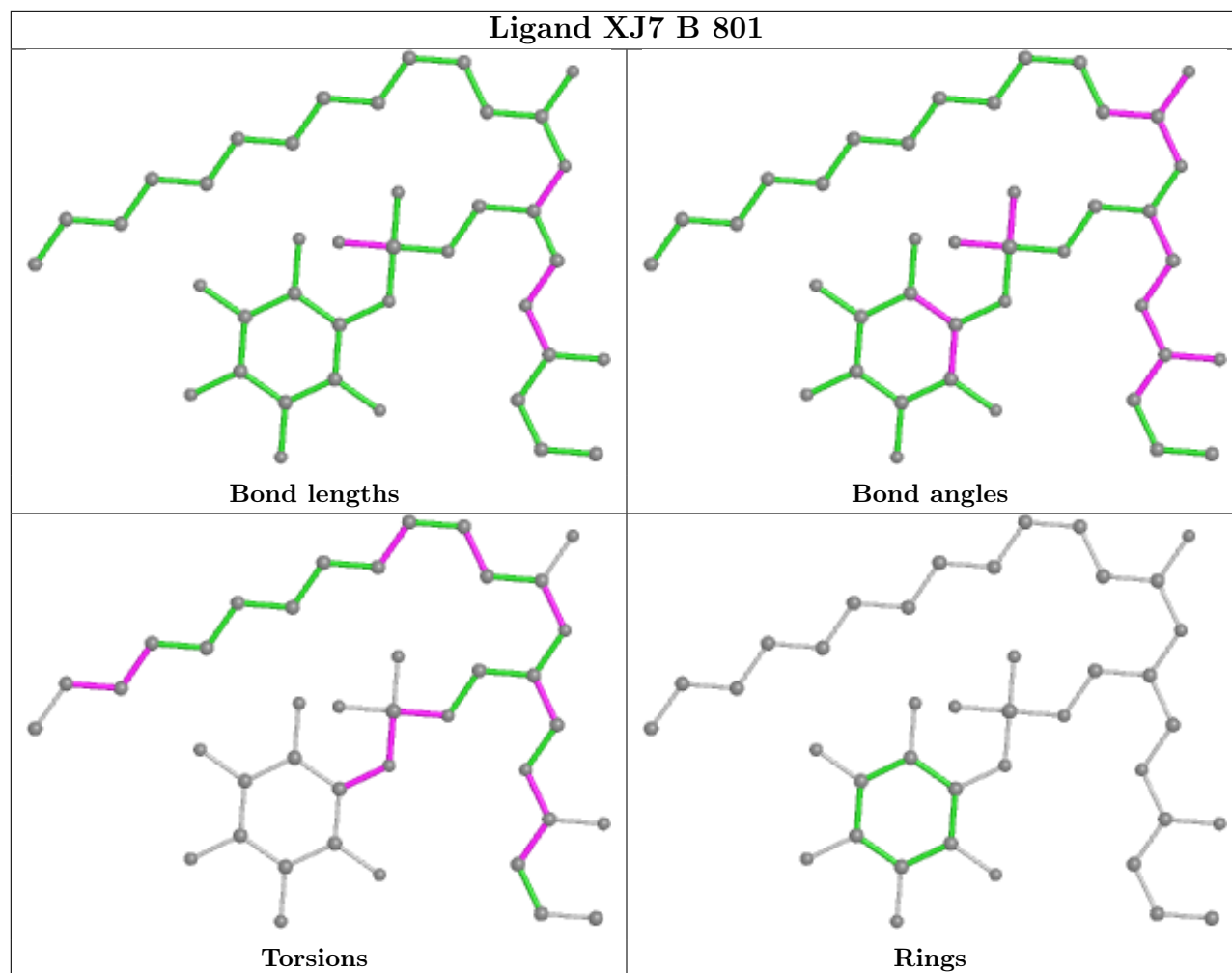
Continued from previous page...

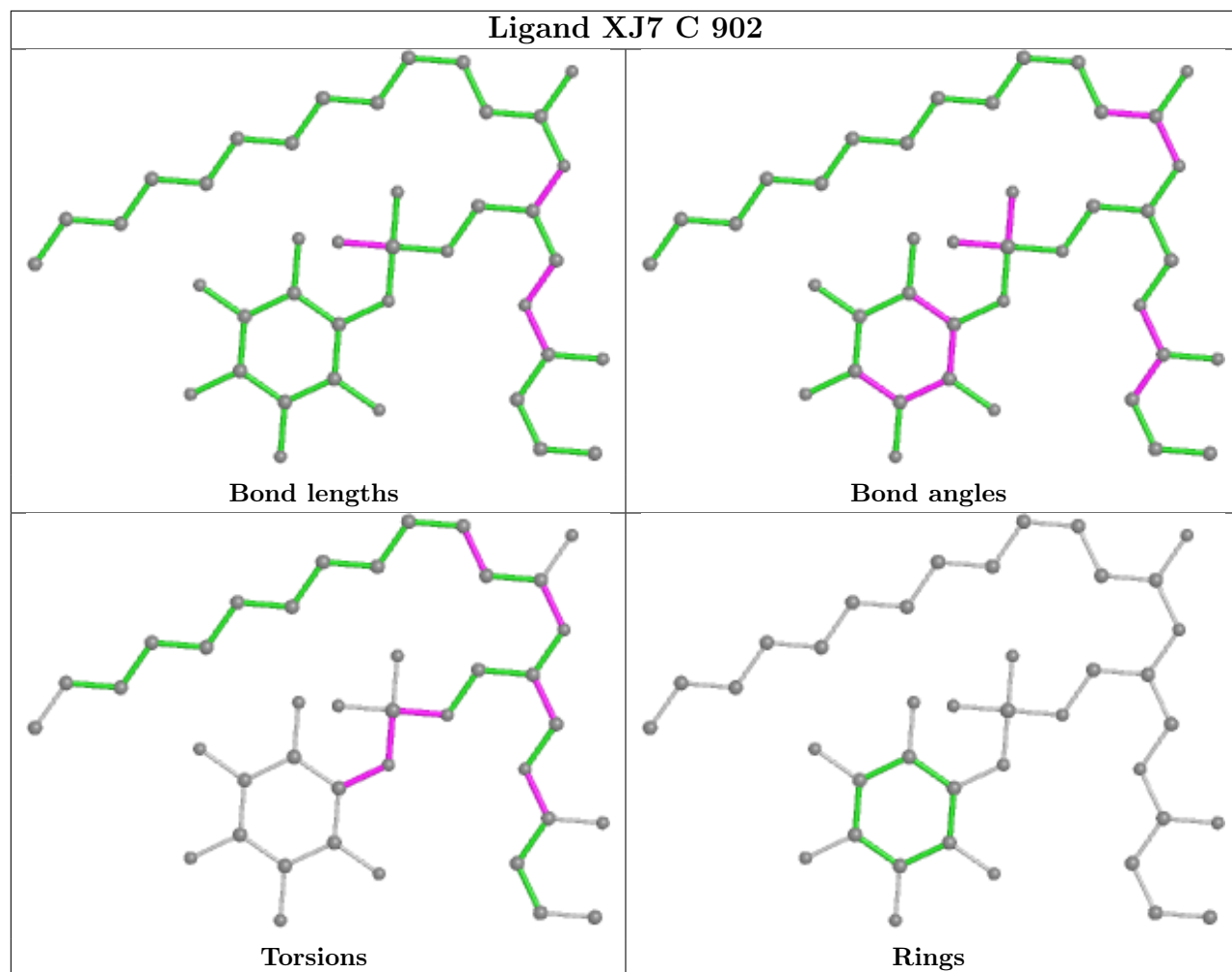
Mol	Chain	Res	Type	Atoms
4	A	802	65I	C12-C13-C14-C15
3	B	801	XJ7	O7-C7-C8-C9
4	F	901	65I	C-C1-C2-C3
3	C	902	XJ7	C2-C3-O3-P
3	A	801	XJ7	O7-C7-C8-C9
4	C	901	65I	O6-C11-C12-C13
3	D	801	XJ7	C13-C14-C15-C16
4	C	901	65I	C12-C13-C14-C15
4	D	802	65I	C12-C11-O6-C7
3	B	801	XJ7	C2-C3-O3-P
3	B	801	XJ7	C24-C3-O3-P
3	C	902	XJ7	C24-C3-O3-P
4	D	802	65I	O1-C6-C7-C8
3	C	902	XJ7	C4-O6-P-O3
4	F	901	65I	C9-O5-P-O4
4	D	802	65I	N-C10-C9-O5
3	D	801	XJ7	O7-C7-C8-C9
4	A	802	65I	C10-C9-O5-P

