wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 12:02 PM EST

PDB ID	:	7N5A
EMDB ID	:	EMD-24184
Title	:	Structure of AtAtm3 in the closed conformation
Authors	:	Fan, C.; Rees, D.C.
Deposited on	:	2021-06-05
Resolution	:	3.95 Å(reported)
Based on initial model	:	6PAR

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 (1)) were used in the production of this report:

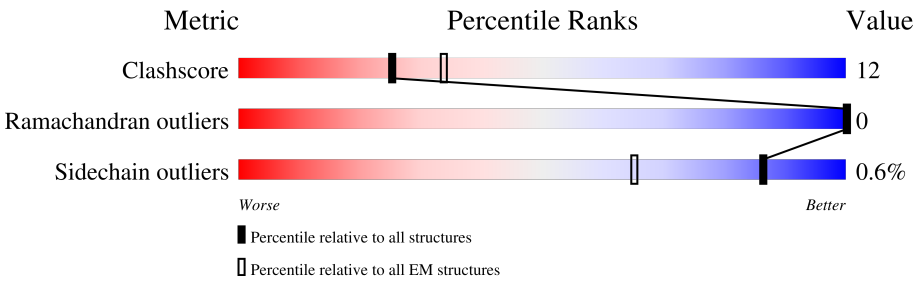
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.95 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	739	13% 57% 22% 20%
1	B	739	13% 58% 21% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9254 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.

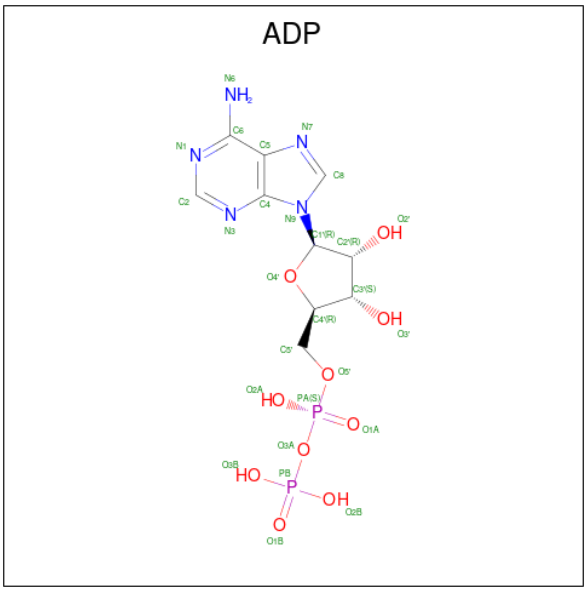
- Molecule 1 is a protein called ABC transporter B family member 25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	589	4594	2933	788	856	17	0	0
1	B	589	4594	2933	788	856	17	0	0

There are 22 discrepancies between the modelled and reference sequences:

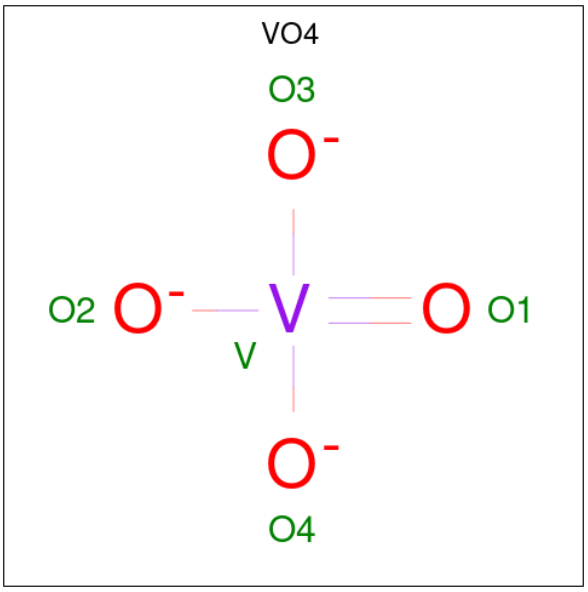
Chain	Residue	Modelled	Actual	Comment	Reference
A	729	ALA	-	expression tag	UNP Q9LVM1
A	730	ALA	-	expression tag	UNP Q9LVM1
A	731	ALA	-	expression tag	UNP Q9LVM1
A	732	LEU	-	expression tag	UNP Q9LVM1
A	733	GLU	-	expression tag	UNP Q9LVM1
A	734	HIS	-	expression tag	UNP Q9LVM1
A	735	HIS	-	expression tag	UNP Q9LVM1
A	736	HIS	-	expression tag	UNP Q9LVM1
A	737	HIS	-	expression tag	UNP Q9LVM1
A	738	HIS	-	expression tag	UNP Q9LVM1
A	739	HIS	-	expression tag	UNP Q9LVM1
B	729	ALA	-	expression tag	UNP Q9LVM1
B	730	ALA	-	expression tag	UNP Q9LVM1
B	731	ALA	-	expression tag	UNP Q9LVM1
B	732	LEU	-	expression tag	UNP Q9LVM1
B	733	GLU	-	expression tag	UNP Q9LVM1
B	734	HIS	-	expression tag	UNP Q9LVM1
B	735	HIS	-	expression tag	UNP Q9LVM1
B	736	HIS	-	expression tag	UNP Q9LVM1
B	737	HIS	-	expression tag	UNP Q9LVM1
B	738	HIS	-	expression tag	UNP Q9LVM1
B	739	HIS	-	expression tag	UNP Q9LVM1

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is VANADATE ION (three-letter code: VO4) (formula: O_4V) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	O	V	0
			5	4	1	

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Mol	Chain	Residues	Atoms			AltConf
			Total	O	V	
3	B	1	5	4	1	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

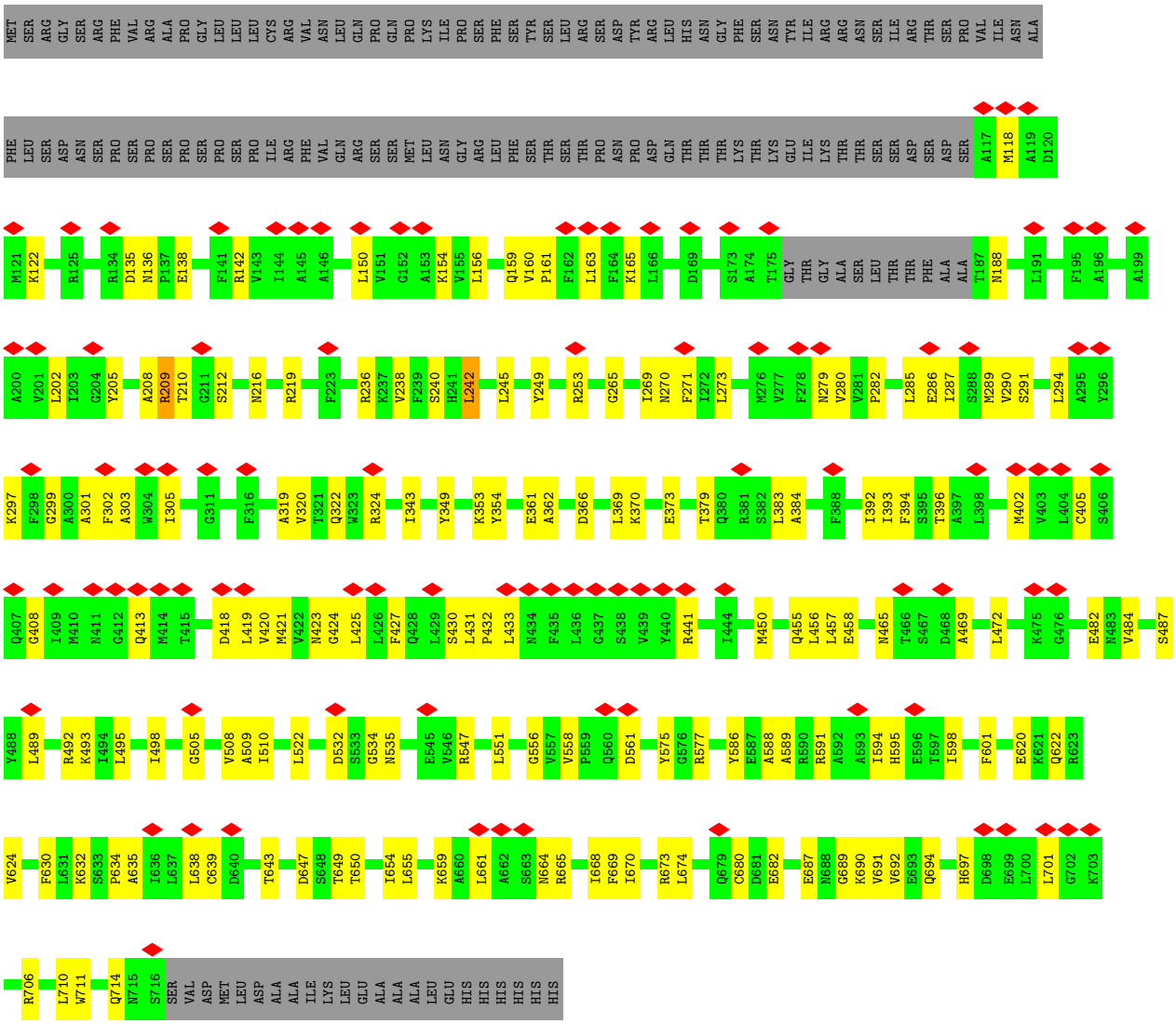
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0
4	B	1	1	1	0

