wwPDB EM Validation Summary Report (i)

Nov 26, 2023 – 10:15 PM JST

PDB ID	:	8I6P
EMDB ID	:	EMD-35202
Title	:	The cryo-EM structure of OsCyc1 tetramer state
Authors	:	Ma, X.L.; Xu, H.F.; Tong, Y.R.; Luo, Y.F.; Dong, Q.H.; Jiang, T.
Deposited on	:	2023-01-29
Resolution	:	3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

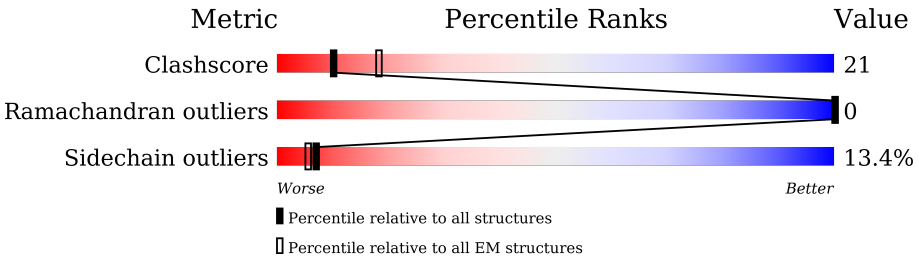
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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	775	44% 40% 5% 11%
1	B	775	45% 39% 5% 11%
1	C	775	46% 38% · 11%
1	D	775	46% 38% · 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 22016 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 Syn-copalyl diphosphate synthase, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	688	Total	C	N	O	S	0	0
			5504	3492	944	1033	35		
1	C	688	Total	C	N	O	S	0	0
			5504	3492	944	1033	35		
1	D	688	Total	C	N	O	S	0	0
			5504	3492	944	1033	35		
1	A	688	Total	C	N	O	S	0	0
			5504	3492	944	1033	35		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	768	GLU	-	expression tag	UNP Q0JF02
B	769	PHE	-	expression tag	UNP Q0JF02
B	770	HIS	-	expression tag	UNP Q0JF02
B	771	HIS	-	expression tag	UNP Q0JF02
B	772	HIS	-	expression tag	UNP Q0JF02
B	773	HIS	-	expression tag	UNP Q0JF02
B	774	HIS	-	expression tag	UNP Q0JF02
B	775	HIS	-	expression tag	UNP Q0JF02
C	768	GLU	-	expression tag	UNP Q0JF02
C	769	PHE	-	expression tag	UNP Q0JF02
C	770	HIS	-	expression tag	UNP Q0JF02
C	771	HIS	-	expression tag	UNP Q0JF02
C	772	HIS	-	expression tag	UNP Q0JF02
C	773	HIS	-	expression tag	UNP Q0JF02
C	774	HIS	-	expression tag	UNP Q0JF02
C	775	HIS	-	expression tag	UNP Q0JF02
D	768	GLU	-	expression tag	UNP Q0JF02
D	769	PHE	-	expression tag	UNP Q0JF02
D	770	HIS	-	expression tag	UNP Q0JF02
D	771	HIS	-	expression tag	UNP Q0JF02
D	772	HIS	-	expression tag	UNP Q0JF02
D	773	HIS	-	expression tag	UNP Q0JF02

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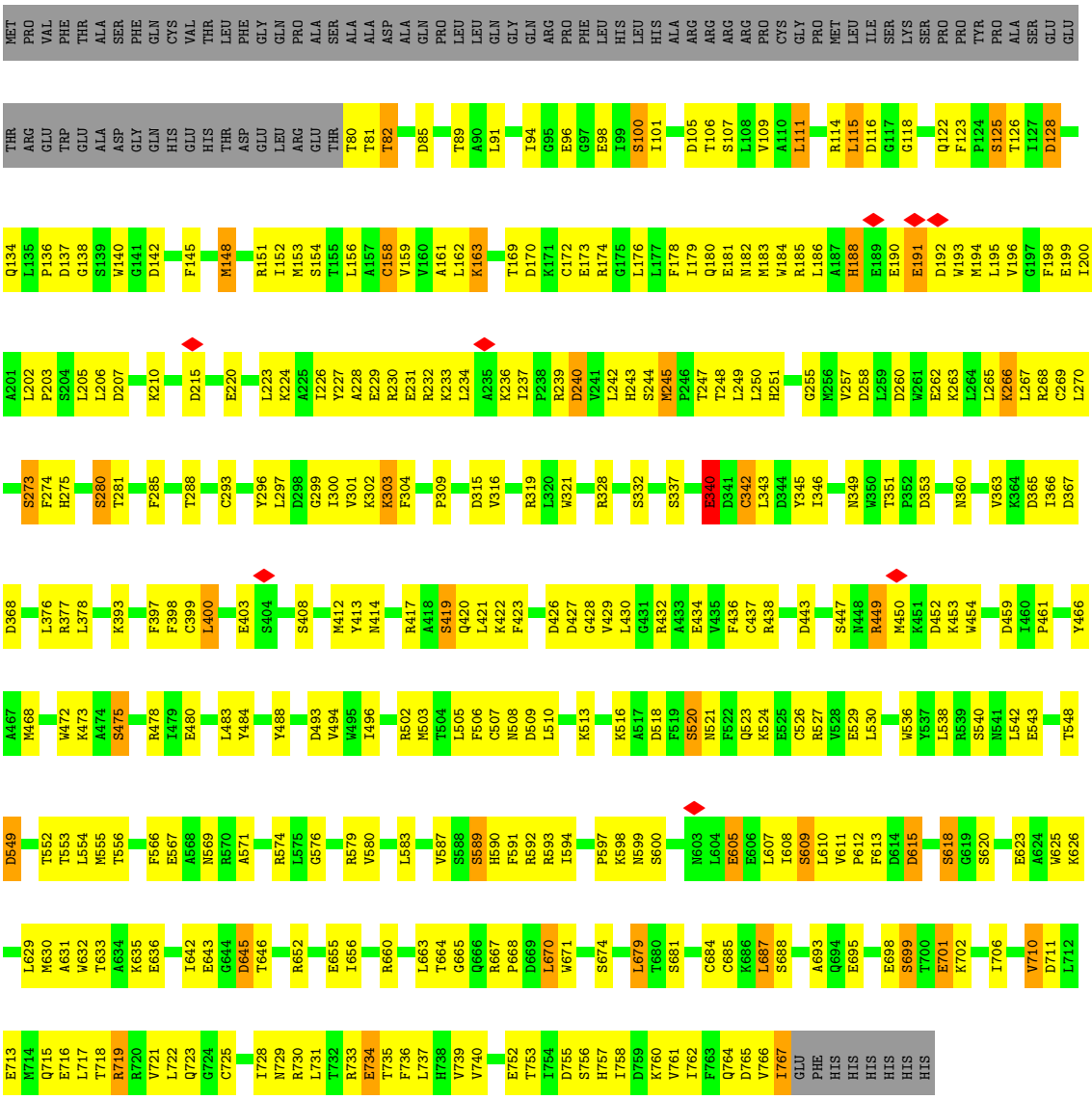
Chain	Residue	Modelled	Actual	Comment	Reference
D	774	HIS	-	expression tag	UNP Q0JF02
D	775	HIS	-	expression tag	UNP Q0JF02
A	768	GLU	-	expression tag	UNP Q0JF02
A	769	PHE	-	expression tag	UNP Q0JF02
A	770	HIS	-	expression tag	UNP Q0JF02
A	771	HIS	-	expression tag	UNP Q0JF02
A	772	HIS	-	expression tag	UNP Q0JF02
A	773	HIS	-	expression tag	UNP Q0JF02
A	774	HIS	-	expression tag	UNP Q0JF02
A	775	HIS	-	expression tag	UNP Q0JF02

