



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:43 PM UTC

PDB ID : 9R5S / pdb_00009r5s
EMDB ID : EMD-53595
Title : Structural characterisation of chromatin remodelling intermediates supports linker DNA dependent product inhibition as a mechanism for nucleosome spacing.
Authors : Sundaramoorthy, R.; Hughes, A.; Owen-hughes, T.A.
Deposited on : 2025-05-09
Resolution : 3.80 Å (reported)
Based on initial models : 6FTX, 3LZ0, 7TN2

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

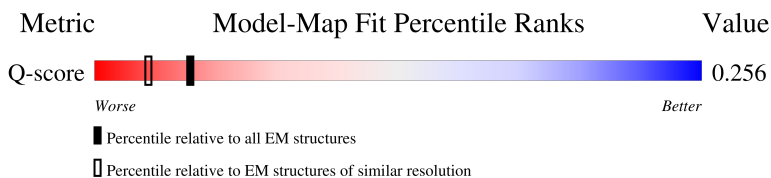
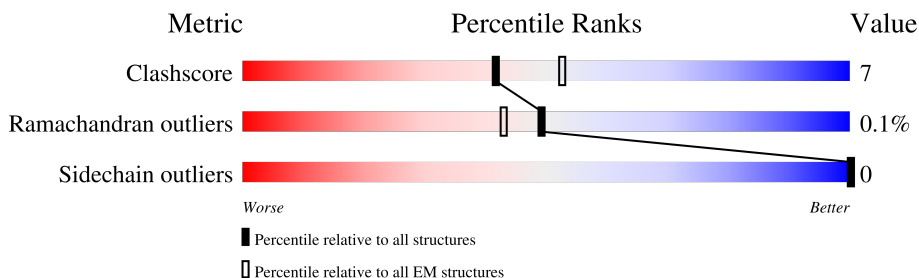
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



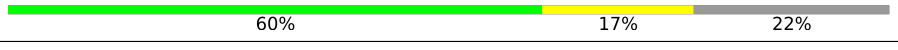
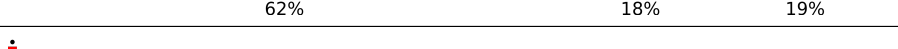
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	I	160	 92% 8%
2	J	160	 5% 86% 14%
3	A	136	 56% 12% 32%
3	E	136	 52% 19% 29%

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Mol	Chain	Length	Quality of chain
4	B	103	
4	F	103	
5	C	130	
5	G	130	
6	D	126	
6	H	126	
7	W	1467	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17423 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 DNA chain called DNA (160-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	160	Total	C	N	O	P	0	0
			3262	1549	590	963	160		

- Molecule 2 is a DNA chain called DNA (160-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	160	Total	C	N	O	P	0	0
			3298	1560	621	957	160		

- Molecule 3 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	92	Total	C	N	O	S	0	0
			749	473	142	132	2		
3	E	97	Total	C	N	O	S	0	0
			794	502	152	138	2		

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
4	F	80	Total	C	N	O	S	0	0
			632	398	122	111	1		

- Molecule 5 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	105	Total	C	N	O	0	0
			798	503	154	141		
5	G	98	Total	C	N	O	0	0
			746	469	146	131		

- Molecule 6 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	94	Total	C	N	O	S	0	0
			734	462	132	138	2		
6	H	92	Total	C	N	O	S	0	0
			718	452	129	135	2		

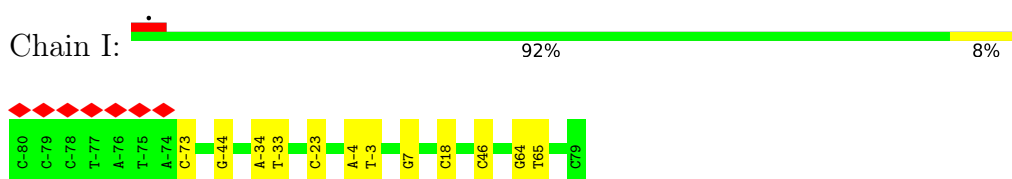
- Molecule 7 is a protein called Chromo domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	652	Total	C	N	O	S	0	0
			5054	3207	877	953	17		

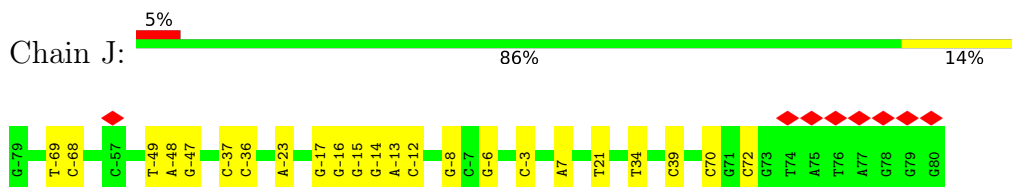
3 Residue-property plots [i](#)

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.

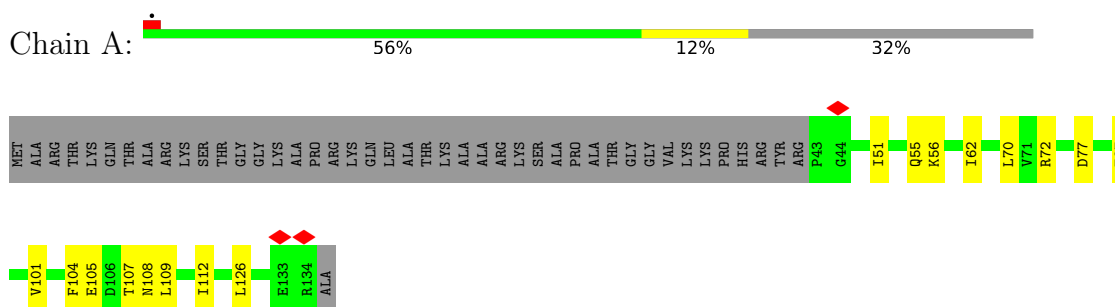
- Molecule 1: DNA (160-MER)



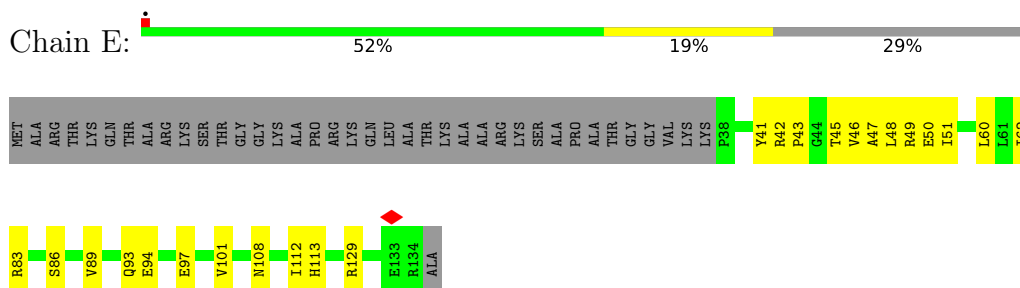
- Molecule 2: DNA (160-MER)



