wwPDB EM Validation Summary Report (i)

Oct 4, 2026 – 04:13 PM JST

PDB ID	:	9X4X / pdb_00009x4x
EMDB ID	:	EMD-66567
Title	:	Cryo-EM structure of HSP90-CDC37-PINK1 complex
Authors	:	Okatsu, K.; Fukai, S.
Deposited on	:	2025-10-12
Resolution	:	3.08 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:

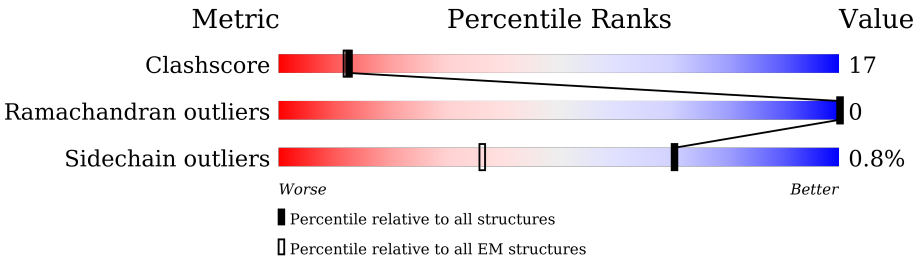
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

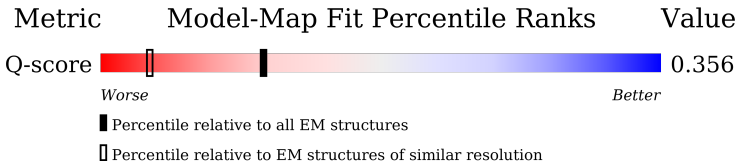
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.08 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	14000 (2.58 - 3.58)

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	C	378	40% 39% 17% 44%
2	D	486	17% 27% 23% 50%
3	A	724	7% 60% 27% 13%
3	B	724	6% 60% 27% • 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14094 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 Hsp90 co-chaperone Cdc37.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	C	213	1806	1132	308	352	1	13	0	0

- Molecule 2 is a protein called Serine/threonine-protein kinase PINK1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	243	1879	1200	328	335	16	0	0

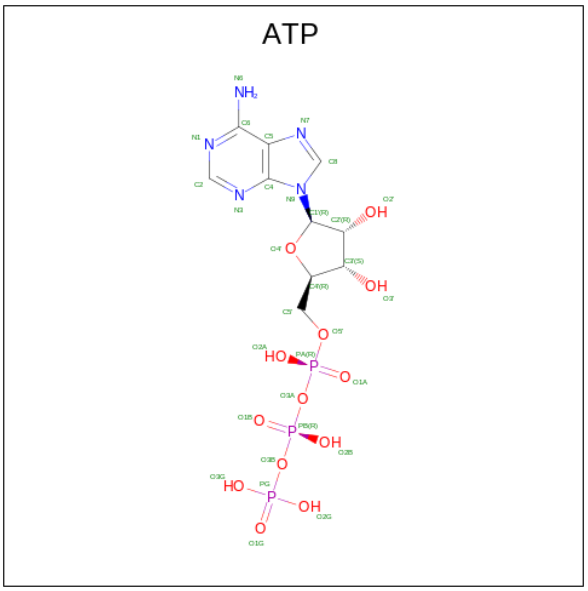
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	104	MET	PHE	engineered mutation	UNP Q9BXM7
D	582	HIS	-	expression tag	UNP Q9BXM7
D	583	HIS	-	expression tag	UNP Q9BXM7
D	584	HIS	-	expression tag	UNP Q9BXM7
D	585	HIS	-	expression tag	UNP Q9BXM7
D	586	HIS	-	expression tag	UNP Q9BXM7
D	587	HIS	-	expression tag	UNP Q9BXM7
D	588	HIS	-	expression tag	UNP Q9BXM7
D	589	HIS	-	expression tag	UNP Q9BXM7

- Molecule 3 is a protein called Heat shock protein HSP 90-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	632	5123	3249	862	989	23	0	0
3	B	644	5222	3310	881	1008	23	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

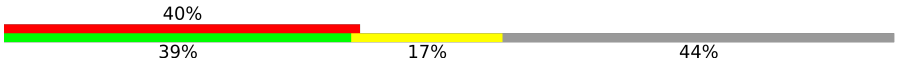
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	

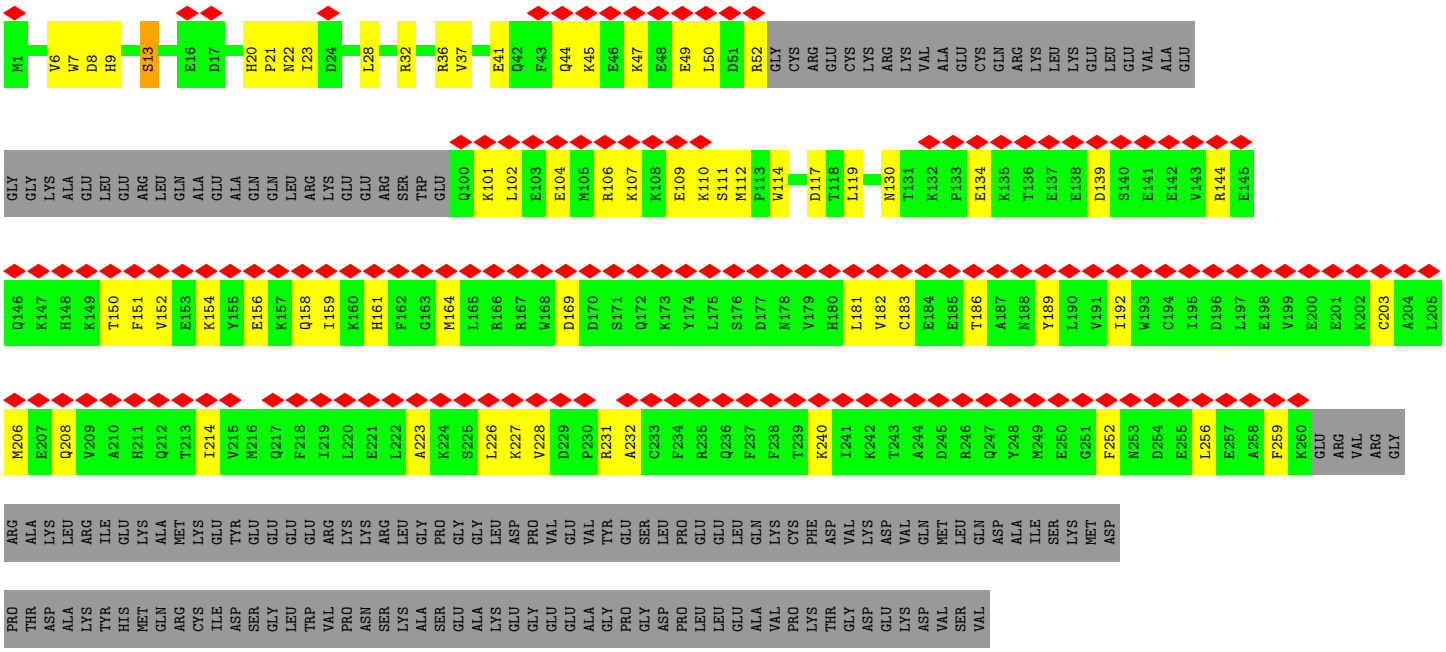
3 Residue-property plots (i)

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: Hsp90 co-chaperone Cdc37

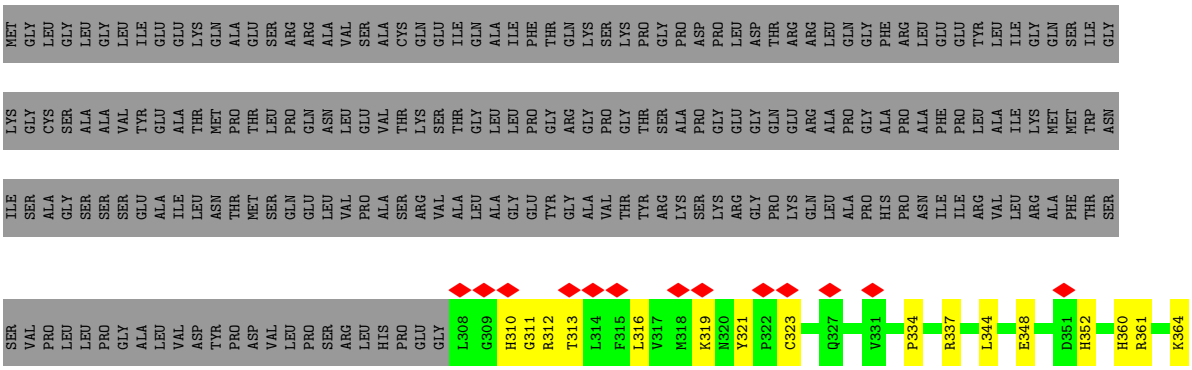
Chain C:

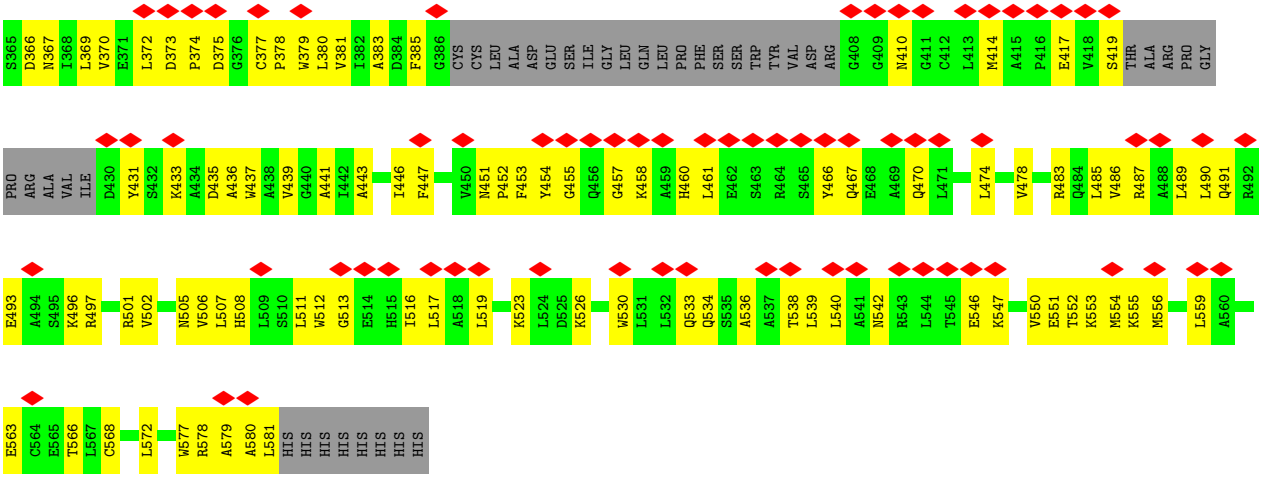




- Molecule 2: Serine/threonine-protein kinase PINK1, mitochondrial

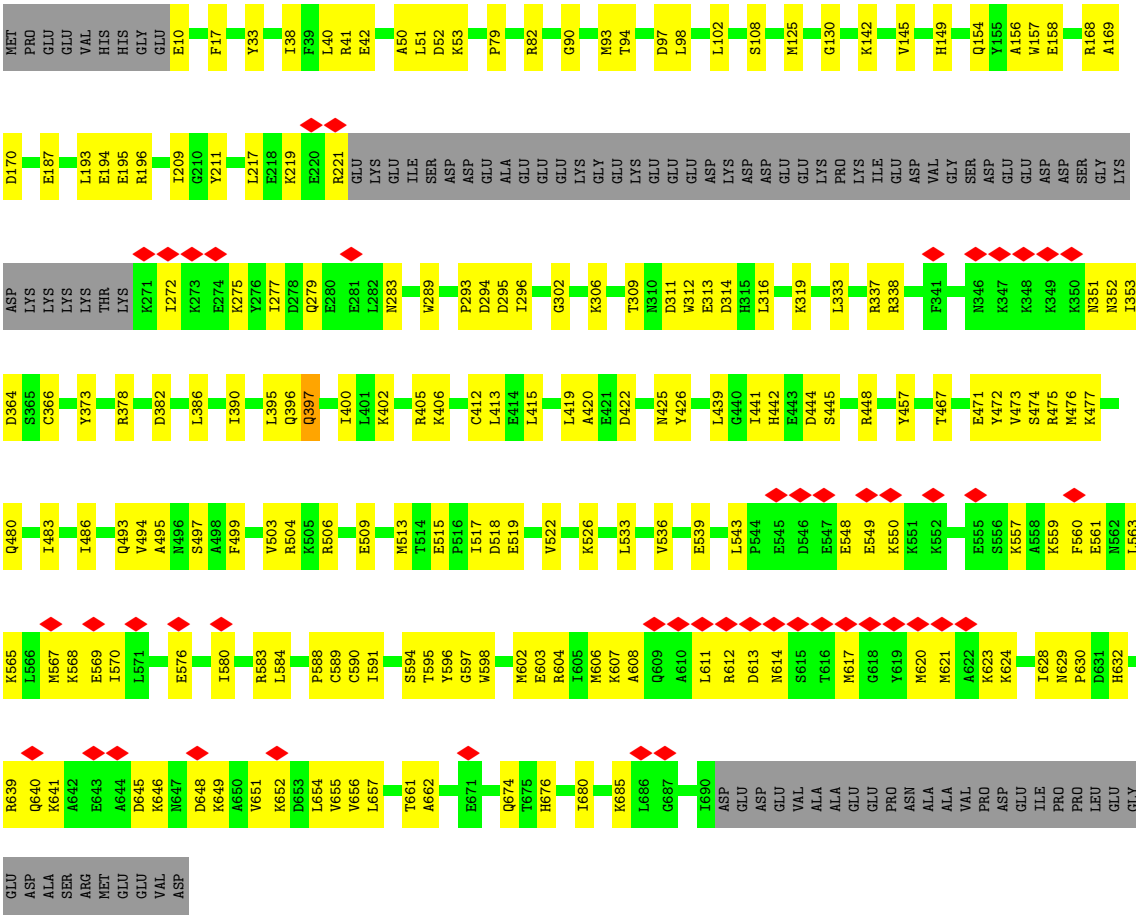
Chain D:





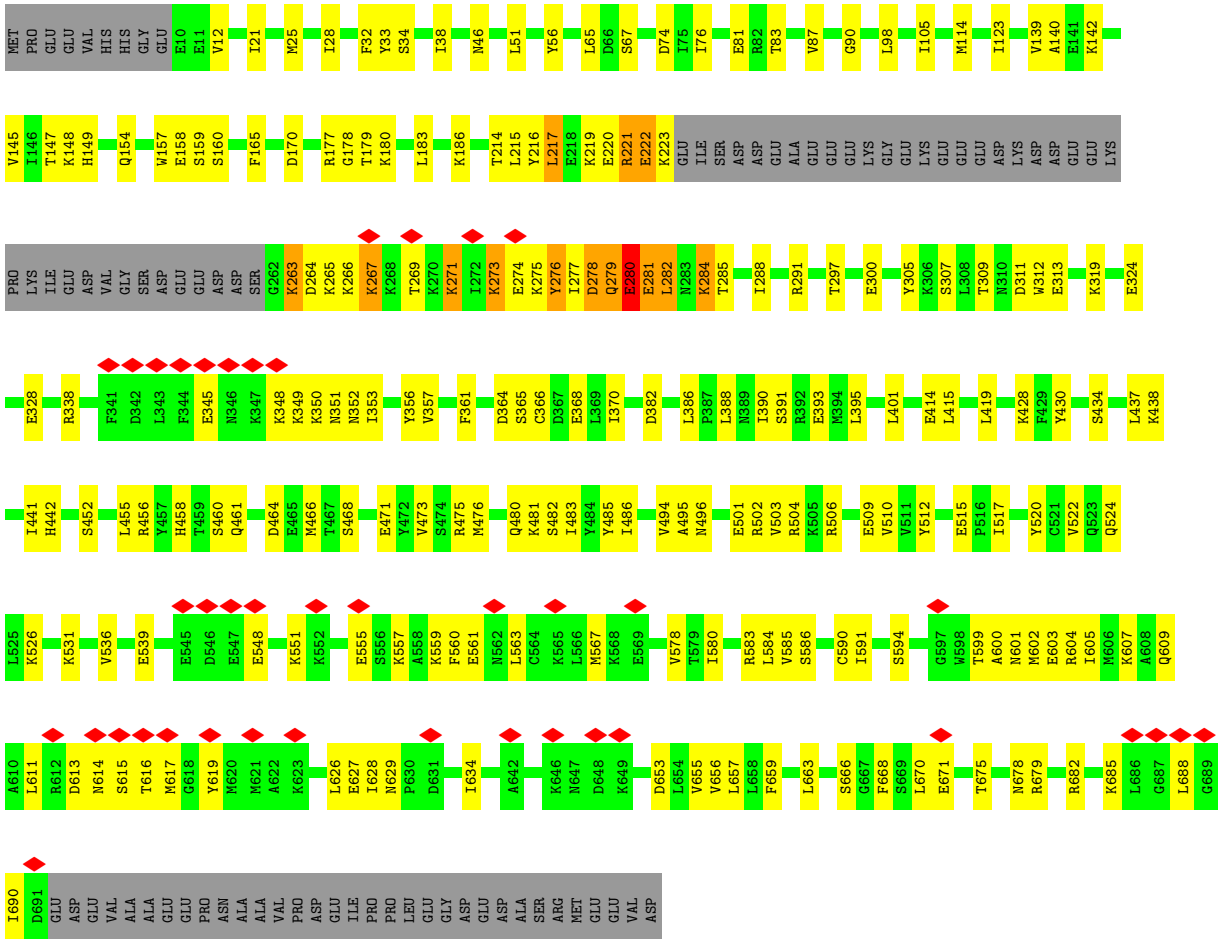
• Molecule 3: Heat shock protein HSP 90-beta

