



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 02:05 AM UTC

PDB ID : 6C66 / pdb_00006c66
EMDB ID : EMD-7347
Title : CRISPR RNA-guided surveillance complex, pre-nicking
Authors : Xiao, Y.; Luo, M.; Liao, M.; Ke, A.
Deposited on : 2018-01-17
Resolution : 3.66 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:

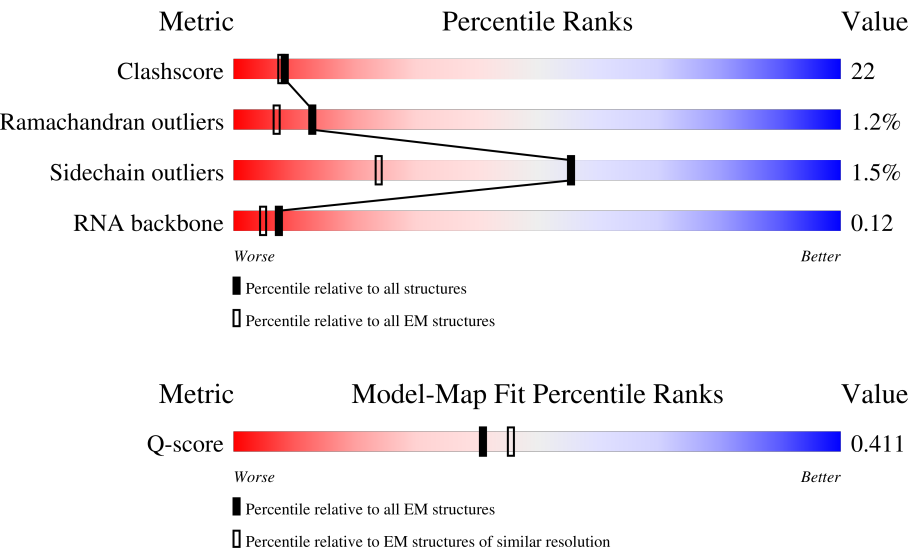
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.66 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.



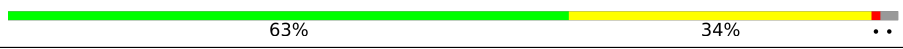
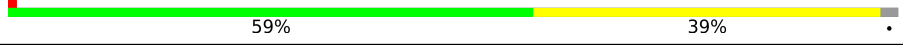
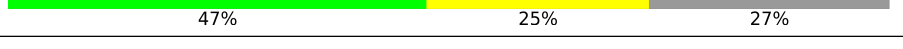
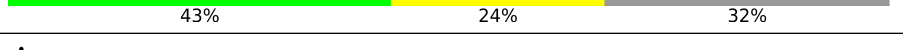
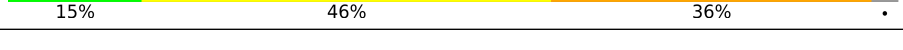
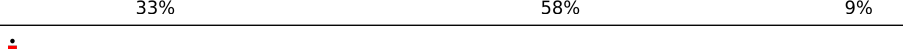
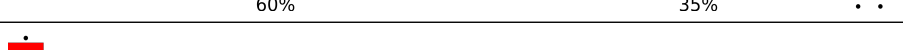
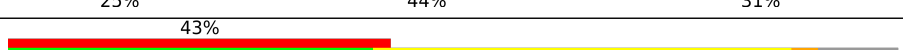
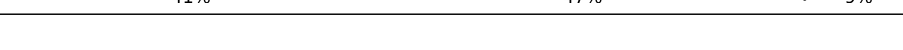
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11491 (3.16 - 4.16)

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	G	944	22% 48% 38% 12%
2	A	549	56% 36% 7%
3	B	373	6% 41% 38% 9% 10%

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Mol	Chain	Length	Quality of chain
3	C	373	
3	D	373	
3	E	373	
3	F	373	
3	H	373	
4	I	244	
4	K	244	
5	J	61	
6	L	55	
7	M	254	
8	N	55	
9	O	232	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 36255 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 helicase, Cas3 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	832	Total	C	N	O	S	0	0
			6467	4104	1153	1185	25		

- Molecule 2 is a protein called CRISPR-associated protein, Cse1 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	511	Total	C	N	O	S	0	0
			4053	2573	740	731	9		

- Molecule 3 is a protein called CRISPR-associated protein, Cse4 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	334	Total	C	N	O	S	0	0
			2501	1573	445	478	5		
3	C	367	Total	C	N	O	S	0	0
			2840	1781	509	545	5		
3	D	367	Total	C	N	O	S	0	0
			2835	1779	508	543	5		
3	E	366	Total	C	N	O	S	0	0
			2825	1770	508	542	5		
3	F	366	Total	C	N	O	S	0	0
			2829	1772	508	544	5		
3	H	329	Total	C	N	O	S	0	0
			2553	1603	460	487	3		

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	177	Total	C	N	O	S	0	0
			1412	887	282	241	2		
4	K	165	Total	C	N	O	S	0	0
			1325	833	264	226	2		

- Molecule 5 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	59	Total	C	N	O	P	0	0
			1267	565	235	409	58		

- Molecule 6 is a DNA chain called Target strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	50	Total	C	N	O	P	0	0
			1012	481	179	302	50		

- Molecule 7 is a protein called CRISPR-associated protein, Cas5e family.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	244	Total	C	N	O	S	0	0
			1916	1215	349	348	4		

- Molecule 8 is a DNA chain called Nontarget strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	38	Total	C	N	O	P	0	0
			766	359	145	224	38		

- Molecule 9 is a protein called CRISPR-associated protein, Cse3 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	212	Total	C	N	O	S	0	0
			1652	1028	322	300	2		

- Molecule 10 is FE (III) ION (CCD ID: FE) (formula: Fe).

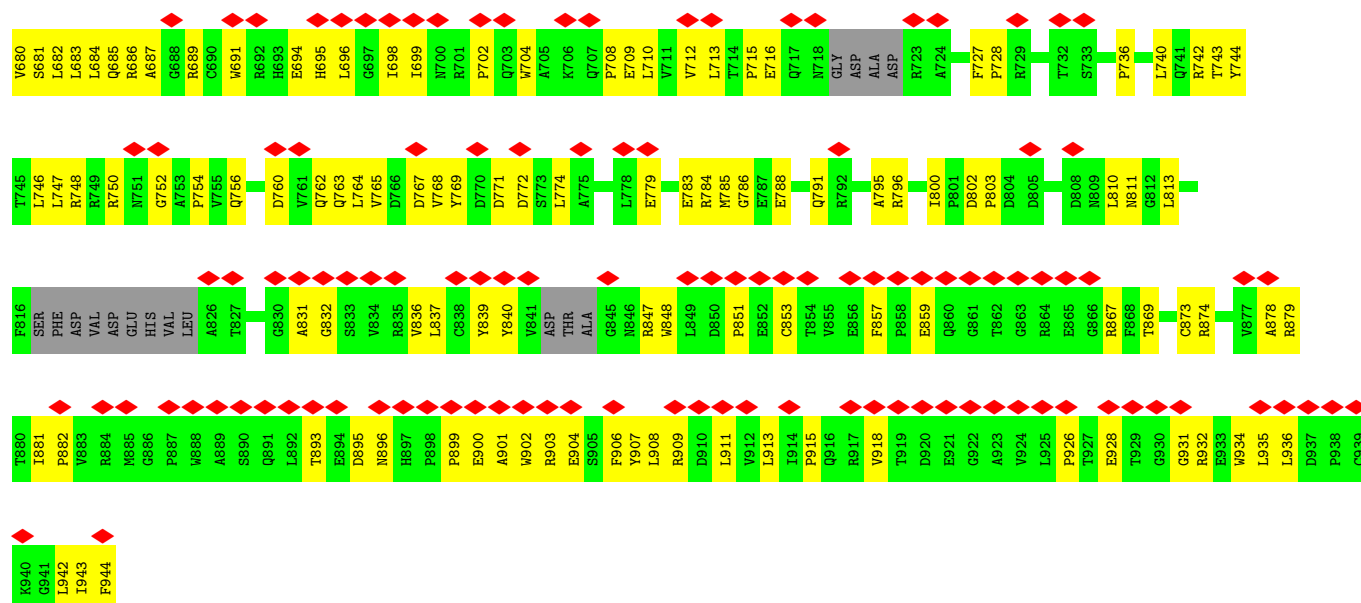
Mol	Chain	Residues	Atoms		AltConf
10	G	2	Total	Fe	0
			2	2	

3 Residue-property plots

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.

