



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:42 AM UTC

PDB ID : 8XRJ / pdb_00008xrj
EMDB ID : EMD-38604
Title : RNA polymerase II elongation complex with upstream nucleosome extracted from human nuclei
Authors : Kujirai, T.; Kato, J.; Yamamoto, K.; Hirai, S.; Negishi, L.; Ogasawara, M.; Takizawa, Y.; Kurumizaka, H.
Deposited on : 2024-01-07
Resolution : 3.60 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

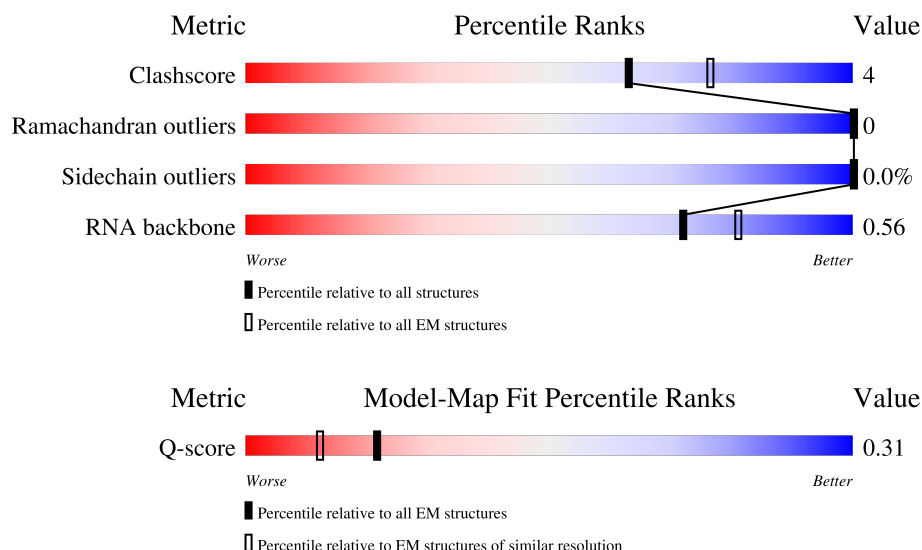
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	1970	
2	B	1174	
3	C	292	

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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	158	
14	P	11	
15	T	158	
16	a	135	
16	e	135	
17	b	102	
17	f	102	
18	c	129	
18	g	129	
19	d	125	
19	h	125	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 43082 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1410	Total	C	N	O	S	0	0
			11173	7032	2001	2070	70		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0
			8932	5657	1571	1640	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	254	Total	C	N	O	S	0	0
			2039	1284	348	401	6		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	MET	-	initiating methionine	UNP P19387
C	-15	HIS	-	expression tag	UNP P19387
C	-14	HIS	-	expression tag	UNP P19387
C	-13	HIS	-	expression tag	UNP P19387
C	-12	HIS	-	expression tag	UNP P19387
C	-11	HIS	-	expression tag	UNP P19387
C	-10	HIS	-	expression tag	UNP P19387
C	-9	ASP	-	expression tag	UNP P19387
C	-8	TYR	-	expression tag	UNP P19387
C	-7	LYS	-	expression tag	UNP P19387
C	-6	ASP	-	expression tag	UNP P19387
C	-5	ASP	-	expression tag	UNP P19387
C	-4	ASP	-	expression tag	UNP P19387
C	-3	ASP	-	expression tag	UNP P19387
C	-2	LYS	-	expression tag	UNP P19387

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P19387
C	0	HIS	-	expression tag	UNP P19387

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S	0	0
			991	624	170	193	4		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	81	Total	C	N	O	S	0	0
			649	414	111	119	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	170	Total	C	N	O	S	0	0
			1329	863	216	243	7		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 13 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	147	Total	C	N	O	P	0	0
			3015	1444	482	943	146		

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	11	Total	C	N	O	P	0	0
			237	106	46	74	11		

- Molecule 15 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	158	Total	C	N	O	P	0	0
			3233	1527	660	888	158		

- Molecule 16 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	95	Total	C	N	O	S	0	0
			783	494	150	135	4		
16	e	95	Total	C	N	O	S	0	0
			783	494	150	135	4		

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	78	Total	C	N	O	S	0	0
			619	391	120	107	1		
17	f	77	Total	C	N	O	S	0	0
			614	389	119	105	1		

- Molecule 18 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	c	104	Total	C	N	O		0	0
			801	505	156	140			
18	g	102	Total	C	N	O		0	0
			787	496	153	138			

- Molecule 19 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
19	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	
20	C	1	Total	Zn	0
			1	1	
20	I	2	Total	Zn	0
			2	2	
20	J	1	Total	Zn	0
			1	1	
20	L	1	Total	Zn	0
			1	1	

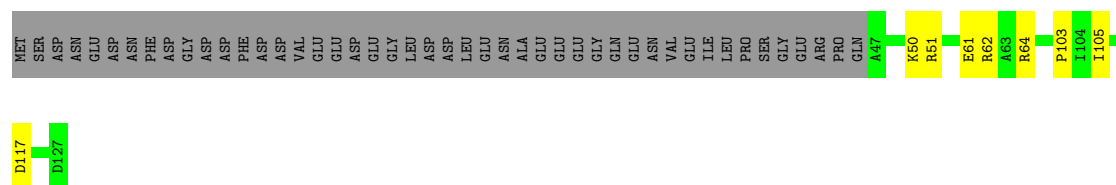
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Mg	0
			1	1	

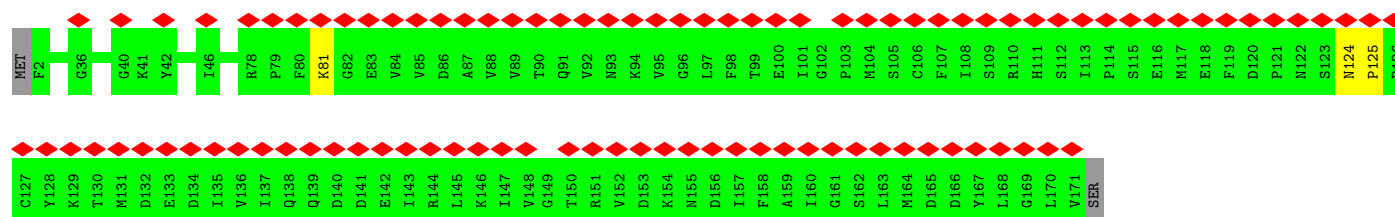
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



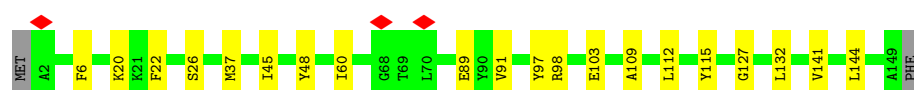
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



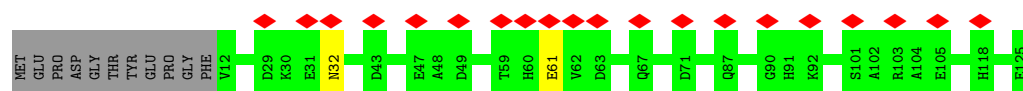
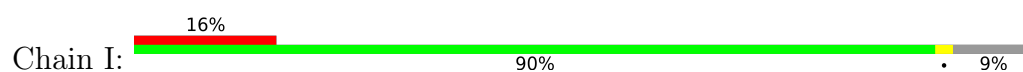
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



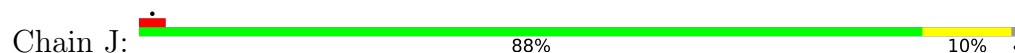
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



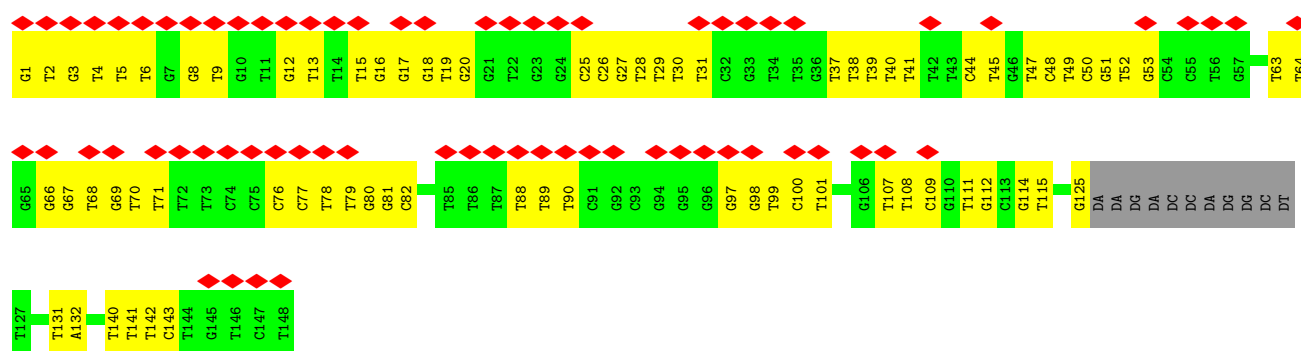
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



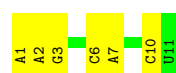
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



