



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 01:52 AM UTC

PDB ID : 9NUF / pdb_00009nuf
EMDB ID : EMD-49803
Title : Cryo-EM structure of the Nipah Virus nucleocapsid complex
Authors : Liu, B.; Yang, G.
Deposited on : 2025-03-19
Resolution : 2.96 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:

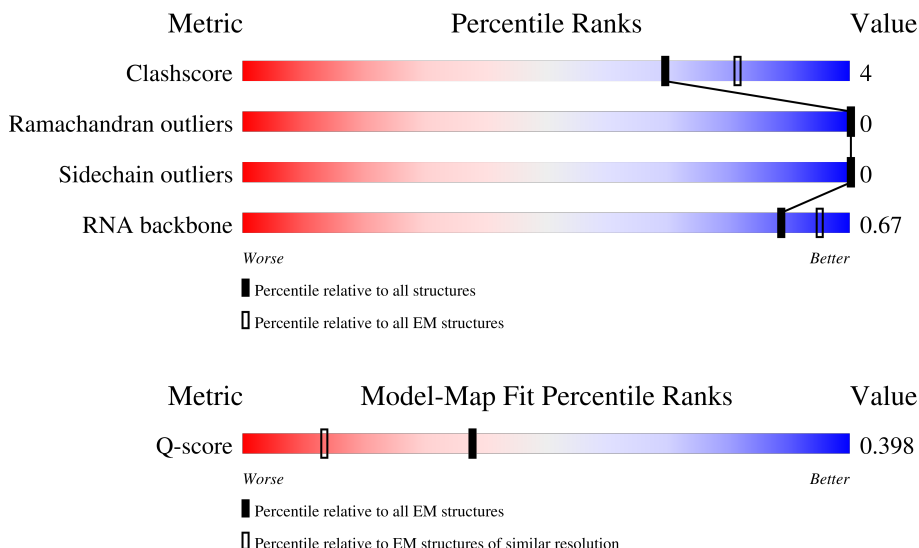
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.96 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.




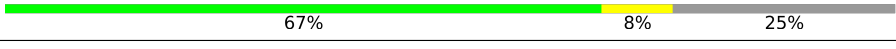
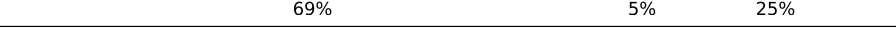
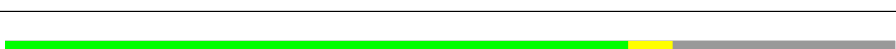



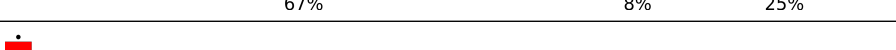




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	D	532	
1	E	532	
1	F	532	

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Mol	Chain	Length	Quality of chain
1	G	532	
1	H	532	
1	I	532	
1	J	532	
1	K	532	
1	L	532	
1	M	532	
1	N	532	
1	O	532	
1	P	532	
1	Q	532	
2	Z	84	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 44996 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	E	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	F	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	G	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	H	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	I	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	J	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	K	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	L	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	M	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	N	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	O	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	P	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		
1	Q	398	Total	C	N	O	S	0	0
			3094	1959	537	582	16		

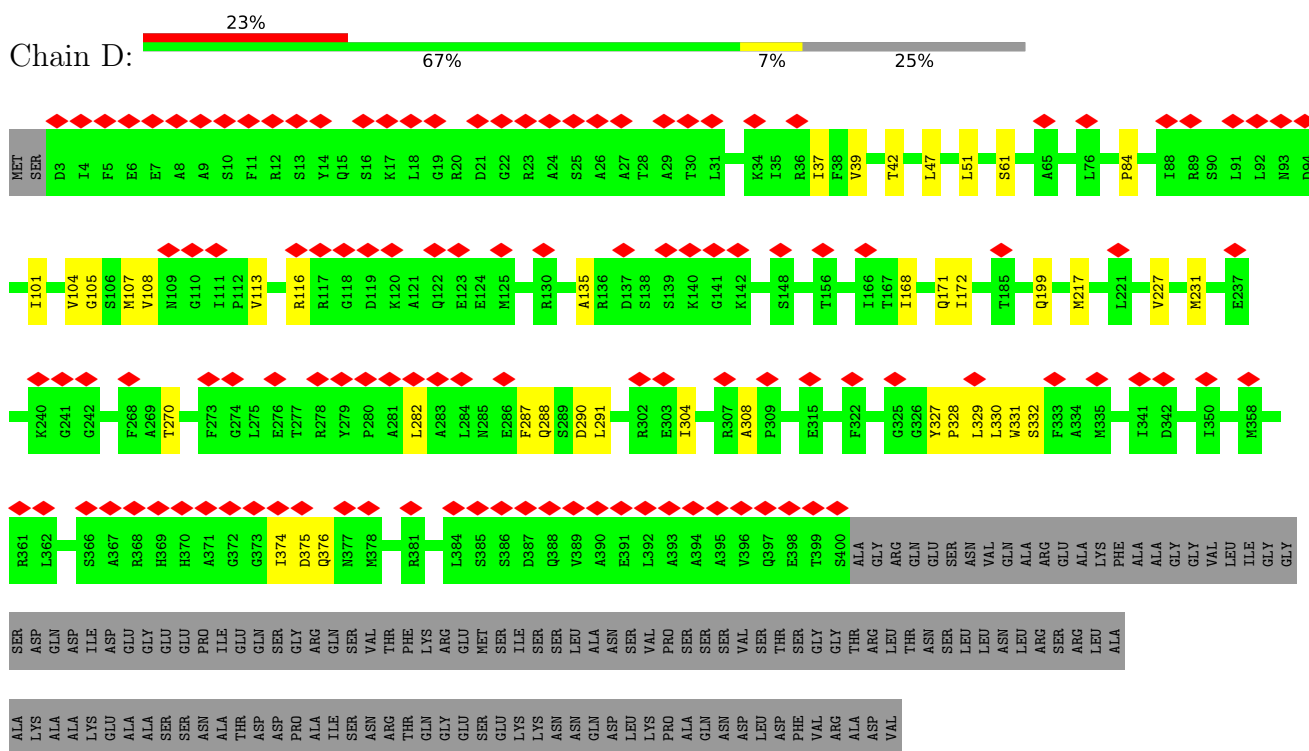
- Molecule 2 is a RNA chain called RNA (84-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	84	Total	C	N	O	P	0	0
			1680	756	168	672	84		

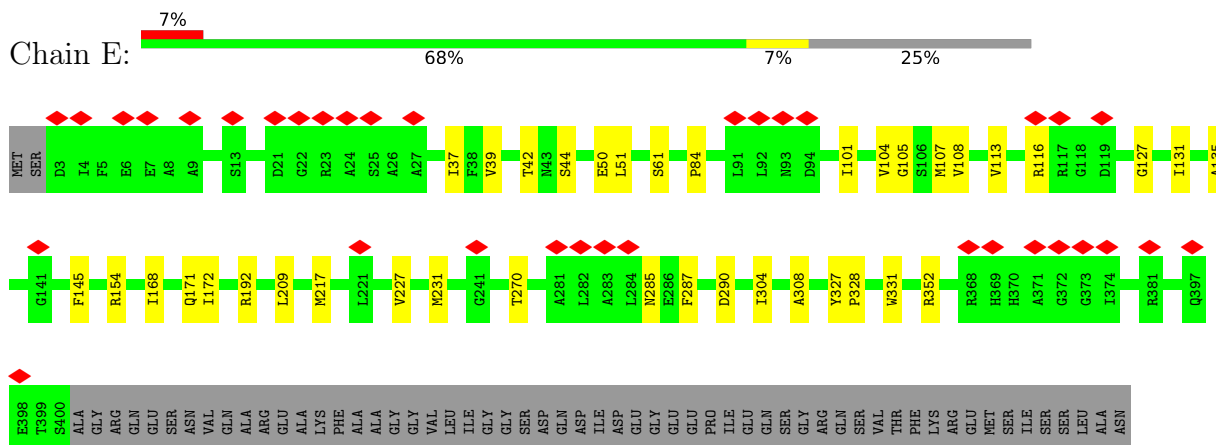
3 Residue-property plots

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.

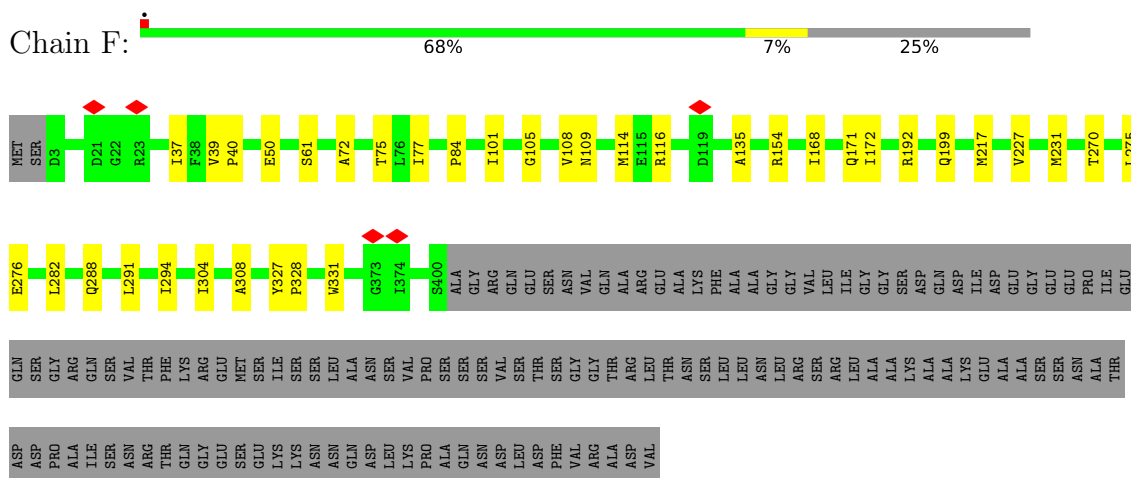
• Molecule 1: Nucleoprotein



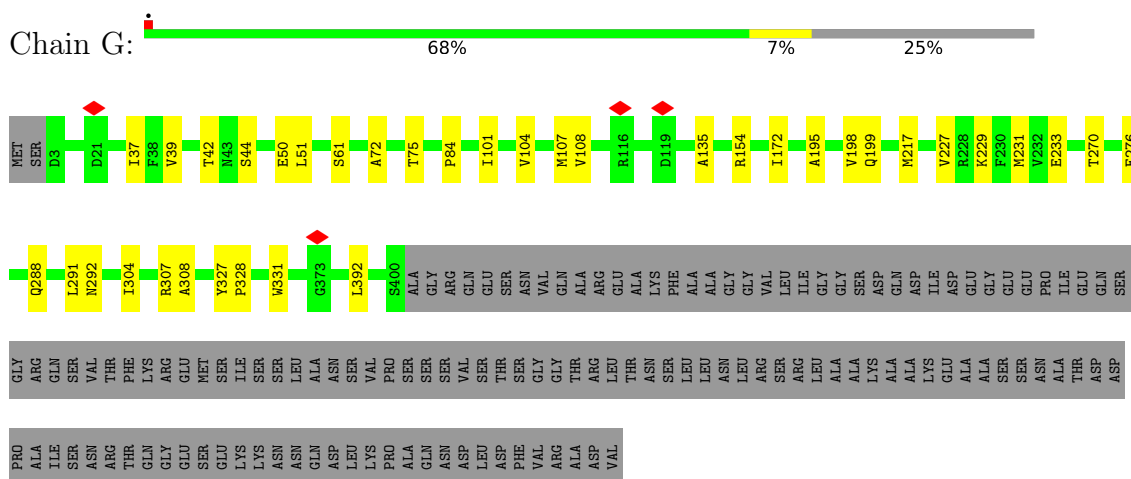
• Molecule 1: Nucleoprotein



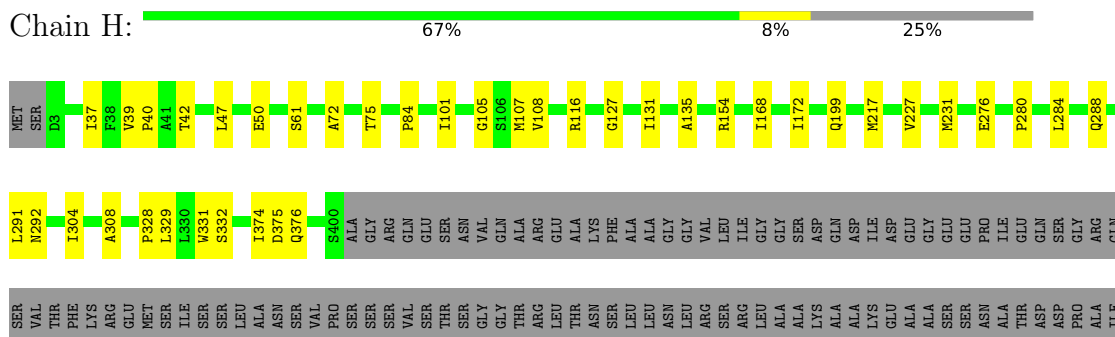
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



