



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 04:36 AM UTC

PDB ID : 7SI3 / pdb_00007si3
EMDB ID : EMD-25137
Title : Consensus structure of ATP7B
Authors : Bitter, R.M.; Oh, S.C.; Hite, R.K.; Yuan, P.
Deposited on : 2021-10-12
Resolution : 3.19 Å(reported)
Based on initial model : 3RFU

This is a wwPDB EM Validation Summary 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

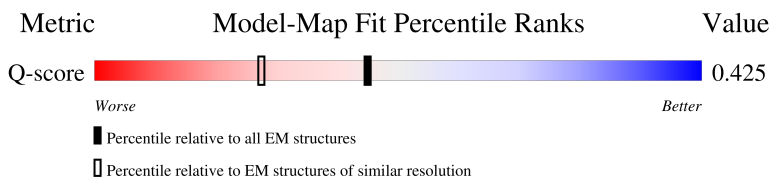
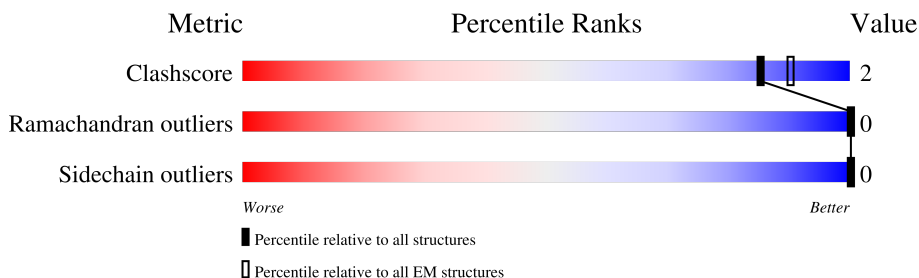
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14455 (2.69 - 3.69)

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	1467	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13500 atoms, of which 6901 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 P-type Cu(+) transporter.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	873	Total	C	H	N	O	S	0	1
			13494	4234	6901	1109	1201	49		

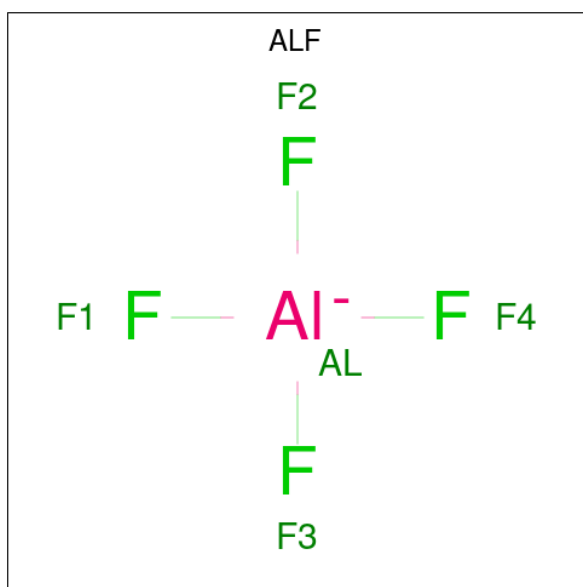
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	HIS	ARG	conflict	UNP A0A6I8R0A5
A	359	ILE	MET	conflict	UNP A0A6I8R0A5
A	497	ILE	ALA	conflict	UNP A0A6I8R0A5

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mg	0
			1	1	

- Molecule 3 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).