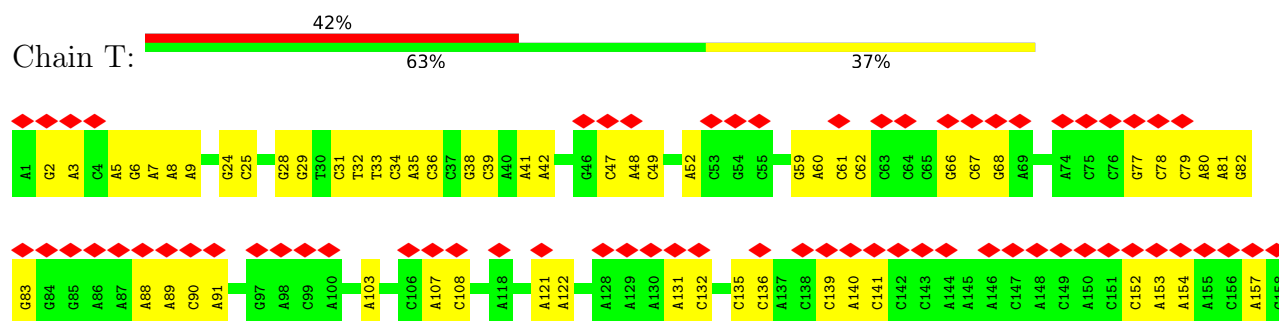
- Molecule 13: DNA



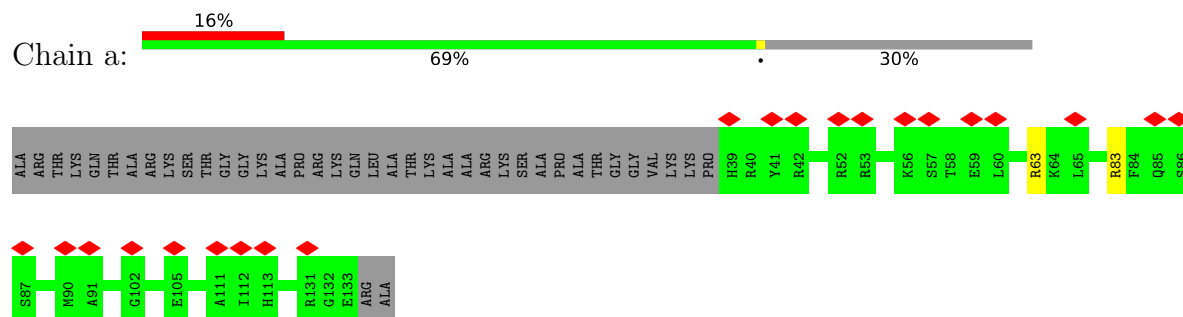
- Molecule 14: RNA



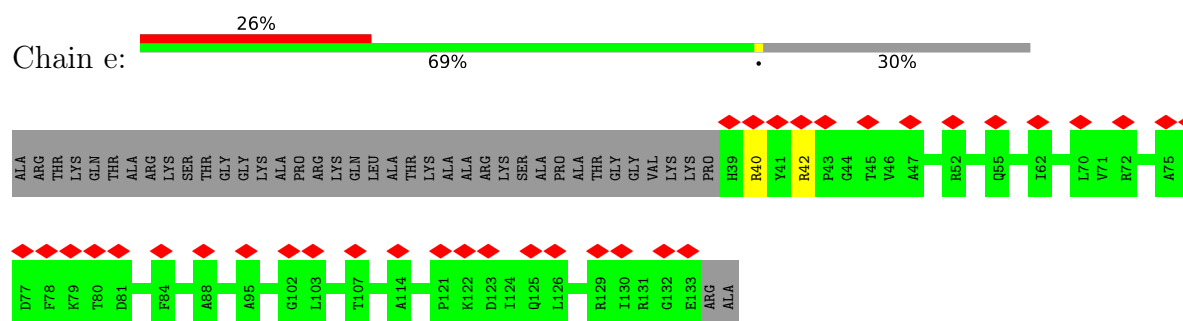
- Molecule 15: DNA



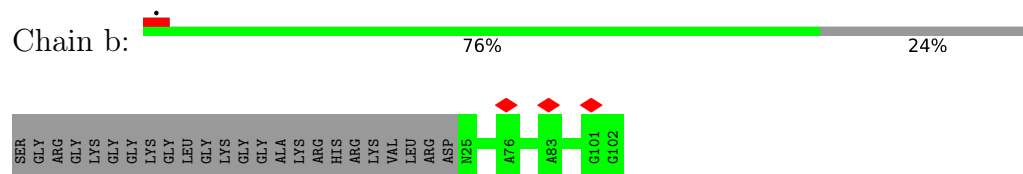
- Molecule 16: Histone H3.1



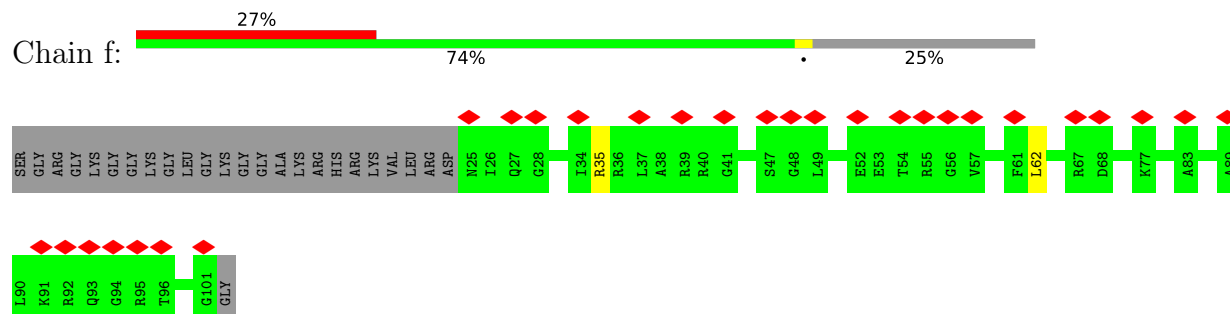
- Molecule 16: Histone H3.1



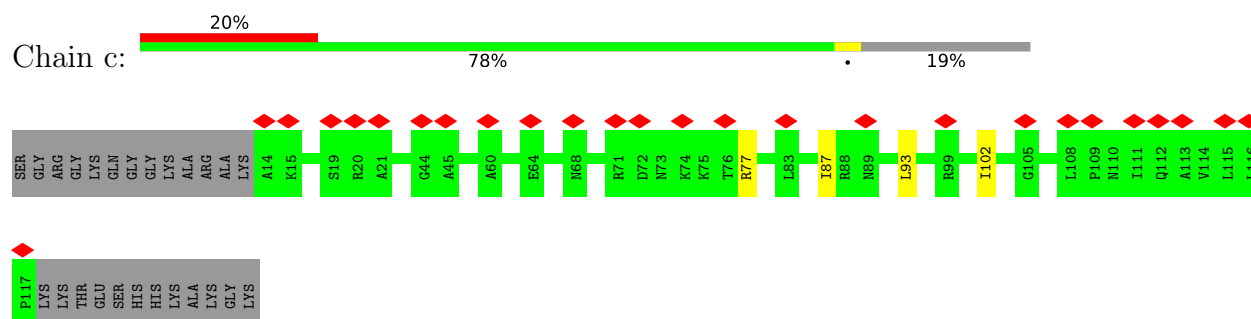
- Molecule 17: Histone H4



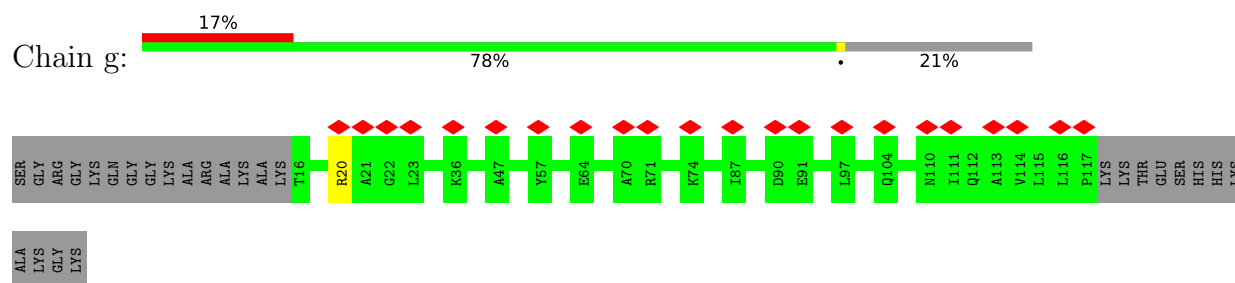
- Molecule 17: Histone H4



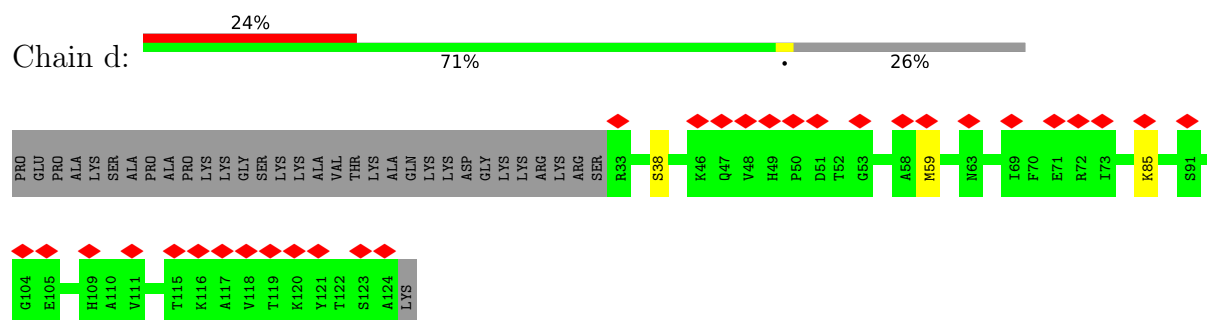
• Molecule 18: Histone H2A type 1-B/E



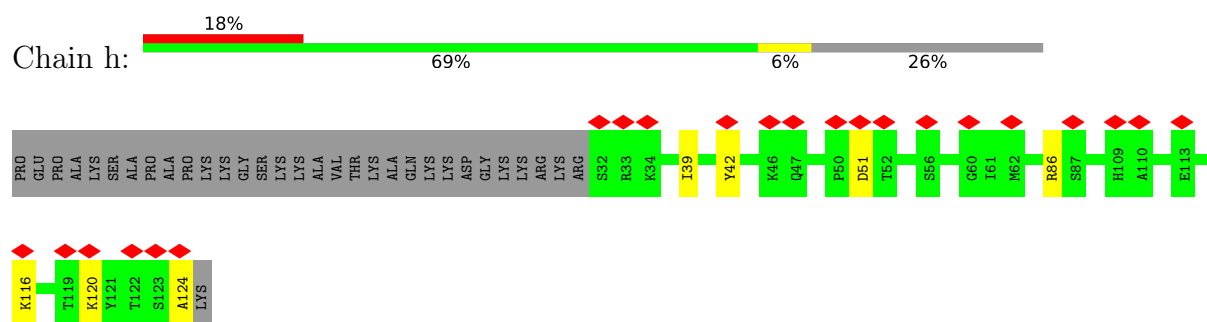
• Molecule 18: Histone H2A type 1-B/E



• Molecule 19: Histone H2B type 1-J



• Molecule 19: Histone H2B type 1-J



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32065	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00744	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	0.24	0/11378	0.50	2/15360 (0.0%)
2	B	0.31	0/9110	0.55	2/12296 (0.0%)
3	C	0.19	0/2082	0.47	0/2829
4	D	0.80	0/1005	1.33	1/1355 (0.1%)
5	E	0.27	0/1745	0.55	0/2358
6	F	0.22	0/659	0.54	2/891 (0.2%)
7	G	0.81	0/1360	1.29	0/1847
8	H	0.29	0/1207	0.59	0/1628
9	I	0.60	0/948	1.00	3/1284 (0.2%)
10	J	0.21	0/533	0.48	0/719
11	K	0.21	0/939	0.47	0/1271
12	L	0.46	0/377	0.77	0/500
13	N	0.34	0/3361	0.75	0/5196
14	P	0.15	0/265	0.44	0/411
15	T	0.32	0/3645	0.64	0/5611
16	a	0.49	0/794	0.82	0/1065
16	e	0.37	0/794	0.71	0/1065
17	b	0.33	0/626	0.57	0/837
17	f	0.31	0/621	0.61	0/832
18	c	0.46	0/811	0.76	0/1096
18	g	0.49	0/797	0.82	0/1078
19	d	0.49	0/730	0.89	0/982
19	h	0.38	0/736	0.82	0/990
All	All	0.36	0/44523	0.66	10/61501 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	935	GLN	CA-C-N	5.70	127.92	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	935	GLN	C-N-CA	5.70	127.92	120.28
4	D	91	LYS	N-CA-C	5.48	117.96	110.24
9	I	61	GLU	CA-C-N	5.42	127.84	120.63
9	I	61	GLU	C-N-CA	5.42	127.84	120.63
2	B	230	ARG	CA-C-N	5.41	125.40	119.89
2	B	230	ARG	C-N-CA	5.41	125.40	119.89
6	F	50	LYS	CA-C-N	5.40	128.77	121.05
6	F	50	LYS	C-N-CA	5.40	128.77	121.05
9	I	32	ASN	N-CA-CB	-5.22	104.05	111.00