SER	ASN	ALA	THR	GLN	GLY	GLU	SER	GLU	LYS	LYS	ASN	ASN	GLN	LEU	LYS	PRO	ALA	GLN	ASN	LEU	ASP	ASP	PHE	VAL	ARG	ALA	ASP	VAL
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● Molecule 1: Nucleoprotein

Chain I: 69%5%25%

PRO	ALA	GLN	ASN	ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																																		
PRO	SER	SER	VAL	SER	THR	SER	GLY	GLY	THR	ARG	LEU	THR	ASN	SER	LEU	ALA	ASN	LEU	ARG	SER	ALA	LYS	ALA	GLY	GLU	GLU	THR	ASP	ASP	PRO	ALA	ILE	ASN	ASN	THR	ARG	ASN	GLN	ASP	LEU	LYS					
S400		ALA	GLY	ARG	GLN	GLU	SER	ASN	VAL	GLN	ALA	ALA	LYS	PHE	ALA	GLY	GLY	GLY	ILE	LEU	VAL	VAL	ASP	GLN	GLY	GLU	GLU	PRO	ILE	GLN	ARG	SER	VAL	THR	PHE	LYS	ARG	GLU	MET	ILE	SER	SER	LEU	ALA	ASN	VAL
MET	SER	D3	V39	E50	L51	S61	I77	P84	V104	M107	V108	V113	R116	A135	R154	I168	I172	M217	V227	M231	E276	P280	A281	L282	M285	E286	F287	Q288	S289	L291	N292	Q364	R368	I374	D375											

● Molecule 1: Nucleoprotein

Chain J: 68%7%25%

SER	GLU	LYS	ASN	ASN	GLN	ASP	LEU	LYS	PRO	ALA	ASN	ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											</
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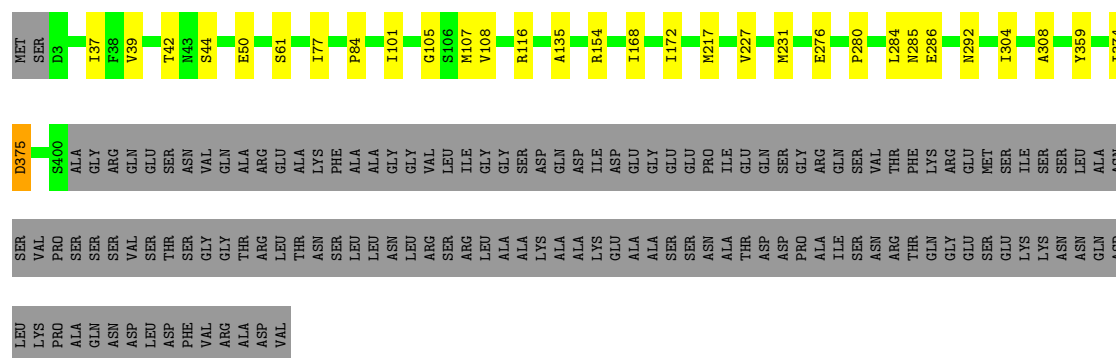
● Molecule 1: Nucleoprotein

Chain K: 70%5%25%

ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					GLN	GLU	SER	MET	
LEU	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					SER	ASN	VAL	GLN	D3
VAL	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					GLY	VAL	ASN	GLN	V39
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					ARG	GLN	ALA	ALA	A41
VAL	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					LEU	ARG	ALA	ALA	T42
VAL	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					THR	GLU	ALA	ALA	S44
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					ASN	LYS	LYS	LYS	E50
LEU	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					LEU	ALA	ALA	ALA	L51
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					ASN	GLY	GLY	GLY	S61
VAL	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					LEU	VAL	VAL	VAL	P84
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					ARG	ILE	GLY	GLY	V104
LEU	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					LEU	GLY	GLY	GLY	M107
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					ALA	SER	SER	SER	V108
VAL	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					LYS	ASP	ASP	GLN	V113
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					ALA	ASP	ASP	GLN	V113
LEU	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					LYS	ILE	ILE	ILE	A135
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					GLU	ASP	ASP	GLY	R154
VAL	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					ALA	GLY	GLY	GLY	I168
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					SER	GLU	GLU	GLU	I172
LEU	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					ASN	PRO	PRO	ILE	M217
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					ALA	THR	THR	GLU	V227
VAL	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					ASP	ASP	SER	GLN	M231
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					PRO	GLY	GLY	ARG	E276
LEU	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					ALA	ILE	GLN	SER	Q288
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					ASN	VAL	VAL	THR	L291
VAL	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					THR	PHE	THR	LYS	M292
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					GLN	GLY	ARG	GLU	I304
LEU	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					GLU	GLY	GLU	MET	A308
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					GLU	SER	SER	ILE	I374
VAL	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					LYS	LYS	SER	SER	D375
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					ASN	LEU	ALA	ALA	Q376
LEU	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					ASP	ASN	ASN	ASN	L392
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					LEU	VAL	VAL	PRO	S400
VAL	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					LYS	GLY	SER	ALA	ALA
ASP	LEU	ASP	PHE	VAL	ARG	ALA	ASP	VAL																					PRO	SER	SER	GLY	ARG
LEU	ASP	PHE	VAL	ARG	ALA	ALA	ASP	VAL																					ASN	SER	SER	ARG	

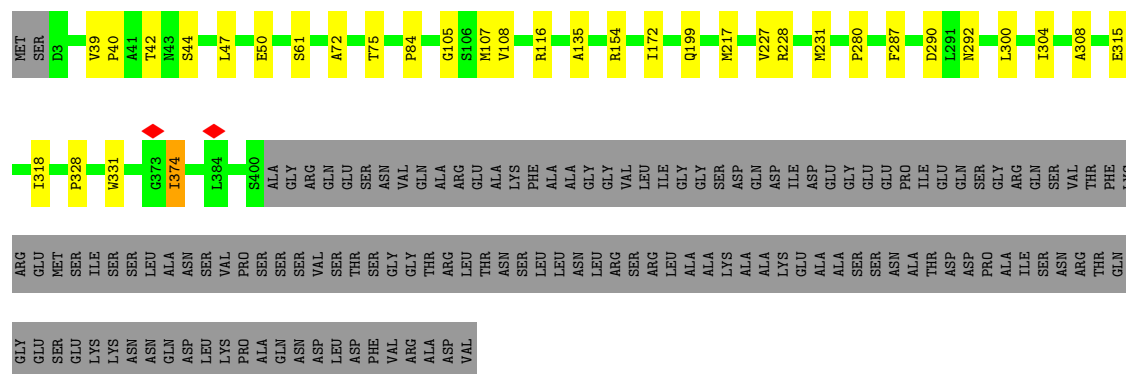
● Molecule 1: Nucleoprotein

Chain L:  69% 6% 25%



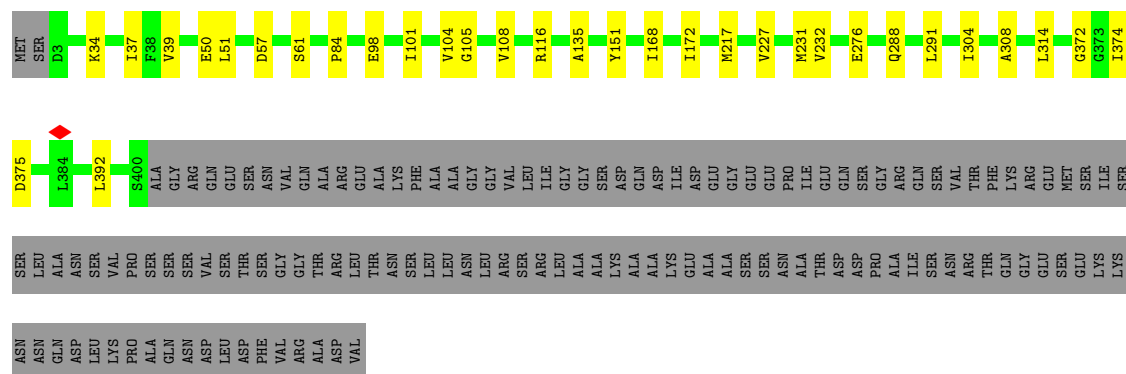
• Molecule 1: Nucleoprotein

Chain M:  68% 6% 25%



• Molecule 1: Nucleoprotein

Chain N:  69% 6% 25%




• Molecule 1: Nucleoprotein

Chain O:  67% 8% 25%



PHE
VAL
ARG
ALA
ASP
VAL

- Molecule 2: RNA (84-MER)

Chain Z:  85% 13% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	138389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.568	Depositor
Minimum map value	-0.240	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	478.08, 478.08, 478.08	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8853333, 0.8853333, 0.8853333	Depositor

5 Model quality

5.1 Standard geometry

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	D	0.21	0/3147	0.51	2/4252 (0.0%)
1	E	0.22	0/3147	0.52	0/4252
1	F	0.22	0/3147	0.51	0/4252
1	G	0.23	0/3147	0.52	0/4252
1	H	0.27	0/3147	0.58	1/4252 (0.0%)
1	I	0.25	0/3147	0.56	1/4252 (0.0%)
1	J	0.27	0/3147	0.59	1/4252 (0.0%)
1	K	0.25	0/3147	0.55	0/4252
1	L	0.26	0/3147	0.56	1/4252 (0.0%)
1	M	0.23	0/3147	0.52	1/4252 (0.0%)
1	N	0.23	0/3147	0.60	3/4252 (0.1%)
1	O	0.25	0/3147	0.55	4/4252 (0.1%)
1	P	0.22	0/3147	0.56	4/4252 (0.1%)
1	Q	0.21	0/3147	0.48	0/4252
2	Z	0.16	0/1847	0.40	0/2852
All	All	0.24	0/45905	0.54	18/62380 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	375	ASP	N-CA-C	-14.26	87.42	109.52
1	N	375	ASP	N-CA-C	-14.11	87.94	109.24
1	J	375	ASP	N-CA-C	-14.03	88.24	109.14
1	L	375	ASP	N-CA-C	-12.23	90.75	108.60
1	I	375	ASP	N-CA-C	-12.07	91.07	109.41
1	N	374	ILE	N-CA-C	10.64	123.01	108.11
1	O	374	ILE	N-CA-C	9.92	123.14	108.45
1	O	375	ASP	N-CA-C	-8.16	93.41	110.80
1	P	374	ILE	N-CA-C	7.84	119.08	108.11
1	D	374	ILE	N-CA-C	7.27	118.36	107.75
1	P	375	ASP	N-CA-C	-6.90	97.72	109.24
1	D	375	ASP	N-CA-C	-6.66	98.54	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	110	GLY	N-CA-C	-6.55	100.31	112.37
1	P	370	HIS	CA-C-N	5.86	129.60	120.82
1	P	370	HIS	C-N-CA	5.86	129.60	120.82
1	M	374	ILE	N-CA-C	5.53	115.65	108.35
1	N	372	GLY	N-CA-C	-5.20	107.55	115.66
1	O	106	SER	N-CA-C	-5.07	105.45	111.69

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	D	3094	0	3141	21	0
1	E	3094	0	3141	22	0
1	F	3094	0	3141	22	0
1	G	3094	0	3141	23	0
1	H	3094	0	3141	29	0
1	I	3094	0	3141	26	0
1	J	3094	0	3141	22	0
1	K	3094	0	3141	18	0
1	L	3094	0	3141	24	0
1	M	3094	0	3141	20	0
1	N	3094	0	3141	16	0
1	O	3094	0	3141	48	0
1	P	3094	0	3141	26	0
1	Q	3094	0	3141	23	0
2	Z	1680	0	841	13	0
All	All	44996	0	44815	319	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 4.

