



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 11:50 PM UTC

PDB ID : 8RKT / pdb_00008rkt
EMDB ID : EMD-19282
Title : Conformational Landscape of the Type V-K CRISPR-associated Transposon Integration Assembly CAST V-K Cas12k domain local-refinement map
Authors : Tenjo-Castano, F.; Mesa, P.; Montoya, G.
Deposited on : 2023-12-30
Resolution : 2.35 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:

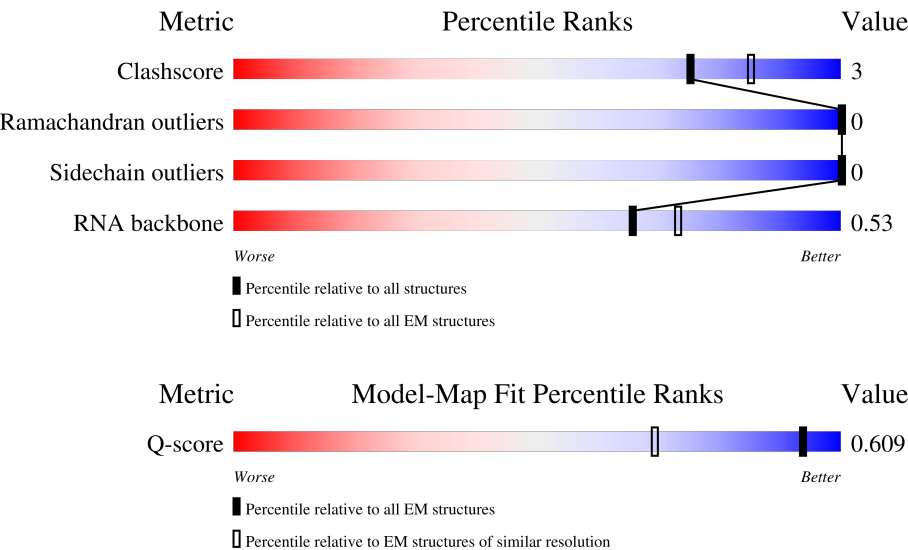
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



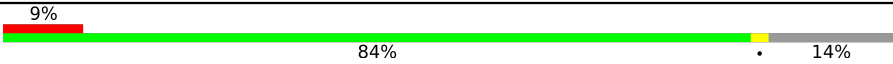
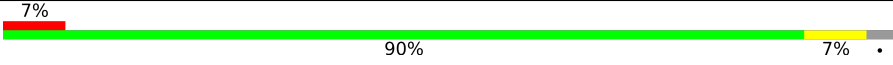
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4607 (1.85 - 2.85)

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	1	261	22% 62% 25% 7% 6%
2	2	68	24% 32% 18% 50%
3	3	133	13% 11% 76%

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Mol	Chain	Length	Quality of chain
4	A	698	
5	B	90	
6	C	179	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13794 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 RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	246	5239	2342	930	1722	245	0	0

- Molecule 2 is a DNA chain called Non-target strand - LE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	34	696	334	125	204	33	0	0

- Molecule 3 is a DNA chain called Target strand - LE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	32	647	311	109	195	32	0	0

- Molecule 4 is a protein called ShCas12k.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	602	4872	3072	882	903	15	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-58	MET	-	initiating methionine	UNP A0A8X6EH11
A	-57	GLY	-	expression tag	UNP A0A8X6EH11
A	-56	SER	-	expression tag	UNP A0A8X6EH11
A	-55	SER	-	expression tag	UNP A0A8X6EH11
A	-54	HIS	-	expression tag	UNP A0A8X6EH11
A	-53	HIS	-	expression tag	UNP A0A8X6EH11
A	-52	HIS	-	expression tag	UNP A0A8X6EH11
A	-51	HIS	-	expression tag	UNP A0A8X6EH11
A	-50	HIS	-	expression tag	UNP A0A8X6EH11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-49	HIS	-	expression tag	UNP A0A8X6EH11
A	-48	SER	-	expression tag	UNP A0A8X6EH11
A	-47	SER	-	expression tag	UNP A0A8X6EH11
A	-46	GLY	-	expression tag	UNP A0A8X6EH11
A	-45	LEU	-	expression tag	UNP A0A8X6EH11
A	-44	VAL	-	expression tag	UNP A0A8X6EH11
A	-43	PRO	-	expression tag	UNP A0A8X6EH11
A	-42	ARG	-	expression tag	UNP A0A8X6EH11
A	-41	GLY	-	expression tag	UNP A0A8X6EH11
A	-40	SER	-	expression tag	UNP A0A8X6EH11
A	-39	HIS	-	expression tag	UNP A0A8X6EH11
A	-38	MET	-	expression tag	UNP A0A8X6EH11
A	-37	ALA	-	expression tag	UNP A0A8X6EH11
A	-36	SER	-	expression tag	UNP A0A8X6EH11
A	-35	TRP	-	expression tag	UNP A0A8X6EH11
A	-34	SER	-	expression tag	UNP A0A8X6EH11
A	-33	HIS	-	expression tag	UNP A0A8X6EH11
A	-32	PRO	-	expression tag	UNP A0A8X6EH11
A	-31	GLN	-	expression tag	UNP A0A8X6EH11
A	-30	PHE	-	expression tag	UNP A0A8X6EH11
A	-29	GLU	-	expression tag	UNP A0A8X6EH11
A	-28	LYS	-	expression tag	UNP A0A8X6EH11
A	-27	GLY	-	expression tag	UNP A0A8X6EH11
A	-26	GLY	-	expression tag	UNP A0A8X6EH11
A	-25	GLY	-	expression tag	UNP A0A8X6EH11
A	-24	SER	-	expression tag	UNP A0A8X6EH11
A	-23	GLY	-	expression tag	UNP A0A8X6EH11
A	-22	GLY	-	expression tag	UNP A0A8X6EH11
A	-21	GLY	-	expression tag	UNP A0A8X6EH11
A	-20	SER	-	expression tag	UNP A0A8X6EH11
A	-19	GLY	-	expression tag	UNP A0A8X6EH11
A	-18	GLY	-	expression tag	UNP A0A8X6EH11
A	-17	SER	-	expression tag	UNP A0A8X6EH11
A	-16	ALA	-	expression tag	UNP A0A8X6EH11
A	-15	TRP	-	expression tag	UNP A0A8X6EH11
A	-14	SER	-	expression tag	UNP A0A8X6EH11
A	-13	HIS	-	expression tag	UNP A0A8X6EH11
A	-12	PRO	-	expression tag	UNP A0A8X6EH11
A	-11	GLN	-	expression tag	UNP A0A8X6EH11
A	-10	PHE	-	expression tag	UNP A0A8X6EH11
A	-9	GLU	-	expression tag	UNP A0A8X6EH11
A	-8	LYS	-	expression tag	UNP A0A8X6EH11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLU	-	expression tag	UNP A0A8X6EH11
A	-6	ASN	-	expression tag	UNP A0A8X6EH11
A	-5	LEU	-	expression tag	UNP A0A8X6EH11
A	-4	TYR	-	expression tag	UNP A0A8X6EH11
A	-3	PHE	-	expression tag	UNP A0A8X6EH11
A	-2	GLN	-	expression tag	UNP A0A8X6EH11
A	-1	GLY	-	expression tag	UNP A0A8X6EH11
A	0	GLY	-	expression tag	UNP A0A8X6EH11
A	1	SER	-	expression tag	UNP A0A8X6EH11

