



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 10:53 PM EST

PDB ID : 6X6A
EMDB ID : EMD-22074
Title : Cryo-EM structure of NLRP1-DPP9 complex
Authors : Hollingsworth, L.R.; Sharif, H.; Griswold, A.R.; Fontana, P.; Mintseris, J.;
Dagbay, K.B.; Paulo, J.A.; Gygi, S.P.; Bachovchin, D.A.; Wu, H.
Deposited on : 2020-05-27
Resolution : 3.60 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.dev43
MolProbity : 4.02b-467
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

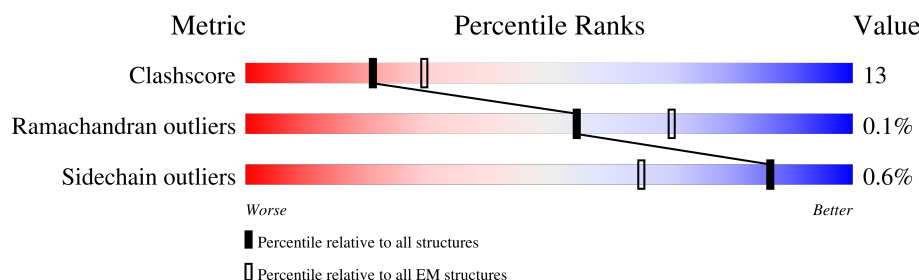
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	863	
1	D	863	
2	B	1212	
2	E	1212	
3	C	261	
3	F	261	
3	G	261	
3	I	261	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20240 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 Dipeptidyl peptidase 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	846	Total	C	N	O	S	0	0
			6816	4378	1164	1245	29		
1	D	846	Total	C	N	O	S	0	0
			6816	4378	1164	1245	29		

- Molecule 2 is a protein called NACHT, LRR and PYD domains-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	134	Total	C	N	O	S	0	0
			1068	696	179	187	6		
2	E	134	Total	C	N	O	S	0	0
			1053	682	178	187	6		

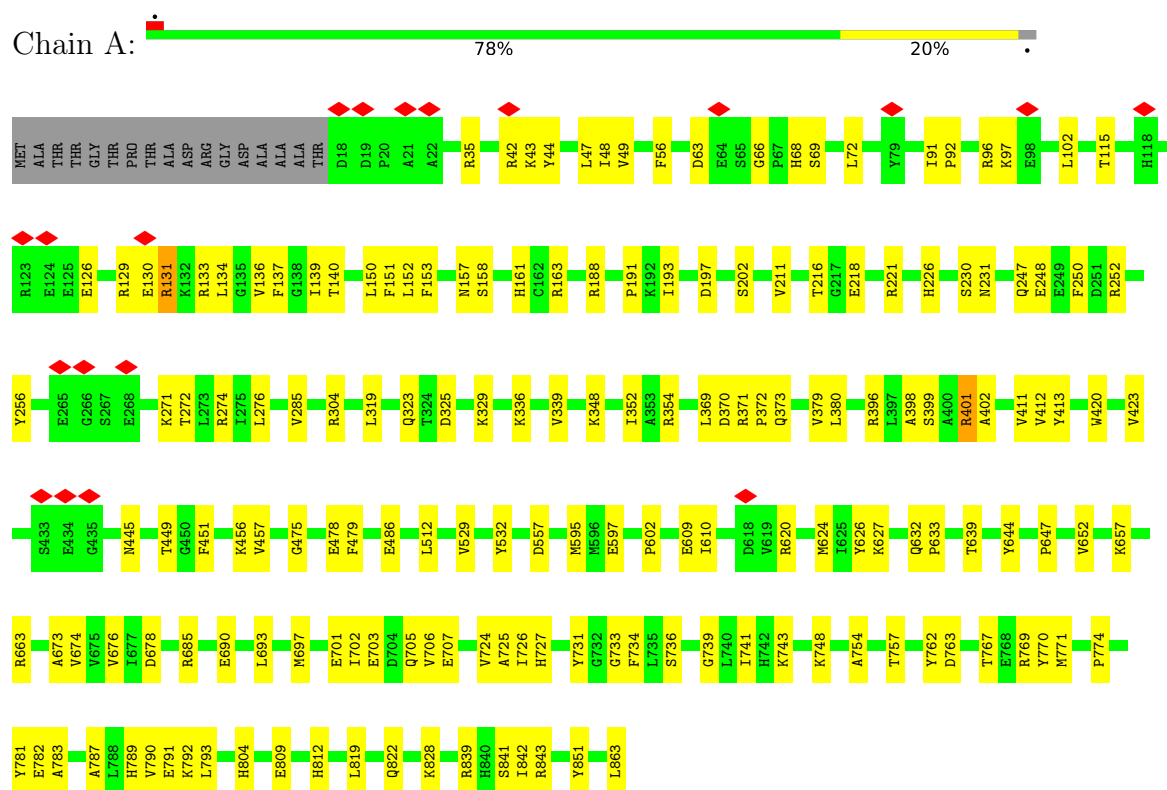
- Molecule 3 is a protein called NACHT, LRR and PYD domains-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	138	Total	C	N	O	S	0	0
			1107	722	183	195	7		
3	C	144	Total	C	N	O	S	0	0
			1136	735	190	203	8		
3	I	138	Total	C	N	O	S	0	0
			1103	719	182	195	7		
3	F	144	Total	C	N	O	S	0	0
			1141	741	189	203	8		

