



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 03:31 PM UTC

PDB ID : 7R7U / pdb_00007r7u
EMDB ID : EMD-24305
Title : D1 and D2 domain structure of the p97(R155H)-p47 complex
Authors : Nandi, P.; Li, S.; Coulmbres, R.C.A.; Wang, F.; Williams, D.R.; Poh, Y.-P.;
Chou, T.-F.; Chiu, P.-L.
Deposited on : 2021-06-25
Resolution : 4.30 Å(reported)
Based on initial model : 5FTK

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:

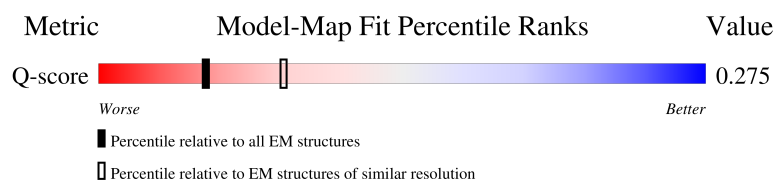
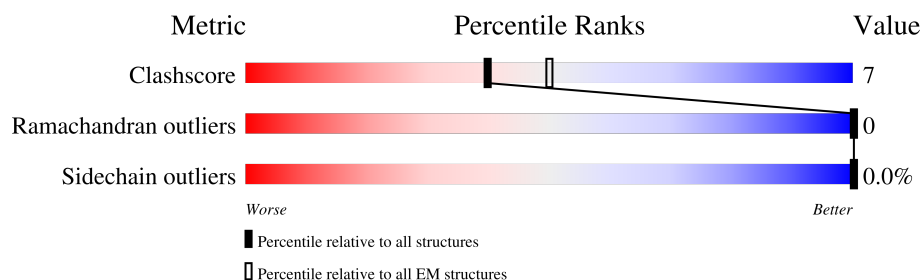
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	806	20% 55% 11% 33%
1	B	806	20% 55% 12% 33%
1	C	806	19% 52% 14% 33%
1	D	806	19% 55% 12% 33%

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Mol	Chain	Length	Quality of chain
1	E	806	17% 53% 14% 33%
1	F	806	17% 55% 12% 33%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25362 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	538	Total	C	N	O	S	0	0
			4215	2656	749	788	22		
1	B	541	Total	C	N	O	S	0	0
			4233	2666	752	793	22		
1	C	538	Total	C	N	O	S	0	0
			4215	2656	749	788	22		
1	D	541	Total	C	N	O	S	0	0
			4233	2666	752	793	22		
1	E	541	Total	C	N	O	S	0	0
			4233	2666	752	793	22		
1	F	541	Total	C	N	O	S	0	0
			4233	2666	752	793	22		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	HIS	ARG	engineered mutation	UNP P55072
B	155	HIS	ARG	engineered mutation	UNP P55072
C	155	HIS	ARG	engineered mutation	UNP P55072
D	155	HIS	ARG	engineered mutation	UNP P55072
E	155	HIS	ARG	engineered mutation	UNP P55072
F	155	HIS	ARG	engineered mutation	UNP P55072

THR
GLY
GLY
SER
SER
VAL
THR
THR
GLU
ASP
ASN
ASP
ASP
LEU
TYR
GLY

• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain B: 

MET
ALA
SER
GLY
ARG
ALA
ASP
SER
LYS
GLY
GLY
ASP
ASP
ASP
LEU
THR
LYS

GLY
LYS
LYS
ARG
GLY
ARG
ALA
THR
GLY
VAL
PHE
LEU
ASP
SER
THR
ASP
LEU
THR
LYS

ASP
THR
VAL
GLY
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THR
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ASN
PHE
VAL
TTR
LEU
LEU
THR
ASP
LEU
THR
LYS

VAL
ILE
HIS
CYS
GLY
GLY
PRO
ILE
ARG
GLU
ASP
GLU
SER
LEU
N199
E200
V201
G202
Y203
D204
D205
I206
G207
G208
C209
R210
A214
K217
E218
W219
E221
L222
R225
F230
I233
G234
P237
P238
R239
G240
Y244
G246
T249
G250
K251
T252
L253

I254
A255
R256
A257
L268
I274
A279
G280
E283
S284
L286
R287
E291
E294
K295
D304
E305
L306
D307
K312
R313
E314
T316
H317
G318
E321
R322
L328
D333
G334
L335
K336
Q337
R338
A339
I342
V343
M344
T347
R346
R349
P350
K351
S352

R358
R359
R365
E366
V367
D368
I369
G370
I371
P372
D373
R377
R387
M388
K389
L390
A391
D392
D393
D395
L396
F402
T403
H404
S416
A419
L420
Q421
A422
I423
R424
K426
M427
D428
L429
I430
D431
L432
GLU
ASP
GLU
THR
ILE
ASP
A439
E440
V441
H442
M443
S444
L445
A446

V447
T448
M449
D450
D451
F452
R453
S457
H460
R465
E466
T467
Q473
V474
T475
W476
I479
G480
G481
L482
E483
D484
V485
K486
R487
E488
L489
Q490
E491
Y495
H499
P500
D501
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L526
L527
A528
K529
Q536
A537
M538
S541

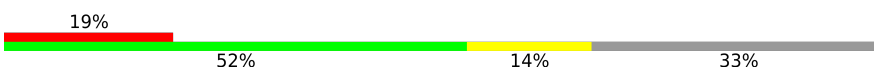
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Q568
A569
A570
P571
C572
V573
L574
F575
E578
L579
D580
S581
I582
A583
K584
A585
R586
G587
G588
ASN
ILE
GLY
GLY
ASP
GLY
GLY
A596
R599
V600
I604
M608
D609
G610
M611

