



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2025 – 02:12 PM JST

PDB ID : 9JUO
EMDB ID : EMD-61832
Title : Structure of Arabidopsis thaliana ABCB1 with AMP-PNP bound in the inward-facing conformation under IAA condition
Authors : Chen, Q.; Su, N.; Guo, J.
Deposited on : 2024-10-08
Resolution : 3.10 Å(reported)

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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

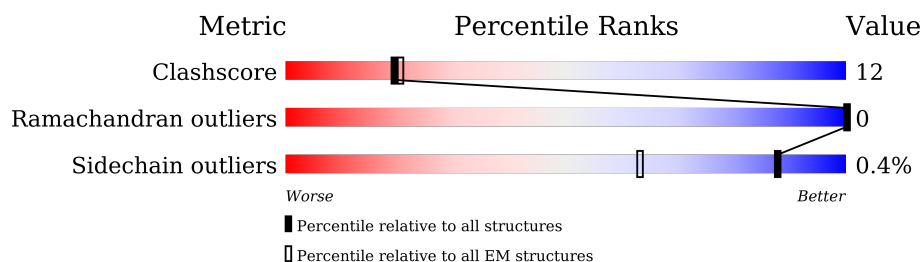
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1327	<div> <div>23%</div> <div>63%</div> <div>23%</div> <div>14%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8858 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 ABC transporter B family member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1144	Total	C	N	O	S	0	0
			8794	5625	1506	1623	40		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	initiating methionine	UNP Q9ZR72
A	-39	ASP	-	expression tag	UNP Q9ZR72
A	-38	TYR	-	expression tag	UNP Q9ZR72
A	-37	LYS	-	expression tag	UNP Q9ZR72
A	-36	ASP	-	expression tag	UNP Q9ZR72
A	-35	ASP	-	expression tag	UNP Q9ZR72
A	-34	ASP	-	expression tag	UNP Q9ZR72
A	-33	ASP	-	expression tag	UNP Q9ZR72
A	-32	LYS	-	expression tag	UNP Q9ZR72
A	-31	TRP	-	expression tag	UNP Q9ZR72
A	-30	SER	-	expression tag	UNP Q9ZR72
A	-29	HIS	-	expression tag	UNP Q9ZR72
A	-28	PRO	-	expression tag	UNP Q9ZR72
A	-27	GLN	-	expression tag	UNP Q9ZR72
A	-26	PHE	-	expression tag	UNP Q9ZR72
A	-25	GLU	-	expression tag	UNP Q9ZR72
A	-24	LYS	-	expression tag	UNP Q9ZR72
A	-23	GLY	-	expression tag	UNP Q9ZR72
A	-22	GLY	-	expression tag	UNP Q9ZR72
A	-21	GLY	-	expression tag	UNP Q9ZR72
A	-20	GLY	-	expression tag	UNP Q9ZR72
A	-19	SER	-	expression tag	UNP Q9ZR72
A	-18	GLY	-	expression tag	UNP Q9ZR72
A	-17	GLY	-	expression tag	UNP Q9ZR72
A	-16	SER	-	expression tag	UNP Q9ZR72
A	-15	ALA	-	expression tag	UNP Q9ZR72
A	-14	TRP	-	expression tag	UNP Q9ZR72
A	-13	SER	-	expression tag	UNP Q9ZR72

Continued on next page...

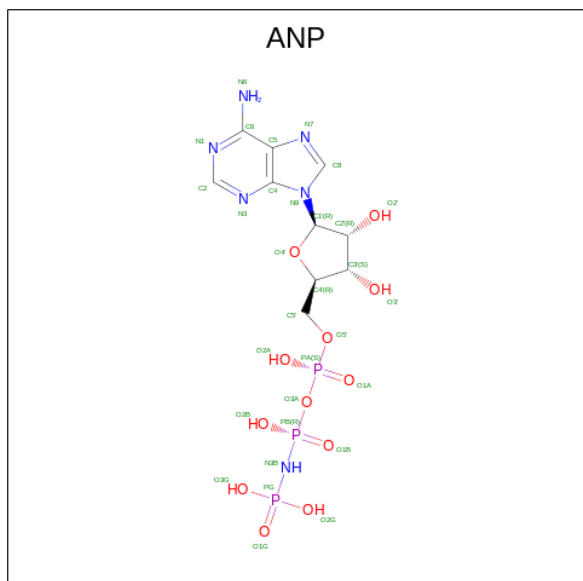
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP Q9ZR72
A	-11	PRO	-	expression tag	UNP Q9ZR72
A	-10	GLN	-	expression tag	UNP Q9ZR72
A	-9	PHE	-	expression tag	UNP Q9ZR72
A	-8	GLU	-	expression tag	UNP Q9ZR72
A	-7	LYS	-	expression tag	UNP Q9ZR72
A	-6	GLU	-	expression tag	UNP Q9ZR72
A	-5	PHE	-	expression tag	UNP Q9ZR72
A	-4	LYS	-	expression tag	UNP Q9ZR72
A	-3	GLY	-	expression tag	UNP Q9ZR72
A	-2	LEU	-	expression tag	UNP Q9ZR72
A	-1	VAL	-	expression tag	UNP Q9ZR72
A	0	ASP	-	expression tag	UNP Q9ZR72

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

Continued on next page...

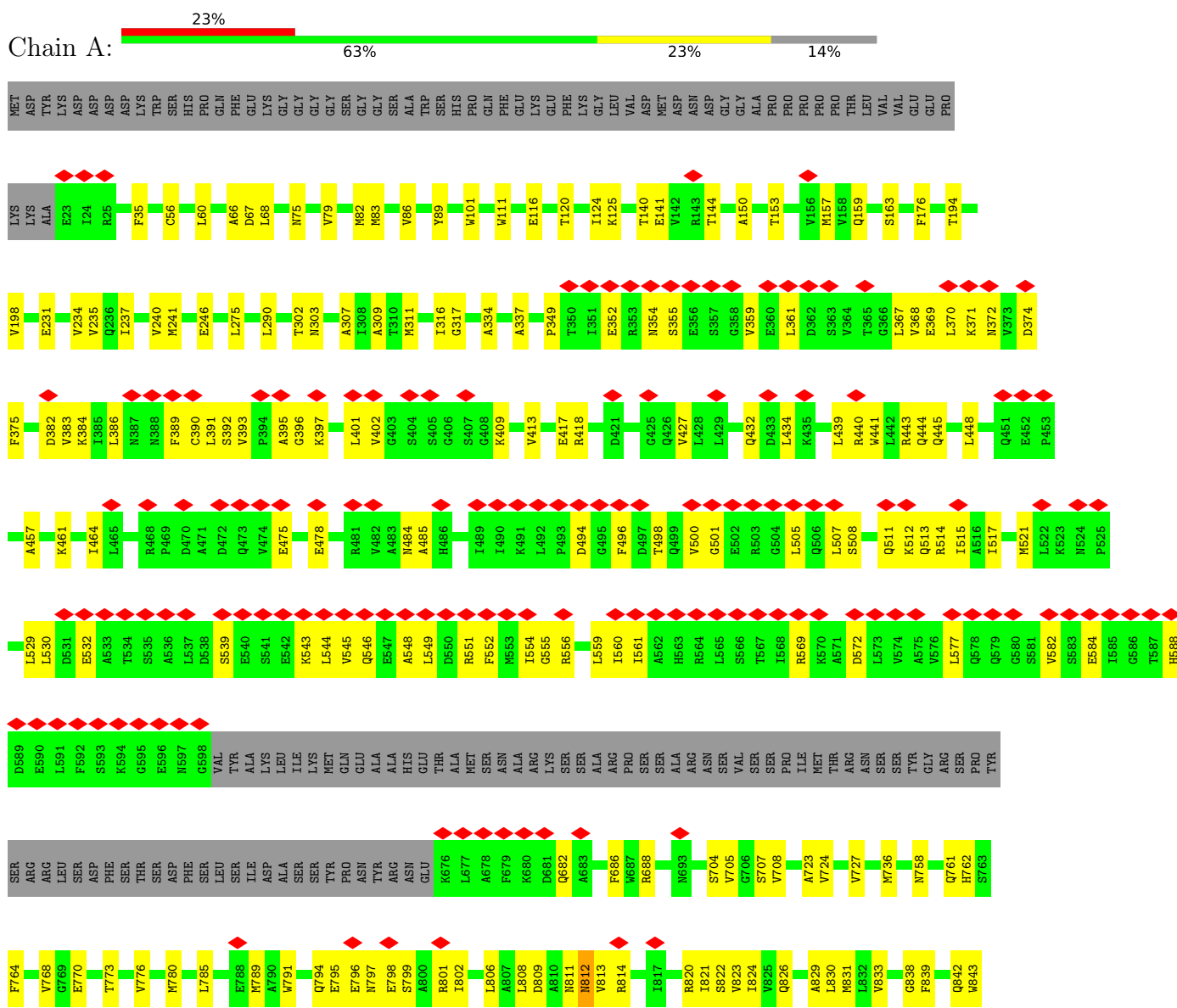
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	31	10	6	12	3	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: ABC transporter B family member 1