Chain A:



• Molecule 3: Heat shock protein HSP 90-beta

Chain B:


MET PRO GLU GLU VAL HIS HIS GLY GLU E10 E11 V12 I21 M25 I28 F32 Y33 S34 I38 N46 L51 Y56 L65 D66 S67 D74 I75 I76 E81 R82 T83 V87 G90 L98 I105 M114 I123 V139 A140 E141 K142
V145 I146 T147 K148 H149 Q154 W157 E158 S159 S160 F165 D170 R177 G178 T179 K180 L183 K186 T214 L215 Y216 L217 E218 K219 E220 R221 E222 K223 GLU ILE SER ASP ASP GLU ALA GLU GLU GLU LYS GLY GLU LYS GLU GLU GLU ASP LYS ASP ASP GLU GLU LYS
PRO LYS ILE GLU ASP VAL GLY SER ASP GLU GLU ASP ASP SER G262 K263 D264 K265 K266 K267 K268 T269 K270 K271 I272 K273 E274 K275 Y276 I277 D278 Q279 E280 E281 L282 N283 K284 T285 I288 R291 T297 E300 Y305 K306 S307 L308 T309 N310 D311 W312 E313 K319 E324
E328 R338 F341 D342 L343 F344 E345 N346 K347 K348 K349 K350 N351 N352 I353 Y356 V357 F361 D364 S365 C366 D367 E368 L369 I370 D382 L386 P387 L388 N389 I390 S391 R392 E393 M394 L395 L401 E414 L415 L419 K428 F429 Y430 S434 L437 K438
I441 H442 S452 L455 R456 Y457 H458 T459 S460 Q461 D464 E465 M466 T467 S468 E471 Y472 V473 S474 R475 M476 Q480 K481 S482 I483 Y484 Y485 I486 V494 A495 N496 E501 R502 V503 R504 K505 R506 E509 V510 V511 Y512 E515 P516 I517 Y520 C521 V522 Q523 Q524
L525 K526 K531 V536 E539 E545 D546 E547 E548 K551 K552 E555 S556 K557 A558 K559 F560 E561 N562 L563 C564 K565 L566 M567 K568 E569 V578 T579 I580 R583 L584 V585 S586 C590 I591 S594 G597 W598 T599 A600 N601 M602 E603 R604 I605 M606 K607 A608 Q609
A610 L611 R612 D613 N614 S615 T616 M617 G618 Y619 M620 M621 A622 K623 L626 E627 I628 N629 P630 D631 I634 A642 K646 N647 D648 K649 D653 L654 V655 V656 L657 L658 F659 L663 S666 G667 F668 S669 L670 E671 T675 N678 R679 R682 K685 L686 G687 L688 G689
I690 D691 GLU ASP GLU VAL ALA ALA GLU GLU PRO ASN ALA ALA VAL PRO ASP GLU ILE PRO PRO LEU GLU GLY ASP GLU ASP ALA SER ARG MET GLU GLU VAL ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	454727	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.363	Depositor
Minimum map value	-0.672	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	173.76, 173.76, 173.76	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.724, 0.724, 0.724	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, MG, ATP

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	C	0.16	0/1830	0.37	0/2452
2	D	0.18	0/1915	0.45	0/2597
3	A	0.30	0/5207	0.57	4/6997 (0.1%)
3	B	0.35	0/5306	0.56	8/7123 (0.1%)
All	All	0.30	0/14258	0.53	12/19169 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	396	GLN	N-CA-C	30.59	143.80	111.07
3	B	282	LEU	N-CA-C	-12.76	97.37	111.28
3	A	397	GLN	N-CA-CB	-10.30	94.08	110.87
3	B	280	GLU	CA-C-N	-8.29	110.59	122.36
3	B	280	GLU	C-N-CA	-8.29	110.59	122.36

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	C	1806	0	1744	48	0
2	D	1879	0	1919	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5123	0	5170	170	0
3	B	5222	0	5285	191	0
4	A	31	0	12	2	0
4	B	31	0	12	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	14094	0	14142	475	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 17.

The worst 5 of 475 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)
2:D:523:LYS:HB3	3:B:223:LYS:NZ	1.55	1.22
2:D:523:LYS:CB	3:B:223:LYS:HZ2	1.60	1.14
2:D:523:LYS:CG	3:B:223:LYS:NZ	2.10	1.14
2:D:523:LYS:CB	3:B:223:LYS:NZ	2.14	1.08
2:D:523:LYS:HG2	3:B:223:LYS:NZ	1.65	1.06

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	C	208/378 (55%)	202 (97%)	6 (3%)	0	100	100
2	D	237/486 (49%)	224 (94%)	13 (6%)	0	100	100
3	A	628/724 (87%)	605 (96%)	23 (4%)	0	100	100
3	B	640/724 (88%)	616 (96%)	24 (4%)	0	100	100
All	All	1713/2312 (74%)	1647 (96%)	66 (4%)	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	C	200/340 (59%)	200 (100%)	0	100	100
2	D	201/397 (51%)	201 (100%)	0	100	100
3	A	571/652 (88%)	571 (100%)	0	100	100
3	B	582/652 (89%)	569 (98%)	13 (2%)	45	68
All	All	1554/2041 (76%)	1541 (99%)	13 (1%)	70	79

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	271	LYS
3	B	273	LYS
3	B	284	LYS
3	B	278	ASP
3	B	280	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	320	HIS
3	A	442	HIS
3	B	614	ASN
3	B	205	HIS
3	B	346	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	C	13	1	8,9,10	1.51	1 (12%)	8,12,14	1.73	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	C	13	1	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	13	SEP	P-O1P	3.32	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	13	SEP	OG-CB-CA	3.18	111.24	108.14
1	C	13	SEP	P-OG-CB	-3.01	110.02	118.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	13	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	13	SEP	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	B	801	5	29,33,33	0.50	0	44,52,52	0.47	0
4	ATP	A	801	5	29,33,33	0.47	0	44,52,52	0.50	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	801	5	-	10/22/38/38	0/3/3/3
4	ATP	A	801	5	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	801	ATP	PB-O3B-PG	2.06	139.88	132.83

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	ATP	PB-O3B-PG-O2G
4	B	801	ATP	C5'-O5'-PA-O1A
4	B	801	ATP	C5'-O5'-PA-O2A
4	B	801	ATP	C5'-O5'-PA-O3A
4	B	801	ATP	O4'-C4'-C5'-O5'

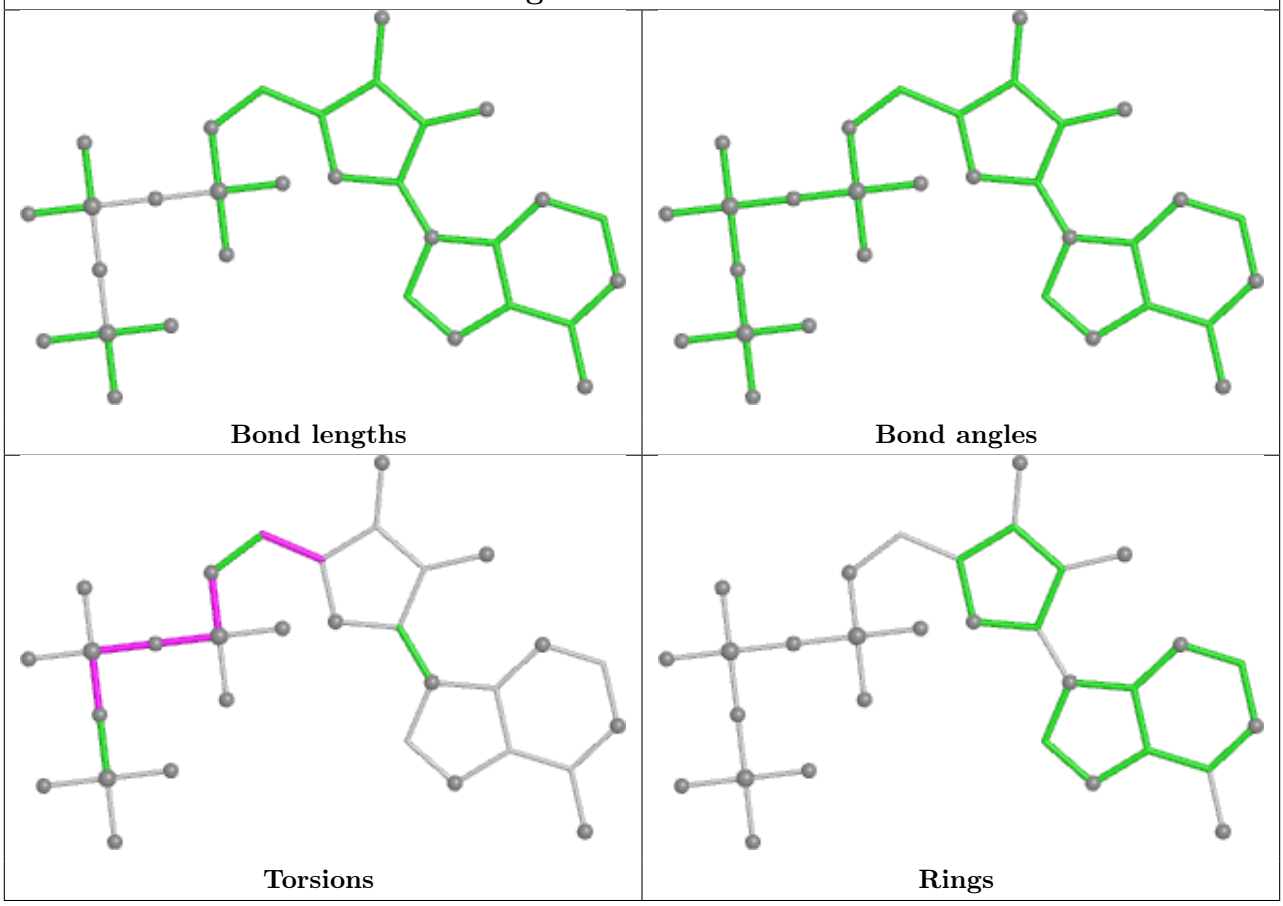
There are no ring outliers.