S612
T613
K614
K615
E616
V617
F618
A622
D627
I628
L629
D630
L634
R635
P636
G637
D640
I643
Y644
P648
K651
S652
R653
L661
R662
K663
V670
D671
F674
L675
A676
K677
M678
T679
N680
L687
T688
I690
L697
A698
T699
R700
S705
R709
E710

R713
GLN
THR
ASN
PRO
SER
ALA
SER
MET
GLU
VAL
GLU
ASP
ASP
D726
I731
D734
M740
R741
F742
A743
R744
R745
N750
R753
R754
T761
Q764
SER
ARG
GLY
PHE
GLY
SER
PHE
ARG
PRO
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GLN
GLY
GLY
R700
S705
R709
E710

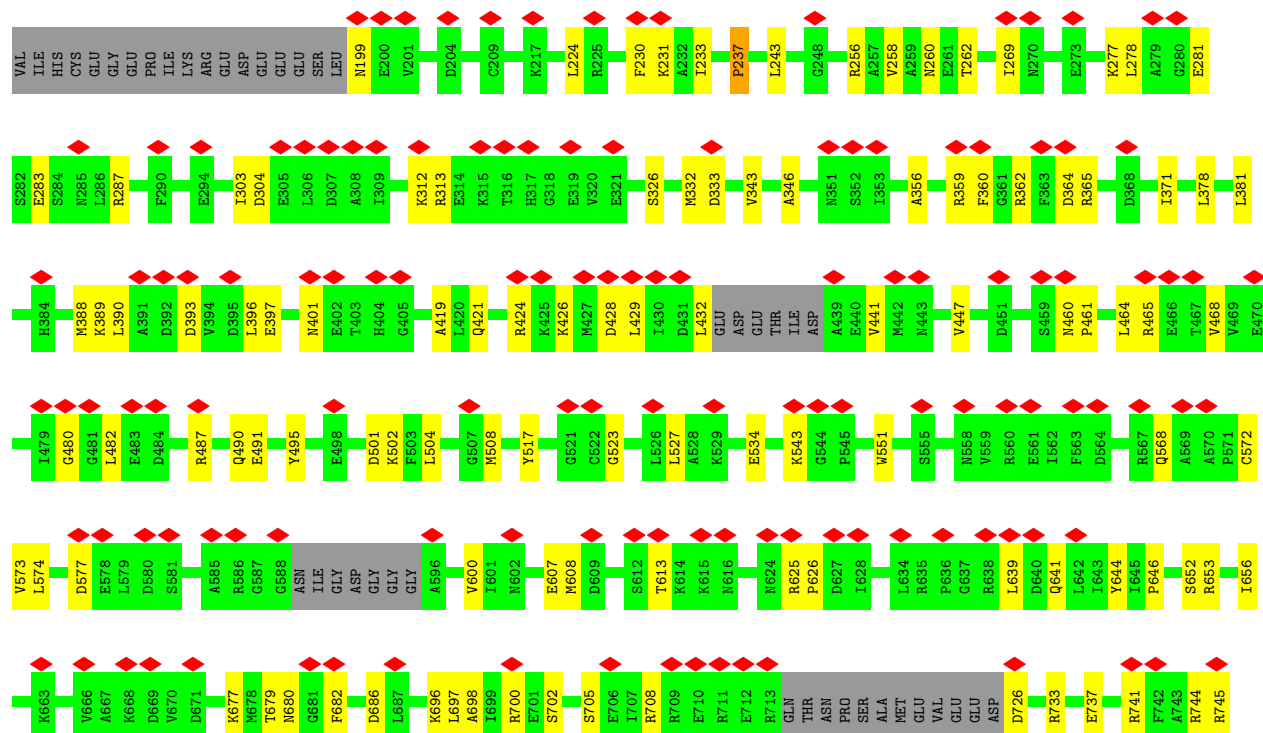
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GLY
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SER
VAL
THR
THR
GLU
GLY
ASP
ASN
ASP
ASP
ASP
LEU
TYR
GLY

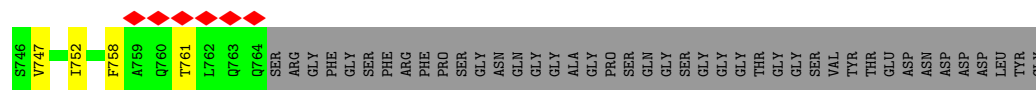
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C: 

