



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 09:10 AM EST

PDB ID : 7TW5
EMDB ID : EMD-26151
Title : Cryo-EM structure of human ankyrin complex (B2P1A2) from red blood cell
Authors : Xia, X.; Liu, S.H.; Zhou, Z.H.
Deposited on : 2022-02-06
Resolution : 5.70 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) : 2.31.3

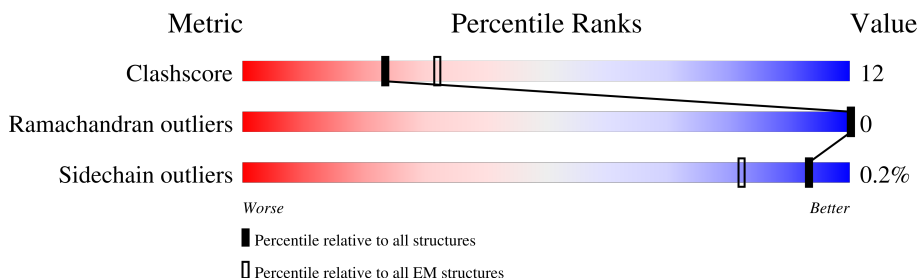
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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	911	<div> <div>9%</div> <div>69%</div> <div>22%</div> <div>9%</div> </div>
1	B	911	<div> <div>65%</div> <div>24%</div> <div>11%</div> </div>
2	E	691	<div> <div>65%</div> <div>31%</div> </div>
3	G	1881	<div> <div>10%</div> <div>26%</div> <div>7%</div> <div>66%</div> </div>
3	H	1881	<div> <div>26%</div> <div>8%</div> <div>66%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27048 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 Band 3 anion transport protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	830	Total	C	N	O	S	0	0
			6563	4300	1087	1151	25		
1	B	814	Total	C	N	O	S	0	0
			6435	4224	1065	1122	24		

- Molecule 2 is a protein called Protein 4.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	665	Total	C	N	O	S	0	0
			5236	3316	929	968	23		

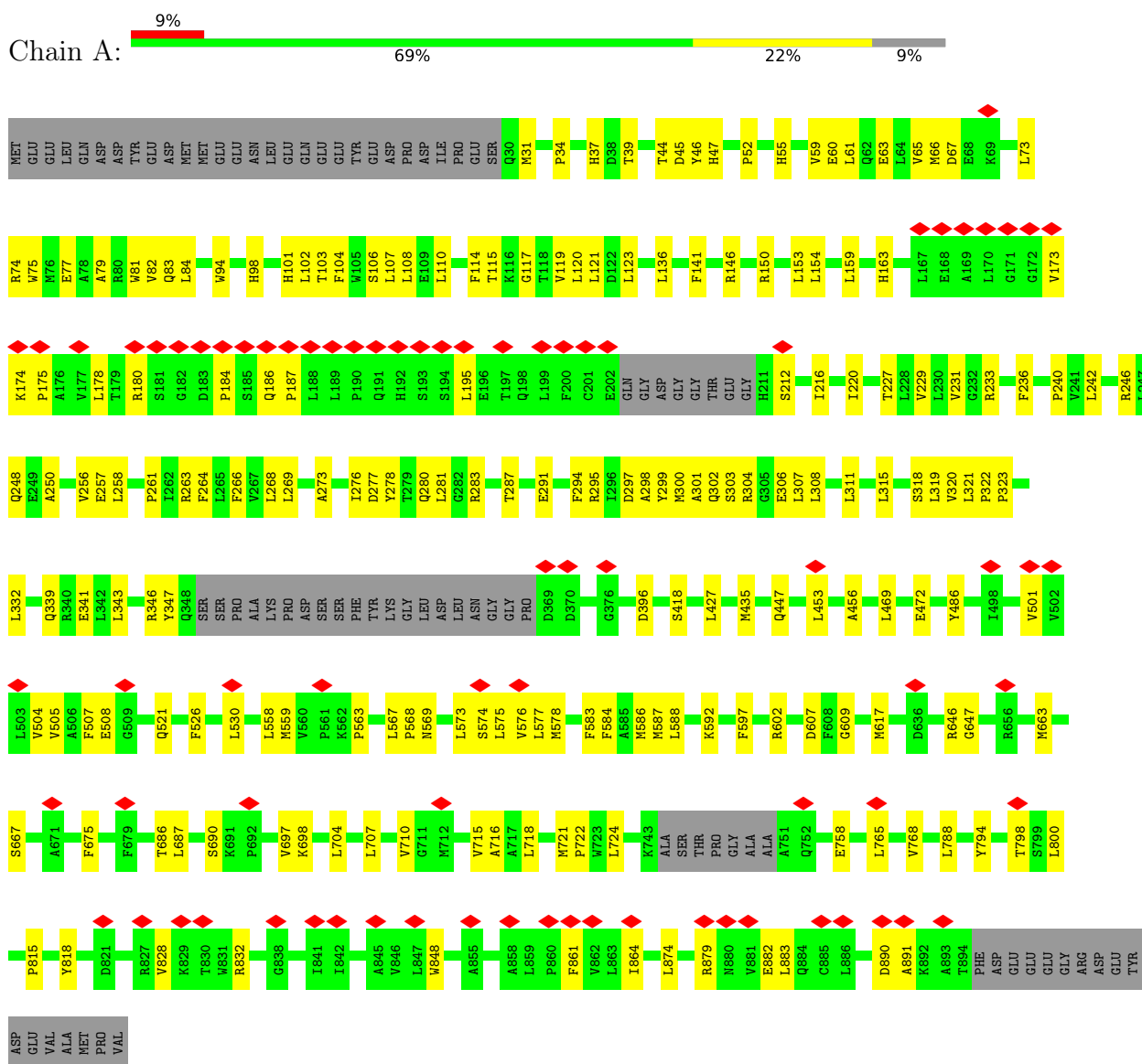
- Molecule 3 is a protein called Ankyrin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	635	Total	C	N	O	S	0	0
			4407	2736	843	814	14		
3	H	635	Total	C	N	O	S	0	0
			4407	2736	843	814	14		

