

wwPDB EM Validation Summary Report (i)

Mar 20, 2024 – 01:20 AM JST

PDB ID	:	6KQ4
EMDB ID	:	EMD-0750
Title	:	323 K cryoEM structure of Sso-KARI in complex with Mg2+ $$
Authors	:	Chen, C.Y.; Chang, Y.C.; Lin, B.L.; Huang, C.H.; Tsai, M.D.
Deposited on		
Resolution	:	2.30 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 (1)) were used in the production of this report:

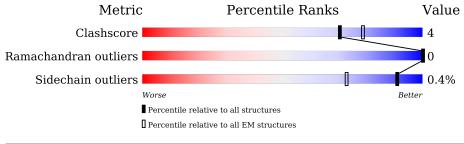
:	0.0.1.dev70
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.13
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.36
	:::::::::::::::::::::::::::::::::::::::

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 2.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
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	А	333	90%	8%	•
1	В	333	90%	8%	·
1	С	333	89%	9%	•
1	D	333	89%	9%	·
1	Е	333	89%	9%	·
1	F	333	89%	10%	·
1	G	333	89%	9%	·
1	Н	333	89%	9%	·

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Mol	Chain	Length	Quality of chain		
1	Ι	333	90%	8%	·
1	J	333	90%	8%	•
1	K	333	89%	9%	•
1	L	333	89%	9%	•



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 62206 atoms, of which 31222 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.

Mol	Chain	Residues		Atoms						Trace					
1	Δ	328	Total	С	Н	Ν	0	S	0	0					
	А	320	5181	1667	2601	423	480	10	0	0					
1	В	200	Total	С	Н	Ν	0	S	0	0					
	D	328	5182	1667	2602	423	480	10	0	0					
1	С	200	Total	С	Н	Ν	0	S	0	0					
	U	328	5180	1667	2600	423	480	10	0	0					
1	D	200	Total	С	Н	Ν	0	S	0	0					
	D	328	5181	1667	2601	423	480	10	0	0					
1	Е	328	Total	С	Η	Ν	0	S	0	0					
	E	320	5181	1667	2601	423	480	10	0	0					
1	Б	F	Б	Б	Б	Г	328	Total	С	Н	Ν	0	S	0	0
	Г	320	5185	1667	2605	423	480	10	0	0					
1	C	С	C	С	С	G	328	Total	С	Η	Ν	0	S	0	0
	G	320	5185	1667	2605	423	480	10	0	U					
1	Н	328	Total	С	Н	Ν	0	S	0	0					
	11	320	5181	1667	2601	423	480	10	0	0					
1	Ι	328	Total	С	Н	Ν	0	S	0	0					
	1	320	5181	1667	2601	423	480	10	0	0					
1	J	328	Total	С	Н	Ν	0	S	0	0					
	J	320	5181	1667	2601	423	480	10	0	0					
1	V	200	Total	С	Н	Ν	0	S	0	0					
1	Κ	328	5184	1667	2604	423	480	10	U	0					
1	т	200	Total	С	Н	Ν	0	S	0	0					
1	L	328	5180	1667	2600	423	480	10	U	0					

• Molecule 1 is a protein called Ketol-acid reductoisomerase.

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	А	2	Total Mg 2 2	0
2	В	2	Total Mg 2 2	0

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Mol	Chain	Residues	Atoms	AltConf
2	С	2	Total Mg 2 2	0
2	D	2	Total Mg 2 2	0
2	Е	2	Total Mg 2 2	0
2	F	2	Total Mg 2 2	0
2	G	2	Total Mg 2 2	0
2	Н	2	Total Mg 2 2	0
2	Ι	2	Total Mg 2 2	0
2	J	2	Total Mg 2 2	0
2	K	2	Total Mg 2 2	0
2	L	2	Total Mg 2 2	0

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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: Ketol-acid reductoisomerase





LYS	ASN	ASP
-----	-----	-----

• Molecule 1: Ketol-acid reductoisomerase

Chain F:		89%		10% •
MET D2 K3 L6 L6 D7 A8 A8 L10 D110 D110 V23	q 30 N 46 V 46 E 57 D 65 R 69 R 69 L 96 C	K98 V122 R130 E134 D138 Q142	1171 1178 1178 1181 1181 1181 1197 1197	E227 E236 1246 F247 Y300 P301



• Molecule 1: Ketol-acid reductoisomerase

Chain G:		8	9%		9% •
MET D2 K3 K3 L10 D11 D11	Y 23 Q 30 N 45 V 46 E57			11/8 11/8 1181 1197 1197 1201 1201	E236 E236 F247 L325 K329 VAL LYS
ASP					