PRO	T1190	C1126	V1058	R994	R844
ASP	S1191	A1127	G1059	S995	L845
GLY	A1192	T1128	P1060	E998	A846
ILE	L1193	E1129	S1061	L999	L847
TYR	D1194	E1130	G1062	L1000	V848
ALA	A1195	E1131	C1063	D1001	L849
ARG	E1196	I1132	G1064	R1002	V850
MET	S1197	I1133	K1065	K1003	T860
LEU	E1198	Q1134	I1069	T1004	L861
GLN	R1199	A1135	I1072	E1005	L862
GLN	S1200	A1136	Q1073	I1006	Q863
ARG	V1201	T1137	R1074	E1007	K864
PHE	Q1202	L1138	F1075	P1008	Q883
THR	E1203	A1139	E1076	D1009	I889
THR	E1204	S1140	E1077	D1010	V905
GLN	A1205	H1141	P1078	D1011	V905
VAL	L1206	H1142	S1079	D1012	T909
ILE	D1207	K1143	S1080	T1013	Y930
GLY	Q1208	F1144	G1081	V1016	G931
NET	A1209	I1145	R1082	P1017	L945
THR	C1210	S1146	V1083	D1018	S949
SER	S1211	A1147	M1084	R1019	W950
SER	G1212	L1148	I1085	L1020	L951
SER	R1212	E1150	D1086	R1021	W952
ARG	V1216	G1151	G1087	G1022	K953
VAL	V1217	Y1152	K1088	E1023	T962
LYS	A1218	K1153	D1089	E1025	I963
GLU	H1219	T1154	I1090	L1026	R964
ASP	R1220	Y1155	K1091	K1027	V965
ASP	L1221	V1156	R1092	H1028	F966
ALA	S1222	G1157	Y1093	I1029	M967
	T1223	E1158	N1094	D1030	L969
	I1224	R1159	L1095	F1031	M970
	R1225	G1160	K1096	S1035	V971
	N1226	V1161	A1097	R1036	S972
	A1227	Q1162	I1098	R1037	A976
	H1228	L1163	R1099	D1038	T979
	V1229	S1164	K1100	I1039	L980
	I1230	G1165	H1101	Q1040	T981
	A1231	G1166	T1104	I1041	L982
	V1232	Q1167	V1105	F1042	A983
	I1233	K1168	P1106	R1043	P984
	D1234	G1169	Q1107	D1044	D985
	D1235	E1170	E1108	L1045	F986
	G1236	R1171	P1109	L1046	I987
	K1237	A1174	T1114	S1046	K988
	V1238	V1178	T1115	L1047	A992
	A1239	R1179	I1116	R1048	M993
	E1240	K1180	Y1117	A1049	
	Q1241	A1181	E1118	R1050	
	G1242	M1184	N1119	A1051	
	S1243	L1185	T1120	G1052	
HIS		L1186	G1123	K1053	
SER		D1187	H1124	T1054	
HIS		E1188	E1125	L1055	
LEU		A1189		A1056	
LEU				L1057	
LYS					
ASN					
HIS					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157897	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	223.2, 223.2, 223.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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: MG, ANP

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	0.31	0/8955	0.48	0/12121

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	8794	0	8936	221	0
2	A	2	0	0	0	0
3	A	62	0	26	0	0
All	All	8858	0	8962	221	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 12.

The worst 5 of 221 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:770:GLU:HG2	1:A:814:ARG:HH21	1.35	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:VAL:HG12	1:A:736:MET:HG3	1.62	0.80
1:A:1095:LEU:HD21	1:A:1099:ARG:HH11	1.46	0.79
1:A:549:LEU:HB3	1:A:552:PHE:HB3	1.65	0.77
1:A:157:MET:HG2	1:A:334:ALA:HA	1.67	0.77

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	1140/1327 (86%)	1080 (95%)	60 (5%)	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	930/1087 (86%)	926 (100%)	4 (0%)	89	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	806	LEU
1	A	812	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1038	ASP
1	A	1159	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	445	GLN
1	A	812	ASN
1	A	826	GLN
1	A	827	ASN
1	A	1142	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ANP	A	1303	2	29,33,33	1.20	5 (17%)	31,52,52	1.17	3 (9%)
3	ANP	A	1304	2	29,33,33	1.22	5 (17%)	31,52,52	1.12	3 (9%)

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	ANP	A	1303	2	-	6/14/38/38	0/3/3/3
3	ANP	A	1304	2	-	3/14/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1304	ANP	PG-O1G	3.26	1.51	1.46
3	A	1303	ANP	PG-O1G	3.12	1.51	1.46
3	A	1303	ANP	PB-O1B	2.98	1.50	1.46
3	A	1304	ANP	PB-O1B	2.93	1.50	1.46
3	A	1304	ANP	PB-O2B	-2.22	1.50	1.56

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1303	ANP	O2B-PB-O1B	4.19	118.71	109.92
3	A	1304	ANP	O2B-PB-O1B	4.06	118.44	109.92
3	A	1304	ANP	C5-C6-N6	2.29	123.83	120.35
3	A	1303	ANP	C5-C6-N6	2.24	123.76	120.35
3	A	1304	ANP	O3G-PG-O1G	-2.08	108.23	113.45