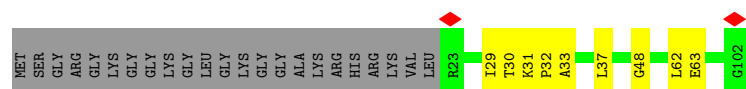
- Molecule 3: Histone H3.2



- Molecule 3: Histone H3.2



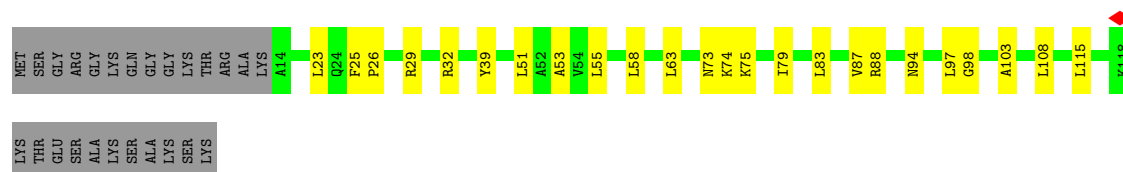
- Molecule 4: Histone H4



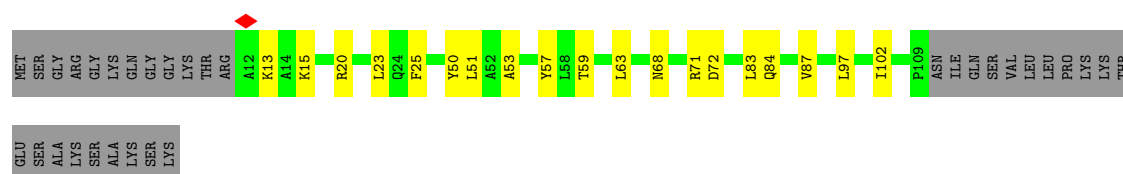
• Molecule 4: Histone H4



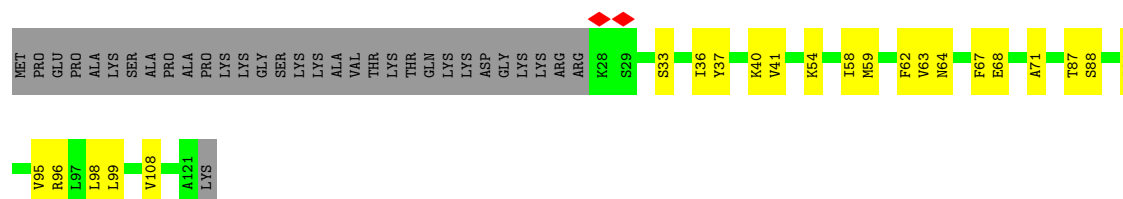
• Molecule 5: Histone H2A type 1



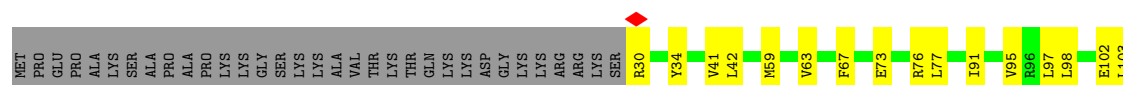
• Molecule 5: Histone H2A type 1



• Molecule 6: Histone H2B 1.1



• Molecule 6: Histone H2B 1.1



LYS	LYS	ASP	HIS
GLY	ARG	CYS	LEU
THR	MET	ARG	TRP
GLY	LYS	HIS	SER
SER	ALA	THR	TYR
PRO	LEU	MET	SER
S1244	PRO	SER	ALA
K1245	LYS	ALA	ASN
G1266	GLY	ILE	PHE
GLY	PRO	TRP	TRP
LEU	ALA	THR	PRO
ASN	ALA	SER	ALA
THR	LEU	LEU	ASP
LYS	ILE	LYS	VAL
SER	ASN	ARG	LYS
PRO	THR	LEU	SER
GLY	ARG	ARG	THR
LYS	LEU	GLY	LYS
LYS	SER	LYS	LEU
LEU	ASP	GLY	ALA
PRO	ILE	SER	TYR
THR	PRO	THR	MET
GLY	LYS	ARG	LYS
PRO	VAL	ILE	ALA
SER	LYS	LEU	LYS
LYS	SER	LYS	THR
ARG	ARG	THR	GLU
ASN	GLN	THR	GLN
GLY	LYS	THR	LYS
THR	THR	ILE	LYS
PRO	ARG	GLY	THR
ALA	GLN	ASN	LEU
ASN	SER	HIS	THR
HIS	SER	ILE	ILE
LYS	ASN	GLU	SER
SER	PRO	SER	ARG
MET	SER	GLN	LYS
THR	GLY	LYS	ALA
PRO	SER	GLY	SER
GLU	ALA	SER	PRO
THR	HIS	SER	GLU
SER	GLU	ARG	LYS
LYS	LYS	LYS	TYR
SER	TYR	SER	ARG
GLY	ASP	MET	LYS
PRO	GLY	GLU	GLU
SER	GLU	LYS	LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.507	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	308.0, 308.0, 308.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.55, 0.55, 0.55	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	I	0.37	0/3654	0.68	0/5633
2	J	0.36	0/3704	0.68	0/5719
3	A	0.18	0/758	0.40	0/1016
3	E	0.17	0/806	0.41	0/1082
4	B	0.19	0/645	0.47	0/862
4	F	0.18	0/639	0.50	0/855
5	C	0.15	0/808	0.36	0/1093
5	G	0.17	0/755	0.36	0/1018
6	D	0.16	0/745	0.43	0/1002
6	H	0.15	0/729	0.45	0/981
7	W	0.17	0/5159	0.32	0/6995
All	All	0.27	0/18402	0.53	0/26256

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	I	3262	0	1797	13	0
2	J	3298	0	1794	31	0
3	A	749	0	787	17	0
3	E	794	0	825	36	0
4	B	638	0	676	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	632	0	665	19	0
5	C	798	0	843	24	0
5	G	746	0	791	23	0
6	D	734	0	758	21	0
6	H	718	0	736	24	0
7	W	5054	0	4662	65	0
All	All	17423	0	14334	214	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 7.