- Molecule 5 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	87	Total	C	N	O	S	0	0
			708	438	141	128	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	expression tag	UNP A0A139X9A4
B	3	ALA	THR	variant	UNP A0A139X9A4
B	7	GLU	GLN	variant	UNP A0A139X9A4
B	14	VAL	SER	variant	UNP A0A139X9A4
B	30	VAL	ILE	variant	UNP A0A139X9A4
B	42	LEU	GLU	variant	UNP A0A139X9A4
B	46	ALA	SER	variant	UNP A0A139X9A4
B	71	ILE	VAL	variant	UNP A0A139X9A4
B	73	LYS	GLN	variant	UNP A0A139X9A4
B	74	ASP	GLY	variant	UNP A0A139X9A4
B	78	LYS	HIS	variant	UNP A0A139X9A4

- Molecule 6 is a protein called TniQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	164	Total	C	N	O	S	0	0
			1306	832	240	220	14		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	168	GLY	-	expression tag	UNP A0A8J0PCL5
C	169	SER	-	expression tag	UNP A0A8J0PCL5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	170	GLU	-	expression tag	UNP A0A8J0PCL5
C	171	PHE	-	expression tag	UNP A0A8J0PCL5
C	172	GLU	-	expression tag	UNP A0A8J0PCL5
C	173	LEU	-	expression tag	UNP A0A8J0PCL5
C	174	GLU	-	expression tag	UNP A0A8J0PCL5
C	175	ASN	-	expression tag	UNP A0A8J0PCL5
C	176	LEU	-	expression tag	UNP A0A8J0PCL5
C	177	TYR	-	expression tag	UNP A0A8J0PCL5
C	178	PHE	-	expression tag	UNP A0A8J0PCL5
C	179	GLN	-	expression tag	UNP A0A8J0PCL5

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

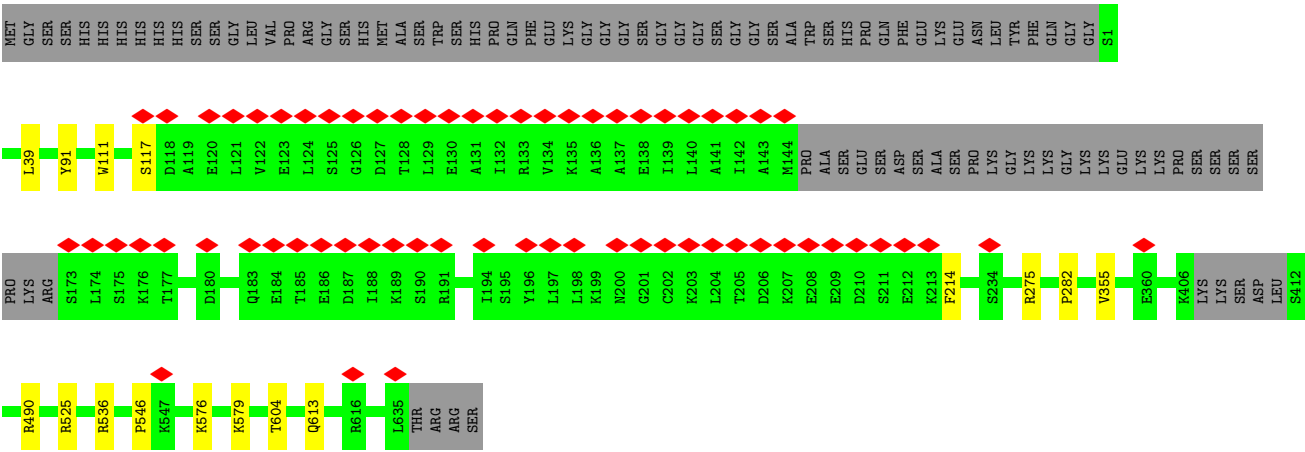
Mol	Chain	Residues	Atoms	AltConf
7	1	1	Total Mg 1 1	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

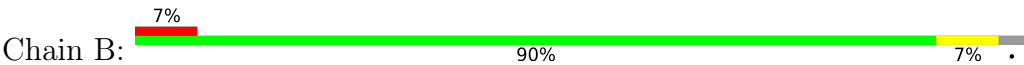
Mol	Chain	Residues	Atoms	AltConf
8	C	2	Total Zn 2 2	0

- Molecule 9 is water.