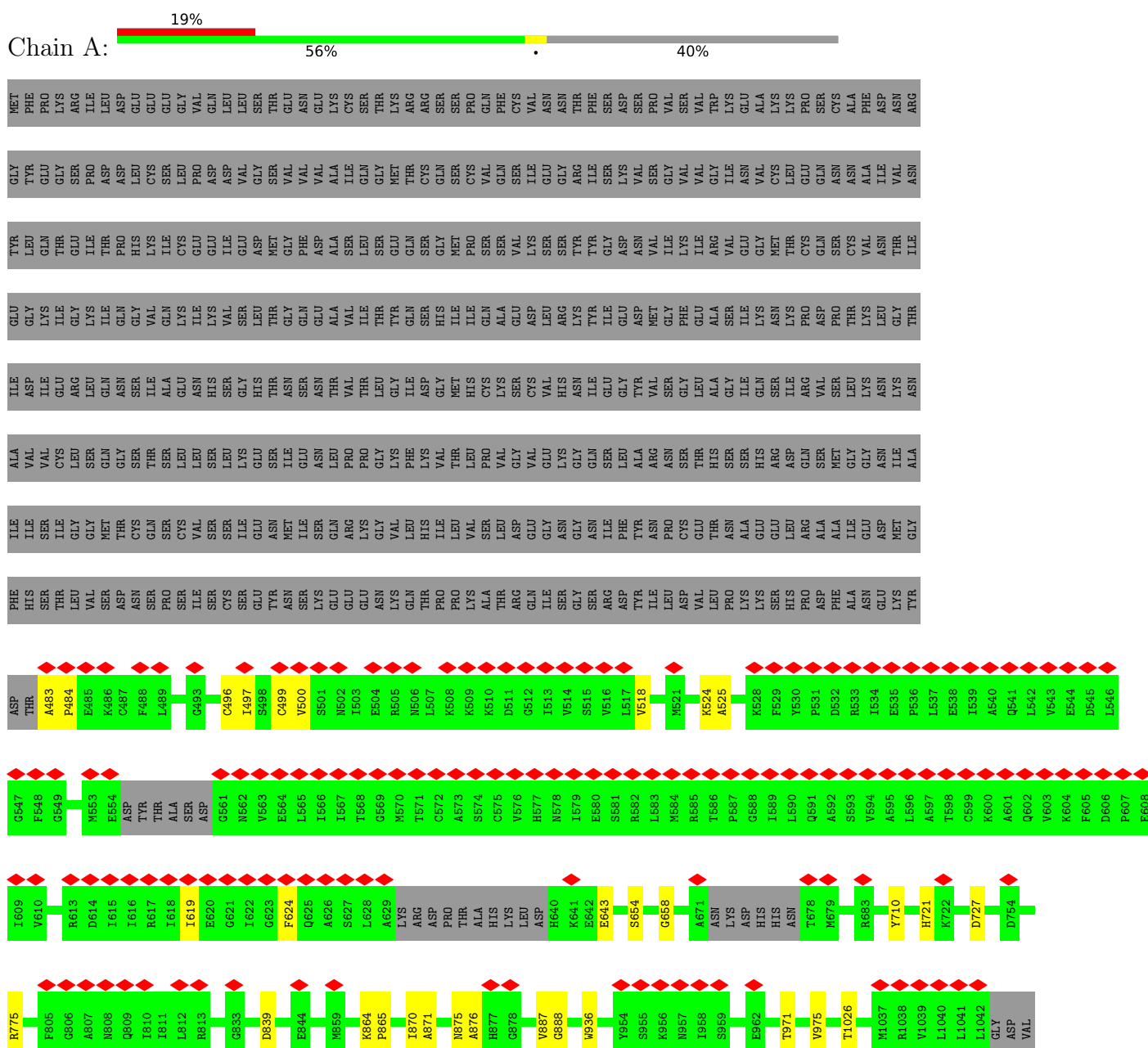


Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
3	A	1	5	1	4	0

3 Residue-property plots

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

- Molecule 1: P-type Cu(+) transporter



TRP	SER	R1389	S1168	S1108	V1046
	LEU	Y1390	T1169	V1109	K1047
	LEU	E1391	D1170	L1110	M1048
	ILE	A1392	V1171	V1111	P1049
	ASN	R1393	D1172	Q1112	L1050
	GLU	A1394	E1173	ASN	K1051
	HIS	Q1395	E1173	GLU	R1052
	THR	Q1396	A1174	GLU	M1053
	GLU	H1397	M1175	LEU	A1055
	ASP	H1397	S1176	GLY	V1057
ILE	GLN	M1398	S1177	LEU	G1058
	MET	K1399	H1178	ASN	T1059
	ASP	P1400	E1179	GLU	A1060
	LEU	L1401	M1180	GLN	E1061
	ASP	T1402	K1181	ASN	A1062
	ASP	P1403	G1182	LEU	S1063
	ASP	S1404	A1185	ILE	S1064
	ASP	G1411	V1186	GLY	E1065
	ASP	M1412	L1187	THR	A1066
	ASP	D1414	Y1188	THR	P1067
LEU	LEU	R1415	A1189	ASP	L1068
	LEU	V1416	T1190	SER	G1069
	LEU	R1417	D1191	SER	M1070
	LEU	ASP	G1192	LEU	
	LEU	LEU	E1193	ILE	
	LEU	LYS	L1194	THR	
	LEU	THR	C1195	PRO	K1074
	LEU	LYS	G1196	GLU	Y1075
	LEU	ALA	A1197	LEU	C1076
	LEU	TRP	I1198	GLY	K1077
LEU	ASP	ASP	A1199	ALA	E1078
	LEU	ILE		GLN	A1079
	SER	SER	I1225	ALA	L1080
	LEU	TYR	D1228	PRO	G1081
	LEU	ILE	N1229	LEU	T1082
	SER	GLN	V1249	ALA	E1083
	SER	VAL	D1312	T1151	L1084
	ALA	ARG	R1326	V1152	L1085
	SER	SER	L1335	L1153	G1086
	SER	GLN	P1357	I1154	Y1087
LEU	LYS	L1335	G1155	G1088	
	PRO	P1358	N1156	T1089	
	LYS	L1339	R1157	D1090	
	ARG	ARG	L1345	E1158	F1091
	GLY	GLY	Q1357	M1159	Q1092
	LEU	LEU	P1358	R1160	A1093
	VAL	VAL	W1359	R1161	V1094
	GLU	GLU	Q1378	N1162	P1095
	GLN	GLN	K1384	G1096	C1097
	ASP	ASP	P1385	L1165	G1098
LEU	LYS	D1386	H1166	T1099	
	LEU	S1387	I1167	S1100	
	LEU	D1388		C1101	
	LEU			K1102	
	LEU			V1103	
	LEU			N1104	
	LEU			M1105	
	LEU			T1106	
	LEU			F1107	
	LEU				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	257208	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	21.203	Depositor
Minimum map value	-13.339	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (Å)	95.200005, 93.5, 147.05	wwPDB
Map dimensions	173, 110, 112	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ALF