3 Residue-property plots

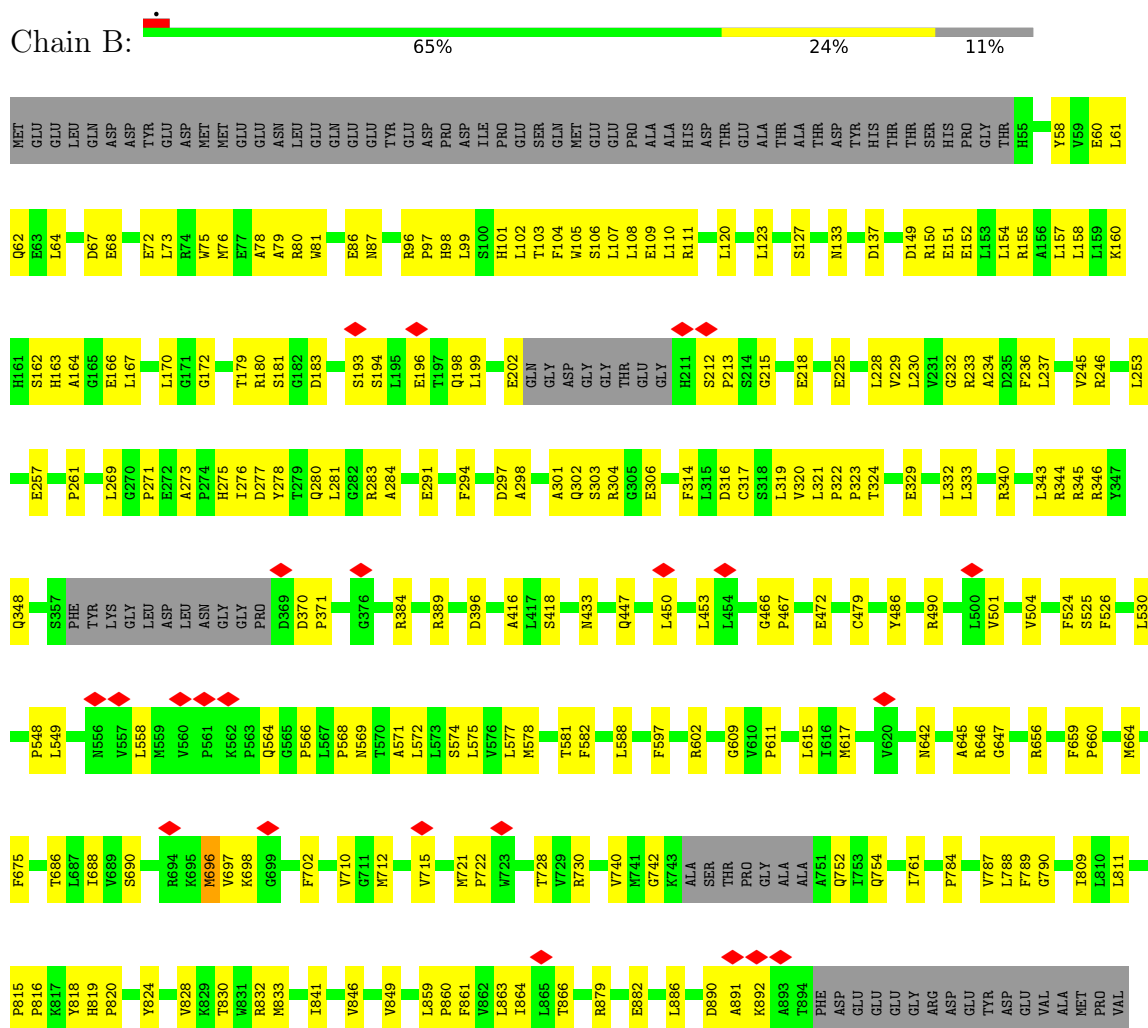
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Band 3 anion transport protein



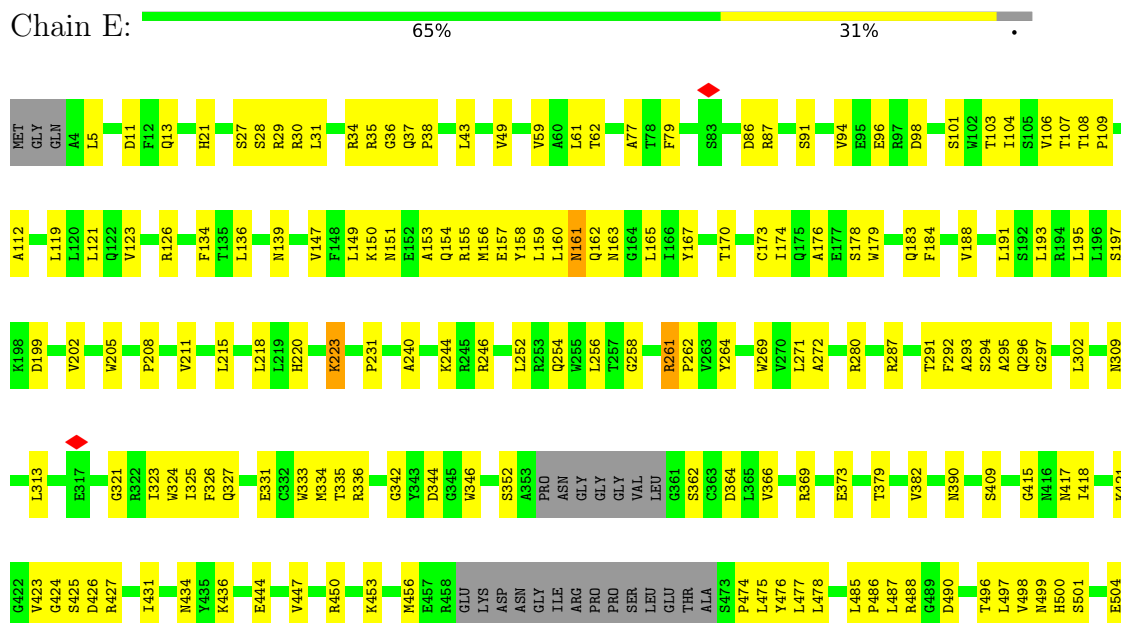
• Molecule 1: Band 3 anion transport protein