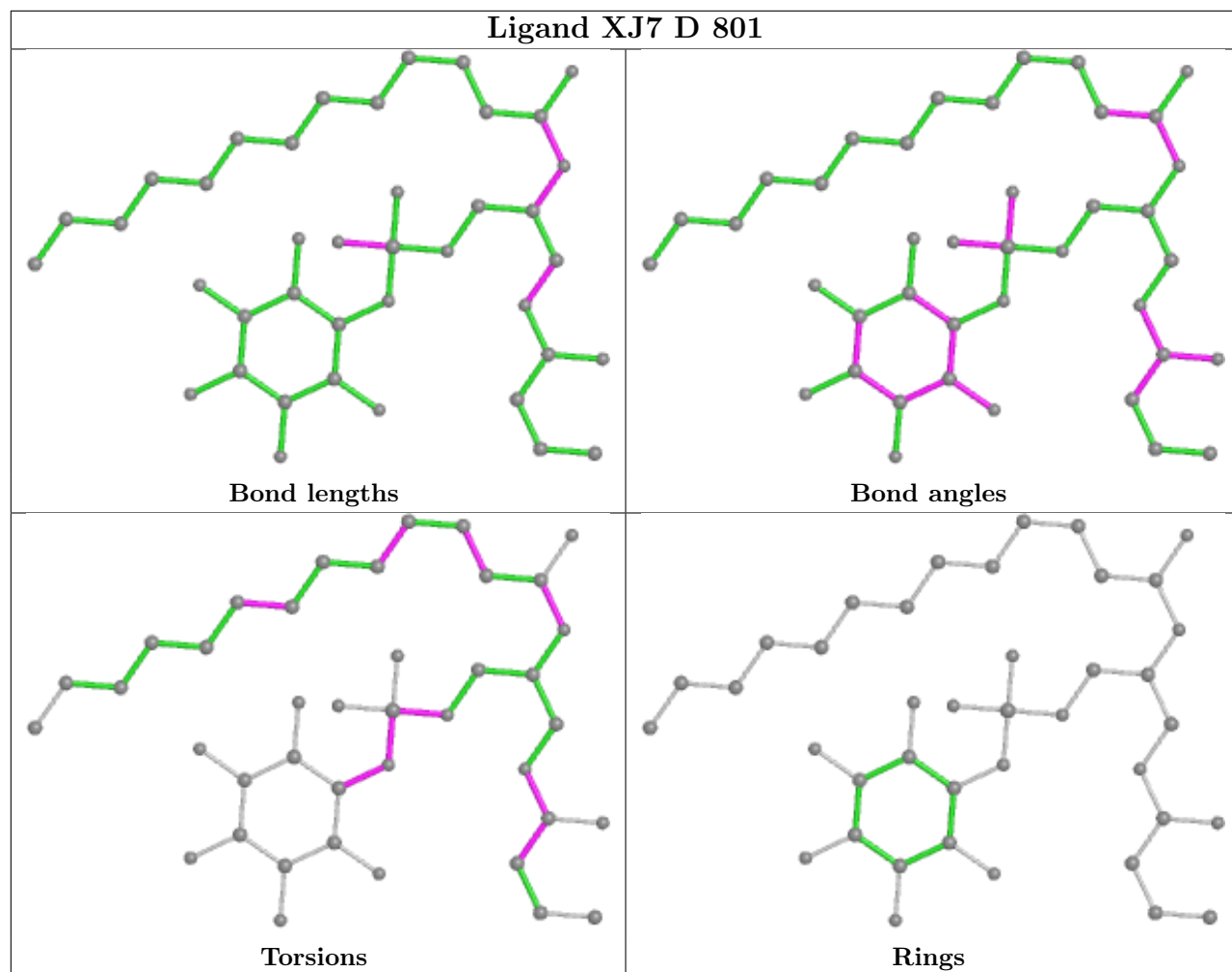
There are no ring outliers.

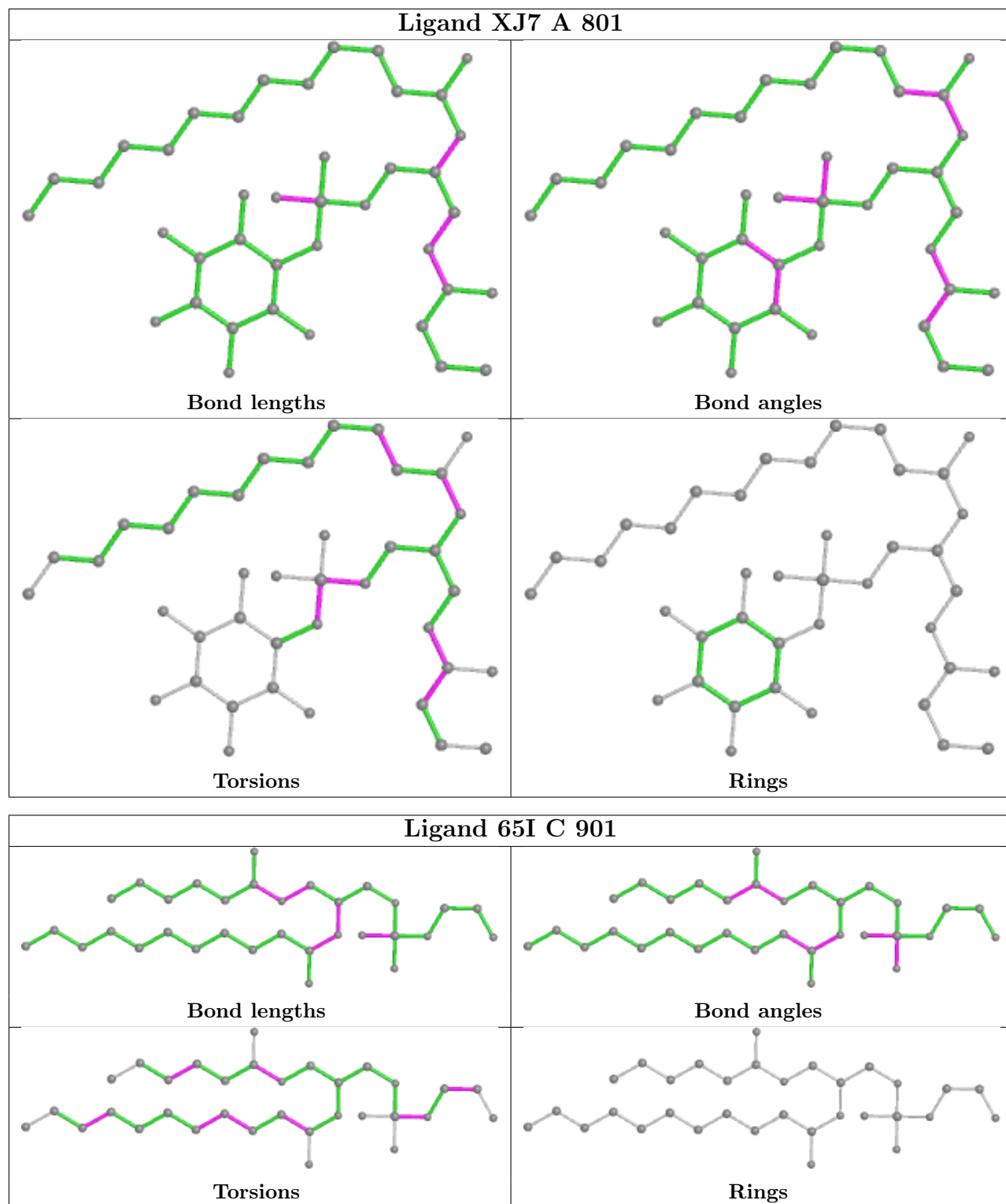
No monomer is involved in short contacts.

