



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:40 AM UTC

PDB ID : 9G44 / pdb_00009g44
EMDB ID : EMD-51023
Title : Structure of the minimal type I-F2 CRISPR-Cas DNA-interference complex.
Authors : Mais, C.N.; Perry, T.N.; Sanchez-Londono, M.; Steinchen, W.; Innis, C.A.;
Randau, L.; Paush, P.; Bange, G.
Deposited on : 2024-07-13
Resolution : 3.20 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

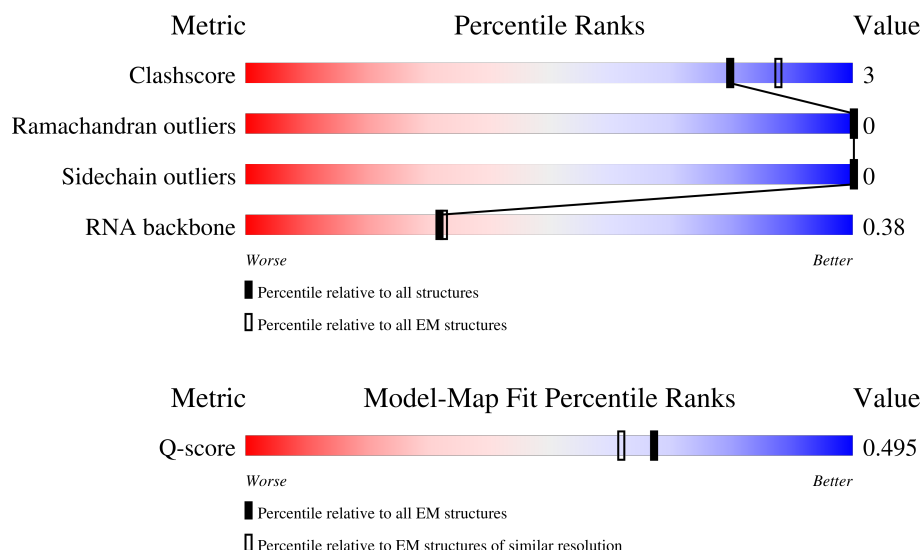
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



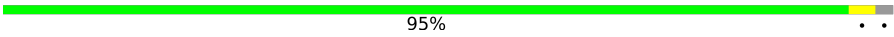

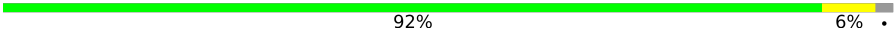
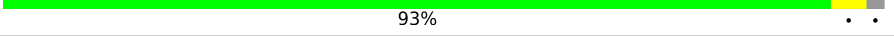

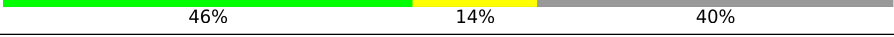


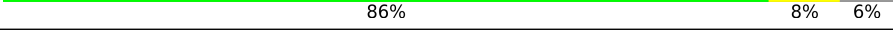
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	C	169	
2	D	322	
2	E	322	

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Mol	Chain	Length	Quality of chain
2	F	322	
2	G	322	
2	H	322	
2	I	322	
3	J	61	
4	K	57	
5	L	57	
6	B	336	
7	A	882	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 28051 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, Csy4 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	169	Total	C	N	O	S	0	0
			1345	866	233	242	4		

- Molecule 2 is a protein called CRISPR-associated protein Cas7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	315	Total	C	N	O	S	0	0
			2507	1584	429	486	8		
2	G	315	Total	C	N	O	S	0	0
			2507	1584	429	486	8		
2	H	315	Total	C	N	O	S	0	0
			2503	1582	429	484	8		
2	I	315	Total	C	N	O	S	0	0
			2501	1582	429	482	8		
2	D	281	Total	C	N	O	S	0	0
			2241	1422	384	427	8		
2	E	308	Total	C	N	O	S	0	0
			2455	1557	419	471	8		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	MET	-	initiating methionine	UNP A4Y6G1
F	-5	GLY	-	expression tag	UNP A4Y6G1
F	-4	HIS	-	expression tag	UNP A4Y6G1
F	-3	HIS	-	expression tag	UNP A4Y6G1
F	-2	HIS	-	expression tag	UNP A4Y6G1
F	-1	HIS	-	expression tag	UNP A4Y6G1
F	0	HIS	-	expression tag	UNP A4Y6G1
G	-6	MET	-	initiating methionine	UNP A4Y6G1
G	-5	GLY	-	expression tag	UNP A4Y6G1
G	-4	HIS	-	expression tag	UNP A4Y6G1
G	-3	HIS	-	expression tag	UNP A4Y6G1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	HIS	-	expression tag	UNP A4Y6G1
G	-1	HIS	-	expression tag	UNP A4Y6G1
G	0	HIS	-	expression tag	UNP A4Y6G1
H	-6	MET	-	initiating methionine	UNP A4Y6G1
H	-5	GLY	-	expression tag	UNP A4Y6G1
H	-4	HIS	-	expression tag	UNP A4Y6G1
H	-3	HIS	-	expression tag	UNP A4Y6G1
H	-2	HIS	-	expression tag	UNP A4Y6G1
H	-1	HIS	-	expression tag	UNP A4Y6G1
H	0	HIS	-	expression tag	UNP A4Y6G1
I	-6	MET	-	initiating methionine	UNP A4Y6G1
I	-5	GLY	-	expression tag	UNP A4Y6G1
I	-4	HIS	-	expression tag	UNP A4Y6G1
I	-3	HIS	-	expression tag	UNP A4Y6G1
I	-2	HIS	-	expression tag	UNP A4Y6G1
I	-1	HIS	-	expression tag	UNP A4Y6G1
I	0	HIS	-	expression tag	UNP A4Y6G1
D	-6	MET	-	initiating methionine	UNP A4Y6G1
D	-5	GLY	-	expression tag	UNP A4Y6G1
D	-4	HIS	-	expression tag	UNP A4Y6G1
D	-3	HIS	-	expression tag	UNP A4Y6G1
D	-2	HIS	-	expression tag	UNP A4Y6G1
D	-1	HIS	-	expression tag	UNP A4Y6G1
D	0	HIS	-	expression tag	UNP A4Y6G1
E	-6	MET	-	initiating methionine	UNP A4Y6G1
E	-5	GLY	-	expression tag	UNP A4Y6G1
E	-4	HIS	-	expression tag	UNP A4Y6G1
E	-3	HIS	-	expression tag	UNP A4Y6G1
E	-2	HIS	-	expression tag	UNP A4Y6G1
E	-1	HIS	-	expression tag	UNP A4Y6G1
E	0	HIS	-	expression tag	UNP A4Y6G1

- Molecule 3 is a RNA chain called RNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	60	Total	C	N	O	P	0	0
			1275	571	234	410	60		

- Molecule 4 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	34	Total	C	N	O	P	0	0
			686	332	109	211	34		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-12	DC	-	expression tag	GB 2321890520
K	-11	DC	-	expression tag	GB 2321890520
K	-10	DC	-	expression tag	GB 2321890520
K	-9	DA	-	expression tag	GB 2321890520
K	-8	DC	-	expression tag	GB 2321890520
K	-7	DG	-	expression tag	GB 2321890520
K	-6	DT	-	expression tag	GB 2321890520
K	-5	DG	-	expression tag	GB 2321890520
K	-4	DC	-	expression tag	GB 2321890520
K	-3	DC	-	expression tag	GB 2321890520
K	-2	DA	-	expression tag	GB 2321890520
K	-1	DC	-	expression tag	GB 2321890520
K	0	DC	-	expression tag	GB 2321890520
K	3	DC	DT	conflict	GB 2321890520
K	34	DC	-	expression tag	GB 2321890520
K	35	DC	-	expression tag	GB 2321890520
K	36	DC	-	expression tag	GB 2321890520
K	37	DC	-	expression tag	GB 2321890520
K	38	DT	-	expression tag	GB 2321890520
K	39	DC	-	expression tag	GB 2321890520
K	40	DC	-	expression tag	GB 2321890520
K	41	DT	-	expression tag	GB 2321890520
K	42	DC	-	expression tag	GB 2321890520
K	43	DG	-	expression tag	GB 2321890520
K	44	DC	-	expression tag	GB 2321890520

- Molecule 5 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	41	Total	C	N	O	P	0	0
			850	403	152	254	41		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-44	DG	-	expression tag	GB 1780508237
L	-43	DC	-	expression tag	GB 1780508237

