wwPDB EM Validation Summary Report (i)

Mar 11, 2024 – 10:40 AM EDT

PDB ID	:	6PUO
EMDB ID	:	EMD-20478
Title	:	Human TRPM2 in the apo state
Authors	:	Du, J.; Lu, W.; Huang, Y.
Deposited on	:	2019-07-18
Resolution	:	3.30 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 (i) 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 (i)) were used in the production of this report:

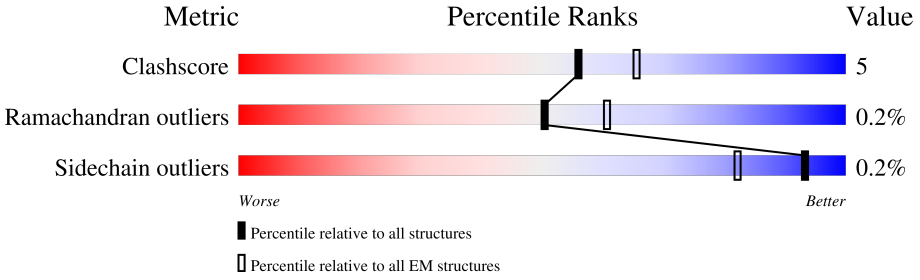
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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 <=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	1512	76% 11% 14%
1	B	1512	76% 11% 14%
1	C	1512	76% 10% 14%
1	D	1512	75% 11% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 37804 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 Transient receptor potential cation channel subfamily M member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1302	9451	6096	1670	1648	37	0	0
1	B	1302	9451	6096	1670	1648	37	0	0
1	C	1302	9451	6096	1670	1648	37	0	0
1	D	1302	9451	6096	1670	1648	37	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP O94759
A	-5	SER	-	expression tag	UNP O94759
A	-4	GLY	-	expression tag	UNP O94759
A	-3	GLY	-	expression tag	UNP O94759
A	-2	ARG	-	expression tag	UNP O94759
A	-1	ALA	-	expression tag	UNP O94759
A	0	THR	-	expression tag	UNP O94759
A	1504	PHE	-	expression tag	UNP O94759
A	1505	GLU	-	expression tag	UNP O94759
B	-6	GLY	-	expression tag	UNP O94759
B	-5	SER	-	expression tag	UNP O94759
B	-4	GLY	-	expression tag	UNP O94759
B	-3	GLY	-	expression tag	UNP O94759
B	-2	ARG	-	expression tag	UNP O94759
B	-1	ALA	-	expression tag	UNP O94759
B	0	THR	-	expression tag	UNP O94759
B	1504	PHE	-	expression tag	UNP O94759
B	1505	GLU	-	expression tag	UNP O94759
C	-6	GLY	-	expression tag	UNP O94759
C	-5	SER	-	expression tag	UNP O94759
C	-4	GLY	-	expression tag	UNP O94759

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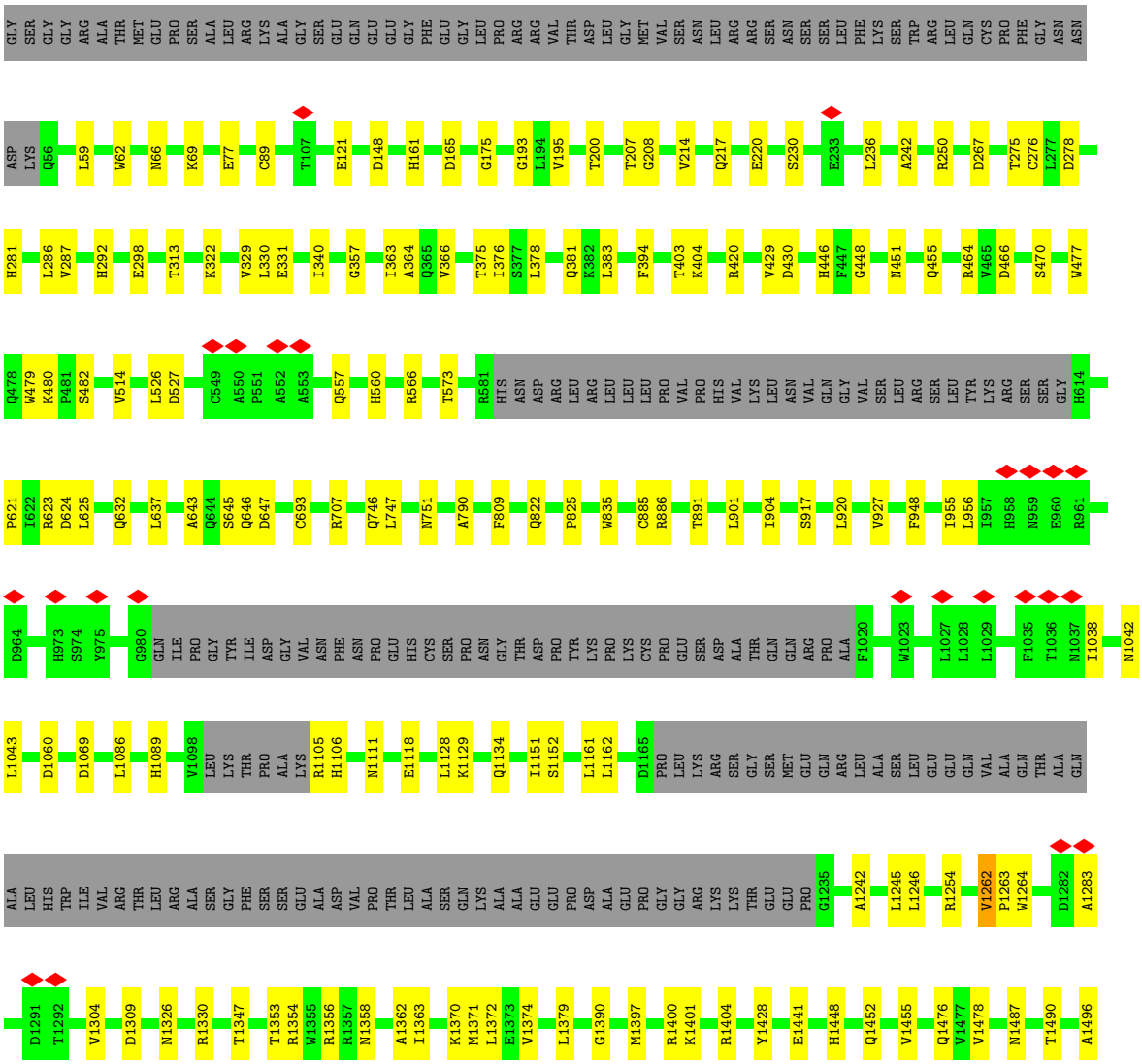
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP O94759
C	-2	ARG	-	expression tag	UNP O94759
C	-1	ALA	-	expression tag	UNP O94759
C	0	THR	-	expression tag	UNP O94759
C	1504	PHE	-	expression tag	UNP O94759
C	1505	GLU	-	expression tag	UNP O94759
D	-6	GLY	-	expression tag	UNP O94759
D	-5	SER	-	expression tag	UNP O94759
D	-4	GLY	-	expression tag	UNP O94759
D	-3	GLY	-	expression tag	UNP O94759
D	-2	ARG	-	expression tag	UNP O94759
D	-1	ALA	-	expression tag	UNP O94759
D	0	THR	-	expression tag	UNP O94759
D	1504	PHE	-	expression tag	UNP O94759
D	1505	GLU	-	expression tag	UNP O94759

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.