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	A	11173	0	11308	76	0
2	B	8932	0	8981	64	0
3	C	2039	0	1993	24	0
4	D	991	0	956	8	0
5	E	1715	0	1733	18	0
6	F	649	0	678	6	0
7	G	1329	0	1325	4	0
8	H	1186	0	1147	12	0
9	I	927	0	859	0	0
10	J	524	0	540	4	0
11	K	920	0	942	8	0
12	L	372	0	378	8	0
13	N	3015	0	1687	70	0
14	P	237	0	121	5	0
15	T	3233	0	1747	55	0
16	a	783	0	818	2	0
16	e	783	0	818	2	0
17	b	619	0	659	0	0
17	f	614	0	656	2	0
18	c	801	0	853	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	g	787	0	835	1	0
19	d	719	0	740	8	0
19	h	725	0	745	16	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
21	A	1	0	0	0	0
All	All	43082	0	40519	347	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 (347) 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)
4:D:15:GLU:HG2	4:D:23:PRO:HD3	1.49	0.93
19:d:38:SER:HA	19:d:59:MET:CE	2.00	0.91
4:D:15:GLU:HG2	4:D:23:PRO:CD	2.05	0.84
15:T:35:DA:H2''	15:T:36:DC:OP2	1.77	0.82
3:C:55:ASN:HB3	12:L:48:ARG:HH22	1.45	0.82
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.61	0.79
13:N:100:DC:H2''	13:N:101:DT:H72	1.65	0.78
4:D:15:GLU:HG2	4:D:23:PRO:N	2.04	0.73
2:B:357:CYS:SG	2:B:361:LYS:NZ	2.62	0.72
2:B:254:GLN:HE21	2:B:254:GLN:N	1.89	0.71
5:E:87:ILE:HD12	5:E:114:ALA:HB1	1.74	0.70
15:T:52:DA:OP1	19:h:86:ARG:HG3	1.92	0.70
13:N:37:DT:H2''	13:N:38:DT:C5	2.27	0.69
13:N:78:DT:H2''	13:N:79:DT:C5	2.28	0.69
2:B:824:ASP:OD2	19:h:42:TYR:HB3	1.93	0.69
2:B:41:ARG:NH2	2:B:45:ASP:OD1	2.24	0.68
19:d:38:SER:HA	19:d:59:MET:HE3	1.76	0.67
13:N:8:DG:H2''	13:N:9:DT:H71	1.76	0.66
19:d:38:SER:HA	19:d:59:MET:HE2	1.76	0.66
13:N:63:DT:H2''	13:N:64:DT:H71	1.78	0.66
1:A:948:ILE:HG12	1:A:1007:ILE:HD11	1.78	0.66
15:T:131:DA:H2''	15:T:132:DC:C5	2.32	0.65
3:C:7:PRO:O	11:K:104:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:52:DA:P	19:h:86:ARG:HD3	2.37	0.64
8:H:98:ARG:HB3	8:H:115:TYR:HB2	1.79	0.64
2:B:533:SER:HB2	2:B:600:GLU:OE2	1.98	0.63
6:F:51:ARG:NH1	6:F:117:ASP:O	2.31	0.63
1:A:465:HIS:HD2	1:A:467:MET:HE2	1.62	0.62
19:d:38:SER:CA	19:d:59:MET:HE2	2.29	0.62
13:N:25:DC:H2''	13:N:26:DC:C5	2.34	0.62
13:N:28:DT:H2''	13:N:29:DT:H71	1.79	0.62
15:T:52:DA:P	19:h:86:ARG:CD	2.88	0.62
1:A:141:LEU:HD13	1:A:1445:HIS:HE1	1.64	0.61
13:N:28:DT:H2''	13:N:29:DT:C7	2.30	0.61
1:A:538:VAL:HG12	1:A:539:GLN:HG2	1.82	0.60
13:N:125:DG:H22	15:T:35:DA:H5'	1.67	0.60
13:N:40:DT:H2'	13:N:41:DT:H71	1.82	0.60
15:T:89:DA:H2''	15:T:90:DC:C5	2.36	0.60
13:N:18:DG:H2''	13:N:19:DT:H71	1.82	0.59
15:T:35:DA:H1'	15:T:36:DC:C6	2.38	0.59
19:d:38:SER:CA	19:d:59:MET:CE	2.79	0.59
2:B:934:LYS:HG2	2:B:1051:LEU:HD12	1.84	0.59
4:D:15:GLU:HA	4:D:21:ILE:O	2.02	0.59
15:T:8:DA:H4'	15:T:9:DA:OP1	2.01	0.59
14:P:2:A:H2'	14:P:3:G:C8	2.38	0.58
13:N:99:DT:H2''	13:N:100:DC:C6	2.37	0.58
13:N:1:DG:H2'	13:N:2:DT:H72	1.84	0.58
1:A:1374:VAL:HG11	1:A:1411:LEU:HD11	1.85	0.58
2:B:953:ASP:OD1	3:C:36:ARG:NH1	2.27	0.57
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.87	0.57
13:N:15:DT:H5'	13:N:15:DT:C6	2.40	0.57
5:E:29:THR:HG23	5:E:32:GLU:H	1.70	0.57
1:A:1213:ARG:NH1	1:A:1215:GLU:OE2	2.38	0.56
13:N:67:DG:H2''	13:N:68:DT:C5	2.41	0.56
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.71	0.56
1:A:958:ARG:HH12	1:A:1014:LYS:HD2	1.71	0.56
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.22	0.56
13:N:69:DG:H2''	13:N:70:DT:C7	2.35	0.56
13:N:111:DT:H2''	13:N:112:DG:C8	2.40	0.56
15:T:52:DA:OP1	19:h:86:ARG:CG	2.54	0.56
2:B:752:TYR:HE1	2:B:809:VAL:HG23	1.70	0.55
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.88	0.55
15:T:139:DC:H2'	15:T:140:DA:C8	2.41	0.55
1:A:863:ARG:NH2	1:A:1129:ASN:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:27:DG:H2''	13:N:28:DT:C5	2.42	0.55
13:N:100:DC:H2''	13:N:101:DT:C7	2.34	0.55
13:N:8:DG:N2	15:T:152:DC:O2	2.39	0.55
1:A:410:ASN:HD22	1:A:430:ARG:HB2	1.73	0.54
13:N:12:DG:H2'	13:N:13:DT:H72	1.89	0.54
1:A:460:ARG:HB2	1:A:501:MET:HE3	1.90	0.54
13:N:78:DT:H2''	13:N:79:DT:C6	2.42	0.54
1:A:339:LEU:HB3	2:B:1165:MET:HE2	1.89	0.54
2:B:585:ASN:OD1	2:B:588:ARG:NH2	2.40	0.54
3:C:98:SER:HA	3:C:165:ALA:O	2.08	0.54
13:N:66:DG:H2''	13:N:67:DG:C8	2.43	0.53
5:E:73:PHE:O	5:E:102:ALA:HA	2.08	0.53
15:T:52:DA:OP1	19:h:86:ARG:CD	2.57	0.53
1:A:517:GLU:OE1	6:F:62:ARG:NH1	2.37	0.53
1:A:1163:HIS:O	1:A:1168:LYS:NZ	2.41	0.53
2:B:274:ARG:NH1	2:B:311:ILE:O	2.41	0.53
5:E:61:LEU:HD13	5:E:73:PHE:HE1	1.74	0.53
1:A:1160:ARG:NH1	1:A:1349:GLU:OE2	2.39	0.53
2:B:677:MET:HE2	2:B:700:PRO:HB3	1.91	0.53
10:J:8:PHE:CD2	10:J:48:MET:HE1	2.44	0.53
13:N:69:DG:H2''	13:N:70:DT:H71	1.91	0.53
1:A:1479:LYS:HD2	6:F:103:PRO:HA	1.91	0.53
8:H:26:SER:HB3	8:H:45:ILE:HD11	1.91	0.53
13:N:1:DG:H2'	13:N:2:DT:C7	2.39	0.53
15:T:52:DA:O5'	19:h:86:ARG:HD2	2.09	0.52
13:N:98:DG:H2''	13:N:99:DT:C5	2.44	0.52
7:G:124:ASN:HB2	7:G:125:PRO:HD3	1.90	0.52
15:T:28:DG:H2'	15:T:29:DG:C8	2.44	0.52
1:A:784:VAL:HG13	2:B:978:ILE:HD11	1.91	0.52
8:H:103:GLU:HB3	8:H:109:ALA:HB2	1.92	0.52
13:N:30:DT:H2'	13:N:31:DT:C5	2.45	0.52
13:N:76:DC:H2''	13:N:77:DC:C6	2.44	0.52
3:C:44:ILE:HD11	3:C:176:TRP:HA	1.92	0.52
15:T:153:DA:H2''	15:T:154:DA:N7	2.24	0.51
1:A:592:PHE:HA	1:A:595:ILE:HD12	1.93	0.51
13:N:68:DT:H2''	13:N:69:DG:C8	2.46	0.51
15:T:2:DG:H2''	15:T:3:DA:C8	2.45	0.51
5:E:110:MET:HE1	5:E:118:LEU:HD11	1.93	0.51
15:T:41:DA:H1'	15:T:42:DA:C8	2.46	0.51
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.93	0.51
13:N:125:DG:H1	15:T:34:DC:H2''	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:830:GLU:OE2	2:B:870:THR:OG1	2.26	0.51
3:C:259:LEU:HD22	11:K:19:ILE:HD11	1.92	0.51
13:N:82:DC:O2	16:e:40:ARG:NH2	2.44	0.50
13:N:125:DG:N2	15:T:35:DA:H5'	2.25	0.50
1:A:1200:PRO:HB2	1:A:1203:ASP:HB3	1.92	0.50
13:N:89:DT:H2''	13:N:90:DT:C5	2.46	0.50
19:d:38:SER:CB	19:d:59:MET:HE2	2.41	0.50
1:A:1208:SER:O	1:A:1260:ARG:NH1	2.44	0.50
3:C:30:VAL:HA	11:K:45:ILE:HD11	1.93	0.50
15:T:38:DG:H1'	15:T:39:DC:C5	2.47	0.50
15:T:80:DA:H2''	15:T:81:DA:C8	2.46	0.50
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.38	0.50
13:N:16:DG:H2''	13:N:17:DG:C8	2.47	0.50
13:N:89:DT:H2''	13:N:90:DT:C7	2.41	0.50
15:T:140:DA:H2''	15:T:141:DC:C5	2.47	0.49
1:A:1468:THR:O	6:F:64:ARG:NH1	2.35	0.49
1:A:545:VAL:HG11	1:A:645:LEU:HD12	1.95	0.49
1:A:1184:THR:HG21	1:A:1193:VAL:HG21	1.94	0.49
14:P:6:C:H2'	14:P:7:A:C8	2.47	0.49
15:T:77:DG:H2''	15:T:78:DC:C5	2.47	0.49
15:T:157:DA:OP1	16:e:42:ARG:NH2	2.38	0.49
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.48	0.49
1:A:1441:GLU:OE2	1:A:1445:HIS:NE2	2.42	0.49
2:B:889:LYS:HE3	19:h:51:ASP:HB2	1.94	0.49
15:T:47:DC:H2''	15:T:48:DA:C8	2.47	0.49
1:A:1199:MET:SD	1:A:1199:MET:N	2.85	0.49
8:H:112:LEU:HB2	8:H:132:LEU:HD23	1.94	0.49
13:N:140:DT:H2'	13:N:141:DT:C6	2.48	0.48
15:T:79:DC:H2''	15:T:80:DA:N7	2.29	0.48
1:A:362:SER:HB2	2:B:1084:LEU:HD12	1.94	0.48
2:B:125:TYR:HB3	2:B:146:LYS:HA	1.95	0.48
13:N:3:DG:H2'	13:N:4:DT:H71	1.95	0.48
13:N:27:DG:H2''	13:N:28:DT:C7	2.44	0.48
2:B:98:HIS:CE1	2:B:106:SER:OG	2.67	0.48
13:N:16:DG:H2''	13:N:17:DG:N7	2.28	0.48
19:d:38:SER:HB2	19:d:59:MET:HE2	1.95	0.48
1:A:1429:LYS:HB2	1:A:1438:VAL:HG11	1.96	0.48
13:N:12:DG:H2'	13:N:13:DT:C7	2.43	0.48
15:T:66:DG:H2'	15:T:67:DC:C5	2.48	0.48
4:D:16:ASP:OD2	7:G:81:LYS:HB3	2.14	0.48
13:N:18:DG:H2''	13:N:19:DT:C7	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:910:THR:HG22	12:L:43:ILE:HA	1.95	0.47
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.96	0.47
2:B:829:PHE:HD2	2:B:917:LYS:HD2	1.78	0.47
13:N:30:DT:H2'	13:N:31:DT:C7	2.43	0.47
13:N:98:DG:H2''	13:N:99:DT:C7	2.44	0.47
2:B:1142:ASN:HD21	2:B:1145:GLN:HG3	1.78	0.47
1:A:1211:LEU:HD11	1:A:1258:ARG:CG	2.45	0.47
13:N:49:DT:H1'	16:a:83:ARG:NH2	2.30	0.47
5:E:82:VAL:HB	5:E:110:MET:HG2	1.95	0.47
13:N:47:DT:H2''	13:N:48:DC:C6	2.50	0.47
15:T:103:DA:H4'	16:a:63:ARG:HD3	1.97	0.47
1:A:1130:ILE:HG21	1:A:1411:LEU:HD23	1.96	0.47
3:C:60:HIS:HD2	3:C:62:GLU:HG2	1.80	0.47
4:D:15:GLU:CG	4:D:23:PRO:HD3	2.32	0.47
5:E:166:ARG:NH1	5:E:168:ASN:OD1	2.48	0.47
2:B:932:GLY:HA3	2:B:1055:VAL:HB	1.97	0.46
4:D:16:ASP:OD1	7:G:81:LYS:HB3	2.15	0.46
13:N:142:DT:H2''	13:N:143:DC:C5	2.50	0.46
1:A:718:GLU:OE2	1:A:722:ASN:ND2	2.49	0.46
2:B:194:LEU:HD23	2:B:467:SER:HB3	1.97	0.46
2:B:780:VAL:HA	2:B:965:ILE:O	2.15	0.46
2:B:1115:GLN:HB3	2:B:1148:LEU:HD11	1.98	0.46
1:A:421:ARG:HG2	1:A:444:TYR:CZ	2.50	0.46
1:A:1246:ILE:HG21	1:A:1258:ARG:NH2	2.30	0.46
2:B:403:LEU:HD21	2:B:447:SER:OG	2.16	0.46
13:N:107:DT:H2''	13:N:108:DT:C5	2.51	0.46
2:B:889:LYS:CE	19:h:51:ASP:HB2	2.46	0.46
13:N:142:DT:H2''	13:N:143:DC:C6	2.51	0.46
1:A:967:ARG:NH2	1:A:1326:GLY:O	2.49	0.46
2:B:109:MET:HE2	2:B:174:LEU:HD13	1.98	0.46
15:T:90:DC:H2''	15:T:91:DA:C8	2.51	0.46
5:E:192:LYS:HE2	5:E:194:ILE:HD11	1.96	0.46
1:A:46:THR:HG22	1:A:47:THR:HG23	1.98	0.46
2:B:710:ILE:HA	2:B:764:MET:HE2	1.98	0.45
1:A:222:HIS:NE2	1:A:226:LYS:HE3	2.30	0.45
2:B:715:ASP:OD1	2:B:715:ASP:N	2.48	0.45
13:N:108:DT:H2''	13:N:109:DC:C5	2.51	0.45
15:T:131:DA:H2''	15:T:132:DC:C6	2.51	0.45
1:A:926:ASN:C	1:A:928:ARG:H	2.24	0.45
2:B:855:ALA:HB3	12:L:49:THR:HB	1.98	0.45
11:K:9:SER:HA	11:K:69:HIS:ND1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:829:PHE:CD2	2:B:917:LYS:HD2	2.52	0.45
3:C:189:ASP:O	3:C:191:ALA:N	2.49	0.45
13:N:50:DC:H2''	13:N:51:DG:H5'	1.98	0.45
15:T:52:DA:OP1	19:h:86:ARG:HD3	2.17	0.45
1:A:1155:LYS:HD2	1:A:1158:LEU:HD23	1.99	0.45
