wwPDB EM Validation Summary Report (i)

Mar 9, 2024 – 12:47 PM EST

PDB ID	:	6O1P
EMDB ID	:	EMD-0594
Title	:	Cryo-EM structure of full length TRPV5 in nanodisc
Authors	:	Dang, S.; van Goor, M.K.; Asarnow, D.; Wang, Y.; Julius, D.; Cheng, Y.; van der Wijst, J.
Deposited on	:	2019-02-21
Resolution	:	3.00 Å(reported)
Based on initial model	:	6O1N

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:

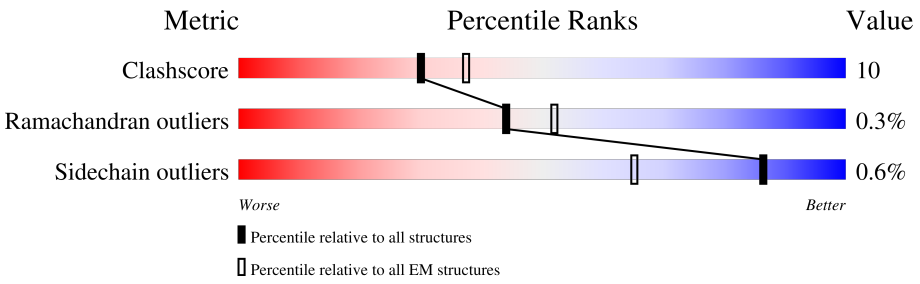
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	730	9% 70% 13% • 16%
1	B	730	11% 69% 14% • 16%
1	C	730	9% 68% 14% • 16%
1	D	730	10% 69% 14% • 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 19608 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 V member 5.

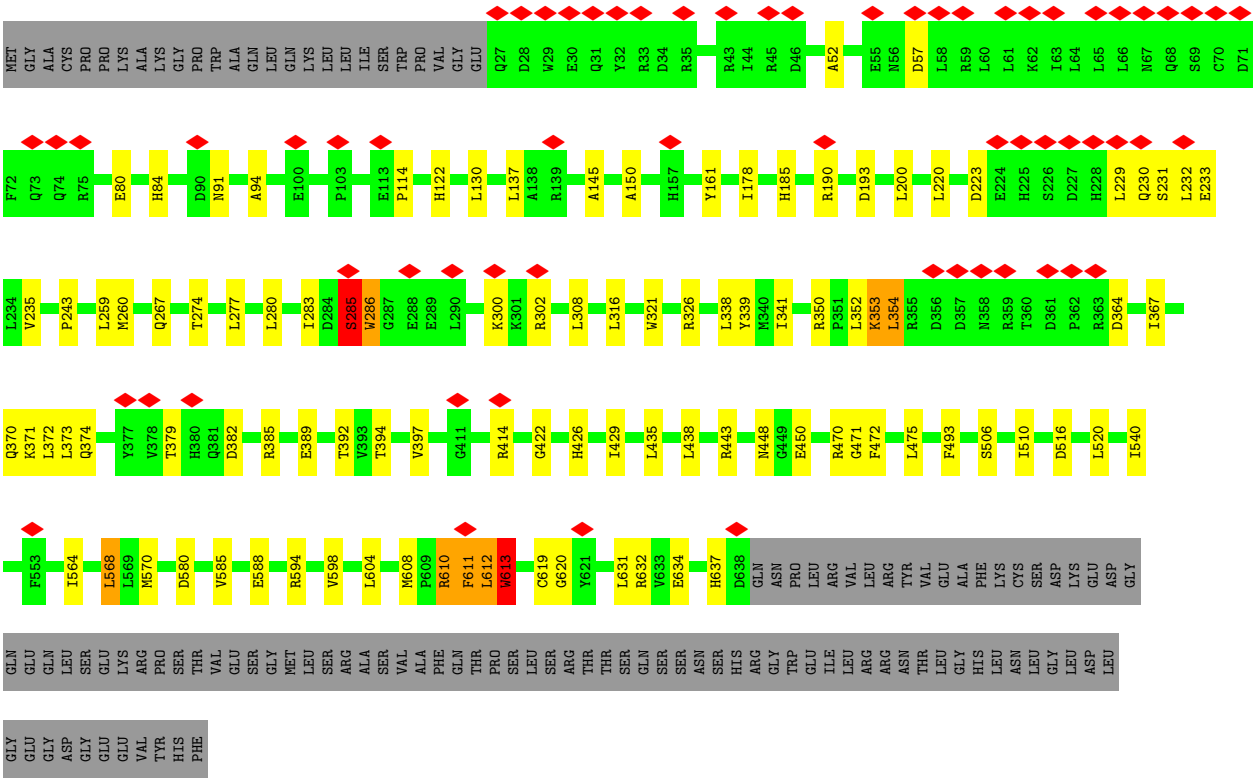
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	612	4902	3165	830	872	35	0	0
1	B	612	4902	3165	830	872	35	0	0
1	C	612	4902	3165	830	872	35	0	0
1	D	612	4902	3165	830	872	35	0	0

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.

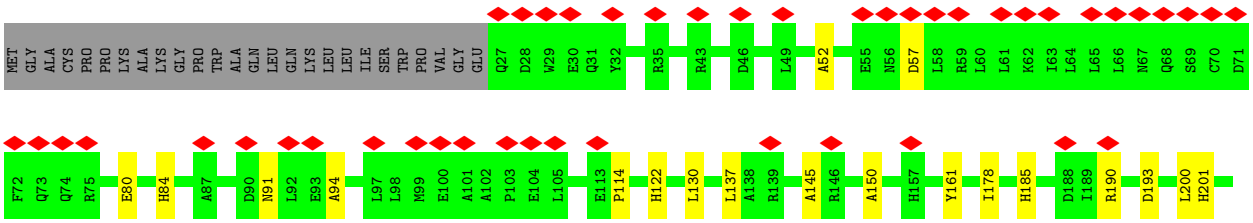
• Molecule 1: Transient receptor potential cation channel subfamily V member 5