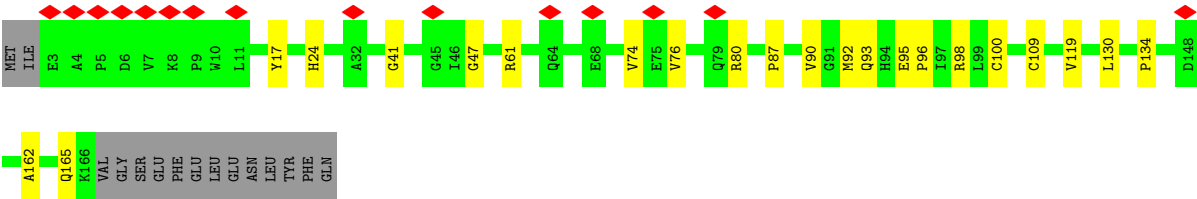
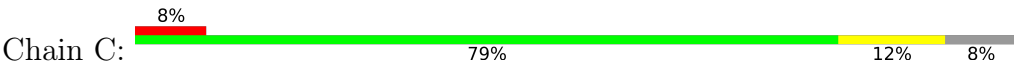
Mol	Chain	Residues	Atoms	AltConf
9	1	160	Total O 160 160	0
9	2	7	Total O 7 7	0
9	3	33	Total O 33 33	0
9	A	93	Total O 93 93	0
9	B	13	Total O 13 13	0
9	C	17	Total O 17 17	0



• Molecule 5: Small ribosomal subunit protein uS15



• Molecule 6: TniQ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144000	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.921	Depositor
Minimum map value	-1.027	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.24	Depositor
Map size (Å)	173.99199, 175.448, 351.624	wwPDB
Map dimensions	239, 241, 483	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7279999, 0.728, 0.728	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: ZN, 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	1	0.32	0/5858	0.68	1/9128 (0.0%)
2	2	0.32	0/780	0.76	0/1203
3	3	0.41	0/722	0.77	1/1110 (0.1%)
4	A	0.22	0/4959	0.46	0/6686
5	B	0.22	0/713	0.46	0/952
6	C	0.29	0/1345	0.51	0/1819
All	All	0.29	0/14377	0.60	2/20898 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	130	DT	P-O3'-C3'	-7.63	108.76	120.20
1	1	196	A	C2'-C3'-O3'	5.74	118.10	109.50

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	1	5239	0	2644	36	0
2	2	696	0	387	8	0
3	3	647	0	364	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4872	0	4938	10	0
5	B	708	0	748	3	0
6	C	1306	0	1285	12	0
7	1	1	0	0	0	0
8	C	2	0	0	0	0
9	1	160	0	0	2	0
9	2	7	0	0	0	0
9	3	33	0	0	0	0
9	A	93	0	0	0	0
9	B	13	0	0	0	0
9	C	17	0	0	0	0
All	All	13794	0	10366	73	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 3.

The worst 5 of 73 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)
1:1:256:G:OP2	6:C:61:ARG:NH1	2.19	0.75
1:1:100:U:H3	1:1:139:A:H2	1.37	0.71
4:A:282:PRO:HB3	4:A:355:VAL:HG22	1.75	0.68
6:C:95:GLU:HB3	6:C:96:PRO:HD3	1.76	0.67
6:C:100:CYS:O	6:C:165:GLN:NE2	2.27	0.66

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
4	A	596/698 (85%)	591 (99%)	5 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	85/90 (94%)	82 (96%)	3 (4%)	0	100	100
6	C	162/179 (90%)	154 (95%)	8 (5%)	0	100	100
All	All	843/967 (87%)	827 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
4	A	531/608 (87%)	531 (100%)	0	100	100
5	B	76/78 (97%)	76 (100%)	0	100	100
6	C	136/150 (91%)	136 (100%)	0	100	100
All	All	743/836 (89%)	743 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	438	GLN
6	C	79	GLN
6	C	152	HIS
6	C	94	HIS
4	A	431	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	245/261 (93%)	46 (18%)	8 (3%)

5 of 46 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	G
1	1	34	C
1	1	38	C
1	1	39	U
1	1	45	U

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	239	A
1	1	238	G
1	1	167	G
1	1	76	A
1	1	196	A

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](#)

Of 3 ligands modelled in this entry, 3 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 ⓘ

There are no chain breaks in this entry.

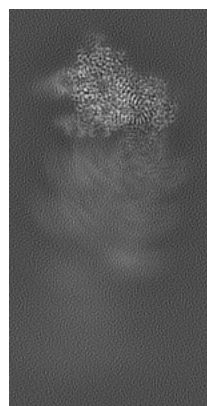
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19282. These allow visual inspection of the internal detail of the map and identification of artifacts.

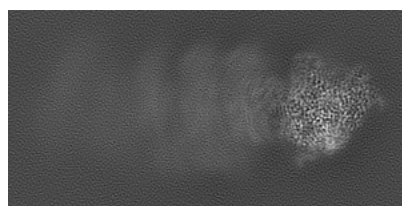
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

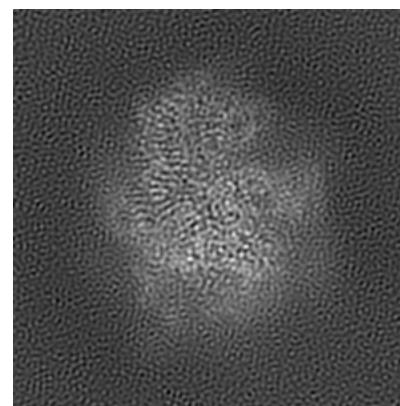
6.1.1 Primary map



X

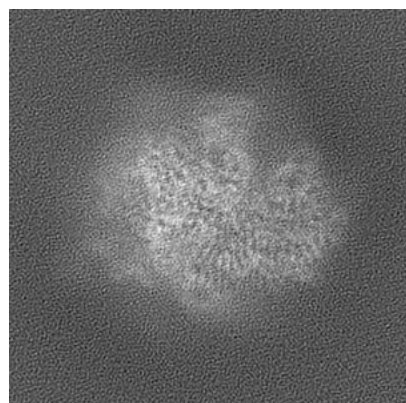


Y

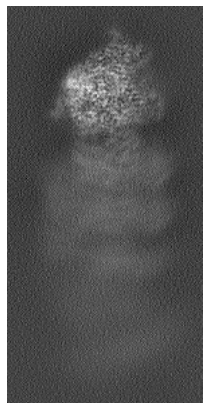


Z

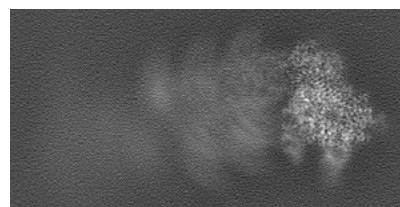
6.1.2 Raw map



X



Y



Z

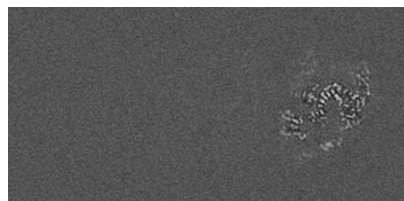
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

