



Full wwPDB EM Validation Report ⓘ

Mar 18, 2026 – 01:00 AM UTC

PDB ID : 9WMU / pdb_00009wmu
EMDB ID : EMD-66105
Title : Co-transcriptional histone H3K36 methylation complex containing RNA polymerase II elongation complex, Set2, and the upstream nucleosome. (temp130, type A)
Authors : Kujirai, T.; Ehara, H.; Ito, T.; Henmi, M.; Sekine, S.; Kurumizaka, H.
Deposited on : 2025-09-03
Resolution : 4.28 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:

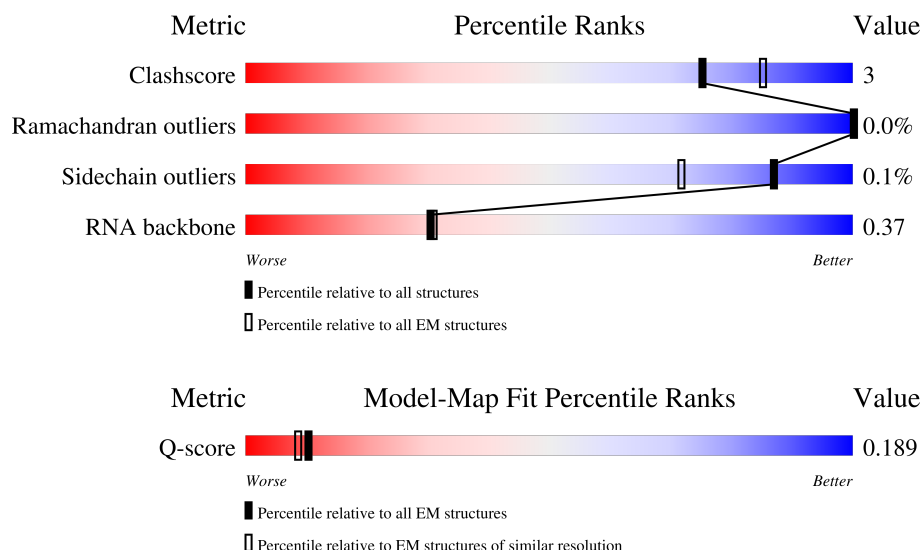
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.28 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	4493 (3.79 - 4.78)

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	

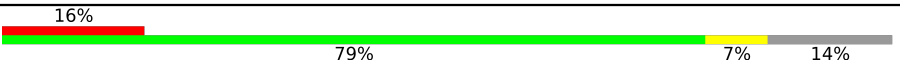
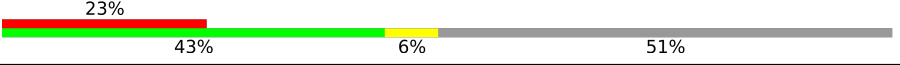
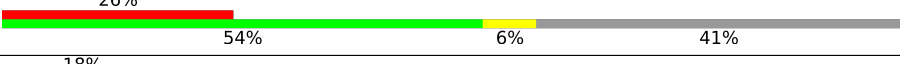
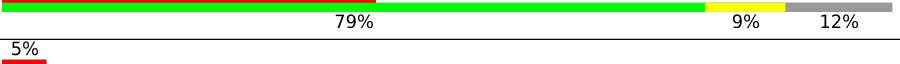
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Mol	Chain	Length	Quality of chain
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	M	113	
14	N	198	
15	P	19	
16	T	198	
17	V	108	
18	W	911	
19	a	139	
19	e	139	
20	b	106	
20	f	106	
21	c	133	
21	g	133	
22	d	129	
22	h	129	
23	m	1503	
24	n	417	

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Mol	Chain	Length	Quality of chain
25	q	1084	
26	r	544	
27	s	725	
28	u	459	
29	v	396	
30	x	395	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 80704 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	1404	Total	C	N	O	S	0	0
			11064	6975	1930	2089	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1164	Total	C	N	O	S	0	0
			9284	5848	1639	1739	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	174	Total	C	N	O	S	0	0
			1349	828	244	274	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1741	1094	312	325	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
			1325	858	214	248	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
			1053	671	169	209	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, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			554	355	97	96	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 protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	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 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	171	Total	C	N	O	P	0	0
			3503	1677	558	1097	171		

- Molecule 15 is a RNA chain called RNA (5'-R(P*UP*CP*CP*UP*UP*UP*UP*GP*UP*GP*CP*GP*GP*CP*CP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	19	Total	C	N	O	P	0	0
			397	177	62	139	19		

- Molecule 16 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	182	Total	C	N	O	P	0	0
			3731	1760	769	1020	182		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	106	Total	C	N	O	S	0	0
			824	512	150	155	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	7	MET	-	initiating methionine	UNP C4R0E6

- Molecule 18 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	535	Total	C	N	O	S	0	0
			4250	2680	754	814	2		

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	104	Total	C	N	O	S	0	0
			841	530	163	145	3		
19	e	91	Total	C	N	O	S	0	0
			739	466	141	130	2		

There are 8 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
a	36	MET	LYS	variant	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243
e	36	MET	LYS	variant	UNP P84243

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	81	Total	C	N	O	S	0	0
			646	407	126	112	1		
20	f	81	Total	C	N	O	S	0	0
			646	407	126	112	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-3	GLY	-	expression tag	UNP P62805

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Chain	Residue	Modelled	Actual	Comment	Reference
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
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	104	Total	C	N	O	0	0
			805	508	157	140		
21	g	106	Total	C	N	O	0	0
			819	517	160	142		

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	93	Total	C	N	O	S	0
			725	456	130	137	2	0
22	h	94	Total	C	N	O	S	0
			735	462	132	139	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-3	GLY	-	expression tag	UNP P06899
d	-2	SER	-	expression tag	UNP P06899
d	-1	HIS	-	expression tag	UNP P06899
h	-3	GLY	-	expression tag	UNP P06899
h	-2	SER	-	expression tag	UNP P06899
h	-1	HIS	-	expression tag	UNP P06899

- Molecule 23 is a protein called Transcription elongation factor Spt6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	m	1178	Total	C	N	O	S	0	0
			9653	6112	1648	1866	27		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	-2	GLY	-	expression tag	UNP C4R7H2
m	-1	PRO	-	expression tag	UNP C4R7H2
m	0	GLY	-	expression tag	UNP C4R7H2

- Molecule 24 is a protein called Protein that interacts with Spt6p and copurifies with Spt5p and RNA polymerase II.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	n	139	Total	C	N	O	S	0	0
			1115	716	193	202	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	-2	GLY	-	expression tag	UNP C4R7L8
n	-1	PRO	-	expression tag	UNP C4R7L8
n	0	GLY	-	expression tag	UNP C4R7L8

- Molecule 25 is a protein called Component of the Paf1p complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	q	930	Total	C	N	O	S	0	0
			7552	4805	1283	1439	25		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	-39	MET	-	initiating methionine	UNP C4R6B2
q	-38	LYS	-	expression tag	UNP C4R6B2
q	-37	ASP	-	expression tag	UNP C4R6B2
q	-36	HIS	-	expression tag	UNP C4R6B2
q	-35	LEU	-	expression tag	UNP C4R6B2
q	-34	ILE	-	expression tag	UNP C4R6B2
q	-33	HIS	-	expression tag	UNP C4R6B2
q	-32	ASN	-	expression tag	UNP C4R6B2

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Chain	Residue	Modelled	Actual	Comment	Reference
q	-31	HIS	-	expression tag	UNP C4R6B2
q	-30	HIS	-	expression tag	UNP C4R6B2
q	-29	LYS	-	expression tag	UNP C4R6B2
q	-28	HIS	-	expression tag	UNP C4R6B2
q	-27	GLU	-	expression tag	UNP C4R6B2
q	-26	HIS	-	expression tag	UNP C4R6B2
q	-25	ALA	-	expression tag	UNP C4R6B2
q	-24	HIS	-	expression tag	UNP C4R6B2
q	-23	ALA	-	expression tag	UNP C4R6B2
q	-22	GLU	-	expression tag	UNP C4R6B2
q	-21	HIS	-	expression tag	UNP C4R6B2
q	-20	ASP	-	expression tag	UNP C4R6B2
q	-19	TYR	-	expression tag	UNP C4R6B2
q	-18	LYS	-	expression tag	UNP C4R6B2
q	-17	ASP	-	expression tag	UNP C4R6B2
q	-16	ASP	-	expression tag	UNP C4R6B2
q	-15	ASP	-	expression tag	UNP C4R6B2
q	-14	ASP	-	expression tag	UNP C4R6B2
q	-13	LYS	-	expression tag	UNP C4R6B2
q	-12	GLU	-	expression tag	UNP C4R6B2
q	-11	HIS	-	expression tag	UNP C4R6B2
q	-10	LEU	-	expression tag	UNP C4R6B2
q	-9	TYR	-	expression tag	UNP C4R6B2
q	-8	PHE	-	expression tag	UNP C4R6B2
q	-7	GLN	-	expression tag	UNP C4R6B2
q	-6	GLY	-	expression tag	UNP C4R6B2
q	-5	SER	-	expression tag	UNP C4R6B2
q	-4	SER	-	expression tag	UNP C4R6B2
q	-3	GLY	-	expression tag	UNP C4R6B2
q	-2	SER	-	expression tag	UNP C4R6B2
q	-1	SER	-	expression tag	UNP C4R6B2
q	0	GLY	-	expression tag	UNP C4R6B2

- Molecule 26 is a protein called RNAPII-associated chromatin remodeling Paf1 complex sub-unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	r	266	Total	C	N	O	S	0	0
			2139	1342	374	412	11		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	-29	MET	-	initiating methionine	UNP F2QQ42
r	-28	LYS	-	expression tag	UNP F2QQ42
r	-27	ASP	-	expression tag	UNP F2QQ42
r	-26	HIS	-	expression tag	UNP F2QQ42
r	-25	LEU	-	expression tag	UNP F2QQ42
r	-24	ILE	-	expression tag	UNP F2QQ42
r	-23	HIS	-	expression tag	UNP F2QQ42
r	-22	ASN	-	expression tag	UNP F2QQ42
r	-21	HIS	-	expression tag	UNP F2QQ42
r	-20	HIS	-	expression tag	UNP F2QQ42
r	-19	LYS	-	expression tag	UNP F2QQ42
r	-18	HIS	-	expression tag	UNP F2QQ42
r	-17	GLU	-	expression tag	UNP F2QQ42
r	-16	HIS	-	expression tag	UNP F2QQ42
r	-15	ALA	-	expression tag	UNP F2QQ42
r	-14	HIS	-	expression tag	UNP F2QQ42
r	-13	ALA	-	expression tag	UNP F2QQ42
r	-12	GLU	-	expression tag	UNP F2QQ42
r	-11	HIS	-	expression tag	UNP F2QQ42
r	-10	LEU	-	expression tag	UNP F2QQ42
r	-9	TYR	-	expression tag	UNP F2QQ42
r	-8	PHE	-	expression tag	UNP F2QQ42
r	-7	GLN	-	expression tag	UNP F2QQ42
r	-6	GLY	-	expression tag	UNP F2QQ42
r	-5	SER	-	expression tag	UNP F2QQ42
r	-4	SER	-	expression tag	UNP F2QQ42
r	-3	GLY	-	expression tag	UNP F2QQ42
r	-2	SER	-	expression tag	UNP F2QQ42
r	-1	SER	-	expression tag	UNP F2QQ42
r	0	GLY	-	expression tag	UNP F2QQ42

- Molecule 27 is a protein called Histone-lysine N-methyltransferase, H3 lysine-36 specific.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	s	431	Total	C	N	O	S	0	0
			3419	2126	593	677	23		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	-2	GLY	-	expression tag	UNP C4QY01
s	-1	PRO	-	expression tag	UNP C4QY01
s	0	GLY	-	expression tag	UNP C4QY01

- Molecule 28 is a protein called Leo1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	u	208	Total	C	N	O	S	0	0
			1707	1063	304	337	3		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	-29	MET	-	initiating methionine	UNP C4R3K1
u	-28	LYS	-	expression tag	UNP C4R3K1
u	-27	ASP	-	expression tag	UNP C4R3K1
u	-26	HIS	-	expression tag	UNP C4R3K1
u	-25	LEU	-	expression tag	UNP C4R3K1
u	-24	ILE	-	expression tag	UNP C4R3K1
u	-23	HIS	-	expression tag	UNP C4R3K1
u	-22	ASN	-	expression tag	UNP C4R3K1
u	-21	HIS	-	expression tag	UNP C4R3K1
u	-20	HIS	-	expression tag	UNP C4R3K1
u	-19	LYS	-	expression tag	UNP C4R3K1
u	-18	HIS	-	expression tag	UNP C4R3K1
u	-17	GLU	-	expression tag	UNP C4R3K1
u	-16	HIS	-	expression tag	UNP C4R3K1
u	-15	ALA	-	expression tag	UNP C4R3K1
u	-14	HIS	-	expression tag	UNP C4R3K1
u	-13	ALA	-	expression tag	UNP C4R3K1
u	-12	GLU	-	expression tag	UNP C4R3K1
u	-11	HIS	-	expression tag	UNP C4R3K1
u	-10	LEU	-	expression tag	UNP C4R3K1
u	-9	TYR	-	expression tag	UNP C4R3K1
u	-8	PHE	-	expression tag	UNP C4R3K1
u	-7	GLN	-	expression tag	UNP C4R3K1
u	-6	GLY	-	expression tag	UNP C4R3K1
u	-5	SER	-	expression tag	UNP C4R3K1
u	-4	SER	-	expression tag	UNP C4R3K1
u	-3	GLY	-	expression tag	UNP C4R3K1
u	-2	SER	-	expression tag	UNP C4R3K1
u	-1	SER	-	expression tag	UNP C4R3K1
u	0	GLY	-	expression tag	UNP C4R3K1

- Molecule 29 is a protein called RNAP II-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	v	349	Total	C	N	O	S	0	0
			2878	1835	510	528	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-2	GLY	-	expression tag	UNP C4R997
v	-1	SER	-	expression tag	UNP C4R997
v	0	ALA	-	expression tag	UNP C4R997

- Molecule 30 is a protein called Constituent of Paf1 complex with RNA polymerase II, Paf1p, Hpr1p, Ctr9, Leo1, Rtf1 and Ccr4p.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	x	205	Total	C	N	O	S	0	0
			1682	1086	287	307	2		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	-29	MET	-	initiating methionine	UNP C4R1E6
x	-28	LYS	-	expression tag	UNP C4R1E6
x	-27	ASP	-	expression tag	UNP C4R1E6
x	-26	HIS	-	expression tag	UNP C4R1E6
x	-25	LEU	-	expression tag	UNP C4R1E6
x	-24	ILE	-	expression tag	UNP C4R1E6
x	-23	HIS	-	expression tag	UNP C4R1E6
x	-22	ASN	-	expression tag	UNP C4R1E6
x	-21	HIS	-	expression tag	UNP C4R1E6
x	-20	HIS	-	expression tag	UNP C4R1E6
x	-19	LYS	-	expression tag	UNP C4R1E6
x	-18	HIS	-	expression tag	UNP C4R1E6
x	-17	GLU	-	expression tag	UNP C4R1E6
x	-16	HIS	-	expression tag	UNP C4R1E6
x	-15	ALA	-	expression tag	UNP C4R1E6
x	-14	HIS	-	expression tag	UNP C4R1E6
x	-13	ALA	-	expression tag	UNP C4R1E6
x	-12	GLU	-	expression tag	UNP C4R1E6
x	-11	HIS	-	expression tag	UNP C4R1E6
x	-10	LEU	-	expression tag	UNP C4R1E6
x	-9	TYR	-	expression tag	UNP C4R1E6
x	-8	PHE	-	expression tag	UNP C4R1E6
x	-7	GLN	-	expression tag	UNP C4R1E6

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Chain	Residue	Modelled	Actual	Comment	Reference
x	-6	GLY	-	expression tag	UNP C4R1E6
x	-5	SER	-	expression tag	UNP C4R1E6
x	-4	SER	-	expression tag	UNP C4R1E6
x	-3	GLY	-	expression tag	UNP C4R1E6
x	-2	SER	-	expression tag	UNP C4R1E6
x	-1	SER	-	expression tag	UNP C4R1E6
x	0	GLY	-	expression tag	UNP C4R1E6

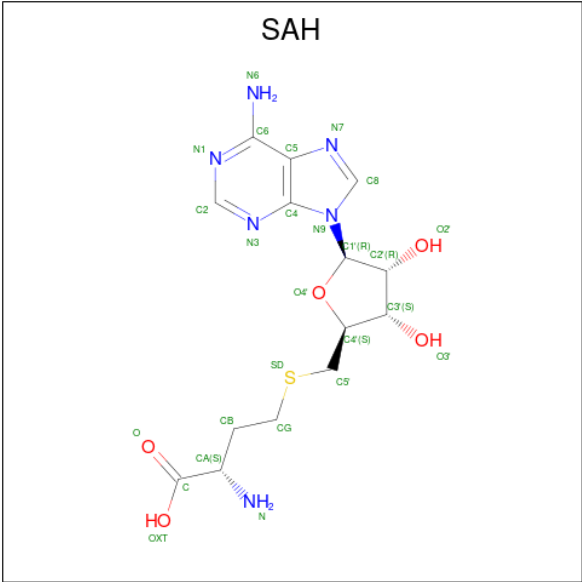
- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total 2	Zn 2	0
31	B	1	Total 1	Zn 1	0
31	C	1	Total 1	Zn 1	0
31	I	2	Total 2	Zn 2	0
31	J	1	Total 1	Zn 1	0
31	L	1	Total 1	Zn 1	0
31	M	1	Total 1	Zn 1	0
31	V	1	Total 1	Zn 1	0
31	s	3	Total 3	Zn 3	0

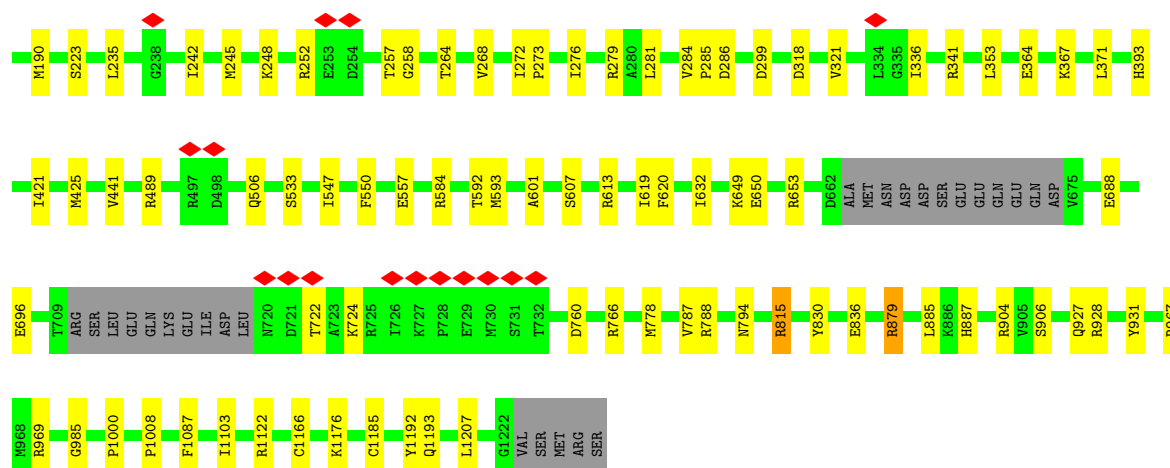
- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 33 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).