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: ABC transporter B family member 25, mitochondrial

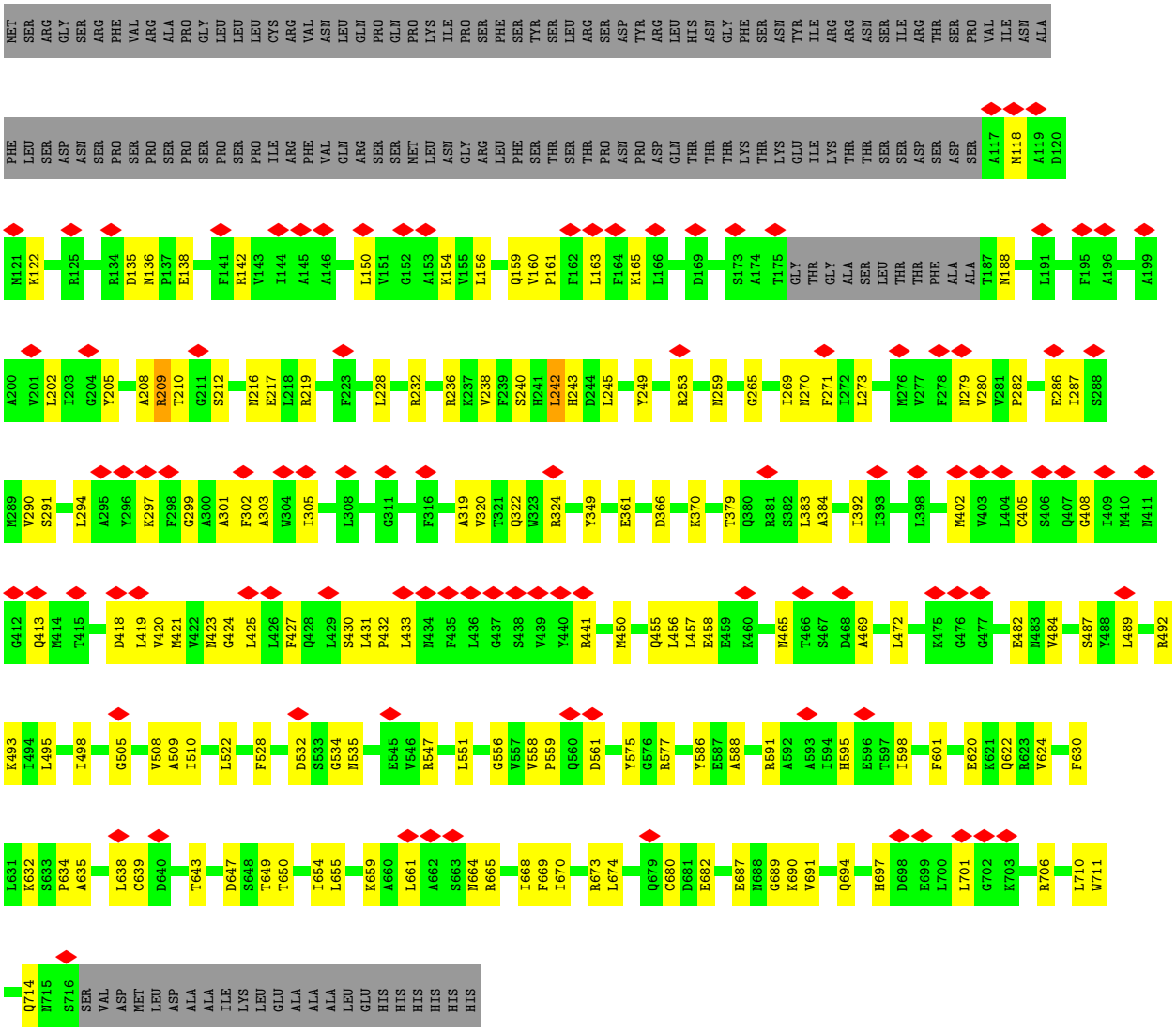
Chain A: 13% 57% 22% 20%



• Molecule 1: ABC transporter B family member 25, mitochondrial

Chain B:

13%
58%
21%
20%


MET SER ARG GLY SER ARG PHE VAL ARG ALA PRO GLY LEU LEU LEU CYS ARG VAL ASN LEU GLN PRO GLN PRO LYS ILE PRO SER PHE SER TYR SER LEU ARG SER ASP TYR ARG LEU HIS ASN GLY PHE SER ASN TYR ILE ARG ARG ASN SER ILE ARG THR SER PRO VAL ILE ASN ALA
PHE LEU SER ASP ASN SER PRO SER PRO SER PRO SER PRO SER PRO ILE ARG PHE VAL GLN ARG SER SER MET LEU ASN GLY ARG LEU PHE SER THR SER THR PRO ASN PRO ASP GLN THR THR THR LYS THR LYS GLU ILE LYS THR THR SER SER ASP SER ASP SER A117 M118 A119 D120
M121 K122 R125 R134 D135 N136 P137 E138 F141 R142 V143 I144 A145 A146 L150 V151 G152 A153 K154 V155 L156 Q159 V160 P161 F162 L163 F164 K165 L166 D169 S173 A174 T175 GLY THR GLY ALA SER LEU THR THR PHE ALA ALA T187 N188 L191 F195 A196 A199
A200 V201 L202 I203 G204 Y205 A208 R209 T210 G211 S212 N216 E217 L218 R219 F223 L228 R232 R236 K237 V238 F239 S240 H241 L242 H243 D244 L245 Y249 R253 N259 G265 I269 N270 F271 I272 L273 M276 V277 F278 N279 V280 V281 P282 E286 I287 S288
M289 V290 S291 L294 A295 Y296 K297 F298 G299 A300 A301 F302 A303 W304 I305 L308 G311 F316 A319 V320 T321 Q322 W323 R324 Y349 E361 D366 K370 T379 Q380 R381 S382 L383 A384 I392 I393 L398 M402 V403 I404 C405 S406 Q407 G408 I409 M410 N411
G412 Q413 M414 T415 D418 L419 V420 M421 V422 N423 G424 L425 L426 F427 Q428 L429 S430 L431 P432 L433 N434 F435 L436 G437 S438 V439 Y440 R441 M450 Q455 L456 L457 E458 E459 K460 N465 T466 S467 D468 A469 L472 K475 G476 G477 E482 N483 V484 S487 Y488 L489 R492
K493 I494 L495 I498 G505 V508 A509 I510 L522 F528 D532 S533 G534 N535 E545 V546 R547 L551 G556 V557 V558 P559 Q560 D561 Y575 G576 R577 Y586 E587 A588 R591 A592 A593 I594 H595 E596 T597 I598 F601 E620 K621 Q622 R623 V624 F630
L631 K632 S633 P634 A635 L638 C639 D640 T643 D647 S648 T649 T650 I654 L655 K659 A660 L661 A662 S663 N664 R665 I668 F669 I670 R673 L674 Q679 C680 D681 E682 E687 N688 G689 K690 V691 Q694 H697 D698 E699 L700 L701 G702 K703 R706 L710 W711
Q714 N715 S716 SER VAL ASP MET LEU ASP ALA ALA ILE LYS LEU GLU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	140569	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.163	Depositor
Minimum map value	-1.106	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	246.0, 246.0, 246.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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: ADP, VO4, MG

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	0.25	0/4674	0.49	0/6322
1	B	0.25	0/4674	0.49	0/6322
All	All	0.25	0/9348	0.49	0/12644

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	4594	0	4662	121	0
1	B	4594	0	4662	116	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	9254	0	9348	214	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 12.