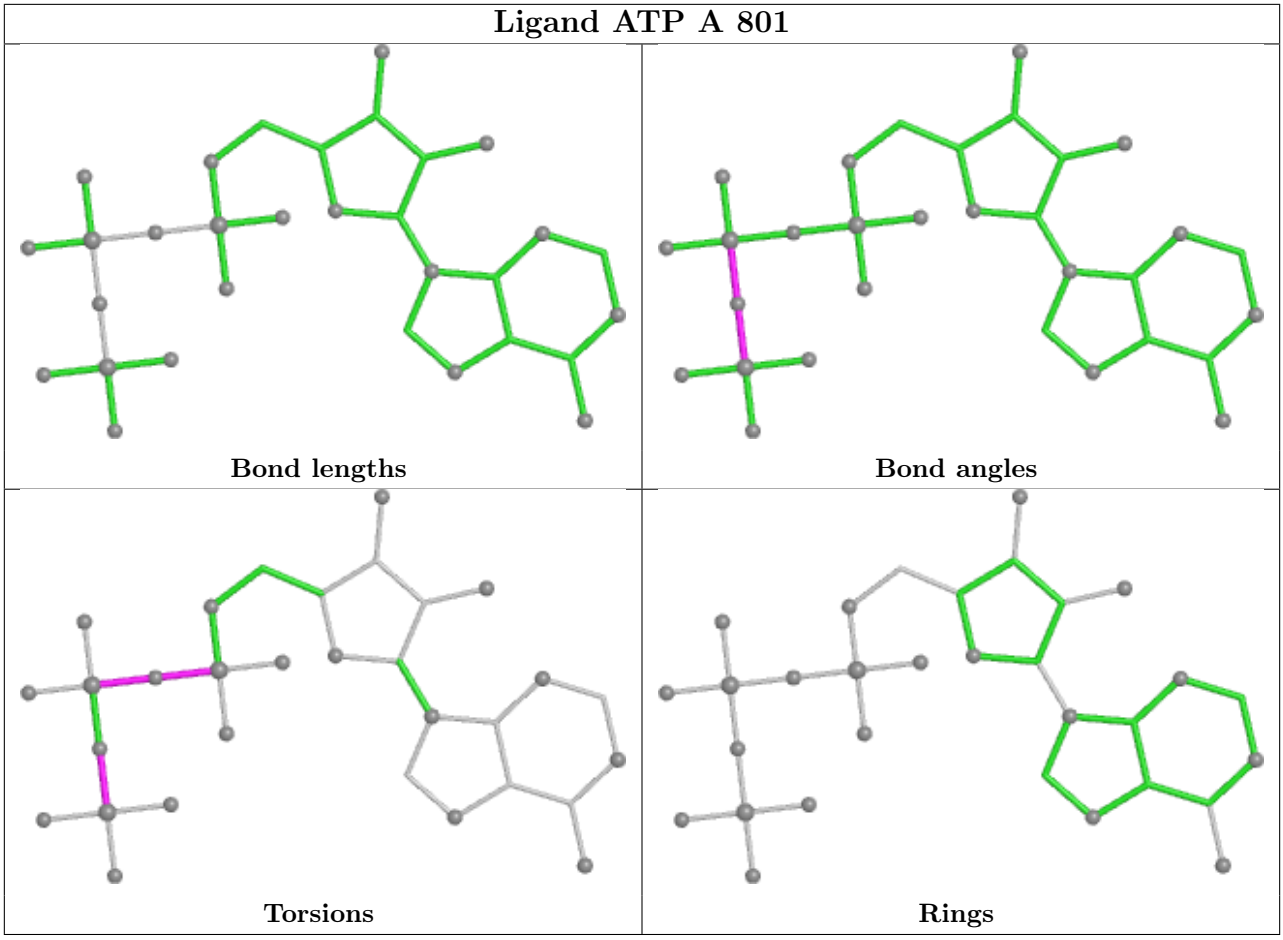
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	ATP	3	0
4	A	801	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP B 801





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.

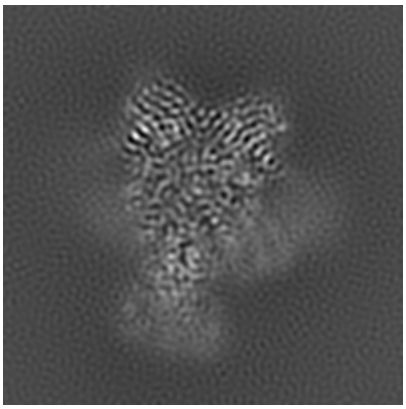
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-66567. These allow visual inspection of the internal detail of the map and identification of artifacts.

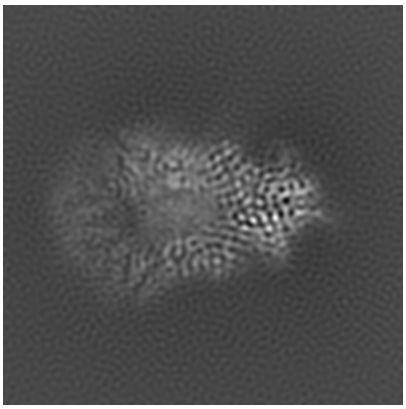
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

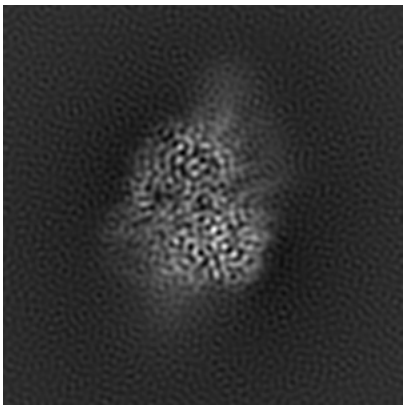
6.1.1 Primary map



X

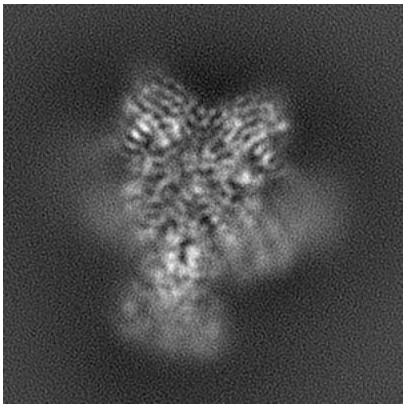


Y

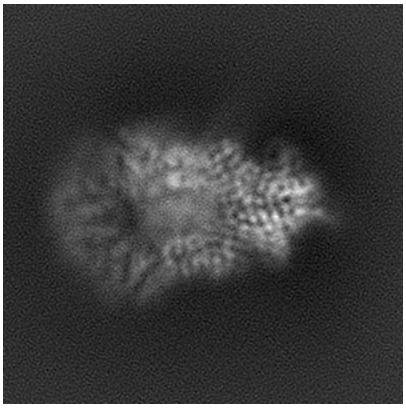


Z

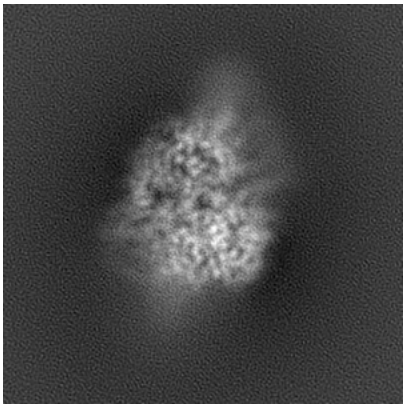
6.1.2 Raw map



X



Y

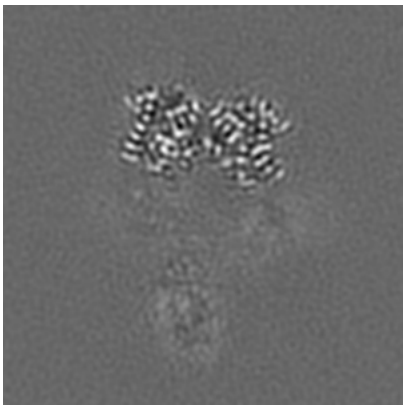


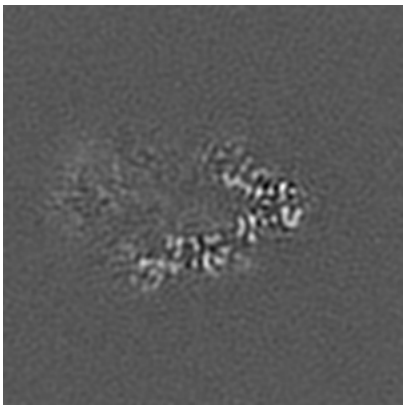
Z

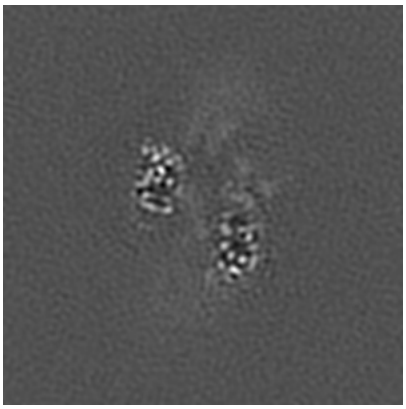
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

