



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 06:36 PM UTC

PDB ID : 6S1K / pdb_00006s1k
EMDB ID : EMD-10050
Title : E. coli Core Signaling Unit, carrying QQQQ receptor mutation
Authors : Cassidy, C.K.
Deposited on : 2019-06-18
Resolution : 8.38 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

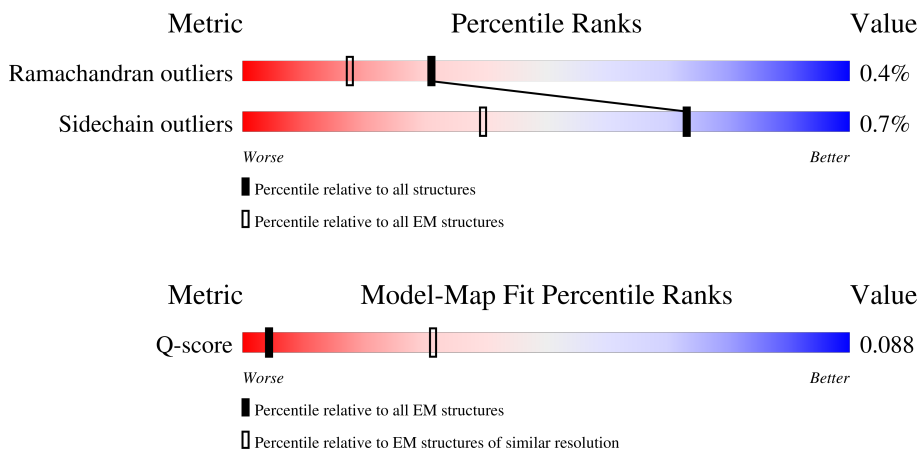
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 8.38 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.



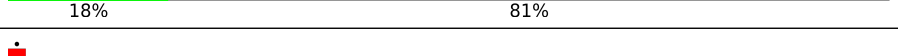
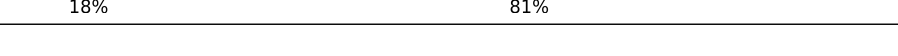
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	298 (7.90 - 8.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	654	29% 57% 41%
1	B	654	30% 56% 41%
2	C	167	56% 82% 5% 13%
2	D	167	53% 83% 13%
3	E	551	18% 81%

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Mol	Chain	Length	Quality of chain
3	F	551	
3	G	551	
3	H	551	
3	I	551	
3	J	551	
3	K	551	
3	L	551	
3	M	551	
3	N	551	
3	O	551	
3	P	551	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16884 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 Chemotaxis protein CheA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	383	Total	C	N	O	S	0	0
			2909	1818	519	559	13		
1	B	383	Total	C	N	O	S	0	0
			2909	1818	519	559	13		

- Molecule 2 is a protein called CheW.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	145	Total	C	N	O	S	0	0
			1117	715	183	217	2		
2	D	145	Total	C	N	O	S	0	0
			1117	715	183	217	2		

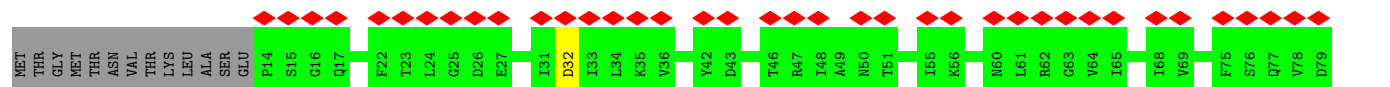
- Molecule 3 is a protein called Methyl-accepting chemotaxis protein I.

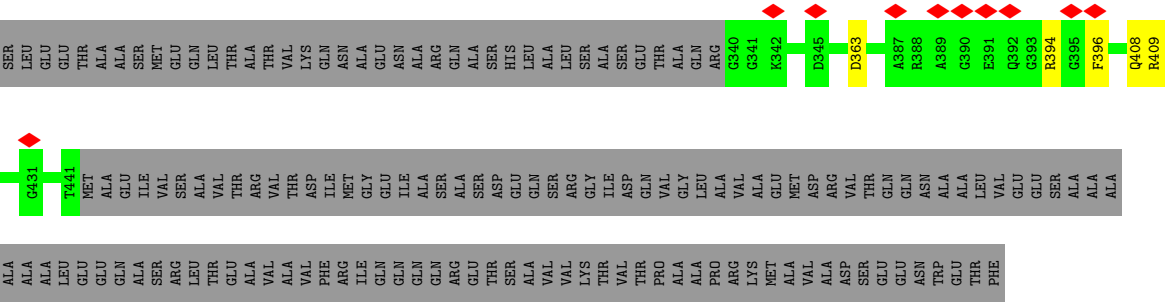
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	F	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	G	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	H	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	I	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	J	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	K	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	L	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	M	102	Total	C	N	O	S	0	0
			736	449	134	152	1		