All (214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:42:ARG:O	3:E:45:THR:HG23	1.49	1.11
5:G:72:ASP:OD2	7:W:137:TYR:HD2	1.53	0.91
3:A:56:LYS:HE2	7:W:141:TYR:HE1	1.46	0.81
5:G:72:ASP:OD2	7:W:137:TYR:CD2	2.33	0.81
1:I:7:DG:H5'	4:F:47:SER:HA	1.66	0.77
2:J:70:DC:OP1	3:E:45:THR:HB	1.85	0.77
3:A:108:ASN:O	3:A:112:ILE:HD12	1.86	0.75
2:J:21:DT:OP1	7:W:523:SER:HB2	1.86	0.75
2:J:-23:DA:H5''	3:E:83:ARG:HD2	1.68	0.74
3:A:109:LEU:HD21	3:E:129:ARG:NH1	2.04	0.72
5:G:63:LEU:HD11	6:H:59:MET:HE2	1.72	0.72
1:I:18:DC:OP1	3:E:63:ARG:HD2	1.90	0.72
4:F:51:TYR:O	4:F:54:THR:HG22	1.91	0.70
1:I:-23:DC:H3'	3:A:72:ARG:HH22	1.56	0.70
2:J:-23:DA:C5'	3:E:83:ARG:HD2	2.21	0.70
4:F:75:HIS:CD2	6:H:77:LEU:HD21	2.28	0.69
3:A:109:LEU:HD21	3:E:129:ARG:CZ	2.23	0.69
7:W:1206:ILE:HG22	7:W:1209:LYS:HD2	1.75	0.69
3:E:42:ARG:C	3:E:45:THR:HG23	2.18	0.68
6:D:54:LYS:O	6:D:58:ILE:HD12	1.93	0.68
2:J:-14:DG:H4'	2:J:-13:DA:OP1	1.94	0.68
3:E:77:ASP:OD1	3:E:78:PHE:N	2.29	0.66
1:I:44:DG:OP1	5:C:32:ARG:NH1	2.28	0.66
4:B:31:LYS:HG3	4:B:32:PRO:HD3	1.78	0.66
5:G:83:LEU:O	5:G:87:VAL:HG23	1.95	0.65
5:G:63:LEU:HD23	6:H:42:LEU:HD13	1.80	0.63
3:A:56:LYS:CE	7:W:141:TYR:HE1	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:72:ASP:CG	7:W:137:TYR:HB2	2.24	0.62
3:E:60:LEU:HD21	3:E:94:GLU:OE2	1.98	0.62
6:H:73:GLU:OE2	6:H:76:ARG:NH2	2.32	0.62
7:W:501:GLU:N	7:W:501:GLU:OE1	2.32	0.62
7:W:510:MET:HE3	7:W:534:VAL:HG21	1.82	0.62
7:W:1141:LYS:O	7:W:1145:ASN:ND2	2.34	0.61
5:G:84:GLN:OE1	5:G:102:ILE:HD12	1.99	0.61
7:W:419:ILE:HG23	7:W:425:ASN:HB3	1.83	0.61
2:J:70:DC:OP1	3:E:45:THR:CB	2.49	0.60
3:A:56:LYS:NZ	7:W:141:TYR:CE1	2.66	0.60
6:D:36:ILE:O	6:D:40:LYS:NZ	2.33	0.60
4:F:64:ASN:O	4:F:67:ARG:HG2	2.02	0.60
5:G:72:ASP:CB	7:W:137:TYR:HB2	2.31	0.60
2:J:7:DA:OP1	4:B:48:GLY:N	2.34	0.59
5:C:25:PHE:CE1	6:D:41:VAL:HG21	2.38	0.59
4:F:71:THR:HB	6:H:97:LEU:HD21	1.85	0.59
4:F:66:ILE:O	4:F:70:VAL:HG23	2.03	0.59
7:W:1170:ASN:O	7:W:1171:TRP:C	2.45	0.59
6:D:91:ILE:O	6:D:95:VAL:HG23	2.02	0.58
3:E:42:ARG:HB2	3:E:45:THR:HG21	1.85	0.58
7:W:401:ASP:OD2	7:W:597:ARG:NH2	2.37	0.58
5:G:57:TYR:HE2	6:H:103:LEU:HD12	1.68	0.57
7:W:284:PHE:HE1	7:W:313:ARG:HB3	1.69	0.57
2:J:-23:DA:H5''	3:E:83:ARG:CD	2.32	0.57
2:J:70:DC:OP1	3:E:45:THR:CG2	2.52	0.57
2:J:70:DC:O3'	3:E:42:ARG:HG3	2.04	0.57
1:I:46:DC:P	5:G:13:LYS:NZ	2.77	0.57
7:W:229:THR:H	7:W:232:SER:HB3	1.68	0.57
6:D:87:THR:HG22	6:D:88:SER:H	1.70	0.57
5:G:25:PHE:CE1	6:H:41:VAL:HG21	2.40	0.56
7:W:183:ILE:O	7:W:277:ARG:NH1	2.33	0.56
3:A:56:LYS:CE	7:W:141:TYR:CE1	2.88	0.56
2:J:21:DT:OP1	7:W:524:SER:N	2.39	0.56
1:I:-4:DA:H2'	1:I:-3:DT:H71	1.86	0.55
1:I:64:DG:OP2	7:W:1002:ALA:HB3	2.06	0.55
2:J:-49:DT:H2''	2:J:-48:DA:C8	2.42	0.55
4:B:31:LYS:CG	4:B:32:PRO:CD	2.83	0.55
6:D:64:ASN:O	6:D:68:GLU:OE1	2.25	0.55
1:I:18:DC:OP1	3:E:63:ARG:CD	2.53	0.55
3:A:62:ILE:HD11	4:B:37:LEU:HD11	1.89	0.55
5:C:63:LEU:HD21	6:D:59:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:71:THR:HG21	6:H:97:LEU:CD2	2.37	0.55
5:G:72:ASP:HB2	7:W:137:TYR:HB2	1.89	0.54
7:W:221:SER:O	7:W:223:LEU:N	2.39	0.54
4:B:31:LYS:HG3	4:B:32:PRO:CD	2.36	0.54
4:F:71:THR:CG2	6:H:97:LEU:HD21	2.38	0.54
3:E:42:ARG:HB2	3:E:45:THR:CG2	2.38	0.54
5:G:72:ASP:OD2	7:W:137:TYR:HB2	2.07	0.53
7:W:345:LYS:HG2	7:W:1038:ASP:HB3	1.89	0.53
5:C:115:LEU:HD11	3:E:112:ILE:HD11	1.90	0.53
3:E:42:ARG:O	3:E:45:THR:CG2	2.41	0.53
3:E:46:VAL:HG12	3:E:50:GLU:OE2	2.08	0.53
4:F:71:THR:CB	6:H:97:LEU:HD21	2.38	0.53
5:C:55:LEU:HD22	6:D:63:VAL:HG13	1.90	0.53
2:J:-69:DT:H4'	7:W:1016:ARG:HH22	1.74	0.53
4:F:70:VAL:O	4:F:74:GLU:OE1	2.28	0.52
1:I:-34:DA:H2''	1:I:-33:DT:H71	1.92	0.52
3:E:86:SER:O	3:E:89:VAL:HG12	2.09	0.52
5:G:68:ASN:OD1	5:G:71:ARG:NH2	2.39	0.52
5:G:59:THR:O	5:G:63:LEU:HD13	2.09	0.52
7:W:217:TRP:HH2	7:W:233:ILE:HD13	1.75	0.52
3:A:101:VAL:O	3:A:105:GLU:OE1	2.28	0.52
3:E:46:VAL:O	3:E:49:ARG:HG2	2.11	0.51
3:A:70:LEU:HD22	4:B:29:ILE:HD11	1.93	0.51
4:F:71:THR:HG21	6:H:97:LEU:HD21	1.91	0.51
5:C:83:LEU:O	5:C:87:VAL:HG23	2.10	0.50
6:H:105:LYS:O	6:H:108:VAL:HG12	2.10	0.50
2:J:-13:DA:H2'	4:F:32:PRO:HG2	1.93	0.50
6:D:87:THR:HG22	6:D:88:SER:N	2.27	0.50
3:A:105:GLU:O	3:A:109:LEU:HD13	2.12	0.49
4:B:31:LYS:CG	4:B:32:PRO:HD3	2.39	0.49
3:E:48:LEU:HD23	3:E:51:ILE:HD12	1.94	0.49
7:W:1009:SER:O	7:W:1044:LYS:NZ	2.42	0.49
7:W:217:TRP:HB2	7:W:220:GLU:HG3	1.93	0.49
1:I:-73:DC:N4	2:J:72:DC:H41	2.10	0.49
5:G:63:LEU:CD1	6:H:59:MET:HE2	2.42	0.49
6:H:34:TYR:HD2	6:H:63:VAL:HG21	1.78	0.49
6:D:96:ARG:HH12	6:D:108:VAL:HG11	1.77	0.49
5:C:29:ARG:NH1	6:D:33:SER:O	2.45	0.49
7:W:368:PRO:HD2	7:W:371:ILE:HD12	1.94	0.49
7:W:308:LEU:CD2	7:W:469:TYR:CE2	2.96	0.48
2:J:-12:DC:H2'	2:J:-12:DC:OP2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:183:ILE:HD11	7:W:216:LYS:HB2	1.93	0.48
7:W:358:ARG:NH1	7:W:391:TRP:O	2.44	0.48
5:C:51:LEU:HD21	6:D:67:PHE:CD1	2.48	0.48
5:C:97:LEU:HD11	6:D:62:PHE:CE2	2.48	0.48
7:W:328:VAL:HG11	7:W:1202:PRO:HB2	1.95	0.48
4:B:30:THR:OG1	4:B:33:ALA:HB2	2.13	0.48
3:E:41:TYR:HB3	3:E:45:THR:OG1	2.14	0.48
6:H:110:GLU:O	6:H:113:LYS:HG2	2.14	0.48
5:C:63:LEU:HD21	6:D:59:MET:SD	2.53	0.48
7:W:286:VAL:O	7:W:312:ARG:HG2	2.14	0.48
1:I:46:DC:P	5:G:13:LYS:HZ3	2.37	0.48
3:E:60:LEU:HD22	3:E:93:GLN:HG2	1.96	0.48
7:W:351:SER:OG	7:W:423:ARG:O	2.22	0.47
2:J:-23:DA:H5'	3:E:83:ARG:HD2	1.94	0.47
5:C:23:LEU:HD11	5:C:53:ALA:N	2.30	0.47
4:F:62:LEU:O	4:F:63:GLU:C	2.56	0.47
1:I:64:DG:C6	1:I:65:DT:H71	2.49	0.47
5:C:63:LEU:HD21	6:D:59:MET:HE1	1.96	0.47
3:A:97:GLU:O	3:A:101:VAL:HG23	2.15	0.47
7:W:539:LEU:HG	7:W:559:LEU:HD21	1.95	0.47
6:H:91:ILE:O	6:H:95:VAL:HG23	2.15	0.47
6:H:73:GLU:HG3	6:H:98:LEU:HD21	1.95	0.47
7:W:1154:ASP:N	7:W:1154:ASP:OD1	2.46	0.47
2:J:70:DC:H3'	3:E:42:ARG:CD	2.44	0.47
6:D:98:LEU:O	6:D:99:LEU:C	2.58	0.47
7:W:284:PHE:CE1	7:W:313:ARG:HB3	2.49	0.47
7:W:288:GLU:HB2	7:W:312:ARG:HD2	1.95	0.46
7:W:308:LEU:HD22	7:W:469:TYR:CE2	2.49	0.46
5:G:51:LEU:HD21	6:H:67:PHE:CD1	2.50	0.46
1:I:46:DC:P	5:G:13:LYS:HZ2	2.39	0.46
7:W:419:ILE:HG12	7:W:425:ASN:HA	1.98	0.46
7:W:290:ILE:O	7:W:341:ARG:NH1	2.48	0.46
2:J:-3:DC:H5'	2:J:-3:DC:C6	2.50	0.46
5:C:94:ASN:O	5:C:98:GLY:N	2.48	0.46
2:J:39:DC:H5'	2:J:39:DC:C6	2.51	0.45
3:E:108:ASN:O	3:E:112:ILE:HG12	2.16	0.45
7:W:1044:LYS:HB2	7:W:1049:TYR:CZ	2.51	0.45
7:W:595:LEU:HD21	7:W:597:ARG:HH12	1.81	0.45
2:J:-8:DG:C8	2:J:-8:DG:H5'	2.51	0.45
6:H:102:GLU:HG3	6:H:105:LYS:HE3	1.99	0.44
7:W:1142:TYR:HA	7:W:1145:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:-37:DC:H2''	2:J:-36:DC:C5	2.52	0.44
3:A:104:PHE:HA	3:A:107:THR:HG22	1.98	0.44
6:H:30:ARG:N	6:H:30:ARG:HE	2.16	0.44
7:W:507:TRP:HB2	7:W:534:VAL:HG22	1.98	0.44
2:J:-15:DG:H1'	2:J:-14:DG:C8	2.52	0.44
2:J:-3:DC:H5'	2:J:-3:DC:H6	1.82	0.44
6:D:64:ASN:O	6:D:67:PHE:HB3	2.17	0.44
6:H:105:LYS:HA	6:H:108:VAL:HG12	1.98	0.44
7:W:564:PHE:HE2	7:W:589:ARG:HB3	1.83	0.44
7:W:383:GLY:O	7:W:387:MET:HG3	2.17	0.44
7:W:389:PHE:CZ	7:W:393:LYS:HD2	2.53	0.44
4:F:68:ASP:HB2	4:F:89:ALA:HB1	2.00	0.44
5:G:23:LEU:HD11	5:G:53:ALA:N	2.32	0.44
4:F:54:THR:HA	4:F:57:VAL:HG22	2.00	0.44
7:W:398:ILE:HG13	7:W:559:LEU:HD11	2.00	0.44
2:J:-23:DA:H4'	3:E:83:ARG:CZ	2.49	0.43
4:B:31:LYS:HG2	4:B:32:PRO:CD	2.48	0.43
7:W:373:GLY:HA3	7:W:447:TRP:CD2	2.52	0.43
3:A:77:ASP:OD1	3:A:77:ASP:N	2.52	0.43
5:C:73:ASN:O	5:C:74:LYS:HB3	2.18	0.43
4:F:70:VAL:HG12	4:F:74:GLU:OE2	2.19	0.43
5:C:74:LYS:HD2	5:C:74:LYS:O	2.17	0.43
3:E:48:LEU:HA	3:E:51:ILE:HD12	2.00	0.43
5:C:88:ARG:HB2	5:C:108:LEU:HD21	2.00	0.43
7:W:567:ASP:OD1	7:W:567:ASP:N	2.51	0.43
3:A:51:ILE:O	3:A:55:GLN:HG3	2.18	0.43
5:G:87:VAL:HG11	5:G:97:LEU:HD12	1.99	0.43
4:F:58:LEU:O	4:F:62:LEU:HD13	2.19	0.43
7:W:308:LEU:CD2	7:W:469:TYR:CD2	3.02	0.42
5:G:50:TYR:CD1	6:H:111:GLY:HA3	2.55	0.42
2:J:-6:DG:H4'	3:E:43:PRO:HG2	2.01	0.42
2:J:-69:DT:H2''	2:J:-68:DC:C6	2.54	0.42
4:B:30:THR:OG1	4:B:33:ALA:CB	2.67	0.42
7:W:472:TYR:HB3	7:W:481:LYS:HB3	2.00	0.42
5:C:115:LEU:HD12	5:C:115:LEU:N	2.35	0.42
7:W:133:LYS:HE2	7:W:133:LYS:HB3	1.88	0.42
5:C:39:TYR:CD2	6:D:71:ALA:HB1	2.54	0.42
5:C:103:ALA:HB2	4:F:100:PHE:CE2	2.54	0.42
3:E:97:GLU:O	3:E:101:VAL:HG23	2.20	0.42
7:W:265:GLU:HA	7:W:268:GLU:HG2	2.01	0.41
7:W:335:VAL:O	7:W:339:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:103:ALA:HB2	4:F:100:PHE:HE2	1.86	0.41
7:W:291:ILE:HD11	7:W:310:LYS:HB2	2.02	0.41
3:E:46:VAL:O	3:E:47:ALA:C	2.63	0.41
7:W:456:TYR:OH	7:W:498:ASP:OD2	2.30	0.41
7:W:1168:VAL:HB	7:W:1171:TRP:CG	2.55	0.41
7:W:288:GLU:HB2	7:W:312:ARG:HA	2.03	0.41
5:C:75:LYS:HE3	5:C:79:ILE:HD13	2.02	0.41
3:E:62:ILE:HD12	3:E:97:GLU:HG3	2.03	0.41
6:H:77:LEU:C	6:H:77:LEU:HD23	2.46	0.41
4:B:62:LEU:O	4:B:63:GLU:C	2.62	0.41
3:A:126:LEU:CD1	3:E:113:HIS:HB2	2.51	0.41
5:C:58:LEU:HD11	6:D:99:LEU:HD11	2.03	0.41
5:G:15:LYS:HB2	5:G:20:ARG:HH21	1.85	0.41
2:J:-23:DA:H5'	3:E:83:ARG:NH1	2.36	0.40
2:J:34:DT:H5'	2:J:34:DT:C6	2.56	0.40
6:H:102:GLU:O	6:H:105:LYS:HG3	2.21	0.40
7:W:221:SER:C	7:W:223:LEU:H	2.25	0.40
5:C:97:LEU:HD11	6:D:62:PHE:HE2	1.86	0.40
7:W:467:ARG:NH1	7:W:501:GLU:HG2	2.36	0.40
2:J:-17:DG:H2''	2:J:-16:DG:C8	2.57	0.40
2:J:-48:DA:H4'	2:J:-47:DG:OP1	2.21	0.40
5:C:26:PRO:HD3	6:D:37:TYR:CG	2.56	0.40
7:W:1210:ILE:HG22	7:W:1212:LEU:HG	2.03	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	
3	A	90/136 (66%)	89 (99%)	1 (1%)	0	100	100
3	E	95/136 (70%)	94 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
4	F	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
5	C	103/130 (79%)	102 (99%)	1 (1%)	0	100	100
5	G	96/130 (74%)	95 (99%)	1 (1%)	0	100	100
6	D	92/126 (73%)	86 (94%)	6 (6%)	0	100	100
6	H	90/126 (71%)	89 (99%)	1 (1%)	0	100	100
7	W	642/1467 (44%)	582 (91%)	58 (9%)	2 (0%)	36	67
All	All	1364/2457 (56%)	1289 (94%)	73 (5%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	W	1171	TRP
7	W	1169	GLN