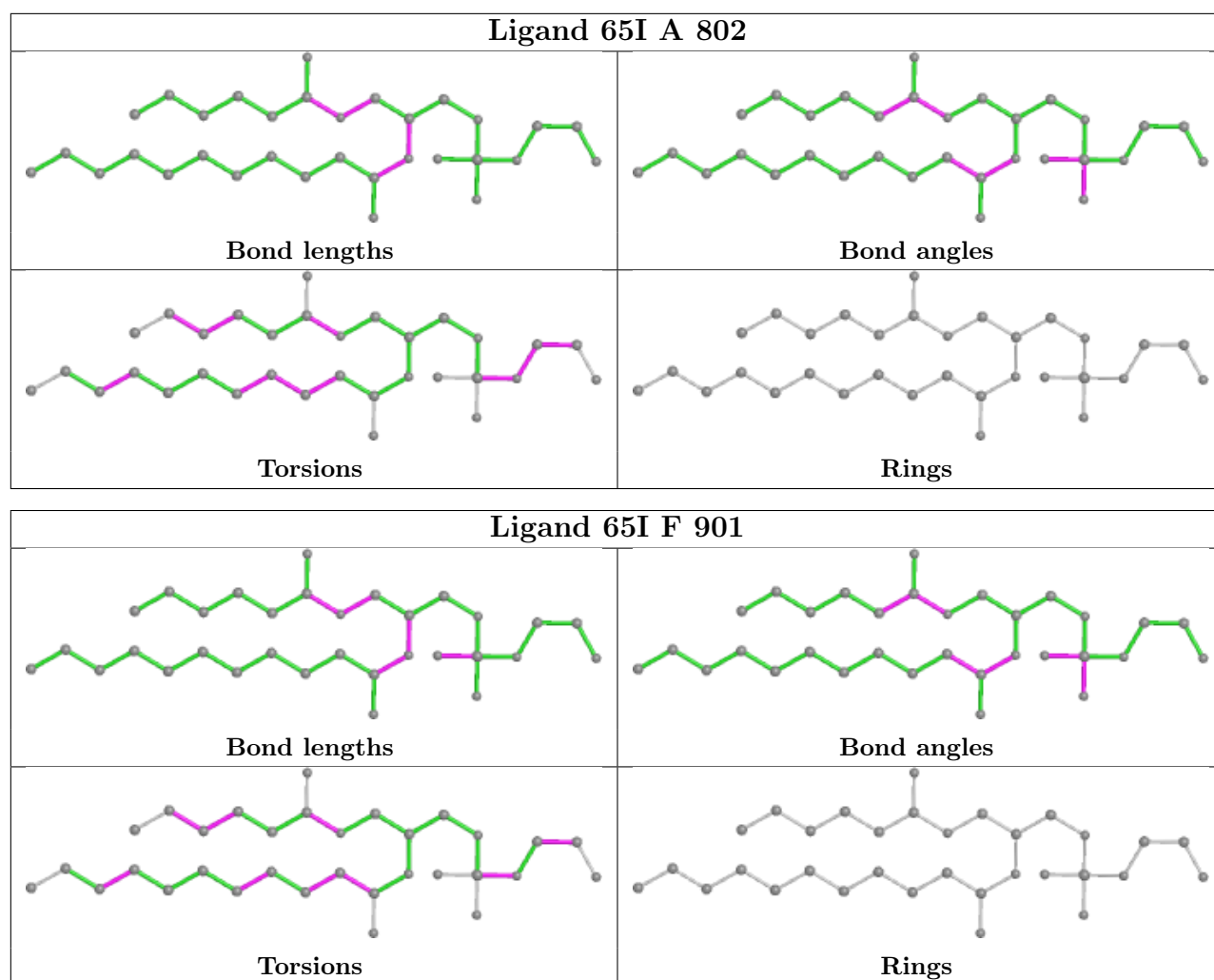
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

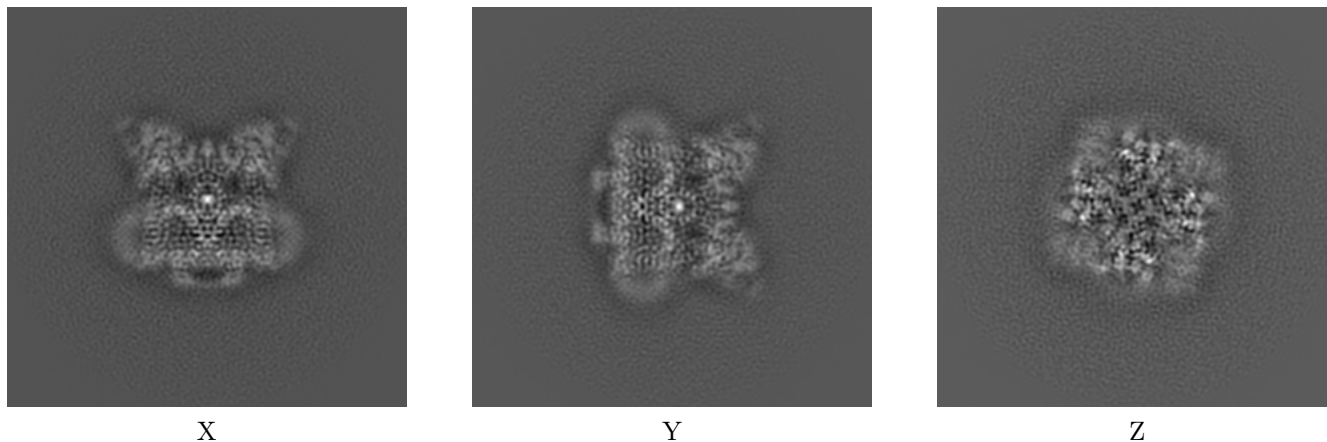
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23138. These allow visual inspection of the internal detail of the map and identification of artifacts.

