



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:06 AM UTC

PDB ID : 8JH2 / pdb_00008jh2
EMDB ID : EMD-36251
Title : RNA polymerase II elongation complex bound with Elf1, Spt4/5 and foreign DNA, stalled at SHL(-1) of the nucleosome
Authors : Akatsu, M.; Fujita, R.; Ogasawara, M.; Ehara, H.; Kujirai, T.; Takizawa, Y.; Sekine, S.; Kurumizaka, H.
Deposited on : 2023-05-22
Resolution : 5.70 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

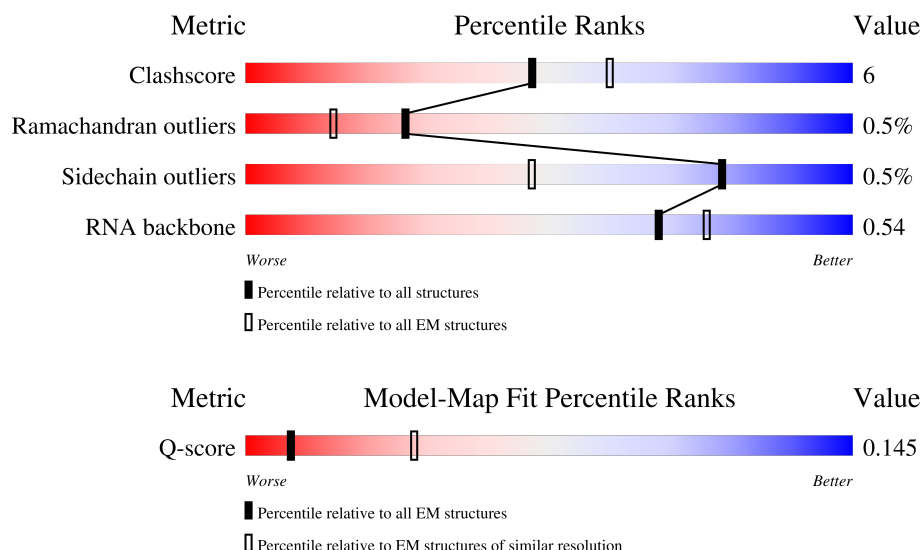
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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	503 (5.20 - 6.20)

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	0	40	
2	1	40	
3	A	1743	

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Mol	Chain	Length	Quality of chain
4	B	1227	
5	C	304	
6	D	186	
7	E	214	
8	F	155	
9	G	171	
10	H	145	
11	I	115	
12	J	72	
13	K	118	
14	L	72	
15	M	110	
16	N	228	
17	P	16	
18	T	228	
19	V	114	
20	W	908	
21	a	136	
21	e	136	
22	b	103	
22	f	103	
23	c	130	
23	g	130	
24	d	126	
24	h	126	

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 47629 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 (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	40	Total	C	N	O	P	0	0
			823	389	175	219	40		

- Molecule 2 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	40	Total	C	N	O	P	0	0
			817	394	122	261	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1411	Total	C	N	O	S	0	0
			11116	7009	1937	2100	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	1157	Total	C	N	O	S	0	0
			9228	5816	1630	1724	58		

- Molecule 5 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	263	Total	C	N	O	S	0	0
			2098	1319	354	413	12		

- Molecule 6 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	168	Total	C	N	O	S	0	0
			1314	812	237	263	2		

- Molecule 7 is a protein called RNA polymerase subunit ABC27.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	213	Total	C	N	O	S	0	0
			1740	1094	312	324	10		

- Molecule 8 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 13 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 14 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 15 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	64	Total	C	N	O	S	0	0
			505	318	82	99	6		

- Molecule 16 is a DNA chain called DNA (218-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	118	Total	C	N	O	P	0	0
			2426	1148	445	715	118		

- Molecule 17 is a RNA chain called RNA (5'-R(P*CP*CP*UP*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*GP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	16	Total	C	N	O	P	0	0
			341	151	56	118	16		

- Molecule 18 is a DNA chain called DNA (218-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	127	Total	C	N	O	P	0	0
			2589	1227	486	750	126		

- Molecule 19 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	102	Total	C	N	O	S	0	0
			792	492	143	150	7		

- Molecule 20 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	275	Total	C	N	O	S	0	0
			2226	1425	397	403	1		

- Molecule 21 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	a	96	Total	C	N	O	S	0	0
			786	497	151	136	2		
21	e	99	Total	C	N	O	S	0	0
			815	515	159	139	2		

- Molecule 22 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	77	Total	C	N	O	S	0	0
			614	389	119	105	1		
22	f	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

- Molecule 23 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	c	101	Total	C	N	O	0	0
			778	492	150	136		
23	g	101	Total	C	N	O	0	0
			778	492	150	136		

- Molecule 24 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	88	Total	C	N	O	S	0	0
			685	433	121	129	2		
24	h	90	Total	C	N	O	S	0	0
			703	444	124	133	2		

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total	Zn	0
			2	2	
25	B	1	Total	Zn	0
			1	1	
25	C	1	Total	Zn	0
			1	1	
25	I	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
25	J	1	Total 1	Zn 1	0
25	L	1	Total 1	Zn 1	0
25	M	1	Total 1	Zn 1	0
25	V	1	Total 1	Zn 1	0

- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

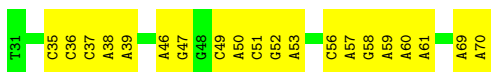
Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total 1	Mg 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

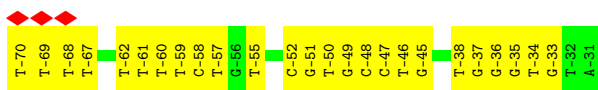
- Molecule 1: DNA (40-MER)

Chain 0: 



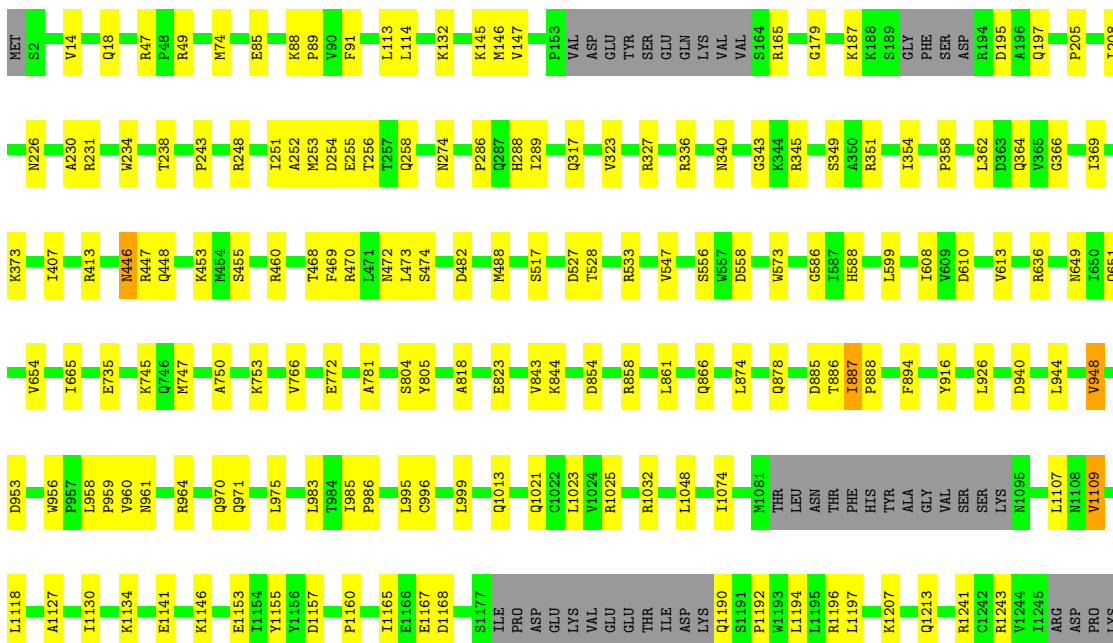
- Molecule 2: DNA (40-MER)

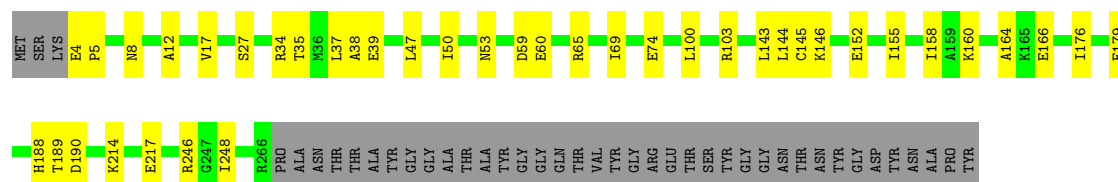
Chain 1: 



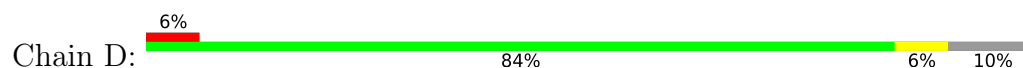
- Molecule 3: DNA-directed RNA polymerase subunit

Chain A: 





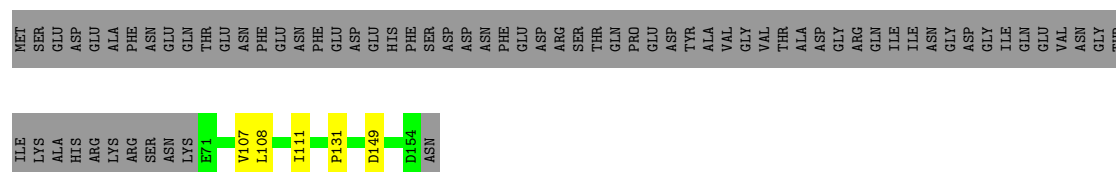
- Molecule 6: RNA polymerase II subunit B32



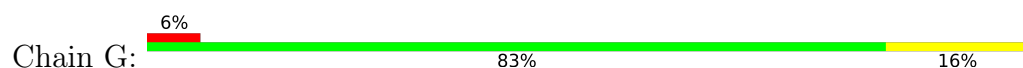
- Molecule 7: RNA polymerase subunit ABC27



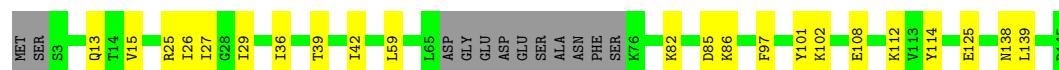
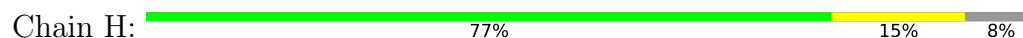
- Molecule 8: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III



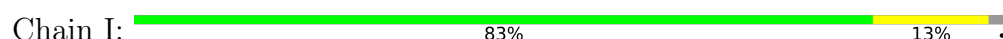
- Molecule 9: RNA polymerase II subunit



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 11: DNA-directed RNA polymerase subunit



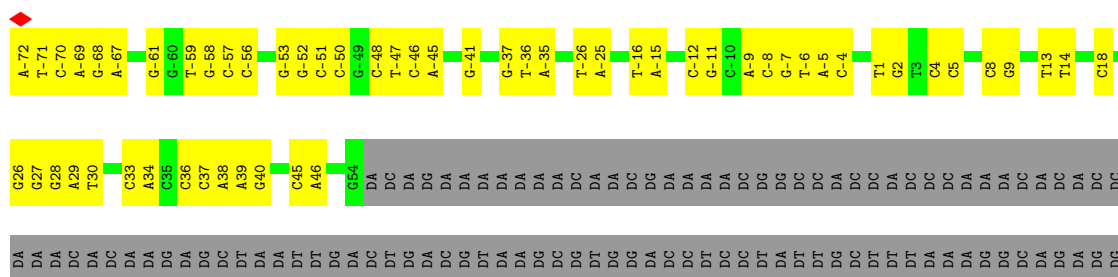
- Molecule 17: RNA (5'-R(P*CP*CP*UP*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*GP*UP*G)-3')

Chain P: 



- Molecule 18: DNA (218-MER)

Chain T: 



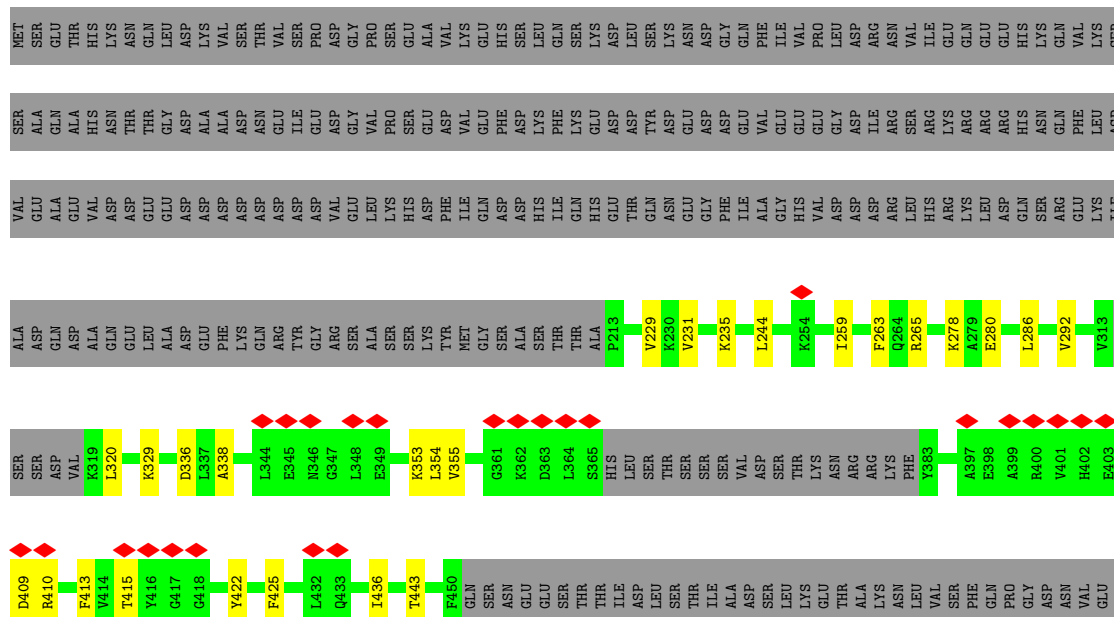
- Molecule 19: Transcription elongation factor SPT4