4:D:16:ASP:CG	7:G:81:LYS:HB3	2.40	0.45
19:h:116:LYS:HG2	19:h:120:LYS:HE2	1.99	0.45
1:A:122:ASN:HA	1:A:127:LYS:HE3	1.97	0.45
2:B:598:VAL:HG12	2:B:600:GLU:H	1.81	0.45
3:C:99:VAL:HG11	3:C:127:VAL:HG21	1.99	0.45
13:N:28:DT:H2''	13:N:29:DT:C5	2.51	0.45
15:T:28:DG:H2'	15:T:29:DG:H8	1.82	0.45
2:B:764:MET:HE1	2:B:938:ARG:NH1	2.32	0.45
19:h:39:ILE:H	19:h:39:ILE:HD12	1.82	0.45
15:T:32:DT:H4'	15:T:33:DT:OP1	2.17	0.45
15:T:121:DA:H2''	15:T:122:DA:N7	2.30	0.45
1:A:199:TYR:CD2	1:A:213:LYS:HE2	2.52	0.45
1:A:461:GLN:NE2	15:T:25:DC:H4'	2.32	0.45
2:B:1165:MET:O	2:B:1166:SER:OG	2.35	0.45
3:C:179:THR:HG21	3:C:182:VAL:HG23	1.99	0.45
1:A:597:PRO:HD3	1:A:668:PHE:CD1	2.52	0.45
2:B:96:PRO:HG2	2:B:120:TYR:CZ	2.52	0.45
1:A:575:PRO:HG3	1:A:594:LEU:HD11	1.99	0.44
1:A:375:ILE:HG12	1:A:666:ARG:HG3	1.99	0.44
13:N:37:DT:H2''	13:N:38:DT:C4	2.51	0.44
13:N:39:DT:H2'	13:N:40:DT:C6	2.52	0.44
5:E:168:ASN:HB2	5:E:172:ARG:HH21	1.82	0.44
11:K:47:LYS:HD3	11:K:61:TYR:HD1	1.82	0.44
13:N:100:DC:H2'	13:N:100:DC:OP2	2.17	0.44
15:T:24:DG:H2'	15:T:25:DC:C6	2.53	0.44
1:A:48:GLU:OE2	1:A:53:LYS:NZ	2.41	0.44
1:A:1441:GLU:HG3	1:A:1445:HIS:HD2	1.83	0.44
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.53	0.44
2:B:526:LEU:HG	2:B:530:ALA:HB3	1.99	0.44
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.53	0.44
11:K:29:ASN:OD1	11:K:79:PRO:HA	2.18	0.44
2:B:719:SER:OG	2:B:720:PRO:HD3	2.18	0.44
5:E:61:LEU:HD13	5:E:73:PHE:CE1	2.52	0.44
10:J:3:ILE:HD12	10:J:4:PRO:HD2	2.00	0.44
13:N:5:DT:H2''	13:N:6:DT:C7	2.48	0.44
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:19:DT:H4'	18:c:77:ARG:NH1	2.33	0.43
15:T:24:DG:H2'	15:T:25:DC:H6	1.83	0.43
1:A:506:PRO:HB2	1:A:511:THR:HG23	1.99	0.43
2:B:761:THR:HG22	2:B:763:SER:H	1.83	0.43
3:C:41:GLU:N	3:C:41:GLU:OE1	2.51	0.43
3:C:101:PHE:CE2	3:C:122:SER:HB3	2.53	0.43
5:E:192:LYS:HE3	5:E:204:ILE:HD13	1.99	0.43
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.53	0.43
13:N:88:DT:H2''	13:N:89:DT:C5	2.53	0.43
13:N:98:DG:H2''	13:N:99:DT:H71	1.98	0.43
15:T:88:DA:C8	15:T:88:DA:H5'	2.54	0.43
15:T:107:DA:H2'	15:T:108:DC:C6	2.52	0.43
15:T:61:DC:H2''	15:T:62:DC:C5	2.53	0.43
3:C:32:ASN:HA	3:C:35:ARG:HG2	2.00	0.43
1:A:996:ILE:HD13	1:A:1060:LEU:HA	1.99	0.43
3:C:235:SER:OG	3:C:239:LEU:O	2.34	0.43
8:H:60:ILE:HG23	8:H:141:VAL:HG13	1.99	0.43
2:B:889:LYS:NZ	19:h:51:ASP:HB2	2.34	0.43
15:T:135:DC:H2'	15:T:136:DC:C6	2.54	0.43
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	2.01	0.43
8:H:6:PHE:HB3	8:H:60:ILE:HB	2.01	0.43
2:B:628:VAL:HG22	2:B:633:LEU:HD23	2.01	0.43
2:B:792:ASP:OD1	2:B:975:ARG:NH2	2.51	0.43
12:L:41:TYR:CZ	12:L:43:ILE:HD12	2.54	0.43
15:T:5:DA:H2''	15:T:6:DG:C8	2.54	0.43
1:A:653:VAL:HG11	1:A:669:TYR:OH	2.19	0.42
2:B:747:LEU:HA	2:B:810:PHE:CE1	2.54	0.42
13:N:131:DT:H2''	13:N:132:DA:C8	2.53	0.42
1:A:601:ASN:HA	1:A:630:VAL:O	2.19	0.42
2:B:33:TYR:HD1	2:B:653:TRP:CE2	2.37	0.42
13:N:81:DG:OP2	17:f:35:ARG:NH1	2.43	0.42
15:T:48:DA:H2''	15:T:49:DC:C6	2.54	0.42
1:A:187:TYR:HB2	1:A:202:TRP:HD1	1.84	0.42
1:A:1471:PHE:CZ	6:F:61:GLU:HA	2.55	0.42
18:c:93:LEU:HD23	18:c:93:LEU:HA	1.92	0.42
1:A:381:PRO:HB3	1:A:480:SER:HA	2.01	0.42
15:T:66:DG:H2'	15:T:67:DC:C6	2.55	0.42
2:B:474:THR:OG1	2:B:732:ALA:O	2.29	0.42
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.52	0.42
2:B:268:PRO:HD2	2:B:271:ILE:HD12	2.01	0.42
3:C:131:THR:HG21	10:J:16:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:LEU:HD21	1:A:973:GLY:HA2	2.01	0.42
2:B:284:ILE:O	2:B:288:ILE:HG12	2.19	0.42
2:B:794:VAL:HG13	2:B:965:ILE:HG23	2.02	0.42
13:N:44:DC:H2'	13:N:45:DT:C6	2.55	0.42
14:P:1:A:H2'	14:P:2:A:C8	2.54	0.42
15:T:135:DC:H2'	15:T:136:DC:C5	2.54	0.42
1:A:370:ASP:HB2	1:A:483:ARG:HG2	2.01	0.42
5:E:111:THR:HG23	5:E:114:ALA:H	1.85	0.42
13:N:97:DG:H2''	13:N:98:DG:C8	2.54	0.42
15:T:31:DC:H2'	15:T:32:DT:H71	2.02	0.42
15:T:82:DG:H2''	15:T:83:DG:C8	2.54	0.42
1:A:92:LYS:NZ	1:A:219:GLU:OE2	2.50	0.42
2:B:192:LYS:HE2	2:B:469:VAL:HG22	2.02	0.42
2:B:854:ILE:O	2:B:907:VAL:HG21	2.19	0.42
12:L:17:TYR:HB3	12:L:44:MET:HB3	2.01	0.42
2:B:198:GLU:OE1	2:B:487:SER:OG	2.30	0.41
2:B:236:TRP:HB2	2:B:259:THR:HB	2.02	0.41
5:E:84:ILE:HD11	5:E:113:SER:HB2	2.02	0.41
14:P:6:C:H2'	14:P:7:A:H8	1.85	0.41
15:T:52:DA:P	19:h:86:ARG:HD2	2.60	0.41
15:T:68:DG:C8	15:T:68:DG:H5'	2.55	0.41
1:A:1181:PRO:HG3	1:A:1207:ILE:HG21	2.01	0.41
8:H:20:LYS:NZ	8:H:22:PHE:O	2.44	0.41
1:A:837:PHE:CE2	1:A:841:MET:HE2	2.55	0.41
2:B:191:GLU:CD	2:B:743:ARG:HH22	2.29	0.41
2:B:399:LEU:HB3	2:B:453:TRP:CZ2	2.55	0.41
5:E:110:MET:HE2	5:E:110:MET:HB3	1.85	0.41
17:f:62:LEU:HD23	17:f:62:LEU:HA	1.83	0.41
2:B:533:SER:HB2	2:B:600:GLU:CD	2.46	0.41
13:N:114:DG:H2'	13:N:115:DT:C5	2.56	0.41
18:c:87:ILE:HD13	18:c:102:ILE:HD11	2.03	0.41
1:A:567:LEU:HB3	1:A:570:TRP:HB2	2.01	0.41
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	2.03	0.41
5:E:116:GLN:HA	5:E:119:VAL:HG12	2.03	0.41
18:g:20:ARG:HG2	19:h:124:ALA:CB	2.50	0.41
8:H:37:MET:HE3	8:H:127:GLY:HA3	2.02	0.41
19:d:85:LYS:HA	19:d:85:LYS:HD3	1.92	0.41
1:A:58:MET:HE2	1:A:65:ILE:HG23	2.03	0.41
2:B:506:TRP:HZ2	2:B:677:MET:HE1	1.85	0.41
2:B:603:MET:HE2	2:B:603:MET:HB2	1.92	0.41
13:N:71:DT:H6	13:N:71:DT:H2'	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLU:OE1	1:A:448:ARG:NH1	2.53	0.41
2:B:1076:GLU:O	2:B:1080:ARG:NH1	2.43	0.41
3:C:260:GLN:HB2	11:K:91:ILE:HG21	2.03	0.41
1:A:1137:PRO:HB2	1:A:1341:VAL:HG23	2.03	0.41
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	2.03	0.41
3:C:69:GLY:HA3	12:L:57:ALA:HB1	2.03	0.41
15:T:35:DA:H1'	15:T:36:DC:O5'	2.21	0.41
19:h:86:ARG:HD3	19:h:86:ARG:HA	1.75	0.41
1:A:428:ASP:OD2	1:A:430:ARG:NH1	2.46	0.41
1:A:1302:GLU:O	1:A:1303:GLN:HG2	2.21	0.41
1:A:1474:LEU:HB2	6:F:105:ILE:HG12	2.01	0.41
8:H:37:MET:HE1	8:H:132:LEU:HD13	2.03	0.41
8:H:48:TYR:OH	8:H:89:GLU:OE1	2.32	0.41
12:L:50:LYS:HD2	12:L:50:LYS:HA	1.91	0.41
13:N:68:DT:H2''	13:N:69:DG:N7	2.36	0.41
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.56	0.40
2:B:115:LEU:HB3	2:B:908:MET:HE2	2.03	0.40
3:C:71:ILE:HD11	3:C:150:ILE:HG12	2.03	0.40
5:E:110:MET:HE1	5:E:118:LEU:CD1	2.51	0.40
11:K:45:ILE:HG23	11:K:94:LEU:HD22	2.02	0.40
13:N:80:DG:H2''	13:N:81:DG:C8	2.57	0.40
15:T:6:DG:H2''	15:T:7:DA:C8	2.56	0.40
15:T:59:DG:H2''	15:T:60:DA:N7	2.36	0.40
1:A:631:GLU:HB3	1:A:992:LYS:HZ3	1.86	0.40
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.37	0.40
5:E:166:ARG:HH22	5:E:168:ASN:HD21	1.69	0.40
13:N:20:DG:C2	15:T:140:DA:C2	3.09	0.40
1:A:370:ASP:OD2	1:A:373:LEU:HG	2.21	0.40
1:A:499:ASP:OD1	14:P:10:C:H4'	2.22	0.40
5:E:35:GLN:NE2	5:E:43:GLN:OE1	2.54	0.40
8:H:91:VAL:HG22	8:H:144:LEU:HD23	2.04	0.40
13:N:26:DC:H2''	13:N:27:DG:C8	2.56	0.40
13:N:52:DT:H2''	13:N:53:DG:H5'	2.03	0.40
3:C:10:ARG:HH12	3:C:24:GLU:CD	2.29	0.40
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.57	0.40
13:N:39:DT:H2'	13:N:40:DT:O4'	2.22	0.40
15:T:140:DA:H2''	15:T:141:DC:C6	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1400/1970 (71%)	1358 (97%)	42 (3%)	0	100	100
2	B	1103/1174 (94%)	1063 (96%)	40 (4%)	0	100	100
3	C	250/292 (86%)	241 (96%)	9 (4%)	0	100	100
4	D	124/142 (87%)	122 (98%)	2 (2%)	0	100	100
5	E	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
6	F	79/127 (62%)	78 (99%)	1 (1%)	0	100	100
7	G	168/172 (98%)	157 (94%)	11 (6%)	0	100	100
8	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
9	I	112/125 (90%)	106 (95%)	6 (5%)	0	100	100
10	J	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
16	a	93/135 (69%)	92 (99%)	1 (1%)	0	100	100
16	e	93/135 (69%)	93 (100%)	0	0	100	100
17	b	76/102 (74%)	74 (97%)	2 (3%)	0	100	100
17	f	75/102 (74%)	74 (99%)	1 (1%)	0	100	100
18	c	102/129 (79%)	99 (97%)	3 (3%)	0	100	100
18	g	100/129 (78%)	96 (96%)	4 (4%)	0	100	100
19	d	90/125 (72%)	89 (99%)	1 (1%)	0	100	100
19	h	91/125 (73%)	91 (100%)	0	0	100	100
All	All	4528/5586 (81%)	4386 (97%)	142 (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	A	1241/1748 (71%)	1241 (100%)	0	100	100
2	B	981/1028 (95%)	980 (100%)	1 (0%)	88	87
3	C	231/268 (86%)	231 (100%)	0	100	100
4	D	105/126 (83%)	105 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	70/111 (63%)	70 (100%)	0	100	100
7	G	147/153 (96%)	147 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	103/112 (92%)	103 (100%)	0	100	100
10	J	55/56 (98%)	55 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
16	a	83/110 (76%)	83 (100%)	0	100	100
16	e	83/110 (76%)	83 (100%)	0	100	100
17	b	63/78 (81%)	63 (100%)	0	100	100
17	f	63/78 (81%)	63 (100%)	0	100	100
18	c	82/99 (83%)	82 (100%)	0	100	100
18	g	81/99 (82%)	81 (100%)	0	100	100
19	d	78/104 (75%)	78 (100%)	0	100	100
19	h	79/104 (76%)	79 (100%)	0	100	100
All	All	4010/4868 (82%)	4009 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
2	B	254	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	143	HIS
1	A	423	ASN
1	A	432	HIS
1	A	465	HIS
1	A	472	HIS
1	A	507	GLN
1	A	620	HIS
1	A	673	GLN
1	A	731	ASN
1	A	861	GLN
1	A	1032	GLN
1	A	1230	GLN
1	A	1417	HIS
2	B	43	GLN
2	B	98	HIS
2	B	145	GLN
2	B	683	GLN
2	B	1117	HIS
2	B	1160	GLN
4	D	34	ASN
4	D	47	GLN
4	D	66	ASN
5	E	169	GLN
6	F	48	ASN
7	G	60	GLN
7	G	139	GLN
9	I	118	HIS
11	K	49	GLN
16	a	85	GLN
16	a	93	GLN
19	d	95	GLN
16	e	76	GLN
16	e	85	GLN
18	g	104	GLN
19	h	67	ASN
19	h	95	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	10/11 (90%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

