



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:18 AM UTC

PDB ID : 6W1X / pdb_00006w1x
EMDB ID : EMD-21516
Title : Cryo-EM structure of anti-CRISPR AcrIF9, bound to the type I-F crRNA-guided CRISPR surveillance complex
Authors : Hirschi, M.; Santiago-Frangos, A.; Wilkinson, R.; Golden, S.M.; Wiedenheft, B.; Lander, G.
Deposited on : 2020-03-04
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation 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

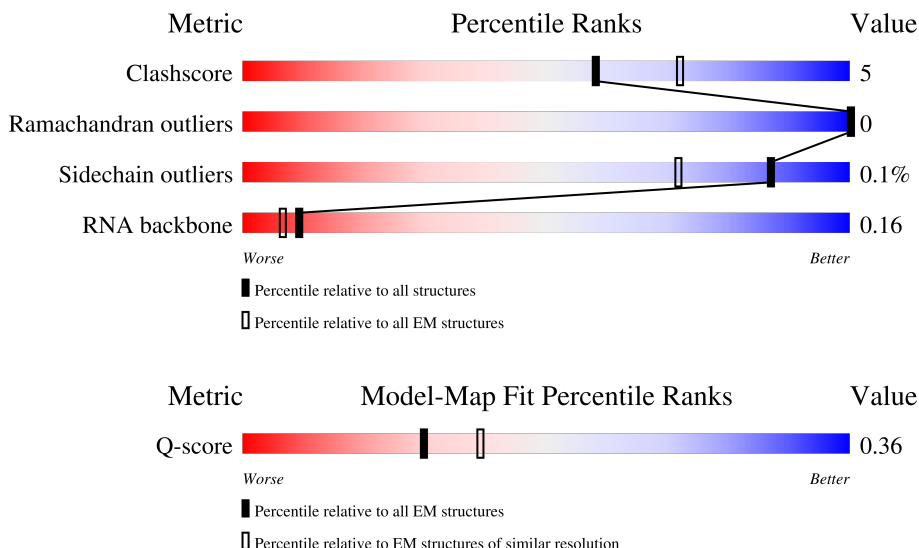
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	360	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	360	83%8%9%
3	E	360	83%9%9%
3	F	360	83%10%7%
3	G	360	81%9%9%
3	H	360	10%84%8%8%
4	M	60	8%25%47%25%.
5	L	187	12%100%
6	I	68	84%10%6%
6	J	68	74%21%6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21735 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	314	Total	C	N	O	0	0
			1817	1134	347	336		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	304	Total	C	N	O	S	0	0
			2129	1359	388	379	3		

- Molecule 3 is a protein called CRISPR-associated protein Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	290	Total	C	N	O	S	0	0
			2111	1345	379	385	2		
3	D	328	Total	C	N	O	S	0	0
			2498	1569	456	471	2		
3	E	329	Total	C	N	O	S	0	0
			2499	1569	458	470	2		
3	F	335	Total	C	N	O	S	0	0
			2528	1586	462	478	2		
3	G	326	Total	C	N	O	S	0	0
			2488	1566	453	467	2		
3	H	333	Total	C	N	O	S	0	0
			2502	1571	450	479	2		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	MET	-	expression tag	UNP A0A444M080
C	3	LYS	-	expression tag	UNP A0A444M080
C	4	SER	-	expression tag	UNP A0A444M080
C	5	SER	-	expression tag	UNP A0A444M080
C	6	HIS	-	expression tag	UNP A0A444M080

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	7	HIS	-	expression tag	UNP A0A444M080
C	8	HIS	-	expression tag	UNP A0A444M080
C	9	HIS	-	expression tag	UNP A0A444M080
C	10	HIS	-	expression tag	UNP A0A444M080
C	11	HIS	-	expression tag	UNP A0A444M080
C	12	GLU	-	expression tag	UNP A0A444M080
C	13	ASN	-	expression tag	UNP A0A444M080
C	14	LEU	-	expression tag	UNP A0A444M080
C	15	TYR	-	expression tag	UNP A0A444M080
C	16	PHE	-	expression tag	UNP A0A444M080
C	17	GLN	-	expression tag	UNP A0A444M080
C	18	SER	-	expression tag	UNP A0A444M080
C	19	ASN	-	expression tag	UNP A0A444M080
C	20	ALA	-	expression tag	UNP A0A444M080
D	2	MET	-	expression tag	UNP A0A444M080
D	3	LYS	-	expression tag	UNP A0A444M080
D	4	SER	-	expression tag	UNP A0A444M080
D	5	SER	-	expression tag	UNP A0A444M080
D	6	HIS	-	expression tag	UNP A0A444M080
D	7	HIS	-	expression tag	UNP A0A444M080
D	8	HIS	-	expression tag	UNP A0A444M080
D	9	HIS	-	expression tag	UNP A0A444M080
D	10	HIS	-	expression tag	UNP A0A444M080
D	11	HIS	-	expression tag	UNP A0A444M080
D	12	GLU	-	expression tag	UNP A0A444M080
D	13	ASN	-	expression tag	UNP A0A444M080
D	14	LEU	-	expression tag	UNP A0A444M080
D	15	TYR	-	expression tag	UNP A0A444M080
D	16	PHE	-	expression tag	UNP A0A444M080
D	17	GLN	-	expression tag	UNP A0A444M080
D	18	SER	-	expression tag	UNP A0A444M080
D	19	ASN	-	expression tag	UNP A0A444M080
D	20	ALA	-	expression tag	UNP A0A444M080
E	2	MET	-	expression tag	UNP A0A444M080
E	3	LYS	-	expression tag	UNP A0A444M080
E	4	SER	-	expression tag	UNP A0A444M080
E	5	SER	-	expression tag	UNP A0A444M080
E	6	HIS	-	expression tag	UNP A0A444M080
E	7	HIS	-	expression tag	UNP A0A444M080
E	8	HIS	-	expression tag	UNP A0A444M080
E	9	HIS	-	expression tag	UNP A0A444M080
E	10	HIS	-	expression tag	UNP A0A444M080

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	11	HIS	-	expression tag	UNP A0A444M080
E	12	GLU	-	expression tag	UNP A0A444M080
E	13	ASN	-	expression tag	UNP A0A444M080
E	14	LEU	-	expression tag	UNP A0A444M080
E	15	TYR	-	expression tag	UNP A0A444M080
E	16	PHE	-	expression tag	UNP A0A444M080
E	17	GLN	-	expression tag	UNP A0A444M080
E	18	SER	-	expression tag	UNP A0A444M080
E	19	ASN	-	expression tag	UNP A0A444M080
E	20	ALA	-	expression tag	UNP A0A444M080
F	2	MET	-	expression tag	UNP A0A444M080
F	3	LYS	-	expression tag	UNP A0A444M080
F	4	SER	-	expression tag	UNP A0A444M080
F	5	SER	-	expression tag	UNP A0A444M080
F	6	HIS	-	expression tag	UNP A0A444M080
F	7	HIS	-	expression tag	UNP A0A444M080
F	8	HIS	-	expression tag	UNP A0A444M080
F	9	HIS	-	expression tag	UNP A0A444M080
F	10	HIS	-	expression tag	UNP A0A444M080
F	11	HIS	-	expression tag	UNP A0A444M080
F	12	GLU	-	expression tag	UNP A0A444M080
F	13	ASN	-	expression tag	UNP A0A444M080
F	14	LEU	-	expression tag	UNP A0A444M080
F	15	TYR	-	expression tag	UNP A0A444M080
F	16	PHE	-	expression tag	UNP A0A444M080
F	17	GLN	-	expression tag	UNP A0A444M080
F	18	SER	-	expression tag	UNP A0A444M080
F	19	ASN	-	expression tag	UNP A0A444M080
F	20	ALA	-	expression tag	UNP A0A444M080
G	2	MET	-	expression tag	UNP A0A444M080
G	3	LYS	-	expression tag	UNP A0A444M080
G	4	SER	-	expression tag	UNP A0A444M080
G	5	SER	-	expression tag	UNP A0A444M080
G	6	HIS	-	expression tag	UNP A0A444M080
G	7	HIS	-	expression tag	UNP A0A444M080
G	8	HIS	-	expression tag	UNP A0A444M080
G	9	HIS	-	expression tag	UNP A0A444M080
G	10	HIS	-	expression tag	UNP A0A444M080
G	11	HIS	-	expression tag	UNP A0A444M080
G	12	GLU	-	expression tag	UNP A0A444M080
G	13	ASN	-	expression tag	UNP A0A444M080
G	14	LEU	-	expression tag	UNP A0A444M080