The worst 5 of 214 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:A:402:MET:HB3	1:B:202:LEU:HD13	1.68	0.75
1:A:419:LEU:O	1:A:423:ASN:ND2	2.28	0.67
1:A:421:MET:O	1:A:425:LEU:N	2.24	0.67
1:B:510:ILE:HB	1:B:670:ILE:HG22	1.77	0.67
1:B:691:VAL:HG12	1:B:694:GLN:HE22	1.60	0.67

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	585/739 (79%)	573 (98%)	12 (2%)	0	100	100
1	B	585/739 (79%)	573 (98%)	12 (2%)	0	100	100
All	All	1170/1478 (79%)	1146 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	498/632 (79%)	495 (99%)	3 (1%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	498/632 (79%)	495 (99%)	3 (1%)	86 91
All	All	996/1264 (79%)	990 (99%)	6 (1%)	86 91

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	188	ASN
1	B	209	ARG
1	B	242	LEU
1	A	209	ARG
1	A	188	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	694	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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	ADP	A	801	4	24,29,29	0.96	1 (4%)	29,45,45	1.42	4 (13%)
3	VO4	B	803	4	1,4,4	4.85	1 (100%)	-		
3	VO4	A	802	4	1,4,4	4.85	1 (100%)	-		
2	ADP	B	802	4	24,29,29	0.95	1 (4%)	29,45,45	1.42	4 (13%)

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
2	ADP	A	801	4	-	7/12/32/32	0/3/3/3
2	ADP	B	802	4	-	7/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	VO4	O1-V	4.85	1.91	1.63
3	B	803	VO4	O1-V	4.85	1.91	1.63
2	A	801	ADP	C5-C4	2.45	1.47	1.40
2	B	802	ADP	C5-C4	2.44	1.47	1.40

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	802	ADP	N3-C2-N1	-3.18	123.70	128.68
2	A	801	ADP	PA-O3A-PB	-3.17	121.95	132.83
2	B	802	ADP	PA-O3A-PB	-3.17	121.96	132.83
2	A	801	ADP	N3-C2-N1	-3.15	123.76	128.68
2	A	801	ADP	C3'-C2'-C1'	3.10	105.64	100.98

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ADP	C5'-O5'-PA-O1A
2	A	801	ADP	C5'-O5'-PA-O2A

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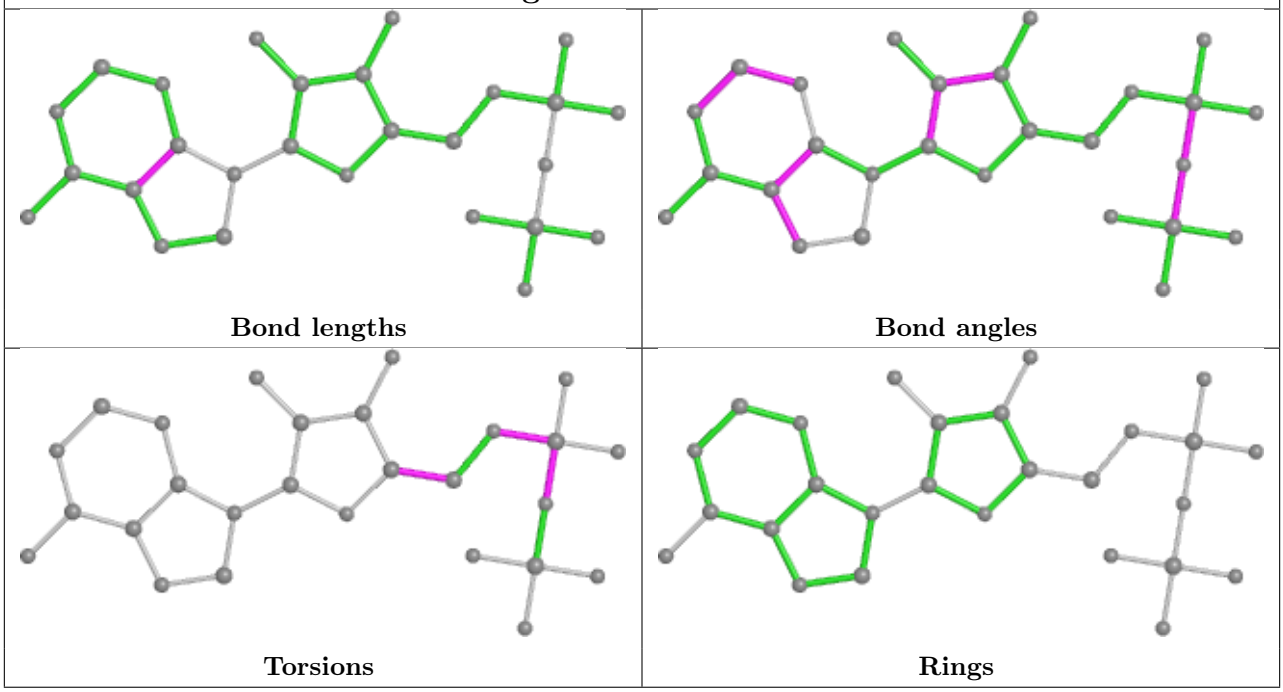
Mol	Chain	Res	Type	Atoms
2	A	801	ADP	C5'-O5'-PA-O3A
2	A	801	ADP	O4'-C4'-C5'-O5'
2	A	801	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

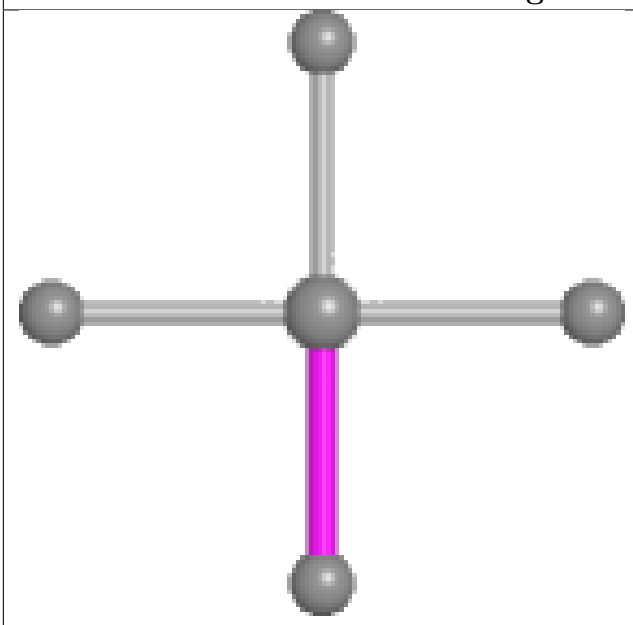
No monomer is involved in short contacts.

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.