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.

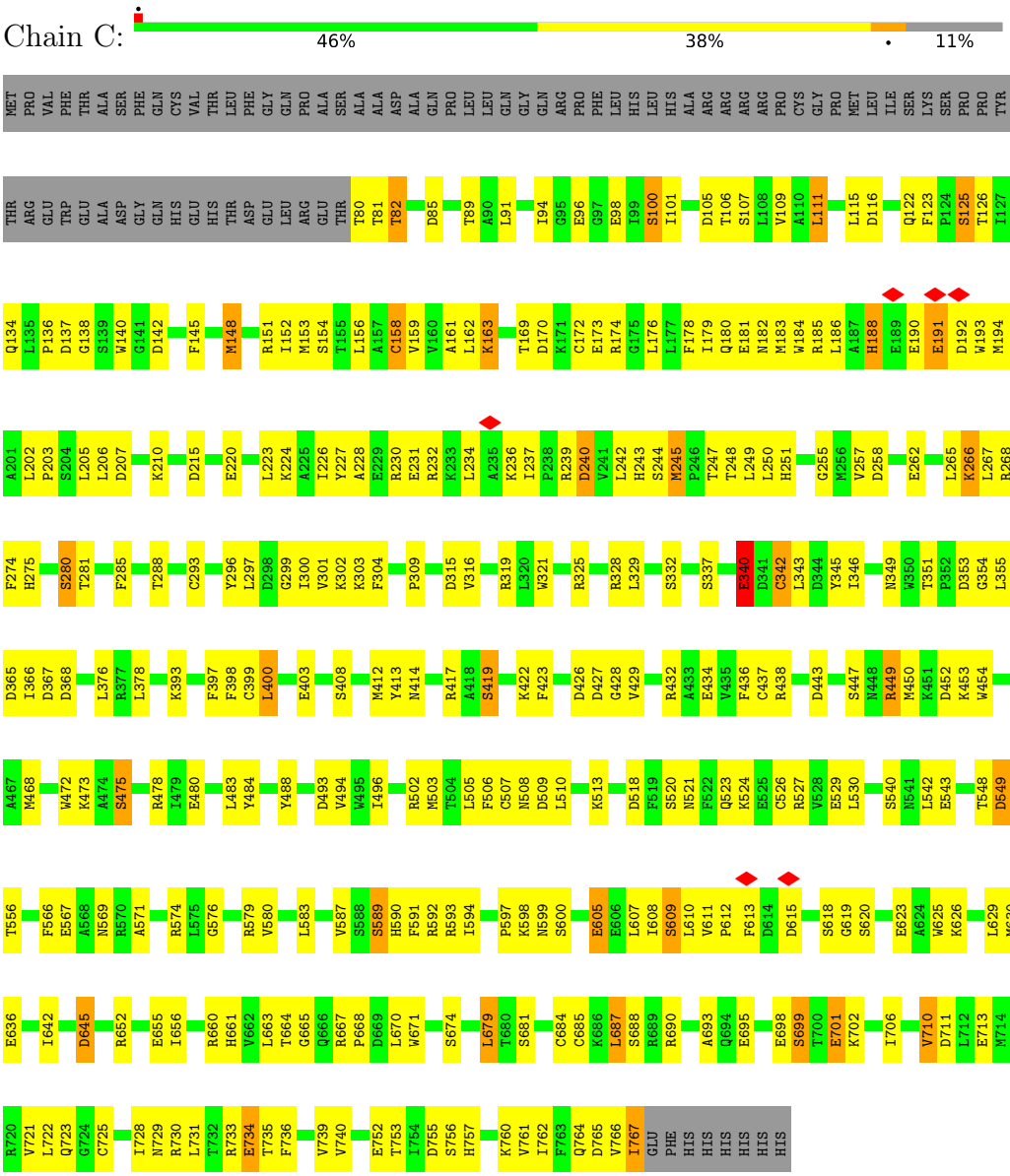
• Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic

Chain B:



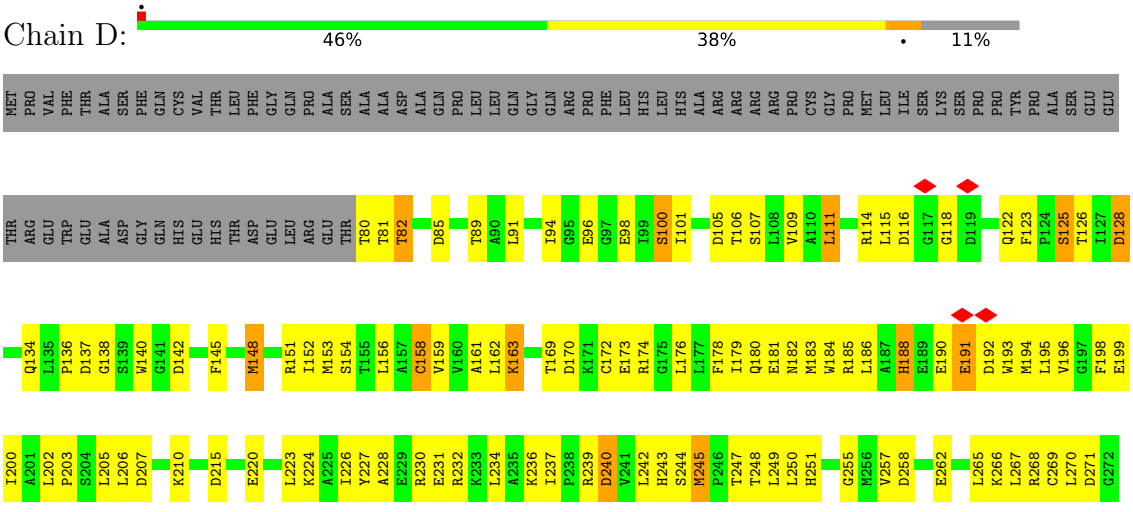
• Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic