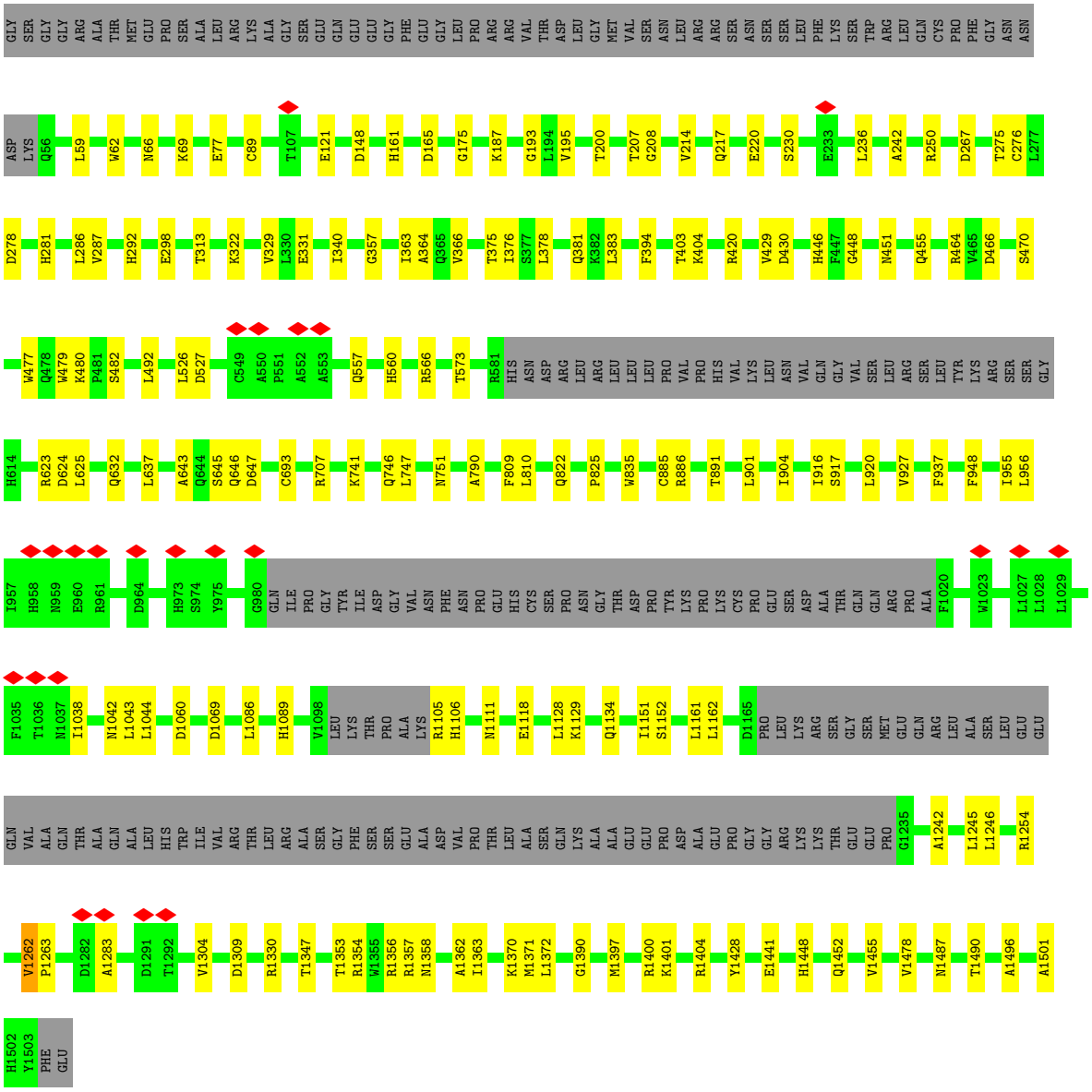
- Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain A: 76% 11% 14%



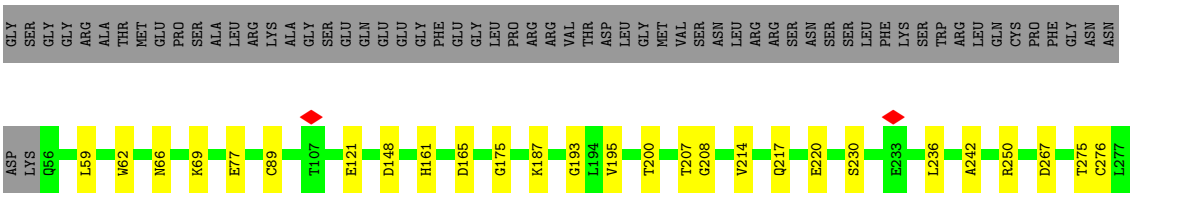
• Molecule 1: Transient receptor potential cation channel subfamily M member 2