All (319) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:51:LEU:CD1	1:O:107:MET:HE1	1.82	1.09
1:O:107:MET:HE3	1:O:113:VAL:CG2	1.84	1.08
1:O:51:LEU:HD13	1:O:107:MET:HE1	1.40	1.03
1:O:107:MET:HG2	1:O:108:VAL:H	1.25	1.01
1:O:107:MET:CE	1:O:113:VAL:HG22	1.92	0.99
1:O:107:MET:HE3	1:O:113:VAL:HG22	0.96	0.96
1:H:280:PRO:HD3	1:H:374:ILE:HD12	1.51	0.93
1:O:51:LEU:HD13	1:O:107:MET:CE	2.03	0.89
1:O:111:ILE:HD13	1:O:136:ARG:NH2	1.88	0.88
1:I:280:PRO:HD3	1:I:374:ILE:HD12	1.58	0.86
1:I:280:PRO:HD3	1:I:374:ILE:CD1	2.07	0.83
1:O:107:MET:CG	1:O:108:VAL:H	1.95	0.80
1:O:280:PRO:HD3	1:O:374:ILE:HD13	1.65	0.78
1:H:280:PRO:CD	1:H:374:ILE:HD12	2.15	0.77
1:H:280:PRO:HD3	1:H:374:ILE:CD1	2.15	0.76
1:O:111:ILE:HD13	1:O:136:ARG:HH22	1.55	0.72
1:O:280:PRO:HD3	1:O:374:ILE:CD1	2.20	0.71
1:O:51:LEU:HD12	1:O:107:MET:HE1	1.74	0.70
1:O:50:GLU:HG2	1:O:108:VAL:HG13	1.73	0.70
1:O:107:MET:HG2	1:O:108:VAL:N	2.04	0.69
1:G:392:LEU:HD21	1:H:284:LEU:HD21	1.74	0.68
1:I:280:PRO:CD	1:I:374:ILE:HD12	2.23	0.68
1:L:280:PRO:HG3	1:L:374:ILE:HD12	1.75	0.67
1:K:392:LEU:HD21	1:L:284:LEU:HD21	1.79	0.65
1:O:111:ILE:CD1	1:O:136:ARG:NH2	2.59	0.65
1:O:111:ILE:HD13	1:O:136:ARG:CZ	2.28	0.63
1:O:111:ILE:HG22	1:O:132:LEU:HD13	1.81	0.62
1:J:280:PRO:HG3	1:J:374:ILE:HD12	1.83	0.61
1:O:111:ILE:CG2	1:O:132:LEU:HD13	2.30	0.61
1:O:111:ILE:HG22	1:O:132:LEU:CD1	2.33	0.59
1:O:51:LEU:CB	1:O:107:MET:HE1	2.32	0.59
1:Q:282:LEU:O	1:Q:288:GLN:NE2	2.36	0.59
1:J:280:PRO:HD3	1:J:374:ILE:HG21	1.83	0.58
1:J:37:ILE:HB	1:J:101:ILE:HG22	1.86	0.58
1:D:282:LEU:O	1:D:288:GLN:NE2	2.35	0.57
1:F:61:SER:HB2	1:F:135:ALA:HB2	1.87	0.57
1:O:109:ASN:HB2	1:O:114:MET:HB3	1.88	0.56
1:P:61:SER:HB2	1:P:135:ALA:HB2	1.88	0.56
1:Q:352:ARG:NH1	2:Z:80:U:OP2	2.38	0.56
1:E:192:ARG:HH12	2:Z:11:U:H5"	1.71	0.55
1:Q:37:ILE:HB	1:Q:101:ILE:HG22	1.89	0.55
1:E:37:ILE:HB	1:E:101:ILE:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:300:LEU:HD21	1:M:318:ILE:HD11	1.89	0.55
1:O:111:ILE:HG21	1:O:132:LEU:HD22	1.89	0.55
1:P:282:LEU:O	1:P:288:GLN:NE2	2.38	0.55
1:J:61:SER:HB2	1:J:135:ALA:HB2	1.89	0.54
1:E:107:MET:HG3	1:E:113:VAL:HA	1.89	0.54
1:D:61:SER:HB2	1:D:135:ALA:HB2	1.89	0.53
1:O:105:GLY:HA2	1:O:116:ARG:HH21	1.72	0.53
1:E:107:MET:HG2	1:E:108:VAL:H	1.73	0.53
1:D:168:ILE:HA	1:D:171:GLN:HE21	1.73	0.53
1:D:37:ILE:HB	1:D:101:ILE:HG22	1.90	0.53
1:M:39:VAL:HG13	1:M:84:PRO:HB2	1.90	0.53
1:M:172:ILE:HD12	1:M:217:MET:HG2	1.89	0.53
1:F:276:GLU:OE1	1:G:292:ASN:ND2	2.42	0.53
1:E:168:ILE:HA	1:E:171:GLN:HE21	1.73	0.53
1:L:39:VAL:HG13	1:L:84:PRO:HB2	1.90	0.52
1:L:42:THR:HG22	1:L:44:SER:H	1.73	0.52
1:H:61:SER:HB2	1:H:135:ALA:HB2	1.91	0.52
1:O:304:ILE:HB	1:O:308:ALA:HB2	1.91	0.52
1:J:42:THR:HG22	1:J:44:SER:H	1.75	0.52
1:P:199:GLN:NE2	2:Z:80:U:O2	2.42	0.52
1:F:105:GLY:HA2	1:F:116:ARG:HH21	1.74	0.52
1:N:51:LEU:HD11	1:N:104:VAL:HG21	1.91	0.52
1:P:51:LEU:HD21	1:P:104:VAL:HG11	1.92	0.52
1:E:61:SER:HB2	1:E:135:ALA:HB2	1.90	0.52
1:F:304:ILE:HB	1:F:308:ALA:HB2	1.92	0.52
1:K:61:SER:HB2	1:K:135:ALA:HB2	1.91	0.52
1:I:39:VAL:HG13	1:I:84:PRO:HB2	1.91	0.52
1:N:37:ILE:HB	1:N:101:ILE:HG22	1.91	0.52
1:L:37:ILE:HB	1:L:101:ILE:HG22	1.91	0.52
1:L:280:PRO:CG	1:L:374:ILE:HD12	2.40	0.52
1:O:375:ASP:OD1	1:P:284:LEU:HA	2.10	0.51
1:G:107:MET:HG2	1:G:108:VAL:H	1.75	0.51
1:K:107:MET:HG3	1:K:113:VAL:HA	1.91	0.51
1:Q:61:SER:HB2	1:Q:135:ALA:HB2	1.93	0.51
1:D:304:ILE:HB	1:D:308:ALA:HB2	1.91	0.51
1:G:51:LEU:HD21	1:G:104:VAL:HG11	1.93	0.51
1:Q:39:VAL:HG13	1:Q:84:PRO:HB2	1.92	0.51
1:G:233:GLU:OE2	1:G:307:ARG:NH2	2.43	0.51
1:G:39:VAL:HG13	1:G:84:PRO:HB2	1.93	0.51
1:H:276:GLU:OE1	1:I:292:ASN:ND2	2.44	0.51
1:I:287:PHE:O	1:I:290:ASP:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:304:ILE:HB	1:Q:308:ALA:HB2	1.91	0.51
1:E:39:VAL:HG23	1:E:84:PRO:HB2	1.93	0.51
1:H:376:GLN:NE2	1:I:285:ASN:OD1	2.44	0.51
1:P:107:MET:HG2	1:P:108:VAL:H	1.77	0.51
1:G:172:ILE:HD12	1:G:217:MET:HG2	1.93	0.50
1:K:51:LEU:HD21	1:K:104:VAL:HG11	1.93	0.50
1:J:276:GLU:OE1	1:K:292:ASN:ND2	2.45	0.50
1:F:37:ILE:HB	1:F:101:ILE:HG22	1.92	0.50
1:N:105:GLY:HA2	1:N:116:ARG:HH21	1.77	0.50
1:P:37:ILE:HB	1:P:101:ILE:HG22	1.93	0.50
1:G:276:GLU:OE1	1:H:292:ASN:ND2	2.42	0.50
1:G:61:SER:HB2	1:G:135:ALA:HB2	1.94	0.50
1:D:199:GLN:NE2	2:Z:8:U:O2	2.44	0.50
1:H:39:VAL:HG13	1:H:84:PRO:HB2	1.94	0.50
1:H:280:PRO:CG	1:H:374:ILE:HD12	2.41	0.50
1:I:50:GLU:OE1	1:I:154:ARG:NH1	2.44	0.50
1:O:61:SER:HB2	1:O:135:ALA:HB2	1.93	0.50
1:N:39:VAL:HG13	1:N:84:PRO:HB2	1.93	0.50
1:F:328:PRO:O	1:F:331:TRP:HB3	2.12	0.50
1:F:270:THR:HG21	1:F:327:TYR:HE2	1.76	0.49
1:I:107:MET:HG3	1:I:113:VAL:HA	1.94	0.49
1:E:304:ILE:HB	1:E:308:ALA:HB2	1.94	0.49
1:H:374:ILE:HD13	1:I:285:ASN:HD21	1.77	0.49
1:N:61:SER:HB2	1:N:135:ALA:HB2	1.94	0.49
1:Q:287:PHE:O	1:Q:290:ASP:HB2	2.12	0.49
1:I:364:GLN:O	1:I:368:ARG:HB3	2.12	0.49
1:I:280:PRO:HD3	1:I:374:ILE:HD13	1.90	0.49
1:K:288:GLN:HA	1:K:291:LEU:HD12	1.95	0.49
1:O:51:LEU:CD1	1:O:107:MET:CE	2.68	0.49
1:L:50:GLU:OE1	1:L:154:ARG:NH1	2.46	0.49
1:N:50:GLU:HG2	1:N:108:VAL:HG22	1.94	0.49
1:D:172:ILE:HD12	1:D:217:MET:HG2	1.95	0.49
1:M:105:GLY:HA2	1:M:116:ARG:HH21	1.78	0.49
1:P:173:TRP:HA	1:P:176:ILE:HD12	1.95	0.48
1:L:280:PRO:HD3	1:L:374:ILE:CD1	2.43	0.48
1:O:107:MET:CG	1:O:108:VAL:N	2.64	0.48
1:E:287:PHE:O	1:E:290:ASP:HB2	2.13	0.48
1:H:50:GLU:OE1	1:H:154:ARG:NH1	2.46	0.48
1:I:107:MET:HG2	1:I:108:VAL:H	1.78	0.48
1:O:352:ARG:HH21	2:Z:69:U:H5	1.62	0.48
1:F:50:GLU:OE1	1:F:154:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:107:MET:SD	1:Q:108:VAL:N	2.84	0.48
1:G:328:PRO:O	1:G:331:TRP:HB3	2.14	0.48
1:H:42:THR:HB	1:H:47:LEU:HD11	1.96	0.48
1:K:107:MET:HG2	1:K:108:VAL:H	1.78	0.48
1:N:304:ILE:HB	1:N:308:ALA:HB2	1.96	0.48
1:F:39:VAL:HG13	1:F:84:PRO:HB2	1.94	0.48
1:H:328:PRO:O	1:H:331:TRP:HB3	2.14	0.48
1:I:282:LEU:O	1:I:288:GLN:NE2	2.47	0.48
1:M:42:THR:HB	1:M:47:LEU:HD11	1.96	0.48
1:N:232:VAL:HG11	1:N:314:LEU:HD11	1.96	0.48
1:P:172:ILE:HD12	1:P:217:MET:HG2	1.96	0.47
1:E:270:THR:HG21	1:E:327:TYR:HE2	1.79	0.47
1:K:276:GLU:OE1	1:L:292:ASN:ND2	2.47	0.47
1:L:172:ILE:HD12	1:L:217:MET:HG2	1.96	0.47
1:O:42:THR:HG22	1:O:44:SER:H	1.79	0.47
1:F:192:ARG:HH12	2:Z:17:U:H5"	1.79	0.47
1:M:61:SER:HB2	1:M:135:ALA:HB2	1.97	0.47
1:H:105:GLY:HA2	1:H:116:ARG:HH21	1.79	0.47
1:L:61:SER:HB2	1:L:135:ALA:HB2	1.95	0.47
1:O:280:PRO:HG3	1:O:374:ILE:HD12	1.95	0.47
1:M:42:THR:HG22	1:M:44:SER:H	1.80	0.47
1:F:50:GLU:HG2	1:F:108:VAL:HG22	1.97	0.47
1:I:61:SER:HB2	1:I:135:ALA:HB2	1.95	0.47
1:K:50:GLU:OE1	1:K:154:ARG:NH1	2.48	0.47
1:D:105:GLY:HA2	1:D:116:ARG:HH21	1.80	0.47
1:F:168:ILE:HA	1:F:171:GLN:HE21	1.79	0.47
1:I:172:ILE:HD12	1:I:217:MET:HG2	1.97	0.47
1:Q:105:GLY:HA2	1:Q:116:ARG:HH21	1.80	0.47
1:M:50:GLU:OE1	1:M:154:ARG:NH1	2.48	0.47
1:N:172:ILE:HD12	1:N:217:MET:HG2	1.97	0.47
1:P:287:PHE:O	1:P:290:ASP:HB2	2.14	0.47
1:Q:51:LEU:HD11	1:Q:104:VAL:HG21	1.97	0.47
1:L:105:GLY:HA2	1:L:116:ARG:HH21	1.79	0.47
1:L:304:ILE:HB	1:L:308:ALA:HB2	1.96	0.47
1:P:39:VAL:HG13	1:P:84:PRO:HB2	1.97	0.47
1:D:107:MET:HG2	1:D:108:VAL:H	1.80	0.46
1:O:172:ILE:HD12	1:O:217:MET:HG2	1.98	0.46
1:Q:149:ARG:O	1:Q:153:LEU:N	2.48	0.46
1:O:104:VAL:HB	1:O:107:MET:HB2	1.97	0.46
1:P:258:TYR:OH	2:Z:79:U:OP2	2.30	0.46
1:O:51:LEU:HA	1:O:107:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:ILE:HD12	1:E:217:MET:HG2	1.97	0.46
1:F:282:LEU:O	1:F:288:GLN:NE2	2.47	0.46
1:G:304:ILE:HB	1:G:308:ALA:HB2	1.97	0.46
1:H:304:ILE:HB	1:H:308:ALA:HB2	1.97	0.46
1:I:77:ILE:HG13	1:I:231:MET:HE1	1.98	0.46
1:J:42:THR:HB	1:J:47:LEU:HD11	1.98	0.46
1:Q:50:GLU:HB3	1:Q:107:MET:HE1	1.98	0.46
1:M:228:ARG:NH1	1:M:315:GLU:OE2	2.41	0.46
1:E:42:THR:HG22	1:E:44:SER:H	1.80	0.46
1:G:199:GLN:HE22	2:Z:26:U:H3	1.64	0.46
1:G:270:THR:HG21	1:G:327:TYR:HE2	1.81	0.46
1:H:172:ILE:HD12	1:H:217:MET:HG2	1.97	0.46
1:G:227:VAL:O	1:G:231:MET:HG2	2.16	0.46
1:L:227:VAL:O	1:L:231:MET:HG2	2.16	0.46
1:H:280:PRO:HG3	1:H:374:ILE:HD12	1.97	0.46
1:H:37:ILE:HB	1:H:101:ILE:HG22	1.98	0.46