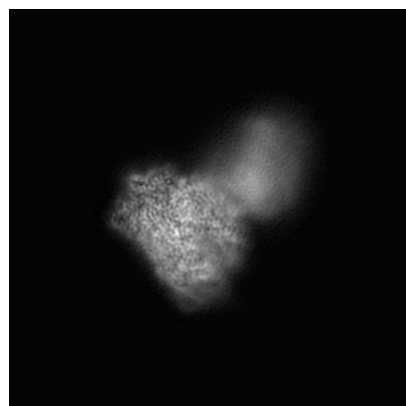
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38604. These allow visual inspection of the internal detail of the map and identification of artifacts.

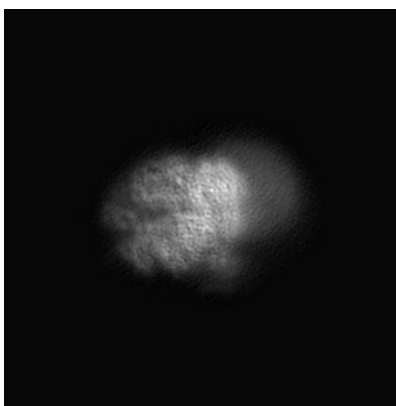
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

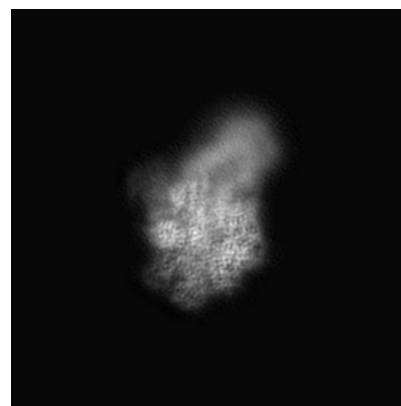
6.1.1 Primary map



X

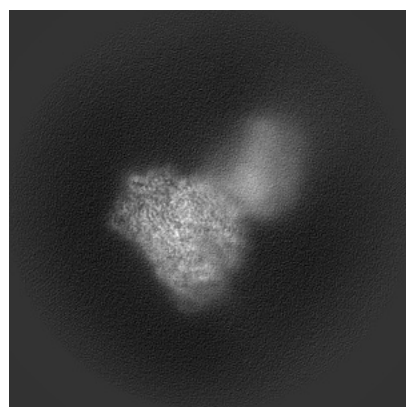


Y

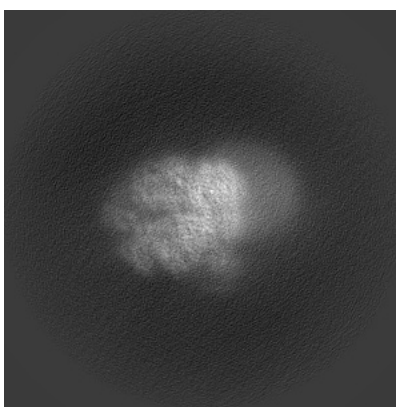


Z

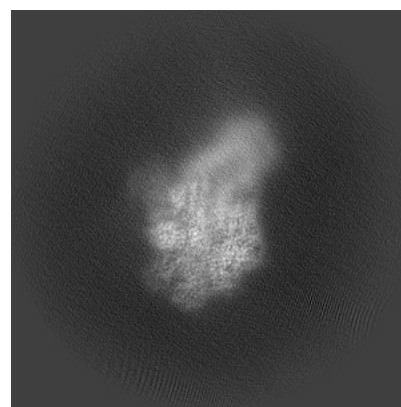
6.1.2 Raw map



X



Y

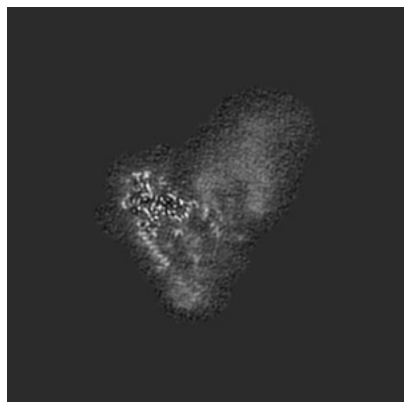


Z

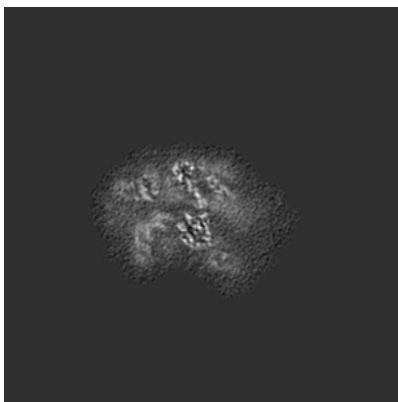
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