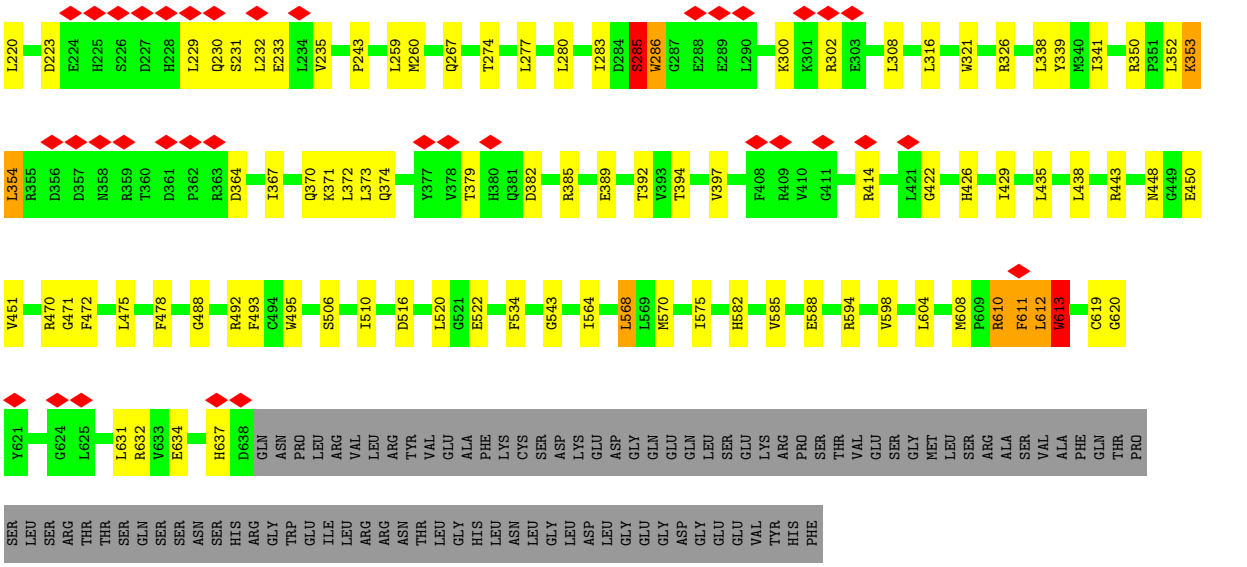
Chain A: 9% 70% 13% • 16%



• Molecule 1: Transient receptor potential cation channel subfamily V member 5

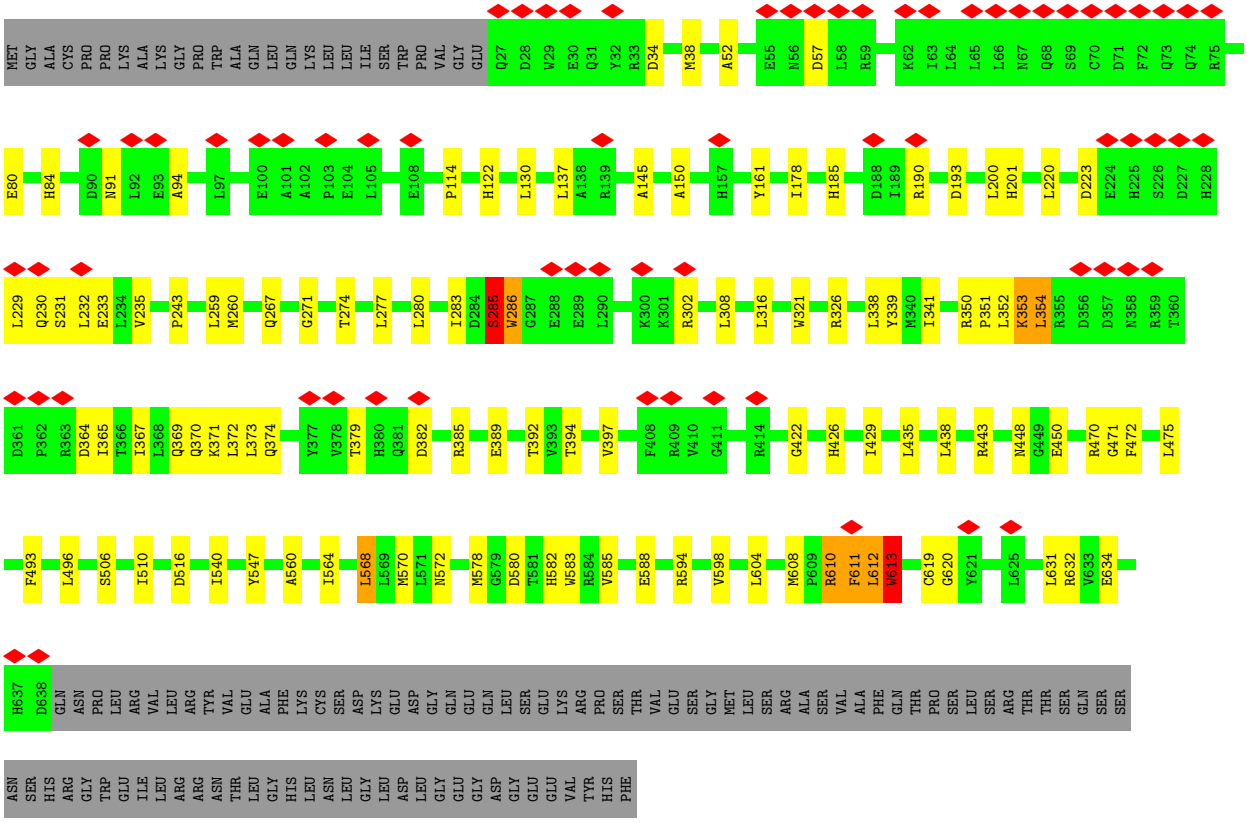
Chain B: 11% 69% 14% • 16%





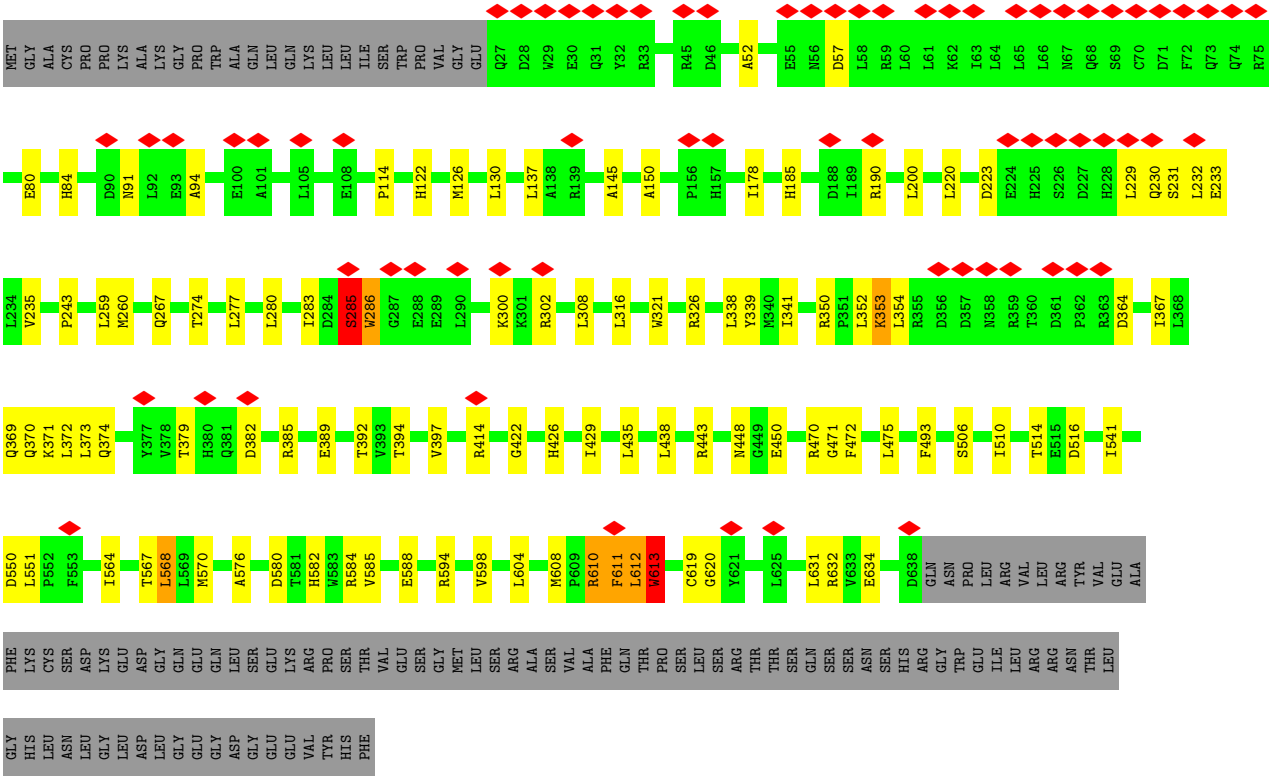
• Molecule 1: Transient receptor potential cation channel subfamily V member 5

Chain C:



• Molecule 1: Transient receptor potential cation channel subfamily V member 5

Chain D:


MET GLY ALA CYS PRO PRO LYS ALA LYS GLY PRO TRP ALA GLN LEU GLN LYS LEU LEU ILE SER TRP PRO VAL GLY GLU
Q27 D28 W29 E30 Q31 Y32 R33
R45 D46
A52
E55 N56 D57 L58 R59 L60 L61 K62 I63 L64 L65 L66 N67 Q68 S69 C70 D71 F72 Q73 Q74 R75
E80 H84 D90 N91 L92 E93 A94 E100 A101 L105 E108 P114 H122 M126 L130 L137 A138 R139 A145 A150 P156 H157 I178 H185 D188 I189 R190 L200 L220 D223 E224 H225 S226 D227 H228 L229 Q230 S231 L232 E233
L234 V235 P243 L259 M260 Q267 T274 L277 L280 I283 D284 S285 W286 G287 E288 E289 L290 K300 K301 R302 L308 L316 W321 R326 L338 Y339 M340 I341 R350 P351 L352 K353 L354 R355 D356 D357 N358 R359 T360 D361 P362 R363 D364 I367 L368
Q369 Q370 K371 L372 L373 Q374 Y377 V378 T379 H380 Q381 D382 R385 E389 T392 V393 T394 V397 R414 G422 H426 I429 L435 L438 R443 N448 G449 E450 R470 G471 F472 L475 F493 S506 I510 T514 E515 D516 I541
D550 L551 P552 F553 I564 T567 L568 L569 M570 A576 D580 T581 H582 W583 R584 V585 E588 R594 V598 L604 M608 P609 R610 F611 L612 W613 C619 G620 Y621 L625 L631 R632 V633 E634 D638 GLN ASN PRO LEU ARG VAL LEU ARG TYR VAL GLU ALA
PHE LYS CYS SER ASP LYS GLU ASP GLY GLN GLU GLN LEU SER GLU LYS ARG PRO SER THR VAL GLU SER GLY MET LEU SER ARG ALA SER VAL ALA PHE GLN THR PRO SER LEU SER ARG THR THR SER GLN SER SER ASN SER HIS ARG GLY TRP GLU ILE LEU ARG ARG ASN THR LEU