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	15	TYR	-	expression tag	UNP A0A444M080
G	16	PHE	-	expression tag	UNP A0A444M080
G	17	GLN	-	expression tag	UNP A0A444M080
G	18	SER	-	expression tag	UNP A0A444M080
G	19	ASN	-	expression tag	UNP A0A444M080
G	20	ALA	-	expression tag	UNP A0A444M080
H	2	MET	-	expression tag	UNP A0A444M080
H	3	LYS	-	expression tag	UNP A0A444M080
H	4	SER	-	expression tag	UNP A0A444M080
H	5	SER	-	expression tag	UNP A0A444M080
H	6	HIS	-	expression tag	UNP A0A444M080
H	7	HIS	-	expression tag	UNP A0A444M080
H	8	HIS	-	expression tag	UNP A0A444M080
H	9	HIS	-	expression tag	UNP A0A444M080
H	10	HIS	-	expression tag	UNP A0A444M080
H	11	HIS	-	expression tag	UNP A0A444M080
H	12	GLU	-	expression tag	UNP A0A444M080
H	13	ASN	-	expression tag	UNP A0A444M080
H	14	LEU	-	expression tag	UNP A0A444M080
H	15	TYR	-	expression tag	UNP A0A444M080
H	16	PHE	-	expression tag	UNP A0A444M080
H	17	GLN	-	expression tag	UNP A0A444M080
H	18	SER	-	expression tag	UNP A0A444M080
H	19	ASN	-	expression tag	UNP A0A444M080
H	20	ALA	-	expression tag	UNP A0A444M080

- Molecule 4 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	60	Total	C	N	O	P	0	0
			1272	569	223	421	59		

- Molecule 5 is a protein called CRISPR-associated endonuclease Cas6/Csy4.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	187	Total	C	N	O	0	0
			920	546	187	187		

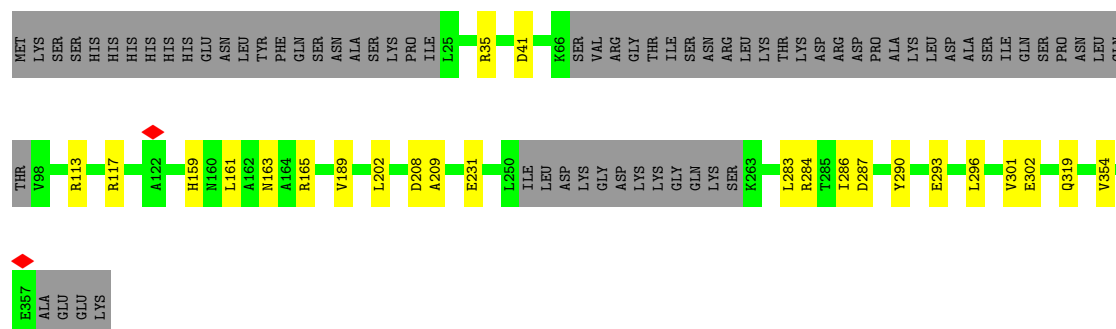
- Molecule 6 is a protein called anti-CRISPR AcrIF9.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	64	Total 489	C 307	N 86	O 96	0	0
6	J	64	Total 482	C 305	N 87	O 90	0	0



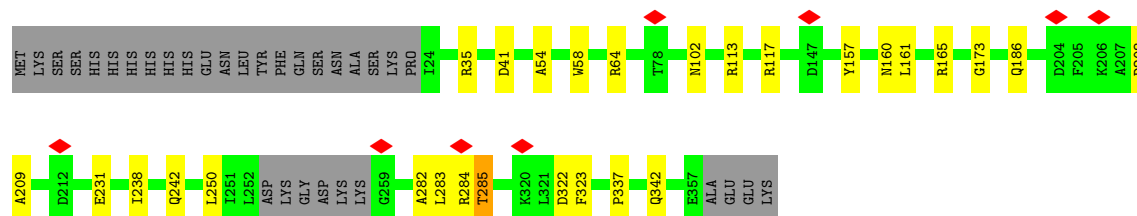
• Molecule 3: CRISPR-associated protein Csy3

Chain C: 74% 7% 19%



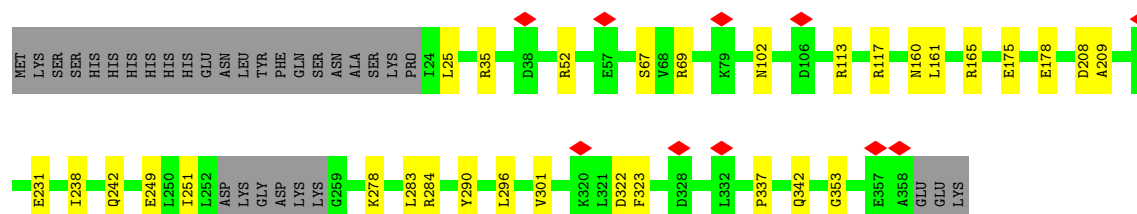
• Molecule 3: CRISPR-associated protein Csy3

Chain D: 83% 8% 9%



• Molecule 3: CRISPR-associated protein Csy3

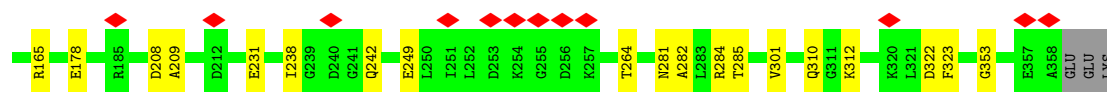
Chain E: 83% 9% 9%



• Molecule 3: CRISPR-associated protein Csy3

Chain F: 83% 10% 7%





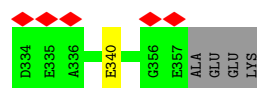
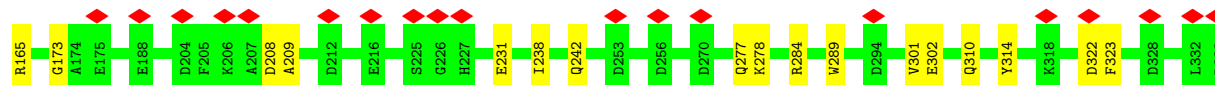
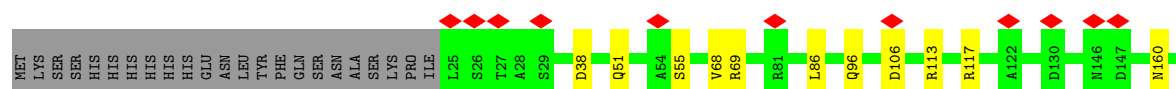
• Molecule 3: CRISPR-associated protein Csy3

Chain G: 81% 9% 9%



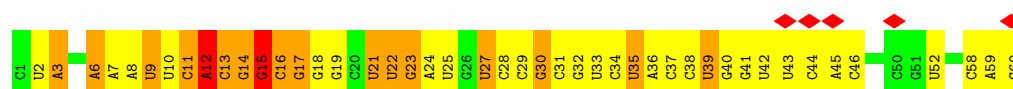
• Molecule 3: CRISPR-associated protein Csy3

Chain H: 10% 84% 8% 8%



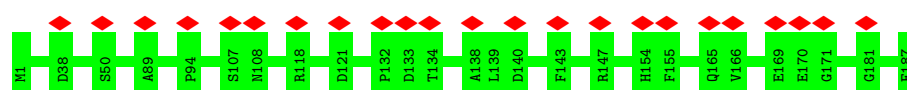
• Molecule 4: RNA (60-MER)

Chain M: 8% 25% 47% 25%



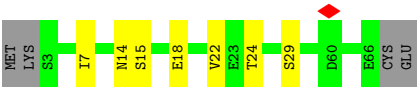
• Molecule 5: CRISPR-associated endonuclease Cas6/Csy4

Chain L: 12% 100%



• Molecule 6: anti-CRISPR AcrIF9

Chain I: 84% 10% 6%



● Molecule 6: anti-CRISPR AcrIF9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	285707	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.061	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	230.0, 230.0, 230.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.15, 1.15, 1.15	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	0.87	0/1857	0.75	0/2582
2	B	0.76	0/2180	0.67	0/2994
3	C	0.77	0/2154	0.68	0/2943
3	D	0.81	0/2544	0.70	0/3457
3	E	0.82	0/2544	0.71	0/3456
3	F	0.82	0/2575	0.71	0/3502
3	G	0.81	0/2534	0.69	0/3445
3	H	0.76	0/2548	0.66	0/3468
4	M	0.58	0/1420	1.10	2/2212 (0.1%)
5	L	0.91	0/919	0.80	0/1276
6	I	0.74	0/497	0.61	0/674
6	J	0.77	0/490	0.87	0/664
All	All	0.79	0/22262	0.74	2/30673 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	15	G	C4'-C3'-O3'	6.10	122.15	113.00
4	M	12	A	C3'-C2'-O2'	5.07	118.30	110.70

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	1817	0	1222	5	0
2	B	2129	0	1928	30	0
3	C	2111	0	1990	20	0
3	D	2498	0	2446	20	0
3	E	2499	0	2458	22	0
3	F	2528	0	2457	26	0
3	G	2488	0	2446	29	0
3	H	2502	0	2420	29	0
4	M	1272	0	644	52	0
5	L	920	0	413	0	0
6	I	489	0	458	5	0
6	J	482	0	455	9	0
All	All	21735	0	19337	191	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 5.