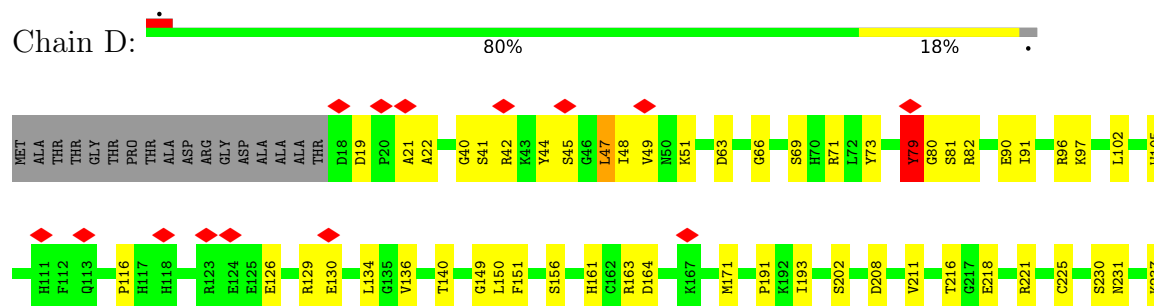
3 Residue-property plots

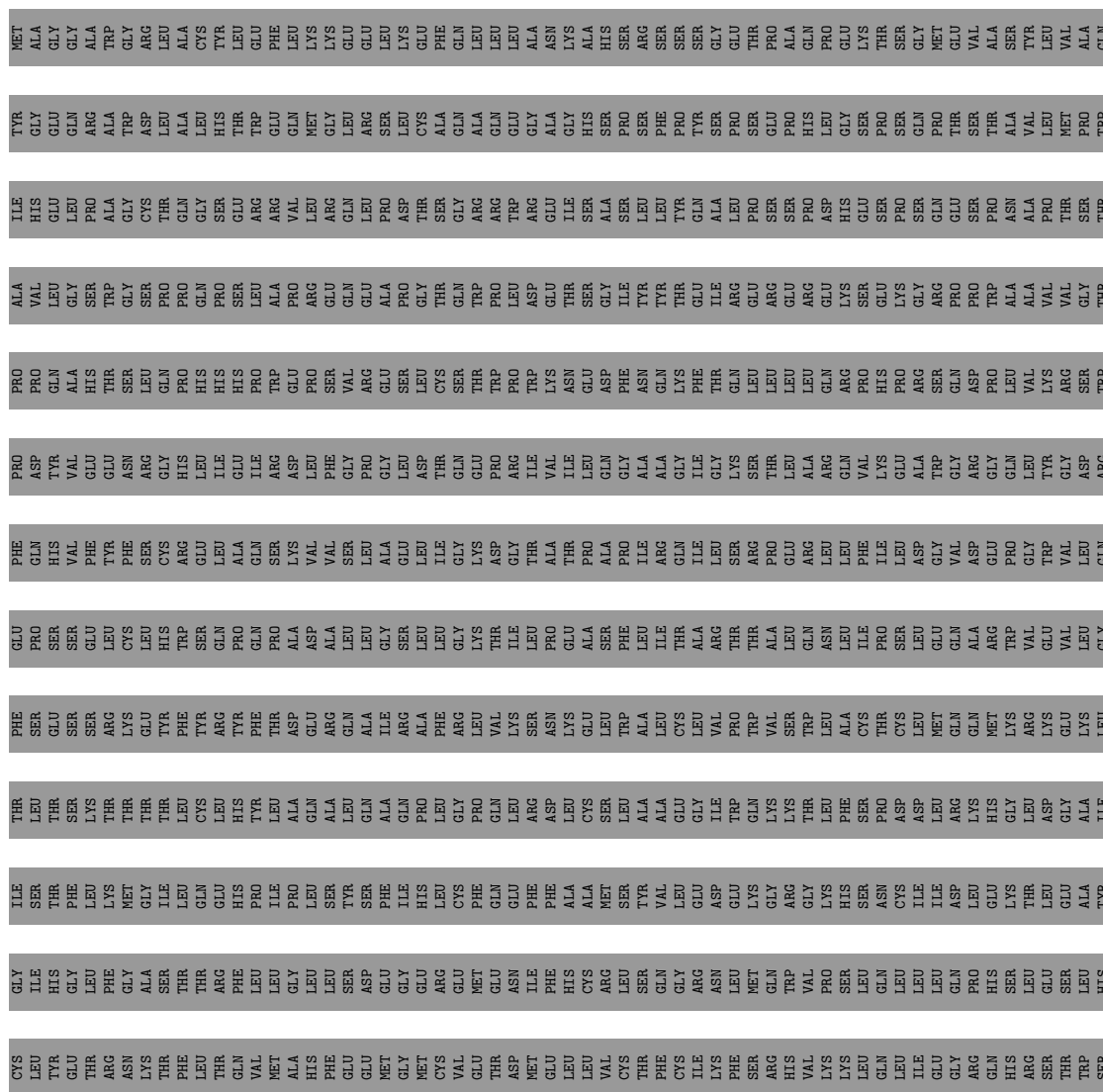
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Dipeptidyl peptidase 9



• Molecule 1: Dipeptidyl peptidase 9







[illegible]