GLY HIS LEU ASN LEU GLY LEU ASP LEU GLY GLU GLY ASP GLY GLU GLU VAL TYR HIS PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	87603	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 ($e^-/Å^2$)	64	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	4.176	Depositor
Minimum map value	-2.492	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	271.104, 271.104, 271.104	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	0.57	3/5016 (0.1%)	0.77	10/6812 (0.1%)
1	B	0.57	3/5016 (0.1%)	0.77	10/6812 (0.1%)
1	C	0.57	3/5016 (0.1%)	0.77	10/6812 (0.1%)
1	D	0.57	3/5016 (0.1%)	0.77	10/6812 (0.1%)
All	All	0.57	12/20064 (0.1%)	0.77	40/27248 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	286	TRP	CB-CG	-8.08	1.35	1.50
1	A	286	TRP	CB-CG	-8.07	1.35	1.50
1	D	286	TRP	CB-CG	-8.06	1.35	1.50
1	B	286	TRP	CB-CG	-8.04	1.35	1.50
1	C	286	TRP	CE3-CZ3	-7.58	1.25	1.38

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	613	TRP	N-CA-CB	-14.12	85.18	110.60
1	D	613	TRP	N-CA-CB	-14.12	85.19	110.60
1	A	613	TRP	N-CA-CB	-14.11	85.20	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	613	TRP	N-CA-CB	-14.11	85.21	110.60
1	D	286	TRP	CA-CB-CG	-11.52	91.81	113.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	SER	Mainchain
1	A	471	GLY	Peptide
1	B	285	SER	Mainchain
1	B	471	GLY	Peptide
1	C	285	SER	Mainchain

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	4902	0	4925	100	0
1	B	4902	0	4925	110	0
1	C	4902	0	4925	113	0
1	D	4902	0	4925	103	0
All	All	19608	0	19700	392	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 10.

