



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 03:16 PM JST

PDB ID : 6M66
EMDB ID : EMD-30114
Title : The Cryo-EM Structure of Human Pannexin 1
Authors : Jin, Q.; Bo, Z.; Xiang, Z.; Xiaokang, Z.; Ye, S.
Deposited on : 2020-03-13
Resolution : 4.10 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:

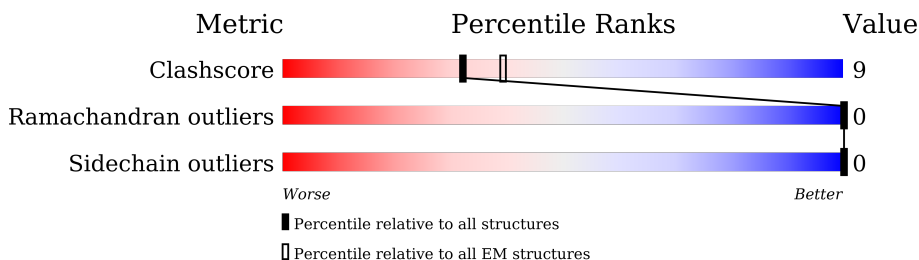
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	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	440	
1	B	440	
1	C	440	
1	D	440	
1	E	440	
1	F	440	
1	G	440	

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 14938 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 Pannexin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	265	2134	1425	329	370	10	0	0
1	B	265	2134	1425	329	370	10	0	0
1	C	265	2134	1425	329	370	10	0	0
1	D	265	2134	1425	329	370	10	0	0
1	E	265	2134	1425	329	370	10	0	0
1	F	265	2134	1425	329	370	10	0	0
1	G	265	2134	1425	329	370	10	0	0

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	427	GLY	-	expression tag	UNP Q96RD7
A	428	SER	-	expression tag	UNP Q96RD7
A	429	GLY	-	expression tag	UNP Q96RD7
A	430	SER	-	expression tag	UNP Q96RD7
A	431	HIS	-	expression tag	UNP Q96RD7
A	432	HIS	-	expression tag	UNP Q96RD7
A	433	HIS	-	expression tag	UNP Q96RD7
A	434	HIS	-	expression tag	UNP Q96RD7
A	435	HIS	-	expression tag	UNP Q96RD7
A	436	HIS	-	expression tag	UNP Q96RD7
A	437	HIS	-	expression tag	UNP Q96RD7
A	438	HIS	-	expression tag	UNP Q96RD7
A	439	HIS	-	expression tag	UNP Q96RD7
A	440	HIS	-	expression tag	UNP Q96RD7
B	427	GLY	-	expression tag	UNP Q96RD7
B	428	SER	-	expression tag	UNP Q96RD7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	429	GLY	-	expression tag	UNP Q96RD7
B	430	SER	-	expression tag	UNP Q96RD7
B	431	HIS	-	expression tag	UNP Q96RD7
B	432	HIS	-	expression tag	UNP Q96RD7
B	433	HIS	-	expression tag	UNP Q96RD7
B	434	HIS	-	expression tag	UNP Q96RD7
B	435	HIS	-	expression tag	UNP Q96RD7
B	436	HIS	-	expression tag	UNP Q96RD7
B	437	HIS	-	expression tag	UNP Q96RD7
B	438	HIS	-	expression tag	UNP Q96RD7
B	439	HIS	-	expression tag	UNP Q96RD7
B	440	HIS	-	expression tag	UNP Q96RD7
C	427	GLY	-	expression tag	UNP Q96RD7
C	428	SER	-	expression tag	UNP Q96RD7
C	429	GLY	-	expression tag	UNP Q96RD7
C	430	SER	-	expression tag	UNP Q96RD7
C	431	HIS	-	expression tag	UNP Q96RD7
C	432	HIS	-	expression tag	UNP Q96RD7
C	433	HIS	-	expression tag	UNP Q96RD7
C	434	HIS	-	expression tag	UNP Q96RD7
C	435	HIS	-	expression tag	UNP Q96RD7
C	436	HIS	-	expression tag	UNP Q96RD7
C	437	HIS	-	expression tag	UNP Q96RD7
C	438	HIS	-	expression tag	UNP Q96RD7
C	439	HIS	-	expression tag	UNP Q96RD7
C	440	HIS	-	expression tag	UNP Q96RD7
D	427	GLY	-	expression tag	UNP Q96RD7
D	428	SER	-	expression tag	UNP Q96RD7
D	429	GLY	-	expression tag	UNP Q96RD7
D	430	SER	-	expression tag	UNP Q96RD7
D	431	HIS	-	expression tag	UNP Q96RD7
D	432	HIS	-	expression tag	UNP Q96RD7
D	433	HIS	-	expression tag	UNP Q96RD7
D	434	HIS	-	expression tag	UNP Q96RD7
D	435	HIS	-	expression tag	UNP Q96RD7
D	436	HIS	-	expression tag	UNP Q96RD7
D	437	HIS	-	expression tag	UNP Q96RD7
D	438	HIS	-	expression tag	UNP Q96RD7
D	439	HIS	-	expression tag	UNP Q96RD7
D	440	HIS	-	expression tag	UNP Q96RD7
E	427	GLY	-	expression tag	UNP Q96RD7
E	428	SER	-	expression tag	UNP Q96RD7

