



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:00 PM UTC

PDB ID : 6J4W / pdb_00006j4w
EMDB ID : EMD-0671
Title : RNA polymerase II elongation complex bound with Elf1 and Spt4/5, stalled at SHL(-5) of the nucleosome
Authors : Ehara, H.; Kujirai, T.; Fujino, Y.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on : 2019-01-10
Resolution : 7.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

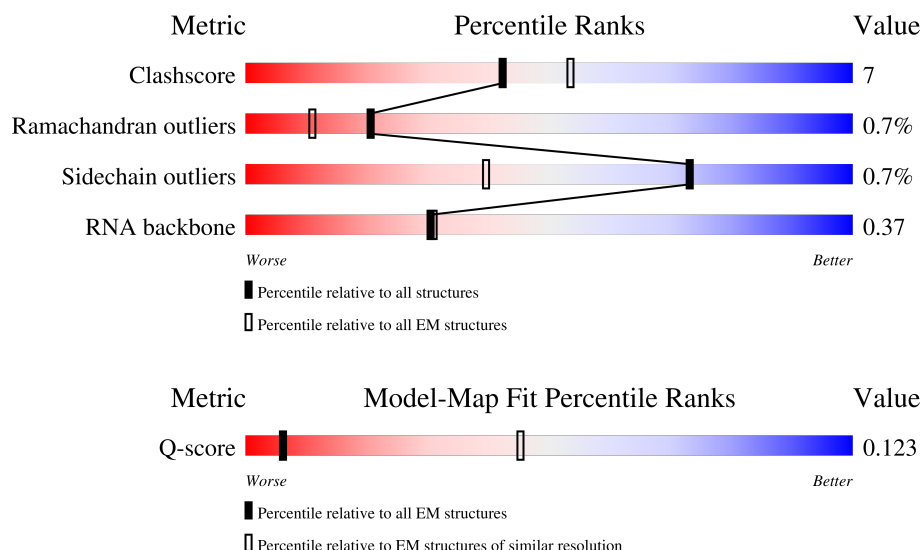
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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

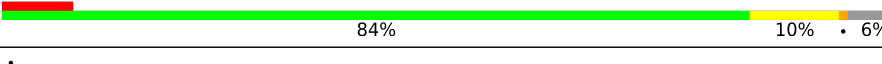
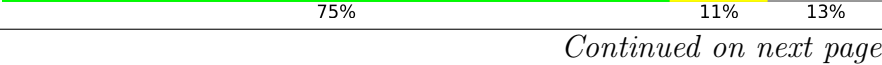
The reported resolution of this entry is 7.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	366 (7.40 - 8.40)

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

Mol	Chain	Length	Quality of chain
1	A	1743	
2	B	1227	
3	C	304	

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Mol	Chain	Length	Quality of chain
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	P	16	
14	T	198	
15	N	198	
16	M	113	
17	V	108	
18	W	911	
19	a	139	
19	e	139	
20	b	106	
20	f	106	
21	c	133	
21	g	133	
22	d	129	
22	h	129	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 48001 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1412	Total	C	N	O	S	0	0
			11123	7014	1938	2101	70		

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

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

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

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

- Molecule 4 is a protein called RNA polymerase II subunit B32.

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

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

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

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

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

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

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

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

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

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

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

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta.

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

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

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

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

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

- Molecule 13 is a RNA chain called RNA (5'-R(P*GP*UP*GP*UP*UP*UP*GP*GP*GP*U P*GP*GP*UP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	16	Total	C	N	O	P	0	0
			347	153	60	118	16		

- Molecule 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	171	Total	C	N	O	P	0	0
			3487	1652	676	989	170		

- Molecule 15 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	165	Total	C	N	O	P	0	0
			3397	1616	592	1024	165		

- Molecule 16 is a protein called Transcription elongation factor 1 homolog.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP C4QZ45
M	-1	PRO	-	expression tag	UNP C4QZ45
M	0	GLY	-	expression tag	UNP C4QZ45

- Molecule 17 is a protein called Transcription elongation factor SPT4.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	7	MET	-	expression tag	UNP C4R0E6

- Molecule 18 is a protein called Spt5.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-2	GLY	-	expression tag	UNP C4R370
W	-1	PRO	-	expression tag	UNP C4R370
W	0	GLY	-	expression tag	UNP C4R370

- Molecule 19 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	97	Total	C	N	O	S	0	0
			797	503	155	137	2		
19	e	97	Total	C	N	O	S	0	0
			796	501	155	138	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P84243
a	-2	SER	-	expression tag	UNP P84243
a	-1	HIS	-	expression tag	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
20	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805

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Chain	Residue	Modelled	Actual	Comment	Reference
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805

- Molecule 21 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	c	103	Total	C	N	O	0	0
			796	502	155	139		
21	g	105	Total	C	N	O	0	0
			810	511	158	141		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908

- Molecule 22 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
22	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899

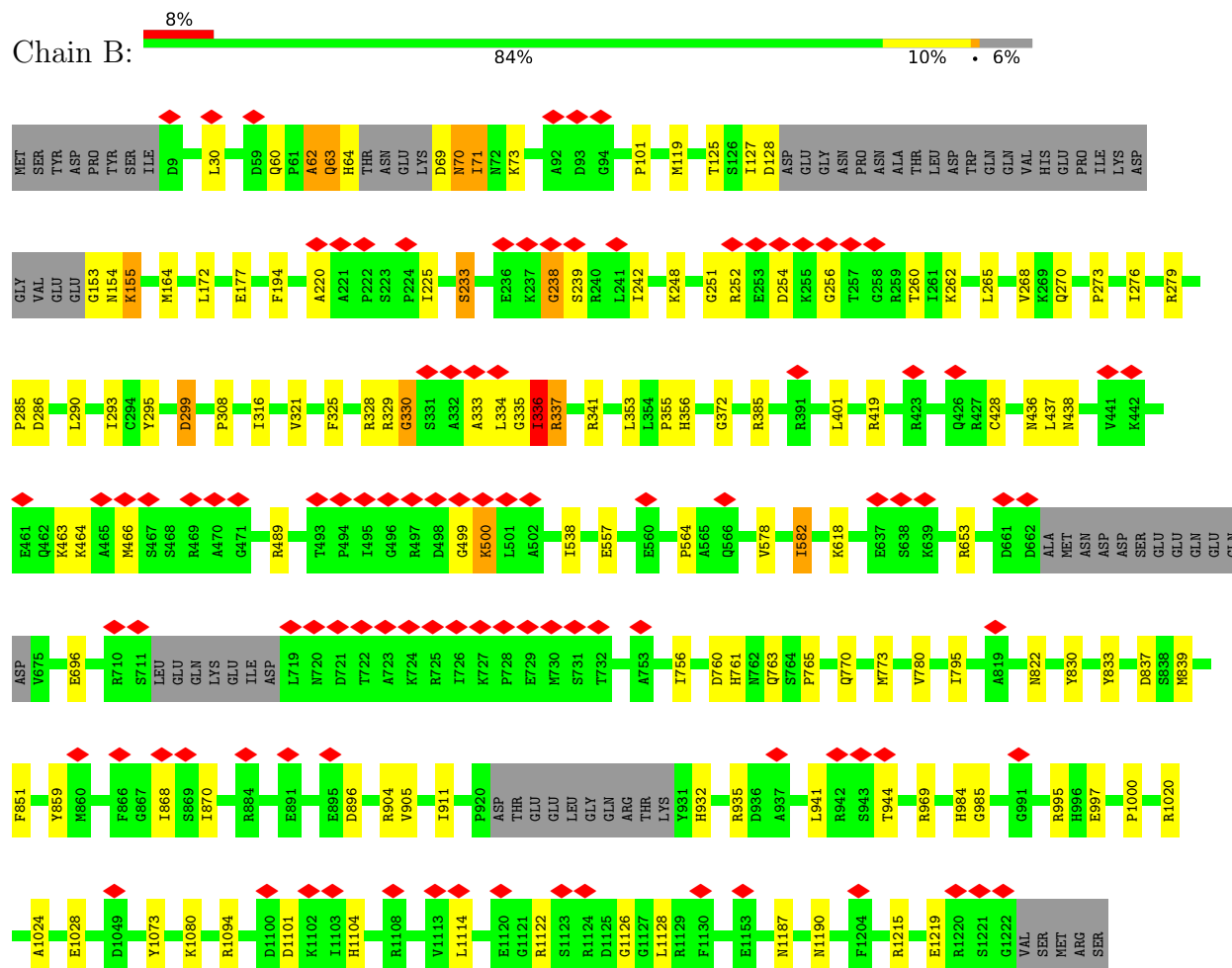
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

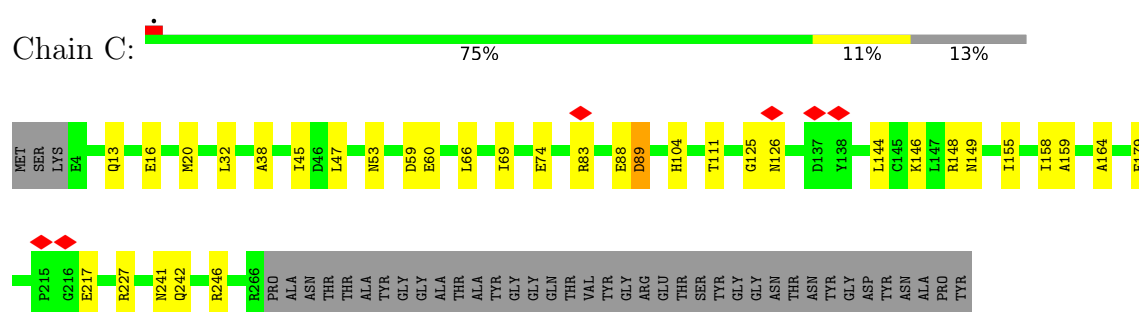
- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

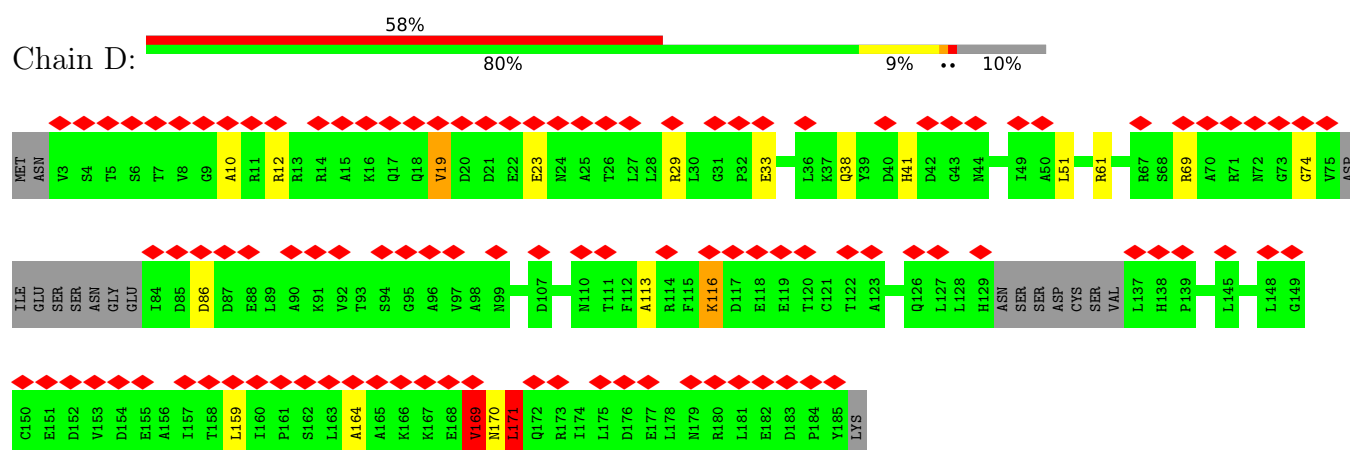
- Molecule 2: DNA-directed RNA polymerase subunit beta



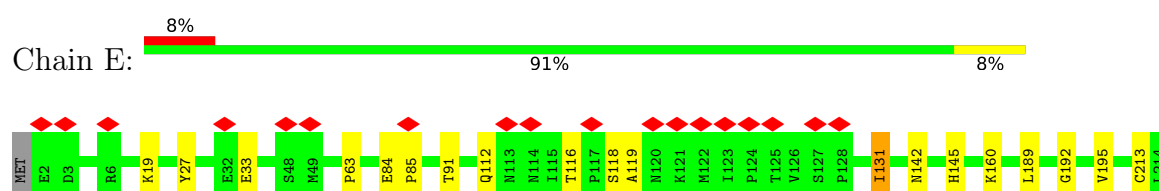
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core



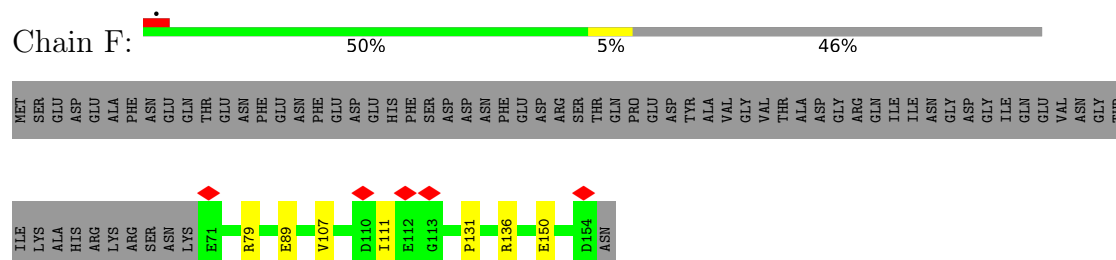
- Molecule 4: RNA polymerase II subunit B32



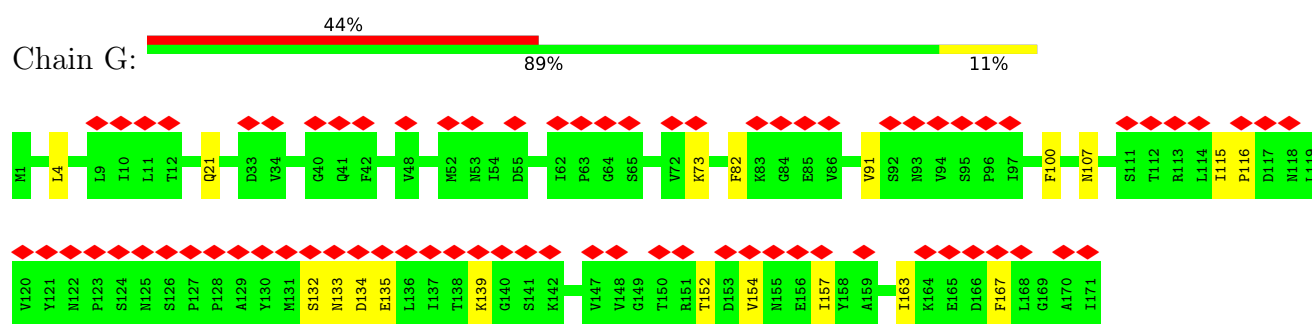
- Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III