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

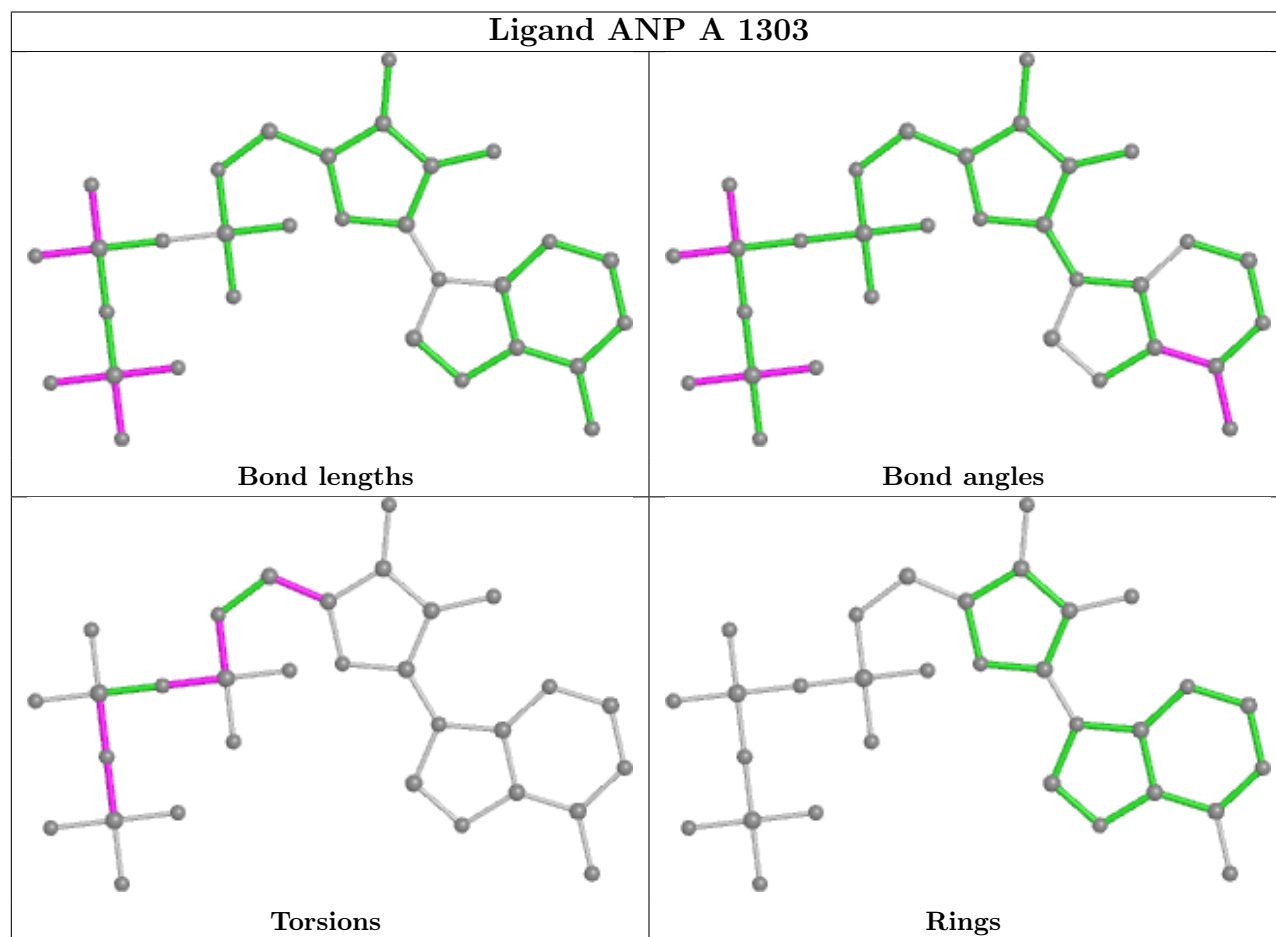
Mol	Chain	Res	Type	Atoms
3	A	1303	ANP	PB-N3B-PG-O1G
3	A	1303	ANP	PG-N3B-PB-O1B
3	A	1303	ANP	PB-O3A-PA-O5'
3	A	1304	ANP	PB-N3B-PG-O1G
3	A	1304	ANP	PG-N3B-PB-O1B

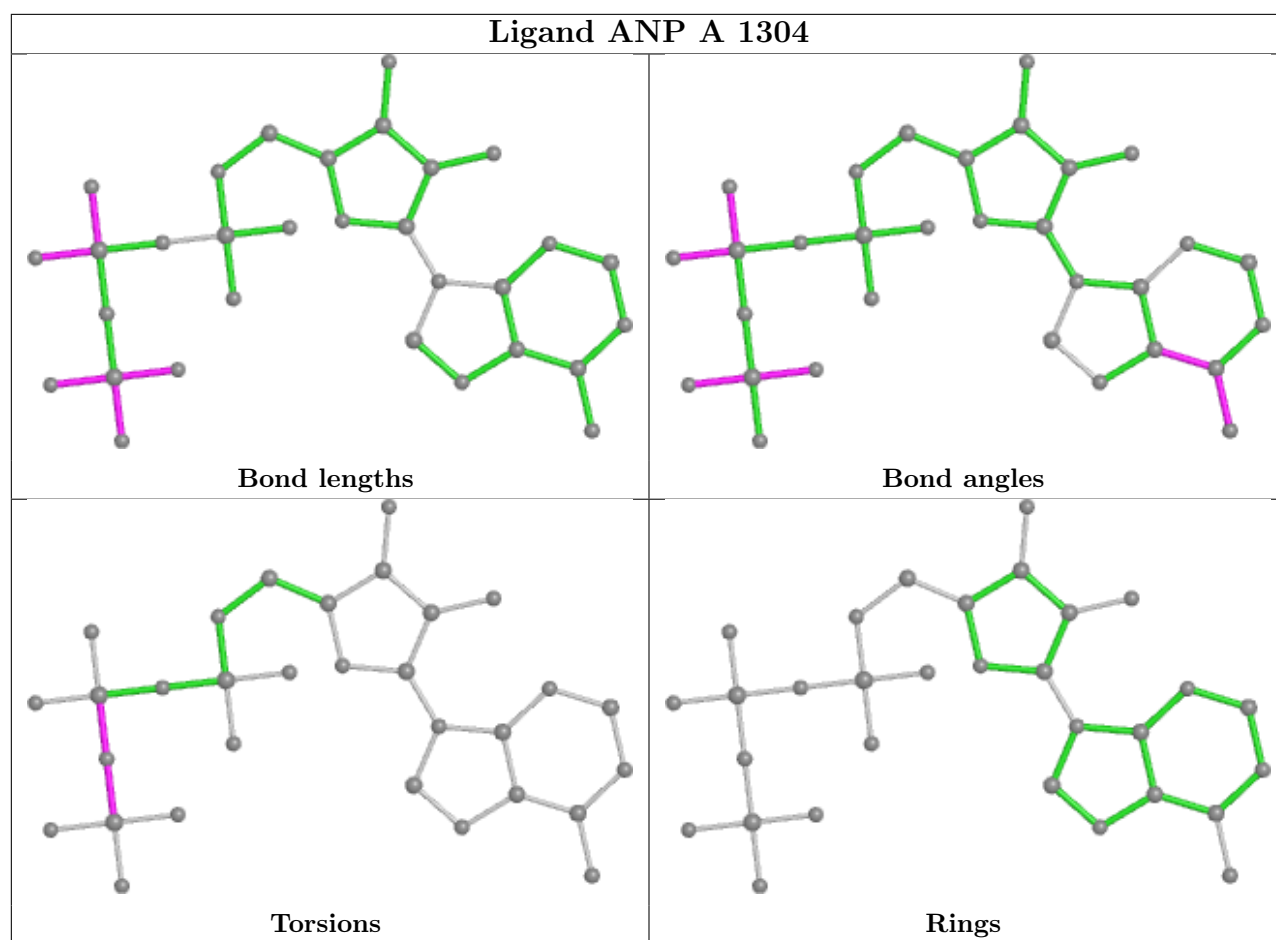
There are no ring outliers.

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.

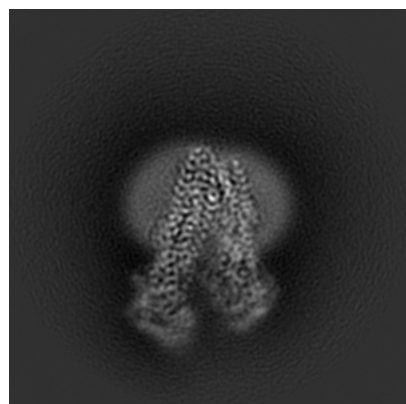
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61832. These allow visual inspection of the internal detail of the map and identification of artifacts.