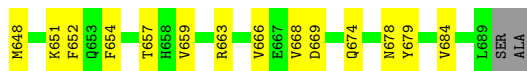
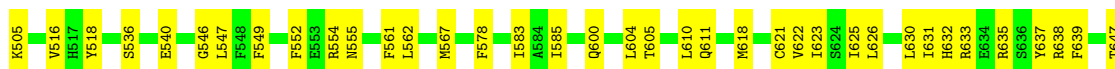
Chain B:



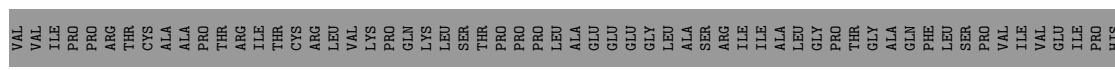
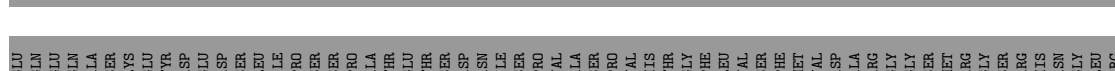
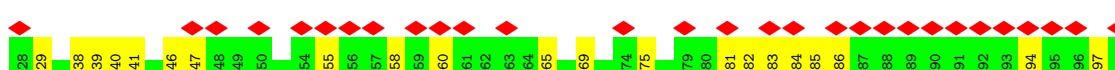
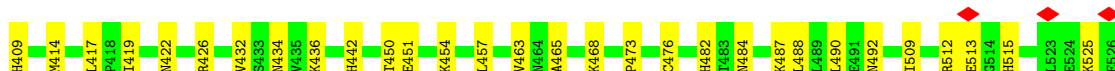
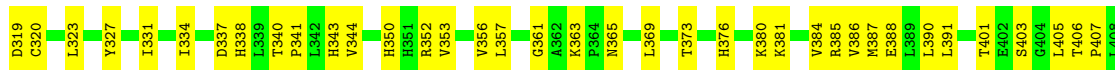
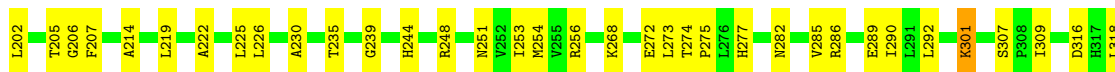
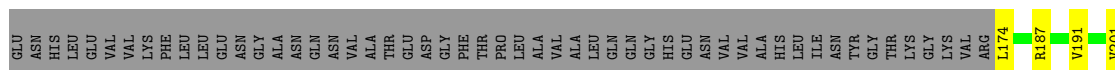
• Molecule 2: Protein 4.2

Chain E:





• Molecule 3: Ankyrin-1



- Molecule 3: Ankyrin-1

[illegible]



LEU	ARG	ALA	GLN
GLU	SER	ASP	PRO
CYS	GLU	GLY	GLU
SER	GLU	ALA	ILE
LYS	LYS	ILE	ARG
ALA	LEU	VAL	LYS
GLU	PRO	SER	VAL
ASP	GLY	SER	GLN
ASP	SER	TYR	GLN
LYS	LYS	ASP	ALA
ALA	ARG	ILE	ARG
THR	GLN	ASP	ASP
GLY	ASP	ALA	ARG
HIS	ASP	GLN	ARG
GLU	THR	GLY	GLN
TRP	THR	GLY	GLN
LYS	GLY	TRP	GLY
LEU	ALA	GLN	ALA
GLU	GLY	GLU	GLU
GLY	GLN	GLU	GLU
ALA	ASP	VAL	GLN
SER	GLU	THR	VAL
SER	GLU	GLN	GLN
GLU	ASN	GLY	GLU
GLU	GLU	PRO	ALA
PRO	VAL	HIS	LYS
ARG	SER	SER	ASN
GLY	LEU	PHE	THR
PRO	VAL	GLY	THR
GLU	SER	GLY	THR
LEU	GLY	THR	GLN
GLY	HIS	SER	VAL
SER	GLN	THR	VAL
LEU	ARG	MET	GLN
GLU	THR	THR	GLY
LEU	GLN	GLU	ASN
VAL	ALA	GLY	GLU
GLU	ARG	LEU	PHE
ASP	ILE	GLU	GLN
THR	THR	PRO	ASN
HIS	THR	GLY	ILE
VAL	PRO	ASP	THR
SER	THR	GLY	GLN
ASP	VAL	GLU	VAL
ALA	ASP	TYR	VAL
THR	ALA	GLN	THR
ASN	THR	LYS	THR
GLY	THR	VAL	GLU
LEU	ARG	LEU	GLN
ILE	ARG	VAL	PHE
THR	SER	VAL	THR
LEU	GLN	VAL	ASP
GLU	ASP	GLU	SER
GLN	ARG	GLN	THR
THR	GLY	GLY	PRO
GLU	LEU	HIS	ASN
GLY	GLN	THR	GLY
TRP	ASP	TRP	ILE
GLN	ASP	THR	VAL
		GLU	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34612	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.274	Depositor
Minimum map value	-0.973	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.35	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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	0.27	0/6720	0.54	0/9136
1	B	0.27	0/6588	0.55	0/8953
2	E	0.27	0/5345	0.56	0/7255
3	G	0.25	0/4479	0.52	0/6115
3	H	0.26	0/4479	0.52	0/6115
All	All	0.27	0/27611	0.54	0/37574