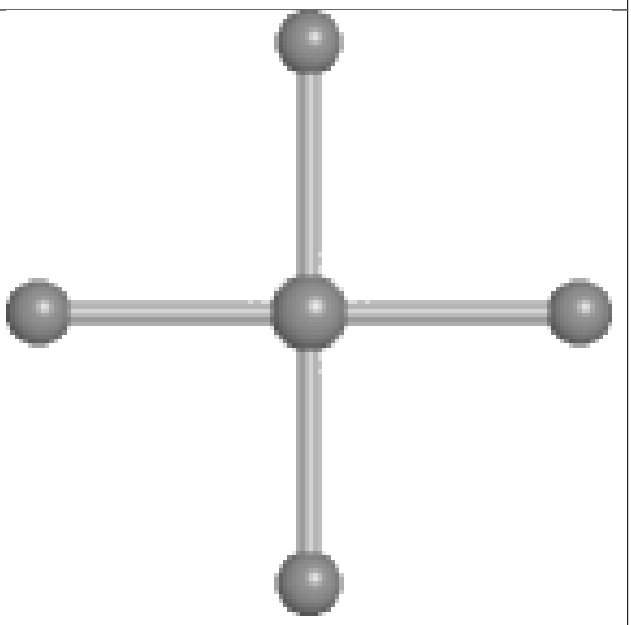
Ligand ADP A 801



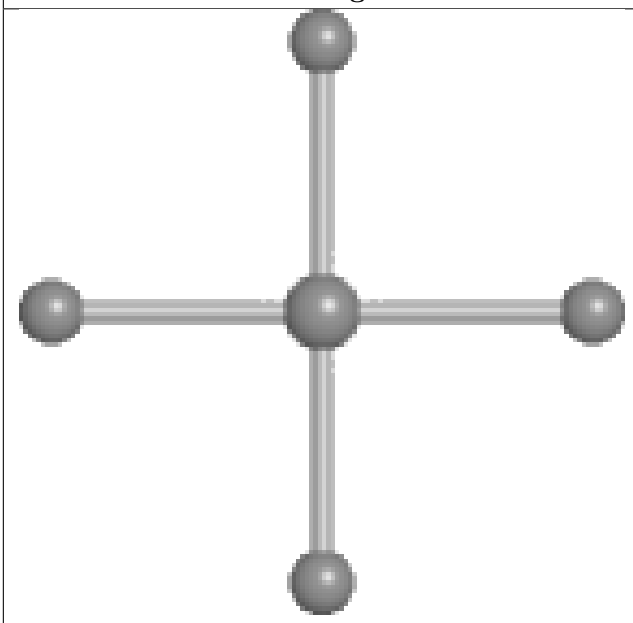
Ligand VO4 B 803



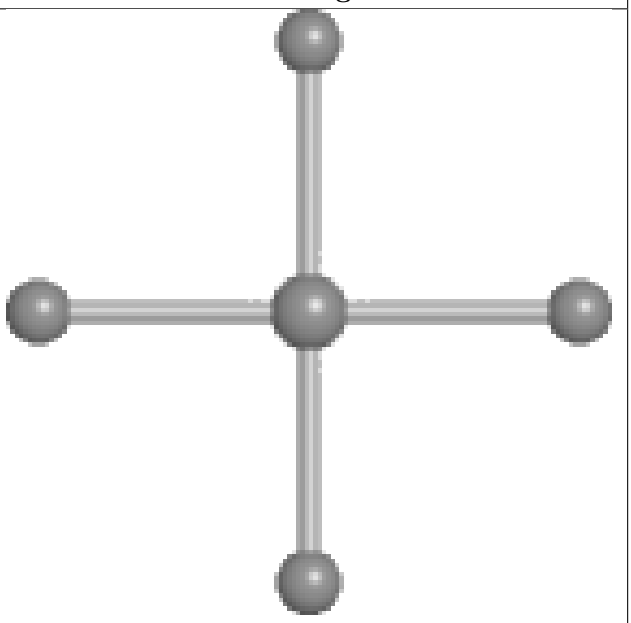
Bond lengths



Bond angles

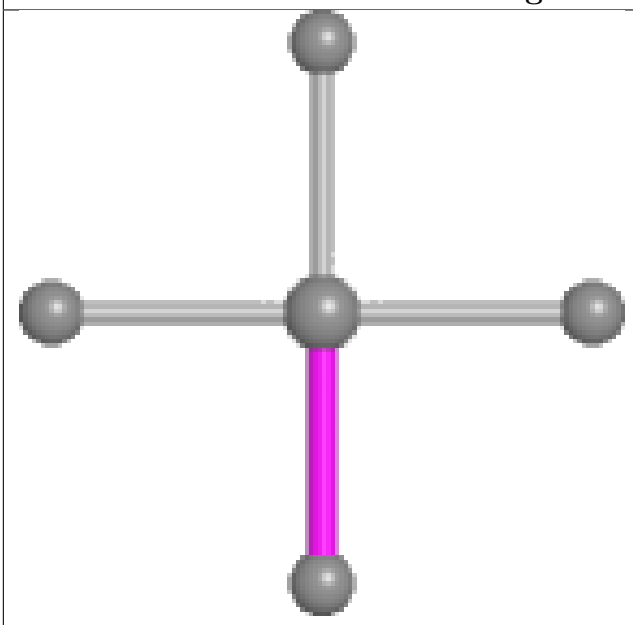


Torsions

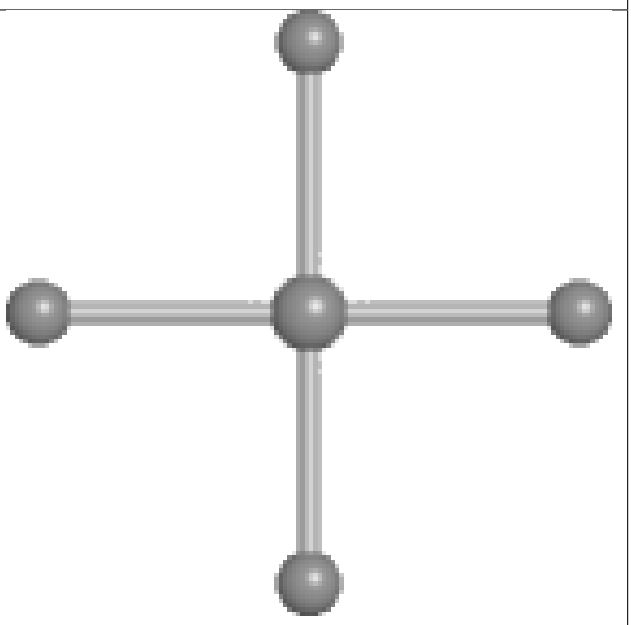


Rings

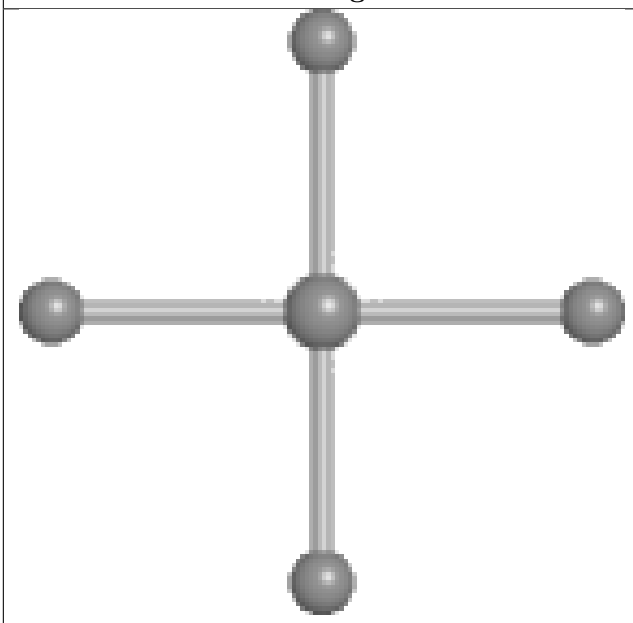
Ligand VO4 A 802



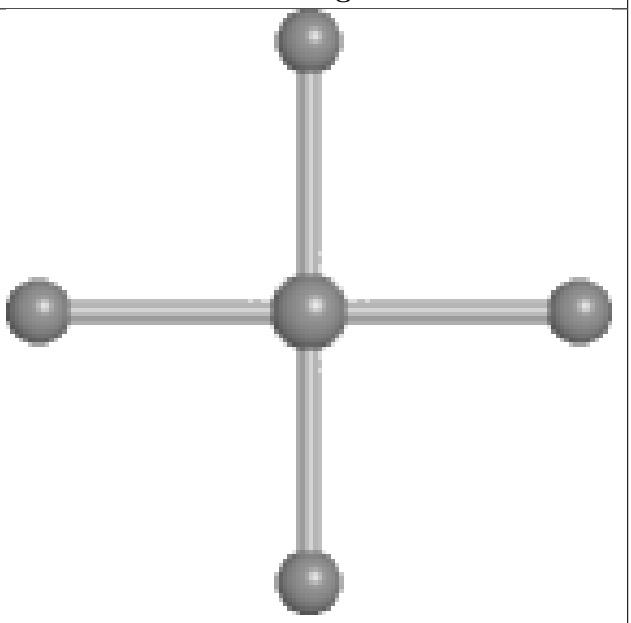
Bond lengths



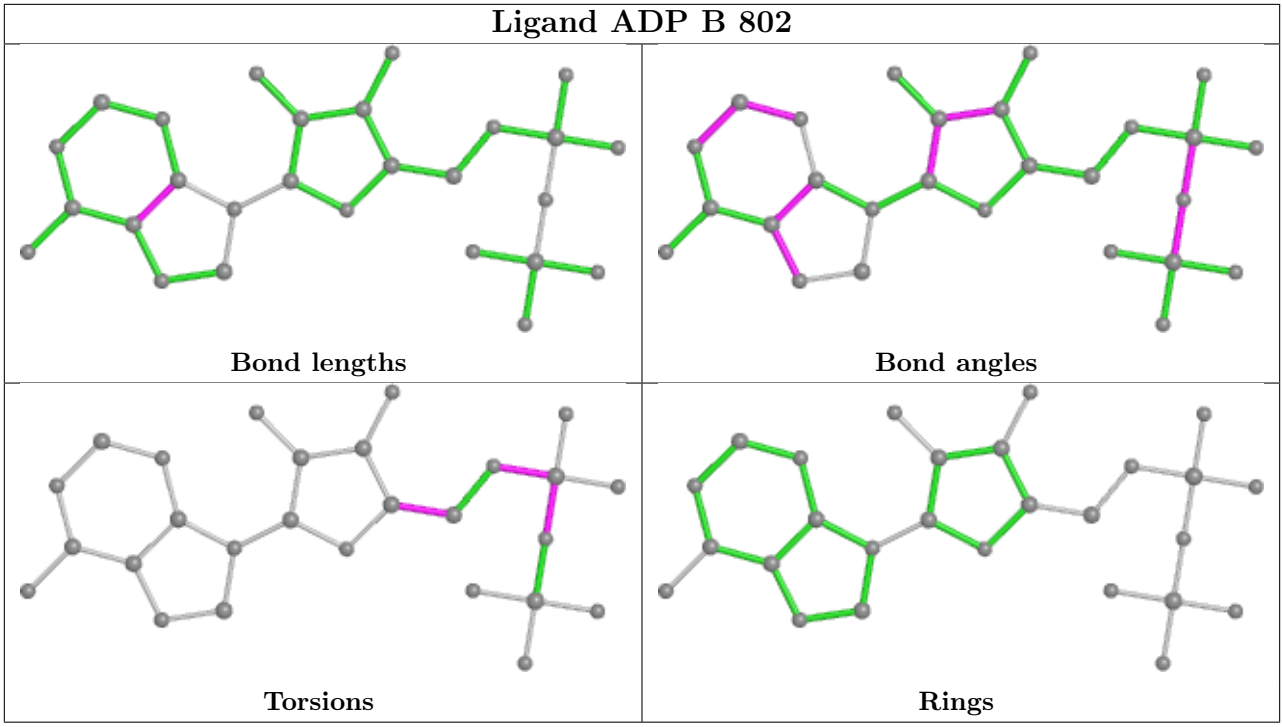
Bond angles



Torsions



Rings



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.