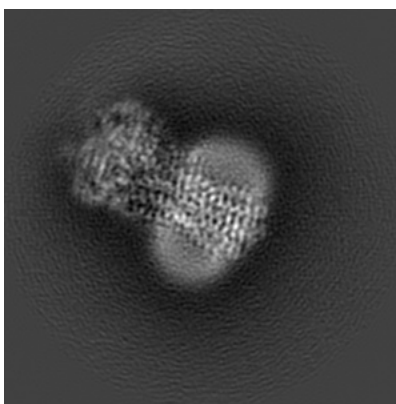
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

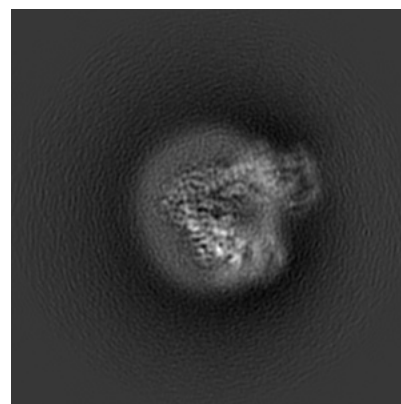
6.1.1 Primary map



X

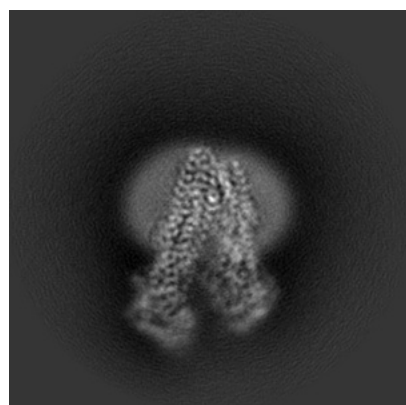


Y

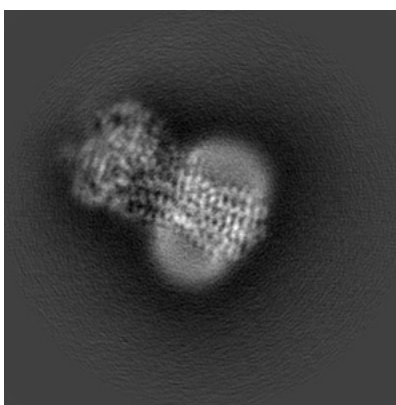


Z

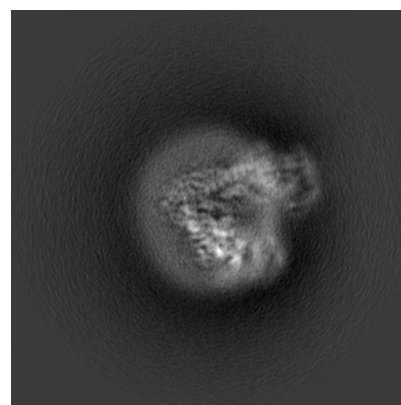
6.1.2 Raw map



X



Y

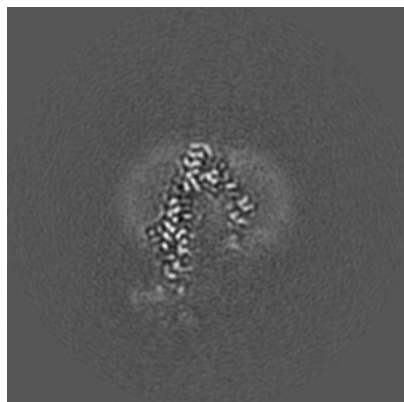


Z

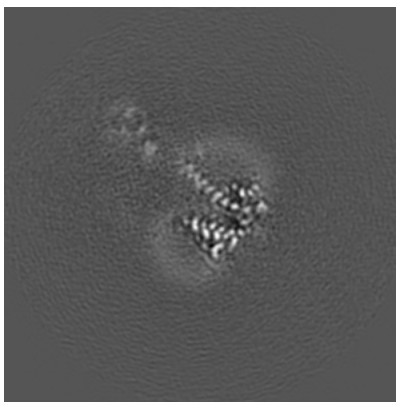
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

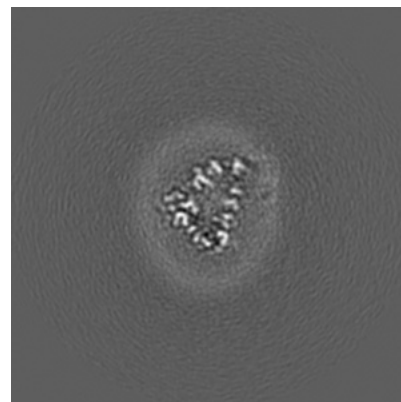
6.2.1 Primary map



X Index: 120

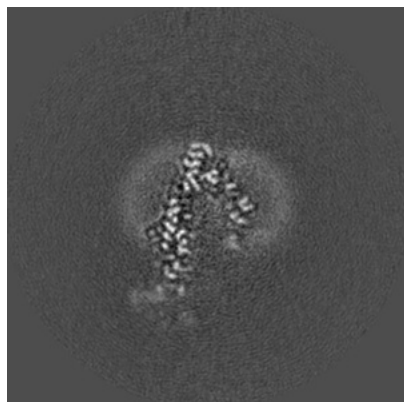


Y Index: 120

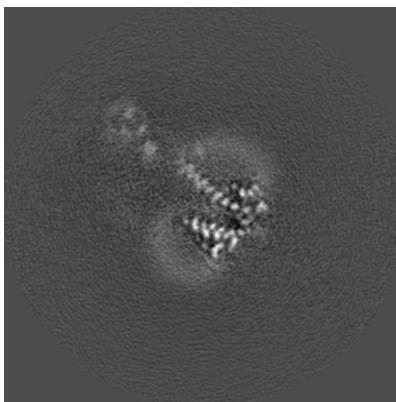


Z Index: 120

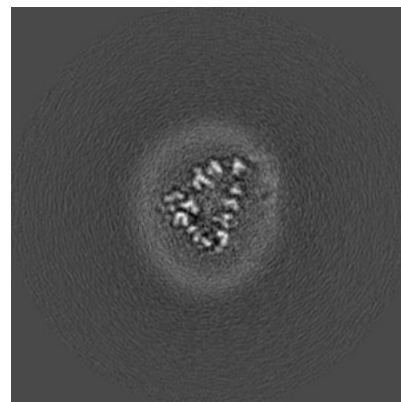
6.2.2 Raw map



X Index: 120



Y Index: 120

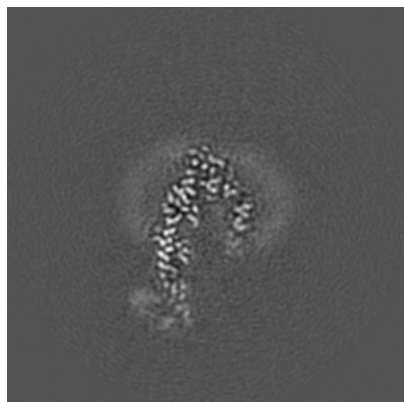


Z Index: 120

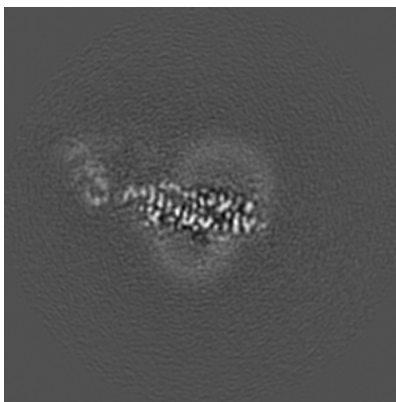
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