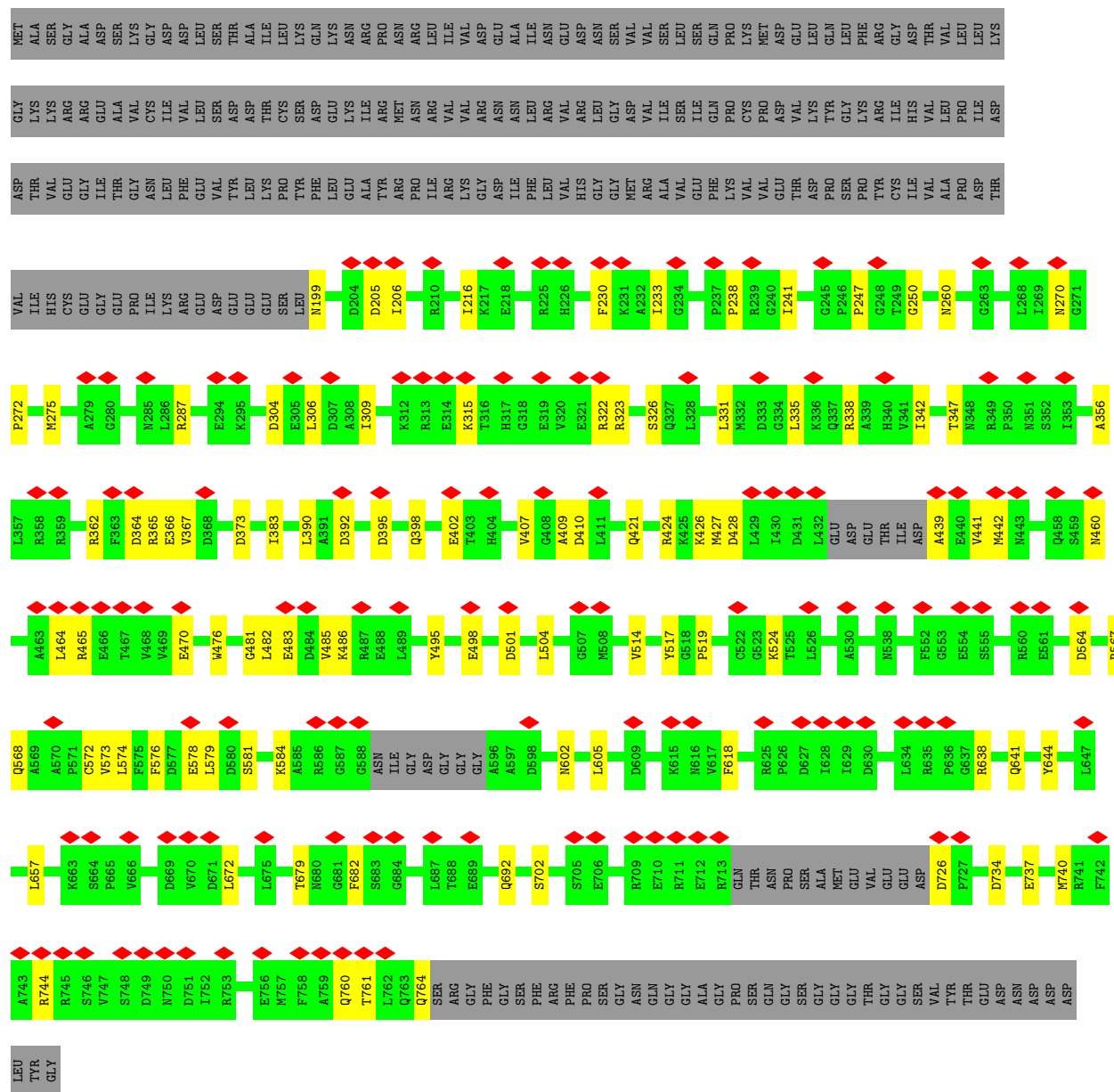
MET
ALA
SER
GLY
ARG
ALA
ASP
SER
LYS
GLY
GLY
ASP
ASP
ASP
LEU
THR
LYS

GLY
LYS
LYS
ARG
GLY
ARG
ALA
THR
GLY
VAL
PHE
LEU
ASP
SER
THR
ASP
LEU
THR
LYS





• Molecule 1: Transitional endoplasmic reticulum ATPase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	203242	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 ($e^-/\text{\AA}^2$)	44.4	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	0.075	Depositor
Minimum map value	-0.039	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0217	Depositor
Map size ($\text{\AA}$)	374.4, 374.4, 374.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.56, 1.56, 1.56	Depositor

5 Model quality

5.1 Standard geometry

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	0.24	0/4283	0.65	1/5775 (0.0%)
1	B	0.23	0/4301	0.65	3/5800 (0.1%)
1	C	0.23	0/4283	0.65	1/5775 (0.0%)
1	D	0.24	0/4301	0.65	1/5800 (0.0%)
1	E	0.25	0/4302	0.67	0/5803
1	F	0.24	0/4301	0.66	0/5800
All	All	0.24	0/25771	0.66	6/34753 (0.0%)

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	B	0	1
1	E	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	441	VAL	N-CA-C	-5.91	107.05	112.96
1	D	474	VAL	N-CA-C	-5.75	108.25	113.71
1	B	679	THR	CA-C-N	5.54	129.14	120.82
1	B	679	THR	C-N-CA	5.54	129.14	120.82
1	C	335	LEU	CA-CB-CG	5.15	134.34	116.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	482	LEU	Peptide
1	E	237	PRO	Peptide
1	E	360	PHE	Peptide

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	4215	0	4279	61	0
1	B	4233	0	4293	62	0
1	C	4215	0	4279	81	0
1	D	4233	0	4293	67	0
1	E	4233	0	4294	75	0
1	F	4233	0	4293	68	0
All	All	25362	0	25731	365	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 7.

The worst 5 of 365 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:E:491:GLU:O	1:E:495:TYR:HB2	1.89	0.71
1:E:397:GLU:O	1:E:401:ASN:HB2	1.91	0.70
1:B:764:GLN:HE22	1:C:683:SER:H	1.40	0.68
1:C:567:ARG:HH22	1:D:460:ASN:HA	1.58	0.68
1:F:206:ILE:HG21	1:F:250:GLY:HA3	1.79	0.64

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	530/806 (66%)	487 (92%)	43 (8%)	0	100	100
1	B	533/806 (66%)	479 (90%)	54 (10%)	0	100	100
1	C	530/806 (66%)	489 (92%)	41 (8%)	0	100	100
1	D	533/806 (66%)	485 (91%)	48 (9%)	0	100	100
1	E	535/806 (66%)	486 (91%)	49 (9%)	0	100	100
1	F	533/806 (66%)	486 (91%)	47 (9%)	0	100	100
All	All	3194/4836 (66%)	2912 (91%)	282 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	451/678 (66%)	451 (100%)	0	100	100
1	B	452/678 (67%)	452 (100%)	0	100	100
1	C	451/678 (66%)	451 (100%)	0	100	100
1	D	452/678 (67%)	452 (100%)	0	100	100
1	E	452/678 (67%)	451 (100%)	1 (0%)	87	85
1	F	452/678 (67%)	452 (100%)	0	100	100
All	All	2710/4068 (67%)	2709 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	641	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	490	GLN
1	E	624	ASN
1	E	538	ASN
1	E	692	GLN
1	B	458	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 oligosaccharides 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.