MET	GLU	K1337	H1276
	GLU	D1338	K1277
	VAL	K1339	P1278
	LEU	K1340	
	ASP	D1341	L1281
	LYS	E1342	T1282
	GLY	T1343	T1283
	HIS	L1344	L1284
	LYS	V1345	V1285
	GLY	W1346	M1286
LEU	E1347	G1287	
LEU	A1348	G1288	
PRO	L1349	L1289	
PRO	V1350	V1290	
ARG	K1351	T1291	
ARG	F1352	V1292	
VAL	G1353	S1293	
LEU	A1354	G1294	
ALA	D1355	S1295	
GLU	L1356	G1296	
ASN	M1356	S1297	
THR	PRO	G1298	
ARG	ALA	M1299	
PRO	SER	L1300	
SER	THR	E1301	
GLN	LEU	I1302	
GLN	ILE	L1303	
MET	PRO	P1304	
ARG	PRO	K1305	
LYS	ALA	E1306	
LEU	PHE	L1307	
LEU	SER	E1308	
SER	GLN	L1309	
SER	SER		
ASP	TRP	G1310	
ARG	ASP	V1311	
LYS	LYS	R1312	
LYS	CYS	S1313	
ASP	ASP	P1314	
GLY	GLN	G1315	
LEU	LEU	E1316	
TYR	TYR	D1317	
GLN	PHE	Q1318	
ALA	ALA	L1319	
LEU	LEU	F1320	
LYS	LYS	S1321	
GLU	TYR	E1322	
THR	THR	F1323	
HIS	SER	V1324	
LEU	VAL	V1325	
ILE	ARG	G1326	
	VAL	G1326	
	THR	H1327	
	SER	L1328	
	VAL	G1329	
		S1330	
		G1331	
		I1332	
		R1333	
		L1334	
		G1335	
		V1336	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	179306	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 ($e^-/\text{\AA}^2$)	67.54, 67.6	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	10500	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0184	Depositor
Map size (\AA)	330.0, 330.0, 330.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.825, 0.825, 0.825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.56	0/7022	0.68	0/9534
1	D	0.56	0/7022	0.70	0/9534
2	B	0.39	0/1104	0.74	0/1506
2	E	0.37	0/1086	0.72	0/1481
3	C	0.35	0/1165	0.72	0/1580
3	F	0.34	0/1171	0.71	0/1589
3	G	0.38	0/1136	0.70	0/1539
3	I	0.34	0/1132	0.73	0/1535
All	All	0.50	0/20838	0.70	0/28298

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	6816	0	6590	153	0
1	D	6816	0	6590	119	0
2	B	1068	0	1032	26	0
2	E	1053	0	1017	39	0
3	C	1136	0	1143	59	0
3	F	1141	0	1148	90	0
3	G	1107	0	1131	48	0
3	I	1103	0	1120	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20240	0	19771	531	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 13.

The worst 5 of 531 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:D:660:LYS:HA	3:F:1219:LEU:CD2	1.49	1.39
1:A:842:ILE:HB	3:C:1218:LEU:CD1	1.54	1.35
3:C:1221:MET:HB3	3:C:1223:HIS:CE1	1.67	1.29
3:G:1238:TYR:CE1	3:G:1267:GLU:HG3	1.75	1.20
1:D:48:ILE:HD11	1:D:602:PRO:CG	1.71	1.19

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	844/863 (98%)	788 (93%)	56 (7%)	0	100	100
1	D	844/863 (98%)	794 (94%)	49 (6%)	1 (0%)	51	83
2	B	132/1212 (11%)	118 (89%)	14 (11%)	0	100	100
2	E	132/1212 (11%)	122 (92%)	10 (8%)	0	100	100
3	C	142/261 (54%)	125 (88%)	17 (12%)	0	100	100
3	F	142/261 (54%)	127 (89%)	15 (11%)	0	100	100
3	G	136/261 (52%)	124 (91%)	12 (9%)	0	100	100
3	I	136/261 (52%)	119 (88%)	15 (11%)	2 (2%)	10	47
All	All	2508/5194 (48%)	2317 (92%)	188 (8%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	1306	GLU
3	I	1303	LEU
1	D	79	TYR

5.3.2 Protein sidechains ⓘ

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	738/753 (98%)	735 (100%)	3 (0%)	91	97
1	D	738/753 (98%)	736 (100%)	2 (0%)	92	97
2	B	114/1056 (11%)	114 (100%)	0	100	100
2	E	112/1056 (11%)	111 (99%)	1 (1%)	78	90
3	C	127/237 (54%)	125 (98%)	2 (2%)	62	83
3	F	128/237 (54%)	125 (98%)	3 (2%)	50	76
3	G	125/237 (53%)	125 (100%)	0	100	100
3	I	124/237 (52%)	122 (98%)	2 (2%)	62	83
All	All	2206/4566 (48%)	2193 (99%)	13 (1%)	86	94

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	1120	ARG
3	I	1320	PHE
3	F	1275	ILE
3	F	1217	VAL
3	F	1221	MET

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	157	ASN
2	E	1140	ASN

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](#)

There are no ligands in this entry.

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.

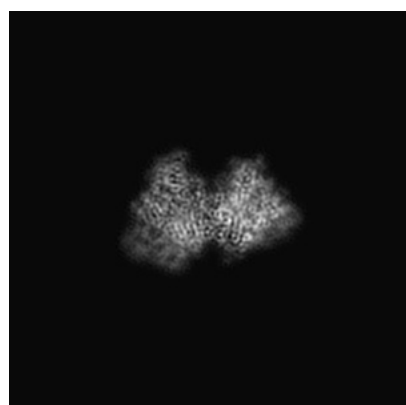
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22074. These allow visual inspection of the internal detail of the map and identification of artifacts.

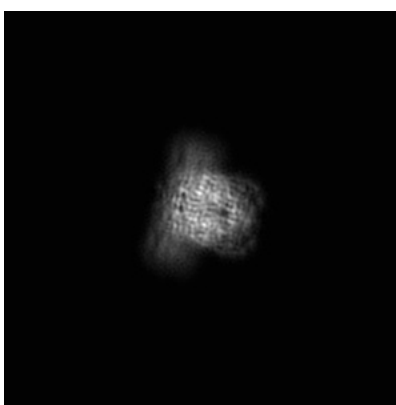
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