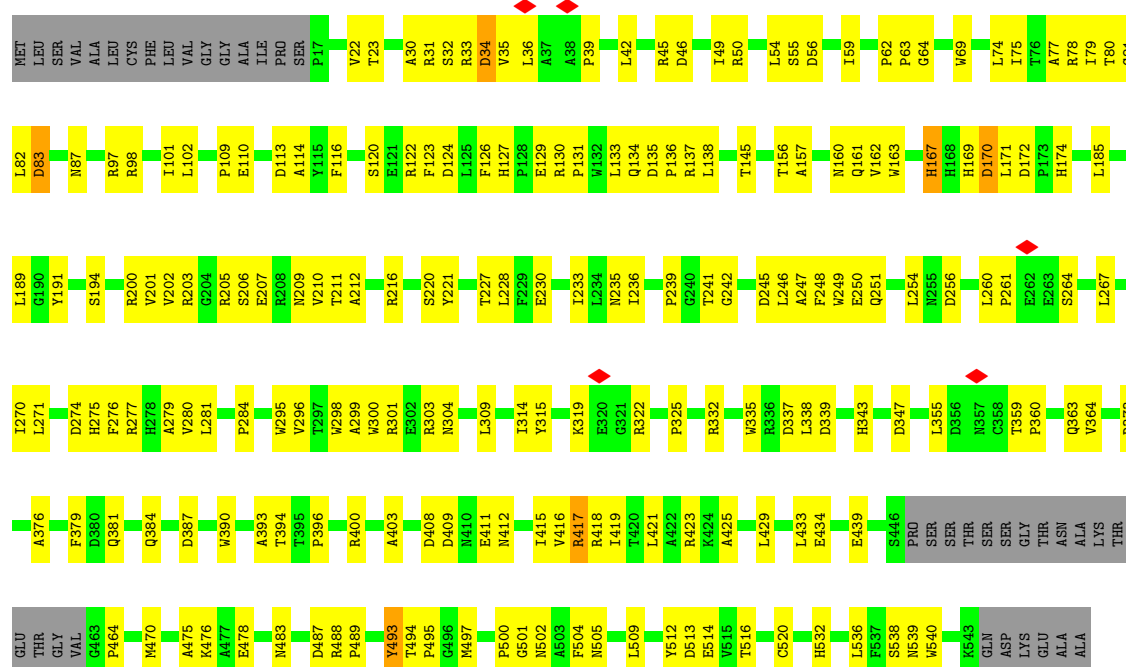
- Molecule 1: CRISPR-associated helicase, Cas3 family





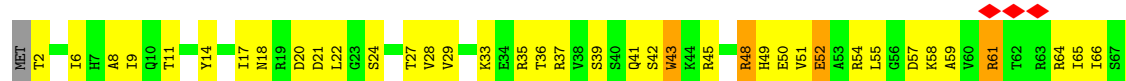
• Molecule 2: CRISPR-associated protein, Cse1 family

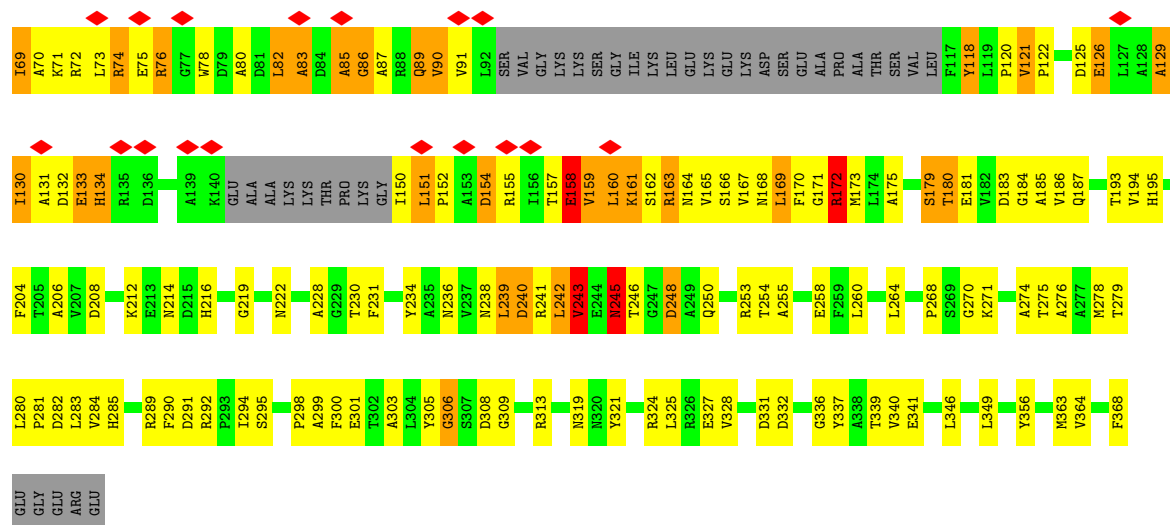
Chain A: 56% 36% 7%



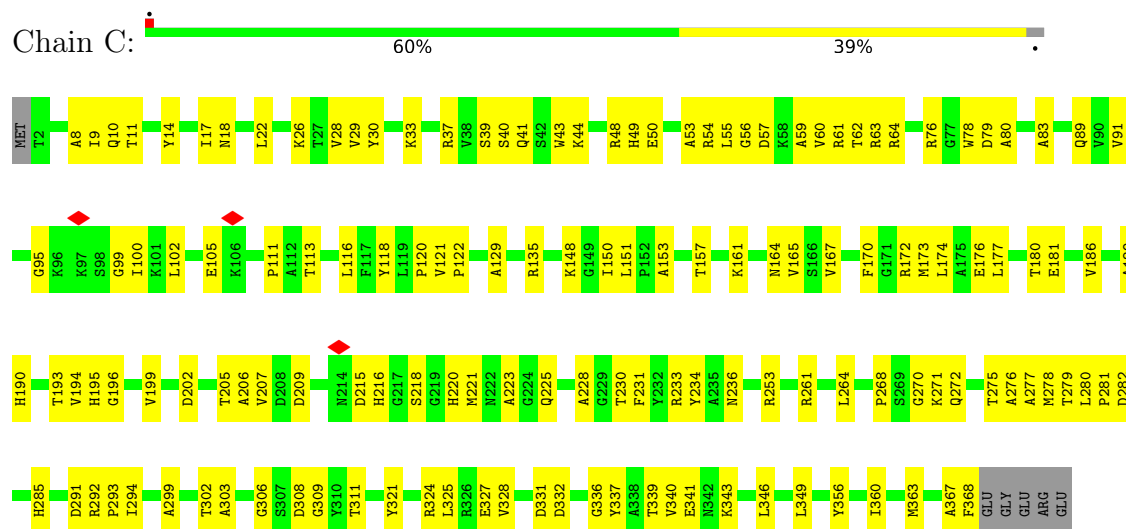
• Molecule 3: CRISPR-associated protein, Cse4 family