All (191) 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)
6:I:24:THR:OG1	6:I:29:SER:OG	1.98	0.81
3:F:284:ARG:NH1	3:F:301:VAL:O	2.14	0.80
3:H:68:VAL:HG21	4:M:13:C:C5	2.19	0.77
3:C:284:ARG:NH1	3:C:301:VAL:O	2.18	0.76
3:H:278:LYS:HD2	4:M:9:U:OP1	1.86	0.76
3:F:160:ASN:OD1	3:F:165:ARG:NH1	2.19	0.76
3:G:52:ARG:NH1	3:G:178:GLU:OE1	2.19	0.76
3:H:160:ASN:OD1	3:H:165:ARG:NH1	2.19	0.75
3:E:160:ASN:OD1	3:E:165:ARG:NH1	2.19	0.75
2:B:144:ILE:O	3:H:117:ARG:NH1	2.21	0.74
3:H:96:GLN:OE1	4:M:13:C:N4	2.19	0.74
2:B:135:GLY:O	3:H:117:ARG:NH1	2.21	0.74
3:D:160:ASN:OD1	3:D:165:ARG:NH1	2.20	0.73
4:M:18:G:O2'	4:M:19:G:O4'	2.07	0.72
3:G:284:ARG:NH1	3:G:301:VAL:O	2.22	0.72
4:M:30:G:O2'	4:M:31:C:O4'	2.08	0.71
3:E:284:ARG:NH1	3:E:301:VAL:O	2.23	0.71
3:G:160:ASN:OD1	3:G:165:ARG:NH1	2.24	0.71
2:B:25:SER:HG	2:B:28:THR:HG1	0.74	0.70
3:F:249:GLU:O	3:F:264:THR:OG1	2.09	0.70
4:M:39:U:O2'	4:M:40:G:N2	2.25	0.70
3:H:68:VAL:HG21	4:M:13:C:H5	1.54	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:LEU:HD13	2:B:15:LEU:HD11	1.74	0.70
1:A:179:TYR:OH	2:B:272:ASP:OD2	2.07	0.69
3:C:159:HIS:O	3:C:163:ASN:ND2	2.27	0.68
4:M:21:U:O2'	4:M:22:U:O4'	2.11	0.67
3:F:69:ARG:HD2	4:M:27:U:H1'	1.78	0.66
3:H:284:ARG:NH2	3:H:302:GLU:OE2	2.30	0.65
2:B:189:ARG:NH1	2:B:288:GLU:OE1	2.30	0.64
3:F:281:ASN:OD1	3:F:284:ARG:NH2	2.31	0.64
3:G:69:ARG:O	4:M:19:G:O2'	2.11	0.64
3:E:35:ARG:N	4:M:24:A:OP1	2.30	0.64
3:D:54:ALA:O	3:D:58:TRP:NE1	2.32	0.62
4:M:8:A:H3'	4:M:9:U:H5''	1.81	0.62
3:G:249:GLU:N	3:G:264:THR:O	2.33	0.61
3:C:35:ARG:N	4:M:36:A:OP1	2.34	0.61
4:M:27:U:H2'	4:M:27:U:O2	2.00	0.61
6:J:29:SER:O	6:J:32:ARG:HG2	2.01	0.61
3:C:165:ARG:NH2	3:C:202:LEU:O	2.35	0.60
3:D:282:ALA:O	3:D:285:THR:OG1	2.18	0.60
6:J:31:LYS:HB3	6:J:64:TRP:CZ2	2.38	0.59
3:C:41:ASP:OD2	3:D:64:ARG:NH2	2.36	0.58
3:C:319:GLN:N	3:C:319:GLN:OE1	2.36	0.58
3:C:354:VAL:HG22	4:M:35:U:H1'	1.85	0.58
1:A:178:LEU:HD11	4:M:3:A:H4'	1.84	0.58
3:D:41:ASP:OD2	3:E:102:ASN:ND2	2.36	0.58
3:G:284:ARG:NH2	4:M:14:G:OP2	2.37	0.58
2:B:12:LEU:HD12	2:B:109:LEU:HB2	1.84	0.57
3:G:286:ILE:HG22	3:G:286:ILE:O	2.04	0.57
4:M:21:U:O2'	4:M:22:U:O5'	2.22	0.56
3:H:96:GLN:CD	4:M:13:C:H41	2.13	0.56
4:M:21:U:H2'	4:M:21:U:O2	2.05	0.56
3:C:284:ARG:NH2	3:C:302:GLU:OE2	2.37	0.56
3:E:113:ARG:NE	3:E:231:GLU:OE2	2.35	0.56
3:G:322:ASP:OD2	3:G:325:THR:OG1	2.16	0.56
3:D:113:ARG:NE	3:D:231:GLU:OE2	2.39	0.56
6:J:7:ILE:HD13	6:J:34:ALA:HB2	1.88	0.56
3:H:69:ARG:HE	4:M:15:G:H21	1.53	0.55
3:D:35:ARG:N	4:M:30:G:OP1	2.37	0.55
3:F:41:ASP:OD2	3:G:64:ARG:NH2	2.40	0.55
3:D:238:ILE:HG22	3:D:242:GLN:HG3	1.89	0.55
4:M:6:A:O2'	4:M:7:A:O4'	2.24	0.55
2:B:86:ASN:ND2	2:B:96:ALA:O	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:353:GLY:O	4:M:17:G:O2'	2.25	0.55
3:H:113:ARG:NE	3:H:231:GLU:OE2	2.37	0.54
3:C:41:ASP:OD2	3:D:102:ASN:ND2	2.40	0.54
2:B:261:LEU:HD23	2:B:262:TYR:N	2.22	0.54
3:C:113:ARG:NE	3:C:231:GLU:OE2	2.39	0.54
3:C:189:VAL:O	3:C:189:VAL:HG23	2.06	0.54
2:B:37:PHE:CD1	2:B:139:LEU:HD11	2.42	0.54
3:C:117:ARG:NH1	3:D:173:GLY:O	2.41	0.54
6:J:15:SER:O	6:J:46:ARG:NH1	2.37	0.54
3:G:113:ARG:NE	3:G:231:GLU:OE2	2.38	0.53
3:G:278:LYS:HA	4:M:14:G:H4'	1.91	0.53
3:H:238:ILE:HG22	3:H:242:GLN:HG3	1.91	0.53
3:G:322:ASP:OD1	3:G:322:ASP:N	2.42	0.53
3:D:250:LEU:N	3:E:67:SER:OG	2.38	0.53
4:M:8:A:C3'	4:M:9:U:H5''	2.38	0.53
3:F:52:ARG:NE	3:F:178:GLU:OE1	2.42	0.52
3:H:284:ARG:NH1	3:H:301:VAL:O	2.43	0.52
3:C:286:ILE:HG22	3:C:286:ILE:O	2.08	0.52
3:E:52:ARG:NE	3:E:178:GLU:OE1	2.42	0.52
3:E:69:ARG:O	4:M:31:C:O2'	2.26	0.52
6:I:18:GLU:N	6:I:18:GLU:OE1	2.42	0.52
3:G:238:ILE:HG22	3:G:242:GLN:HG3	1.92	0.51
2:B:45:GLN:NE2	2:B:54:ILE:O	2.36	0.51
3:C:117:ARG:NH1	3:D:238:ILE:HG23	2.26	0.51
6:J:38:GLN:HG3	6:J:45:LEU:HD21	1.92	0.51
3:G:34:GLU:HA	4:M:12:A:OP1	2.10	0.51
3:G:117:ARG:NH1	3:H:173:GLY:O	2.44	0.51
3:H:289:TRP:NE1	3:H:340:GLU:OE1	2.43	0.51
2:B:11:LEU:HD13	2:B:110:LEU:HD21	1.93	0.51
3:E:278:LYS:HD2	4:M:27:U:OP1	2.11	0.50
3:H:208:ASP:OD1	3:H:209:ALA:N	2.44	0.50
3:G:278:LYS:HD2	4:M:15:G:H5'	1.93	0.50
3:H:51:GLN:O	3:H:55:SER:N	2.42	0.50
3:F:86:LEU:O	3:F:86:LEU:HD23	2.12	0.50
1:A:268:LEU:HD21	2:B:29:TRP:CZ3	2.46	0.49
3:F:310:GLN:HB3	3:F:312:LYS:HZ2	1.77	0.49
3:D:117:ARG:NH1	3:E:238:ILE:HG23	2.26	0.49
4:M:27:U:O2	4:M:27:U:C2'	2.61	0.49
2:B:9:LEU:HD23	2:B:112:GLY:HA2	1.94	0.49
1:A:178:LEU:HD11	4:M:3:A:C4'	2.43	0.49
3:F:134:ARG:NH1	3:G:310:GLN:OE1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:208:ASP:OD1	3:F:209:ALA:N	2.46	0.49
3:C:35:ARG:NH1	4:M:37:C:OP1	2.45	0.49
3:E:208:ASP:OD1	3:E:209:ALA:N	2.46	0.48
4:M:21:U:O2	4:M:21:U:C2'	2.61	0.48
3:F:69:ARG:HD2	4:M:27:U:C1'	2.42	0.48
3:F:30:VAL:N	3:F:129:ASN:OD1	2.44	0.48
3:G:277:GLN:HG2	4:M:14:G:H5'	1.94	0.48
3:E:290:TYR:OH	3:E:296:LEU:N	2.47	0.48
3:D:208:ASP:OD1	3:D:209:ALA:N	2.47	0.48
3:E:238:ILE:HG22	3:E:242:GLN:HG3	1.95	0.48
3:E:251:ILE:HD12	3:E:251:ILE:N	2.28	0.48
3:G:208:ASP:OD1	3:G:209:ALA:N	2.47	0.48
3:H:310:GLN:NE2	3:H:314:TYR:OH	2.47	0.47
3:H:68:VAL:CG2	4:M:13:C:C5	2.93	0.47
3:F:117:ARG:NH1	3:G:238:ILE:HG23	2.30	0.47
3:C:208:ASP:OD1	3:C:209:ALA:N	2.48	0.47
3:F:90:ILE:C	3:F:90:ILE:HD12	2.40	0.47
1:A:189:LEU:HD11	2:B:277:LEU:CB	2.44	0.47
3:C:290:TYR:HE1	3:C:293:GLU:CB	2.27	0.47
3:G:277:GLN:CG	4:M:14:G:H5'	2.45	0.47
2:B:25:SER:OG	2:B:28:THR:OG1	1.88	0.47
3:E:117:ARG:NH1	3:F:238:ILE:HG23	2.30	0.46
6:I:7:ILE:CD1	6:I:22:VAL:HG21	2.45	0.46
3:G:289:TRP:NE1	3:G:340:GLU:OE1	2.48	0.46
6:I:7:ILE:HD12	6:I:22:VAL:HG21	1.97	0.46
2:B:37:PHE:HD1	2:B:139:LEU:HD11	1.80	0.46
4:M:11:C:H6	4:M:11:C:H2'	1.59	0.46
2:B:138:ARG:O	4:M:2:U:N3	2.45	0.46
3:D:186:GLN:N	3:E:175:GLU:OE2	2.47	0.46
3:F:238:ILE:HG22	3:F:242:GLN:HG3	1.97	0.45
3:H:69:ARG:HE	4:M:15:G:N2	2.13	0.45
3:E:337:PRO:O	3:E:342:GLN:NE2	2.47	0.45
2:B:59:VAL:HG13	2:B:59:VAL:O	2.17	0.45
3:C:161:LEU:HD23	3:C:283:LEU:HD22	1.98	0.45
3:F:322:ASP:OD1	3:F:323:PHE:N	2.50	0.44
3:C:296:LEU:C	3:C:296:LEU:HD23	2.43	0.44
3:G:186:GLN:N	3:G:186:GLN:OE1	2.50	0.44
4:M:35:U:H6	4:M:35:U:H2'	1.54	0.44
6:J:29:SER:HA	6:J:32:ARG:NH1	2.32	0.44
3:E:353:GLY:O	4:M:23:G:O2'	2.33	0.44
3:F:78:THR:HG22	3:F:79:LYS:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:117:ARG:NH1	3:H:238:ILE:HG23	2.32	0.44
4:M:15:G:C2	4:M:16:C:N4	2.86	0.44
3:G:351:ARG:NH2	4:M:13:C:H5''	2.32	0.44
3:H:69:ARG:HD2	4:M:15:G:N3	2.33	0.43
2:B:78:THR:HG23	2:B:78:THR:O	2.18	0.43
2:B:192:LEU:O	2:B:196:HIS:ND1	2.38	0.43
3:D:161:LEU:HD23	3:D:283:LEU:HD22	2.00	0.43
3:D:337:PRO:O	3:D:342:GLN:NE2	2.51	0.43
3:H:277:GLN:OE1	3:H:277:GLN:N	2.46	0.43
3:E:249:GLU:OE1	3:F:67:SER:N	2.51	0.43
3:F:76:LEU:HD12	3:F:76:LEU:N	2.34	0.43
3:G:30:VAL:N	3:G:129:ASN:OD1	2.46	0.43
4:M:13:C:H6	4:M:13:C:H2'	1.65	0.42
3:C:287:ASP:HB2	3:C:301:VAL:HG22	2.02	0.42
4:M:13:C:N3	6:J:11:GLN:OE1	2.51	0.42
3:H:68:VAL:HG21	4:M:13:C:C6	2.54	0.42
2:B:7:GLU:O	2:B:160:LEU:HD12	2.19	0.42
4:M:24:A:O2'	4:M:25:U:O4'	2.26	0.42
3:G:214:LEU:O	3:G:214:LEU:HD23	2.20	0.42
6:I:14:ASN:O	6:I:15:SER:OG	2.34	0.42
2:B:181:LEU:N	2:B:182:PRO:CD	2.83	0.41
2:B:261:LEU:HD23	2:B:261:LEU:C	2.45	0.41
2:B:143:SER:OG	3:H:38:ASP:OD2	2.32	0.41
3:D:322:ASP:OD1	3:D:323:PHE:N	2.53	0.41
3:E:161:LEU:HD23	3:E:283:LEU:HD22	2.03	0.41
3:F:282:ALA:O	3:F:285:THR:HG23	2.20	0.41
3:H:96:GLN:CD	4:M:13:C:N4	2.74	0.41
3:H:322:ASP:OD1	3:H:323:PHE:N	2.54	0.41
3:E:322:ASP:OD1	3:E:323:PHE:N	2.53	0.41
6:J:24:THR:HG21	6:J:30:ALA:HB2	2.02	0.41
3:D:157:TYR:HE1	3:D:284:ARG:HG2	1.85	0.41
3:D:285:THR:H	3:D:285:THR:HG1	1.59	0.41
3:E:25:LEU:HD12	3:E:25:LEU:N	2.36	0.41
2:B:80:VAL:HG12	2:B:81:PHE:N	2.35	0.40
2:B:216:LEU:HD12	2:B:216:LEU:C	2.45	0.40
2:B:251:ILE:O	2:B:285:GLY:N	2.54	0.40
6:J:31:LYS:HA	6:J:47:ILE:HD11	2.02	0.40
2:B:11:LEU:HD11	2:B:180:LEU:HD21	2.03	0.40
3:F:78:THR:HG22	3:F:79:LYS:N	2.37	0.40
3:H:106:ASP:OD1	3:H:106:ASP:N	2.54	0.40
3:F:113:ARG:NE	3:F:231:GLU:OE2	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:86:LEU:C	3:H:86:LEU:HD23	2.47	0.40
2:B:305:HIS:ND1	2:B:305:HIS:O	2.54	0.40
3:F:35:ARG:NH2	4:M:18:G:OP2	2.54	0.40
3:G:337:PRO:O	3:G:342:GLN:NE2	2.54	0.40
3:G:268:VAL:O	3:G:268:VAL:HG23	2.21	0.40