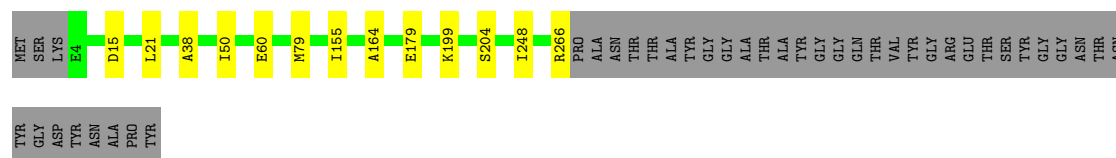


Mol	Chain	Residues	Atoms					AltConf
33	s	1	Total	C	N	O	S	0
			26	14	6	5	1	



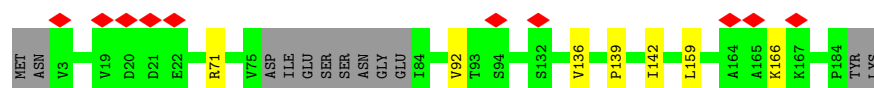
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core

Chain C: 82% 13%



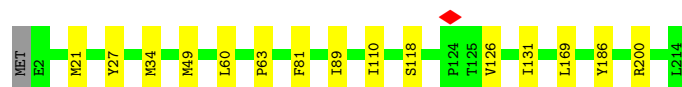
- Molecule 4: RNA polymerase II subunit B32

Chain D: 5% 90% 6%



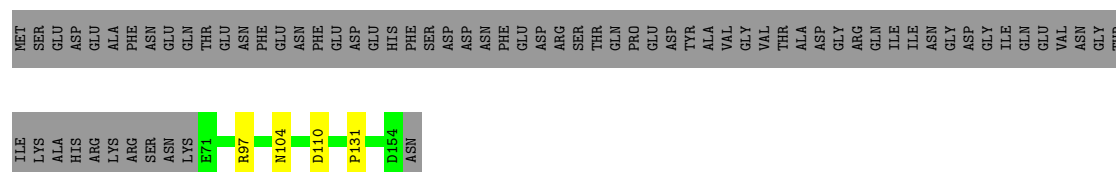
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 93% 7%



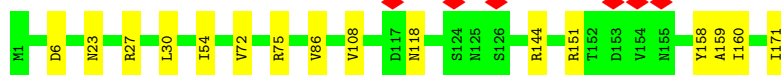
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

Chain F: 52% 46%



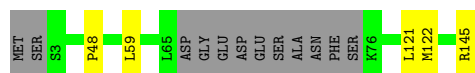
- Molecule 7: RNA polymerase II subunit

Chain G:  91% 9%



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

Chain H:  88% 8%



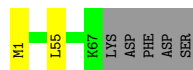
- Molecule 9: DNA-directed RNA polymerase subunit

Chain I:  83% 13%



- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J:  90% 7%



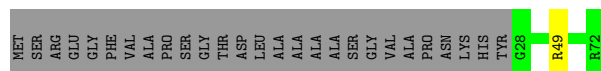
- Molecule 11: RNA polymerase II subunit B12.5

Chain K:  84% 12%



- Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L:  61% 38%



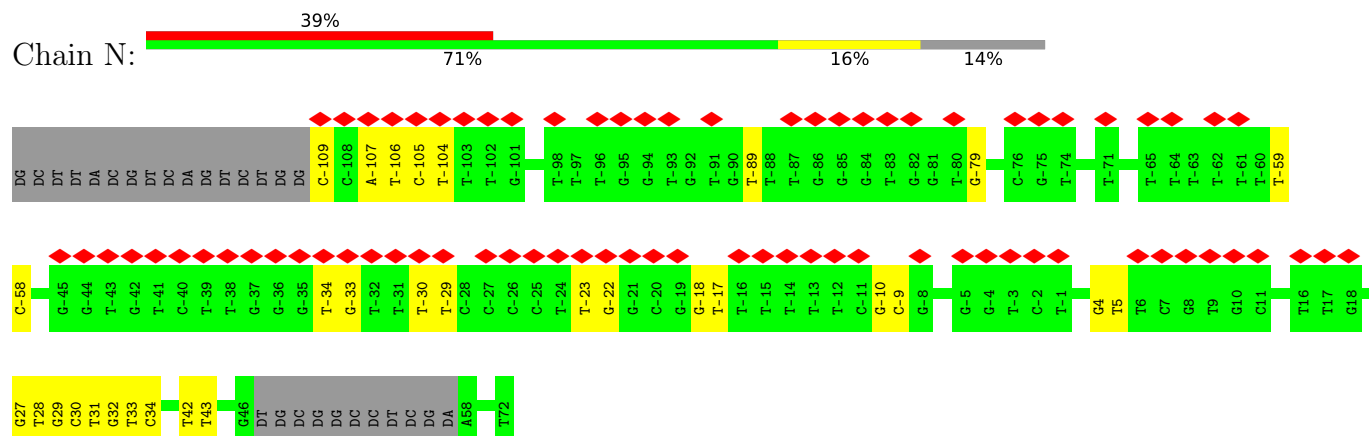
- Molecule 13: Transcription elongation factor 1 homolog

Chain M:  51% 5% 43%



ASP
ASP
TYR
ASP
ASP
GLU
PHE

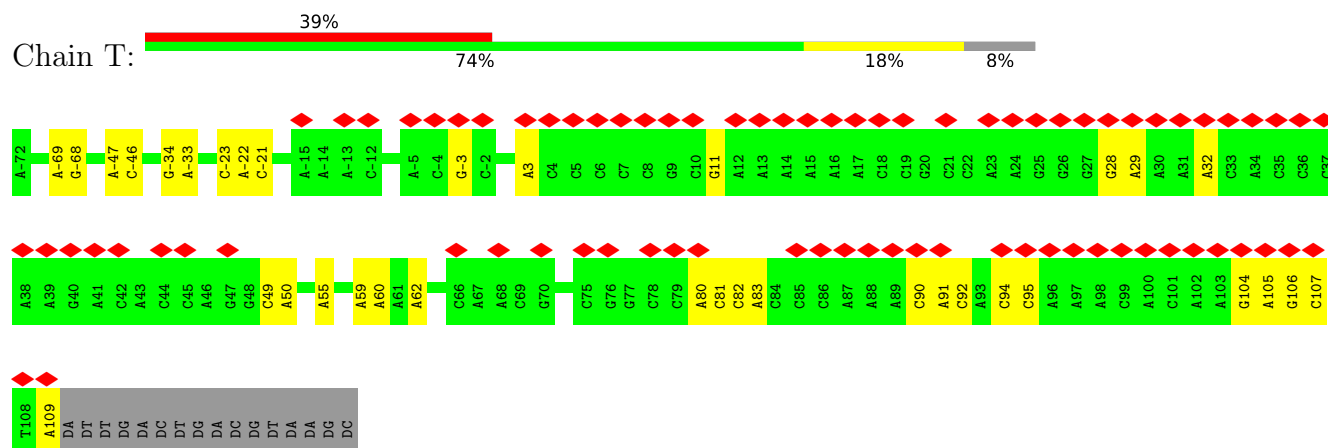
• Molecule 14: DNA (198-MER)



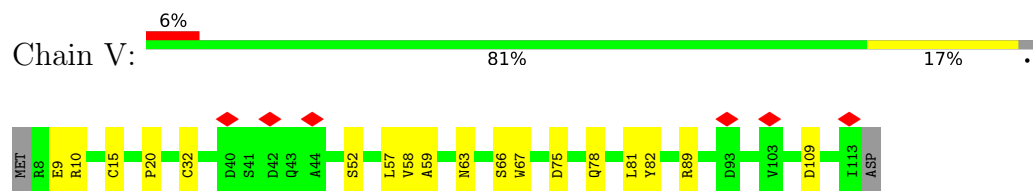
• Molecule 15: RNA (5'-R(P*UP*CP*CP*UP*UP*UP*UP*GP*UP*GP*CP*GP*GP*CP*CP*UP*CP*GP*A)-3')



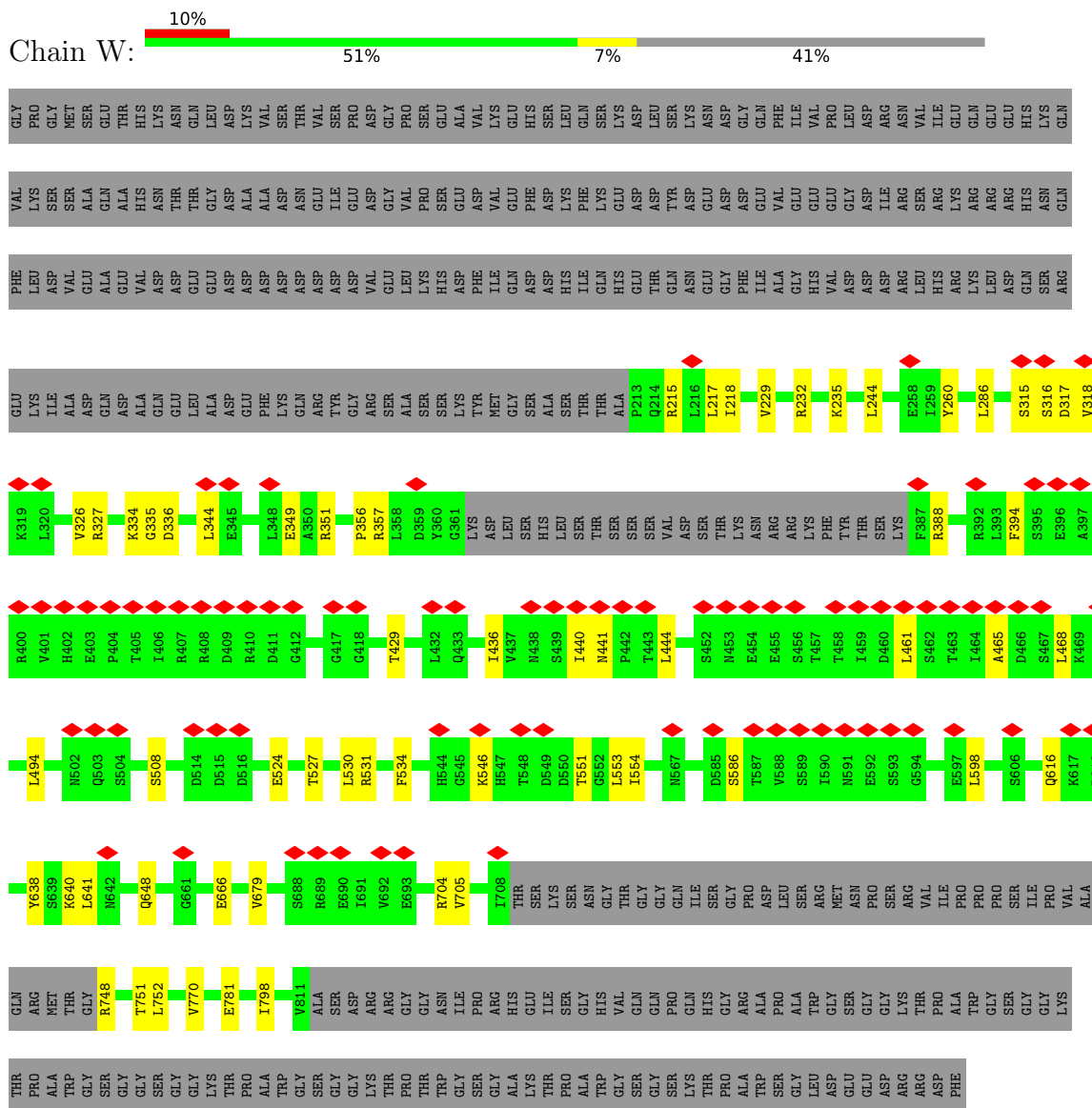
• Molecule 16: DNA (198-MER)



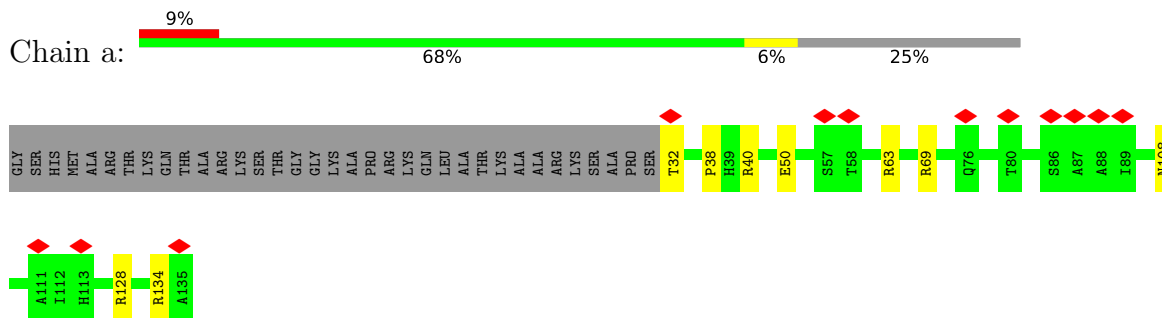
• Molecule 17: Transcription elongation factor SPT4



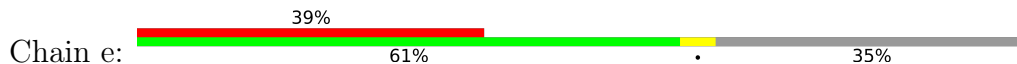
• Molecule 18: Transcription elongation factor SPT5