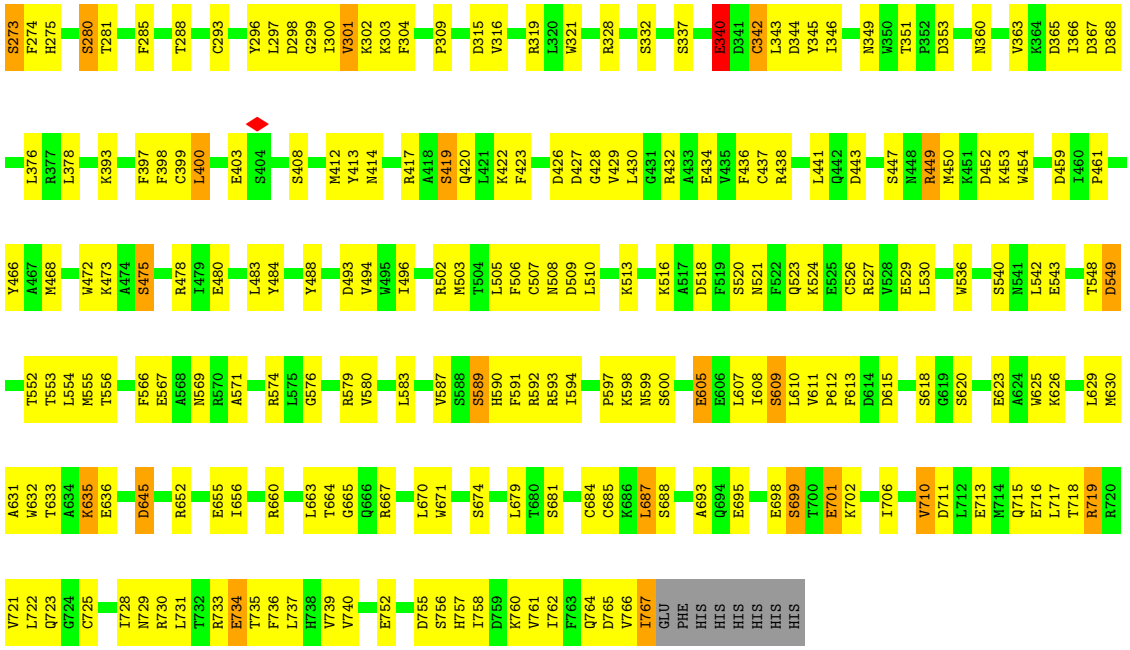
Chain C:



• Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic

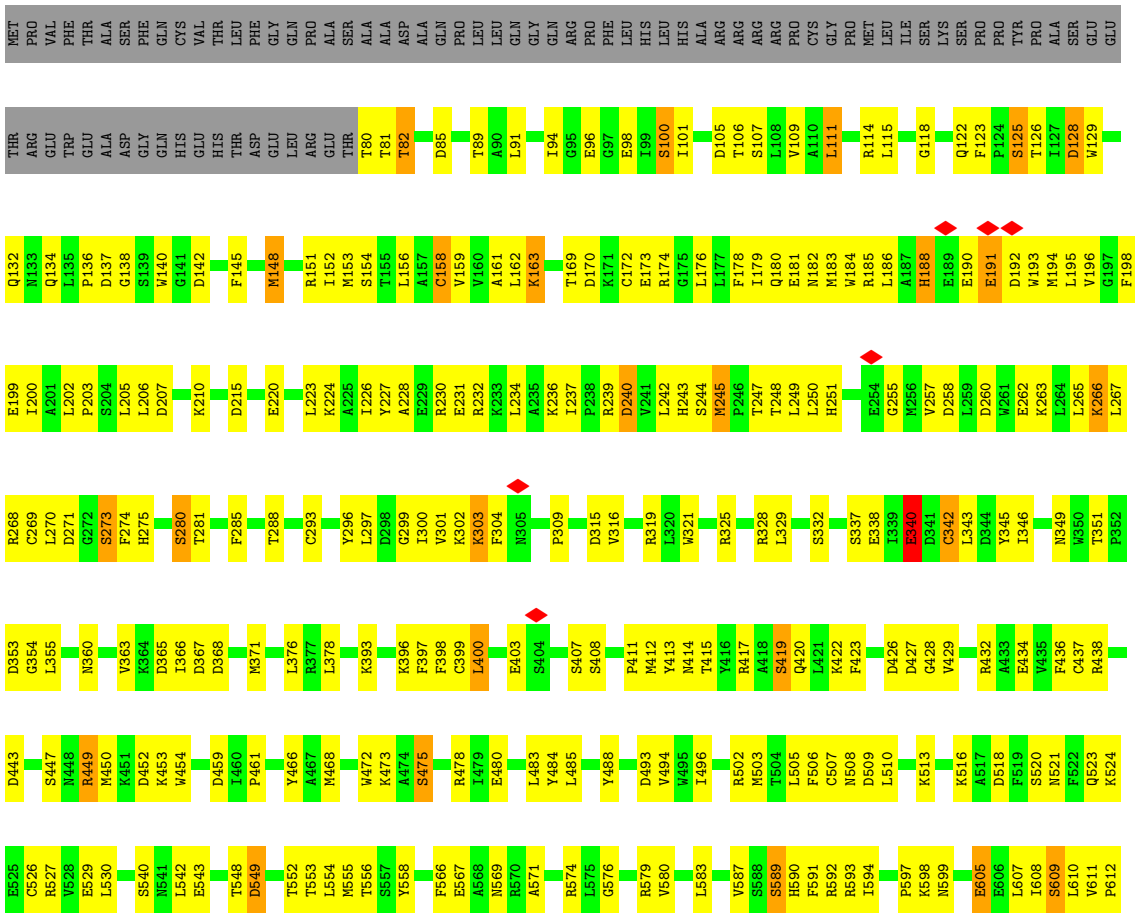
Chain D:





• Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic

Chain A:




F613 D614 D615 S618 G619 S620 E623 A624 W625 K626 L629 M630 A631 W632 T633 A634 K635 E636 D645 R652 E655 I656 R660 L663 T664 G665 Q666 R667 P668 D669 L670 W671 E672 Y673 S674 L679 T680 S681 C684 C685 K686 L687 S688 R689 R690 A693 Q694 E695
E698 S699 T700 E701 K702 I706 V710 D711 L712 E713 M714 Q715 E716 L717 T718 R719 R720 V721 L722 Q723 G724 C725 I728 N729 R730 L731 T732 R733 E734 T735 F736 L737 H738 V739 V740 E752 D755 S756 H757 I758 D759 K760 V761 I762 F763 Q764 D765 V766 I767 GLU PHE HIS HIS HIS HIS
HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	149837	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0137	Depositor
Map size (Å)	299.6, 299.6, 299.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0.34	0/5627	0.47	1/7615 (0.0%)
1	B	0.34	0/5627	0.47	1/7615 (0.0%)
1	C	0.34	0/5627	0.47	1/7615 (0.0%)
1	D	0.34	0/5627	0.47	1/7615 (0.0%)
All	All	0.34	0/22508	0.47	4/30460 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	340	GLU	CA-CB-CG	5.32	125.10	113.40
1	C	340	GLU	CA-CB-CG	5.31	125.08	113.40
1	A	340	GLU	CA-CB-CG	5.31	125.08	113.40
1	D	340	GLU	CA-CB-CG	5.30	125.06	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5504	0	5413	237	0
1	B	5504	0	5413	249	0
1	C	5504	0	5413	229	0
1	D	5504	0	5413	236	0
All	All	22016	0	21652	938	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 21.

The worst 5 of 938 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:297:LEU:O	1:D:301:VAL:CG1	1.94	1.16
1:D:297:LEU:O	1:D:301:VAL:HG12	1.44	1.11
1:D:631:ALA:C	1:D:635:LYS:HE2	1.77	1.05
1:A:631:ALA:C	1:A:635:LYS:HE2	1.82	0.98
1:B:631:ALA:O	1:B:635:LYS:HE3	1.67	0.93

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	686/775 (88%)	647 (94%)	39 (6%)	0	100	100
1	B	686/775 (88%)	647 (94%)	39 (6%)	0	100	100
1	C	686/775 (88%)	647 (94%)	39 (6%)	0	100	100
1	D	686/775 (88%)	646 (94%)	40 (6%)	0	100	100
All	All	2744/3100 (88%)	2587 (94%)	157 (6%)	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	597/672 (89%)	517 (87%)	80 (13%)	4 21
1	B	597/672 (89%)	518 (87%)	79 (13%)	4 21
1	C	597/672 (89%)	517 (87%)	80 (13%)	4 21
1	D	597/672 (89%)	516 (86%)	81 (14%)	3 20
All	All	2388/2688 (89%)	2068 (87%)	320 (13%)	7 21

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	688	SER
1	A	493	ASP
1	D	734	GLU
1	A	245	MET
1	A	615	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	709	GLN
1	A	531	ASN
1	D	723	GLN
1	A	291	GLN
1	A	678	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

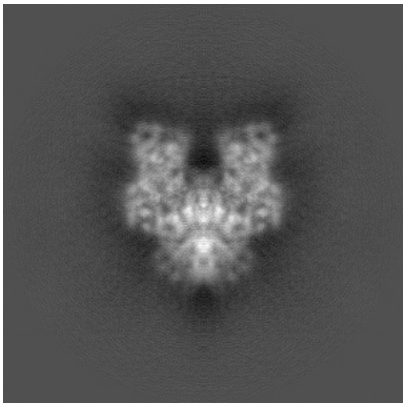
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35202. These allow visual inspection of the internal detail of the map and identification of artifacts.

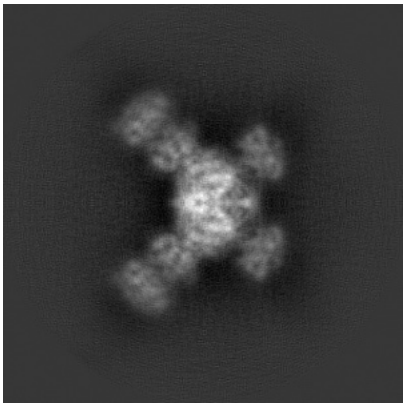
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

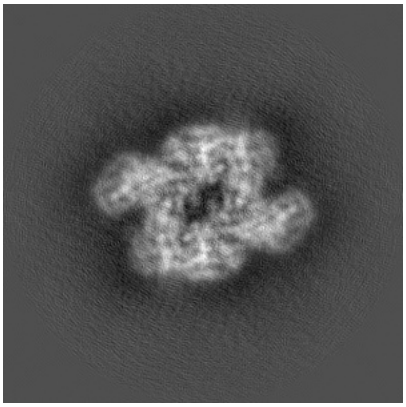
6.1.1 Primary map



X



Y

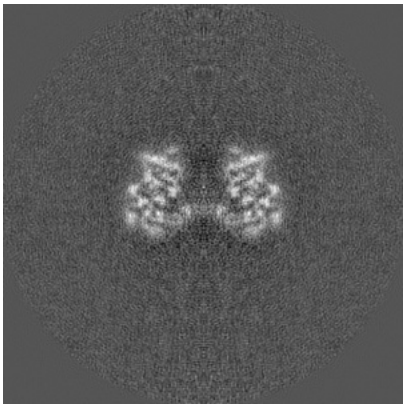


Z

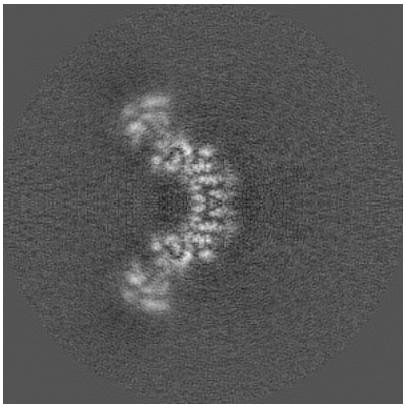
The images above show the map projected in three orthogonal directions.