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	310/434 (71%)	308 (99%)	2 (1%)	0	100	100
2	B	300/327 (92%)	297 (99%)	3 (1%)	0	100	100
3	C	284/360 (79%)	284 (100%)	0	0	100	100
3	D	324/360 (90%)	323 (100%)	1 (0%)	0	100	100
3	E	325/360 (90%)	325 (100%)	0	0	100	100
3	F	333/360 (92%)	333 (100%)	0	0	100	100
3	G	322/360 (89%)	322 (100%)	0	0	100	100
3	H	331/360 (92%)	329 (99%)	2 (1%)	0	100	100
5	L	185/187 (99%)	185 (100%)	0	0	100	100
6	I	62/68 (91%)	62 (100%)	0	0	100	100
6	J	62/68 (91%)	62 (100%)	0	0	100	100
All	All	2838/3244 (88%)	2830 (100%)	8 (0%)	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	
1	A	77/365 (21%)	77 (100%)	0	100	100
2	B	183/270 (68%)	183 (100%)	0	100	100
3	C	190/290 (66%)	190 (100%)	0	100	100
3	D	249/290 (86%)	248 (100%)	1 (0%)	84	83
3	E	249/290 (86%)	249 (100%)	0	100	100
3	F	248/290 (86%)	248 (100%)	0	100	100
3	G	249/290 (86%)	249 (100%)	0	100	100
3	H	246/290 (85%)	246 (100%)	0	100	100
6	I	50/61 (82%)	50 (100%)	0	100	100
6	J	47/61 (77%)	47 (100%)	0	100	100
All	All	1788/2497 (72%)	1787 (100%)	1 (0%)	87	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	285	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	HIS
2	B	86	ASN
2	B	131	GLN
2	B	173	GLN
3	C	342	GLN
3	D	182	ASN
3	D	227	HIS
3	D	248	GLN
3	E	242	GLN
3	E	343	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	182	ASN
3	F	342	GLN
3	G	91	GLN
3	G	148	GLN
3	G	182	ASN
3	G	242	GLN
3	G	343	HIS
3	H	74	ASN
3	H	310	GLN
3	H	342	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	M	59/60 (98%)	33 (55%)	14 (23%)