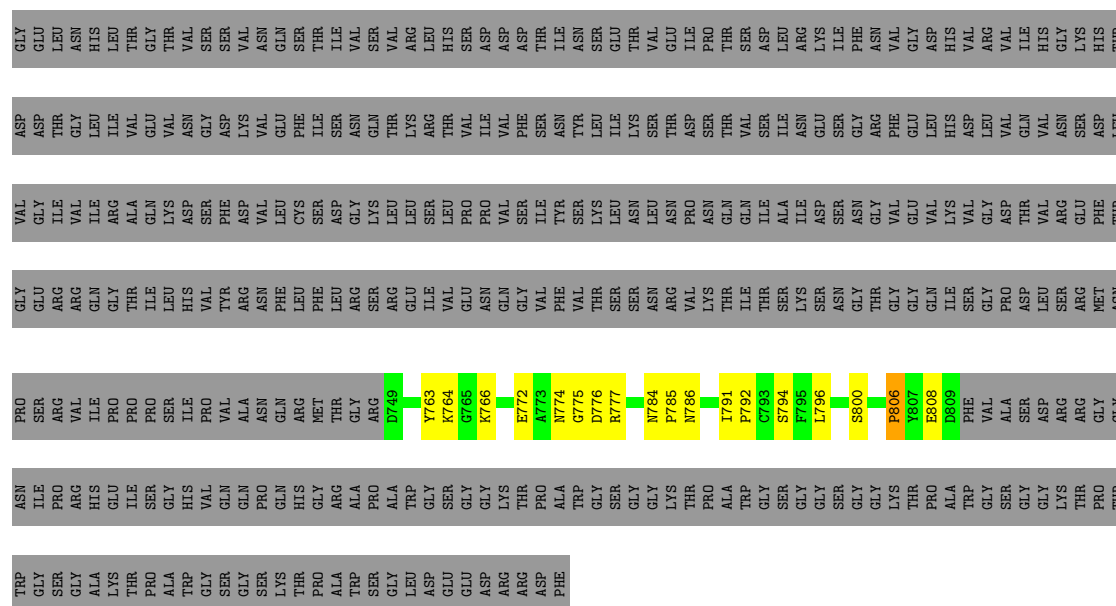
Chain V: 



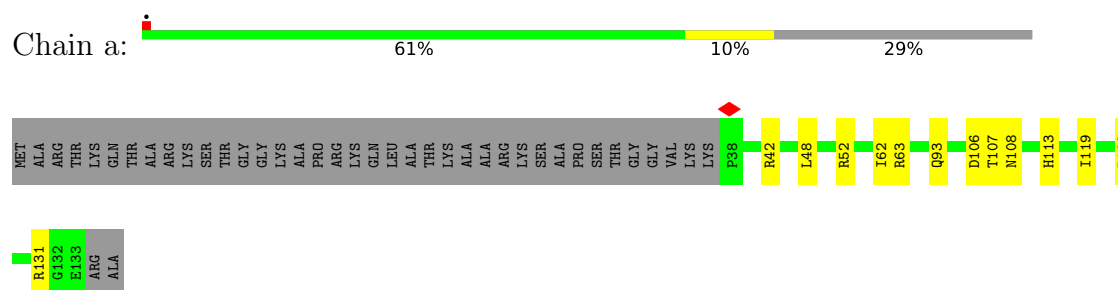
- Molecule 20: Transcription elongation factor SPT5

Chain W: 

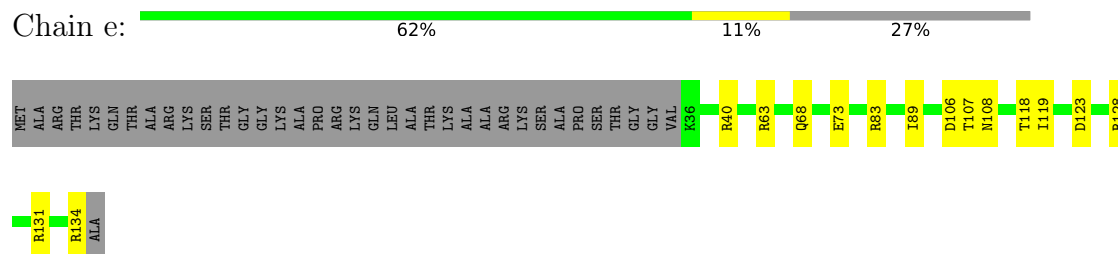




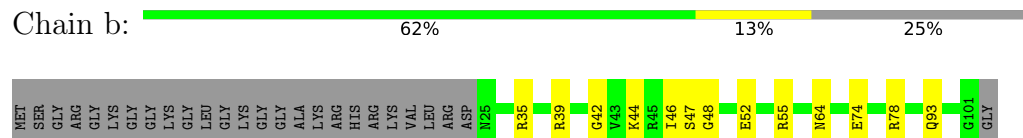
- Molecule 21: Histone H3.3



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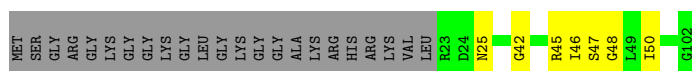


- Molecule 22: Histone H4

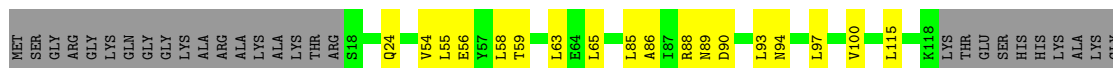


- Molecule 22: Histone H4





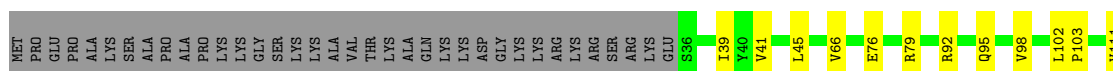
- Molecule 23: Histone H2A type 1-B/E



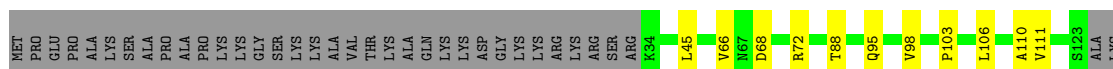
- Molecule 23: Histone H2A type 1-B/E



- Molecule 24: Histone H2B type 1-J



- Molecule 24: 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	74079	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.84	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	0.025	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00307	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.19	0/930	0.37	0/1430
2	1	0.22	0/908	0.41	0/1402
3	A	0.06	0/11322	0.18	0/15300
4	B	0.06	0/9407	0.18	0/12685
5	C	0.06	0/2139	0.17	0/2895
6	D	0.05	0/1326	0.15	0/1788
7	E	0.06	0/1772	0.17	0/2385
8	F	0.05	0/687	0.15	0/931
9	G	0.06	0/1353	0.17	0/1837
10	H	0.05	0/1069	0.17	0/1444
11	I	0.05	0/934	0.17	0/1257
12	J	0.04	0/554	0.13	0/742
13	K	0.06	0/953	0.17	0/1291
14	L	0.04	0/365	0.17	0/484
15	M	0.06	0/513	0.19	0/693
16	N	0.15	0/2719	0.31	0/4195
17	P	0.05	0/379	0.12	0/589
18	T	0.14	0/2905	0.28	0/4477
19	V	0.05	0/808	0.15	0/1097
20	W	0.06	0/2267	0.18	0/3048
21	a	0.06	0/798	0.15	0/1071
21	e	0.06	0/827	0.15	0/1108
22	b	0.08	0/621	0.20	0/832
22	f	0.06	0/645	0.16	0/862
23	c	0.06	0/788	0.16	0/1065
23	g	0.06	0/788	0.16	0/1065
24	d	0.06	0/696	0.15	0/938
24	h	0.06	0/714	0.14	0/961
All	All	0.08	0/49187	0.21	0/67872

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 ⓘ

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	0	823	0	442	16	0
2	1	817	0	463	30	0
3	A	11116	0	11137	129	0
4	B	9228	0	9232	129	0
5	C	2098	0	2058	27	0
6	D	1314	0	1314	8	0
7	E	1740	0	1754	13	0
8	F	677	0	693	4	0
9	G	1324	0	1342	16	0
10	H	1052	0	1050	12	0
11	I	917	0	867	14	0
12	J	545	0	560	5	0
13	K	932	0	944	11	0
14	L	359	0	358	7	0
15	M	505	0	495	4	0
16	N	2426	0	1327	41	0
17	P	341	0	170	5	0
18	T	2589	0	1420	54	0
19	V	792	0	757	10	0
20	W	2226	0	2273	28	0
21	a	786	0	822	10	0
21	e	815	0	860	14	0
22	b	614	0	656	11	0
22	f	638	0	676	6	0
23	c	778	0	828	13	0
23	g	778	0	828	12	0
24	d	685	0	703	9	0
24	h	703	0	722	7	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	1	0	0	0	0
25	V	1	0	0	0	0
26	A	1	0	0	0	0
All	All	47629	0	44751	550	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 6.