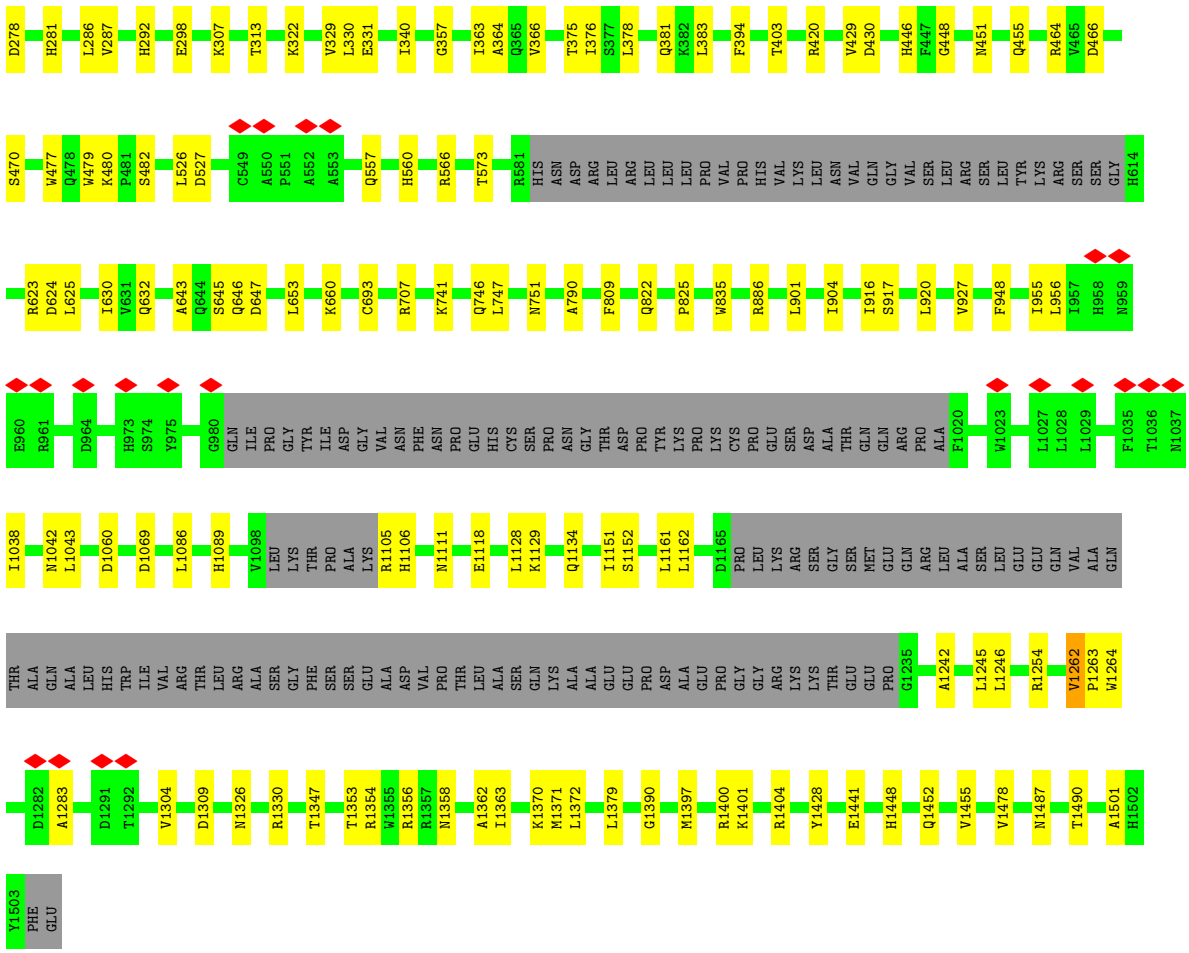
Chain B:



• Molecule 1: Transient receptor potential cation channel subfamily M member 2

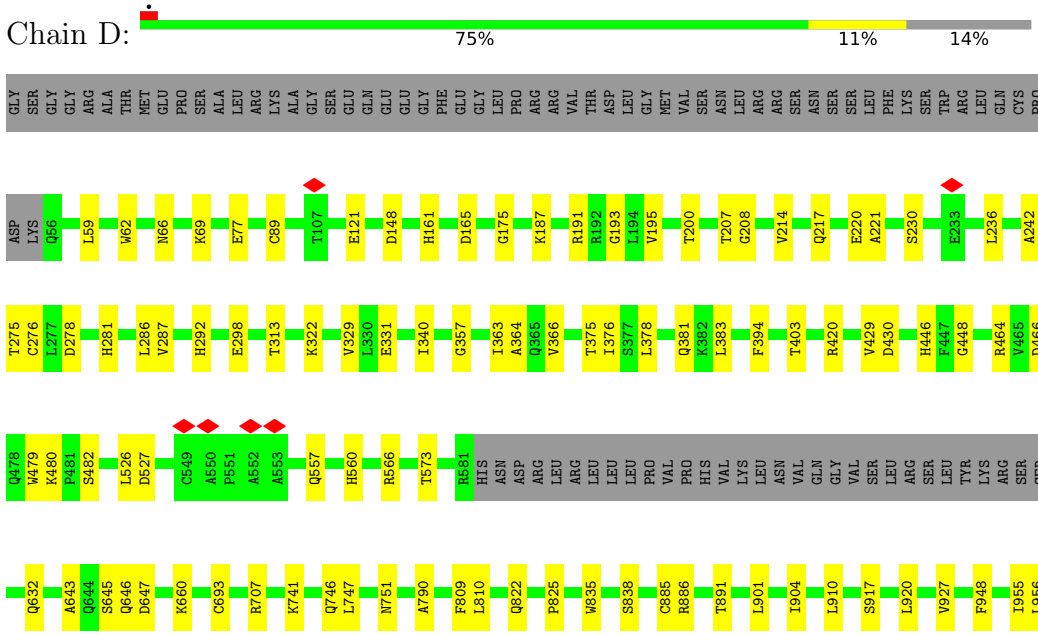
Chain C:

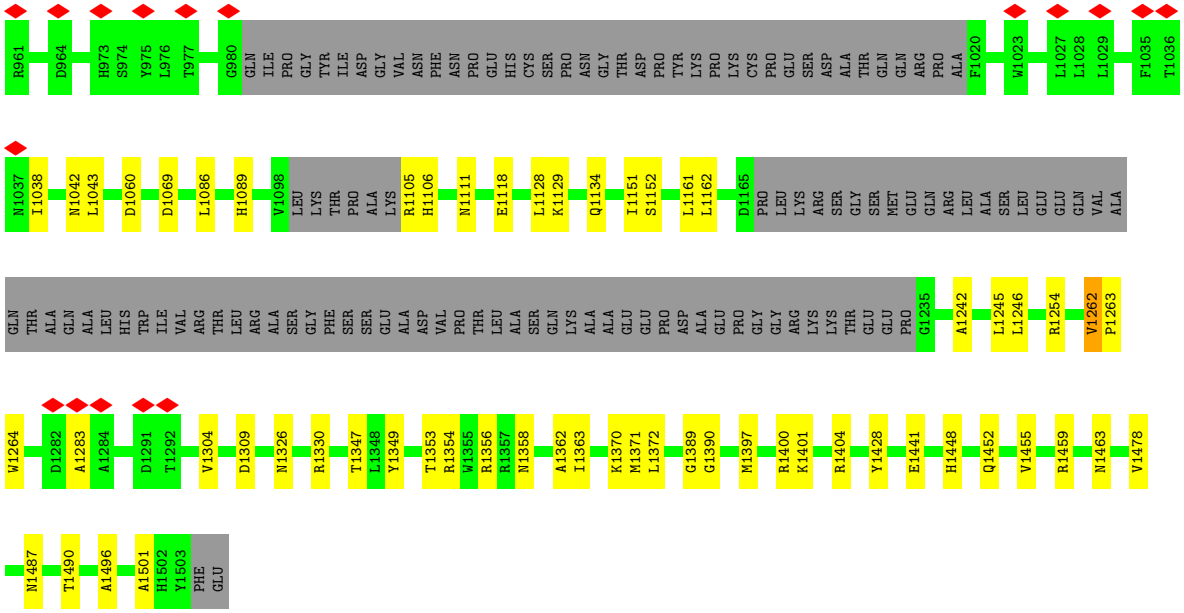




• Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain D:




R961
D964
H973
S974
Y975
L976
T977
G990
GLN ILE PRO GLY TYR ILE ASP GLY VAL ASN PHE ASN PRO GLU HIS CYS SER PRO ASN GLY THR ASP PRO TYR LYS PRO LYS CYS PRO GLU SER ASP ALA THR GLN GLN ARG PRO ALA
F1020
W1023
L1027
L1028
L1029
F1035
T1036
N1037
I1038
N1042
L1043
D1060
D1069
L1086
H1089
V1098
LEU LYS THR PRO ALA LYS
R1105
H1106
N1111
E1118
L1128
K1129
Q1134
I1151
S1152
L1161
L1162
D1165
PRO LEU LYS ARG SER GLY SER MET GLU GLN ARG LEU ALA SER LEU GLU GLU GLN VAL ALA
GLN THR ALA GLN ALA LEU HIS TRP ILE VAL ARG THR LEU ARG ALA SER GLY PHE SER SER GLU ALA ASP VAL PRO THR LEU ALA SER GLN LYS ALA ALA GLU GLU PRO ASP ALA GLU PRO GLY GLY ARG LYS LYS THR GLU GLU PRO
G1235
A1242
L1245
L1246
R1254
V1262
P1263
W1264
D1282
A1283
A1284
D1291
T1292
V1304
D1309
N1326
R1330
T1347
L1348
Y1349
T1353
R1354
W1355
R1356
R1357
N1358
A1362
I1363
K1370
M1371
L1372
G1389
G1390
M1397
R1400
K1401
R1404
Y1428
E1441
H1448
Q1452
V1455
R1459
N1463
V1478
N1487
T1490
A1496
A1501
H1502
Y1503
PHE GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161360	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 ($e^-/Å^2$)	6.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	322.2, 322.2, 322.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	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	0.40	0/9675	0.53	0/13228
1	B	0.40	0/9675	0.53	0/13228
1	C	0.40	0/9675	0.53	0/13228
1	D	0.40	0/9675	0.53	0/13228
All	All	0.40	0/38700	0.53	0/52912

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	9451	0	8720	98	0
1	B	9451	0	8720	100	0
1	C	9451	0	8720	99	0
1	D	9451	0	8720	100	0
All	All	37804	0	34880	381	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 5.

The worst 5 of 381 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:466:ASP:O	1:D:470:SER:HB3	1.85	0.77
1:C:466:ASP:O	1:C:470:SER:HB3	1.85	0.77
1:B:466:ASP:O	1:B:470:SER:HB3	1.85	0.77
1:A:466:ASP:O	1:A:470:SER:HB3	1.85	0.76
1:B:1372:LEU:O	1:B:1478:VAL:HG23	1.86	0.76

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	1292/1512 (85%)	1195 (92%)	95 (7%)	2 (0%)	47	77
1	B	1292/1512 (85%)	1195 (92%)	95 (7%)	2 (0%)	47	77
1	C	1292/1512 (85%)	1195 (92%)	95 (7%)	2 (0%)	47	77
1	D	1292/1512 (85%)	1195 (92%)	95 (7%)	2 (0%)	47	77
All	All	5168/6048 (85%)	4780 (92%)	380 (7%)	8 (0%)	50	77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1455	VAL
1	B	1455	VAL
1	C	1455	VAL
1	D	1455	VAL
1	A	1283	ALA

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	855/1323 (65%)	853 (100%)	2 (0%)	93	97
1	B	855/1323 (65%)	853 (100%)	2 (0%)	93	97
1	C	855/1323 (65%)	853 (100%)	2 (0%)	93	97
1	D	855/1323 (65%)	853 (100%)	2 (0%)	93	97
All	All	3420/5292 (65%)	3412 (100%)	8 (0%)	93	97

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1262	VAL
1	D	948	PHE
1	C	948	PHE
1	B	1262	VAL
1	C	1262	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	120	GLN
1	C	560	HIS
1	D	732	HIS
1	C	281	HIS
1	C	381	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.

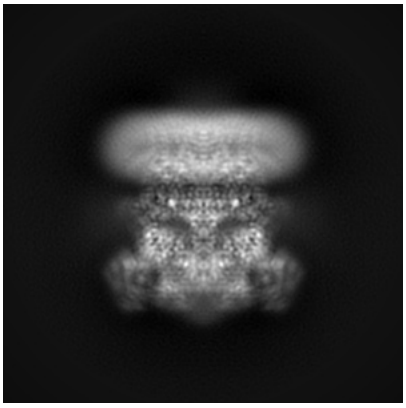
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20478. These allow visual inspection of the internal detail of the map and identification of artifacts.

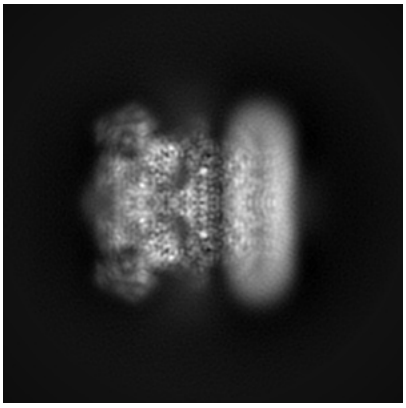
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