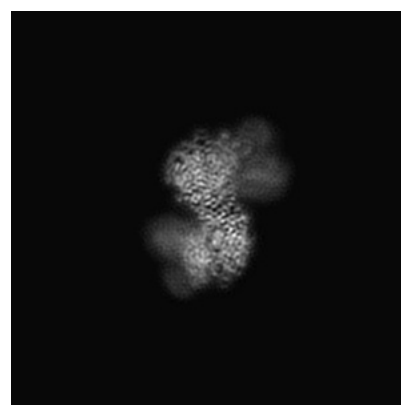
6.1.1 Primary map



X



Y

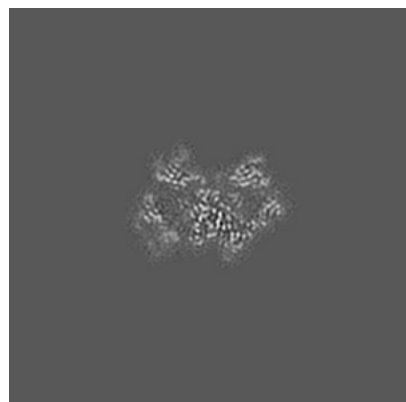


Z

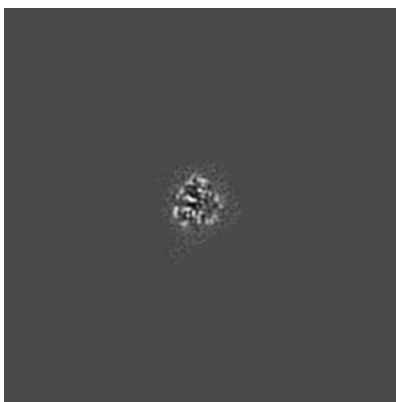
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200



Y Index: 200

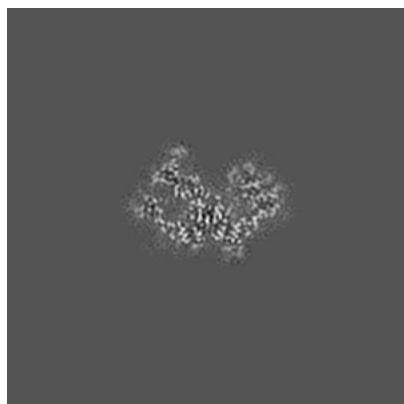


Z Index: 200

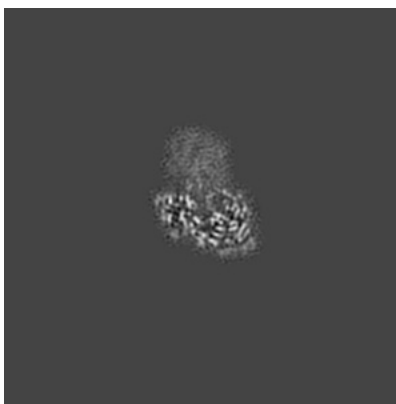
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 208



Y Index: 232

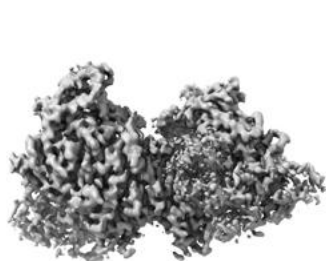


Z Index: 199

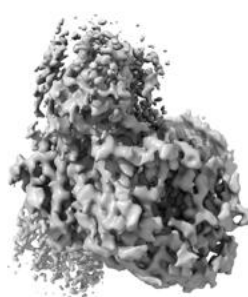
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0184. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