All (550) 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:B:995:ARG:NH1	4:B:997:GLU:OE2	1.94	1.00
16:N:-18:DG:N2	18:T:18:DC:O2	2.00	0.94
4:B:279:ARG:NH1	4:B:316:ILE:O	2.05	0.90
3:A:885:ASP:OD2	3:A:1032:ARG:NH1	2.04	0.90
2:1:-69:DT:H2''	2:1:-68:DT:C7	2.02	0.88
2:1:-69:DT:H2''	2:1:-68:DT:H71	1.55	0.86
3:A:1146:LYS:NZ	4:B:254:ASP:OD2	2.13	0.82
4:B:896:ASP:OD2	14:L:60:LYS:NZ	2.13	0.81
19:V:15:CYS:HB3	19:V:32:CYS:SG	2.22	0.79
16:N:41:DC:N3	18:T:-41:DG:N1	2.30	0.78
4:B:688:GLU:OE2	4:B:740:HIS:NE2	2.17	0.78
4:B:822:ASN:O	12:J:47:ARG:NH1	2.16	0.77
3:A:468:THR:OG1	3:A:470:ARG:NH1	2.19	0.76
16:N:41:DC:O2	18:T:-41:DG:N2	2.13	0.75
3:A:1155:TYR:OH	11:I:42:LYS:NZ	2.20	0.74
2:1:-69:DT:H2''	2:1:-68:DT:C5	2.23	0.74
4:B:350:GLN:O	4:B:367:LYS:NZ	2.21	0.73
3:A:636:ARG:NH1	3:A:878:GLN:OE1	2.22	0.72
19:V:85:ARG:NH1	19:V:87:ASP:OD1	2.22	0.72
3:A:781:ALA:N	4:B:696:GLU:OE2	2.22	0.71
3:A:854:ASP:OD2	3:A:858:ARG:NH2	2.24	0.71
4:B:969:ARG:NH1	5:C:60:GLU:OE1	2.24	0.70
18:T:37:DC:H2'	18:T:38:DA:H8	1.57	0.70
18:T:27:DG:N2	18:T:28:DG:O6	2.26	0.69
3:A:1118:LEU:HD11	3:A:1315:ASN:H	1.57	0.68
3:A:1194:LEU:HD11	3:A:1241:ARG:HB3	1.75	0.68
21:e:106:ASP:OD2	21:e:131:ARG:NE	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:284:VAL:HG23	4:B:285:PRO:HD3	1.77	0.67
18:T:9:DG:N3	21:e:40:ARG:NH2	2.43	0.67
3:A:866:GLN:NE2	3:A:1376:ASP:OD2	2.23	0.67
1:0:51:DC:N4	1:0:52:DG:O6	2.27	0.66
2:1:-55:DT:H5''	23:g:77:ARG:NH1	2.12	0.65
2:1:-38:DT:H2''	2:1:-37:DG:OP2	1.96	0.64
4:B:427:ARG:HH21	20:W:235:LYS:NZ	1.96	0.64
18:T:26:DG:H2''	18:T:27:DG:H5''	1.79	0.64
2:1:-47:DC:H2''	2:1:-46:DT:C5	2.32	0.64
7:E:60:LEU:HD11	7:E:76:THR:HB	1.80	0.64
4:B:56:LEU:HD11	4:B:418:THR:HG23	1.79	0.63
21:a:106:ASP:OD2	21:a:131:ARG:NE	2.31	0.63
20:W:772:GLU:OE2	20:W:774:ASN:ND2	2.31	0.63
5:C:146:LYS:NZ	12:J:57:GLU:OE2	2.26	0.62
6:D:11:ARG:HH12	6:D:32:PRO:HG3	1.64	0.62
3:A:327:ARG:HG3	3:A:1409:VAL:HG21	1.80	0.62
10:H:36:ILE:HA	10:H:125:GLU:O	1.99	0.62
16:N:46:DG:H2''	16:N:47:DA:N7	2.14	0.62
2:1:-61:DT:H3'	2:1:-60:DT:H71	1.80	0.62
3:A:343:GLY:O	4:B:1129:ARG:NH1	2.33	0.62
4:B:1082:MET:HA	5:C:189:THR:HA	1.80	0.62
11:I:19:ASP:O	11:I:23:GLN:HA	2.00	0.62
1:0:70:DA:O3'	21:a:42:ARG:HD2	2.00	0.62
3:A:1160:PRO:HB3	3:A:1190:GLN:HE21	1.64	0.62
3:A:14:VAL:H	3:A:1435:GLN:HE22	1.48	0.61
3:A:995:LEU:HD22	3:A:1048:LEU:HD22	1.81	0.61
4:B:271:ASP:O	4:B:329:ARG:NH1	2.33	0.61
4:B:997:GLU:HB2	5:C:34:ARG:HG2	1.83	0.61
22:b:47:SER:OG	22:b:48:GLY:N	2.33	0.61
3:A:1280:PRO:O	3:A:1315:ASN:ND2	2.34	0.60
4:B:49:LEU:HD22	4:B:411:ARG:HB2	1.83	0.60
13:K:29:ASN:ND2	13:K:78:GLU:O	2.34	0.60
23:c:54:VAL:HG21	24:d:98:VAL:HG21	1.84	0.60
3:A:1168:ASP:OD2	3:A:1196:ARG:NE	2.34	0.60
4:B:1163:CYS:HB3	4:B:1166:CYS:SG	2.41	0.60
3:A:448:GLN:NE2	4:B:1134:GLU:OE2	2.34	0.59
5:C:69:ILE:HD11	5:C:144:LEU:HD21	1.84	0.59
3:A:447:ARG:HB2	3:A:488:MET:HG2	1.84	0.59
4:B:74:ARG:HB2	4:B:124:PHE:HB2	1.83	0.59
4:B:931:TYR:O	4:B:932:HIS:ND1	2.35	0.59
10:H:15:VAL:HG22	10:H:26:ILE:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:409:ASP:OD2	20:W:415:THR:OG1	2.19	0.59
2:1:-69:DT:C2'	2:1:-68:DT:H71	2.30	0.59
18:T:-68:DG:H2''	18:T:-67:DA:C8	2.38	0.59
2:1:-69:DT:C2'	2:1:-68:DT:C7	2.79	0.58
3:A:996:CYS:O	3:A:1021:GLN:NE2	2.35	0.58
16:N:-25:DC:H2''	16:N:-24:DT:C5	2.38	0.58
3:A:88:LYS:HZ1	3:A:205:PRO:HD2	1.68	0.58
2:1:-61:DT:H2'	2:1:-60:DT:C6	2.38	0.58
3:A:588:HIS:HA	3:A:608:ILE:O	2.03	0.58
3:A:610:ASP:OD1	3:A:971:GLN:NE2	2.36	0.58
3:A:772:GLU:N	3:A:823:GLU:OE2	2.29	0.58
11:I:29:CYS:SG	11:I:30:ARG:N	2.77	0.58
23:g:65:LEU:HB3	23:g:86:ALA:HB1	1.85	0.58
4:B:351:LYS:O	4:B:353:LEU:N	2.37	0.58
4:B:413:LEU:HB3	4:B:446:ILE:HG12	1.84	0.58
4:B:810:GLU:OE2	4:B:815:ARG:NE	2.36	0.58
16:N:17:DA:H4'	21:a:63:ARG:HD2	1.84	0.58
4:B:590:VAL:HG21	4:B:610:ARG:HD2	1.86	0.58
23:g:90:ASP:HB3	23:g:93:LEU:HB2	1.86	0.57
4:B:337:ARG:HE	4:B:339:GLU:HB3	1.69	0.57
4:B:427:ARG:HH21	20:W:235:LYS:HZ3	1.51	0.57
10:H:27:ILE:HG12	10:H:39:THR:HG23	1.86	0.57
9:G:114:LEU:HD13	9:G:162:SER:HB2	1.85	0.57
21:a:119:ILE:HD11	22:b:46:ILE:HG23	1.87	0.57
20:W:763:TYR:HB3	20:W:766:LYS:HD2	1.86	0.57
23:c:88:ARG:NH1	23:c:94:ASN:OD1	2.36	0.57
3:A:195:ASP:OD1	3:A:195:ASP:N	2.38	0.57
2:1:-62:DT:H2''	2:1:-61:DT:H71	1.86	0.57
17:P:6:G:O6	18:T:38:DA:N6	2.38	0.57
3:A:146:MET:HB3	3:A:187:LYS:NZ	2.19	0.56
22:b:35:ARG:HD2	22:b:46:ILE:HD12	1.86	0.56
23:c:90:ASP:HB3	23:c:93:LEU:HB2	1.87	0.56
3:A:588:HIS:NE2	3:A:971:GLN:OE1	2.38	0.56
2:1:-70:DT:H2''	2:1:-69:DT:C5	2.40	0.56
4:B:190:MET:SD	4:B:190:MET:N	2.79	0.56
4:B:792:MET:SD	4:B:857:ARG:NH2	2.79	0.56
5:C:248:ILE:HG21	13:K:102:ASP:HB2	1.87	0.56
16:N:26:DA:H2''	16:N:27:DG:C8	2.41	0.56
4:B:835:GLN:O	4:B:838:SER:OG	2.23	0.56
23:g:54:VAL:HG21	24:h:98:VAL:HG21	1.87	0.56
11:I:19:ASP:O	11:I:23:GLN:CA	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1074:ILE:HD13	3:A:1374:LEU:HD22	1.87	0.56
18:T:-47:DT:H2''	18:T:-46:DC:C5	2.41	0.56
3:A:197:GLN:HE22	15:M:50:LYS:HB3	1.70	0.56
20:W:229:VAL:HG21	20:W:286:LEU:HD11	1.88	0.55
3:A:1445:ASP:HB3	3:A:1447:MET:HE3	1.87	0.55
4:B:760:ASP:OD1	4:B:760:ASP:N	2.39	0.55
9:G:152:THR:HA	9:G:157:ILE:HG22	1.88	0.55
10:H:112:LYS:HG2	10:H:125:GLU:HG2	1.88	0.55
18:T:-6:DT:H2'	18:T:-6:DT:OP2	2.07	0.55
3:A:369:ILE:HG22	3:A:373:LYS:NZ	2.22	0.55
21:a:108:ASN:ND2	22:b:42:GLY:O	2.40	0.55
22:b:64:ASN:O	22:b:93:GLN:NE2	2.39	0.55
11:I:19:ASP:O	11:I:23:GLN:N	2.40	0.55
2:1:-34:DT:H2''	2:1:-33:DG:C8	2.41	0.55
4:B:1008:PRO:HB3	4:B:1087:PHE:HE1	1.71	0.55
21:a:62:ILE:O	21:a:93:GLN:NE2	2.40	0.55
21:e:108:ASN:ND2	22:f:42:GLY:O	2.39	0.55
5:C:214:LYS:HB2	5:C:217:GLU:HB2	1.89	0.55
10:H:102:LYS:HB3	10:H:114:TYR:HB2	1.89	0.55
3:A:113:LEU:O	3:A:165:ARG:NH2	2.40	0.55
4:B:776:GLN:NE2	17:P:8:G:O2'	2.40	0.55
5:C:50:ILE:O	14:L:62:ARG:NH2	2.40	0.55
4:B:1106:ARG:HH11	4:B:1126:GLY:HA2	1.70	0.55
20:W:329:LYS:HD2	20:W:436:ILE:HB	1.89	0.55
1:0:36:DC:H2''	1:0:37:DC:C5	2.42	0.55
1:0:69:DA:H2''	1:0:70:DA:H5'	1.89	0.55
9:G:123:PRO:HA	9:G:128:PRO:HB3	1.89	0.54
16:N:-8:DG:H2''	16:N:-7:DG:H5'	1.88	0.54
18:T:4:DC:H2''	18:T:5:DC:OP2	2.06	0.54
1:0:56:DC:H2''	1:0:57:DA:N7	2.22	0.54
2:1:-59:DT:H2''	2:1:-58:DC:C5	2.43	0.54
3:A:887:ILE:H	3:A:888:PRO:HD2	1.72	0.54
4:B:242:ILE:HG21	4:B:355:PRO:HG3	1.88	0.54
3:A:608:ILE:HG12	3:A:613:VAL:HG22	1.89	0.54
2:1:-37:DG:OP2	2:1:-37:DG:H2'	2.08	0.54
16:N:62:DG:H2''	16:N:63:DG:OP2	2.07	0.54
17:P:-3:U:O4	17:P:-2:G:N2	2.41	0.54
18:T:-8:DC:H2''	18:T:-7:DG:C8	2.43	0.54
1:0:58:DG:H2''	1:0:59:DA:N7	2.22	0.54
7:E:8:ILE:HG21	7:E:42:ARG:HG2	1.90	0.54
3:A:88:LYS:NZ	3:A:205:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1439:MET:HE1	4:B:1139:ILE:HG12	1.90	0.54
5:C:35:THR:HG23	5:C:39:GLU:HB2	1.89	0.53
4:B:436:ASN:O	4:B:438:ASN:N	2.40	0.53
9:G:132:SER:HB2	9:G:135:GLU:HB2	1.89	0.53
3:A:146:MET:HB3	3:A:187:LYS:HZ2	1.72	0.53
4:B:30:LEU:O	4:B:489:ARG:NH1	2.41	0.53
4:B:910:ILE:HD13	4:B:940:PRO:HB3	1.91	0.53
4:B:257:THR:OG1	4:B:258:GLY:N	2.38	0.53
16:N:-19:DG:H2''	16:N:-18:DG:H8	1.74	0.53
5:C:38:ALA:HA	5:C:164:ALA:HB3	1.90	0.53
5:C:100:LEU:HB3	5:C:155:ILE:HG13	1.91	0.53
7:E:54:ARG:HH12	7:E:112:GLN:HG2	1.74	0.53
2:1:-51:DG:H2'	2:1:-50:DT:H71	1.91	0.53
4:B:759:PRO:HD2	4:B:1046:PRO:HB3	1.90	0.53
5:C:47:LEU:HB2	5:C:158:ILE:HB	1.91	0.53
3:A:1192:PRO:HG3	11:I:18:GLU:OE2	2.08	0.53
16:N:-19:DG:H2''	16:N:-18:DG:C8	2.44	0.53
14:L:43:ASN:O	14:L:45:SER:N	2.39	0.52
18:T:8:DC:H5'	18:T:8:DC:H6	1.74	0.52
3:A:1153:GLU:OE2	11:I:45:ARG:NH1	2.42	0.52
19:V:58:VAL:HG13	20:W:263:PHE:HB3	1.91	0.52
4:B:225:ILE:O	4:B:252:ARG:NH2	2.42	0.52
23:c:58:LEU:HD21	24:d:102:LEU:HD21	1.91	0.52
3:A:74:MET:O	4:B:1116:ARG:NH2	2.42	0.52
23:c:55:LEU:HD22	24:d:66:VAL:HG13	1.90	0.52
21:a:107:THR:HG23	21:a:123:ASP:HB2	1.91	0.52
2:1:-58:DC:H2''	2:1:-57:DT:OP2	2.09	0.52
3:A:349:SER:HB2	4:B:1128:LEU:HD12	1.92	0.52
3:A:474:SER:OG	3:A:651:GLN:NE2	2.43	0.52
12:J:66:GLU:HG2	14:L:32:THR:HG21	1.92	0.52
3:A:286:PRO:O	3:A:288:HIS:N	2.42	0.52
3:A:1402:ARG:NH2	3:A:1420:GLU:OE1	2.43	0.52
4:B:974:PRO:HA	4:B:978:ASP:OD2	2.08	0.52
16:N:55:DC:H2''	16:N:56:DG:C8	2.45	0.52
3:A:1130:ILE:HG12	3:A:1134:LYS:HE2	1.90	0.52
5:C:65:ARG:NH2	5:C:143:LEU:O	2.40	0.52
7:E:85:PRO:HA	7:E:112:GLN:HB2	1.92	0.52
22:b:52:GLU:O	22:b:55:ARG:HB2	2.10	0.52
7:E:19:LYS:NZ	7:E:33:GLU:O	2.43	0.52
14:L:33:CYS:HB3	14:L:38:HIS:H	1.75	0.52
1:0:46:DA:N1	2:1:-45:DG:N2	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:-46:DT:H2''	2:1:-45:DG:C8	2.45	0.51