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	
3	A	79/111 (71%)	79 (100%)	0	100	100
3	E	83/111 (75%)	83 (100%)	0	100	100
4	B	65/79 (82%)	65 (100%)	0	100	100
4	F	64/79 (81%)	64 (100%)	0	100	100
5	C	81/100 (81%)	81 (100%)	0	100	100
5	G	74/100 (74%)	74 (100%)	0	100	100
6	D	80/106 (76%)	80 (100%)	0	100	100
6	H	78/106 (74%)	78 (100%)	0	100	100
7	W	499/1312 (38%)	499 (100%)	0	100	100
All	All	1103/2104 (52%)	1103 (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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	76	GLN
5	C	31	HIS
5	C	104	GLN
6	D	44	GLN
3	E	55	GLN
7	W	138	ASN
7	W	340	ASN
7	W	459	ASN
7	W	460	GLN
7	W	546	GLN
7	W	1145	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

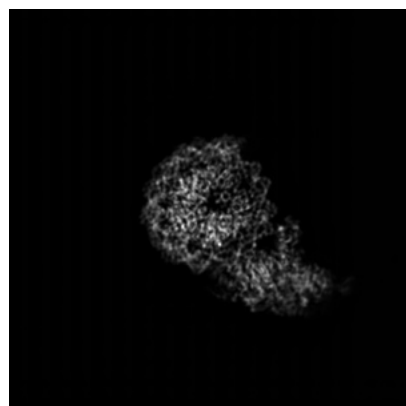
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53595. These allow visual inspection of the internal detail of the map and identification of artifacts.

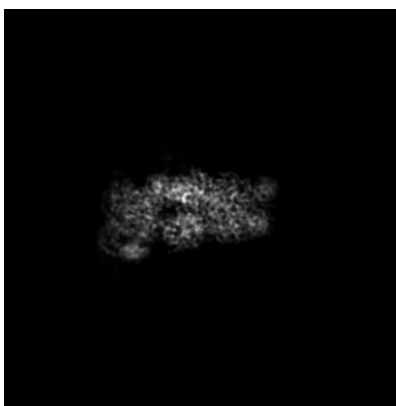
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

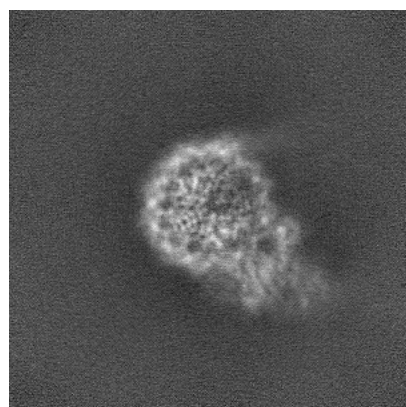


Y

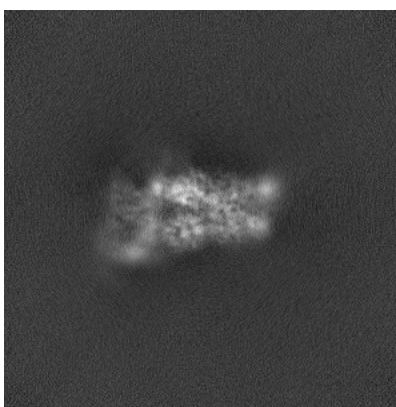


Z

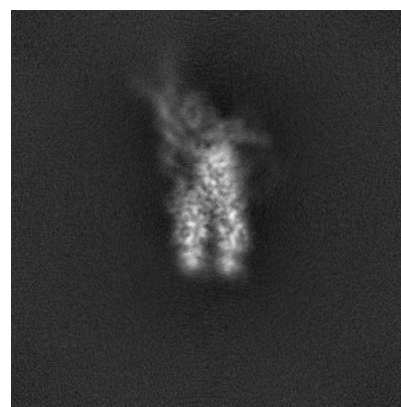
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