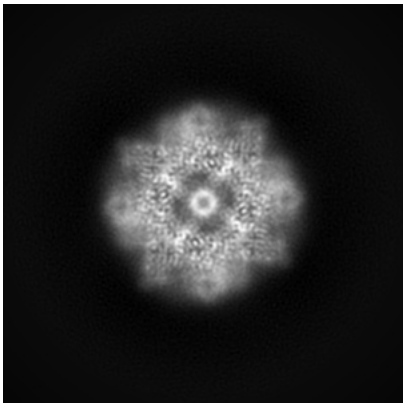
6.1.1 Primary map



X



Y

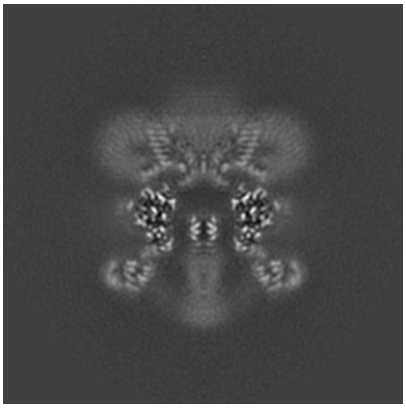


Z

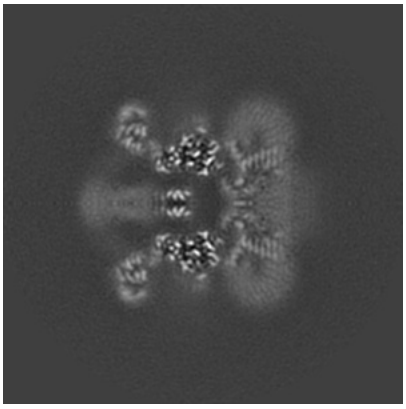
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

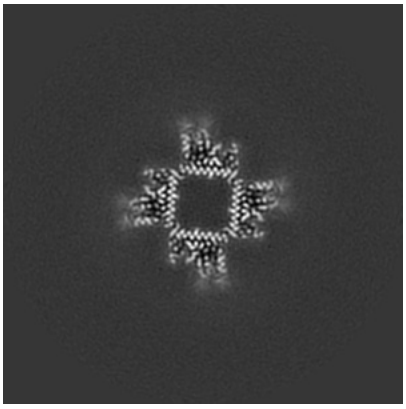
6.2.1 Primary map



X Index: 150



Y Index: 150

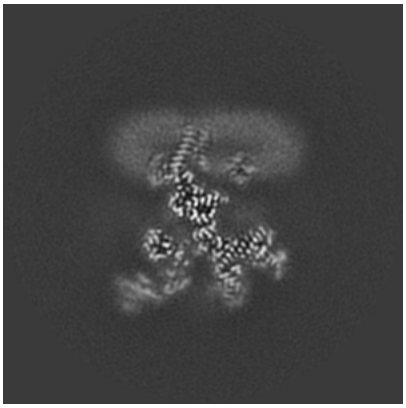


Z Index: 150

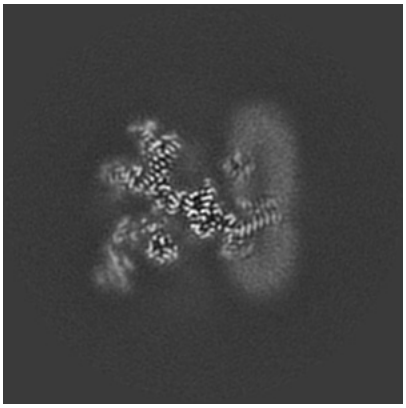
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

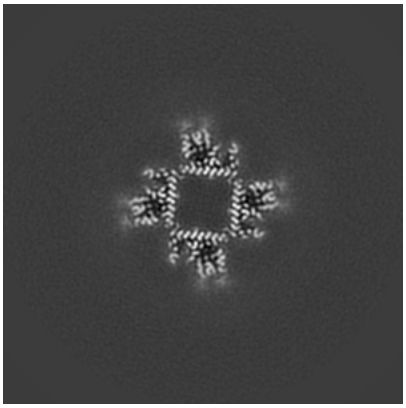
6.3.1 Primary map



X Index: 180



Y Index: 120

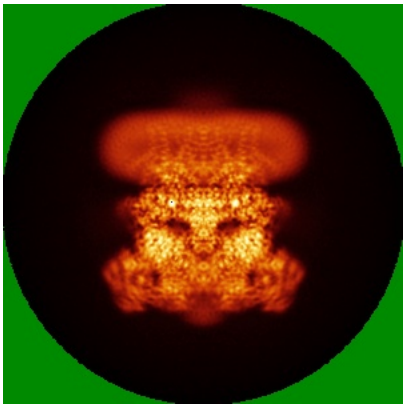


Z Index: 149

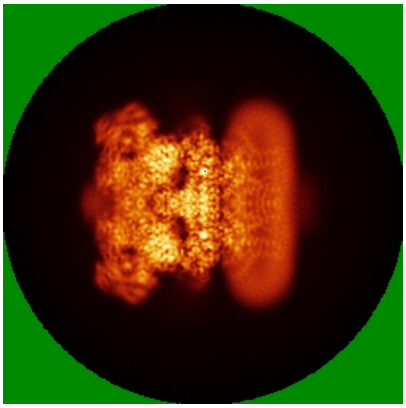
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

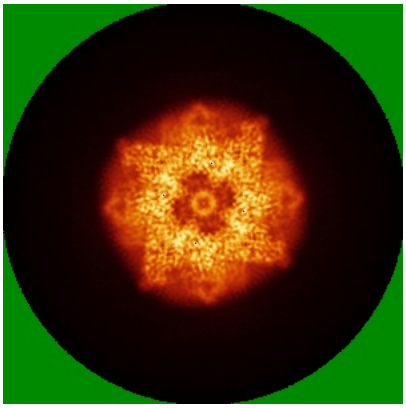
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