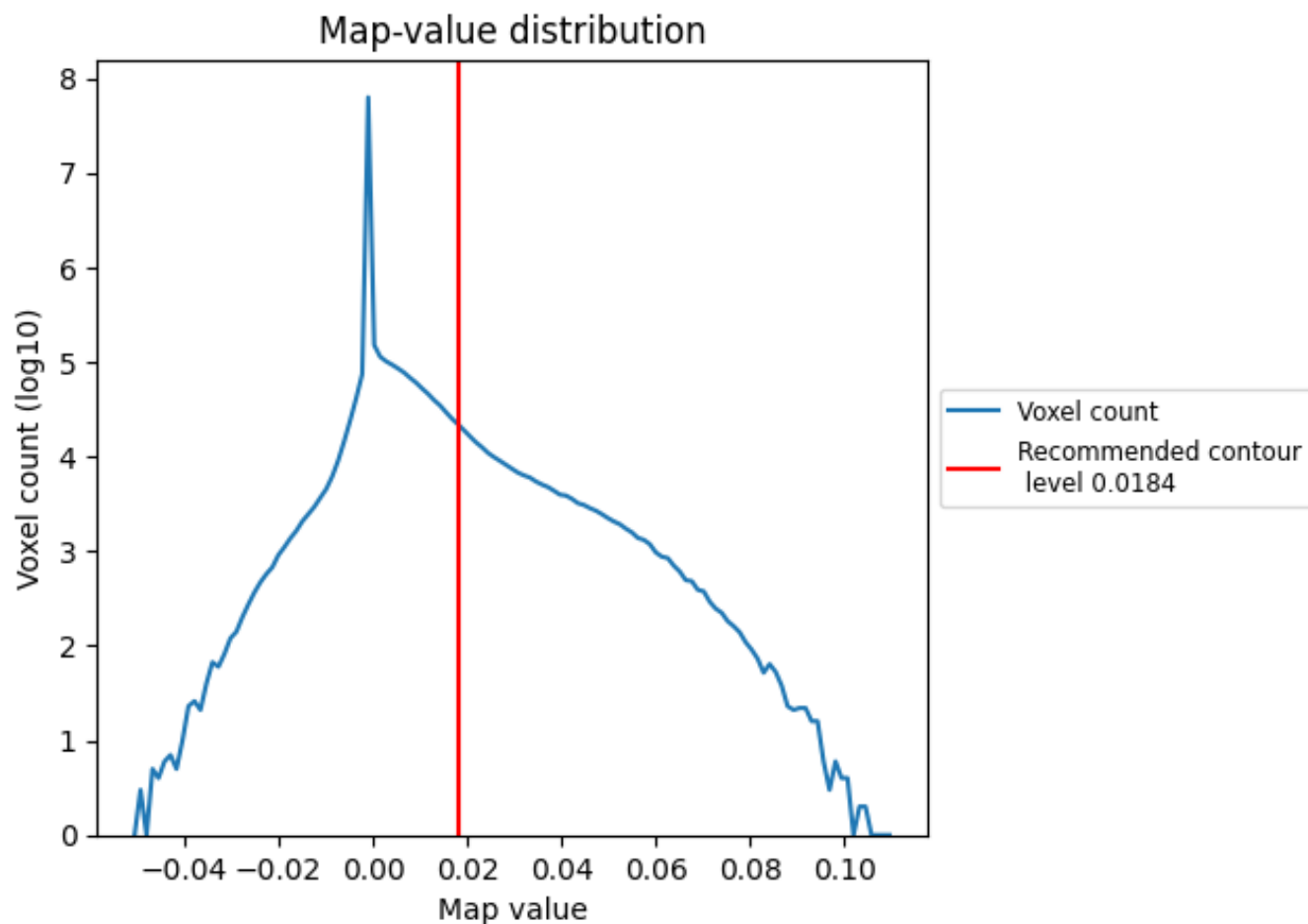
6.5 Mask visualisation

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

7 Map analysis [i](#)

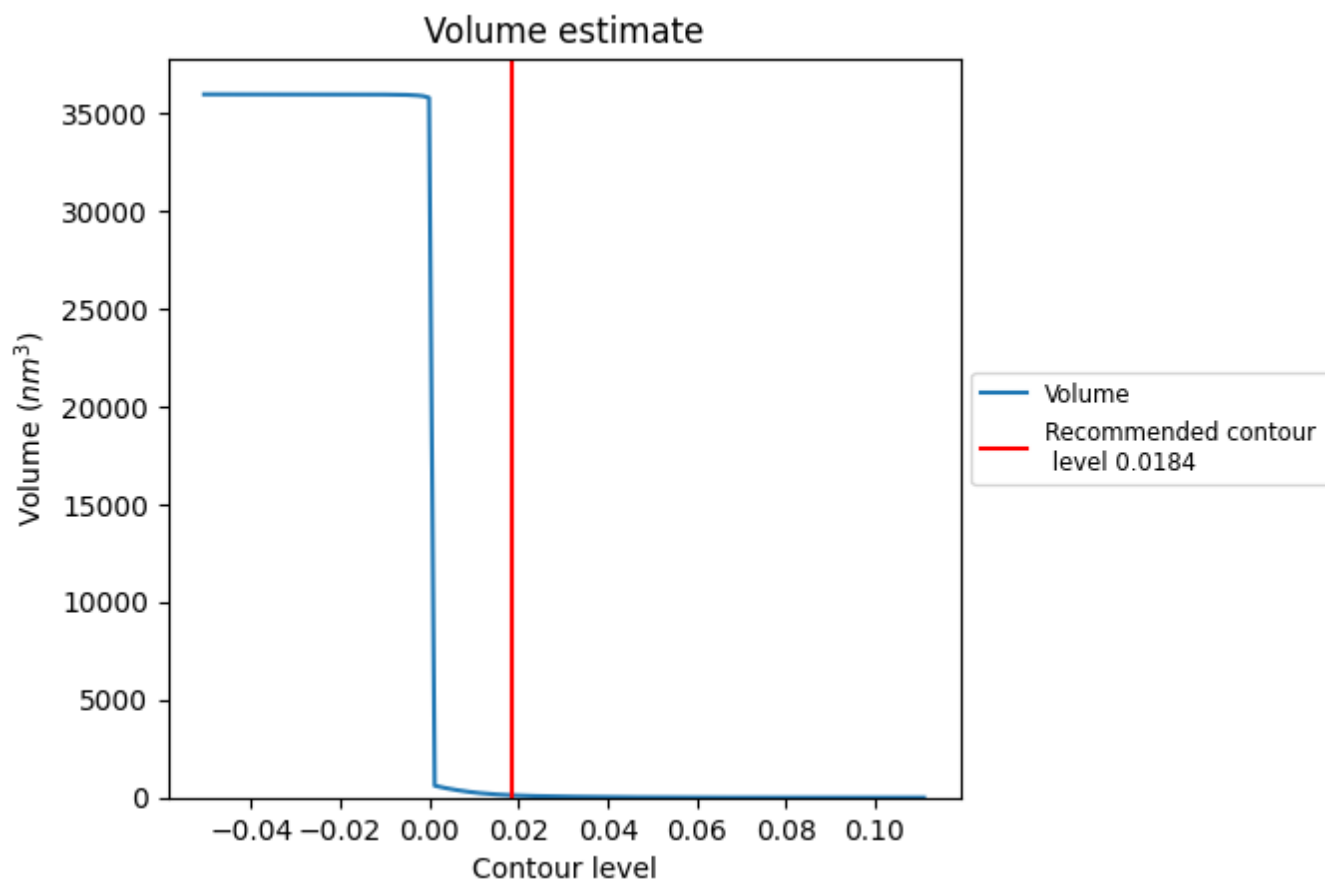
This section contains the results of statistical analysis of the map.

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.