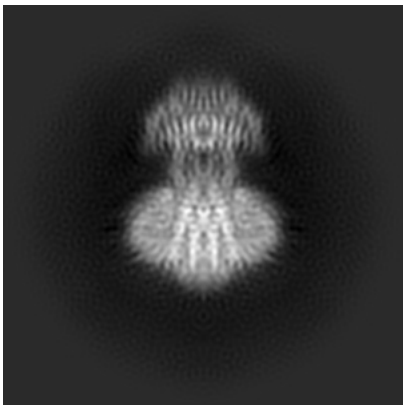
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24184. These allow visual inspection of the internal detail of the map and identification of artifacts.

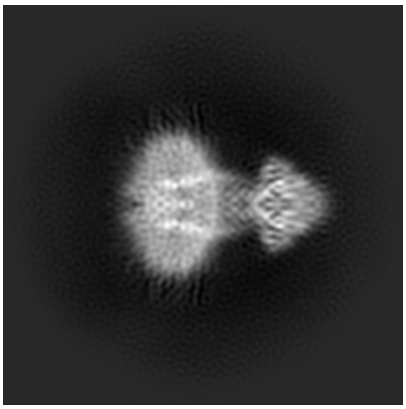
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

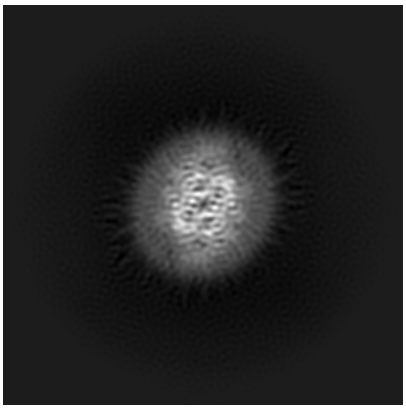
6.1.1 Primary map



X

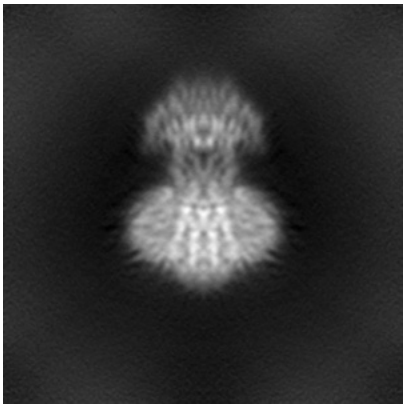


Y

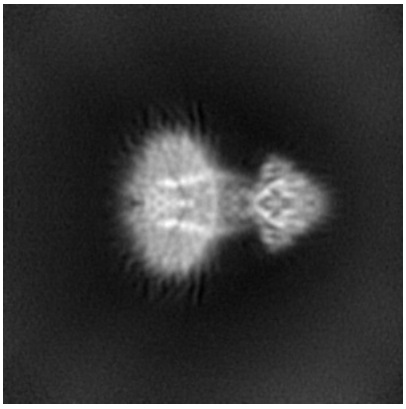


Z

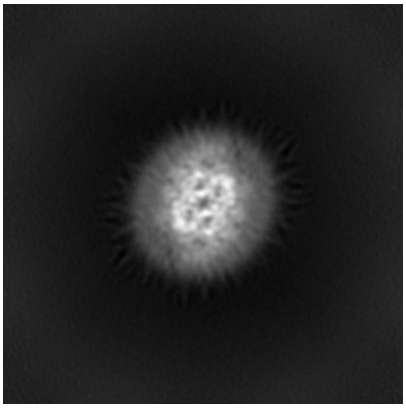
6.1.2 Raw map



X



Y

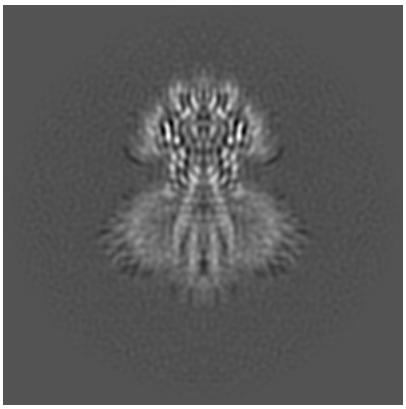


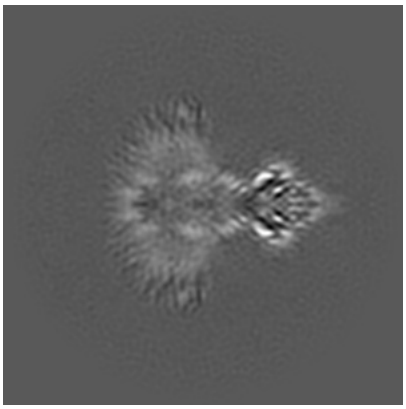
Z

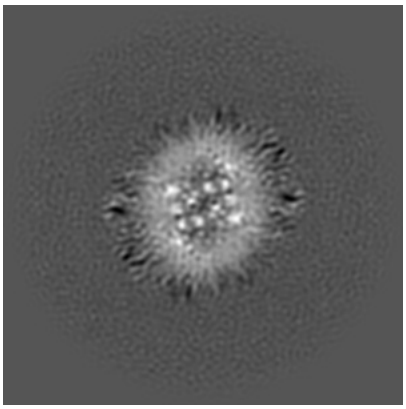
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

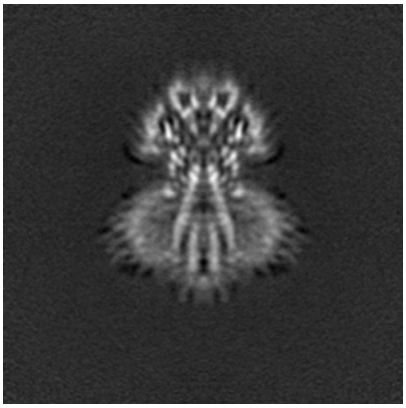
6.2.1 Primary map

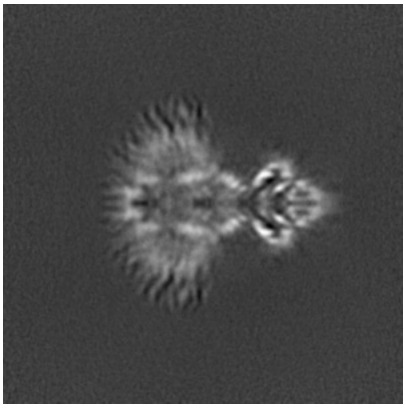

X Index: 150

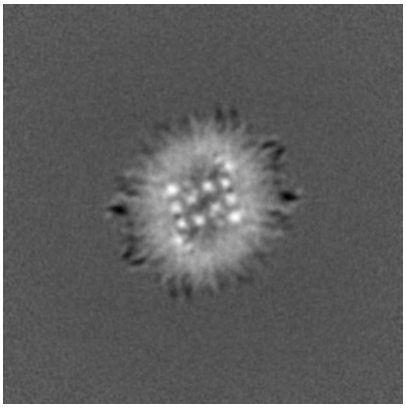

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

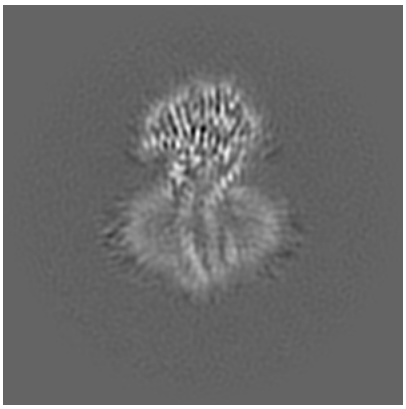

Y Index: 150

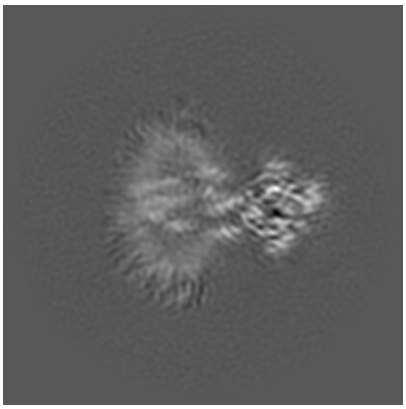

Z Index: 150

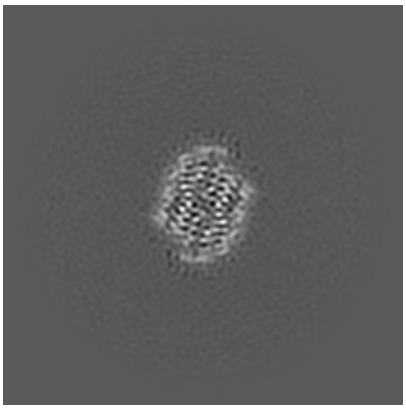
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