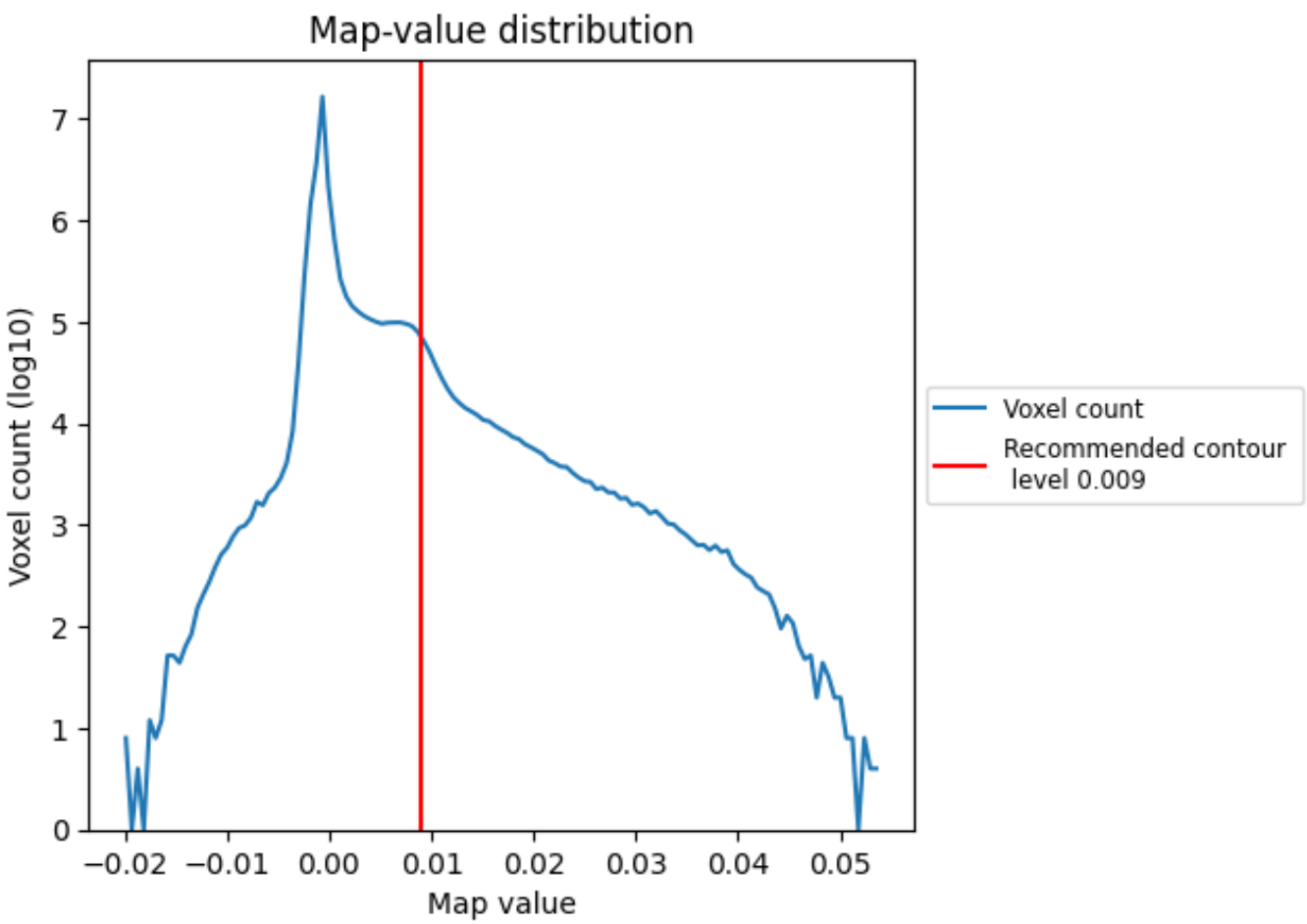
6.6 Mask visualisation (i)

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

7 Map analysis (i)

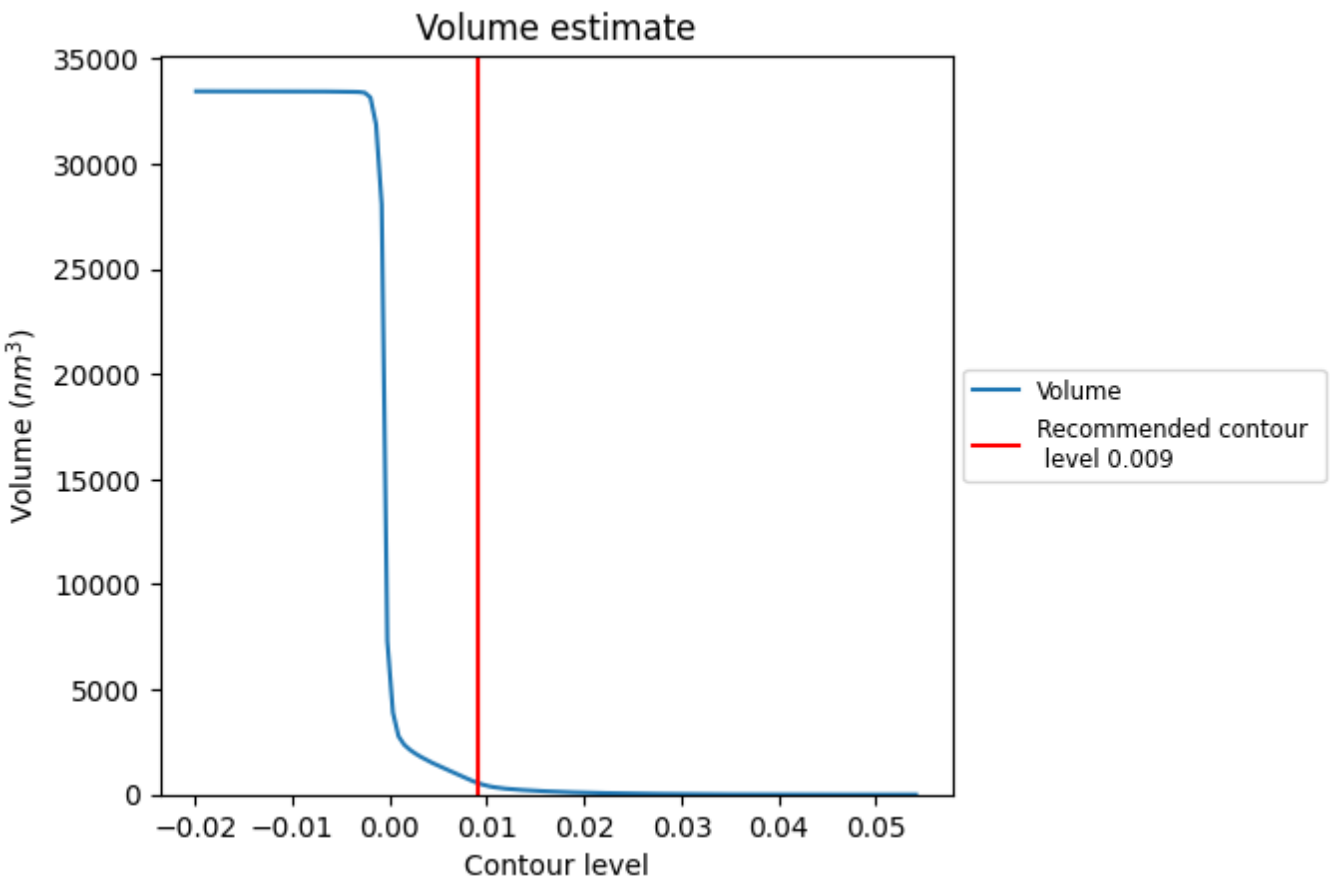
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