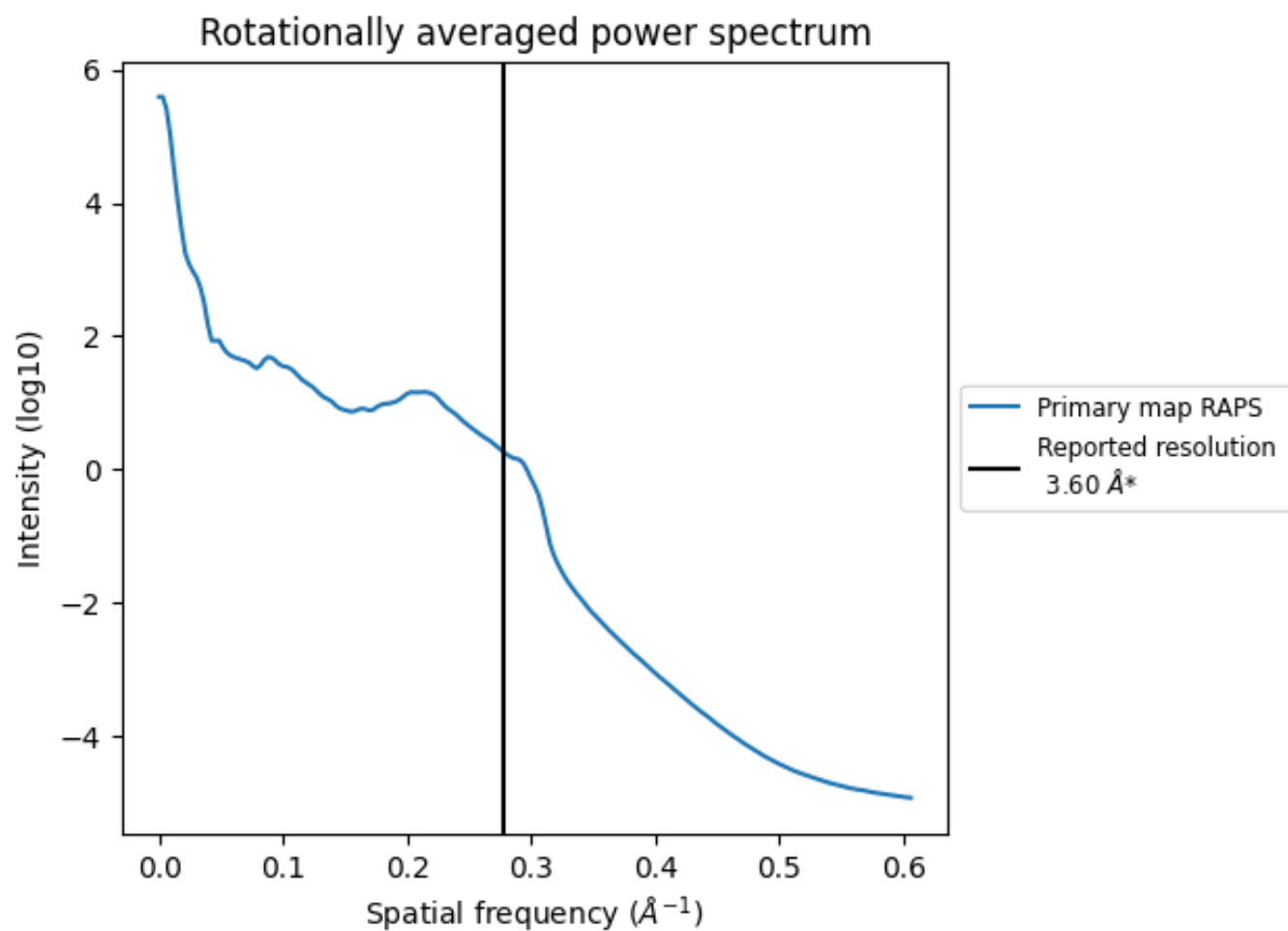
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm³; this corresponds to an approximate mass of 107 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 ⓘ