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	6563	0	6753	167	0
1	B	6435	0	6652	174	0
2	E	5236	0	5248	159	0
3	G	4407	0	4091	98	0
3	H	4407	0	4091	99	0
All	All	27048	0	26835	659	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 659 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:581:THR:CG2	1:B:790:GLY:HA3	1.97	0.94
1:B:581:THR:HG21	1:B:790:GLY:HA3	1.56	0.87
1:A:31:MET:HE2	2:E:651:LYS:HB2	1.60	0.83
2:E:35:ARG:O	2:E:139:ASN:ND2	2.12	0.82
2:E:610:LEU:HD21	2:E:648:MET:HB3	1.59	0.82

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	822/911 (90%)	806 (98%)	16 (2%)	0	100	100
1	B	806/911 (88%)	787 (98%)	19 (2%)	0	100	100
2	E	659/691 (95%)	646 (98%)	13 (2%)	0	100	100
3	G	631/1881 (34%)	596 (94%)	35 (6%)	0	100	100
3	H	631/1881 (34%)	595 (94%)	36 (6%)	0	100	100
All	All	3549/6275 (57%)	3430 (97%)	119 (3%)	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	719/786 (92%)	719 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	707/786 (90%)	706 (100%)	1 (0%)	93	96
2	E	568/588 (97%)	565 (100%)	3 (0%)	88	93
3	G	391/1594 (24%)	390 (100%)	1 (0%)	92	94
3	H	391/1594 (24%)	391 (100%)	0	100	100
All	All	2776/5348 (52%)	2771 (100%)	5 (0%)	93	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	696	MET
2	E	161	ASN
2	E	223	LYS
2	E	261	ARG
3	G	301	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	161	ASN
3	G	482	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 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.

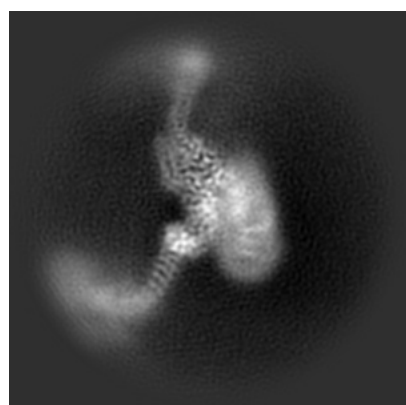
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26151. These allow visual inspection of the internal detail of the map and identification of artifacts.

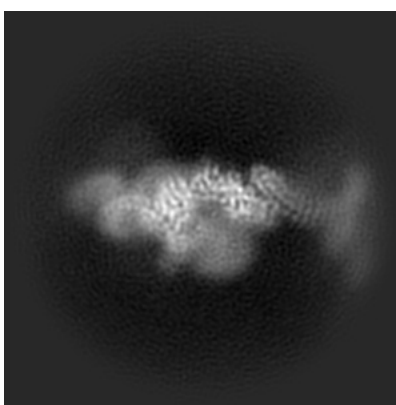
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

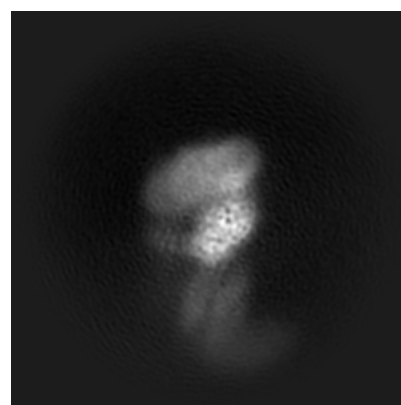
6.1.1 Primary map



X



Y

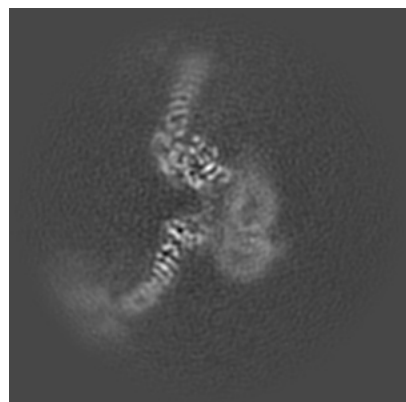


Z

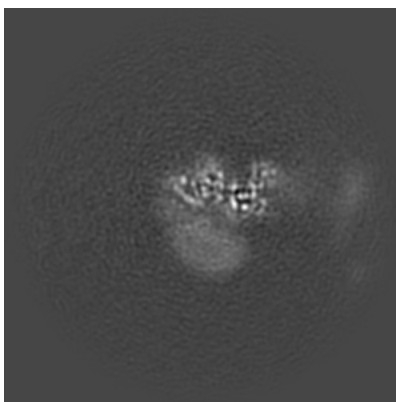
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