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	0.07	0/6692	0.20	0/9062

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

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	6593	6901	6899	30	0
2	A	1	0	0	0	0
3	A	5	0	0	1	0
All	All	6599	6901	6899	30	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 2.

The worst 5 of 30 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:496:CYS:SG	1:A:499:CYS:N	2.54	0.81

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LYS:NZ	1:A:525:ALA:O	2.19	0.75
1:A:643:GLU:OE1	1:A:710:TYR:OH	2.07	0.72
1:A:727:ASP:OD2	1:A:775:ARG:NH1	2.23	0.71
1:A:1326:ARG:NH1	1:A:1378:GLN:OE1	2.24	0.70

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	858/1467 (58%)	845 (98%)	13 (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	723/1254 (58%)	723 (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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1213	HIS
1	A	1397	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	ALF	A	1502	-	4,4,4	1.37	0	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

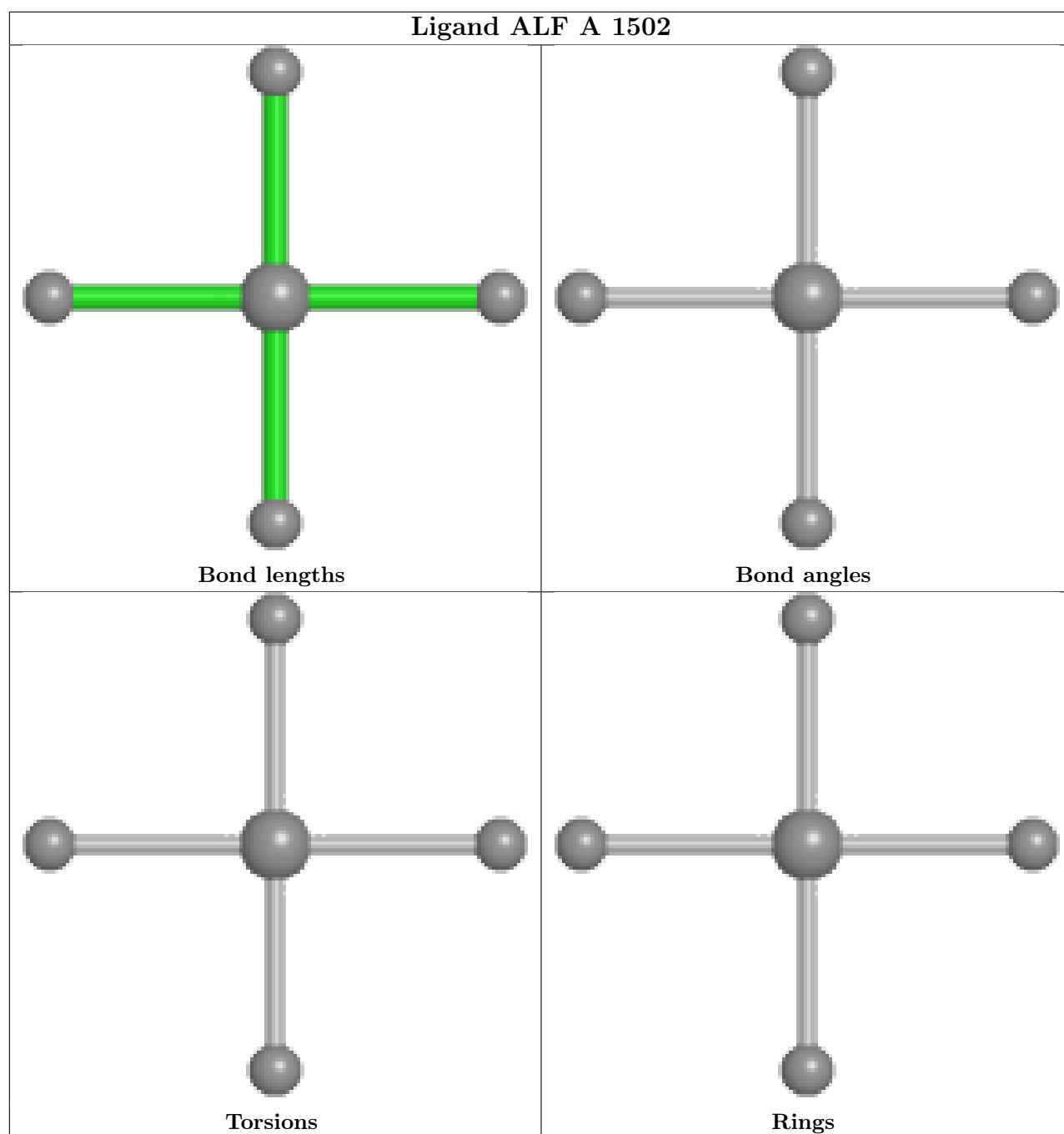
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1502	ALF	1	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	575:CYS	C	576:VAL	N	3.90

