



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 07:21 PM EDT

PDB ID : 9MU9 / pdb_00009mu9
EMDB ID : EMD-48626
Title : Structure of a native *Drosophila melanogaster* Nucleosome Elongation Complex (Pol II EC-nucleosome). Composite map
Authors : Venette-Smith, N.L.; Vishwakarma, R.K.; Dollinger, R.; Schultz, J.; Venkatakrishnan, V.; Babitzke, P.; Anand, G.; Gilmour, D.S.; Armache, J.-P.; Murakami, K.S.
Deposited on : 2025-01-13
Resolution : 7.80 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:

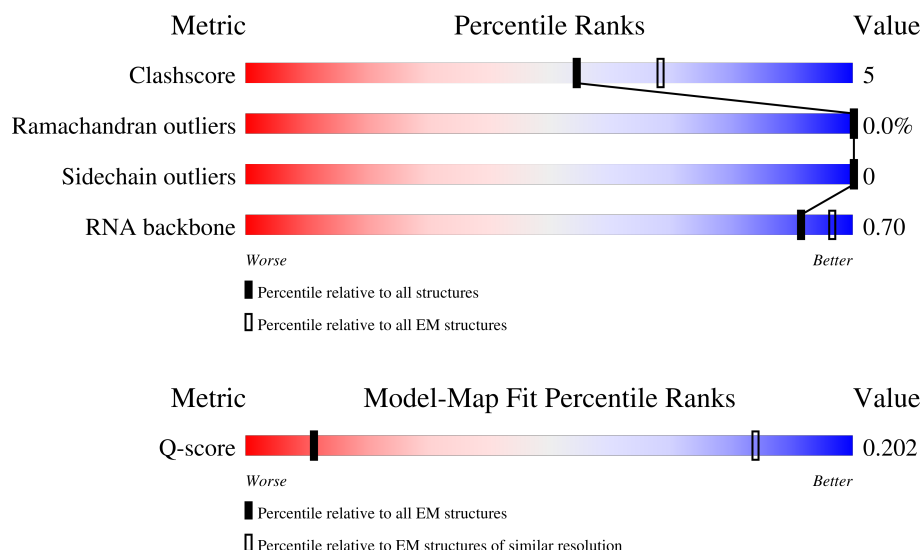
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 7.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	370 (7.30 - 8.30)

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

Mol	Chain	Length	Quality of chain
1	R	10	 60% 40%
2	T	174	 5% 90% 10%
3	N	163	 5% 88% 12%

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Mol	Chain	Length	Quality of chain
4	c	106	 6% 81% 18%
4	g	106	 1% 82% 18%
5	d	97	 76% 24%
5	h	97	 89% 11%
6	a	100	 1% 84% 16%
6	e	100	 1% 79% 13% 8%
7	b	80	 1% 88% 12%
7	f	80	 86% 14%
8	A	1470	 1% 85% 15%
9	B	1164	 1% 86% 14%
10	C	269	 5% 84% 16%
11	F	84	 1% 81% 19%
12	H	147	 7% 78% 22%
13	I	116	 1% 85% 15%
14	J	67	 81% 19%
15	K	116	 1% 82% 18%
16	L	46	 70% 30%
17	E	210	 87% 13%

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 42423 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	10	Total	C	N	O	P	0	0
			220	100	50	60	10		

- Molecule 2 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	174	Total	C	N	O	P	0	0
			3522	1695	567	1087	173		

- Molecule 3 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	163	Total	C	N	O	P	0	0
			3376	1598	673	942	163		

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	106	Total	C	N	O	S	0	0
			809	511	157	140	1		
4	c	105	Total	C	N	O	S	0	0
			803	506	156	140	1		

- Molecule 5 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	97	Total	C	N	O	S	0	0
			753	474	135	142	2		
5	d	97	Total	C	N	O	S	0	0
			753	474	135	142	2		

- Molecule 6 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	92	Total	C	N	O	S	0	0
			749	471	142	133	3		
6	a	100	Total	C	N	O	S	0	0
			817	514	158	142	3		

- Molecule 7 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	80	Total	C	N	O	S	0	0
			630	395	123	111	1		
7	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	1470	Total	C	N	O	S	0	0
			11565	7261	2052	2163	89		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	1164	Total	C	N	O	S	0	0
			9257	5851	1633	1709	64		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	269	Total	C	N	O	S	0	0
			2156	1354	362	432	8		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	84	Total	C	N	O	S	0	0
			674	430	115	123	6		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	147	Total	C	N	O	S	0	0
			1186	748	200	228	10		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	116	Total	C	N	O	S	0	0
			947	588	164	183	12		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	67	Total	C	N	O	S	0	0
			530	342	89	93	6		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	116	Total	C	N	O	S	0	0
			935	603	153	176	3		

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	46	Total	C	N	O	S	0	0
			390	239	78	66	7		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	210	Total	C	N	O	S	0	0
			1705	1081	290	322	12		

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
18	L	1	1	1	0

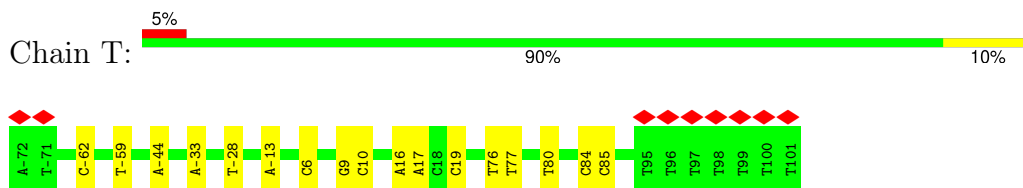
3 Residue-property plots [i](#)