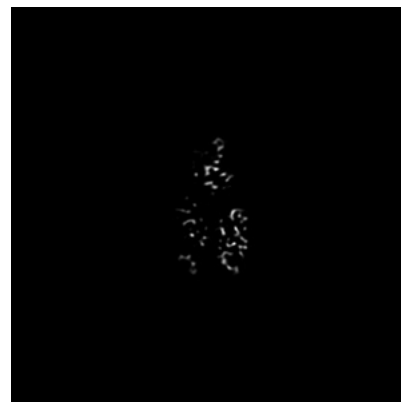
6.2.1 Primary map



X Index: 280

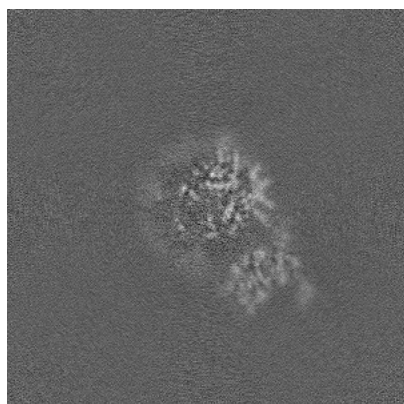


Y Index: 280

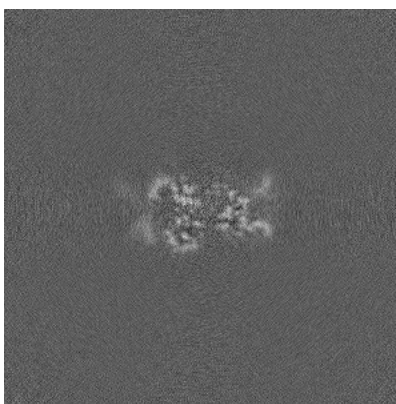


Z Index: 280

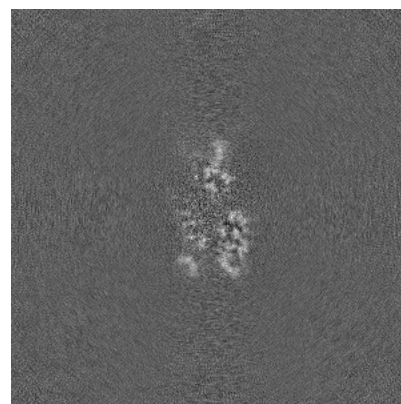
6.2.2 Raw map



X Index: 280



Y Index: 280



Z Index: 280

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

6.3 Largest variance slices [i](#)

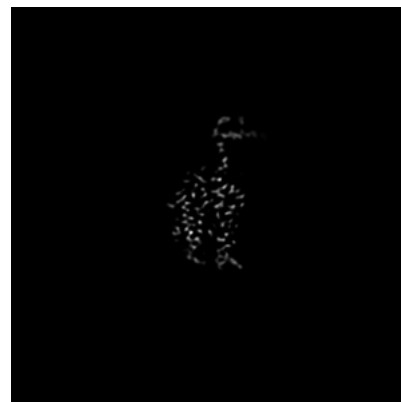
6.3.1 Primary map



X Index: 301

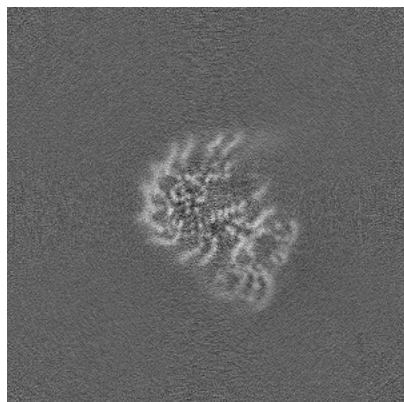


Y Index: 259

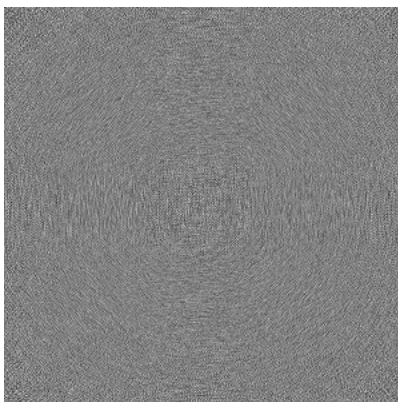


Z Index: 252

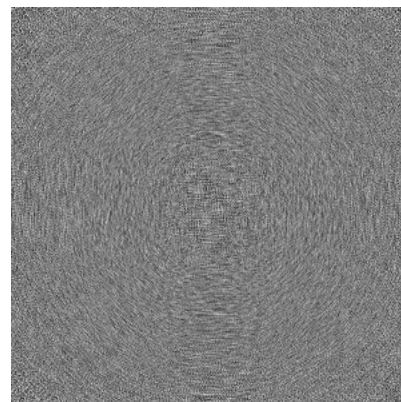
6.3.2 Raw map



X Index: 301



Y Index: 0

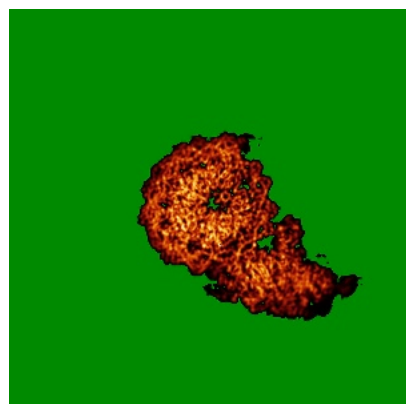


Z Index: 0

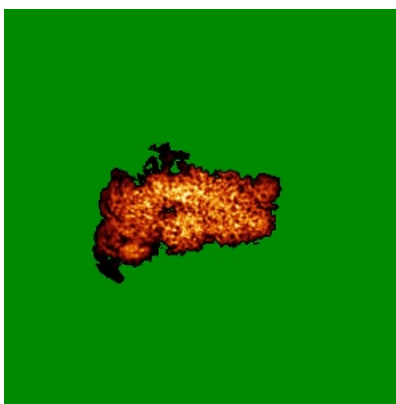
The images above show the largest variance slices of the map in three orthogonal directions.

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

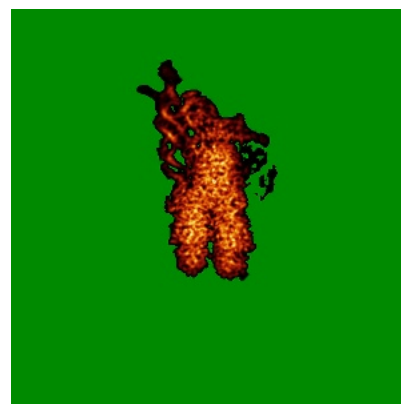
6.4.1 Primary map



X

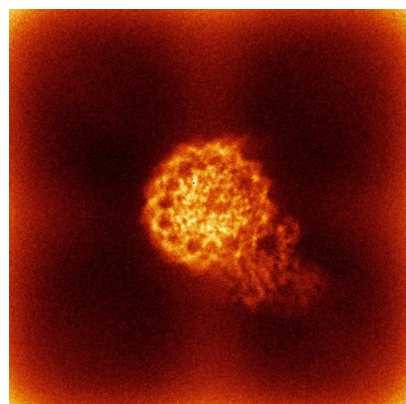


Y

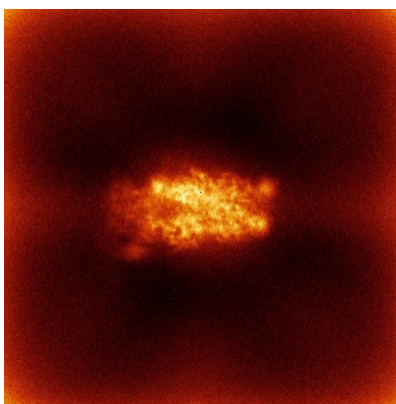


Z

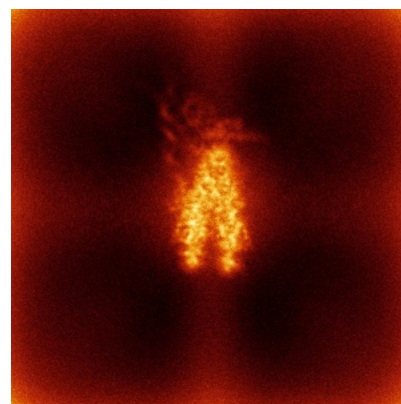
6.4.2 Raw map



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](#)

This section was not generated.