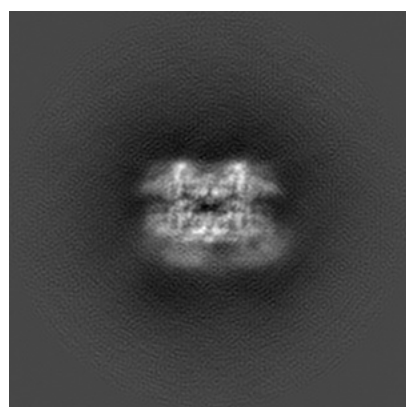
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24305. These allow visual inspection of the internal detail of the map and identification of artifacts.

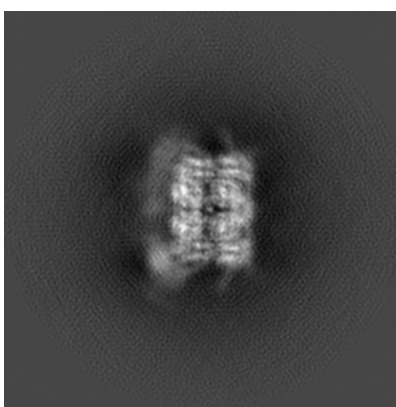
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

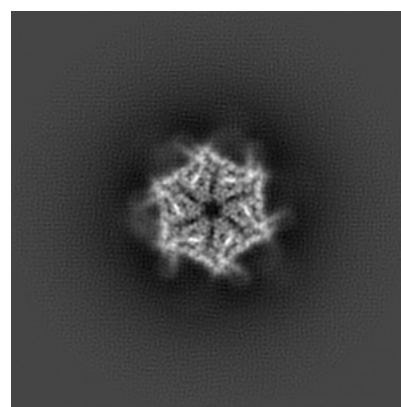
6.1.1 Primary map



X



Y

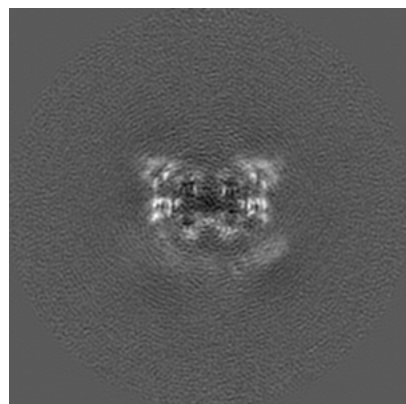


Z

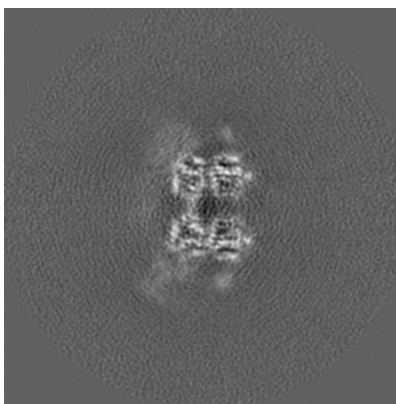
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

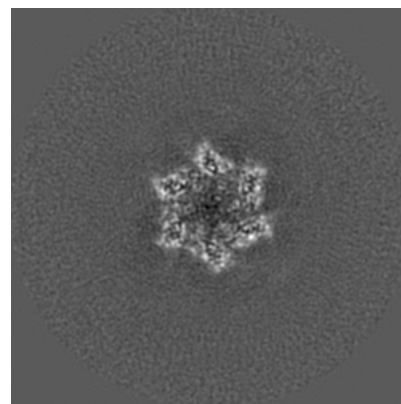
6.2.1 Primary map



X Index: 120



Y Index: 120

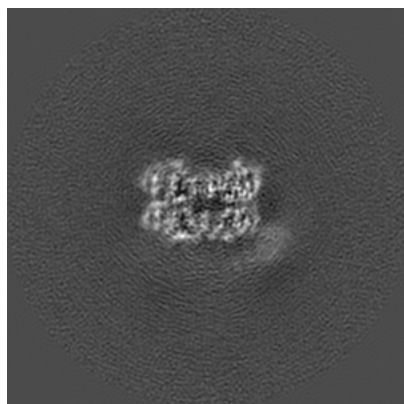


Z Index: 120

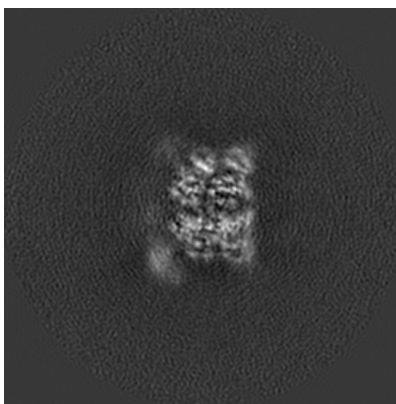
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