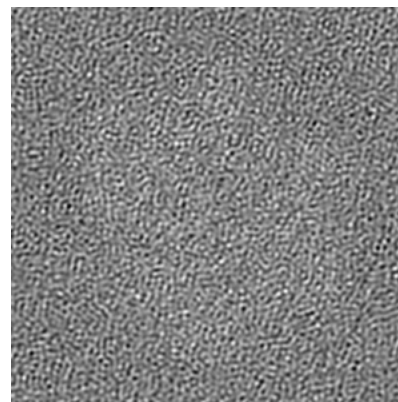
6.2.1 Primary map



X Index: 119

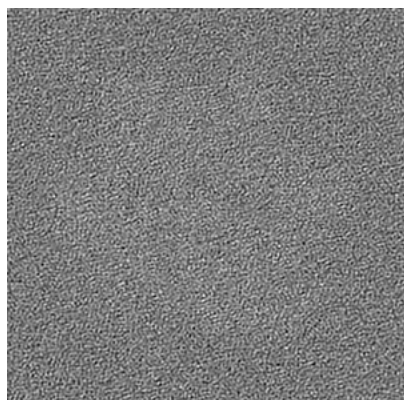


Y Index: 120

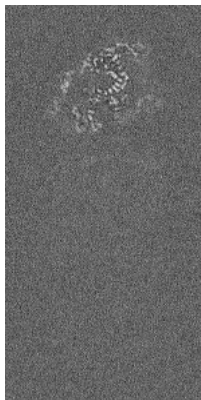


Z Index: 241

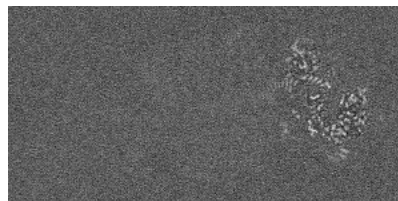
6.2.2 Raw map



X Index: 241



Y Index: 120

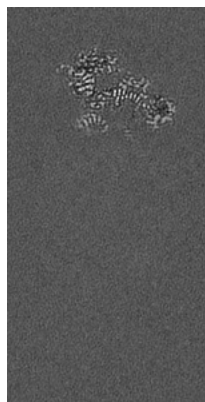


Z Index: 119

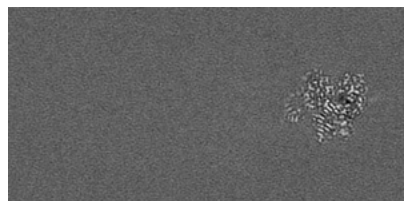
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

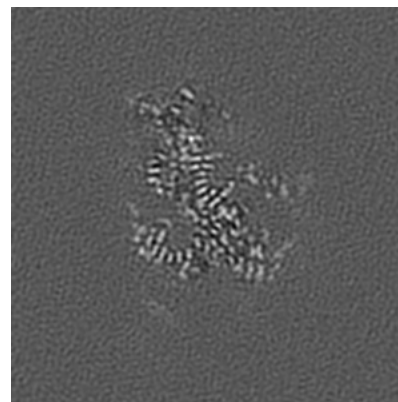
6.3.1 Primary map



X Index: 113

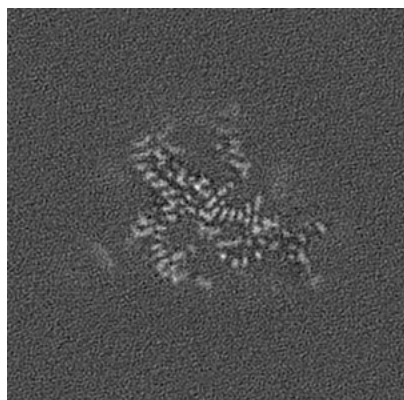


Y Index: 92

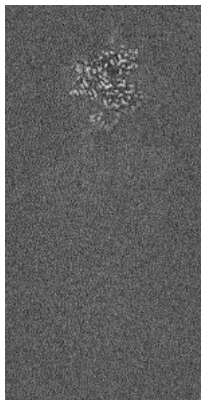


Z Index: 377

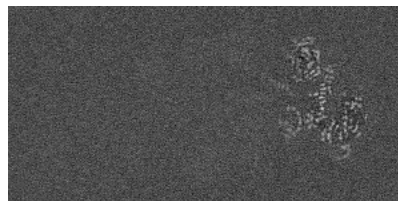
6.3.2 Raw map



X Index: 378



Y Index: 92

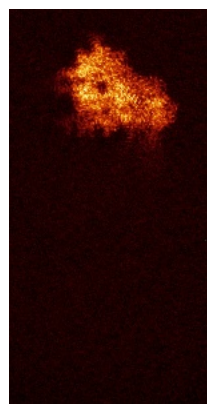


Z Index: 115

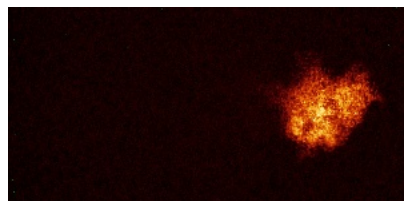
The images above show the largest variance slices of the map in three orthogonal directions.