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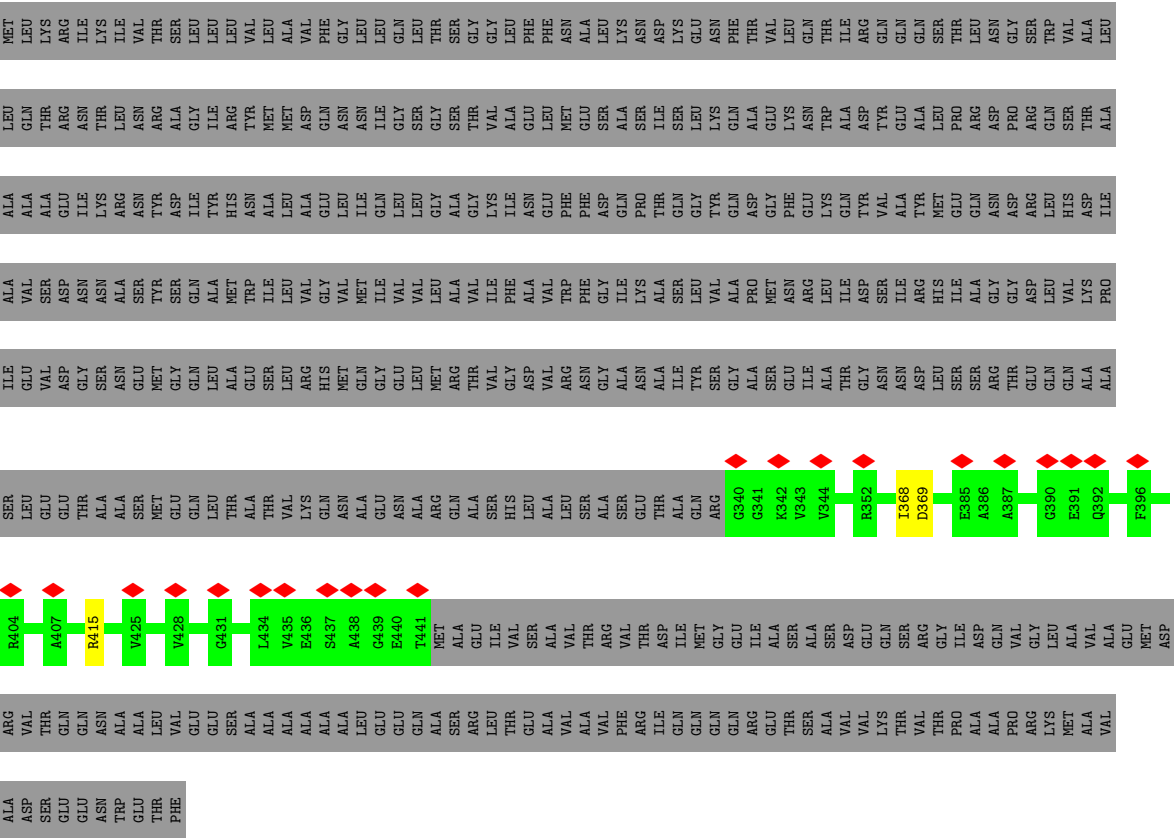
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	O	102	Total	C	N	O	S	0	0
			736	449	134	152	1		
3	P	102	Total	C	N	O	S	0	0
			736	449	134	152	1		

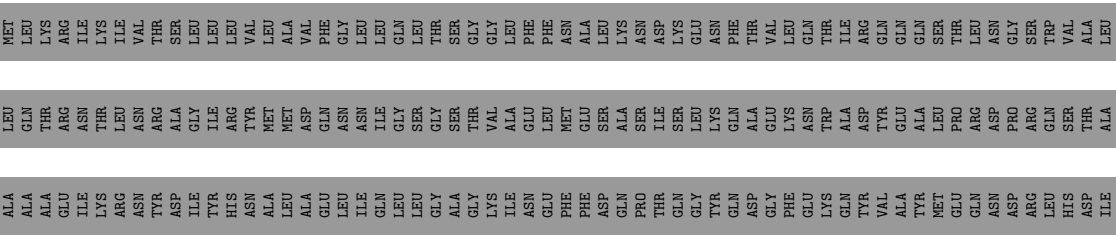




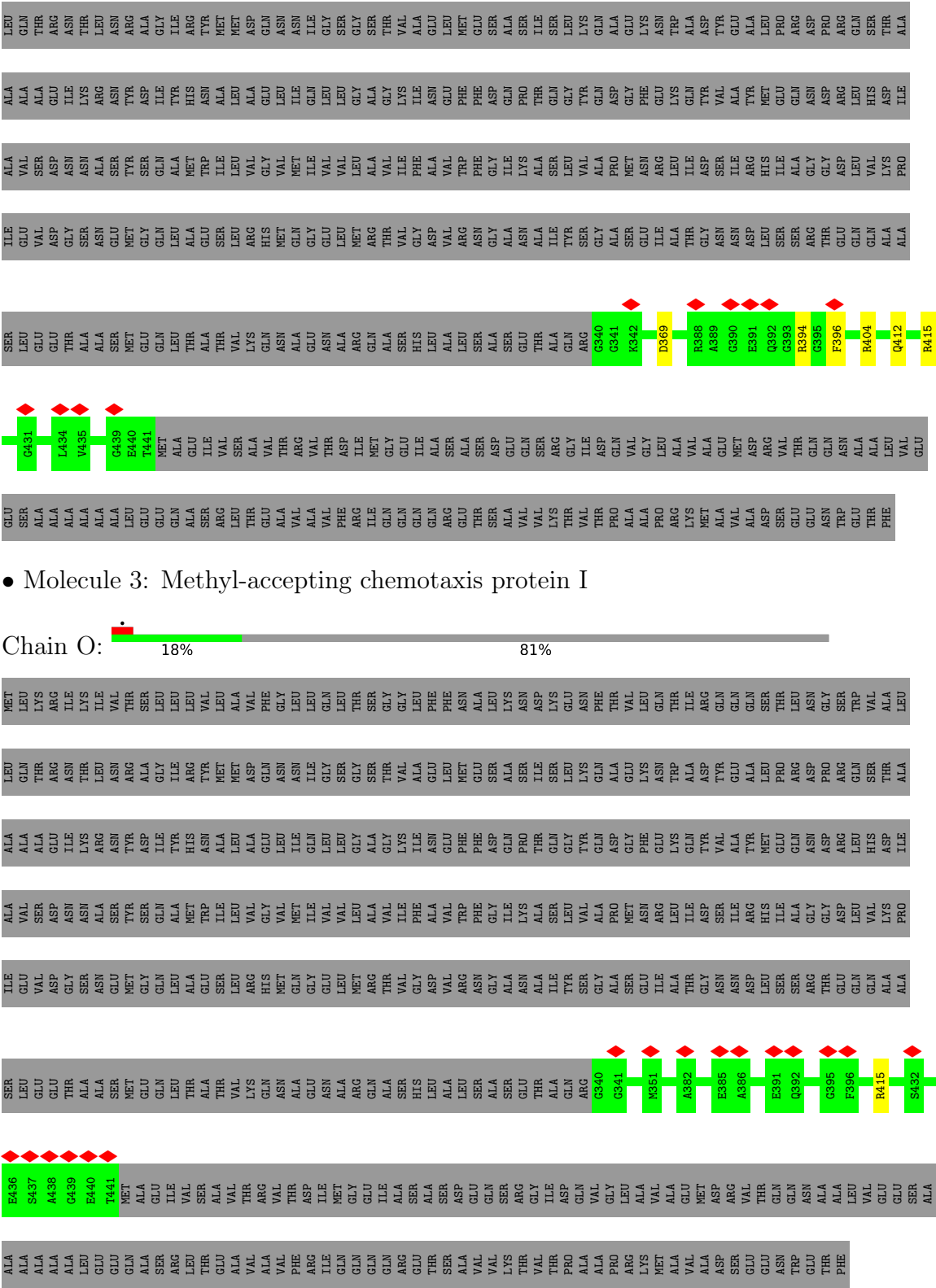
● Molecule 3: Methyl-accepting chemotaxis protein I