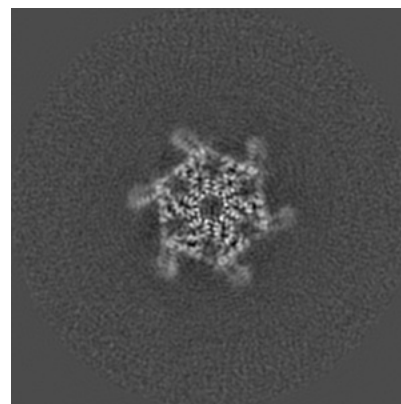
6.3.1 Primary map



X Index: 128



Y Index: 102

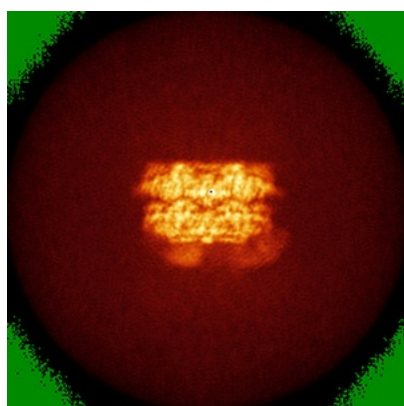


Z Index: 131

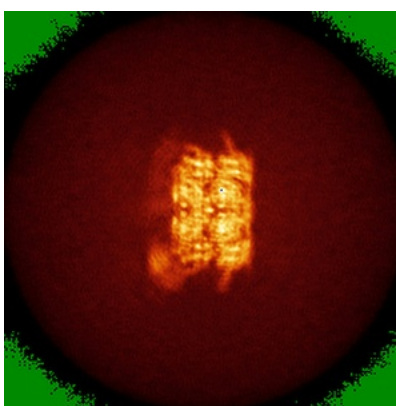
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

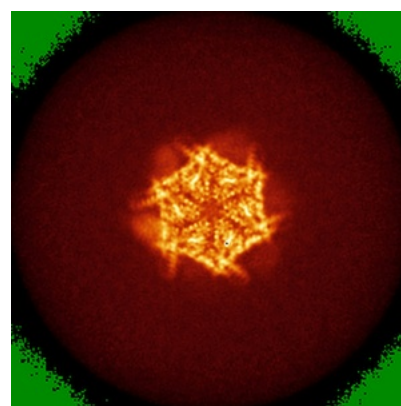
6.4.1 Primary map



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 0.0217. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

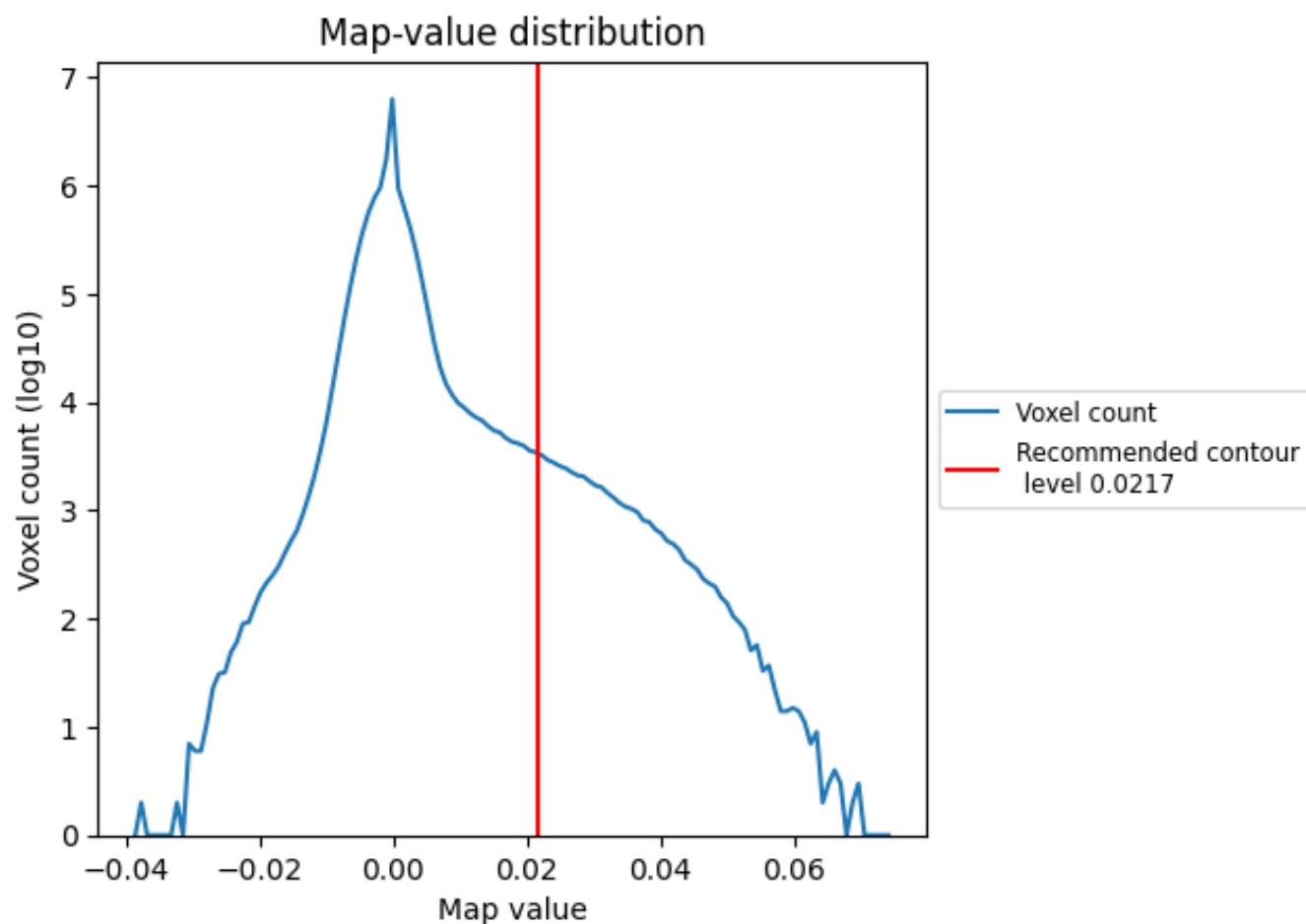
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