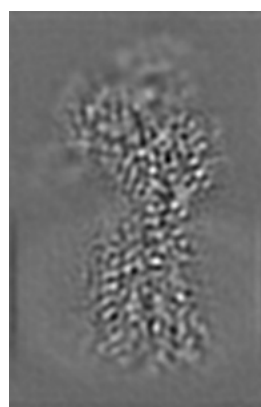
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25137. These allow visual inspection of the internal detail of the map and identification of artifacts.

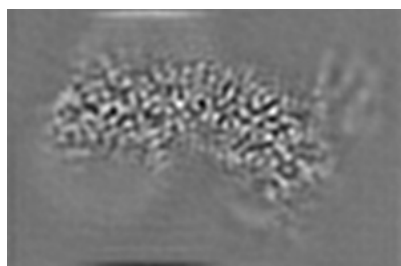
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

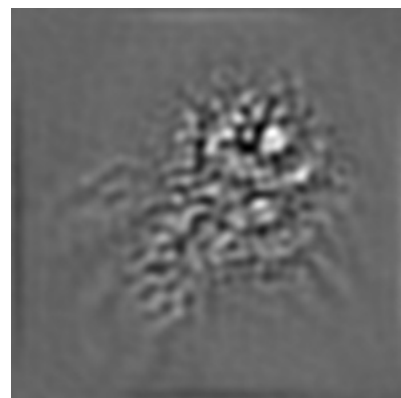
6.1.1 Primary map



X



Y

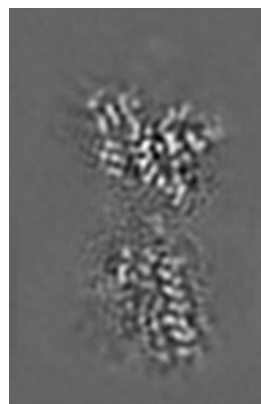


Z

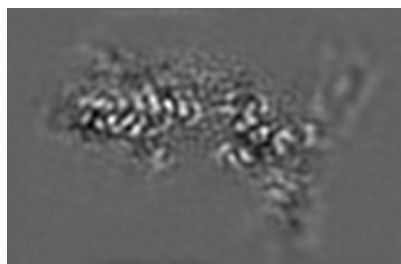
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

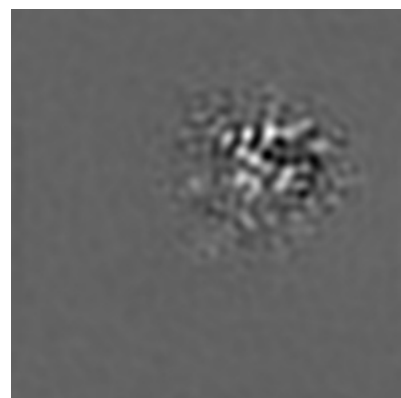
6.2.1 Primary map



X Index: 56



Y Index: 55

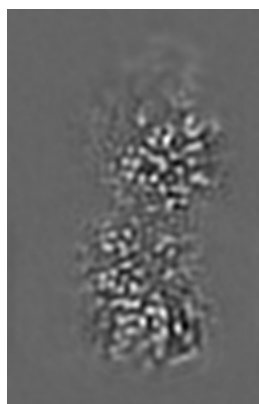


Z Index: 86

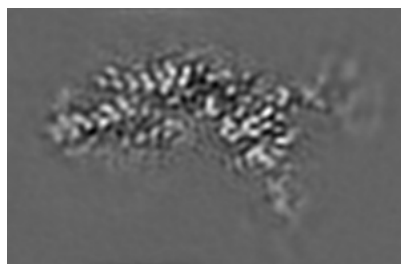
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

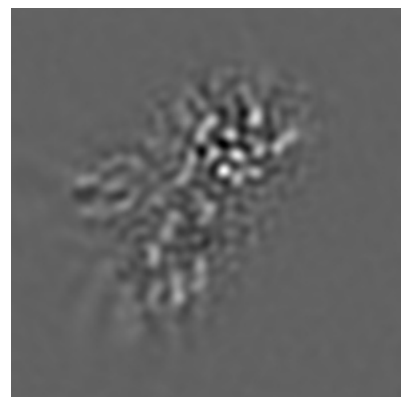
6.3.1 Primary map



X Index: 63



Y Index: 66

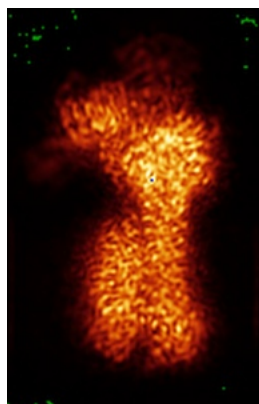


Z Index: 116

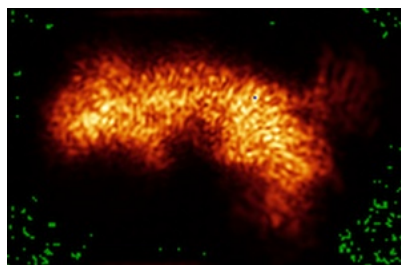
The images above show the largest variance slices of the map in three orthogonal directions.