• Molecule 1: Ketol-acid reductoisomerase

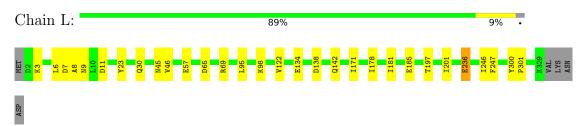
Chain H:	89%	9% •
MET MET 74 74 75 76 10 11 11 72 86 73 72 86 73 72 86 73 72 86 73 72 86 75 86 86 86 86 86 86 86 86 86 86 86 86 86	K98 V122 R130 D138 D138 D138 D138 T171 117 117 117 117 117 117 117 117 11	E227 E236 E236 F247 F247 K329 VAL
LYS ASN ASP		
• Molecule 1: Ketol-acid reductoisor	nerase	
Chain I:	90%	8% •
MET MET K3 K3 K3 M8 M45 K11 M45 K23 K69 K69 K69 K69 K69 K69 K69 K69 K69 K69	1122 1128 1134 1138 1138 1171 1171 1171 1171 1171 1171	1246 F247 K329 VAL LYS ASN ASP
• Molecule 1: Ketol-acid reductoisor	nerase	
Chain J:	90%	8% •
MET MET K3 K3 K3 K3 M45 K9 M45 K9 M45 K9 M45 K9 M45 K9 M45 K9 M45 K9 M45 K9 M45 K9 M45 K9 M45 K3 K3 K3 K3 K3 K3 K3 K3 K3 K3 K3 K3 K3	1171 1178 1178 1178 1178 1178 1178 1178	K329 VAL LYS ASN ASP

• Molecule 1: Ketol-acid reductoisomerase



Cha	ii	n	K	:	•												89%	6												90	%	•			
MET D2 K3		L6	D7	A8	6N	L10	D11	Y 23	1 30	N45	V46	E57	D65	R69	L95	 K98	V122		E134	D138	0142	1171	1178	1181	<u>т185</u>	T197	1201	E236	-	1246 F247	-	L322	L325	K329 VAL	LYS
ASN ASP																																			

• Molecule 1: Ketol-acid reductoisomerase





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87458	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	10.568	Depositor
Minimum map value	-3.452	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.417	Depositor
Recommended contour level	1.56	Depositor
Map size (Å)	295.68, 295.68, 295.68	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: 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
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.37	0/2633	0.46	0/3555
1	В	0.37	0/2633	0.46	0/3555
1	С	0.37	0/2633	0.46	0/3555
1	D	0.37	0/2633	0.46	0/3555
1	Е	0.37	0/2633	0.46	0/3555
1	F	0.37	0/2633	0.46	0/3555
1	G	0.37	0/2633	0.46	0/3555
1	Н	0.37	0/2633	0.46	0/3555
1	Ι	0.37	0/2633	0.46	0/3555
1	J	0.37	0/2633	0.46	0/3555
1	Κ	0.37	0/2633	0.46	0/3555
1	L	0.37	0/2633	0.46	0/3555
All	All	0.37	0/31596	0.46	0/42660

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	А	2580	2601	2604	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	2580	2602	2604	17	0
1	С	2580	2600	2604	22	0
1	D	2580	2601	2604	21	0
1	Ε	2580	2601	2604	21	0
1	F	2580	2605	2604	22	0
1	G	2580	2605	2604	21	0
1	Н	2580	2601	2604	21	0
1	Ι	2580	2601	2604	18	0
1	J	2580	2601	2604	17	0
1	Κ	2580	2604	2604	19	0
1	L	2580	2600	2604	19	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0
2	Ε	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	Н	2	0	0	0	0
2	Ι	2	0	0	0	0
2	J	2	0	0	0	0
2	Κ	2	0	0	0	0
2	L	2	0	0	0	0
All	All	30984	31222	31248	224	0

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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 4.