6.2 Central slices

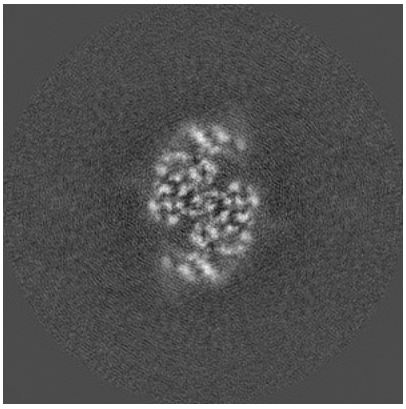
6.2.1 Primary map



X Index: 140



Y Index: 140

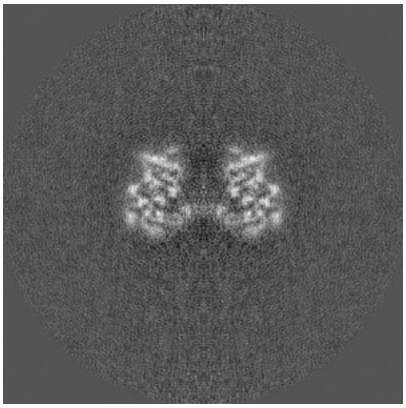


Z Index: 140

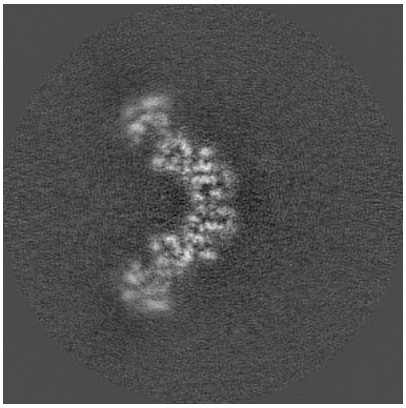
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

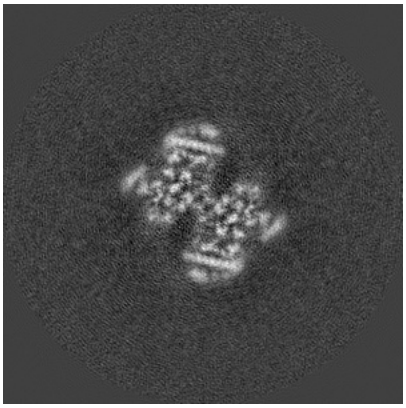
6.3.1 Primary map



X Index: 140



Y Index: 141

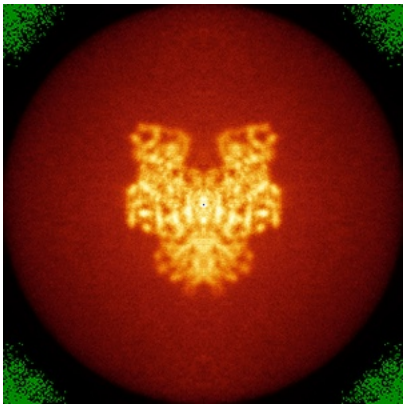


Z Index: 133

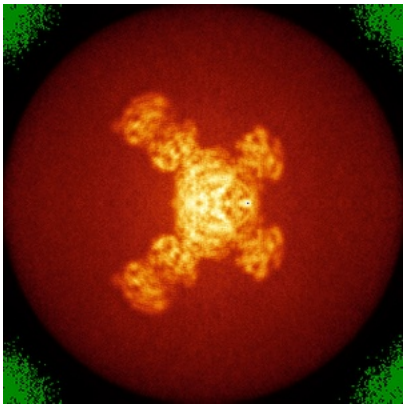
The images above show the largest variance slices of the map in three orthogonal directions.

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

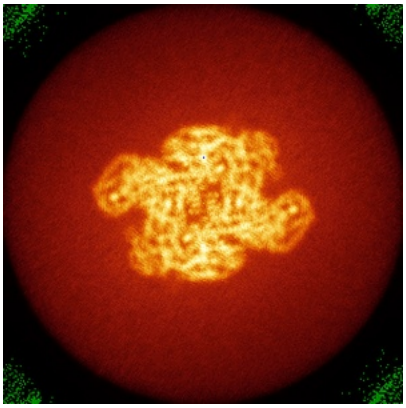
6.4.1 Primary map



X



Y

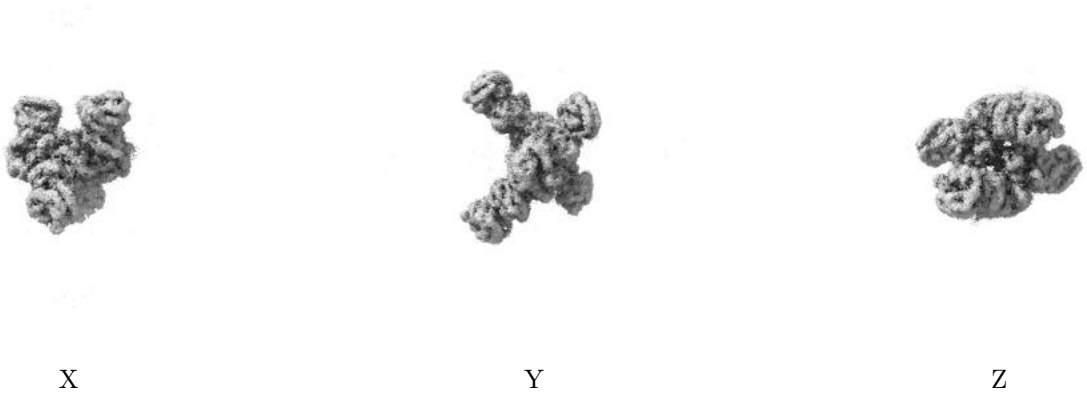


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0137. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