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

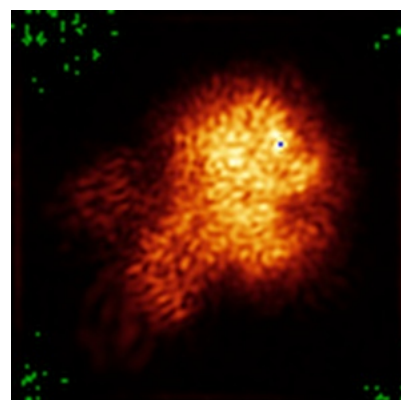
6.4.1 Primary map



X



Y

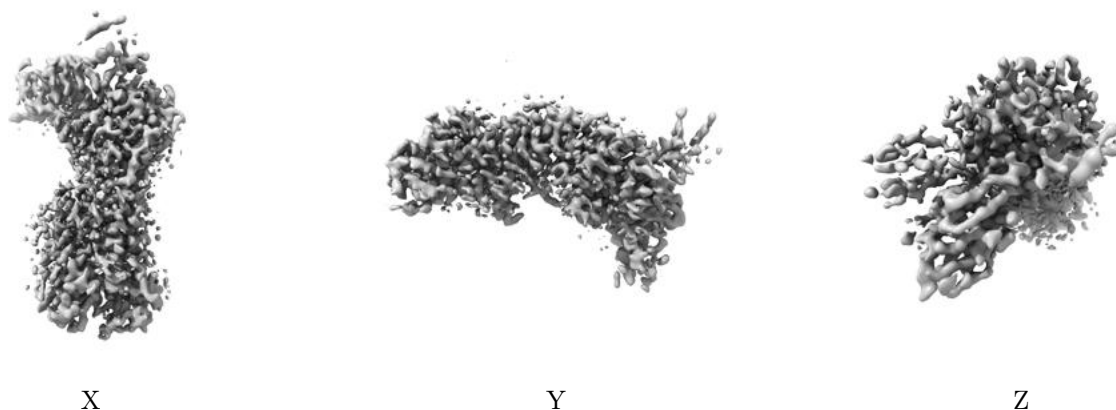


Z

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 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

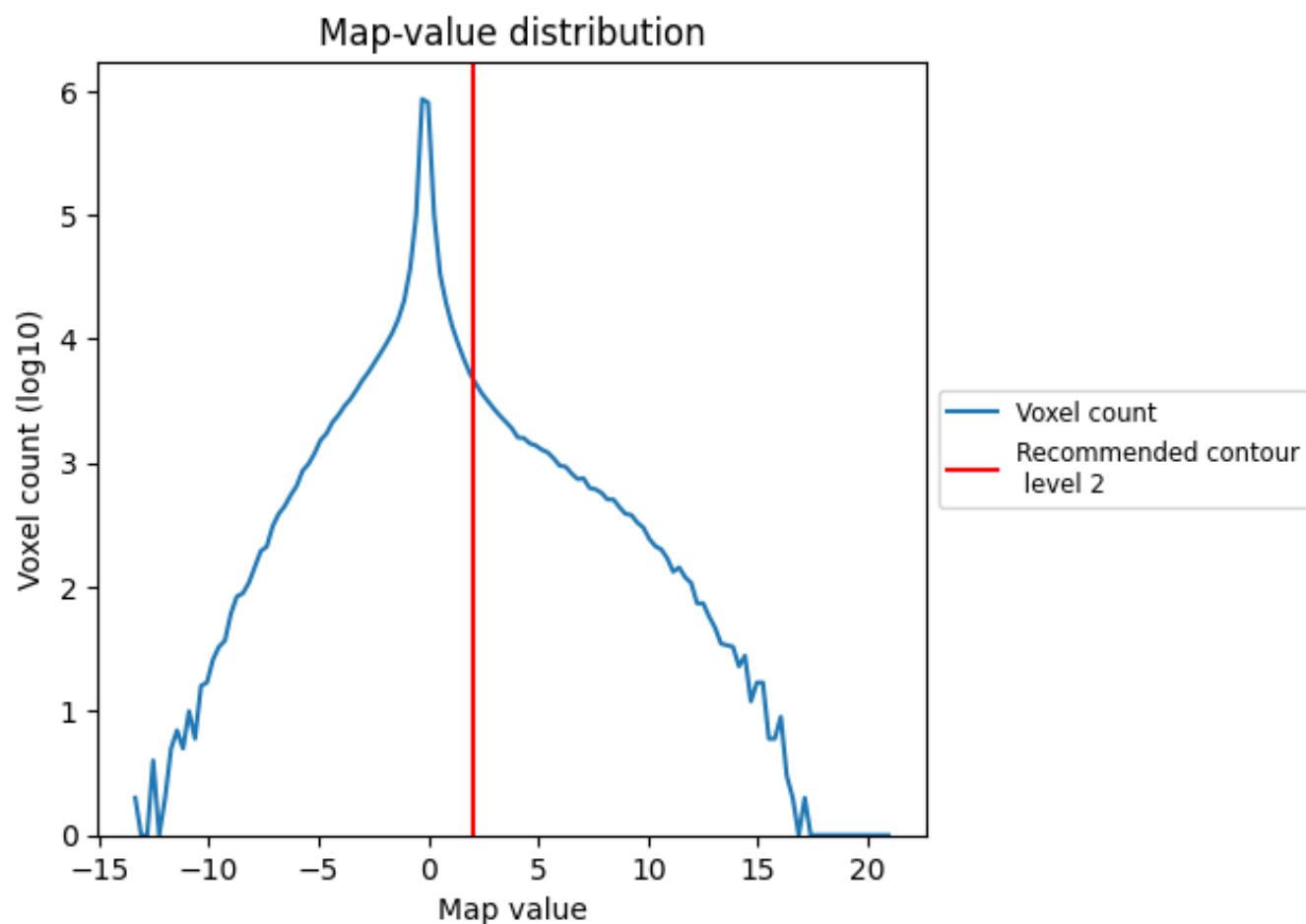
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