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

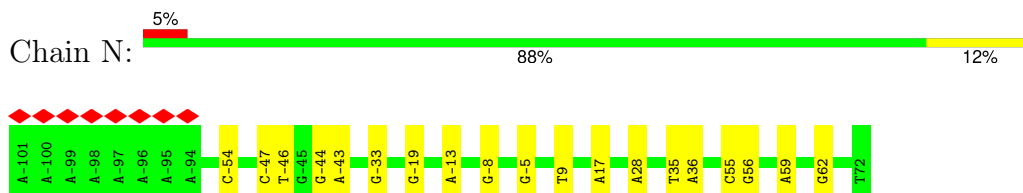
- Molecule 1: RNA



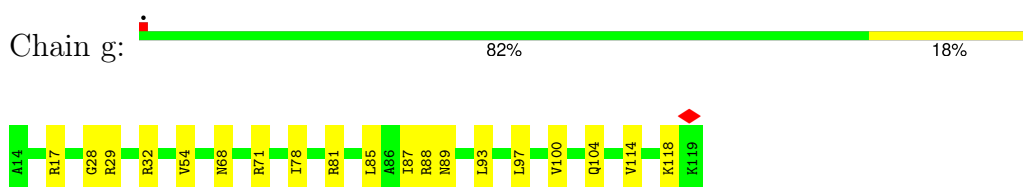
- Molecule 2: Template DNA



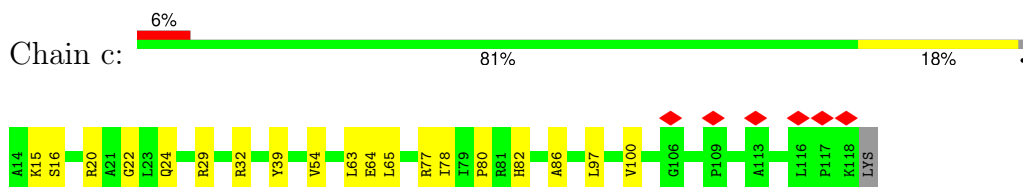
- Molecule 3: Non-template DNA



- Molecule 4: Histone H2A

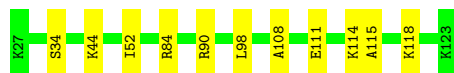


- Molecule 4: Histone H2A



- Molecule 5: Histone H2B

Chain h:  89% 11%



- Molecule 5: Histone H2B

Chain d:  76% 24%



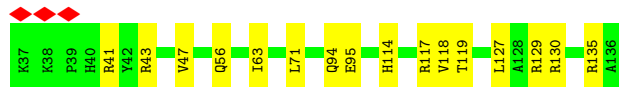
- Molecule 6: Histone H3

Chain e:  79% 13% 8%



- Molecule 6: Histone H3

Chain a:  84% 16%



- Molecule 7: Histone H4

Chain f:  86% 14%



- Molecule 7: Histone H4

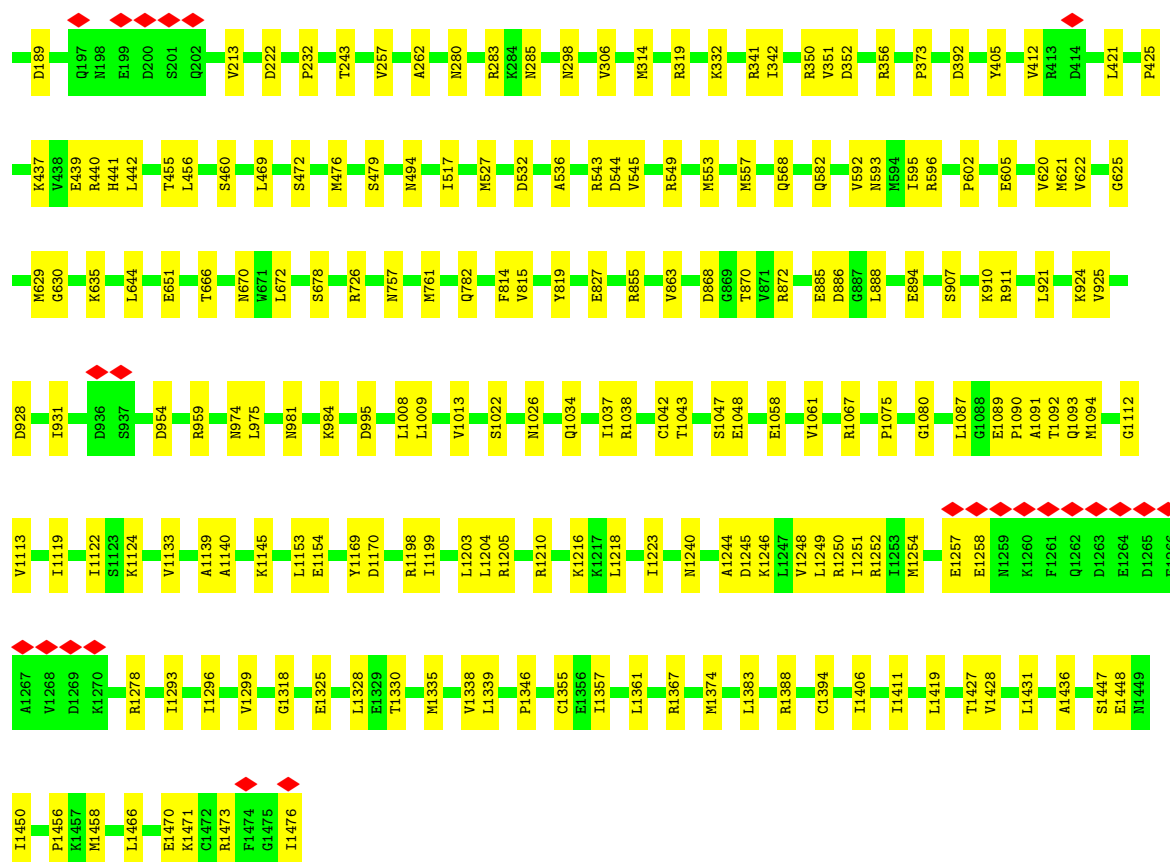
Chain b:  88% 12%



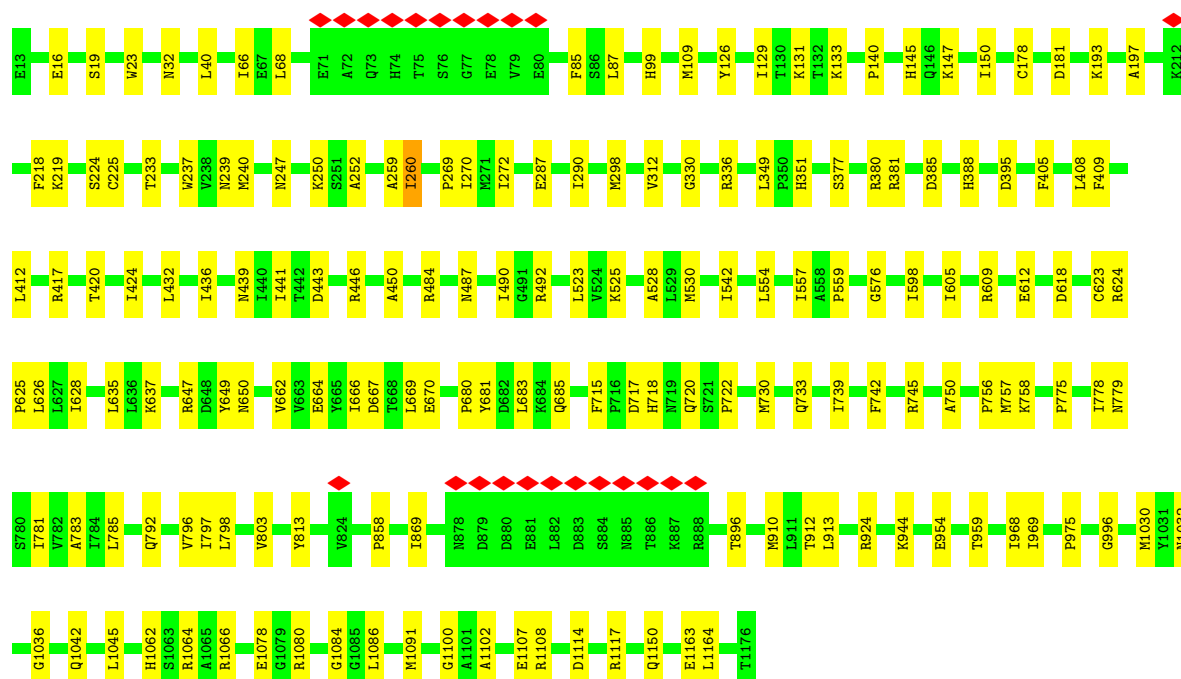
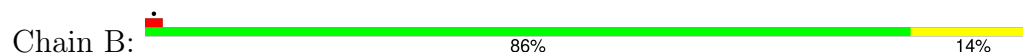
- Molecule 8: DNA-directed RNA polymerase II subunit RPB1

Chain A:  85% 15%

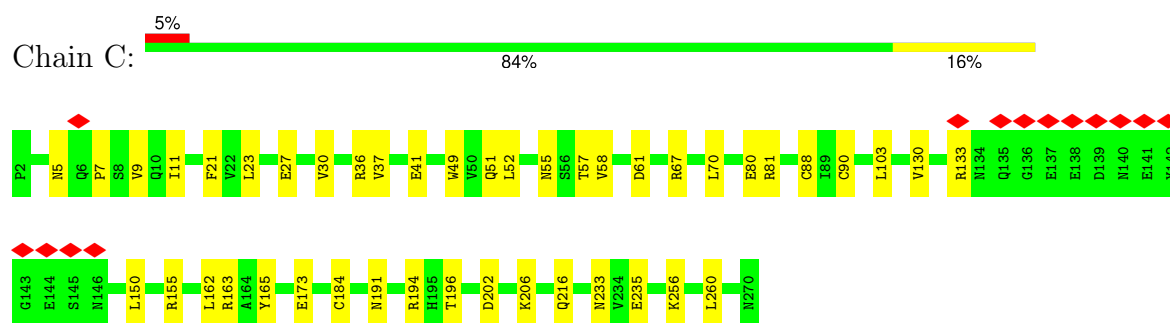




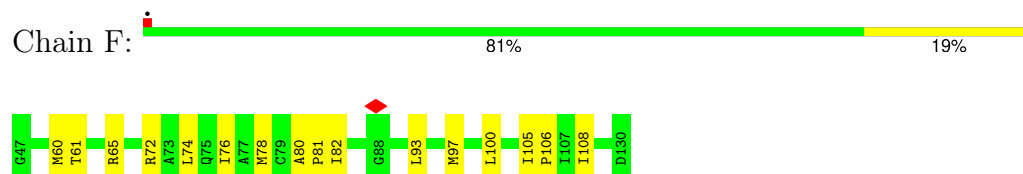
• Molecule 9: DNA-directed RNA polymerase II subunit RPB2



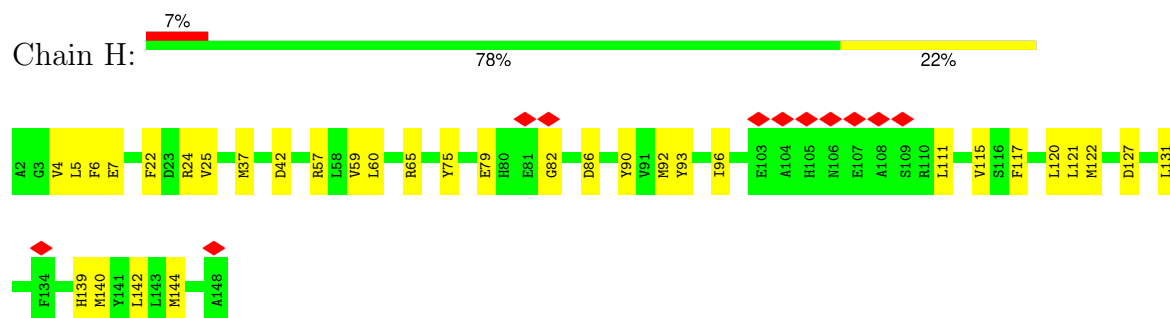
• Molecule 10: DNA-directed RNA polymerase II subunit RPB3



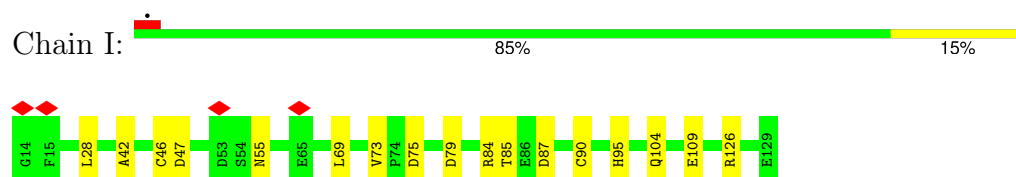
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC2



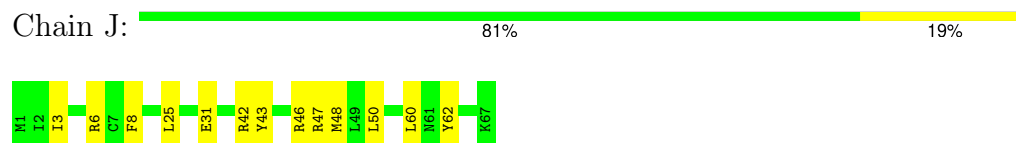
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC3



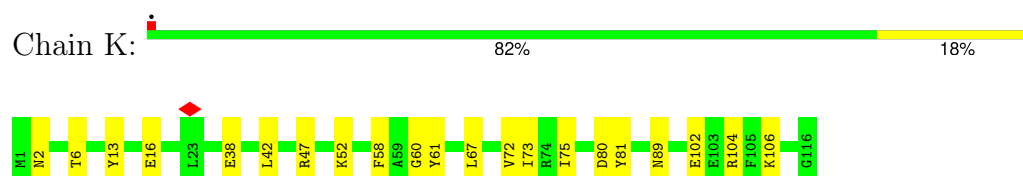
- Molecule 13: DNA-directed RNA polymerase II subunit RPB9



- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 15: DNA-directed RNA polymerase II subunit RPB11



- Molecule 16: DNA-directed RNA polymerase II subunit RPB12

Chain L:  70% 30%



- Molecule 17: DNA-directed RNA polymerase II subunit RPB5

Chain E:  87% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36552	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; 'Patch CTF Estimation' in cryoSPARC	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.572	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	415.368, 415.368, 415.368	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1538, 1.1538, 1.1538	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: 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	R	0.08	0/249	0.16	0/386
2	T	0.21	0/3927	0.50	0/6056
3	N	0.20	0/3805	0.40	0/5871
4	c	0.15	0/813	0.38	0/1097
4	g	0.15	0/819	0.35	0/1104
5	d	0.16	0/764	0.41	0/1027
5	h	0.15	0/764	0.35	0/1027
6	a	0.17	0/829	0.41	0/1112
6	e	0.16	0/757	0.41	0/1013
7	b	0.16	0/645	0.36	0/862
7	f	0.16	0/637	0.37	0/854
8	A	0.21	1/11779 (0.0%)	0.44	0/15904
9	B	0.15	0/9444	0.40	2/12756 (0.0%)
10	C	0.14	0/2201	0.35	0/2989
11	F	0.18	0/685	0.47	0/923
12	H	0.15	0/1211	0.45	0/1627
13	I	0.16	0/968	0.42	0/1311
14	J	0.13	0/539	0.34	0/726
15	K	0.17	0/954	0.40	0/1286
16	L	0.15	0/397	0.42	0/527
17	E	0.16	0/1735	0.44	0/2339
All	All	0.18	1/43922 (0.0%)	0.42	2/60797 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	150	CYS	C-N	9.06	1.46	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	260	ILE	CA-C-N	5.86	137.62	120.97
9	B	260	ILE	C-N-CA	5.86	137.62	120.97

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	R	220	0	111	3	0
2	T	3522	0	1987	17	0
3	N	3376	0	1821	17	0
4	c	803	0	853	17	0
4	g	809	0	862	14	0
5	d	753	0	767	20	0
5	h	753	0	767	10	0
6	a	817	0	847	15	0
6	e	749	0	787	10	0
7	b	638	0	676	8	0
7	f	630	0	654	9	0
8	A	11565	0	11557	141	0
9	B	9257	0	9229	108	0
10	C	2156	0	2084	32	0
11	F	674	0	702	11	0
12	H	1186	0	1132	20	0
13	I	947	0	878	10	0
14	J	530	0	542	11	0
15	K	935	0	946	17	0
16	L	390	0	386	9	0
17	E	1705	0	1718	16	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	42423	0	39306	414	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 5.