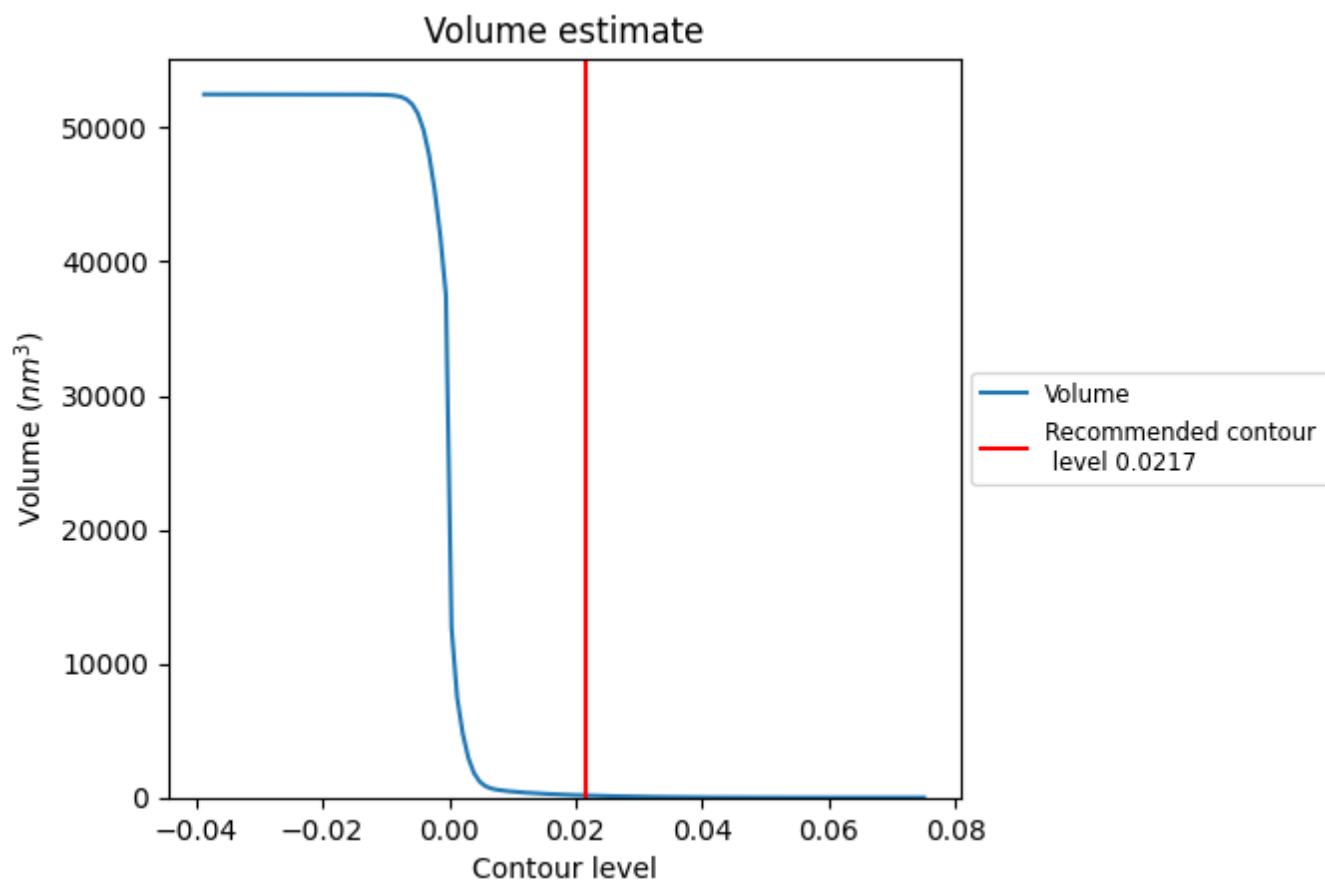
This section contains the results of statistical analysis of the map.

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.

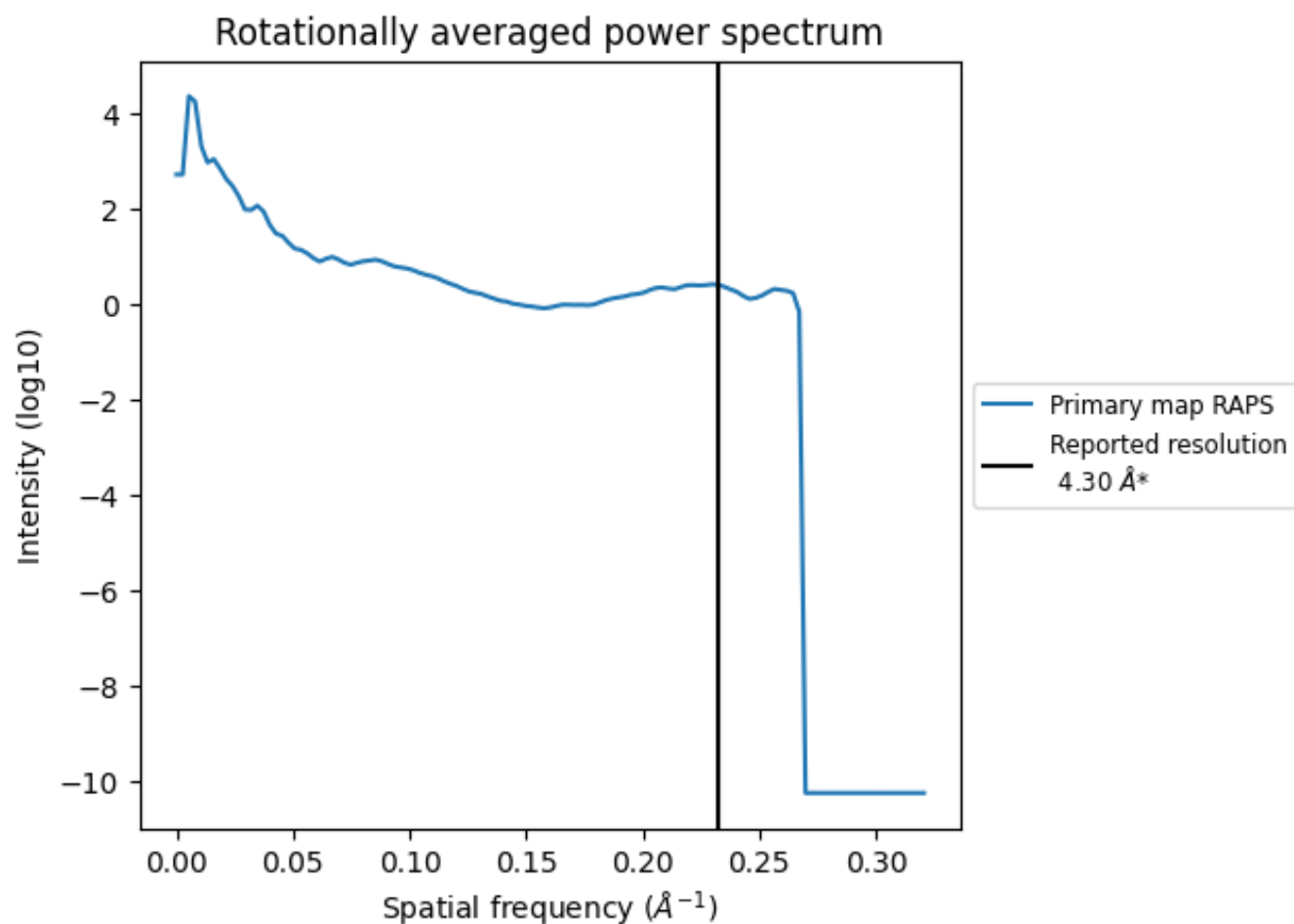
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 157 nm³; this corresponds to an approximate mass of 142 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 0.233 Å⁻¹