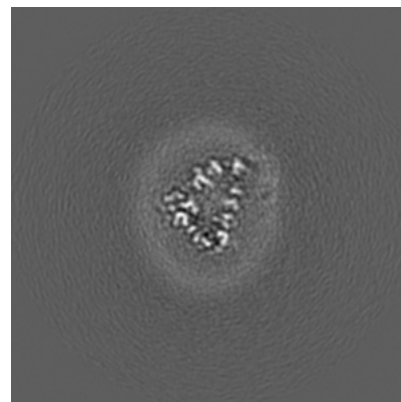
6.3.1 Primary map



X Index: 123

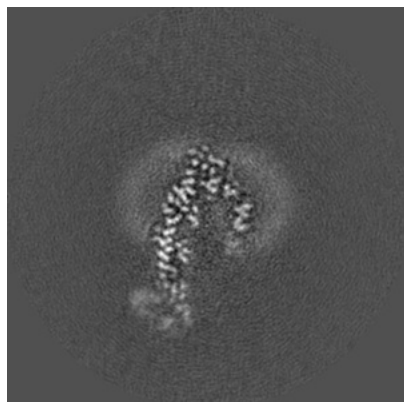


Y Index: 107

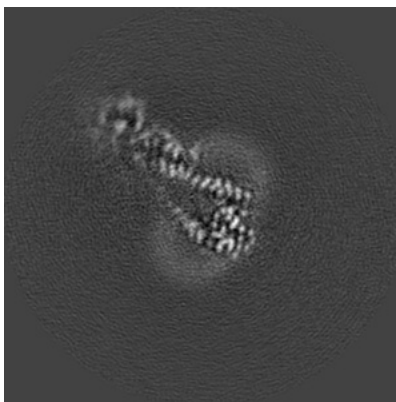


Z Index: 120

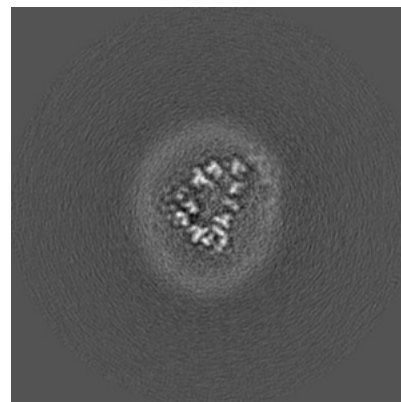
6.3.2 Raw map



X Index: 123



Y Index: 130

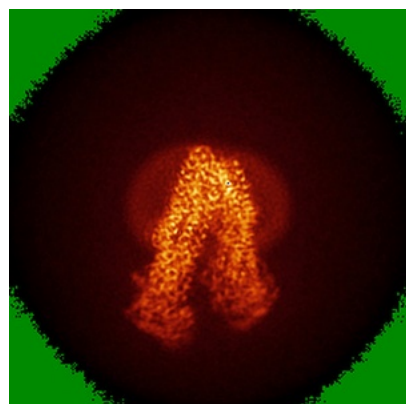


Z Index: 119

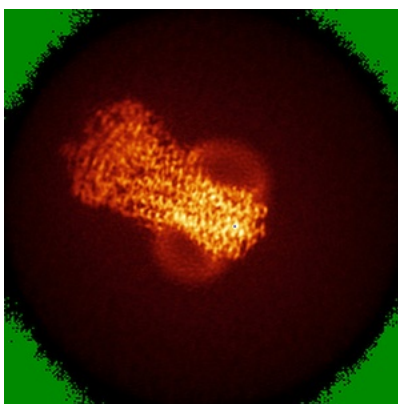
The images above show the largest variance slices of the map in three orthogonal directions.

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

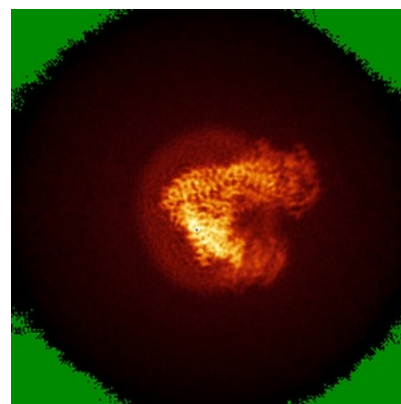
6.4.1 Primary map



X

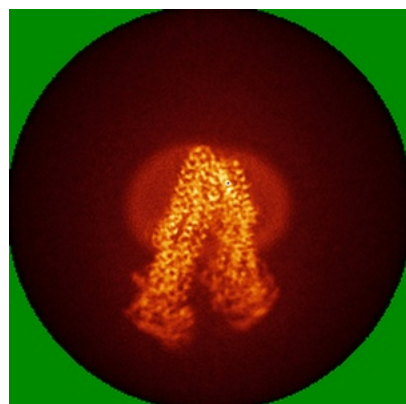


Y

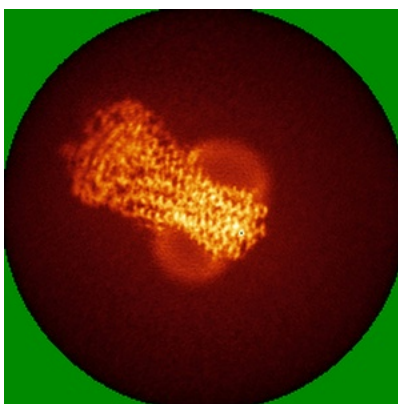


Z

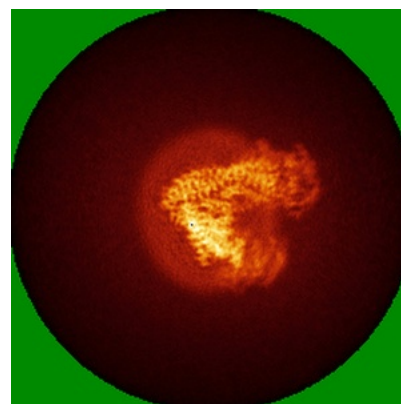
6.4.2 Raw map



X



Y

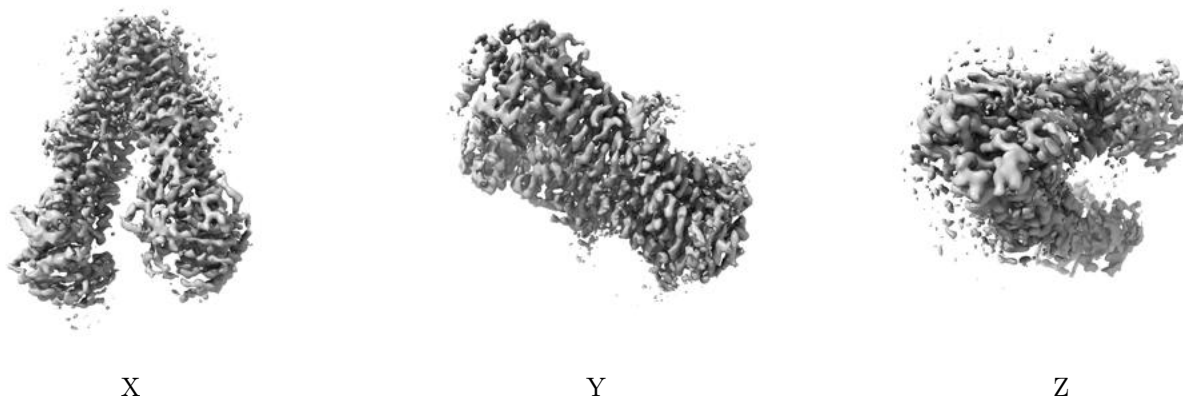


Z

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.

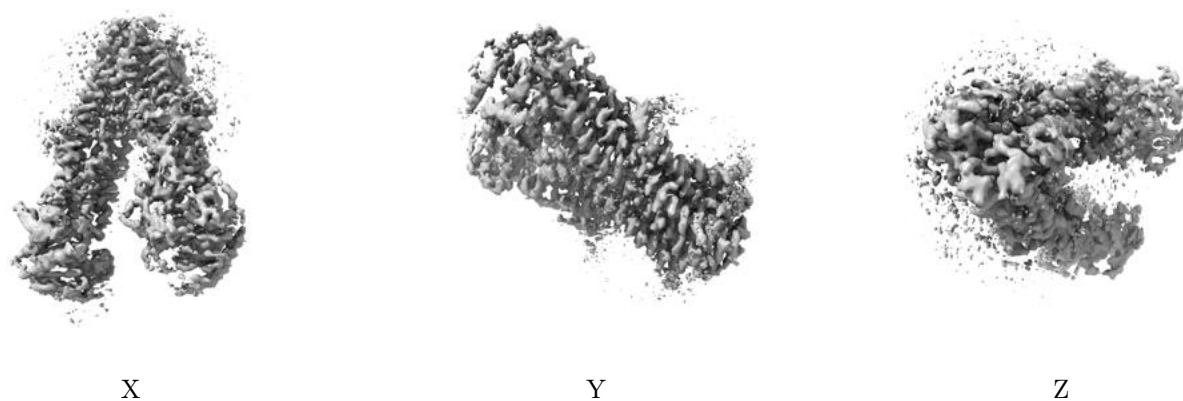
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