The worst 5 of 224 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:F:142:GLN:N	1:F:142:GLN:OE1	2.17	0.78
1:L:142:GLN:N	1:L:142:GLN:OE1	2.17	0.78
1:J:9:ASN:ND2	1:J:11:ASP:OD1	2.17	0.78
1:B:9:ASN:ND2	1:B:11:ASP:OD1	2.17	0.78
1:A:9:ASN:ND2	1:A:11:ASP:OD1	2.17	0.78

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	Perce	ntiles
1	А	326/333~(98%)	312 (96%)	14 (4%)	0	100	100
1	В	326/333~(98%)	312 (96%)	14 (4%)	0	100	100
1	С	326/333~(98%)	312 (96%)	14 (4%)	0	100	100
1	D	326/333~(98%)	312 (96%)	14 (4%)	0	100	100
1	Е	326/333~(98%)	312 (96%)	14 (4%)	0	100	100
1	F	326/333~(98%)	312 (96%)	14 (4%)	0	100	100
1	G	326/333~(98%)	312 (96%)	14 (4%)	0	100	100
1	Η	326/333~(98%)	312 (96%)	14 (4%)	0	100	100
1	Ι	326/333~(98%)	312 (96%)	14 (4%)	0	100	100
1	J	326/333~(98%)	312 (96%)	14 (4%)	0	100	100
1	Κ	326/333~(98%)	312 (96%)	14 (4%)	0	100	100
1	L	326/333~(98%)	312 (96%)	14 (4%)	0	100	100
All	All	3912/3996~(98%)	3744 (96%)	168 (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	А	267/272~(98%)	266 (100%)	1 (0%)	91 96
1	В	267/272~(98%)	266 (100%)	1 (0%)	91 96

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	С	267/272~(98%)	266 (100%)	1 (0%)	91	96
1	D	267/272~(98%)	266 (100%)	1 (0%)	91	96
1	Ε	267/272~(98%)	266 (100%)	1 (0%)	91	96
1	\mathbf{F}	267/272~(98%)	266 (100%)	1 (0%)	91	96
1	G	267/272~(98%)	266 (100%)	1 (0%)	91	96
1	Η	267/272~(98%)	266 (100%)	1 (0%)	91	96
1	Ι	267/272~(98%)	266 (100%)	1 (0%)	91	96
1	J	267/272~(98%)	266 (100%)	1 (0%)	91	96
1	Κ	267/272~(98%)	266 (100%)	1 (0%)	91	96
1	L	267/272~(98%)	266 (100%)	1 (0%)	91	96
All	All	3204/3264~(98%)	3192 (100%)	12~(0%)	91	96

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

Mol	Chain	\mathbf{Res}	Type
1	Н	236	GLU
1	Ι	236	GLU
1	L	236	GLU
1	J	236	GLU
1	D	236	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
1	С	278	ASN
1	Ι	278	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.



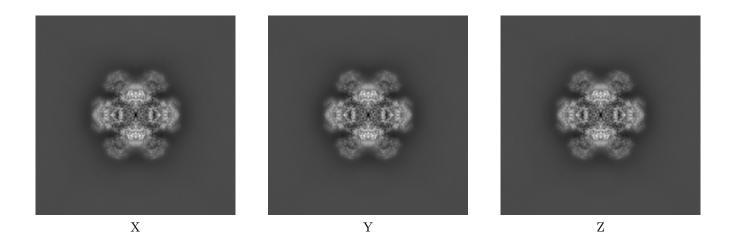
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0750. 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)

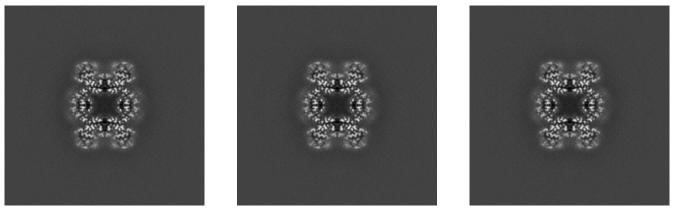
6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 176

Y Index: 176

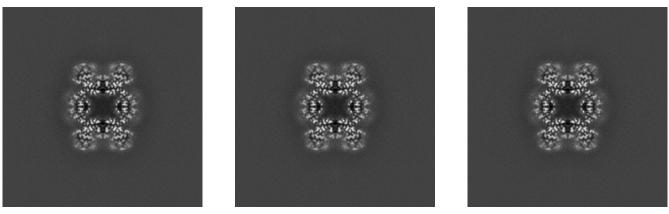


Z Index: 176

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: 176

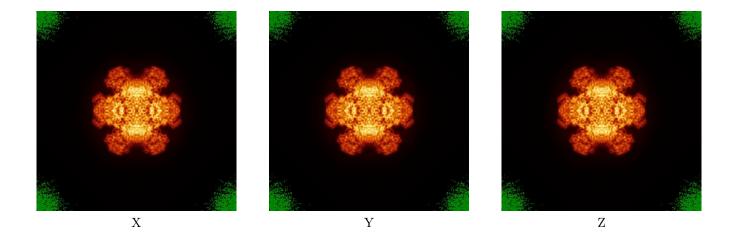
Y Index: 176

Z Index: 176

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

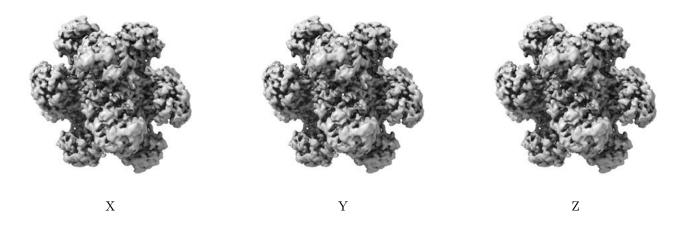


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



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 1.56. 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)