3:A:1213:GLN:OE1	3:A:1277:ARG:NH2	2.43	0.51
6:D:11:ARG:NH1	6:D:32:PRO:HG3	2.25	0.51
6:D:183:ASP:N	6:D:183:ASP:OD1	2.43	0.51
22:b:74:GLU:O	24:d:92:ARG:NH2	2.42	0.51
22:f:47:SER:OG	22:f:48:GLY:N	2.43	0.51
4:B:878:THR:O	4:B:882:THR:OG1	2.27	0.51
5:C:145:CYS:SG	5:C:146:LYS:N	2.84	0.51
6:D:125:ASP:OD1	6:D:129:HIS:ND1	2.43	0.51
16:N:20:DG:H2''	16:N:21:DG:H5''	1.92	0.51
3:A:482:ASP:OD1	3:A:482:ASP:N	2.43	0.51
9:G:153:ASP:O	9:G:155:ASN:N	2.43	0.51
4:B:941:LEU:HD21	4:B:968:MET:HE2	1.92	0.51
7:E:27:TYR:HA	7:E:63:PRO:HA	1.91	0.51
3:A:364:GLN:HE21	3:A:460:ARG:HH12	1.58	0.51
5:C:53:ASN:ND2	5:C:59:ASP:OD1	2.38	0.51
11:I:82:ASP:OD2	11:I:104:LEU:HD12	2.11	0.51
4:B:27:GLU:OE2	4:B:679:SER:OG	2.22	0.50
16:N:4:DG:H2''	16:N:5:DT:C5	2.45	0.50
18:T:36:DC:H2'	18:T:37:DC:C6	2.46	0.50
23:c:63:LEU:HD13	24:d:45:LEU:HB2	1.93	0.50
23:g:55:LEU:HD22	24:h:66:VAL:HG13	1.94	0.50
23:g:42:ARG:HB2	24:h:88:THR:HG22	1.93	0.50
4:B:291:GLN:NE2	4:B:563:ASP:OD1	2.45	0.50
4:B:316:ILE:HG23	4:B:321:VAL:HG23	1.94	0.50
16:N:35:DT:H2''	16:N:36:DA:N7	2.26	0.50
18:T:33:DC:H2'	18:T:34:DA:C8	2.47	0.50
3:A:407:ILE:HG12	3:A:413:ARG:HG2	1.94	0.50
15:M:53:ASN:OD1	21:e:83:ARG:NH1	2.44	0.50
19:V:9:GLU:HA	19:V:20:PRO:HA	1.94	0.50
5:C:100:LEU:HD22	5:C:155:ILE:HD11	1.92	0.50
16:N:67:DT:H2''	16:N:68:DC:C5	2.46	0.50
4:B:1156:ASP:OD1	4:B:1156:ASP:N	2.44	0.50
18:T:37:DC:H2'	18:T:38:DA:C8	2.44	0.50
3:A:1157:ASP:HB3	3:A:1243:ARG:HH12	1.77	0.49
18:T:-50:DC:H5'	18:T:-50:DC:C6	2.47	0.49
1:0:38:DA:H2''	1:0:39:DA:C8	2.47	0.49
2:1:-52:DC:H2''	2:1:-51:DG:H8	1.77	0.49
3:A:818:ALA:HA	4:B:764:SER:HB3	1.93	0.49
23:g:85:LEU:O	23:g:89:ASN:ND2	2.45	0.49
4:B:273:PRO:HD2	4:B:276:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:318:ASP:OD1	4:B:318:ASP:N	2.45	0.49
13:K:55:ASP:OD2	13:K:81:THR:HG21	2.12	0.49
18:T:-36:DT:H2''	18:T:-35:DA:C8	2.47	0.49
3:A:999:LEU:O	3:A:1013:GLN:NE2	2.42	0.49
4:B:59:ASP:OD1	4:B:59:ASP:N	2.45	0.49
13:K:63:VAL:HG22	13:K:71:PHE:HB3	1.95	0.49
16:N:61:DC:H1'	16:N:62:DG:H5'	1.95	0.49
18:T:1:DT:H2''	18:T:2:DG:C8	2.47	0.49
19:V:62:ASP:HB3	19:V:66:SER:HB2	1.94	0.49
3:A:1127:ALA:HB1	3:A:1306:LEU:HB3	1.94	0.49
4:B:25:PHE:HZ	4:B:534:LEU:HG	1.76	0.49
5:C:12:ALA:HA	5:C:17:VAL:HG22	1.93	0.49
5:C:103:ARG:HB2	5:C:152:GLU:HG3	1.95	0.49
3:A:89:PRO:HB3	3:A:238:THR:HG22	1.93	0.49
4:B:1101:ASP:C	4:B:1122:ARG:HH12	2.20	0.48
3:A:766:VAL:HG23	3:A:804:SER:HA	1.94	0.48
4:B:240:ARG:HH12	4:B:415:ARG:HH21	1.60	0.48
2:1:-33:DG:C8	2:1:-33:DG:H5'	2.48	0.48
3:A:231:ARG:HB3	3:A:234:TRP:CD2	2.47	0.48
3:A:317:GLN:HG2	3:A:323:VAL:HG22	1.94	0.48
13:K:50:LEU:HD11	13:K:87:LEU:HD13	1.96	0.48
18:T:-57:DC:H2''	18:T:-56:DC:C5	2.48	0.48
23:g:84:GLN:NE2	23:g:106:GLY:O	2.46	0.48
3:A:49:ARG:NH1	20:W:443:THR:HG22	2.29	0.48
4:B:827:ILE:HG12	4:B:1012:ILE:HD11	1.95	0.48
12:J:10:CYS:SG	12:J:11:GLY:N	2.86	0.48
3:A:351:ARG:HB2	4:B:1128:LEU:HD11	1.96	0.48
3:A:446:ASN:ND2	3:A:447:ARG:H	2.11	0.48
3:A:556:SER:OG	3:A:649:ASN:ND2	2.47	0.48
3:A:1343:GLY:O	3:A:1347:THR:OG1	2.28	0.48
19:V:15:CYS:SG	19:V:16:GLY:N	2.87	0.48
21:e:73:GLU:OE1	22:f:25:ASN:ND2	2.45	0.48
3:A:874:LEU:HD13	3:A:959:PRO:HG3	1.95	0.48
16:N:27:DG:OP2	16:N:27:DG:H2'	2.13	0.48
16:N:36:DA:H2''	16:N:37:DC:C5	2.49	0.48
18:T:-26:DT:H2''	18:T:-25:DA:C8	2.49	0.48
1:0:46:DA:H2''	1:0:47:DG:N7	2.28	0.48
1:0:61:DA:H2'	1:0:61:DA:OP2	2.14	0.48
3:A:358:PRO:HG3	3:A:473:LEU:HD22	1.94	0.48
18:T:-25:DA:H8	18:T:-25:DA:OP2	1.96	0.48
18:T:13:DT:H2''	18:T:14:DT:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:h:68:ASP:OD2	24:h:72:ARG:NH2	2.47	0.48
3:A:252:ALA:HA	3:A:258:GLN:HA	1.96	0.47
6:D:117:ASP:OD1	6:D:117:ASP:N	2.41	0.47
3:A:364:GLN:HE21	3:A:460:ARG:NH1	2.12	0.47
20:W:775:GLY:O	20:W:777:ARG:N	2.47	0.47
3:A:886:THR:HG22	3:A:894:PHE:HE1	1.79	0.47
4:B:480:THR:HG23	4:B:483:SER:H	1.79	0.47
4:B:262:LYS:HB3	4:B:271:ASP:HB3	1.96	0.47
13:K:57:THR:OG1	13:K:76:GLN:O	2.26	0.47
21:e:68:GLN:HG3	21:e:89:ILE:HD13	1.96	0.47
3:A:254:ASP:HB2	4:B:864:LYS:NZ	2.29	0.47
3:A:753:LYS:HG3	4:B:1019:SER:HB3	1.96	0.47
4:B:483:SER:HA	4:B:775:LYS:HG2	1.96	0.47
4:B:974:PRO:HG3	4:B:1094:ARG:HH12	1.80	0.47
20:W:231:VAL:HG12	20:W:292:VAL:HG22	1.95	0.47
20:W:338:ALA:HB2	20:W:354:LEU:HD22	1.96	0.47
2:1:-50:DT:H2''	2:1:-49:DG:N7	2.30	0.47
18:T:40:DG:H5'	18:T:40:DG:H8	1.80	0.47
4:B:27:GLU:OE1	4:B:678:TRP:N	2.48	0.47
4:B:755:ILE:HA	4:B:809:MET:HE2	1.96	0.47
2:1:-51:DG:H8	2:1:-51:DG:H5'	1.80	0.47
3:A:926:LEU:HD21	3:A:985:ILE:HD12	1.96	0.47
4:B:984:HIS:NE2	4:B:1028:GLU:OE1	2.34	0.47
5:C:74:GLU:O	5:C:246:ARG:NH2	2.48	0.47
20:W:353:LYS:HG3	20:W:425:PHE:HB3	1.97	0.47
4:B:240:ARG:HH12	4:B:415:ARG:NH2	2.13	0.46
14:L:29:VAL:HG11	14:L:60:LYS:NZ	2.31	0.46
3:A:446:ASN:HD21	3:A:455:SER:HB3	1.80	0.46
3:A:533:ARG:HD3	3:A:750:ALA:HB2	1.97	0.46
4:B:252:ARG:HA	4:B:252:ARG:HD3	1.61	0.46
18:T:-12:DC:H2''	18:T:-11:DG:C8	2.50	0.46
20:W:791:ILE:HG13	20:W:792:PRO:HD2	1.97	0.46
21:a:108:ASN:HD21	23:g:115:LEU:HD11	1.80	0.46
23:c:24:GLN:N	23:c:56:GLU:OE1	2.49	0.46
1:0:35:DC:OP2	1:0:35:DC:H2'	2.14	0.46
7:E:150:PRO:HB3	7:E:199:ARG:HG3	1.97	0.46
3:A:226:ASN:HB3	3:A:230:ALA:H	1.79	0.46
3:A:336:ARG:HH22	4:B:1114:LEU:HD21	1.79	0.46
3:A:599:LEU:HG	10:H:25:ARG:NH1	2.30	0.46
18:T:-47:DT:H2'	18:T:-47:DT:OP2	2.14	0.46
4:B:904:ARG:HH22	20:W:786:ASN:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:366:GLY:HA3	3:A:470:ARG:HB2	1.97	0.46
6:D:49:ILE:HG21	9:G:4:LEU:HD12	1.97	0.46
9:G:165:GLU:HB2	9:G:168:LEU:HD12	1.96	0.46
20:W:784:ASN:HB2	20:W:785:PRO:HD3	1.96	0.46
2:1:-68:DT:H2''	2:1:-67:DT:C6	2.50	0.46
3:A:805:TYR:O	4:B:761:HIS:ND1	2.45	0.46
8:F:107:VAL:HG21	8:F:111:ILE:HD11	1.97	0.46
22:b:39:ARG:NH1	22:b:44:LYS:O	2.48	0.46
16:N:43:DA:H2'	16:N:44:DT:H71	1.97	0.46
7:E:71:TYR:OH	7:E:154:ARG:O	2.29	0.46
10:H:13:GLN:HE22	10:H:29:ILE:HD12	1.81	0.46
10:H:82:LYS:HB2	10:H:85:ASP:OD2	2.16	0.46
4:B:878:THR:HG1	4:B:881:THR:HG1	1.61	0.45
10:H:101:TYR:CZ	10:H:114:TYR:HB3	2.51	0.45
3:A:1153:GLU:OE2	11:I:42:LYS:NZ	2.48	0.45
4:B:807:GLN:O	4:B:810:GLU:HB2	2.16	0.45
4:B:466:MET:N	4:B:466:MET:SD	2.90	0.45
16:N:-46:DT:H2''	16:N:-45:DG:C8	2.51	0.45
18:T:5:DC:OP2	18:T:5:DC:H2'	2.16	0.45
4:B:159:GLY:HA2	4:B:443:SER:HB2	1.98	0.45
3:A:586:GLY:HA2	3:A:971:GLN:HE22	1.81	0.45
3:A:1332:SER:HB3	3:A:1338:ILE:HD11	1.98	0.45
4:B:175:LEU:HB3	4:B:179:ASP:HB2	1.97	0.45
18:T:38:DA:H2''	18:T:39:DA:H8	1.81	0.45
4:B:999:MET:HE3	4:B:1008:PRO:HG2	1.99	0.45
16:N:56:DG:H2''	16:N:57:DG:N7	2.31	0.45
18:T:-48:DC:H2''	18:T:-47:DT:C2	2.51	0.45
23:c:115:LEU:HD11	21:e:108:ASN:HD21	1.81	0.45
3:A:354:ILE:HG22	3:A:469:PHE:HB2	1.98	0.45
4:B:1073:TYR:HE2	5:C:179:GLU:HA	1.81	0.45
14:L:29:VAL:HG11	14:L:60:LYS:HZ1	1.81	0.45
22:b:52:GLU:HG2	22:b:55:ARG:NH1	2.31	0.45
3:A:1345:GLU:OE1	7:E:199:ARG:NH1	2.50	0.45
4:B:371:LEU:HD23	4:B:371:LEU:HA	1.89	0.45
4:B:156:VAL:HG13	4:B:438:ASN:HD22	1.82	0.45
4:B:447:THR:HG22	4:B:451:LYS:HD2	1.99	0.45
18:T:-16:DT:H2''	18:T:-15:DA:N7	2.32	0.45
19:V:59:ALA:HB1	20:W:244:LEU:HB2	1.99	0.45
20:W:794:SER:O	20:W:794:SER:OG	2.33	0.45
3:A:970:GLN:HG2	3:A:975:LEU:HD12	1.99	0.44
4:B:252:ARG:HB3	4:B:255:LYS:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:735:HIS:HB3	11:I:70:ARG:HH11	1.82	0.44
9:G:116:PRO:HA	9:G:164:LYS:NZ	2.30	0.44
10:H:86:LYS:HE2	10:H:86:LYS:HB3	1.86	0.44
18:T:-69:DA:H8	18:T:-69:DA:OP2	2.00	0.44
24:d:95:GLN:HG3	24:d:111:VAL:HG22	2.00	0.44
1:O:35:DC:H2''	1:O:36:DC:C5	2.52	0.44
3:A:1456:LEU:HD21	8:F:108:LEU:HG	1.98	0.44
4:B:319:LYS:HE2	4:B:323:LEU:HD11	2.00	0.44
4:B:1080:LYS:HB2	5:C:188:HIS:HB3	1.99	0.44
3:A:1165:ILE:HG22	3:A:1167:GLU:H	1.82	0.44
4:B:104:ALA:HA	4:B:109:LEU:HB2	1.99	0.44
4:B:170:CYS:SG	4:B:171:SER:N	2.90	0.44
16:N:-28:DC:H42	18:T:29:DA:H61	1.65	0.44
18:T:-5:DA:H2''	18:T:-4:DC:C5	2.52	0.44
4:B:501:LEU:HD12	4:B:501:LEU:HA	1.92	0.44
5:C:37:LEU:HG	5:C:176:ILE:HD12	2.00	0.44
5:C:166:GLU:HA	13:K:6:ARG:HB3	2.00	0.44
23:c:88:ARG:HA	23:c:88:ARG:HD3	1.74	0.44
24:d:76:GLU:OE1	24:d:79:ARG:NH1	2.50	0.44
5:C:160:LYS:NZ	20:W:764:LYS:O	2.50	0.44
16:N:32:DG:H2''	16:N:33:DT:H5'	1.99	0.44
20:W:336:ASP:HB2	20:W:354:LEU:HD21	2.00	0.44
20:W:410:ARG:HB2	20:W:413:PHE:HB3	2.00	0.44
3:A:1109:VAL:HG13	3:A:1335:PHE:HE1	1.81	0.44
3:A:1282:ILE:HG23	3:A:1311:THR:HB	1.98	0.44
4:B:840:ILE:HG12	4:B:992:VAL:HG12	2.00	0.44
21:a:113:HIS:NE2	21:e:123:ASP:OD1	2.40	0.44
23:c:65:LEU:HB3	23:c:86:ALA:HB1	1.98	0.44
4:B:230:GLU:HG3	4:B:246:GLN:HG2	1.99	0.44
3:A:517:SER:OG	3:A:1365:TYR:O	2.29	0.44