1:Q:168:ILE:HA	1:Q:171:GLN:HE21	1.80	0.45
1:G:37:ILE:HB	1:G:101:ILE:HG22	1.97	0.45
1:P:80:TYR:HD2	1:Q:30:THR:HG22	1.81	0.45
1:E:328:PRO:O	1:E:331:TRP:HB3	2.16	0.45
1:P:168:ILE:HA	1:P:171:GLN:HE21	1.82	0.45
1:O:37:ILE:HB	1:O:101:ILE:HG22	1.98	0.45
1:H:227:VAL:O	1:H:231:MET:HG2	2.17	0.45
1:P:352:ARG:HH21	2:Z:75:U:H5	1.64	0.45
1:F:40:PRO:HG2	1:F:84:PRO:HG2	1.99	0.45
1:J:107:MET:HG2	1:J:108:VAL:H	1.82	0.45
1:P:291:LEU:HD12	1:P:330:LEU:HD22	1.98	0.45
1:J:172:ILE:HD12	1:J:217:MET:HG2	1.99	0.45
1:P:50:GLU:OE1	1:P:154:ARG:NH1	2.50	0.45
1:Q:270:THR:HG21	1:Q:327:TYR:HE2	1.82	0.45
1:L:280:PRO:CD	1:L:374:ILE:HD12	2.47	0.45
1:K:40:PRO:HA	1:K:104:VAL:HG22	1.99	0.44
1:G:288:GLN:O	1:G:291:LEU:HB2	2.16	0.44
1:I:227:VAL:O	1:I:231:MET:HG2	2.17	0.44
1:D:107:MET:HE3	1:D:113:VAL:HG22	1.99	0.44
1:K:304:ILE:HB	1:K:308:ALA:HB2	1.99	0.44
1:H:107:MET:HG2	1:H:108:VAL:H	1.83	0.44
1:K:227:VAL:O	1:K:231:MET:HG2	2.18	0.44
1:N:392:LEU:HD21	1:O:284:LEU:HD11	1.98	0.44
1:M:227:VAL:O	1:M:231:MET:HG2	2.18	0.44
1:I:280:PRO:CG	1:I:374:ILE:HD12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:304:ILE:HB	1:J:308:ALA:HB2	2.00	0.44
1:G:288:GLN:HA	1:G:291:LEU:HD12	1.99	0.43
1:J:227:VAL:O	1:J:231:MET:HG2	2.18	0.43
1:N:288:GLN:HA	1:N:291:LEU:HD12	1.99	0.43
1:Q:328:PRO:O	1:Q:331:TRP:HB3	2.18	0.43
1:F:227:VAL:O	1:F:231:MET:HG2	2.18	0.43
1:K:172:ILE:HD12	1:K:217:MET:HG2	2.00	0.43
1:P:227:VAL:O	1:P:231:MET:HG2	2.17	0.43
1:F:77:ILE:HG13	1:F:231:MET:HE1	2.00	0.43
1:D:291:LEU:HD12	1:D:330:LEU:HD22	2.00	0.43
1:K:374:ILE:HD13	1:L:285:ASN:HD21	1.84	0.43
1:O:104:VAL:HB	1:O:107:MET:SD	2.58	0.43
1:O:227:VAL:O	1:O:231:MET:HG2	2.18	0.43
1:P:265:ALA:O	1:P:269:ALA:HB2	2.18	0.43
1:Q:172:ILE:HD12	1:Q:217:MET:HG2	2.00	0.43
1:D:51:LEU:HD21	1:D:104:VAL:HG11	2.00	0.43
1:E:50:GLU:OE1	1:E:154:ARG:NH1	2.52	0.43
1:H:288:GLN:HA	1:H:291:LEU:HD12	1.99	0.43
1:D:39:VAL:HG13	1:D:84:PRO:HB2	2.01	0.43
1:E:227:VAL:O	1:E:231:MET:HG2	2.18	0.43
1:F:172:ILE:HD12	1:F:217:MET:HG2	2.01	0.43
1:F:275:LEU:HD11	1:F:294:ILE:HG21	2.01	0.43
1:N:227:VAL:O	1:N:231:MET:HG2	2.18	0.43
1:F:199:GLN:HE22	2:Z:20:U:H3	1.67	0.43
1:L:107:MET:HG2	1:L:108:VAL:H	1.83	0.43
1:D:42:THR:HB	1:D:47:LEU:HD11	2.01	0.43
1:E:105:GLY:HA2	1:E:116:ARG:HH21	1.84	0.43
1:J:270:THR:HG21	1:J:327:TYR:HE2	1.84	0.43
1:J:40:PRO:HA	1:J:104:VAL:HG22	2.01	0.43
1:J:328:PRO:O	1:J:331:TRP:HB3	2.19	0.43
1:N:57:ASP:OD2	1:N:151:TYR:OH	2.37	0.42
1:D:227:VAL:O	1:D:231:MET:HG2	2.18	0.42
1:D:328:PRO:O	1:D:331:TRP:HB3	2.19	0.42
1:H:199:GLN:HE22	2:Z:32:U:H3	1.67	0.42
1:N:34:LYS:HA	1:N:98:GLU:O	2.18	0.42
1:Q:40:PRO:HG2	1:Q:84:PRO:HG2	2.01	0.42
1:Q:227:VAL:O	1:Q:231:MET:HG2	2.19	0.42
1:L:280:PRO:HD3	1:L:374:ILE:HD12	2.02	0.42
1:F:72:ALA:HA	1:F:75:THR:HG22	2.02	0.42
1:F:288:GLN:HA	1:F:291:LEU:HD12	2.00	0.42
1:P:196:LYS:NZ	1:P:200:GLN:OE1	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:280:PRO:HG3	1:I:374:ILE:HD12	2.01	0.42
1:P:270:THR:HG21	1:P:327:TYR:HE2	1.85	0.42
1:J:105:GLY:HA2	1:J:116:ARG:HH21	1.84	0.42
1:J:107:MET:HE3	1:J:113:VAL:HG22	2.01	0.42
1:L:276:GLU:OE1	1:M:292:ASN:ND2	2.52	0.42
1:E:51:LEU:HD11	1:E:104:VAL:HG21	2.02	0.42
1:M:107:MET:HG2	1:M:108:VAL:H	1.83	0.42
1:P:265:ALA:O	1:P:269:ALA:CB	2.68	0.42
1:E:352:ARG:HH21	2:Z:9:U:H5	1.68	0.42
1:L:77:ILE:HG13	1:L:231:MET:HE1	2.02	0.42
1:N:276:GLU:HB3	1:O:289:SER:HB3	2.02	0.42
1:G:392:LEU:HD12	1:H:280:PRO:HB2	2.02	0.42
1:I:276:GLU:OE1	1:J:292:ASN:ND2	2.53	0.42
1:I:285:ASN:HA	1:I:288:GLN:HG2	2.01	0.42
1:L:168:ILE:O	1:L:172:ILE:HG12	2.20	0.42
1:M:40:PRO:HG2	1:M:84:PRO:HG2	2.02	0.42
1:Q:168:ILE:O	1:Q:172:ILE:HG12	2.20	0.42
1:O:51:LEU:HB2	1:O:107:MET:HE1	2.00	0.41
1:P:304:ILE:HB	1:P:308:ALA:HB2	2.01	0.41
1:E:145:PHE:HA	1:E:209:LEU:HA	2.02	0.41
1:P:328:PRO:O	1:P:331:TRP:HB3	2.20	0.41
1:I:51:LEU:HD21	1:I:104:VAL:HG11	2.02	0.41
1:K:42:THR:HG22	1:K:44:SER:H	1.84	0.41
1:L:374:ILE:HG12	1:L:375:ASP:N	2.36	0.41
1:O:51:LEU:HB2	1:O:107:MET:CE	2.50	0.41
1:P:168:ILE:O	1:P:172:ILE:HG12	2.21	0.41
1:Q:42:THR:HG22	1:Q:44:SER:H	1.85	0.41
1:J:232:VAL:HG11	1:J:314:LEU:HD11	2.03	0.41
1:G:229:LYS:O	1:G:233:GLU:HG2	2.21	0.41
1:I:374:ILE:HD13	1:J:285:ASN:HD21	1.85	0.41
1:D:287:PHE:O	1:D:290:ASP:HB2	2.19	0.41
1:H:168:ILE:O	1:H:172:ILE:HG12	2.21	0.41
1:J:39:VAL:HG13	1:J:84:PRO:HB2	2.01	0.41
1:J:287:PHE:O	1:J:290:ASP:HB2	2.20	0.41
1:M:287:PHE:O	1:M:290:ASP:HB2	2.19	0.41
1:M:304:ILE:HB	1:M:308:ALA:HB2	2.01	0.41
1:M:328:PRO:O	1:M:331:TRP:HB3	2.20	0.41
1:D:376:GLN:NE2	1:E:285:ASN:OD1	2.50	0.41
1:G:195:ALA:HA	1:G:198:VAL:HG12	2.02	0.41
1:H:40:PRO:HG2	1:H:84:PRO:HG2	2.02	0.41
1:I:168:ILE:O	1:I:172:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:376:GLN:NE2	1:L:285:ASN:OD1	2.49	0.41
1:D:329:LEU:O	1:D:332:SER:OG	2.30	0.41
1:E:127:GLY:O	1:E:131:ILE:HG12	2.21	0.41
1:I:374:ILE:CD1	1:J:285:ASN:HD21	2.33	0.41
1:M:280:PRO:HG3	1:M:374:ILE:HD13	2.02	0.41
1:N:168:ILE:O	1:N:172:ILE:HG12	2.21	0.41
1:O:51:LEU:HD13	1:O:107:MET:SD	2.60	0.41
1:O:291:LEU:HD12	1:O:330:LEU:HD22	2.02	0.41
1:P:40:PRO:HA	1:P:104:VAL:HG22	2.03	0.41
1:Q:50:GLU:OE1	1:Q:154:ARG:NH1	2.54	0.41
1:E:168:ILE:O	1:E:172:ILE:HG12	2.22	0.41
1:G:72:ALA:HA	1:G:75:THR:HG22	2.03	0.41
1:M:154:ARG:HA	1:M:154:ARG:HD3	1.95	0.41
1:D:168:ILE:O	1:D:172:ILE:HG12	2.21	0.40
1:F:109:ASN:HB3	1:F:114:MET:HB3	2.03	0.40
1:G:42:THR:HG22	1:G:44:SER:H	1.86	0.40
1:G:50:GLU:OE1	1:G:154:ARG:NH1	2.54	0.40
1:H:329:LEU:O	1:H:332:SER:OG	2.31	0.40
1:K:39:VAL:HG13	1:K:84:PRO:HB2	2.03	0.40
1:O:177:ALA:HB2	1:O:259:VAL:HG22	2.01	0.40
1:H:72:ALA:HA	1:H:75:THR:HG22	2.03	0.40
1:H:127:GLY:O	1:H:131:ILE:HG12	2.21	0.40
1:O:40:PRO:HG2	1:O:84:PRO:HG2	2.02	0.40
1:O:287:PHE:O	1:O:290:ASP:HB2	2.21	0.40
1:Q:329:LEU:O	1:Q:332:SER:OG	2.30	0.40
1:M:72:ALA:HA	1:M:75:THR:HG22	2.03	0.40
1:O:112:PRO:HG3	1:O:129:MET:HG2	2.04	0.40
1:D:270:THR:HG21	1:D:327:TYR:HE2	1.87	0.40
1:K:168:ILE:O	1:K:172:ILE:HG12	2.22	0.40
1:M:199:GLN:HE22	2:Z:62:U:H3	1.68	0.40
1:L:286:GLU:OE1	1:L:359:TYR:OH	2.31	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	D	396/532 (74%)	382 (96%)	14 (4%)	0	100	100
1	E	396/532 (74%)	383 (97%)	13 (3%)	0	100	100
1	F	396/532 (74%)	384 (97%)	12 (3%)	0	100	100
1	G	396/532 (74%)	384 (97%)	12 (3%)	0	100	100
1	H	396/532 (74%)	381 (96%)	15 (4%)	0	100	100
1	I	396/532 (74%)	385 (97%)	11 (3%)	0	100	100
1	J	396/532 (74%)	387 (98%)	9 (2%)	0	100	100
1	K	396/532 (74%)	384 (97%)	12 (3%)	0	100	100
1	L	396/532 (74%)	383 (97%)	13 (3%)	0	100	100
1	M	396/532 (74%)	384 (97%)	12 (3%)	0	100	100
1	N	396/532 (74%)	386 (98%)	10 (2%)	0	100	100
1	O	396/532 (74%)	385 (97%)	11 (3%)	0	100	100
1	P	396/532 (74%)	383 (97%)	13 (3%)	0	100	100
1	Q	396/532 (74%)	383 (97%)	13 (3%)	0	100	100
All	All	5544/7448 (74%)	5374 (97%)	170 (3%)	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	D	328/436 (75%)	328 (100%)	0	100	100
1	E	328/436 (75%)	328 (100%)	0	100	100
1	F	328/436 (75%)	328 (100%)	0	100	100
1	G	328/436 (75%)	328 (100%)	0	100	100
1	H	328/436 (75%)	328 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	328/436 (75%)	328 (100%)	0	100	100
1	J	328/436 (75%)	328 (100%)	0	100	100
1	K	328/436 (75%)	328 (100%)	0	100	100
1	L	328/436 (75%)	328 (100%)	0	100	100
1	M	328/436 (75%)	328 (100%)	0	100	100
1	N	328/436 (75%)	328 (100%)	0	100	100
1	O	328/436 (75%)	328 (100%)	0	100	100
1	P	328/436 (75%)	328 (100%)	0	100	100
1	Q	328/436 (75%)	328 (100%)	0	100	100
All	All	4592/6104 (75%)	4592 (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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	109	ASN
1	D	388	GLN
1	E	199	GLN
1	E	223	GLN
1	E	376	GLN
1	E	377	ASN
1	F	376	GLN
1	F	388	GLN
1	G	377	ASN
1	G	388	GLN
1	H	376	GLN
1	H	377	ASN
1	I	285	ASN
1	M	376	GLN
1	N	199	GLN
1	N	376	GLN
1	N	377	ASN
1	O	109	ASN
1	O	199	GLN
1	P	369	HIS
1	Q	257	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Z	83/84 (98%)	3 (3%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Z	9	U
2	Z	75	U
2	Z	81	U

