



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:25 PM UTC

PDB ID : 7JZY / pdb_00007jzy
EMDB ID : EMD-22584
Title : CryoEM structure of a CRISPR-Cas complex
Authors : Chang, L.; Li, Z.; Gabel, C.
Deposited on : 2020-09-02
Resolution : 3.60 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:

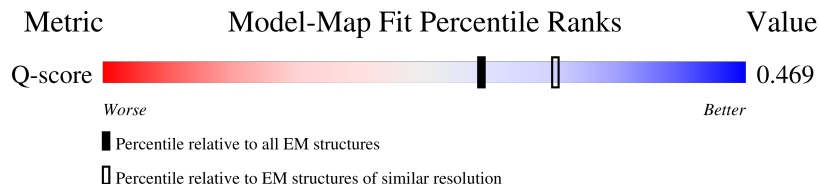
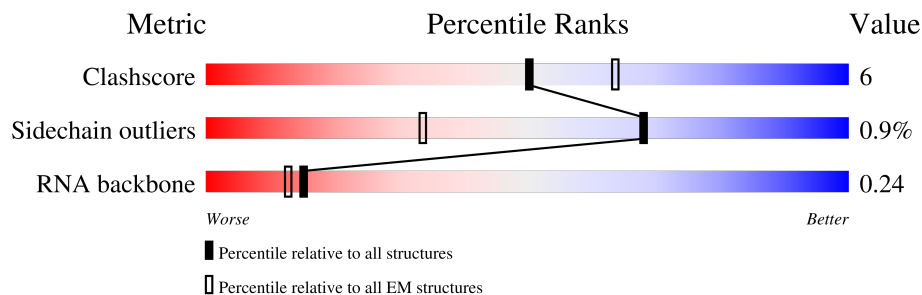
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.60 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	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	434	
2	B	327	
3	C	189	
4	M	61	

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Mol	Chain	Length	Quality of chain
5	D	342	
5	E	342	
5	F	342	
5	G	342	
5	H	342	
5	I	342	
6	J	68	
6	K	68	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 24539 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 CRISPR-associated protein Csy1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	427	Total	C	N	O	S	0	0
			3088	1939	582	564	3		

- Molecule 2 is a protein called Type I-F CRISPR-associated protein Csy2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	306	Total	C	N	O	S	0	0
			2411	1529	445	432	5		

- Molecule 3 is a protein called Type I-F CRISPR-associated endoribonuclease Cas6/Csy4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	187	Total	C	N	O	S	1	0
			1448	922	264	257	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	PHE	-	expression tag	UNP A0A643HZS6
C	0	THR	-	expression tag	UNP A0A643HZS6

- Molecule 4 is a RNA chain called RNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	61	Total	C	N	O	P	0	0
			1273	569	223	421	60		

There are 2 discrepancies between the modelled and reference sequences:

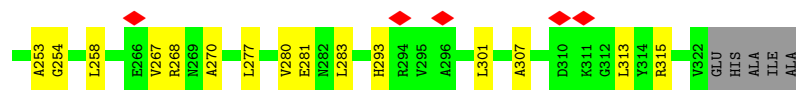
Chain	Residue	Modelled	Actual	Comment	Reference
M	41	A	G	conflict	GB 313291946
M	53	A	G	conflict	GB 313291946

- Molecule 5 is a protein called CRISPR type I-F/YPEST-associated protein Csy3.

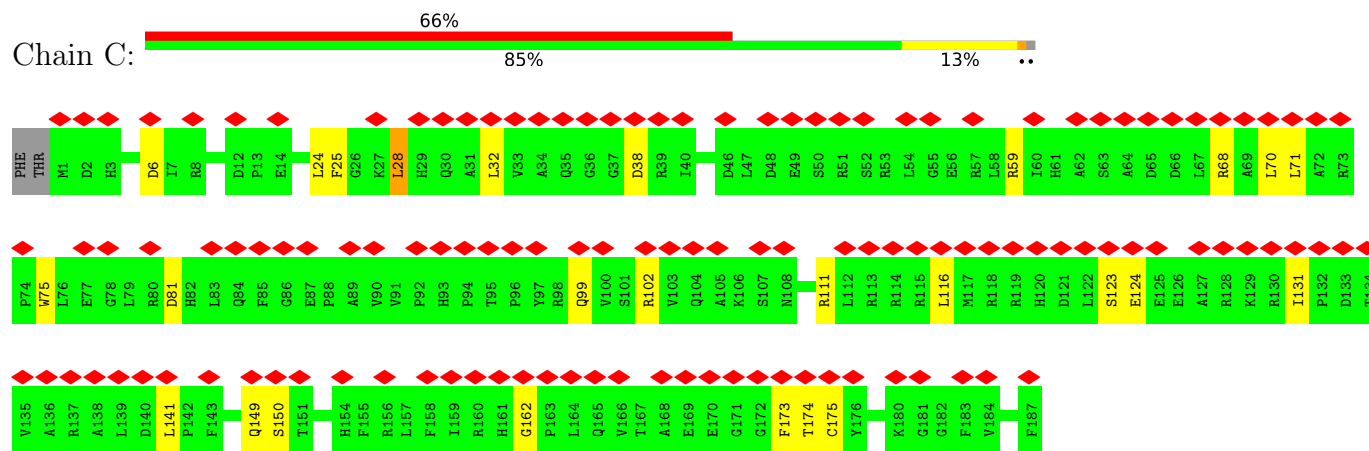
Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	298	Total	C	N	O	S	0	0
			2307	1453	415	437	2		
5	E	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		
5	F	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		
5	G	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		
5	H	330	Total	C	N	O	S	0	0
			2554	1604	464	484	2		
5	I	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		

- Molecule 6 is a protein called AcrF9.