3:A:861:LEU:HD21	3:A:1397:THR:HA	2.00	0.44
3:A:940:ASP:OD2	3:A:1025:ARG:NE	2.51	0.44
5:C:27:SER:OG	13:K:48:GLU:OE1	2.30	0.44
20:W:806:PRO:HG2	20:W:808:GLU:HG2	2.00	0.44
4:B:291:GLN:HE21	4:B:564:PRO:HD2	1.82	0.44
16:N:41:DC:N4	18:T:-41:DG:O6	2.36	0.44
16:N:58:DC:H2''	16:N:59:DA:N7	2.33	0.44
3:A:1452:LEU:HD22	8:F:131:PRO:HB3	2.00	0.43
11:I:94:ASP:OD1	11:I:94:ASP:N	2.49	0.43
16:N:15:DT:H2''	16:N:16:DA:C8	2.53	0.43
6:D:23:GLU:HB3	9:G:82:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:58:SER:HA	7:E:79:VAL:O	2.17	0.43
9:G:116:PRO:HA	9:G:164:LYS:HZ1	1.83	0.43
21:e:118:THR:HA	22:f:45:ARG:HB3	2.00	0.43
2:1:-37:DG:H2''	2:1:-36:DG:N7	2.33	0.43
9:G:115:ILE:HG12	9:G:163:ILE:HD11	2.00	0.43
10:H:97:PHE:HE1	10:H:138:ASN:HB3	1.83	0.43
18:T:38:DA:H2''	18:T:39:DA:C8	2.54	0.43
1:0:52:DG:H2''	1:0:53:DA:OP2	2.19	0.43
3:A:1389:ARG:NH1	3:A:1407:GLU:OE2	2.51	0.43
18:T:-52:DG:C4	18:T:-51:DC:C5	3.06	0.43
3:A:1287:MET:HE2	3:A:1287:MET:HB2	1.92	0.43
6:D:33:GLU:O	6:D:38:GLN:NE2	2.51	0.43
18:T:-26:DT:H2''	18:T:-25:DA:OP2	2.18	0.43
18:T:-9:DA:C8	18:T:-9:DA:H5'	2.53	0.43
19:V:46:VAL:O	19:V:50:THR:OG1	2.35	0.43
3:A:1107:LEU:HD22	3:A:1387:ILE:HG13	2.00	0.43
4:B:827:ILE:HG22	4:B:1014:PRO:HG3	2.01	0.43
5:C:4:GLU:HB3	5:C:5:PRO:HD3	2.01	0.43
16:N:15:DT:H2''	16:N:16:DA:N7	2.34	0.43
1:0:60:DA:H2''	1:0:61:DA:H8	1.83	0.43
3:A:843:VAL:HG11	4:B:1136:ASP:OD2	2.19	0.43
3:A:844:LYS:HD2	3:A:844:LYS:HA	1.80	0.43
9:G:56:VAL:HG12	9:G:72:VAL:HG13	2.01	0.43
18:T:-48:DC:H2''	18:T:-47:DT:C6	2.53	0.43
3:A:1141:GLU:OE2	3:A:1207:LYS:NZ	2.52	0.43
3:A:1431:VAL:HG11	4:B:1135:ARG:HH11	1.83	0.43
4:B:1082:MET:HG3	5:C:190:ASP:HB2	2.01	0.43
18:T:5:DC:OP2	18:T:5:DC:H6	2.02	0.43
20:W:265:ARG:HD2	20:W:265:ARG:HA	1.77	0.43
3:A:132:LYS:NZ	3:A:1420:GLU:OE2	2.52	0.43
3:A:243:PRO:HG2	3:A:248:ARG:NH1	2.34	0.43
3:A:547:VAL:HG21	3:A:573:TRP:HB2	2.01	0.43
7:E:176:ARG:HD3	7:E:214:LEU:HD21	1.99	0.43
9:G:5:LYS:HD3	9:G:5:LYS:HA	1.73	0.43
11:I:90:GLN:HE21	11:I:92:ARG:HG3	1.84	0.43
4:B:1017:ILE:H	4:B:1018:PRO:HD2	1.84	0.42
3:A:1153:GLU:CD	11:I:45:ARG:HH11	2.27	0.42
4:B:119:MET:O	4:B:153:GLY:N	2.52	0.42
4:B:203:LEU:HD22	4:B:472:VAL:HG12	2.01	0.42
9:G:43:GLY:HA3	9:G:80:LYS:HB2	2.01	0.42
12:J:1:MET:HA	12:J:55:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:-12:DC:H2''	18:T:-11:DG:H8	1.85	0.42
3:A:18:GLN:HB3	4:B:1215:ARG:HB2	2.00	0.42
10:H:59:LEU:HD23	10:H:139:LEU:HD13	2.02	0.42
3:A:243:PRO:HG2	3:A:248:ARG:HH11	1.84	0.42
4:B:55:ARG:HD3	4:B:78:ARG:NH1	2.34	0.42
4:B:408:ASN:OD1	4:B:411:ARG:NH1	2.42	0.42
16:N:48:DG:H3'	24:d:39:ILE:HD13	2.01	0.42
4:B:885:LEU:HD23	4:B:936:ASP:HB2	2.01	0.42
18:T:45:DC:H2''	18:T:46:DA:C8	2.55	0.42
22:b:44:LYS:HB2	23:g:115:LEU:HD13	2.00	0.42
3:A:254:ASP:O	3:A:256:THR:N	2.53	0.42
3:A:665:ILE:HD12	3:A:747:MET:HE1	2.01	0.42
3:A:1284:LYS:HD2	3:A:1284:LYS:HA	1.88	0.42
4:B:401:LEU:HB3	4:B:402:ALA:H	1.61	0.42
4:B:721:ASP:OD2	4:B:724:LYS:N	2.46	0.42
16:N:26:DA:H2''	16:N:27:DG:N7	2.34	0.42
16:N:27:DG:OP2	16:N:27:DG:H8	2.03	0.42
1:0:53:DA:OP2	1:0:53:DA:H2'	2.19	0.42
3:A:453:LYS:O	4:B:1141:HIS:NE2	2.52	0.42
3:A:528:THR:O	3:A:654:VAL:HG11	2.19	0.42
3:A:558:ASP:OD1	3:A:558:ASP:N	2.52	0.42
3:A:1320:MET:HE2	7:E:141:VAL:HG11	2.00	0.42
1:0:49:DC:H2''	1:0:50:DA:C8	2.55	0.42
4:B:55:ARG:HD2	4:B:76:GLU:OE2	2.19	0.42
4:B:219:LYS:HD3	4:B:219:LYS:HA	1.90	0.42
4:B:721:ASP:HB3	4:B:724:LYS:HG2	2.00	0.42
18:T:-59:DT:H2''	18:T:-58:DG:C8	2.55	0.42
21:e:128:ARG:HH22	21:e:134:ARG:HE	1.68	0.42
2:1:-69:DT:H2''	2:1:-68:DT:C6	2.54	0.42
3:A:961:ASN:HD22	3:A:964:ARG:NH1	2.18	0.42
9:G:29:LYS:HE3	9:G:33:ASP:OD2	2.18	0.42
19:V:91:PRO:HD2	19:V:94:ILE:HD12	2.02	0.42
23:g:63:LEU:HD13	24:h:45:LEU:HB2	2.00	0.42
23:g:54:VAL:HG22	24:h:110:ALA:HB1	2.01	0.42
13:K:55:ASP:OD1	13:K:55:ASP:N	2.53	0.41
13:K:75:LEU:HG	13:K:83:PRO:HB3	2.01	0.41
15:M:38:LEU:HD22	15:M:60:ILE:HD13	2.02	0.41
15:M:47:LEU:HG	15:M:69:ILE:HD13	2.01	0.41
23:c:59:THR:HG21	24:d:41:VAL:HG22	2.02	0.41
23:c:85:LEU:O	23:c:89:ASN:ND2	2.53	0.41
21:e:119:ILE:HD11	22:f:46:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:-36:DG:H2''	2:1:-35:DG:C8	2.55	0.41
3:A:286:PRO:HD2	3:A:289:ILE:HB	2.02	0.41
4:B:70:ASN:OD1	4:B:70:ASN:N	2.52	0.41
8:F:149:ASP:OD1	8:F:149:ASP:N	2.52	0.41
19:V:42:ASP:OD1	19:V:42:ASP:N	2.50	0.41
3:A:345:ARG:NH1	4:B:1129:ARG:HB2	2.35	0.41
4:B:955:THR:OG1	4:B:956:THR:N	2.51	0.41
16:N:-9:DC:H2''	16:N:-8:DG:H8	1.85	0.41
16:N:28:DA:H5''	22:b:78:ARG:HG2	2.02	0.41
18:T:-53:DG:C2	18:T:-52:DG:C5	3.09	0.41
18:T:-53:DG:H2''	18:T:-52:DG:H8	1.86	0.41
21:e:63:ARG:HD3	21:e:63:ARG:HA	1.74	0.41
21:e:107:THR:HG23	21:e:123:ASP:HB2	2.02	0.41
24:h:95:GLN:HG3	24:h:111:VAL:HG22	2.01	0.41
18:T:30:DT:H6	18:T:30:DT:H2'	1.63	0.41
3:A:91:PHE:HZ	3:A:208:ILE:HD12	1.85	0.41
3:A:362:LEU:HA	3:A:472:ASN:HD22	1.86	0.41
4:B:293:ILE:HG12	4:B:372:GLY:HA2	2.02	0.41
16:N:-11:DC:H2''	16:N:-10:DG:H8	1.86	0.41
18:T:-58:DG:H2''	18:T:-57:DC:C5	2.56	0.41
3:A:340:ASN:ND2	4:B:1117:GLN:OE1	2.48	0.41
4:B:471:GLY:HA3	17:P:6:G:H5'	2.02	0.41
16:N:62:DG:N1	18:T:-61:DG:O6	2.53	0.41
18:T:-37:DG:H4'	18:T:-36:DT:H5'	2.03	0.41
2:1:-48:DC:H6	2:1:-48:DC:H2'	1.70	0.41
4:B:563:ASP:OD2	4:B:565:ALA:HB3	2.21	0.41
11:I:59:VAL:HG23	11:I:62:ILE:HB	2.02	0.41
18:T:-72:DA:C8	18:T:-71:DT:H72	2.56	0.41
20:W:791:ILE:HG21	20:W:796:LEU:HD21	2.03	0.41
2:1:-37:DG:H2''	2:1:-36:DG:C8	2.56	0.41
3:A:735:GLU:OE2	3:A:745:LYS:HE3	2.21	0.41
3:A:944:LEU:HD23	3:A:948:VAL:HG21	2.03	0.41
3:A:953:ASP:O	3:A:956:TRP:NE1	2.52	0.41
3:A:985:ILE:N	3:A:986:PRO:HD2	2.36	0.41
4:B:288:GLU:O	4:B:292:HIS:ND1	2.47	0.41
4:B:357:ILE:HG12	4:B:578:VAL:HG23	2.02	0.41
4:B:886:LYS:HA	17:P:-1:G:H1	1.86	0.41
9:G:165:GLU:HB3	9:G:166:ASP:H	1.64	0.41
16:N:-40:DC:OP2	16:N:-40:DC:H2'	2.20	0.41
16:N:-5:DG:H2''	16:N:-4:DG:OP2	2.21	0.41
18:T:-51:DC:N3	18:T:-50:DC:N4	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:-46:DC:H2''	18:T:-45:DA:C8	2.56	0.41
23:c:97:LEU:HD22	23:c:100:VAL:HG21	2.02	0.41
2:1:-36:DG:H2''	2:1:-35:DG:N7	2.36	0.40
3:A:527:ASP:HB2	4:B:835:GLN:CD	2.45	0.40
4:B:101:PRO:HG2	4:B:172:LEU:HD11	2.03	0.40
4:B:337:ARG:HG3	4:B:339:GLU:H	1.86	0.40
4:B:547:ILE:HG21	4:B:619:ILE:HG21	2.03	0.40
7:E:123:ILE:HB	7:E:124:PRO:HD3	2.03	0.40
16:N:-42:DG:H2''	16:N:-41:DT:H71	2.03	0.40
18:T:-70:DC:H2''	18:T:-69:DA:C8	2.56	0.40
3:A:446:ASN:HD22	3:A:447:ARG:H	1.68	0.40
4:B:832:GLY:HA2	4:B:835:GLN:HE21	1.87	0.40
20:W:278:LYS:HD2	20:W:280:GLU:OE2	2.21	0.40
20:W:413:PHE:HD1	20:W:422:TYR:HB2	1.86	0.40
3:A:243:PRO:O	3:A:248:ARG:NH1	2.53	0.40
3:A:369:ILE:HG22	3:A:373:LYS:HZ2	1.85	0.40
3:A:958:LEU:HD13	3:A:1023:LEU:HD22	2.03	0.40
4:B:220:ALA:O	4:B:252:ARG:NH2	2.54	0.40
4:B:413:LEU:HD13	4:B:446:ILE:HG23	2.03	0.40
21:a:48:LEU:HB3	21:a:52:ARG:NH1	2.36	0.40
3:A:916:TYR:OH	3:A:983:LEU:O	2.30	0.40
4:B:974:PRO:HG3	4:B:1094:ARG:NH1	2.35	0.40
13:K:103:HIS:NE2	13:K:107:GLU:OE2	2.55	0.40
16:N:27:DG:H2''	16:N:28:DA:N7	2.37	0.40
3:A:85:GLU:O	3:A:274:ASN:ND2	2.53	0.40
3:A:114:LEU:HD13	3:A:145:LYS:HB3	2.03	0.40
16:N:-4:DG:H2''	16:N:-3:DA:N7	2.37	0.40
16:N:35:DT:H2''	16:N:36:DA:C8	2.57	0.40
20:W:336:ASP:HB3	20:W:354:LEU:HD11	2.03	0.40
20:W:354:LEU:HD12	20:W:355:VAL:H	1.87	0.40
21:e:119:ILE:HG13	22:f:50:ILE:HG13	2.04	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	1399/1743 (80%)	1301 (93%)	90 (6%)	8 (1%)	21	59
4	B	1145/1227 (93%)	1064 (93%)	75 (7%)	6 (0%)	24	63
5	C	261/304 (86%)	243 (93%)	18 (7%)	0	100	100
6	D	162/186 (87%)	149 (92%)	12 (7%)	1 (1%)	21	59
7	E	211/214 (99%)	203 (96%)	5 (2%)	3 (1%)	9	39
8	F	82/155 (53%)	78 (95%)	4 (5%)	0	100	100
9	G	169/171 (99%)	158 (94%)	9 (5%)	2 (1%)	10	43
10	H	129/145 (89%)	126 (98%)	2 (2%)	1 (1%)	16	53
11	I	109/115 (95%)	95 (87%)	14 (13%)	0	100	100
12	J	64/72 (89%)	59 (92%)	5 (8%)	0	100	100
13	K	111/118 (94%)	107 (96%)	4 (4%)	0	100	100
14	L	43/72 (60%)	37 (86%)	6 (14%)	0	100	100
15	M	62/110 (56%)	55 (89%)	7 (11%)	0	100	100
19	V	100/114 (88%)	94 (94%)	6 (6%)	0	100	100
20	W	265/908 (29%)	238 (90%)	23 (9%)	4 (2%)	8	39
21	a	94/136 (69%)	91 (97%)	3 (3%)	0	100	100
21	e	97/136 (71%)	95 (98%)	2 (2%)	0	100	100
22	b	75/103 (73%)	70 (93%)	5 (7%)	0	100	100
22	f	78/103 (76%)	73 (94%)	5 (6%)	0	100	100
23	c	99/130 (76%)	97 (98%)	2 (2%)	0	100	100
23	g	99/130 (76%)	96 (97%)	3 (3%)	0	100	100
24	d	86/126 (68%)	82 (95%)	3 (4%)	1 (1%)	10	43
24	h	88/126 (70%)	84 (96%)	3 (3%)	1 (1%)	11	45
All	All	5028/6644 (76%)	4695 (93%)	306 (6%)	27 (0%)	26	63

