



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 08:20 AM UTC

PDB ID : 8HAH / pdb_00008hah
EMDB ID : EMD-34589
Title : Cryo-EM structure of the p300 catalytic core bound to the H4K12acK16ac nucleosome, class 2 (3.9 angstrom resolution)
Authors : Kikuchi, M.; Morita, S.; Wakamori, M.; Shin, S.; Uchikubo-Kamo, T.; Shirouzu, M.; Umehara, T.
Deposited on : 2022-10-26
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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

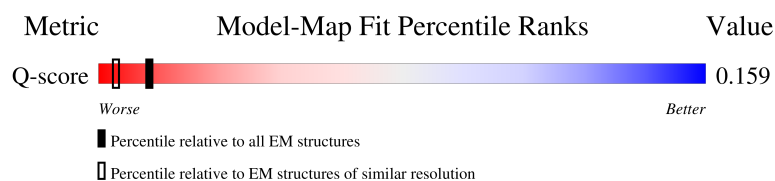
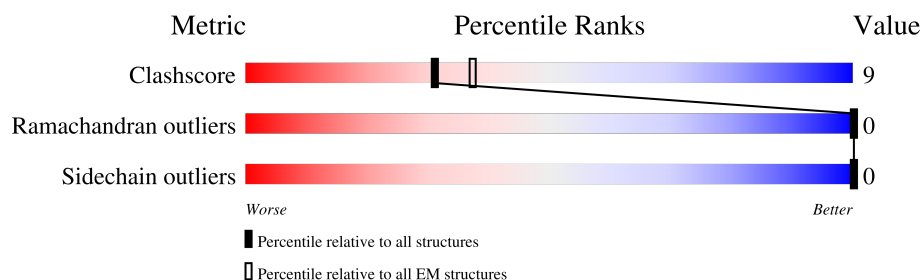
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



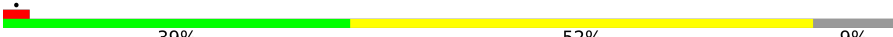
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	135	 59% 18% 24%
1	E	135	 51% 22% 27%
2	B	102	 69% 10% 22%
2	F	102	 69% 13% 19%

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Mol	Chain	Length	Quality of chain
3	C	129	
3	G	129	
4	D	125	
4	H	125	
5	I	180	
5	J	180	
6	K	796	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17096 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 Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	103	Total	C	N	O	S	0	0
			838	527	163	144	4		
1	E	99	Total	C	N	O	S	0	0
			816	514	158	140	4		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
2	F	83	Total	C	N	O	S	0	0
			662	418	129	114	1		

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	107	Total	C	N	O	S	0	0
			824	520	161	143			
3	G	105	Total	C	N	O	S	0	0
			810	511	158	141			

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	97	Total	C	N	O	S	0	0
			761	477	141	141	2		
4	H	96	Total	C	N	O	S	0	0
			756	474	140	140	2		

- Molecule 5 is a DNA chain called DNA (180-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	164	Total	C	N	O	P	0	0
			3365	1605	615	981	164		
5	J	164	Total	C	N	O	P	0	0
			3359	1604	604	987	164		

- Molecule 6 is a protein called Histone acetyltransferase p300.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	517	Total	C	N	O	S	0	0
			4267	2729	729	776	33		

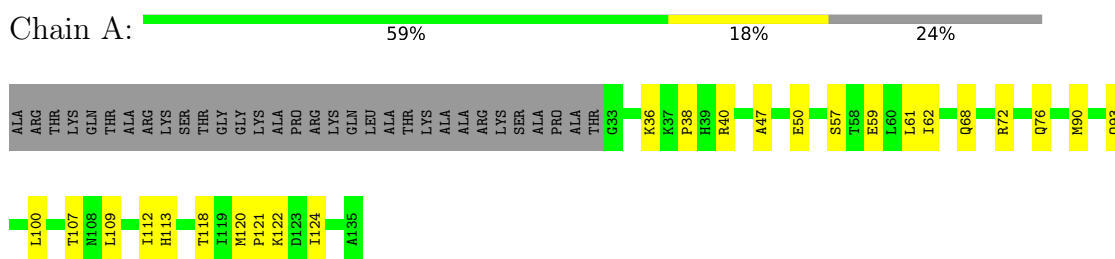
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1041	GLY	-	expression tag	UNP Q09472
K	1042	SER	-	expression tag	UNP Q09472
K	1043	SER	-	expression tag	UNP Q09472
K	1044	GLY	-	expression tag	UNP Q09472
K	1045	SER	-	expression tag	UNP Q09472
K	1046	SER	-	expression tag	UNP Q09472
K	1047	GLY	-	expression tag	UNP Q09472

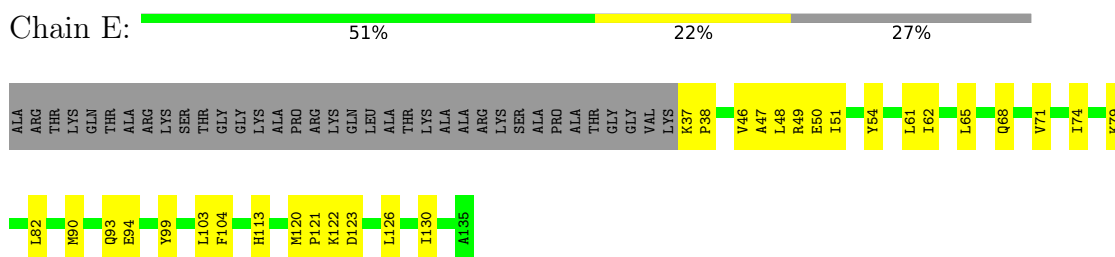
3 Residue-property plots [i](#)

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.

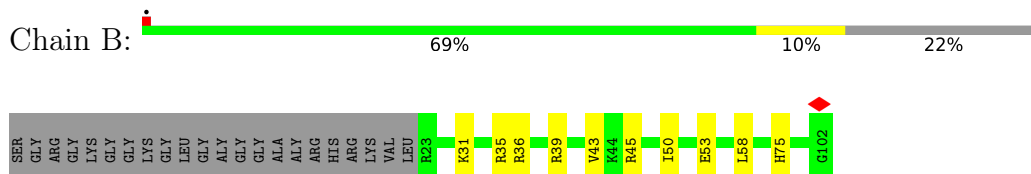
- Molecule 1: Histone H3.1



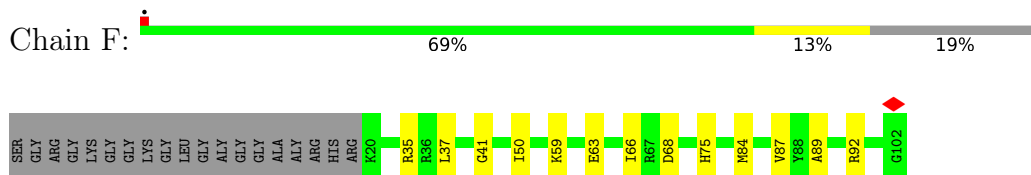
- Molecule 1: Histone H3.1



- Molecule 2: Histone H4



- Molecule 2: Histone H4



- Molecule 3: Histone H2A type 1-B/E

HIS	SER
LYS	GLY
ALA	ARG
LYS	GLY
GLY	LYS
LYS	GLN
	GLY
	GLY
	LYS
	ALA
	ARG
	A12
	R29
	L33
	K36
	G37
	N38
	Y39
	S40
	F41
	R42
	V43
	Y50
	Y57
	N68
	A69
	A70
	K74
	I79
	H82
	L83
	Q84
	R88
	N89
	D90
	N94
	R99
	G106
	L116
	F117
	K118
	LYS
	THR
	GLU
	SER
	TRP

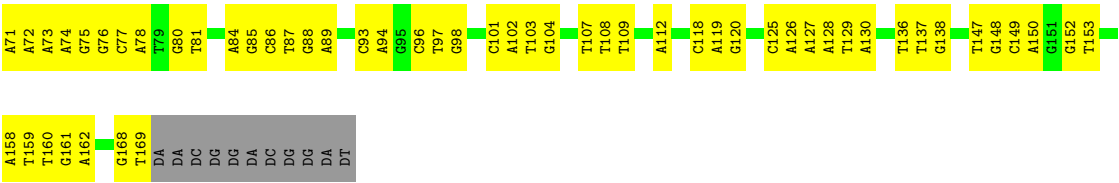
SER	GLY	ARG	GLY	LYS	GLN	GLY	GLY	LYS	ALA	ARG	ALA	LYS	A14	A21	Q24	V27	R35	N38	Y39	S40	V49	L58	I62	R88	L108	Q112	X118	LYS	THR	GLU	SER	SER	HIS	HIS	LYS	ALA	LYS	GLY	GLY
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E105	E113	E114	E115	E116	E117	E118	E119	T122	S123	A124	LYS														
PRO	GLU	PRO	ALA	LYS	SER	ALA	PRO	PRO	ALA	LYS	GLY	SER	LYS	ALA	VAL	THR	LYS	ALA	GLN	LYS	LYS	ASP	GLY	LYS	K28
Y40	Y41	Y42	K43	K44	L45	K46	P50	K57	A58	D68	R72	R79	L80	Y83	R86	S87	T88	T89	T90	S91	R92	E93			