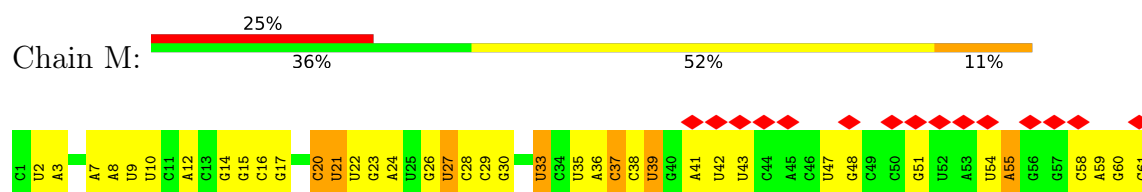
Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	68	Total	C	N	O	S	0	0
			545	339	98	104	4		
6	K	68	Total	C	N	O	S	0	0
			545	339	98	104	4		



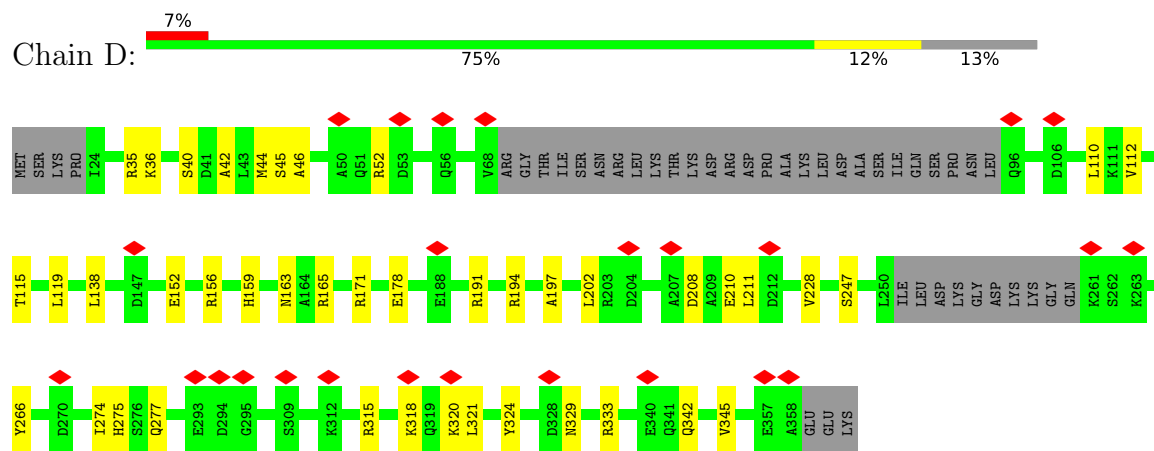
• Molecule 3: Type I-F CRISPR-associated endoribonuclease Cas6/Csy4



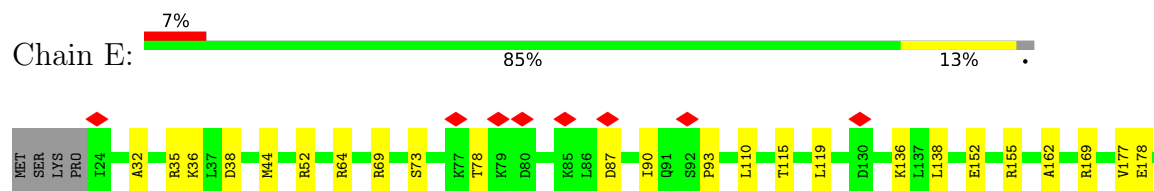
• Molecule 4: RNA (61-MER)



• Molecule 5: CRISPR type I-F/YPEST-associated protein Csy3



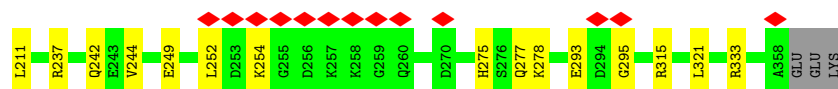
• Molecule 5: CRISPR type I-F/YPEST-associated protein Csy3





- Molecule 5: CRISPR type I-F/YPEST-associated protein Csy3

Chain F: 85% 13%



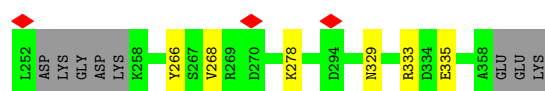
- Molecule 5: CRISPR type I-F/YPEST-associated protein Csy3

Chain G: 6% 88% 10%



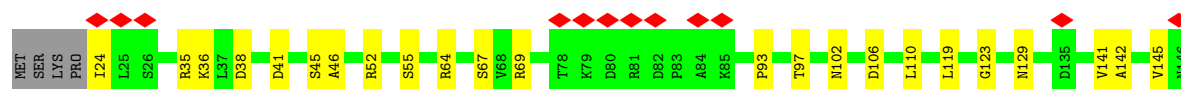
- Molecule 5: CRISPR type I-F/YPEST-associated protein Csy3

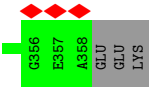
Chain H: 87% 10%



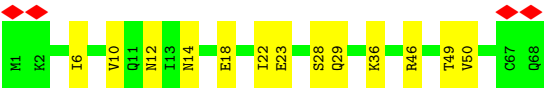
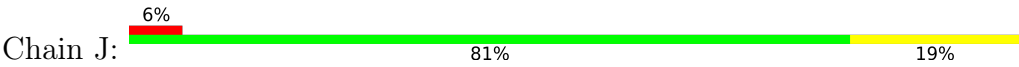
- Molecule 5: CRISPR type I-F/YPEST-associated protein Csy3