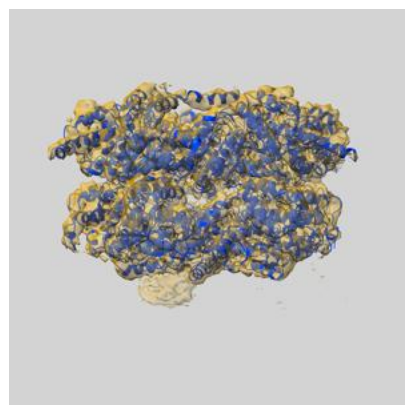
8 Fourier-Shell correlation

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

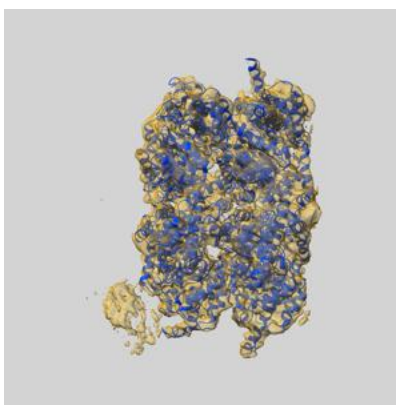
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24305 and PDB model 7R7U. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

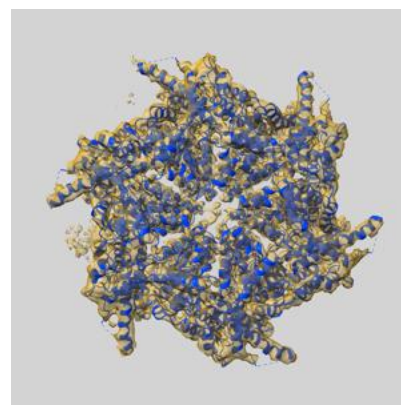
9.1 Map-model overlay [i](#)