● Molecule 3: Methyl-accepting chemotaxis protein I







• Molecule 3: Methyl-accepting chemotaxis protein I

• Molecule 3: Methyl-accepting chemotaxis protein I

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	91636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	14.403	Depositor
Minimum map value	-7.622	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.175	Depositor
Recommended contour level	2.15	Depositor
Map size (Å)	627.50397, 627.50397, 627.50397	wwPDB
Map dimensions	204, 204, 204	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.0759997, 3.0759997, 3.0759997	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	0.89	0/2939	1.45	2/3975 (0.1%)
1	B	0.88	0/2939	1.45	9/3975 (0.2%)
2	C	0.87	0/1130	1.34	4/1537 (0.3%)
2	D	0.87	0/1130	1.33	1/1537 (0.1%)
3	E	0.89	0/737	1.67	1/994 (0.1%)
3	F	0.88	0/737	1.68	2/994 (0.2%)
3	G	0.88	0/737	1.67	3/994 (0.3%)
3	H	0.89	0/737	1.63	1/994 (0.1%)
3	I	0.88	0/737	1.65	0/994
3	J	0.88	0/737	1.62	1/994 (0.1%)
3	K	0.88	0/737	1.67	2/994 (0.2%)
3	L	0.89	0/737	1.65	0/994
3	M	0.89	0/737	1.67	0/994
3	N	0.89	0/737	1.67	2/994 (0.2%)
3	O	0.89	0/737	1.67	0/994
3	P	0.90	0/737	1.66	1/994 (0.1%)
All	All	0.88	0/16982	1.55	29/22952 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
3	F	0	2
3	G	0	1
3	H	0	1
3	I	0	1
3	J	0	2
3	M	0	2
3	N	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	O	0	1
3	P	0	1
All	All	0	25

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	369	ASP	CA-CB-CG	7.65	120.25	112.60
3	N	396	PHE	CA-CB-CG	6.51	120.31	113.80
3	H	396	PHE	CA-CB-CG	6.34	120.14	113.80
2	C	32	ASP	CA-CB-CG	6.14	118.74	112.60
3	E	369	ASP	CA-CB-CG	6.05	118.65	112.60

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	ARG	Sidechain
1	A	379	ARG	Sidechain
1	A	480	ARG	Sidechain
1	A	518	ARG	Sidechain
1	A	538	ARG	Sidechain

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	2909	0	3009	0	0
1	B	2909	0	3009	0	0
2	C	1117	0	1152	0	0
2	D	1117	0	1152	0	0
3	E	736	0	750	0	0
3	F	736	0	750	0	0
3	G	736	0	750	0	0
3	H	736	0	750	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	736	0	750	0	0
3	J	736	0	750	0	0
3	K	736	0	750	0	0
3	L	736	0	750	0	0
3	M	736	0	750	0	0
3	N	736	0	750	0	0
3	O	736	0	750	0	0
3	P	736	0	750	0	0
All	All	16884	0	17322	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	381/654 (58%)	368 (97%)	10 (3%)	3 (1%)	16	54
1	B	381/654 (58%)	372 (98%)	7 (2%)	2 (0%)	24	63
2	C	143/167 (86%)	135 (94%)	6 (4%)	2 (1%)	9	40
2	D	143/167 (86%)	135 (94%)	6 (4%)	2 (1%)	9	40
3	E	100/551 (18%)	100 (100%)	0	0	100	100
3	F	100/551 (18%)	100 (100%)	0	0	100	100
3	G	100/551 (18%)	100 (100%)	0	0	100	100
3	H	100/551 (18%)	100 (100%)	0	0	100	100
3	I	100/551 (18%)	100 (100%)	0	0	100	100
3	J	100/551 (18%)	100 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	100/551 (18%)	100 (100%)	0	0	100	100
3	L	100/551 (18%)	100 (100%)	0	0	100	100
3	M	100/551 (18%)	100 (100%)	0	0	100	100
3	N	100/551 (18%)	100 (100%)	0	0	100	100
3	O	100/551 (18%)	100 (100%)	0	0	100	100
3	P	100/551 (18%)	100 (100%)	0	0	100	100
All	All	2248/8254 (27%)	2210 (98%)	29 (1%)	9 (0%)	31	67