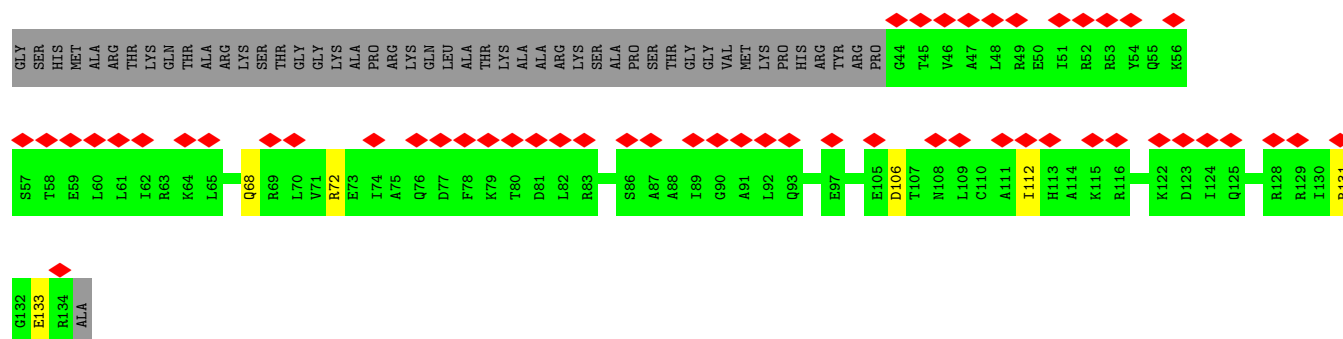


- Molecule 19: Histone H3.3

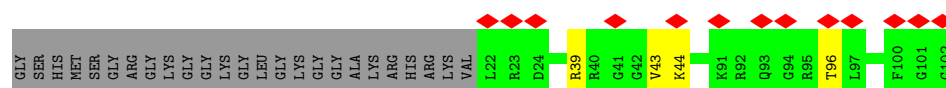


- Molecule 19: Histone H3.3

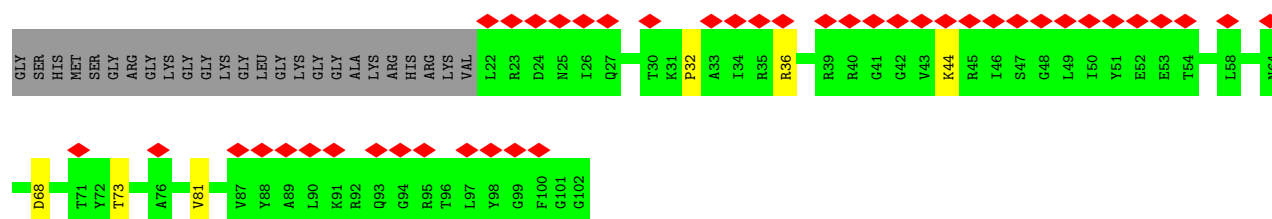




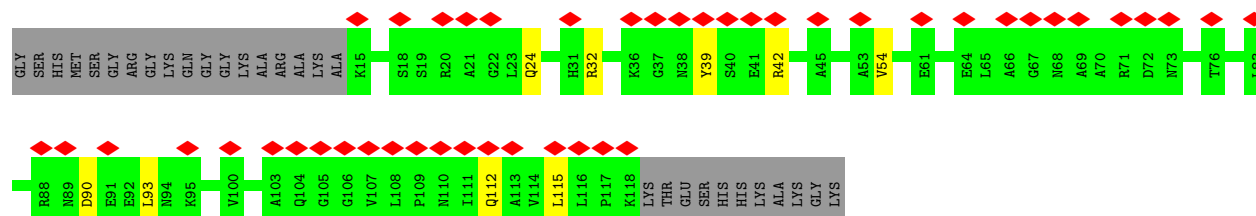
• Molecule 20: Histone H4



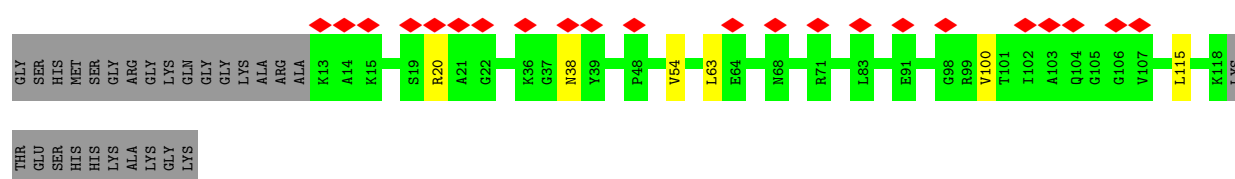
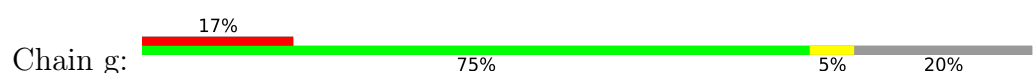
• Molecule 20: Histone H4



• Molecule 21: Histone H2A type 1-B/E



• Molecule 21: Histone H2A type 1-B/E



Chain d:

24%

67%

5%

28%

GLY
SER
HIS
MET
PRO
GLU
PRO
ALA
LYS
SER
ALA
PRO
PRO
LYS
LYS
GLY
SER
LYS
LYS
ALA
VAL
THR
LYS
LYS
ALA
GLN
LYS
LYS
ASP
GLY
LYS
LYS
ARG
LYS
ARG
S32
R33
K34
E35
S36
Y37
L45
K46
Q47
V48
H49
P50
D51
T52
G53
S56
N67
A74
S78
S79

Chain h:

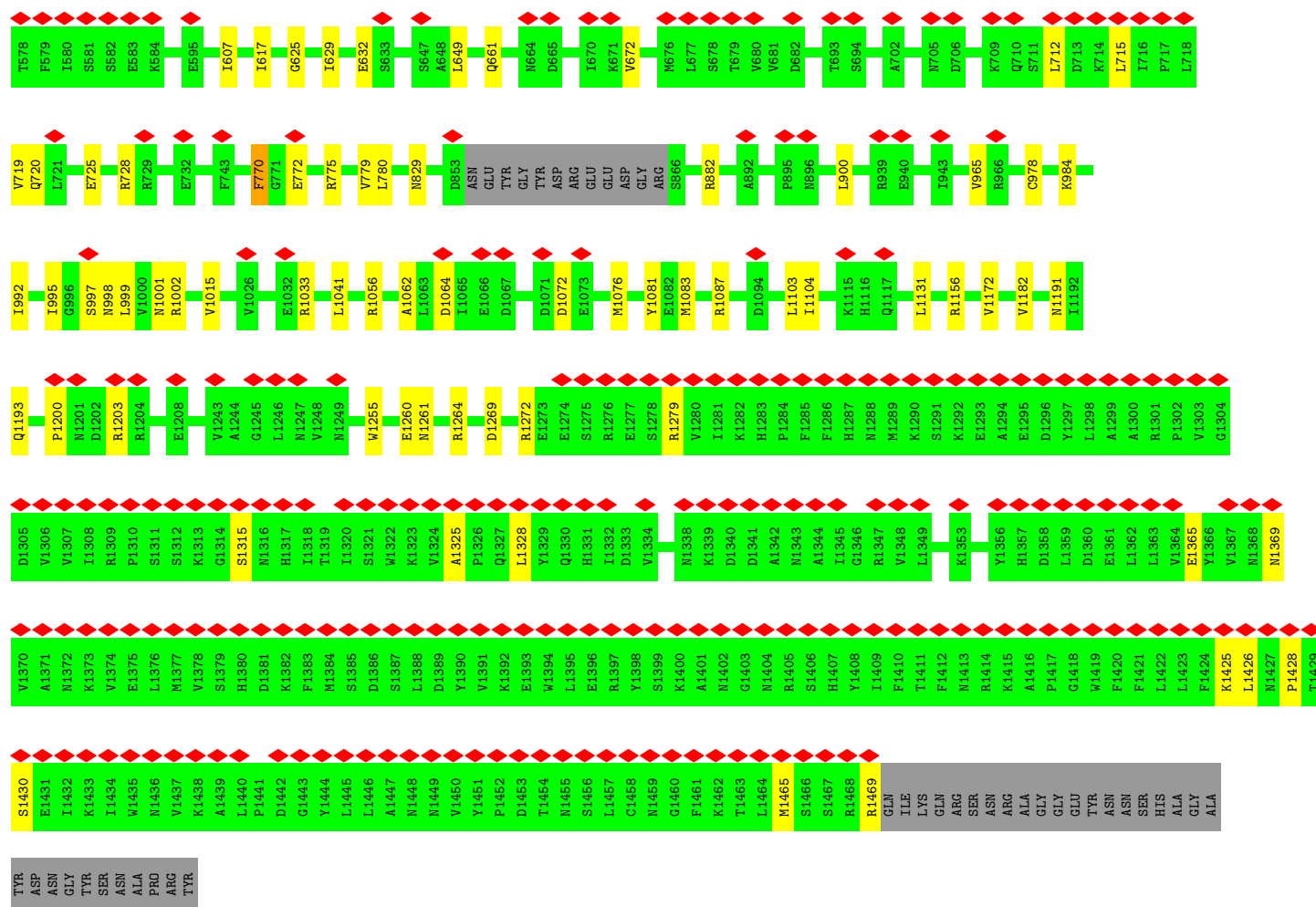
26% 66% 7% 27%

GLY SER HIS MET PRO GLU PRO ALA LYS SER LYS GLY LYS VAL THR LYS ALA GLN LYS LYS ASP GLY LYS LYS ARG LYS ARG S32 R33 K34 V41 Y42 K43 V44 L45 K46 Q47 V48 H49 F50 D51 G60 S64 F70 A77 S78 S79

Chain m:

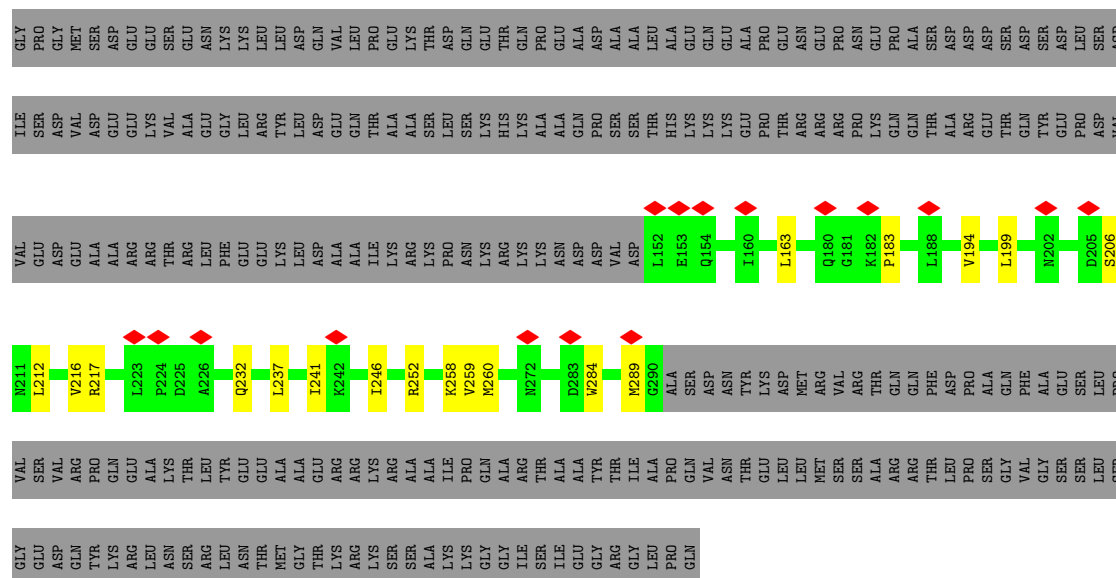
72% 6% 22%

21%

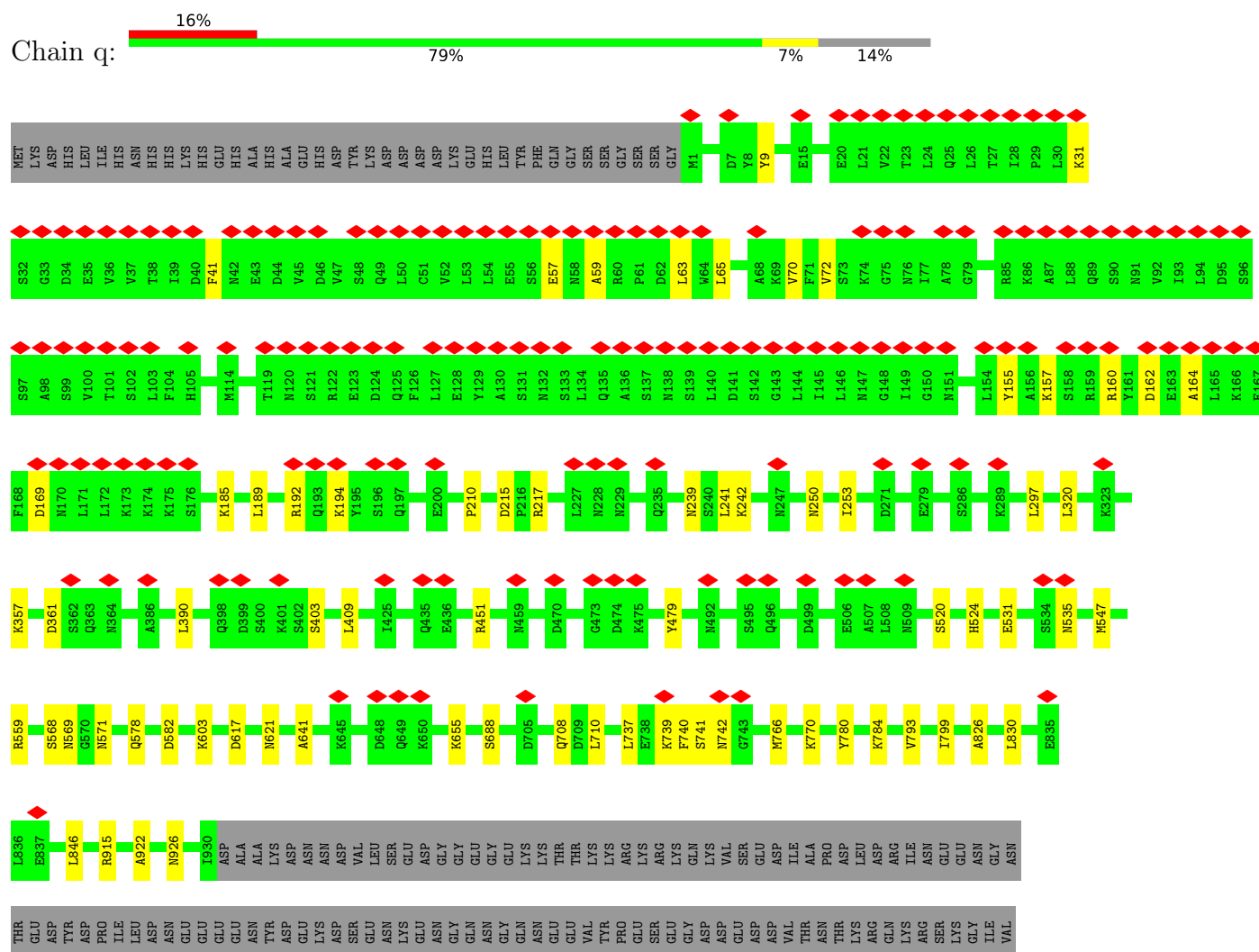


- Molecule 24: Protein that interacts with Spt6p and copurifies with Spt5p and RNA polymerase II