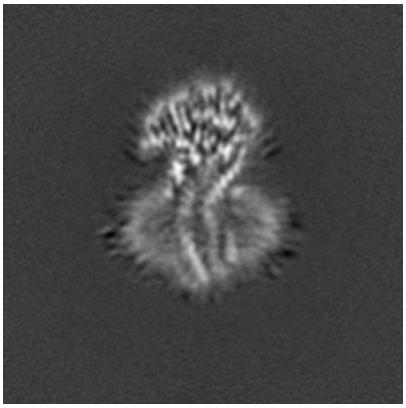
6.3.1 Primary map

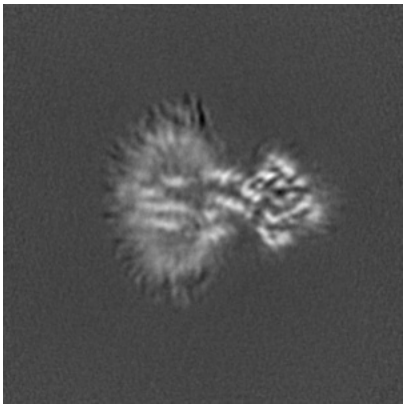

X Index: 143

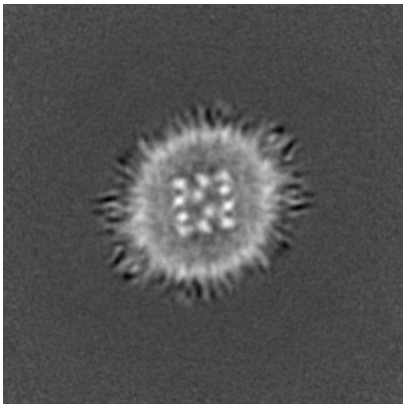

Y Index: 142


Z Index: 206

6.3.2 Raw map


X Index: 143

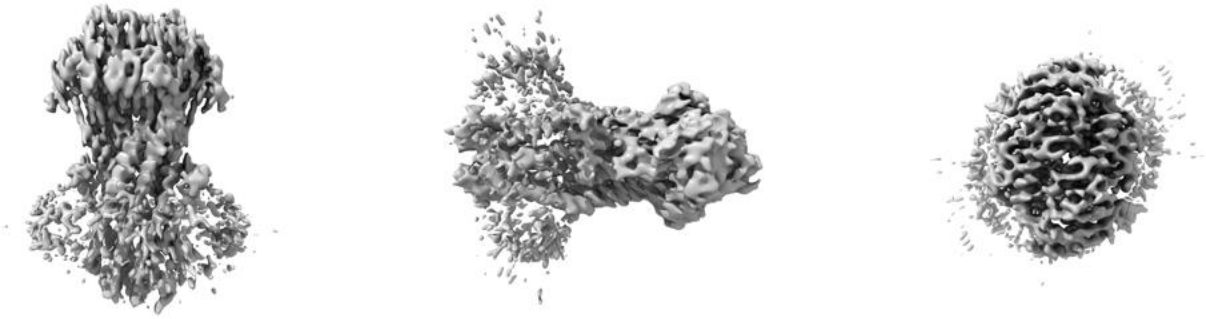

Y Index: 157


Z Index: 136

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

6.4 Orthogonal surface views (i)

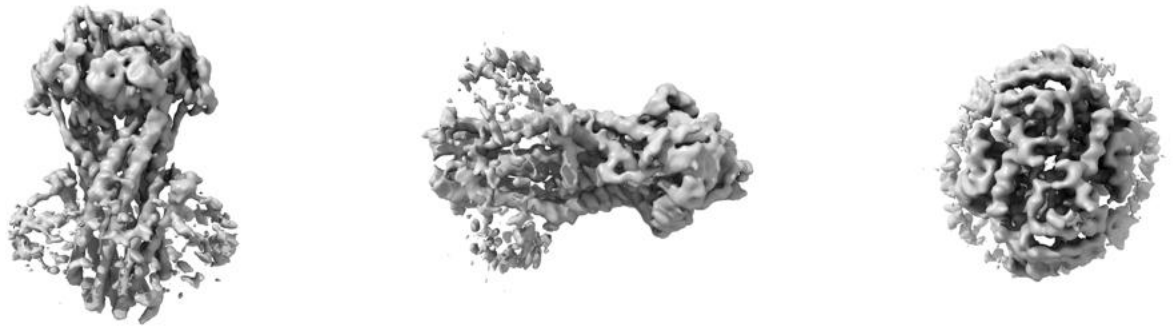
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

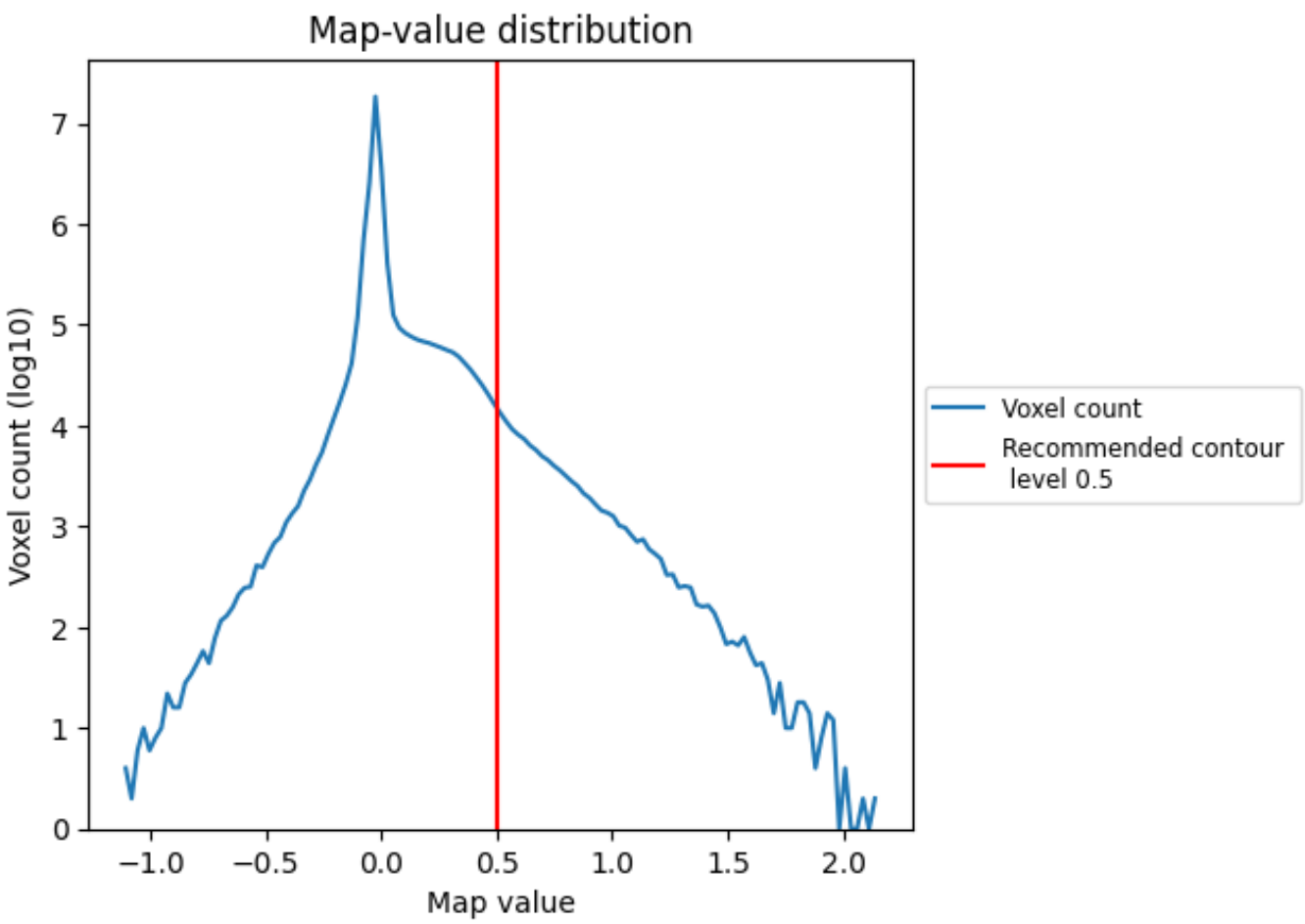
6.5 Mask visualisation (i)