The worst 5 of 392 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:285:SER:O	1:D:286:TRP:HD1	1.08	1.28
1:A:285:SER:O	1:A:286:TRP:HD1	1.08	1.27
1:B:285:SER:O	1:B:286:TRP:HD1	1.08	1.27
1:C:285:SER:O	1:C:286:TRP:HD1	1.08	1.26
1:D:285:SER:O	1:D:286:TRP:CD1	1.90	1.25

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	610/730 (84%)	566 (93%)	42 (7%)	2 (0%)	41	76
1	B	610/730 (84%)	566 (93%)	42 (7%)	2 (0%)	41	76
1	C	610/730 (84%)	566 (93%)	42 (7%)	2 (0%)	41	76
1	D	610/730 (84%)	566 (93%)	42 (7%)	2 (0%)	41	76
All	All	2440/2920 (84%)	2264 (93%)	168 (7%)	8 (0%)	44	76

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	LYS
1	B	353	LYS
1	C	353	LYS
1	D	353	LYS
1	A	364	ASP

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	530/631 (84%)	527 (99%)	3 (1%)	86	95
1	B	530/631 (84%)	527 (99%)	3 (1%)	86	95
1	C	530/631 (84%)	527 (99%)	3 (1%)	86	95
1	D	530/631 (84%)	527 (99%)	3 (1%)	86	95
All	All	2120/2524 (84%)	2108 (99%)	12 (1%)	86	95

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	610	ARG
1	C	613	TRP
1	D	613	TRP
1	D	594	ARG
1	B	594	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	51	GLN
1	C	238	HIS
1	D	446	ASN
1	C	228	HIS
1	C	446	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.

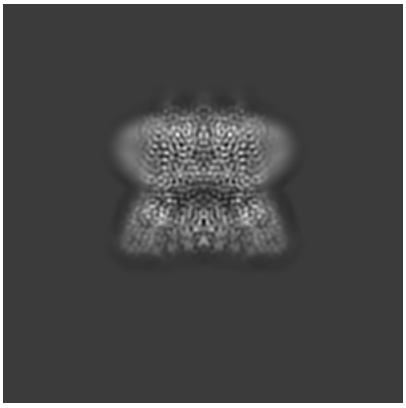
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0594. These allow visual inspection of the internal detail of the map and identification of artifacts.

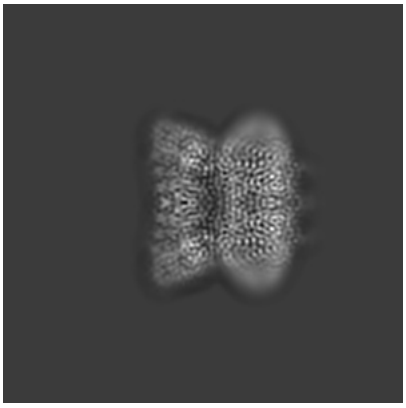
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

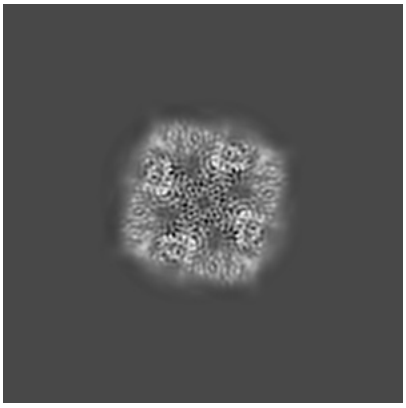
6.1.1 Primary map



X



Y



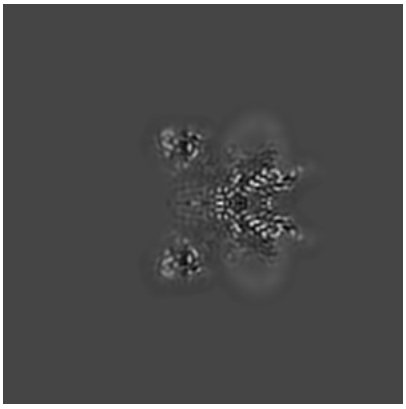
Z

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

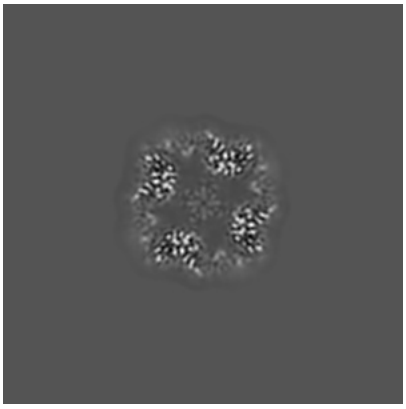
6.2 Central slices (i)

6.2.1 Primary map

X Index: 128



Y Index: 128

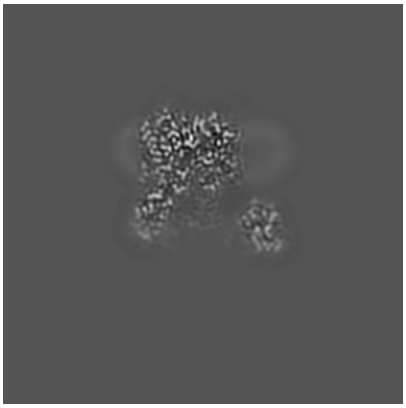


Z Index: 128

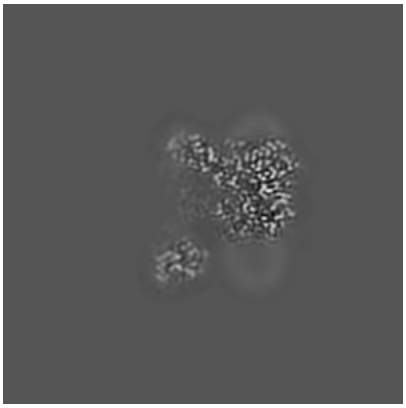
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