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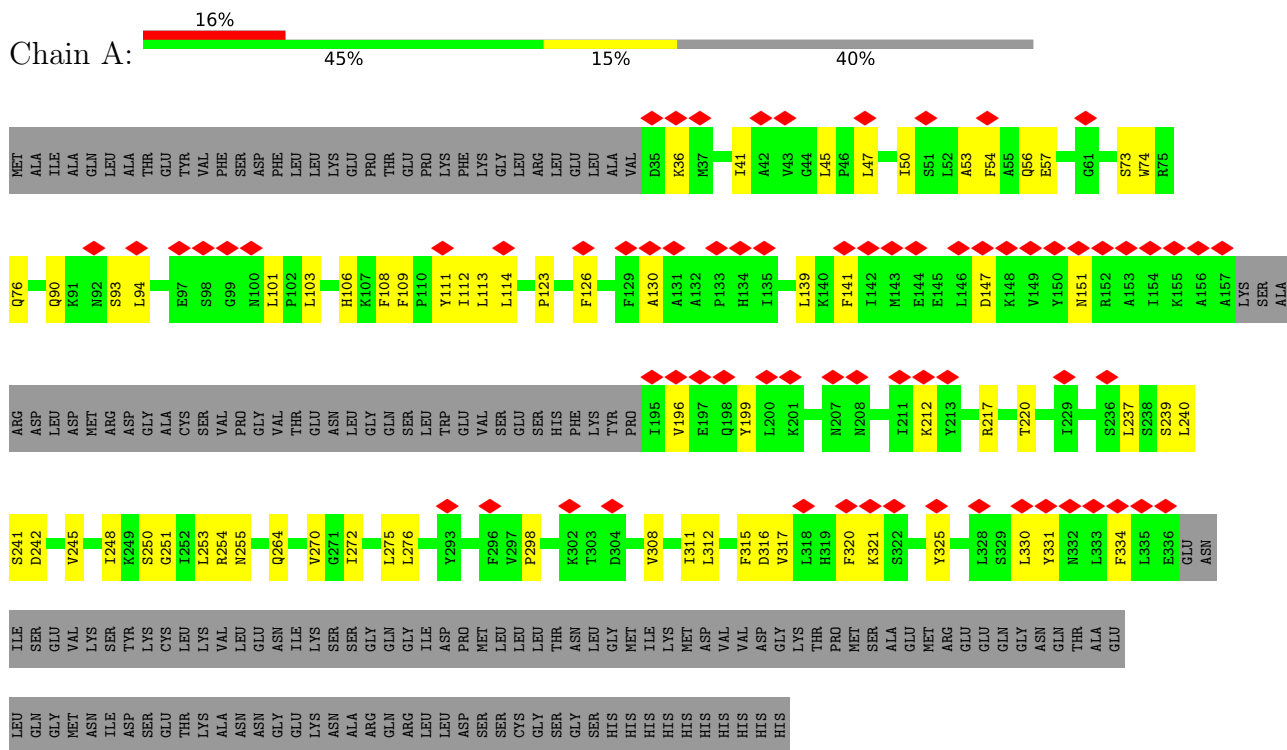
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Chain	Residue	Modelled	Actual	Comment	Reference
E	429	GLY	-	expression tag	UNP Q96RD7
E	430	SER	-	expression tag	UNP Q96RD7
E	431	HIS	-	expression tag	UNP Q96RD7
E	432	HIS	-	expression tag	UNP Q96RD7
E	433	HIS	-	expression tag	UNP Q96RD7
E	434	HIS	-	expression tag	UNP Q96RD7
E	435	HIS	-	expression tag	UNP Q96RD7
E	436	HIS	-	expression tag	UNP Q96RD7
E	437	HIS	-	expression tag	UNP Q96RD7
E	438	HIS	-	expression tag	UNP Q96RD7
E	439	HIS	-	expression tag	UNP Q96RD7
E	440	HIS	-	expression tag	UNP Q96RD7
F	427	GLY	-	expression tag	UNP Q96RD7
F	428	SER	-	expression tag	UNP Q96RD7
F	429	GLY	-	expression tag	UNP Q96RD7
F	430	SER	-	expression tag	UNP Q96RD7
F	431	HIS	-	expression tag	UNP Q96RD7
F	432	HIS	-	expression tag	UNP Q96RD7
F	433	HIS	-	expression tag	UNP Q96RD7
F	434	HIS	-	expression tag	UNP Q96RD7
F	435	HIS	-	expression tag	UNP Q96RD7
F	436	HIS	-	expression tag	UNP Q96RD7
F	437	HIS	-	expression tag	UNP Q96RD7
F	438	HIS	-	expression tag	UNP Q96RD7
F	439	HIS	-	expression tag	UNP Q96RD7
F	440	HIS	-	expression tag	UNP Q96RD7
G	427	GLY	-	expression tag	UNP Q96RD7
G	428	SER	-	expression tag	UNP Q96RD7
G	429	GLY	-	expression tag	UNP Q96RD7
G	430	SER	-	expression tag	UNP Q96RD7
G	431	HIS	-	expression tag	UNP Q96RD7
G	432	HIS	-	expression tag	UNP Q96RD7
G	433	HIS	-	expression tag	UNP Q96RD7
G	434	HIS	-	expression tag	UNP Q96RD7
G	435	HIS	-	expression tag	UNP Q96RD7
G	436	HIS	-	expression tag	UNP Q96RD7
G	437	HIS	-	expression tag	UNP Q96RD7
G	438	HIS	-	expression tag	UNP Q96RD7
G	439	HIS	-	expression tag	UNP Q96RD7
G	440	HIS	-	expression tag	UNP Q96RD7

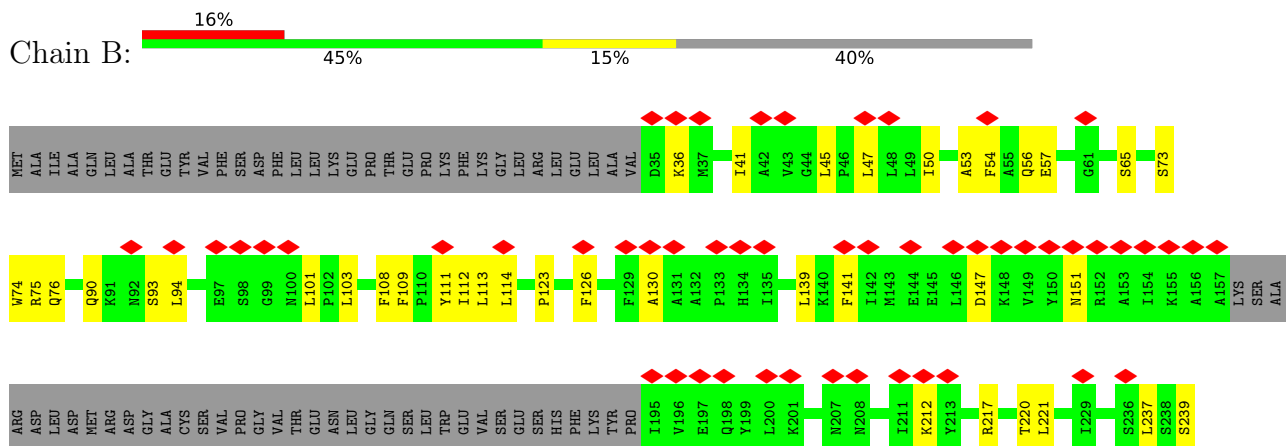
3 Residue-property plots [i](#)