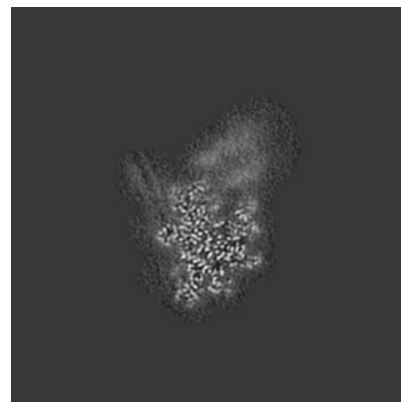
6.2.1 Primary map



X Index: 180

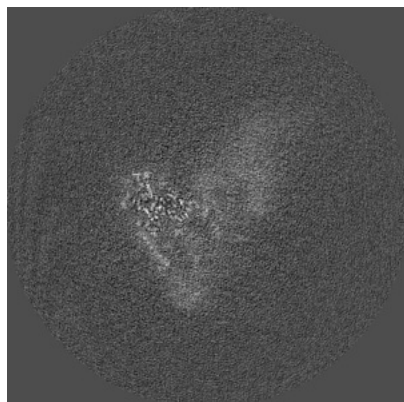


Y Index: 180

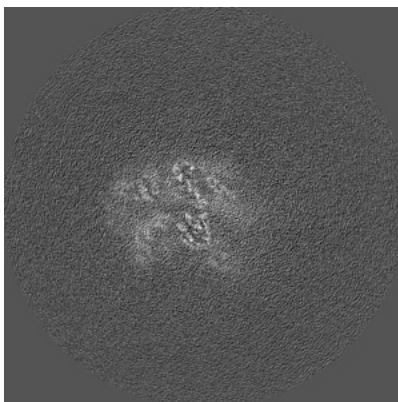


Z Index: 180

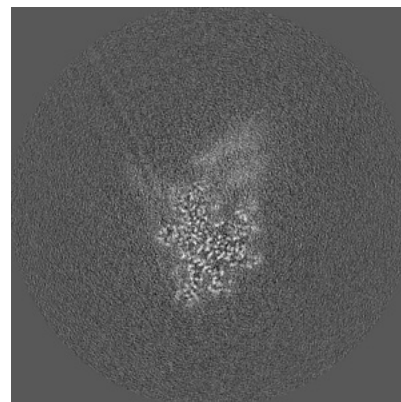
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

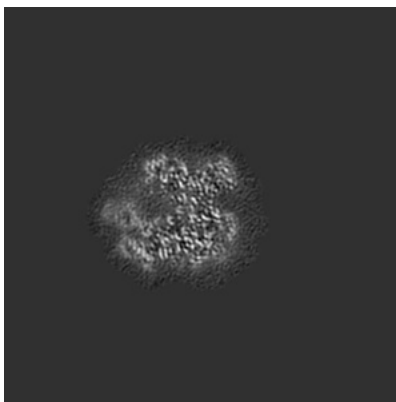
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

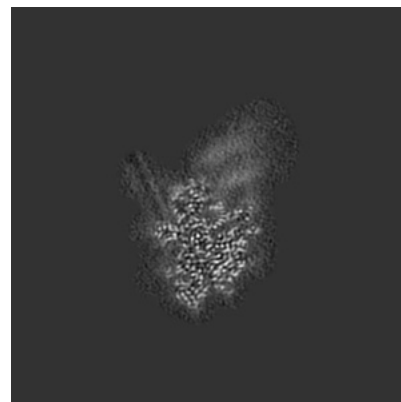
6.3.1 Primary map



X Index: 191

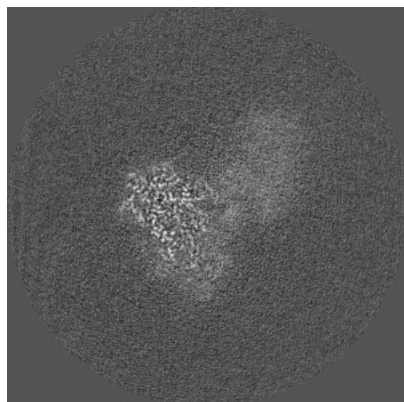


Y Index: 155

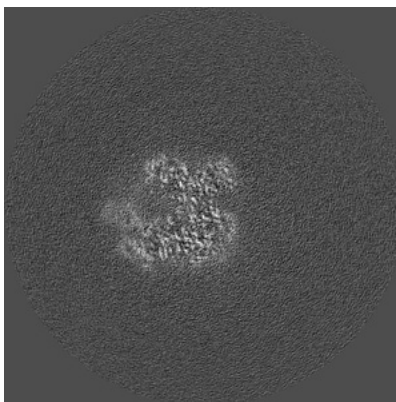


Z Index: 176

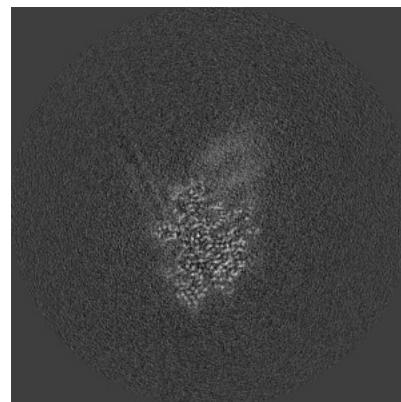
6.3.2 Raw map



X Index: 196



Y Index: 155

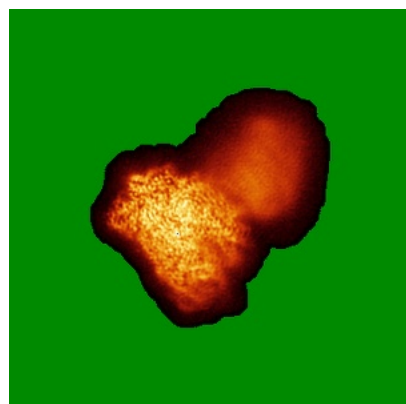


Z Index: 176

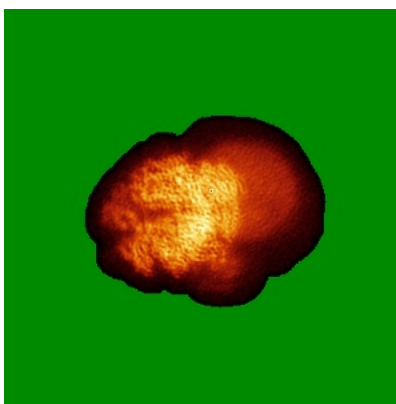
The images above show the largest variance slices of the map in three orthogonal directions.

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

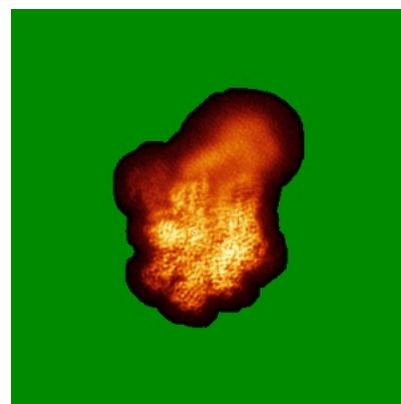
6.4.1 Primary map



X

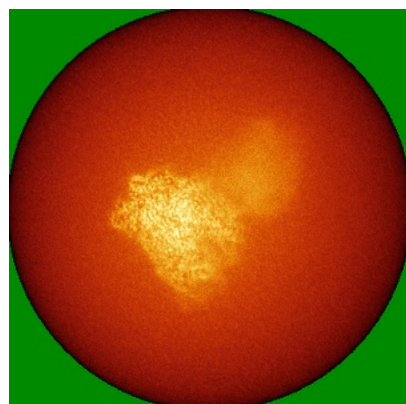


Y

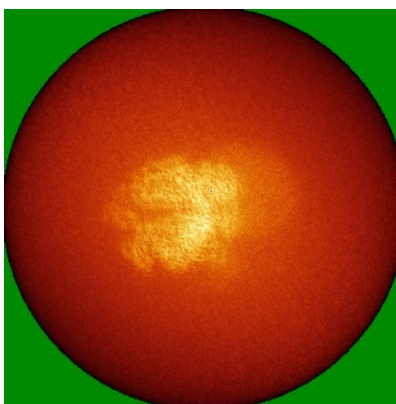


Z

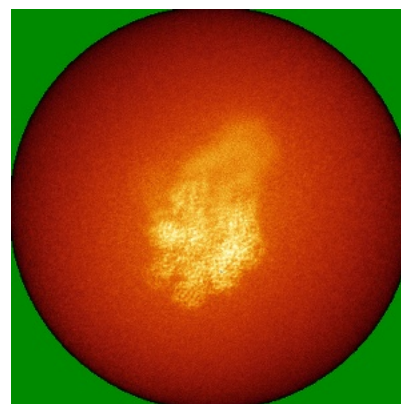
6.4.2 Raw map



X



Y

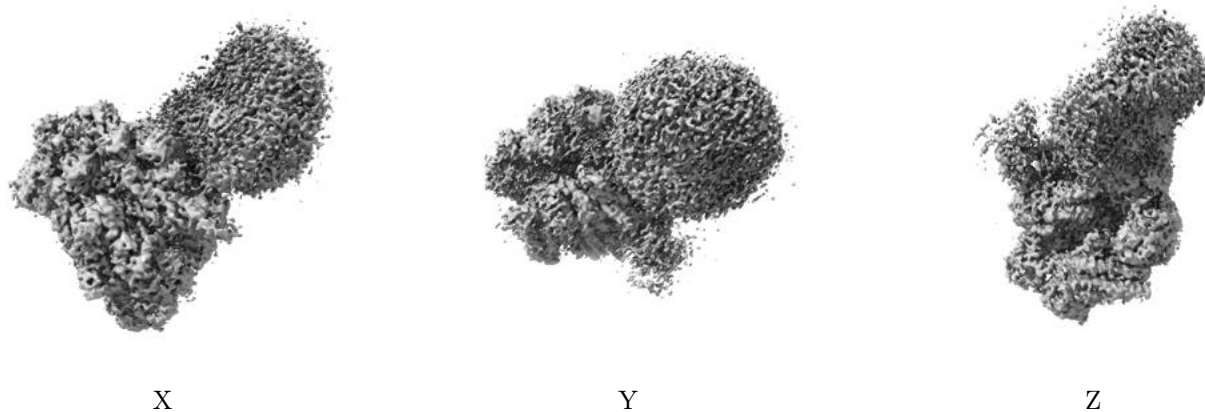


Z

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.

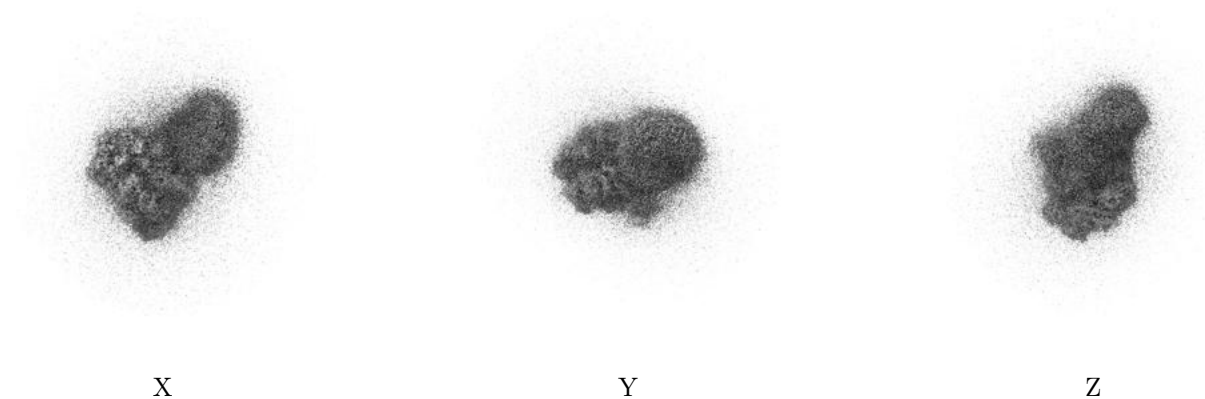
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00744. 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.