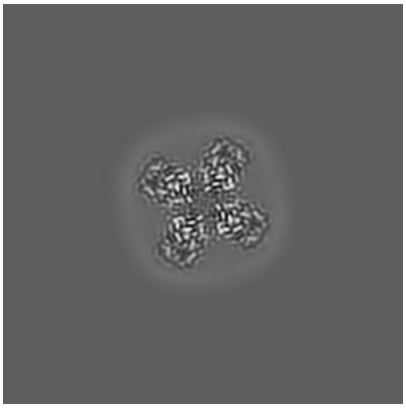
6.3.1 Primary map



X Index: 118



Y Index: 118

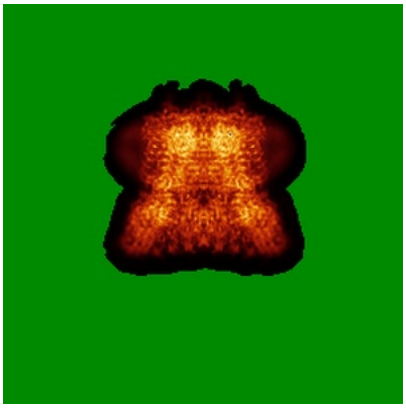


Z Index: 172

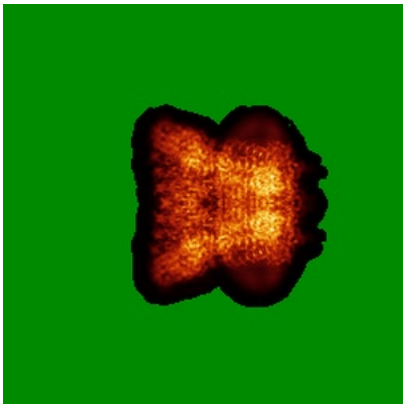
The images above show the largest variance slices of the map in three orthogonal directions.

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

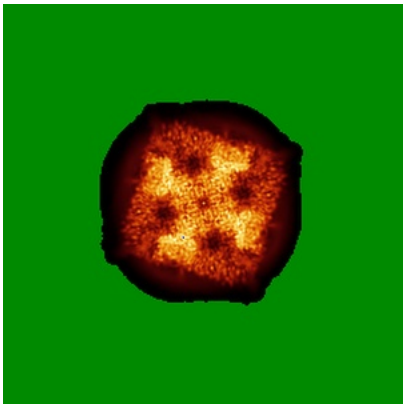
6.4.1 Primary map



X



Y

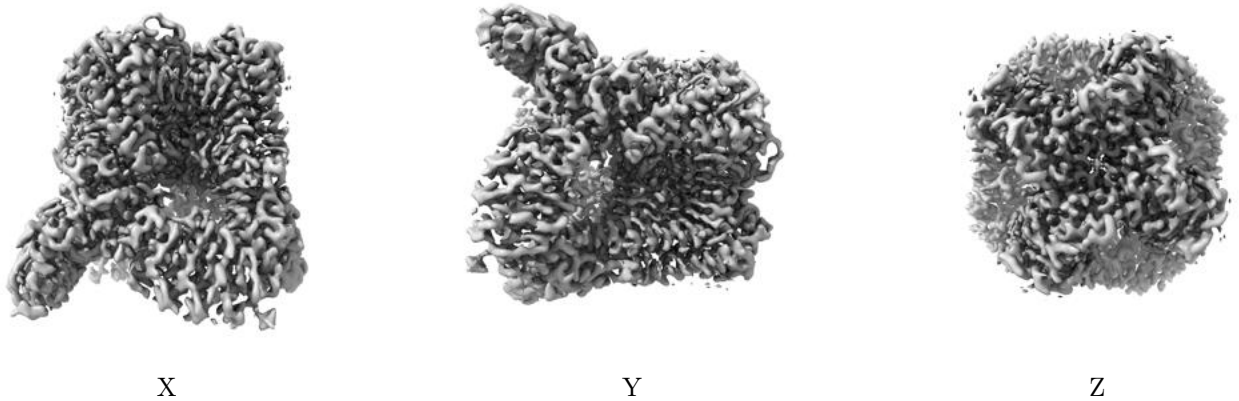


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

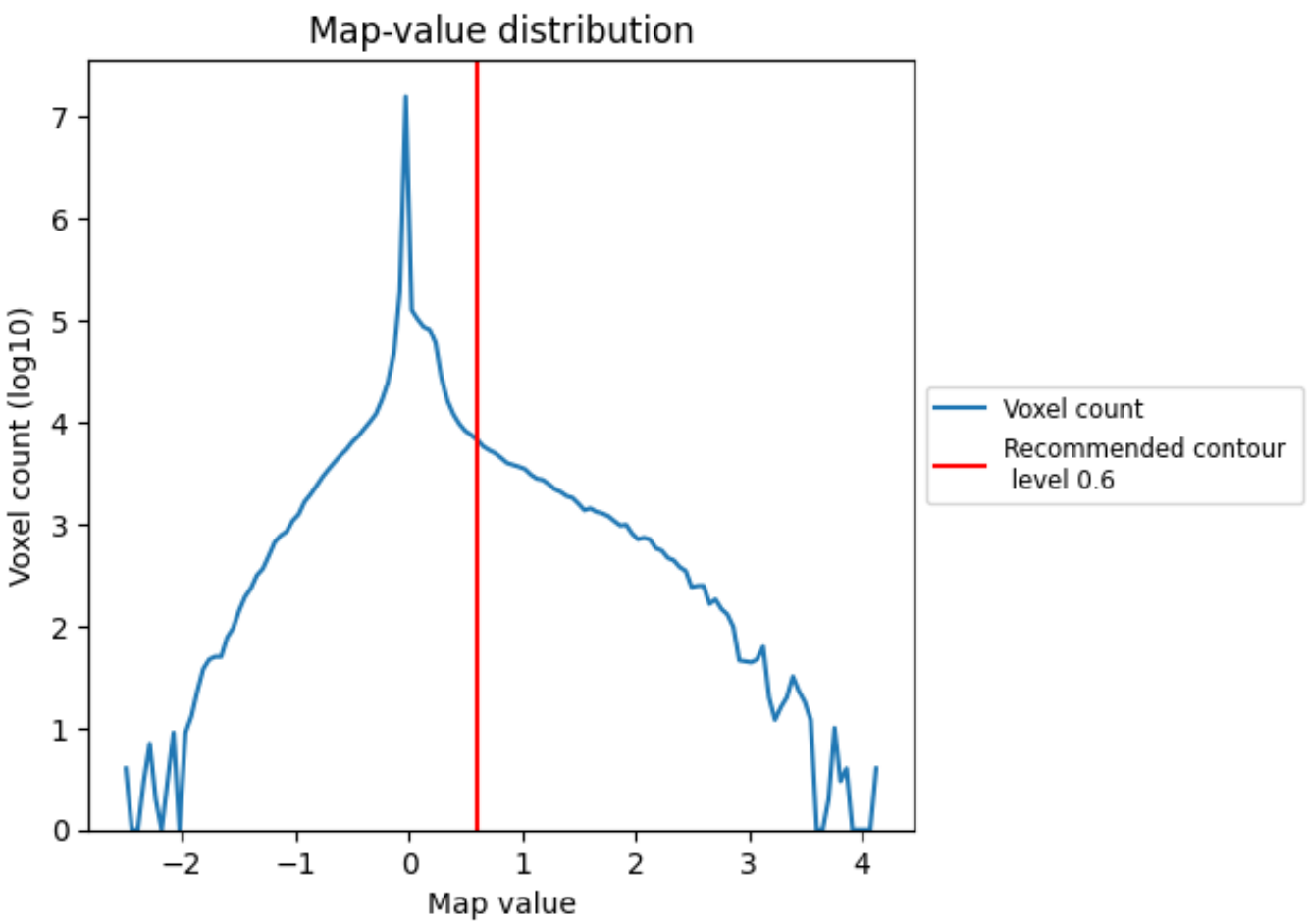
6.6 Mask visualisation (i)