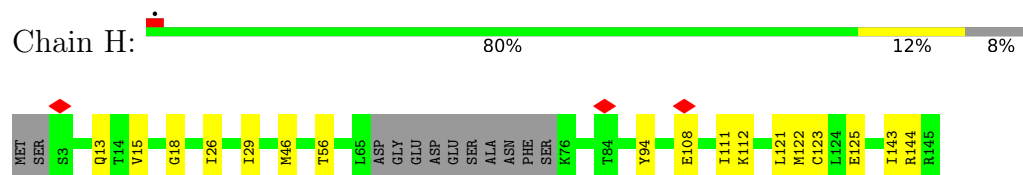
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III



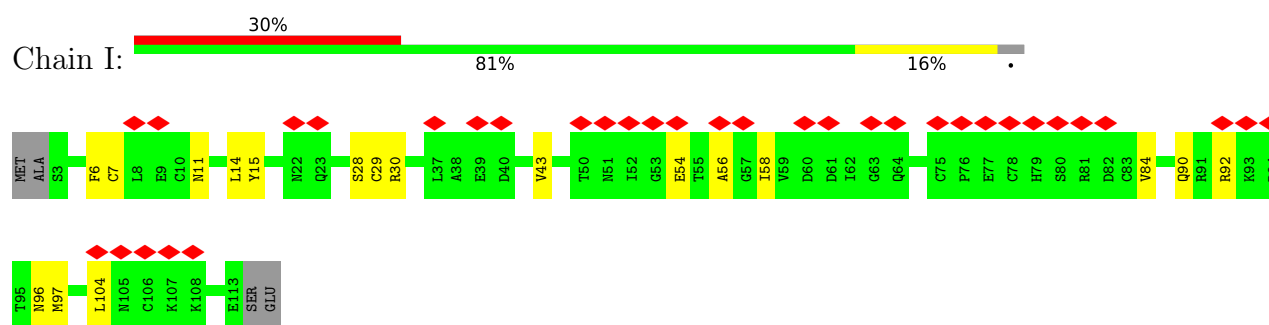
- Molecule 7: RNA polymerase II subunit



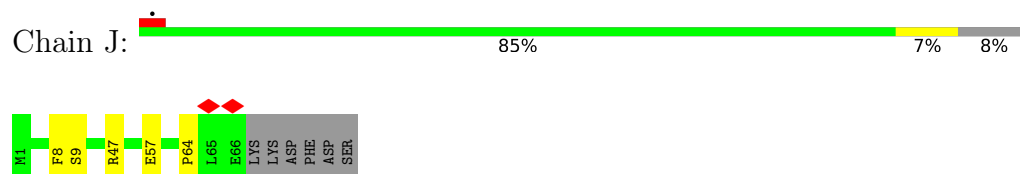
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



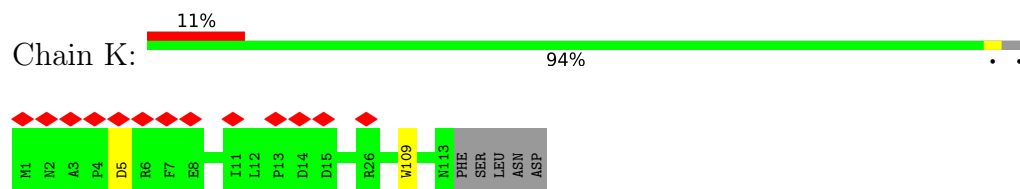
- Molecule 9: DNA-directed RNA polymerase subunit



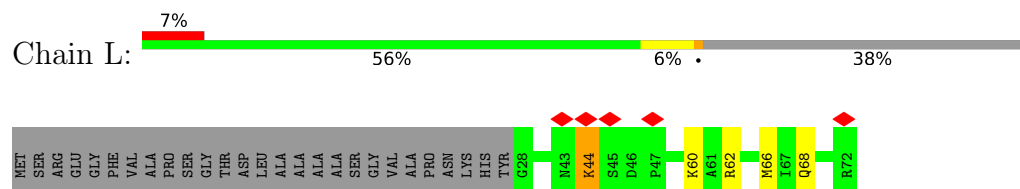
- Molecule 10: RNA polymerase subunit ABC10-beta



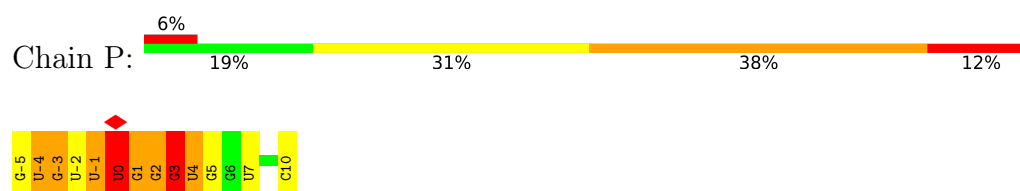
- Molecule 11: RNA polymerase II subunit B12.5



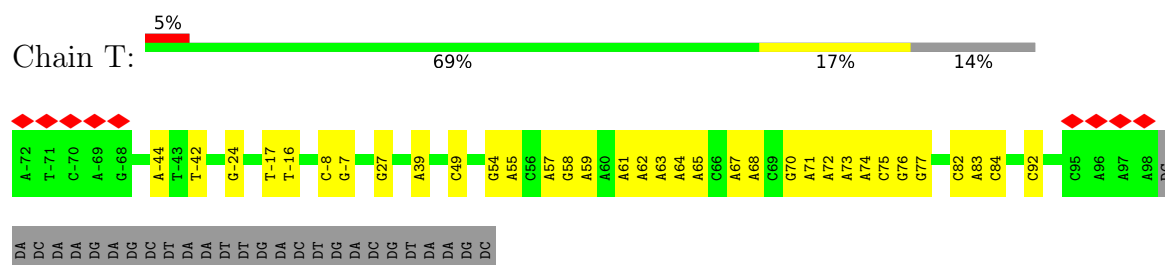
- Molecule 12: RNA polymerase subunit ABC10-alpha



- Molecule 13: RNA (5'-R(P*GP*UP*GP*UP*UP*UP*GP*GP*GP*UP*GP*GP*UP*GP*GP*C)-3')

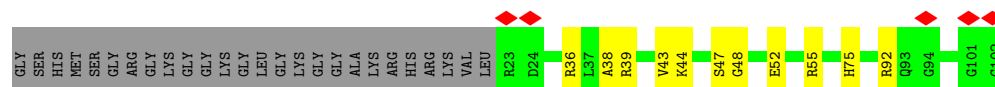


- Molecule 14: DNA (198-MER)

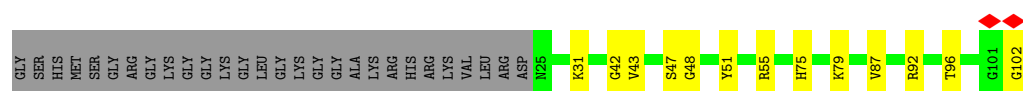




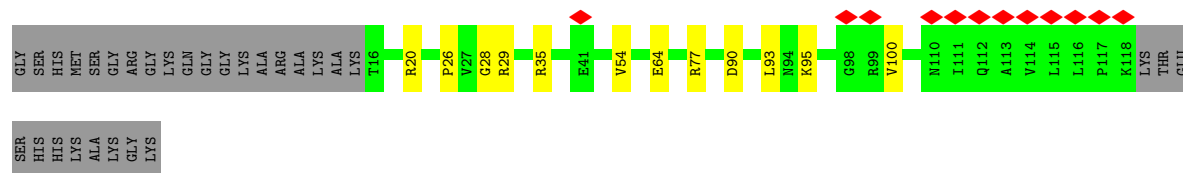
- Molecule 20: Histone H4



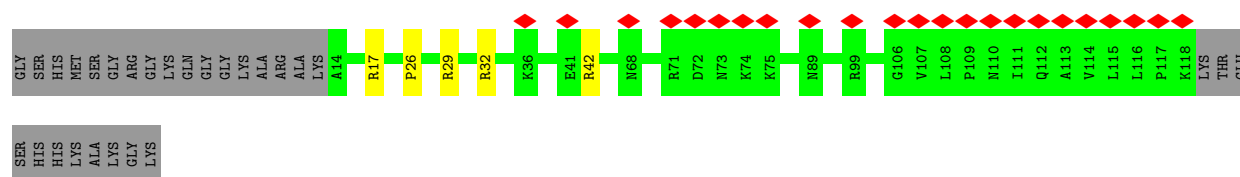
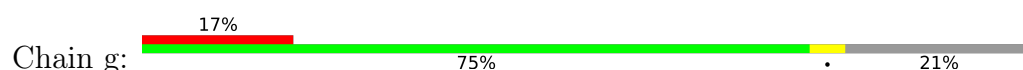
- Molecule 20: Histone H4



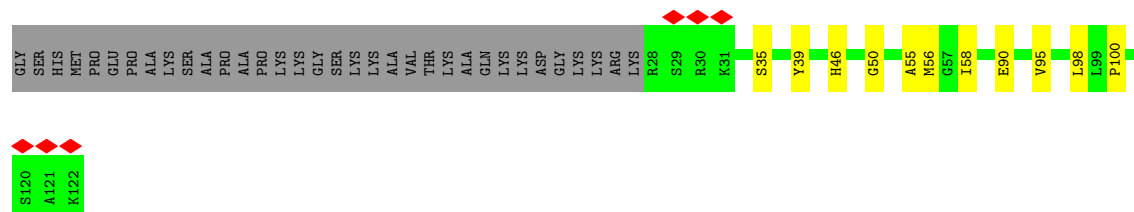
- Molecule 21: Histone H2A type 1-B/E



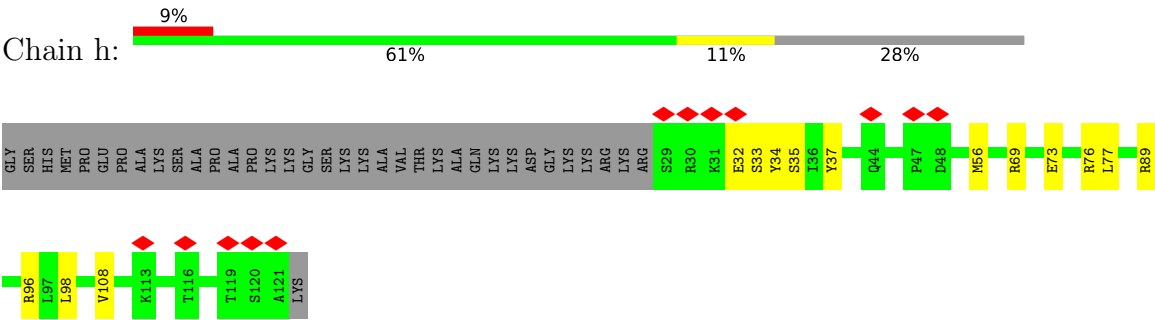
- Molecule 21: Histone H2A type 1-B/E



- Molecule 22: Histone H2B type 1-J



● Molecule 22: Histone H2B type 1-J



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12112	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	357.6, 357.6, 357.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.49, 1.49, 1.49	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/11329	0.74	3/15310 (0.0%)
2	B	0.43	0/9407	0.79	11/12685 (0.1%)
3	C	0.42	0/2139	0.76	4/2895 (0.1%)
4	D	0.30	0/1326	0.79	4/1788 (0.2%)
5	E	0.36	0/1772	0.73	0/2385
6	F	0.39	0/687	0.68	0/931
7	G	0.31	0/1353	0.79	2/1837 (0.1%)
8	H	0.35	0/1069	0.72	0/1444
9	I	0.31	0/934	0.89	4/1257 (0.3%)
10	J	0.46	0/554	0.80	0/742
11	K	0.40	0/953	0.73	0/1291
12	L	0.38	0/365	0.85	1/484 (0.2%)
13	P	1.02	7/387 (1.8%)	0.65	0/603
14	T	0.43	0/3920	0.64	0/6038
15	N	0.43	1/3801 (0.0%)	0.65	0/5872
16	M	0.16	0/513	0.36	0/693
17	V	0.60	2/808 (0.2%)	0.91	1/1097 (0.1%)
18	W	0.50	1/2267 (0.0%)	0.86	3/3048 (0.1%)
19	a	0.30	0/809	0.57	0/1085
19	e	0.33	0/807	0.58	0/1081
20	b	0.32	0/645	0.61	0/862
20	f	0.33	0/626	0.61	0/837
21	c	0.31	0/806	0.55	0/1089
21	g	0.29	0/820	0.54	0/1107
22	d	0.31	0/757	0.54	0/1015
22	h	0.31	0/736	0.54	0/990
All	All	0.41	11/49590 (0.0%)	0.73	33/68466 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	29	CYS	C-N	8.20	1.43	1.33
13	P	2	G	C1'-N9	-7.46	1.36	1.48
18	W	440	ILE	CA-C	-7.41	1.43	1.52
13	P	3	G	C1'-N9	-7.18	1.37	1.48
13	P	4	U	C1'-N1	6.97	1.58	1.48
13	P	-5	G	C1'-N9	-6.83	1.36	1.47
13	P	-3	G	C1'-N9	-6.41	1.38	1.48
15	N	-69	DG	C1'-N9	-6.26	1.33	1.46
17	V	63	ASN	C-N	-6.22	1.24	1.33
13	P	7	U	C1'-N1	5.63	1.56	1.48
13	P	0	U	C1'-N1	5.36	1.55	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	GLN	N-CA-C	-9.59	92.34	108.26
18	W	389	PRO	CA-N-CD	-8.91	99.53	112.00
2	B	63	GLN	N-CA-CB	-8.60	96.75	110.77
17	V	29	CYS	O-C-N	-8.25	114.30	121.31
18	W	388	ARG	CA-C-N	7.15	128.78	119.84
18	W	388	ARG	C-N-CA	7.15	128.78	119.84
2	B	336	ILE	CA-CB-CG2	6.96	122.32	110.50
7	G	133	ASN	CA-C-N	6.51	133.98	121.54
7	G	133	ASN	C-N-CA	6.51	133.98	121.54
4	D	170	ASN	CA-C-N	6.37	133.71	121.54
4	D	170	ASN	C-N-CA	6.37	133.71	121.54
2	B	238	GLY	CA-C-N	6.06	133.12	121.54
2	B	238	GLY	C-N-CA	6.06	133.12	121.54
2	B	60	GLN	CA-C-N	5.88	127.19	119.84
2	B	60	GLN	C-N-CA	5.88	127.19	119.84
1	A	1108	ASN	CA-C-N	5.75	132.32	121.97
1	A	1108	ASN	C-N-CA	5.75	132.32	121.97
1	A	473	LEU	CA-CB-CG	-5.70	96.36	116.30
2	B	330	GLY	N-CA-C	5.63	126.51	113.18
2	B	932	HIS	N-CA-C	-5.60	98.88	110.80
12	L	44	LYS	N-CA-C	5.54	122.61	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	88	GLU	CA-C-N	5.40	131.85	121.54
3	C	88	GLU	C-N-CA	5.40	131.85	121.54
4	D	169	VAL	CA-CB-CG1	5.20	119.24	110.40
4	D	169	VAL	CB-CA-C	5.19	119.80	111.29
3	C	89	ASP	CA-C-N	-5.18	111.62	122.03
3	C	89	ASP	C-N-CA	-5.18	111.62	122.03
2	B	336	ILE	CA-CB-CG1	5.13	119.12	110.40
9	I	58	ILE	CA-C-N	-5.11	115.09	122.45
9	I	58	ILE	C-N-CA	-5.11	115.09	122.45
2	B	499	GLY	N-CA-C	-5.11	101.08	113.18
9	I	54	GLU	CA-C-N	5.05	132.41	121.64
9	I	54	GLU	C-N-CA	5.05	132.41	121.64