X



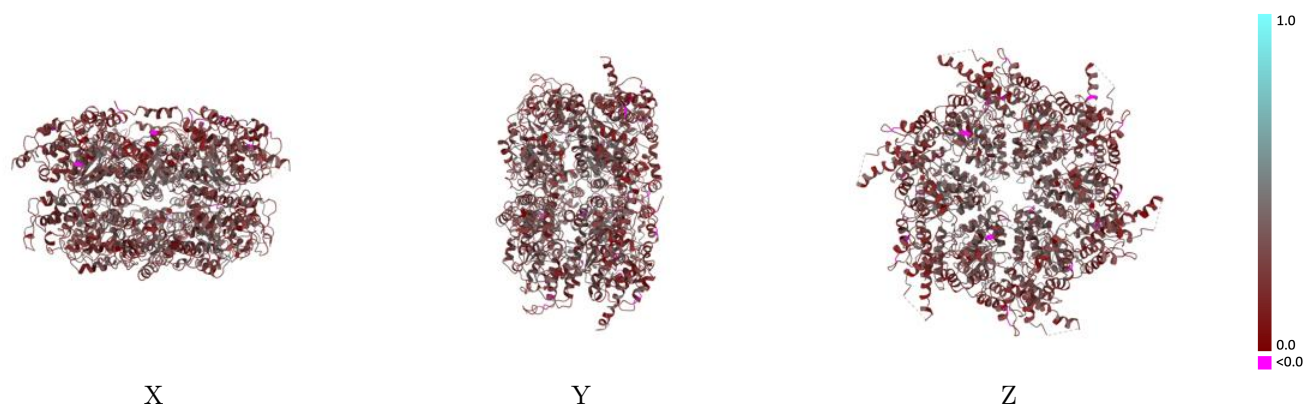
Y



Z

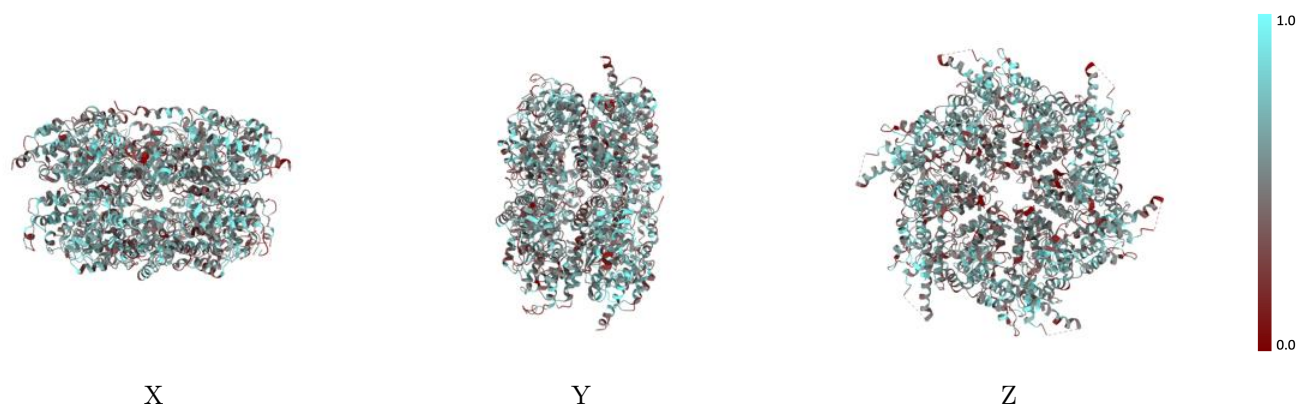
The images above show the 3D surface view of the map at the recommended contour level 0.0217 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



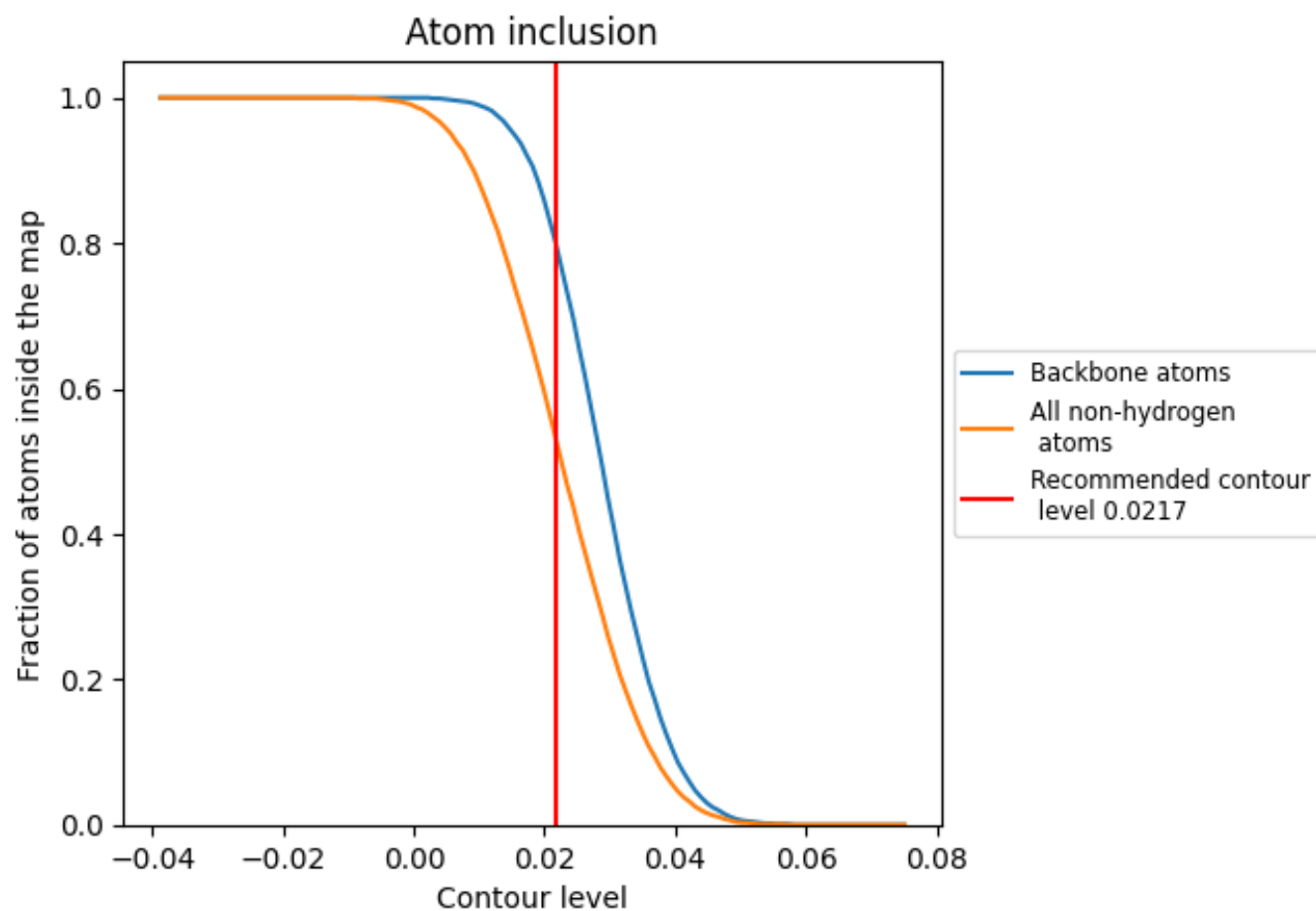
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0217).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 53% 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 (0.0217) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5320	0.2750
A	0.5300	0.2760
B	0.5200	0.2820
C	0.5310	0.2710
D	0.5250	0.2760
E	0.5400	0.2740
F	0.5430	0.2720

1.0

0.0

<0.0