Chain I: 8% 85% 13%

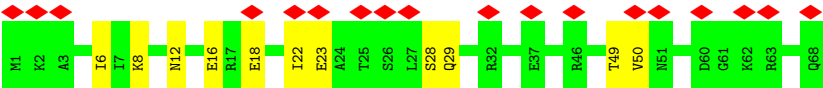
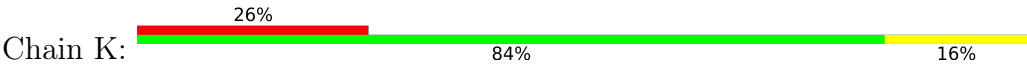




● Molecule 6: AcrF9



● Molecule 6: AcrF9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150697	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 ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	270.9, 270.9, 270.9	wwPDB
Map dimensions	258, 258, 258	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.30	0/3153	0.64	2/4299 (0.0%)
2	B	0.38	0/2471	0.60	0/3365
3	C	0.26	0/1490	0.57	0/2024
4	M	0.42	0/1421	0.47	0/2211
5	D	0.33	0/2350	0.55	0/3190
5	E	0.41	0/2639	0.54	0/3579
5	F	0.46	0/2639	0.58	0/3579
5	G	0.48	0/2639	0.60	0/3579
5	H	0.46	0/2600	0.56	2/3527 (0.1%)
5	I	0.42	0/2639	0.58	0/3579
6	J	0.39	0/552	0.59	0/740
6	K	0.40	0/552	0.59	0/740
All	All	0.40	0/25145	0.58	4/34412 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	GLN	CA-C-N	5.80	129.53	120.82
1	A	124	GLN	C-N-CA	5.80	129.53	120.82
5	H	77	LYS	CA-C-N	5.53	132.11	121.54
5	H	77	LYS	C-N-CA	5.53	132.11	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3088	0	2773	42	0
2	B	2411	0	2408	37	0
3	C	1448	0	1394	36	0
4	M	1273	0	646	28	0
5	D	2307	0	2275	27	0
5	E	2592	0	2581	31	0
5	F	2592	0	2581	29	0
5	G	2592	0	2581	24	0
5	H	2554	0	2543	26	0
5	I	2592	0	2581	32	0
6	J	545	0	547	5	0
6	K	545	0	547	2	0
All	All	24539	0	23457	270	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 6.

The worst 5 of 270 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)
3:C:25:PHE:HA	3:C:28:LEU:CD2	1.57	1.33
3:C:25:PHE:CA	3:C:28:LEU:HD21	1.85	1.06
3:C:25:PHE:HA	3:C:28:LEU:HD21	0.94	0.94
1:A:145:LEU:HD23	1:A:145:LEU:H	1.32	0.93
3:C:25:PHE:O	3:C:28:LEU:HG	1.73	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	264/365 (72%)	264 (100%)	0	100	100
2	B	255/270 (94%)	254 (100%)	1 (0%)	84	81
3	C	146/162 (90%)	145 (99%)	1 (1%)	76	78
5	D	234/273 (86%)	233 (100%)	1 (0%)	84	81
5	E	266/273 (97%)	265 (100%)	1 (0%)	84	81
5	F	266/273 (97%)	266 (100%)	0	100	100
5	G	174/273 (64%)	174 (100%)	0	100	100
5	H	246/273 (90%)	246 (100%)	0	100	100
5	I	266/273 (97%)	266 (100%)	0	100	100
6	J	58/58 (100%)	50 (86%)	8 (14%)	3	20
6	K	58/58 (100%)	50 (86%)	8 (14%)	3	20
All	All	2233/2551 (88%)	2213 (99%)	20 (1%)	68	76

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	K	22	ILE
6	K	29	GLN
6	K	50	VAL
6	K	49	THR
6	J	22	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
5	H	159	HIS
5	I	94	ASN
5	I	96	GLN
5	H	260	GLN
5	D	248	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	M	59/61 (96%)	24 (40%)	0

5 of 24 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	M	3	A
4	M	9	U
4	M	10	U
4	M	15	G
4	M	16	C

There are no RNA pucker outliers to report.

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.

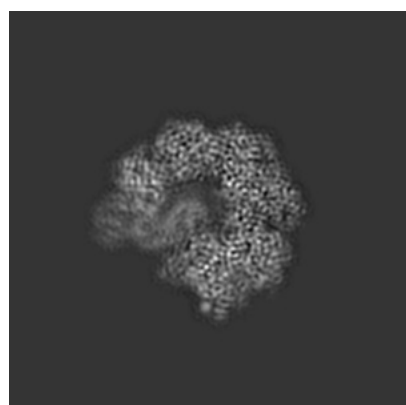
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22584. These allow visual inspection of the internal detail of the map and identification of artifacts.

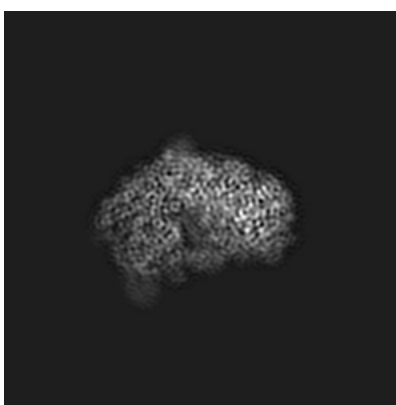
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