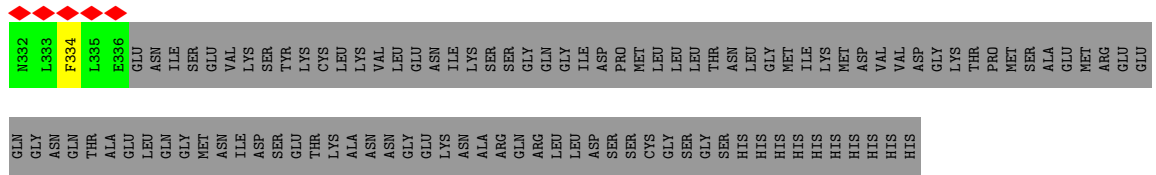
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Pannexin-1

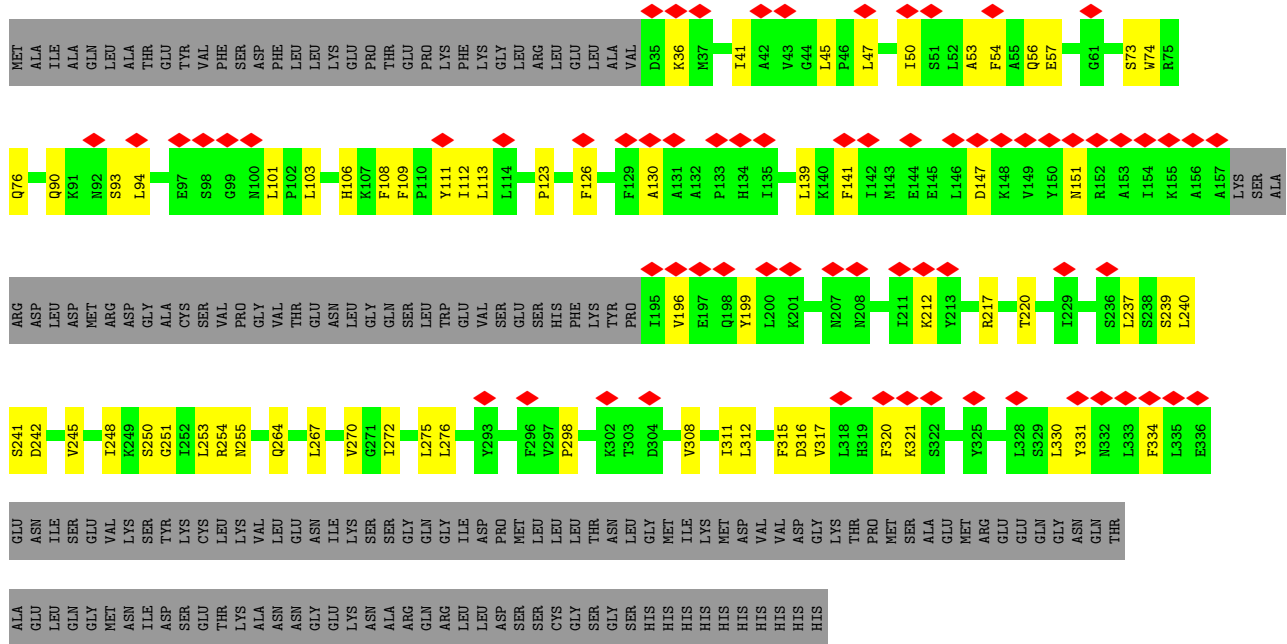


- Molecule 1: Pannexin-1

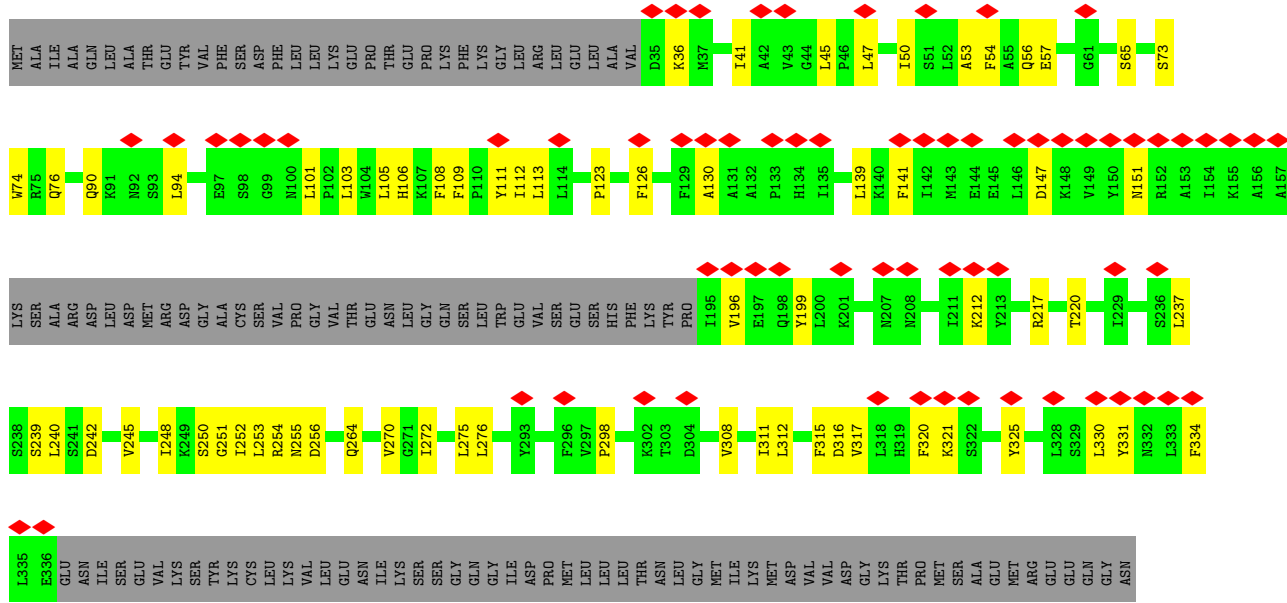




● Molecule 1: Pannexin-1



● Molecule 1: Pannexin-1



GLN	THR	ALA	ALA	GLU	GLU	GLN	GLY	GLY	MET	ASN	ILE	ASP	ASP	GLU	THR	LYS	ALA	ASN	GLY	GLU	LYS	ASN	GLU	LYS	ASN	ALA	ALA	GLN	ARG	LEU	LEU	ASP	SER	GLY	CYS	GLY	SER	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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● Molecule 1: Pannexin-1