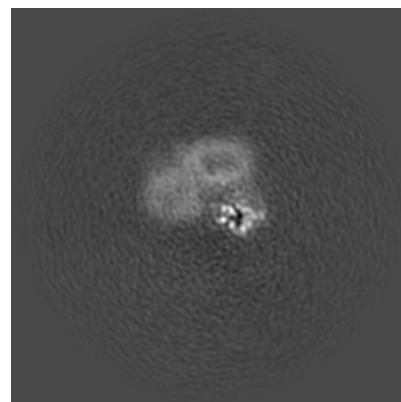
6.2.1 Primary map



X Index: 192



Y Index: 192

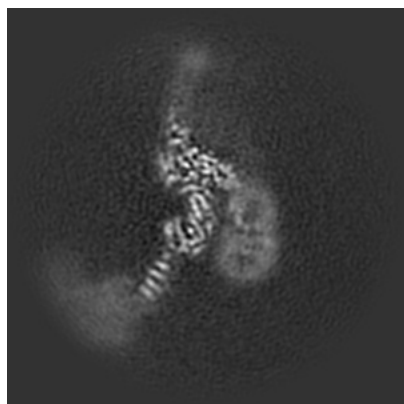


Z Index: 192

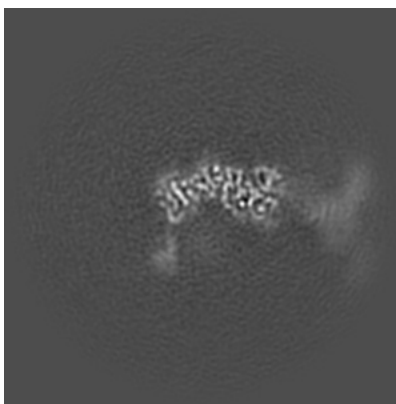
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

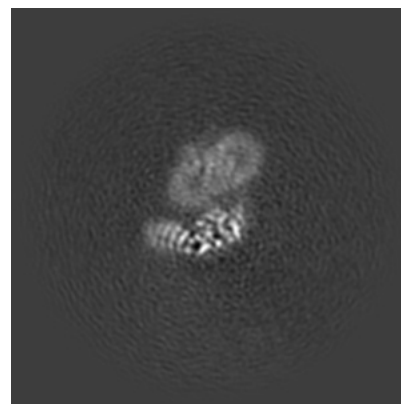
6.3.1 Primary map



X Index: 203



Y Index: 176



Z Index: 161

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

6.4 Orthogonal surface views [i](#)

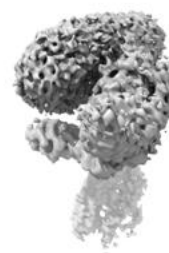
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