Chain B: 41% 38% 9% 10%

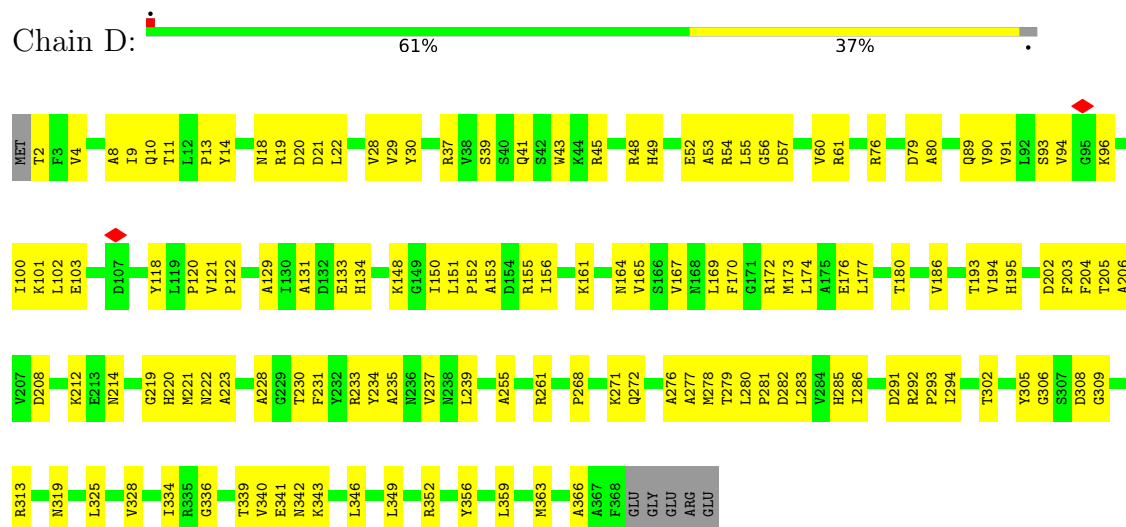




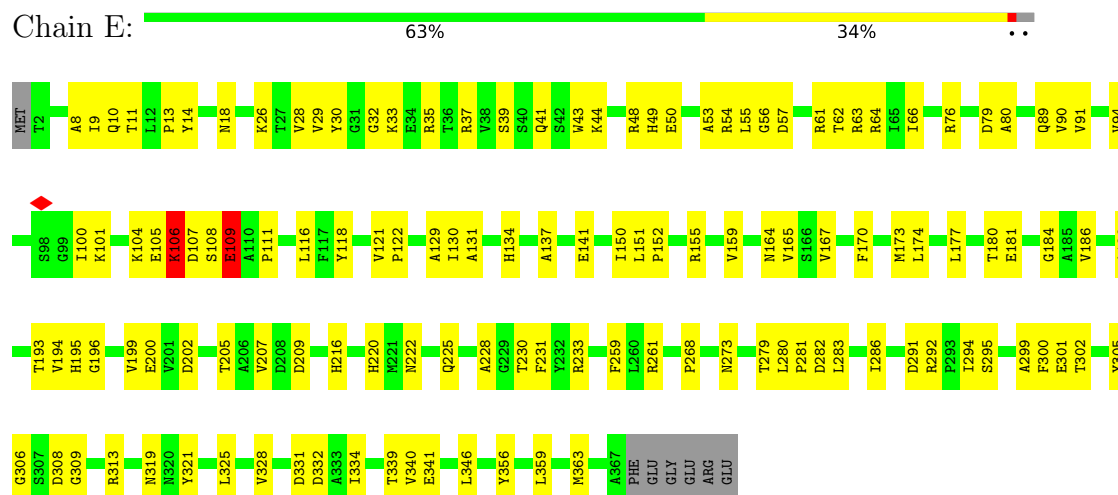
• Molecule 3: CRISPR-associated protein, Cse4 family



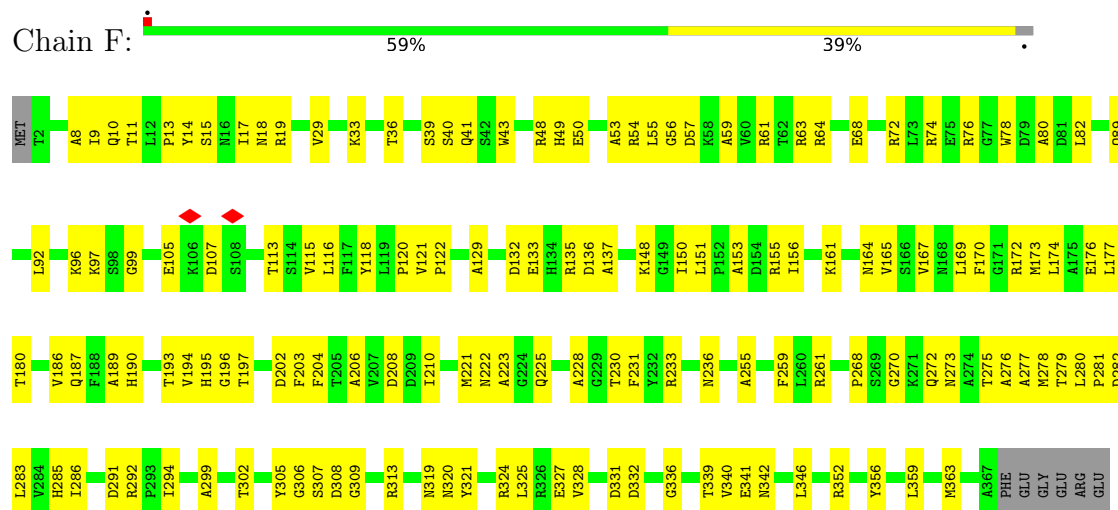
• Molecule 3: CRISPR-associated protein, Cse4 family



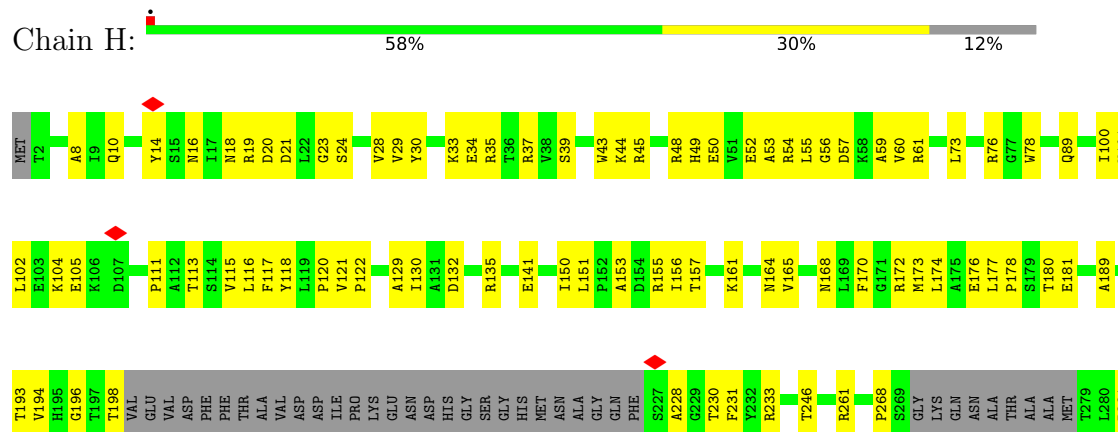
• Molecule 3: CRISPR-associated protein, Cse4 family