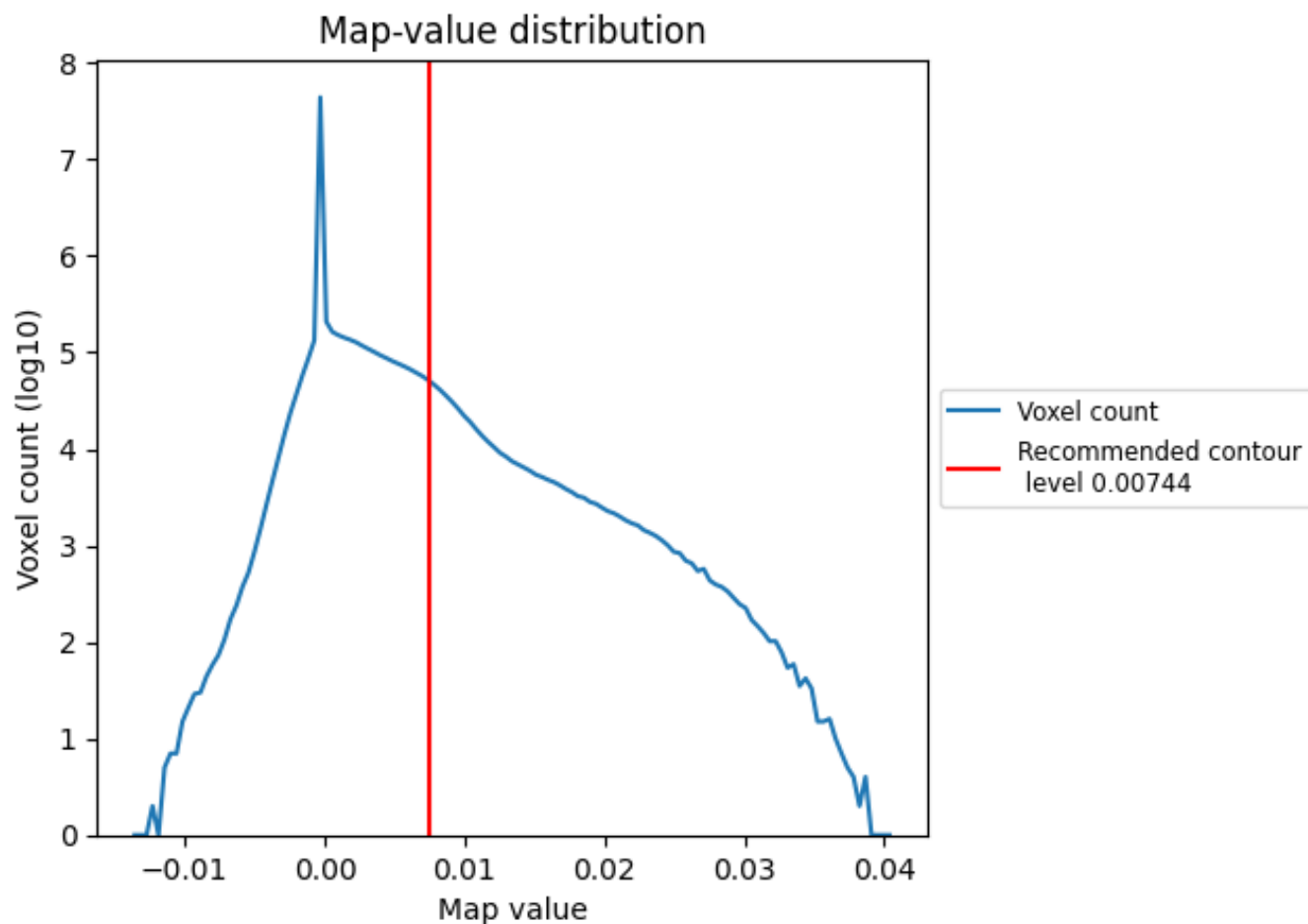
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

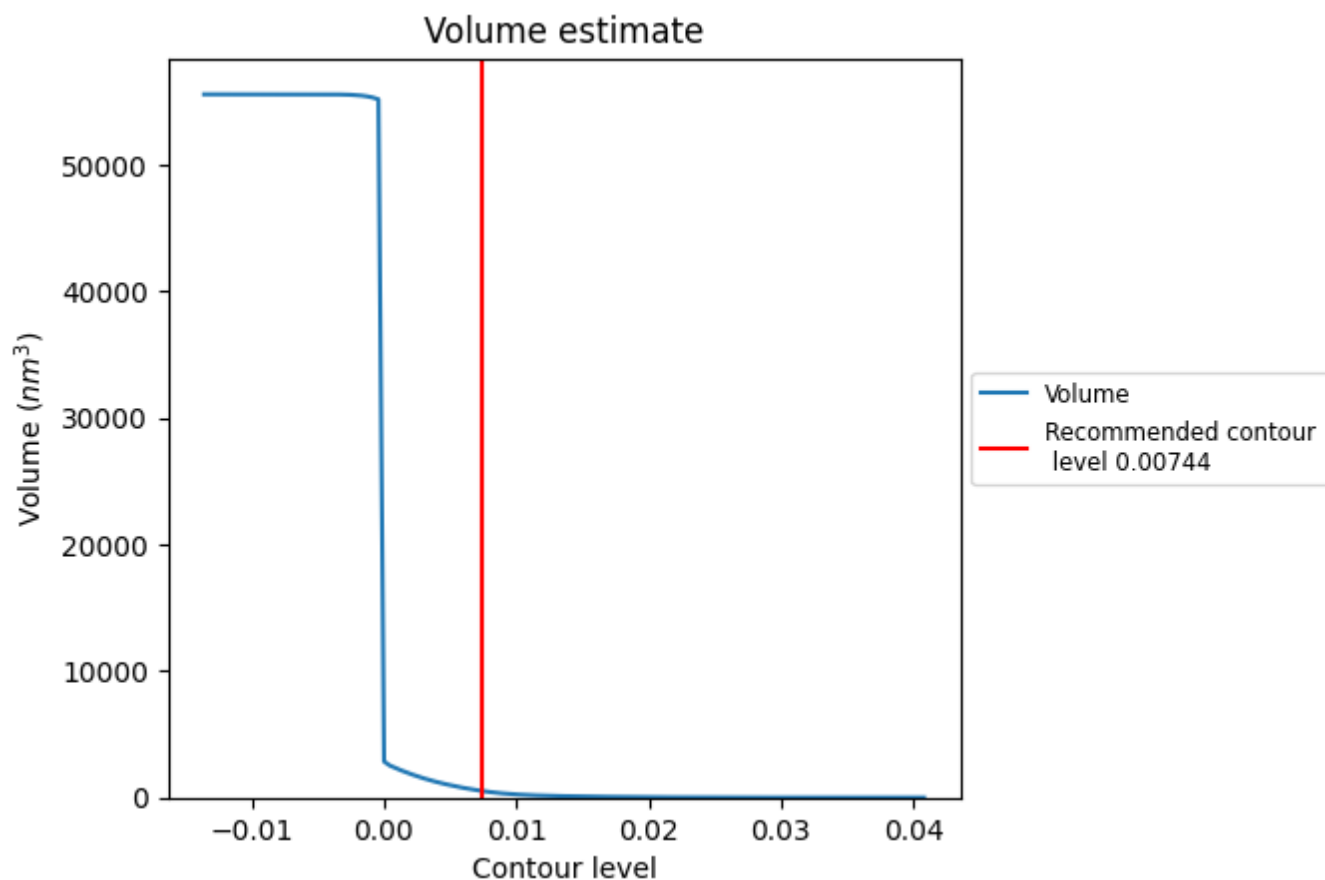
This section contains the results of statistical analysis of the map.

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.

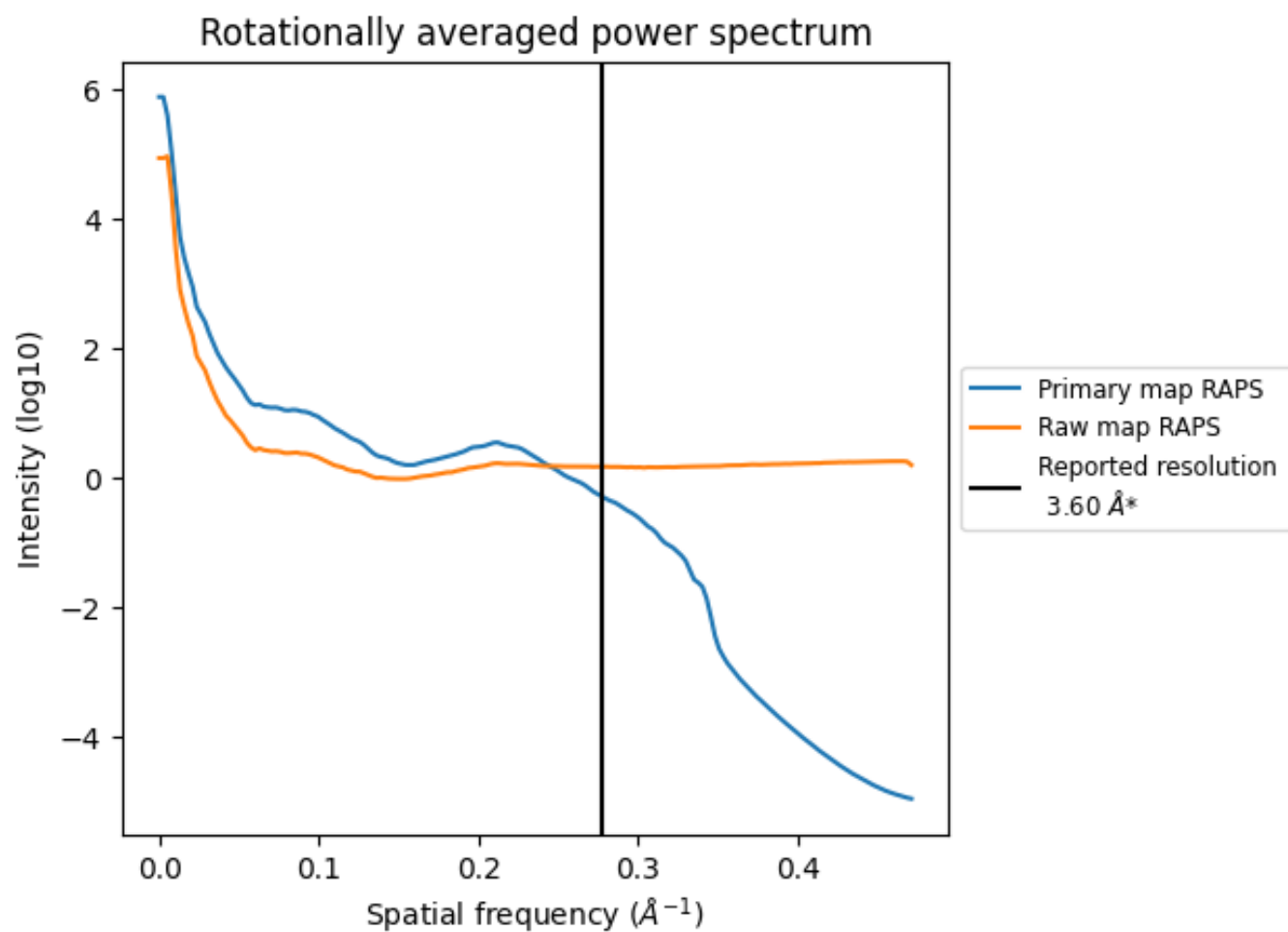
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 518 nm³; this corresponds to an approximate mass of 468 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 ⓘ