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	336	ILE	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11123	0	11147	102	0
2	B	9228	0	9232	124	0
3	C	2098	0	2059	20	0
4	D	1314	0	1314	11	0
5	E	1740	0	1754	25	0
6	F	677	0	693	5	0
7	G	1324	0	1342	11	0
8	H	1052	0	1050	8	0
9	I	917	0	868	9	0
10	J	545	0	561	4	0
11	K	932	0	944	2	0
12	L	359	0	358	3	0
13	P	347	0	170	22	0
14	T	3487	0	1904	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	3397	0	1872	100	0
16	M	505	0	496	24	0
17	V	792	0	757	7	0
18	W	2226	0	2273	144	0
19	a	797	0	835	6	0
19	e	796	0	832	8	0
20	b	638	0	676	7	0
20	f	619	0	659	10	0
21	c	796	0	848	12	0
21	g	810	0	866	5	0
22	d	746	0	771	10	0
22	h	725	0	745	10	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	V	1	0	0	0	0
24	A	1	0	0	0	0
All	All	48001	0	45026	598	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (598) 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)
18:W:333:PHE:CD1	18:W:354:LEU:HD21	1.73	1.24
1:A:288:HIS:CD2	18:W:299:PHE:CZ	2.26	1.23
2:B:337:ARG:HD2	16:M:78:GLU:OE1	1.39	1.20
2:B:463:LYS:HD2	15:N:-84:DG:N2	1.56	1.20
18:W:409:ASP:HB2	18:W:413:PHE:CD2	1.73	1.20
18:W:333:PHE:CG	18:W:354:LEU:HD21	1.80	1.16
14:T:62:DA:N6	15:N:-62:DT:H3	1.45	1.15
18:W:332:LYS:HD2	18:W:389:PRO:HD3	1.24	1.12
14:T:73:DA:C2'	14:T:74:DA:H5''	1.79	1.11
2:B:419:ARG:HH11	15:N:-83:DT:H1'	1.14	1.10
5:E:118:SER:OG	15:N:-61:DT:O3'	1.70	1.09
18:W:399:ALA:HB1	18:W:406:ILE:HD11	1.27	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:73:DA:H2''	14:T:74:DA:C5'	1.82	1.08
18:W:352:LEU:HD11	18:W:435:LEU:HD11	1.31	1.08
1:A:976:ASP:O	1:A:977:ARG:HB2	1.51	1.07
18:W:409:ASP:HB2	18:W:413:PHE:HD2	1.04	1.07
18:W:320:LEU:HD22	18:W:432:LEU:HD13	1.37	1.05
2:B:419:ARG:NH1	15:N:-83:DT:H1'	1.71	1.05
14:T:61:DA:H1'	14:T:62:DA:OP2	1.57	1.04
14:T:74:DA:N6	15:N:-74:DT:O4	1.91	1.03
18:W:320:LEU:HD22	18:W:432:LEU:CD1	1.88	1.03
18:W:399:ALA:CB	18:W:406:ILE:HD11	1.90	1.00
1:A:288:HIS:CD2	18:W:299:PHE:CE1	2.49	1.00
14:T:62:DA:H61	15:N:-62:DT:H3	1.02	0.99
2:B:62:ALA:O	2:B:70:ASN:HA	1.62	0.98
18:W:396:GLU:OE2	18:W:414:VAL:HG23	1.64	0.98
18:W:399:ALA:HB1	18:W:406:ILE:CD1	1.95	0.96
14:T:92:DC:H5''	18:W:330:ASN:HD21	1.25	0.95
5:E:118:SER:OG	15:N:-60:DT:P	2.23	0.95
2:B:62:ALA:HB3	2:B:71:ILE:CG2	1.97	0.95
15:N:-58:DC:H2''	15:N:-57:DT:H71	1.49	0.94
18:W:409:ASP:CB	18:W:413:PHE:CD2	2.50	0.94
2:B:62:ALA:CB	2:B:71:ILE:CG2	2.46	0.93
1:A:286:PRO:CG	18:W:268:PHE:CZ	2.51	0.93
2:B:337:ARG:CD	16:M:78:GLU:OE1	2.16	0.93
1:A:288:HIS:NE2	18:W:299:PHE:CZ	2.36	0.92
18:W:399:ALA:C	18:W:406:ILE:CD1	2.43	0.92
18:W:409:ASP:CB	18:W:413:PHE:HD2	1.81	0.92
18:W:394:PHE:HE2	18:W:396:GLU:HG2	1.37	0.90
14:T:68:DA:N6	15:N:-69:DG:O6	2.03	0.90
2:B:463:LYS:HD2	15:N:-84:DG:H22	1.34	0.89
1:A:288:HIS:NE2	18:W:299:PHE:CE1	2.41	0.89
1:A:197:GLN:NE2	16:M:50:LYS:HB3	1.87	0.88
2:B:62:ALA:CB	2:B:71:ILE:HG23	2.03	0.88
14:T:58:DG:C6	14:T:59:DA:N6	2.42	0.88
17:V:85:ARG:NH1	17:V:87:ASP:OD1	2.07	0.88
2:B:463:LYS:CD	15:N:-84:DG:N2	2.36	0.87
5:E:118:SER:OG	15:N:-60:DT:OP1	1.93	0.86
18:W:333:PHE:CG	18:W:354:LEU:CD2	2.59	0.86
5:E:118:SER:HG	15:N:-60:DT:P	1.97	0.85
18:W:409:ASP:O	18:W:410:ARG:HG3	1.75	0.85
18:W:320:LEU:CD2	18:W:432:LEU:HD13	2.05	0.85
18:W:357:ARG:C	18:W:389:PRO:HG2	2.02	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:68:DA:N6	15:N:-69:DG:C6	2.45	0.85
18:W:329:LYS:HD2	18:W:436:ILE:HG13	1.59	0.84
18:W:332:LYS:HD2	18:W:388:ARG:HB2	1.59	0.84
18:W:399:ALA:CB	18:W:406:ILE:CD1	2.55	0.84
14:T:61:DA:C1'	14:T:62:DA:OP2	2.24	0.84
14:T:62:DA:C2	15:N:-61:DT:O2	2.31	0.84
18:W:399:ALA:C	18:W:406:ILE:HD11	2.02	0.84
2:B:62:ALA:HB3	2:B:71:ILE:HG22	1.59	0.83
13:P:10:C:O2	14:T:77:DG:N2	2.09	0.83
14:T:58:DG:C2	14:T:59:DA:C6	2.66	0.83
18:W:352:LEU:HD11	18:W:435:LEU:CD1	2.07	0.83
1:A:197:GLN:HE22	16:M:50:LYS:HB3	1.40	0.83
18:W:388:ARG:HB2	18:W:389:PRO:HD3	1.58	0.83
2:B:62:ALA:CB	2:B:71:ILE:HG22	2.09	0.82
14:T:62:DA:N1	15:N:-62:DT:O2	2.11	0.82
2:B:500:LYS:H	2:B:500:LYS:HD3	1.42	0.82
16:M:33:SER:HA	16:M:50:LYS:HE2	1.63	0.81
1:A:286:PRO:HG2	18:W:268:PHE:CZ	2.14	0.81
1:A:286:PRO:HG2	18:W:268:PHE:CE2	2.16	0.80
15:N:-84:DG:OP2	15:N:-84:DG:H2'	1.82	0.79
2:B:328:ARG:HD3	16:M:68:ASP:OD1	1.81	0.79
18:W:328:VAL:HA	18:W:435:LEU:HD23	1.64	0.78
18:W:357:ARG:HB3	18:W:389:PRO:HD2	1.64	0.78
18:W:394:PHE:CE2	18:W:396:GLU:HG2	2.18	0.78
2:B:328:ARG:CD	16:M:68:ASP:OD1	2.32	0.78
5:E:118:SER:HB2	15:N:-60:DT:C5'	2.14	0.78
14:T:92:DC:H5''	18:W:330:ASN:ND2	1.99	0.78
2:B:419:ARG:NH1	15:N:-83:DT:C1'	2.45	0.78
14:T:72:DA:N1	15:N:-72:DT:O2	2.17	0.77
15:N:-58:DC:H2''	15:N:-57:DT:C7	2.15	0.77
1:A:288:HIS:CE1	18:W:299:PHE:CE1	2.74	0.76
13:P:1:G:H2'	13:P:2:G:C8	2.21	0.76
5:E:116:THR:CG2	15:N:-61:DT:H5''	2.14	0.76
1:A:286:PRO:CD	18:W:268:PHE:CZ	2.69	0.75
18:W:319:LYS:O	18:W:320:LEU:CB	2.33	0.75
14:T:-24:DG:N2	15:N:24:DC:O2	2.18	0.75
14:T:54:DG:C4	14:T:55:DA:N7	2.54	0.75
14:T:54:DG:C2	14:T:55:DA:C4	2.75	0.75
1:A:288:HIS:CE1	18:W:299:PHE:HE1	2.04	0.75
14:T:57:DA:H1'	14:T:58:DG:H5'	1.68	0.75
2:B:463:LYS:CE	15:N:-84:DG:H21	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:NZ	15:N:-68:DT:OP1	2.20	0.74
14:T:54:DG:N3	14:T:55:DA:C8	2.55	0.74
1:A:45:ARG:O	1:A:45:ARG:HG2	1.88	0.73
2:B:868:ILE:HG12	15:N:-90:DG:OP1	1.89	0.73
5:E:116:THR:HB	15:N:-61:DT:H5''	1.71	0.73
14:T:54:DG:C4	14:T:55:DA:C8	2.77	0.73
18:W:328:VAL:HG22	18:W:435:LEU:HD21	1.70	0.73
18:W:396:GLU:OE2	18:W:414:VAL:CG2	2.36	0.72
15:N:-84:DG:H1'	15:N:-83:DT:C7	2.19	0.72
14:T:61:DA:C2'	14:T:62:DA:OP2	2.37	0.72
15:N:-85:DG:OP1	18:W:233:LEU:HD13	1.90	0.71
18:W:326:VAL:HG21	18:W:435:LEU:HD13	1.71	0.71
18:W:388:ARG:HB2	18:W:389:PRO:CD	2.19	0.71
13:P:3:G:N1	14:T:84:DC:N3	2.37	0.71
18:W:323:GLY:HA2	18:W:339:GLN:HE21	1.54	0.70
2:B:500:LYS:HD3	2:B:500:LYS:N	2.06	0.70
1:A:1160:PRO:HB3	1:A:1190:GLN:HE21	1.56	0.70
14:T:61:DA:C6	14:T:62:DA:N6	2.59	0.70
14:T:-24:DG:N1	15:N:24:DC:N3	2.38	0.70
15:N:-71:DT:H2''	15:N:-70:DC:C5	2.27	0.70
1:A:14:VAL:H	1:A:1435:GLN:HE22	1.40	0.70
2:B:71:ILE:HD12	2:B:127:ILE:HG23	1.73	0.70
18:W:320:LEU:HD22	18:W:432:LEU:HD11	1.74	0.70
18:W:357:ARG:HB3	18:W:389:PRO:CD	2.22	0.70
18:W:332:LYS:HG3	18:W:388:ARG:CB	2.22	0.69
2:B:935:ARG:NH2	13:P:0:U:C4	2.61	0.68
18:W:357:ARG:O	18:W:389:PRO:HG2	1.94	0.68
15:N:-73:DT:H2''	15:N:-72:DT:H5''	1.76	0.68
2:B:935:ARG:NH2	13:P:0:U:C5	2.62	0.68
18:W:357:ARG:HB3	18:W:389:PRO:HG2	1.75	0.68
18:W:329:LYS:CD	18:W:436:ILE:HG13	2.24	0.67
2:B:463:LYS:HD2	15:N:-84:DG:H21	1.54	0.67
14:T:58:DG:N2	14:T:59:DA:C2	2.62	0.67
18:W:399:ALA:CA	18:W:406:ILE:HD11	2.23	0.67
15:N:-58:DC:C2	15:N:-57:DT:C4	2.82	0.67
14:T:61:DA:H2''	14:T:62:DA:OP2	1.94	0.67
5:E:118:SER:HB2	15:N:-60:DT:H5''	1.75	0.67
14:T:54:DG:H2''	14:T:55:DA:OP2	1.94	0.67
2:B:63:GLN:OE1	18:W:249:ALA:HA	1.96	0.66
5:E:116:THR:CB	15:N:-61:DT:H5''	2.25	0.66
13:P:3:G:O6	14:T:84:DC:N4	2.19	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PRO:O	1:A:248:ARG:NH1	2.28	0.66
12:L:68:GLN:HB3	18:W:784:ASN:HD21	1.61	0.66
18:W:332:LYS:CD	18:W:388:ARG:HB2	2.24	0.66
1:A:466:TYR:HB2	1:A:470:ARG:HH22	1.61	0.66
14:T:58:DG:N1	14:T:59:DA:C6	2.64	0.66
18:W:329:LYS:HD2	18:W:436:ILE:CG1	2.25	0.66
18:W:409:ASP:O	18:W:410:ARG:CG	2.43	0.66
14:T:73:DA:H2''	14:T:74:DA:H5''	0.85	0.65
7:G:132:SER:HB2	7:G:135:GLU:HB2	1.78	0.65
18:W:351:ARG:HG2	18:W:429:THR:HG22	1.78	0.65
1:A:197:GLN:HE22	16:M:50:LYS:CB	2.09	0.65
18:W:352:LEU:CD1	18:W:435:LEU:HD11	2.19	0.65
18:W:396:GLU:CD	18:W:414:VAL:CG2	2.70	0.64
18:W:409:ASP:CB	18:W:413:PHE:CE2	2.80	0.64
18:W:333:PHE:CD1	18:W:354:LEU:CD2	2.65	0.64
2:B:463:LYS:CD	15:N:-84:DG:H21	2.08	0.64
2:B:896:ASP:OD2	12:L:60:LYS:NZ	2.30	0.64
2:B:70:ASN:O	2:B:127:ILE:HA	1.97	0.64
2:B:335:GLY:HA2	16:M:74:ILE:HD13	1.78	0.64
13:P:5:G:C2	14:T:83:DA:C2	2.85	0.64
1:A:286:PRO:CG	18:W:268:PHE:CE2	2.80	0.64
4:D:159:LEU:HD21	7:G:167:PHE:HB2	1.80	0.64
14:T:62:DA:N6	15:N:-62:DT:N3	2.23	0.64
2:B:63:GLN:OE1	18:W:249:ALA:CA	2.46	0.63
18:W:329:LYS:CG	18:W:436:ILE:HG13	2.29	0.63
14:T:61:DA:C2	14:T:62:DA:C5	2.87	0.63
14:T:83:DA:H2''	14:T:84:DC:H5''	1.81	0.63
18:W:332:LYS:HG3	18:W:388:ARG:HB3	1.79	0.63
2:B:62:ALA:HB3	2:B:71:ILE:HG23	1.70	0.63
14:T:62:DA:N1	15:N:-62:DT:C2	2.67	0.63
18:W:437:VAL:O	18:W:437:VAL:HG22	1.98	0.63
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.32	0.63
1:A:197:GLN:CD	16:M:50:LYS:HB3	2.24	0.62
2:B:62:ALA:HB3	2:B:71:ILE:H	1.64	0.62
1:A:286:PRO:HD3	18:W:268:PHE:CZ	2.34	0.62
14:T:61:DA:N1	14:T:62:DA:C6	2.68	0.62
16:M:25:CYS:SG	16:M:54:LEU:HD21	2.39	0.62
16:M:54:LEU:HD12	16:M:54:LEU:C	2.24	0.62
1:A:288:HIS:CG	18:W:299:PHE:CE1	2.87	0.61
1:A:982:ASP:O	1:A:1041:ARG:NH2	2.33	0.61
2:B:220:ALA:O	2:B:252:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:357:ARG:HB3	18:W:389:PRO:CG	2.31	0.61
4:D:19:VAL:O	4:D:29:ARG:NH1	2.33	0.61
14:T:67:DA:N6	15:N:-68:DT:O4	2.33	0.61
2:B:328:ARG:HD3	16:M:68:ASP:HA	1.83	0.61
9:I:29:CYS:SG	9:I:30:ARG:N	2.74	0.61
19:e:108:ASN:ND2	20:f:42:GLY:O	2.33	0.61
1:A:288:HIS:NE2	18:W:299:PHE:HZ	1.97	0.61
4:D:41:HIS:HB3	7:G:73:LYS:HD3	1.82	0.61
20:b:92:ARG:HH21	22:d:98:LEU:HA	1.65	0.61
5:E:118:SER:CB	15:N:-61:DT:O3'	2.49	0.60
17:V:44:ALA:O	17:V:48:GLU:HG2	2.01	0.60
20:f:92:ARG:HH21	22:h:98:LEU:HA	1.67	0.60
18:W:328:VAL:HG22	18:W:435:LEU:CD2	2.30	0.60
2:B:969:ARG:NH1	3:C:60:GLU:OE1	2.35	0.60
8:H:56:THR:HB	8:H:144:ARG:HB3	1.83	0.60
15:N:58:DC:H5'	21:c:77:ARG:HH21	1.65	0.60
1:A:318:LYS:HG2	15:N:-85:DG:O6	2.02	0.60
13:P:1:G:N2	13:P:2:G:C2	2.69	0.60
14:T:62:DA:H2''	14:T:63:DA:C8	2.37	0.60
15:N:-63:DT:H2''	15:N:-62:DT:H6	1.67	0.60
3:C:69:ILE:HD11	3:C:144:LEU:HD21	1.84	0.60
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.35	0.59
2:B:859:TYR:HD2	2:B:911:ILE:HD11	1.67	0.59
5:E:84:GLU:OE1	5:E:91:THR:OG1	2.20	0.59
5:E:85:PRO:HA	5:E:112:GLN:HB2	1.85	0.59
5:E:118:SER:CB	15:N:-60:DT:OP1	2.51	0.59
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.35	0.59
18:W:397:ALA:O	18:W:401:VAL:HG23	2.03	0.59
18:W:399:ALA:O	18:W:406:ILE:CD1	2.50	0.59
1:A:976:ASP:O	1:A:977:ARG:CB	2.37	0.59
18:W:328:VAL:HA	18:W:435:LEU:CD2	2.33	0.59
18:W:394:PHE:CE2	18:W:396:GLU:CG	2.86	0.58
5:E:118:SER:OG	15:N:-61:DT:C3'	2.51	0.58
8:H:112:LYS:HG2	8:H:125:GLU:HG2	1.85	0.58
1:A:42:ASP:O	1:A:43:GLU:HG3	2.03	0.58
18:W:319:LYS:O	18:W:320:LEU:HB3	2.02	0.58
18:W:394:PHE:HE2	18:W:396:GLU:CG	2.14	0.58
19:a:62:ILE:O	19:a:93:GLN:NE2	2.37	0.58
20:f:75:HIS:HA	22:h:89:ARG:HH12	1.69	0.58
2:B:233:SER:HG	2:B:356:HIS:HD1	1.50	0.58
18:W:389:PRO:HD2	18:W:389:PRO:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:ARG:HD2	16:M:68:ASP:OD1	2.02	0.58
14:T:58:DG:C2	14:T:59:DA:N1	2.72	0.58
14:T:61:DA:N1	14:T:62:DA:N6	2.52	0.58
18:W:396:GLU:CD	18:W:414:VAL:HG21	2.27	0.58
18:W:413:PHE:CE1	18:W:420:GLU:HB3	2.38	0.58
14:T:54:DG:C2	14:T:55:DA:C5	2.92	0.57
2:B:295:TYR:HD1	2:B:564:PRO:HB3	1.69	0.57
19:e:48:LEU:HD23	19:e:51:ILE:HD12	1.86	0.57
2:B:337:ARG:HB2	16:M:75:ASP:OD1	2.04	0.57
18:W:319:LYS:O	18:W:320:LEU:HB2	2.03	0.57
2:B:30:LEU:O	2:B:489:ARG:NH1	2.38	0.57
3:C:20:MET:SD	3:C:227:ARG:NH2	2.75	0.57
5:E:116:THR:HG21	15:N:-61:DT:H5''	1.87	0.57
5:E:118:SER:CB	15:N:-60:DT:P	2.91	0.57
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.34	0.57
15:N:-83:DT:O5'	15:N:-83:DT:H6	1.88	0.57
1:A:570:LYS:HB3	8:H:46:MET:HE1	1.86	0.57
1:A:351:ARG:HB2	2:B:1128:LEU:HD11	1.87	0.56
1:A:1459:ASP:OD1	1:A:1459:ASP:N	2.34	0.56
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.87	0.56
8:H:13:GLN:HE22	8:H:29:ILE:HD12	1.70	0.56
18:W:332:LYS:CG	18:W:388:ARG:HB2	2.35	0.56
1:A:1201:ARG:NH2	1:A:1235:ALA:O	2.39	0.56
13:P:-1:U:H2'	13:P:-1:U:O2	2.05	0.56
14:T:62:DA:N1	15:N:-61:DT:O2	2.38	0.56
15:N:-64:DT:H2''	15:N:-63:DT:H71	1.87	0.56
2:B:268:VAL:HA	2:B:330:GLY:HA2	1.88	0.56
1:A:50:GLU:CD	18:W:444:LEU:HD11	2.31	0.56
14:T:58:DG:N1	14:T:59:DA:N6	2.53	0.56
15:N:22:DT:H2''	15:N:23:DG:H5''	1.88	0.56
2:B:935:ARG:NH2	13:P:0:U:O4	2.39	0.56
14:T:-42:DT:OP1	21:c:20:ARG:NH2	2.39	0.56
17:V:43:GLN:NE2	17:V:47:ASN:OD1	2.39	0.56
2:B:334:LEU:HD22	16:M:67:ILE:CD1	2.37	0.55
18:W:344:LEU:CD1	18:W:349:GLU:HB2	2.35	0.55
18:W:409:ASP:OD2	18:W:415:THR:OG1	2.21	0.55
2:B:822:ASN:O	10:J:47:ARG:NH1	2.39	0.55
15:N:-63:DT:H2'	15:N:-62:DT:C7	2.36	0.55
13:P:-2:U:O2'	13:P:-1:U:H5	1.90	0.55
14:T:61:DA:C2	14:T:62:DA:C6	2.94	0.55
2:B:62:ALA:HB1	2:B:71:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:ARG:HG2	18:W:762:GLY:HA2	1.88	0.54
20:b:52:GLU:OE2	20:b:55:ARG:NH1	2.40	0.54
1:A:409:ASP:OD1	1:A:409:ASP:N	2.40	0.54
2:B:270:GLN:HB3	2:B:329:ARG:HD3	1.89	0.54
15:N:-85:DG:OP1	18:W:233:LEU:CD1	2.55	0.54
2:B:904:ARG:NH1	18:W:782:LEU:O	2.41	0.54
15:N:-63:DT:H2'	15:N:-62:DT:H72	1.90	0.54
19:e:62:ILE:O	19:e:93:GLN:NE2	2.38	0.54
13:P:1:G:O2'	13:P:2:G:O4'	2.23	0.54
18:W:352:LEU:HD11	18:W:435:LEU:HD21	1.90	0.53
22:h:73:GLU:OE1	22:h:76:ARG:NH2	2.41	0.53
14:T:92:DC:C5'	18:W:330:ASN:HD21	2.11	0.53
15:N:-85:DG:H4'	15:N:-84:DG:O5'	2.08	0.53
21:c:26:PRO:HG3	21:c:29:ARG:HD3	1.90	0.53
10:J:8:PHE:HB2	10:J:47:ARG:HH22	1.73	0.53
1:A:50:GLU:OE1	18:W:444:LEU:HD11	2.09	0.53
1:A:286:PRO:CD	18:W:268:PHE:CE1	2.92	0.53
1:A:288:HIS:CD2	18:W:299:PHE:HZ	2.18	0.53
9:I:90:GLN:HE21	9:I:92:ARG:HG3	1.74	0.53
18:W:772:GLU:OE2	18:W:774:ASN:ND2	2.42	0.53
1:A:1452:LEU:HD22	6:F:131:PRO:HB3	1.90	0.53
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.91	0.52
22:h:96:ARG:HE	22:h:108:VAL:HG21	1.74	0.52
17:V:41:SER:HB2	17:V:45:THR:HB	1.91	0.52
18:W:396:GLU:CD	18:W:414:VAL:HG23	2.30	0.52
18:W:413:PHE:HZ	18:W:420:GLU:CD	2.17	0.52
3:C:104:HIS:ND1	3:C:111:THR:OG1	2.38	0.52
19:a:123:ASP:OD1	19:e:113:HIS:NE2	2.29	0.52
21:g:32:ARG:NH2	22:h:32:GLU:OE1	2.38	0.52
14:T:61:DA:H1'	14:T:62:DA:P	2.49	0.52
1:A:336:ARG:HH22	2:B:1114:LEU:HD21	1.74	0.52
2:B:944:THR:HG21	2:B:1122:ARG:HE	1.75	0.52
15:N:-58:DC:C4	15:N:-57:DT:O4	2.63	0.51
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.92	0.51
4:D:113:ALA:O	4:D:116:LYS:NZ	2.43	0.51
19:a:122:LYS:HG3	19:e:113:HIS:HE1	1.75	0.51
1:A:1402:ARG:NH2	1:A:1420:GLU:OE1	2.43	0.51
2:B:242:ILE:HG21	2:B:355:PRO:HG3	1.93	0.51
2:B:333:ALA:HB3	2:B:336:ILE:HD11	1.92	0.51
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.93	0.51
2:B:62:ALA:HB2	2:B:71:ILE:HG23	1.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:OE1	1:A:231:ARG:NH1	2.44	0.51
2:B:760:ASP:OD1	2:B:760:ASP:N	2.38	0.51
2:B:62:ALA:HB3	2:B:71:ILE:N	2.26	0.51