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	81	ASP
2	D	81	ASP
1	A	618	PRO
1	B	579	GLN
1	B	618	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/552 (58%)	319 (99%)	2 (1%)	78	83
1	B	321/552 (58%)	320 (100%)	1 (0%)	86	86
2	C	126/143 (88%)	123 (98%)	3 (2%)	43	64
2	D	126/143 (88%)	123 (98%)	3 (2%)	43	64
3	E	77/438 (18%)	77 (100%)	0	100	100
3	F	77/438 (18%)	76 (99%)	1 (1%)	61	74
3	G	77/438 (18%)	77 (100%)	0	100	100
3	H	77/438 (18%)	77 (100%)	0	100	100
3	I	77/438 (18%)	76 (99%)	1 (1%)	61	74
3	J	77/438 (18%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	77/438 (18%)	77 (100%)	0	100	100
3	L	77/438 (18%)	77 (100%)	0	100	100
3	M	77/438 (18%)	76 (99%)	1 (1%)	61	74
3	N	77/438 (18%)	76 (99%)	1 (1%)	61	74
3	O	77/438 (18%)	77 (100%)	0	100	100
3	P	77/438 (18%)	77 (100%)	0	100	100
All	All	1818/6646 (27%)	1805 (99%)	13 (1%)	73	81

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

Mol	Chain	Res	Type
2	D	115	GLN
2	D	126	LEU
3	N	412	GLN
3	I	349	GLN
3	M	365	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10050. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

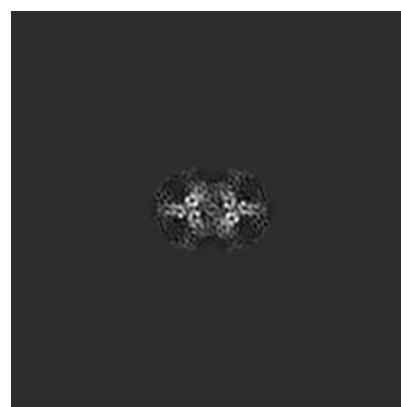
6.1.1 Primary map



X



Y



Z

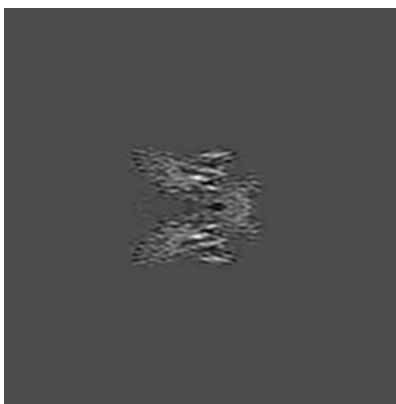
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 102



Y Index: 102



Z Index: 102

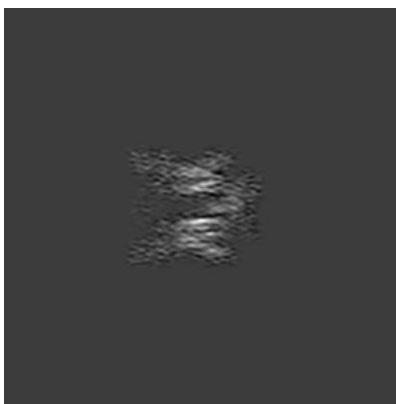
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

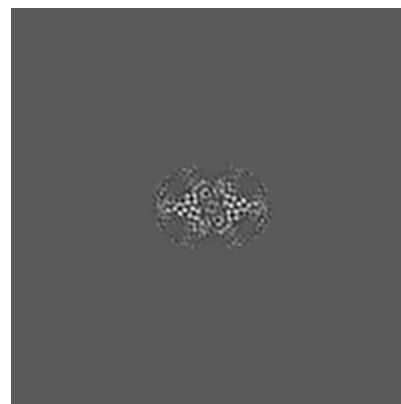
6.3.1 Primary map



X Index: 110



Y Index: 100

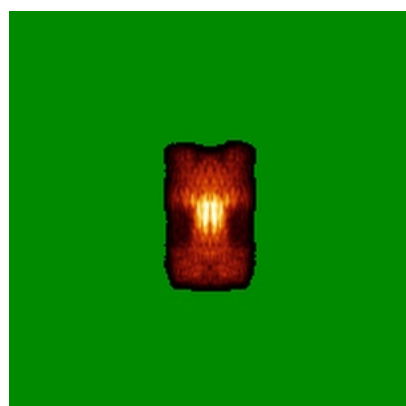


Z Index: 105

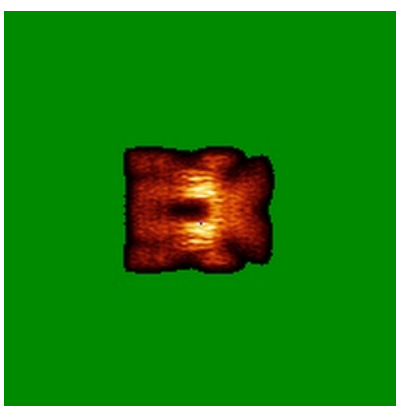
The images above show the largest variance slices of the map in three orthogonal directions.