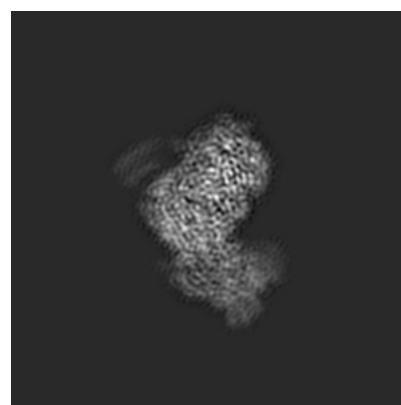
6.1.1 Primary map



X



Y

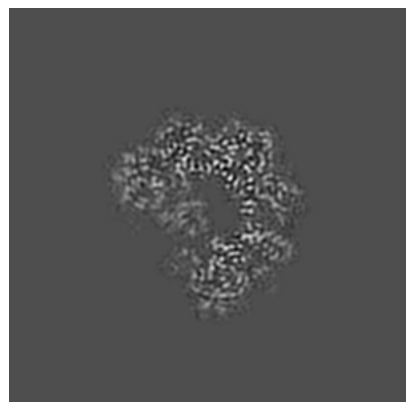


Z

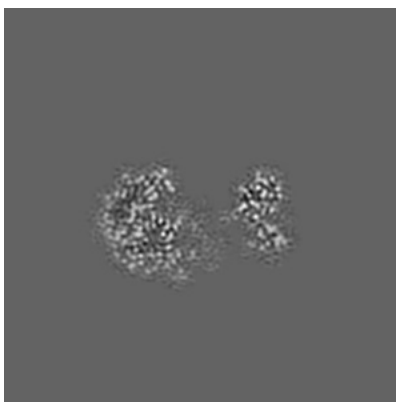
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

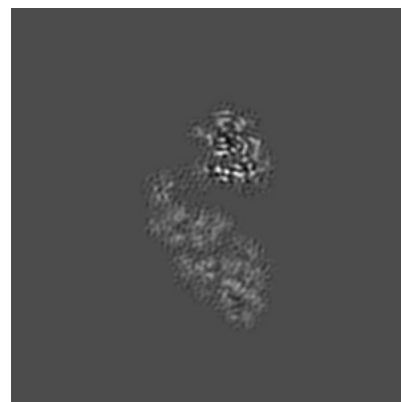
6.2.1 Primary map



X Index: 129



Y Index: 129

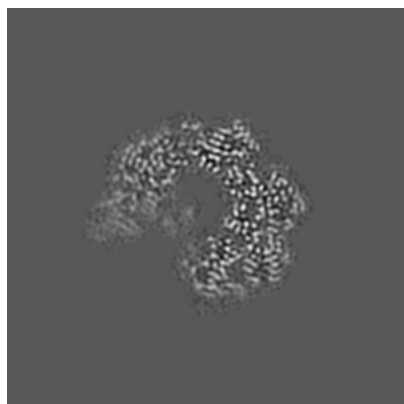


Z Index: 129

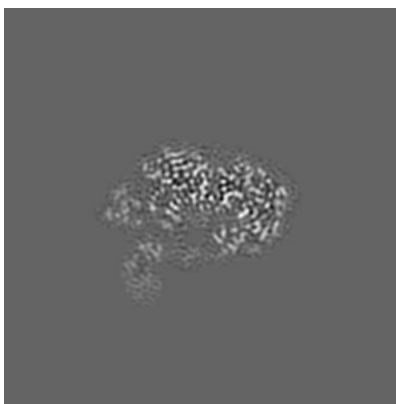
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

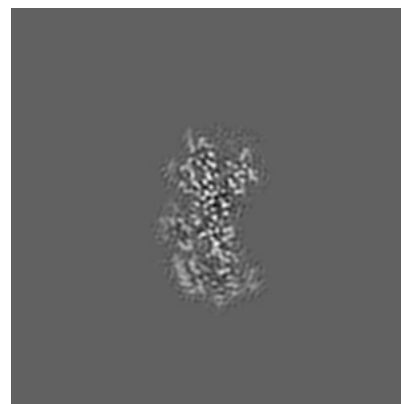
6.3.1 Primary map



X Index: 139



Y Index: 151

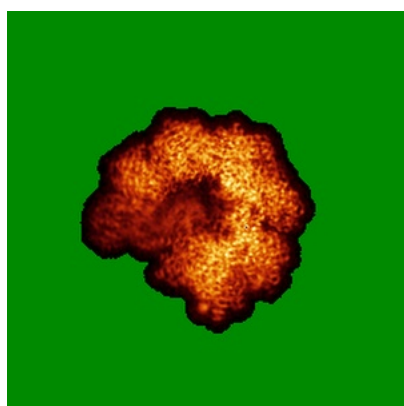


Z Index: 157

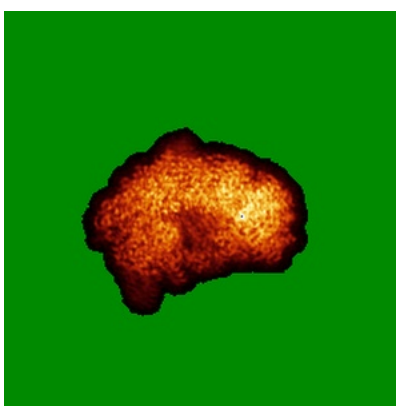
The images above show the largest variance slices of the map in three orthogonal directions.