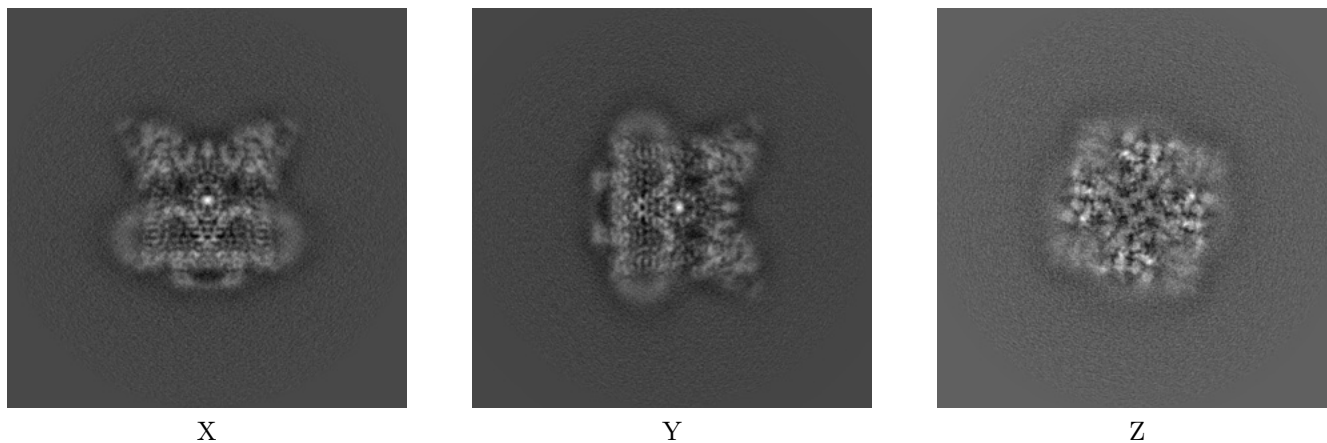
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



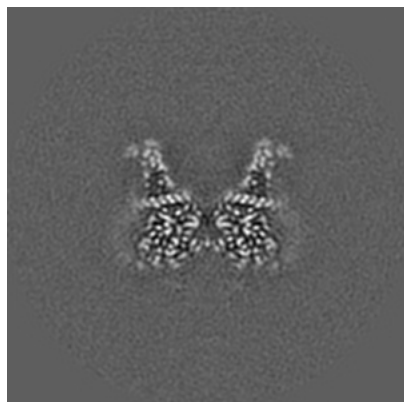
6.1.2 Raw map



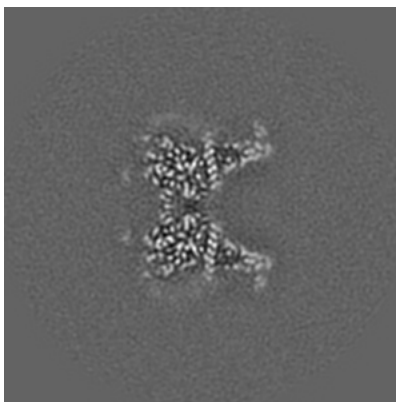
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

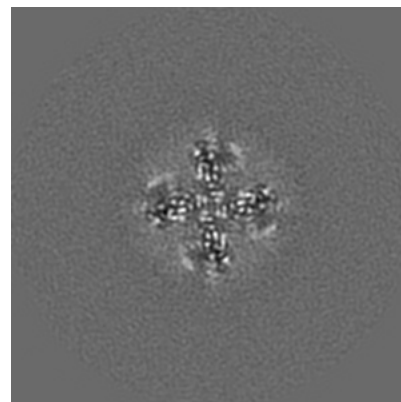
6.2.1 Primary map



X Index: 160

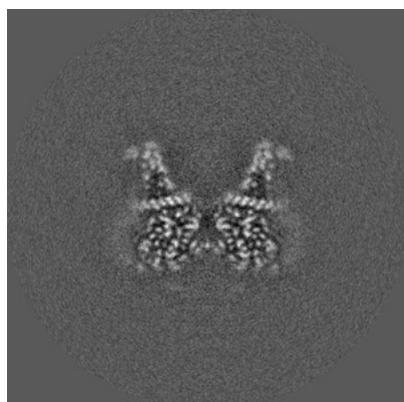


Y Index: 160

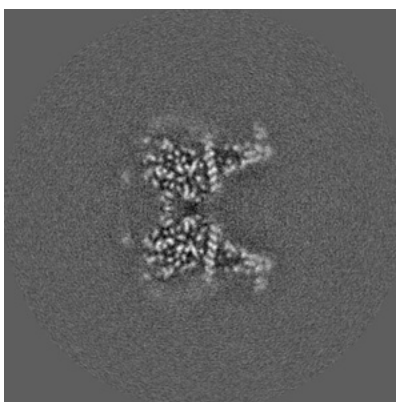


Z Index: 160

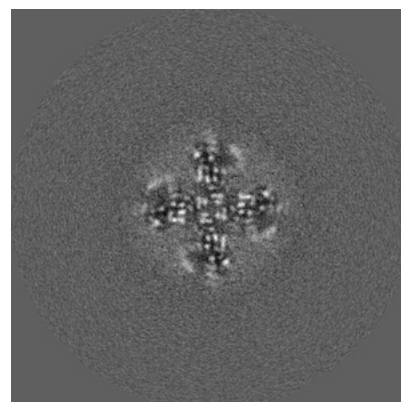
6.2.2 Raw map



X Index: 160



Y Index: 160

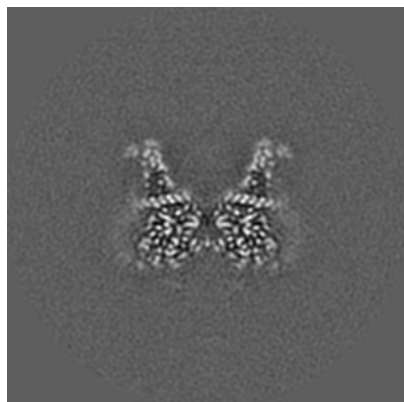


Z Index: 160

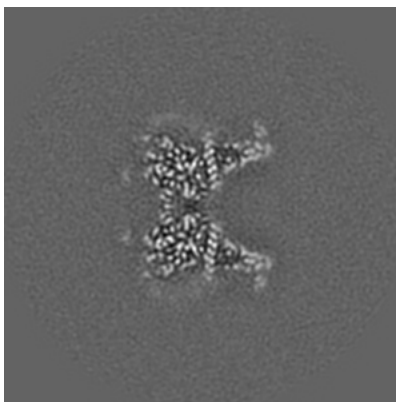
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