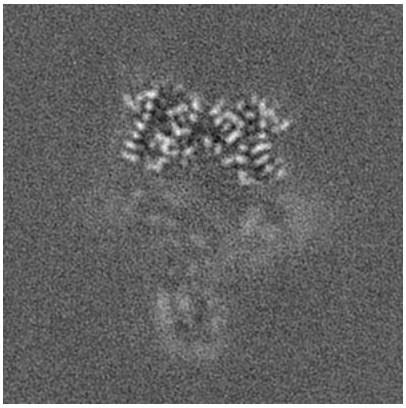
6.2.1 Primary map

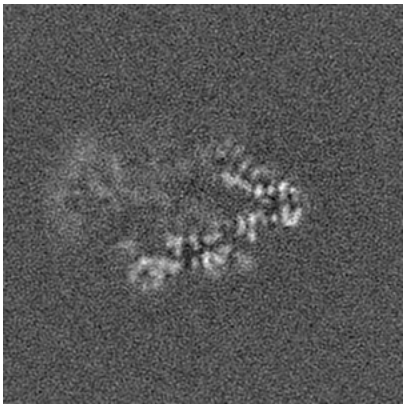

X Index: 120

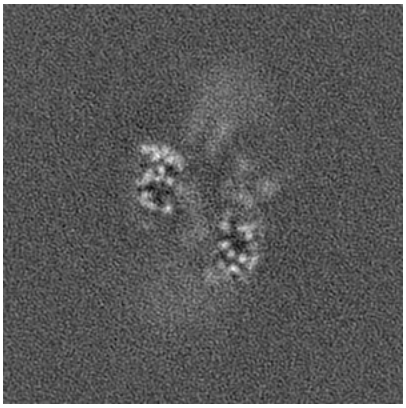

Y Index: 120


Z Index: 120

6.2.2 Raw map


X Index: 120

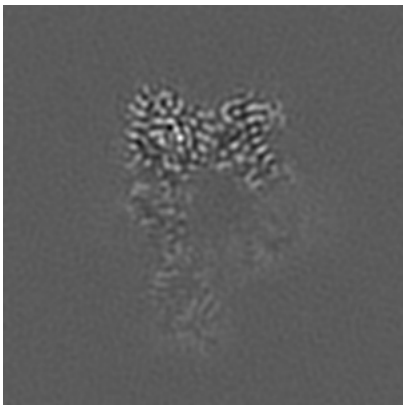

Y Index: 120

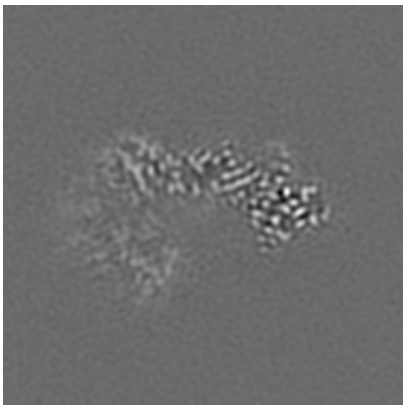

Z Index: 120

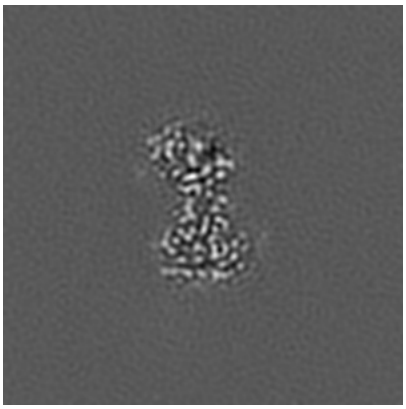
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

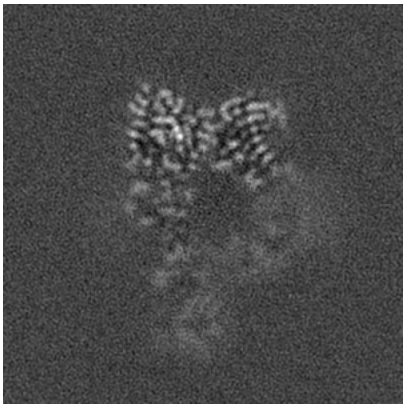
6.3.1 Primary map

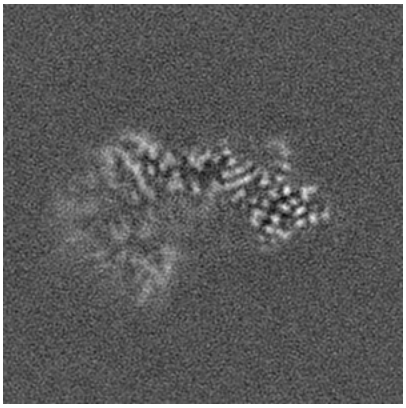

X Index: 127

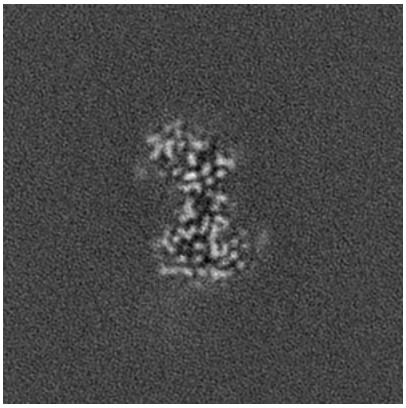

Y Index: 100


Z Index: 162

6.3.2 Raw map


X Index: 127

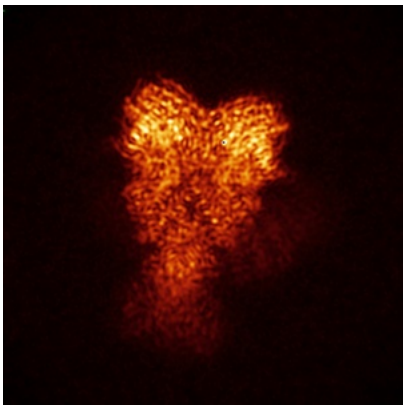

Y Index: 100


Z Index: 162

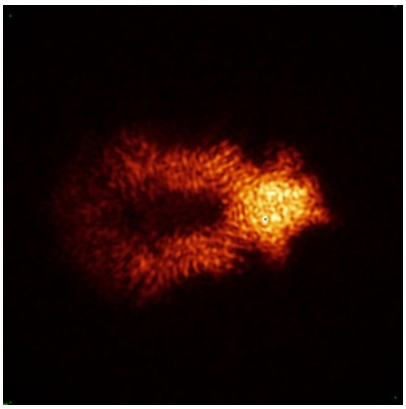
The images above show the largest variance slices of the map in three orthogonal directions.

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

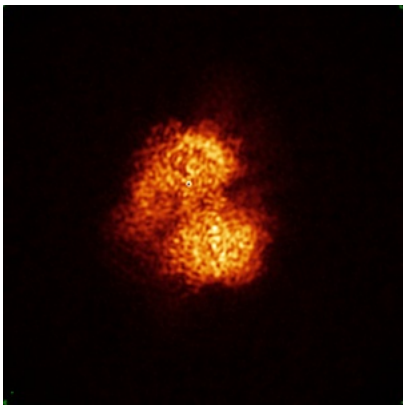
6.4.1 Primary map



X

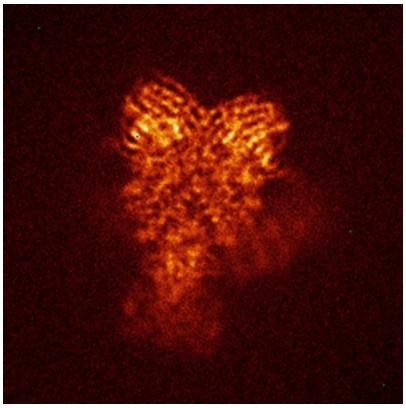


Y

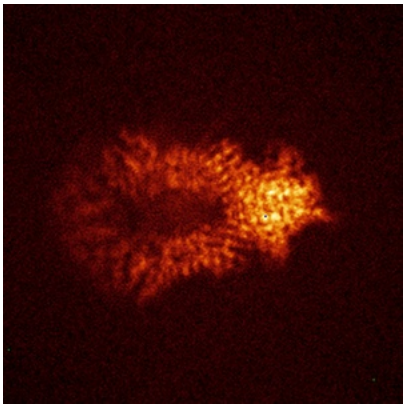


Z

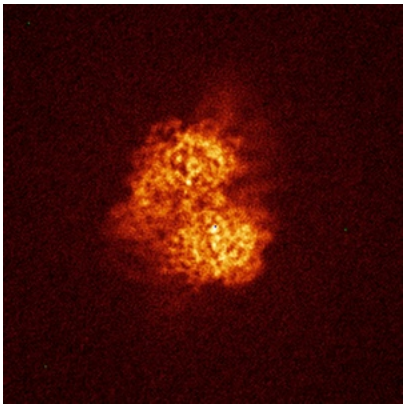
6.4.2 Raw map



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.