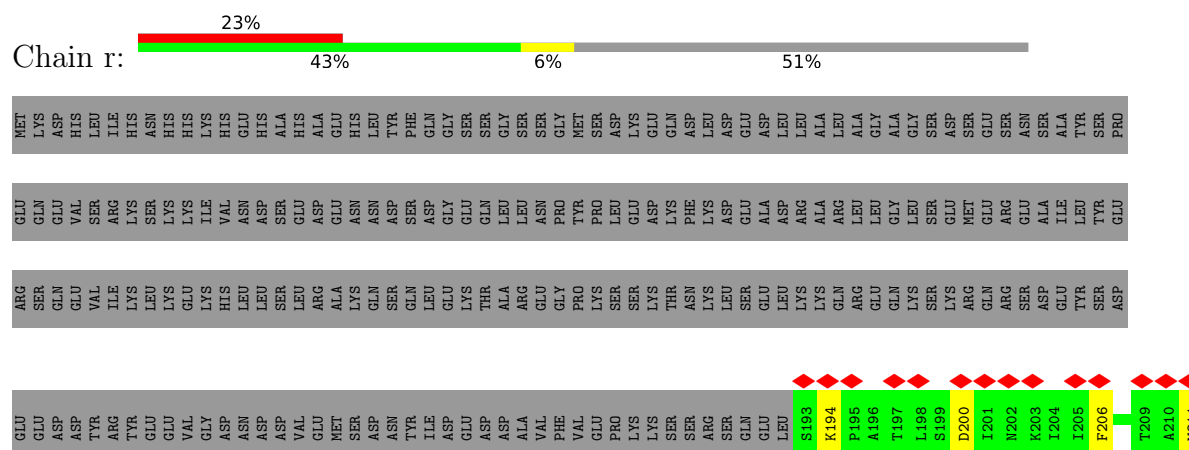
Chain n: 29% 5% 67%

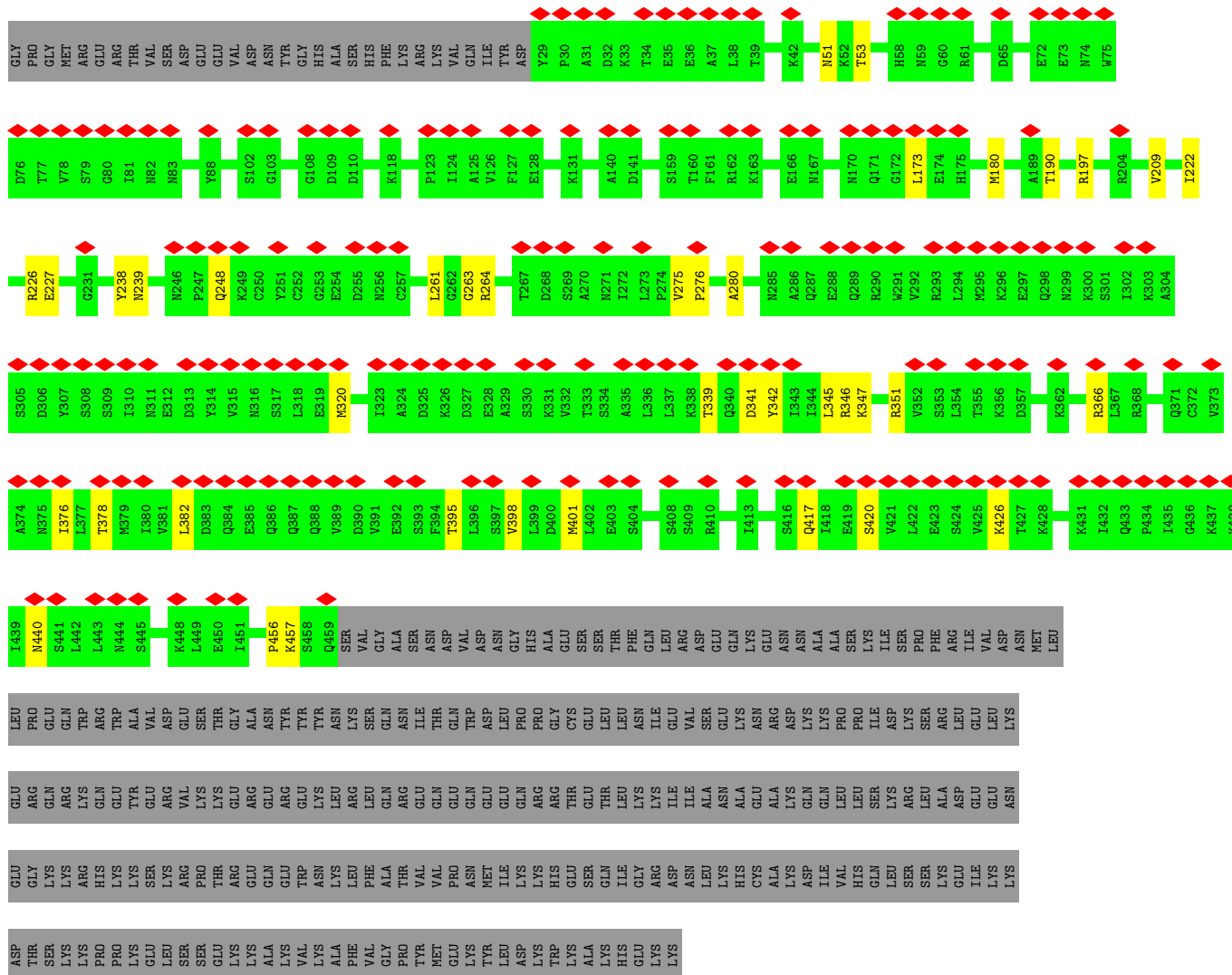


- Molecule 25: Component of the Paf1p complex



- Molecule 26: RNAPII-associated chromatin remodeling Paf1 complex subunit





Chain u:

Chain v: 42% 79% 9% 12%

- Molecule 30: Constituent of Paf1 complex with RNA polymerase II, Paf1p, Hpr1p, Ctr9, Leo1, Rtf1 and Ccr4p



MET LYS ASP HIS ILE HIS ASN HIS HIS HIS HIS HIS ALA ALA GLU HIS LEU TYR PHE GLN GLY SER SER GLY MET GLU PRO LEU ILE ALA LEU ARG GLN ALA ILE ILE LYS ASP LYS LYS PRO VAL GLY VAL ASN GLU THR ILE GLY ASN ALA LYS

VAL LEU ASN ILE GLY LYS GLN TYR LEU ASP ALA PRO THR SER PHE VAL ILE ASN GLY LYS PHE ASN LEU VAL ILE TYR GLN CYS TRP VAL PHE ARG ASP SER SER SER GLN ASP TYR ILE THR THR CYS GLU LYS VAL GLU ASN GLY THR ARG

SER GLU LEU ILE SER TRP LEU LYS GLY GLU ILE THR SER SER ALA PHE ILE LYS GLY GLU VAL ILE THR GLU ASN GLY ASN LYS LYS ARG LYS LEU SER D135 R147 V155 I156 R157 G158 I159 R160 P161 R179 PRO ALA ASN

ALA LYS SER SER ASP SER ASN GLY ARG SER THR SER VAL SER SER SER LYS ASP ALA ARG ASN K206 K222 K226 K239 E240 P241 A242 S243 S244 I250 K271 D291 W292 K296 D301 F302 Q303 Q307 G311 G318 A323 V330 E339

K364 S365

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15255	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.1	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size ($\text{\AA}$)	531.0, 531.0, 531.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.475, 1.475, 1.475	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: SAH, 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	0.22	0/11267	0.50	0/15222
2	B	0.22	0/9464	0.51	0/12763
3	C	0.22	0/2139	0.46	0/2895
4	D	0.17	0/1361	0.45	0/1837
5	E	0.21	0/1773	0.54	0/2385
6	F	0.21	0/687	0.47	0/931
7	G	0.16	0/1354	0.38	0/1837
8	H	0.21	0/1070	0.43	0/1444
9	I	0.14	0/934	0.41	0/1257
10	J	0.21	0/563	0.52	0/753
11	K	0.22	0/953	0.49	0/1291
12	L	0.22	0/365	0.57	0/484
13	M	0.16	0/513	0.37	0/693
14	N	0.31	0/3904	0.64	0/6033
15	P	0.32	0/440	0.65	0/682
16	T	0.29	0/4209	0.57	0/6481
17	V	0.17	0/840	0.46	0/1140
18	W	0.20	0/4319	0.51	0/5838
19	a	0.24	0/853	0.63	0/1144
19	e	0.25	0/747	0.65	0/1001
20	b	0.26	0/653	0.67	0/873
20	f	0.25	0/653	0.67	0/873
21	c	0.23	0/815	0.60	0/1100
21	g	0.26	0/829	0.62	0/1118
22	d	0.23	0/736	0.61	0/990
22	h	0.26	0/746	0.60	0/1001
23	m	0.19	0/9847	0.46	0/13321
24	n	0.19	0/1132	0.45	0/1526
25	q	0.17	0/7689	0.40	0/10368
26	r	0.18	0/2169	0.43	0/2901
27	s	0.24	0/3473	0.55	0/4676
28	u	0.16	0/1740	0.38	0/2347

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	v	0.17	0/2944	0.44	0/3973
30	x	0.15	0/1716	0.39	0/2310
All	All	0.22	0/82897	0.50	0/113488

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11064	0	11090	61	0
2	B	9284	0	9282	62	0
3	C	2098	0	2057	10	0
4	D	1349	0	1345	4	0
5	E	1741	0	1754	10	0
6	F	677	0	693	4	0
7	G	1325	0	1342	10	0
8	H	1053	0	1050	3	0
9	I	917	0	864	9	0
10	J	554	0	573	1	0
11	K	932	0	944	11	0
12	L	359	0	358	1	0
13	M	505	0	495	3	0
14	N	3503	0	1960	27	0
15	P	397	0	203	17	0
16	T	3731	0	2010	27	0
17	V	824	0	795	11	0
18	W	4250	0	4296	52	0
19	a	841	0	883	9	0
19	e	739	0	778	4	0
20	b	646	0	687	4	0
20	f	646	0	687	5	0
21	c	805	0	861	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	g	819	0	879	9	0
22	d	725	0	745	7	0
22	h	735	0	758	11	0
23	m	9653	0	9500	66	0
24	n	1115	0	1186	15	0
25	q	7552	0	7545	46	0
26	r	2139	0	2155	19	0
27	s	3419	0	3351	24	0
28	u	1707	0	1676	20	0
29	v	2878	0	2873	28	0
30	x	1682	0	1731	8	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	V	1	0	0	0	0
31	s	3	0	0	0	0
32	A	1	0	0	0	0
33	s	26	0	19	1	0
All	All	80704	0	77425	482	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 3.