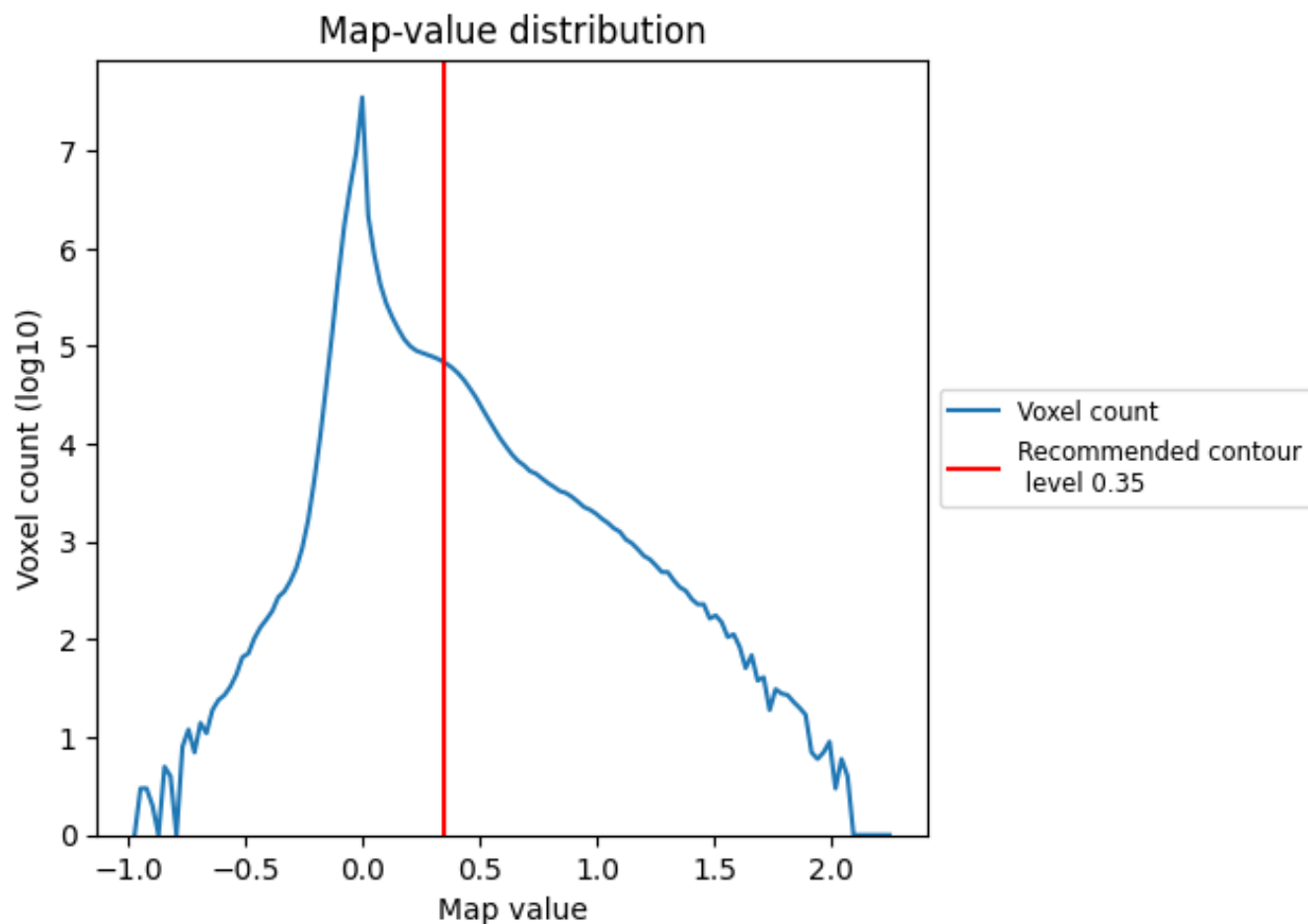
6.5 Mask visualisation

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

7 Map analysis [i](#)

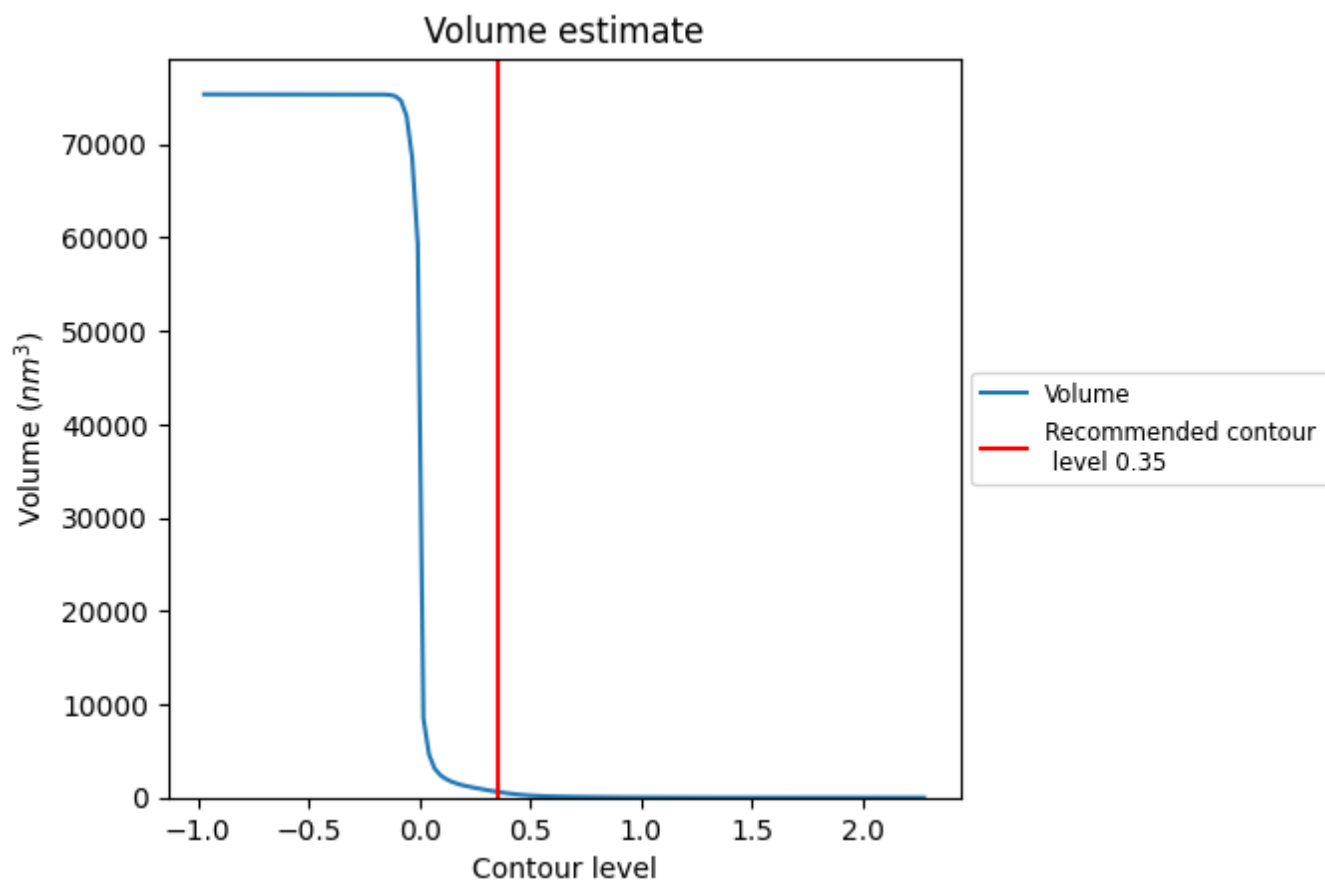
This section contains the results of statistical analysis of the map.

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.