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

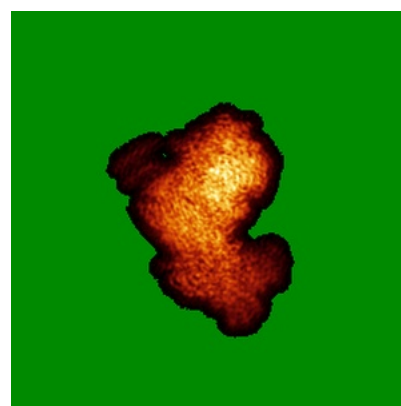
6.4.1 Primary map



X



Y

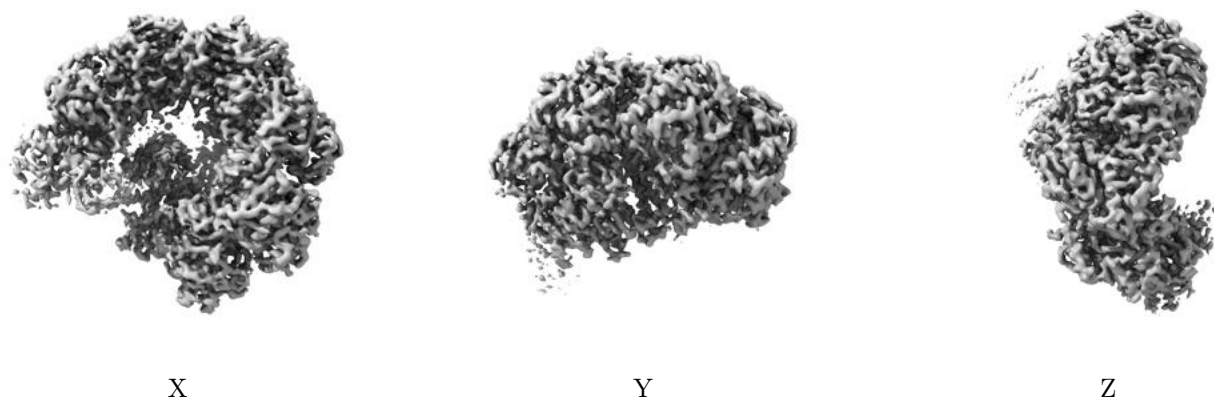


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

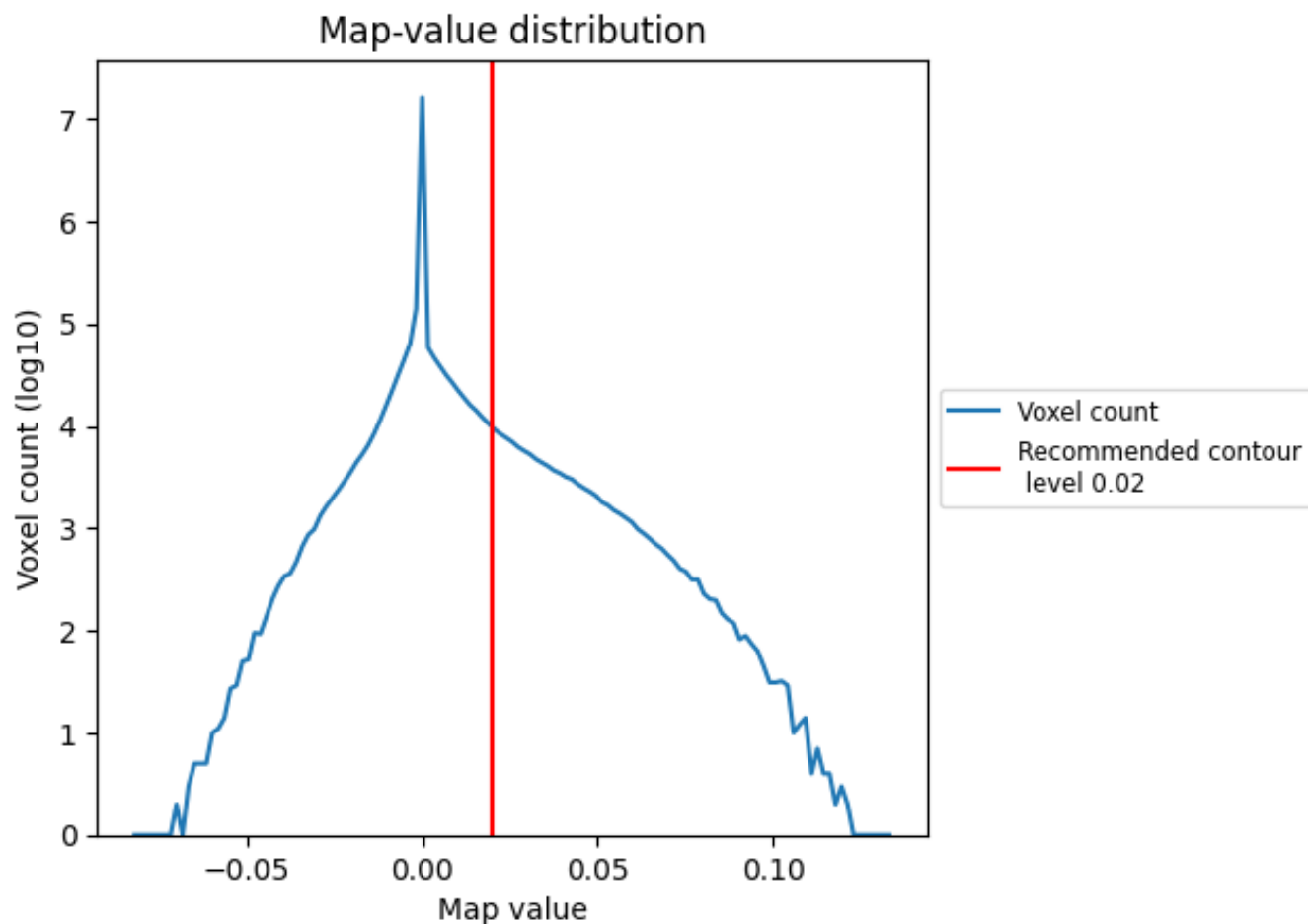
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