All (482) 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)
1:A:445:PHE:CE2	1:A:471:LEU:HD21	2.24	0.72
14:N:-89:DT:H73	21:c:32:ARG:NH1	2.05	0.72
18:W:218:ILE:CD1	24:n:289:MET:HE1	2.22	0.69
18:W:444:LEU:HG	23:m:284:PHE:CE1	2.28	0.69
18:W:461:LEU:HD13	23:m:278:THR:HA	1.74	0.68
14:N:5:DT:H5'	22:h:33:ARG:HG2	1.75	0.67
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.35	0.67
18:W:444:LEU:HD12	23:m:284:PHE:CD2	2.30	0.67
15:P:-3:U:H4'	15:P:-2:U:OP2	1.95	0.67
1:A:483:PHE:CD2	2:B:836:GLU:HB2	2.29	0.67
14:N:-109:DC:H42	16:T:109:DA:H61	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:-4:U:OP2	15:P:-4:U:H3'	1.95	0.66
1:A:445:PHE:HE2	1:A:471:LEU:HD21	1.60	0.66
14:N:-107:DA:H61	16:T:107:DC:H42	1.45	0.65
23:m:337:GLN:HG2	23:m:458:ARG:HH12	1.62	0.65
18:W:487:ILE:HD11	18:W:531:ARG:HB2	1.79	0.64
16:T:62:DA:OP2	19:a:69:ARG:NH1	2.31	0.64
19:e:68:GLN:HE21	19:e:72:ARG:HH11	1.46	0.63
15:P:-5:C:H5'	23:m:775:ARG:HH11	1.63	0.63
21:c:115:LEU:HD21	19:e:112:ILE:HD11	1.79	0.63
1:A:285:SER:HB2	1:A:290:ILE:HD11	1.80	0.63
14:N:-105:DC:H42	16:T:105:DA:H61	1.46	0.63
21:g:63:LEU:HD13	22:h:45:LEU:HB2	1.81	0.62
14:N:-89:DT:H73	21:c:32:ARG:HH11	1.62	0.62
18:W:444:LEU:HB2	23:m:284:PHE:CE2	2.35	0.62
23:m:473:ASN:HA	23:m:525:ARG:HH12	1.64	0.62
3:C:266:ARG:HH12	11:K:82:ARG:HH12	1.48	0.62
19:a:38:PRO:HD3	27:s:180:MET:HB3	1.82	0.61
23:m:331:ARG:HH11	23:m:368:LYS:HB3	1.65	0.61
25:q:793:VAL:HG11	25:q:830:LEU:HG	1.83	0.61
1:A:1211:MET:SD	1:A:1211:MET:N	2.73	0.61
9:I:33:ASP:OD1	28:u:75:HIS:N	2.35	0.60
2:B:1103:ILE:O	2:B:1122:ARG:NH2	2.34	0.60
23:m:1072:ASP:OD2	27:s:366:ARG:NH2	2.35	0.60
2:B:969:ARG:NH2	3:C:60:GLU:OE1	2.35	0.60
17:V:57:LEU:HD11	17:V:81:LEU:HD22	1.85	0.59
21:c:39:TYR:HB3	22:d:78:SER:HB2	1.83	0.59
1:A:831:LYS:NZ	1:A:1079:THR:O	2.34	0.59
16:T:3:DA:OP1	21:g:20:ARG:NH1	2.35	0.59
17:V:15:CYS:HB3	17:V:32:CYS:SG	2.42	0.59
7:G:27:ARG:NH2	7:G:54:ILE:O	2.36	0.59
24:n:206:SER:O	24:n:210:ASN:ND2	2.35	0.59
25:q:169:ASP:OD1	25:q:185:LYS:NZ	2.35	0.59
2:B:1176:LYS:HD2	18:W:598:LEU:HD23	1.86	0.58
1:A:1262:MET:SD	1:A:1265:ARG:NH1	2.76	0.58
2:B:887:HIS:HA	15:P:-2:U:C4	2.39	0.58
2:B:778:MET:HE3	2:B:794:ASN:HB3	1.84	0.58
25:q:253:ILE:HG12	25:q:297:LEU:HD21	1.84	0.58
25:q:922:ALA:O	25:q:926:ASN:ND2	2.35	0.58
27:s:248:GLN:HB3	27:s:261:LEU:HD12	1.86	0.58
27:s:320:MET:HE3	27:s:347:LYS:HB3	1.84	0.58
27:s:426:LYS:NZ	27:s:440:ASN:OD1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:m:672:VAL:O	23:m:720:GLN:NE2	2.37	0.58
26:r:269:ASP:HB3	26:r:349:LEU:HD21	1.85	0.58
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.85	0.57
2:B:190:MET:SD	2:B:190:MET:N	2.77	0.57
2:B:815:ARG:HD2	29:v:135:SER:HB3	1.86	0.57
8:H:48:PRO:O	8:H:145:ARG:NH2	2.37	0.57
23:m:725:GLU:OE2	23:m:728:ARG:NH1	2.36	0.57
29:v:267:TYR:HB3	29:v:297:TYR:HB3	1.87	0.57
2:B:489:ARG:NH1	2:B:533:SER:O	2.37	0.57
4:D:71:ARG:HE	4:D:92:VAL:HG13	1.70	0.57
22:d:79:ARG:NH2	22:d:83:TYR:OH	2.38	0.57
25:q:569:ASN:O	25:q:603:LYS:NZ	2.36	0.57
27:s:238:TYR:O	27:s:239:ASN:C	2.47	0.57
2:B:50:VAL:HG21	2:B:82:ILE:HD11	1.86	0.57
18:W:218:ILE:HG13	24:n:289:MET:HE1	1.86	0.57
28:u:121:PHE:HB3	28:u:153:ARG:HB3	1.86	0.57
1:A:127:ARG:O	1:A:129:ARG:NH2	2.38	0.57
18:W:444:LEU:HG	23:m:284:PHE:CZ	2.39	0.57
29:v:233:GLY:O	29:v:244:ASN:ND2	2.38	0.57
10:J:1:MET:HA	10:J:55:LEU:HB2	1.86	0.57
25:q:793:VAL:HG13	25:q:826:ALA:HB1	1.87	0.57
13:M:49:CYS:SG	13:M:52:CYS:HB2	2.45	0.56
25:q:531:GLU:O	25:q:535:ASN:N	2.38	0.56
1:A:1207:LYS:O	1:A:1277:ARG:NH1	2.39	0.56
26:r:200:ASP:HB3	26:r:319:VAL:HG11	1.88	0.56
1:A:473:LEU:HD23	2:B:836:GLU:HG3	1.88	0.56
18:W:616:GLN:OE1	18:W:619:SER:OG	2.23	0.56
21:c:115:LEU:HB3	20:f:44:LYS:HD2	1.88	0.56
23:m:1056:ARG:HB3	23:m:1076:MET:HB3	1.88	0.56
28:u:209:LEU:HB2	29:v:252:PHE:HB2	1.88	0.56
1:A:1201:ARG:NH1	1:A:1235:ALA:O	2.39	0.56
2:B:281:LEU:HD12	2:B:364:GLU:HB2	1.88	0.56
23:m:1261:ASN:OD1	23:m:1264:ARG:NH1	2.39	0.56
5:E:126:VAL:HG11	5:E:131:ILE:HG12	1.88	0.55
28:u:145:ILE:O	28:u:149:THR:OG1	2.21	0.55
2:B:421:ILE:HD11	2:B:441:VAL:HG22	1.89	0.55
9:I:73:LYS:NZ	9:I:112:ASP:OD2	2.39	0.55
9:I:20:LYS:O	9:I:23:GLN:NE2	2.39	0.54
26:r:490:VAL:HG22	26:r:495:ARG:HE	1.72	0.54
18:W:524:GLU:O	24:n:232:GLN:NE2	2.40	0.54
18:W:327:ARG:NH2	18:W:335:GLY:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:59:LEU:HD21	8:H:122:MET:HE1	1.88	0.54
30:x:292:TRP:HA	30:x:295:LYS:HE2	1.89	0.54
9:I:100:PHE:HE1	9:I:111:ARG:HE	1.56	0.54
1:A:40:ILE:HG23	1:A:54:ASN:HD22	1.72	0.54
2:B:557:GLU:OE2	2:B:584:ARG:NH2	2.40	0.54
3:C:248:ILE:HG21	11:K:102:ASP:HB2	1.88	0.54
27:s:280:ALA:O	27:s:351:ARG:NH2	2.39	0.54
4:D:159:LEU:HD22	7:G:86:VAL:HG11	1.90	0.54
2:B:879:ARG:HD2	2:B:885:LEU:HD12	1.91	0.53
23:m:607:ILE:HG22	23:m:719:VAL:HG11	1.89	0.53
28:u:199:LEU:HD11	29:v:211:PHE:HB3	1.91	0.53
13:M:33:SER:HA	13:M:50:LYS:HE2	1.91	0.53
1:A:1124:ARG:NH1	1:A:1304:GLU:OE2	2.39	0.53
17:V:89:ARG:NH2	17:V:109:ASP:OD2	2.41	0.53
25:q:157:LYS:NZ	29:v:71:ASP:OD1	2.40	0.53
2:B:927:GLN:HB2	2:B:931:TYR:HB3	1.89	0.53
21:g:20:ARG:NH2	22:h:125:LYS:OXT	2.42	0.53
23:m:1426:LEU:HD13	23:m:1469:ARG:HH21	1.75	0.52
30:x:157:ARG:HB3	30:x:161:PRO:HB3	1.91	0.52
1:A:976:ASP:O	1:A:979:LYS:NZ	2.42	0.52
2:B:235:LEU:HD23	2:B:242:ILE:HG13	1.91	0.52
23:m:1083:MET:HE1	23:m:1131:LEU:HD23	1.91	0.52
9:I:14:LEU:HB3	9:I:27:TYR:HB3	1.92	0.52
25:q:830:LEU:HD22	25:q:846:LEU:HB3	1.91	0.52
27:s:378:THR:HG23	27:s:382:LEU:HD12	1.91	0.52
14:N:29:DG:H1'	14:N:30:DC:O4'	2.10	0.52
23:m:236:GLU:OE2	24:n:252:ARG:NH1	2.43	0.52
25:q:688:SER:HG	29:v:16:TYR:HH	1.56	0.52
2:B:906:SER:OG	18:W:781:GLU:OE1	2.27	0.52
14:N:-104:DT:H3	16:T:104:DG:H1	1.57	0.52
25:q:59:ALA:HB1	25:q:63:LEU:HD12	1.91	0.52
18:W:232:ARG:HH22	18:W:235:LYS:HE3	1.73	0.52
25:q:155:TYR:HB2	25:q:164:ALA:HB2	1.90	0.52
25:q:766:MET:HG3	25:q:770:LYS:HE3	1.92	0.52
28:u:114:LEU:HD11	28:u:150:VAL:HG23	1.92	0.52
1:A:63:ARG:NH1	15:P:0:G:OP1	2.42	0.52
2:B:393:HIS:NE2	2:B:696:GLU:OE2	2.42	0.52
9:I:45:ARG:NH1	9:I:47:GLU:OE2	2.42	0.52
7:G:6:ASP:OD1	7:G:75:ARG:NH2	2.43	0.51
23:m:532:VAL:HG22	23:m:565:MET:HE2	1.91	0.51
25:q:451:ARG:NH2	29:v:35:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:356:PRO:HG2	18:W:394:PHE:HB2	1.92	0.51
25:q:239:ASN:HA	25:q:242:LYS:HD2	1.92	0.51
2:B:10:ASP:HB3	2:B:649:LYS:HG3	1.93	0.51
2:B:353:LEU:O	2:B:367:LYS:NZ	2.38	0.51
25:q:578:GLN:NE2	25:q:582:ASP:OD1	2.43	0.51
2:B:257:THR:OG1	2:B:258:GLY:N	2.42	0.51
27:s:226:ARG:NH2	27:s:227:GLU:O	2.43	0.51
1:A:1195:LEU:HB2	1:A:1263:LEU:HD21	1.93	0.51
1:A:447:ARG:HB2	1:A:488:MET:HE3	1.93	0.51
11:K:25:SER:O	30:x:307:GLN:NE2	2.41	0.51
18:W:218:ILE:CG1	24:n:289:MET:HE1	2.41	0.51
2:B:245:MET:HE1	2:B:371:LEU:HD21	1.93	0.50
23:m:1033:ARG:HH22	23:m:1087:ARG:HH22	1.58	0.50
23:m:1191:ASN:OD1	23:m:1193:GLN:NE2	2.43	0.50
24:n:207:ILE:HG23	24:n:212:LEU:HB3	1.92	0.50
25:q:215:ASP:OD1	25:q:217:ARG:NH2	2.43	0.50
25:q:357:LYS:NZ	25:q:361:ASP:OD1	2.43	0.50
2:B:879:ARG:HH21	15:P:-3:U:H1'	1.76	0.50
14:N:-89:DT:C7	21:c:32:ARG:NH1	2.75	0.50
18:W:229:VAL:HG21	18:W:286:LEU:HD11	1.92	0.50
23:m:1200:PRO:O	23:m:1203:ARG:NH2	2.43	0.50
18:W:666:GLU:HG2	18:W:705:VAL:HG12	1.93	0.50
5:E:49:MET:SD	5:E:49:MET:N	2.76	0.50
16:T:32:DA:H5''	20:f:32:PRO:HG2	1.92	0.50
24:n:260:MET:HG3	24:n:284:TRP:HZ3	1.77	0.50
25:q:31:LYS:HB2	25:q:57:GLU:HA	1.94	0.50
1:A:286:PRO:HG2	1:A:289:ILE:HD12	1.93	0.50
20:b:96:THR:HB	21:g:100:VAL:HG12	1.93	0.50
23:m:1041:LEU:HD11	23:m:1081:TYR:HD2	1.77	0.50
23:m:1425:LYS:HE3	23:m:1428:PRO:HA	1.94	0.50
14:N:4:DG:O3'	22:h:33:ARG:HD2	2.12	0.50
1:A:363:ASP:OD1	1:A:363:ASP:N	2.45	0.49
15:P:-5:C:H5'	23:m:775:ARG:NH1	2.26	0.49
18:W:351:ARG:HA	18:W:429:THR:HA	1.94	0.49
19:e:106:ASP:OD2	19:e:131:ARG:NH2	2.41	0.49
28:u:191:THR:HG22	28:u:219:VAL:HG22	1.94	0.49
30:x:226:LYS:HG3	30:x:250:ILE:HG22	1.93	0.49
1:A:1190:GLN:HA	1:A:1245:ILE:HA	1.95	0.49
24:n:163:LEU:HD11	24:n:194:VAL:HG22	1.94	0.49
21:c:42:ARG:HB2	22:d:88:THR:HG22	1.94	0.49
2:B:268:VAL:HG11	2:B:272:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:-34:DG:H2''	16:T:-33:DA:C8	2.48	0.49
16:T:11:DG:OP1	22:h:88:THR:OG1	2.22	0.49
29:v:210:VAL:HG13	29:v:334:VAL:HG21	1.95	0.49
1:A:807:ARG:NH2	2:B:724:LYS:O	2.43	0.49
27:s:275:VAL:O	27:s:276:PRO:C	2.54	0.49
25:q:250:ASN:HA	25:q:253:ILE:HD12	1.93	0.49
27:s:51:ASN:OD1	27:s:53:THR:OG1	2.27	0.49
2:B:613:ARG:HH11	9:I:62:ILE:HD11	1.76	0.49
17:V:9:GLU:HA	17:V:20:PRO:HA	1.95	0.49
24:n:216:VAL:HG13	24:n:237:LEU:HD13	1.94	0.49
1:A:599:LEU:O	8:H:121:LEU:HD12	2.13	0.49
5:E:60:LEU:O	25:q:915:ARG:NH2	2.39	0.49
14:N:-58:DC:H5'	19:a:63:ARG:HH11	1.77	0.49
18:W:317:ASP:O	18:W:318:VAL:C	2.55	0.49
23:m:1172:VAL:HA	23:m:1182:VAL:HG12	1.93	0.49
2:B:336:ILE:O	2:B:341:ARG:NH2	2.46	0.49
18:W:666:GLU:HA	18:W:705:VAL:HA	1.94	0.49
1:A:9:ALA:O	2:B:1193:GLN:NE2	2.44	0.48
2:B:279:ARG:NH1	2:B:286:ASP:OD1	2.46	0.48
18:W:640:LYS:NZ	18:W:641:LEU:O	2.46	0.48
25:q:479:TYR:HD1	29:v:30:LEU:HB3	1.78	0.48
17:V:10:ARG:HA	17:V:52:SER:HA	1.95	0.48
18:W:704:ARG:NH2	23:m:632:GLU:OE2	2.46	0.48
14:N:-18:DG:H2''	14:N:-17:DT:H71	1.96	0.48
18:W:327:ARG:NH1	18:W:441:ASN:O	2.46	0.48
18:W:465:ALA:HA	18:W:468:LEU:HD12	1.95	0.48
1:A:253:MET:SD	16:T:-47:DA:H2''	2.54	0.48
11:K:14:ASP:N	11:K:14:ASP:OD1	2.47	0.48
15:P:-7:U:C2	15:P:-6:C:C2	3.01	0.48
23:m:1255:TRP:NE1	23:m:1260:GLU:OE1	2.42	0.48
28:u:173:TRP:NE1	28:u:179:SER:OG	2.37	0.48
1:A:1199:LEU:HD13	1:A:1204:MET:HG3	1.96	0.48
3:C:15:ASP:OD1	3:C:15:ASP:N	2.44	0.48
16:T:32:DA:OP1	20:f:36:ARG:NH1	2.47	0.48
30:x:311:GLY:HA3	30:x:330:VAL:HG12	1.95	0.48
1:A:204:THR:OG1	1:A:207:GLU:OE1	2.31	0.47
2:B:601:ALA:HA	28:u:239:SER:HB3	1.96	0.47
16:T:-3:DG:H21	22:h:33:ARG:HH22	1.60	0.47
16:T:55:DA:H5'	19:a:40:ARG:HG2	1.96	0.47
19:a:32:THR:OG1	27:s:173:LEU:O	2.31	0.47
25:q:390:LEU:HB3	25:q:409:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:GLU:OE2	7:G:23:ASN:ND2	2.47	0.47
2:B:879:ARG:NH2	15:P:-3:U:H1'	2.29	0.47
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.95	0.47
1:A:106:ILE:HD13	1:A:215:ILE:HD11	1.96	0.47
22:h:79:ARG:NH2	22:h:83:TYR:OH	2.44	0.47
23:m:998:ASN:HD22	23:m:999:LEU:N	2.12	0.47
28:u:108:VAL:HG22	28:u:219:VAL:HB	1.96	0.47
2:B:248:LYS:NZ	2:B:264:THR:OG1	2.46	0.47
15:P:-5:C:O3'	15:P:-4:U:H2'	2.15	0.47
16:T:-23:DC:H2''	16:T:-22:DA:C8	2.49	0.47
25:q:559:ARG:NH1	29:v:24:PRO:O	2.47	0.47
26:r:223:VAL:HG22	26:r:325:GLN:HG2	1.95	0.47
1:A:1227:PHE:HB2	1:A:1245:ILE:HD11	1.97	0.47
14:N:-23:DT:H2''	14:N:-22:DG:H5''	1.96	0.47
23:m:625:GLY:O	23:m:629:ILE:HG12	2.14	0.47
25:q:72:VAL:HG21	29:v:75:LEU:HD13	1.97	0.47
26:r:493:ASN:HB2	26:r:502:ILE:HD11	1.96	0.47
29:v:263:TRP:HE1	29:v:356:ASN:HD21	1.61	0.47
5:E:34:MET:HE2	5:E:34:MET:HB2	1.80	0.47
14:N:-106:DT:H3	16:T:106:DG:H1	1.63	0.47
18:W:326:VAL:HA	18:W:440:ILE:HD13	1.96	0.47
25:q:210:PRO:O	25:q:217:ARG:NH1	2.39	0.47
25:q:708:GLN:OE1	25:q:739:LYS:NZ	2.48	0.47
1:A:261:ASP:OD1	1:A:262:ASP:N	2.48	0.47
23:m:1279:ARG:NH2	23:m:1315:SER:O	2.48	0.47
21:c:112:GLN:HB2	21:c:115:LEU:HG	1.97	0.47
17:V:58:VAL:N	17:V:82:TYR:O	2.45	0.47
20:b:44:LYS:HB2	21:g:115:LEU:HD11	1.96	0.47
28:u:80:TYR:CZ	29:v:356:ASN:HB2	2.49	0.47
23:m:882:ARG:HH12	23:m:1156:ARG:HH11	1.62	0.46
26:r:211:MET:HB3	26:r:286:LEU:HD23	1.97	0.46
2:B:81:LYS:NZ	28:u:247:TYR:O	2.44	0.46
18:W:494:LEU:HD21	24:n:183:PRO:HG3	1.96	0.46
23:m:1269:ASP:OD1	23:m:1272:ARG:NH2	2.46	0.46
11:K:55:ASP:OD1	11:K:55:ASP:N	2.41	0.46
15:P:-5:C:H4'	15:P:-4:U:C6	2.51	0.46
21:c:39:TYR:O	21:g:38:ASN:ND2	2.48	0.46
7:G:160:ILE:HD12	18:W:553:LEU:HD12	1.97	0.46
16:T:-22:DA:H2''	16:T:-21:DC:C6	2.50	0.46
25:q:65:LEU:HD13	29:v:81:ILE:HG12	1.96	0.46
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:550:PHE:HB3	2:B:593:MET:HE1	1.96	0.46
27:s:339:THR:HG22	27:s:341:ASP:H	1.80	0.46
15:P:-2:U:C6	15:P:-2:U:H5''	2.51	0.46
18:W:215:ARG:NH2	23:m:234:TYR:CE1	2.84	0.46
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.80	0.46
5:E:89:ILE:HD13	5:E:118:SER:HB2	1.98	0.46
7:G:151:ARG:HB3	7:G:158:TYR:HB2	1.98	0.46
11:K:29:ASN:ND2	11:K:78:GLU:O	2.49	0.46
21:c:24:GLN:HE21	22:d:47:GLN:HE21	1.63	0.46
23:m:712:LEU:HA	23:m:715:LEU:HB2	1.98	0.46
1:A:599:LEU:HD12	1:A:599:LEU:HA	1.73	0.46
15:P:-4:U:H1'	15:P:-3:U:C2	2.51	0.46
16:T:-69:DA:H2''	16:T:-68:DG:C8	2.51	0.46
16:T:59:DA:H1'	16:T:60:DA:H5'	1.97	0.46
23:m:527:ASP:OD1	23:m:528:ALA:N	2.47	0.45
16:T:80:DA:H2''	16:T:81:DC:C5	2.51	0.45
19:e:133:GLU:OE1	19:e:133:GLU:N	2.49	0.45
14:N:-30:DT:H2''	14:N:-29:DT:C6	2.51	0.45
17:V:66:SER:HB2	18:W:260:TYR:HB3	1.98	0.45
18:W:638:TYR:CZ	23:m:882:ARG:HG3	2.52	0.45
19:a:50:GLU:HG3	20:b:39:ARG:HG2	1.99	0.45
23:m:780:LEU:HD12	23:m:900:LEU:HB3	1.97	0.45
23:m:984:LYS:HE2	23:m:1015:VAL:HG21	1.99	0.45
25:q:520:SER:O	25:q:524:HIS:ND1	2.48	0.45
12:L:49:ARG:HD3	26:r:339:VAL:HG11	1.98	0.45
13:M:46:LEU:HD11	13:M:55:SER:HB3	1.99	0.45
21:c:90:ASP:HB3	21:c:93:LEU:HB2	1.98	0.45
25:q:737:LEU:O	25:q:742:ASN:N	2.47	0.45
26:r:366:GLU:HG2	28:u:252:VAL:HG22	1.99	0.45
1:A:864:ILE:HD12	5:E:169:LEU:HD11	1.99	0.45
1:A:1423:ASP:OD1	1:A:1423:ASP:N	2.41	0.45
4:D:139:PRO:HA	4:D:142:ILE:HD12	1.99	0.45
16:T:49:DC:H2''	16:T:50:DA:C8	2.52	0.45
21:c:54:VAL:HG21	22:d:98:VAL:HG21	1.99	0.45
1:A:134:ARG:HH11	1:A:224:GLY:HA2	1.81	0.45
1:A:466:TYR:HB2	1:A:470:ARG:NH1	2.32	0.45
6:F:110:ASP:OD1	6:F:110:ASP:N	2.38	0.45
14:N:-89:DT:C7	21:c:32:ARG:HH11	2.28	0.45
23:m:992:ILE:HG22	23:m:997:SER:HA	1.99	0.45
23:m:1064:ASP:OD1	27:s:457:LYS:NZ	2.46	0.45
25:q:189:LEU:HD22	25:q:194:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:r:276:PHE:HB2	26:r:279:GLN:HB2	1.99	0.45
27:s:342:TYR:CZ	27:s:346:ARG:HD2	2.51	0.45
27:s:345:LEU:HD13	27:s:376:ILE:HG23	1.99	0.45
14:N:32:DG:H1'	14:N:33:DT:H5'	1.98	0.45
18:W:527:THR:HA	18:W:530:LEU:HD12	1.99	0.45
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.98	0.45
14:N:-59:DT:O3'	19:a:63:ARG:NH1	2.49	0.45
18:W:215:ARG:NH1	23:m:234:TYR:CE1	2.85	0.45
1:A:1452:LEU:HD22	6:F:131:PRO:HB3	1.98	0.45
18:W:751:THR:HG23	18:W:798:ILE:HG12	1.99	0.45
20:f:73:THR:HG21	20:f:81:VAL:HG22	1.99	0.45
25:q:320:LEU:HD13	26:r:514:LEU:HD11	1.99	0.45
16:T:90:DC:H2''	16:T:91:DA:C8	2.52	0.44
18:W:508:SER:HA	18:W:524:GLU:HA	1.99	0.44
25:q:568:SER:O	25:q:571:ASN:ND2	2.50	0.44
27:s:190:THR:O	27:s:197:ARG:NH1	2.50	0.44
1:A:41:MET:HG2	1:A:44:SER:HA	1.98	0.44
1:A:870:GLY:C	1:A:872:ASP:H	2.24	0.44
23:m:1104:ILE:HD12	27:s:456:PRO:HB2	1.98	0.44
7:G:144:ARG:HB2	7:G:171:ILE:HD13	1.99	0.44
18:W:546:LYS:NZ	23:m:291:GLU:OE1	2.48	0.44
29:v:262:LYS:HD3	29:v:305:GLN:HE21	1.81	0.44
1:A:948:VAL:O	5:E:200:ARG:NH2	2.50	0.44
27:s:395:THR:HA	27:s:398:VAL:HG12	1.98	0.44
1:A:231:ARG:HB3	1:A:234:TRP:CD2	2.53	0.44
2:B:284:VAL:N	2:B:285:PRO:HD2	2.32	0.44
18:W:444:LEU:HD12	23:m:284:PHE:CG	2.52	0.44
16:T:91:DA:H2''	16:T:92:DC:C5	2.52	0.44
28:u:97:HIS:NE2	29:v:203:ASP:OD2	2.47	0.44
29:v:312:LYS:HB3	29:v:315:GLU:HG2	1.99	0.44
5:E:21:MET:HE2	5:E:186:TYR:HA	2.00	0.44
16:T:28:DG:H2''	16:T:29:DA:C8	2.52	0.44
28:u:90:LEU:HB2	29:v:362:MET:HE1	1.99	0.44
4:D:136:VAL:O	4:D:166:LYS:NZ	2.50	0.44
17:V:67:TRP:NE1	18:W:217:LEU:O	2.51	0.44
26:r:244:LYS:NZ	26:r:305:GLU:OE2	2.46	0.44
14:N:-10:DG:H2''	14:N:-9:DC:C5	2.53	0.44
16:T:94:DC:H2'	16:T:95:DC:C6	2.53	0.44
18:W:315:SER:O	18:W:316:SER:C	2.61	0.44
21:g:63:LEU:HD11	22:h:41:VAL:HG13	2.00	0.44
25:q:641:ALA:HB1	25:q:655:LYS:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:v:258:ASN:OD1	29:v:261:ASN:N	2.44	0.44
2:B:86:ARG:NH1	26:r:369:GLU:OE1	2.50	0.43
1:A:835:THR:HG21	1:A:1079:THR:HA	1.99	0.43
1:A:1343:GLY:O	1:A:1347:THR:OG1	2.29	0.43
3:C:179:GLU:OE2	3:C:204:SER:OG	2.36	0.43
17:V:59:ALA:HB1	18:W:244:LEU:HD13	2.01	0.43
15:P:-5:C:H4'	15:P:-4:U:C5	2.53	0.43
25:q:617:ASP:OD1	25:q:621:ASN:ND2	2.51	0.43
1:A:188:LYS:HE3	1:A:199:GLU:HB2	2.01	0.43
7:G:30:LEU:HD22	7:G:72:VAL:HG11	2.00	0.43
9:I:23:GLN:O	9:I:24:ARG:NE	2.51	0.43
14:N:-79:DG:OP1	22:d:88:THR:OG1	2.25	0.43
16:T:105:DA:H2'	16:T:106:DG:C8	2.54	0.43
18:W:628:LYS:HE3	23:m:661:GLN:HE22	1.82	0.43
23:m:1062:ALA:HB2	23:m:1103:LEU:HD11	1.99	0.43
11:K:99:LYS:HB2	11:K:99:LYS:HE2	1.73	0.43
20:f:68:ASP:OD1	20:f:68:ASP:N	2.52	0.43
23:m:770:PHE:HB3	23:m:779:VAL:HG22	2.00	0.43
2:B:273:PRO:HG2	2:B:276:ILE:HD12	2.00	0.43
14:N:27:DG:H2'	14:N:28:DT:H72	2.00	0.43
17:V:78:GLN:O	17:V:82:TYR:OH	2.23	0.43
18:W:534:PHE:HB3	18:W:554:ILE:HD13	2.00	0.43
18:W:752:LEU:HD23	18:W:770:VAL:HG12	1.99	0.43
19:a:108:ASN:HB2	20:b:43:VAL:HG22	2.00	0.43
1:A:465:PRO:O	1:A:470:ARG:NH1	2.52	0.43
2:B:788:ARG:O	2:B:967:ARG:NH2	2.52	0.43
14:N:33:DT:H2''	14:N:34:DC:C6	2.54	0.43
23:m:242:GLY:HA3	24:n:258:LYS:HG2	2.00	0.43
27:s:401:MET:HE3	27:s:401:MET:HB3	1.90	0.43
28:u:200:VAL:HA	28:u:211:THR:HA	2.00	0.43
9:I:17:LYS:N	9:I:26:LEU:O	2.50	0.43
21:g:54:VAL:HG21	22:h:98:VAL:HG21	1.99	0.43
23:m:1426:LEU:HD21	23:m:1465:MET:HE2	1.99	0.43
26:r:277:PRO:HB2	26:r:305:GLU:HB3	2.01	0.43
29:v:104:PRO:HA	29:v:107:ARG:HD3	2.00	0.43
15:P:-6:C:C2	15:P:-5:C:N4	2.87	0.43
23:m:1365:GLU:O	23:m:1369:ASN:ND2	2.49	0.43
30:x:222:MET:HE3	30:x:222:MET:HB3	1.85	0.43
14:N:-34:DT:H2''	14:N:-33:DG:C8	2.55	0.42
18:W:334:LYS:HB3	18:W:388:ARG:HH22	1.84	0.42
18:W:472:ALA:O	18:W:476:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:h:43:LYS:HE3	22:h:43:LYS:HB2	1.89	0.42
27:s:263:GLY:O	27:s:264:ARG:C	2.62	0.42
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	2.01	0.42
18:W:327:ARG:HB3	18:W:436:ILE:HB	2.01	0.42
26:r:245:VAL:HG23	26:r:298:GLU:HG2	2.01	0.42
1:A:547:VAL:HG22	1:A:578:LEU:HD21	2.01	0.42
25:q:41:PHE:CG	25:q:70:VAL:HG11	2.55	0.42
25:q:155:TYR:HB3	25:q:160:ARG:HB2	2.01	0.42
28:u:208:ILE:HG22	29:v:253:LYS:HG3	2.01	0.42
1:A:318:LYS:HE3	16:T:-46:DC:C5	2.54	0.42
17:V:63:ASN:HB3	17:V:75:ASP:HA	2.01	0.42
3:C:199:LYS:HB3	3:C:199:LYS:HE2	1.80	0.42
23:m:1425:LYS:NZ	23:m:1430:SER:O	2.41	0.42
3:C:79:MET:HE2	3:C:79:MET:HB3	1.87	0.42
18:W:344:LEU:HD12	18:W:349:GLU:HB2	2.01	0.42
18:W:461:LEU:HD12	23:m:278:THR:HG23	2.01	0.42
23:m:1325:ALA:HB3	23:m:1328:LEU:HB3	2.02	0.42
1:A:823:GLU:OE2	2:B:506:GLN:NE2	2.53	0.42
1:A:1448:ILE:HD11	1:A:1453:LEU:HD11	2.01	0.42
2:B:928:ARG:NH1	23:m:775:ARG:O	2.52	0.42
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.88	0.42
2:B:299:ASP:OD1	2:B:299:ASP:N	2.52	0.42
5:E:81:PHE:HE1	5:E:110:ILE:HD13	1.84	0.42
23:m:545:ASN:ND2	23:m:553:HIS:O	2.53	0.42
24:n:217:ARG:HG3	24:n:259:VAL:HG21	2.02	0.42
26:r:206:PHE:H	26:r:229:LEU:HD21	1.85	0.42
2:B:83:TYR:HB2	2:B:116:TYR:HB2	2.01	0.42
2:B:223:SER:O	2:B:252:ARG:NH1	2.41	0.42
2:B:547:ILE:HG21	2:B:619:ILE:HG21	2.00	0.42
23:m:295:THR:OG1	23:m:298:ASP:OD2	2.37	0.42
23:m:338:LEU:HD23	23:m:338:LEU:HA	1.86	0.42
23:m:380:GLU:HB3	23:m:978:CYS:SG	2.60	0.42
2:B:318:ASP:HB3	2:B:321:VAL:HG22	2.02	0.42
7:G:108:VAL:HG22	7:G:159:ALA:HB3	2.02	0.42
25:q:737:LEU:HD12	25:q:741:SER:HB2	2.01	0.42
2:B:592:THR:HA	28:u:226:PHE:HZ	1.85	0.41
2:B:607:SER:HB2	2:B:620:PHE:HB2	2.02	0.41
25:q:710:LEU:HD13	25:q:740:PHE:HB2	2.01	0.41
30:x:301:ASP:OD1	30:x:303:GLN:NE2	2.53	0.41
18:W:551:THR:HG21	18:W:586:SER:HA	2.03	0.41
1:A:983:LEU:HD13	1:A:1041:ARG:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:648:GLN:NE2	18:W:679:VAL:H	2.18	0.41
2:B:766:ARG:NH1	2:B:985:GLY:O	2.53	0.41
19:a:128:ARG:HH11	19:a:134:ARG:HH11	1.68	0.41
1:A:203:LEU:HB3	1:A:208:ILE:HD11	2.01	0.41
2:B:760:ASP:OD1	2:B:760:ASP:N	2.48	0.41
2:B:887:HIS:HA	15:P:-2:U:C5	2.56	0.41
25:q:241:LEU:HD23	25:q:241:LEU:HA	1.95	0.41
26:r:194:LYS:HB2	26:r:316:LEU:HD12	2.03	0.41
2:B:815:ARG:NH2	29:v:132:GLN:O	2.54	0.41
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	2.01	0.41
2:B:184:LYS:HB3	2:B:787:VAL:HG21	2.03	0.41
2:B:632:ILE:HD11	2:B:688:GLU:HB3	2.01	0.41
24:n:241:ILE:HG23	24:n:246:ILE:HD12	2.03	0.41
27:s:417:GLN:O	27:s:420:SER:OG	2.31	0.41
3:C:21:LEU:HD22	11:K:101:LEU:HD11	2.03	0.41
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.86	0.41
23:m:772:GLU:O	23:m:829:ASN:ND2	2.48	0.41
23:m:992:ILE:HA	23:m:995:ILE:HG12	2.02	0.41
25:q:766:MET:HE1	25:q:799:ILE:HG23	2.02	0.41
1:A:557:TRP:O	11:K:26:ARG:NH2	2.54	0.41
1:A:677:MET:HG3	2:B:722:THR:HB	2.03	0.41
2:B:650:GLU:OE1	2:B:653:ARG:NH1	2.49	0.41
3:C:50:ILE:HG12	3:C:155:ILE:HG22	2.03	0.41
5:E:27:TYR:HA	5:E:63:PRO:HA	2.03	0.41
6:F:104:ASN:HD22	6:F:104:ASN:HA	1.70	0.41
7:G:118:ASN:OD1	7:G:118:ASN:N	2.53	0.41
14:N:4:DG:O3'	22:h:33:ARG:HB3	2.21	0.41
18:W:336:ASP:OD2	18:W:357:ARG:NE	2.47	0.41
21:c:24:GLN:HE21	22:d:47:GLN:NE2	2.19	0.41
21:g:63:LEU:HD23	21:g:63:LEU:HA	1.91	0.41
23:m:449:THR:HG21	23:m:543:ARG:HD2	2.03	0.41
23:m:1001:ASN:OD1	23:m:1002:ARG:N	2.54	0.41
25:q:9:TYR:OH	29:v:106:ASP:OD2	2.28	0.41
25:q:162:ASP:OD1	25:q:192:ARG:NH1	2.51	0.41
26:r:345:MET:O	26:r:348:SER:OG	2.33	0.41
27:s:209:VAL:HG22	27:s:222:ILE:HG12	2.03	0.41
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.55	0.41
16:T:82:DC:H2''	16:T:83:DA:C8	2.56	0.41
26:r:263:SER:OG	26:r:264:LYS:N	2.53	0.41
14:N:32:DG:H2''	14:N:33:DT:OP2	2.20	0.40
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:42:DT:C6	14:N:43:DT:H72	2.56	0.40
27:s:238:TYR:OH	33:s:1904:SAH:H5'2	2.20	0.40
28:u:180:LEU:HB2	28:u:189:MET:HE3	2.03	0.40
29:v:199:HIS:O	29:v:328:ALA:N	2.54	0.40
14:N:30:DC:H2''	14:N:31:DT:O5'	2.22	0.40
25:q:403:SER:OG	29:v:56:LYS:NZ	2.54	0.40
29:v:29:LEU:N	30:x:147:ARG:O	2.52	0.40
1:A:109:ASN:HD21	24:n:199:LEU:HB3	1.85	0.40
1:A:1412:LEU:HD13	2:B:1207:LEU:HD21	2.02	0.40
23:m:617:ILE:HG13	23:m:649:LEU:HD11	2.04	0.40
23:m:965:VAL:HG21	23:m:992:ILE:HG21	2.02	0.40
1:A:215:ILE:O	1:A:231:ARG:NH1	2.47	0.40
1:A:363:ASP:HB3	1:A:509:PRO:HD3	2.03	0.40
1:A:554:VAL:HB	1:A:557:TRP:HB2	2.04	0.40
15:P:-5:C:O2	18:W:748:ARG:HD3	2.21	0.40
23:m:243:ASP:OD1	23:m:243:ASP:N	2.55	0.40
25:q:547:MET:HE3	25:q:547:MET:HB2	1.97	0.40
25:q:780:TYR:O	25:q:784:LYS:N	2.50	0.40
26:r:230:ARG:NH2	26:r:292:SER:OG	2.45	0.40
28:u:89:SER:HB3	29:v:365:ARG:HE	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1392/1743 (80%)	1355 (97%)	36 (3%)	1 (0%)	48	83
2	B	1154/1227 (94%)	1127 (98%)	27 (2%)	0	100	100
3	C	261/304 (86%)	259 (99%)	2 (1%)	0	100	100
4	D	170/186 (91%)	168 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
6	F	82/155 (53%)	79 (96%)	3 (4%)	0	100	100
7	G	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
8	H	129/145 (89%)	125 (97%)	4 (3%)	0	100	100
9	I	109/115 (95%)	105 (96%)	4 (4%)	0	100	100
10	J	65/72 (90%)	65 (100%)	0	0	100	100
11	K	111/118 (94%)	109 (98%)	2 (2%)	0	100	100
12	L	43/72 (60%)	41 (95%)	2 (5%)	0	100	100
13	M	62/113 (55%)	62 (100%)	0	0	100	100
17	V	104/108 (96%)	102 (98%)	2 (2%)	0	100	100
18	W	529/911 (58%)	506 (96%)	23 (4%)	0	100	100
19	a	102/139 (73%)	100 (98%)	2 (2%)	0	100	100
19	e	89/139 (64%)	89 (100%)	0	0	100	100
20	b	79/106 (74%)	76 (96%)	3 (4%)	0	100	100
20	f	79/106 (74%)	76 (96%)	3 (4%)	0	100	100
21	c	102/133 (77%)	100 (98%)	2 (2%)	0	100	100
21	g	104/133 (78%)	101 (97%)	3 (3%)	0	100	100
22	d	91/129 (70%)	88 (97%)	3 (3%)	0	100	100
22	h	92/129 (71%)	90 (98%)	2 (2%)	0	100	100
23	m	1170/1503 (78%)	1152 (98%)	18 (2%)	0	100	100
24	n	137/417 (33%)	136 (99%)	1 (1%)	0	100	100
25	q	928/1084 (86%)	923 (100%)	5 (0%)	0	100	100
26	r	260/544 (48%)	254 (98%)	6 (2%)	0	100	100
27	s	429/725 (59%)	417 (97%)	12 (3%)	0	100	100
28	u	206/459 (45%)	206 (100%)	0	0	100	100
29	v	341/396 (86%)	330 (97%)	11 (3%)	0	100	100
30	x	201/395 (51%)	200 (100%)	1 (0%)	0	100	100
All	All	9001/12191 (74%)	8814 (98%)	186 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	960	VAL