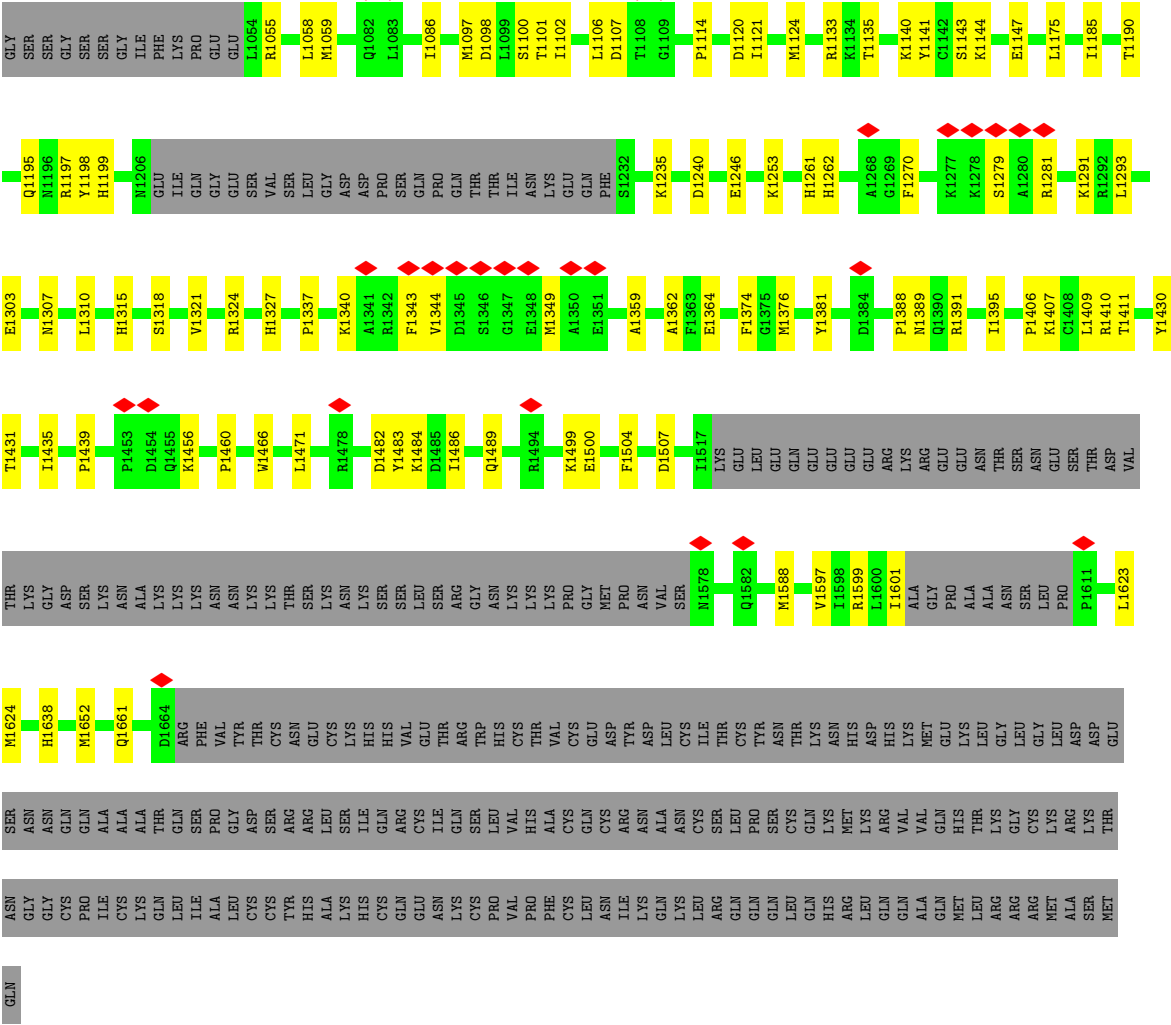
PRO	GLU	PRO	ALA	LYS	SER	ALA	PRO	PRO	ALA	ALA	LYS	LYS	GLY	LYS	LYS	ALA	VAL	THR	LYS	ALA	ALA	GLN	LYS	LYS	ASP	GLY	LYS	LYS	R29	Y37	Y40	Y41	Y42	K43	K46	K57	A58	T61	M62	R92	Q95	T96	R99	L100	E105	L106	K120	A124	LYS
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T110	G111	A112	T113	G114	G115	A116	C124	A125	A126	A127	T129	A130	C131	A132	C133	T134	T135	T136	T137	C146	T147	G148	C149	A150	A156	T157	A158	G161	A162	T163	G164	T169	A170	A171	C172	G173	G174	A175	DC	DG	DG	DA	DT
DA	DT	DC	DC	DG	DT	DC	DG	DT	A12	C20	A21	T31	G32	T40	A41	A46	T51	A52	T55	G56	G57	A58	A59	T62	G63	G66	C67	G77	A78	T79	A84	G85	G93	A94	G95	G98	C101	A102	T103	G104	C105	C106	T107

DA	DT	DC	DC	DC	DG	T6	C7	C8	G9	T10	T11	A12	G13	C14	G15	C20	A21	C26	C27	T31	G32	G35	T37	T38	C39	T40	A41	C42	C43	A44	A45	A46	A47	G48	T49	G50	T51	A52	T53	T54	T55	G56	G57	A58	A59	A60	G61	T62	G63	C66	C67	A68	T69
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• Molecule 6: Histone acetyltransferase p300



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74692	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	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0035	Depositor
Map size (Å)	281.86, 281.86, 281.86	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82899994, 0.82899994, 0.82899994	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/850	0.34	0/1137
1	E	0.12	0/828	0.35	0/1109
2	B	0.10	0/645	0.34	0/862
2	F	0.11	0/669	0.31	0/894
3	C	0.12	0/834	0.32	0/1125
3	G	0.11	0/820	0.31	0/1107
4	D	0.15	0/772	0.42	0/1036
4	H	0.14	0/767	0.37	0/1029
5	I	0.17	0/3776	0.36	0/5826
5	J	0.16	0/3766	0.36	0/5810
6	K	0.10	0/4382	0.30	0/5923
All	All	0.14	0/18109	0.34	0/25858

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	A	838	0	877	18	0
1	E	816	0	856	22	0
2	B	638	0	676	9	0
2	F	662	0	709	11	0
3	C	824	0	884	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	810	0	866	10	0
4	D	761	0	786	23	0
4	H	756	0	784	13	0
5	I	3365	0	1850	49	0
5	J	3359	0	1853	76	0
6	K	4267	0	4176	57	0
All	All	17096	0	14317	274	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 9.