MET	ALA	ILE	ALA	GLN	LEU	ALA	THR	GLU	TYR	VAL	PHE	SER	ASP	PHE	LEU	LEU	LYS	ASN	GLY	PRO	THR	GLU	VAL	D35	K36	I41	A42	V43	G44	L45	P46	L47	L48	L49	I50	S51	L52	A53	F54	A55	Q56	E57	G61	F67	S73
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W74	E75	Q76	Q90	K91	N92	L94	E97	S98	G99	N100	L101	L103	H106	K107	F108	F109	P110	Y111	I112	L113	L114	P123	F126	F129	A130	A131	A132	F133	H134	I135	L139	K140	F141	I142	M143	E144	E145	L146	D147	K148	V149	Y150	N151	R152	A153	I154	K155	A156	A157	LYS
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SER	ALA	ARG	ASP	LEU	ASP	MET	ARG	ASP	GLY	ALA	CYS	SER	VAL	PRO	GLY	VAL	THR	GLU	ASN	LEU	GLY	GLN	SER	LEU	TRP	GLU	VAL	VAL	GLU	SER	GLY	HIS	PHE	TYR	I195	V196	E197	Q198	Y199	L200	K201	N207	N208	I211	K212	Y213	R217	T220	I229	S236	L237	S238
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S239	L240	S241	D242	V245	I248	K249	S250	G251	L252	R254	N255	Q264	L267	V270	G271	I272	L275	L276	Y293	F296	V297	P298	K302	T303	D304	V308	I311	F315	D316	V317	L318	H319	F320	K321	S322	Y325	L328	S329	L330	Y331	N332	L333	F334	L335
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E336	GLU	ASN	ILE	SER	GLU	VAL	LYS	TYR	LYS	CYS	LEU	VAL	LEU	GLU	ASN	ILE	LYS	SER	SER	GLY	GLN	GLY	ILE	ASP	PRO	MET	LEU	LEU	LEU	THR	ASN	GLY	MET	ILE	LYS	MET	MET	ASP	VAL	VAL	ASP	GLY	LYS	THR	PRO	MET	SER	ALA	GLU	MET	ARG	GLU	GLN	GLY	ASN	GLN
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THR	ALA	GLU	LEU	GLN	GLY	MET	ASN	ILE	ASP	GLU	LYS	ASN	GLU	LYS	ASN	ARG	GLY	GLN	ARG	LEU	LEU	ASP	ASP	SER	SER	CYS	GLY	SER	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145716	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 ($e^-/\text{\AA}^2$)	57.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.334	Depositor
Minimum map value	-0.984	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.577	Depositor
Map size (Å)	270.08, 270.08, 270.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	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	0.32	0/2187	0.59	0/2975
1	B	0.32	0/2187	0.59	0/2975
1	C	0.32	0/2187	0.59	0/2975
1	D	0.32	0/2187	0.59	0/2975
1	E	0.32	0/2187	0.59	0/2975
1	F	0.32	0/2187	0.59	0/2975
1	G	0.32	0/2187	0.59	0/2975
All	All	0.32	0/15309	0.59	0/20825

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	2134	0	2201	45	0
1	B	2134	0	2201	46	0
1	C	2134	0	2201	43	0
1	D	2134	0	2201	42	0
1	E	2134	0	2201	45	0
1	F	2134	0	2201	46	0
1	G	2134	0	2201	46	0
All	All	14938	0	15407	286	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 9.

The worst 5 of 286 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:G:298:PRO:HB3	1:G:308:VAL:HG21	1.71	0.73
1:A:298:PRO:HB3	1:A:308:VAL:HG21	1.71	0.73
1:F:298:PRO:HB3	1:F:308:VAL:HG21	1.70	0.73
1:B:298:PRO:HB3	1:B:308:VAL:HG21	1.70	0.72
1:C:298:PRO:HB3	1:C:308:VAL:HG21	1.70	0.72

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	261/440 (59%)	238 (91%)	23 (9%)	0	100	100
1	B	261/440 (59%)	238 (91%)	23 (9%)	0	100	100
1	C	261/440 (59%)	238 (91%)	23 (9%)	0	100	100
1	D	261/440 (59%)	238 (91%)	23 (9%)	0	100	100
1	E	261/440 (59%)	237 (91%)	24 (9%)	0	100	100
1	F	261/440 (59%)	239 (92%)	22 (8%)	0	100	100
1	G	261/440 (59%)	238 (91%)	23 (9%)	0	100	100
All	All	1827/3080 (59%)	1666 (91%)	161 (9%)	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	241/393 (61%)	241 (100%)	0	100	100
1	B	241/393 (61%)	241 (100%)	0	100	100
1	C	241/393 (61%)	241 (100%)	0	100	100
1	D	241/393 (61%)	241 (100%)	0	100	100
1	E	241/393 (61%)	241 (100%)	0	100	100
1	F	241/393 (61%)	241 (100%)	0	100	100
1	G	241/393 (61%)	241 (100%)	0	100	100
All	All	1687/2751 (61%)	1687 (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. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	319	HIS
1	F	319	HIS
1	G	319	HIS
1	G	56	GLN
1	C	56	GLN

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.

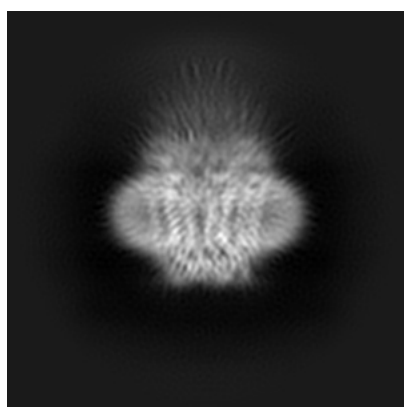
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30114. These allow visual inspection of the internal detail of the map and identification of artifacts.

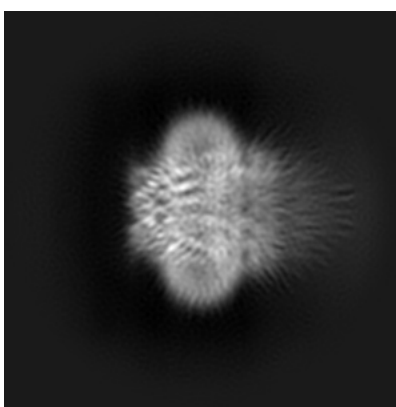
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