15:N:-63:DT:H2''	15:N:-62:DT:C6	2.43	0.51
18:W:409:ASP:HB2	18:W:413:PHE:CE2	2.35	0.51
21:c:77:ARG:HG2	22:d:50:GLY:HA3	1.93	0.51
18:W:286:LEU:HD22	18:W:292:VAL:HG21	1.93	0.50
2:B:63:GLN:OE1	18:W:249:ALA:HB1	2.11	0.50
7:G:100:PHE:HB3	7:G:107:ASN:HD21	1.75	0.50
18:W:349:GLU:HG2	18:W:431:ARG:HA	1.92	0.50
3:C:74:GLU:O	3:C:246:ARG:NH2	2.33	0.50
20:f:47:SER:OG	20:f:48:GLY:N	2.42	0.50
2:B:463:LYS:CD	15:N:-84:DG:H22	2.14	0.50
1:A:351:ARG:NE	1:A:487:GLU:OE1	2.44	0.50
14:T:27:DG:OP2	20:f:79:LYS:NZ	2.45	0.50
15:N:-61:DT:H2''	15:N:-60:DT:C6	2.46	0.50
4:D:33:GLU:O	4:D:38:GLN:NE2	2.45	0.50
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.94	0.50
18:W:403:GLU:O	18:W:403:GLU:HG3	2.12	0.50
1:A:310:ALA:HB2	14:T:72:DA:OP1	2.12	0.50
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.92	0.50
2:B:1187:ASN:HD21	2:B:1190:ASN:HB3	1.77	0.50
14:T:62:DA:C2	15:N:-62:DT:O2	2.64	0.50
1:A:354:ILE:HG22	1:A:469:PHE:HB2	1.93	0.49
2:B:260:THR:HG22	2:B:308:PRO:HB2	1.93	0.49
15:N:68:DC:H2''	15:N:69:DT:H5'	1.95	0.49
2:B:419:ARG:NH1	15:N:-83:DT:C2	2.74	0.49
18:W:413:PHE:HE1	18:W:420:GLU:HB3	1.78	0.49
22:h:35:SER:HA	22:h:56:MET:HE2	1.95	0.49
2:B:859:TYR:HE2	2:B:941:LEU:HD12	1.77	0.49
15:N:-88:DT:OP1	18:W:334:LYS:HE3	2.12	0.49
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.95	0.49
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.46	0.49
5:E:27:TYR:HA	5:E:63:PRO:HA	1.95	0.49
14:T:64:DA:H2'	14:T:65:DA:C8	2.47	0.49
1:A:841:ARG:NH2	1:A:1108:ASN:OD1	2.46	0.49
1:A:1153:GLU:OE1	1:A:1196:ARG:NH1	2.45	0.49
18:W:357:ARG:CB	18:W:389:PRO:HG2	2.42	0.49
18:W:399:ALA:O	18:W:406:ILE:HD12	2.13	0.49
2:B:1101:ASP:O	2:B:1122:ARG:NH1	2.45	0.48
5:E:19:LYS:NZ	5:E:33:GLU:O	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:28:GLY:HA3	17:V:33:ASP:CG	2.38	0.48
14:T:49:DC:OP1	21:g:29:ARG:NH2	2.42	0.48
14:T:74:DA:H2''	14:T:75:DC:H5'	1.94	0.48
1:A:122:MET:HE1	1:A:138:VAL:HG13	1.96	0.48
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.36	0.48
1:A:43:GLU:OE2	18:W:335:GLY:O	2.31	0.48
1:A:14:VAL:H	1:A:1435:GLN:NE2	2.10	0.48
13:P:-4:U:H4'	13:P:-4:U:OP1	2.14	0.48
14:T:63:DA:H2'	14:T:64:DA:C8	2.49	0.48
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.95	0.48
2:B:780:VAL:HG22	2:B:795:ILE:HG23	1.96	0.48
3:C:47:LEU:HB2	3:C:158:ILE:HB	1.96	0.48
15:N:68:DC:H2'	15:N:69:DT:C6	2.48	0.48
18:W:409:ASP:OD2	18:W:413:PHE:CE2	2.66	0.48
22:d:55:ALA:HA	22:d:58:ILE:HD12	1.94	0.48
3:C:74:GLU:HG3	3:C:242:GLN:HE22	1.77	0.48
14:T:68:DA:N1	15:N:-69:DG:N1	2.62	0.48
18:W:308:ASP:HA	18:W:311:ARG:HG3	1.96	0.48
19:a:61:LEU:HD22	20:b:36:ARG:HB3	1.96	0.48
1:A:113:LEU:O	1:A:165:ARG:NH2	2.47	0.47
1:A:1193:TRP:HZ3	9:I:43:VAL:HG21	1.79	0.47
21:c:64:GLU:HA	22:d:46:HIS:HE1	1.78	0.47
19:e:108:ASN:HB2	20:f:43:VAL:HG22	1.96	0.47
14:T:62:DA:N1	15:N:-61:DT:C2	2.83	0.47
15:N:-71:DT:C2	15:N:-70:DC:C4	3.02	0.47
17:V:91:PRO:HB2	17:V:93:ASP:OD1	2.14	0.47
19:e:79:LYS:HD3	19:e:82:LEU:HD21	1.96	0.47
2:B:273:PRO:HD2	2:B:276:ILE:HD12	1.97	0.47
5:E:160:LYS:NZ	5:E:192:GLY:O	2.44	0.47
10:J:9:SER:OG	10:J:47:ARG:NH2	2.47	0.47
15:N:-64:DT:C2'	15:N:-63:DT:H71	2.44	0.47
18:W:388:ARG:CB	18:W:389:PRO:CD	2.88	0.47
1:A:283:ASP:OD1	1:A:283:ASP:N	2.46	0.47
2:B:401:LEU:HD13	2:B:538:ILE:HG21	1.96	0.47
22:d:35:SER:O	22:d:39:TYR:HB2	2.15	0.47
1:A:115:LEU:HB2	1:A:122:MET:HE2	1.96	0.47
2:B:63:GLN:OE1	18:W:249:ALA:CB	2.62	0.47
15:N:4:DG:H4'	15:N:5:DT:H5'	1.97	0.47
18:W:437:VAL:O	18:W:437:VAL:CG2	2.61	0.47
20:b:47:SER:OG	20:b:48:GLY:N	2.47	0.47
1:A:254:ASP:OD1	1:A:254:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:52:CYS:O	16:M:53:ASN:HB2	2.15	0.47
5:E:189:LEU:HD13	5:E:213:CYS:HB2	1.96	0.46
18:W:399:ALA:CB	18:W:406:ILE:HD13	2.44	0.46
20:b:38:ALA:HB1	20:b:43:VAL:HB	1.97	0.46
21:c:90:ASP:HB3	21:c:93:LEU:HB2	1.96	0.46
1:A:286:PRO:HG3	18:W:268:PHE:CZ	2.46	0.46
5:E:142:ASN:HB3	5:E:145:HIS:HD2	1.80	0.46
14:T:70:DG:H2'	14:T:71:DA:C8	2.50	0.46
21:c:100:VAL:HG22	20:f:96:THR:HB	1.97	0.46
1:A:542:ILE:HD12	1:A:578:LEU:HD13	1.98	0.46
1:A:912:ASP:OD1	1:A:912:ASP:N	2.42	0.46
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.47	0.46
13:P:-2:U:H6	13:P:-2:U:O5'	1.98	0.46
1:A:1227:PHE:HB2	1:A:1245:ILE:HD11	1.97	0.46
2:B:969:ARG:HH22	3:C:59:ASP:HB2	1.80	0.46
3:C:13:GLN:HE21	3:C:16:GLU:HG2	1.79	0.46
15:N:-72:DT:H5''	15:N:-72:DT:H6	1.79	0.46
1:A:1109:VAL:HG13	1:A:1335:PHE:HE2	1.80	0.46
11:K:5:ASP:OD1	18:W:787:LYS:NZ	2.48	0.46
22:h:69:ARG:HB3	22:h:98:LEU:HD21	1.97	0.46
2:B:225:ILE:HD13	2:B:248:LYS:HD3	1.97	0.46
22:h:33:SER:OG	22:h:34:TYR:N	2.47	0.46
1:A:887:ILE:O	1:A:945:ARG:NH2	2.41	0.46
2:B:557:GLU:HB2	2:B:582:ILE:HD12	1.97	0.46
13:P:-1:U:H2'	13:P:0:U:H5''	1.97	0.46
15:N:-83:DT:O4	15:N:-82:DG:C2	2.68	0.46
20:b:39:ARG:NH1	20:b:44:LYS:O	2.49	0.46
1:A:358:PRO:HD2	2:B:833:TYR:CE1	2.51	0.46
8:H:94:TYR:HD2	8:H:143:ILE:HD12	1.81	0.46
6:F:79:ARG:NH1	6:F:150:GLU:OE2	2.49	0.45
13:P:2:G:O5'	13:P:2:G:H8	1.99	0.45
18:W:409:ASP:C	18:W:410:ARG:HG3	2.37	0.45
2:B:164:MET:HB2	2:B:194:PHE:HE1	1.80	0.45
3:C:45:ILE:HA	3:C:159:ALA:HA	1.99	0.45
13:P:-2:U:O5'	13:P:-2:U:C6	2.69	0.45
15:N:-63:DT:C6	15:N:-62:DT:H72	2.52	0.45
15:N:2:DG:H1'	15:N:3:DC:H5'	1.98	0.45
1:A:599:LEU:HD13	8:H:123:CYS:HB2	1.98	0.45
2:B:419:ARG:NH1	15:N:-83:DT:N1	2.59	0.45
2:B:436:ASN:O	2:B:438:ASN:N	2.48	0.45
2:B:464:LYS:HZ3	15:N:-81:DG:N2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:5:G:H1	14:T:82:DC:H42	1.64	0.45
15:N:-58:DC:C2	15:N:-57:DT:N3	2.85	0.45
18:W:352:LEU:CD1	18:W:435:LEU:HD21	2.46	0.45
1:A:979:LYS:O	1:A:980:ALA:C	2.58	0.45
2:B:299:ASP:OD2	2:B:385:ARG:NH1	2.37	0.45
9:I:96:ASN:OD1	9:I:97:MET:N	2.48	0.45
15:N:-71:DT:H2''	15:N:-70:DC:H5	1.79	0.45
1:A:119:ASN:HB3	1:A:122:MET:HB3	1.98	0.45
2:B:1219:GLU:O	4:D:12:ARG:NH2	2.49	0.45
13:P:1:G:N2	13:P:2:G:N3	2.64	0.45
15:N:20:DG:H2''	15:N:21:DG:H5''	1.98	0.45
2:B:64:HIS:O	2:B:64:HIS:CG	2.70	0.45
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.99	0.45
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.40	0.45
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.99	0.45
14:T:68:DA:C6	15:N:-69:DG:N1	2.85	0.45
19:e:79:LYS:HB3	19:e:82:LEU:HD11	1.99	0.45
1:A:1162:SER:OG	1:A:1163:THR:N	2.49	0.44
7:G:116:PRO:HD2	7:G:163:ILE:HG13	1.99	0.44
18:W:322:ARG:HD3	18:W:342:GLU:HA	1.99	0.44
21:c:54:VAL:HG21	22:d:95:VAL:HG21	1.99	0.44
2:B:276:ILE:HD11	16:M:63:LEU:HD21	2.00	0.44
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.52	0.44
2:B:62:ALA:HB1	2:B:71:ILE:CG2	2.42	0.44
13:P:3:G:N2	14:T:84:DC:O2	2.49	0.44
18:W:409:ASP:OD2	18:W:413:PHE:HE2	2.00	0.44
2:B:325:PHE:CE1	16:M:63:LEU:HB3	2.52	0.44
1:A:286:PRO:O	1:A:288:HIS:N	2.50	0.44
1:A:1146:LYS:NZ	2:B:254:ASP:OD2	2.38	0.44
14:T:54:DG:N3	14:T:55:DA:N9	2.65	0.44
14:T:62:DA:H2''	14:T:63:DA:O4'	2.17	0.44
15:N:-71:DT:H2''	15:N:-70:DC:C6	2.52	0.44
21:g:26:PRO:HG3	22:h:37:TYR:CZ	2.53	0.44
2:B:870:ILE:HG13	18:W:387:PHE:CZ	2.52	0.44
4:D:23:GLU:HB3	7:G:82:PHE:HD1	1.83	0.44
4:D:51:LEU:HD11	7:G:4:LEU:HG	1.99	0.44
5:E:119:ALA:N	15:N:-60:DT:OP1	2.51	0.44
15:N:-58:DC:C5	15:N:-57:DT:O4	2.71	0.44
20:b:75:HIS:CE1	22:d:90:GLU:HG3	2.53	0.44
1:A:1168:ASP:OD2	1:A:1196:ARG:NE	2.49	0.44
2:B:334:LEU:HD22	16:M:67:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:46:VAL:HG22	19:a:49:ARG:HH22	1.82	0.44
2:B:70:ASN:HB2	2:B:128:ASP:O	2.18	0.44
2:B:935:ARG:CZ	13:P:0:U:O4	2.66	0.44
18:W:399:ALA:O	18:W:406:ILE:HD11	2.14	0.43
1:A:240:LEU:HD12	1:A:240:LEU:HA	1.88	0.43
18:W:333:PHE:CD2	18:W:354:LEU:CD2	3.00	0.43
18:W:344:LEU:HD11	18:W:349:GLU:HB2	2.00	0.43
1:A:1461:ALA:HB1	7:G:21:GLN:HB2	1.99	0.43
2:B:265:LEU:HD22	2:B:353:LEU:HD13	1.99	0.43
18:W:442:PRO:HB2	18:W:447:LEU:CD1	2.48	0.43
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	2.01	0.43
7:G:91:VAL:HG23	7:G:139:LYS:HA	2.01	0.43
14:T:58:DG:C2	14:T:59:DA:C5	3.07	0.43
15:N:-73:DT:H2''	15:N:-72:DT:C5'	2.45	0.43
18:W:421:TYR:HA	18:W:425:PHE:O	2.19	0.43
1:A:891:ASP:HA	1:A:941:ARG:HH12	1.83	0.43
2:B:1073:TYR:HE2	3:C:179:GLU:HA	1.83	0.43
3:C:148:ARG:HG2	3:C:149:ASN:H	1.83	0.43
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.77	0.43
18:W:332:LYS:HE3	18:W:357:ARG:HB2	2.01	0.43
1:A:1263:LEU:HD12	1:A:1263:LEU:HA	1.93	0.43
2:B:71:ILE:HG12	2:B:73:LYS:HE3	2.00	0.43
14:T:75:DC:H3'	14:T:75:DC:H6	1.83	0.43
15:N:-85:DG:H2''	15:N:-84:DG:C8	2.53	0.43
18:W:344:LEU:HD12	18:W:349:GLU:HB2	2.00	0.43
18:W:792:PRO:HG2	18:W:795:PHE:CD2	2.54	0.43
1:A:407:ILE:HG12	1:A:413:ARG:HG2	2.00	0.43
4:D:61:ARG:NH1	4:D:86:ASP:OD1	2.52	0.43
14:T:76:DG:N1	14:T:77:DG:C6	2.87	0.43
21:c:64:GLU:HA	22:d:46:HIS:CE1	2.54	0.43
2:B:334:LEU:HD22	16:M:67:ILE:HD13	2.00	0.42
2:B:336:ILE:H	2:B:341:ARG:HH21	1.67	0.42
14:T:58:DG:N3	14:T:59:DA:C5	2.87	0.42
21:c:95:LYS:HD2	22:d:100:PRO:HG3	2.01	0.42
20:f:87:VAL:HG11	20:f:102:GLY:HA3	2.01	0.42
2:B:463:LYS:HE3	15:N:-84:DG:H21	1.82	0.42
6:F:107:VAL:HG11	6:F:111:ILE:HD11	2.00	0.42
14:T:-8:DC:H2''	14:T:-7:DG:C8	2.54	0.42
15:N:-84:DG:O3'	15:N:-83:DT:H71	2.19	0.42
15:N:44:DT:H2''	15:N:45:DT:C5	2.54	0.42
18:W:352:LEU:HD11	18:W:435:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	2.01	0.42
7:G:115:ILE:HG23	7:G:163:ILE:HD11	2.01	0.42
1:A:468:THR:OG1	1:A:470:ARG:NH1	2.52	0.42
2:B:154:ASN:OD1	2:B:155:LYS:N	2.45	0.42
2:B:839:MET:HE2	2:B:839:MET:HB3	1.91	0.42
9:I:15:TYR:N	9:I:28:SER:O	2.37	0.42
14:T:58:DG:N2	14:T:59:DA:N1	2.67	0.42
19:a:68:GLN:HE21	19:a:72:ARG:HH21	1.66	0.42
1:A:519:LYS:NZ	1:A:625:SER:O	2.46	0.42
2:B:119:MET:O	2:B:153:GLY:N	2.53	0.42
6:F:89:GLU:OE2	6:F:136:ARG:NE	2.51	0.42
14:T:-17:DT:H2''	14:T:-16:DT:C6	2.54	0.42
1:A:168:CYS:SG	1:A:170:ASN:ND2	2.93	0.42
15:N:55:DC:H2''	15:N:56:DG:C8	2.55	0.42
1:A:615:PHE:HB3	8:H:121:LEU:HD21	2.01	0.42
1:A:1445:ASP:HB3	1:A:1447:MET:HE3	2.01	0.42
2:B:101:PRO:HG2	2:B:172:LEU:HD11	2.01	0.42
14:T:39:DA:H5''	21:g:42:ARG:HG2	2.01	0.42
1:A:286:PRO:O	1:A:288:HIS:ND1	2.52	0.42
7:G:152:THR:HA	7:G:157:ILE:HG22	2.02	0.42
9:I:84:VAL:HG22	9:I:104:LEU:HD21	2.01	0.42
14:T:58:DG:C6	14:T:59:DA:C6	3.07	0.42
15:N:-55:DT:H2''	15:N:-54:DC:C5	2.54	0.42
15:N:-43:DT:OP2	21:g:17:ARG:NH2	2.34	0.42
15:N:39:DA:OP2	21:c:35:ARG:NH2	2.52	0.42
16:M:60:ILE:HB	16:M:64:SER:OG	2.20	0.42
17:V:15:CYS:HB3	17:V:32:CYS:SG	2.59	0.42
1:A:292:GLU:OE1	18:W:271:HIS:HE1	2.02	0.41
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.77	0.41
1:A:883:THR:O	1:A:1027:ARG:NH2	2.52	0.41
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.02	0.41
4:D:169:VAL:C	4:D:171:LEU:H	2.28	0.41
14:T:76:DG:C6	14:T:77:DG:C6	3.08	0.41
18:W:278:LYS:HD2	18:W:280:GLU:OE2	2.20	0.41
20:f:31:LYS:HG3	20:f:51:TYR:CZ	2.55	0.41
2:B:251:GLY:HA2	2:B:256:GLY:HA3	2.02	0.41
5:E:189:LEU:HD11	5:E:195:VAL:HG13	2.01	0.41
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.55	0.41
13:P:3:G:H2'	13:P:4:U:O4'	2.19	0.41
18:W:352:LEU:HD21	18:W:435:LEU:CD1	2.50	0.41
1:A:1444:PHE:CZ	6:F:89:GLU:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:LEU:HD22	9:I:6:PHE:HZ	1.85	0.41
1:A:341:LEU:HD23	1:A:341:LEU:HA	1.78	0.41
2:B:63:GLN:OE1	18:W:249:ALA:O	2.38	0.41
2:B:233:SER:OG	2:B:356:HIS:ND1	2.43	0.41
5:E:118:SER:HB2	15:N:-60:DT:P	2.59	0.41
14:T:74:DA:C6	15:N:-74:DT:O4	2.66	0.41
18:W:784:ASN:HB2	18:W:785:PRO:HD3	2.02	0.41
2:B:325:PHE:CZ	16:M:63:LEU:HD23	2.55	0.41
1:A:781:ALA:N	2:B:696:GLU:OE2	2.45	0.41
14:T:54:DG:N2	14:T:55:DA:C4	2.88	0.41
18:W:228:GLY:HA3	18:W:299:PHE:CZ	2.55	0.41
18:W:322:ARG:CD	18:W:342:GLU:HG3	2.51	0.41
22:d:35:SER:HA	22:d:56:MET:HE2	2.02	0.41
1:A:591:ARG:HH11	1:A:591:ARG:HD3	1.74	0.41
4:D:69:ARG:HG2	4:D:74:GLY:HA2	2.03	0.41
14:T:-44:DA:H3'	21:c:28:GLY:HA3	2.01	0.41
14:T:71:DA:H2'	14:T:72:DA:C8	2.55	0.41
15:N:-85:DG:H2''	15:N:-84:DG:O5'	2.21	0.41
15:N:35:DT:H4'	15:N:36:DA:H5'	2.02	0.41
18:W:322:ARG:CD	18:W:342:GLU:HA	2.51	0.41
20:f:51:TYR:HB3	20:f:55:ARG:HH12	1.86	0.41
2:B:71:ILE:O	2:B:73:LYS:HG3	2.20	0.41
2:B:262:LYS:HA	2:B:273:PRO:HA	2.03	0.41
3:C:125:GLY:HA2	3:C:126:ASN:HA	1.75	0.41
3:C:241:ASN:HD22	11:K:109:TRP:NE1	2.19	0.41
14:T:70:DG:C6	14:T:71:DA:C6	3.08	0.41
1:A:447:ARG:HB2	1:A:488:MET:HG2	2.03	0.40
2:B:653:ARG:HE	2:B:653:ARG:HB3	1.70	0.40
3:C:32:LEU:HD12	3:C:32:LEU:HA	1.83	0.40
12:L:66:MET:HE2	12:L:66:MET:HB3	1.91	0.40
1:A:122:MET:HE3	1:A:126:ILE:HD11	2.02	0.40
1:A:1351:LEU:HD12	1:A:1351:LEU:HA	1.83	0.40
2:B:285:PRO:HB2	9:I:11:ASN:HB3	2.04	0.40
2:B:463:LYS:CE	15:N:-84:DG:N2	2.71	0.40
18:W:229:VAL:HG21	18:W:286:LEU:HD11	2.03	0.40
1:A:285:SER:O	1:A:285:SER:OG	2.30	0.40
1:A:844:LYS:HA	1:A:844:LYS:HD2	1.93	0.40
2:B:904:ARG:HG2	2:B:905:VAL:N	2.36	0.40
3:C:66:LEU:HD11	3:C:155:ILE:HD12	2.02	0.40
18:W:265:ARG:HA	18:W:265:ARG:HD2	1.71	0.40
22:h:77:LEU:HD23	22:h:77:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASP:N	1:A:195:ASP:OD1	2.53	0.40
1:A:970:GLN:HA	1:A:975:LEU:HB2	2.03	0.40
2:B:293:ILE:HG12	2:B:372:GLY:HA2	2.04	0.40
18:W:354:LEU:HD23	18:W:426:LEU:HD23	2.03	0.40
18:W:799:GLU:HB3	18:W:804:TRP:CZ3	2.56	0.40
1:A:197:GLN:OE1	16:M:50:LYS:HB3	2.21	0.40
1:A:262:ASP:OD1	1:A:317:GLN:NE2	2.54	0.40
1:A:841:ARG:NE	1:A:1387:ILE:O	2.44	0.40
1:A:1356:LEU:HD13	1:A:1371:MET:HE1	2.02	0.40
14:T:54:DG:C4	14:T:55:DA:C5	3.08	0.40
14:T:55:DA:C2	15:N:-54:DC:C2	3.10	0.40
15:N:-85:DG:H4'	15:N:-84:DG:OP1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1400/1743 (80%)	1343 (96%)	47 (3%)	10 (1%)	18	56
2	B	1145/1227 (93%)	1082 (94%)	55 (5%)	8 (1%)	18	56
3	C	261/304 (86%)	253 (97%)	6 (2%)	2 (1%)	16	54
4	D	162/186 (87%)	149 (92%)	9 (6%)	4 (2%)	4	26
5	E	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	160 (95%)	7 (4%)	2 (1%)	10	44
8	H	129/145 (89%)	125 (97%)	2 (2%)	2 (2%)	7	38
9	I	109/115 (95%)	102 (94%)	6 (6%)	1 (1%)	14	51
10	J	64/72 (89%)	61 (95%)	2 (3%)	1 (2%)	7	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
12	L	43/72 (60%)	42 (98%)	0	1 (2%)	5	28
16	M	62/113 (55%)	58 (94%)	4 (6%)	0	100	100
17	V	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
18	W	265/911 (29%)	246 (93%)	17 (6%)	2 (1%)	16	54
19	a	95/139 (68%)	92 (97%)	3 (3%)	0	100	100
19	e	95/139 (68%)	90 (95%)	5 (5%)	0	100	100
20	b	78/106 (74%)	75 (96%)	3 (4%)	0	100	100
20	f	76/106 (72%)	72 (95%)	4 (5%)	0	100	100
21	c	101/133 (76%)	95 (94%)	6 (6%)	0	100	100
21	g	103/133 (77%)	97 (94%)	6 (6%)	0	100	100
22	d	93/129 (72%)	90 (97%)	3 (3%)	0	100	100
22	h	91/129 (70%)	88 (97%)	3 (3%)	0	100	100
All	All	5045/6668 (76%)	4814 (95%)	198 (4%)	33 (1%)	20	56