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-42	DG	-	expression tag	GB 1780508237
L	-41	DA	-	expression tag	GB 1780508237
L	-40	DG	-	expression tag	GB 1780508237
L	-39	DG	-	expression tag	GB 1780508237
L	-38	DA	-	expression tag	GB 1780508237
L	-37	DG	-	expression tag	GB 1780508237
L	-36	DG	-	expression tag	GB 1780508237
L	-35	DG	-	expression tag	GB 1780508237
L	-34	DG	-	expression tag	GB 1780508237
L	-33	DA	-	expression tag	GB 1780508237
L	0	DG	-	expression tag	GB 1780508237
L	1	DG	-	expression tag	GB 1780508237
L	2	DT	-	expression tag	GB 1780508237
L	3	DG	-	expression tag	GB 1780508237
L	4	DG	-	expression tag	GB 1780508237
L	5	DC	-	expression tag	GB 1780508237
L	6	DA	-	expression tag	GB 1780508237
L	7	DC	-	expression tag	GB 1780508237
L	8	DG	-	expression tag	GB 1780508237
L	9	DT	-	expression tag	GB 1780508237
L	10	DG	-	expression tag	GB 1780508237
L	11	DG	-	expression tag	GB 1780508237
L	12	DG	-	expression tag	GB 1780508237

- Molecule 6 is a protein called Cas5fv helical domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	331	Total	C	N	O	S	0	0
			2614	1667	431	502	14		

- Molecule 7 is a protein called DEAD-like helicases-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	828	Total	C	N	O	S	0	0
			6565	4186	1114	1245	20		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	MET	-	initiating methionine	UNP A4Y6G0
A	99	GLY	-	expression tag	UNP A4Y6G0
A	100	HIS	-	expression tag	UNP A4Y6G0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	101	HIS	-	expression tag	UNP A4Y6G0
A	102	HIS	-	expression tag	UNP A4Y6G0
A	103	HIS	-	expression tag	UNP A4Y6G0
A	104	HIS	-	expression tag	UNP A4Y6G0
A	105	HIS	-	expression tag	UNP A4Y6G0
A	163	GLN	ASP	conflict	UNP A4Y6G0

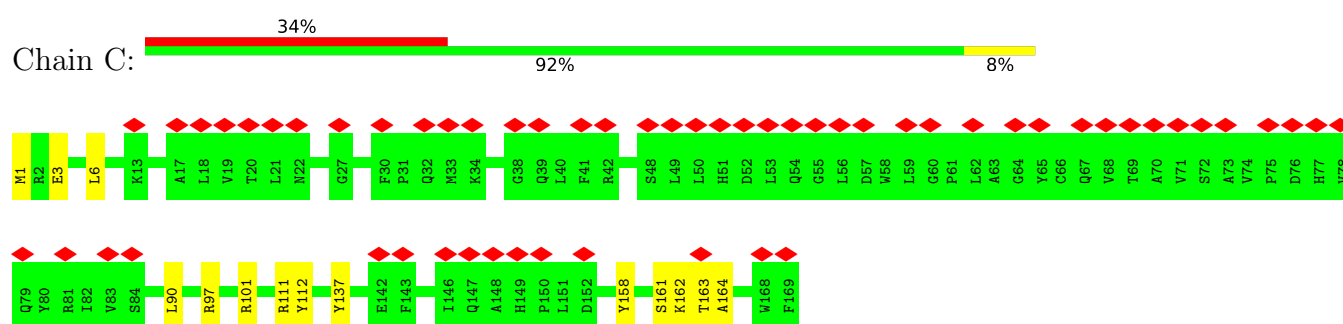
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	Mg	0
			2	2	

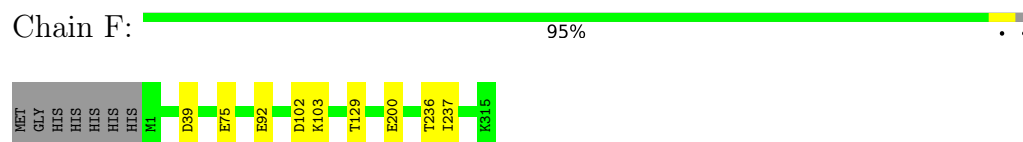
3 Residue-property plots

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.

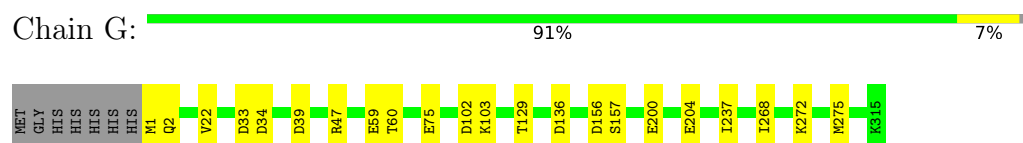
- Molecule 1: CRISPR-associated protein, Csy4 family



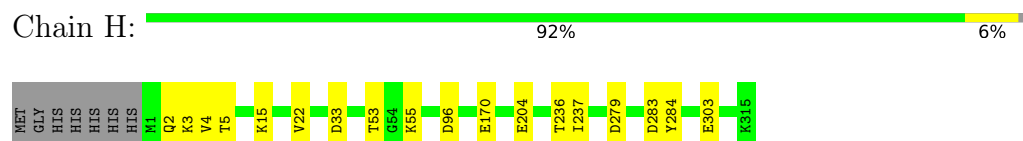
- Molecule 2: CRISPR-associated protein Cas7



- Molecule 2: CRISPR-associated protein Cas7



- Molecule 2: CRISPR-associated protein Cas7

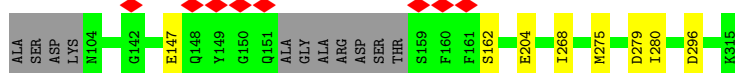
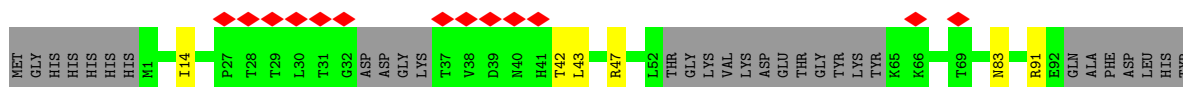
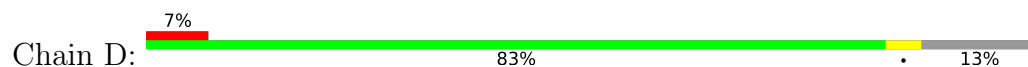


- Molecule 2: CRISPR-associated protein Cas7

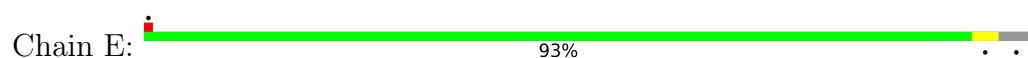




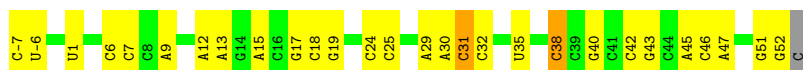
- Molecule 2: CRISPR-associated protein Cas7



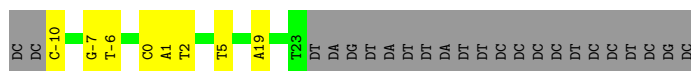
- Molecule 2: CRISPR-associated protein Cas7



- Molecule 3: RNA (61-MER)



- Molecule 4: DNA (39-MER)



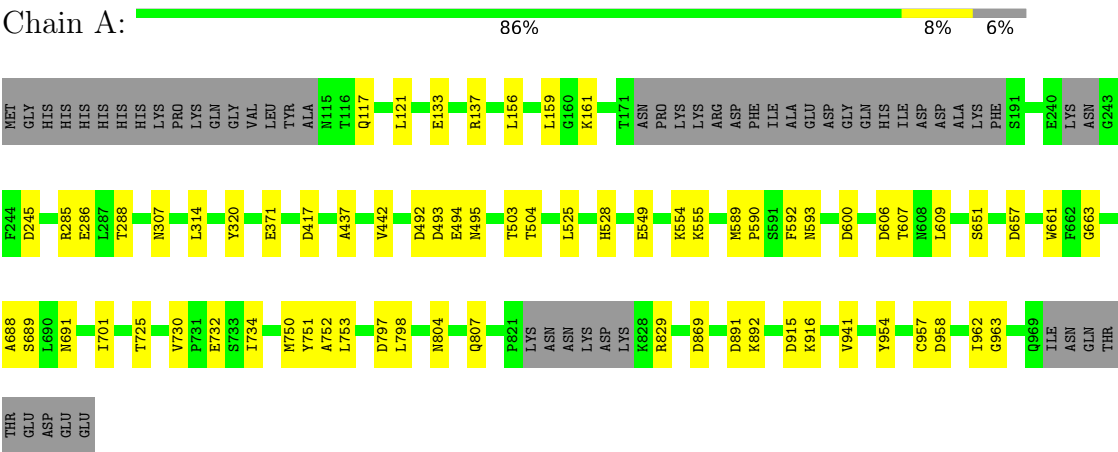
- Molecule 5: DNA (41-MER)



- Molecule 6: Cas5fv helical domain-containing protein



● Molecule 7: DEAD-like helicases-like protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	250975	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.773	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	279.0, 279.0, 279.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	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: 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	C	0.10	0/1377	0.34	0/1852
2	D	0.15	0/2280	0.29	0/3071
2	E	0.19	0/2502	0.33	0/3373
2	F	0.20	0/2555	0.32	0/3446
2	G	0.21	0/2555	0.34	0/3446
2	H	0.21	0/2551	0.34	0/3441
2	I	0.20	0/2549	0.34	0/3438
3	J	0.21	0/1425	0.39	0/2217
4	K	0.23	0/764	0.49	0/1175
5	L	0.27	0/952	0.51	0/1471
6	B	0.16	0/2657	0.33	0/3572
7	A	0.15	0/6703	0.33	0/9087
All	All	0.18	0/28870	0.35	0/39589

There are no bond length outliers.