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 ⓘ

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.

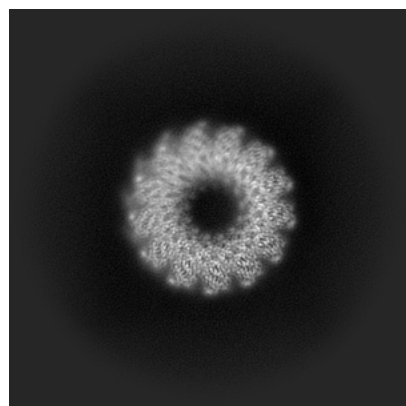
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49803. These allow visual inspection of the internal detail of the map and identification of artifacts.

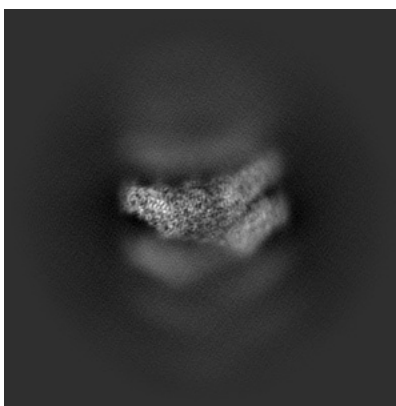
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

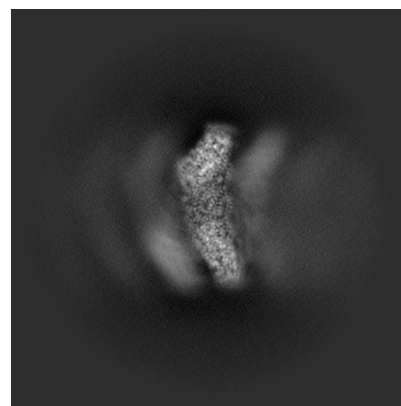
6.1.1 Primary map



X

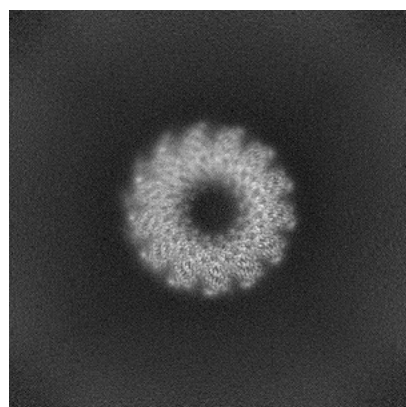


Y

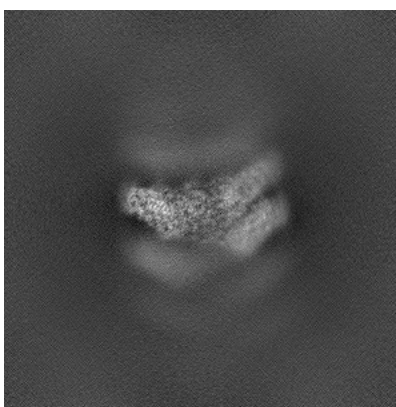


Z

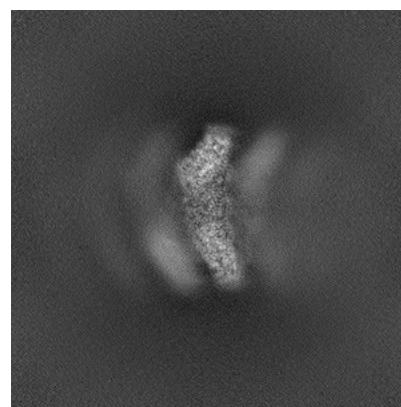
6.1.2 Raw map



X



Y

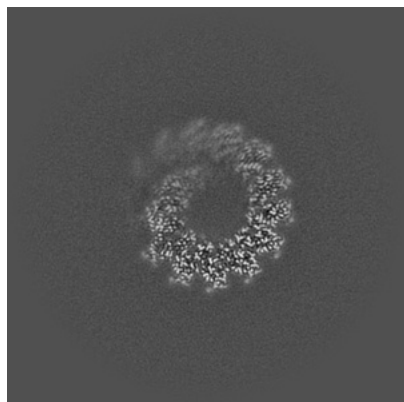


Z

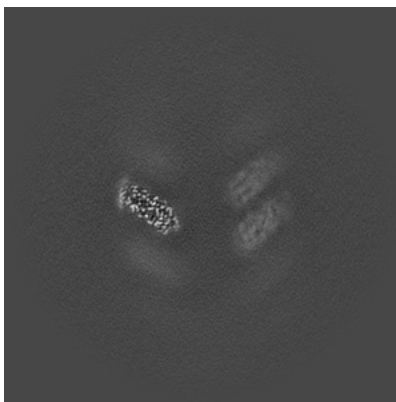
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