All (33) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	M	3	A
4	M	6	A
4	M	9	U
4	M	10	U
4	M	11	C
4	M	12	A
4	M	13	C
4	M	14	G
4	M	15	G
4	M	16	C
4	M	17	G
4	M	22	U
4	M	23	G
4	M	27	U
4	M	28	C
4	M	29	C
4	M	30	G
4	M	32	G
4	M	33	U
4	M	34	C
4	M	35	U
4	M	38	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	M	39	U
4	M	41	G
4	M	42	U
4	M	43	U
4	M	44	C
4	M	45	A
4	M	46	C
4	M	52	U
4	M	58	C
4	M	59	A
4	M	60	G

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	M	9	U
4	M	10	U
4	M	11	C
4	M	12	A
4	M	13	C
4	M	14	G
4	M	15	G
4	M	21	U
4	M	27	U
4	M	28	C
4	M	29	C
4	M	33	U
4	M	34	C
4	M	35	U

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

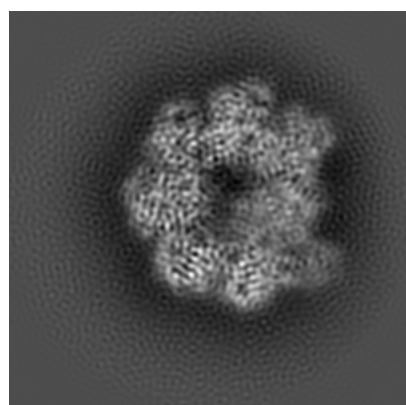
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21516. These allow visual inspection of the internal detail of the map and identification of artifacts.

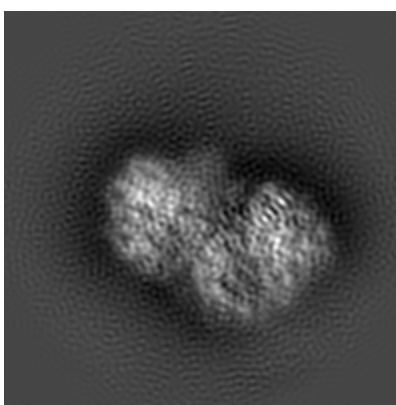
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

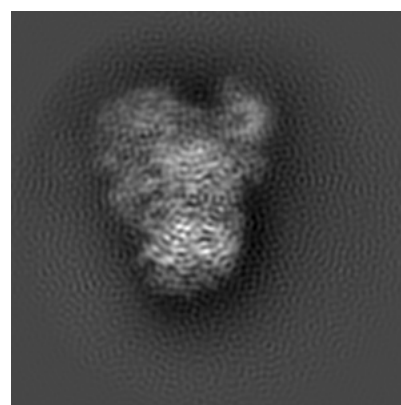
6.1.1 Primary map



X



Y

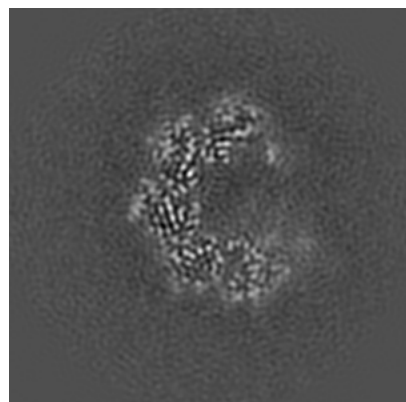


Z

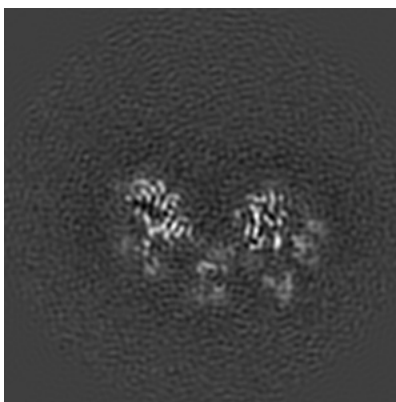
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

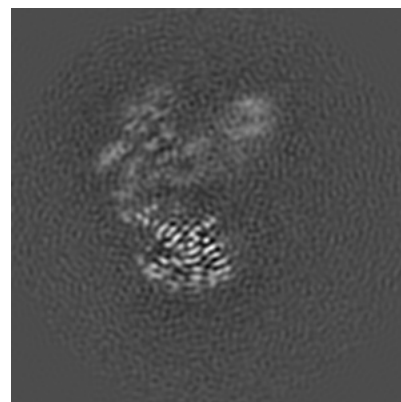
6.2.1 Primary map



X Index: 100



Y Index: 100

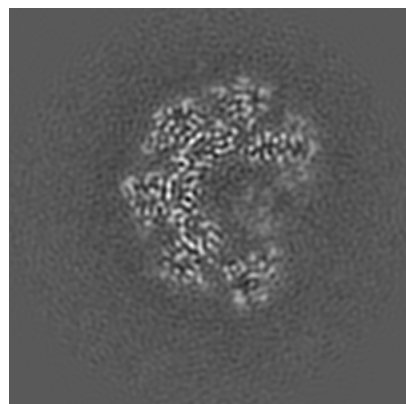


Z Index: 100

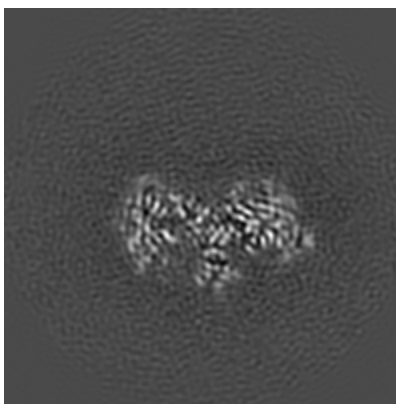
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