• Molecule 3: CRISPR-associated protein, Cse4 family

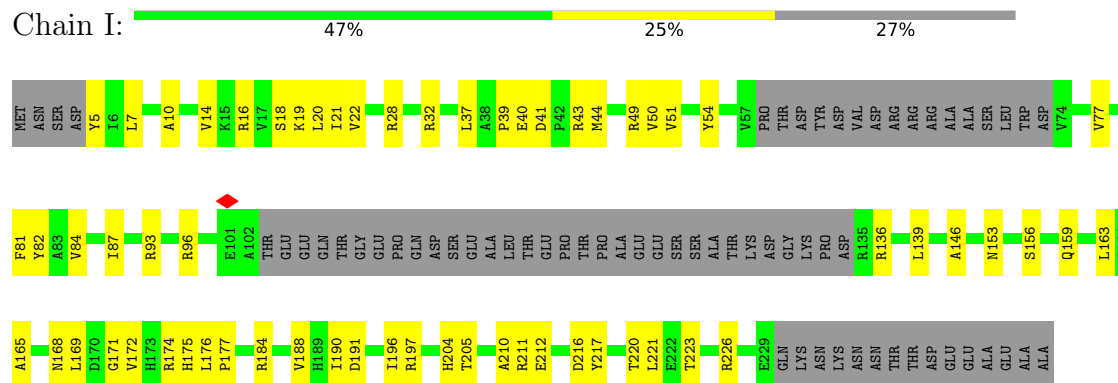


• Molecule 3: CRISPR-associated protein, Cse4 family

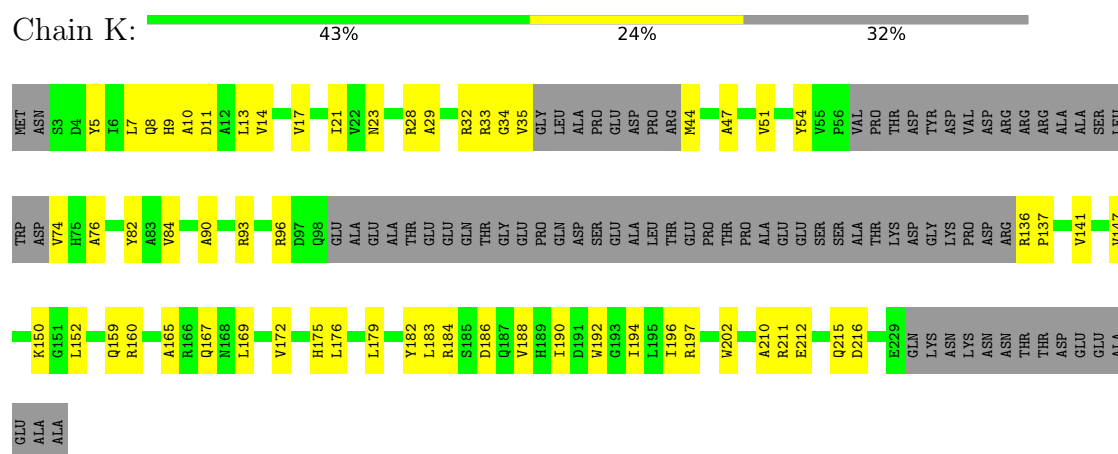




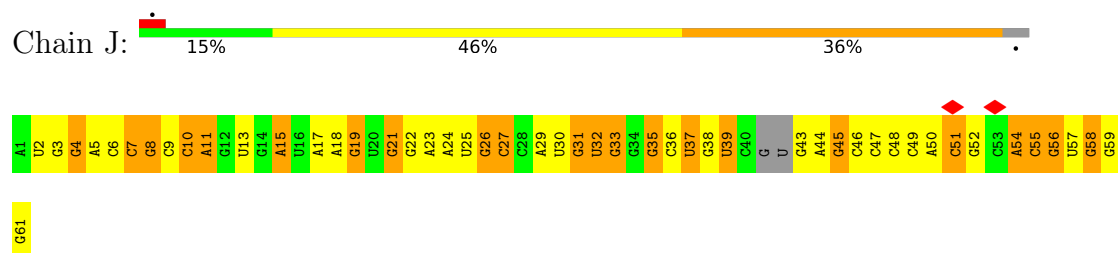
- Molecule 4: Uncharacterized protein



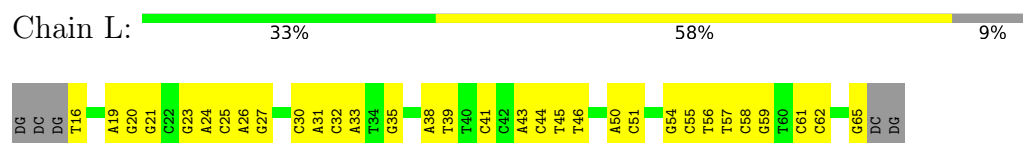
- Molecule 4: Uncharacterized protein



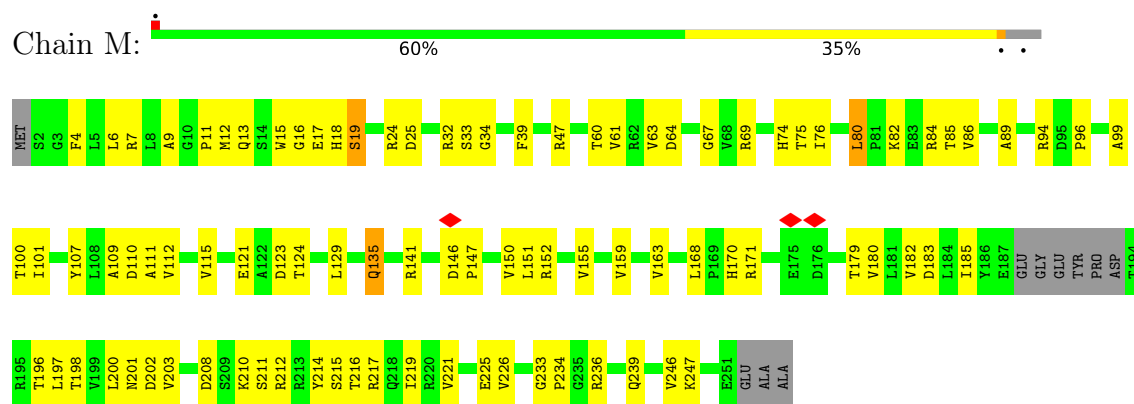
- Molecule 5: crRNA



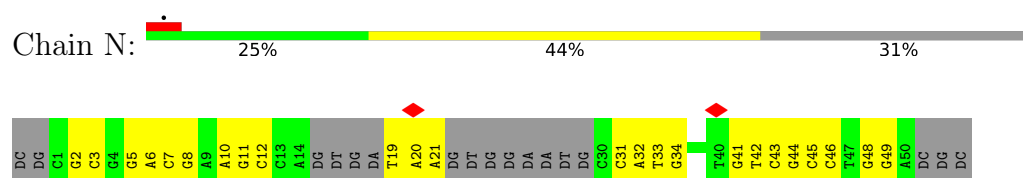
- Molecule 6: Target strand



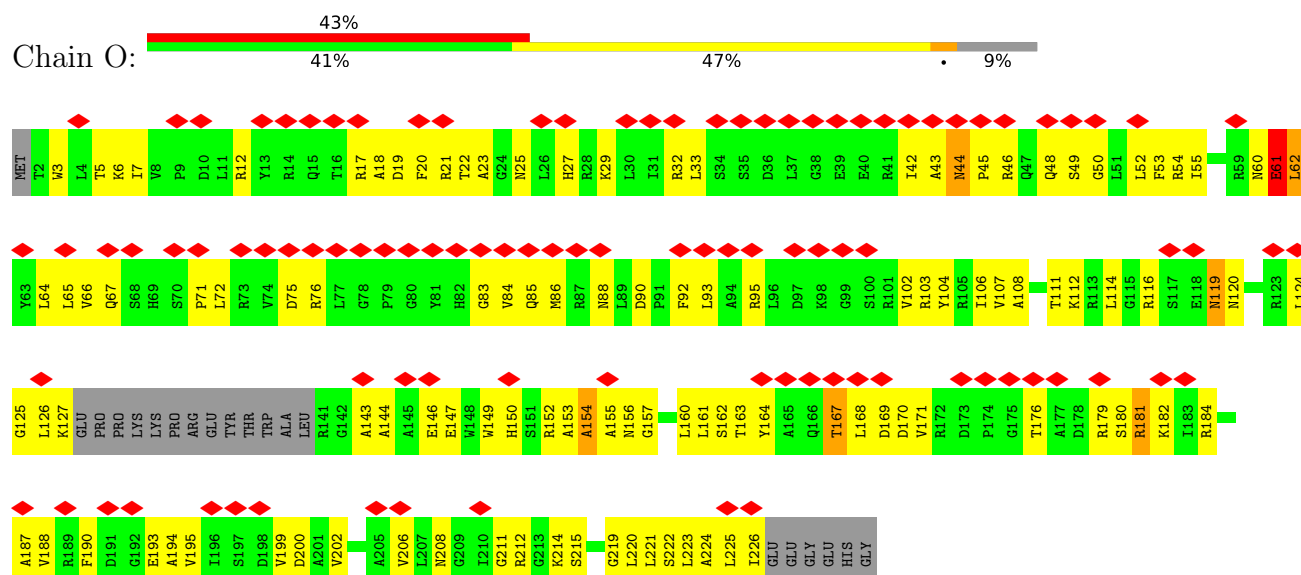
- Molecule 7: CRISPR-associated protein, Cas5e family



- Molecule 8: Nontarget strand



- Molecule 9: CRISPR-associated protein, Cse3 family



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51889	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 ($e^-/\text{\AA}^2$)	8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.212	Depositor
Minimum map value	-0.102	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	317.44, 317.44, 317.44	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	G	0.22	0/6620	0.62	2/9016 (0.0%)
2	A	0.35	0/4175	0.75	2/5705 (0.0%)
3	B	0.37	0/2551	0.77	3/3476 (0.1%)
3	C	0.36	0/2894	0.66	1/3927 (0.0%)
3	D	0.37	0/2889	0.64	0/3920
3	E	0.38	0/2878	0.67	0/3906
3	F	0.38	0/2882	0.64	0/3911
3	H	0.31	0/2598	0.62	0/3524
4	I	0.40	0/1441	0.76	0/1957
4	K	0.36	0/1351	0.68	0/1832
5	J	0.39	0/1417	0.60	0/2208
6	L	0.39	0/1131	0.52	0/1740
7	M	0.37	0/1959	0.71	0/2665
8	N	0.29	0/857	0.49	0/1317
9	O	0.24	0/1680	0.87	5/2270 (0.2%)
All	All	0.34	0/37323	0.67	13/51374 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	222	ASP	CA-C-N	7.46	135.13	121.70
1	G	222	ASP	C-N-CA	7.46	135.13	121.70
9	O	119	ASN	CA-C-N	6.56	133.51	121.70
9	O	119	ASN	C-N-CA	6.56	133.51	121.70
9	O	167	THR	CA-C-N	5.46	131.52	121.70