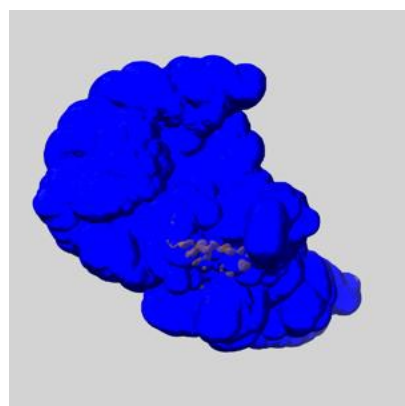
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

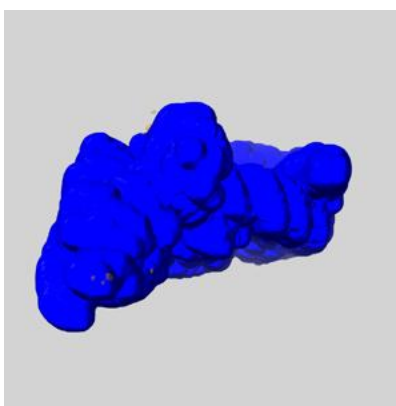
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

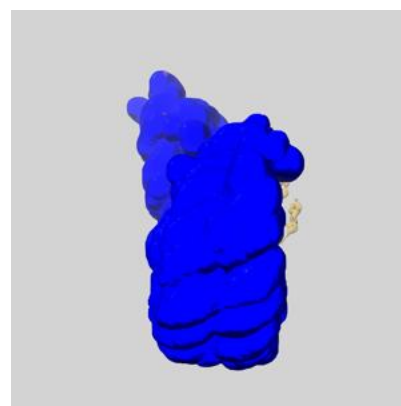
6.6.1 emd_53595_msk_1.map [i](#)



X



Y

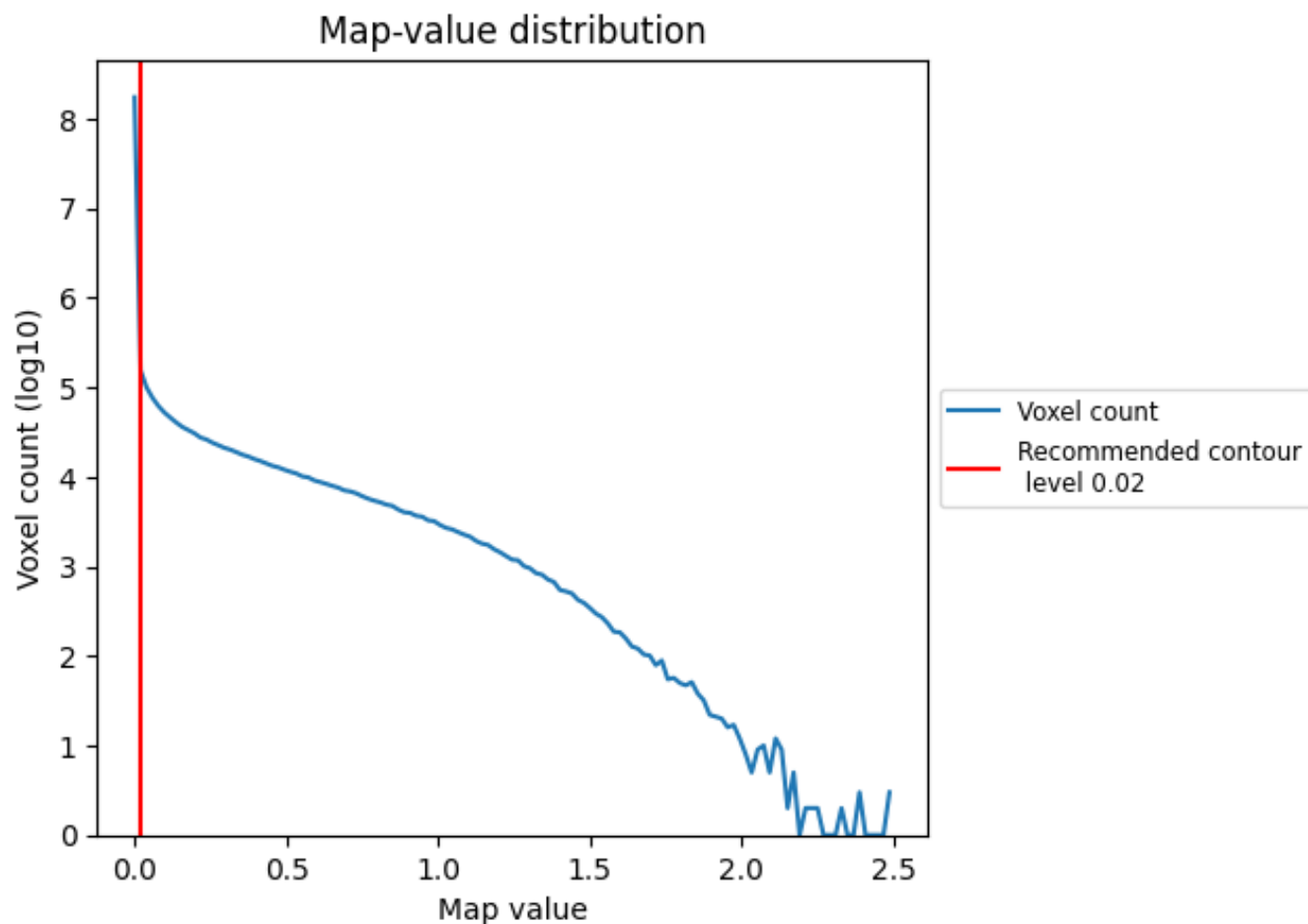


Z

7 Map analysis [i](#)

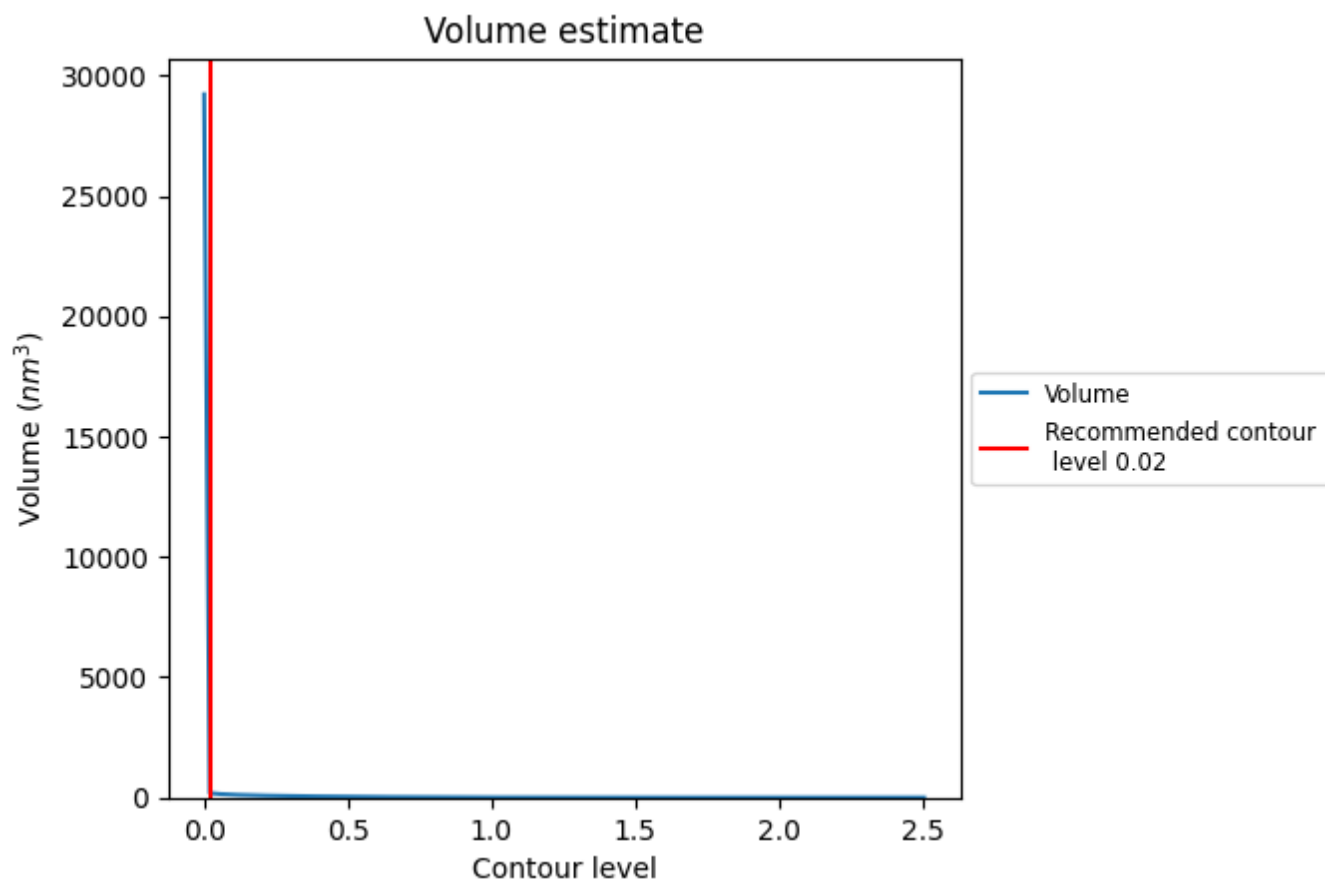
This section contains the results of statistical analysis of the map.