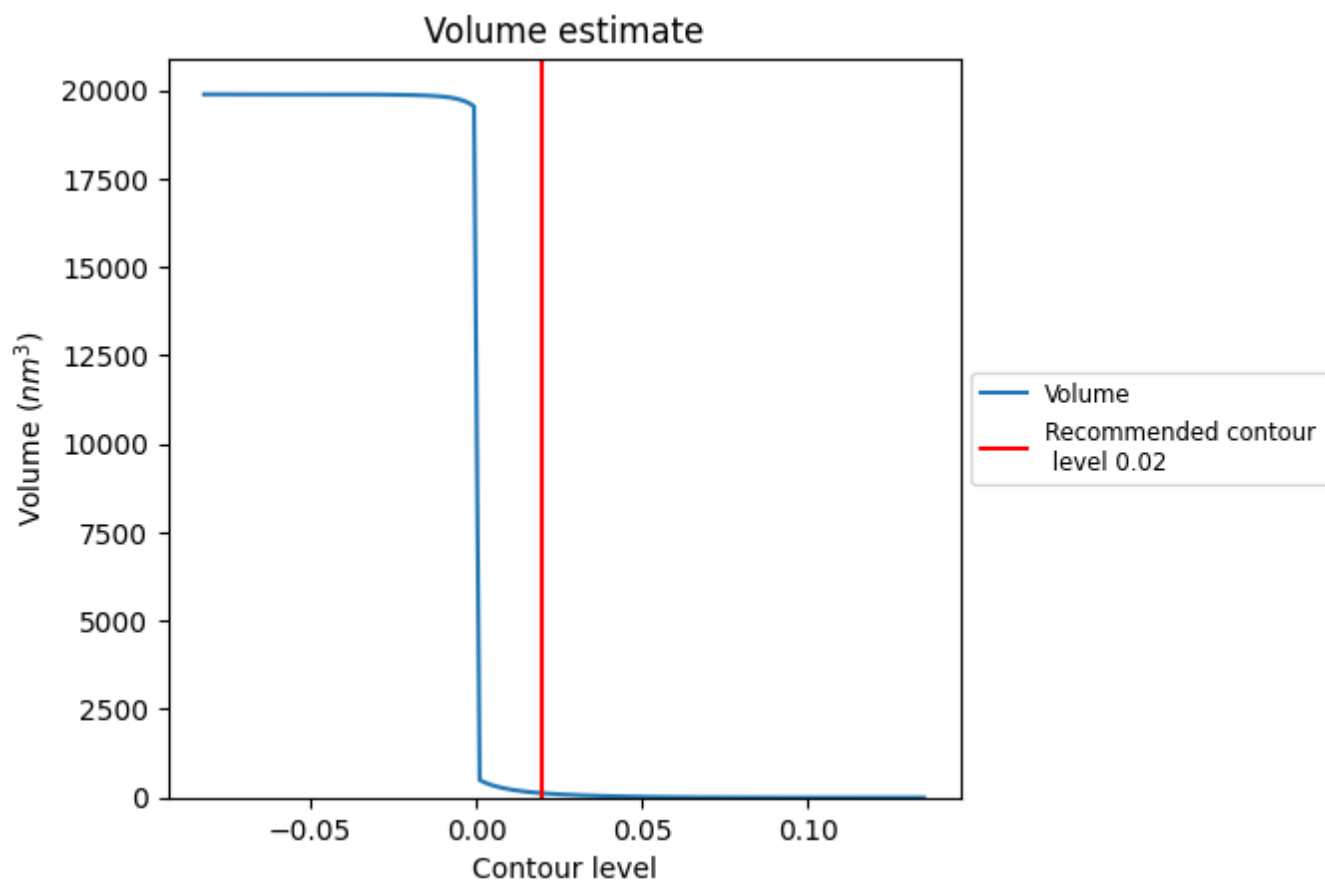
This section contains the results of statistical analysis of the map.

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.

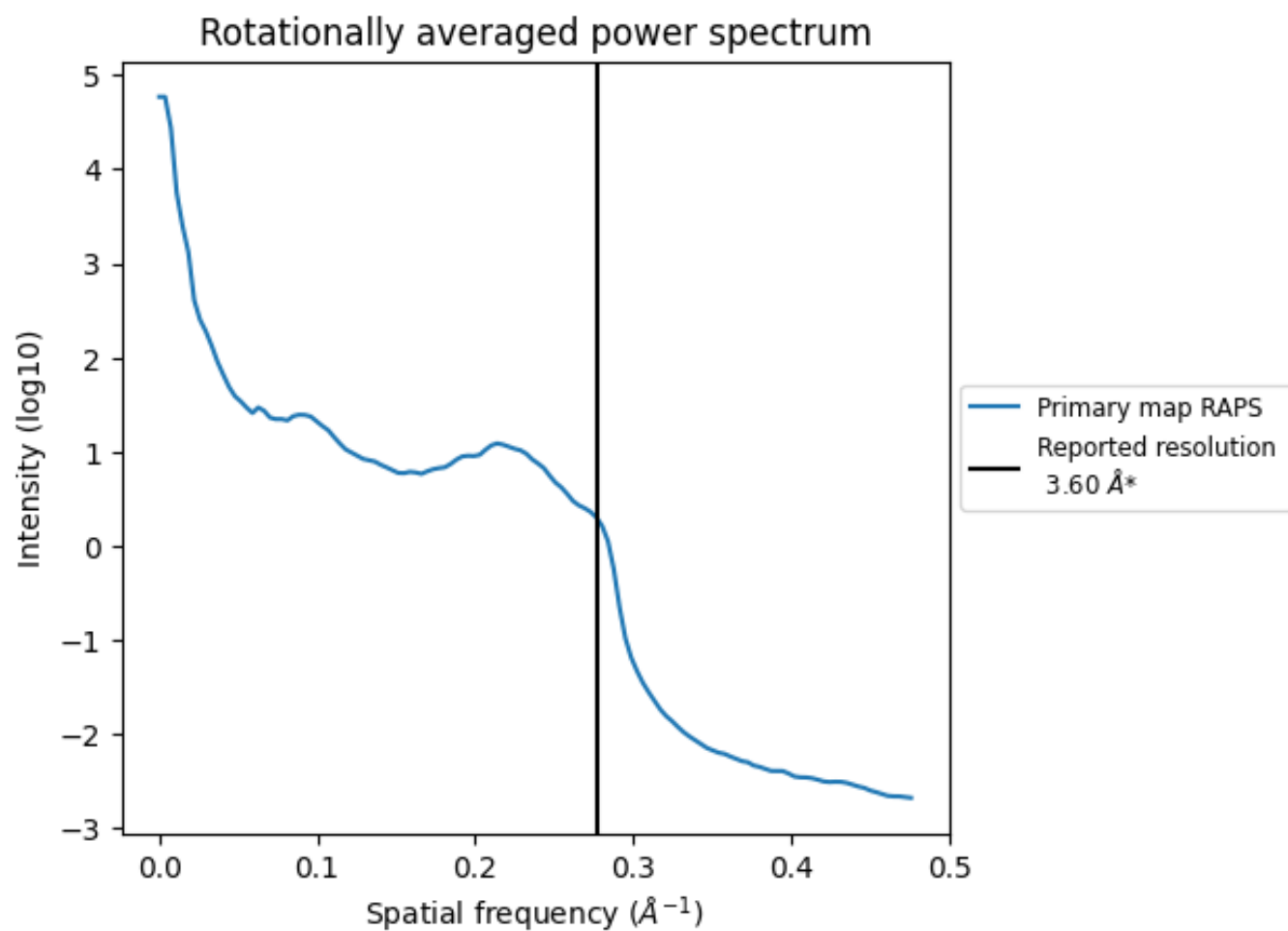
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 122 nm³; this corresponds to an approximate mass of 111 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