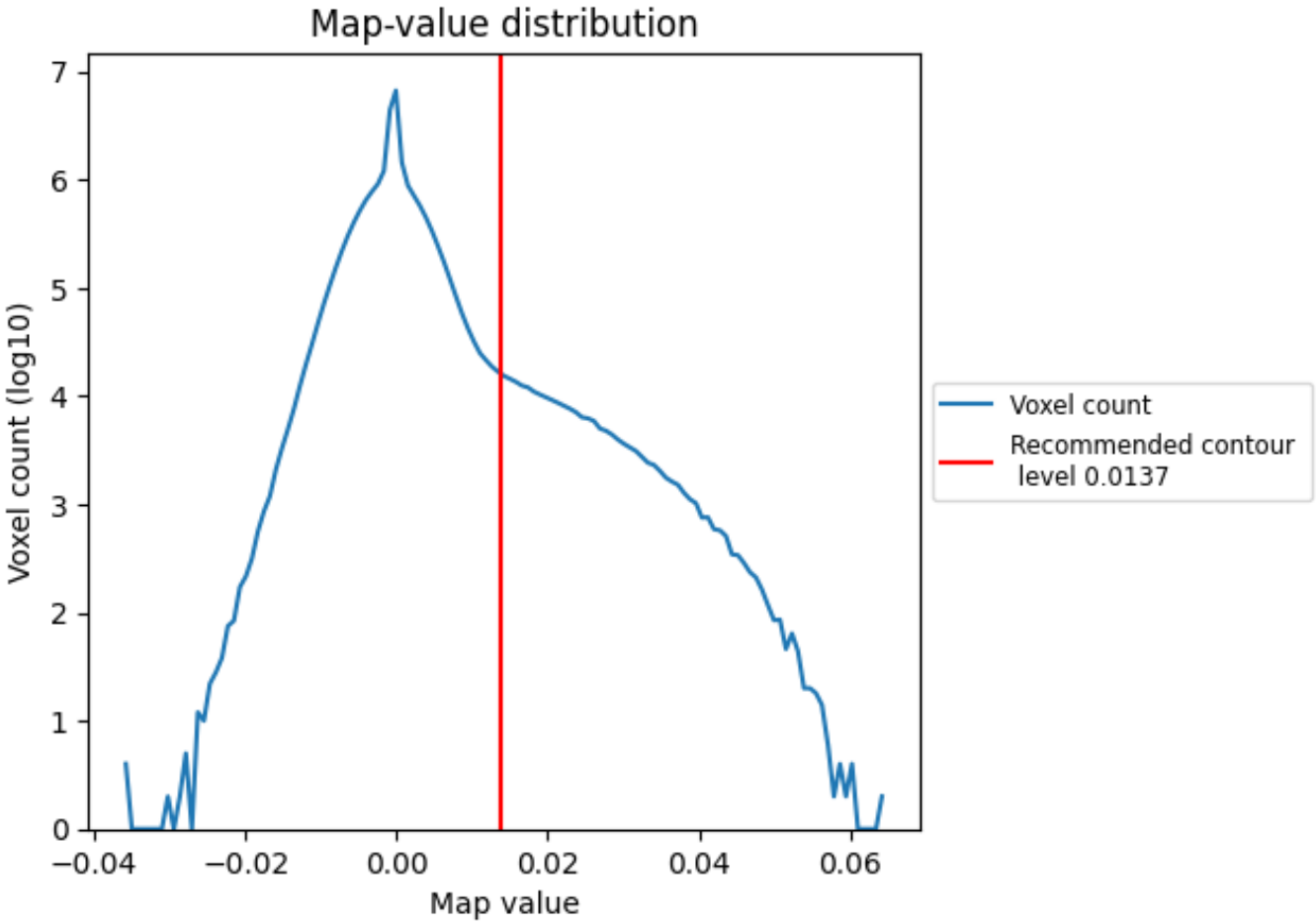
6.6 Mask visualisation (i)

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

7 Map analysis

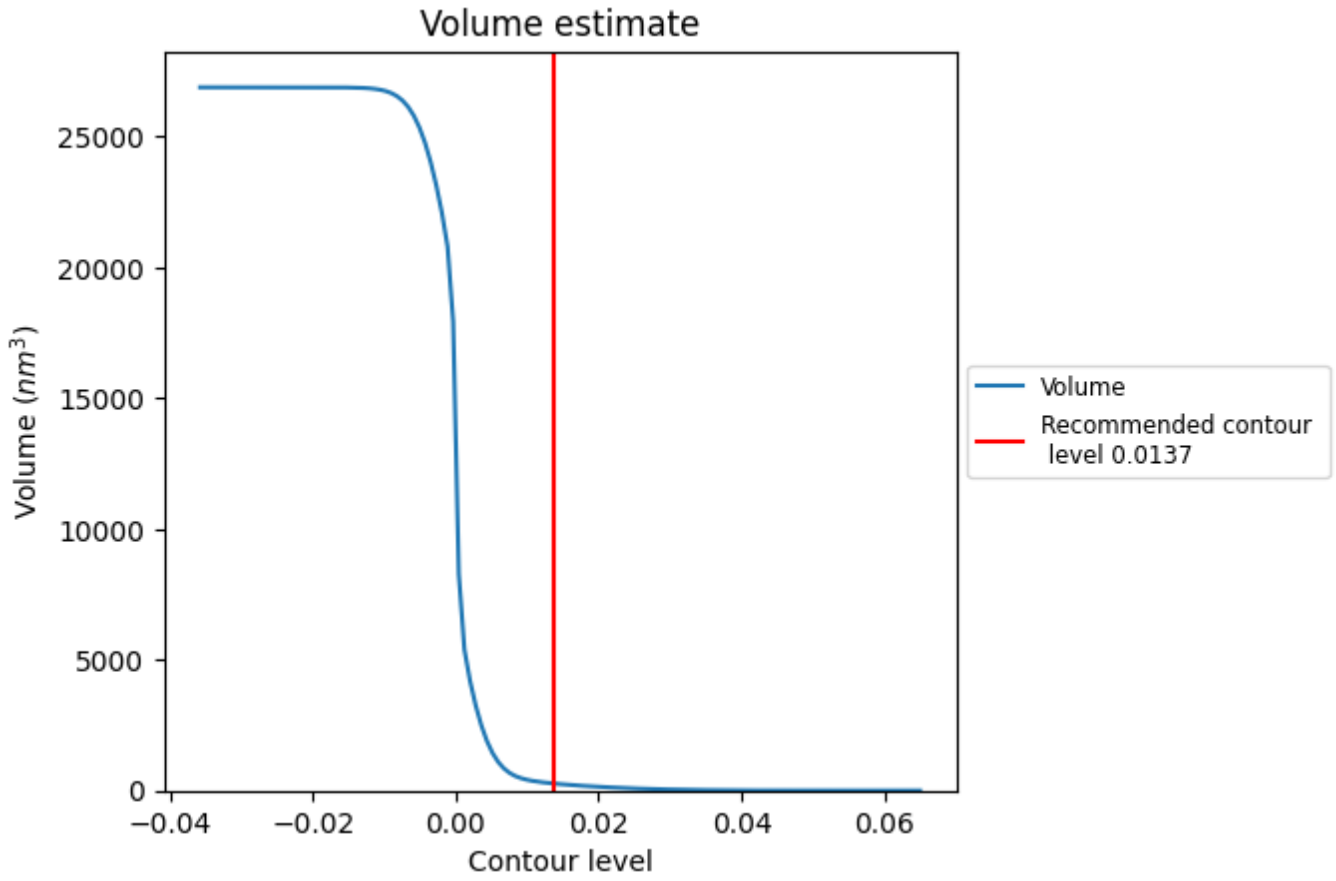
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