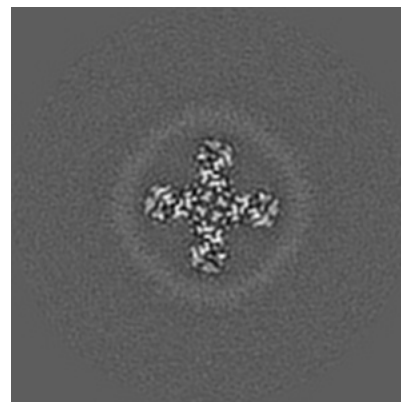
6.3.1 Primary map



X Index: 160

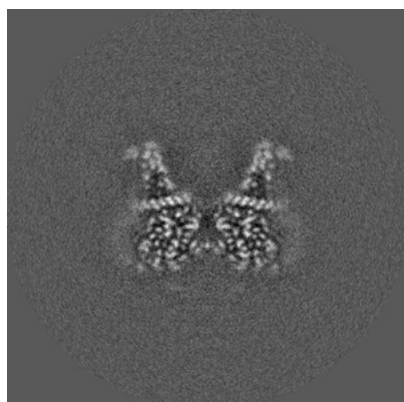


Y Index: 160

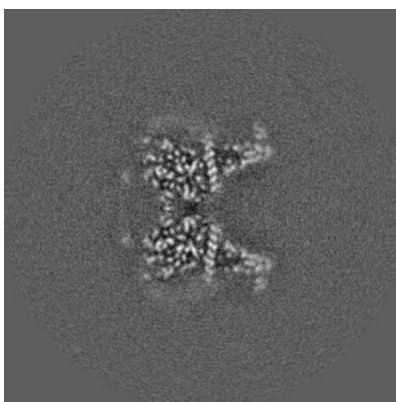


Z Index: 134

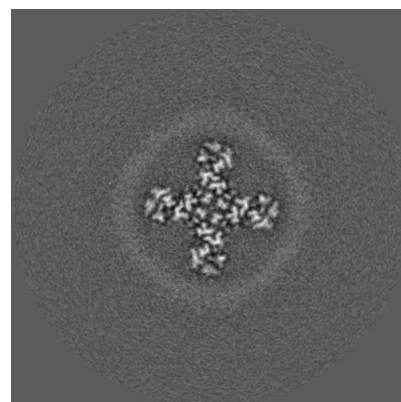
6.3.2 Raw map



X Index: 160



Y Index: 160

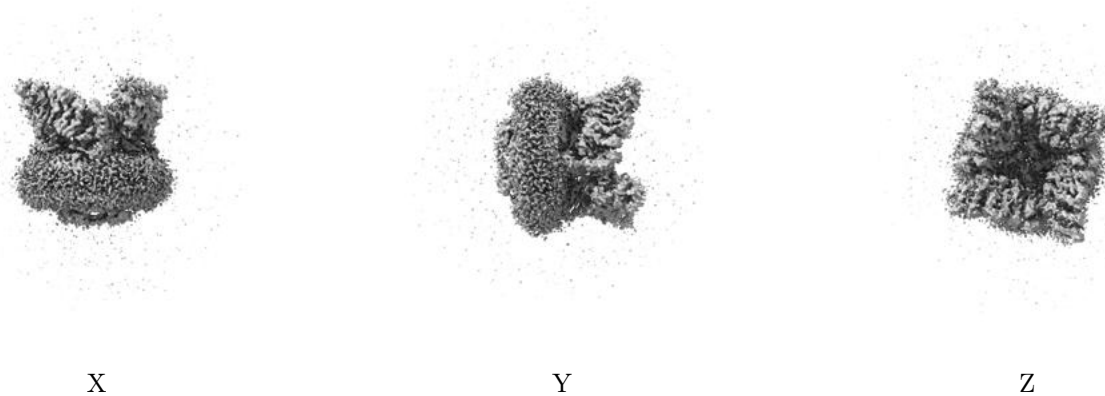


Z Index: 134

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

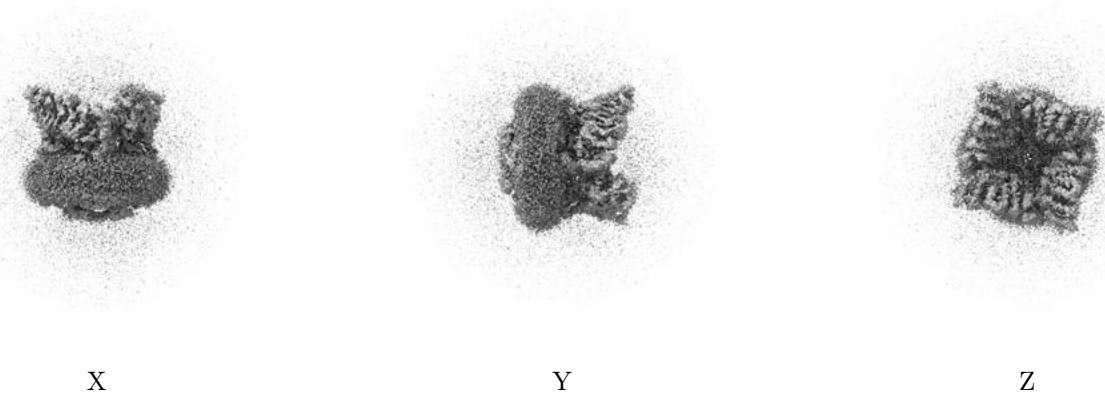
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

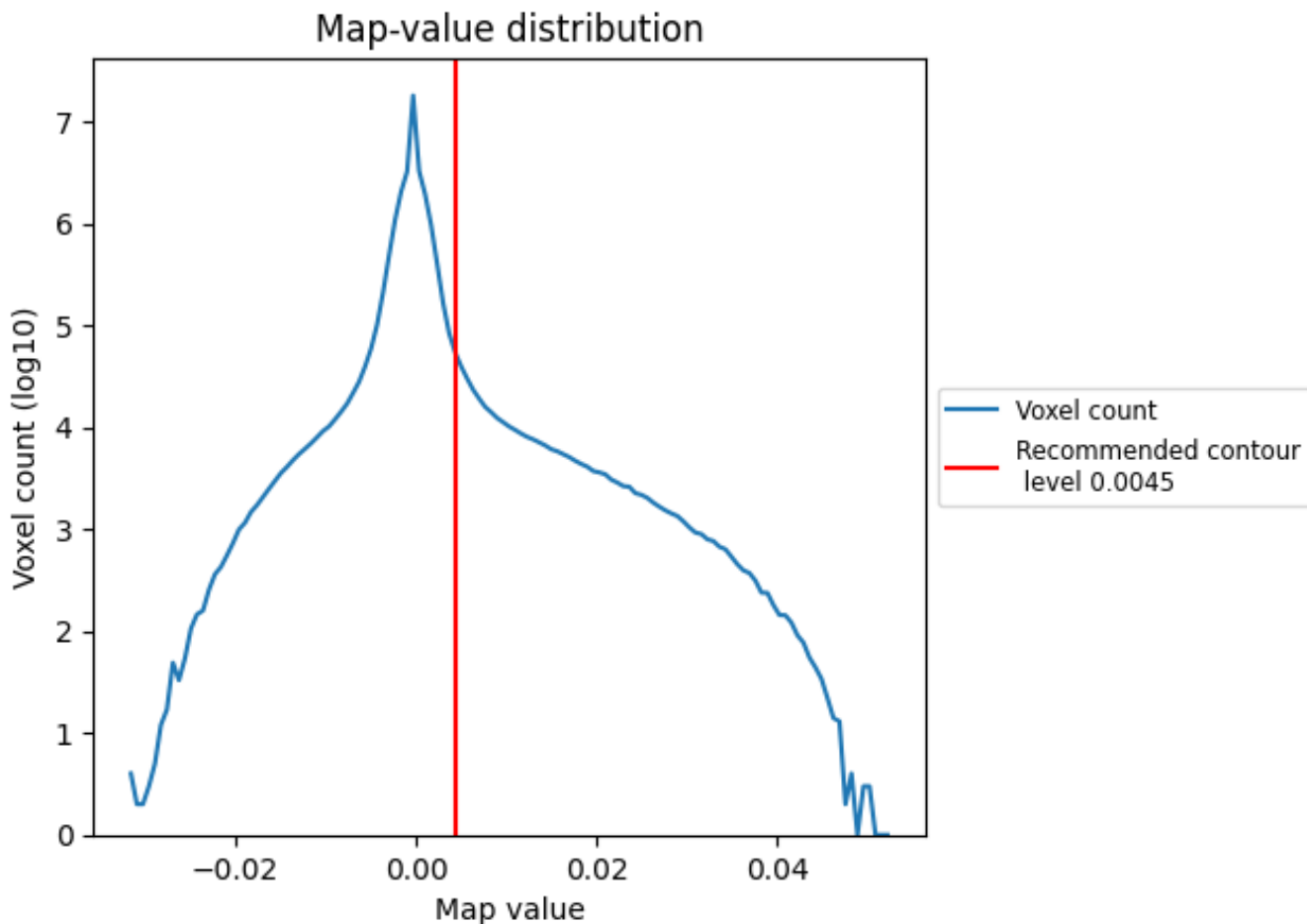
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