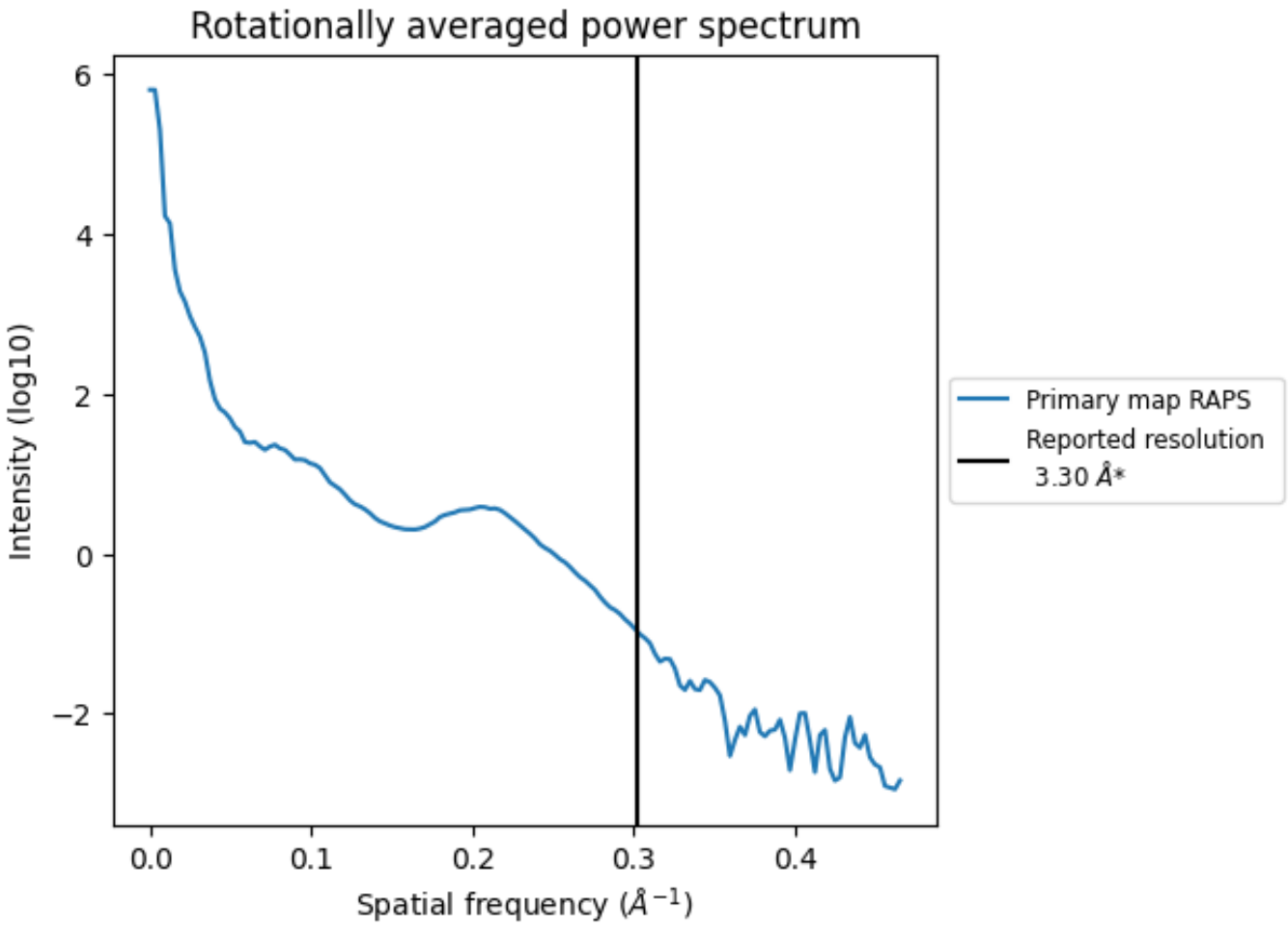
7.2 Volume estimate (i)



The volume at the recommended contour level is 561 nm^3; this corresponds to an approximate mass of 507 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 0.303 Å^{-1}

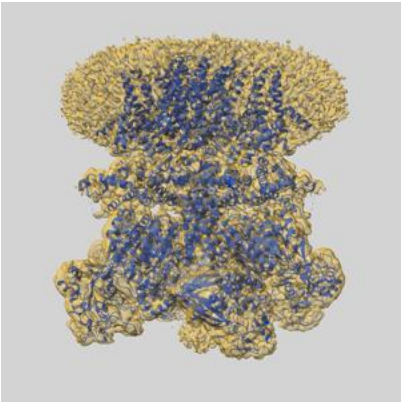
8 Fourier-Shell correlation (i)

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

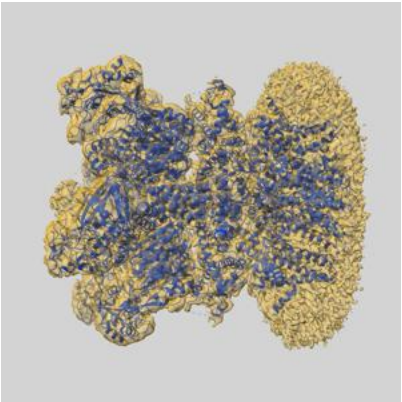
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20478 and PDB model 6PUO. Per-residue inclusion information can be found in section 3 on page 5.

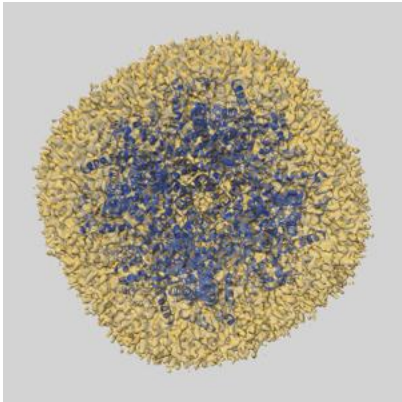
9.1 Map-model overlay (i)