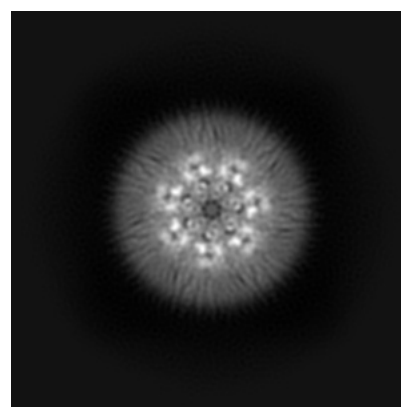
6.1.1 Primary map



X



Y

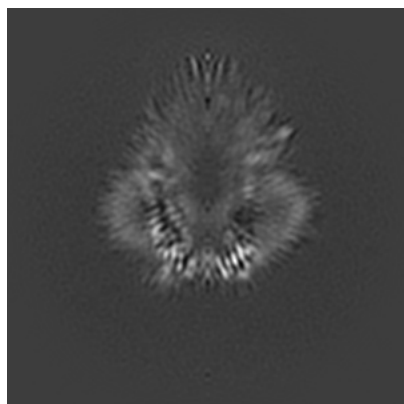


Z

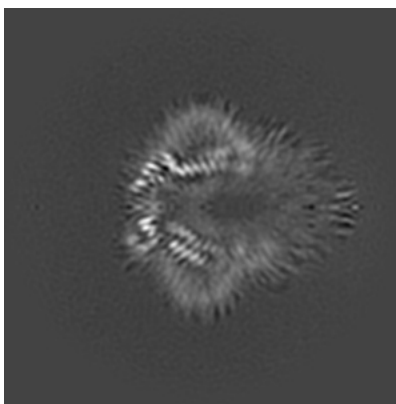
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

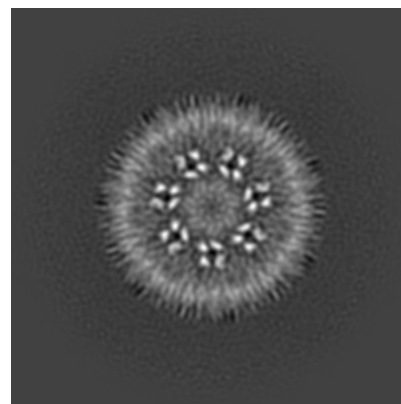
6.2.1 Primary map



X Index: 128



Y Index: 128

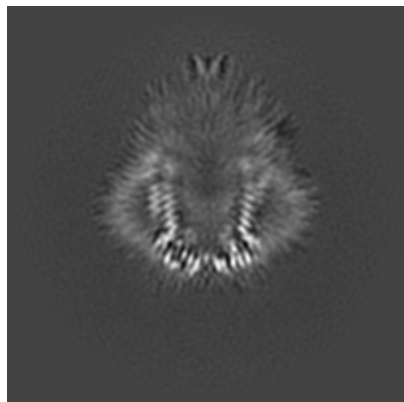


Z Index: 128

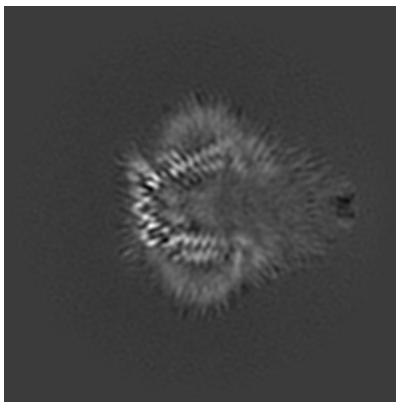
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

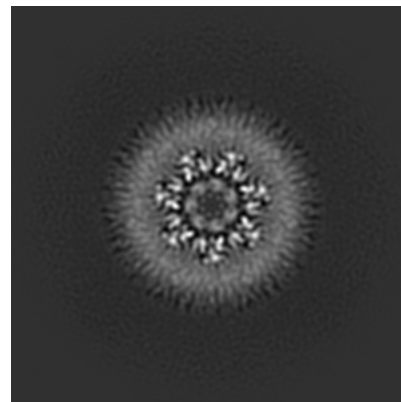
6.3.1 Primary map



X Index: 122



Y Index: 139

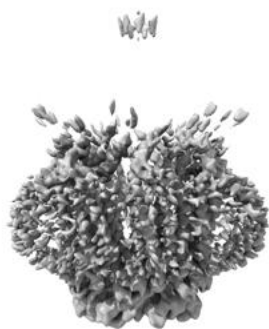


Z Index: 109

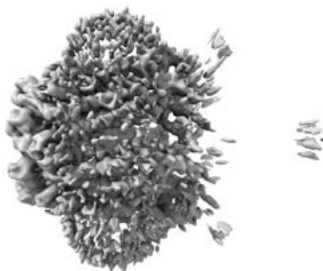
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

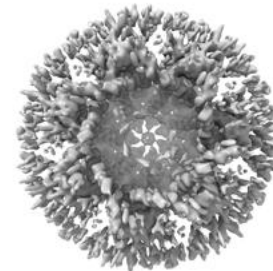
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.577. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