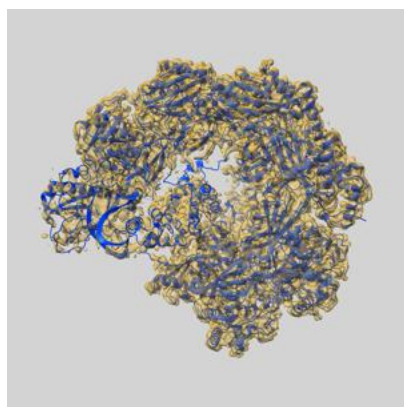
8 Fourier-Shell correlation

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

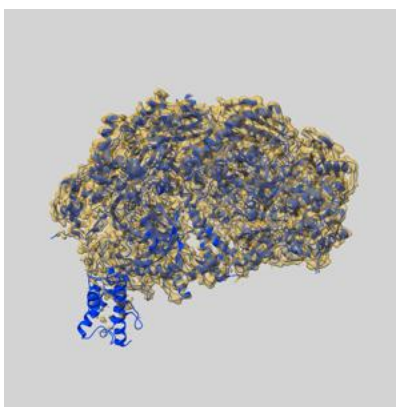
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22584 and PDB model 7JZY. Per-residue inclusion information can be found in section [3](#) on page [6](#).

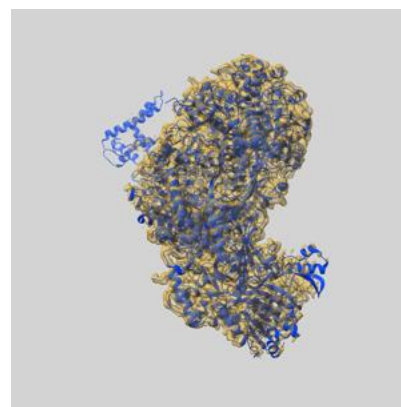
9.1 Map-model overlay [i](#)