There are no bond angle outliers.

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	C	1345	0	1358	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2241	0	2220	11	0
2	E	2455	0	2421	8	0
2	F	2507	0	2468	7	0
2	G	2507	0	2468	18	0
2	H	2503	0	2464	12	0
2	I	2501	0	2464	9	0
3	J	1275	0	653	14	0
4	K	686	0	390	6	0
5	L	850	0	465	7	0
6	B	2614	0	2645	20	0
7	A	6565	0	6503	43	0
8	A	2	0	0	0	0
All	All	28051	0	26519	149	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.

All (149) 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)
2:I:93:GLN:OE1	2:I:113:THR:OG1	1.98	0.82
2:G:59:GLU:N	2:G:59:GLU:OE2	2.16	0.78
2:G:75:GLU:N	2:G:75:GLU:OE2	2.18	0.77
7:A:417:ASP:OD2	7:A:555:LYS:NZ	2.18	0.76
2:F:75:GLU:N	2:F:75:GLU:OE2	2.17	0.75
7:A:320:TYR:OH	7:A:549:GLU:OE2	2.05	0.74
2:G:200:GLU:OE1	2:G:200:GLU:N	2.19	0.73
2:G:2:GLN:N	2:G:2:GLN:OE1	2.26	0.69
2:I:127:LYS:NZ	3:J:-7:C:OP2	2.24	0.68
2:H:303:GLU:N	2:H:303:GLU:OE1	2.28	0.67
2:E:200:GLU:N	2:E:200:GLU:OE1	2.28	0.66
2:F:39:ASP:O	2:F:39:ASP:OD1	2.13	0.65
7:A:117:GLN:N	7:A:117:GLN:OE1	2.31	0.63
7:A:797:ASP:OD1	7:A:798:LEU:N	2.32	0.63
2:I:72:ASN:ND2	2:I:75:GLU:OE1	2.32	0.63
1:C:162:LYS:O	1:C:163:THR:OG1	2.12	0.62
2:D:47:ARG:NH1	2:E:145:ASN:OD1	2.33	0.61
3:J:43:G:O2'	3:J:47:A:N6	2.34	0.61
6:B:112:ASP:OD1	6:B:113:GLN:N	2.32	0.61
2:F:129:THR:HG22	3:J:15:A:H4'	1.82	0.60
2:G:39:ASP:OD2	2:G:39:ASP:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:315:LYS:HE2	2:E:315:LYS:HA	1.83	0.60
2:G:272:LYS:NZ	3:J:17:G:OP2	2.29	0.59
2:I:296:ASP:OD2	2:I:296:ASP:O	2.20	0.59
6:B:302:ASP:OD1	6:B:303:ARG:N	2.36	0.58
7:A:688:ALA:O	7:A:689:SER:OG	2.21	0.58
6:B:210:THR:O	6:B:212:ILE:N	2.37	0.58
2:D:14:ILE:HG22	2:D:280:ILE:HG22	1.85	0.58
2:F:92:GLU:OE1	2:F:92:GLU:N	2.37	0.57
7:A:657:ASP:OD2	7:A:954:TYR:OH	2.23	0.57
2:G:156:ASP:OD1	2:G:157:SER:N	2.38	0.56
2:E:39:ASP:OD1	2:E:39:ASP:O	2.21	0.56
1:C:158:TYR:OH	3:J:52:G:OP2	2.19	0.56
2:I:1:MET:SD	2:I:2:GLN:N	2.79	0.56
7:A:957:CYS:SG	7:A:958:ASP:N	2.79	0.56
3:J:35:U:O2'	2:D:91:ARG:NH1	2.36	0.56
2:F:102:ASP:OD2	2:F:103:LYS:N	2.38	0.55
7:A:915:ASP:OD1	7:A:916:LYS:N	2.39	0.55
7:A:494:GLU:OE1	7:A:495:ASN:N	2.36	0.55
2:I:156:ASP:OD1	2:I:157:SER:N	2.36	0.55
2:H:204:GLU:OE1	2:H:204:GLU:N	2.36	0.55
6:B:150:ILE:O	6:B:225:ARG:NH2	2.40	0.55
5:L:-9:DT:H2'	5:L:-8:DG:C8	2.41	0.55
7:A:751:TYR:OH	7:A:804:ASN:OD1	2.18	0.55
1:C:97:ARG:NH1	3:J:42:C:OP2	2.37	0.54
1:C:3:GLU:N	1:C:3:GLU:OE1	2.40	0.54
2:D:268:ILE:HG22	2:D:275:MET:HE3	1.87	0.54
2:I:261:GLU:C	2:I:261:GLU:OE2	2.51	0.54
2:H:33:ASP:OD2	2:H:33:ASP:C	2.49	0.54
7:A:732:GLU:N	7:A:732:GLU:OE1	2.41	0.54
2:D:296:ASP:N	2:D:296:ASP:OD1	2.41	0.53
7:A:121:LEU:HD21	7:A:161:LYS:HB2	1.91	0.53
2:H:283:ASP:OD1	2:H:284:TYR:N	2.42	0.53
3:J:31:C:OP1	2:D:83:ASN:ND2	2.42	0.53
1:C:1:MET:HE3	1:C:6:LEU:HD23	1.92	0.52
7:A:437:ALA:HB1	7:A:442:VAL:HG11	1.92	0.52
1:C:101:ARG:NE	3:J:45:A:OP1	2.39	0.52
2:G:34:ASP:C	2:G:34:ASP:OD1	2.52	0.52
7:A:307:ASN:O	7:A:307:ASN:ND2	2.43	0.52
7:A:829:ARG:NH2	7:A:869:ASP:O	2.43	0.51
7:A:371:GLU:N	7:A:371:GLU:OE1	2.44	0.51
6:B:151:ILE:C	6:B:151:ILE:HD12	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:279:ASP:OD2	2:H:279:ASP:C	2.54	0.50
2:F:200:GLU:N	2:F:200:GLU:OE1	2.44	0.50
3:J:35:U:O2	2:D:91:ARG:NH1	2.45	0.50
7:A:288:THR:HG22	7:A:288:THR:O	2.11	0.50
6:B:210:THR:O	6:B:211:PRO:C	2.55	0.50
2:D:204:GLU:OE1	2:D:204:GLU:N	2.45	0.49
7:A:701:ILE:HG21	7:A:734:ILE:CD1	2.43	0.49
2:G:1:MET:SD	2:G:1:MET:C	2.96	0.48
6:B:8:ASP:OD1	6:B:8:ASP:C	2.55	0.48
7:A:661:TRP:O	7:A:663:GLY:N	2.46	0.48
2:G:268:ILE:HD12	2:G:275:MET:HE3	1.95	0.48
7:A:525:LEU:O	7:A:554:LYS:NZ	2.45	0.48
2:G:102:ASP:OD1	2:G:103:LYS:N	2.48	0.47
2:G:129:THR:HG22	3:J:9:A:H4'	1.96	0.47
1:C:111:ARG:CZ	1:C:111:ARG:HA	2.44	0.47
7:A:606:ASP:O	7:A:607:THR:OG1	2.27	0.47
6:B:189:VAL:HA	6:B:192:VAL:HG12	1.96	0.47
1:C:90:LEU:HD22	1:C:112:TYR:CE1	2.49	0.47
2:H:15:LYS:NZ	2:H:170:GLU:OE2	2.44	0.47
6:B:183:SER:OG	6:B:185:ASP:OD1	2.23	0.47
7:A:156:LEU:HD13	7:A:159:LEU:HD22	1.97	0.47
7:A:701:ILE:HG21	7:A:734:ILE:HD11	1.96	0.47
2:D:279:ASP:OD1	2:D:280:ILE:N	2.48	0.47
4:K:2:DT:O2	4:K:2:DT:O4'	2.34	0.46
6:B:318:VAL:HG12	6:B:319:SER:N	2.30	0.46
3:J:40:G:C6	3:J:51:G:O6	2.69	0.46
5:L:-5:DC:H4'	5:L:-4:DG:OP1	2.15	0.46
1:C:137:TYR:HB3	3:J:38:C:O2	2.16	0.46
2:G:204:GLU:N	2:G:204:GLU:OE1	2.46	0.46
7:A:941:VAL:HG22	7:A:941:VAL:O	2.16	0.46
1:C:161:SER:OG	1:C:164:ALA:O	2.22	0.45
7:A:133:GLU:OE2	7:A:137:ARG:NH2	2.47	0.45
2:E:102:ASP:OD1	2:E:103:LYS:N	2.49	0.45
2:H:236:THR:HG22	2:H:237:ILE:N	2.32	0.45
6:B:304:ASP:OD1	6:B:305:LYS:N	2.49	0.45
2:G:60:THR:O	2:G:60:THR:HG22	2.17	0.45
2:H:4:VAL:HG22	2:H:5:THR:H	1.82	0.45
2:H:22:VAL:HG12	2:H:22:VAL:O	2.16	0.45
2:G:47:ARG:NH2	2:G:136:ASP:OD2	2.46	0.45
2:G:33:ASP:O	2:G:34:ASP:CG	2.61	0.44
7:A:730:VAL:HG13	7:A:734:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:891:ASP:OD1	7:A:892:LYS:N	2.48	0.44
7:A:691:ASN:O	7:A:691:ASN:ND2	2.50	0.44
5:L:-28:DA:N7	5:L:-27:DT:H73	2.33	0.44
2:F:236:THR:HG22	2:F:237:ILE:N	2.32	0.44
6:B:196:TYR:CD1	6:B:196:TYR:N	2.85	0.44
5:L:5:DC:H2''	5:L:6:DA:C8	2.53	0.44
6:B:100:GLU:C	6:B:287:MET:HE3	2.43	0.44
7:A:962:ILE:HG22	7:A:963:GLY:N	2.32	0.44
7:A:492:ASP:OD1	7:A:492:ASP:N	2.50	0.43
7:A:807:GLN:O	7:A:807:GLN:OE1	2.35	0.43
6:B:210:THR:N	6:B:211:PRO:CD	2.81	0.43
4:K:19:DA:H5'	7:A:651:SER:HB3	2.00	0.43
2:G:237:ILE:HG12	2:H:96:ASP:OD2	2.18	0.43
2:H:53:THR:HG23	2:H:55:LYS:H	1.84	0.43
6:B:64:ASP:OD1	6:B:65:GLN:N	2.51	0.43
7:A:600:ASP:OD2	7:A:725:THR:OG1	2.26	0.43
5:L:-10:DC:C6	5:L:-9:DT:H72	2.53	0.43
2:D:147:GLU:O	2:D:162:SER:OG	2.23	0.43
2:I:60:THR:HG23	2:I:62:TYR:H	1.83	0.43
4:K:0:DC:C2	4:K:1:DA:C2	3.07	0.43
3:J:29:A:O2'	2:E:150:GLY:O	2.36	0.43
6:B:8:ASP:OD1	6:B:9:SER:N	2.52	0.42
6:B:190:LEU:C	6:B:190:LEU:HD23	2.45	0.42
5:L:-9:DT:H2''	5:L:-8:DG:O5'	2.19	0.42
7:A:245:ASP:O	7:A:314:LEU:HD11	2.20	0.42
6:B:209:ILE:C	6:B:211:PRO:CD	2.93	0.42
4:K:5:DT:O2	4:K:5:DT:H2'	2.19	0.42
7:A:503:THR:HG22	7:A:504:THR:O	2.20	0.42
7:A:442:VAL:HG12	7:A:528:HIS:CD2	2.55	0.42
7:A:493:ASP:OD1	7:A:494:GLU:N	2.53	0.42
7:A:592:PHE:O	7:A:593:ASN:OD1	2.37	0.42
6:B:261:THR:HG23	6:B:261:THR:O	2.20	0.41
4:K:-10:DC:P	5:L:10:DG:H22	2.42	0.41
7:A:285:ARG:O	7:A:286:GLU:HB2	2.20	0.41
7:A:609:LEU:C	7:A:609:LEU:HD12	2.46	0.41
2:I:297:GLU:OE1	2:I:297:GLU:C	2.63	0.41
2:E:33:ASP:OD2	2:E:33:ASP:C	2.64	0.41
2:E:47:ARG:NH2	2:E:136:ASP:OD2	2.50	0.41
2:H:2:GLN:O	2:H:3:LYS:HB2	2.21	0.41
7:A:589:MET:HE3	7:A:590:PRO:O	2.20	0.41
7:A:750:MET:HA	7:A:750:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:62:ILE:O	6:B:62:ILE:HG22	2.21	0.40
2:D:42:THR:C	2:D:43:LEU:HD22	2.47	0.40
7:A:752:ALA:O	7:A:753:LEU:HB3	2.22	0.40
2:G:22:VAL:O	2:G:22:VAL:HG12	2.21	0.40
4:K:-7:DG:H2'	4:K:-6:DT:H72	2.02	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	C	167/169 (99%)	163 (98%)	4 (2%)	0	100	100
2	D	271/322 (84%)	271 (100%)	0	0	100	100
2	E	304/322 (94%)	298 (98%)	6 (2%)	0	100	100
2	F	313/322 (97%)	304 (97%)	9 (3%)	0	100	100
2	G	313/322 (97%)	302 (96%)	11 (4%)	0	100	100
2	H	313/322 (97%)	309 (99%)	4 (1%)	0	100	100
2	I	313/322 (97%)	310 (99%)	3 (1%)	0	100	100
6	B	327/336 (97%)	312 (95%)	15 (5%)	0	100	100
7	A	820/882 (93%)	785 (96%)	35 (4%)	0	100	100
All	All	3141/3319 (95%)	3054 (97%)	87 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	C	146/146 (100%)	146 (100%)	0	100	100
2	D	245/278 (88%)	245 (100%)	0	100	100
2	E	266/278 (96%)	266 (100%)	0	100	100
2	F	272/278 (98%)	272 (100%)	0	100	100
2	G	272/278 (98%)	272 (100%)	0	100	100
2	H	271/278 (98%)	271 (100%)	0	100	100
2	I	270/278 (97%)	270 (100%)	0	100	100
6	B	291/296 (98%)	291 (100%)	0	100	100
7	A	719/771 (93%)	719 (100%)	0	100	100
All	All	2752/2881 (96%)	2752 (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. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	82	GLN
2	F	98	HIS
2	F	140	GLN
2	F	288	HIS
2	F	305	HIS
2	G	140	GLN
2	G	305	HIS
2	H	23	ASN
2	H	82	GLN
2	H	98	HIS
2	H	215	GLN
2	H	305	HIS
2	I	288	HIS
2	I	302	ASN
6	B	13	ASN
6	B	20	ASN
6	B	49	ASN
6	B	175	ASN
7	A	233	HIS
7	A	897	HIS
7	A	960	GLN