All (274) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:1327:HIS:HB2	6:K:1624:MET:HE3	1.61	0.83
6:K:1097:MET:HE1	6:K:1102:ILE:HG13	1.67	0.76
6:K:1055:ARG:NH1	6:K:1059:MET:HG3	2.05	0.71
5:J:59:DA:H2'	5:J:60:DA:C8	2.27	0.69
4:D:106:LEU:O	4:D:109:HIS:HB2	1.95	0.67
3:C:40:SER:HA	3:G:38:ASN:HD21	1.60	0.67
3:G:24:GLN:HB3	4:H:43:LYS:HE2	1.79	0.65
5:I:113:DT:H2''	5:I:114:DG:C8	2.31	0.65
2:B:75:HIS:O	4:D:92:ARG:NH2	2.30	0.65
1:A:61:LEU:HD11	2:B:36:ARG:HE	1.62	0.65
6:K:1343:PHE:HB2	6:K:1349:MET:HE2	1.80	0.64
5:J:47:DA:H2''	5:J:48:DG:H8	1.63	0.63
4:H:29:ARG:NH2	5:J:120:DG:OP1	2.32	0.63
6:K:1407:LYS:HG3	6:K:1410:ARG:HH12	1.63	0.63
3:C:42:ARG:NH2	3:C:43:VAL:O	2.33	0.62
6:K:1195:GLN:HE21	6:K:1197:ARG:HD3	1.64	0.62
5:I:104:DG:H2''	5:I:105:DC:C5	2.35	0.61
5:J:11:DT:H2''	5:J:12:DA:C8	2.35	0.61
6:K:1195:GLN:HG2	6:K:1197:ARG:HG2	1.81	0.61
1:E:74:ILE:HG22	2:F:66:ILE:HD13	1.80	0.61
6:K:1055:ARG:HH11	6:K:1059:MET:HG3	1.66	0.61
6:K:1262:HIS:HB2	6:K:1652:MET:HE1	1.83	0.60
1:A:68:GLN:HE21	1:A:72:ARG:HE	1.49	0.60
6:K:1321:VAL:HG22	6:K:1364:GLU:HG3	1.84	0.60
5:J:40:DT:H2'	5:J:41:DA:H8	1.67	0.59
5:I:51:DT:H2'	5:I:52:DA:C8	2.36	0.59
5:J:20:DC:H2''	5:J:21:DA:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:LEU:HD23	3:C:36:LYS:HZ3	1.68	0.58
5:I:31:DT:H2''	5:I:32:DG:C8	2.39	0.58
6:K:1133:ARG:NH1	6:K:1135:THR:OG1	2.36	0.58
5:J:31:DT:H2''	5:J:32:DG:C8	2.38	0.58
6:K:1327:HIS:HB3	6:K:1359:ALA:HB3	1.85	0.58
5:I:161:DG:H2''	5:I:162:DA:C8	2.38	0.58
5:J:125:DC:H2''	5:J:126:DA:C8	2.38	0.58
6:K:1121:ILE:HA	6:K:1124:MET:HE2	1.85	0.58
6:K:1439:PRO:HG3	6:K:1460:PRO:HG3	1.86	0.57
6:K:1059:MET:HE3	6:K:1106:LEU:HD23	1.86	0.57
6:K:1504:PHE:HB2	6:K:1507:ASP:HB2	1.86	0.57
5:J:101:DC:H2'	5:J:102:DA:C8	2.38	0.57
6:K:1391:ARG:HD2	6:K:1430:TYR:HA	1.87	0.57
3:C:84:GLN:NE2	3:C:106:GLY:O	2.37	0.57
3:C:29:ARG:NH1	4:D:40:TYR:OH	2.38	0.56
5:I:169:DT:H2''	5:I:170:DA:C8	2.40	0.56
4:D:68:ASP:OD2	4:D:72:ARG:NH1	2.39	0.56
4:D:105:GLU:HA	4:D:108:LYS:HE2	1.87	0.56
2:F:68:ASP:HB3	2:F:89:ALA:HB1	1.88	0.56
1:A:112:ILE:HD13	3:G:112:GLN:HG3	1.89	0.55
6:K:1293:LEU:O	6:K:1324:ARG:NH1	2.39	0.55
6:K:1489:GLN:HG2	6:K:1597:VAL:HG11	1.87	0.55
5:J:26:DC:H2'	5:J:27:DC:C6	2.41	0.55
5:J:168:DG:H2''	5:J:169:DT:H5'	1.88	0.55
5:J:147:DT:H2''	5:J:148:DG:N7	2.22	0.55
6:K:1141:TYR:HD1	6:K:1144:LYS:HZ3	1.55	0.55
5:J:46:DA:H2''	5:J:47:DA:C8	2.41	0.55
5:J:46:DA:H2''	5:J:47:DA:H8	1.73	0.54
6:K:1411:THR:HG23	6:K:1466:TRP:HE1	1.72	0.54
6:K:1086:ILE:HG13	6:K:1086:ILE:O	2.06	0.54
6:K:1362:ALA:HB3	6:K:1374:PHE:HB3	1.89	0.54
1:E:48:LEU:HA	1:E:51:ILE:HG22	1.90	0.54
4:D:113:GLU:O	4:D:116:LYS:HG2	2.08	0.54
2:B:75:HIS:CD2	4:D:80:LEU:HD12	2.43	0.53
5:I:163:DT:H2''	5:I:164:DG:C8	2.44	0.53
5:J:160:DT:H2''	5:J:161:DG:C8	2.43	0.53
6:K:1337:PRO:HA	6:K:1340:LYS:HB2	1.90	0.53
4:D:90:THR:N	4:D:93:GLU:OE2	2.38	0.53
5:I:105:DC:H2''	5:I:106:DC:C5	2.43	0.53
5:I:172:DC:H2''	5:I:173:DG:C8	2.42	0.53
5:J:72:DA:H2''	5:J:73:DA:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:1140:LYS:O	6:K:1144:LYS:HG2	2.09	0.53
5:I:93:DC:H2''	5:I:94:DA:C8	2.44	0.53
5:I:20:DC:H2''	5:I:21:DA:C8	2.44	0.52
2:F:35:ARG:HH12	5:I:98:DG:P	2.31	0.52
6:K:1395:ILE:HD12	6:K:1435:ILE:HG12	1.90	0.52
5:I:125:DC:H2''	5:I:126:DA:C8	2.44	0.52
3:G:21:ALA:O	4:H:120:LYS:NZ	2.42	0.52
5:I:147:DT:H2''	5:I:148:DG:N7	2.24	0.52
6:K:1310:LEU:HD21	6:K:1318:SER:HB2	1.92	0.52
1:A:118:THR:HG22	2:B:45:ARG:HD3	1.91	0.52
3:C:90:ASP:O	3:C:94:ASN:ND2	2.43	0.52
5:I:135:DT:O4	5:J:45:DA:N6	2.41	0.52
5:J:159:DT:H2'	5:J:160:DT:H71	1.91	0.52
5:I:55:DT:H2''	5:I:56:DG:N7	2.24	0.52
5:J:40:DT:H2'	5:J:41:DA:C8	2.44	0.52
5:J:136:DT:H2''	5:J:137:DT:C5	2.45	0.52
5:J:55:DT:H2''	5:J:56:DG:N7	2.24	0.51
5:J:58:DA:H2''	5:J:59:DA:C8	2.45	0.51
1:A:36:LYS:HZ1	1:A:40:ARG:HH21	1.59	0.51
6:K:1198:TYR:O	6:K:1199:HIS:ND1	2.43	0.51
1:A:120:MET:HE3	1:A:120:MET:HA	1.92	0.51
3:C:116:LEU:O	3:C:118:LYS:NZ	2.41	0.51
1:E:79:LYS:HB3	1:E:82:LEU:HD11	1.91	0.51
4:H:42:TYR:O	4:H:46:LYS:HG2	2.11	0.51
5:I:79:DT:OP1	6:K:1140:LYS:NZ	2.34	0.51
5:J:47:DA:H2''	5:J:48:DG:C8	2.45	0.51
5:J:88:DG:H2''	5:J:89:DA:C8	2.45	0.51
6:K:1143:SER:O	6:K:1147:GLU:HG2	2.11	0.51
1:E:121:PRO:HG3	2:F:50:ILE:HG22	1.93	0.50
5:I:106:DC:H2''	5:I:107:DT:C5	2.46	0.50
3:C:57:TYR:CE2	4:D:109:HIS:HB3	2.47	0.50
5:I:101:DC:H2''	5:I:102:DA:C8	2.47	0.50
6:K:1279:SER:HB2	6:K:1281:ARG:HE	1.76	0.50
1:A:122:LYS:HG3	1:E:113:HIS:HE1	1.76	0.50
5:J:56:DG:H2''	5:J:57:DG:C8	2.45	0.50
5:J:136:DT:H2''	5:J:137:DT:C4	2.47	0.50
6:K:1623:LEU:HD13	6:K:1661:GLN:HE22	1.76	0.50
5:I:94:DA:H2''	5:I:95:DG:N7	2.26	0.49
5:J:38:DT:H2'	5:J:39:DC:H6	1.77	0.49
5:J:62:DT:H2''	5:J:63:DG:C8	2.47	0.49
5:I:84:DA:H2''	5:I:85:DG:N7	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:127:DA:H2''	5:J:128:DA:C8	2.47	0.49
5:J:86:DC:H2''	5:J:87:DT:C5	2.47	0.49
5:I:125:DC:H2''	5:I:126:DA:N7	2.27	0.49
6:K:1303:GLU:O	6:K:1307:ASN:ND2	2.46	0.49
1:E:126:LEU:O	1:E:130:ILE:HG12	2.13	0.49
5:I:157:DT:H2''	5:I:158:DA:C8	2.47	0.49
5:I:46:DA:H5'	5:I:46:DA:C8	2.48	0.49
5:I:132:DA:H2'	5:I:133:DC:C6	2.47	0.49
5:I:131:DC:H2'	5:I:132:DA:C8	2.48	0.49
5:J:137:DT:H2''	5:J:138:DG:C8	2.47	0.49
6:K:1246:GLU:HB2	6:K:1253:LYS:HE2	1.95	0.48
5:I:156:DA:H2''	5:I:157:DT:O5'	2.13	0.48
5:J:55:DT:H2''	5:J:56:DG:C8	2.48	0.48
5:J:71:DA:H2''	5:J:72:DA:C8	2.48	0.48
1:E:65:LEU:O	1:E:68:GLN:HG3	2.13	0.48
5:I:93:DC:H2''	5:I:94:DA:N7	2.29	0.48
5:J:51:DT:H2''	5:J:52:DA:C8	2.48	0.48
5:J:129:DT:H2''	5:J:130:DA:H8	1.79	0.48
6:K:1388:PRO:HD3	6:K:1499:LYS:HE2	1.96	0.48
1:A:36:LYS:HZ3	1:A:38:PRO:HD2	1.79	0.48
5:I:103:DT:H2''	5:I:104:DG:C8	2.48	0.48
2:F:75:HIS:O	4:H:92:ARG:NH2	2.45	0.48
3:G:58:LEU:O	3:G:62:ILE:HG12	2.14	0.48
5:I:66:DC:H2''	5:I:67:DC:C5	2.49	0.47
5:J:97:DT:H2''	5:J:98:DG:C8	2.49	0.47
1:E:61:LEU:HD11	2:F:37:LEU:HG	1.95	0.47
5:I:115:DG:H2''	5:I:116:DA:N7	2.28	0.47
5:J:112:DA:C8	5:J:112:DA:H5''	2.50	0.47
2:F:92:ARG:HD3	4:H:100:LEU:HD21	1.97	0.47
5:I:136:DT:H2'	5:I:137:DT:C5	2.49	0.47
5:J:14:DC:H2''	5:J:15:DG:C8	2.50	0.47
5:J:80:DG:H2'	5:J:81:DT:H71	1.97	0.47
4:H:57:LYS:O	4:H:61:ILE:HG12	2.15	0.47
5:I:57:DG:H2''	5:I:58:DA:C8	2.50	0.47
5:I:126:DA:H2''	5:I:127:DA:C8	2.50	0.47
5:J:161:DG:H2''	5:J:162:DA:C8	2.50	0.47
6:K:1315:HIS:HB3	6:K:1318:SER:HB3	1.96	0.47
6:K:1374:PHE:HE2	6:K:1376:MET:HE2	1.80	0.47
3:G:35:ARG:NH2	5:I:129:DT:OP1	2.47	0.47
1:E:99:TYR:CZ	1:E:103:LEU:HD11	2.51	0.46