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	1219/1528 (80%)	1219 (100%)	0	100	100
2	B	1018/1077 (94%)	1014 (100%)	4 (0%)	84	82
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	149/160 (93%)	149 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
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%)	120 (100%)	0	100	100
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	61/66 (92%)	61 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	38 (100%)	0	100	100
13	M	61/99 (62%)	61 (100%)	0	100	100
17	V	90/92 (98%)	90 (100%)	0	100	100
18	W	482/796 (61%)	482 (100%)	0	100	100
19	a	87/112 (78%)	87 (100%)	0	100	100
19	e	77/112 (69%)	77 (100%)	0	100	100
20	b	66/81 (82%)	66 (100%)	0	100	100
20	f	66/81 (82%)	66 (100%)	0	100	100
21	c	83/102 (81%)	83 (100%)	0	100	100
21	g	84/102 (82%)	84 (100%)	0	100	100
22	d	79/107 (74%)	79 (100%)	0	100	100
22	h	80/107 (75%)	80 (100%)	0	100	100
23	m	1079/1354 (80%)	1078 (100%)	1 (0%)	88	88
24	n	125/361 (35%)	125 (100%)	0	100	100
25	q	824/962 (86%)	824 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	r	239/485 (49%)	239 (100%)	0	100	100
27	s	380/649 (59%)	380 (100%)	0	100	100
28	u	192/406 (47%)	192 (100%)	0	100	100
29	v	325/369 (88%)	325 (100%)	0	100	100
30	x	190/354 (54%)	190 (100%)	0	100	100
All	All	8079/10712 (75%)	8074 (100%)	5 (0%)	87	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	425	MET
2	B	815	ARG
2	B	879	ARG
2	B	904	ARG
23	m	770	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	278	GLN
1	A	288	HIS
1	A	291	ASN
1	A	387	HIS
1	A	661	ASN
1	A	690	GLN
1	A	769	GLN
1	A	839	GLN
1	A	1080	GLN
2	B	157	HIS
2	B	477	ASN
2	B	492	ASN
2	B	524	GLN
2	B	549	ASN
2	B	996	HIS
2	B	1074	ASN
2	B	1084	GLN
2	B	1179	GLN
3	C	8	ASN