X



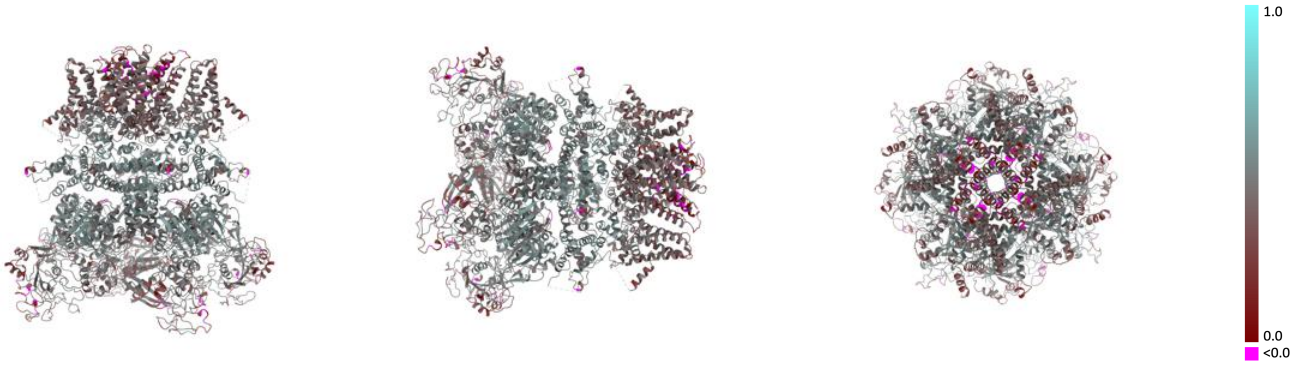
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

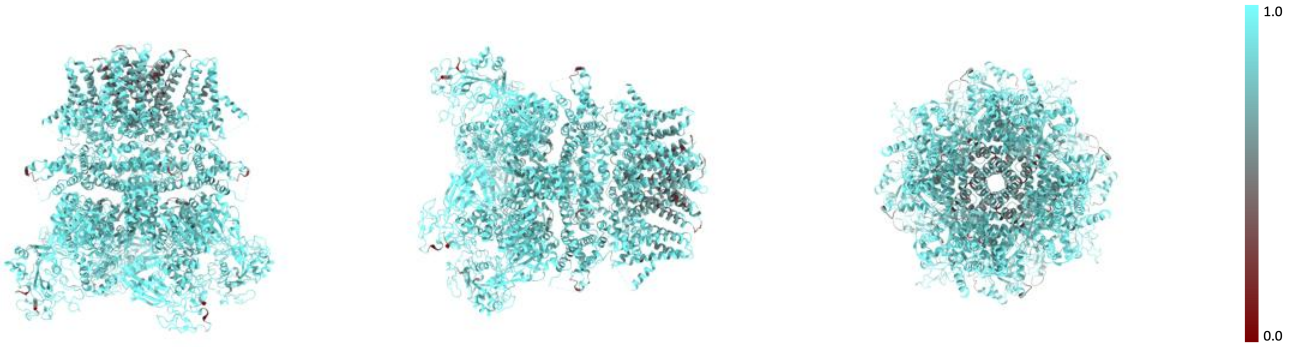
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

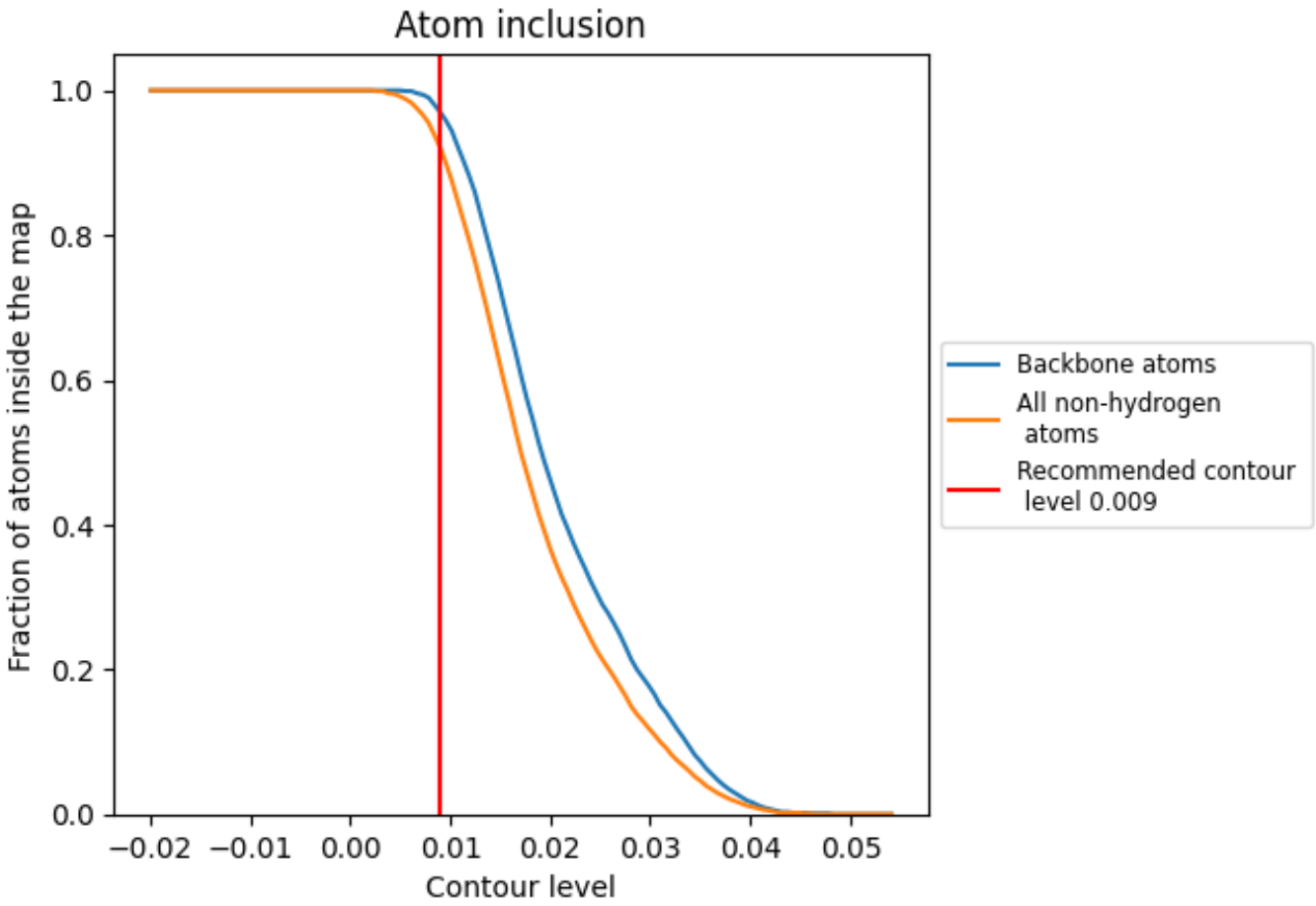
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9220	0.4570
A	0.9220	0.4570
B	0.9220	0.4570
C	0.9220	0.4570
D	0.9210	0.4570