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

7 Map analysis (i)

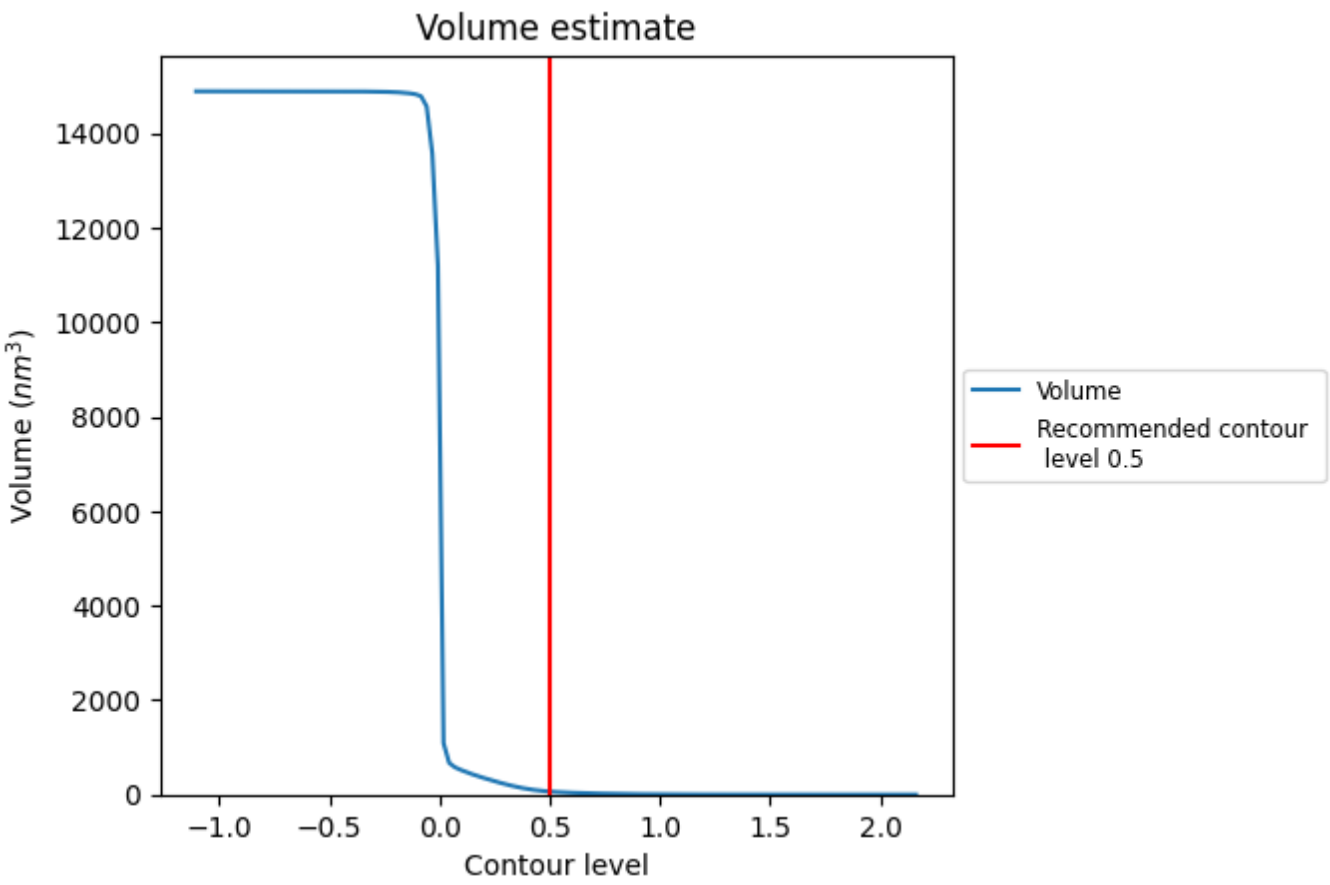
This section contains the results of statistical analysis of the map.

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.

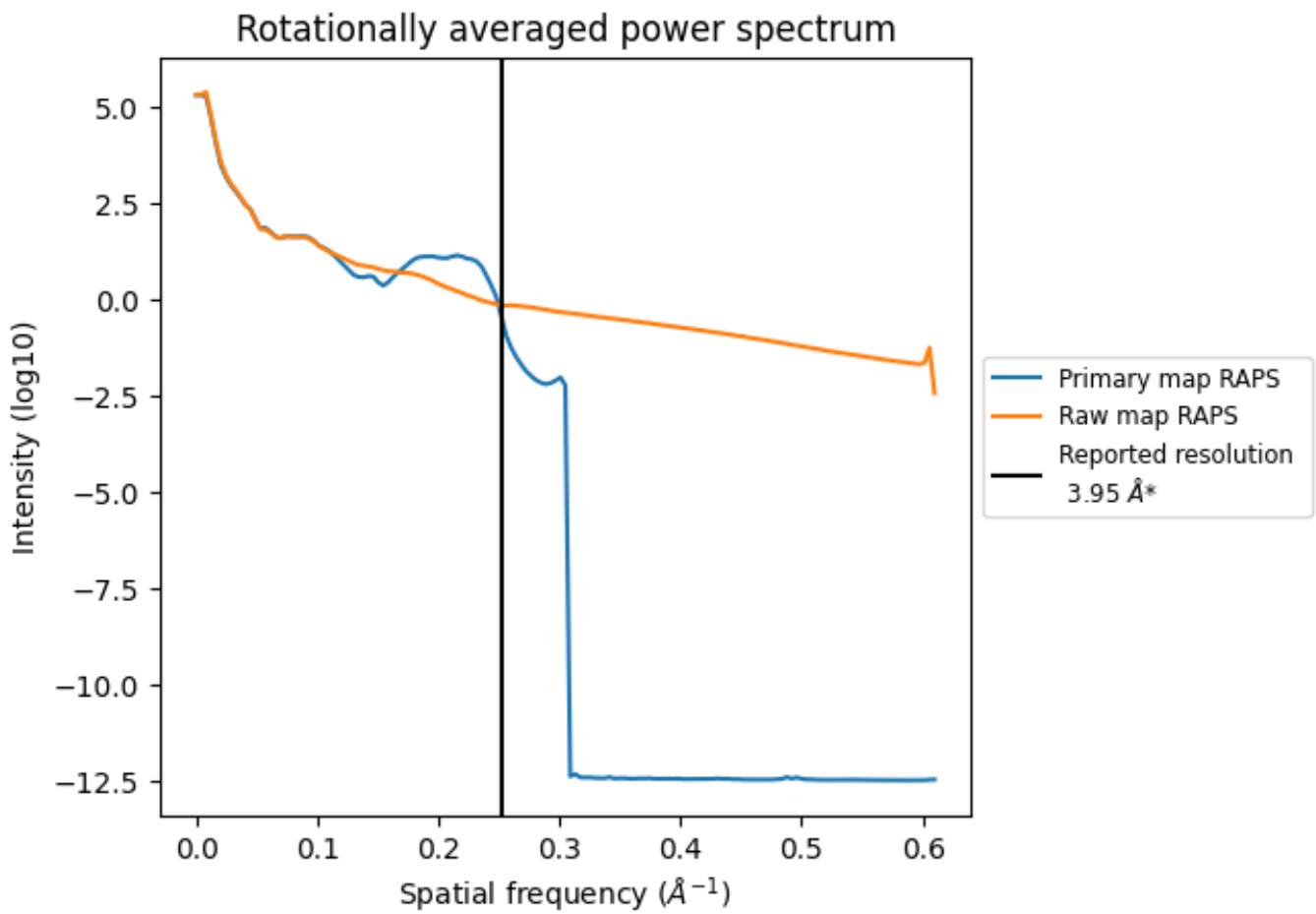
7.2 Volume estimate (i)



The volume at the recommended contour level is 63 nm^3; this corresponds to an approximate mass of 57 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)