1:E:68:GLN:HA	1:E:71:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:118:DC:H2''	5:J:119:DA:H8	1.80	0.46
6:K:1190:THR:HG22	6:K:1235:LYS:HG3	1.97	0.46
1:A:109:LEU:HA	1:A:112:ILE:HG12	1.96	0.46
5:J:49:DT:H2''	5:J:50:DG:H8	1.81	0.46
1:A:62:ILE:HB	1:A:93:GLN:HE21	1.81	0.46
3:C:68:ASN:OD1	3:C:69:ALA:N	2.49	0.46
5:J:84:DA:H2''	5:J:85:DG:N7	2.31	0.45
5:J:126:DA:H2''	5:J:127:DA:C8	2.50	0.45
6:K:1102:ILE:HD11	6:K:1120:ASP:HB3	1.97	0.45
3:C:38:ASN:HD21	3:G:40:SER:HA	1.81	0.45
4:D:57:LYS:HD2	4:D:58:ALA:N	2.31	0.45
5:J:96:DC:OP1	6:K:1456:LYS:NZ	2.39	0.45
1:E:79:LYS:HD2	1:E:79:LYS:HA	1.84	0.45
3:C:99:ARG:HA	3:C:99:ARG:HD3	1.82	0.45
6:K:1058:LEU:HD11	6:K:1114:PRO:HB3	1.99	0.45
6:K:1388:PRO:HG3	6:K:1500:GLU:HA	1.97	0.45
5:I:110:DT:H2''	5:I:111:DG:H5'	1.98	0.45
1:A:90:MET:HA	1:A:90:MET:HE2	1.99	0.45
2:F:75:HIS:HB2	4:H:96:THR:HG21	1.98	0.45
5:I:20:DC:N4	5:J:160:DT:O4	2.50	0.45
1:E:37:LYS:NZ	5:J:162:DA:OP1	2.36	0.45
5:J:74:DA:H2''	5:J:75:DG:N7	2.32	0.45
6:K:1055:ARG:NE	6:K:1107:ASP:OD1	2.47	0.45
2:B:35:ARG:O	2:B:39:ARG:HG2	2.17	0.45
4:H:96:THR:OG1	4:H:99:ARG:NH1	2.50	0.45
1:E:46:VAL:HA	1:E:49:ARG:HD3	1.98	0.45
3:G:27:VAL:HG21	3:G:49:VAL:HG22	1.99	0.45
5:J:74:DA:H2''	5:J:75:DG:C8	2.51	0.45
5:I:62:DT:H2'	5:I:63:DG:C8	2.52	0.45
5:J:149:DC:H2''	5:J:150:DA:C8	2.51	0.45
6:K:1175:LEU:HB2	6:K:1185:ILE:HB	1.99	0.45
3:C:70:ALA:HA	3:C:82:HIS:CE1	2.52	0.44
5:I:113:DT:O4	5:J:67:DC:N4	2.50	0.44
5:I:129:DT:H2''	5:I:130:DA:C8	2.52	0.44
4:D:46:LYS:NZ	4:D:50:PRO:O	2.43	0.44
5:J:128:DA:H2'	5:J:129:DT:H71	1.99	0.44
4:D:41:VAL:O	4:D:45:LEU:HD23	2.16	0.44
5:J:57:DG:H2''	5:J:58:DA:H8	1.82	0.44
1:E:120:MET:HB2	1:E:122:LYS:HG2	2.00	0.44
4:H:58:ALA:O	4:H:62:MET:HG2	2.17	0.44
5:J:68:DA:H2'	5:J:69:DT:H71	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:39:DC:H2'	5:J:40:DT:H71	2.00	0.44
1:E:62:ILE:HB	1:E:93:GLN:HE21	1.81	0.44
5:I:124:DC:H2''	5:I:125:DC:C5	2.52	0.44
5:I:127:DA:H2''	5:I:128:DA:N7	2.33	0.44
2:B:39:ARG:NH2	2:B:43:VAL:O	2.49	0.44
1:E:104:PHE:HB3	2:F:41:GLY:HA3	1.99	0.44
4:H:105:GLU:OE2	4:H:106:LEU:HG	2.18	0.43
5:J:54:DT:H2''	5:J:55:DT:C6	2.53	0.43
6:K:1098:ASP:OD2	6:K:1100:SER:OG	2.34	0.43
6:K:1406:PRO:HG2	6:K:1409:LEU:HB2	2.00	0.43
1:A:120:MET:HE3	1:A:121:PRO:HD3	1.99	0.43
5:J:87:DT:H2''	5:J:88:DG:N7	2.33	0.43
5:J:119:DA:H2''	5:J:120:DG:H8	1.83	0.43
6:K:1340:LYS:HA	6:K:1344:VAL:HB	2.00	0.43
2:B:31:LYS:NZ	2:B:35:ARG:HE	2.16	0.43
2:F:59:LYS:O	2:F:63:GLU:HG2	2.18	0.43
6:K:1240:ASP:HB2	6:K:1638:HIS:HE1	1.82	0.43
4:D:115:THR:O	4:D:118:VAL:HG12	2.19	0.43
5:J:48:DG:H2'	5:J:49:DT:C6	2.54	0.43
1:A:57:SER:HB2	1:A:59:GLU:OE1	2.18	0.43
5:I:58:DA:H2''	5:I:59:DA:C8	2.54	0.43
5:J:66:DC:H2''	5:J:67:DC:C5	2.54	0.43
1:A:72:ARG:O	1:A:76:GLN:HG3	2.18	0.43
5:J:158:DA:H2'	5:J:159:DT:H71	2.01	0.43
6:K:1486:ILE:HG23	6:K:1588:MET:SD	2.59	0.43
5:J:76:DG:H2''	5:J:77:DC:C6	2.54	0.42
5:J:161:DG:H2''	5:J:162:DA:H8	1.84	0.42
6:K:1097:MET:HE2	6:K:1101:THR:HB	2.00	0.42
5:J:43:DC:H2''	5:J:44:DA:N7	2.34	0.42
5:J:129:DT:C2	5:J:130:DA:N7	2.88	0.42
4:D:41:VAL:HA	4:D:44:VAL:HG12	2.00	0.42
5:J:108:DT:H2'	5:J:109:DT:H72	2.01	0.42
1:E:47:ALA:HA	1:E:50:GLU:OE2	2.19	0.42
5:J:96:DC:H2''	5:J:97:DT:C5	2.54	0.42
5:J:107:DT:H2''	5:J:108:DT:H72	2.02	0.42
4:D:90:THR:HG23	4:D:92:ARG:H	1.84	0.42
5:J:152:DG:H2'	5:J:153:DT:H71	2.02	0.42
3:C:40:SER:HA	3:G:38:ASN:ND2	2.32	0.42
6:K:1381:TYR:CD2	6:K:1389:ASN:HB3	2.55	0.42
1:A:47:ALA:O	1:A:50:GLU:HG3	2.20	0.42
1:A:107:THR:HG21	1:A:124:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:ARG:O	4:D:89:ILE:HD13	2.19	0.42
5:J:77:DC:H2''	5:J:78:DA:C8	2.55	0.42
3:C:79:ILE:HG22	3:C:82:HIS:ND1	2.35	0.42
3:C:74:LYS:O	3:C:74:LYS:HG3	2.20	0.41
4:D:86:ARG:HG3	4:D:88:THR:H	1.84	0.41
4:H:37:TYR:HA	4:H:40:TYR:HD2	1.84	0.41
1:E:90:MET:O	1:E:94:GLU:HG3	2.20	0.41
3:G:88:ARG:HB3	3:G:108:LEU:HD11	2.01	0.41
6:K:1482:ASP:OD2	6:K:1484:LYS:NZ	2.53	0.41
4:D:106:LEU:HA	4:D:109:HIS:HD2	1.86	0.41
5:J:20:DC:H2''	5:J:21:DA:N7	2.35	0.41
1:E:61:LEU:H	1:E:61:LEU:HD23	1.85	0.41
4:H:95:GLN:HG3	4:H:99:ARG:NE	2.35	0.41
1:A:100:LEU:HD21	2:B:58:LEU:HD13	2.02	0.41
4:D:42:TYR:O	4:D:46:LYS:HG2	2.21	0.41
5:I:149:DC:H2''	5:I:150:DA:C8	2.55	0.41
3:C:88:ARG:C	3:C:94:ASN:HD21	2.29	0.41
2:F:84:MET:HA	2:F:87:VAL:HG12	2.03	0.41
5:I:146:DC:H2''	5:I:147:DT:C6	2.56	0.41
6:K:1431:THR:HG23	6:K:1601:ILE:H	1.85	0.41
5:I:40:DT:H2''	5:I:41:DA:O4'	2.21	0.41
5:I:77:DC:H2''	5:I:78:DA:C8	2.56	0.41
5:I:101:DC:H2''	5:I:102:DA:H8	1.84	0.41
5:J:127:DA:H2''	5:J:128:DA:H8	1.86	0.41
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.54	0.41
2:B:50:ILE:HA	2:B:53:GLU:OE2	2.21	0.41
4:D:79:ARG:HG2	4:D:83:TYR:CE2	2.56	0.41
1:E:37:LYS:HA	1:E:38:PRO:HD3	1.95	0.41
5:J:62:DT:H2''	5:J:63:DG:H8	1.85	0.41
6:K:1291:LYS:HE2	6:K:1291:LYS:HB2	1.85	0.41
6:K:1471:LEU:HB3	6:K:1483:TYR:CD1	2.56	0.41
5:I:149:DC:H2''	5:I:150:DA:N7	2.36	0.40
5:J:35:DG:H2''	5:J:36:DA:C8	2.56	0.40
5:J:93:DC:H2''	5:J:94:DA:C8	2.56	0.40
6:K:1261:HIS:CD2	6:K:1270:PHE:HB2	2.56	0.40
3:C:50:TYR:CE2	4:D:114:GLY:HA3	2.56	0.40
1:E:50:GLU:HB2	1:E:54:TYR:CE2	2.57	0.40
3:C:57:TYR:HE2	4:D:109:HIS:HB3	1.85	0.40
6:K:1482:ASP:OD1	6:K:1599:ARG:HB3	2.22	0.40
3:C:33:LEU:HA	3:C:36:LYS:HG2	2.02	0.40
4:D:119:THR:O	4:D:122:THR:OG1	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:103:DT:H2''	5:J:104:DG:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	101/135 (75%)	96 (95%)	5 (5%)	0	100	100
1	E	97/135 (72%)	95 (98%)	2 (2%)	0	100	100
2	B	78/102 (76%)	77 (99%)	1 (1%)	0	100	100
2	F	81/102 (79%)	78 (96%)	3 (4%)	0	100	100
3	C	105/129 (81%)	103 (98%)	2 (2%)	0	100	100
3	G	103/129 (80%)	101 (98%)	2 (2%)	0	100	100
4	D	95/125 (76%)	91 (96%)	4 (4%)	0	100	100
4	H	94/125 (75%)	90 (96%)	4 (4%)	0	100	100
6	K	509/796 (64%)	499 (98%)	10 (2%)	0	100	100
All	All	1263/1778 (71%)	1230 (97%)	33 (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	A	87/110 (79%)	87 (100%)	0	100	100
1	E	86/110 (78%)	86 (100%)	0	100	100
2	B	65/76 (86%)	65 (100%)	0	100	100
2	F	68/76 (90%)	68 (100%)	0	100	100
3	C	84/99 (85%)	84 (100%)	0	100	100
3	G	83/99 (84%)	83 (100%)	0	100	100
4	D	82/104 (79%)	82 (100%)	0	100	100
4	H	82/104 (79%)	82 (100%)	0	100	100
6	K	475/726 (65%)	475 (100%)	0	100	100
All	All	1112/1504 (74%)	1112 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
2	B	64	ASN
3	G	38	ASN
6	K	1195	GLN
6	K	1307	ASN
6	K	1377	HIS
6	K	1661	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 [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.