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.

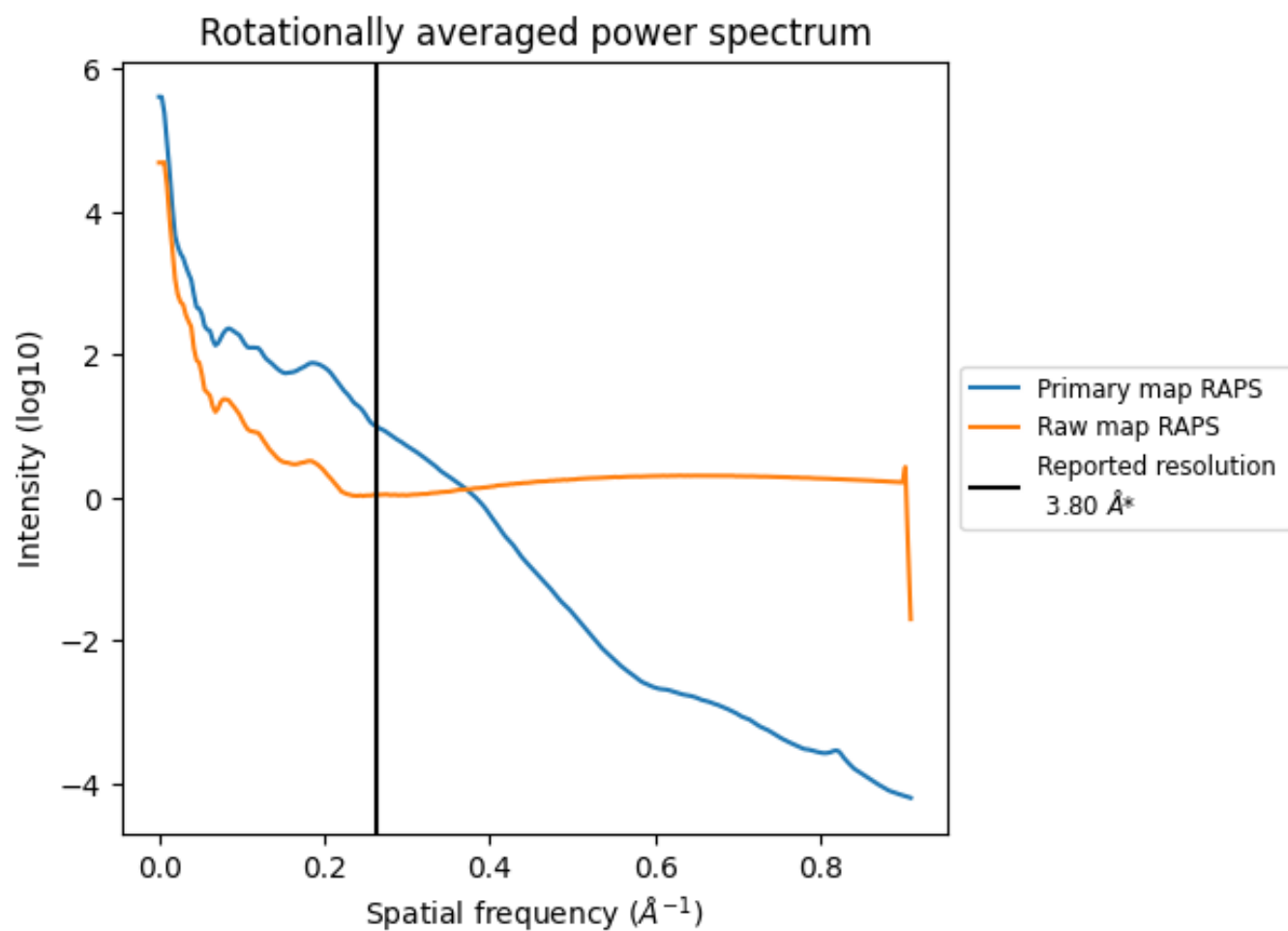
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 182 nm^3 ; this corresponds to an approximate mass of 165 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 ⓘ

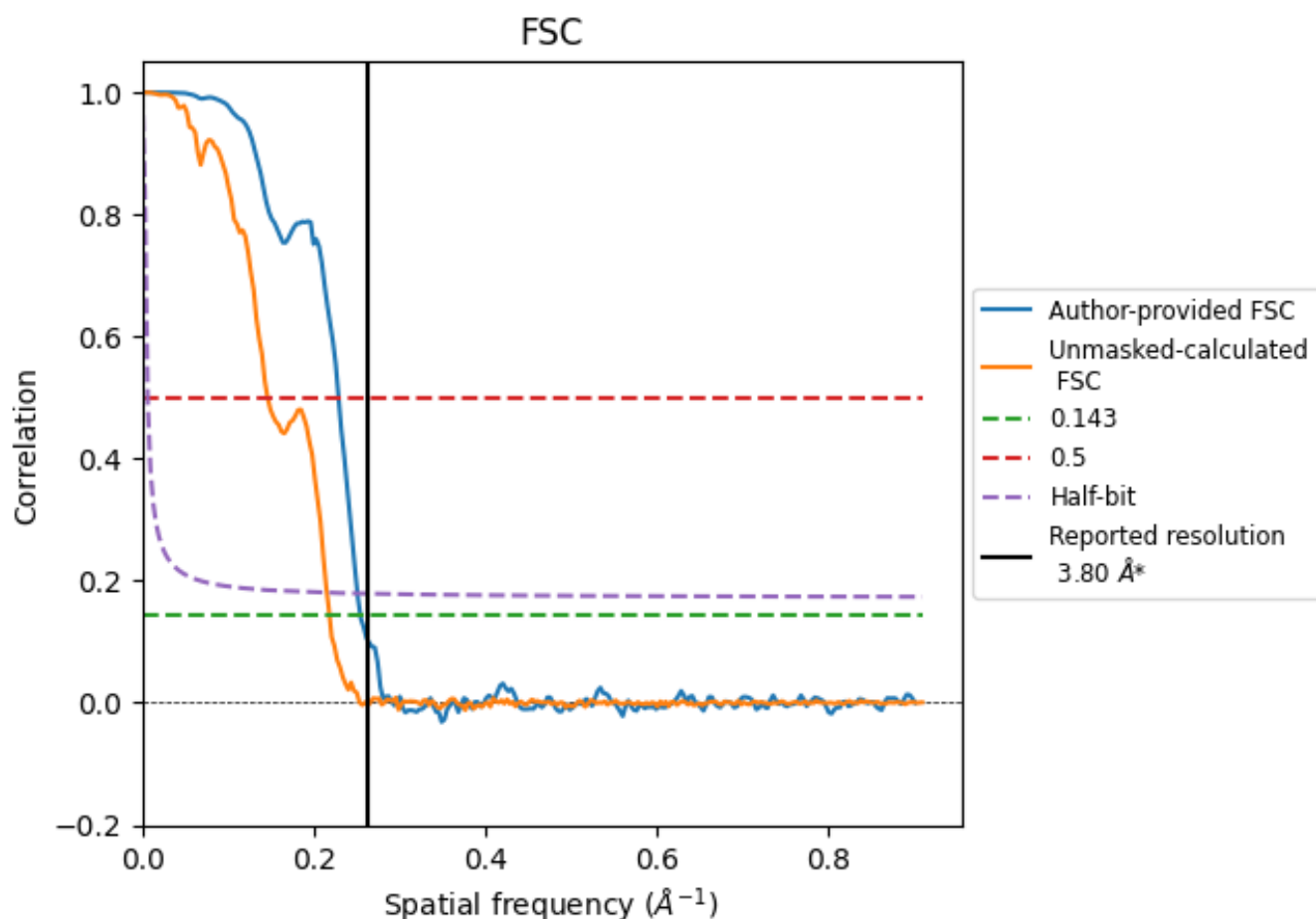


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

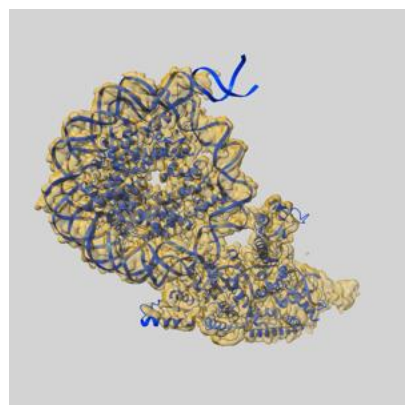
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.93	4.37	3.98
Unmasked-calculated*	4.58	6.84	4.64

*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 4.58 differs from the reported value 3.8 by more than 10 %

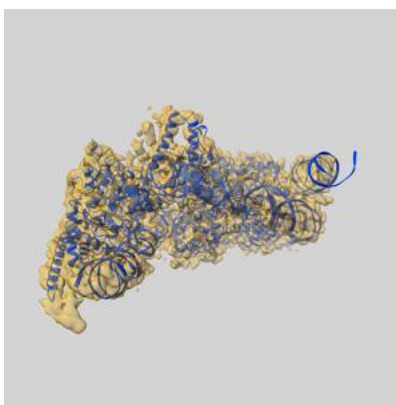
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53595 and PDB model 9R5S. Per-residue inclusion information can be found in section [3](#) on page [6](#).