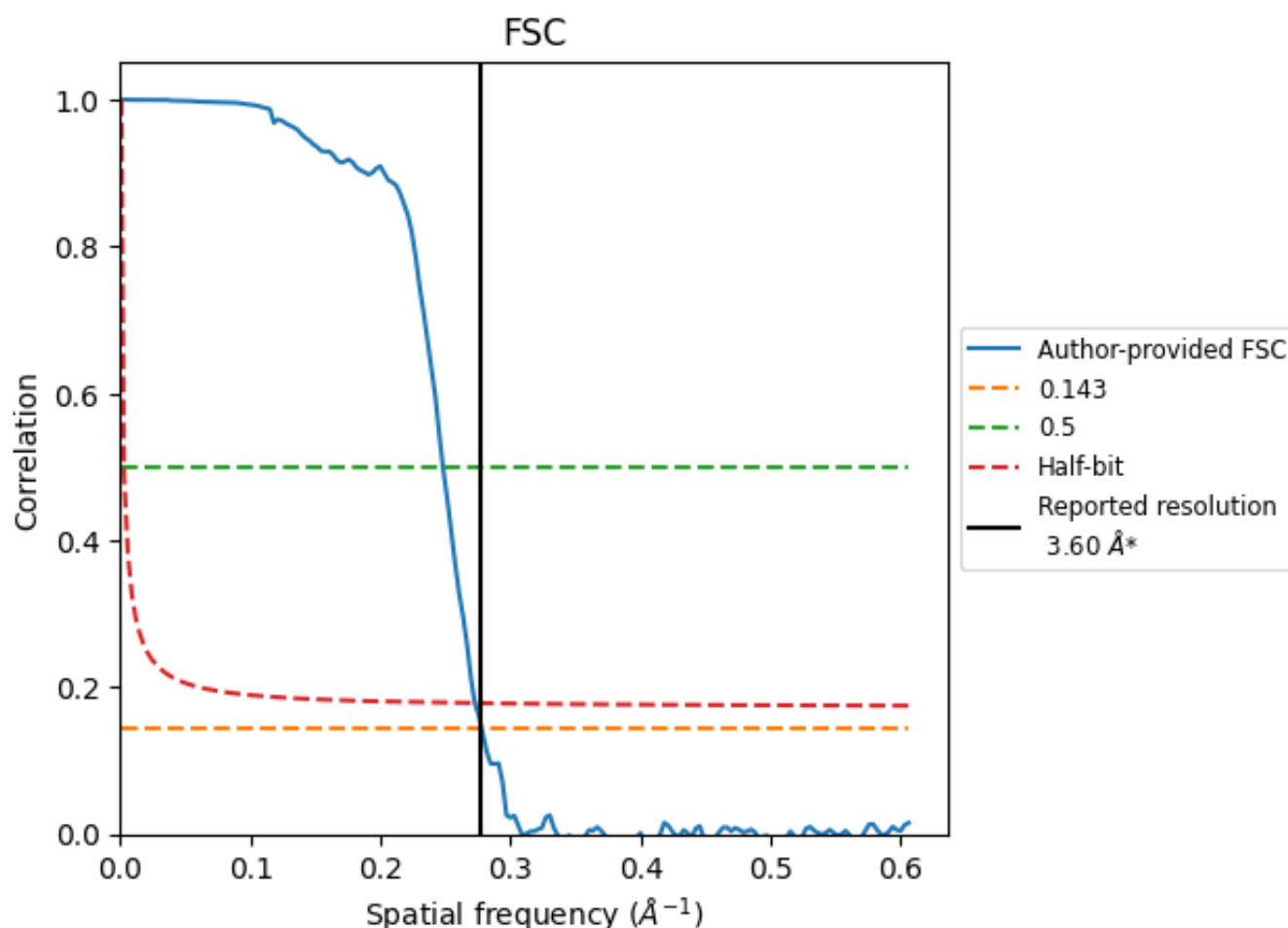


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

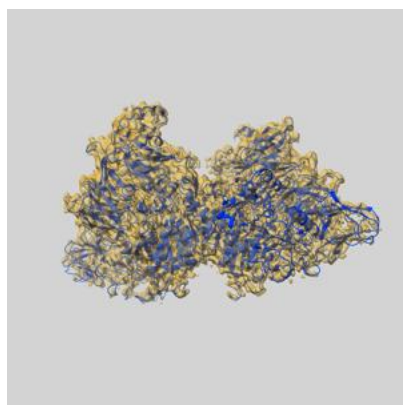
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.03	3.67
Unmasked-calculated*	-	-	-

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

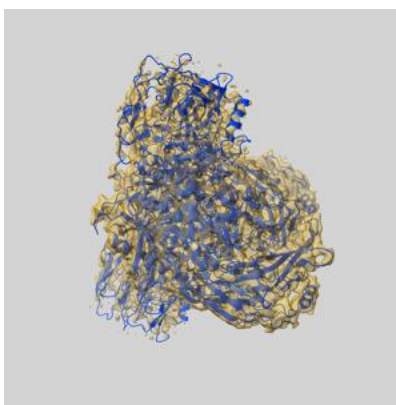
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22074 and PDB model 6X6A. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

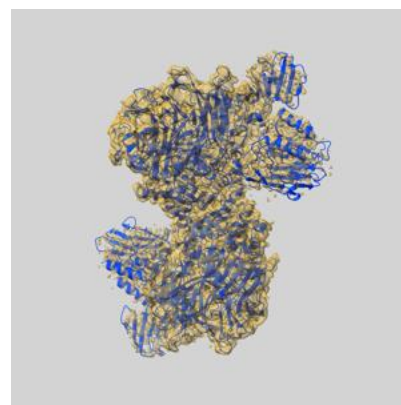
9.1 Map-model overlay [i](#)