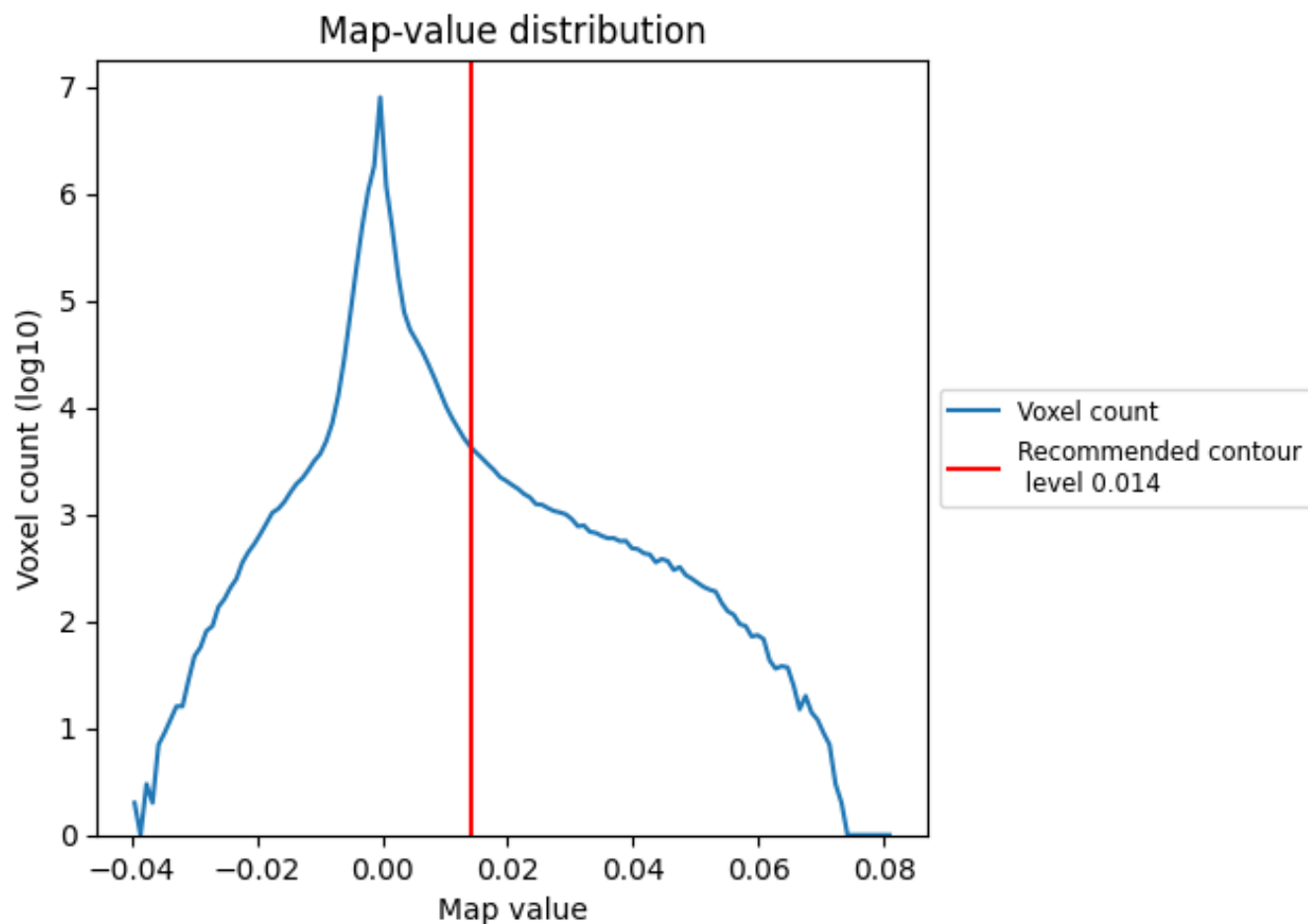
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

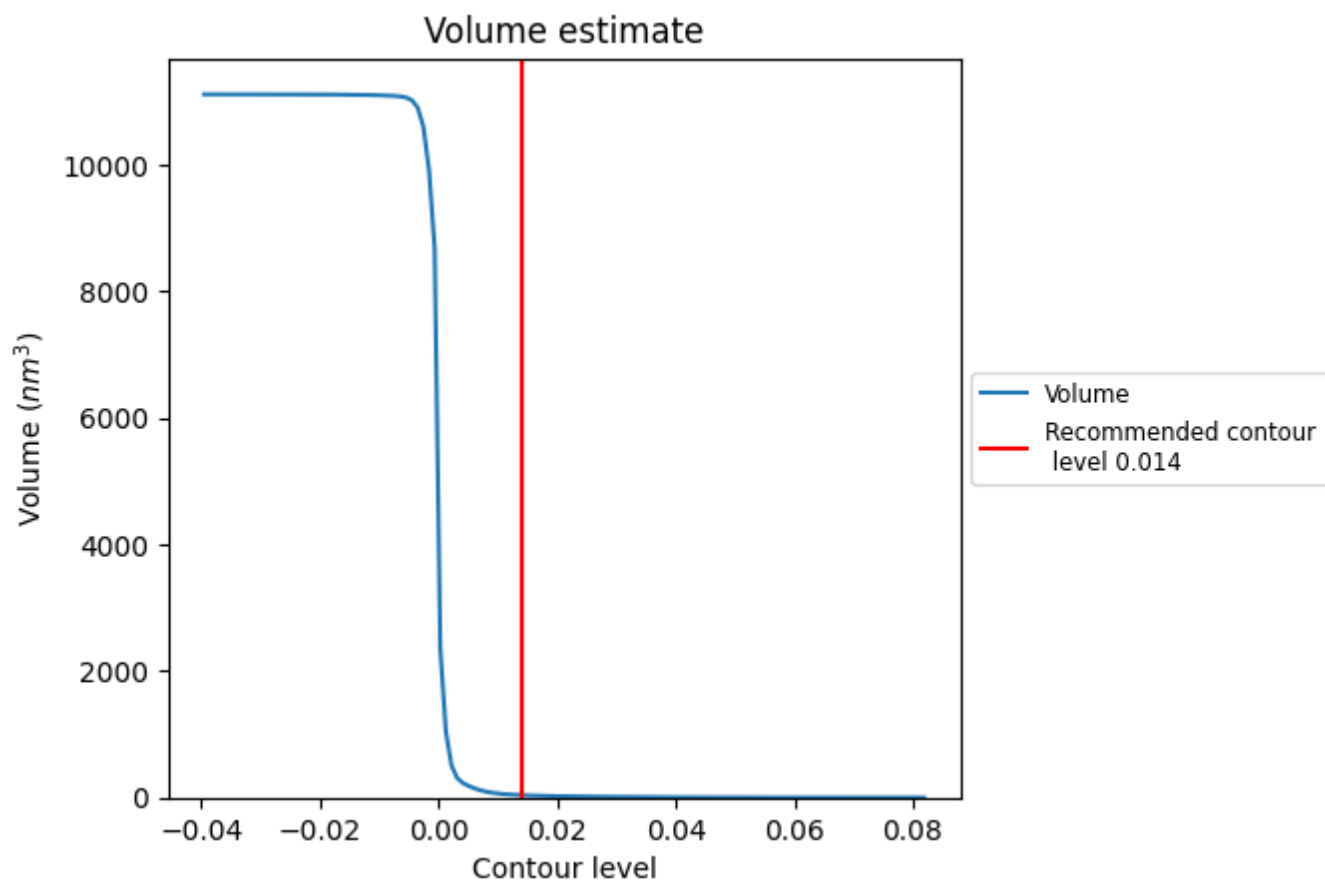
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