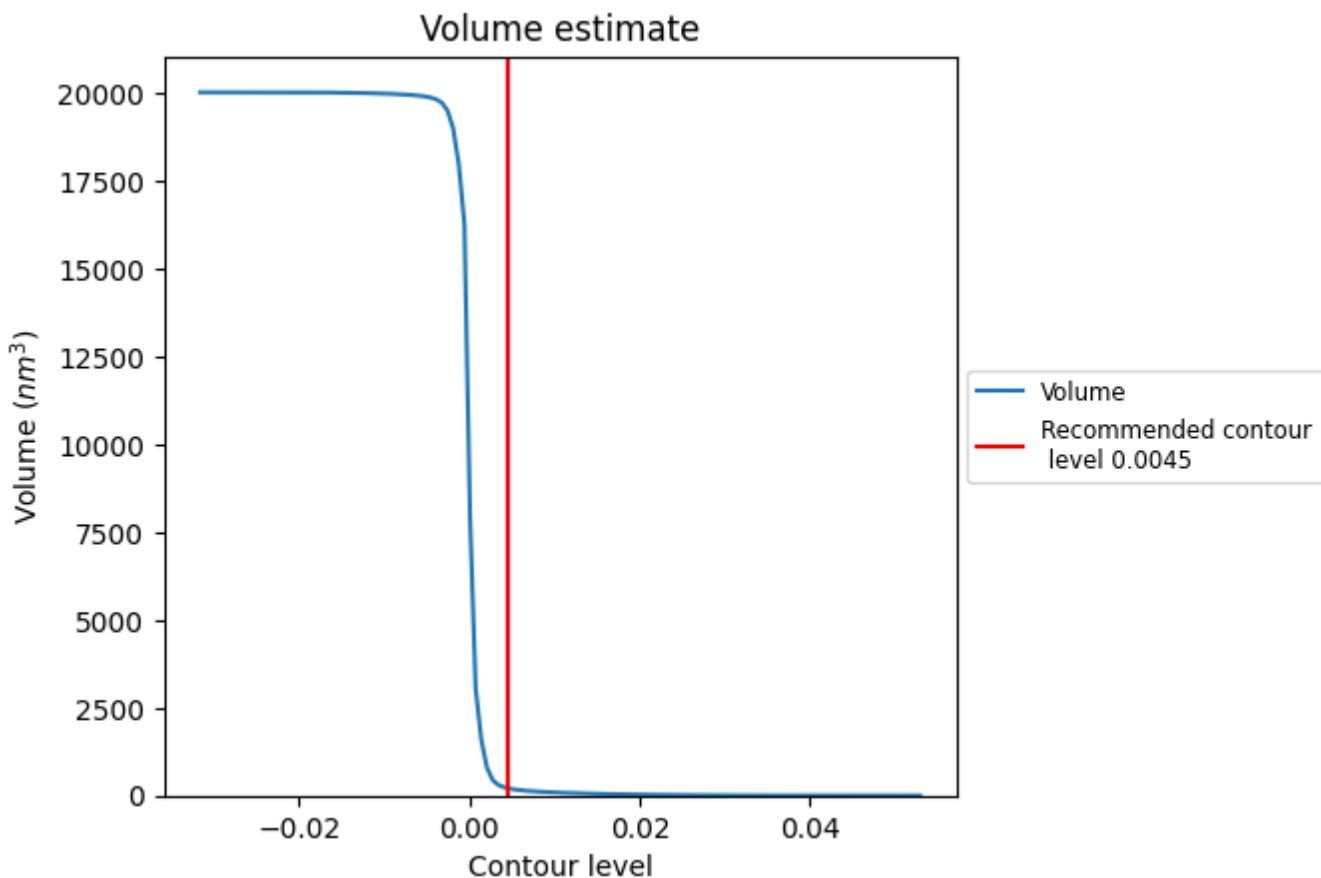
This section contains the results of statistical analysis of the map.

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.

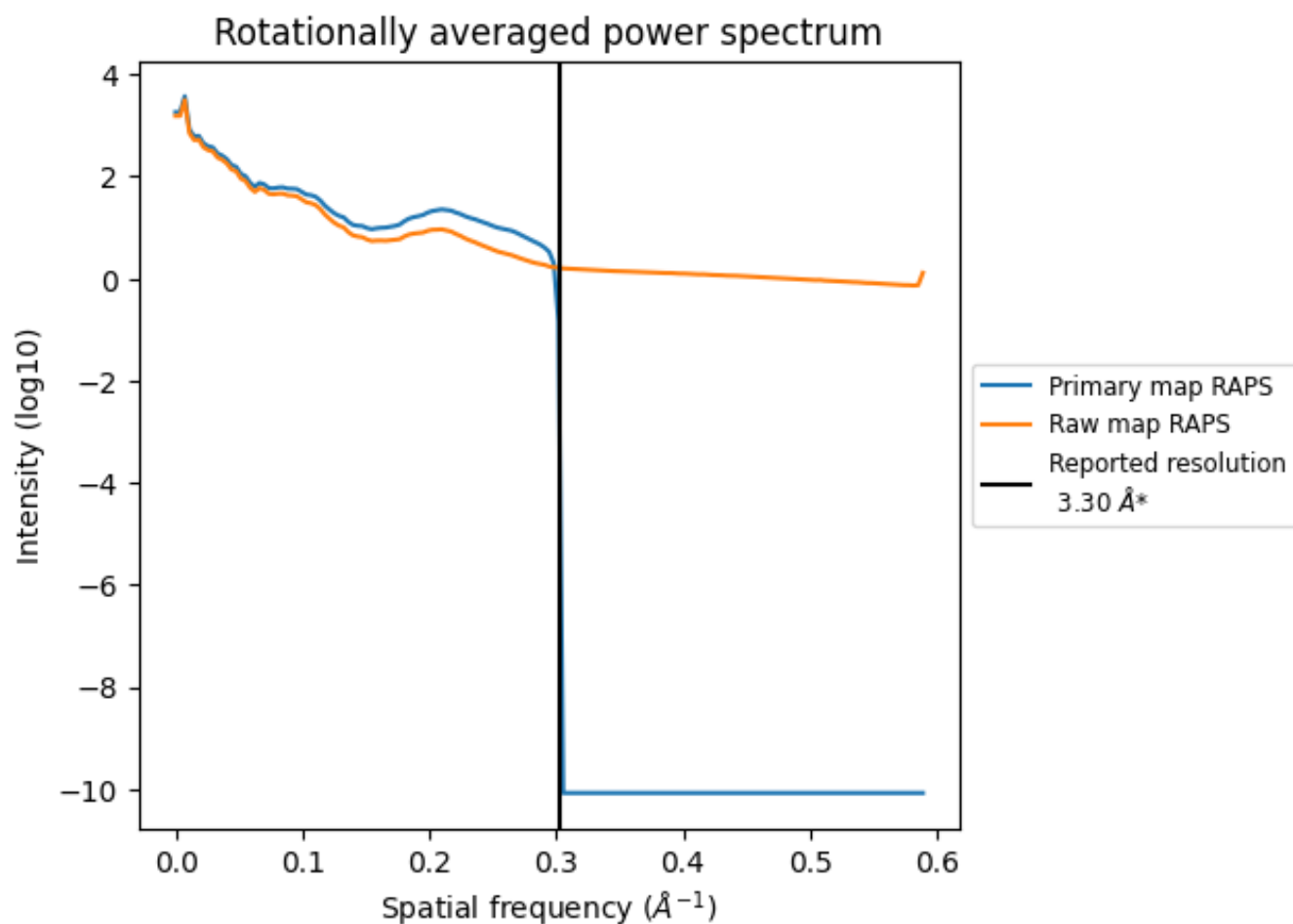
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm³; this corresponds to an approximate mass of 193 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](#)