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	G	6467	0	6433	324	0
2	A	4053	0	3928	176	0
3	B	2501	0	2352	170	0
3	C	2840	0	2809	127	0
3	D	2835	0	2800	125	0
3	E	2825	0	2796	110	0
3	F	2829	0	2800	123	0
3	H	2553	0	2550	100	0
4	I	1412	0	1427	60	0
4	K	1325	0	1339	47	0
5	J	1267	0	642	86	0
6	L	1012	0	562	41	0
7	M	1916	0	1941	90	0
8	N	766	0	415	24	0
9	O	1652	0	1647	115	0
10	G	2	0	0	0	0
All	All	36255	0	34441	1520	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 22.

The worst 5 of 1520 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)
9:O:167:THR:HB	9:O:168:LEU:HB2	1.46	0.98
5:J:61:G:H2'	9:O:180:SER:HB2	1.45	0.97
5:J:49:C:H2'	5:J:50:A:H8	1.32	0.95
4:K:84:VAL:HG11	4:K:196:ILE:HG12	1.50	0.93
9:O:171:VAL:O	9:O:182:LYS:HA	1.69	0.91

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	G	814/944 (86%)	764 (94%)	43 (5%)	7 (1%)	14	43
2	A	507/549 (92%)	457 (90%)	47 (9%)	3 (1%)	21	51
3	B	328/373 (88%)	243 (74%)	59 (18%)	26 (8%)	1	7
3	C	365/373 (98%)	346 (95%)	18 (5%)	1 (0%)	36	64
3	D	365/373 (98%)	345 (94%)	19 (5%)	1 (0%)	36	64
3	E	364/373 (98%)	337 (93%)	23 (6%)	4 (1%)	11	39
3	F	364/373 (98%)	342 (94%)	21 (6%)	1 (0%)	36	64
3	H	323/373 (87%)	300 (93%)	23 (7%)	0	100	100
4	I	171/244 (70%)	165 (96%)	6 (4%)	0	100	100
4	K	157/244 (64%)	153 (98%)	4 (2%)	0	100	100
7	M	240/254 (94%)	225 (94%)	15 (6%)	0	100	100
9	O	208/232 (90%)	180 (86%)	22 (11%)	6 (3%)	3	22
All	All	4206/4705 (89%)	3857 (92%)	300 (7%)	49 (1%)	13	38

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	221	GLU
1	G	223	PHE
1	G	224	LEU
3	B	70	ALA
3	B	72	ARG

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	G	684/779 (88%)	673 (98%)	11 (2%)	55	66
2	A	416/452 (92%)	412 (99%)	4 (1%)	68	72
3	B	241/299 (81%)	211 (88%)	30 (12%)	4	20
3	C	294/299 (98%)	294 (100%)	0	100	100
3	D	292/299 (98%)	292 (100%)	0	100	100
3	E	292/299 (98%)	289 (99%)	3 (1%)	68	72
3	F	293/299 (98%)	293 (100%)	0	100	100
3	H	265/299 (89%)	265 (100%)	0	100	100
4	I	142/200 (71%)	142 (100%)	0	100	100
4	K	135/200 (68%)	135 (100%)	0	100	100
7	M	204/211 (97%)	201 (98%)	3 (2%)	57	67
9	O	168/193 (87%)	166 (99%)	2 (1%)	63	70
All	All	3426/3829 (90%)	3373 (98%)	53 (2%)	55	67

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	133	GLU
3	B	162	SER
7	M	80	LEU
3	B	154	ASP
3	B	159	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	7	HIS
4	I	208	HIS
3	F	134	HIS
3	H	89	GLN
4	K	167	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	J	57/61 (93%)	28 (49%)	0

5 of 28 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	J	4	G
5	J	7	C
5	J	8	G
5	J	9	C
5	J	10	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](#)

Of 2 ligands modelled in this entry, 2 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.

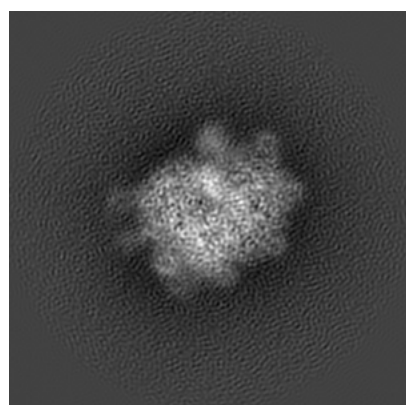
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7347. These allow visual inspection of the internal detail of the map and identification of artifacts.

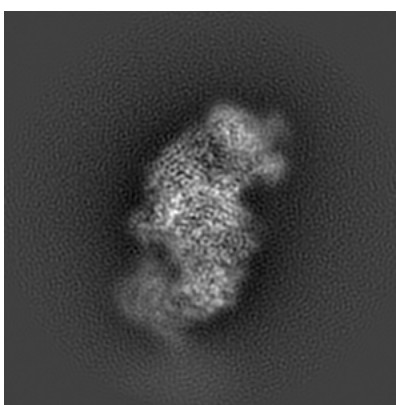
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

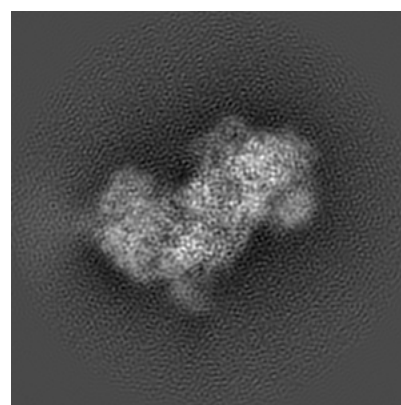
6.1.1 Primary map



X



Y

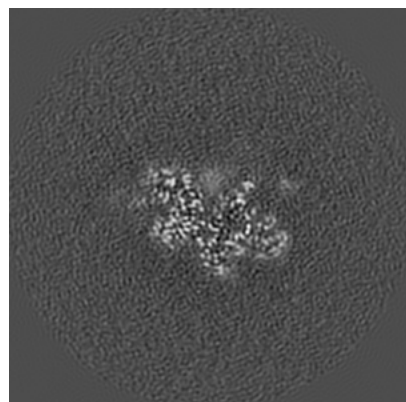


Z

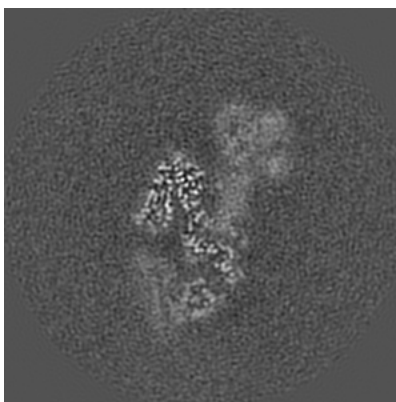
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