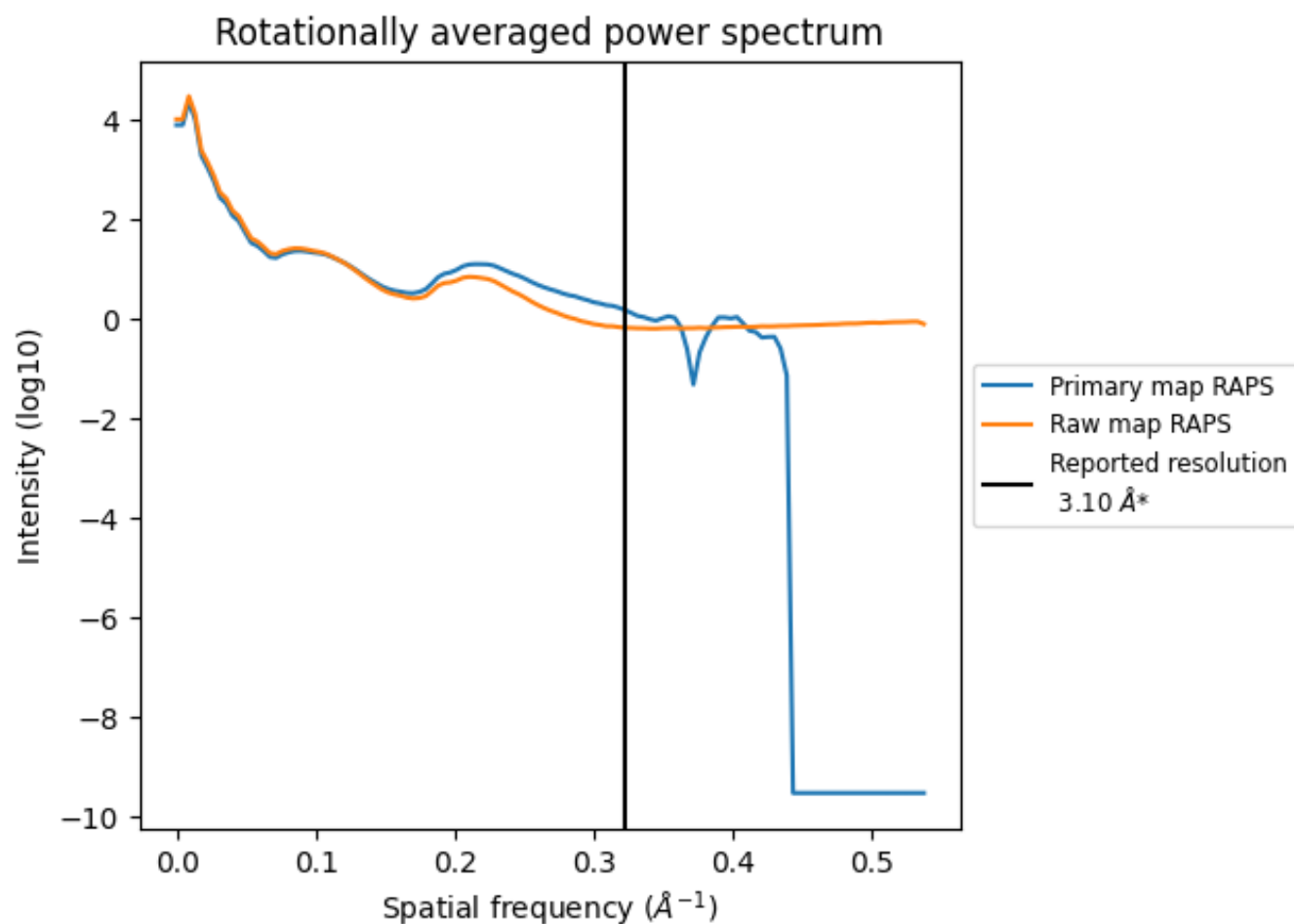
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38 nm^3 ; this corresponds to an approximate mass of 34 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

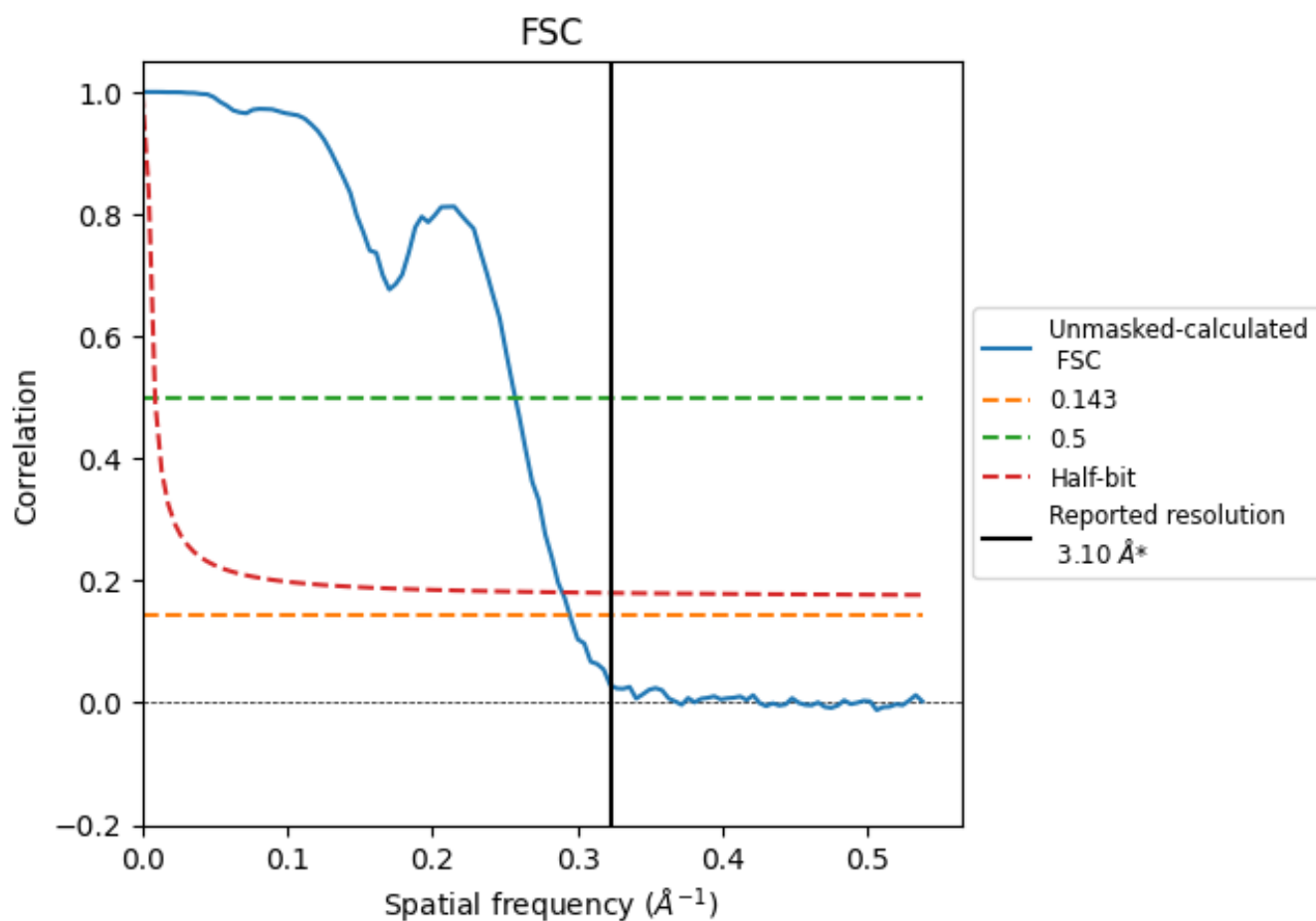


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

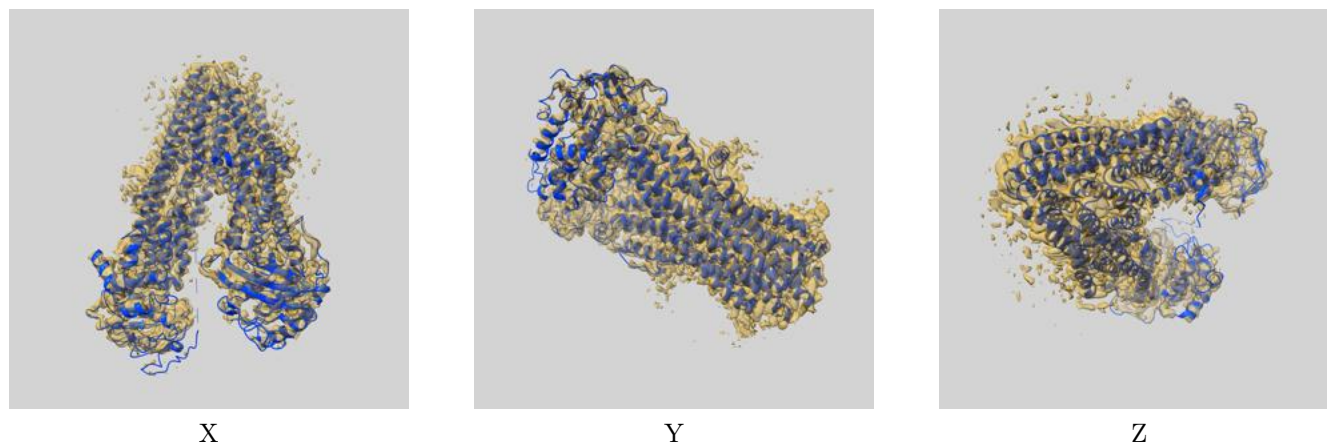
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.39	3.89	3.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