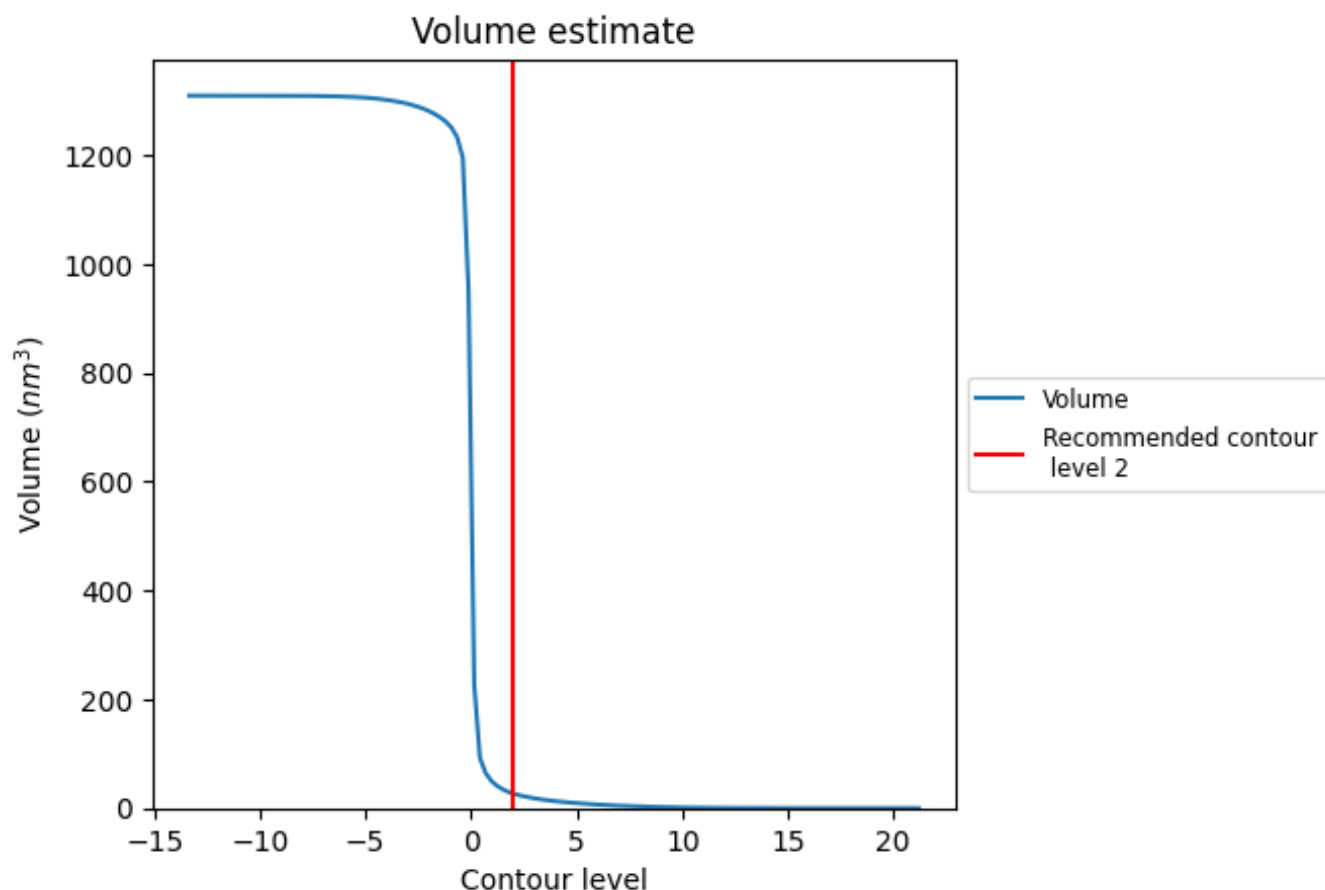
This section contains the results of statistical analysis of the map.