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

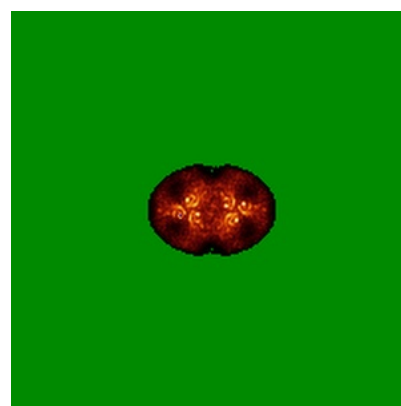
6.4.1 Primary map



X



Y

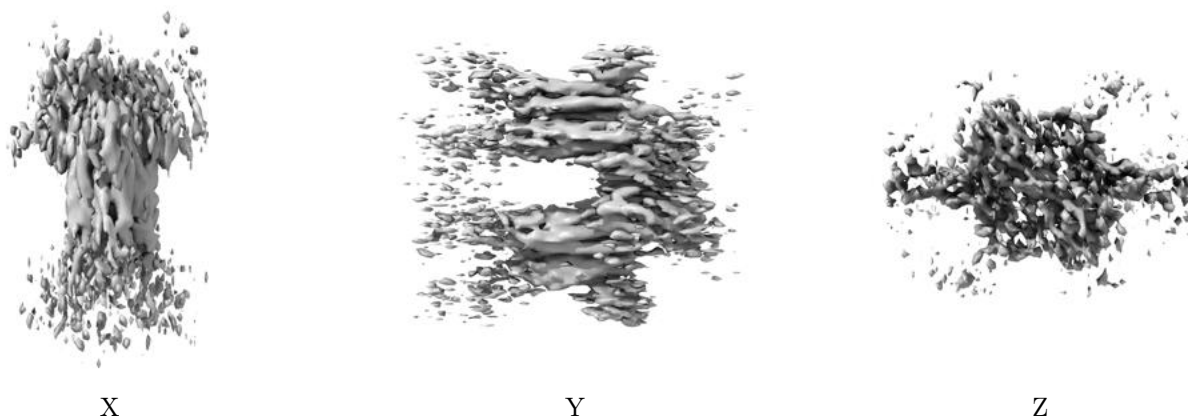


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

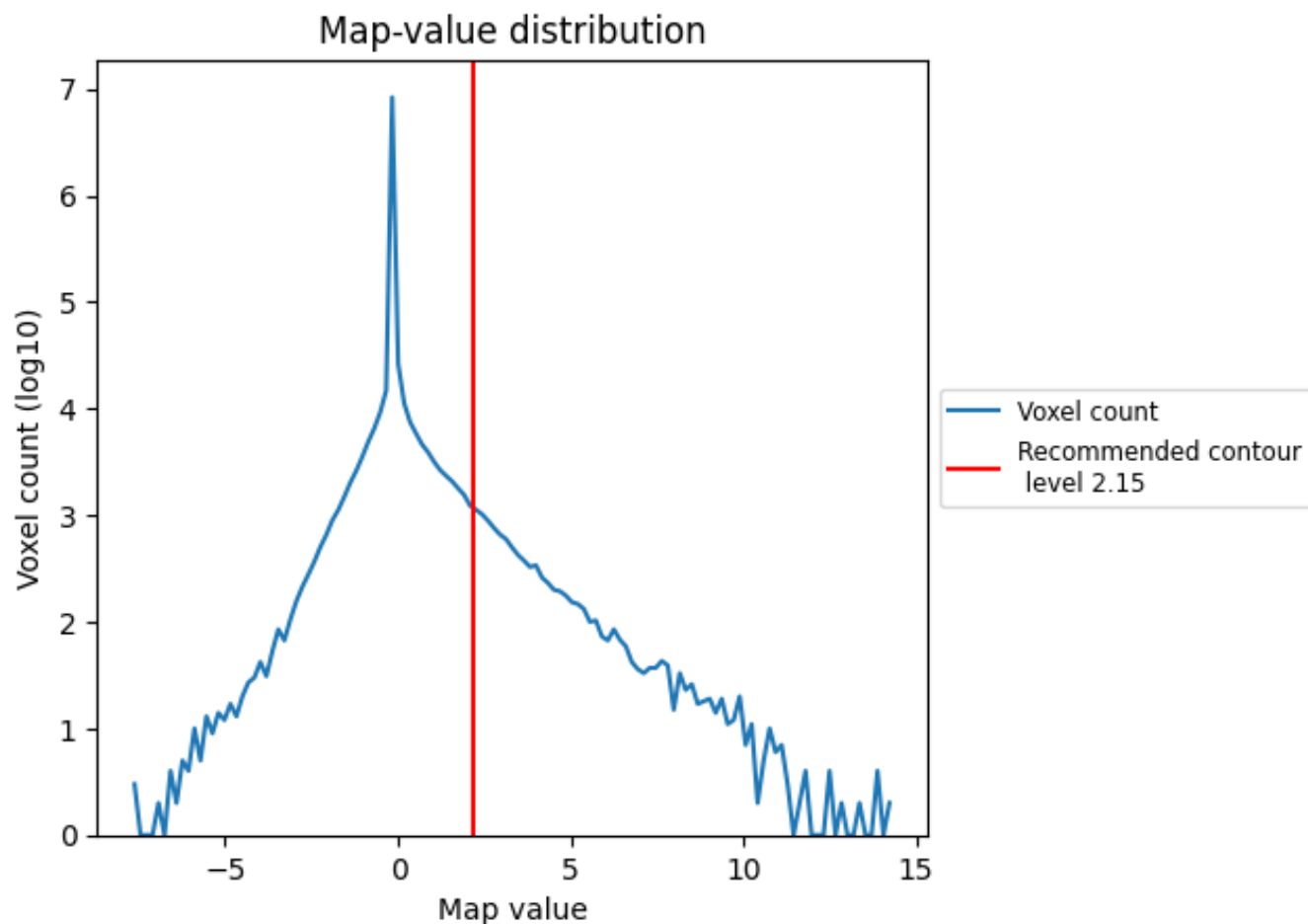
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