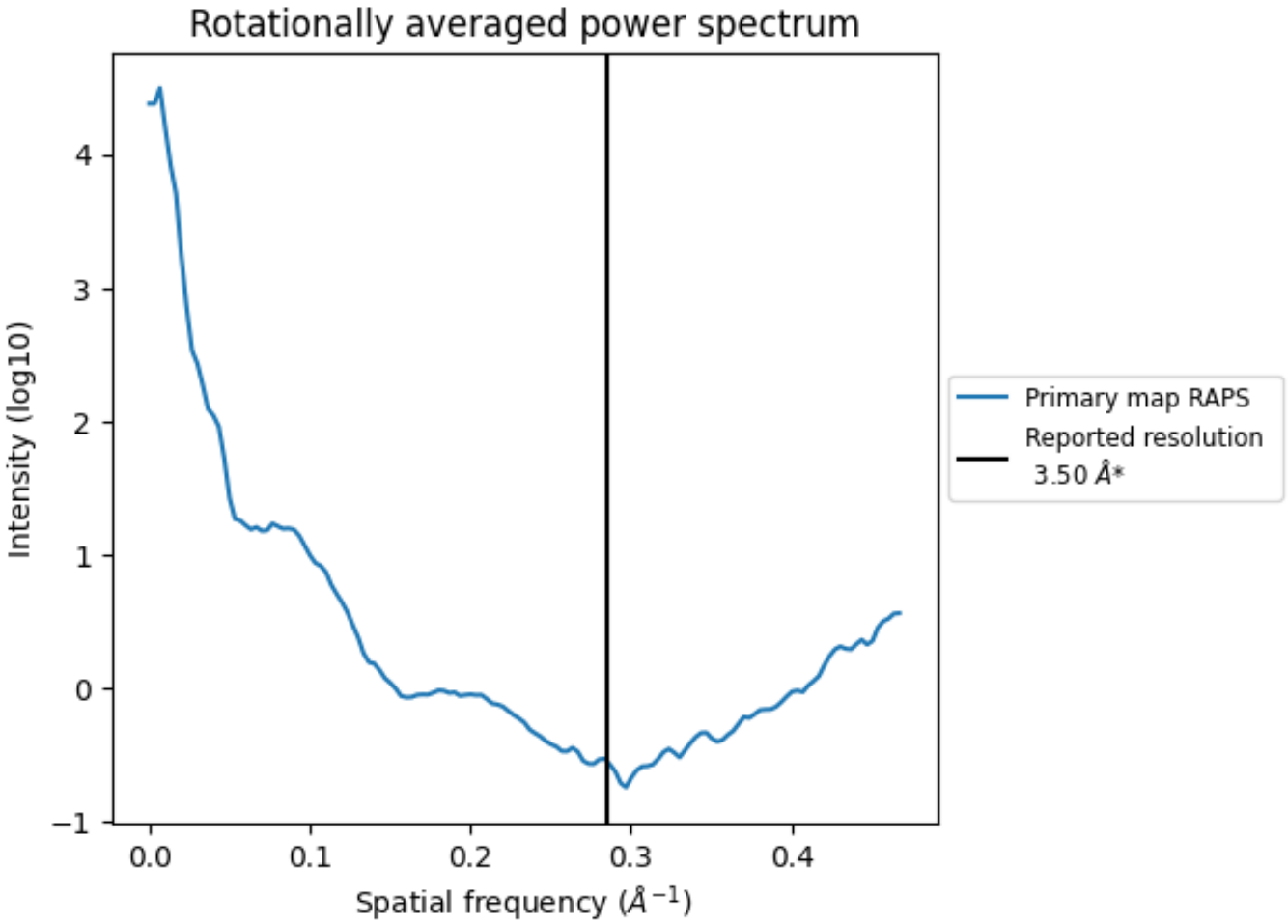
7.2 Volume estimate (i)



The volume at the recommended contour level is 270 nm^3; this corresponds to an approximate mass of 244 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 0.286 $Å^{-1}$

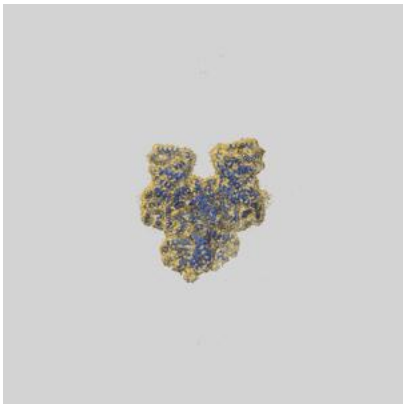
8 Fourier-Shell correlation (i)

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

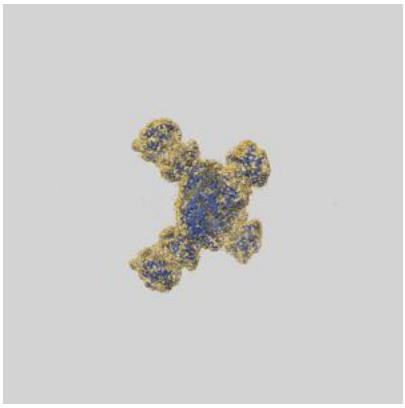
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35202 and PDB model 8I6P. Per-residue inclusion information can be found in section 3 on page 5.

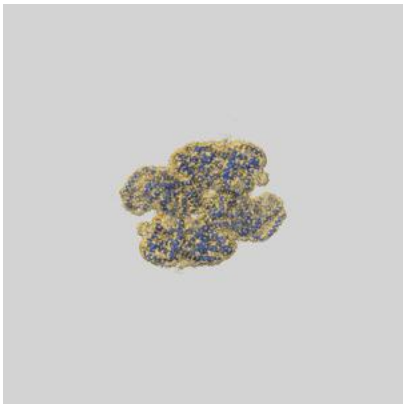
9.1 Map-model overlay



X



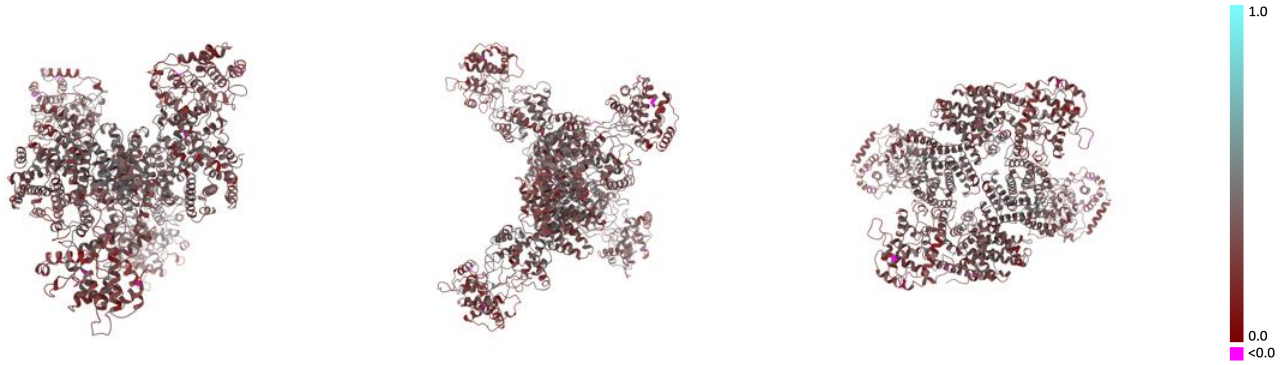
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0137 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.