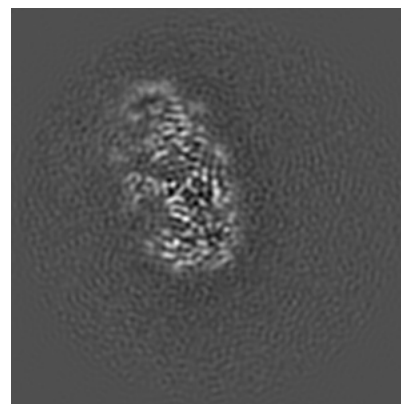
6.3.1 Primary map



X Index: 86



Y Index: 91

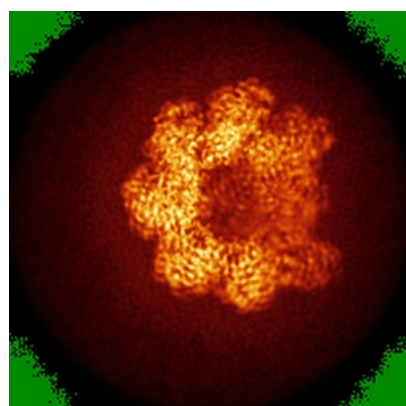


Z Index: 135

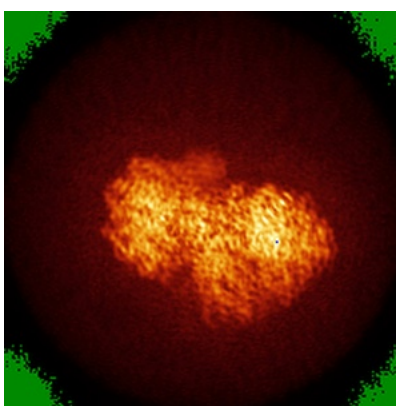
The images above show the largest variance slices of the map in three orthogonal directions.

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

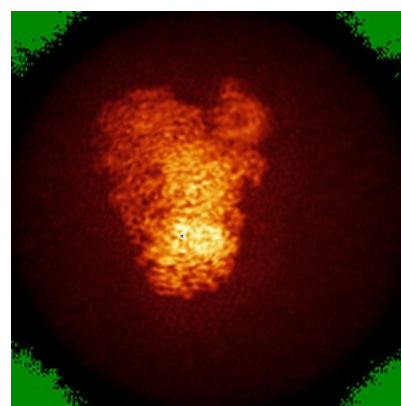
6.4.1 Primary map



X



Y

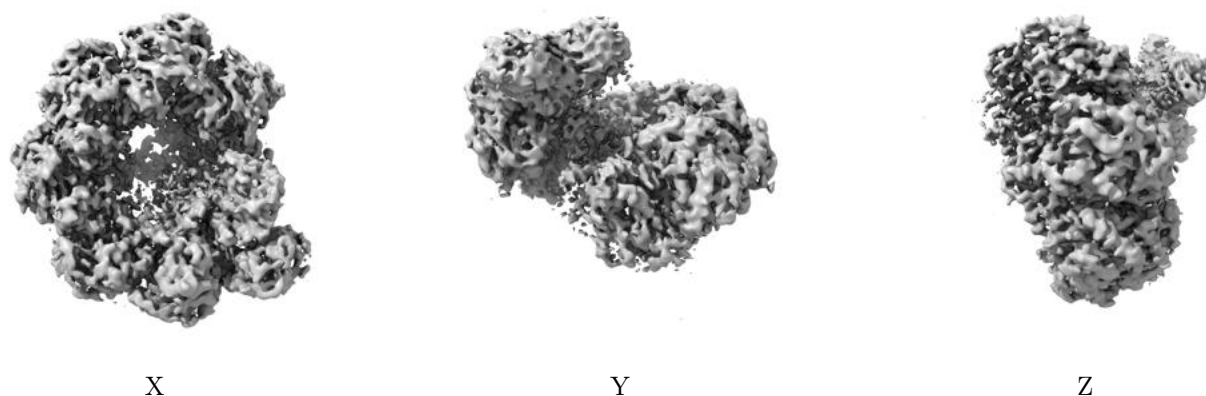


Z

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

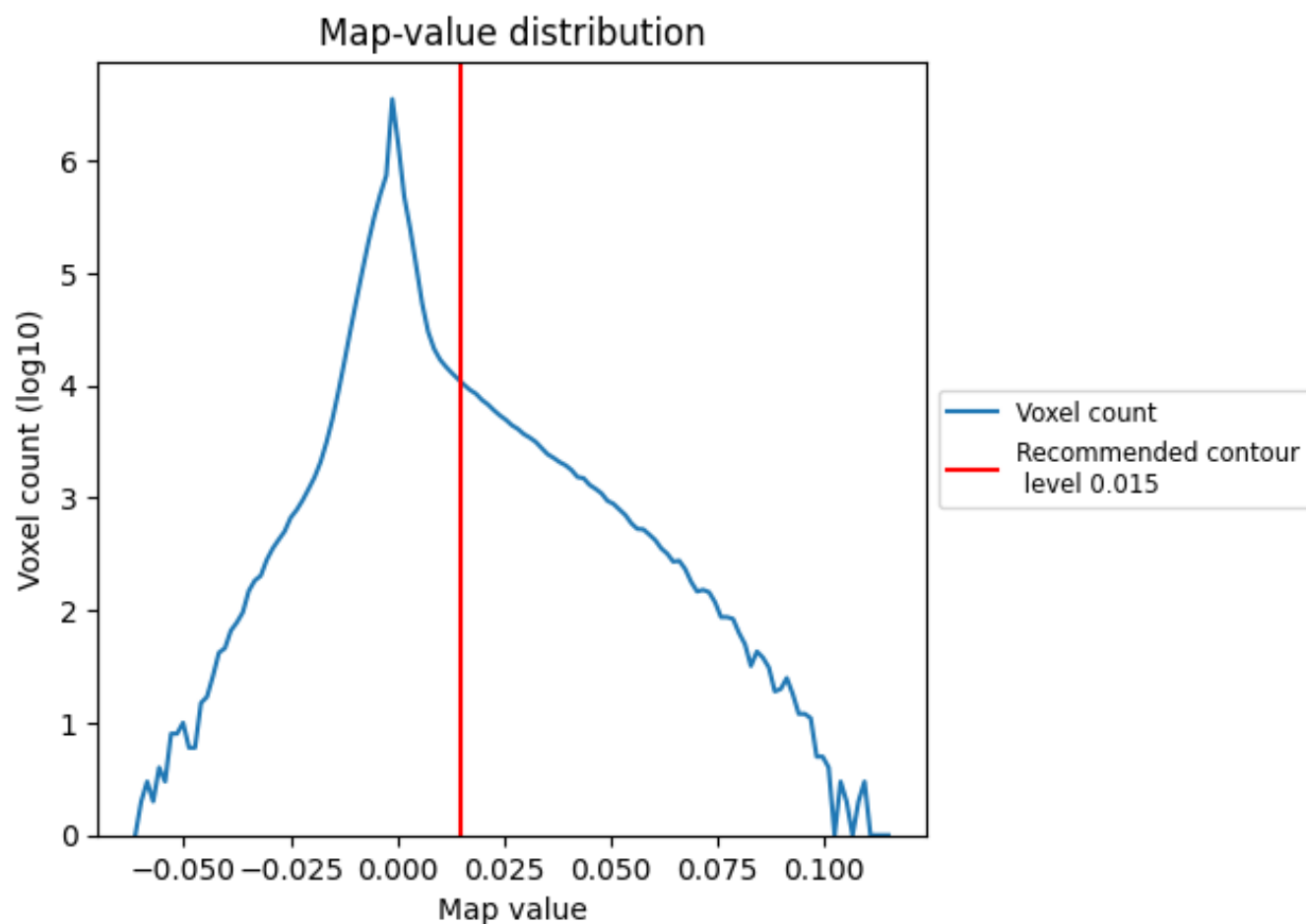
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