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Mol	Chain	Res	Type
2	E	23	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	J	59/61 (96%)	15 (25%)	0

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	J	-6	U
3	J	1	U
3	J	6	C
3	J	7	C
3	J	12	A
3	J	13	A
3	J	18	C
3	J	19	G
3	J	24	C
3	J	25	C
3	J	30	A
3	J	31	C
3	J	32	C
3	J	38	C
3	J	46	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

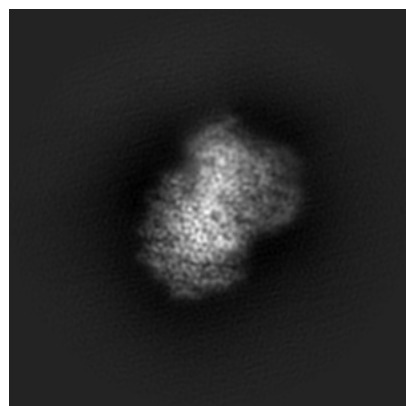
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51023. These allow visual inspection of the internal detail of the map and identification of artifacts.

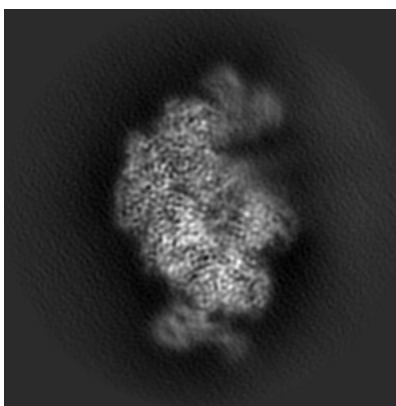
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