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

7 Map analysis (i)

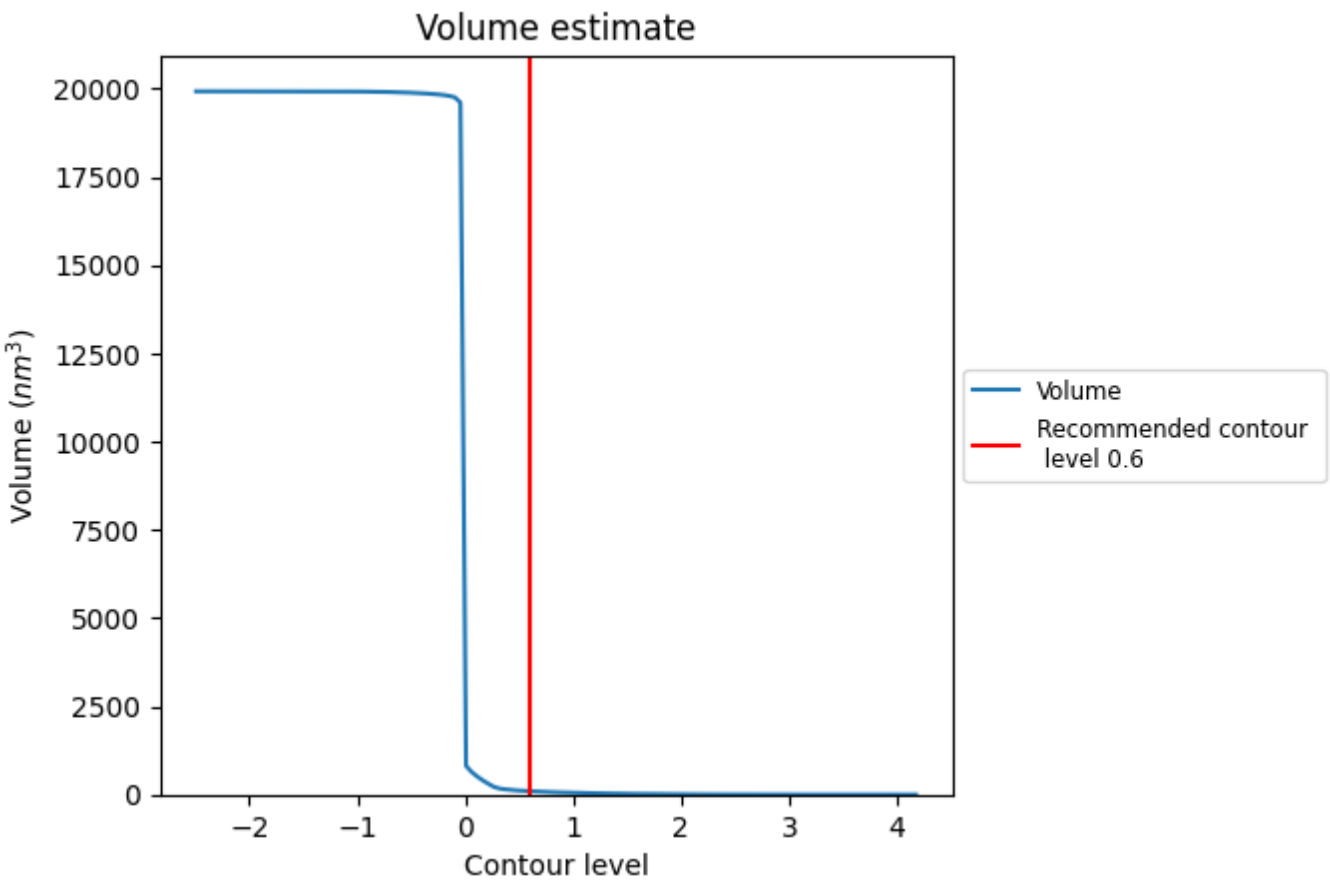
This section contains the results of statistical analysis of the map.

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.