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLU
1	A	287	GLN
1	A	960	VAL
1	A	1109	VAL
2	B	155	LYS
2	B	239	SER
2	B	337	ARG
3	C	89	ASP
7	G	134	ASP
8	H	108	GLU
12	L	44	LYS
18	W	320	LEU
1	A	284	GLY
1	A	977	ARG
1	A	1223	SER
2	B	62	ALA
2	B	177	GLU
2	B	299	ASP
4	D	169	VAL

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Mol	Chain	Res	Type
4	D	171	LEU
7	G	154	VAL
8	H	18	GLY
1	A	979	LYS
4	D	10	ALA
4	D	164	ALA
9	I	56	ALA
1	A	47	ARG
2	B	437	LEU
3	C	217	GLU
1	A	43	GLU
2	B	238	GLY
10	J	64	PRO
18	W	806	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	
1	A	1225/1528 (80%)	1219 (100%)	6 (0%)	81	83
2	B	1012/1077 (94%)	1002 (99%)	10 (1%)	68	78
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	143/160 (89%)	140 (98%)	3 (2%)	47	65
5	E	196/197 (100%)	195 (100%)	1 (0%)	81	83
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	118 (98%)	2 (2%)	53	69
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	37 (97%)	1 (3%)	40	62
16	M	61/99 (62%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	V	86/92 (94%)	85 (99%)	1 (1%)	63	75
18	W	241/796 (30%)	236 (98%)	5 (2%)	47	65
19	a	83/112 (74%)	82 (99%)	1 (1%)	63	75
19	e	82/112 (73%)	82 (100%)	0	100	100
20	b	65/81 (80%)	65 (100%)	0	100	100
20	f	63/81 (78%)	63 (100%)	0	100	100
21	c	82/102 (80%)	82 (100%)	0	100	100
21	g	83/102 (81%)	83 (100%)	0	100	100
22	d	81/107 (76%)	81 (100%)	0	100	100
22	h	79/107 (74%)	79 (100%)	0	100	100
All	All	4469/5772 (77%)	4439 (99%)	30 (1%)	73	81