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 27 nm³; this corresponds to an approximate mass of 24 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

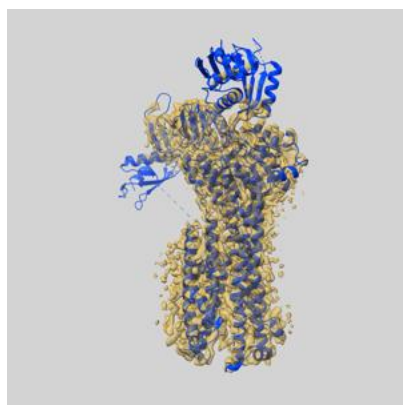
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

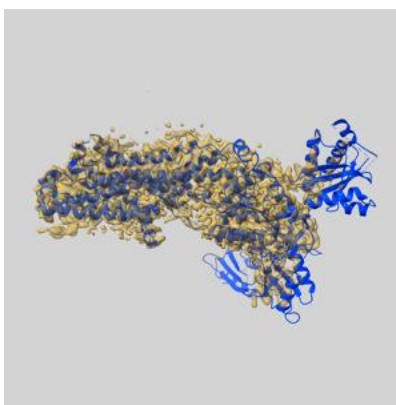
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25137 and PDB model 7SI3. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

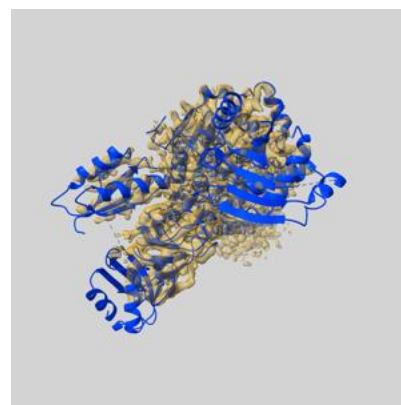
9.1 Map-model overlay [i](#)