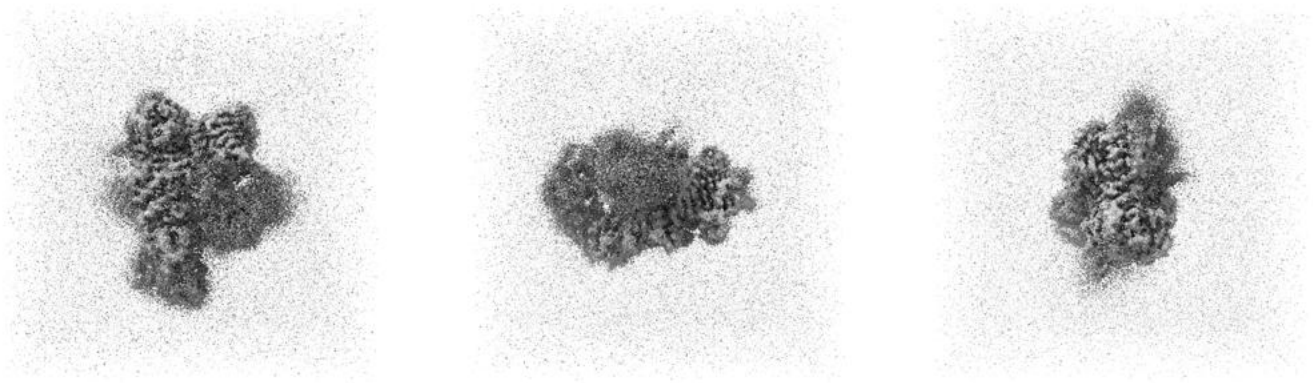
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

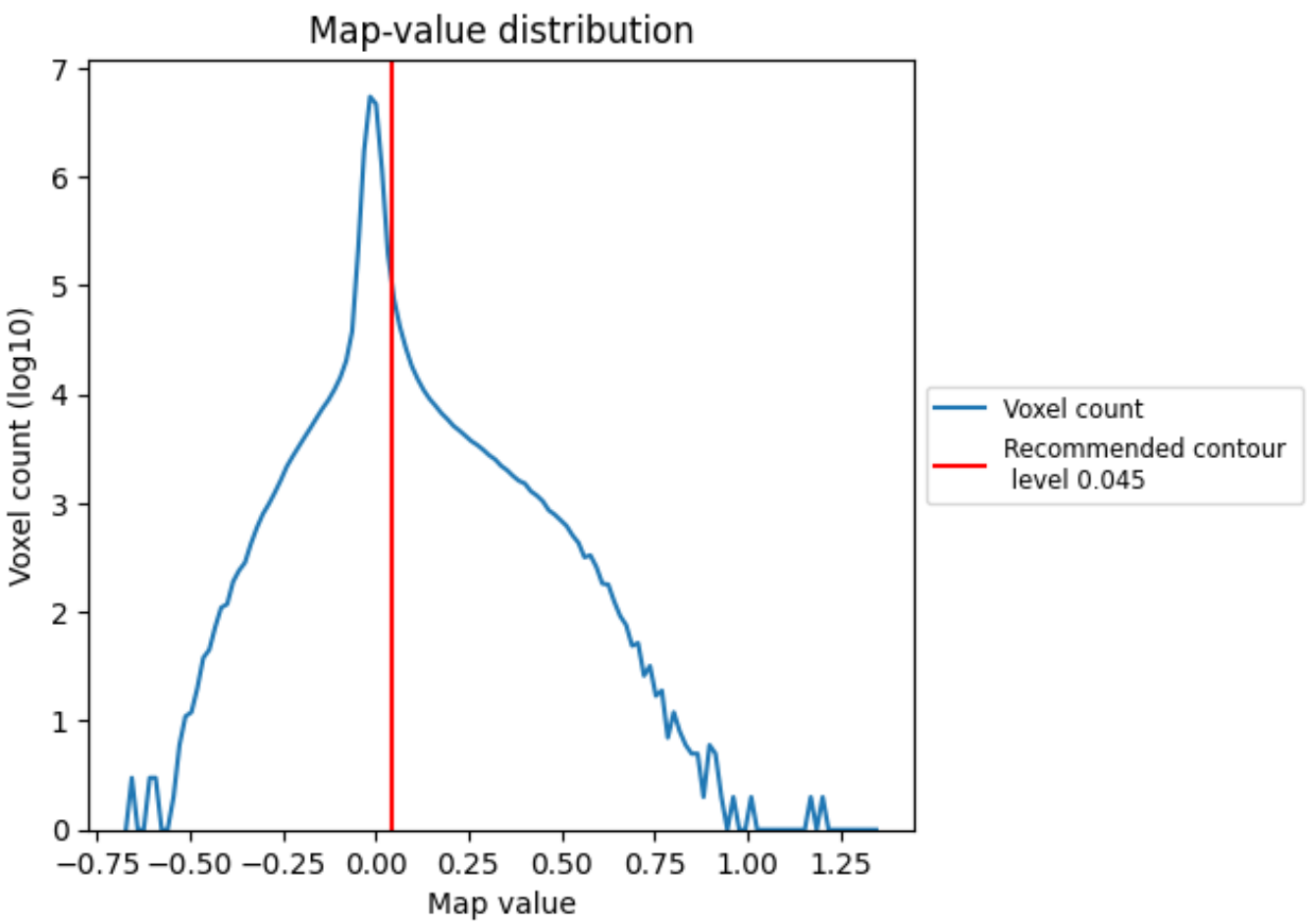
6.6 Mask visualisation (i)

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

7 Map analysis (i)

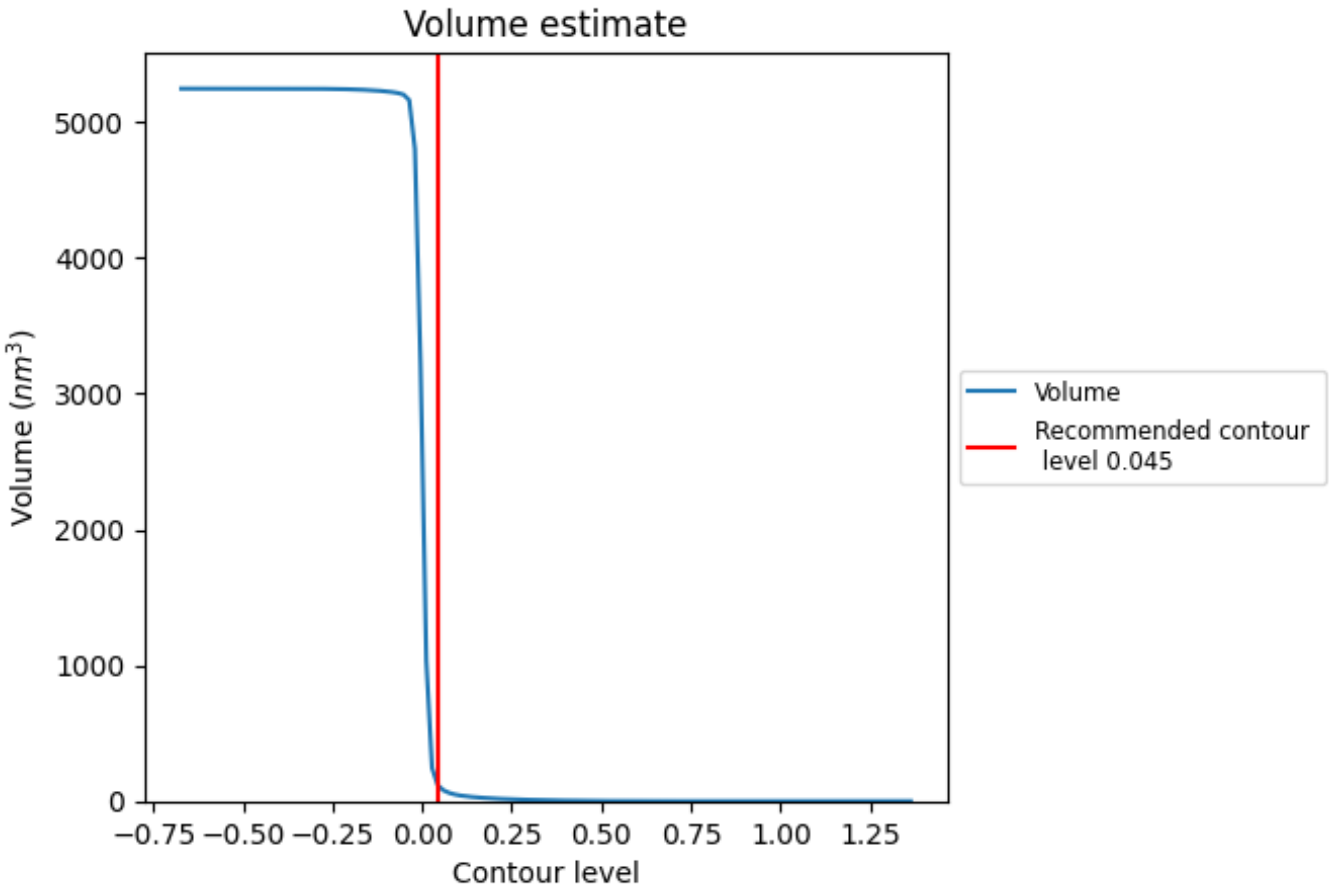
This section contains the results of statistical analysis of the map.