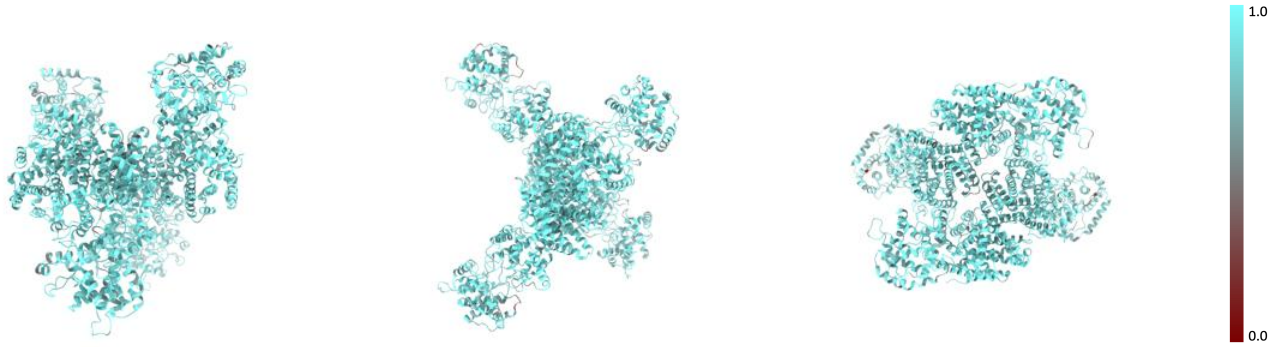
9.2 Q-score mapped to coordinate model (i)



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.

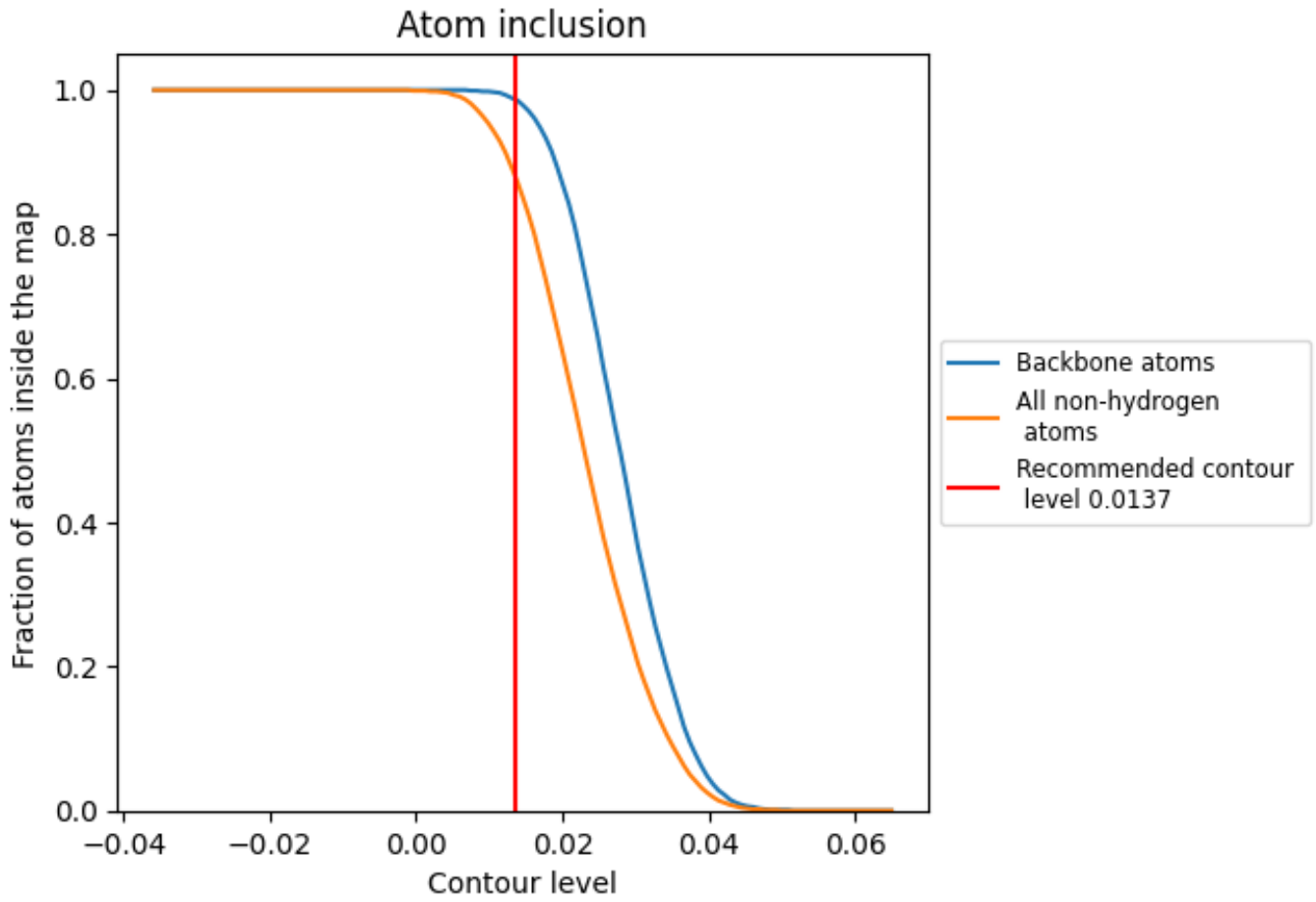
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0137).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 88% 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 (0.0137) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8770	0.3190
A	0.8840	0.3140
B	0.8700	0.3210
C	0.8700	0.3270
D	0.8860	0.3130