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	948	VAL
4	B	830	TYR
20	W	806	PRO
3	A	253	MET

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Mol	Chain	Res	Type
3	A	255	GLU
4	B	555	GLY
20	W	320	LEU
20	W	776	ASP
3	A	887	ILE
4	B	352	GLU
6	D	10	ALA
9	G	46	VAL
10	H	108	GLU
3	A	47	ARG
3	A	960	VAL
4	B	257	THR
4	B	1039	GLY
20	W	800	SER
3	A	179	GLY
4	B	1017	ILE
7	E	113	ASN
24	h	103	PRO
3	A	1109	VAL
9	G	154	VAL
7	E	123	ILE
7	E	150	PRO
24	d	103	PRO

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	1224/1528 (80%)	1220 (100%)	4 (0%)	86	85
4	B	1012/1077 (94%)	1002 (99%)	10 (1%)	68	77
5	C	236/264 (89%)	235 (100%)	1 (0%)	84	83
6	D	143/160 (89%)	142 (99%)	1 (1%)	76	80
7	E	196/197 (100%)	196 (100%)	0	100	100
8	F	75/137 (55%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	G	148/148 (100%)	146 (99%)	2 (1%)	59	71
10	H	120/130 (92%)	119 (99%)	1 (1%)	73	79
11	I	106/109 (97%)	106 (100%)	0	100	100
12	J	60/66 (91%)	59 (98%)	1 (2%)	53	68
13	K	104/109 (95%)	103 (99%)	1 (1%)	68	77
14	L	38/56 (68%)	38 (100%)	0	100	100
15	M	61/98 (62%)	61 (100%)	0	100	100
19	V	86/97 (89%)	86 (100%)	0	100	100
20	W	241/795 (30%)	240 (100%)	1 (0%)	84	83
21	a	82/110 (74%)	82 (100%)	0	100	100
21	e	85/110 (77%)	85 (100%)	0	100	100
22	b	63/79 (80%)	63 (100%)	0	100	100
22	f	65/79 (82%)	65 (100%)	0	100	100
23	c	80/100 (80%)	80 (100%)	0	100	100
23	g	80/100 (80%)	80 (100%)	0	100	100
24	d	75/105 (71%)	75 (100%)	0	100	100
24	h	77/105 (73%)	76 (99%)	1 (1%)	61	73
All	All	4457/5759 (77%)	4434 (100%)	23 (0%)	78	82

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	147	VAL
3	A	251	ILE
3	A	446	ASN
3	A	1197	LEU
4	B	44	THR
4	B	231	ILE
4	B	261	ILE
4	B	284	VAL
4	B	647	ILE
4	B	719	LEU
4	B	764	SER
4	B	795	ILE
4	B	992	VAL
4	B	1010	LEU

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Mol	Chain	Res	Type
5	C	8	ASN
6	D	19	VAL
9	G	87	VAL
9	G	157	ILE
10	H	42	ILE
12	J	3	ILE
13	K	72	VAL
20	W	259	ILE
24	h	106	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	172	GLN
3	A	197	GLN
3	A	260	GLN
3	A	287	GLN
3	A	364	GLN
3	A	446	ASN
3	A	649	ASN
3	A	651	GLN
3	A	661	ASN
3	A	737	ASN
3	A	769	GLN
3	A	927	GLN
3	A	961	ASN
3	A	1147	ASN
3	A	1190	GLN
3	A	1261	GLN
3	A	1435	GLN
4	B	102	GLN
4	B	206	GLN
4	B	291	GLN
4	B	438	ASN
4	B	477	ASN
4	B	524	GLN
4	B	776	GLN
4	B	794	ASN
4	B	835	GLN
4	B	996	HIS
4	B	1062	ASN
4	B	1076	HIS

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Mol	Chain	Res	Type
4	B	1097	HIS
4	B	1174	ASN
5	C	8	ASN
5	C	13	GLN
5	C	126	ASN
5	C	150	HIS
5	C	242	GLN
6	D	38	GLN
6	D	46	HIS
6	D	110	ASN
7	E	4	ASN
7	E	112	GLN
7	E	120	ASN
7	E	145	HIS
7	E	193	GLN
9	G	21	GLN
9	G	125	ASN
10	H	13	GLN
10	H	44	ASN
10	H	136	GLN
11	I	12	ASN
11	I	31	ASN
11	I	90	GLN
11	I	105	ASN
14	L	38	HIS
15	M	65	GLN
19	V	43	GLN
19	V	78	GLN
20	W	434	ASN
20	W	783	HIS
20	W	784	ASN
21	a	85	GLN
21	a	108	ASN
22	b	25	ASN
23	c	24	GLN
23	c	38	ASN
23	c	73	ASN
23	c	104	GLN
24	d	82	HIS
24	d	84	ASN
21	e	108	ASN
23	g	112	GLN

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Mol	Chain	Res	Type
24	h	47	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	P	15/16 (93%)	1 (6%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	P	-4	C

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 11 ligands modelled in this entry, 11 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 ⓘ

There are no chain breaks in this entry.

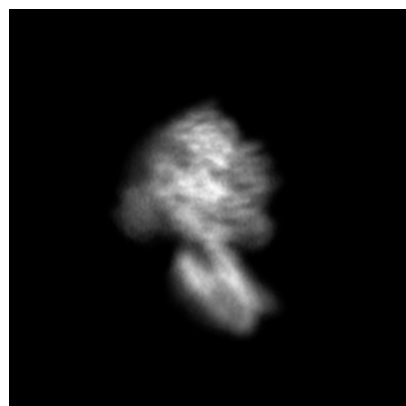
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36251. These allow visual inspection of the internal detail of the map and identification of artifacts.

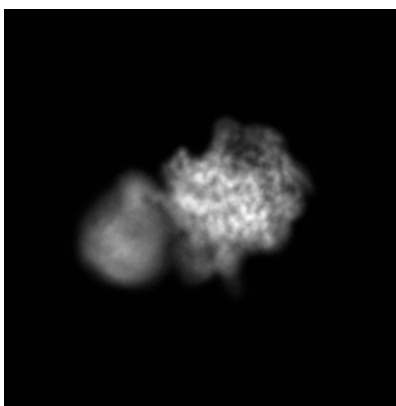
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

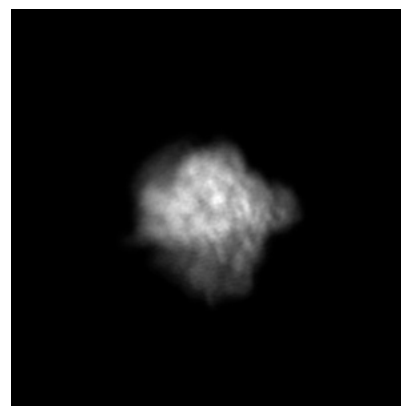
6.1.1 Primary map



X

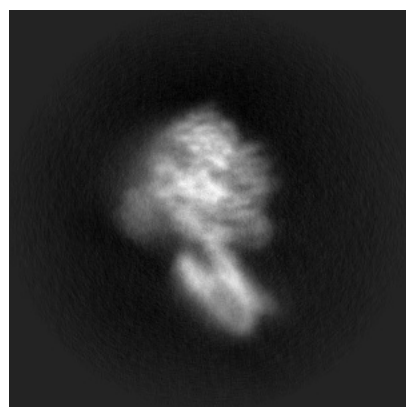


Y

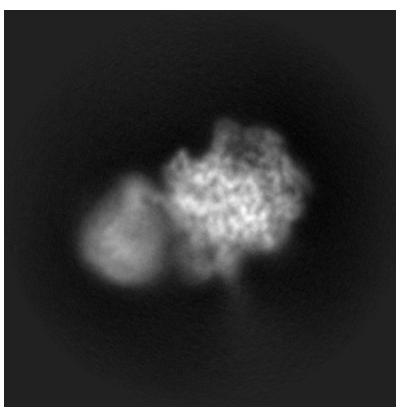


Z

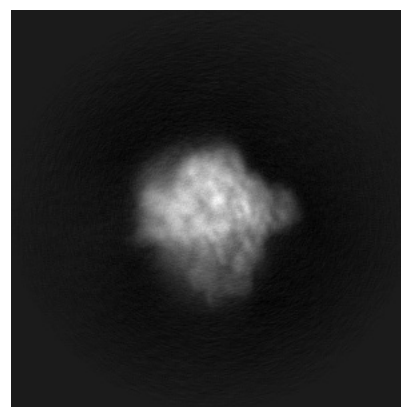
6.1.2 Raw map



X



Y

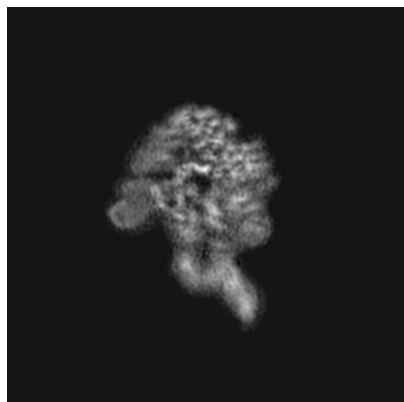


Z

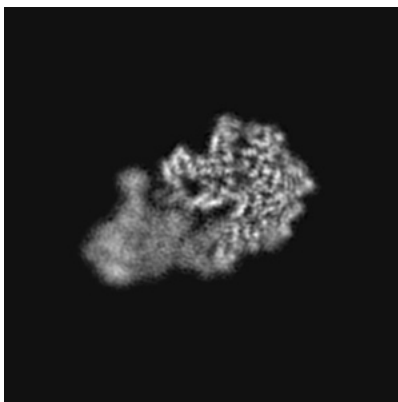
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

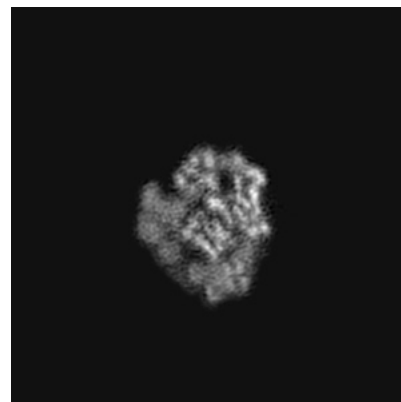
6.2.1 Primary map



X Index: 180

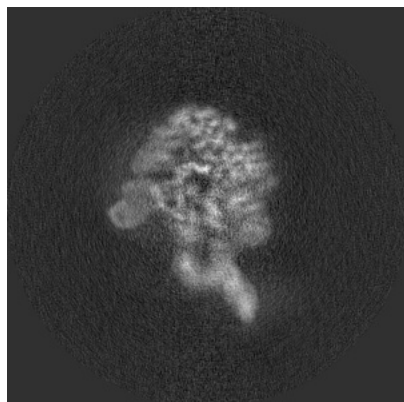


Y Index: 180

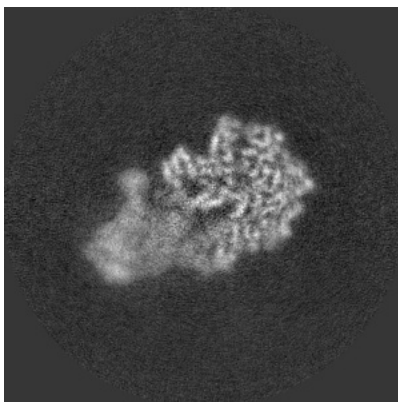


Z Index: 180

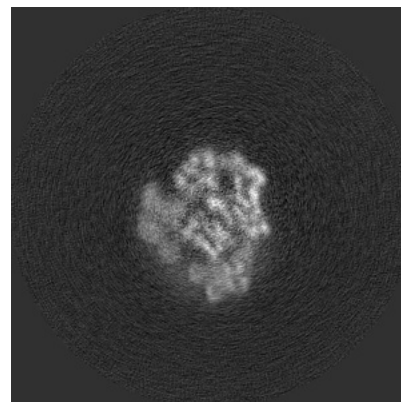
6.2.2 Raw map



X Index: 180



Y Index: 180

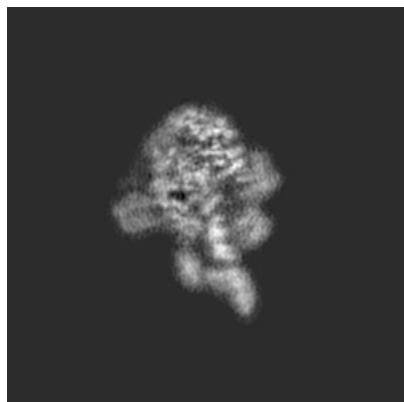


Z Index: 180

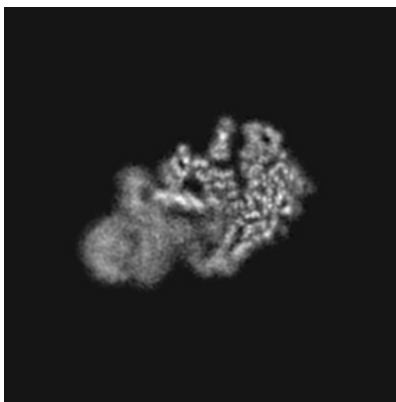
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

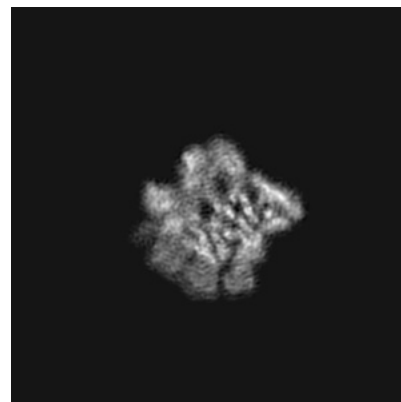
6.3.1 Primary map



X Index: 188

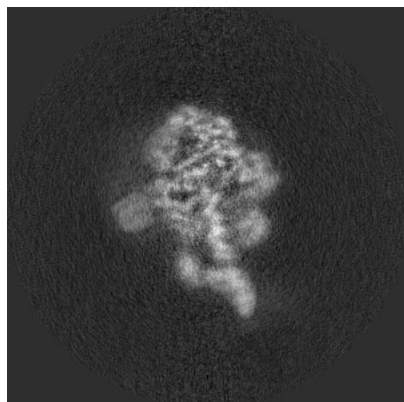


Y Index: 188

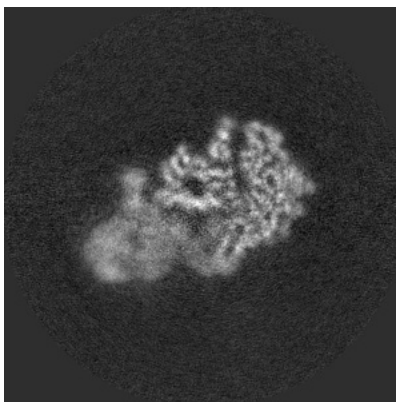


Z Index: 195

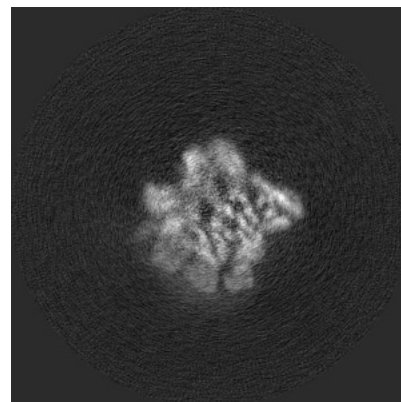
6.3.2 Raw map



X Index: 186



Y Index: 185

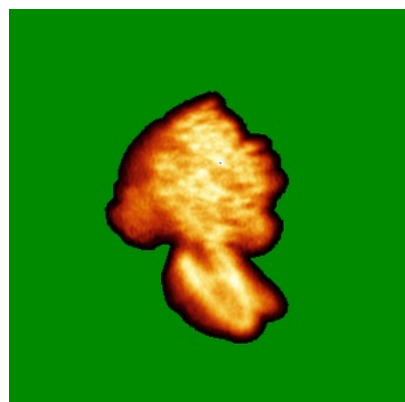


Z Index: 196

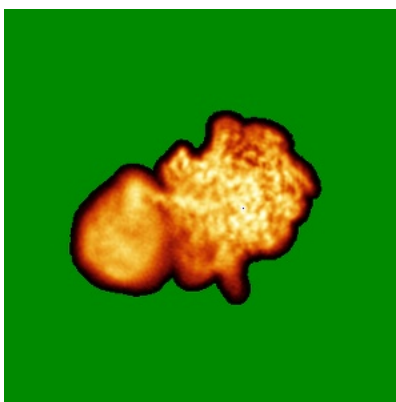
The images above show the largest variance slices of the map in three orthogonal directions.