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

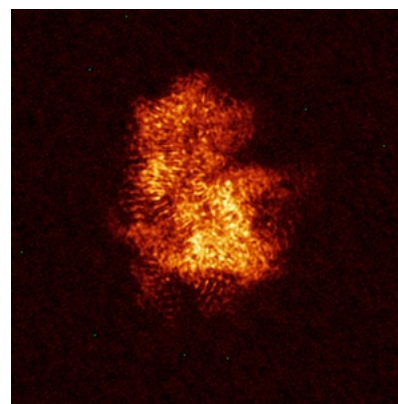
6.4.1 Primary map



X

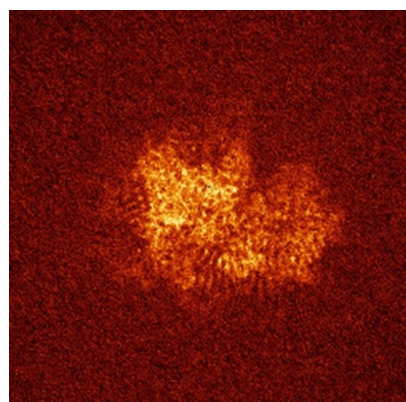


Y

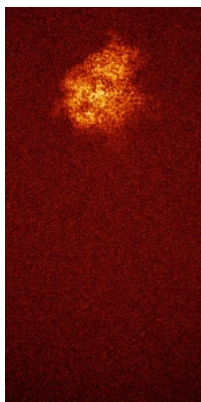


Z

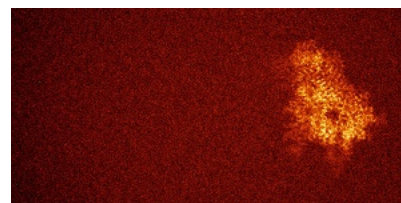
6.4.2 Raw map



X



Y

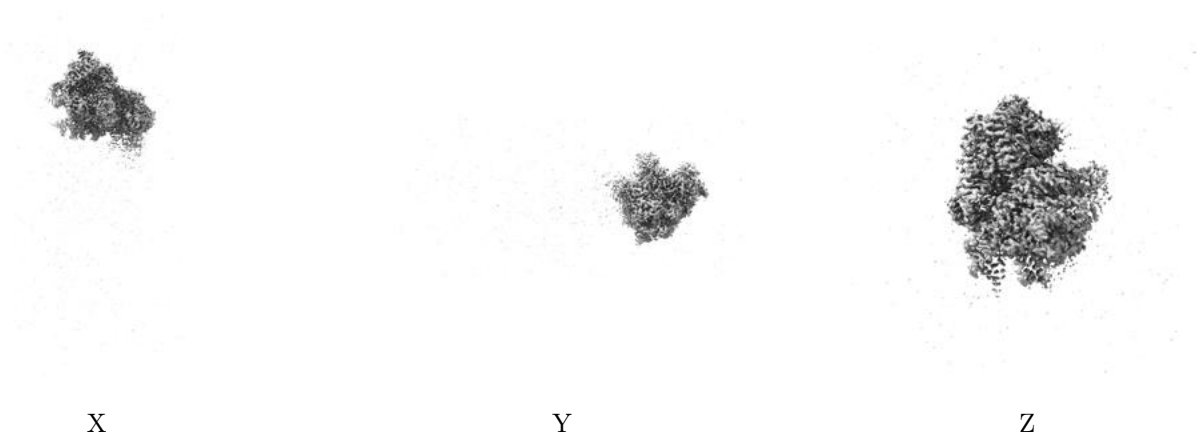


Z

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

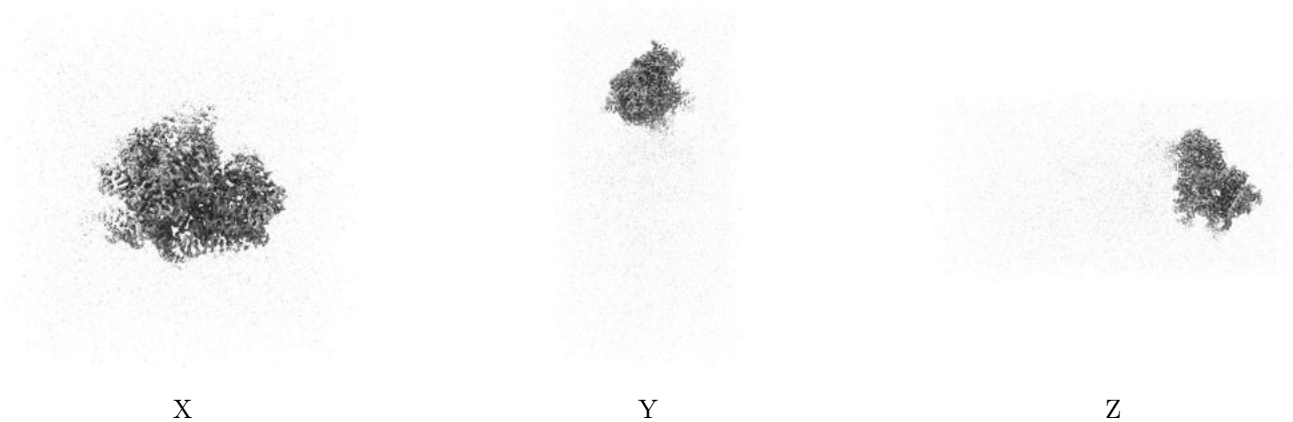
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

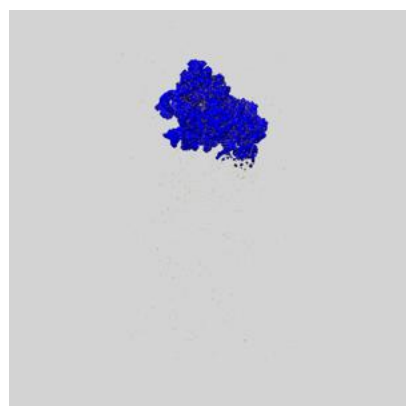
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

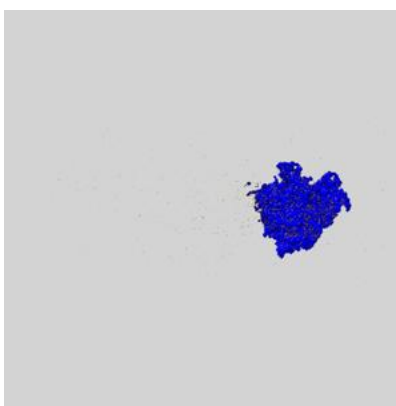
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