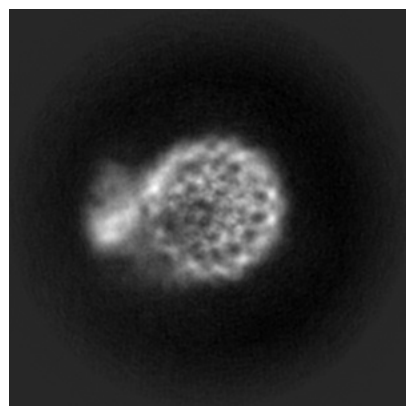
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34589. These allow visual inspection of the internal detail of the map and identification of artifacts.

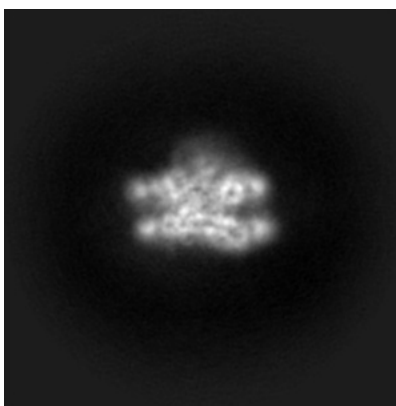
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

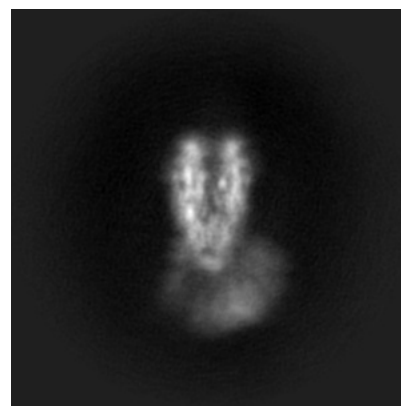
6.1.1 Primary map



X

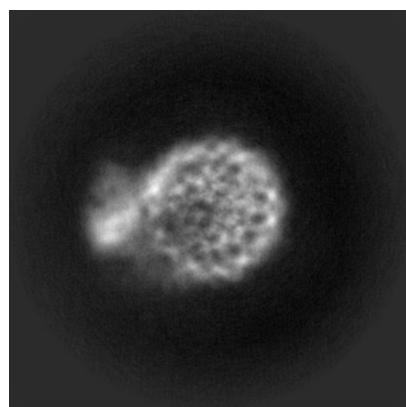


Y

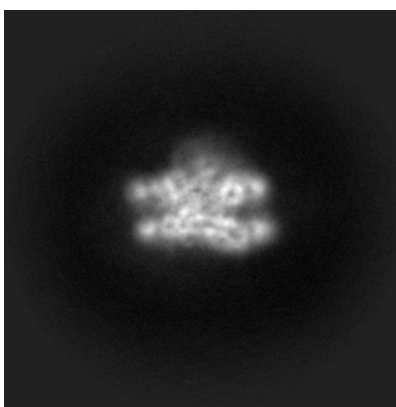


Z

6.1.2 Raw map



X



Y

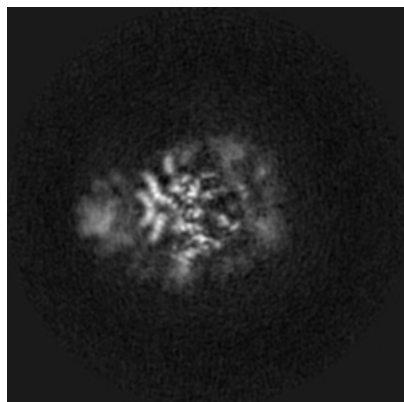


Z

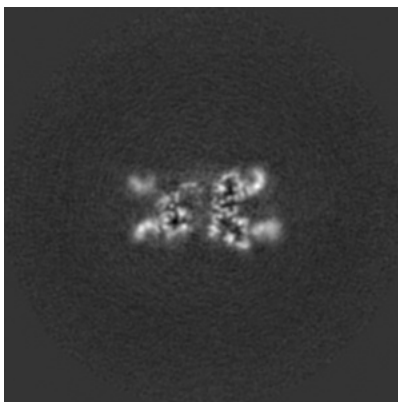
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

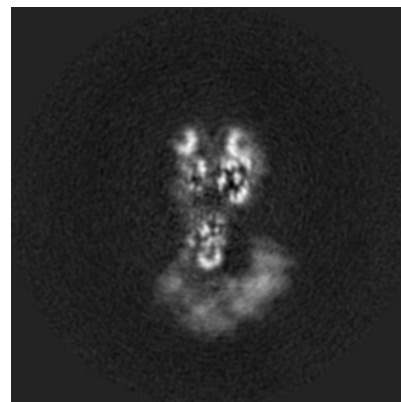
6.2.1 Primary map



X Index: 170

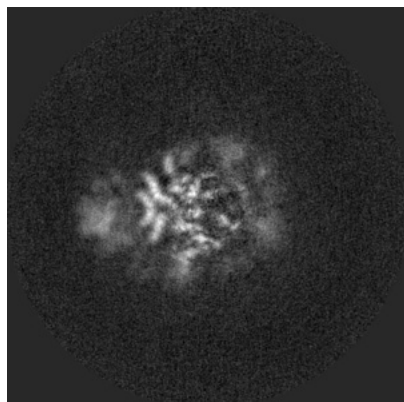


Y Index: 170

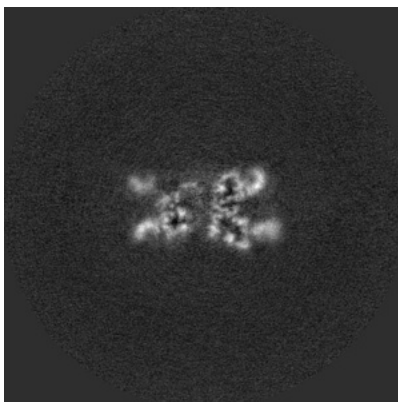


Z Index: 170

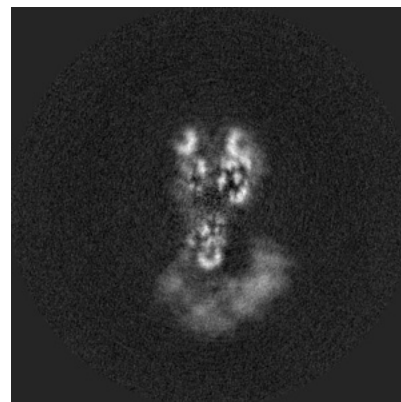
6.2.2 Raw map



X Index: 170



Y Index: 170

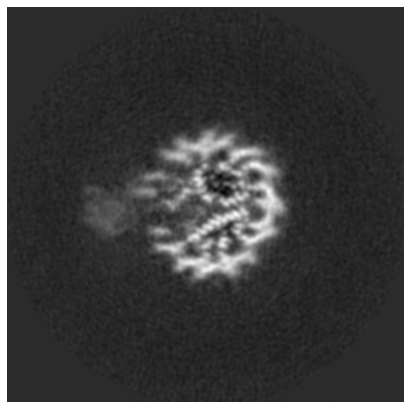


Z Index: 170

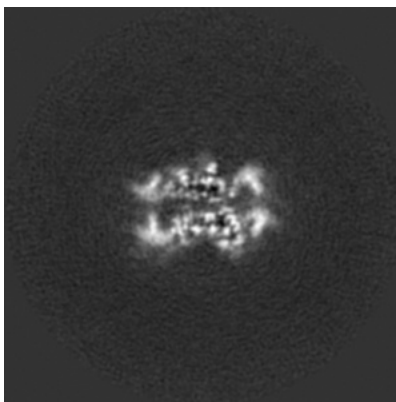
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

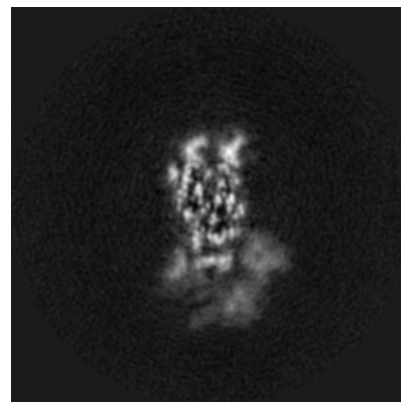
6.3.1 Primary map



X Index: 152

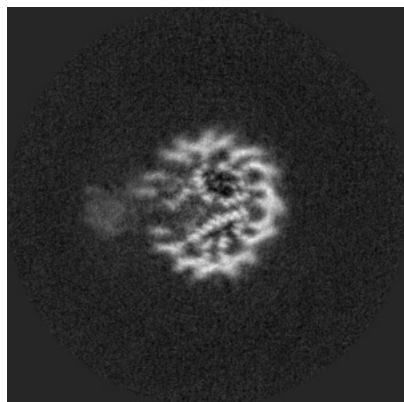


Y Index: 197

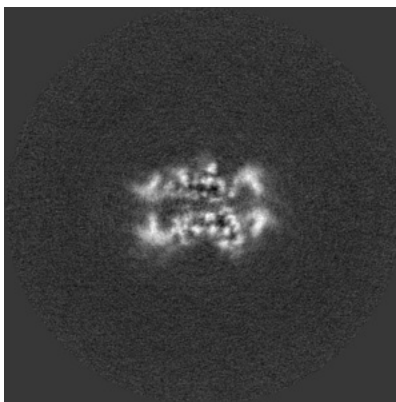


Z Index: 187

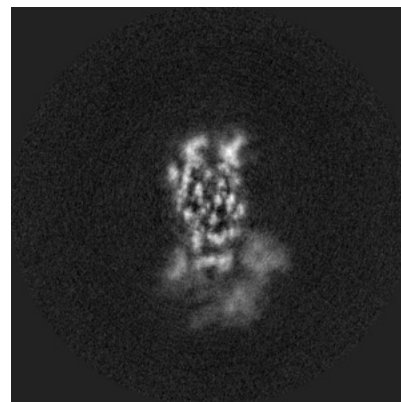
6.3.2 Raw map



X Index: 152



Y Index: 197

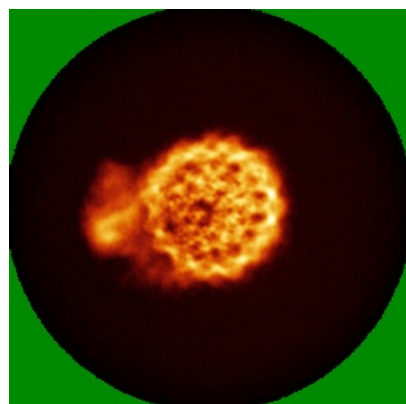


Z Index: 187

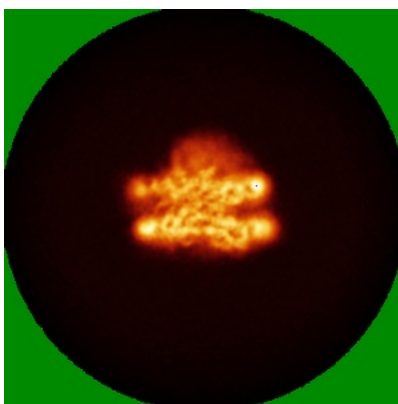
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