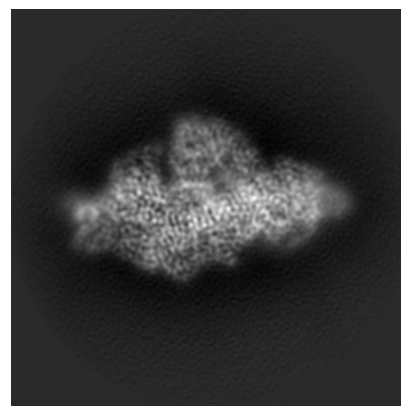
6.1.1 Primary map



X

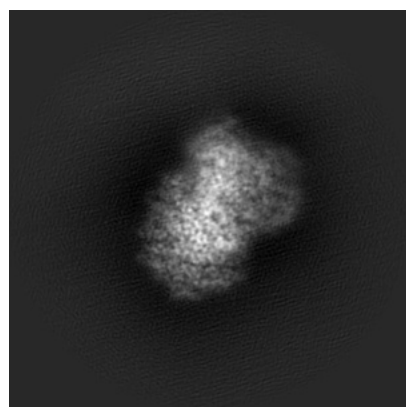


Y

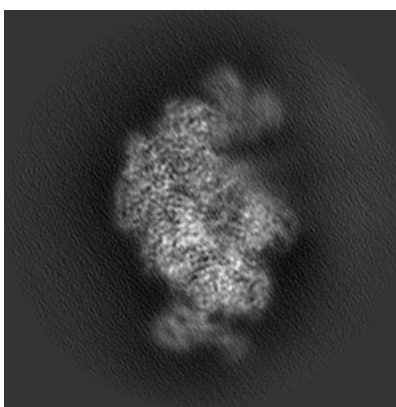


Z

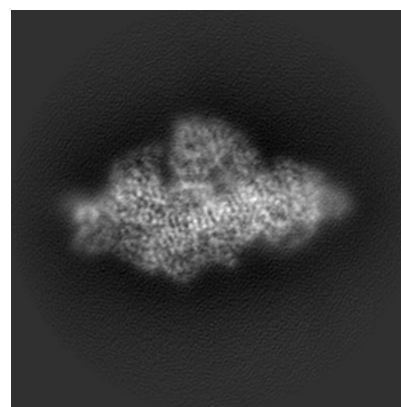
6.1.2 Raw map



X



Y

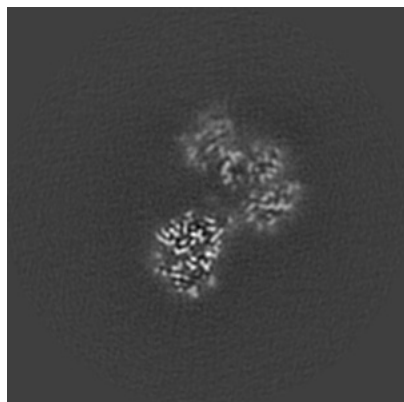


Z

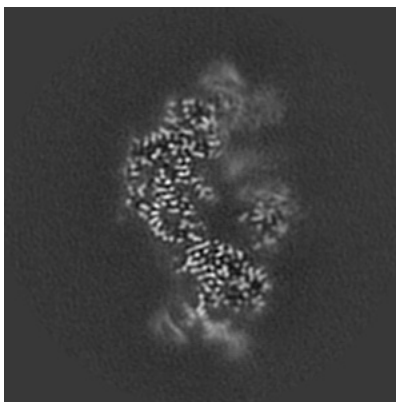
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

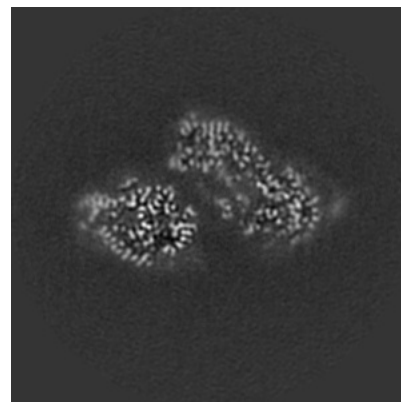
6.2.1 Primary map



X Index: 150

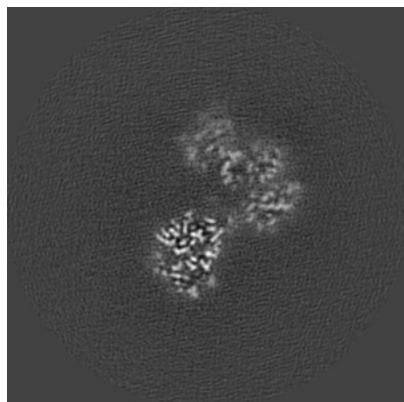


Y Index: 150

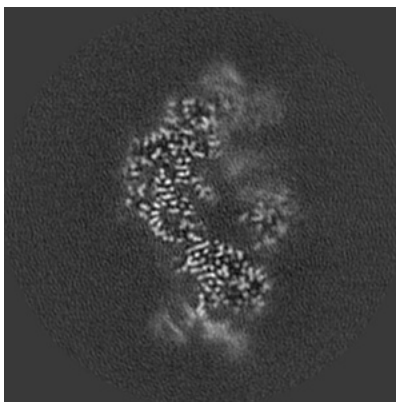


Z Index: 150

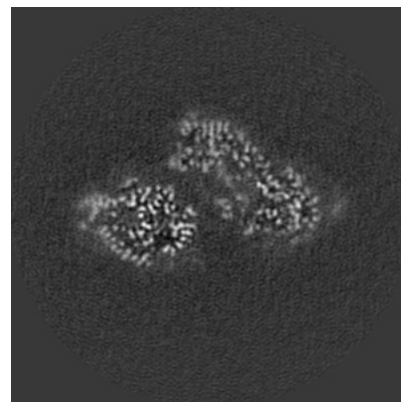
6.2.2 Raw map



X Index: 150



Y Index: 150

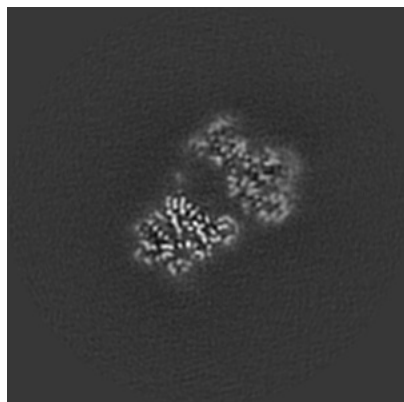


Z Index: 150

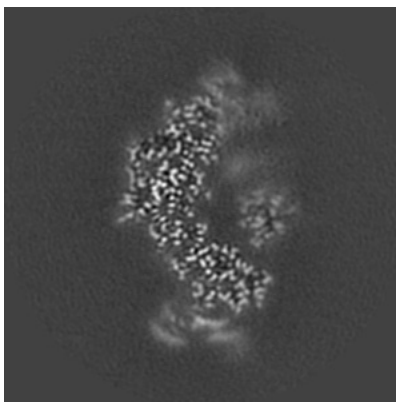
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