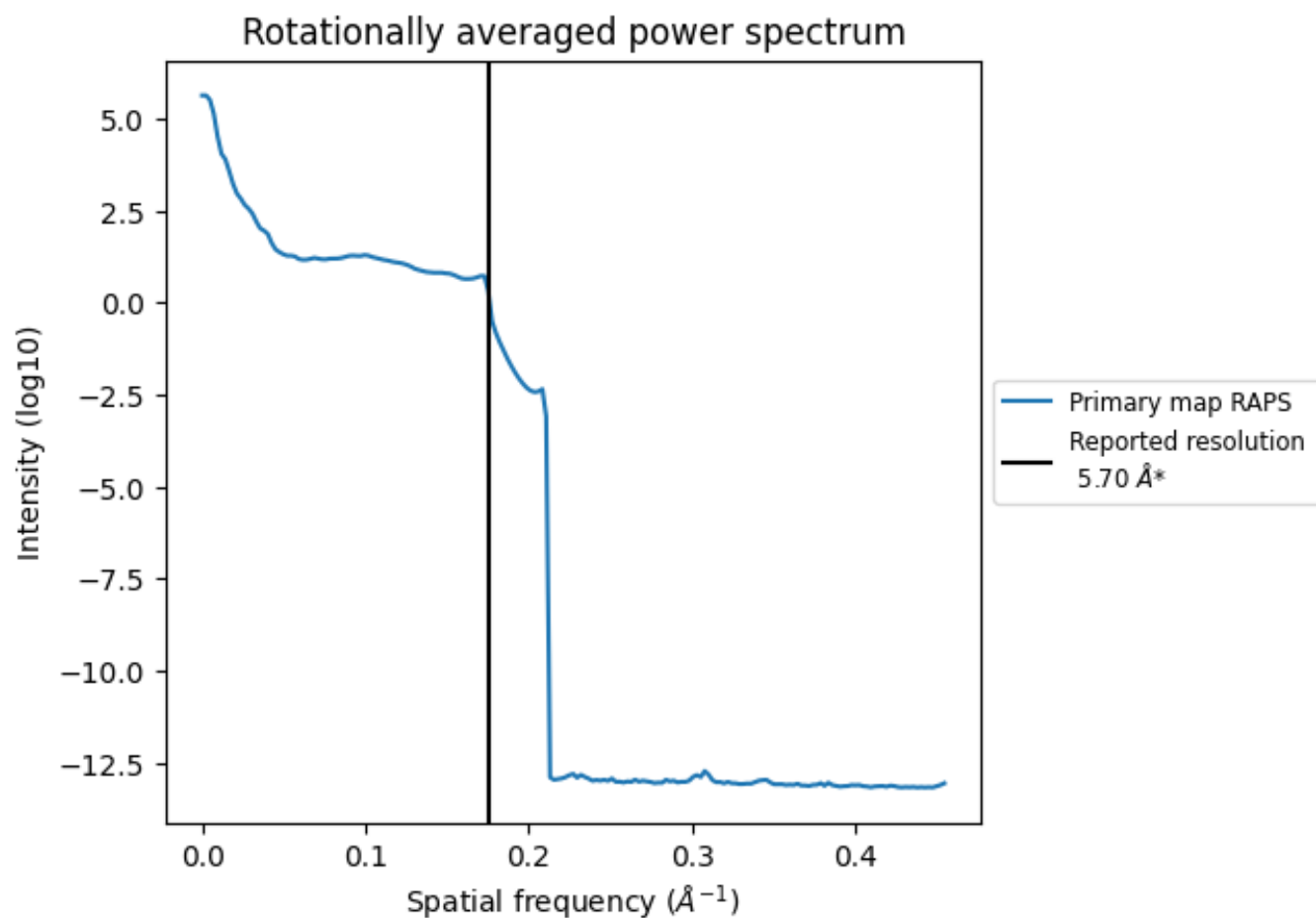
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 617 nm³; this corresponds to an approximate mass of 557 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 0.175 Å⁻¹

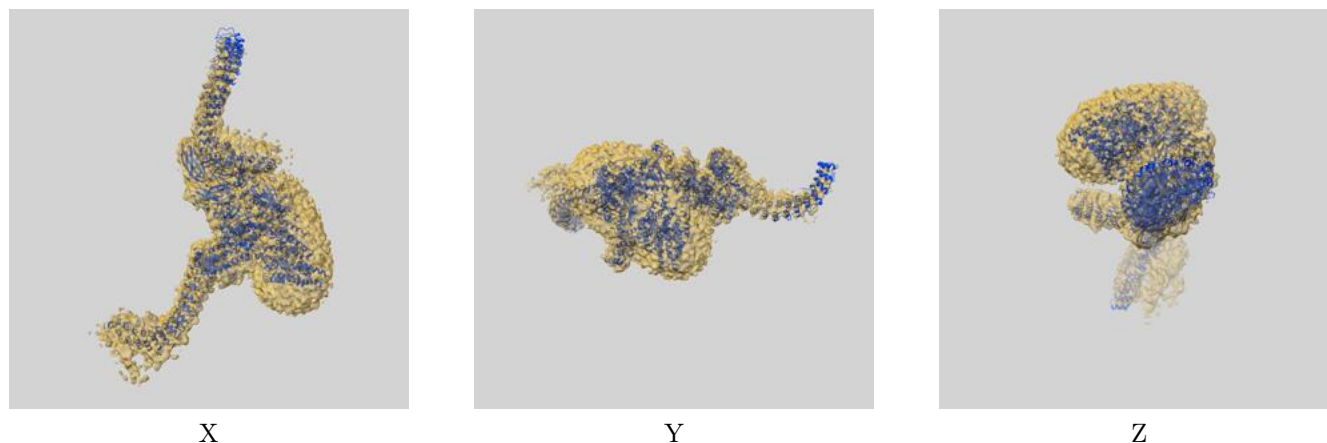
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

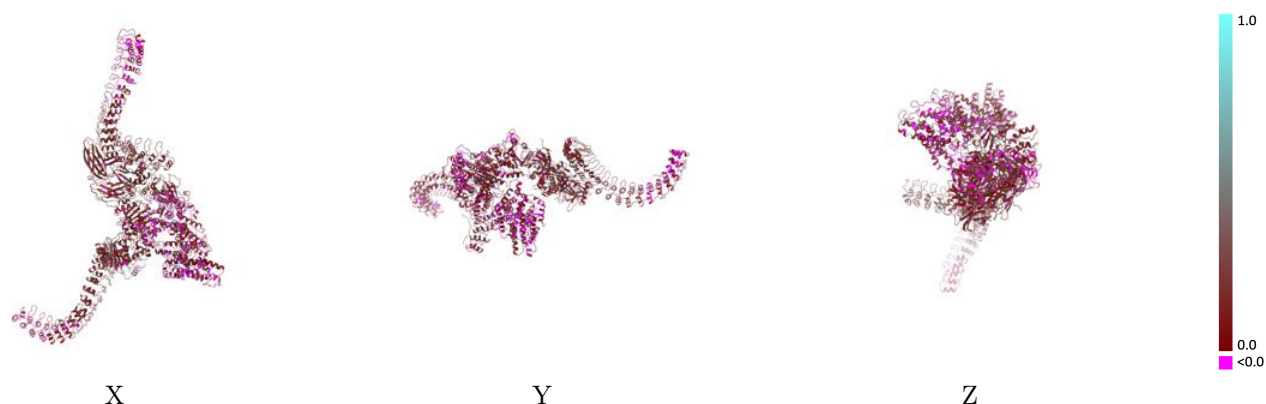
This section contains information regarding the fit between EMDB map EMD-26151 and PDB model 7TW5. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