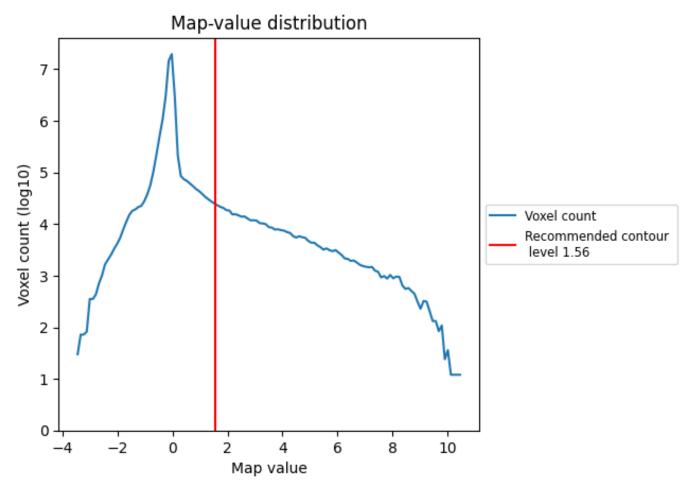
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

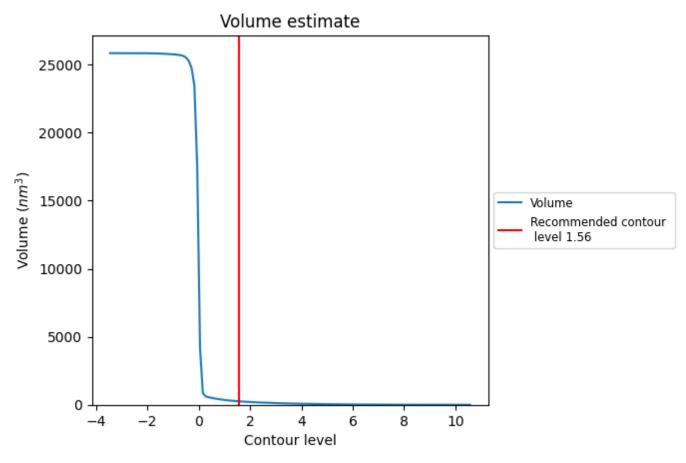
7.1 Map-value distribution (i)



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)

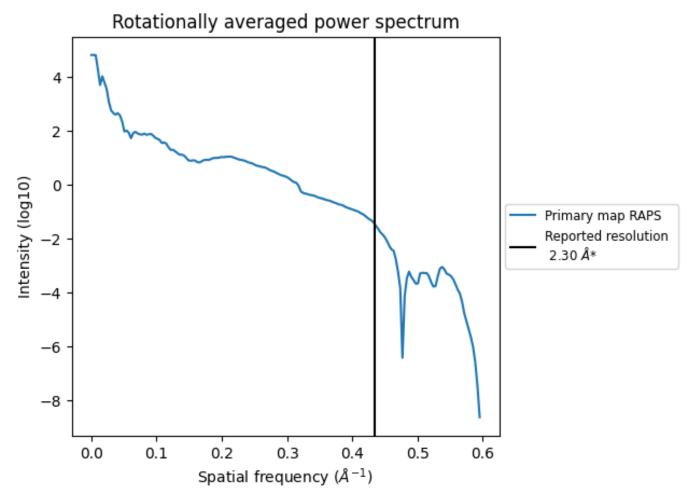


The volume at the recommended contour level is 256 nm^3 ; this corresponds to an approximate mass of 232 kDa.