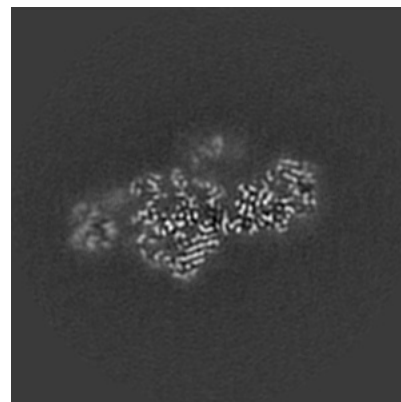
6.3.1 Primary map



X Index: 128

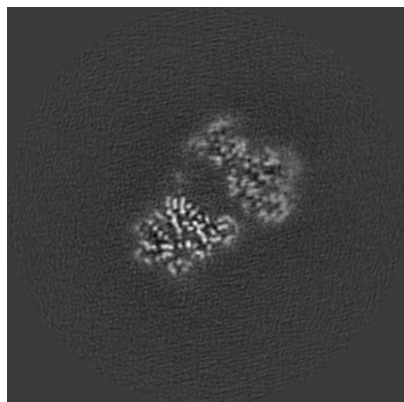


Y Index: 146

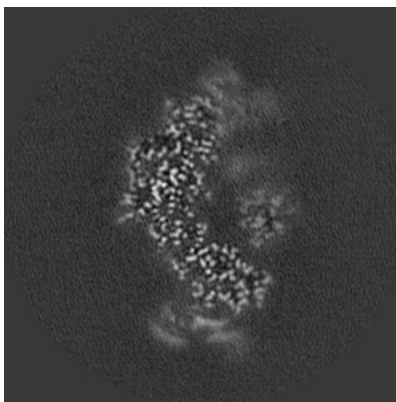


Z Index: 133

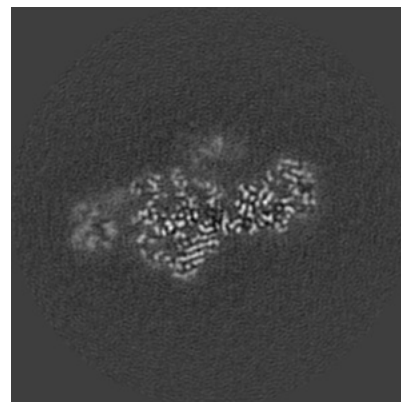
6.3.2 Raw map



X Index: 128



Y Index: 146

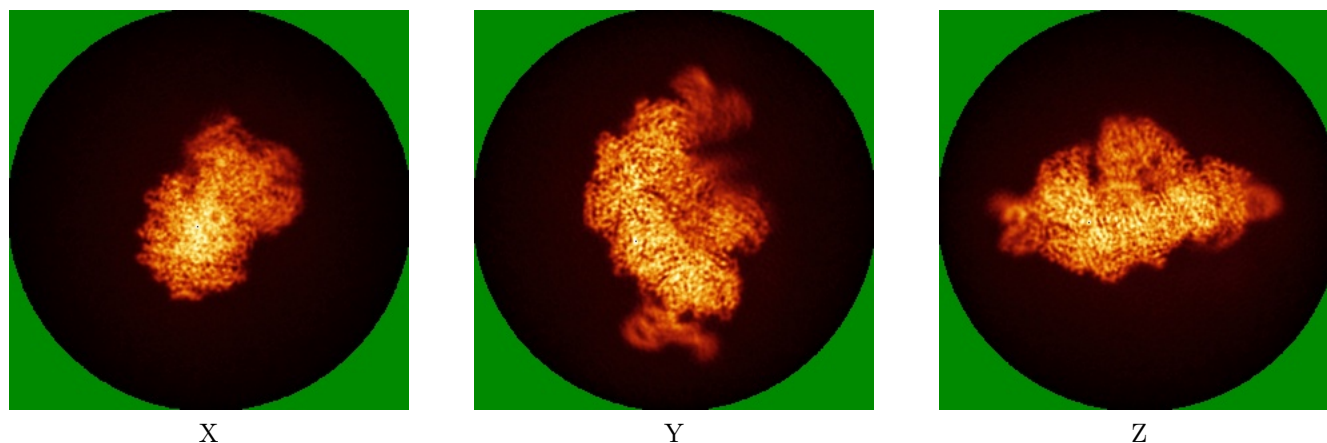


Z Index: 133

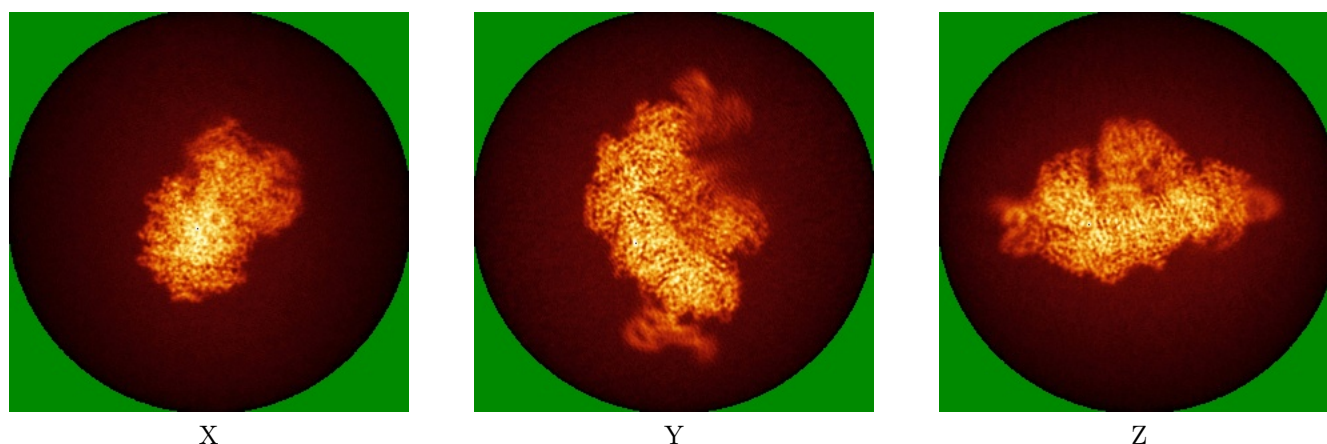
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

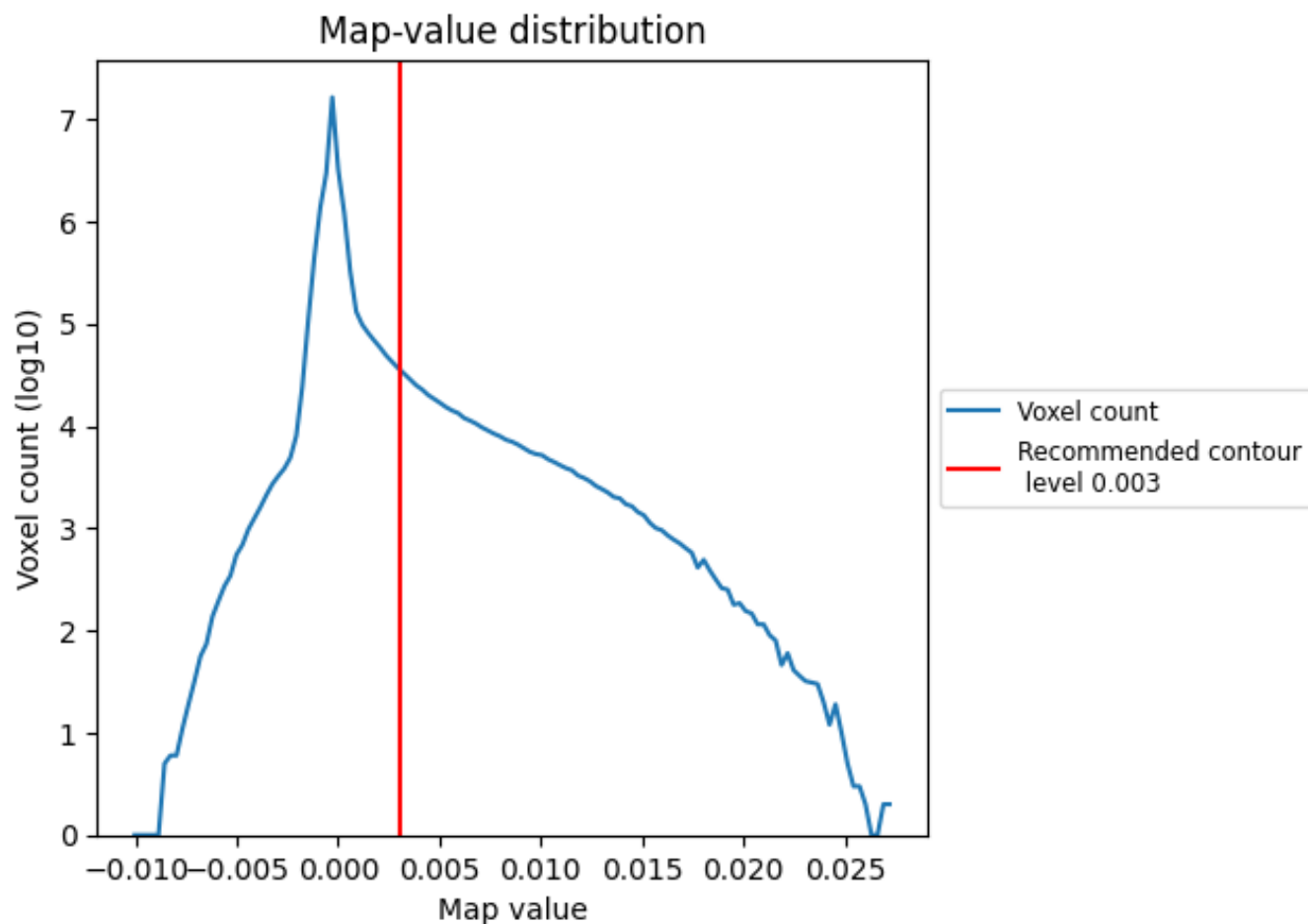
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