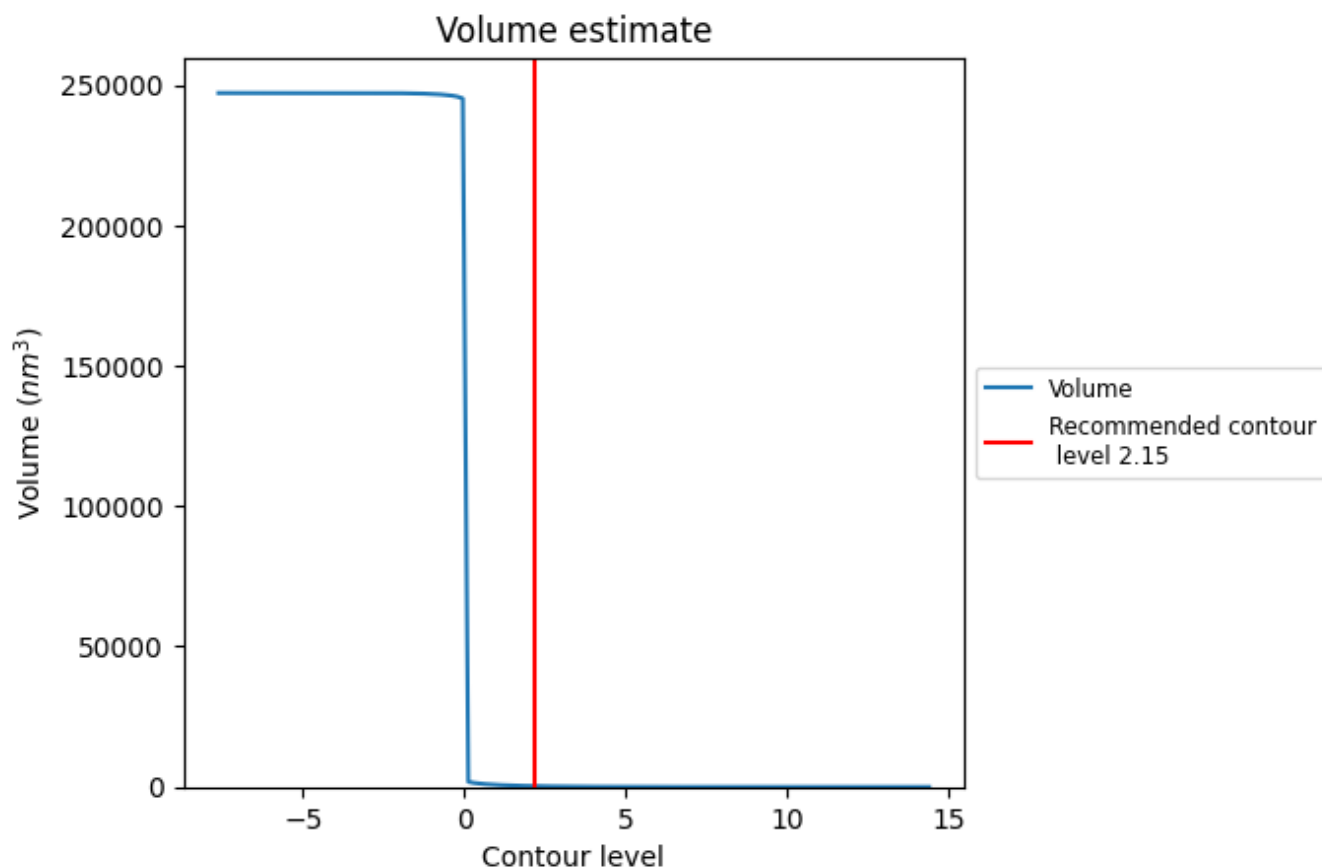
This section contains the results of statistical analysis of the map.

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.

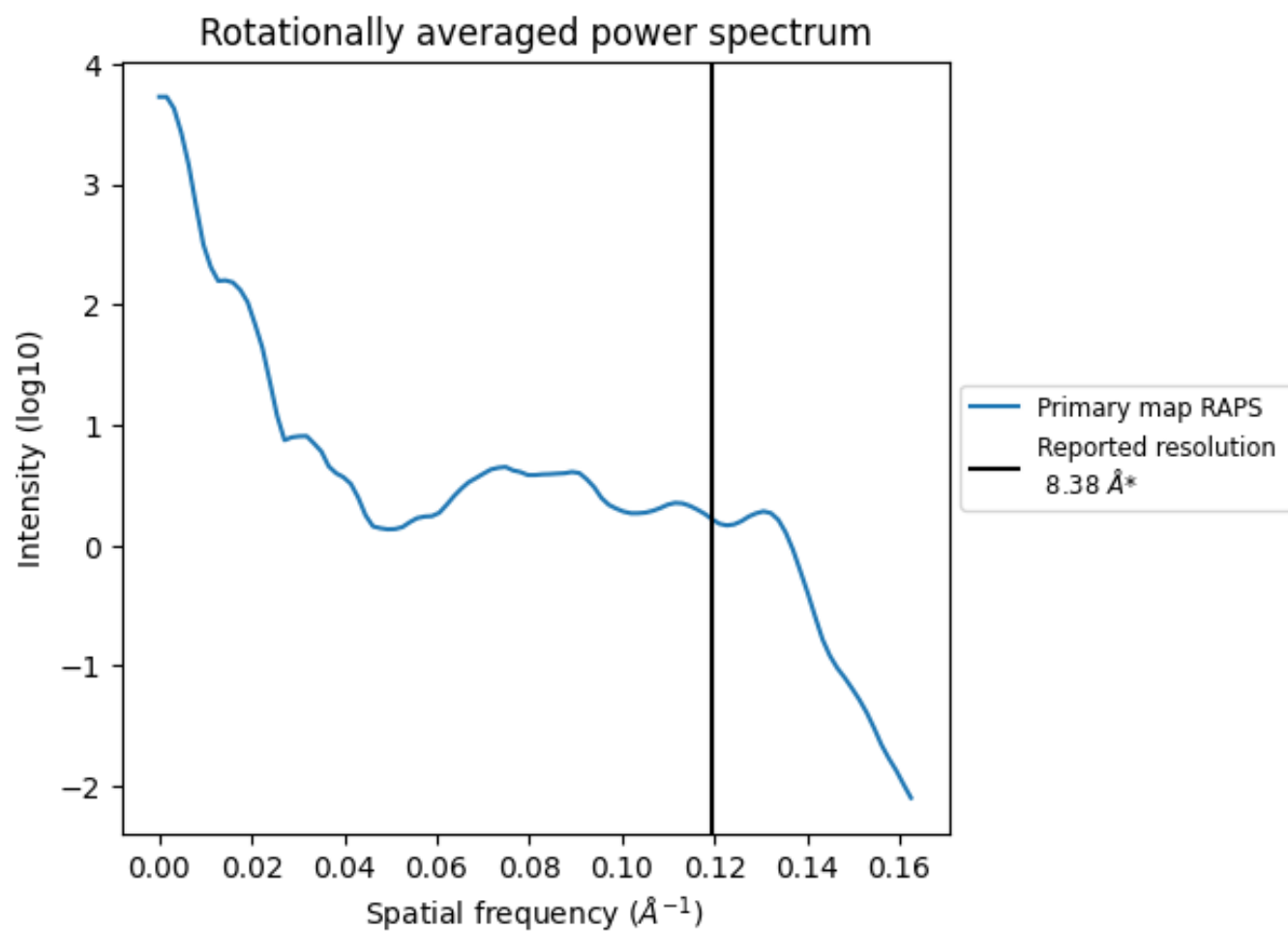
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 305 nm^3 ; this corresponds to an approximate mass of 275 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 0.119 Å⁻¹