All (414) 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)
8:A:34:GLU:OE1	8:A:57:ARG:NH1	1.94	1.01
2:T:19:DC:H42	3:N:-19:DG:H1	1.42	0.68
1:R:39:A:H61	2:T:84:DC:H42	1.42	0.68
9:B:756:PRO:HB2	9:B:775:PRO:HG2	1.78	0.65
2:T:-62:DC:H42	3:N:62:DG:H1	1.45	0.65
8:A:1091:ALA:HA	8:A:1094:MET:HE3	1.79	0.65
9:B:609:ARG:HE	13:I:104:GLN:HE21	1.46	0.62
8:A:1367:ARG:HG2	8:A:1394:CYS:HB3	1.82	0.62
17:E:55:ARG:HH21	17:E:76:PHE:HB3	1.65	0.62
10:C:49:TRP:HB3	10:C:165:TYR:HB2	1.82	0.61
5:d:106:LYS:O	5:d:109:VAL:HB	2.01	0.60
12:H:37:MET:HE1	12:H:127:ASP:H	1.65	0.60
8:A:1119:ILE:CB	8:A:1374:MET:HE2	2.31	0.60
8:A:1008:LEU:HD12	8:A:1061:VAL:HG23	1.84	0.60
13:I:46:CYS:SG	13:I:47:ASP:N	2.75	0.60
8:A:472:SER:HB3	15:K:2:ASN:HB2	1.84	0.59
4:c:64:GLU:HA	5:d:47:HIS:HE1	1.67	0.59
10:C:184:CYS:HB2	10:C:233:ASN:HB3	1.85	0.59
8:A:595:ILE:HG23	8:A:621:MET:HE1	1.85	0.58
8:A:544:ASP:HB3	12:H:22:PHE:HB3	1.83	0.58
8:A:621:MET:HB2	8:A:629:MET:HB3	1.84	0.58
8:A:568:GLN:HA	12:H:75:TYR:HB2	1.85	0.58
8:A:1133:VAL:HB	8:A:1328:LEU:HB2	1.84	0.57
17:E:165:LEU:HD23	17:E:169:MET:HE2	1.86	0.57
12:H:90:TYR:HB3	12:H:144:MET:HB3	1.86	0.57
6:a:127:LEU:HD12	6:a:130:ARG:HE	1.70	0.56
9:B:797:ILE:HB	9:B:968:ILE:HG22	1.86	0.56
12:H:65:ARG:HH22	12:H:79:GLU:HB3	1.70	0.56
6:e:128:ALA:O	6:e:132:ARG:HB2	2.05	0.56
8:A:89:PRO:HB3	8:A:243:THR:HG22	1.87	0.56
9:B:628:ILE:HD11	9:B:664:GLU:HB2	1.86	0.56
10:C:55:ASN:ND2	10:C:61:ASP:OD1	2.36	0.56
8:A:553:MET:HG3	15:K:47:ARG:HH21	1.71	0.56
12:H:7:GLU:HG3	12:H:57:ARG:HH12	1.70	0.56
8:A:412:VAL:O	8:A:437:LYS:HB3	2.06	0.56
13:I:28:LEU:HA	13:I:42:ALA:O	2.05	0.56
5:h:90:ARG:NH2	7:f:75:GLU:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:115:VAL:HG23	8:A:122:ILE:HD11	1.87	0.56
9:B:150:ILE:HG22	9:B:436:ILE:HG21	1.88	0.56
8:A:1456:PRO:HD2	9:B:1102:ALA:HB1	1.88	0.55
8:A:352:ASP:OD1	9:B:1064:ARG:NH1	2.39	0.55
9:B:32:ASN:HB3	9:B:647:ARG:HH22	1.72	0.55
9:B:178:CYS:HB3	9:B:181:ASP:HB2	1.88	0.55
9:B:484:ARG:NH2	9:B:528:ALA:O	2.39	0.55
11:F:74:LEU:HG	11:F:78:MET:HE1	1.89	0.55
3:N:-43:DA:H5''	4:c:16:SER:HA	1.88	0.55
8:A:48:PRO:HB2	8:A:56:PRO:HD3	1.89	0.55
8:A:925:VAL:HG21	8:A:1048:GLU:HG3	1.89	0.55
9:B:68:LEU:HD12	9:B:85:PHE:HB2	1.88	0.55
16:L:35:CYS:HB3	16:L:40:TYR:H	1.71	0.55
9:B:66:ILE:HD12	9:B:417:ARG:HE	1.72	0.54
13:I:73:VAL:HG12	13:I:75:ASP:H	1.72	0.54
9:B:757:MET:HB2	9:B:778:ILE:HA	1.90	0.54
11:F:93:LEU:HD23	11:F:97:MET:HE1	1.88	0.54
7:b:40:ARG:NH1	7:b:44:VAL:O	2.37	0.54
10:C:260:LEU:HD11	15:K:42:LEU:HD13	1.89	0.54
8:A:100:ILE:HA	8:A:103:LEU:HB2	1.88	0.54
8:A:341:ARG:NH1	9:B:1163:GLU:OE2	2.40	0.54
9:B:781:ILE:HG12	14:J:47:ARG:HE	1.73	0.54
4:c:24:GLN:HE22	5:d:38:TYR:HB3	1.72	0.54
3:N:17:DA:H4'	6:e:64:ARG:HD2	1.89	0.54
15:K:60:GLY:O	15:K:73:ILE:HA	2.07	0.54
8:A:342:ILE:HG13	8:A:1427:THR:HG21	1.89	0.54
8:A:455:THR:HG23	8:A:460:SER:HB2	1.89	0.54
10:C:67:ARG:NH1	14:J:3:ILE:O	2.40	0.54
2:T:-28:DT:H3	3:N:28:DA:H61	1.56	0.53
5:d:100:LEU:HB2	5:d:105:ALA:HB2	1.90	0.53
9:B:487:ASN:OD1	9:B:492:ARG:NH2	2.41	0.53
4:g:68:ASN:OD1	4:g:71:ARG:NH2	2.41	0.53
4:g:81:ARG:NH2	6:a:56:GLN:O	2.40	0.53
8:A:332:LYS:HG3	8:A:1428:VAL:HG21	1.90	0.53
9:B:530:MET:HG3	9:B:625:PRO:HD2	1.91	0.53
8:A:761:MET:HE2	9:B:975:PRO:HG2	1.89	0.53
9:B:542:ILE:HG12	9:B:598:ILE:HG12	1.90	0.53
8:A:593:ASN:ND2	8:A:981:ASN:OD1	2.42	0.53
9:B:1042:GLN:OE1	10:C:196:THR:OG1	2.27	0.53
8:A:1199:ILE:HG22	8:A:1254:MET:HG3	1.91	0.53
12:H:92:MET:HB2	12:H:142:LEU:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:120:ILE:HD11	7:f:47:ILE:HG23	1.91	0.53
9:B:330:GLY:O	9:B:336:ARG:NH1	2.42	0.53
8:A:1335:MET:HA	8:A:1338:VAL:HB	1.90	0.53
8:A:1431:LEU:HD13	9:B:1164:LEU:HD21	1.90	0.53
17:E:15:LYS:NZ	17:E:33:LEU:O	2.41	0.53
6:e:109:ASN:HB2	7:f:44:VAL:HG22	1.91	0.52
9:B:605:ILE:HD11	9:B:669:LEU:HB3	1.91	0.52
2:T:-59:DT:H3	3:N:59:DA:H61	1.56	0.52
4:g:29:ARG:NH1	5:h:34:SER:O	2.42	0.52
8:A:568:GLN:O	8:A:582:GLN:NE2	2.41	0.52
10:C:9:VAL:HB	15:K:104:ARG:HH11	1.73	0.52
4:g:78:ILE:HB	5:h:52:ILE:HG13	1.91	0.52
8:A:1205:ARG:HA	8:A:1249:LEU:O	2.09	0.52
9:B:681:TYR:O	9:B:685:GLN:NE2	2.43	0.52
10:C:191:ASN:O	10:C:194:ARG:NH1	2.41	0.52
8:A:870:THR:OG1	8:A:872:ARG:NH1	2.43	0.52
8:A:1124:LYS:HA	8:A:1355:CYS:SG	2.50	0.52
11:F:100:LEU:HD13	11:F:105:ILE:HD12	1.91	0.52
13:I:90:CYS:HB3	13:I:95:HIS:H	1.74	0.52
8:A:888:LEU:O	8:A:1388:ARG:NH1	2.43	0.52
8:A:1170:ASP:OD2	8:A:1252:ARG:NH2	2.43	0.52
8:A:1476:ILE:H	11:F:81:PRO:HB3	1.75	0.52
9:B:779:ASN:O	14:J:47:ARG:NH1	2.43	0.52
3:N:-8:DG:H21	6:a:41:ARG:HH12	1.57	0.52
9:B:869:ILE:HB	9:B:896:THR:HB	1.92	0.52
9:B:959:THR:HG22	9:B:1030:MET:HG2	1.92	0.52
9:B:66:ILE:HB	9:B:87:LEU:HB2	1.91	0.51
10:C:67:ARG:NH2	10:C:150:LEU:O	2.43	0.51
12:H:6:PHE:HB3	12:H:60:LEU:HB2	1.91	0.51
4:c:15:LYS:O	4:c:20:ARG:NH2	2.43	0.51
8:A:1089:GLU:OE2	8:A:1093:GLN:NE2	2.43	0.51
6:e:119:THR:OG1	7:f:46:ARG:NH1	2.42	0.51
9:B:287:GLU:HB3	9:B:559:PRO:HB2	1.91	0.51
9:B:219:LYS:HE3	9:B:239:ASN:HD21	1.75	0.51
10:C:202:ASP:OD1	10:C:202:ASP:N	2.44	0.51
3:N:-33:DG:OP2	5:d:84:ARG:NH2	2.43	0.51
8:A:90:VAL:HG21	8:A:306:VAL:HG21	1.92	0.51
8:A:356:ARG:NH1	8:A:494:ASN:OD1	2.43	0.51
9:B:717:ASP:N	9:B:717:ASP:OD1	2.43	0.51
16:L:26:GLU:O	16:L:36:ARG:NH2	2.43	0.51
8:A:666:THR:O	8:A:670:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1047:SER:OG	8:A:1048:GLU:OE1	2.29	0.51
9:B:412:LEU:HD11	9:B:436:ILE:HG23	1.92	0.51
8:A:819:TYR:O	9:B:718:HIS:ND1	2.42	0.51
8:A:885:GLU:OE2	17:E:195:ARG:NH1	2.42	0.51
8:A:532:ASP:OD1	9:B:792:GLN:NE2	2.44	0.51
11:F:76:ILE:HD13	11:F:80:ALA:HB3	1.92	0.51
5:d:98:LEU:O	7:b:93:ARG:NH2	2.42	0.51
8:A:1299:VAL:HG13	8:A:1330:THR:HG22	1.93	0.51
5:d:116:VAL:O	5:d:119:TYR:HB3	2.10	0.50
8:A:678:SER:O	8:A:757:ASN:ND2	2.44	0.50
8:A:928:ASP:HA	8:A:931:ILE:HD12	1.93	0.50
12:H:96:ILE:HG13	12:H:115:VAL:HG22	1.93	0.50
8:A:1470:GLU:O	8:A:1473:ARG:NH1	2.44	0.50
9:B:758:LYS:O	9:B:779:ASN:ND2	2.44	0.50
10:C:235:GLU:OE1	14:J:42:ARG:NH2	2.43	0.50
3:N:9:DT:OP1	6:e:45:GLY:N	2.45	0.50
8:A:439:GLU:OE2	9:B:1066:ARG:NH2	2.45	0.50
8:A:975:LEU:HD21	8:A:1037:ILE:HD13	1.94	0.50
12:H:5:LEU:HD12	12:H:140:MET:HE1	1.92	0.50
9:B:380:ARG:O	9:B:609:ARG:NH2	2.42	0.50
9:B:439:ASN:O	9:B:443:ASP:HB2	2.12	0.50
8:A:959:ARG:NH2	8:A:1318:GLY:O	2.42	0.50
13:I:85:THR:OG1	13:I:87:ASP:OD1	2.30	0.50
9:B:443:ASP:OD1	9:B:446:ARG:NH2	2.45	0.50
10:C:37:VAL:HG23	10:C:41:GLU:HB2	1.94	0.50
9:B:785:LEU:HG	9:B:968:ILE:HD11	1.92	0.50
12:H:42:ASP:HB2	12:H:121:LEU:H	1.77	0.50
17:E:18:MET:HE3	17:E:28:VAL:HG22	1.94	0.50
8:A:543:ARG:HG2	12:H:25:VAL:HG21	1.94	0.50
8:A:596:ARG:HH21	8:A:635:LYS:HB3	1.76	0.50
8:A:1278:ARG:HD2	9:B:252:ALA:HB1	1.94	0.50
9:B:783:ALA:HB2	9:B:1045:LEU:HD12	1.94	0.50
9:B:954:GLU:O	10:C:36:ARG:NH1	2.45	0.50
4:c:78:ILE:HA	4:c:82:HIS:HD1	1.77	0.49
8:A:62:ASP:OD1	8:A:62:ASP:N	2.44	0.49
10:C:155:ARG:NH1	14:J:60:LEU:O	2.45	0.49
2:T:77:DT:H4'	9:B:1091:MET:HE1	1.94	0.49