X



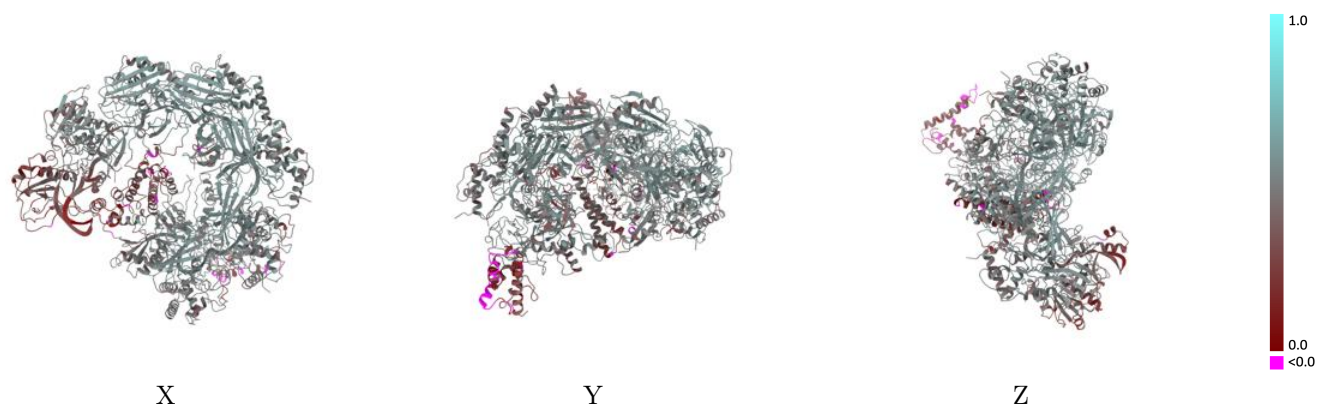
Y



Z

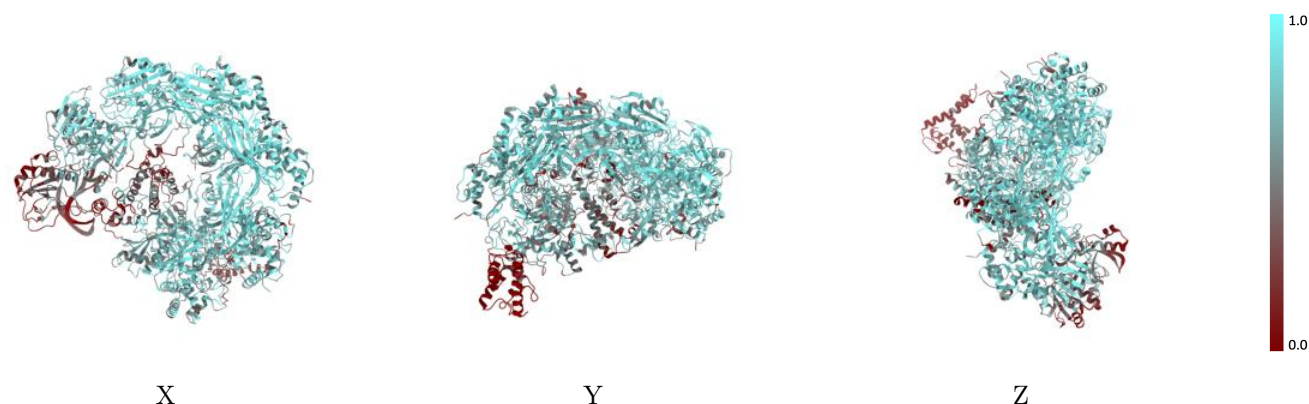
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



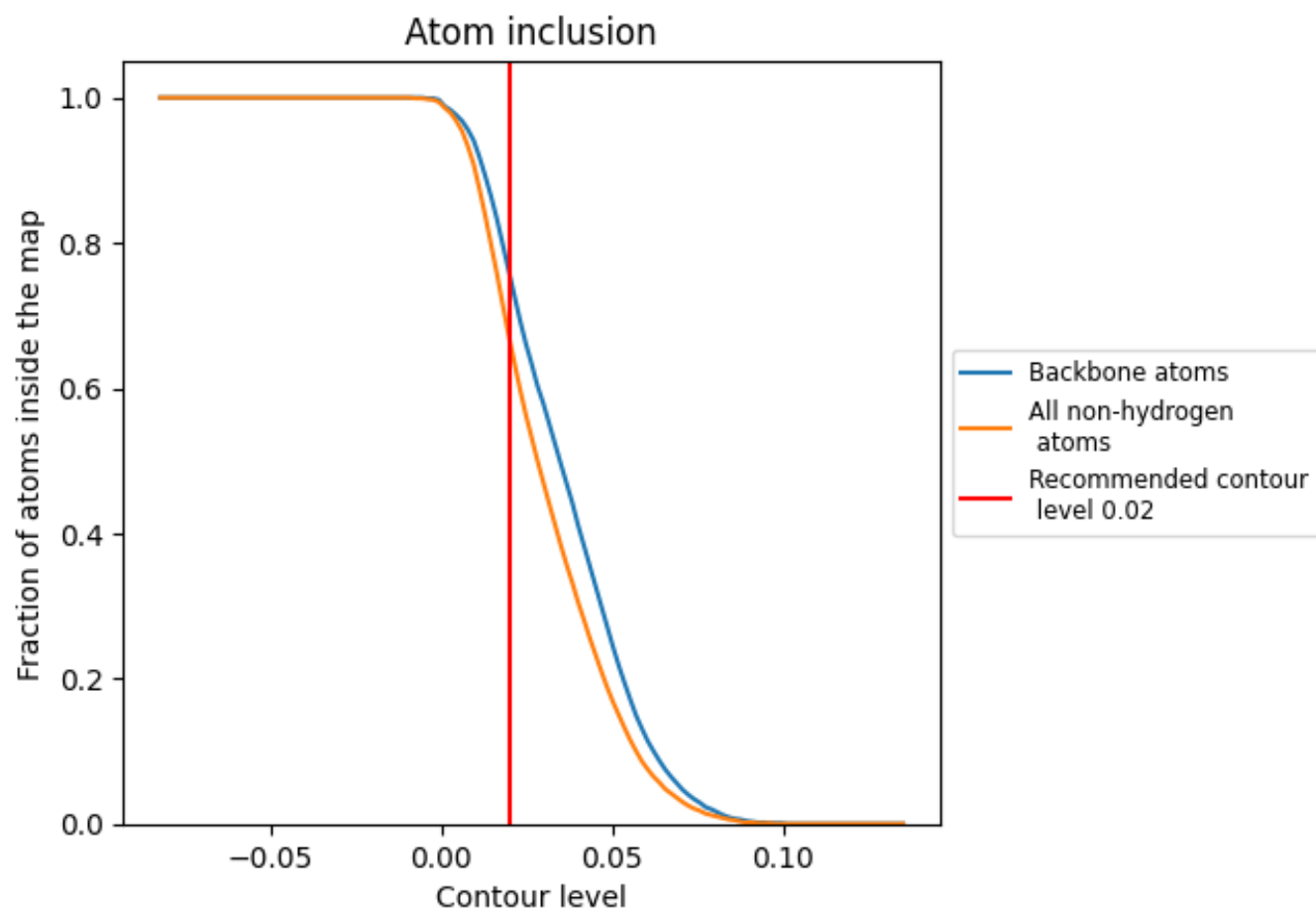
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 67% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6670	0.4690
A	0.3990	0.3420
B	0.6880	0.4830
C	0.3140	0.3250
D	0.6990	0.4800
E	0.7520	0.5110
F	0.7870	0.5280
G	0.7780	0.5120
H	0.7850	0.5230
I	0.7190	0.4950
J	0.6850	0.4810
K	0.5230	0.4560
M	0.6980	0.4410

1.0

0.0

<0.0