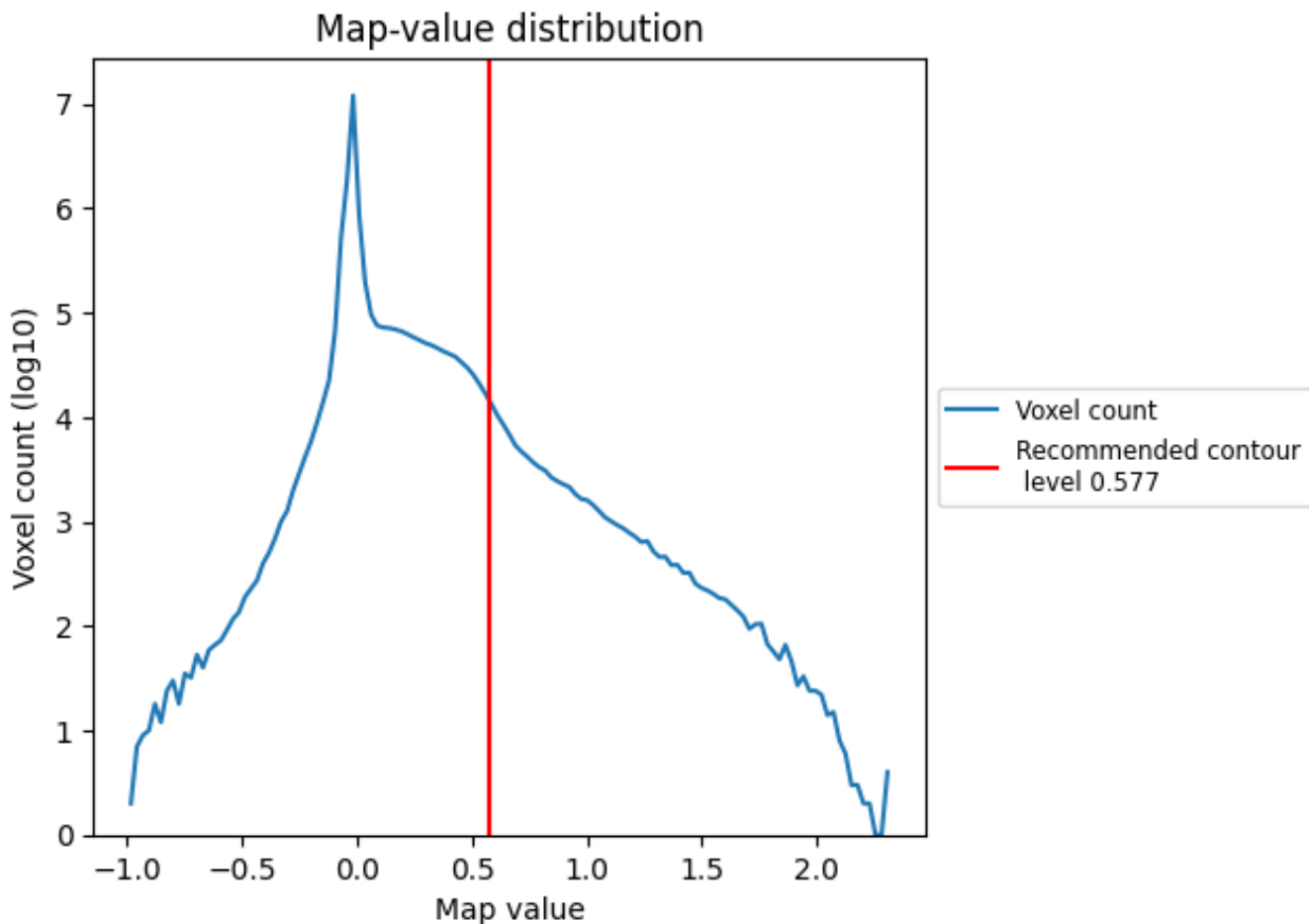
6.5 Mask visualisation

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

7 Map analysis [i](#)

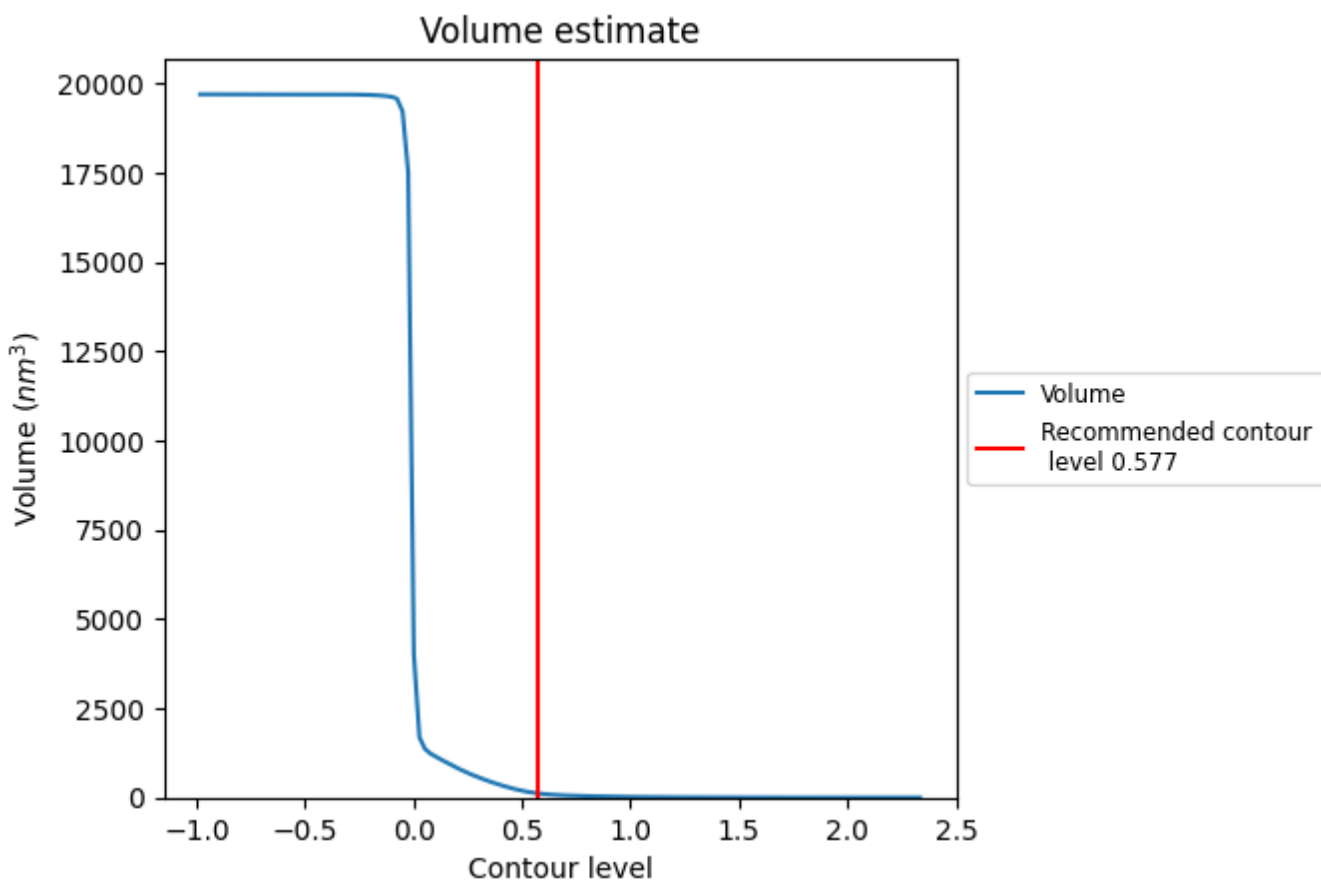
This section contains the results of statistical analysis of the map.

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.