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	248	ARG
1	A	473	LEU
1	A	661	ASN
1	A	977	ARG
1	A	1459	ASP
2	B	69	ASP
2	B	70	ASN
2	B	71	ILE
2	B	233	SER
2	B	428	CYS
2	B	466	MET
2	B	500	LYS
2	B	578	VAL
2	B	582	ILE
2	B	618	LYS
4	D	19	VAL
4	D	116	LYS
4	D	171	LEU
5	E	131	ILE
8	H	111	ILE
8	H	122	MET
12	L	62	ARG

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Mol	Chain	Res	Type
17	V	33	ASP
18	W	246	LYS
18	W	264	GLN
18	W	313	VAL
18	W	342	GLU
18	W	343	VAL
19	a	74	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	197	GLN
1	A	287	GLN
1	A	340	ASN
1	A	400	HIS
1	A	446	ASN
1	A	452	HIS
1	A	563	GLN
1	A	651	GLN
1	A	661	ASN
1	A	1190	GLN
1	A	1261	GLN
1	A	1435	GLN
2	B	735	HIS
2	B	794	ASN
2	B	887	HIS
2	B	1062	ASN
2	B	1097	HIS
2	B	1174	ASN
3	C	8	ASN
3	C	13	GLN
3	C	126	ASN
3	C	242	GLN
4	D	179	ASN
5	E	4	ASN
5	E	51	ASN
5	E	94	ASN
5	E	112	GLN
5	E	120	ASN
5	E	145	HIS
5	E	193	GLN

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Mol	Chain	Res	Type
7	G	21	GLN
7	G	125	ASN
8	H	13	GLN
8	H	136	GLN
9	I	90	GLN
9	I	105	ASN
18	W	264	GLN
18	W	330	ASN
18	W	339	GLN
18	W	402	HIS
18	W	434	ASN
18	W	784	ASN
19	a	68	GLN
20	b	27	GLN
21	c	24	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	15/16 (93%)	6 (40%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	-4	U
13	P	-3	G
13	P	-1	U
13	P	0	U
13	P	1	G
13	P	3	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

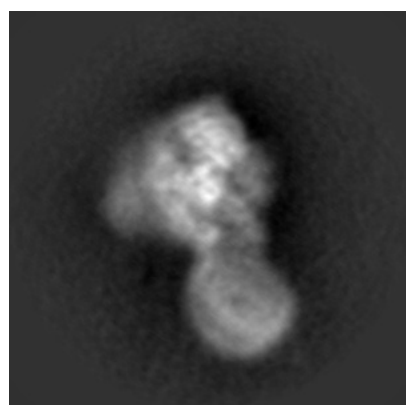
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0671. These allow visual inspection of the internal detail of the map and identification of artifacts.