6:a:63:ILE:O	6:a:94:GLN:NE2	2.45	0.49
10:C:70:LEU:HD22	14:J:6:ARG:HD2	1.95	0.49
8:A:1419:LEU:HB2	8:A:1448:GLU:HG2	1.95	0.49
10:C:173:GLU:HG2	16:L:57:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:8:TYR:OH	17:E:12:ARG:NH2	2.45	0.49
4:c:54:VAL:HG21	5:d:96:VAL:HG21	1.95	0.49
8:A:651:GLU:OE2	8:A:1067:ARG:NH1	2.44	0.49
10:C:155:ARG:NH1	14:J:62:TYR:O	2.46	0.49
10:C:256:LYS:NZ	15:K:38:GLU:OE1	2.46	0.49
12:H:115:VAL:HB	12:H:122:MET:HB2	1.93	0.49
9:B:40:LEU:O	9:B:484:ARG:NH1	2.44	0.49
9:B:1114:ASP:N	9:B:1114:ASP:OD1	2.45	0.49
4:g:85:LEU:O	4:g:89:ASN:ND2	2.46	0.49
8:A:1245:ASP:OD1	8:A:1245:ASP:N	2.45	0.49
9:B:730:MET:HA	9:B:733:GLN:HG3	1.94	0.49
3:N:-44:DG:OP1	4:c:32:ARG:NH1	2.46	0.49
4:c:65:LEU:HB3	4:c:86:ALA:HB1	1.95	0.49
9:B:272:ILE:HG23	9:B:312:VAL:HG11	1.94	0.49
12:H:7:GLU:OE2	12:H:57:ARG:NH2	2.45	0.49
6:e:61:LEU:HD13	6:e:94:GLN:HG2	1.94	0.49
9:B:490:ILE:O	9:B:492:ARG:NH1	2.46	0.49
5:h:108:ALA:HA	5:h:111:GLU:HG2	1.94	0.48
4:g:104:GLN:NE2	6:a:95:GLU:OE2	2.47	0.48
8:A:1154:GLU:OE2	8:A:1216:LYS:NZ	2.46	0.48
10:C:11:ILE:HG12	10:C:21:PHE:HB3	1.96	0.48
10:C:27:GLU:HB2	10:C:30:VAL:HG23	1.94	0.48
15:K:58:PHE:O	15:K:75:ILE:HA	2.13	0.48
4:g:88:ARG:NH2	4:g:100:VAL:O	2.44	0.48
5:d:90:ARG:NH2	7:b:75:GLU:O	2.46	0.48
8:A:392:ASP:OD1	8:A:392:ASP:N	2.45	0.48
9:B:796:VAL:HG12	9:B:969:ILE:HG22	1.95	0.48
2:T:16:DA:H1'	2:T:17:DA:C8	2.49	0.48
5:d:94:THR:HG21	7:b:76:HIS:HB2	1.95	0.48
6:e:80:LYS:HD3	6:e:83:LEU:HD21	1.96	0.48
8:A:1466:LEU:HB2	11:F:108:ILE:HB	1.95	0.48
8:A:1042:CYS:SG	8:A:1043:THR:N	2.87	0.48
12:H:4:VAL:HG13	12:H:59:VAL:HG13	1.95	0.48
4:c:29:ARG:HG3	4:c:32:ARG:HH12	1.79	0.48
9:B:99:HIS:HB2	9:B:109:MET:HE2	1.96	0.48
9:B:624:ARG:HE	9:B:626:LEU:HD21	1.77	0.48
9:B:666:ILE:HG23	9:B:670:GLU:HB3	1.95	0.48
4:c:29:ARG:NH1	5:d:34:SER:O	2.47	0.48
4:c:54:VAL:HG22	5:d:108:ALA:HB1	1.96	0.48
9:B:16:GLU:HB3	9:B:637:LYS:HB3	1.95	0.48
9:B:1117:ARG:HG3	9:B:1150:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:76:ILE:HD12	11:F:82:ILE:HG13	1.96	0.47
10:C:130:VAL:HG22	10:C:133:ARG:HD3	1.96	0.47
2:T:-33:DA:OP2	5:h:84:ARG:NH2	2.44	0.47
9:B:269:PRO:HD2	9:B:272:ILE:HD12	1.96	0.47
5:h:111:GLU:HA	5:h:114:LYS:HG2	1.96	0.47
16:L:24:GLU:OE2	16:L:46:LYS:NZ	2.43	0.47
8:A:114:LEU:O	8:A:147:LYS:NZ	2.46	0.47
8:A:1339:LEU:HD22	8:A:1346:PRO:HA	1.97	0.47
15:K:61:TYR:HA	15:K:72:VAL:O	2.15	0.47
8:A:1140:ALA:HB1	8:A:1325:GLU:HB3	1.96	0.47
6:a:117:ARG:NH1	6:a:119:THR:O	2.48	0.47
8:A:440:ARG:NH1	8:A:441:HIS:O	2.42	0.47
8:A:98:LYS:O	8:A:101:LYS:HB2	2.15	0.47
8:A:549:ARG:O	8:A:553:MET:HB2	2.15	0.47
10:C:88:CYS:HB3	10:C:90:CYS:SG	2.55	0.47
17:E:6:GLU:HB3	17:E:48:PRO:HG2	1.95	0.47
8:A:1471:LYS:HB3	11:F:106:PRO:HB3	1.95	0.47
16:L:23:HIS:ND1	16:L:25:ASN:OD1	2.45	0.47
9:B:420:THR:O	9:B:424:ILE:HB	2.15	0.46
3:N:-54:DC:OP1	4:c:77:ARG:NH1	2.48	0.46
8:A:476:MET:SD	8:A:476:MET:N	2.88	0.46
9:B:858:PRO:HG2	16:L:47:ARG:HA	1.98	0.46
8:A:1458:MET:HE1	9:B:1100:GLY:HA2	1.98	0.46
9:B:290:ILE:HD12	9:B:298:MET:HG2	1.96	0.46
10:C:51:GLN:OE1	10:C:163:ARG:NH2	2.48	0.46
10:C:80:GLU:HG2	10:C:81:ARG:HG3	1.98	0.46
8:A:421:LEU:HD13	8:A:425:PRO:HG3	1.97	0.46
8:A:782:GLN:HA	8:A:814:PHE:HA	1.98	0.46
8:A:1198:ARG:HH21	8:A:1257:GLU:H	1.62	0.46
1:R:37:A:H2'	1:R:38:A:H8	1.81	0.46
8:A:93:ILE:O	8:A:96:ILE:HB	2.15	0.46
9:B:408:LEU:HB3	9:B:441:ILE:HG12	1.96	0.46
10:C:7:PRO:HG2	15:K:104:ARG:HE	1.80	0.46
7:f:60:LYS:O	7:f:64:GLU:HB2	2.15	0.46
8:A:1022:SER:OG	17:E:162:ARG:NE	2.47	0.46
8:A:1199:ILE:HD12	8:A:1252:ARG:HD3	1.98	0.46
9:B:649:TYR:HD2	9:B:650:ASN:HD22	1.63	0.46
8:A:257:VAL:HA	8:A:262:ALA:HA	1.98	0.46
8:A:622:VAL:HG21	8:A:644:LEU:HD11	1.97	0.46
8:A:1169:TYR:O	13:I:55:ASN:ND2	2.47	0.46
9:B:259:ALA:HB2	9:B:270:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:469:LEU:HD23	15:K:67:LEU:HD12	1.98	0.46
9:B:193:LYS:HE3	9:B:450:ALA:HA	1.97	0.46
8:A:1153:LEU:HD22	8:A:1338:VAL:HG22	1.96	0.46
9:B:385:ASP:HB3	9:B:388:HIS:HB2	1.98	0.46
9:B:739:ILE:HG21	9:B:745:ARG:HD3	1.98	0.46
9:B:910:MET:HE1	16:L:42:ILE:HG23	1.98	0.46
7:f:88:VAL:HG23	7:f:98:LEU:HB3	1.97	0.45
12:H:82:GLY:N	12:H:86:ASP:OD2	2.47	0.45
17:E:19:GLN:OE1	17:E:138:ASN:ND2	2.49	0.45
8:A:21:ILE:HD11	8:A:1436:ALA:HA	1.98	0.45
8:A:1210:ARG:NH2	8:A:1244:ALA:O	2.40	0.45
2:T:10:DC:H5'	6:a:41:ARG:HG3	1.99	0.45
5:d:44:LYS:HD3	5:d:44:LYS:HA	1.77	0.45
12:H:111:LEU:HB3	12:H:131:LEU:HD12	1.98	0.45
16:L:18:CYS:HA	16:L:43:MET:HG2	1.97	0.45
8:A:592:VAL:HB	8:A:625:GLY:HA2	1.98	0.45
5:h:44:LYS:HA	5:h:44:LYS:HD3	1.81	0.45
8:A:189:ASP:OD1	8:A:189:ASP:N	2.47	0.45
9:B:133:LYS:O	9:B:140:PRO:HA	2.16	0.45
16:L:18:CYS:SG	16:L:21:CYS:HB2	2.56	0.45
9:B:129:ILE:HB	9:B:145:HIS:HB2	1.98	0.45
9:B:237:TRP:HB2	9:B:260:ILE:HB	1.98	0.45
10:C:52:LEU:HD23	10:C:162:LEU:HB3	1.99	0.45
3:N:-5:DG:OP1	6:a:43:ARG:NH2	2.49	0.45
6:a:71:LEU:HD11	7:b:60:LYS:HE3	1.98	0.45
8:A:103:LEU:HD21	8:A:213:VAL:HG13	1.99	0.45
8:A:1346:PRO:HB3	17:E:137:ILE:HD12	1.99	0.45
8:A:350:ARG:NE	9:B:1078:GLU:OE2	2.49	0.45
13:I:69:LEU:O	13:I:126:ARG:NE	2.41	0.45
2:T:-13:DA:OP1	7:f:37:ARG:NH1	2.45	0.45
4:c:22:GLY:HA3	5:d:118:LYS:HE2	1.98	0.45
8:A:373:PRO:HB3	8:A:472:SER:HA	1.99	0.45
10:C:206:LYS:NZ	10:C:216:GLN:O	2.48	0.45
8:A:1058:GLU:HA	8:A:1061:VAL:HG12	1.98	0.44
9:B:750:ALA:HB3	9:B:813:TYR:HB2	1.99	0.44
9:B:1062:HIS:NE2	9:B:1084:GLY:O	2.48	0.44
15:K:102:GLU:HG2	15:K:106:LYS:HD2	1.99	0.44
6:e:124:ASP:OD1	6:a:114:HIS:NE2	2.43	0.44
8:A:1240:ASN:HB2	8:A:1248:VAL:H	1.82	0.44
9:B:742:PHE:O	9:B:924:ARG:NH1	2.50	0.44
2:T:-44:DA:H3'	4:g:28:GLY:HA3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:863:VAL:HB	8:A:1080:GLY:HA3	1.99	0.44
8:A:1198:ARG:NH2	8:A:1258:GLU:OE1	2.48	0.44
8:A:1009:LEU:HD13	8:A:1034:GLN:HG2	1.99	0.44
13:I:79:ASP:O	13:I:84:ARG:NH1	2.39	0.44
17:E:41:LYS:HG2	17:E:46:ASP:HB3	1.99	0.44
8:A:356:ARG:HD2	9:B:1086:LEU:HD11	1.99	0.44
12:H:93:TYR:HH	12:H:139:HIS:CE1	2.35	0.44
11:F:60:MET:HE2	11:F:65:ARG:HD3	2.00	0.44
3:N:-47:DC:H2''	3:N:-46:DT:C5	2.52	0.43
7:b:32:LYS:HD3	7:b:36:ARG:HH21	1.82	0.43
8:A:1090:PRO:HB3	8:A:1383:LEU:HD13	2.00	0.43
8:A:726:ARG:HH21	13:I:109:GLU:HB2	1.83	0.43
9:B:131:LYS:HD2	9:B:432:LEU:HD21	2.00	0.43
2:T:-44:DA:OP1	4:g:32:ARG:NH1	2.43	0.43
8:A:593:ASN:HA	8:A:622:VAL:O	2.18	0.43
9:B:126:TYR:HB3	9:B:147:LYS:HA	2.01	0.43
9:B:240:MET:HE1	9:B:377:SER:HB3	2.00	0.43
10:C:103:LEU:HB3	10:C:162:LEU:HG	2.01	0.43
14:J:8:PHE:H	14:J:48:MET:HE3	1.83	0.43
3:N:35:DT:H2''	3:N:36:DA:C8	2.53	0.43
8:A:479:SER:HB3	8:A:527:MET:HB2	2.00	0.43
8:A:921:LEU:HA	8:A:924:LYS:HG2	2.00	0.43
8:A:984:LYS:HA	8:A:984:LYS:HD3	1.88	0.43
6:a:118:VAL:HB	7:b:45:LYS:HD3	2.01	0.43
9:B:618:ASP:N	9:B:618:ASP:OD1	2.50	0.43
12:H:117:PHE:HB2	12:H:120:LEU:HB2	2.01	0.43
8:A:351:VAL:HG11	9:B:1108:ARG:HD3	2.01	0.43
10:C:57:THR:OG1	10:C:58:VAL:N	2.50	0.43
8:A:545:VAL:HA	12:H:24:ARG:HH21	1.83	0.43
9:B:554:LEU:HG	9:B:576:GLY:HA2	2.00	0.43