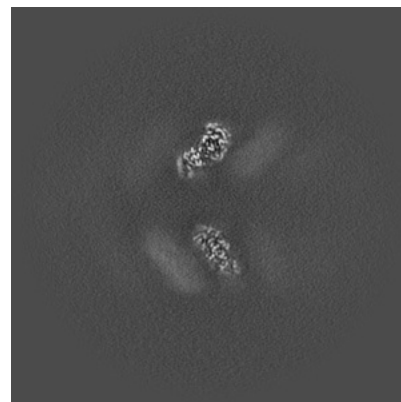
6.2.1 Primary map



X Index: 270

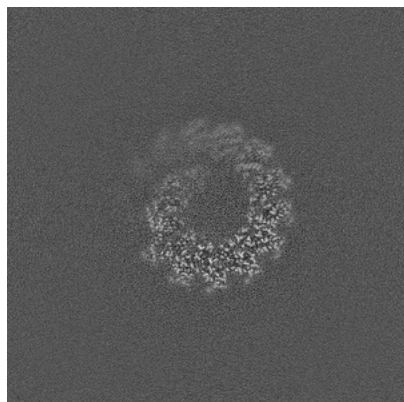


Y Index: 270

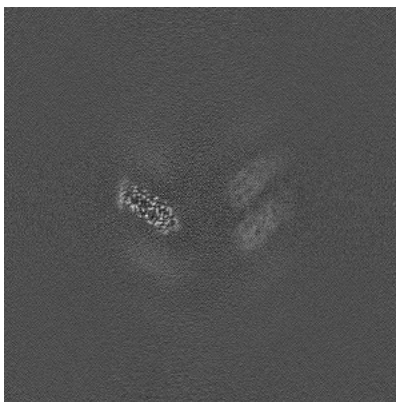


Z Index: 270

6.2.2 Raw map



X Index: 270



Y Index: 270

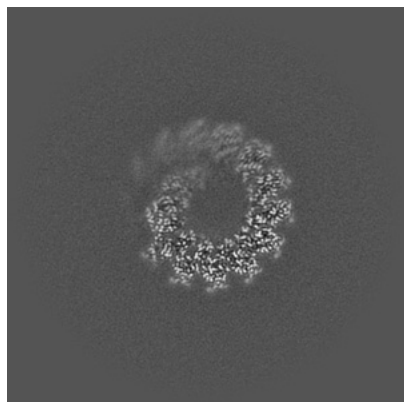


Z Index: 270

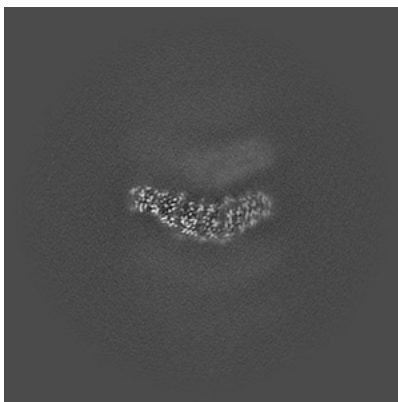
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

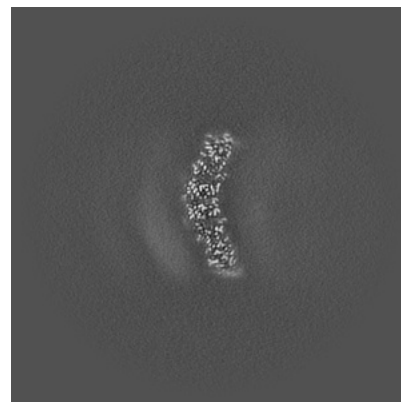
6.3.1 Primary map



X Index: 269

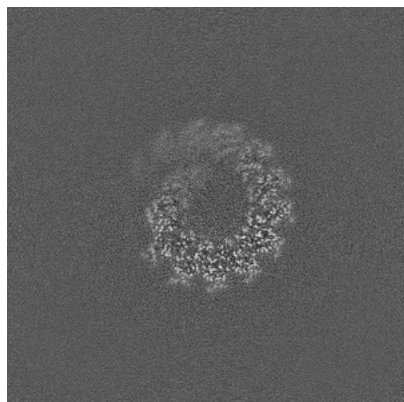


Y Index: 331

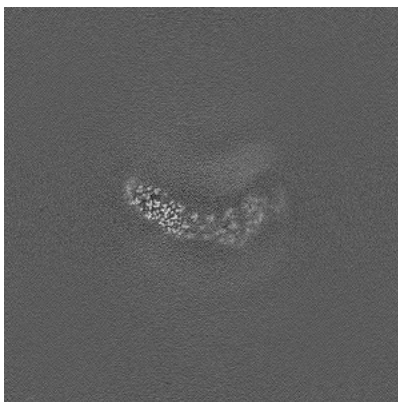


Z Index: 212

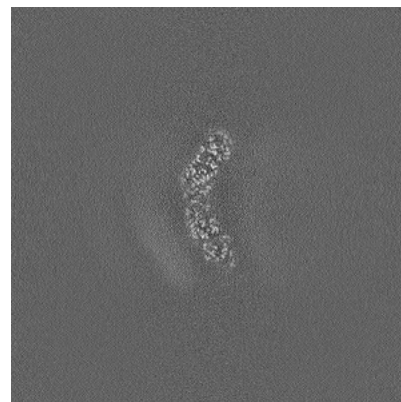
6.3.2 Raw map



X Index: 269



Y Index: 317

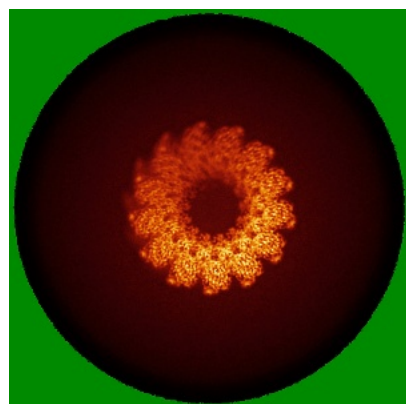


Z Index: 226

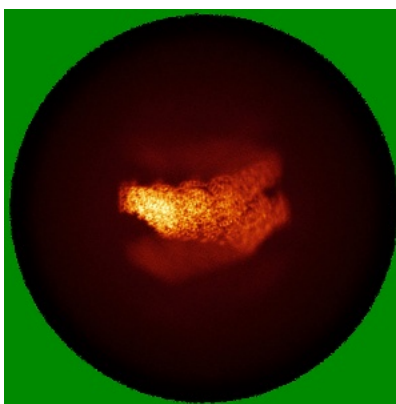
The images above show the largest variance slices of the map in three orthogonal directions.

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

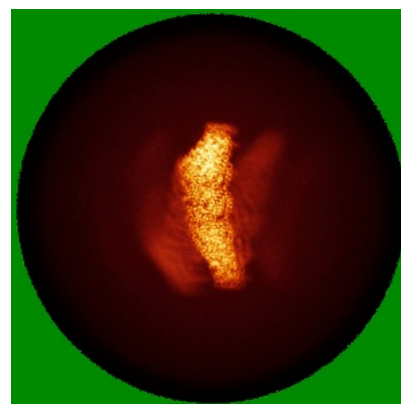
6.4.1 Primary map



X

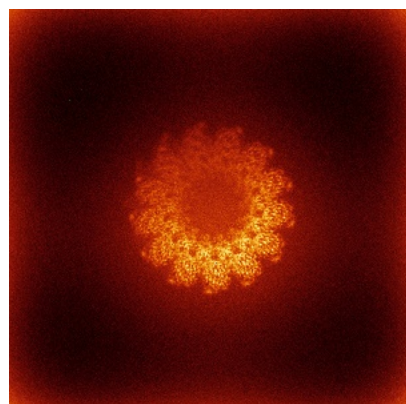


Y

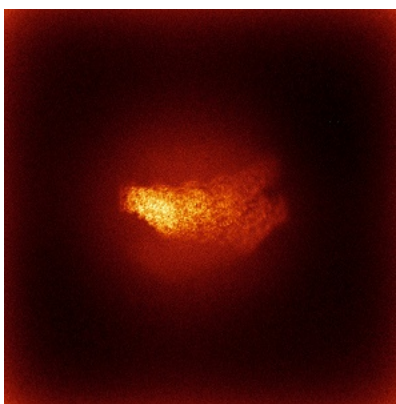


Z

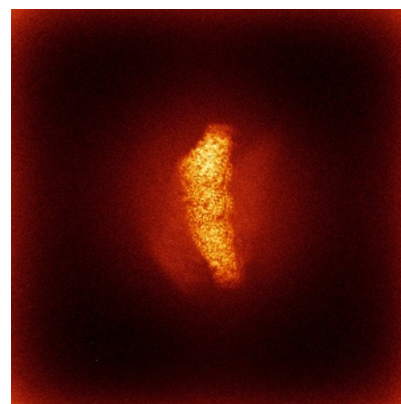
6.4.2 Raw map



X



Y

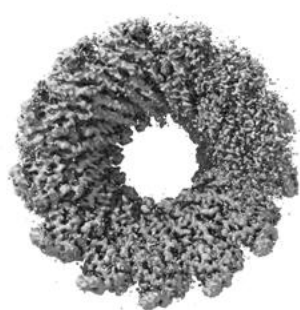


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



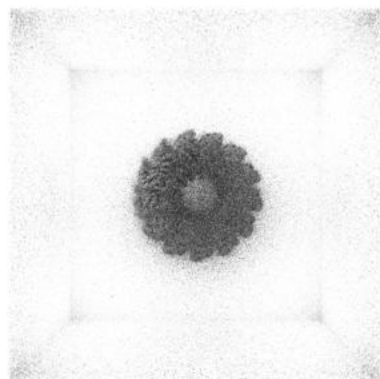
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