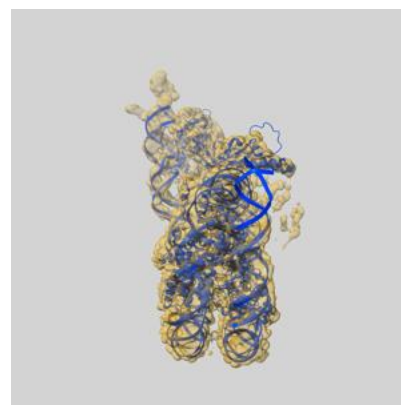
9.1 Map-model overlay [i](#)



X



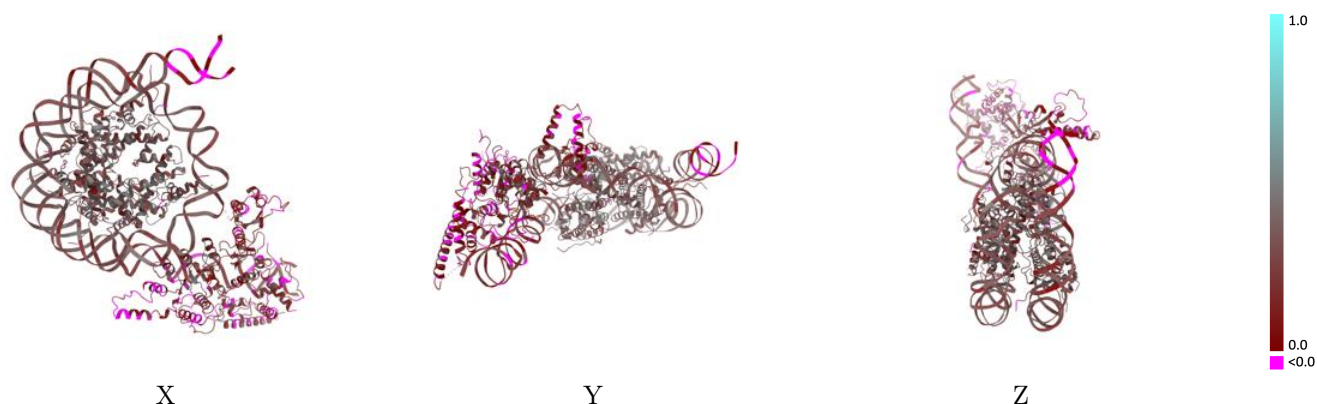
Y



Z

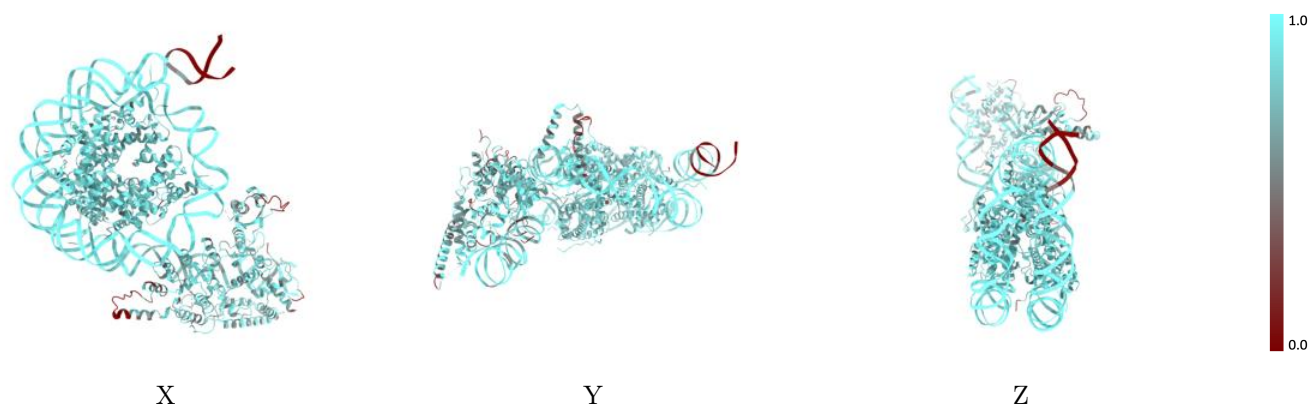
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



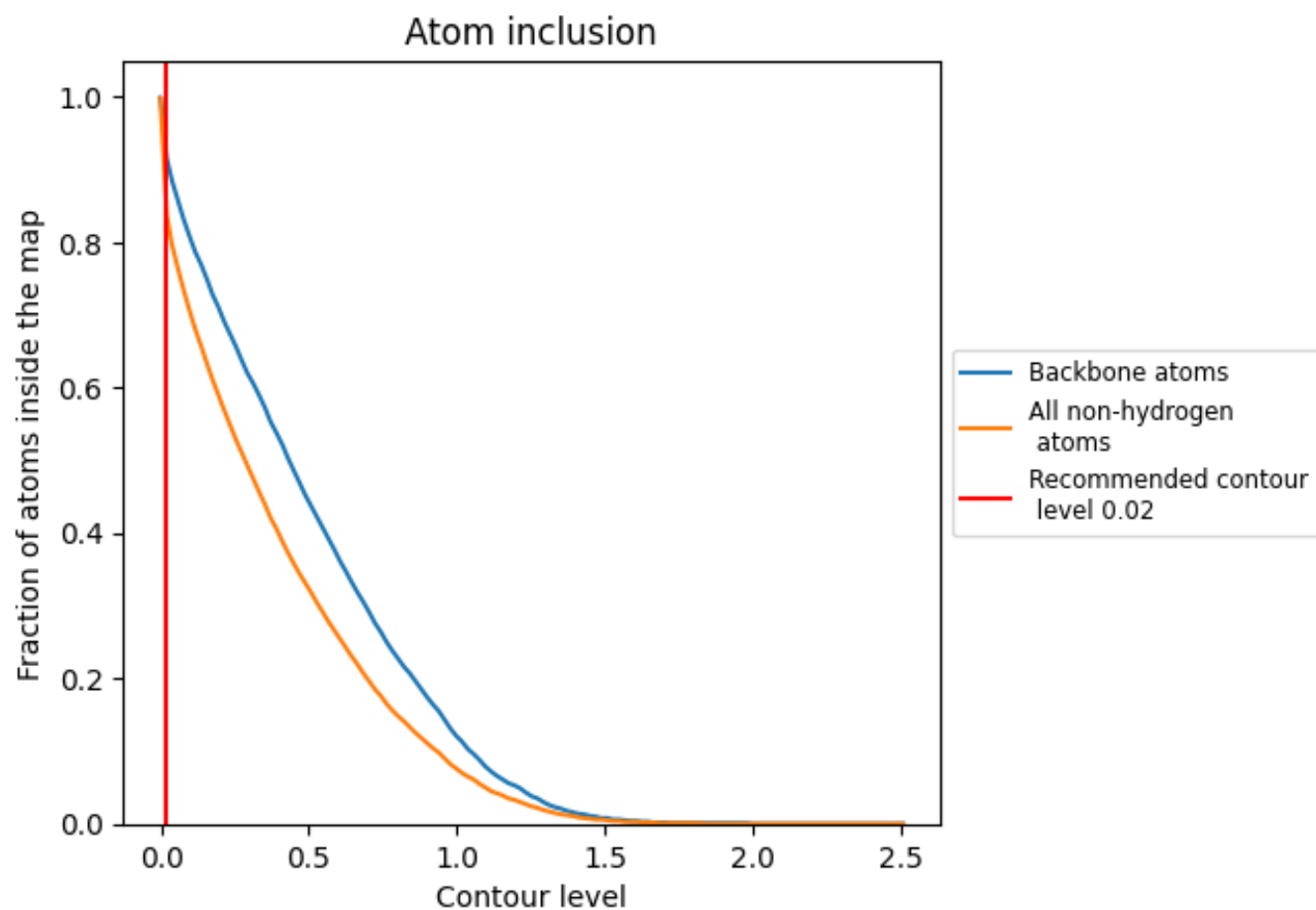
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8370	 0.2560
A	 0.8820	 0.3500
B	 0.8770	 0.3510
C	 0.8760	 0.3410
D	 0.8800	 0.3200
E	 0.8690	 0.2940
F	 0.8930	 0.3470
G	 0.8740	 0.3530
H	 0.8660	 0.3100
I	 0.8830	 0.2730
J	 0.8700	 0.2610
W	 0.7390	 0.1530