X



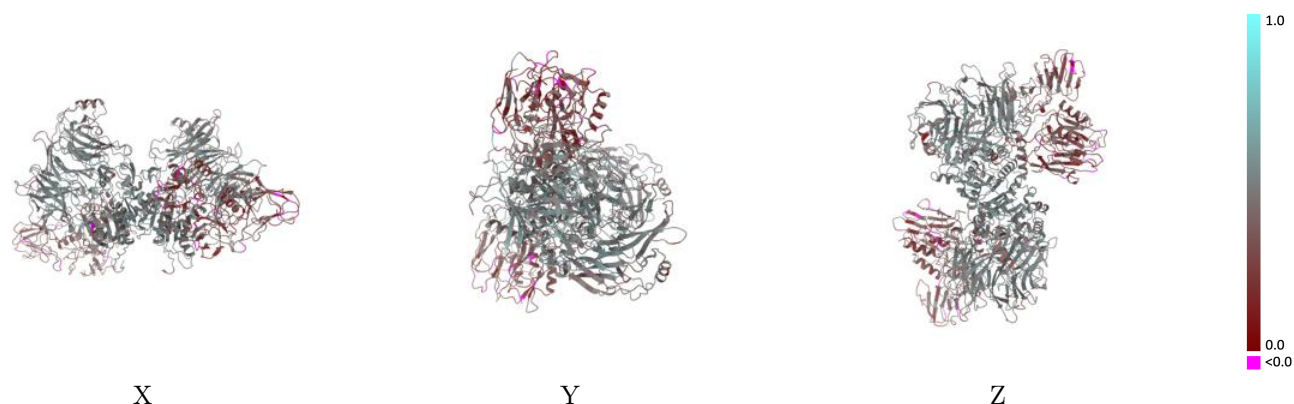
Y



Z

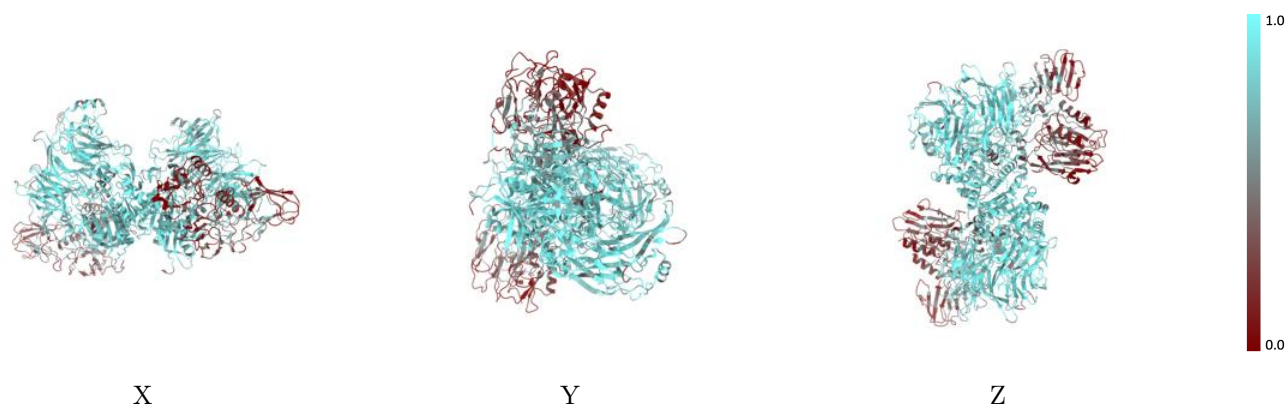
The images above show the 3D surface view of the map at the recommended contour level 0.0184 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



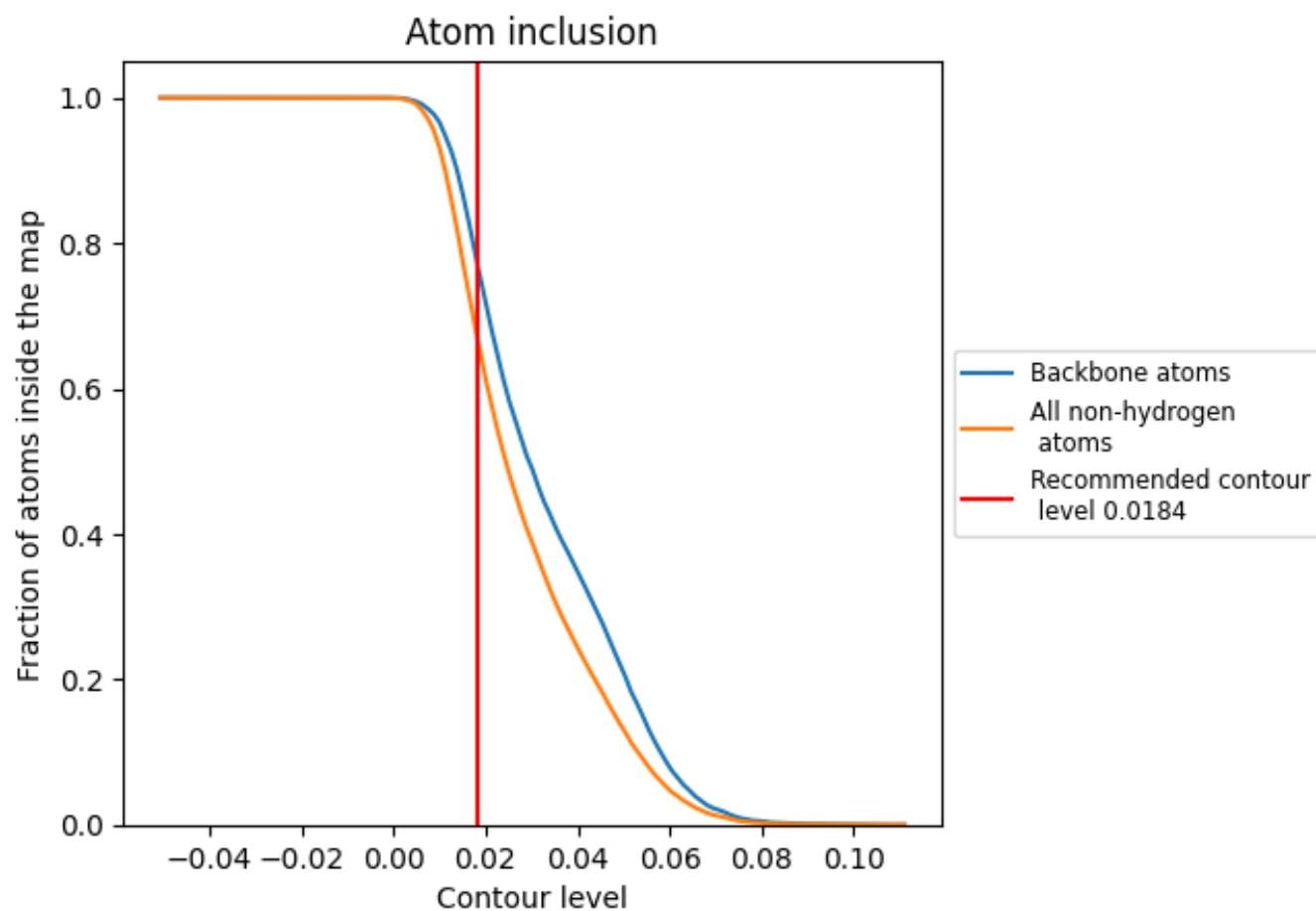
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0184).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 66% 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 (0.0184) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6638	<div></div> 0.4200
A	<div></div> 0.8438	<div></div> 0.4900
B	<div></div> 0.3966	<div></div> 0.3140
C	<div></div> 0.2484	<div></div> 0.2540
D	<div></div> 0.8326	<div></div> 0.4840
E	<div></div> 0.3731	<div></div> 0.3120
F	<div></div> 0.2313	<div></div> 0.2480
G	<div></div> 0.2947	<div></div> 0.2880
I	<div></div> 0.2957	<div></div> 0.2780

1.0

0.0

<0.0