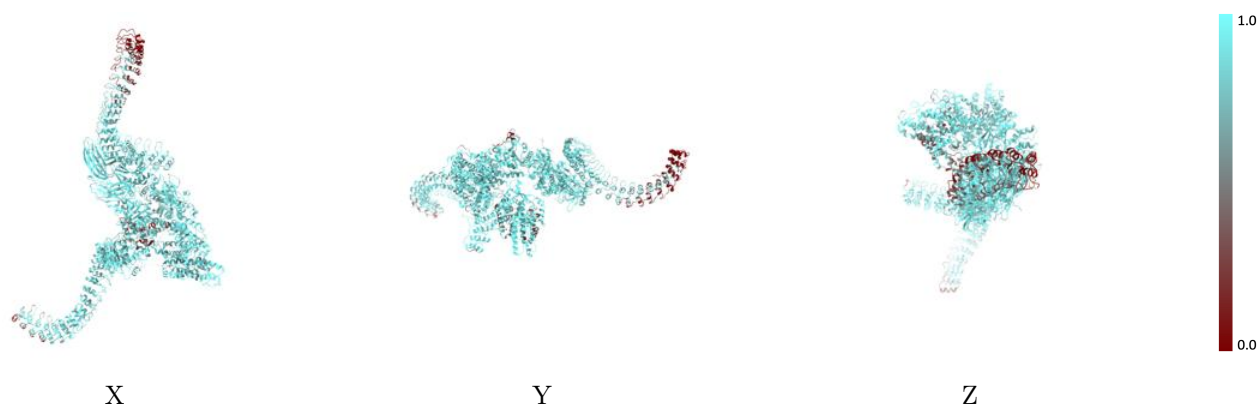
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



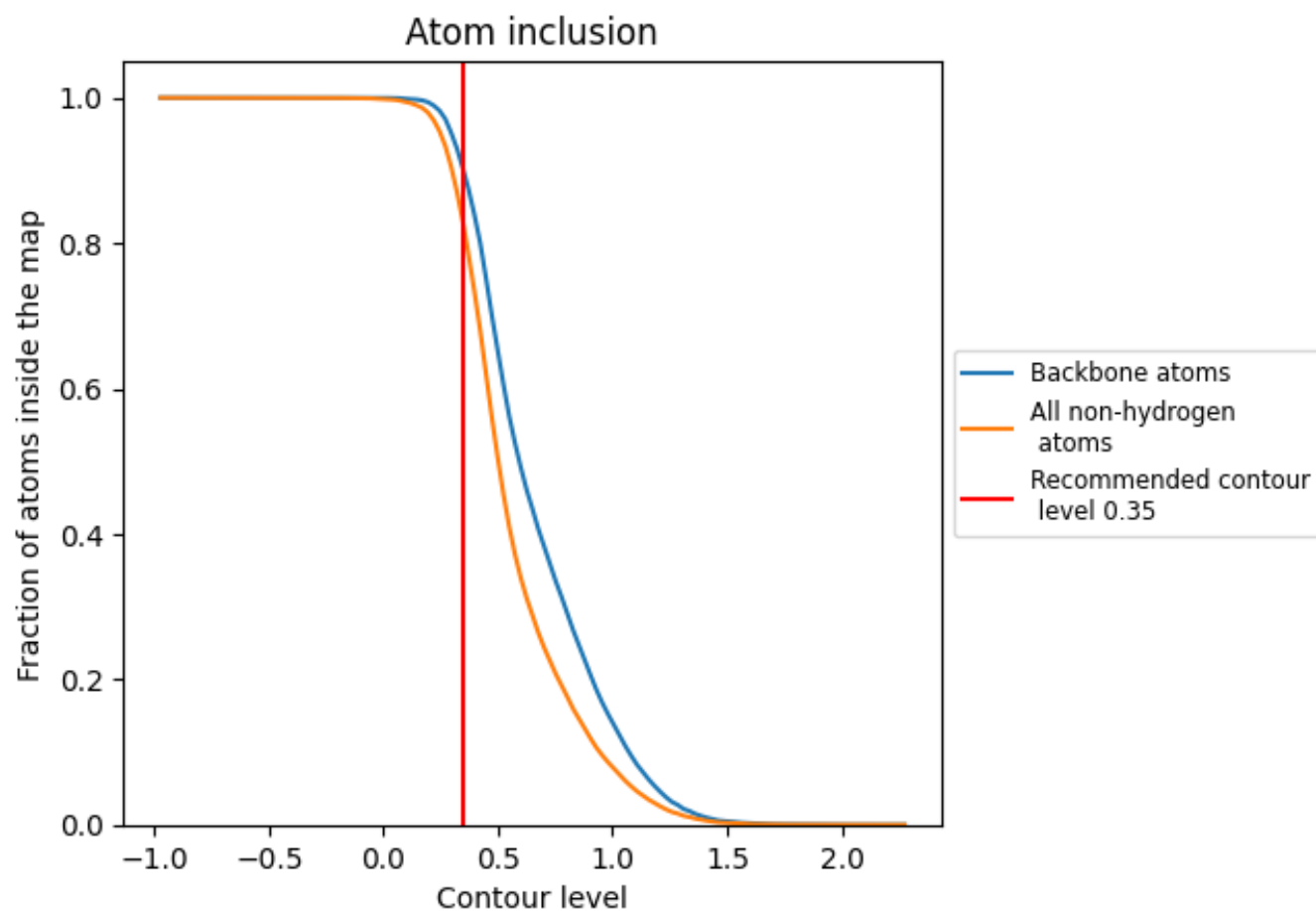
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 82% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8243	<div></div> 0.1640
A	<div></div> 0.8287	<div></div> 0.1230
B	<div></div> 0.8810	<div></div> 0.1450
E	<div></div> 0.9018	<div></div> 0.2290
G	<div></div> 0.6492	<div></div> 0.1680
H	<div></div> 0.8199	<div></div> 0.1740