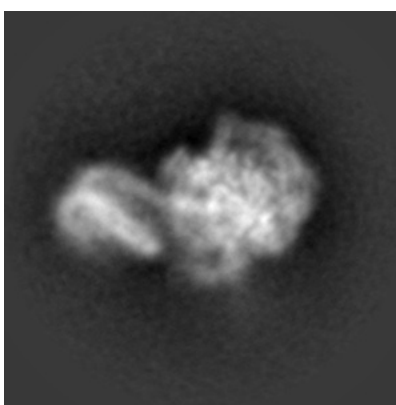
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

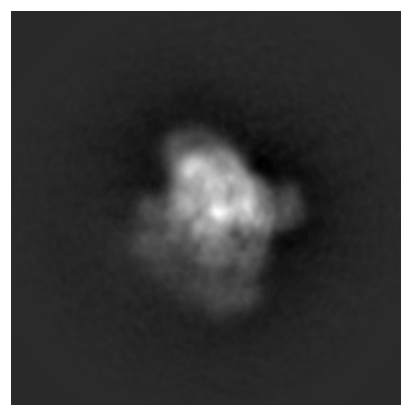
6.1.1 Primary map



X



Y

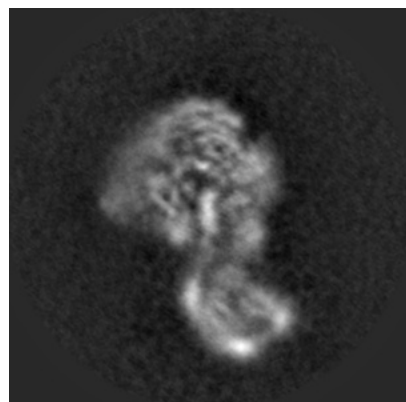


Z

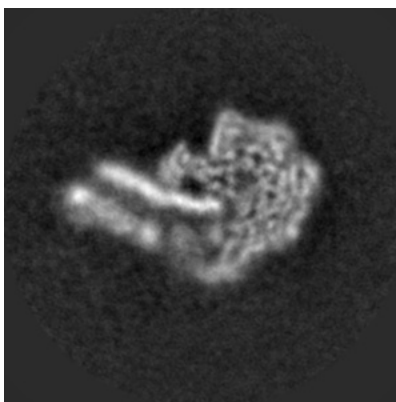
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

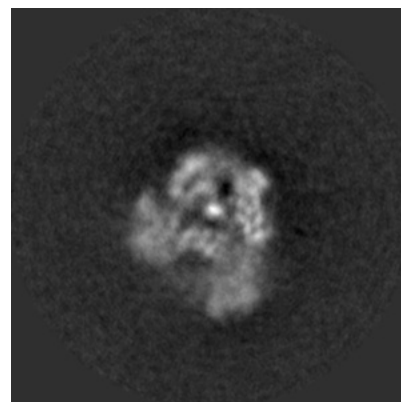
6.2.1 Primary map



X Index: 120



Y Index: 120

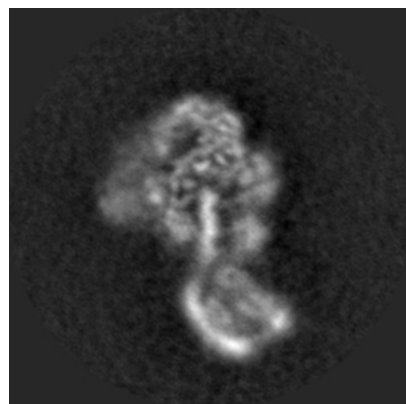


Z Index: 120

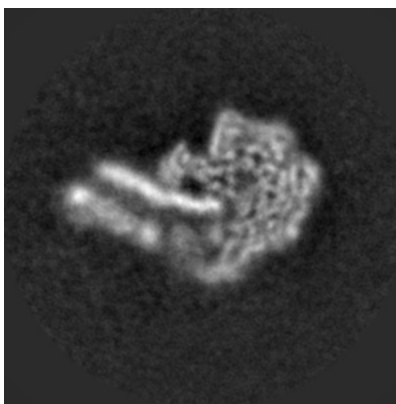
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

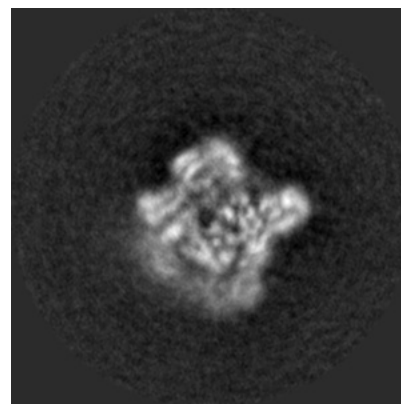
6.3.1 Primary map



X Index: 123



Y Index: 120

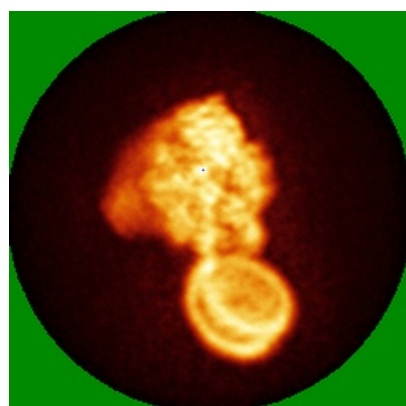


Z Index: 133

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

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

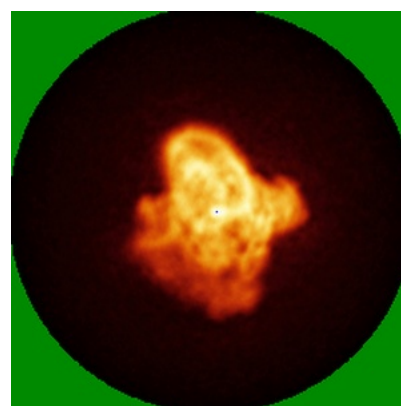
6.4.1 Primary map



X



Y

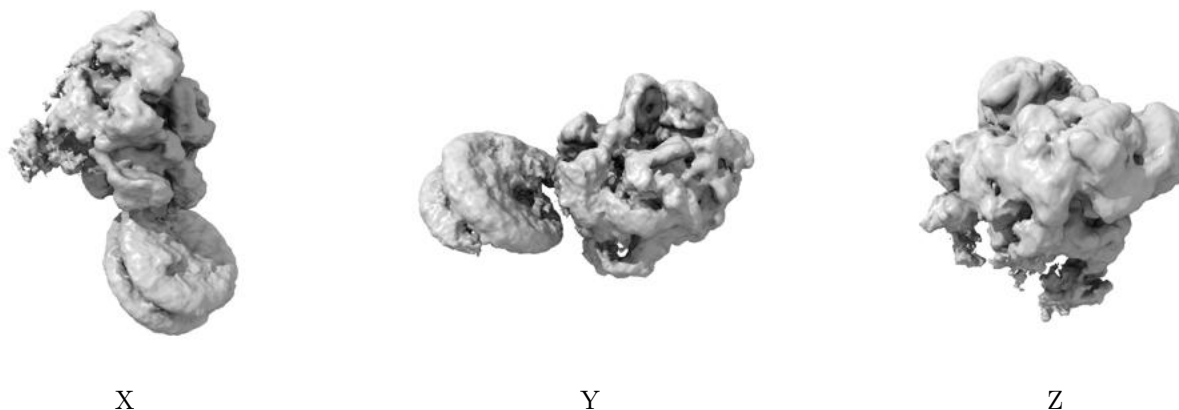


Z

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

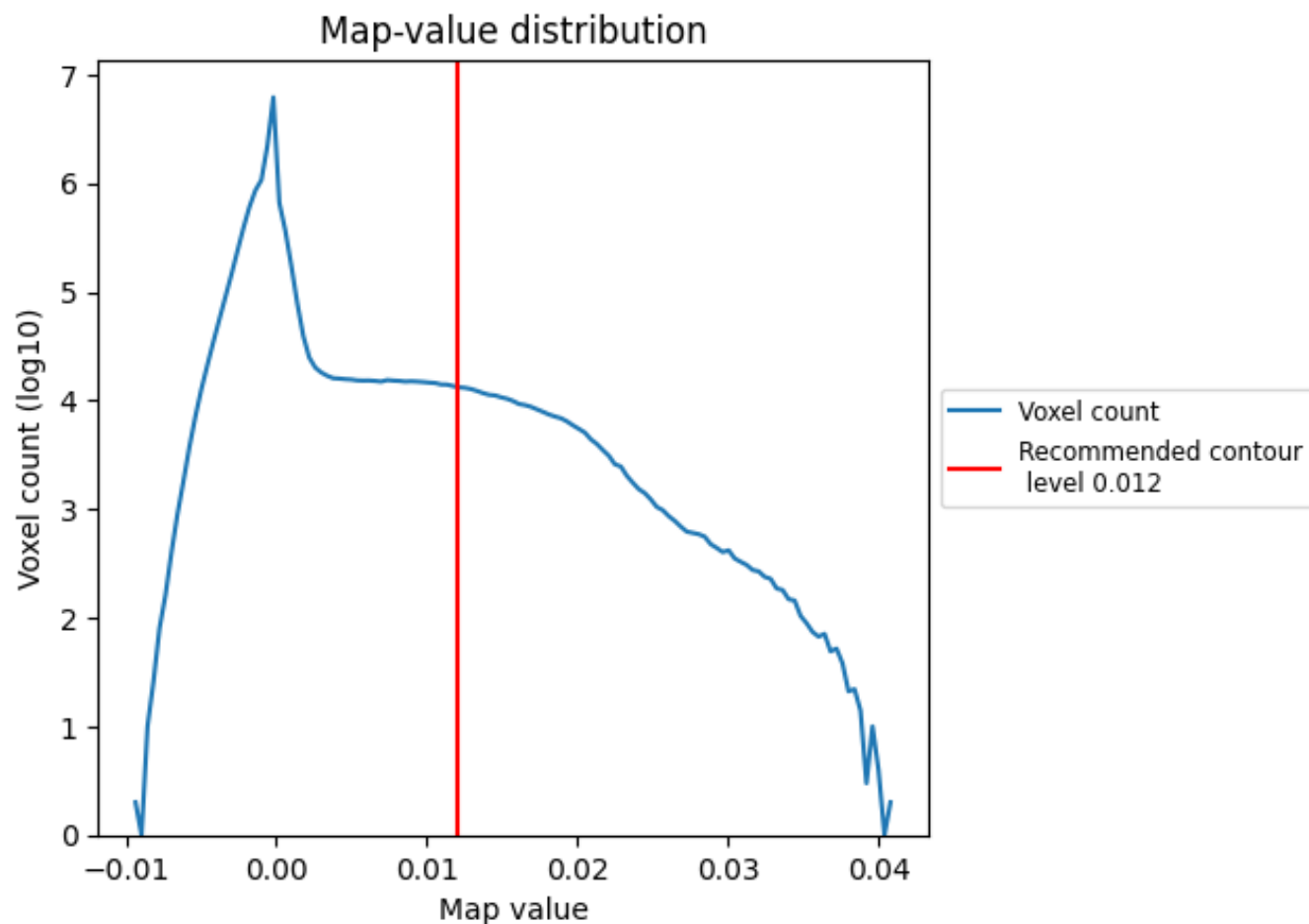
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

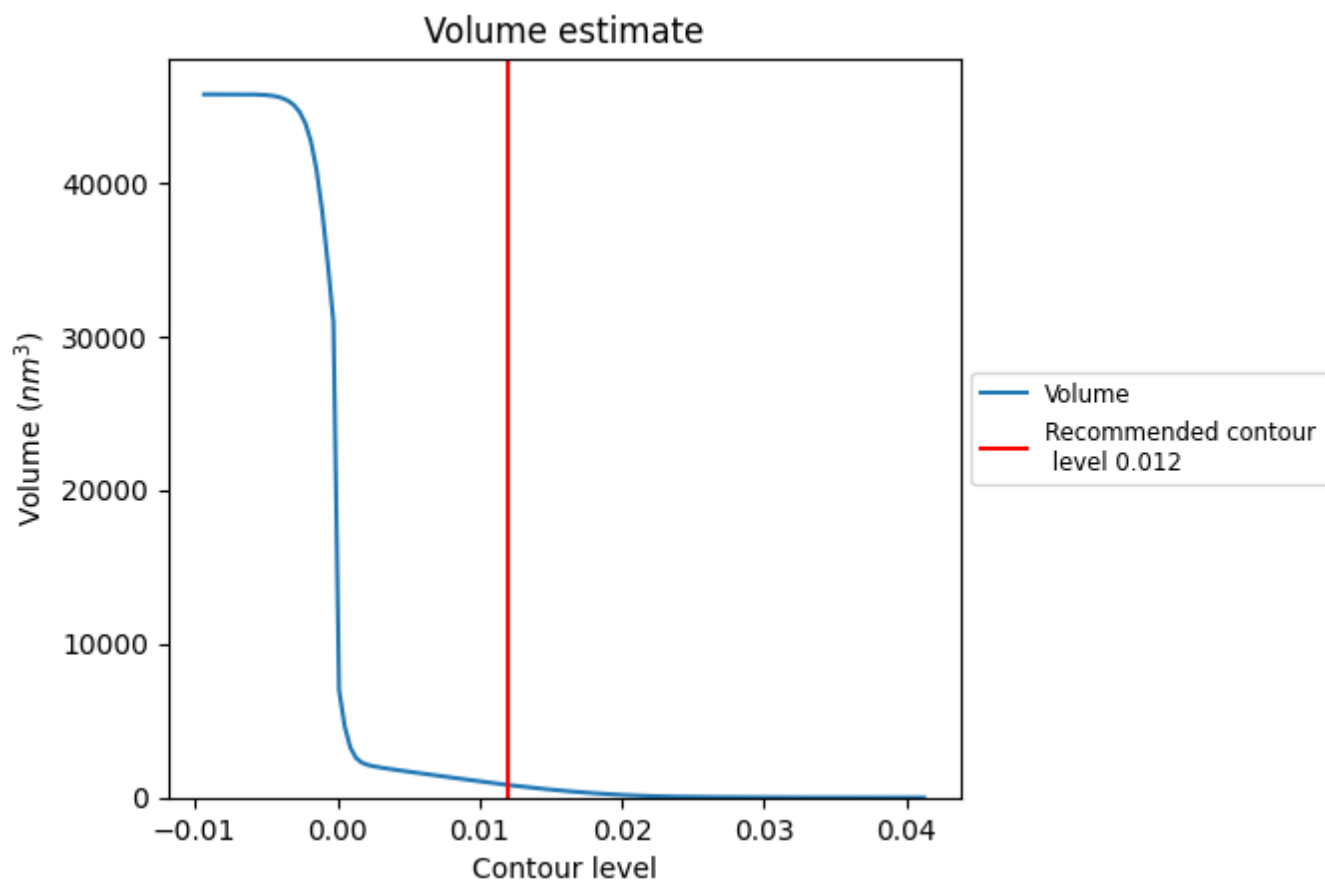
This section contains the results of statistical analysis of the map.

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.