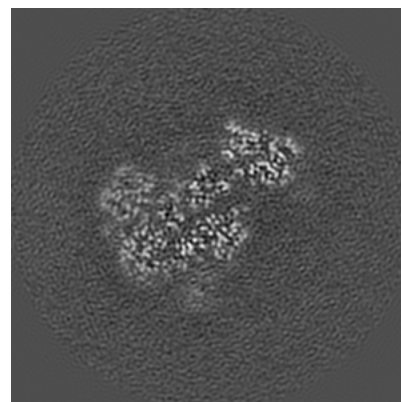
6.2.1 Primary map



X Index: 128



Y Index: 128

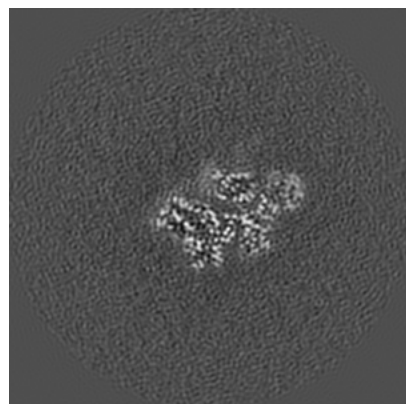


Z Index: 128

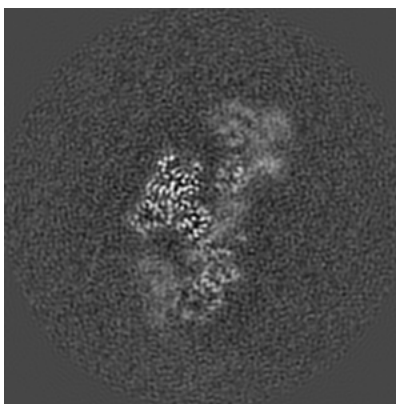
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

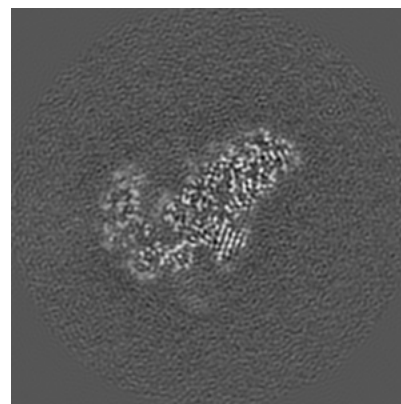
6.3.1 Primary map



X Index: 141



Y Index: 132

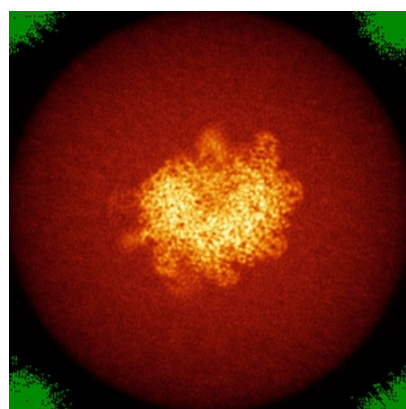


Z Index: 122

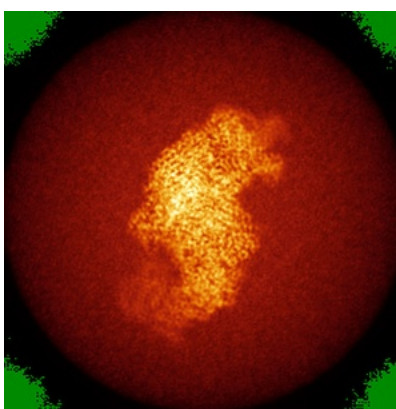
The images above show the largest variance slices of the map in three orthogonal directions.

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

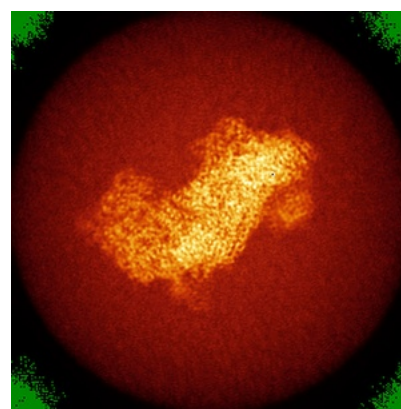
6.4.1 Primary map



X



Y

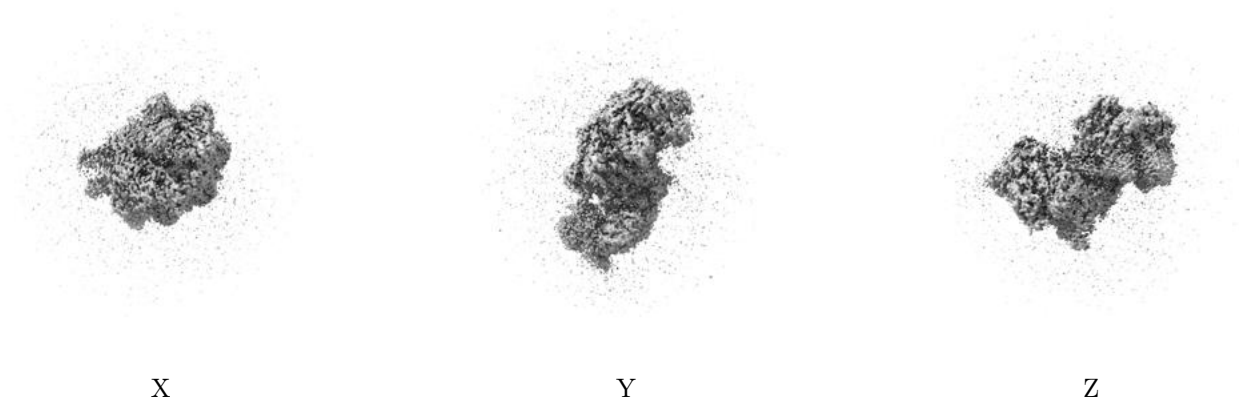


Z

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

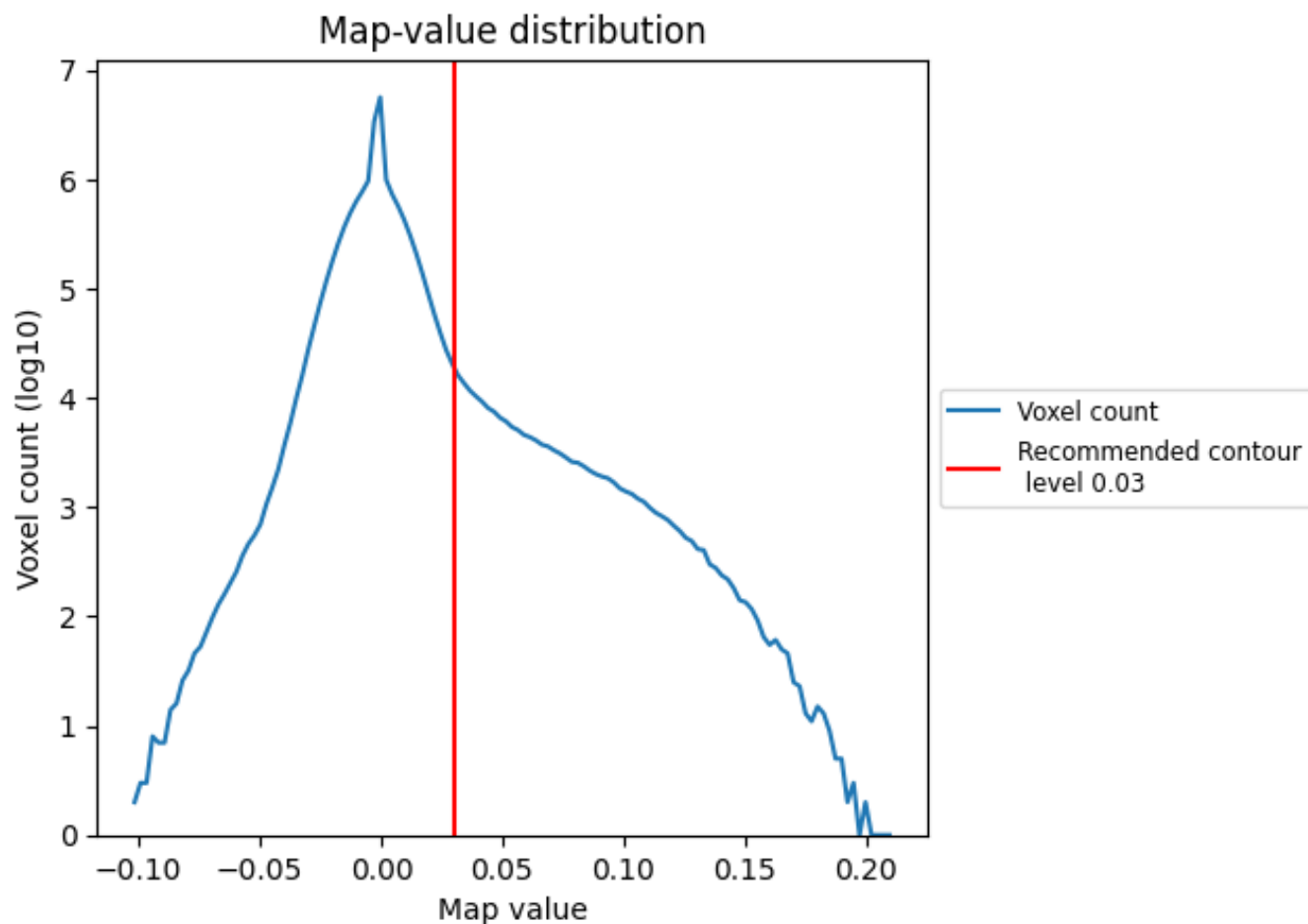
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