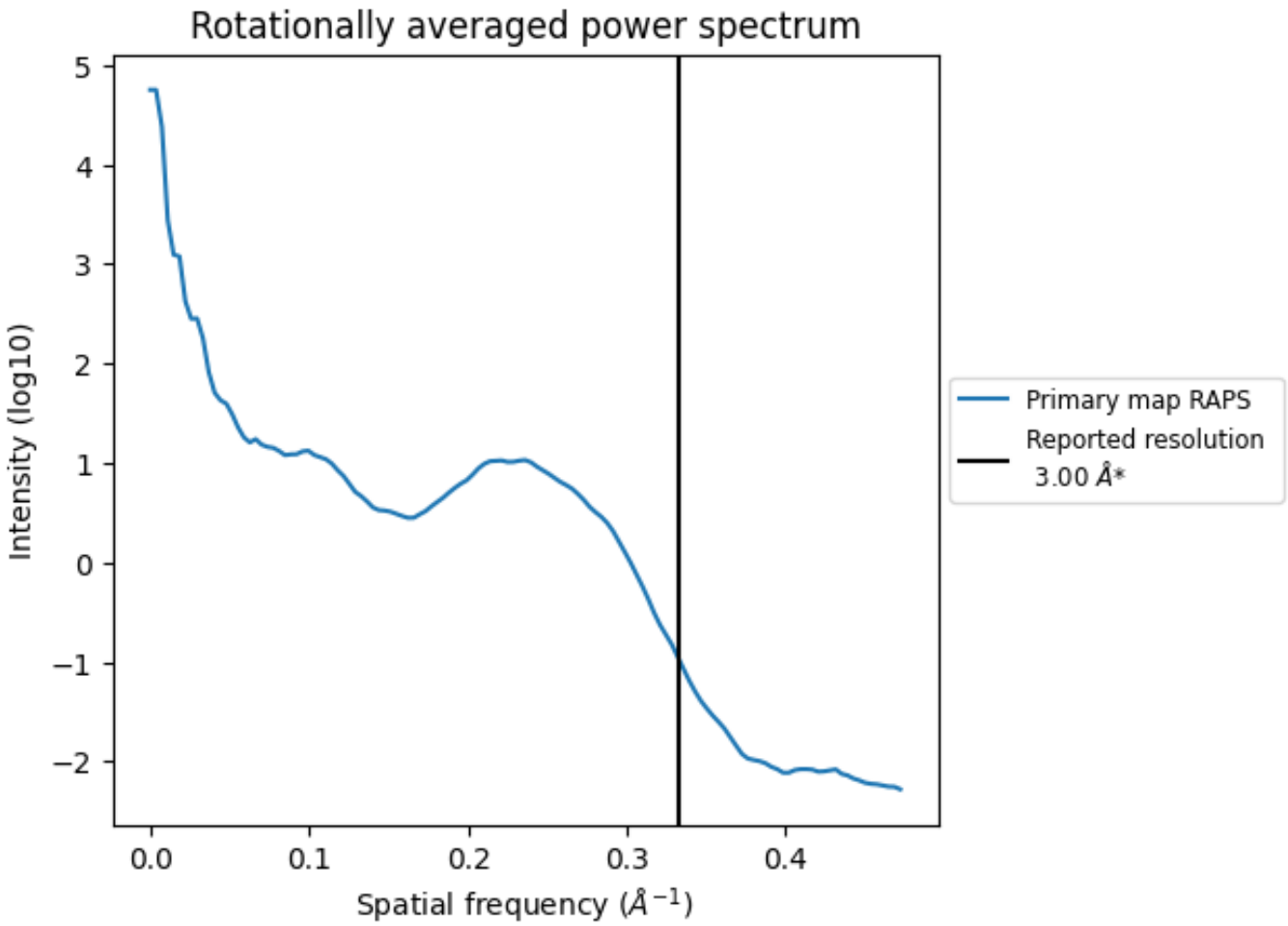
7.2 Volume estimate (i)



The volume at the recommended contour level is 96 nm^3; this corresponds to an approximate mass of 87 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 0.333 Å^{-1}

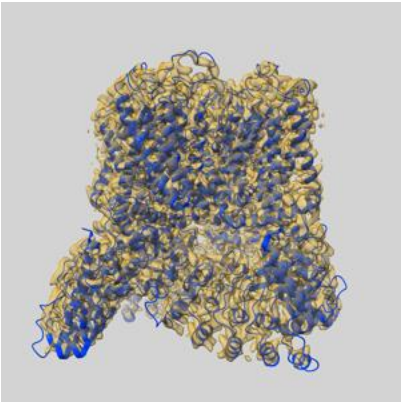
8 Fourier-Shell correlation (i)

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

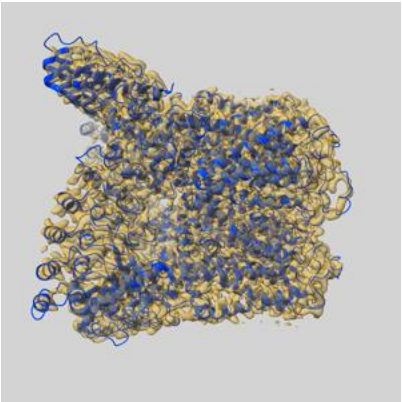
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0594 and PDB model 6O1P. Per-residue inclusion information can be found in section 3 on page 4.

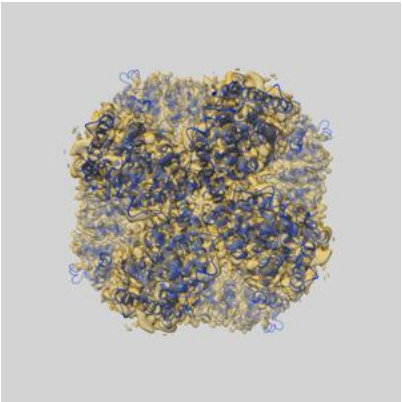
9.1 Map-model overlay (i)



X



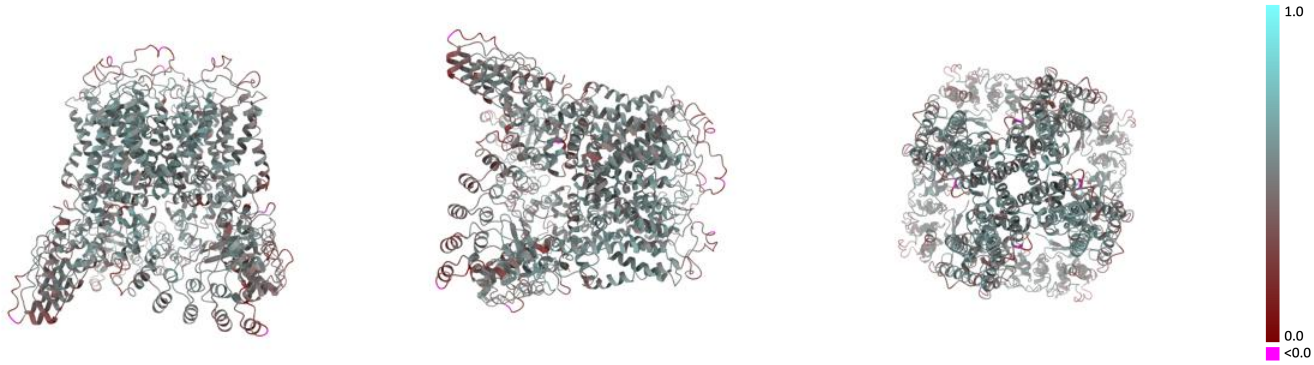
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