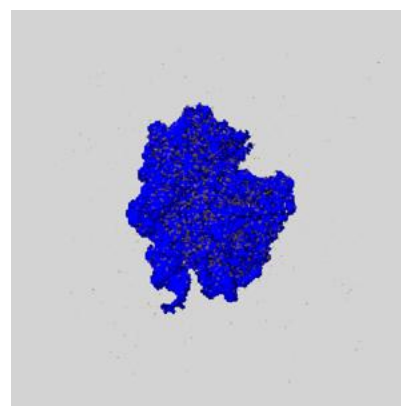
6.6.1 emd_19282_msk_1.map [i](#)



X



Y

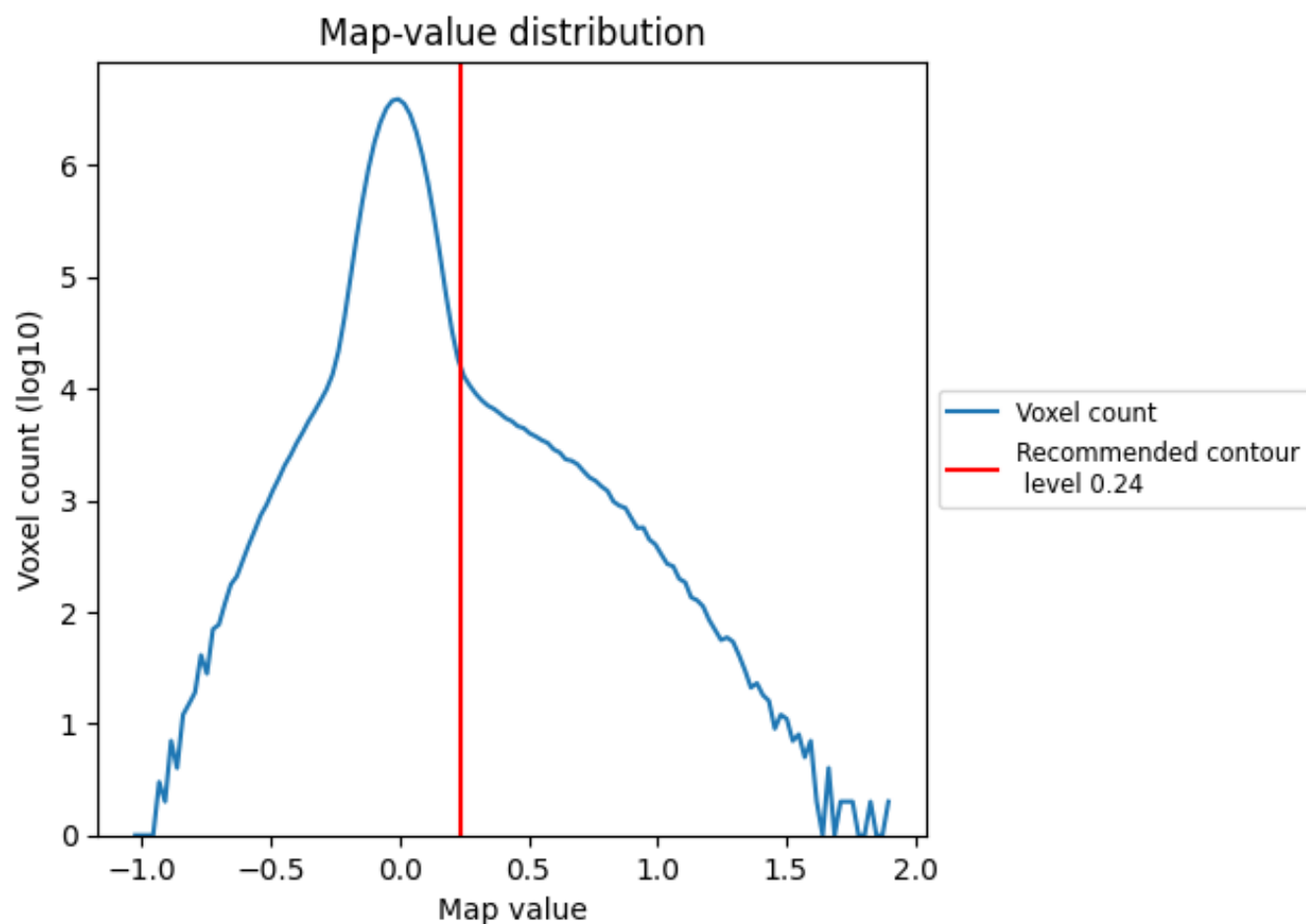


Z

7 Map analysis [i](#)

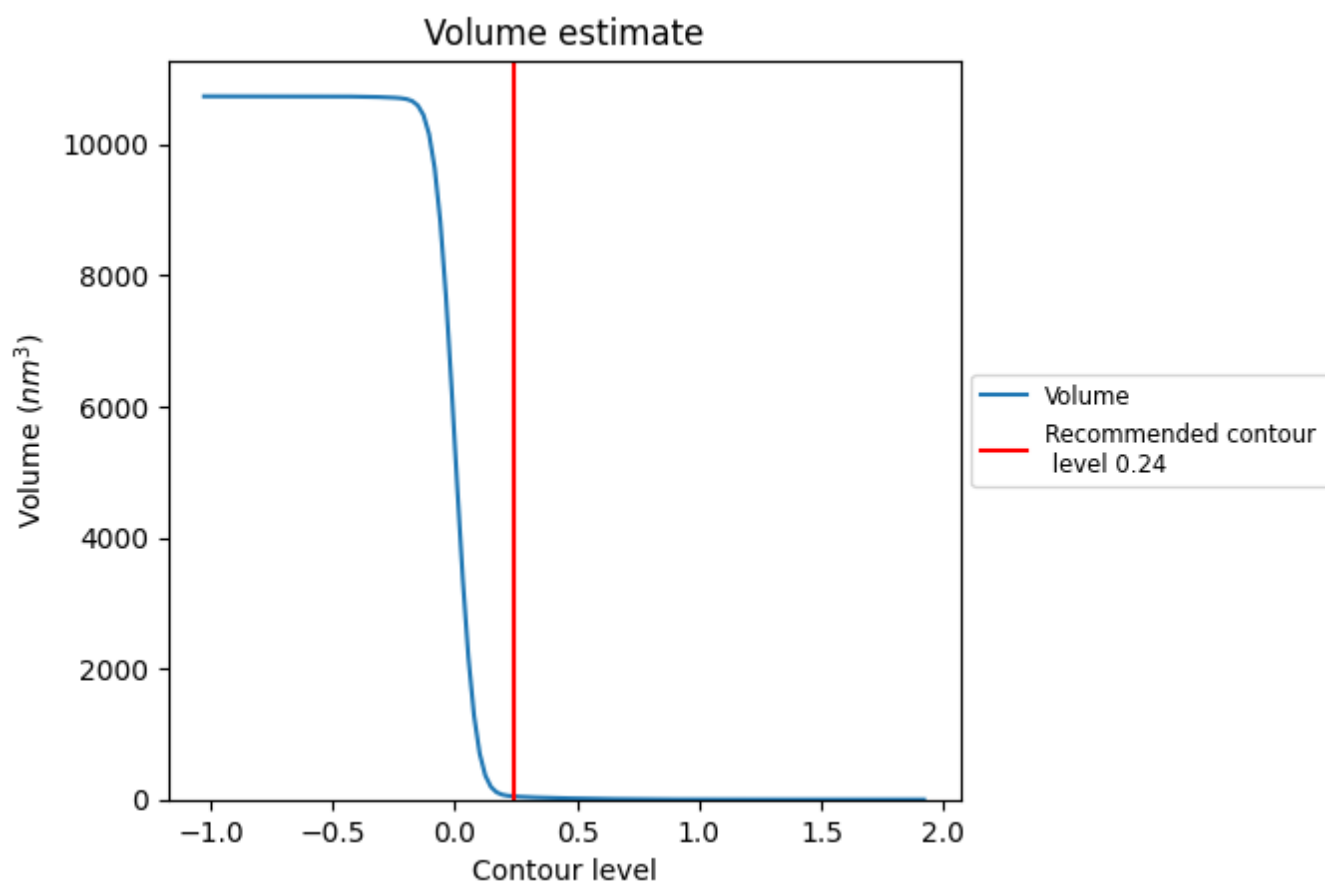
This section contains the results of statistical analysis of the map.

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 49 nm³; this corresponds to an approximate