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)



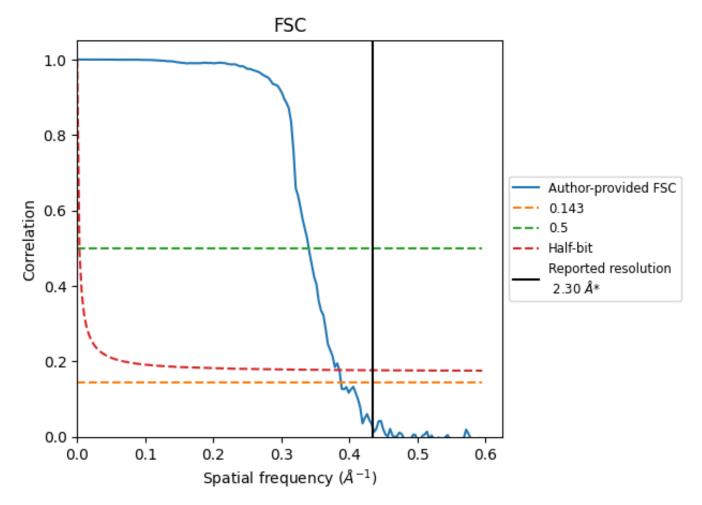
*Reported resolution corresponds to spatial frequency of 0.435 \AA^{-1}



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 0.435 \AA^{-1}



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estim	ation	criterion (FSC cut-off)
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.58	2.94	2.60
Unmasked-calculated*	-	-	-

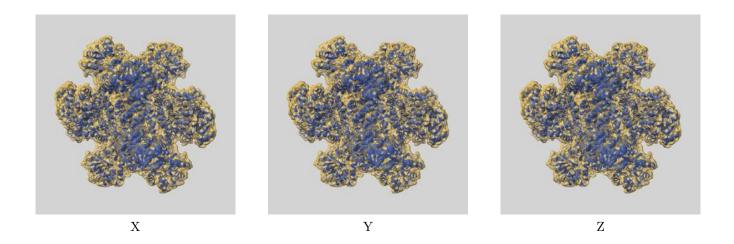
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.58 differs from the reported value 2.3 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0750 and PDB model 6KQ4. Per-residue inclusion information can be found in section 3 on page 6.

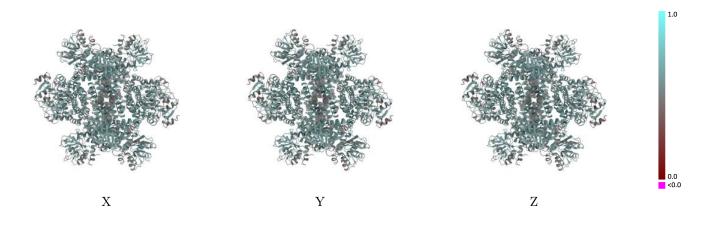
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 1.56 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.

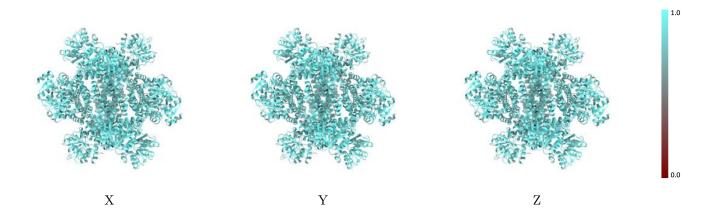


9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according 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.

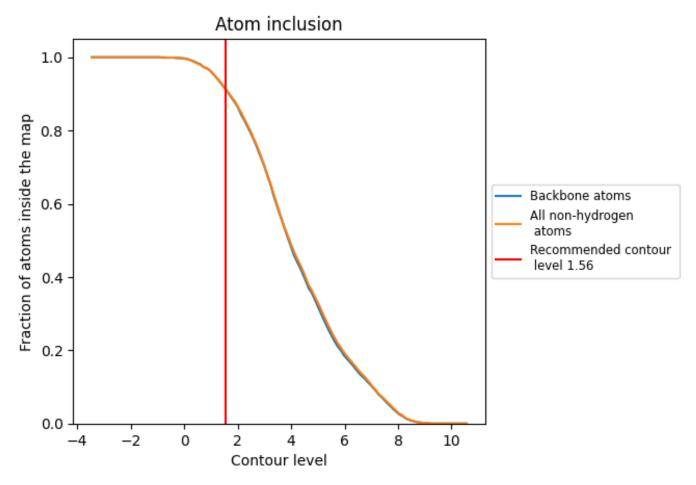
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.56).



9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (1.56) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.9120	0.5700	1.0
А	0.9160	0.5710	1.0
В	0.9160	0.5730	
С	0.9170	0.5700	
D	0.9160	0.5710	
E	0.9190	0.5730	
F	0.9180	0.5710	
G	0.9190	0.5680	
Н	0.9180	0.5700	
Ι	0.9160	0.5730	0.0
J	0.9180	0.5680	<0.0
K	0.9150	0.5680]
L	0.9160	0.5670	