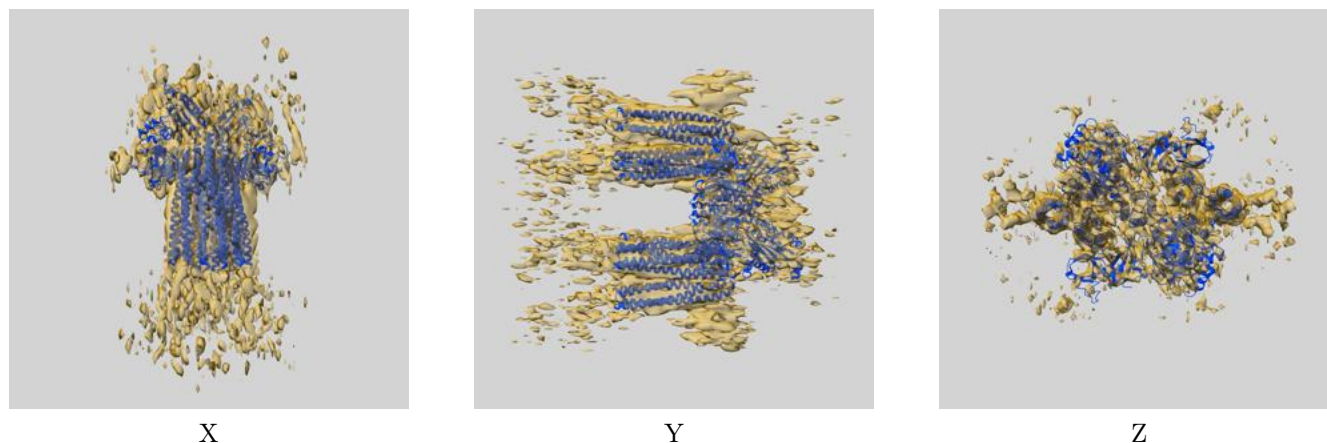
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

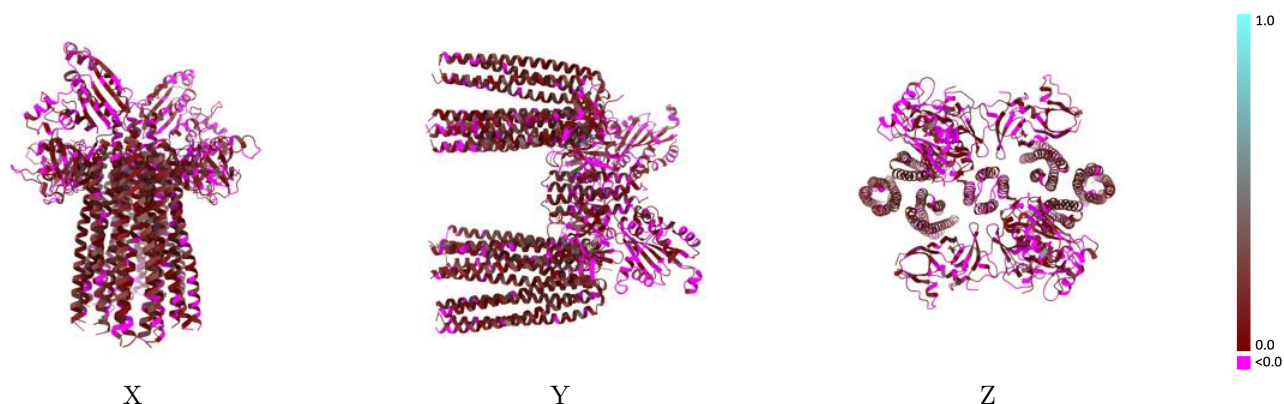
This section contains information regarding the fit between EMDB map EMD-10050 and PDB model 6S1K. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