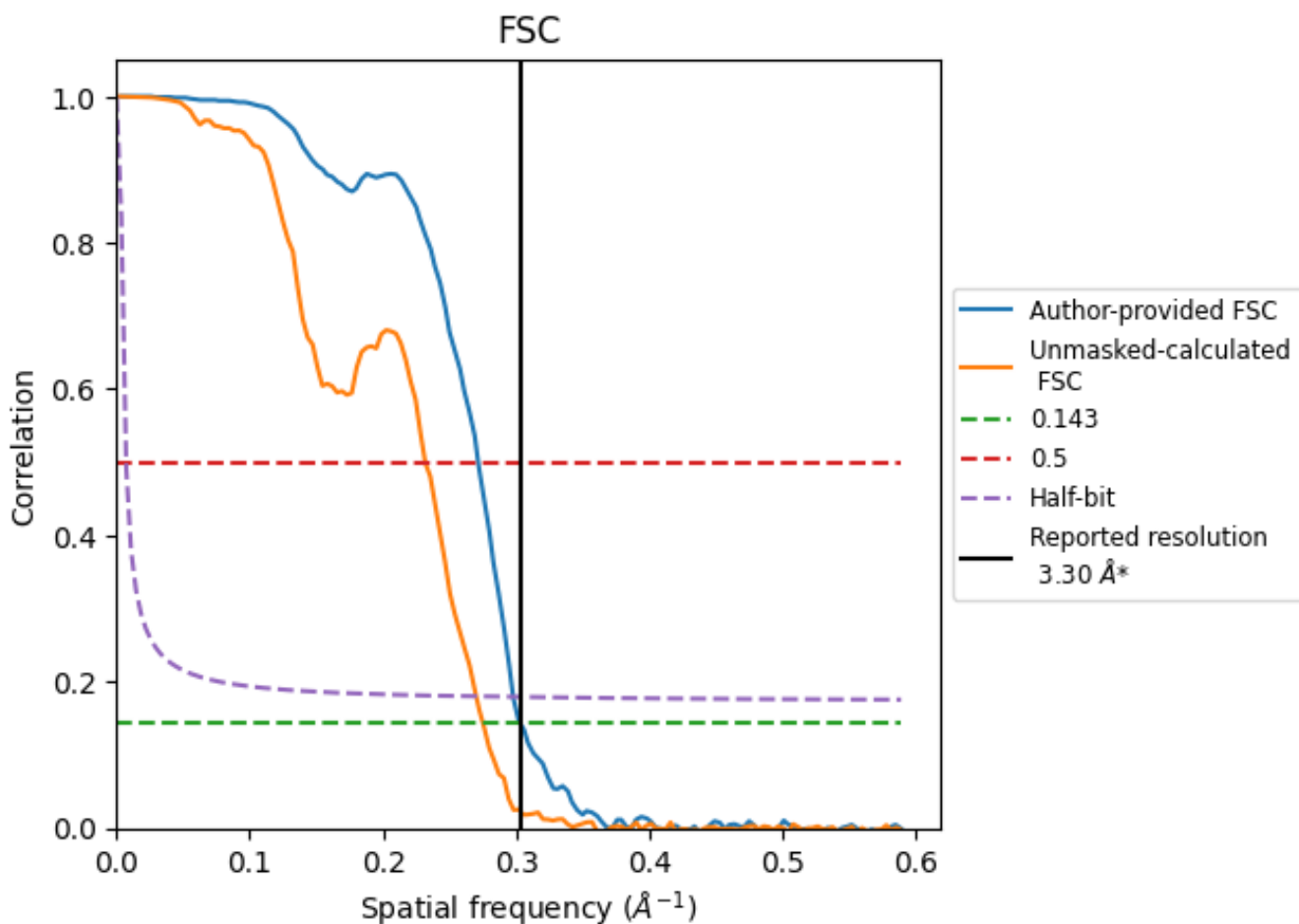


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

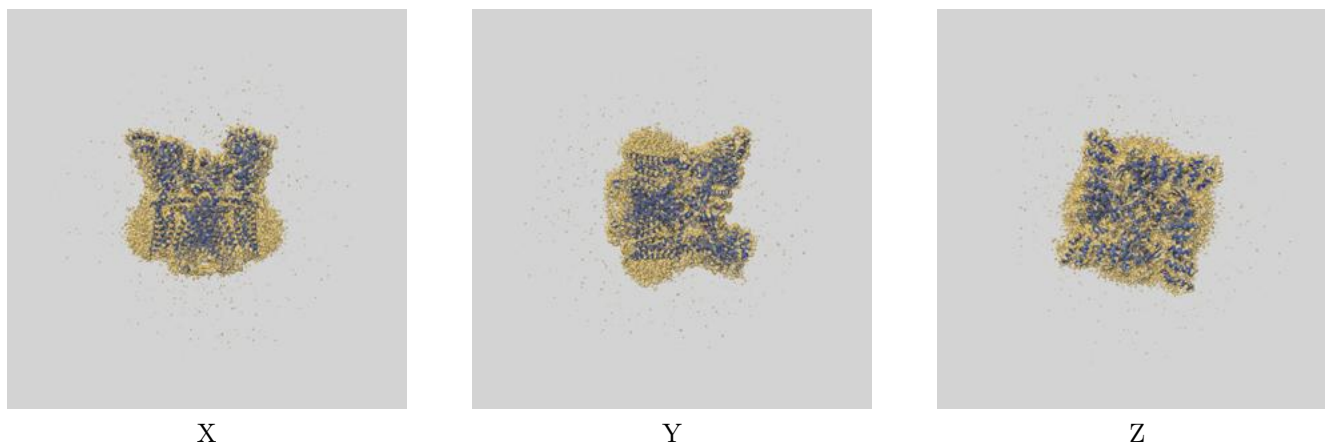
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.68	3.36
Unmasked-calculated*	3.63	4.31	3.70

*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 3.63 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