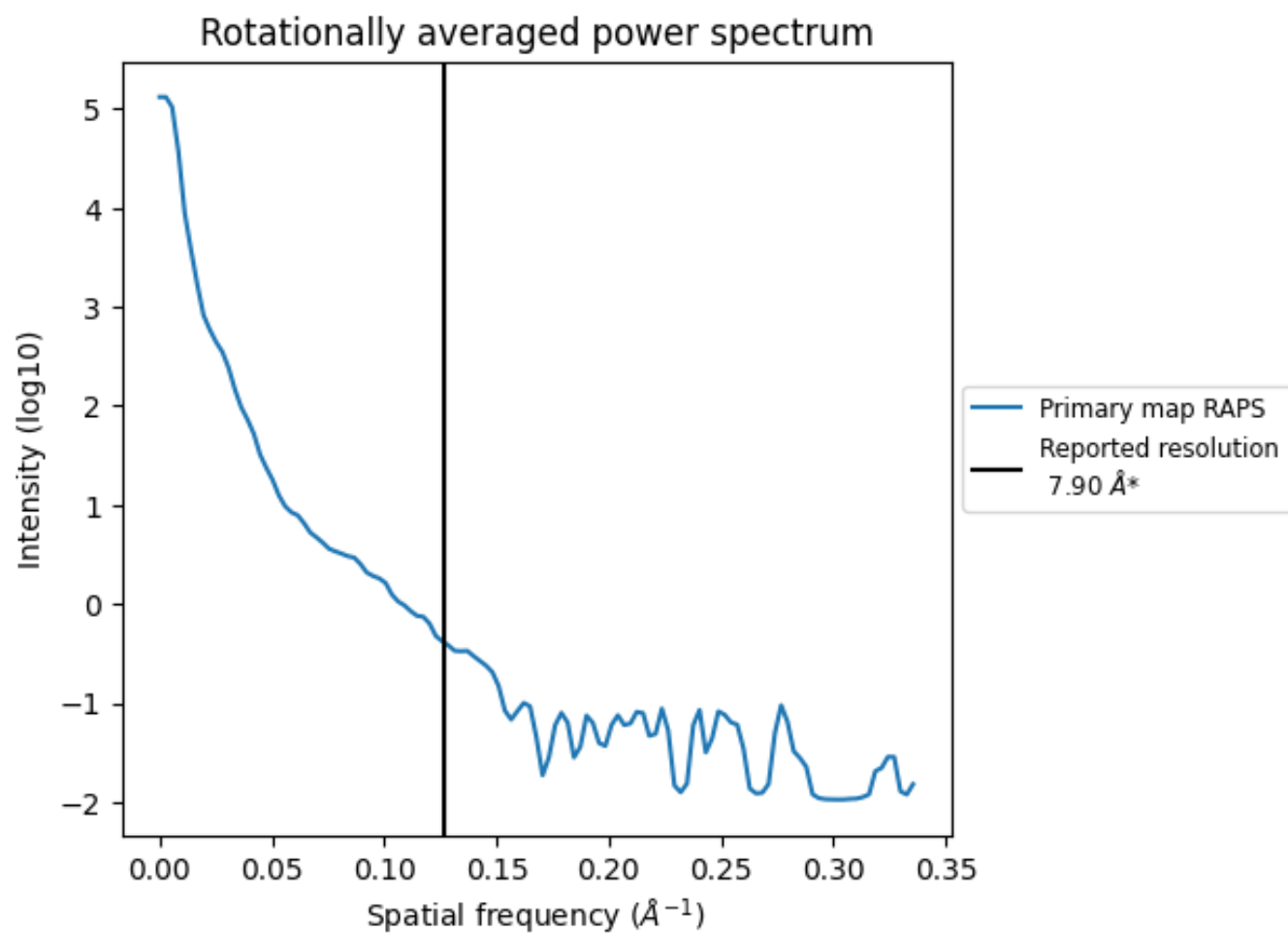
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 821 nm³; this corresponds to an approximate mass of 742 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 ⓘ

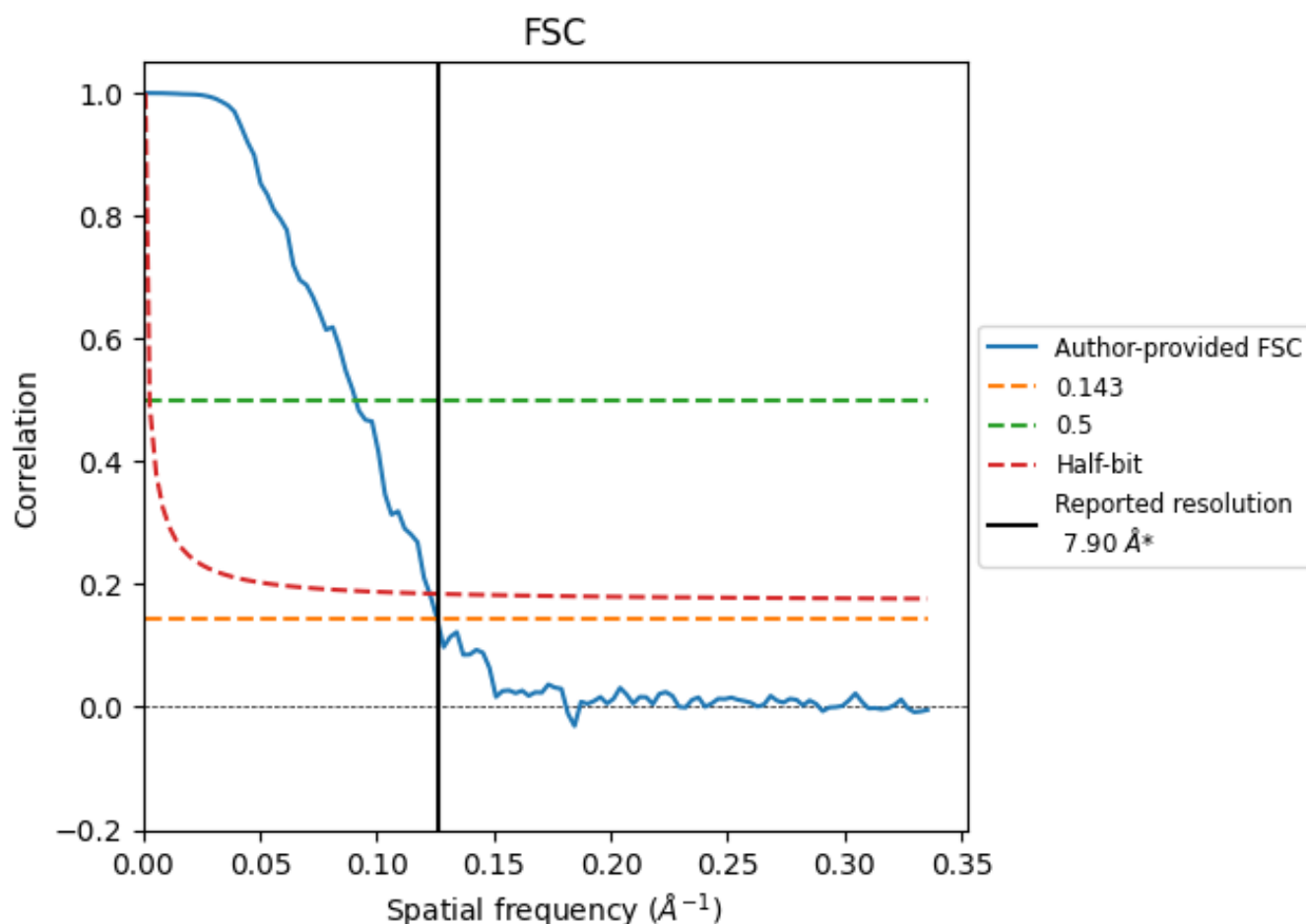


*Reported resolution corresponds to spatial frequency of 0.127 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.127 Å⁻¹

8.2 Resolution estimates [i](#)

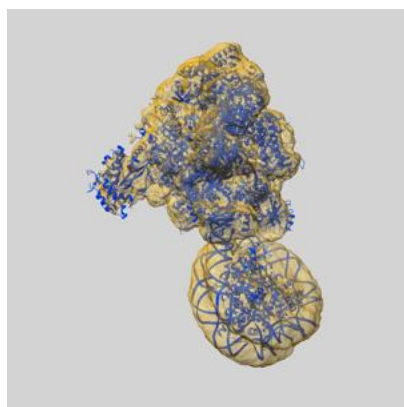
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.90	-	-
Author-provided FSC curve	7.94	11.00	8.15
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

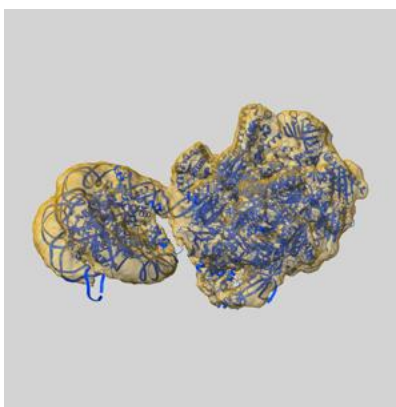
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0671 and PDB model 6J4W. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

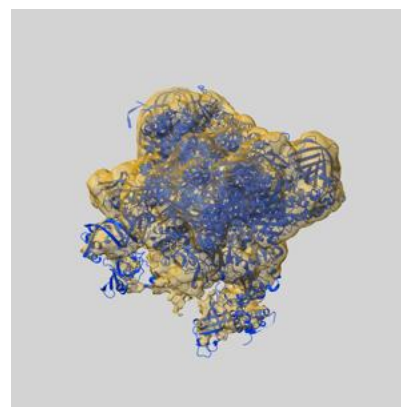
9.1 Map-model overlay [i](#)



X



Y



Z

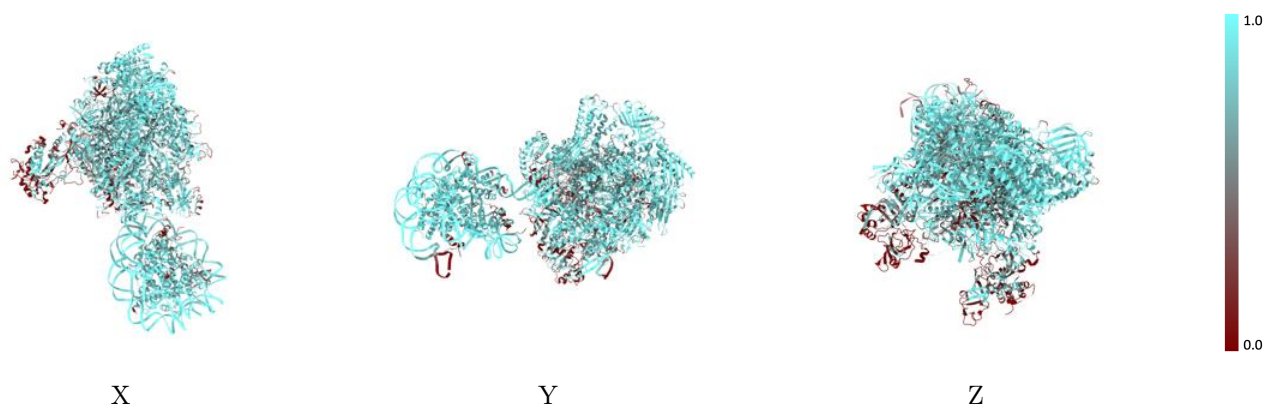
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



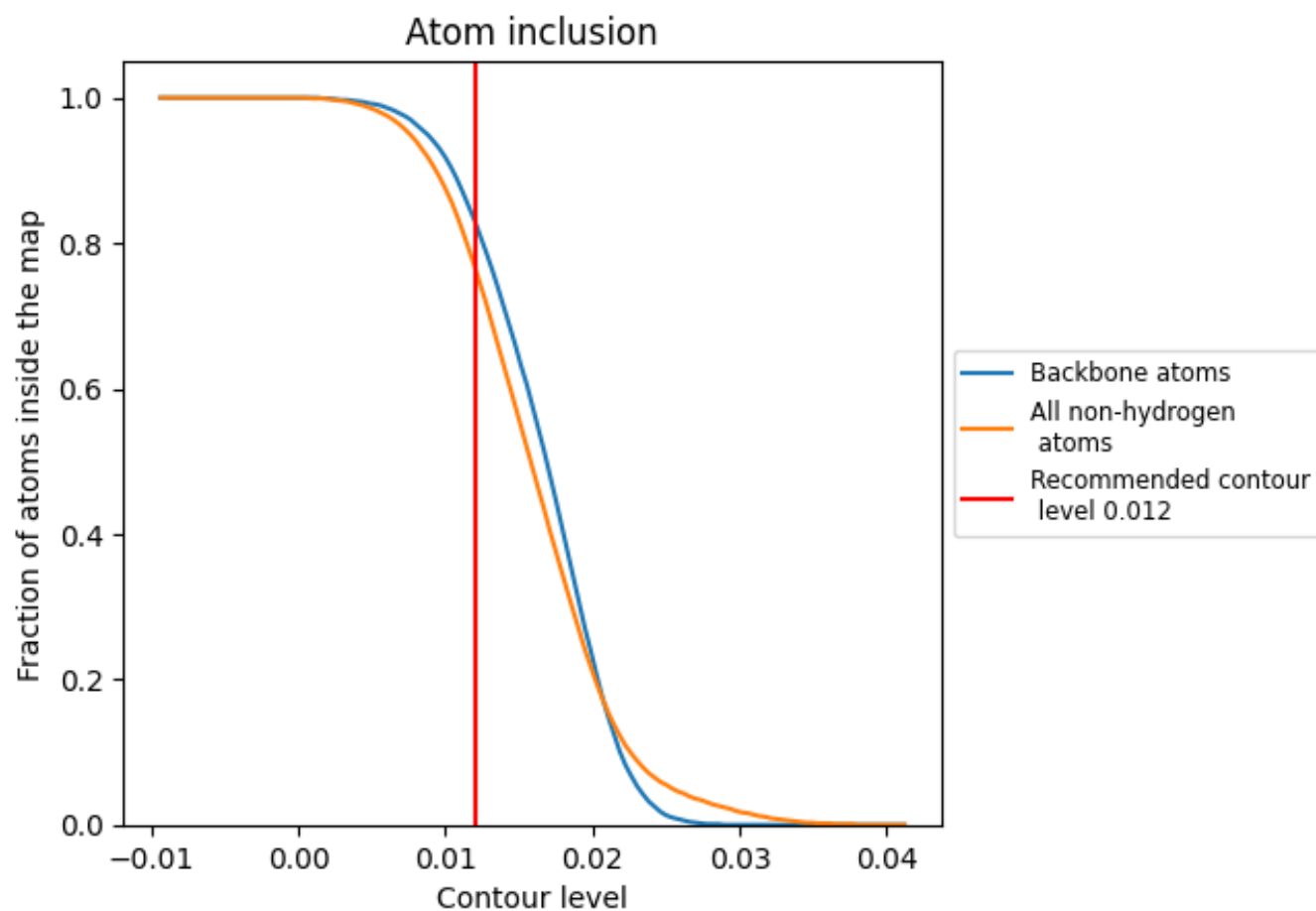
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7680	 0.1230
A	 0.7780	 0.1490
B	 0.8070	 0.1420
C	 0.9110	 0.1490
D	 0.3350	 0.0590
E	 0.8400	 0.1480
F	 0.8620	 0.1560
G	 0.4830	 0.0840
H	 0.9170	 0.1530
I	 0.6880	 0.0580
J	 0.9020	 0.1460
K	 0.8320	 0.1470
L	 0.8560	 0.1170
M	 0.3510	 0.0630
N	 0.8810	 0.1090
P	 0.8210	 0.1770
T	 0.8840	 0.1250
V	 0.3940	 0.0320
W	 0.3320	 0.0560
a	 0.7660	 0.0880
b	 0.9100	 0.0970
c	 0.8530	 0.1160
d	 0.8860	 0.1190
e	 0.8130	 0.0680
f	 0.9280	 0.0850
g	 0.7260	 0.0790
h	 0.8180	 0.0810