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

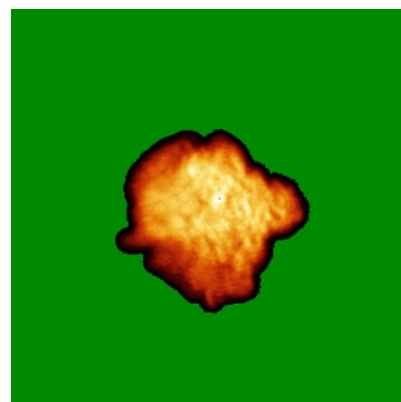
6.4.1 Primary map



X

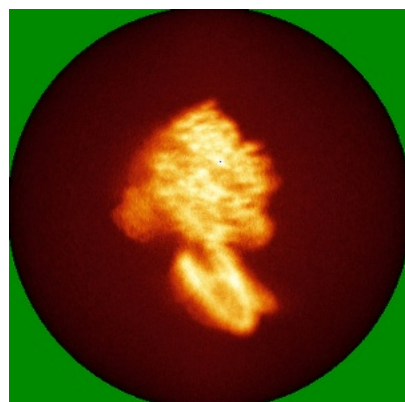


Y

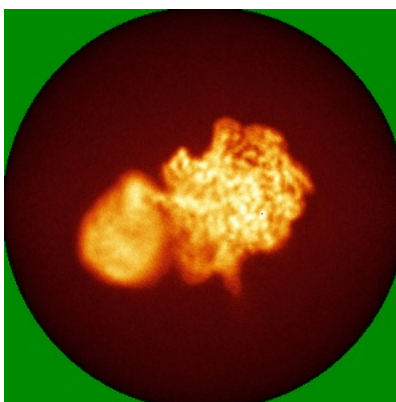


Z

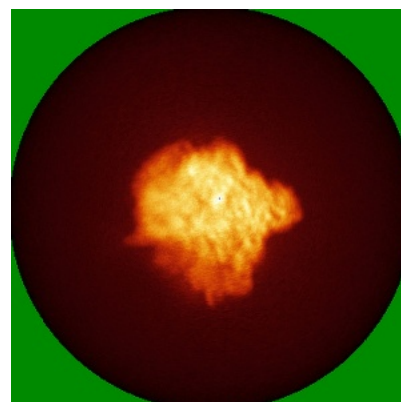
6.4.2 Raw map



X



Y

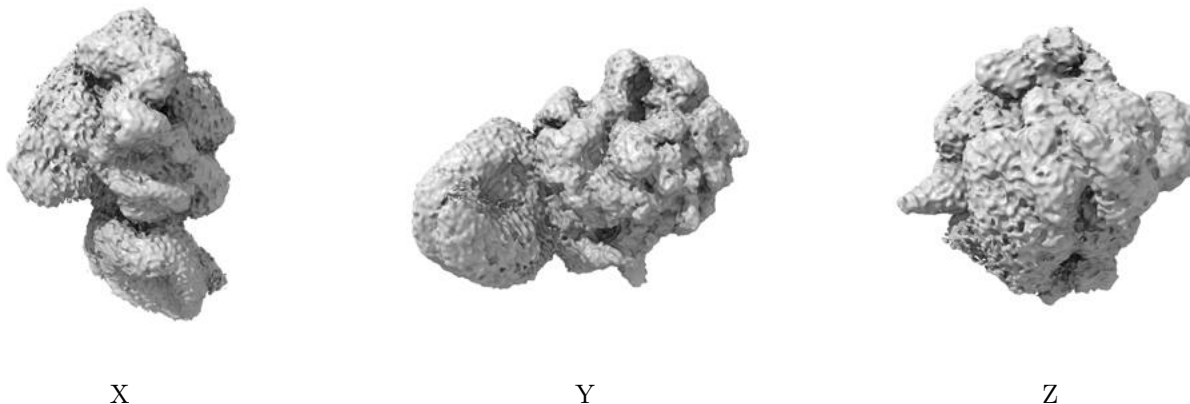


Z

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 0.00307. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

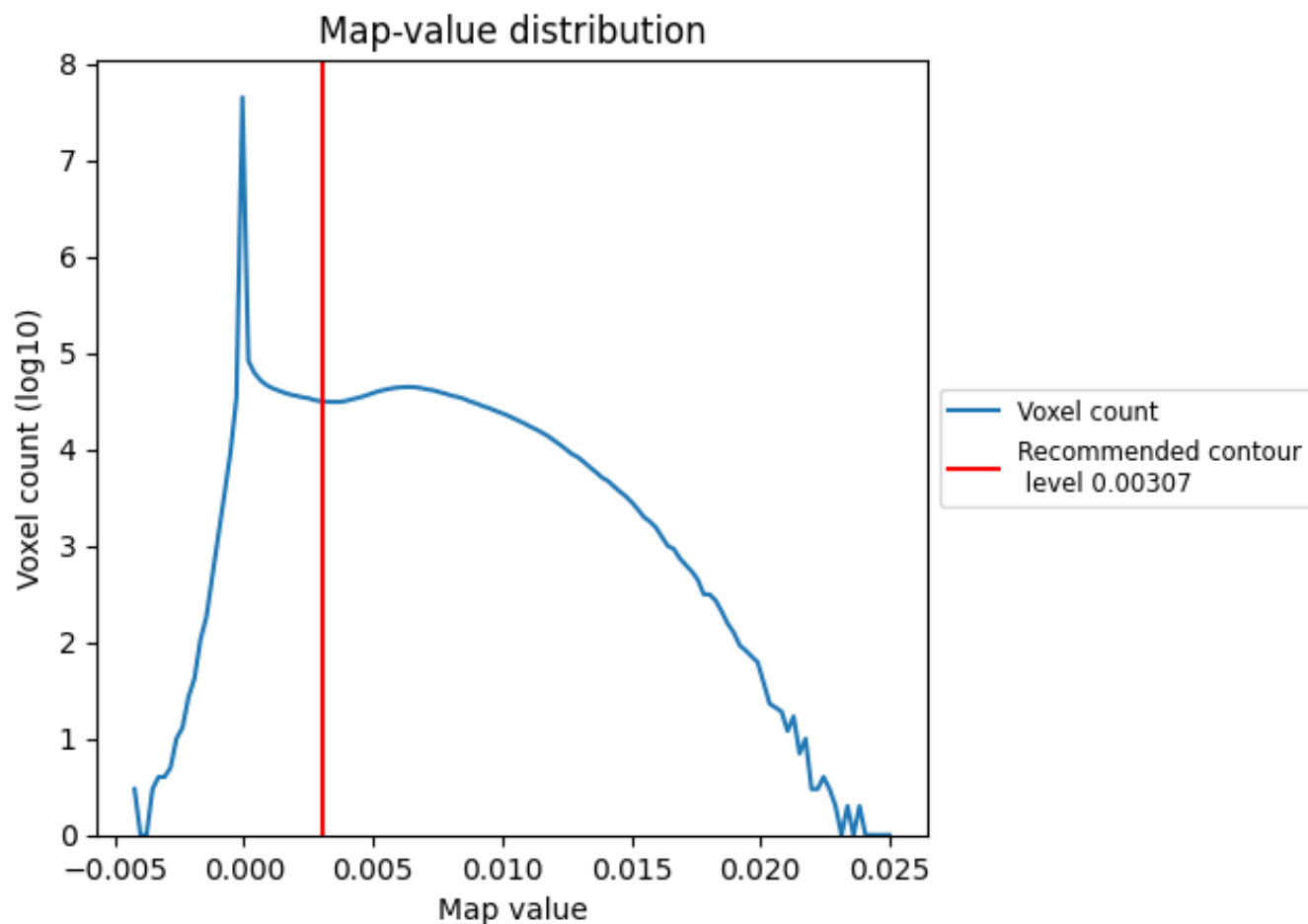
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

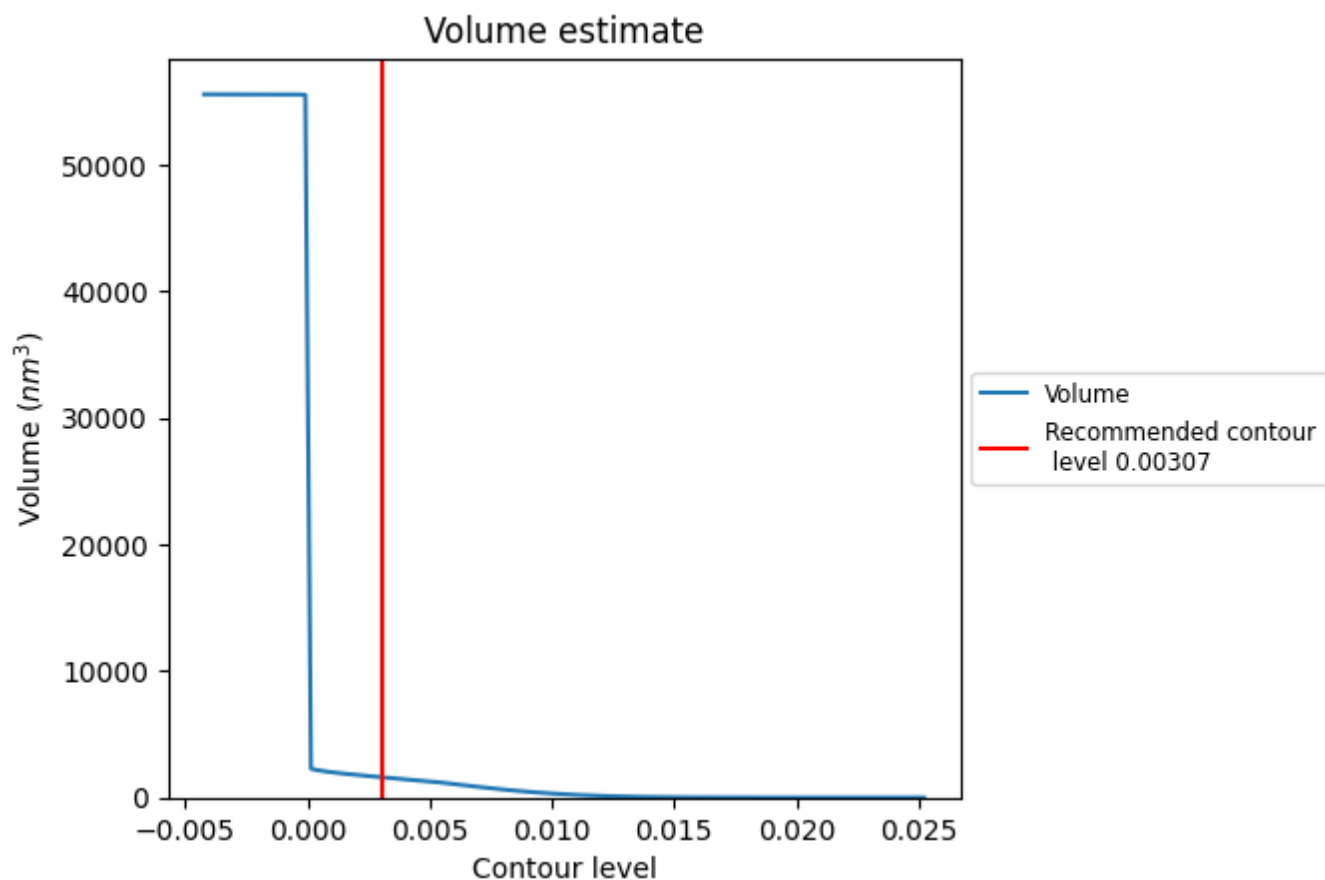
This section contains the results of statistical analysis of the map.

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.