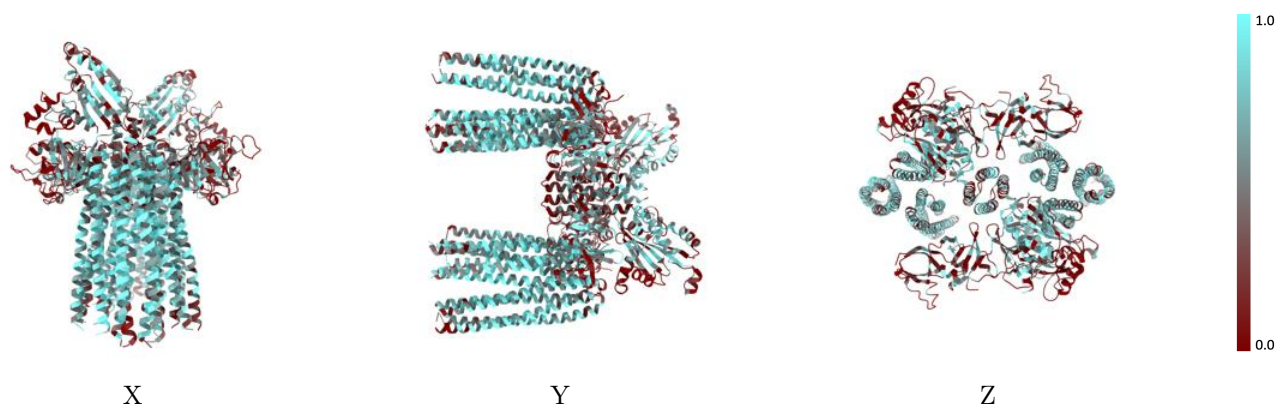
The images above show the 3D surface view of the map at the recommended contour level 2.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



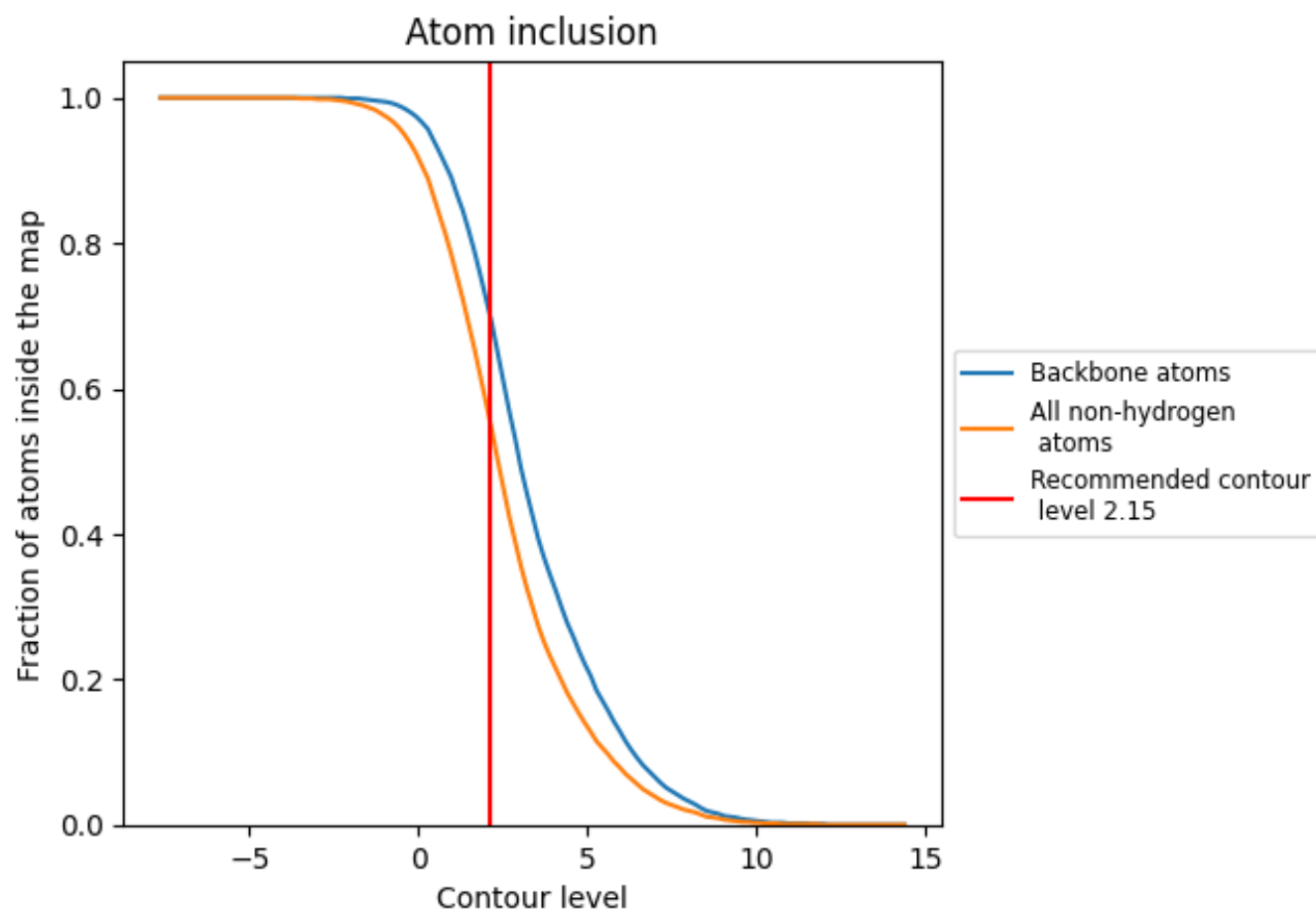
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 55% 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 (2.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5500	0.0880
A	0.4200	0.0390
B	0.4140	0.0380
C	0.3040	0.0660
D	0.3050	0.0480
E	0.6880	0.1330
F	0.7570	0.1300
G	0.6330	0.1230
H	0.7670	0.1270
I	0.6630	0.1200
J	0.7110	0.1200
K	0.6800	0.1340
L	0.7680	0.1470
M	0.6130	0.1220
N	0.7460	0.1350
O	0.6600	0.1160
P	0.7140	0.1240

1.0

0.0

<0.0