mass of 45 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

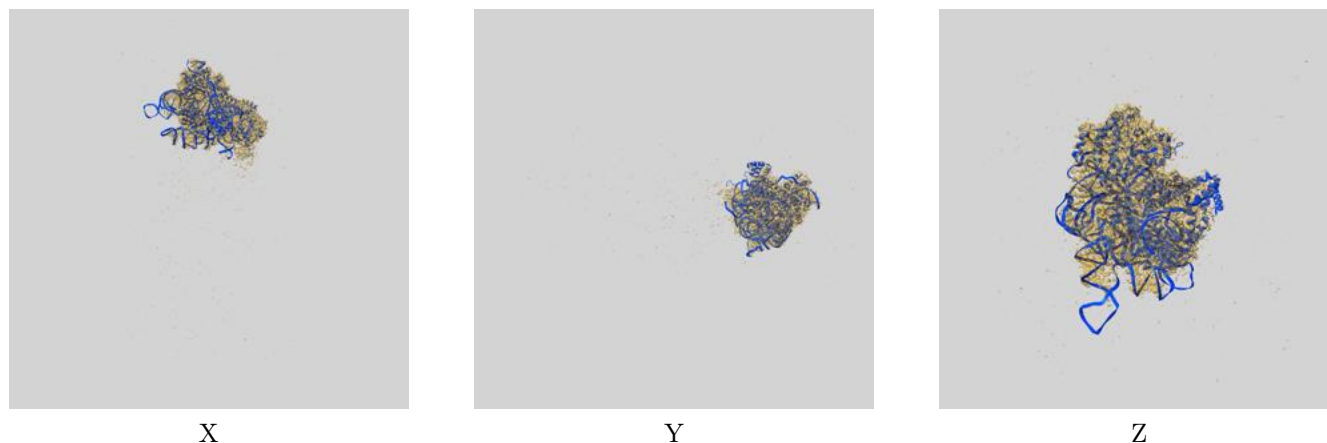
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

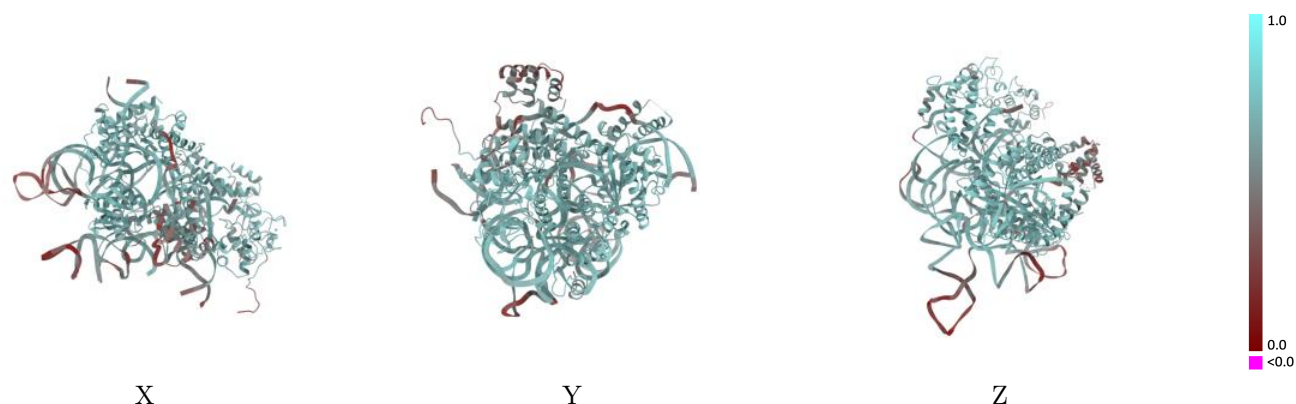
This section contains information regarding the fit between EMDB map EMD-19282 and PDB model 8RKT. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