9:B:623:CYS:HA	9:B:667:ASP:HA	2.00	0.43
9:B:680:PRO:HA	9:B:683:LEU:HD13	2.01	0.43
9:B:715:PHE:HB3	9:B:718:HIS:HD2	1.83	0.43
11:F:72:ARG:HG2	11:F:105:ILE:HD13	2.00	0.43
5:d:74:GLU:OE1	5:d:77:ARG:NH2	2.52	0.43
8:A:907:SER:O	8:A:911:ARG:CB	2.67	0.43
9:B:554:LEU:HD23	9:B:557:ILE:HD11	1.99	0.43
8:A:1139:ALA:HB2	8:A:1145:LYS:HD2	1.99	0.43
1:R:45:A:H5'	9:B:733:GLN:HE22	1.84	0.43
2:T:6:DC:H6	2:T:6:DC:H2'	1.68	0.43
4:c:97:LEU:HD22	4:c:100:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1075:PRO:HD2	11:F:61:THR:HG21	2.01	0.43
9:B:730:MET:HE3	9:B:944:LYS:HD3	2.01	0.43
10:C:173:GLU:O	15:K:6:THR:OG1	2.31	0.43
4:g:17:ARG:HH21	4:g:28:GLY:HA2	1.84	0.42
9:B:1091:MET:SD	9:B:1091:MET:N	2.91	0.42
4:g:97:LEU:HD23	4:g:100:VAL:HG11	2.01	0.42
8:A:152:GLY:HA3	8:A:175:GLY:N	2.34	0.42
5:d:105:ALA:O	5:d:109:VAL:N	2.52	0.42
9:B:523:LEU:O	9:B:525:LYS:NZ	2.43	0.42
9:B:798:LEU:HD13	9:B:803:VAL:HG21	2.00	0.42
15:K:80:ASP:OD1	15:K:80:ASP:N	2.52	0.42
2:T:85:DC:OP1	9:B:446:ARG:NH1	2.52	0.42
8:A:886:ASP:HB3	17:E:200:ALA:HB2	2.01	0.42
8:A:894:GLU:OE2	8:A:974:ASN:N	2.52	0.42
4:g:114:VAL:O	4:g:118:LYS:NZ	2.49	0.42
9:B:218:PHE:HB2	9:B:240:MET:HE3	2.01	0.42
9:B:1107:GLU:HG2	9:B:1108:ARG:HE	1.84	0.42
2:T:9:DG:H3'	6:a:47:VAL:HG21	2.01	0.42
5:h:115:ALA:HA	5:h:118:LYS:HG2	2.01	0.42
8:A:157:ASP:OD1	8:A:157:ASP:N	2.53	0.42
8:A:285:ASN:ND2	8:A:298:ASN:OD1	2.40	0.42
8:A:1204:LEU:HB3	8:A:1251:ILE:HB	2.01	0.42
14:J:43:TYR:HA	14:J:46:ARG:HD3	2.00	0.42
2:T:80:DT:H5''	9:B:1080:ARG:HG3	2.02	0.42
8:A:815:VAL:HG22	8:A:827:GLU:HB2	2.02	0.42
8:A:1357:ILE:HG23	8:A:1361:LEU:HD12	2.01	0.42
9:B:996:GLY:HA2	14:J:50:LEU:HD11	2.02	0.42
8:A:620:VAL:HA	8:A:630:GLY:HA3	2.02	0.42
9:B:225:CYS:HB3	9:B:233:THR:HG23	2.01	0.42
10:C:5:ASN:OD1	15:K:52:LYS:NZ	2.44	0.42
10:C:23:LEU:HD22	15:K:104:ARG:HH12	1.85	0.42
3:N:-5:DG:H5'	6:a:43:ARG:HH21	1.85	0.42
3:N:55:DC:H2''	3:N:56:DG:C8	2.54	0.42
6:a:127:LEU:HA	6:a:130:ARG:HE	1.83	0.42
7:f:85:MET:HA	7:f:88:VAL:HG12	2.01	0.42
8:A:1112:GLY:O	8:A:1113:VAL:C	2.59	0.42
6:e:117:ARG:NH1	6:e:119:THR:O	2.53	0.42
9:B:247:ASN:HB2	9:B:250:LYS:HB2	2.02	0.42
4:g:87:ILE:HG23	4:g:93:LEU:HB3	2.02	0.41
8:A:1293:ILE:HD13	8:A:1296:ILE:HD12	2.02	0.41
8:A:405:TYR:OH	8:A:442:LEU:O	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:868:ASP:OD1	8:A:868:ASP:N	2.50	0.41
8:A:995:ASP:OD1	8:A:995:ASP:N	2.52	0.41
5:d:34:SER:OG	5:d:35:TYR:N	2.52	0.41
9:B:405:PHE:O	9:B:409:PHE:HB2	2.20	0.41
3:N:-13:DA:OP2	7:b:37:ARG:NH1	2.38	0.41
8:A:557:MET:SD	8:A:557:MET:N	2.94	0.41
8:A:855:ARG:HB3	8:A:1406:ILE:HG22	2.02	0.41
4:c:63:LEU:HD12	5:d:42:VAL:HG12	2.03	0.41
8:A:907:SER:HA	8:A:910:LYS:HG2	2.03	0.41
8:A:1218:LEU:HD13	8:A:1223:ILE:HD11	2.03	0.41
9:B:197:ALA:HA	9:B:395:ASP:O	2.20	0.41
4:g:54:VAL:HG22	5:h:108:ALA:HB1	2.01	0.41
17:E:44:PHE:HB3	17:E:53:PRO:HB3	2.02	0.41
8:A:1406:ILE:HG23	8:A:1411:ILE:HD11	2.03	0.41
9:B:381:ARG:NH1	9:B:612:GLU:OE2	2.53	0.41
9:B:912:THR:OG1	9:B:913:LEU:N	2.52	0.41
4:c:39:TYR:HB3	5:d:76:SER:HB2	2.01	0.41
8:A:456:LEU:HD13	8:A:1092:THR:HG21	2.02	0.41
8:A:954:ASP:OD2	8:A:1038:ARG:NE	2.44	0.41
9:B:247:ASN:HD22	9:B:247:ASN:HA	1.74	0.41
9:B:720:GLN:HG2	9:B:722:PRO:HD2	2.02	0.41
4:c:80:PRO:HG2	5:d:55:LYS:HG3	2.02	0.41
8:A:280:ASN:HA	8:A:283:ARG:HG2	2.03	0.41
8:A:314:MET:O	8:A:319:ARG:NH1	2.45	0.41
8:A:1013:VAL:HG12	8:A:1026:ASN:HD21	1.85	0.41
8:A:1203:LEU:HD21	8:A:1250:ARG:HG2	2.02	0.41
8:A:1240:ASN:ND2	8:A:1246:LYS:O	2.54	0.41
14:J:25:LEU:HD21	14:J:31:GLU:HG3	2.03	0.41
15:K:13:TYR:HB2	15:K:16:GLU:HG3	2.02	0.41
17:E:95:GLN:HG3	17:E:125:TYR:HE2	1.85	0.41
2:T:76:DT:H2'	2:T:77:DT:C6	2.56	0.41
8:A:602:PRO:HG2	8:A:605:GLU:HB2	2.03	0.41
8:A:1087:LEU:HD12	8:A:1087:LEU:HA	1.93	0.41
8:A:1447:SER:HA	8:A:1450:ILE:HB	2.03	0.41
5:h:98:LEU:O	7:f:93:ARG:NH2	2.54	0.40
9:B:349:LEU:HD22	9:B:351:HIS:HE1	1.85	0.40
17:E:82:ILE:HB	17:E:110:MET:HG2	2.03	0.40
6:a:129:ARG:HB3	6:a:135:ARG:HG3	2.03	0.40
8:A:222:ASP:HB3	8:A:232:PRO:HG3	2.03	0.40
9:B:224:SER:OG	9:B:351:HIS:ND1	2.41	0.40
9:B:1032:ASN:HB3	9:B:1036:GLY:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:105:CYS:HB3	8:A:113:MET:HE1	2.03	0.40
9:B:19:SER:O	9:B:23:TRP:N	2.52	0.40
9:B:635:LEU:HB3	9:B:662:VAL:HG12	2.04	0.40
8:A:517:ILE:HA	8:A:527:MET:HE1	2.03	0.40
8:A:1335:MET:N	8:A:1335:MET:SD	2.88	0.40
17:E:54:ALA:HB3	17:E:57:ASP:HB2	2.03	0.40
8:A:536:ALA:HB2	8:A:672:LEU:HD13	2.04	0.40
15:K:81:TYR:OH	15:K:89:ASN:OD1	2.36	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	
4	c	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
4	g	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
5	d	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
5	h	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
6	a	98/100 (98%)	98 (100%)	0	0	100	100
6	e	90/100 (90%)	88 (98%)	2 (2%)	0	100	100
7	b	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
7	f	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
8	A	1468/1470 (100%)	1419 (97%)	48 (3%)	1 (0%)	48	83
9	B	1162/1164 (100%)	1120 (96%)	42 (4%)	0	100	100
10	C	267/269 (99%)	254 (95%)	13 (5%)	0	100	100
11	F	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
12	H	145/147 (99%)	135 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	I	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
14	J	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
15	K	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
16	L	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
17	E	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
All	All	4410/4455 (99%)	4264 (97%)	145 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	A	1122	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	c	81/82 (99%)	81 (100%)	0	100	100
4	g	81/82 (99%)	81 (100%)	0	100	100
5	d	80/84 (95%)	80 (100%)	0	100	100
5	h	80/84 (95%)	80 (100%)	0	100	100
6	a	85/87 (98%)	85 (100%)	0	100	100
6	e	79/87 (91%)	79 (100%)	0	100	100
7	b	65/65 (100%)	65 (100%)	0	100	100
7	f	63/65 (97%)	63 (100%)	0	100	100
8	A	1269/1290 (98%)	1269 (100%)	0	100	100
9	B	1003/1015 (99%)	1003 (100%)	0	100	100
10	C	244/244 (100%)	244 (100%)	0	100	100
11	F	74/75 (99%)	74 (100%)	0	100	100
12	H	127/127 (100%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	I	106/108 (98%)	106 (100%)	0	100	100
14	J	56/57 (98%)	56 (100%)	0	100	100
15	K	102/102 (100%)	102 (100%)	0	100	100
16	L	42/42 (100%)	42 (100%)	0	100	100
17	E	190/192 (99%)	190 (100%)	0	100	100
All	All	3827/3888 (98%)	3827 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
4	c	38	ASN
6	a	77	GLN
6	a	109	ASN
7	b	26	ASN
8	A	68	GLN
8	A	173	HIS
8	A	196	HIS
8	A	293	HIS
8	A	345	ASN
8	A	433	GLN
8	A	509	ASN
8	A	523	ASN
8	A	554	ASN
8	A	756	ASN
8	A	1026	ASN
8	A	1070	GLN
8	A	1100	HIS
8	A	1305	GLN
9	B	57	GLN
9	B	501	GLN
9	B	779	ASN
9	B	830	ASN
9	B	1011	GLN
10	C	209	HIS
10	C	216	GLN
10	C	222	ASN
11	F	94	GLN
12	H	129	ASN