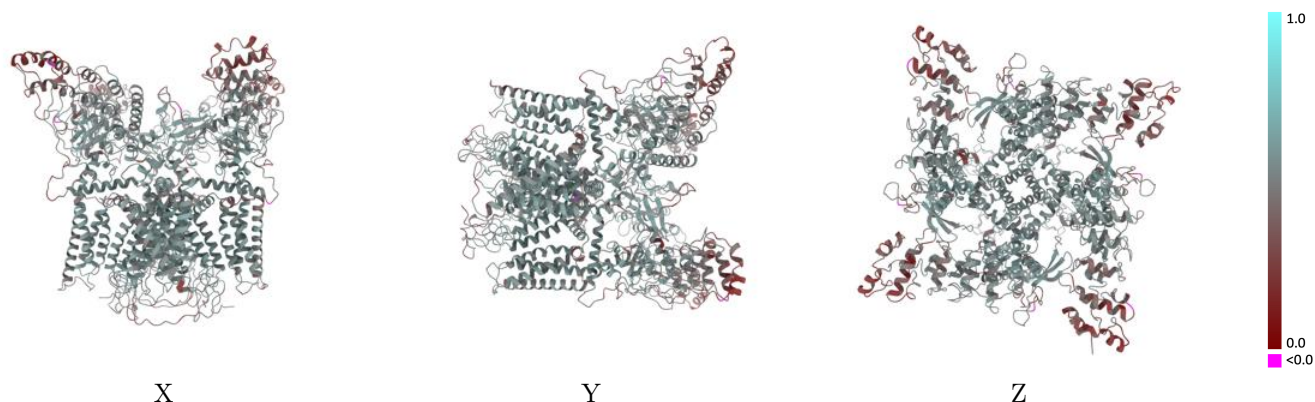
This section contains information regarding the fit between EMDB map EMD-23138 and PDB model 7L2R. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



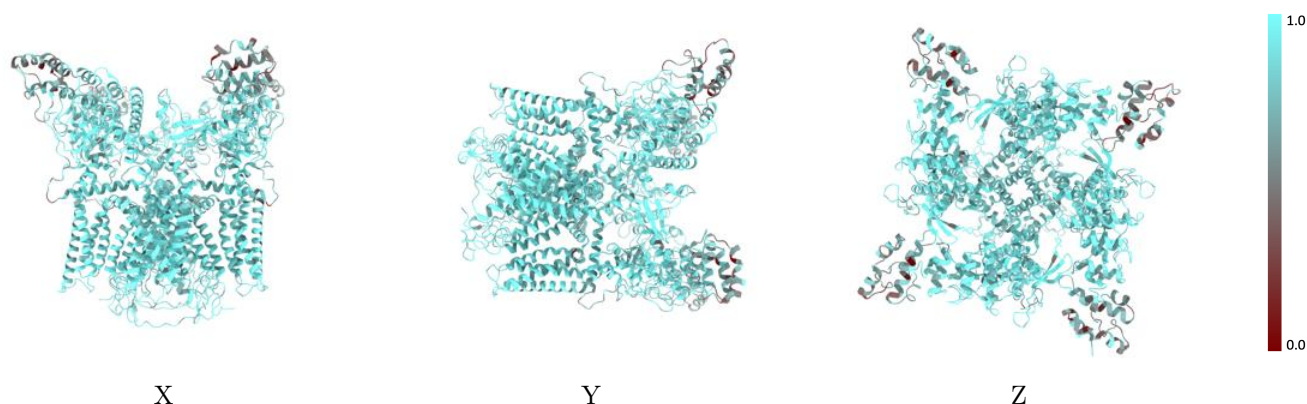
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



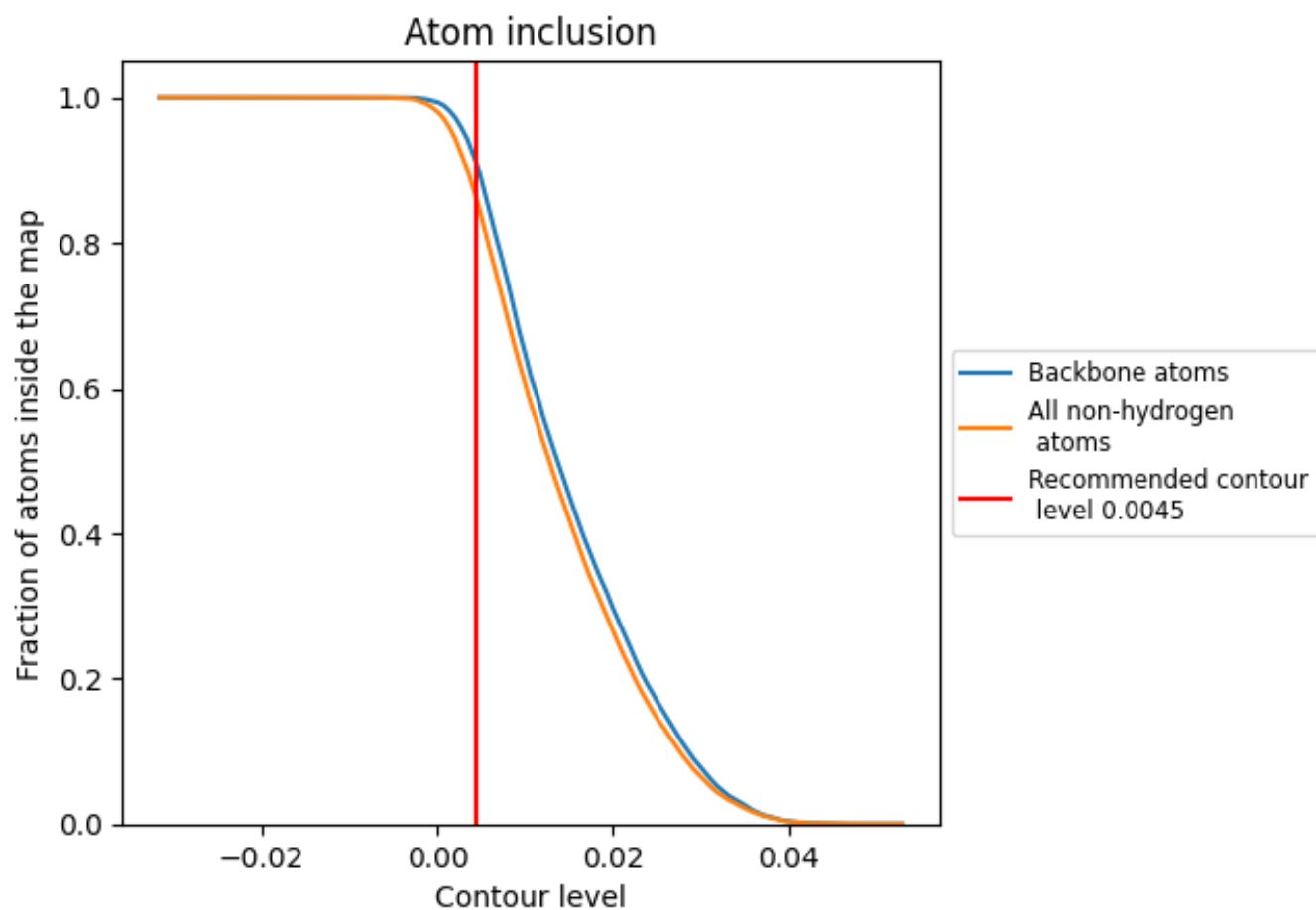
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0045).















9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8583	 0.4930
A	 0.8591	 0.4950
B	 0.8601	 0.4960
C	 0.8647	 0.4940
D	 0.8639	 0.4920
E	 0.8814	 0.4620
F	 0.8941	 0.4730