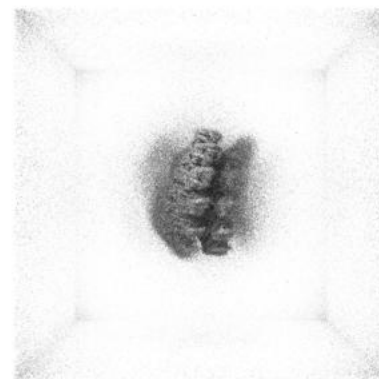
6.5.2 Raw map



X



Y



Z

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

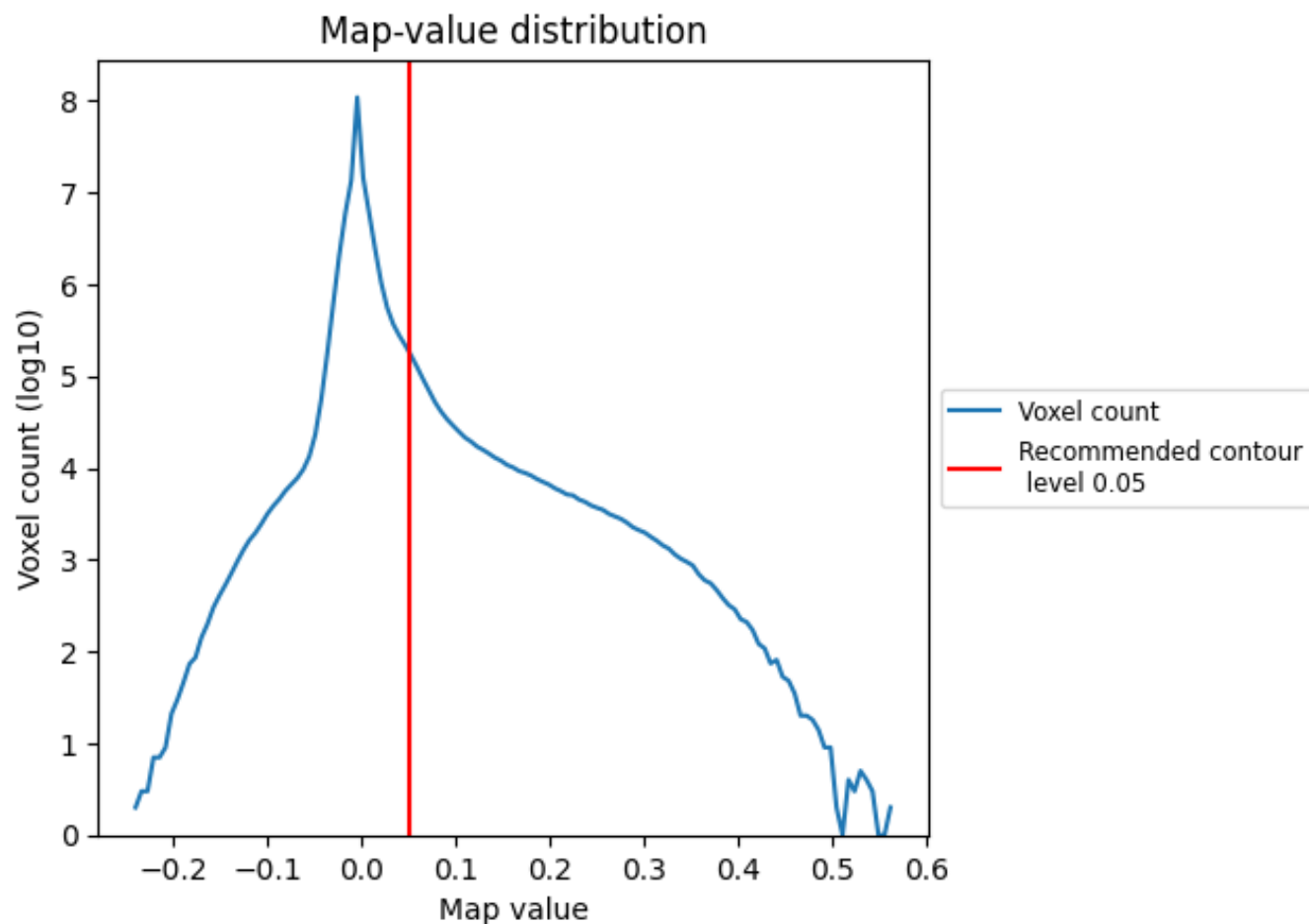
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

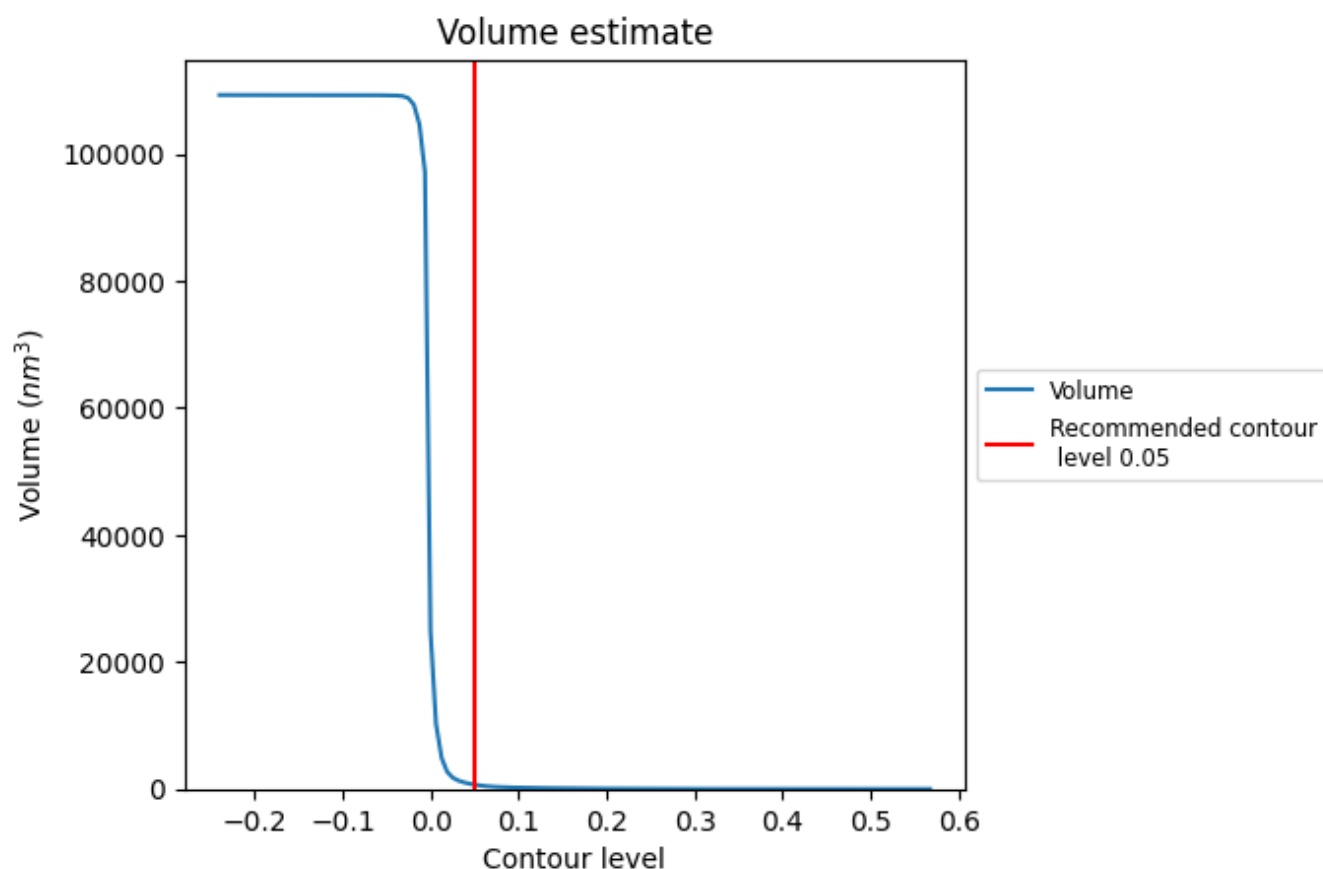
This section contains the results of statistical analysis of the map.

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.

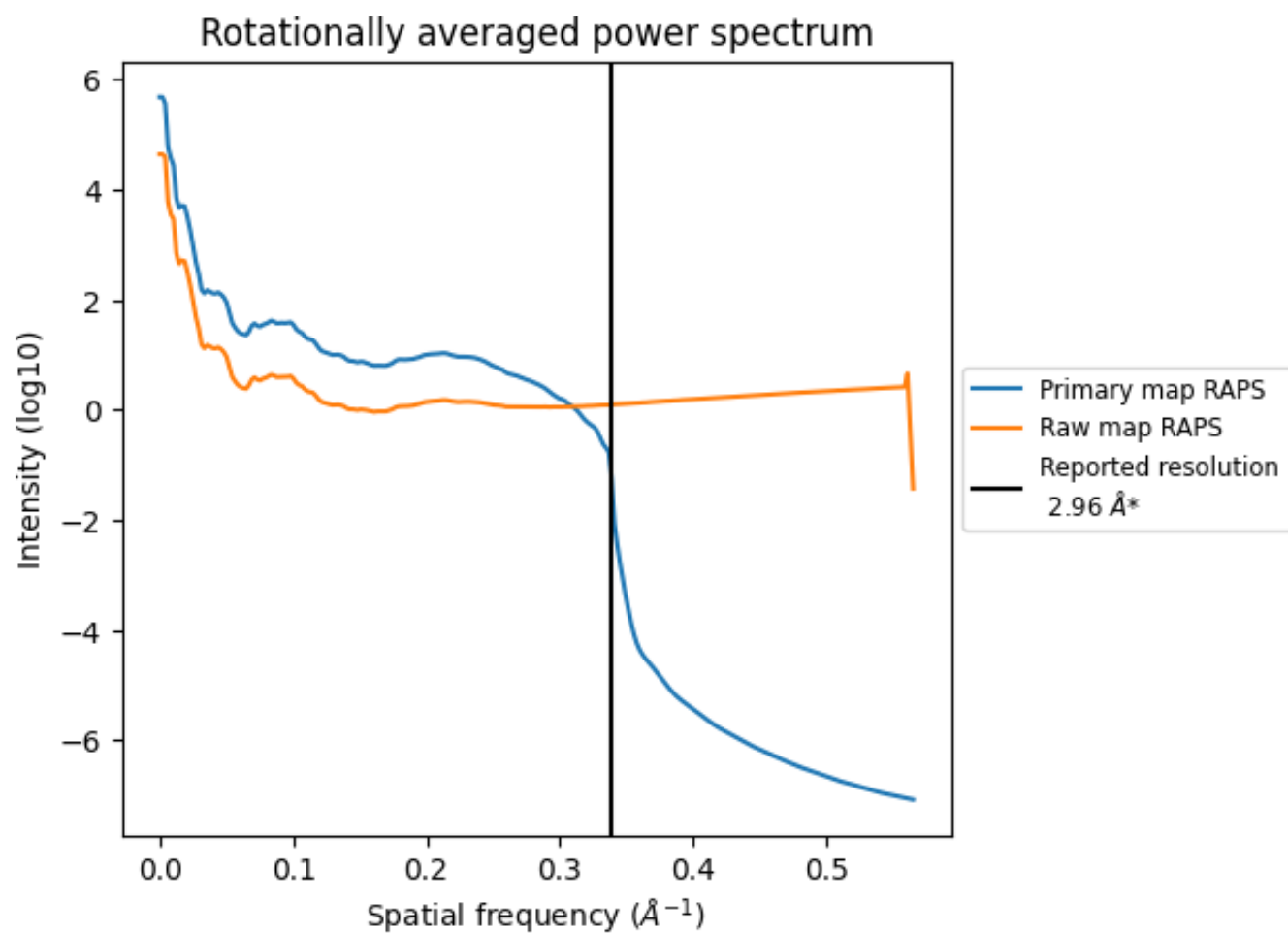
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 682 nm³; this corresponds to an approximate mass of 616 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 ⓘ