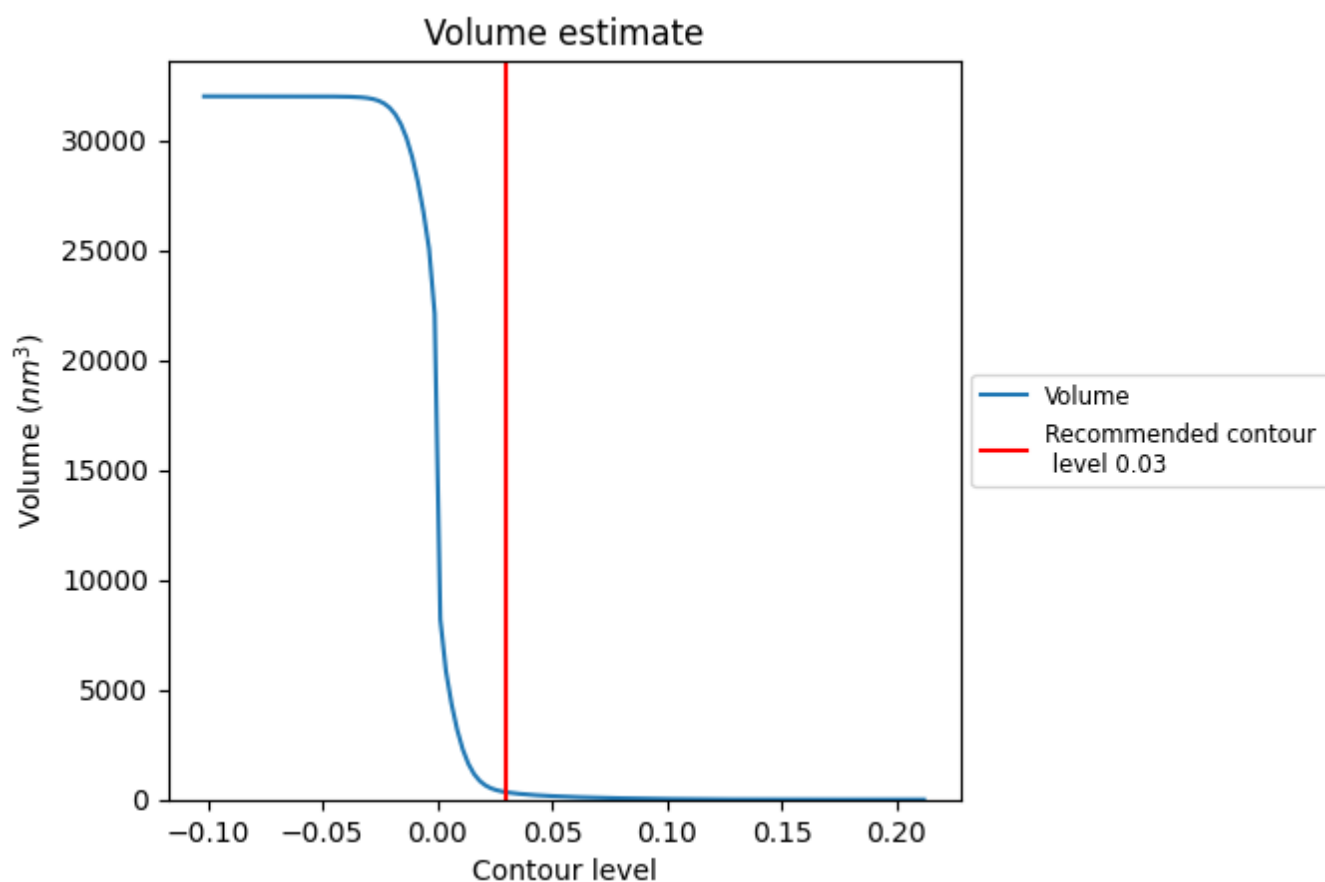
This section contains the results of statistical analysis of the map.

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.

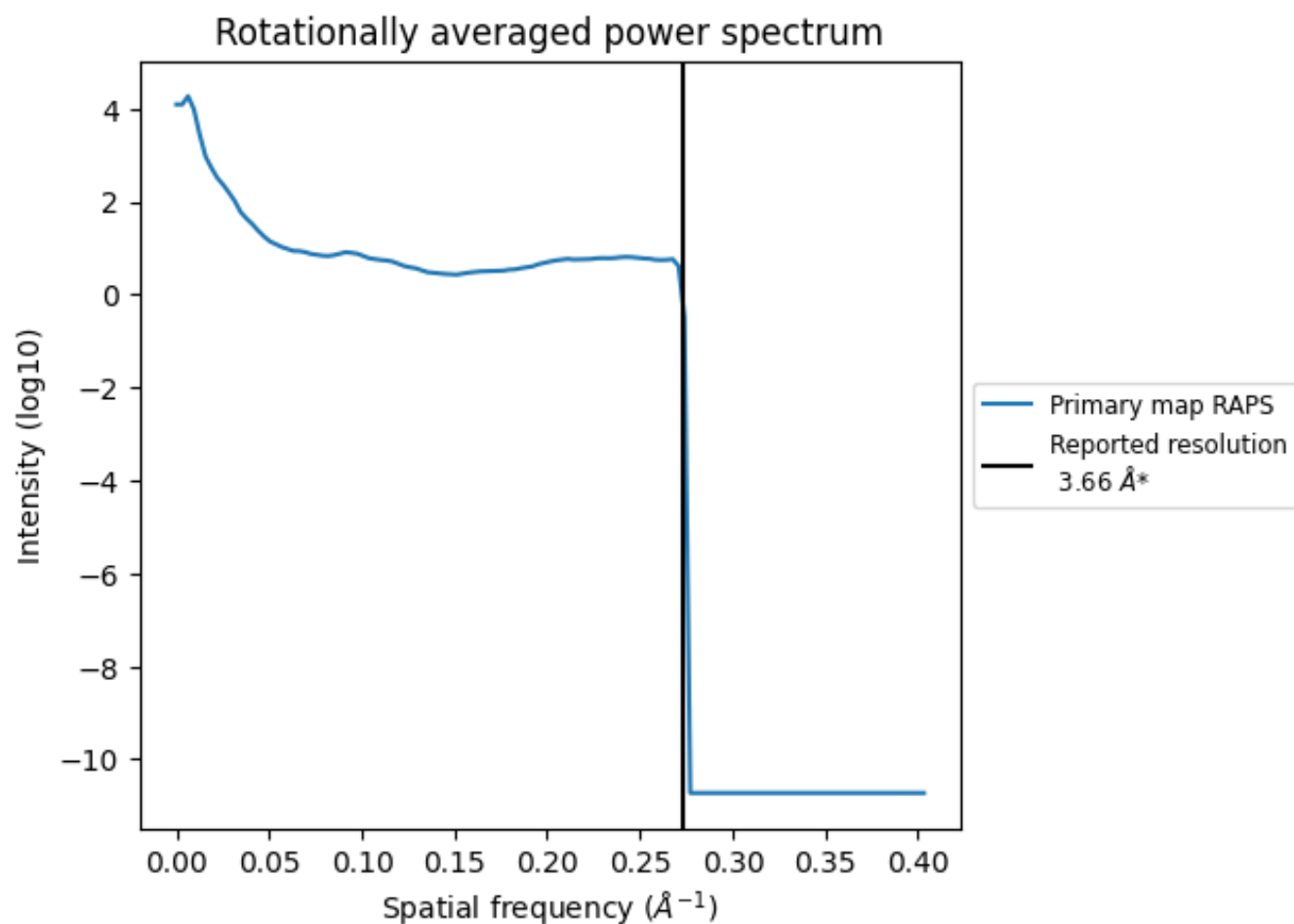
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 336 nm^3 ; this corresponds to an approximate mass of 304 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 0.273 $\text{\AA}^{-1}$