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Mol	Chain	Res	Type
12	H	130	ASN
12	H	138	GLN
15	K	36	ASN
15	K	84	GLN
17	E	22	HIS
17	E	157	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/10 (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 8 ligands modelled in this entry, 8 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	-87:DA	O3'	-75:DA	P	23.10

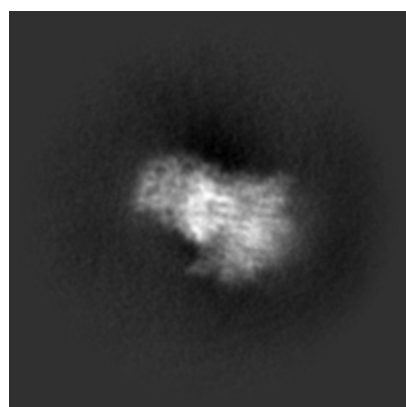
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48626. These allow visual inspection of the internal detail of the map and identification of artifacts.

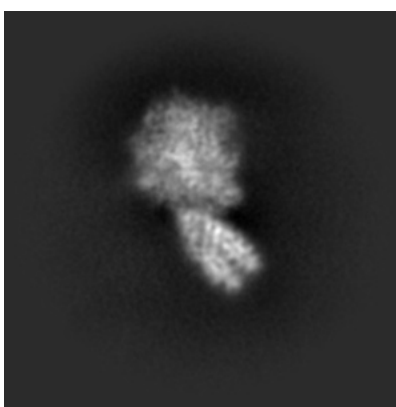
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

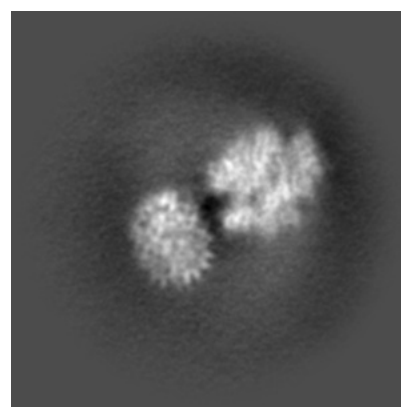
6.1.1 Primary map



X



Y

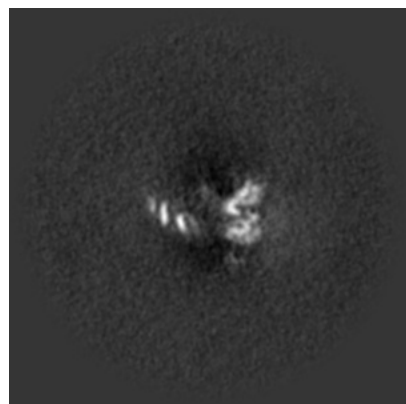


Z

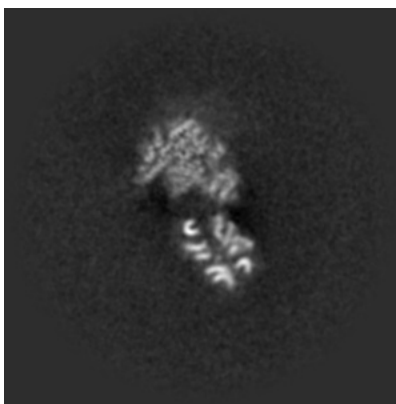
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

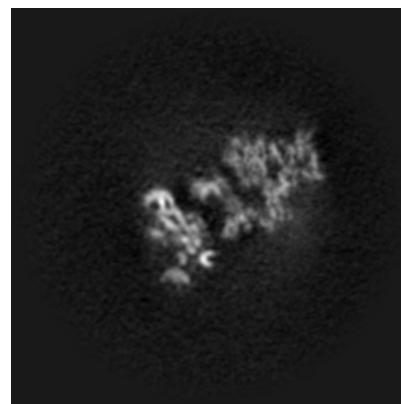
6.2.1 Primary map



X Index: 180



Y Index: 180

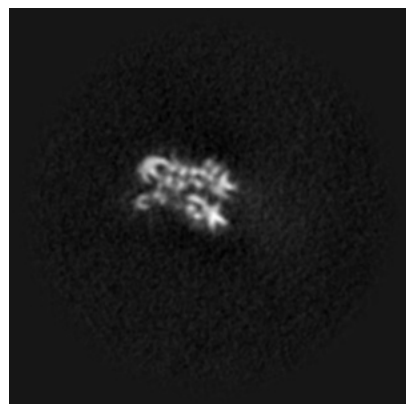


Z Index: 180

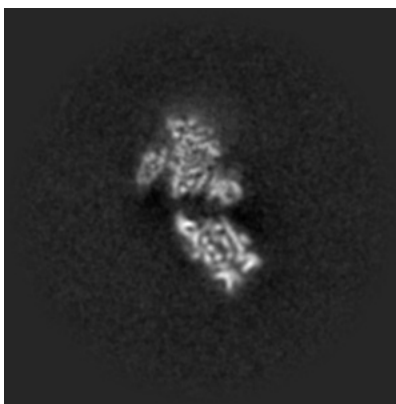
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

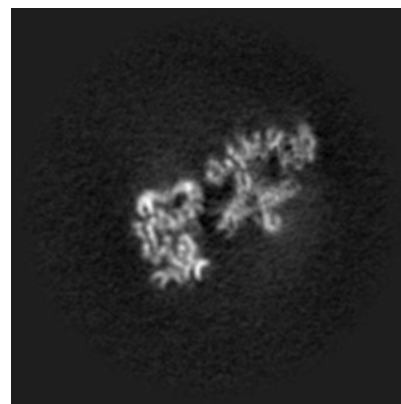
6.3.1 Primary map



X Index: 145



Y Index: 173

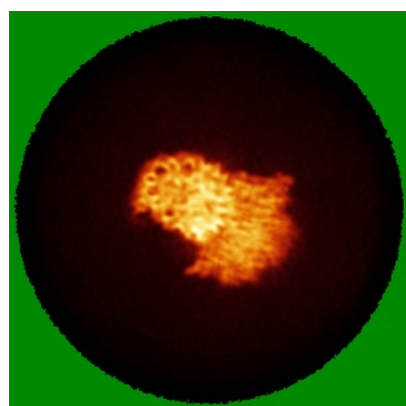


Z Index: 190

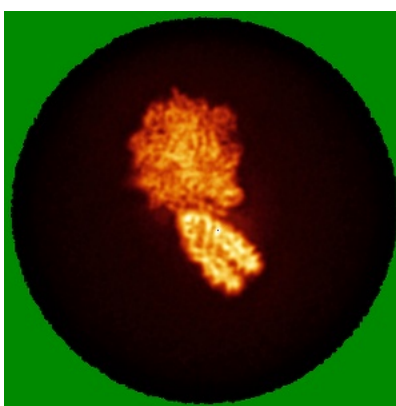
The images above show the largest variance slices of the map in three orthogonal directions.