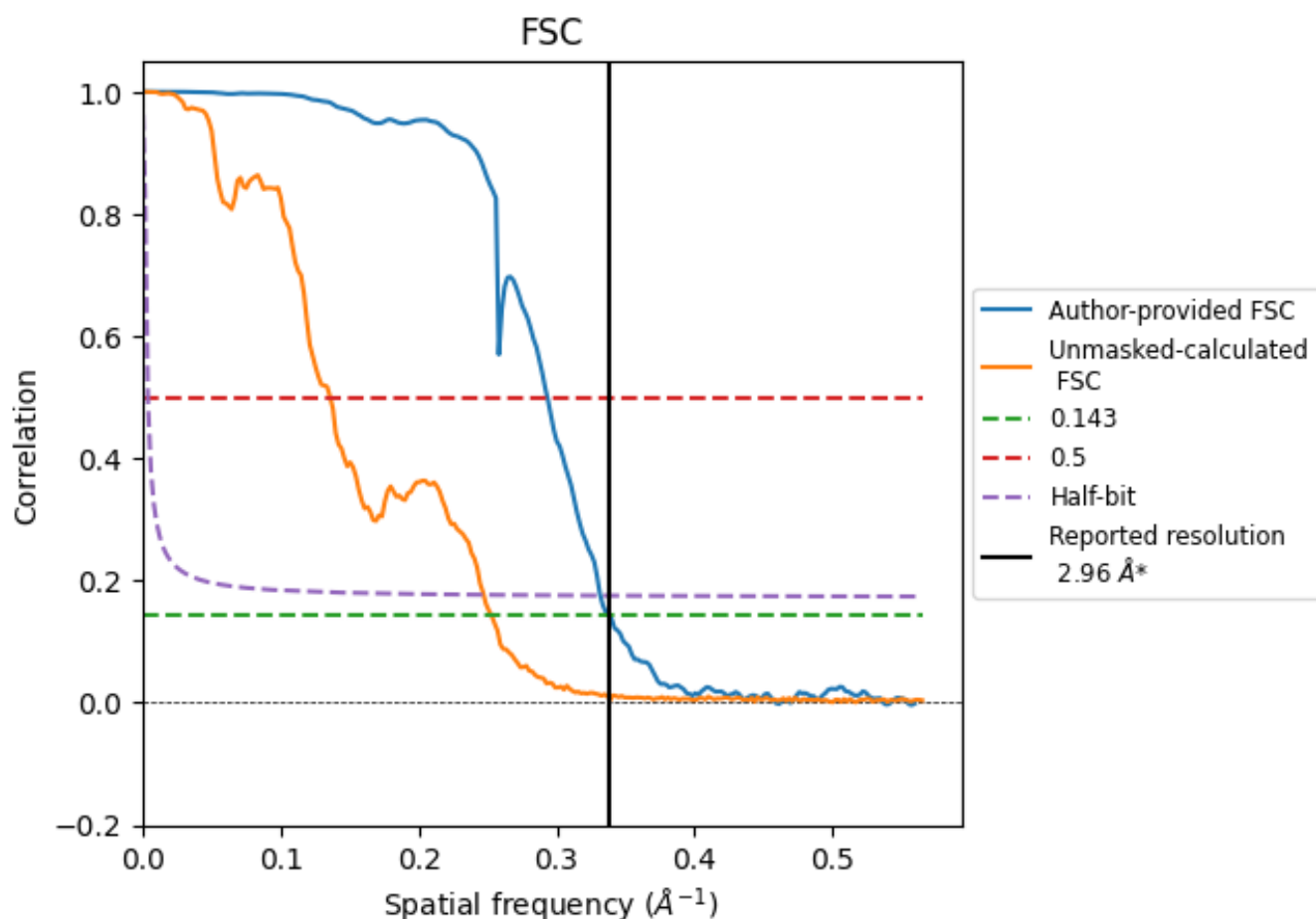


*Reported resolution corresponds to spatial frequency of 0.338 \AA^{-1}

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 0.338 \AA^{-1}

8.2 Resolution estimates [i](#)

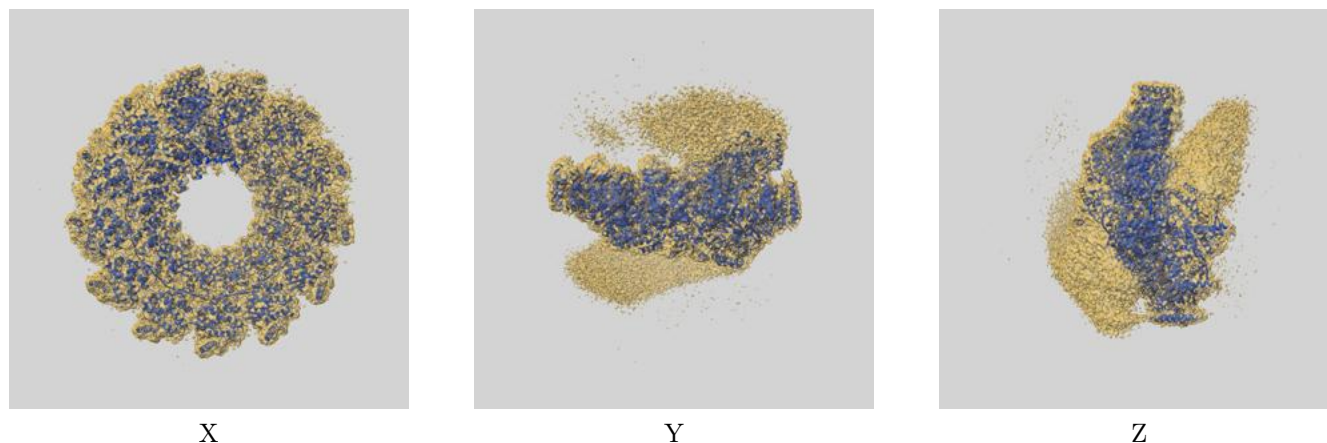
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.41	3.01
Unmasked-calculated*	3.95	7.35	4.04

*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 3.95 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

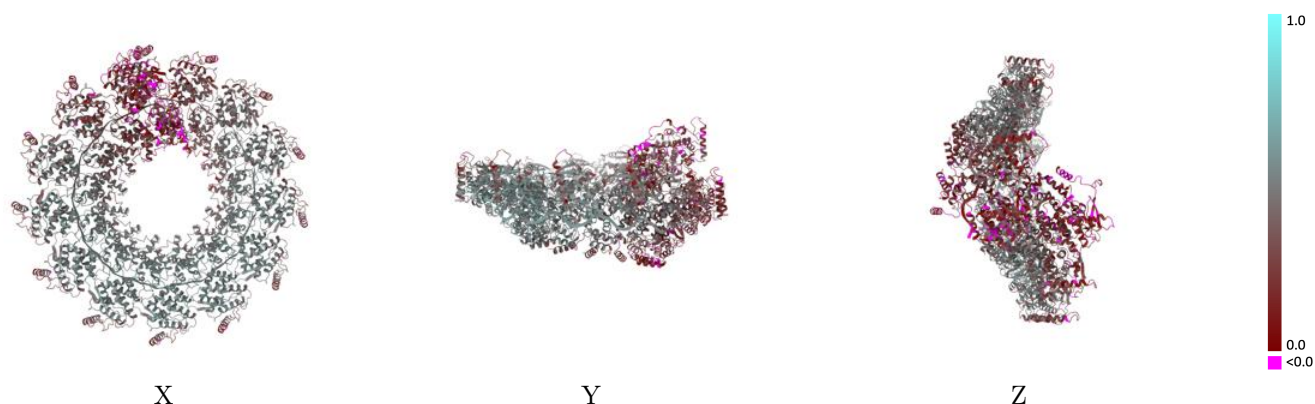
This section contains information regarding the fit between EMDB map EMD-49803 and PDB model 9NUF. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



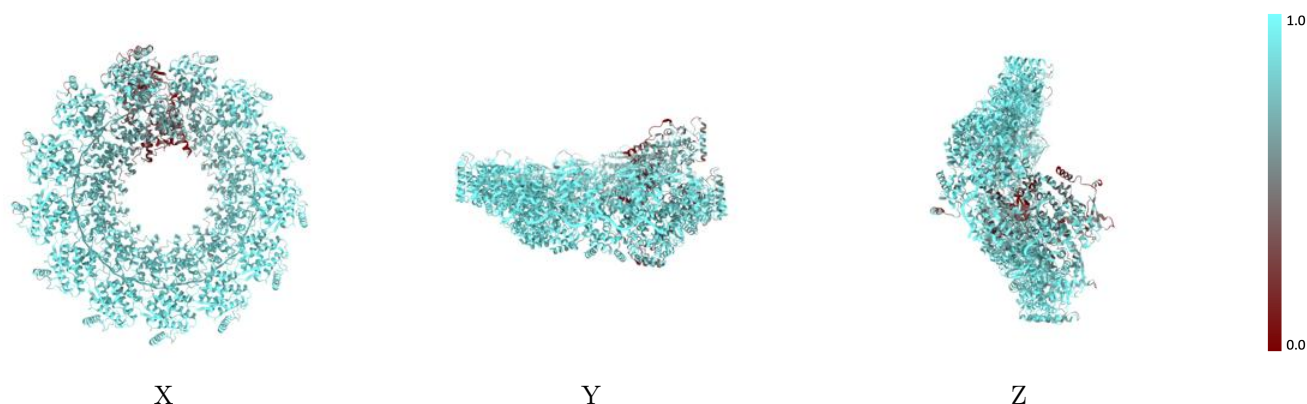
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



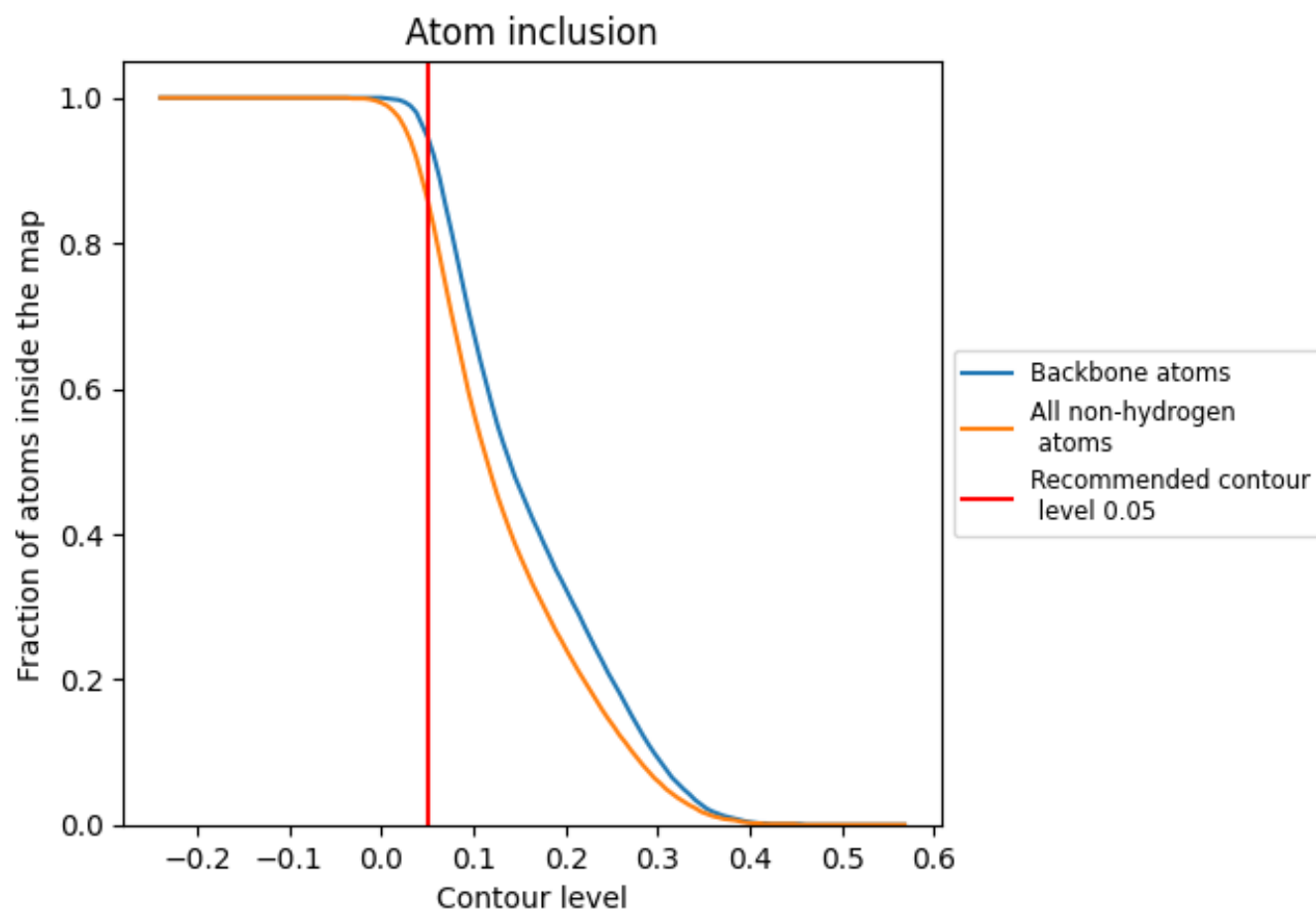
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

































9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 86% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8610	 0.3980
D	 0.5800	 0.1560
E	 0.7510	 0.2840
F	 0.8600	 0.4080
G	 0.9000	 0.4590
H	 0.9210	 0.4850
I	 0.9280	 0.4980
J	 0.9390	 0.5050
K	 0.9390	 0.5030
L	 0.9390	 0.4940
M	 0.9330	 0.4740
N	 0.9170	 0.4420
O	 0.8860	 0.3860
P	 0.8120	 0.2730
Q	 0.6790	 0.1660
Z	 0.9910	 0.4720