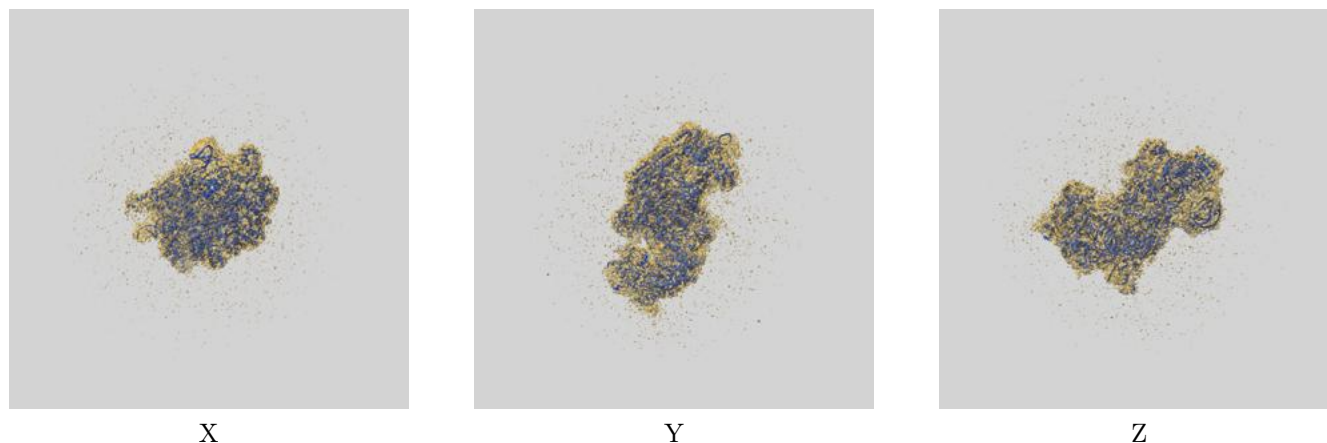
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

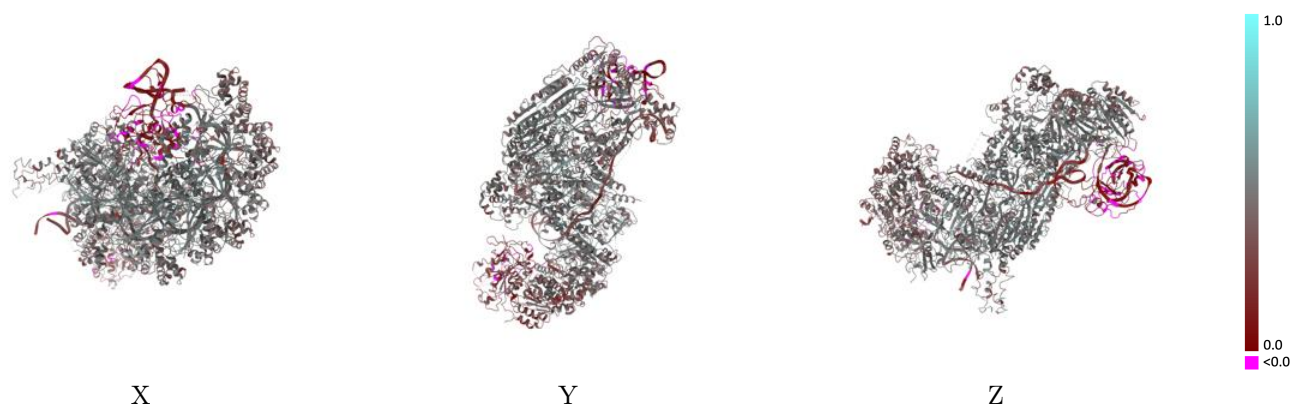
This section contains information regarding the fit between EMDB map EMD-7347 and PDB model 6C66. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.03 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](#)



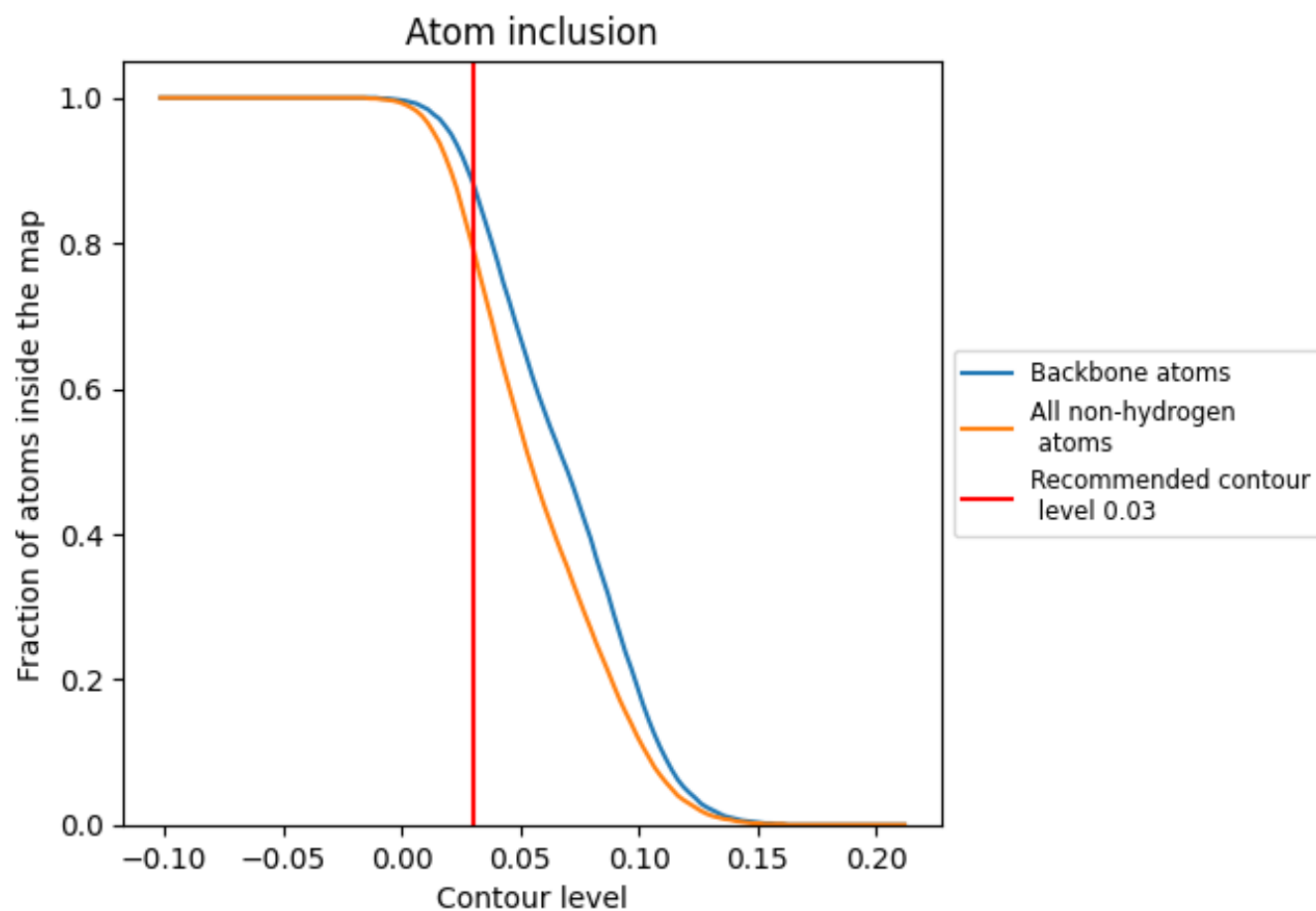
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7950	 0.4110
A	 0.8520	 0.4530
B	 0.8150	 0.4670
C	 0.8780	 0.4570
D	 0.8730	 0.4690
E	 0.8750	 0.4760
F	 0.8570	 0.4740
G	 0.5970	 0.3130
H	 0.8500	 0.4220
I	 0.8820	 0.4780
J	 0.8530	 0.3670
K	 0.8820	 0.4730
L	 0.9310	 0.4110
M	 0.8710	 0.4740
N	 0.7870	 0.2520
O	 0.4470	 0.1120