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

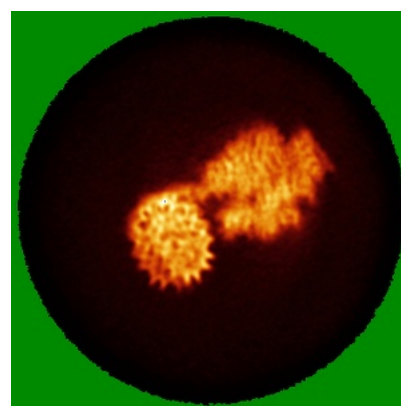
6.4.1 Primary map



X



Y

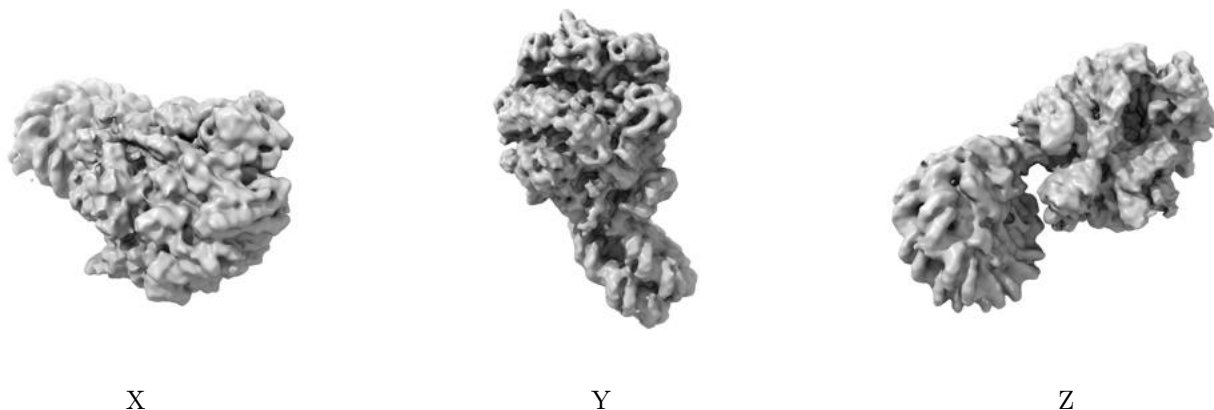


Z

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

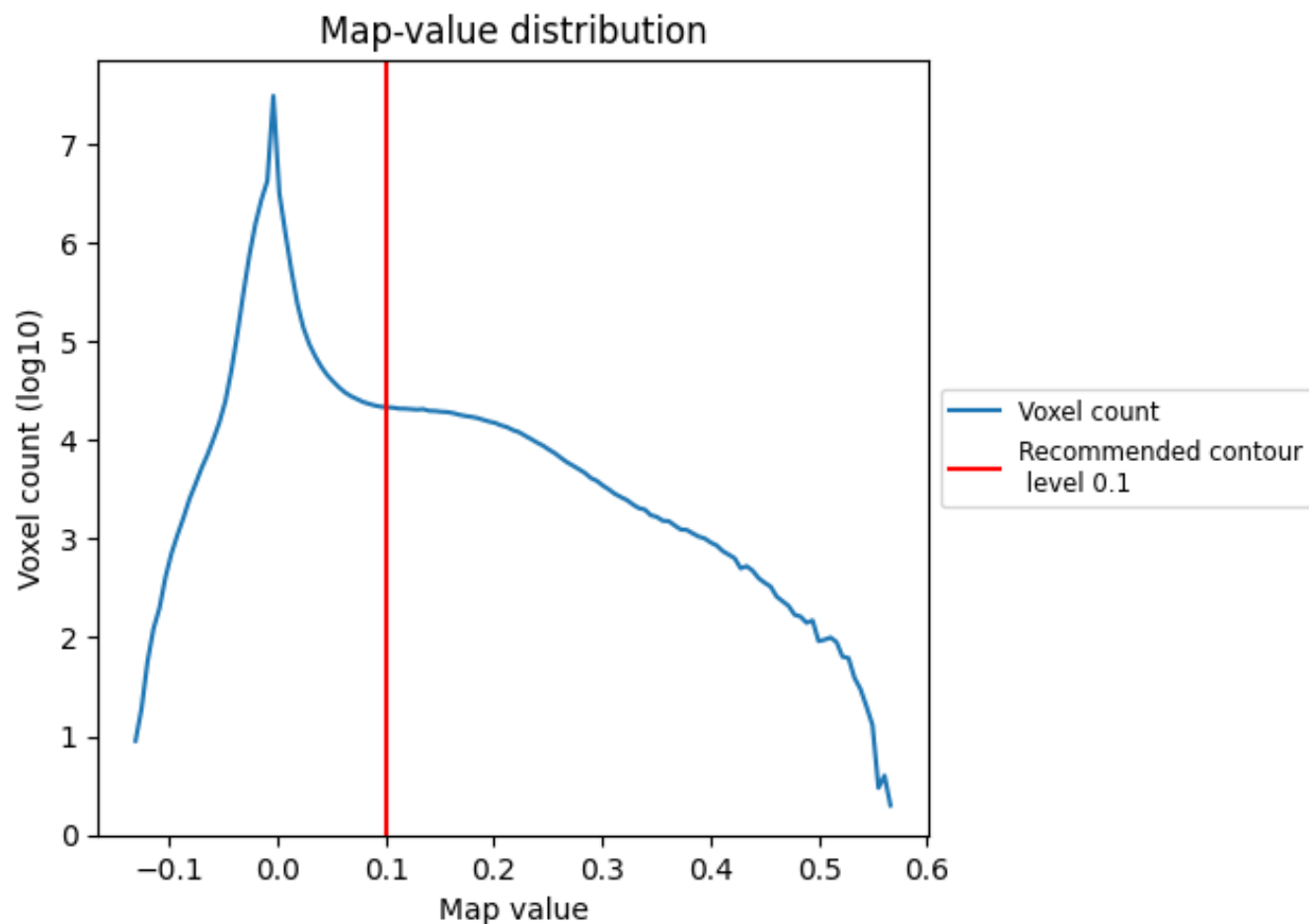
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

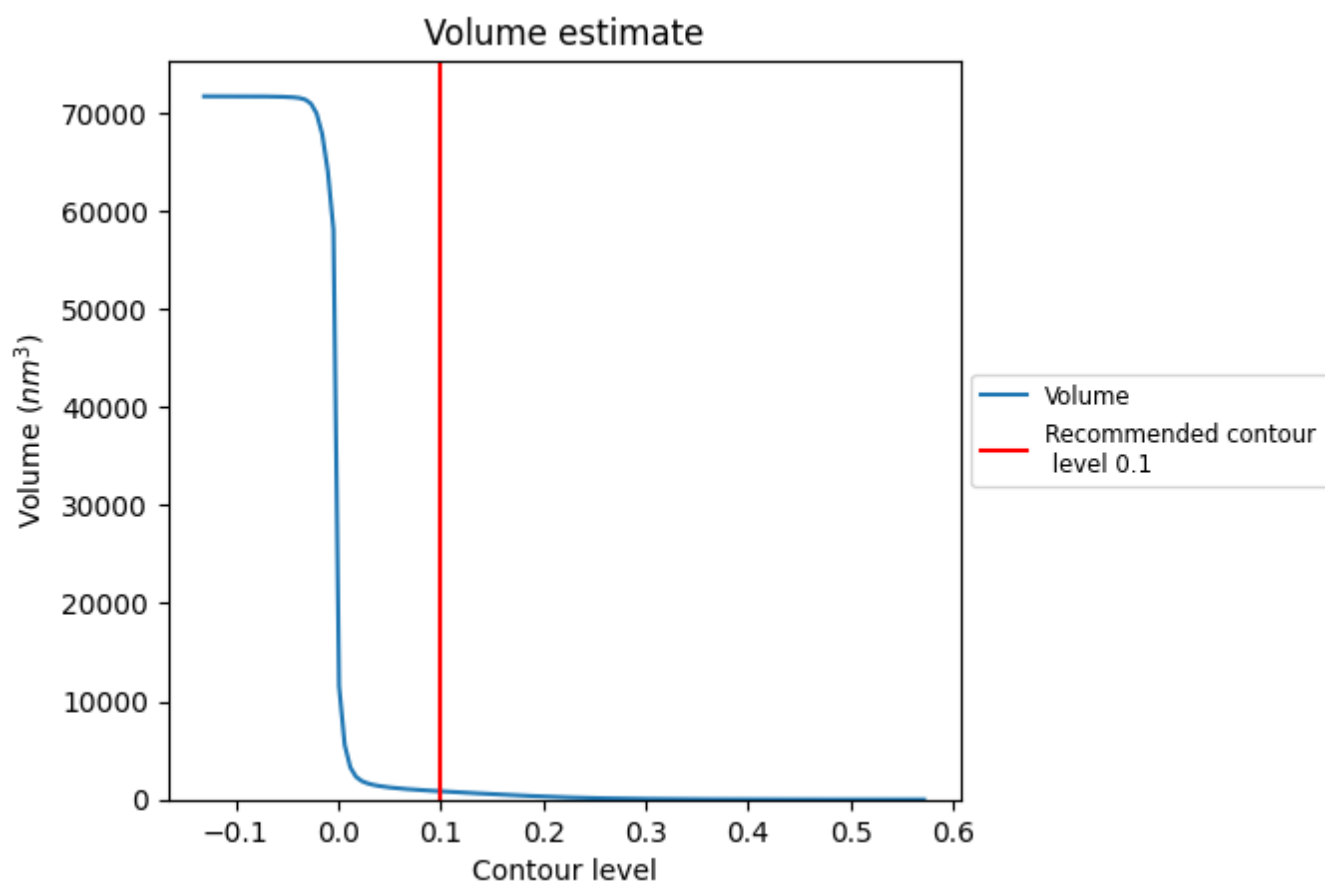
This section contains the results of statistical analysis of the map.

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.

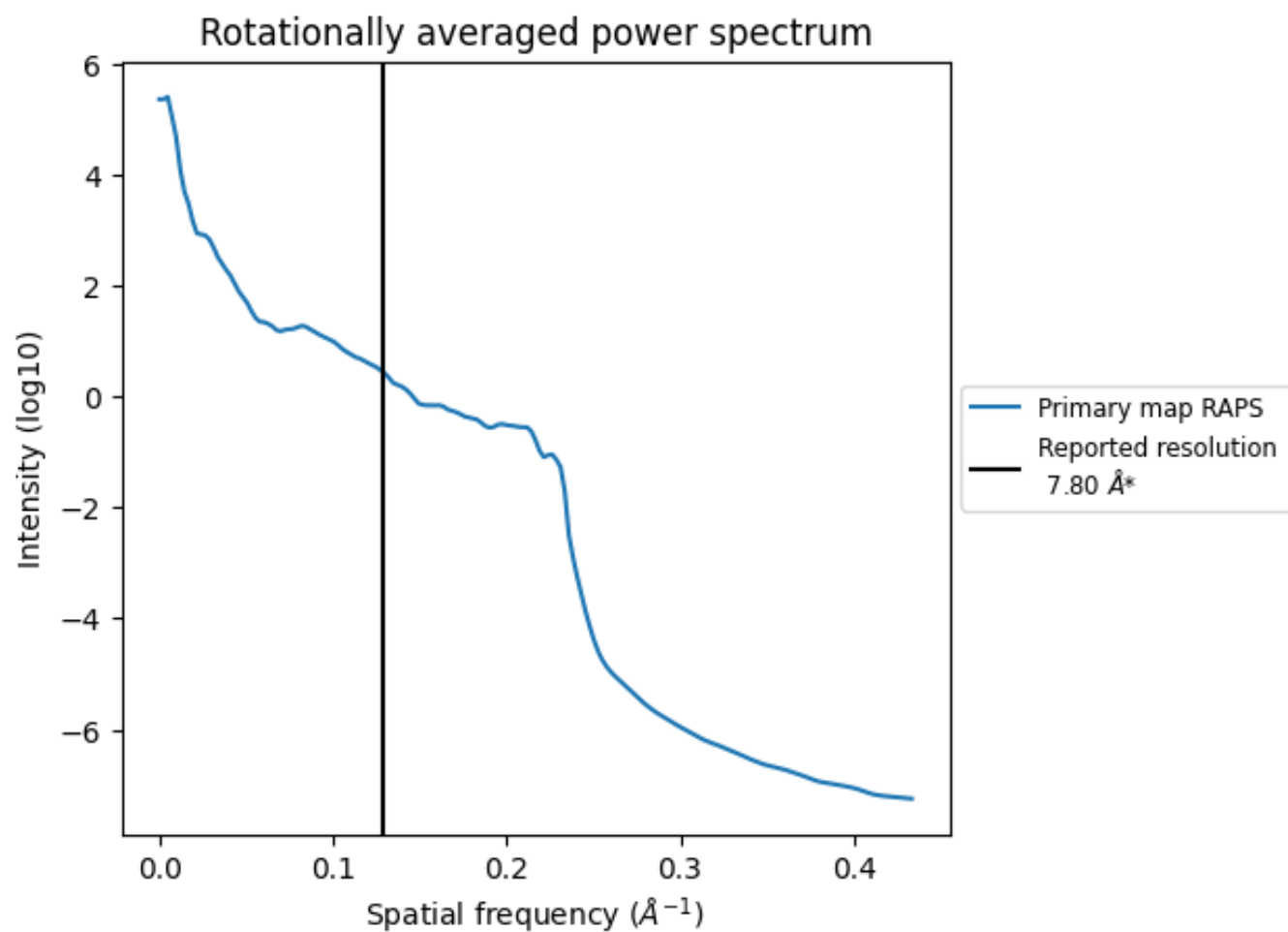
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 844 nm³; this corresponds to an approximate mass of 762 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 0.128 Å⁻¹