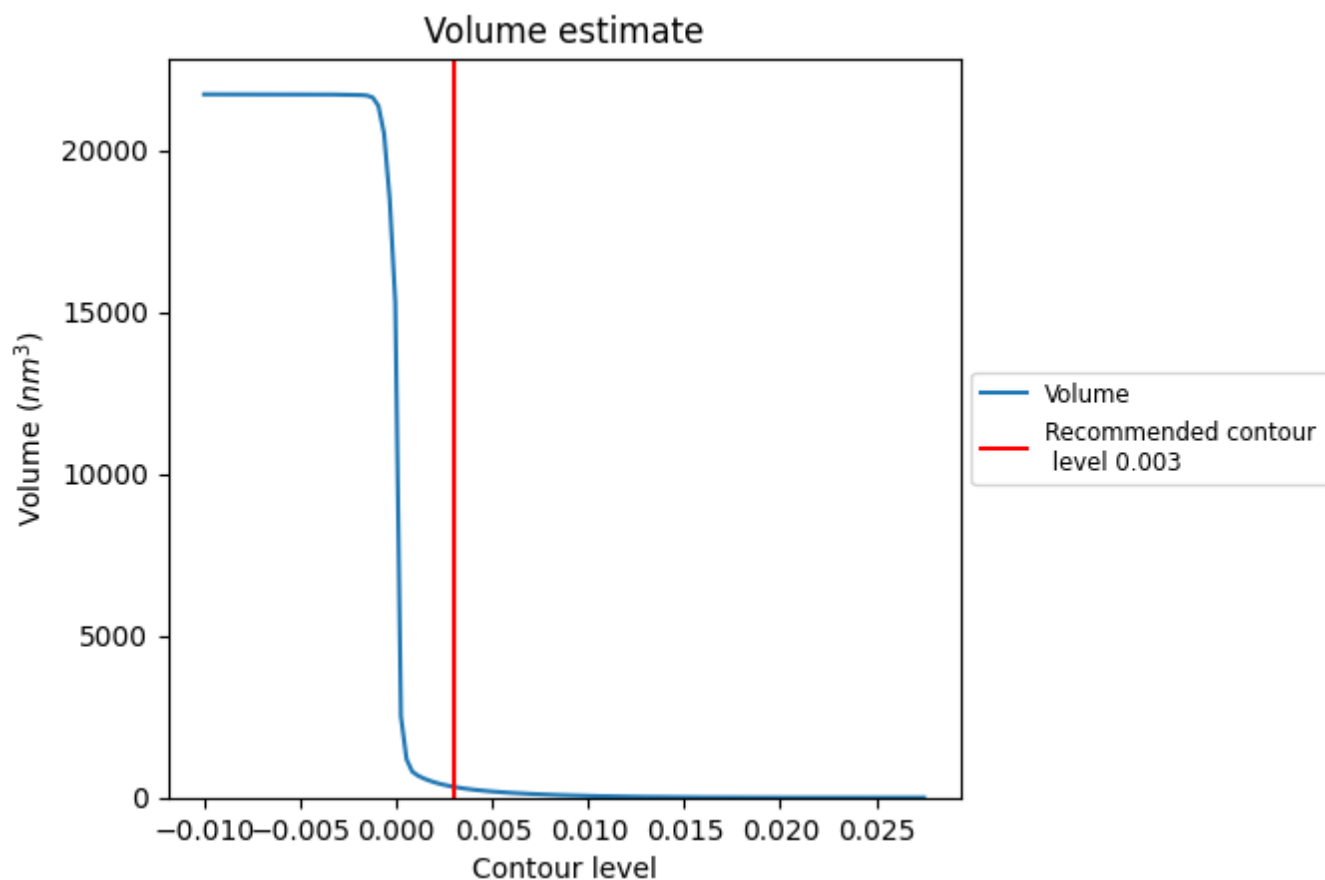
This section contains the results of statistical analysis of the map.

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.

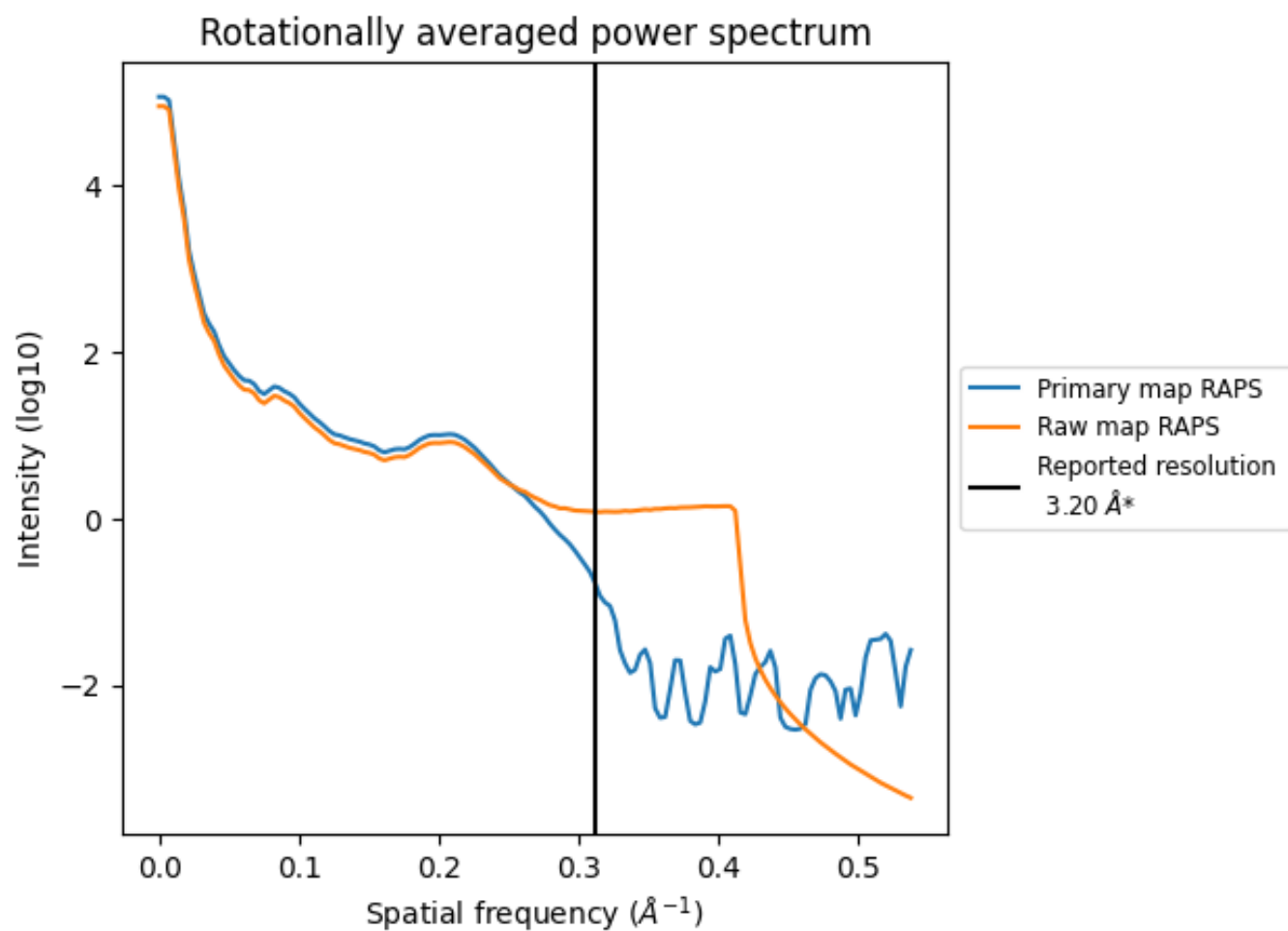
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 329 nm³; this corresponds to an approximate mass of 297 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 ⓘ

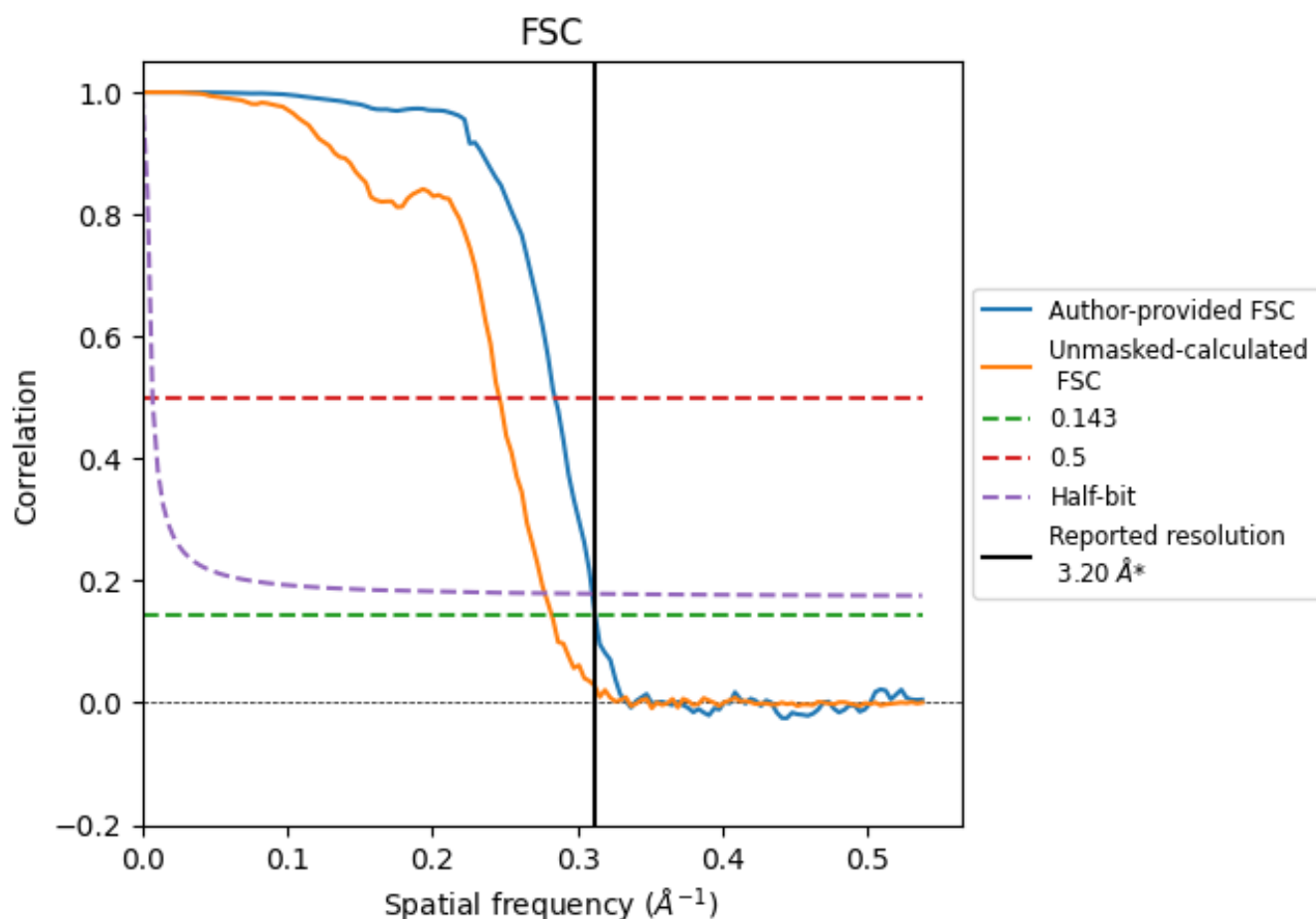


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.51	3.22
Unmasked-calculated*	3.54	4.06	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.54 differs from the reported value 3.2 by more than 10 %