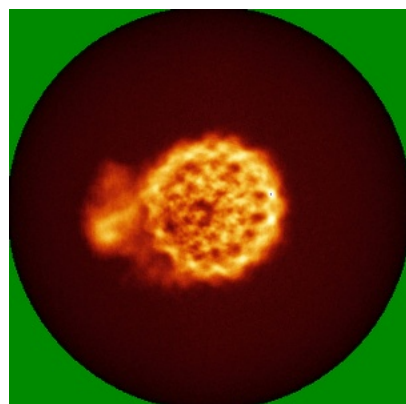


Y

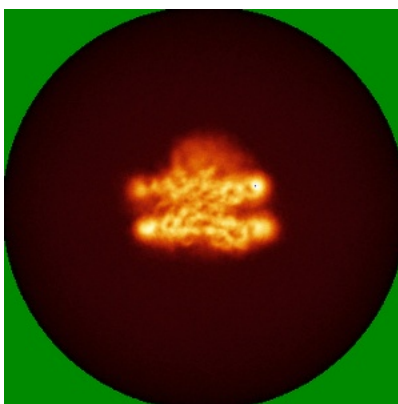


Z

6.4.2 Raw map



X



Y

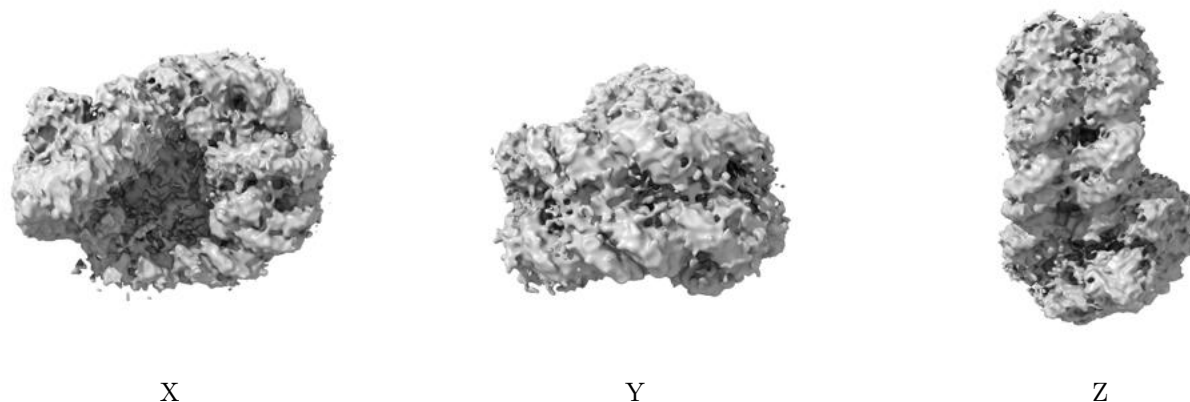


Z

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.

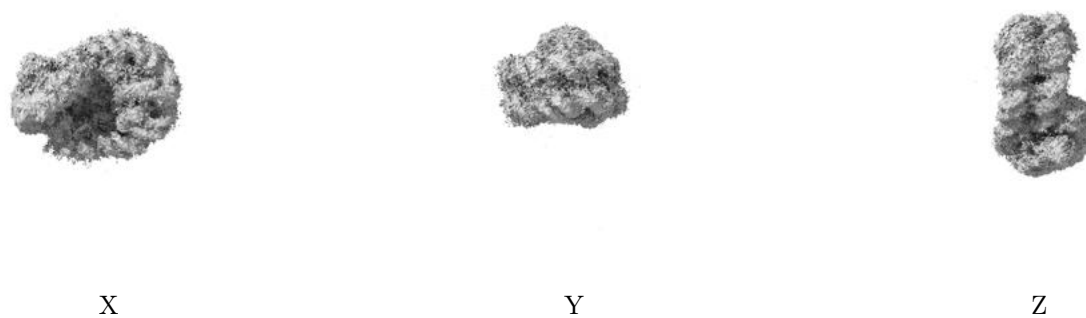
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0035. 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



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.

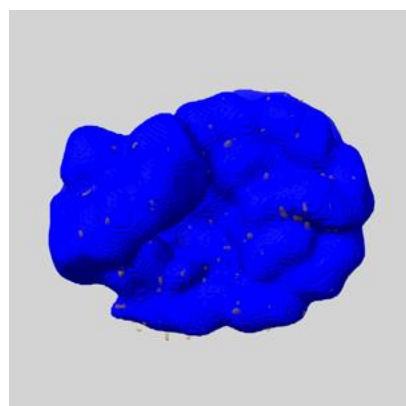
6.6 Mask visualisation [i](#)

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

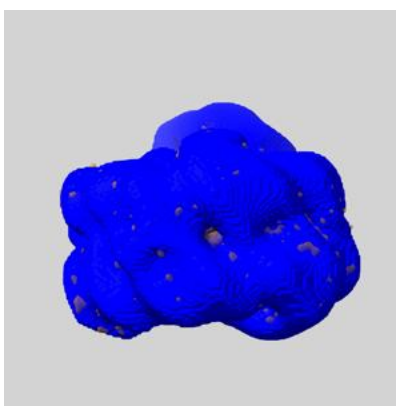
A mask typically either:

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

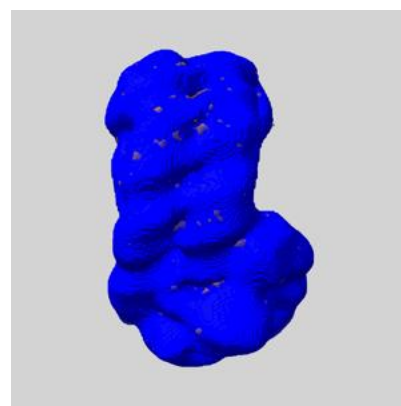
6.6.1 emd_34589_msk_1.map [i](#)