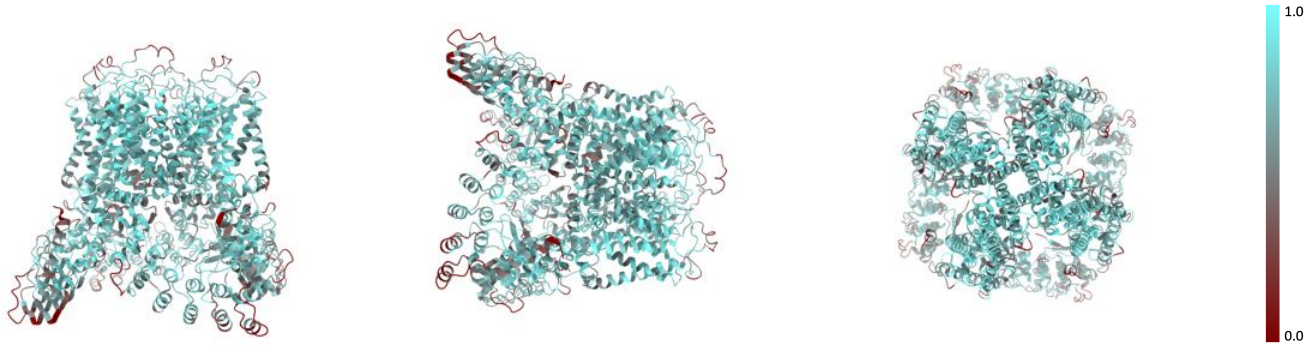
9.2 Q-score mapped to coordinate model (i)



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.

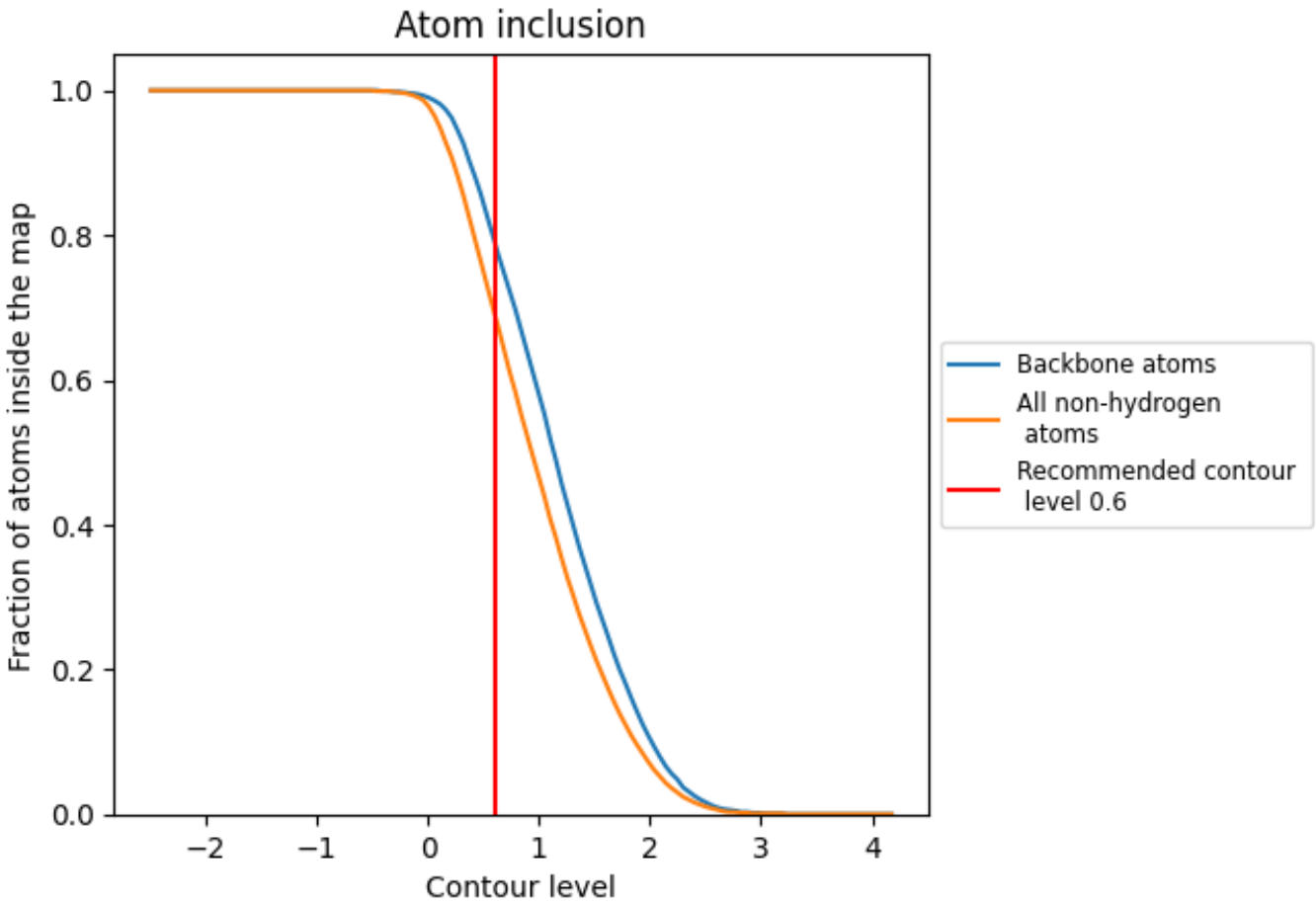
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 69% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6920	0.4780
A	0.7030	0.4920
B	0.6710	0.4450
C	0.6990	0.4930
D	0.6970	0.4810