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Mol	Chain	Res	Type
3	C	25	ASN
4	D	46	HIS
4	D	130	ASN
4	D	170	ASN
5	E	53	GLN
5	E	162	GLN
6	F	104	ASN
6	F	119	GLN
6	F	127	GLN
8	H	43	ASN
9	I	23	GLN
11	K	113	ASN
12	L	55	HIS
13	M	32	ASN
13	M	65	GLN
18	W	283	ASN
18	W	402	HIS
18	W	558	ASN
18	W	568	GLN
18	W	786	ASN
19	a	39	HIS
19	a	55	GLN
20	b	64	ASN
21	c	24	GLN
21	c	84	GLN
22	d	82	HIS
19	e	68	GLN
19	e	125	GLN
20	f	25	ASN
21	g	38	ASN
21	g	73	ASN
21	g	94	ASN
22	h	95	GLN
23	m	428	HIS
23	m	473	ASN
23	m	553	HIS
23	m	661	GLN
23	m	819	ASN
23	m	869	HIS
23	m	886	HIS
23	m	899	GLN
23	m	998	ASN

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Mol	Chain	Res	Type
23	m	1191	ASN
23	m	1193	GLN
23	m	1242	GLN
23	m	1338	ASN
23	m	1436	ASN
24	n	156	GLN
24	n	232	GLN
25	q	58	ASN
25	q	132	ASN
25	q	147	ASN
25	q	170	ASN
25	q	187	GLN
25	q	319	ASN
25	q	325	ASN
25	q	397	ASN
25	q	398	GLN
25	q	503	GLN
25	q	526	ASN
25	q	615	HIS
25	q	625	HIS
26	r	279	GLN
26	r	493	ASN
27	s	50	GLN
27	s	82	ASN
27	s	83	ASN
27	s	114	GLN
27	s	139	GLN
27	s	171	GLN
27	s	311	ASN
27	s	375	ASN
28	u	103	GLN
28	u	138	GLN
28	u	172	GLN
28	u	261	GLN
29	v	64	ASN
29	v	199	HIS
29	v	283	ASN
29	v	381	GLN
30	x	246	ASN
30	x	251	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	18/19 (94%)	8 (44%)	1 (5%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	-6	C
15	P	-5	C
15	P	-4	U
15	P	-3	U
15	P	-2	U
15	P	-1	U
15	P	0	G
15	P	1	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	-4	U

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 15 ligands modelled in this entry, 14 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
33	SAH	s	1904	-	27,28,28	0.60	0	36,40,40	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	SAH	s	1904	-	-	2/15/31/31	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

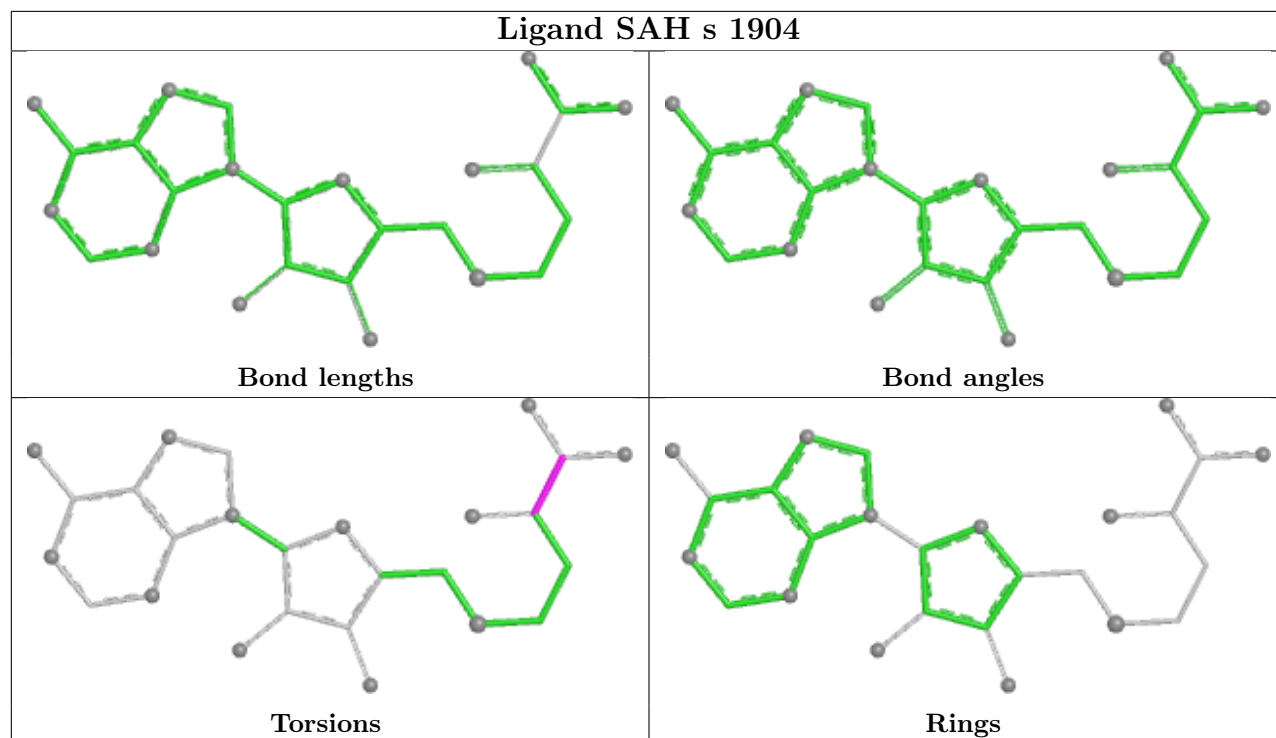
Mol	Chain	Res	Type	Atoms
33	s	1904	SAH	O-C-CA-N
33	s	1904	SAH	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	s	1904	SAH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

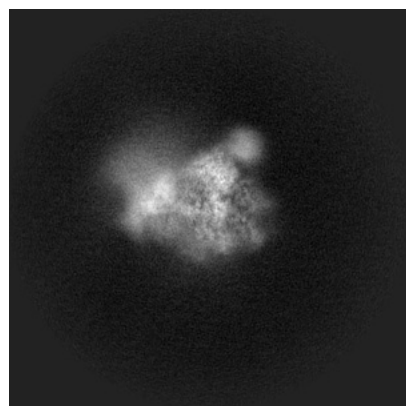
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66105. These allow visual inspection of the internal detail of the map and identification of artifacts.

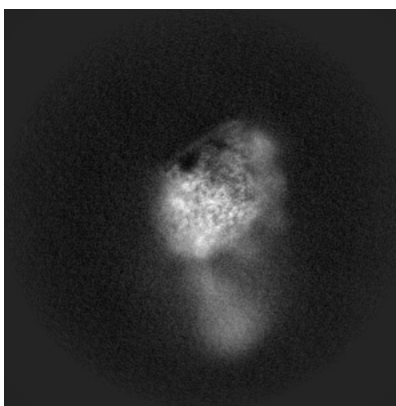
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

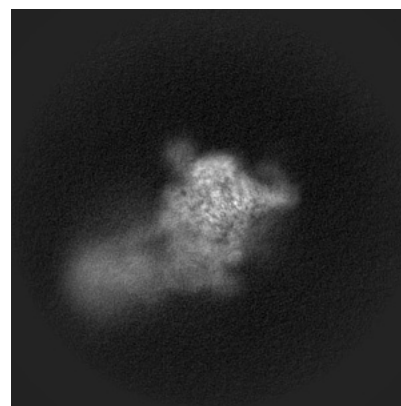
6.1.1 Primary map



X

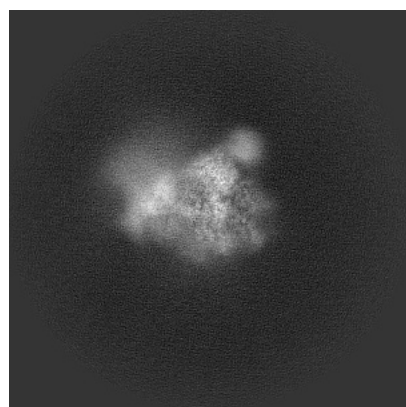


Y

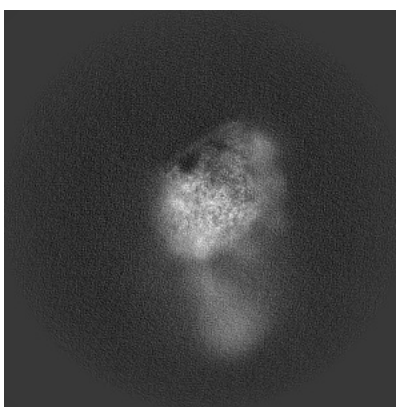


Z

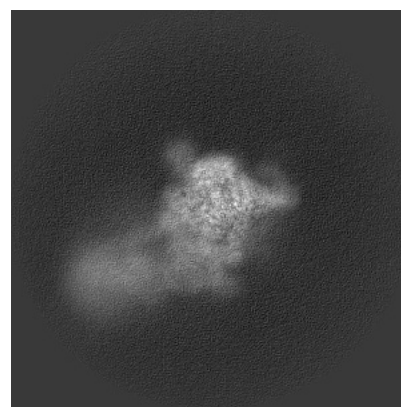
6.1.2 Raw map



X



Y

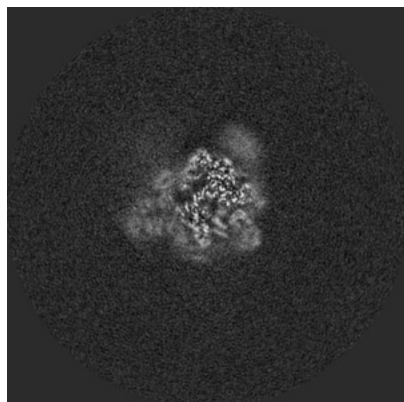


Z

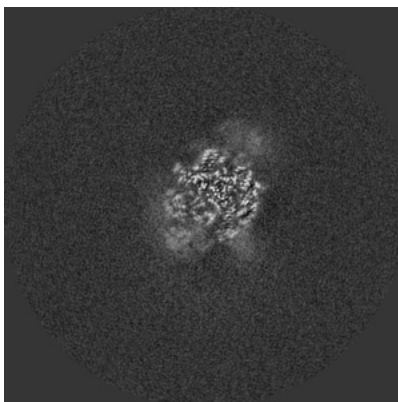
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

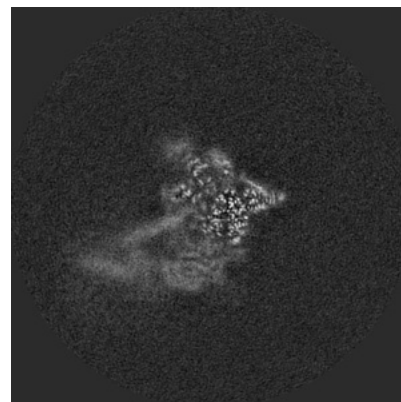
6.2.1 Primary map



X Index: 180

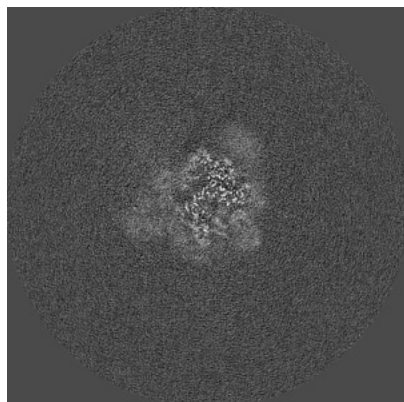


Y Index: 180

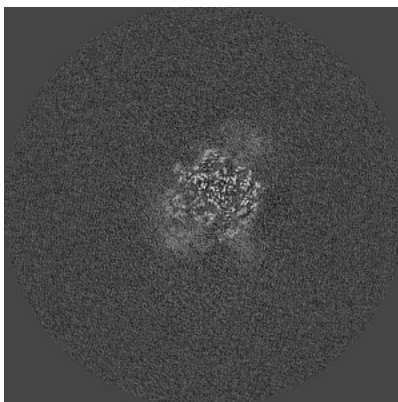


Z Index: 180

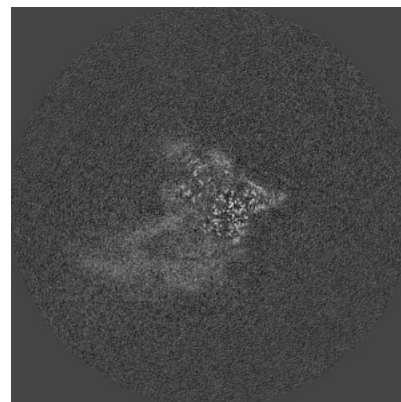
6.2.2 Raw map



X Index: 180



Y Index: 180

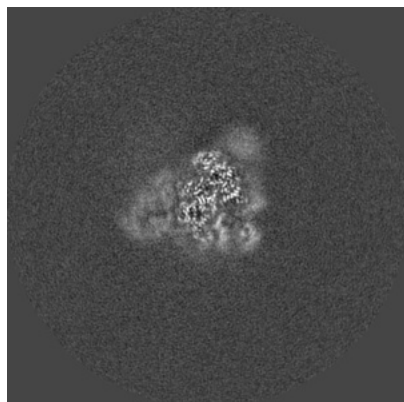


Z Index: 180

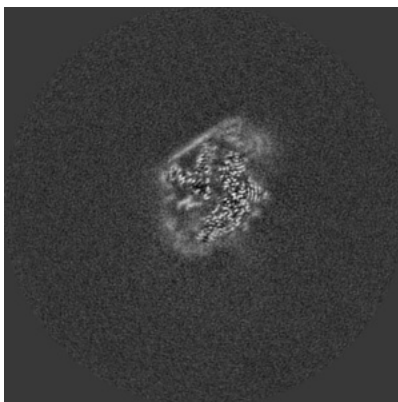
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

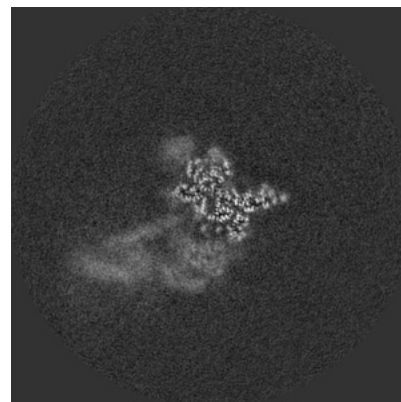
6.3.1 Primary map



X Index: 185

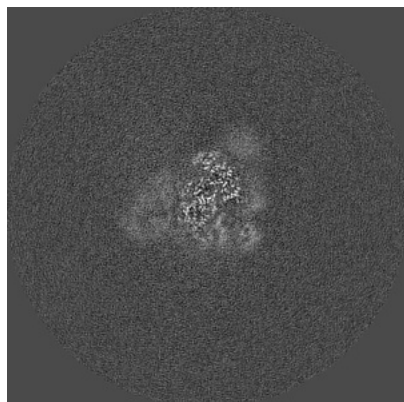


Y Index: 189

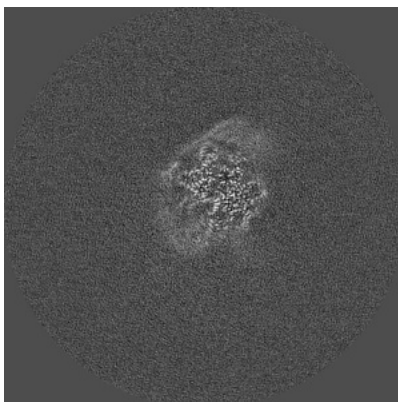


Z Index: 184

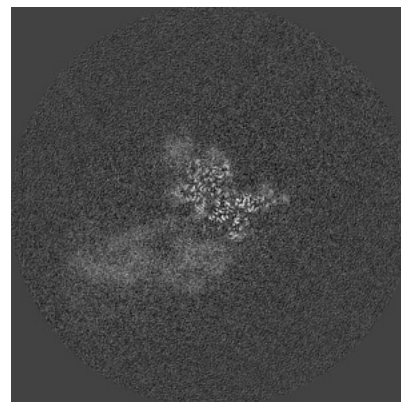
6.3.2 Raw map



X Index: 185



Y Index: 186

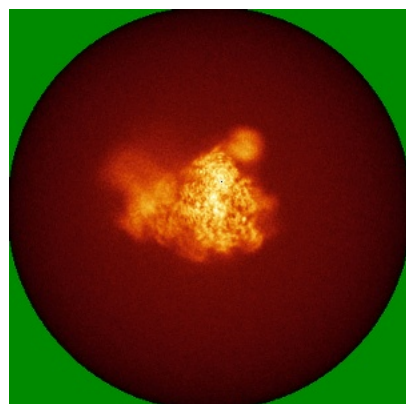


Z Index: 185

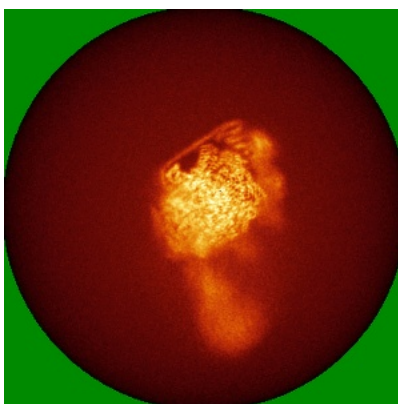
The images above show the largest variance slices of the map in three orthogonal directions.