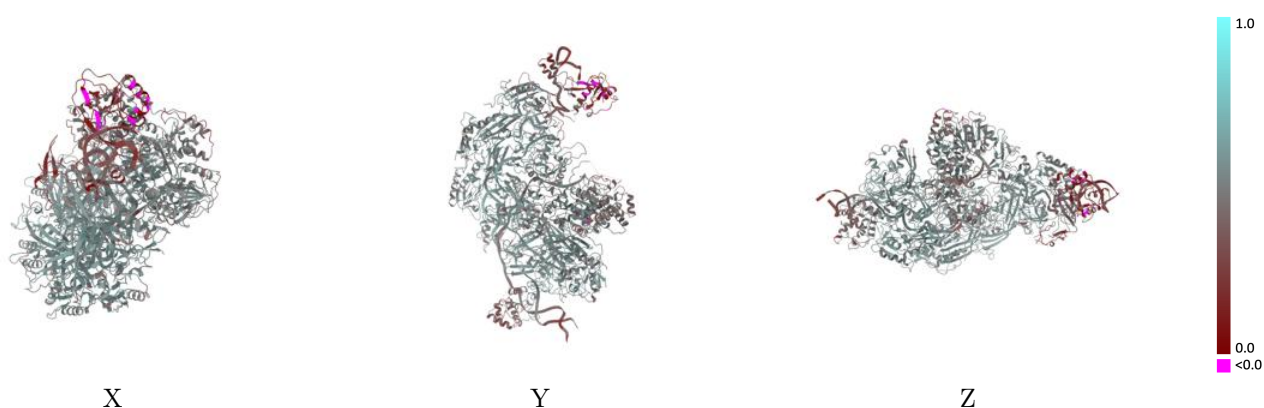
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-51023 and PDB model 9G44. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

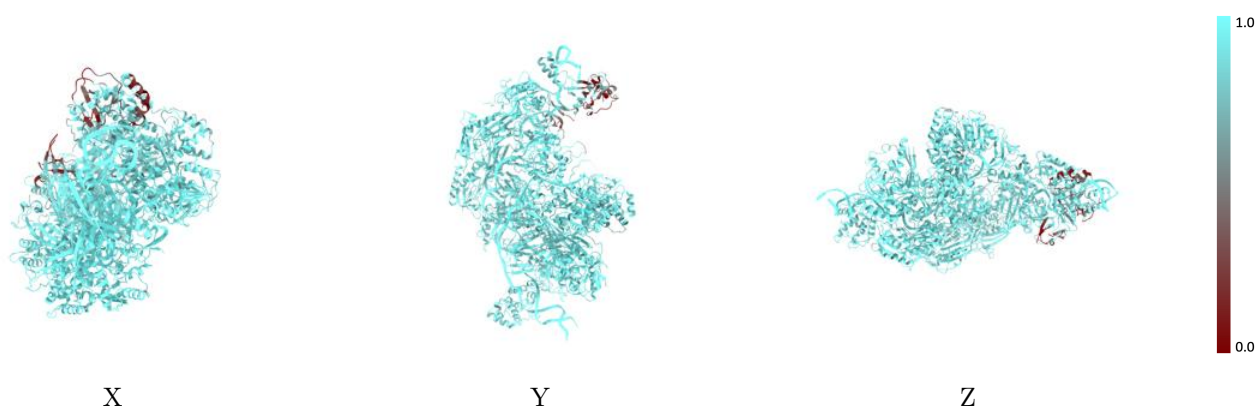
This section was not generated.

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



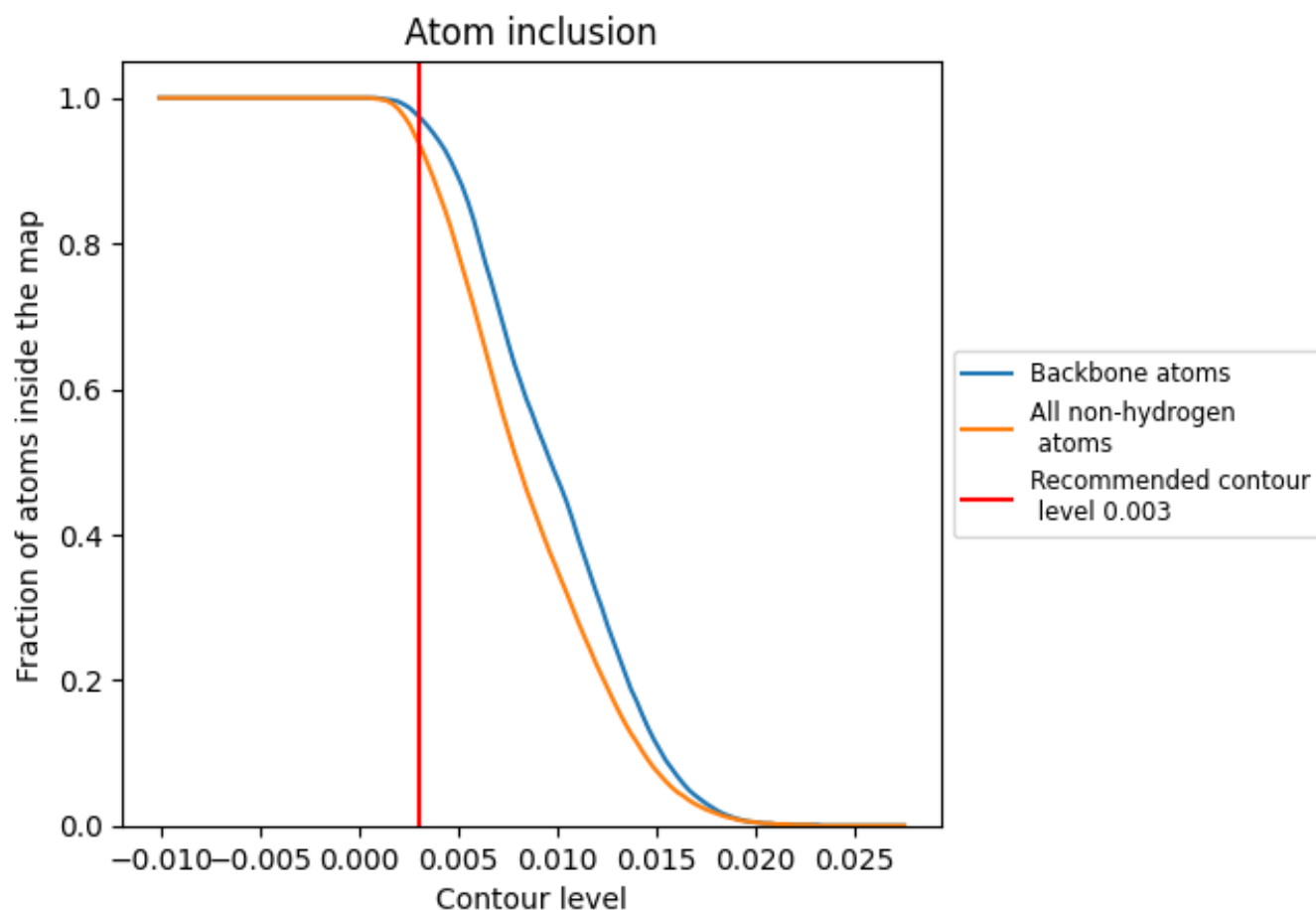
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9390	<div></div> 0.4950
A	<div></div> 0.9330	<div></div> 0.4800
B	<div></div> 0.9510	<div></div> 0.4740
C	<div></div> 0.6120	<div></div> 0.2160
D	<div></div> 0.8860	<div></div> 0.4770
E	<div></div> 0.9660	<div></div> 0.5320
F	<div></div> 0.9730	<div></div> 0.5430
G	<div></div> 0.9770	<div></div> 0.5480
H	<div></div> 0.9700	<div></div> 0.5520
I	<div></div> 0.9740	<div></div> 0.5450
J	<div></div> 0.9870	<div></div> 0.4690
K	<div></div> 0.9870	<div></div> 0.4270
L	<div></div> 0.9990	<div></div> 0.5220