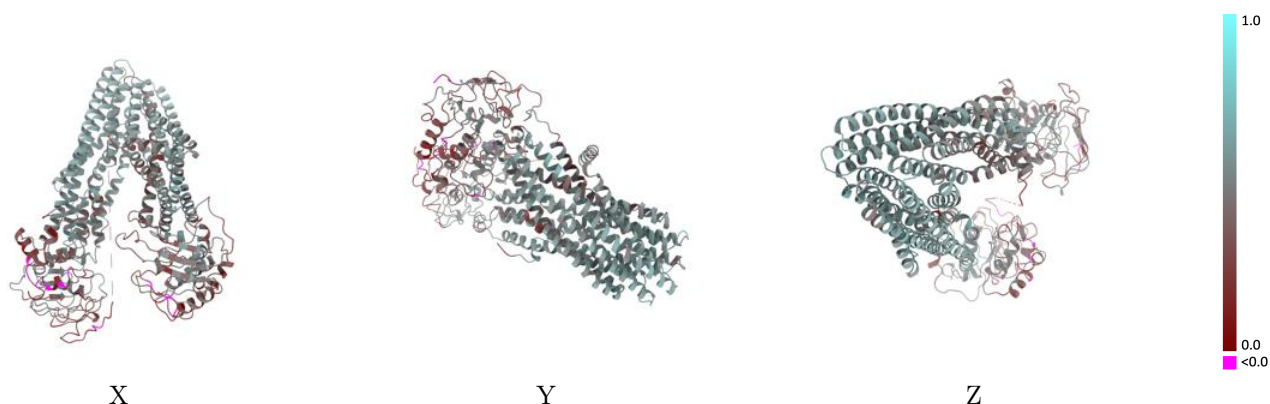
This section contains information regarding the fit between EMDB map EMD-61832 and PDB model 9JUO. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



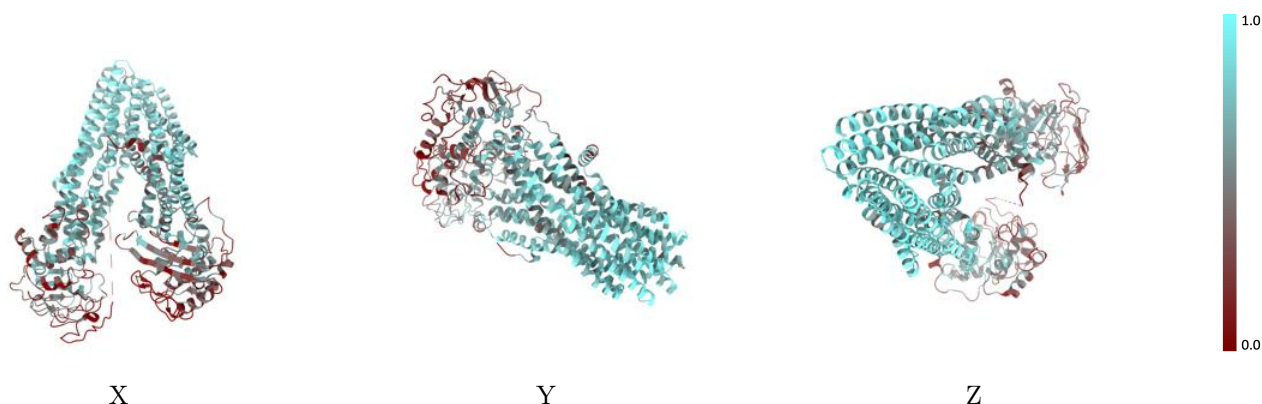
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



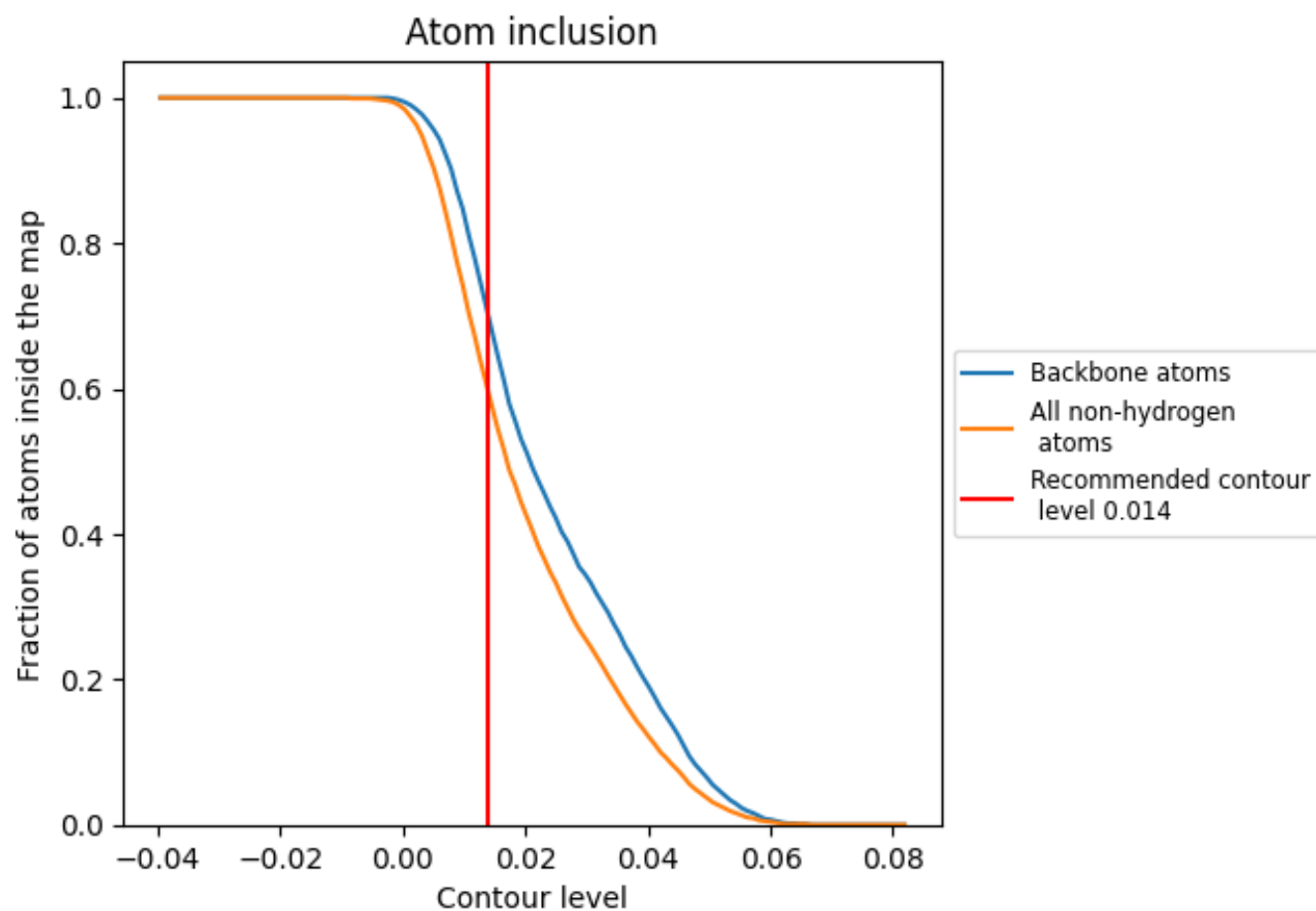
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 59% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5940	<div></div> 0.4610
A	<div></div> 0.5940	<div></div> 0.4610