X



Y

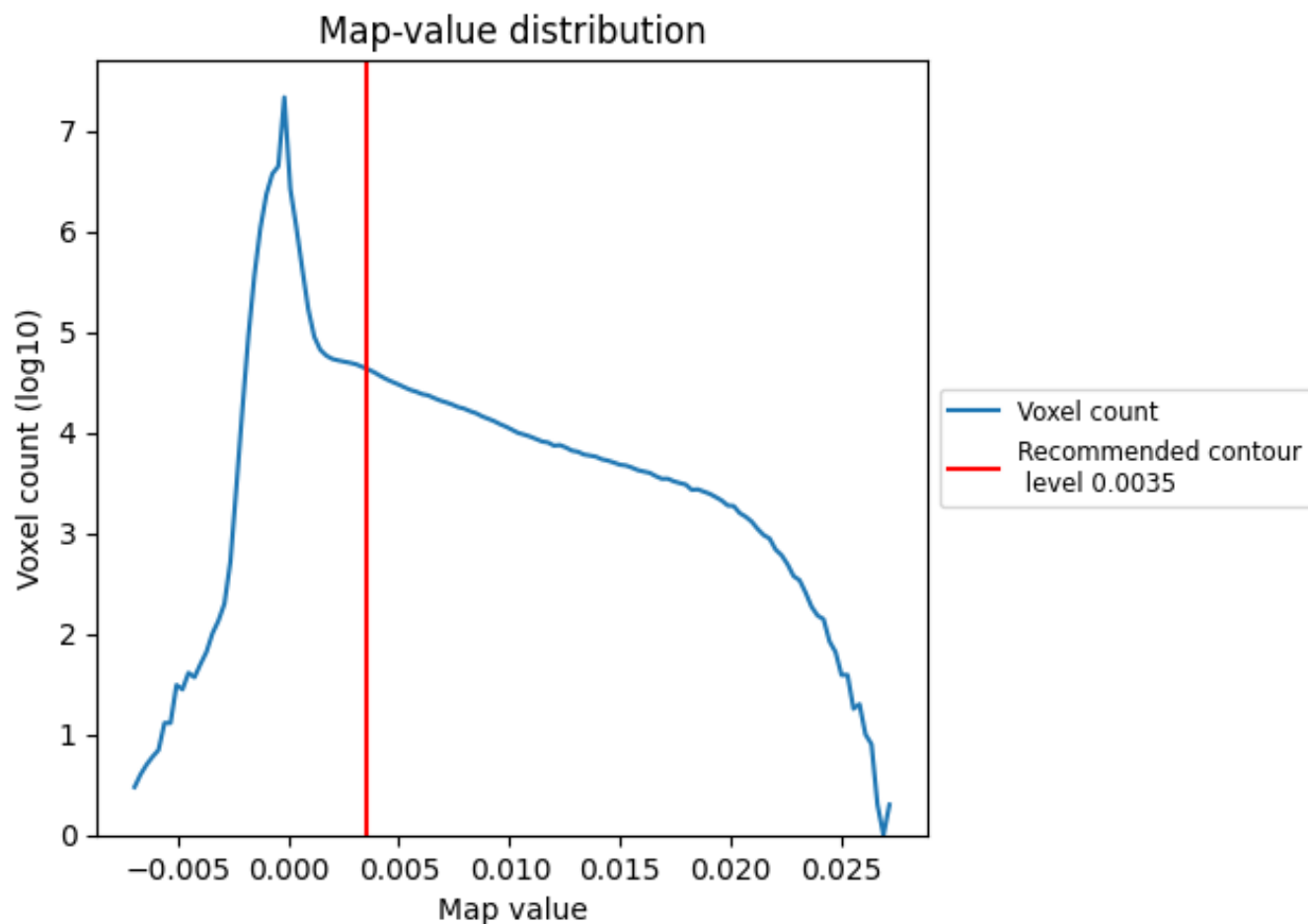


Z

7 Map analysis [i](#)

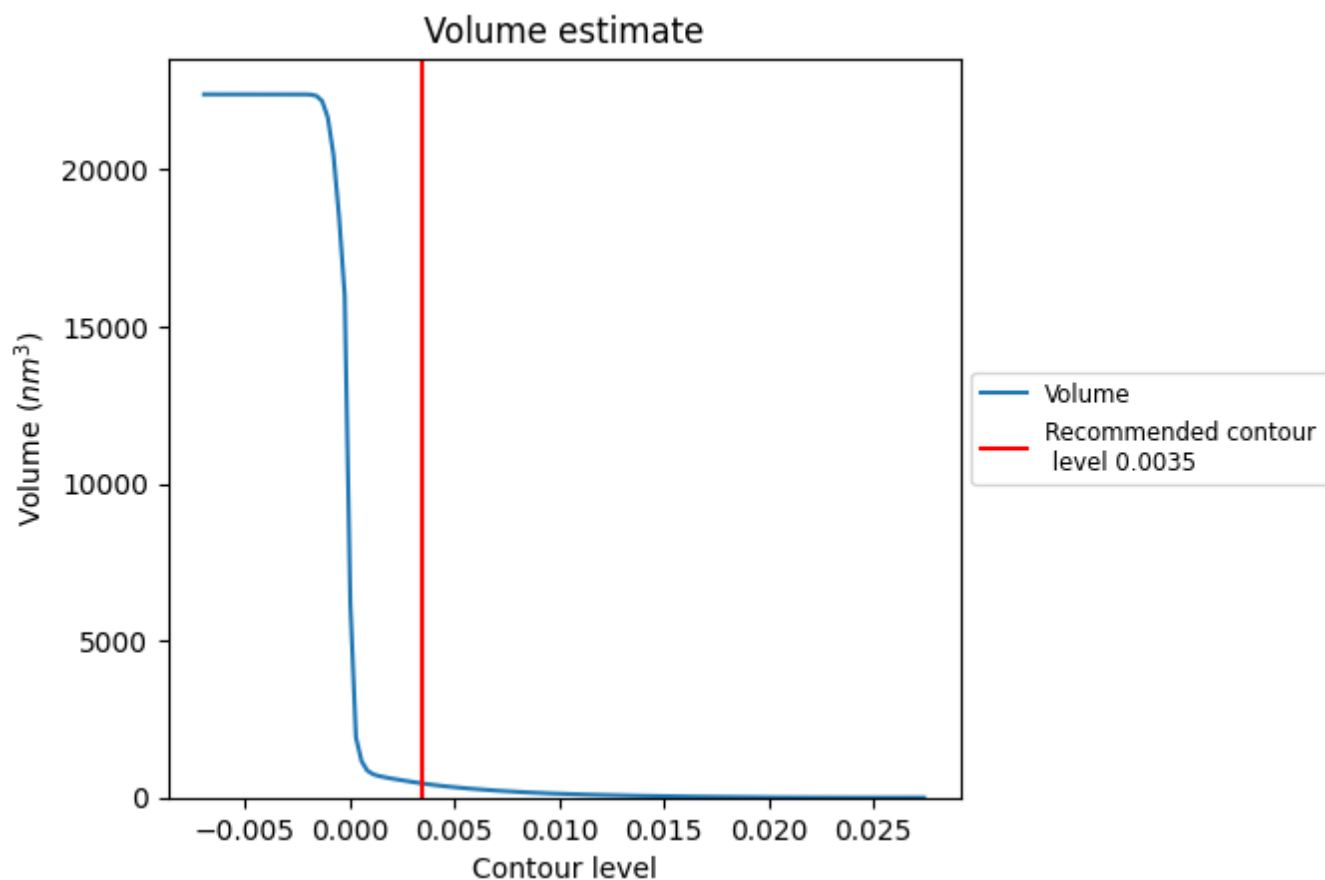
This section contains the results of statistical analysis of the map.

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.

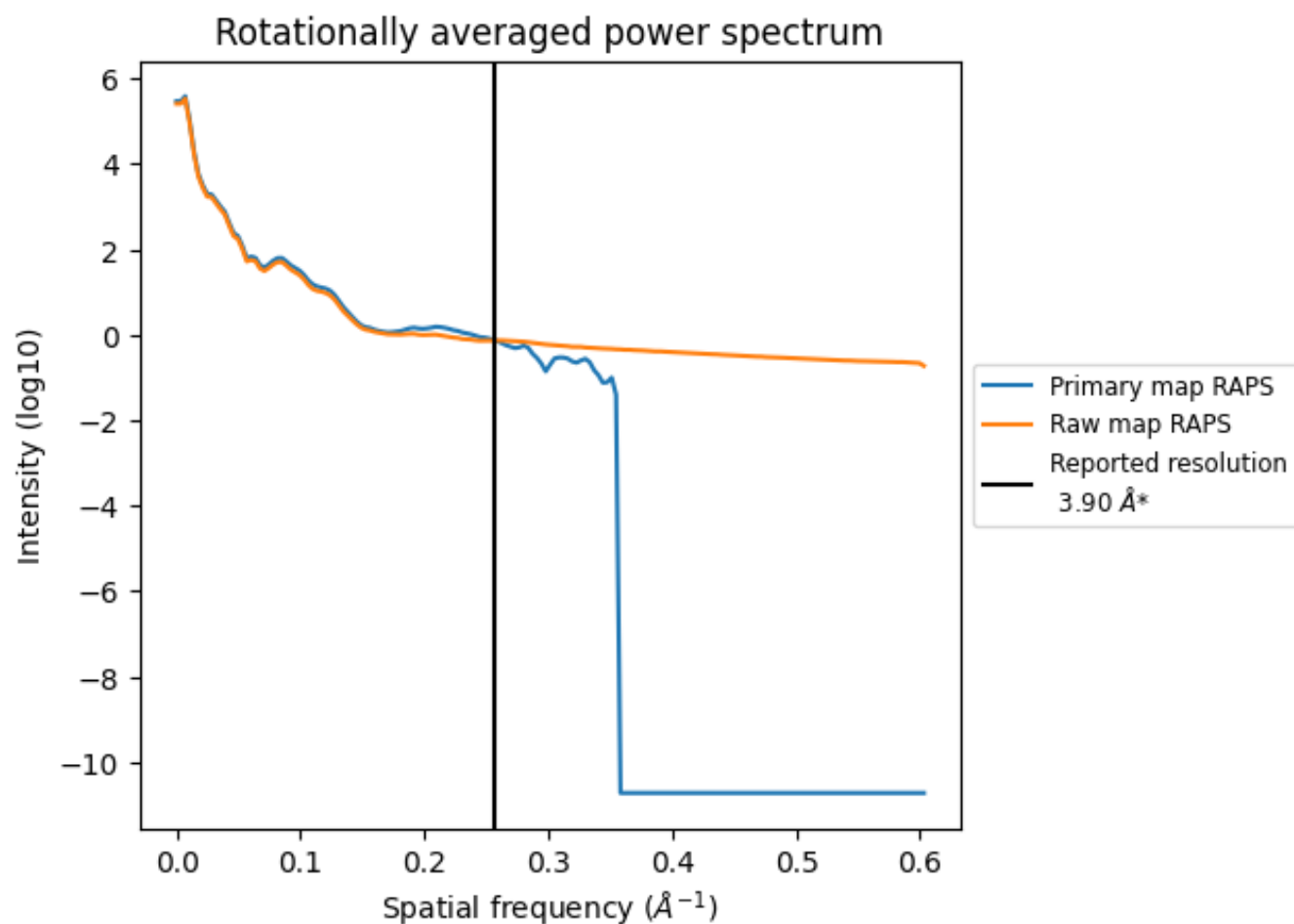
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 448 nm³; this corresponds to an approximate mass of 404 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

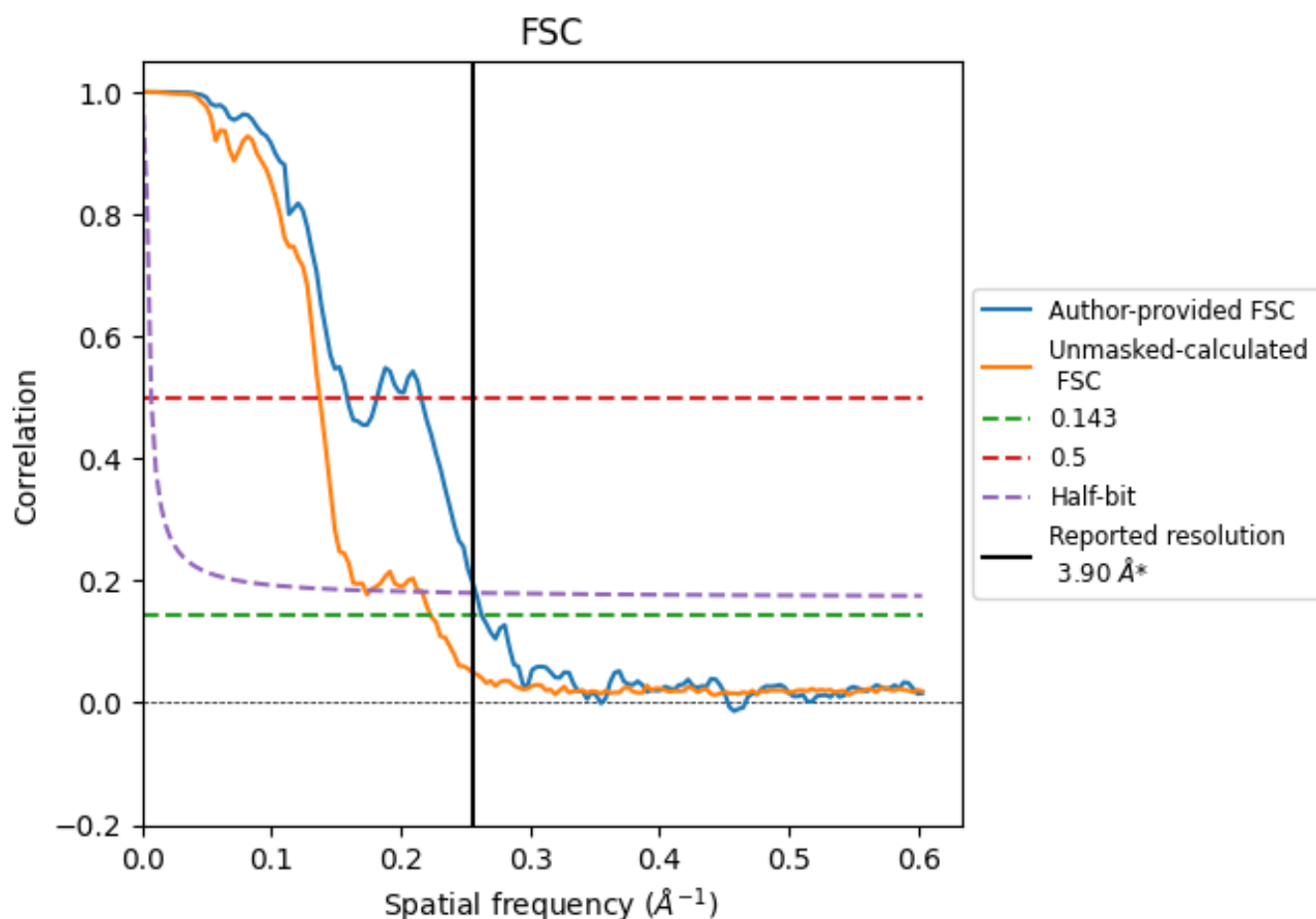


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

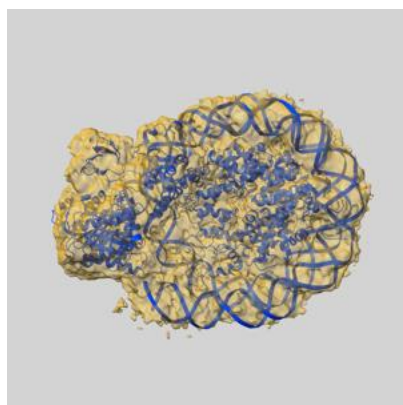
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.81	6.31	3.87
Unmasked-calculated*	4.48	7.29	5.79