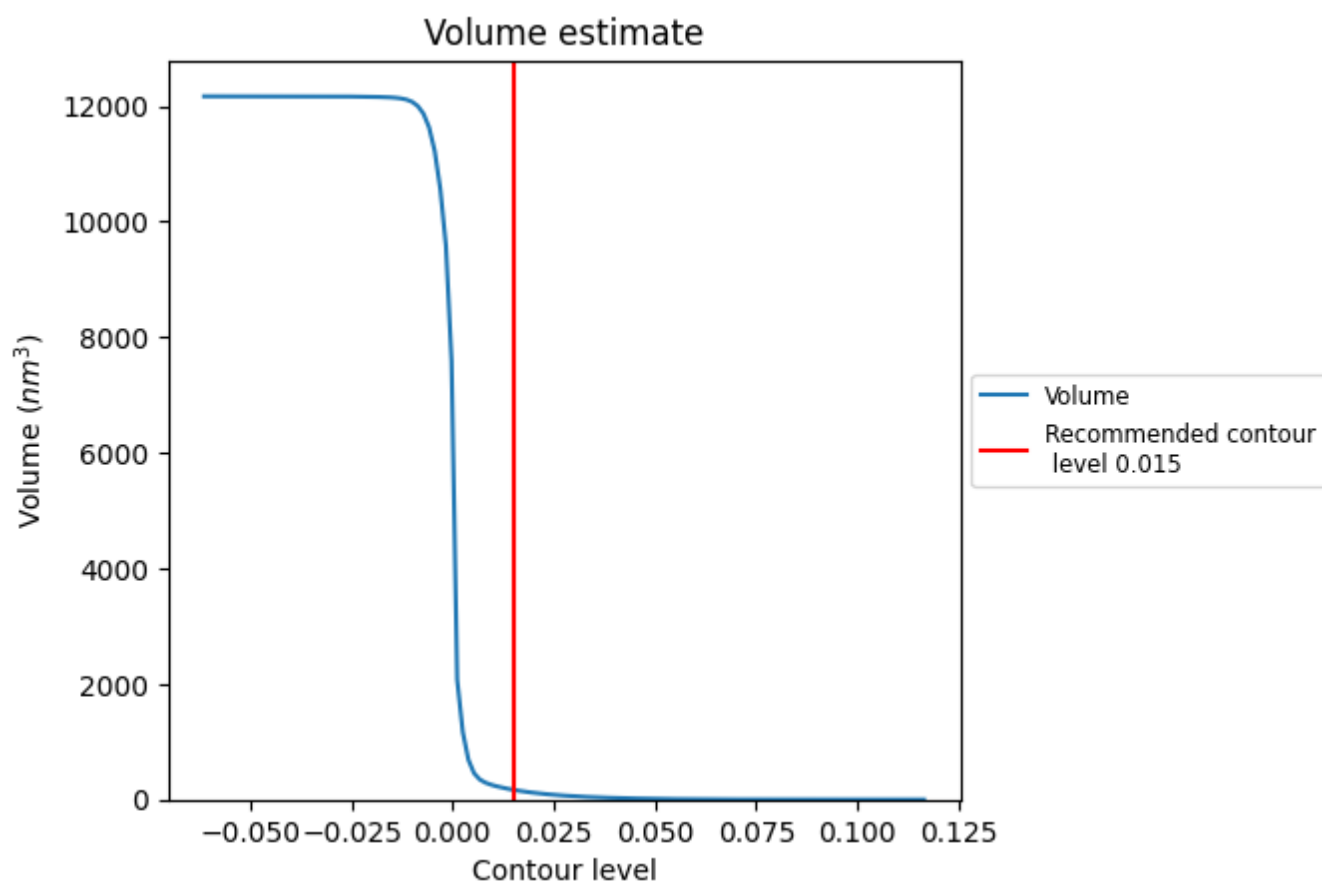
This section contains the results of statistical analysis of the map.

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.

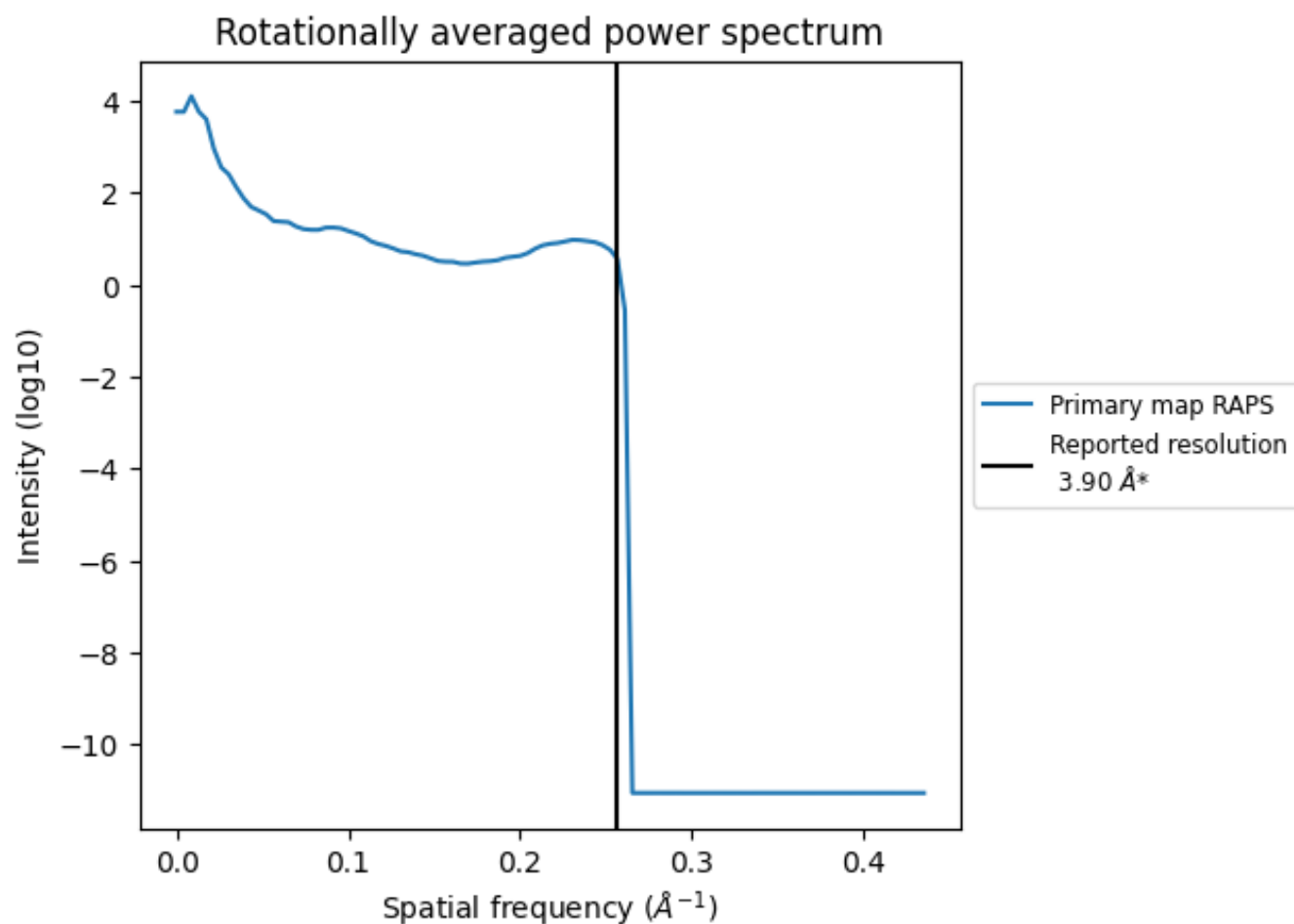
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm³; this corresponds to an approximate mass of 153 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 0.256 Å⁻¹

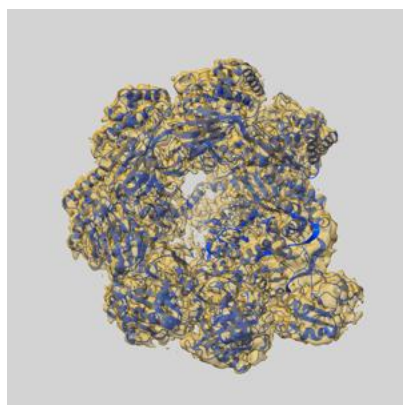
8 Fourier-Shell correlation ⓘ

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

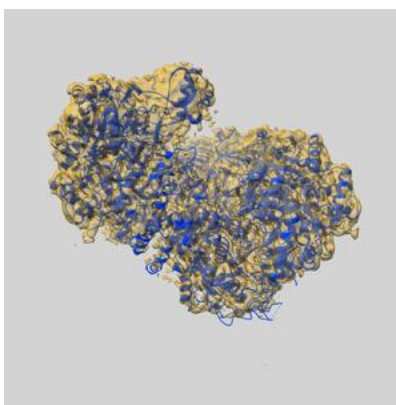
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21516 and PDB model 6W1X. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