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.

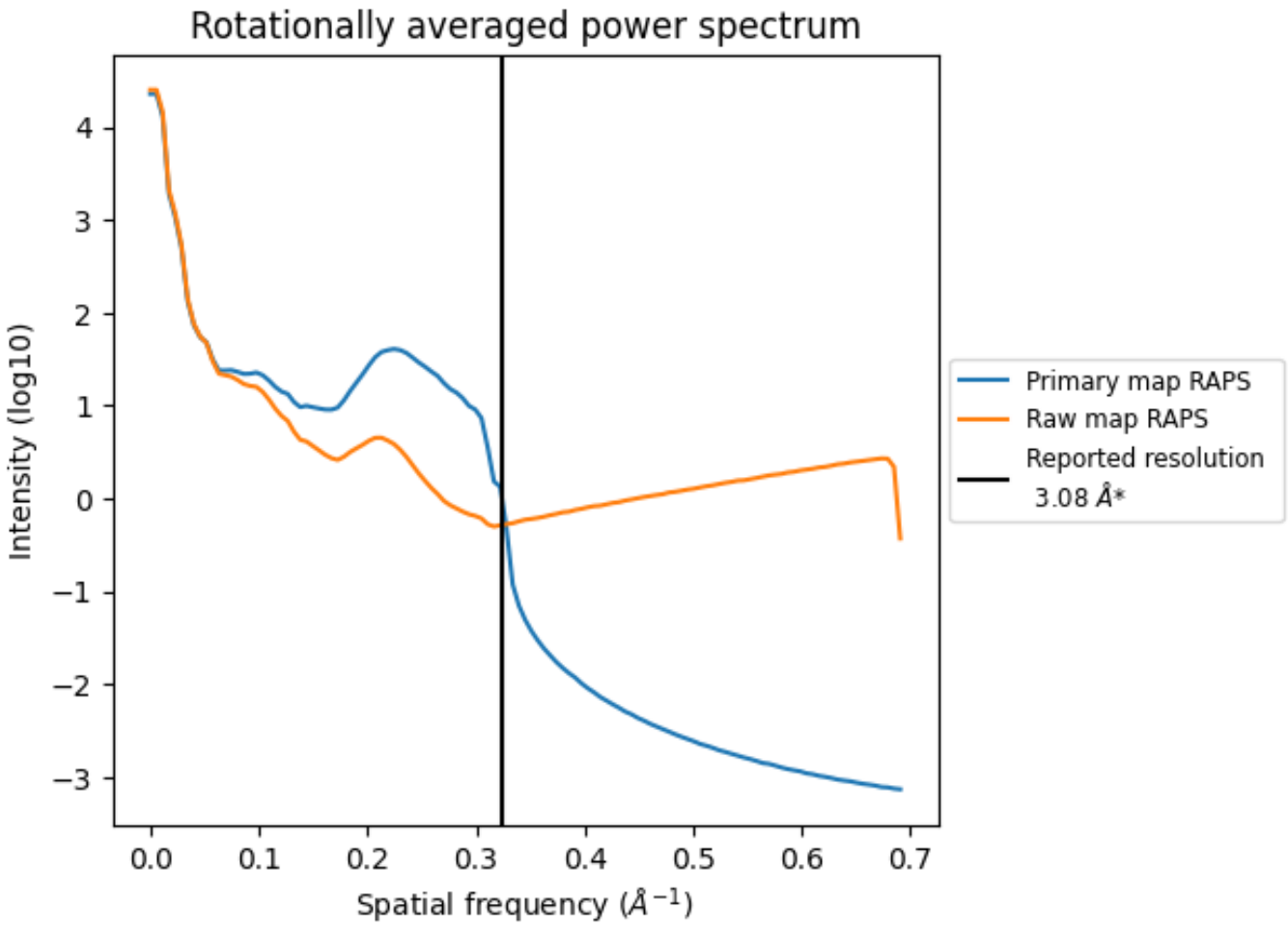
7.2 Volume estimate (i)



The volume at the recommended contour level is 114 nm^3; 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)

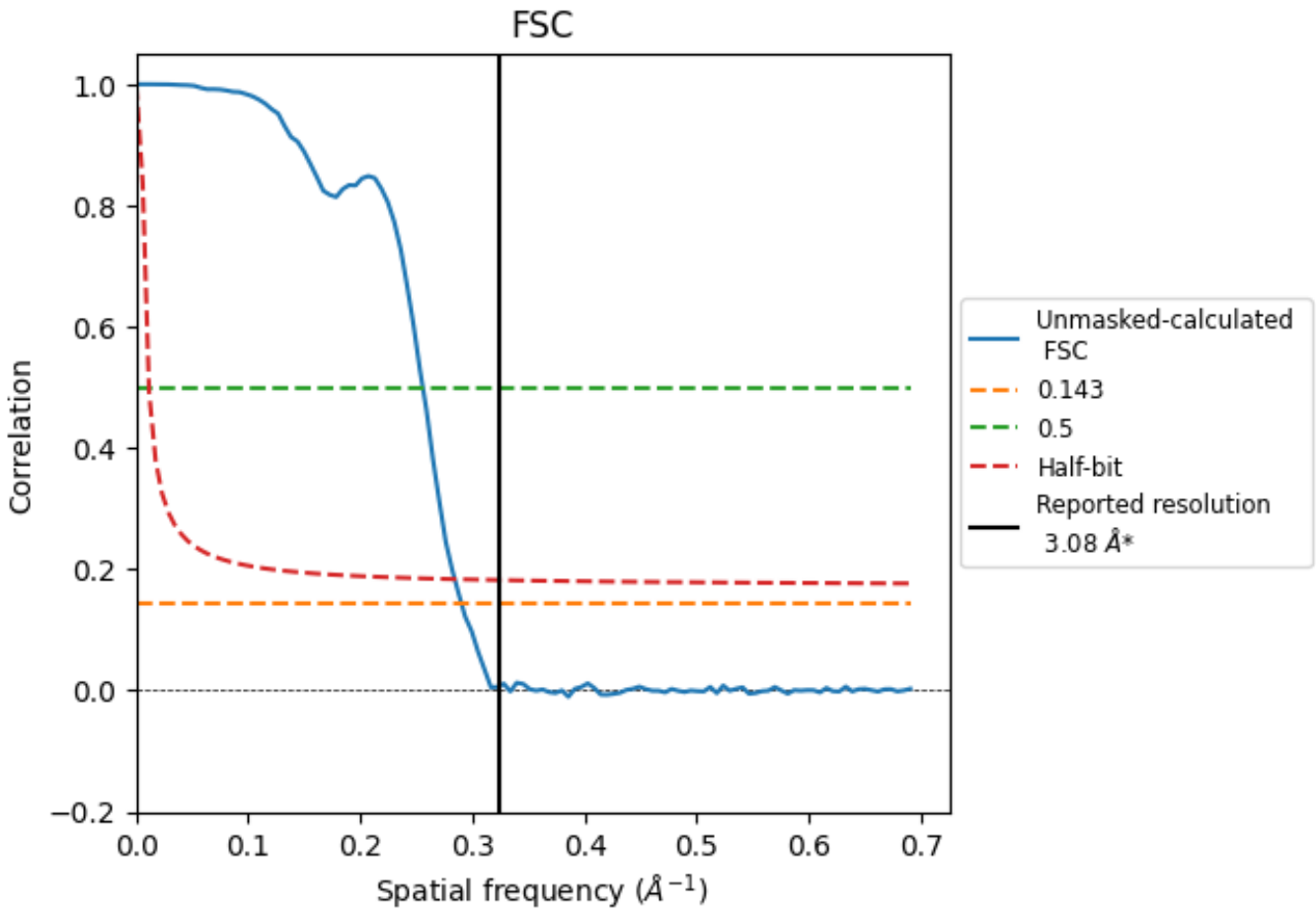


*Reported resolution corresponds to spatial frequency of 0.325 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.325 Å^{-1}