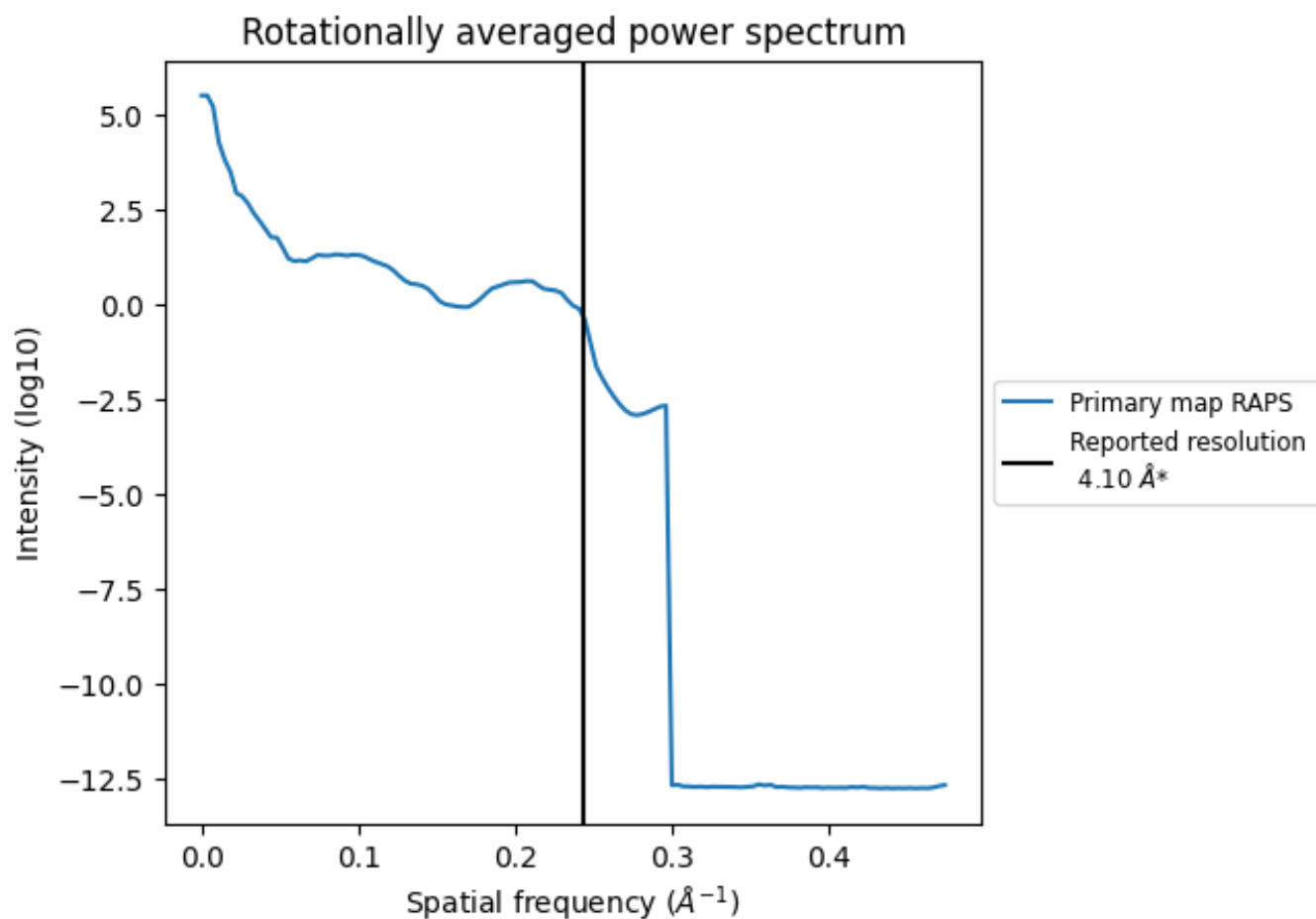
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm³; this corresponds to an approximate mass of 103 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 \AA^{-1}

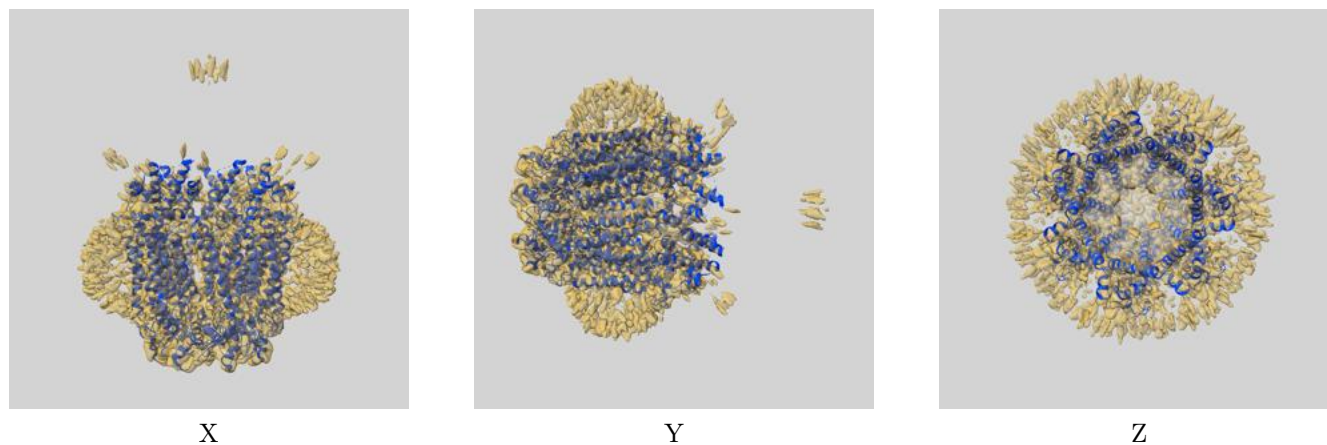
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

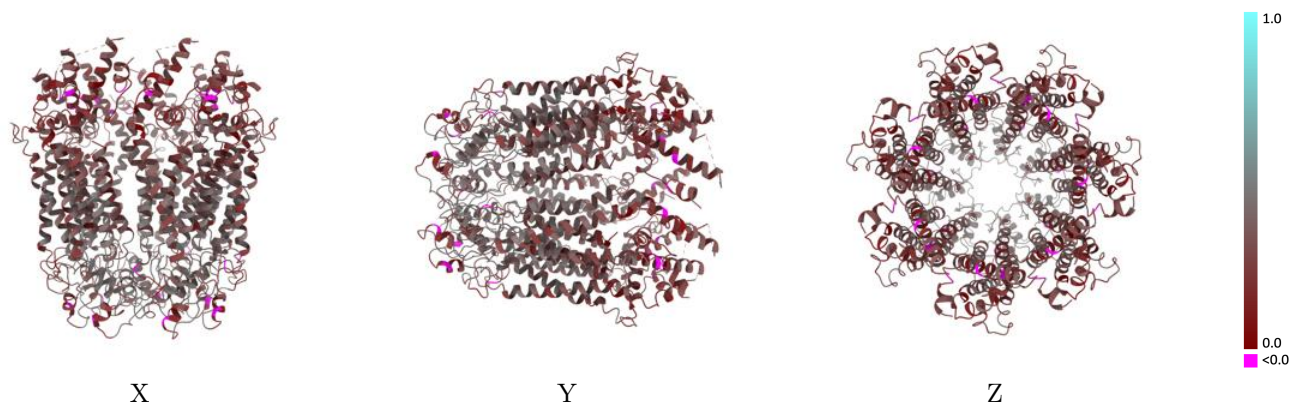
This section contains information regarding the fit between EMDB map EMD-30114 and PDB model 6M66. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