X



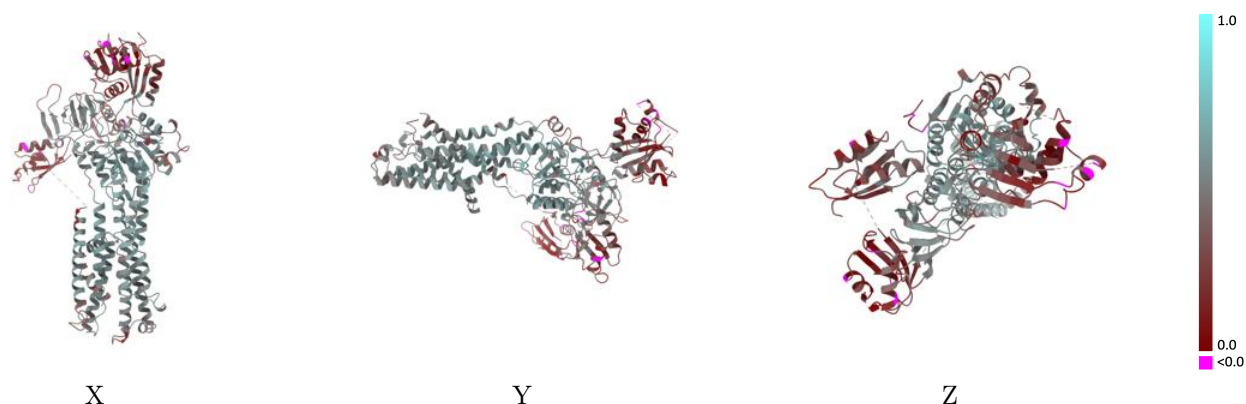
Y



Z

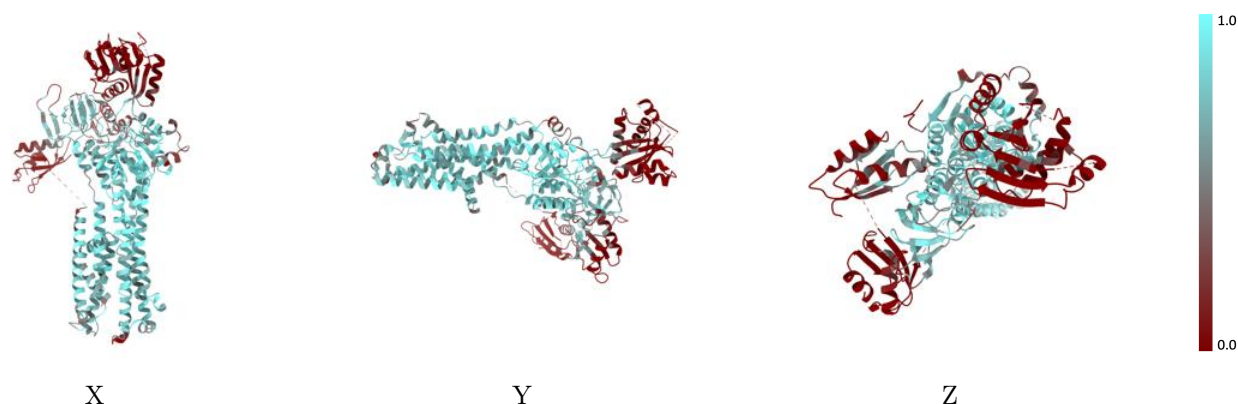
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



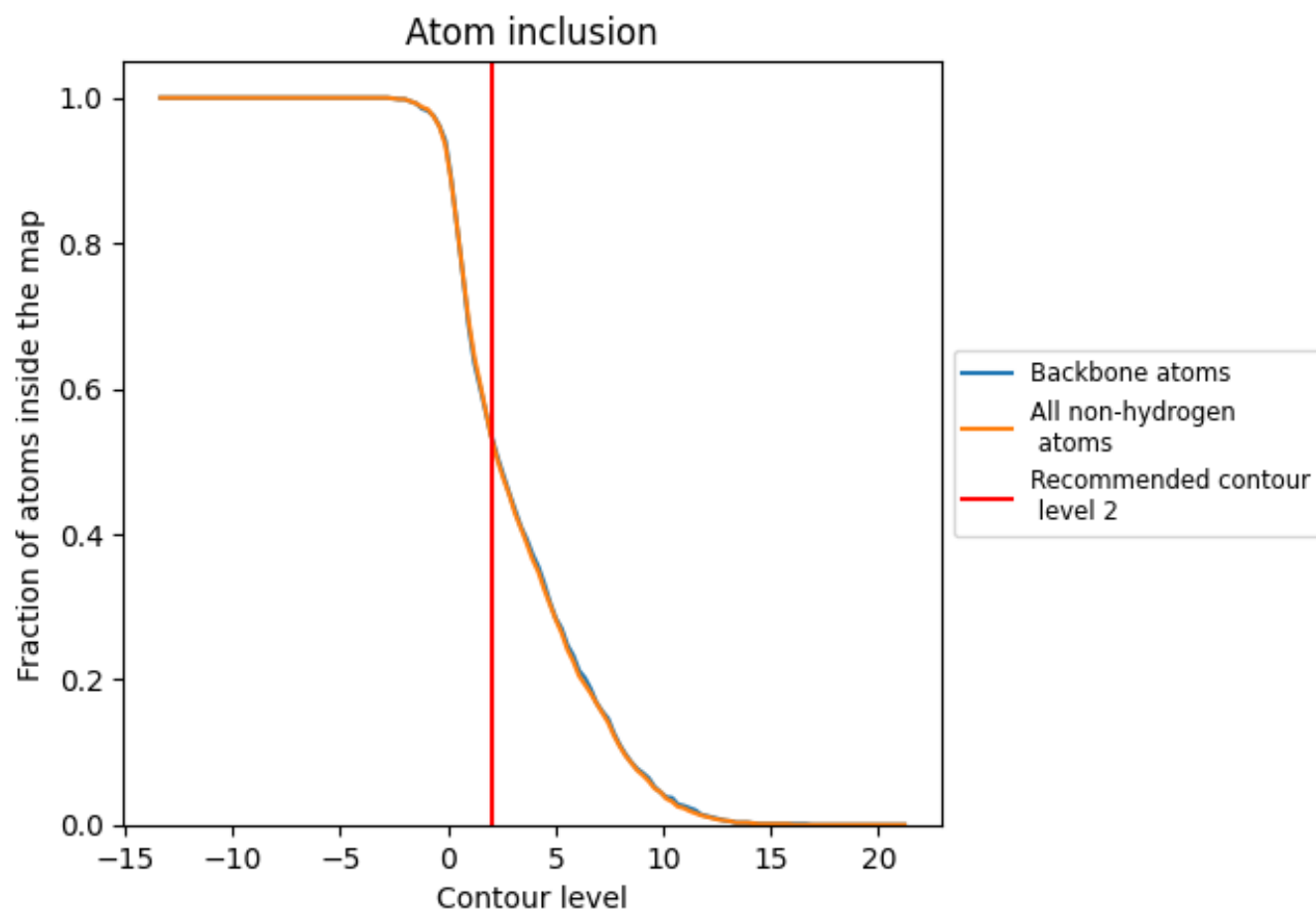
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 54% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5350	0.4250
A	0.5420	0.4250