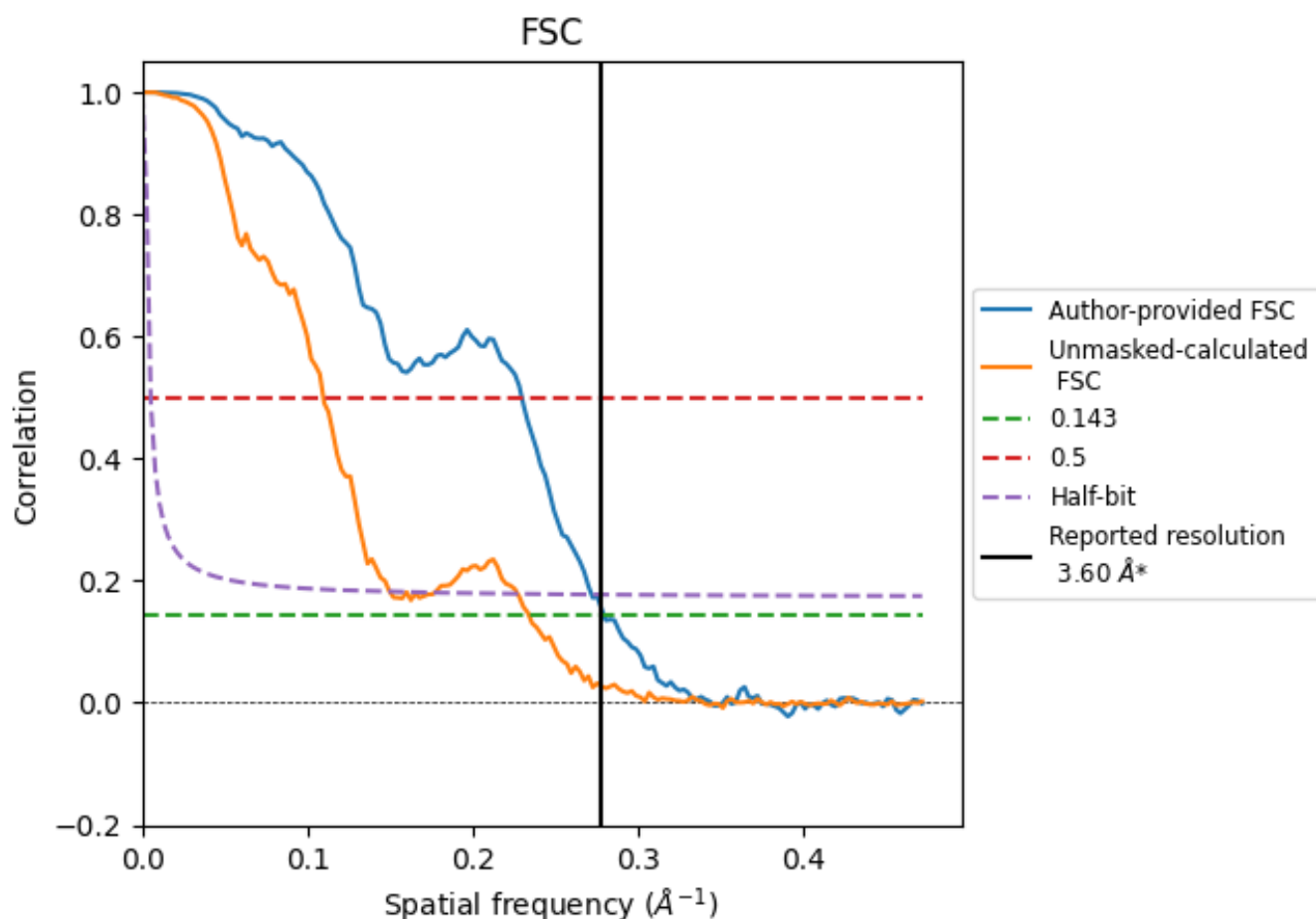


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

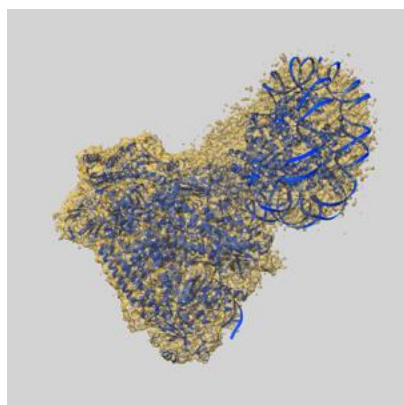
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.36	3.68
Unmasked-calculated*	4.28	9.12	6.68

*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 4.28 differs from the reported value 3.6 by more than 10 %

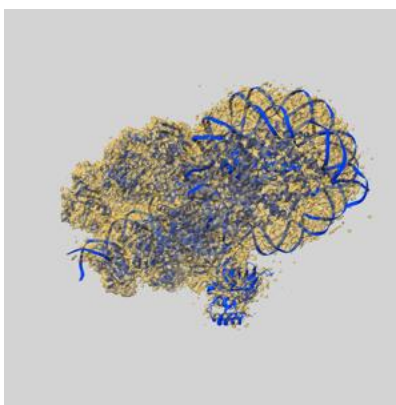
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38604 and PDB model 8XRJ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

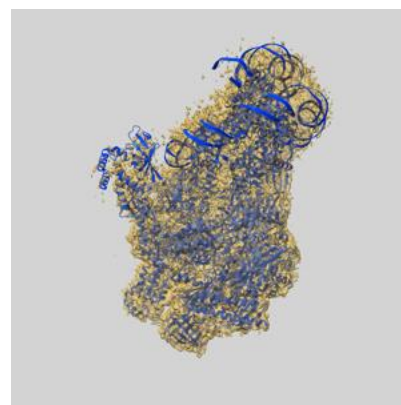
9.1 Map-model overlay [i](#)



X



Y



Z

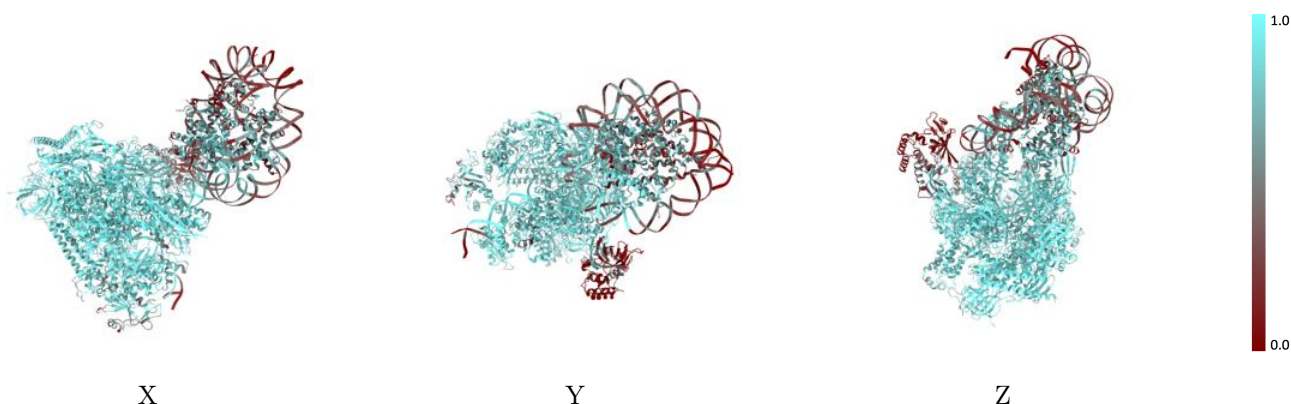
The images above show the 3D surface view of the map at the recommended contour level 0.00744 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



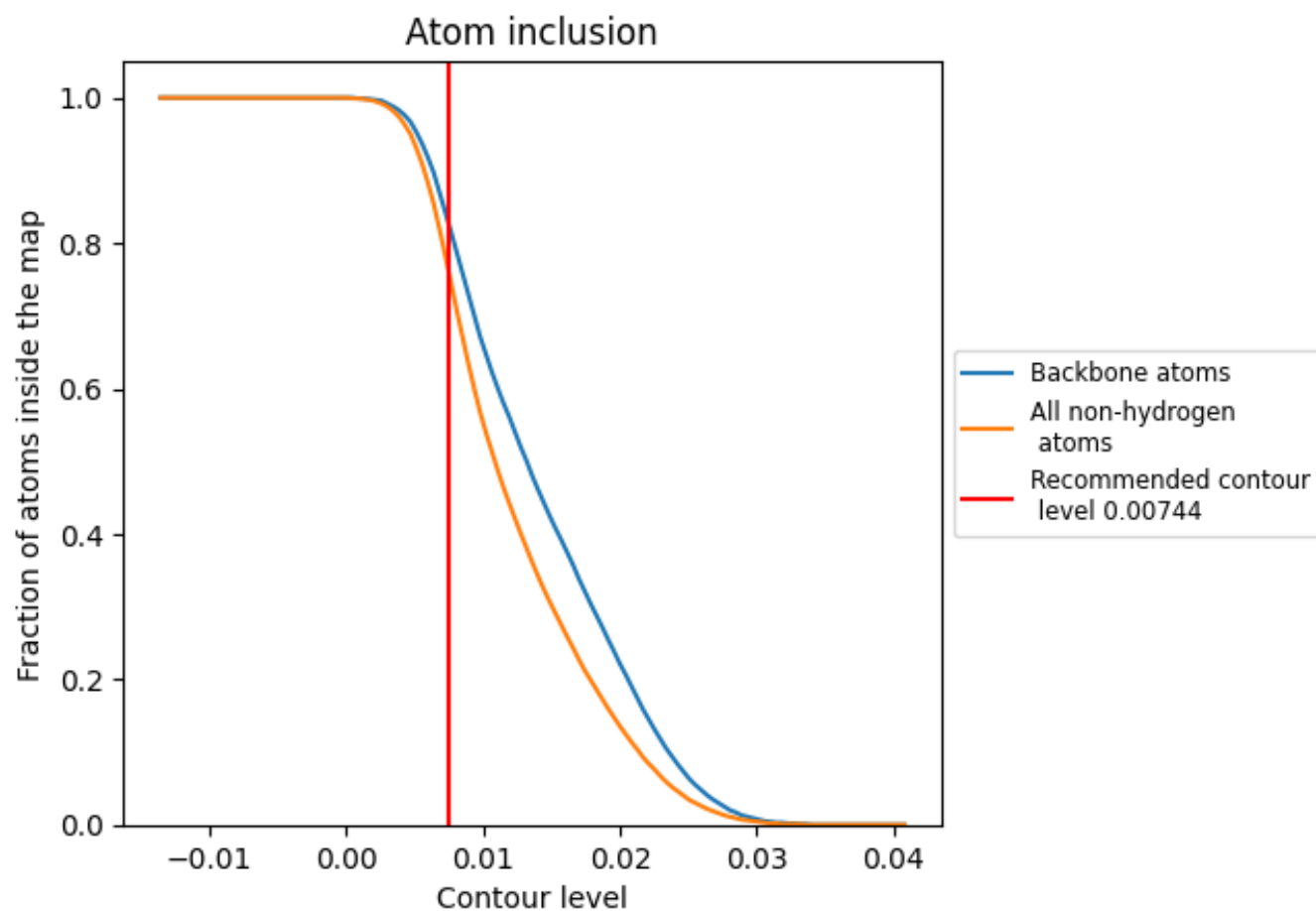
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00744).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.00744) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7650	 0.3100
A	 0.8900	 0.4190
B	 0.9180	 0.4460
C	 0.9060	 0.4590
D	 0.1720	 0.1080
E	 0.9030	 0.4170
F	 0.9330	 0.4710
G	 0.4110	 0.2110
H	 0.8680	 0.4480
I	 0.6730	 0.2800
J	 0.9240	 0.4870
K	 0.9180	 0.4760
L	 0.7860	 0.3240
N	 0.4800	 0.0510
P	 0.9710	 0.4720
T	 0.5220	 0.1010
a	 0.6410	 0.0050
b	 0.8560	 0.0690
c	 0.5610	 0.0380
d	 0.5330	 -0.0060
e	 0.4830	 0.0320
f	 0.5240	 0.0590
g	 0.6300	 -0.0080
h	 0.6060	 0.0400