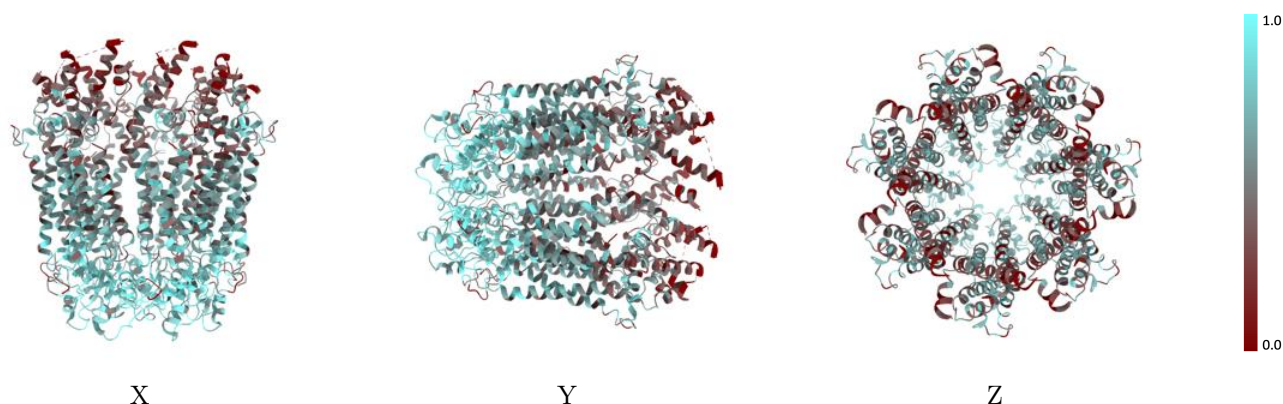
The images above show the 3D surface view of the map at the recommended contour level 0.577 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



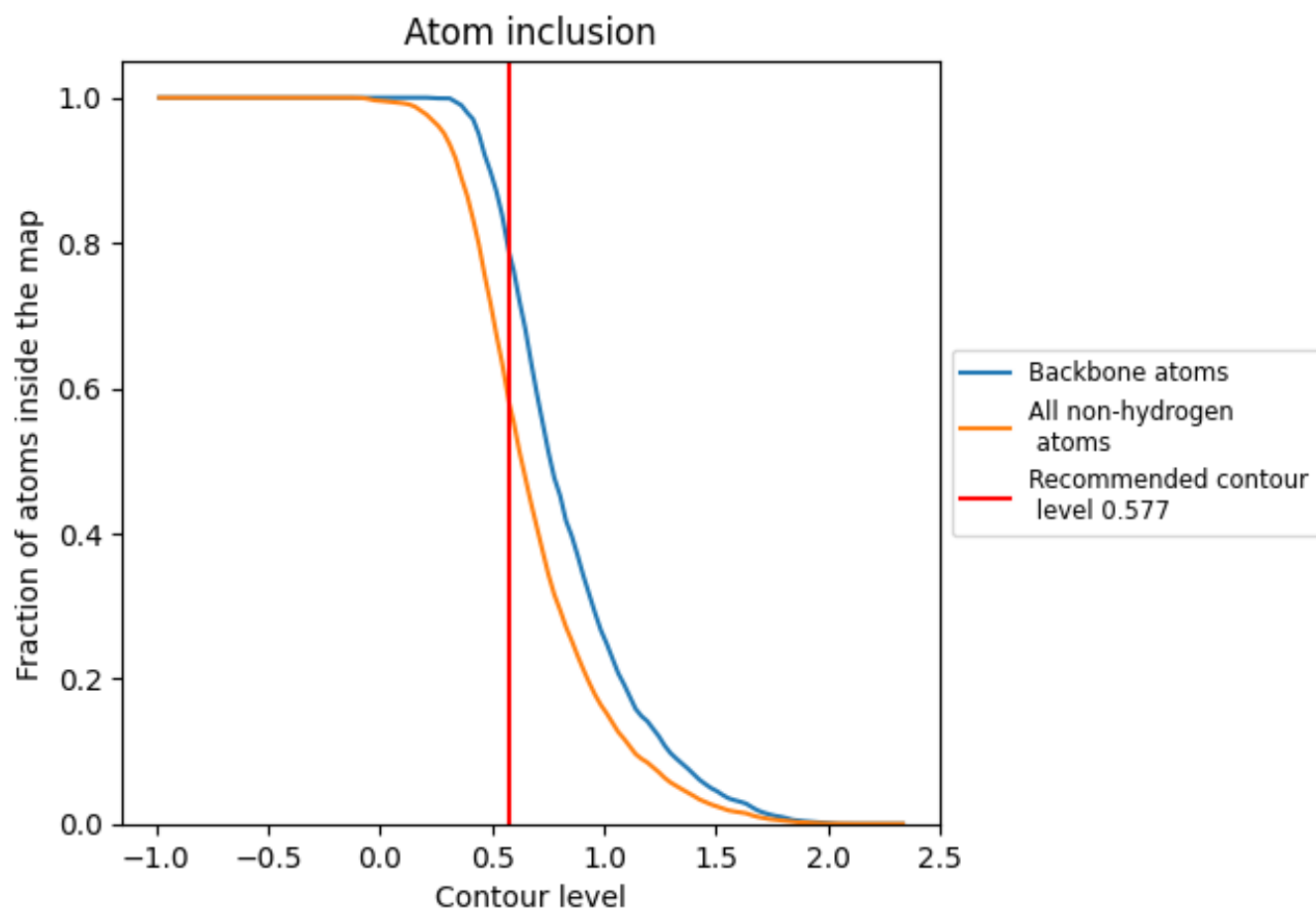
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.577).

















9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 58% 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 (0.577) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5794	 0.3150
A	 0.5789	 0.3140
B	 0.5784	 0.3150
C	 0.5798	 0.3150
D	 0.5794	 0.3140
E	 0.5803	 0.3150
F	 0.5779	 0.3160
G	 0.5813	 0.3150