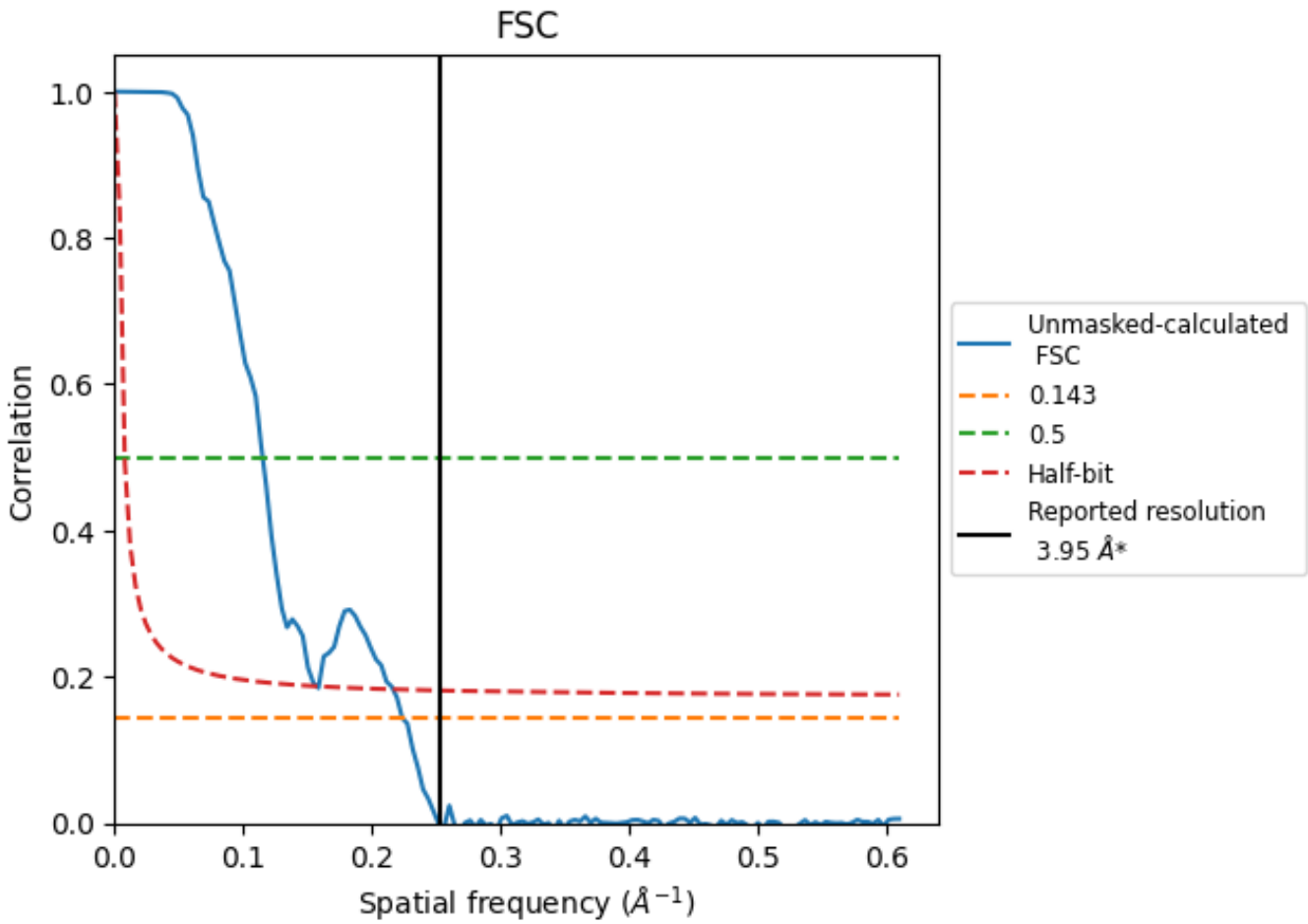


*Reported resolution corresponds to spatial frequency of 0.253 Å^{-1}

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 0.253 Å^{-1}

8.2 Resolution estimates (i)

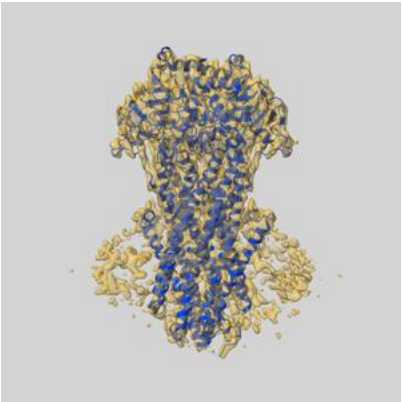
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.95	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.47	8.69	6.36

*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 4.47 differs from the reported value 3.95 by more than 10 %

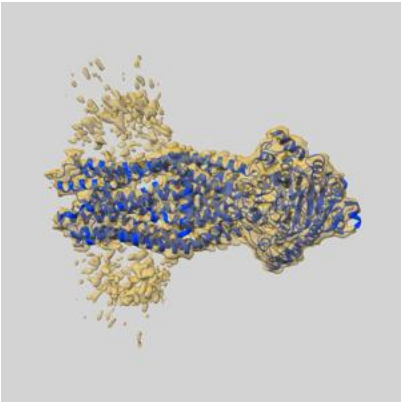
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24184 and PDB model 7N5A. Per-residue inclusion information can be found in section 3 on page 6.

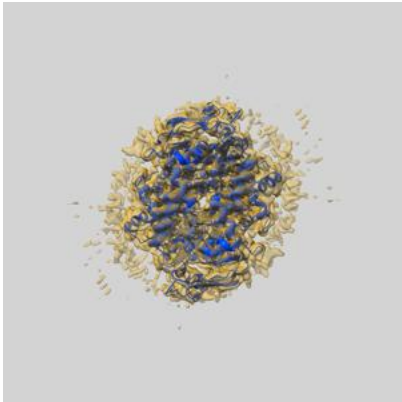
9.1 Map-model overlay (i)



X



Y



Z

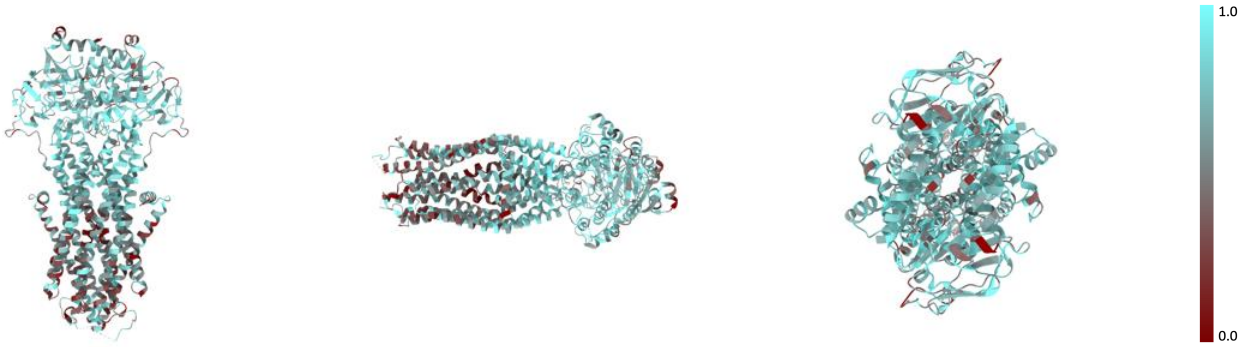
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

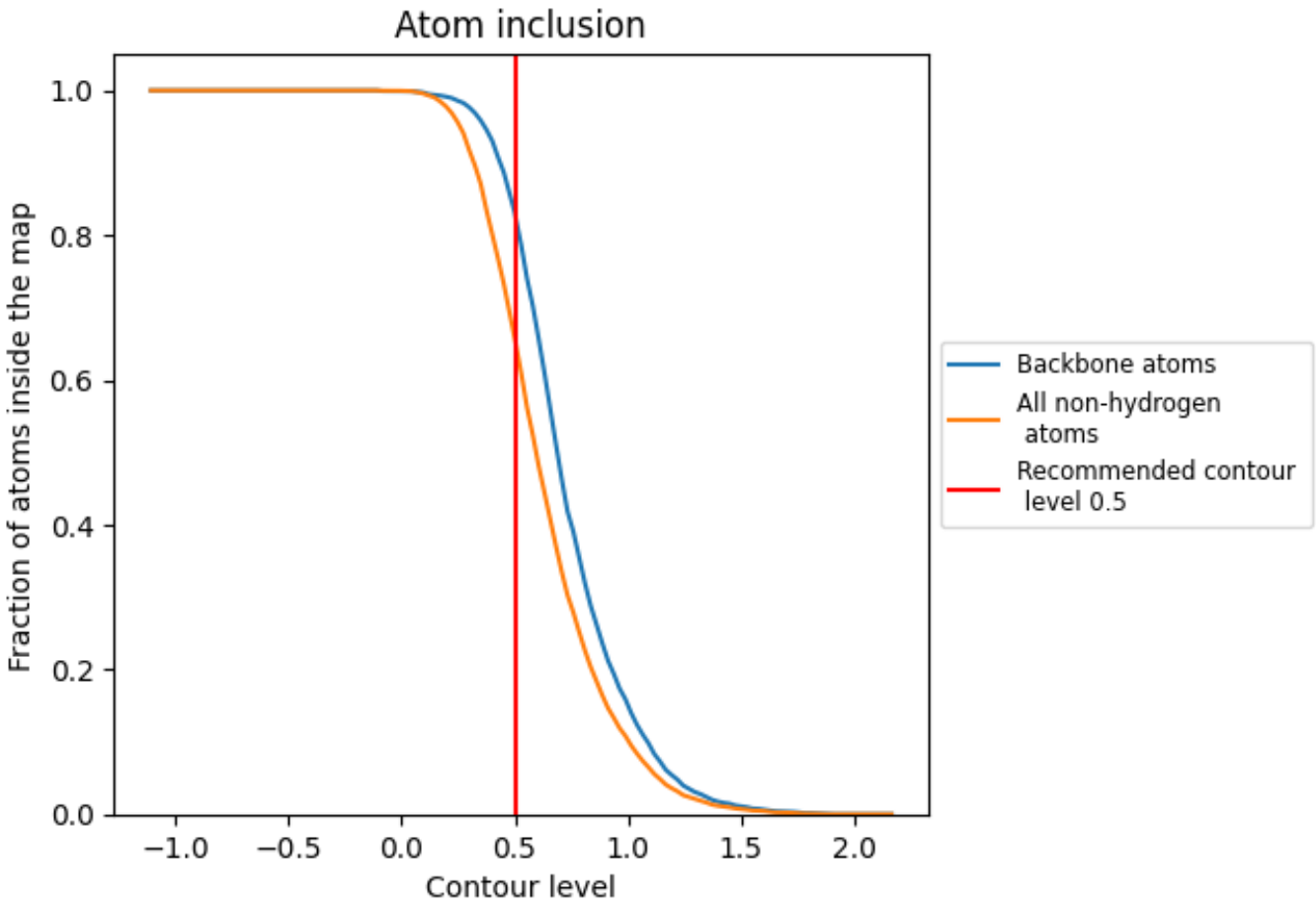
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 66% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6570	0.3640
A	0.6569	0.3650
B	0.6571	0.3630