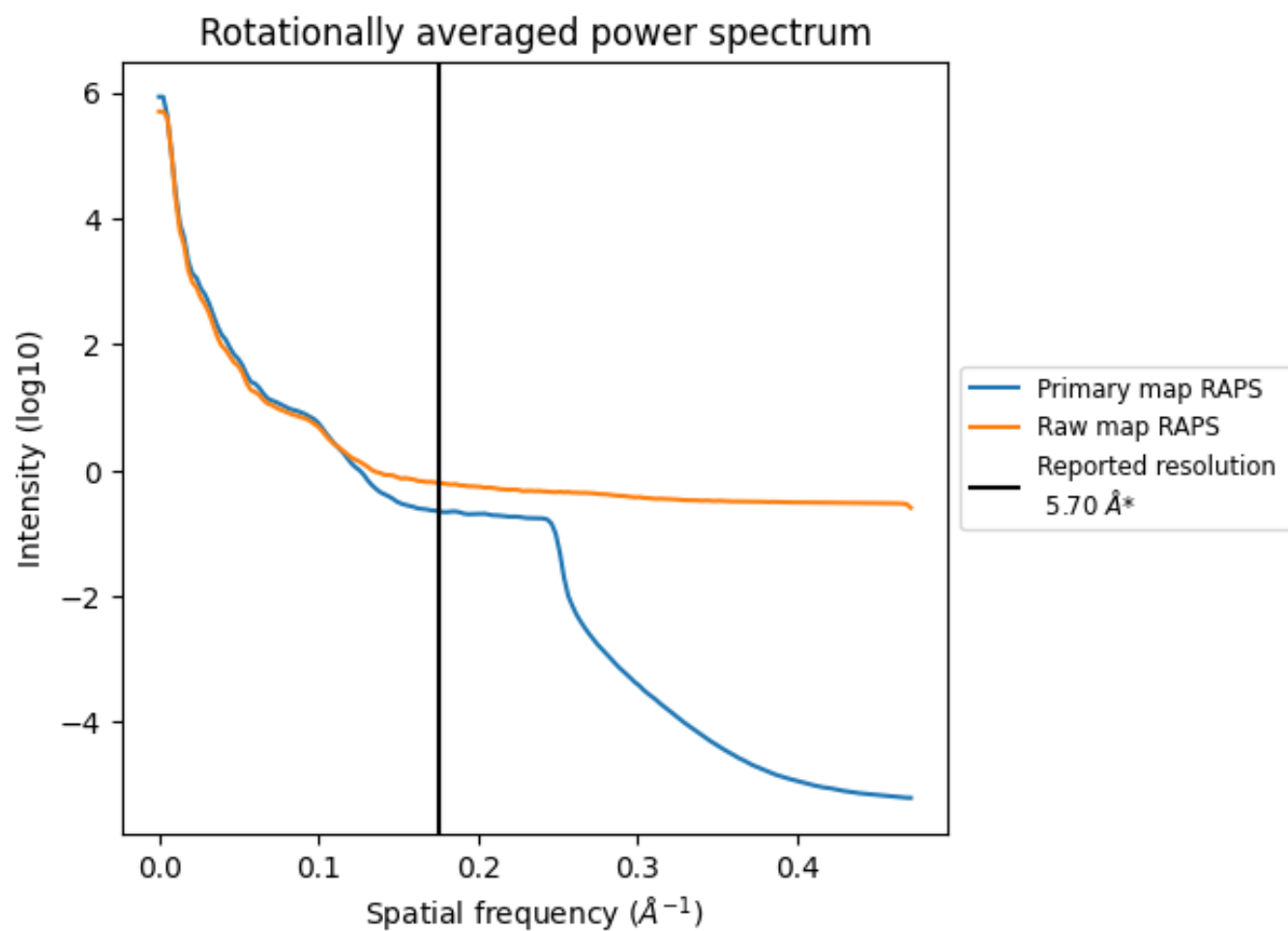
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1603 nm³; this corresponds to an approximate mass of 1448 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 ⓘ

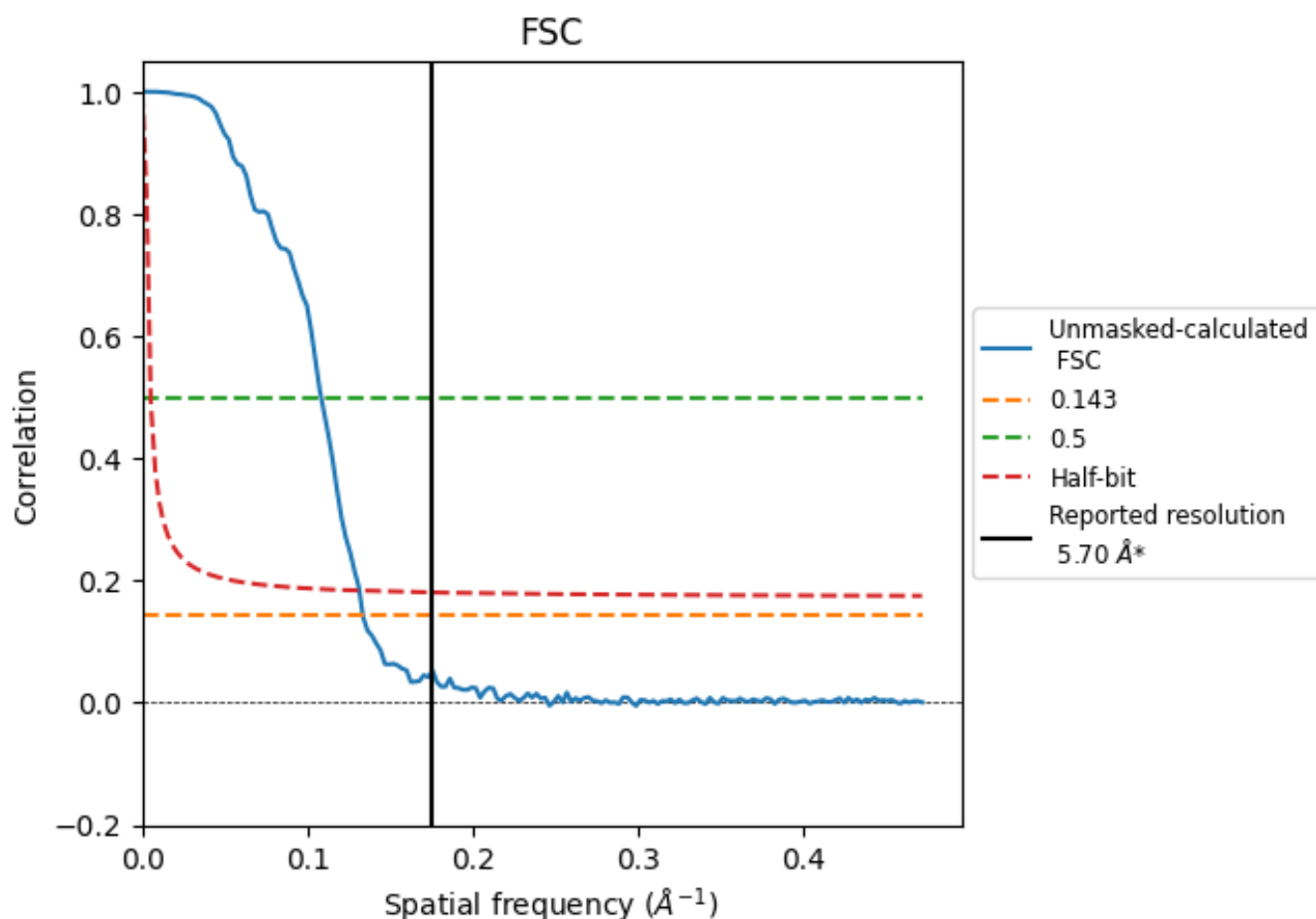


*Reported resolution corresponds to spatial frequency of 0.175 $\text{\AA}^{-1}$

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 0.175 Å⁻¹

8.2 Resolution estimates [i](#)

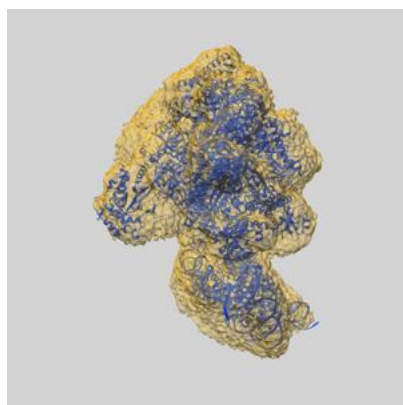
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.49	9.24	7.62

*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 7.49 differs from the reported value 5.7 by more than 10 %

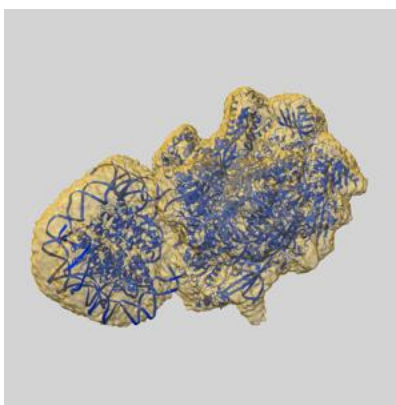
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36251 and PDB model 8JH2. Per-residue inclusion information can be found in section [3](#) on page [9](#).

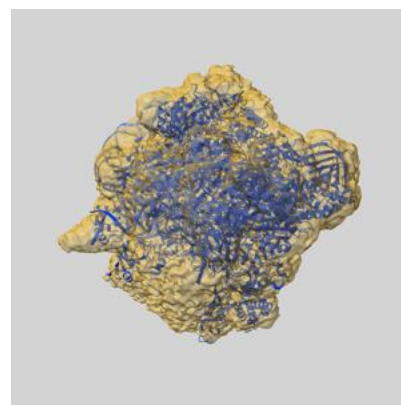
9.1 Map-model overlay [i](#)



X



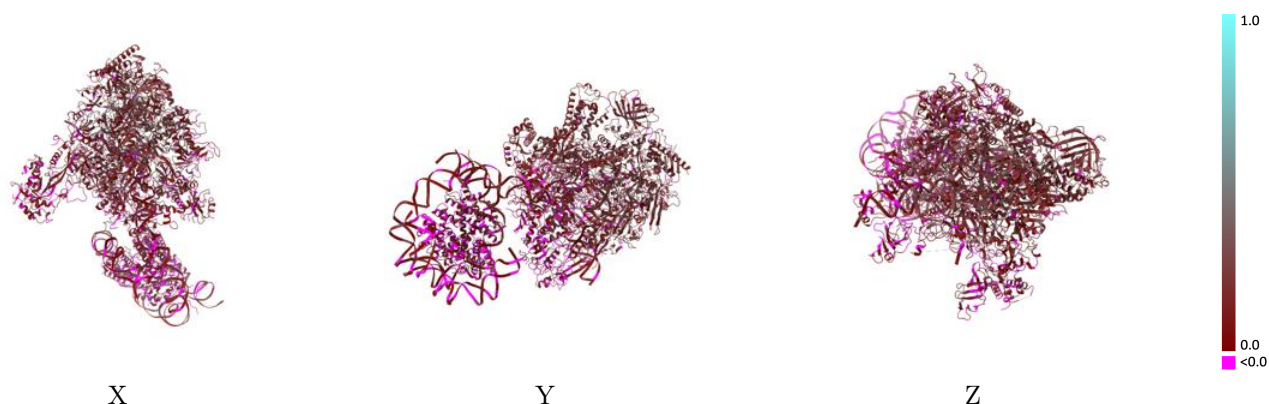
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00307 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](#)

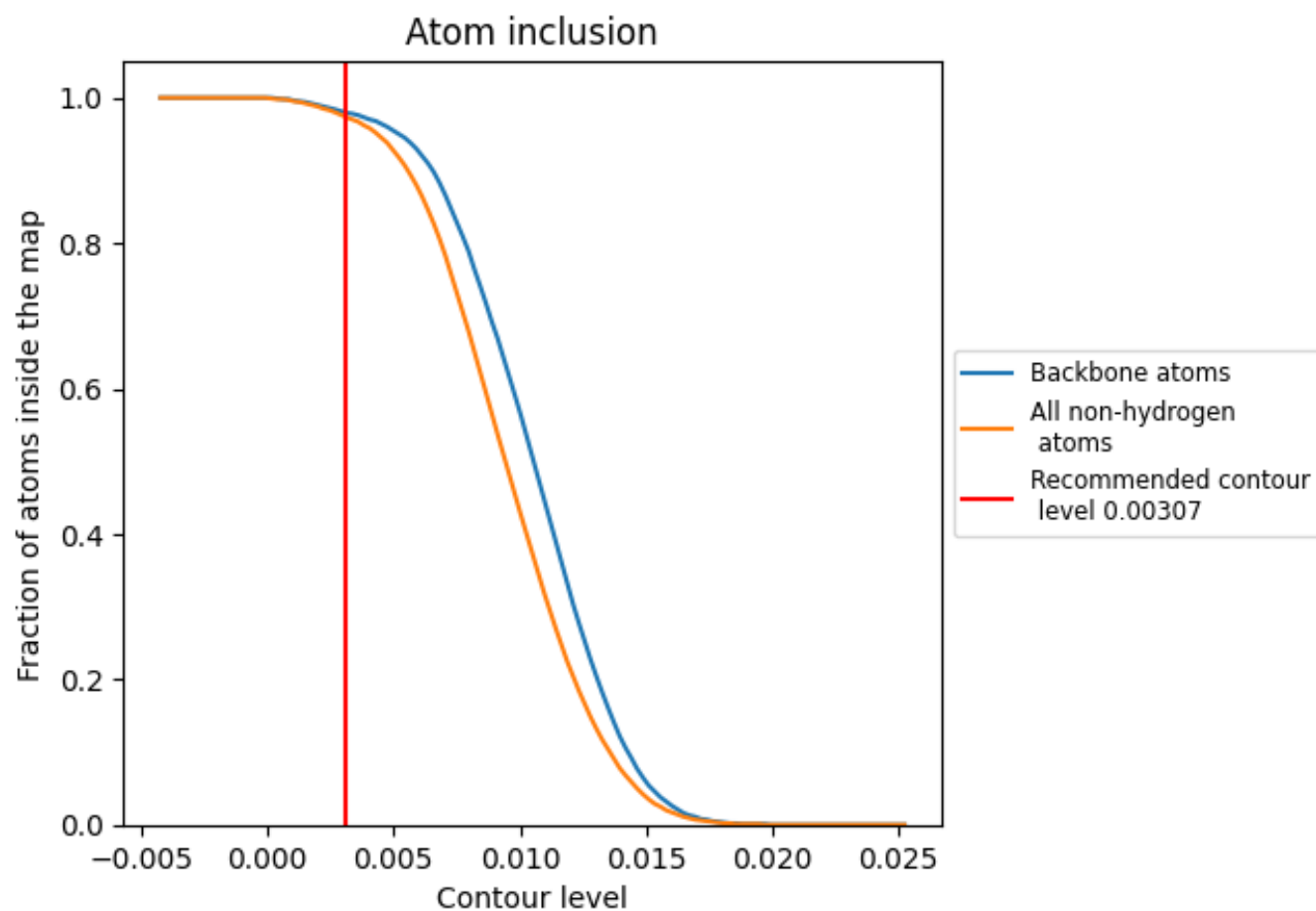


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.00307) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9740	 0.1450
0	 0.8540	 0.0410
1	 0.8000	 0.0240
A	 0.9910	 0.1950
B	 0.9910	 0.1980
C	 0.9900	 0.2100
D	 0.9030	 0.0840
E	 0.9940	 0.1840
F	 0.9990	 0.1890
G	 0.9320	 0.0990
H	 0.9810	 0.2210
I	 0.9870	 0.1020
J	 1.0000	 0.1980
K	 0.9920	 0.1840
L	 1.0000	 0.2090
M	 0.9740	 0.0510
N	 0.9960	 0.0820
P	 1.0000	 0.1830
T	 0.9780	 0.1150
V	 0.8820	 0.0460
W	 0.8850	 0.0560
a	 0.9920	 0.0700
b	 1.0000	 0.0430
c	 0.9960	 0.0380
d	 1.0000	 0.0320
e	 1.0000	 0.0750
f	 0.9950	 0.0640
g	 0.9800	 0.0430
h	 0.9960	 0.0510