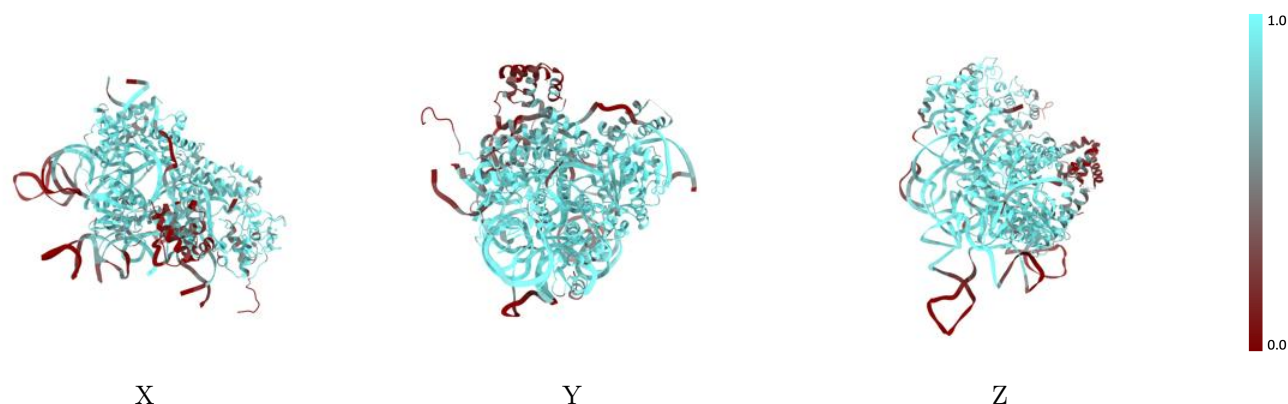
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



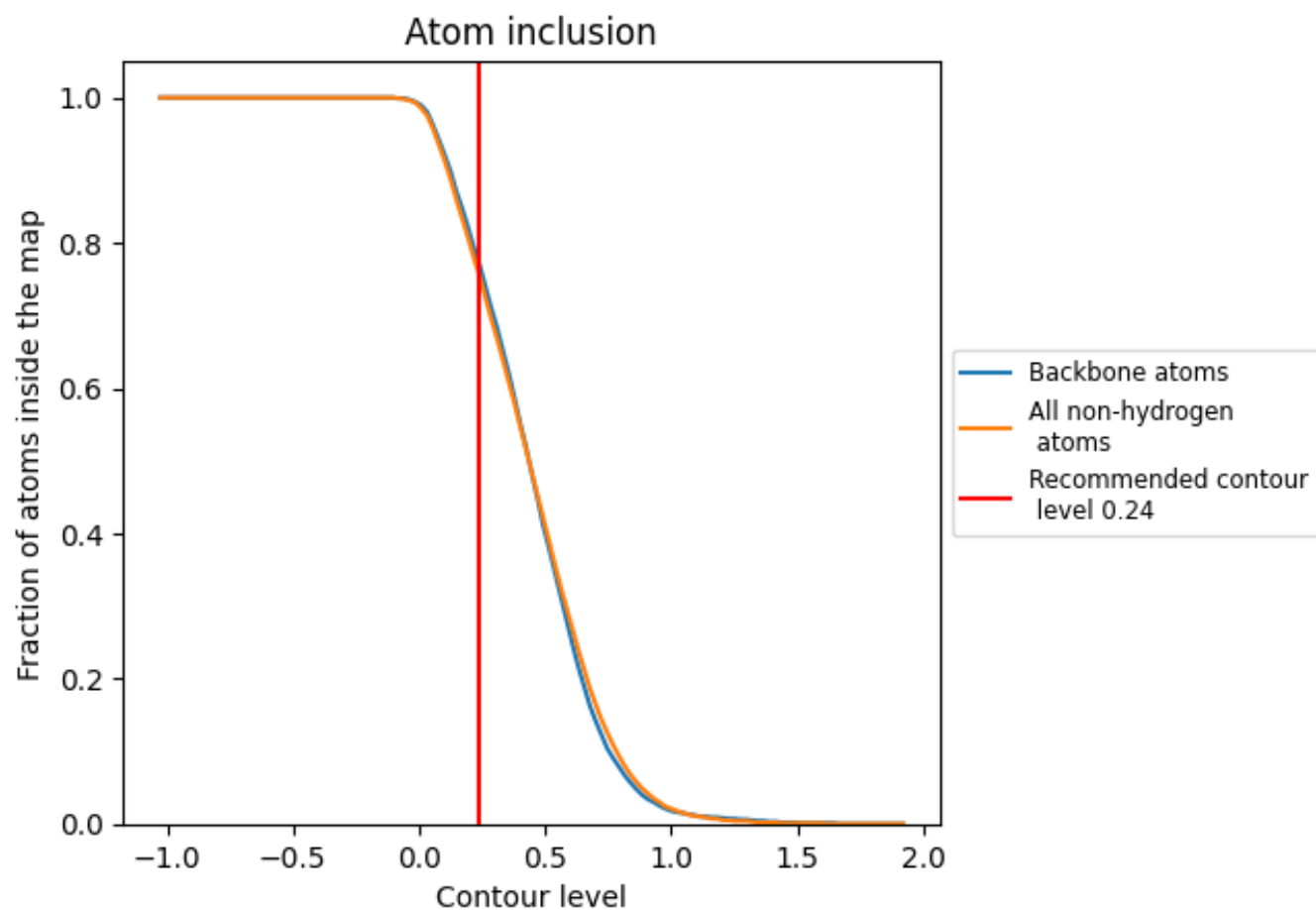
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.6090
1	0.7120	0.5710
2	0.4600	0.4800
3	0.8360	0.6440
A	0.8110	0.6480
B	0.8470	0.6570
C	0.8100	0.6370

1.0

0.0

<0.0