*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 4.48 differs from the reported value 3.9 by more than 10 %

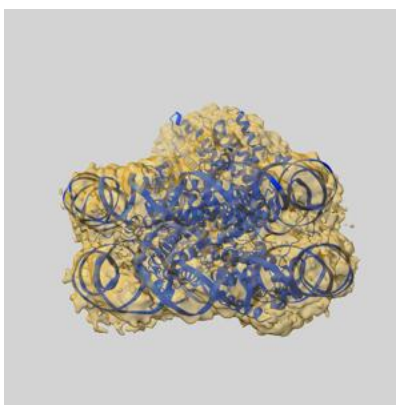
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34589 and PDB model 8HAH. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

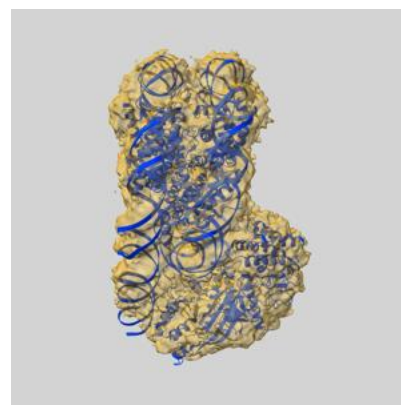
9.1 Map-model overlay [i](#)



X



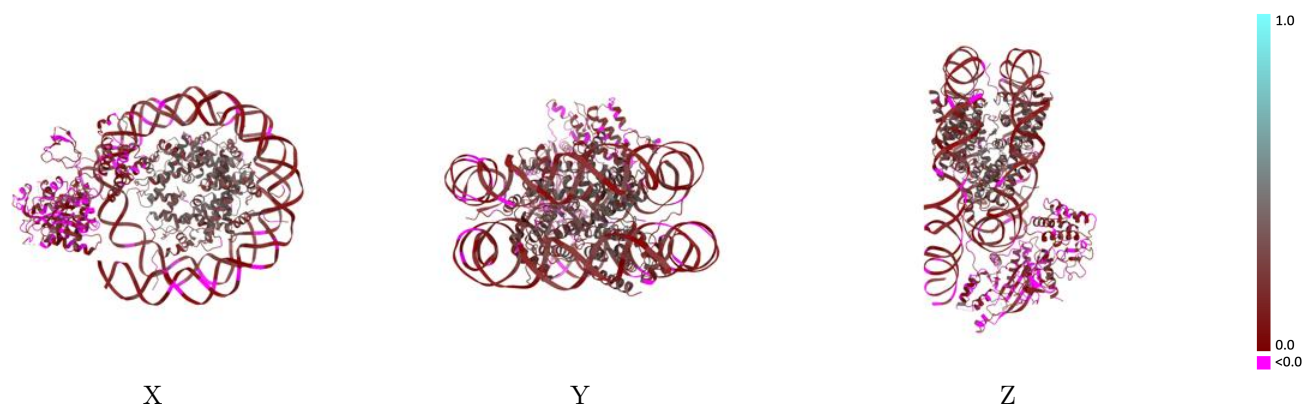
Y



Z

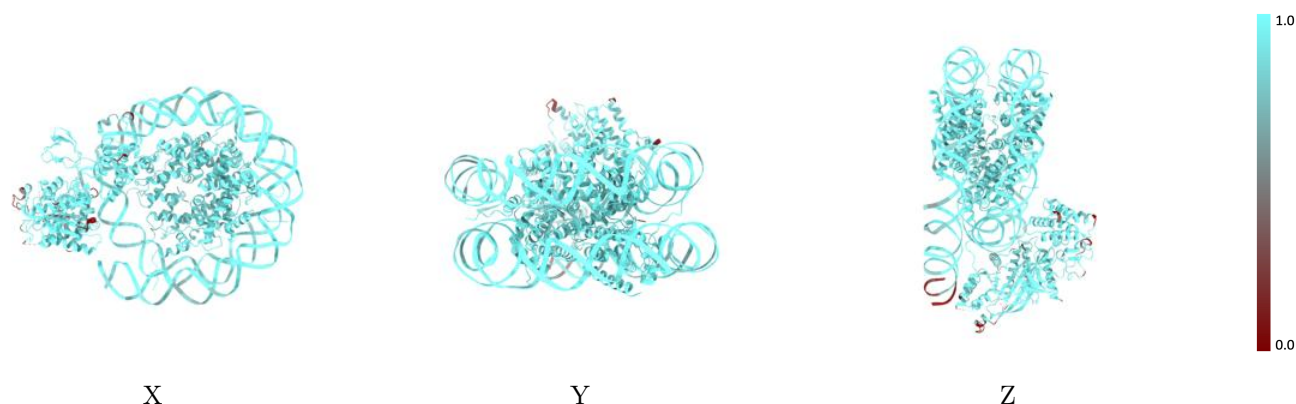
The images above show the 3D surface view of the map at the recommended contour level 0.0035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



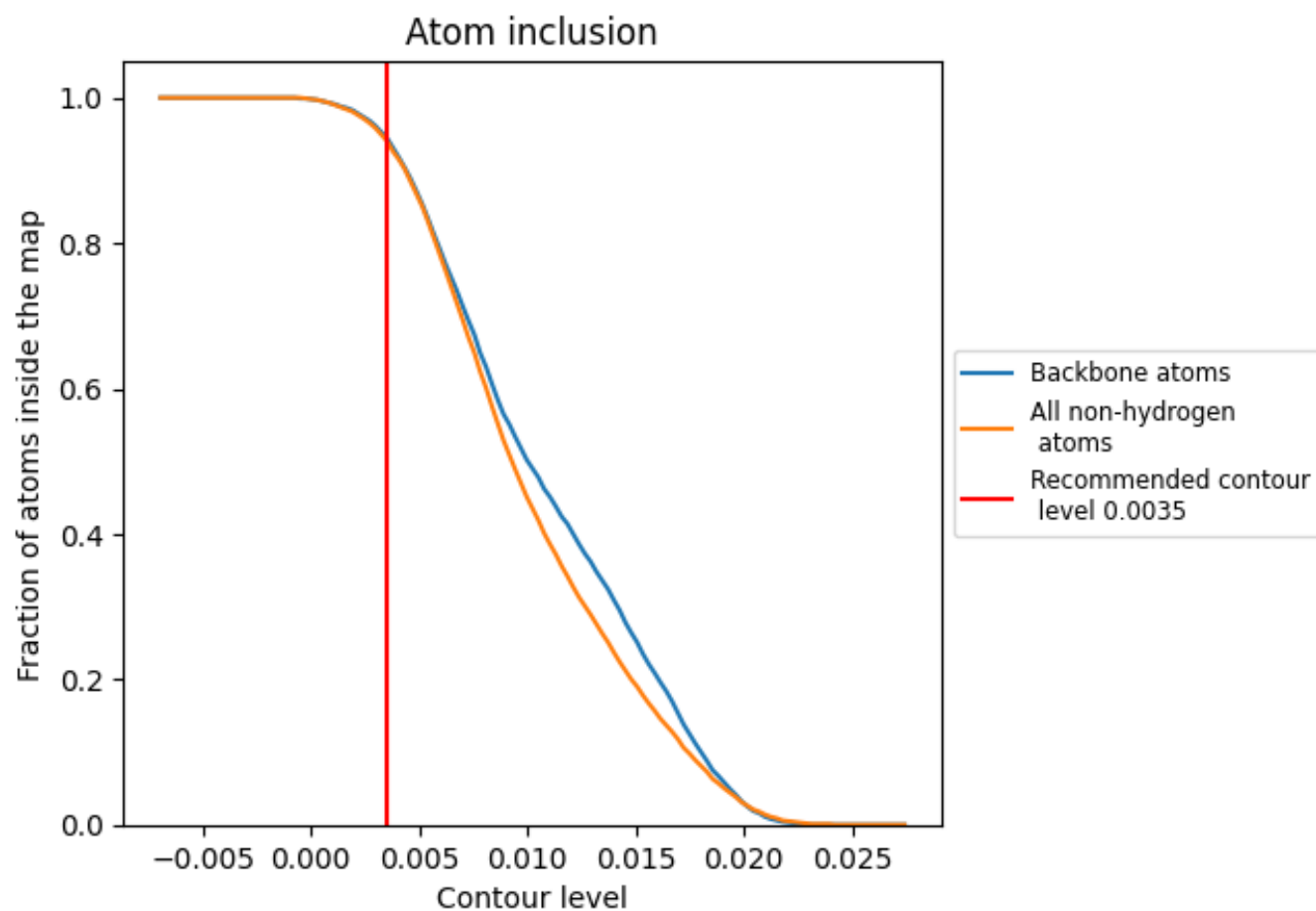
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% 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 (0.0035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9410	0.1590
A	0.9860	0.2500
B	0.9890	0.3260
C	0.9750	0.2730
D	0.9920	0.2960
E	0.9850	0.2590
F	0.9890	0.2970
G	0.9890	0.2660
H	0.9960	0.2940
I	0.9050	0.1070
J	0.9100	0.1130
K	0.9270	0.0620

1.0

0.0

<0.0