8.2 Resolution estimates (i)

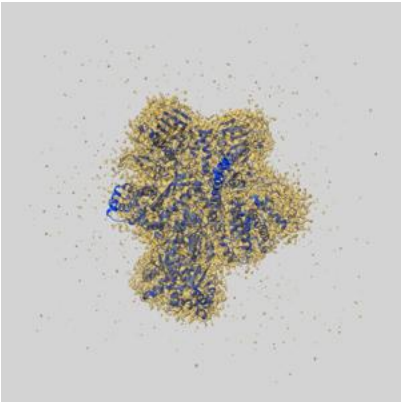
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.45	3.91	3.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.45 differs from the reported value 3.08 by more than 10 %

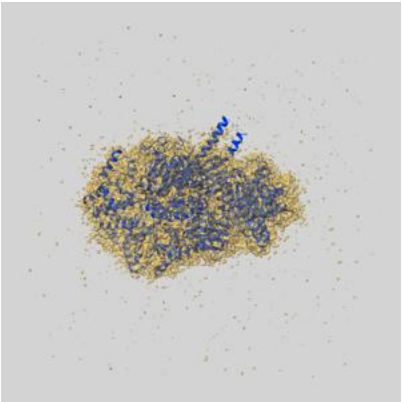
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-66567 and PDB model 9X4X. Per-residue inclusion information can be found in section 3 on page 5.

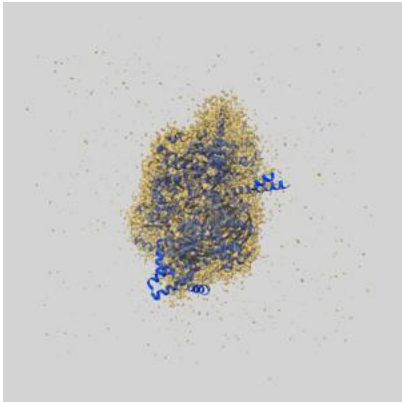
9.1 Map-model overlay (i)



X



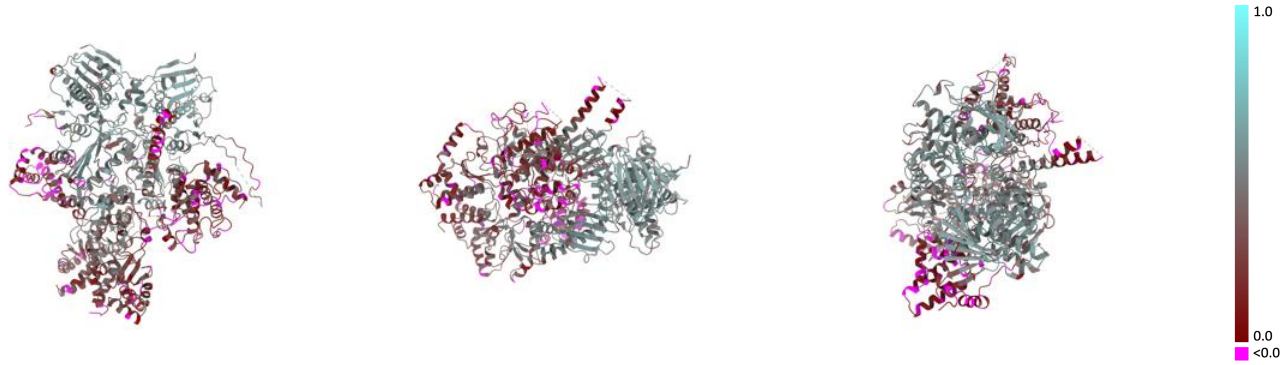
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

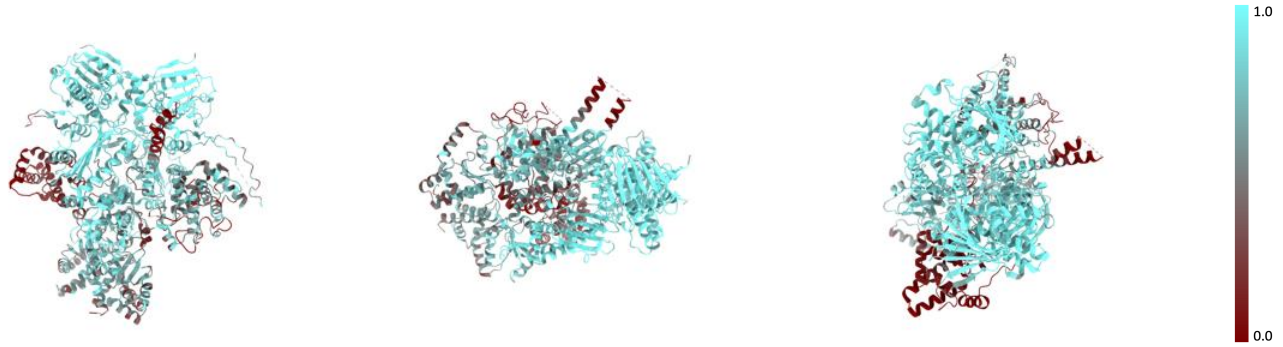
9.2 Q-score mapped to coordinate model (i)



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.

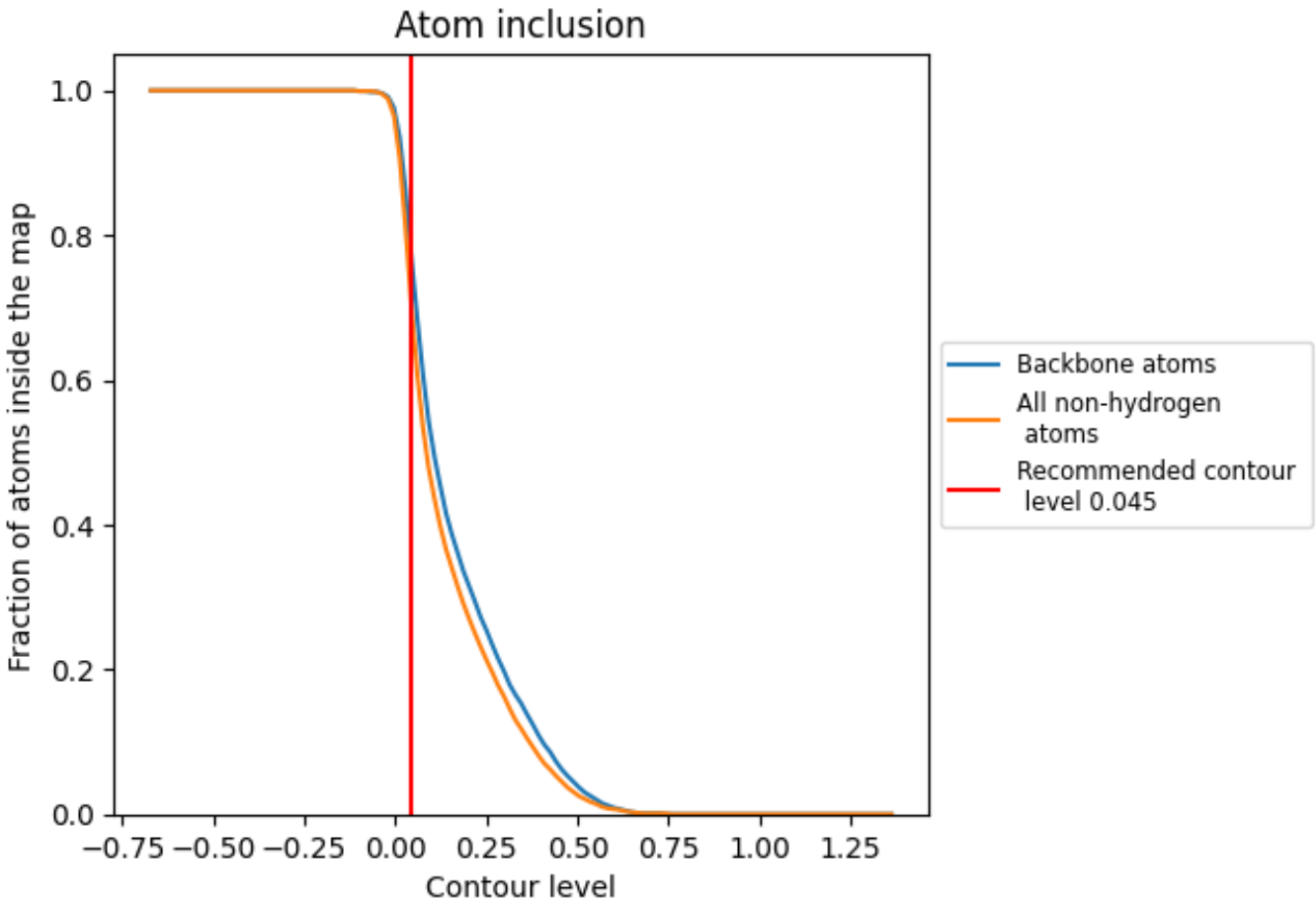
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 76% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6930	0.3560
A	0.7930	0.4150
B	0.8010	0.4290
C	0.2730	0.1500
D	0.5180	0.1860