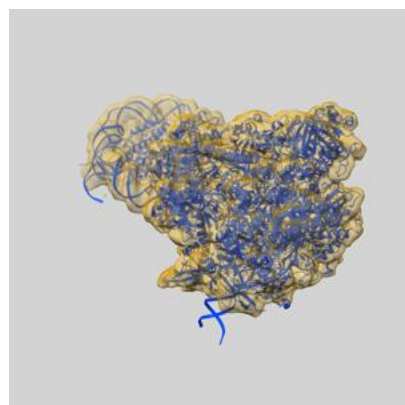
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

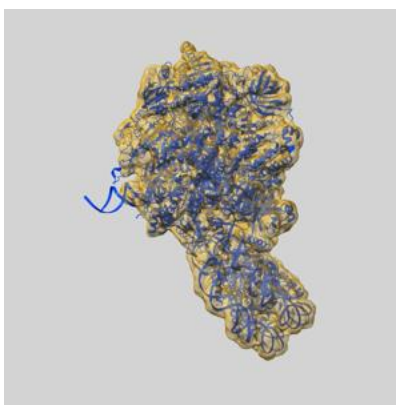
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48626 and PDB model 9MU9. Per-residue inclusion information can be found in section [3](#) on page [8](#).

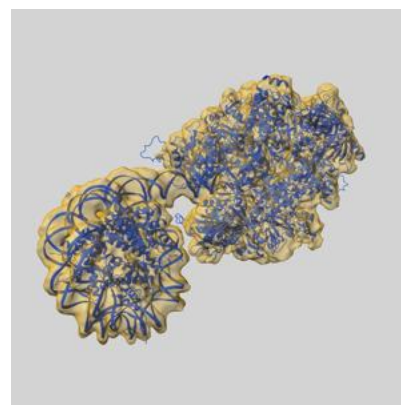
9.1 Map-model overlay [i](#)



X



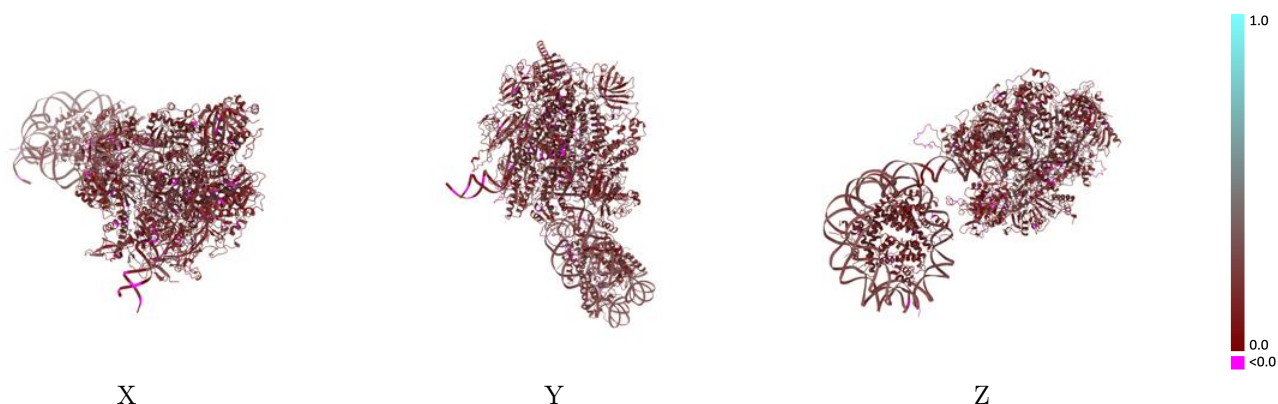
Y



Z

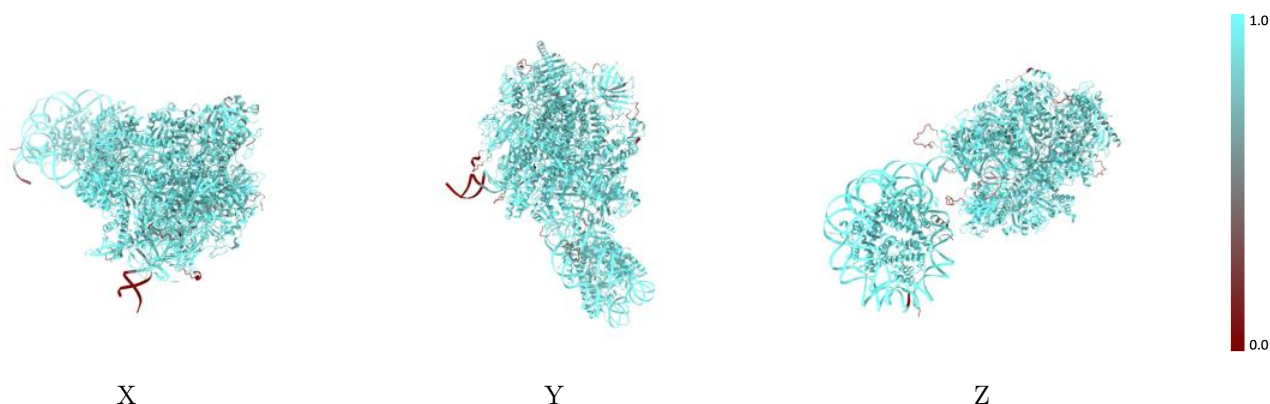
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



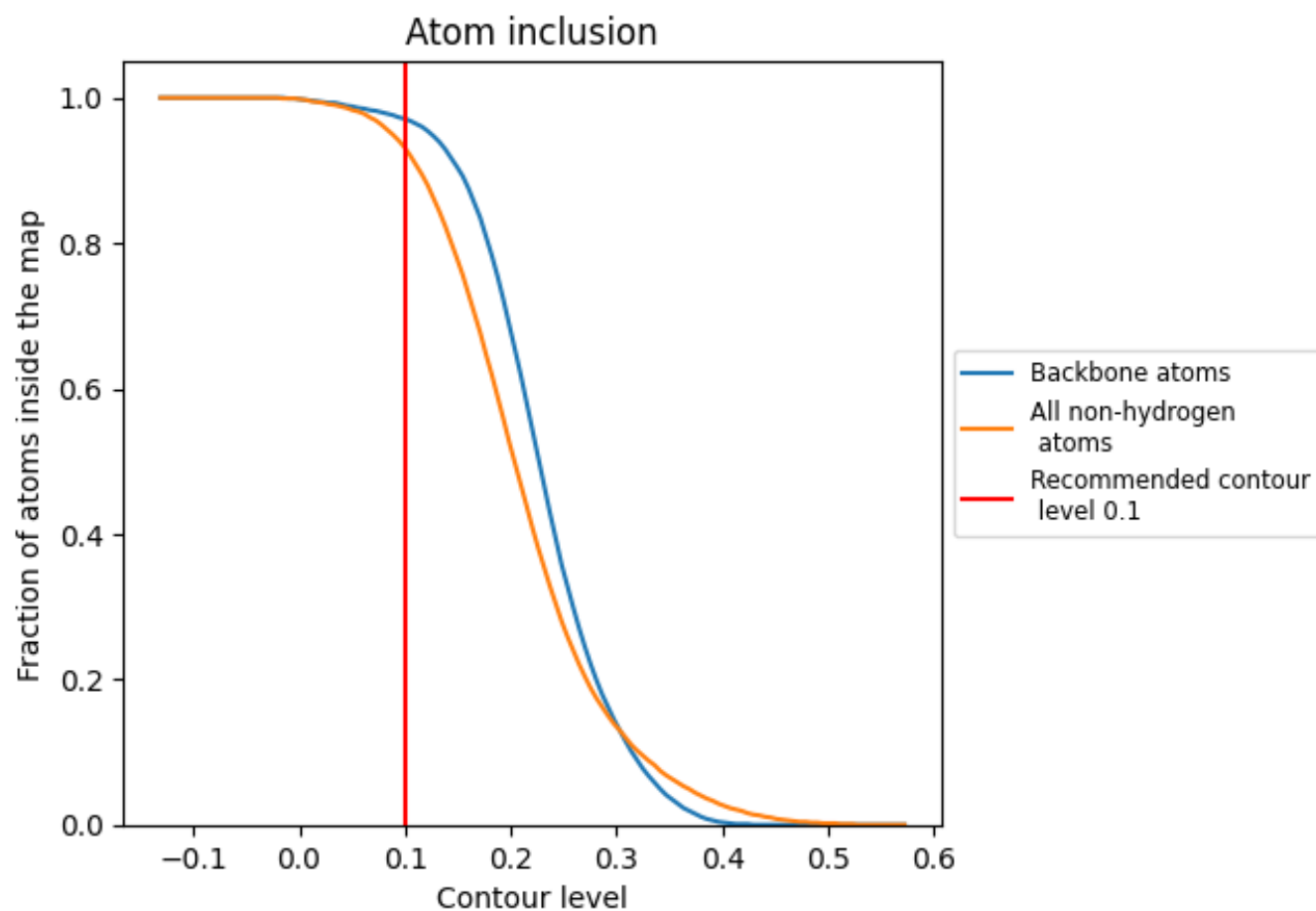
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9310	 0.2020
A	 0.9120	 0.1960
B	 0.9490	 0.1980
C	 0.8550	 0.2050
E	 0.9430	 0.1990
F	 0.9250	 0.1890
H	 0.8280	 0.2100
I	 0.9390	 0.1940
J	 0.9630	 0.2010
K	 0.8540	 0.1960
L	 0.9570	 0.2180
N	 0.9420	 0.2540
R	 1.0000	 0.2790
T	 0.9350	 0.2510
a	 0.9810	 0.1500
b	 0.9890	 0.1440
c	 0.9280	 0.1600
d	 0.9880	 0.1740
e	 0.9630	 0.1510
f	 0.9900	 0.1570
g	 0.9860	 0.1670
h	 0.9990	 0.1720