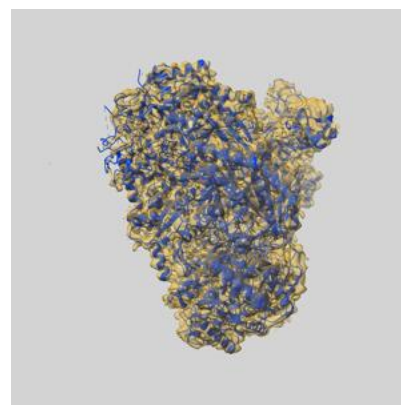
9.1 Map-model overlay [i](#)



X



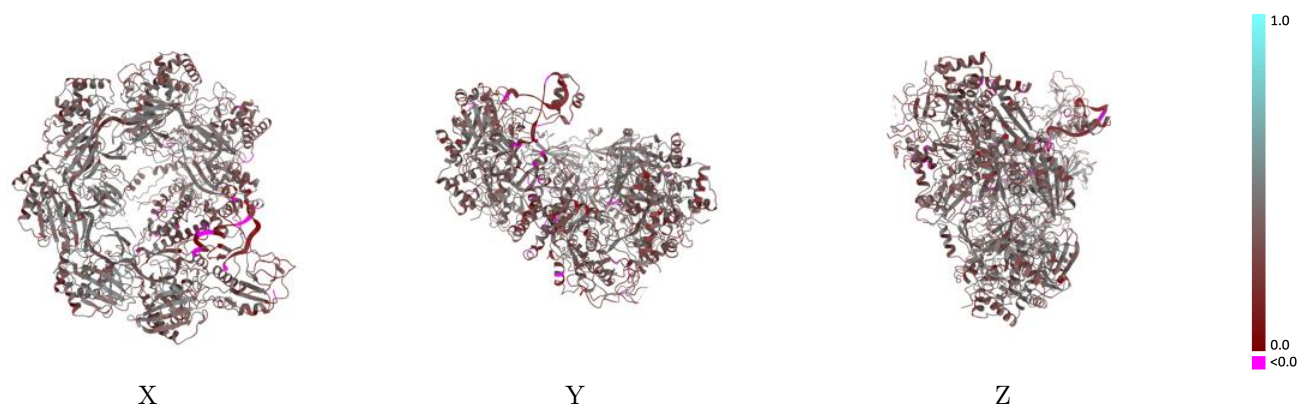
Y



Z

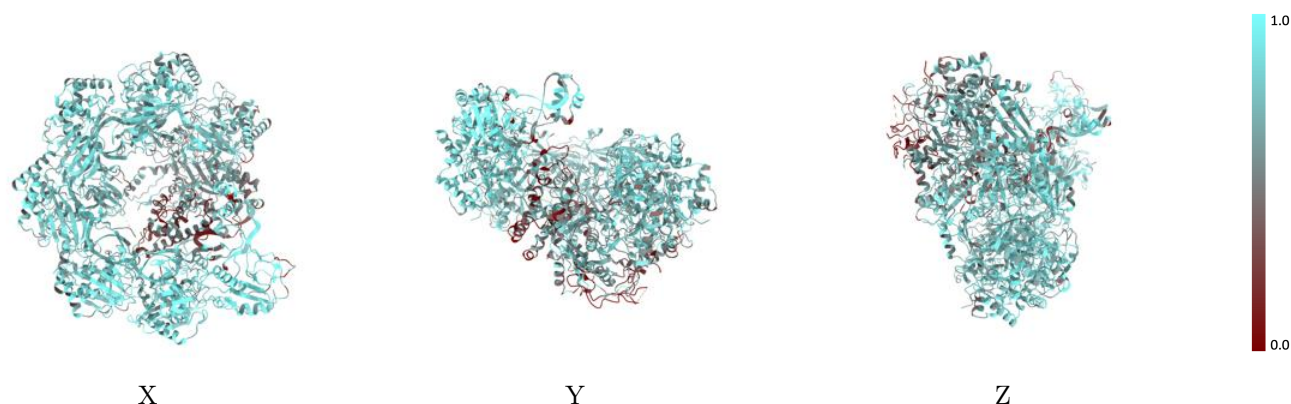
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



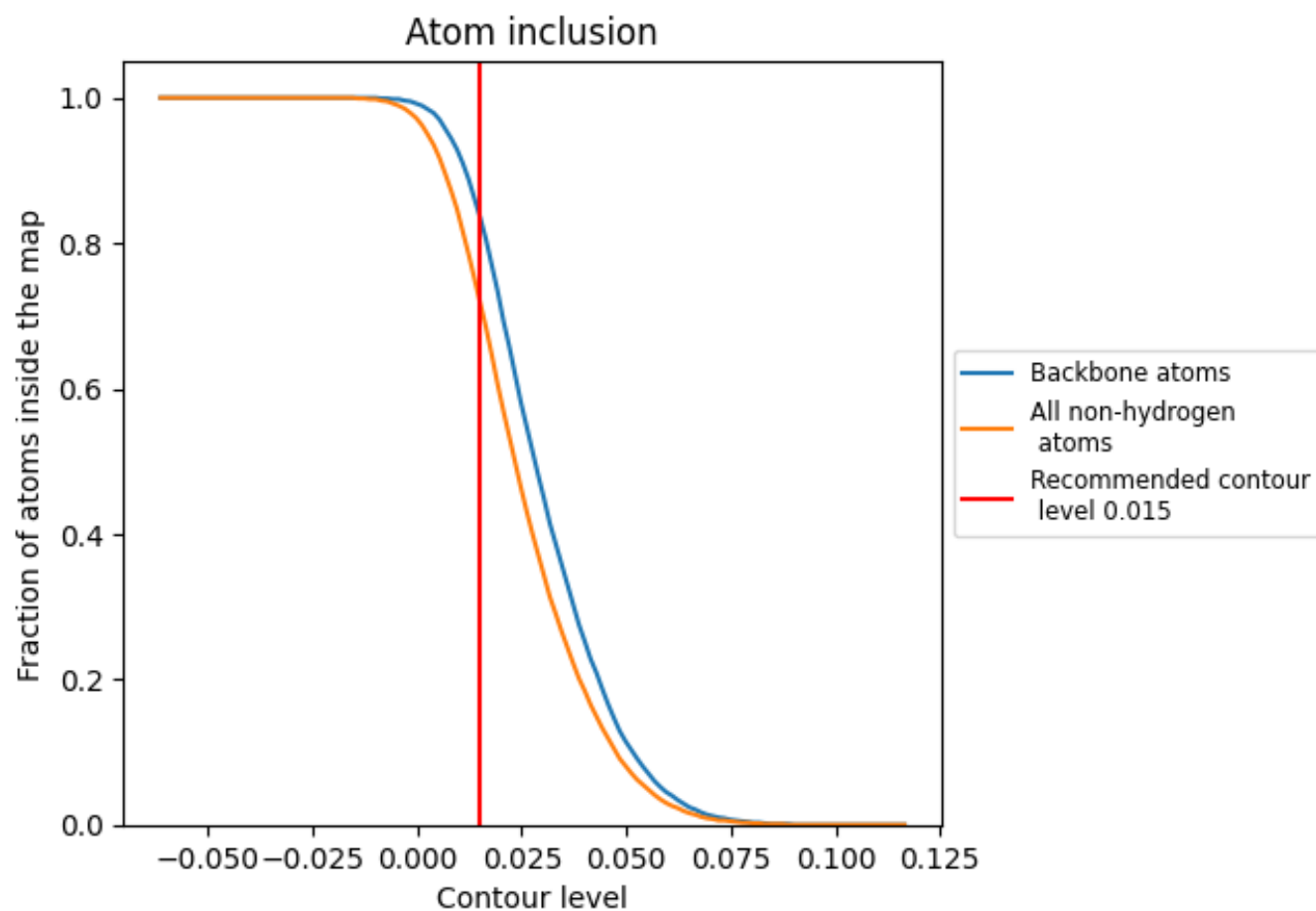
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 72% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7190	0.3600
A	0.4080	0.2980
B	0.6000	0.3440
C	0.8100	0.3750
D	0.7920	0.3840
E	0.7760	0.3900
F	0.7680	0.3890
G	0.7540	0.3730
H	0.7030	0.3570
I	0.7620	0.3990
J	0.7280	0.3980
L	0.7990	0.3090
M	0.7510	0.2720