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

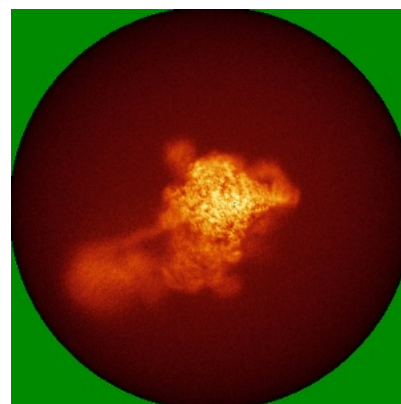
6.4.1 Primary map



X

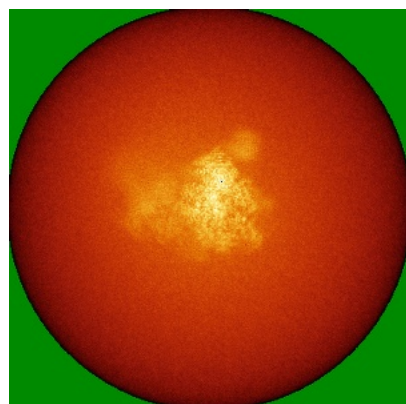


Y

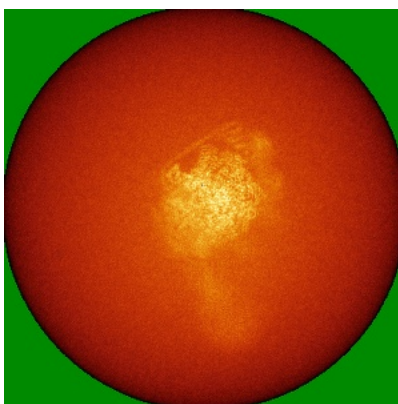


Z

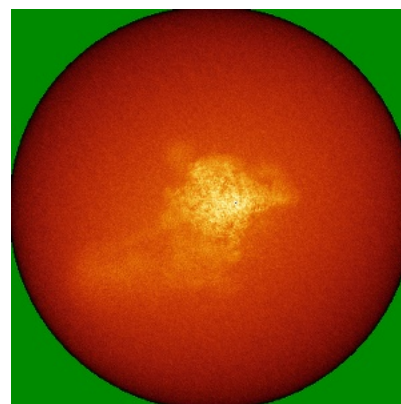
6.4.2 Raw map



X



Y

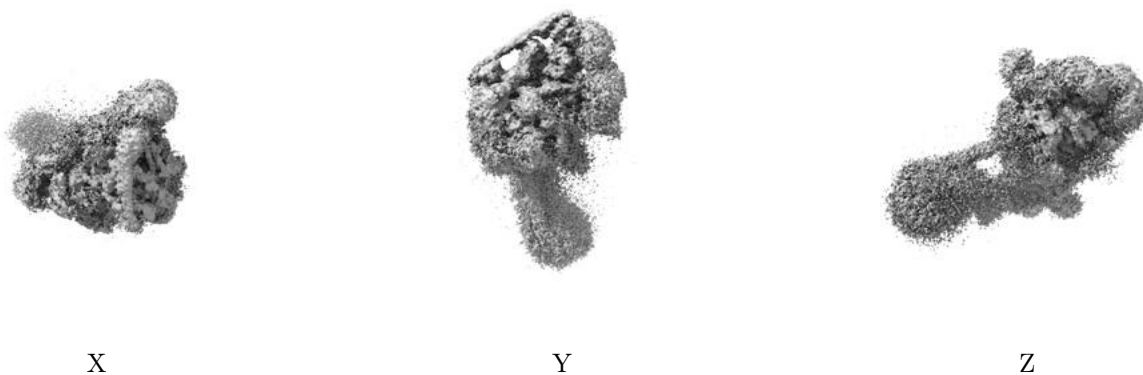


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

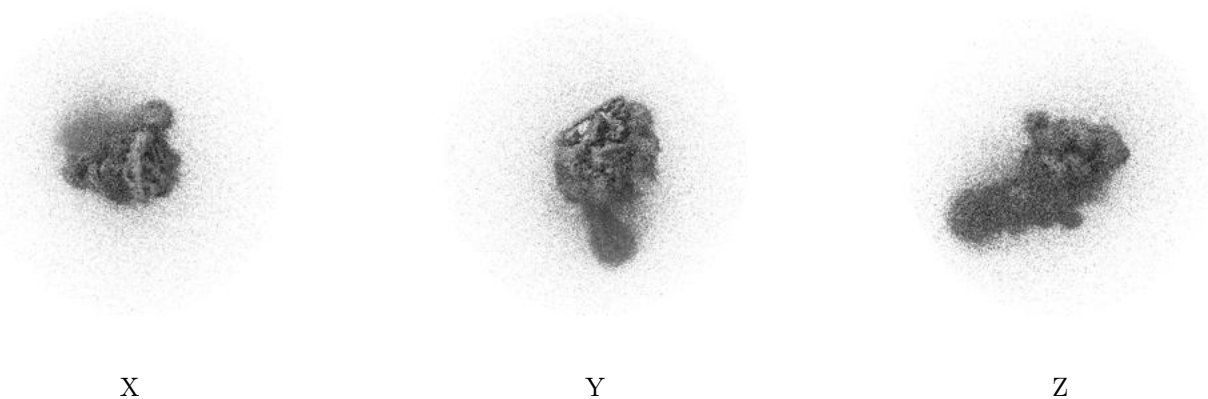
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

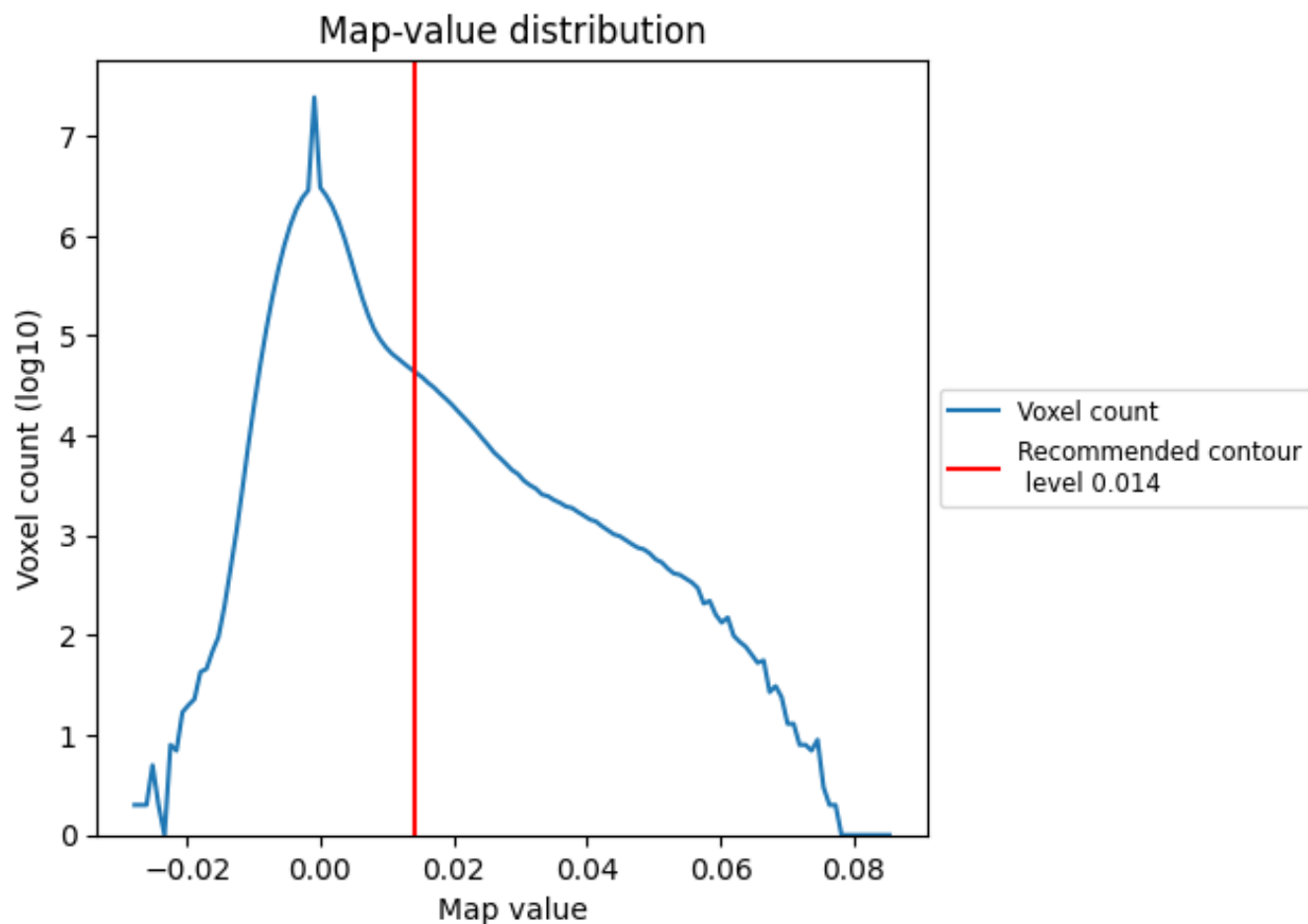
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

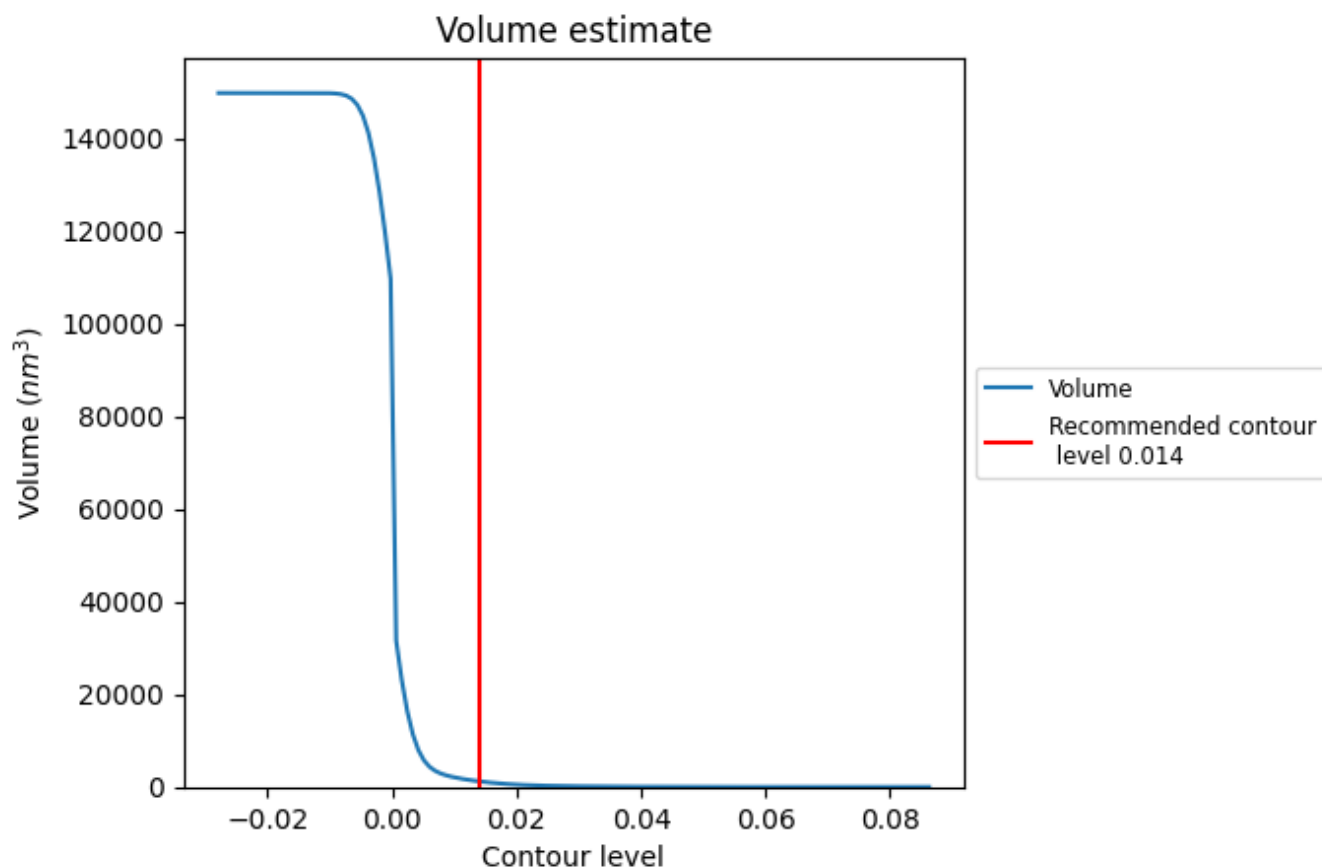
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

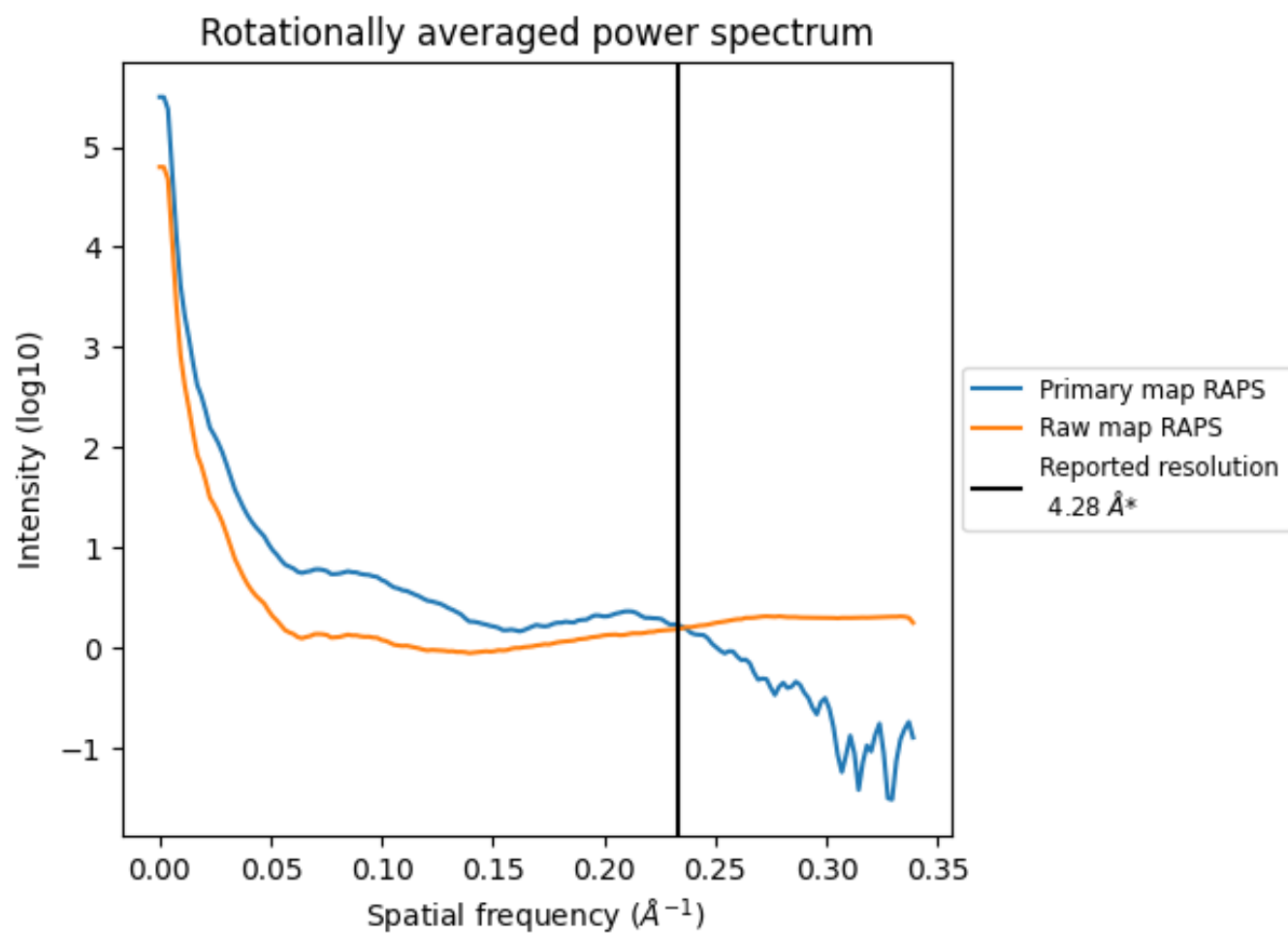
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1212 nm^3 ; this corresponds to an approximate mass of 1095 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 ⓘ

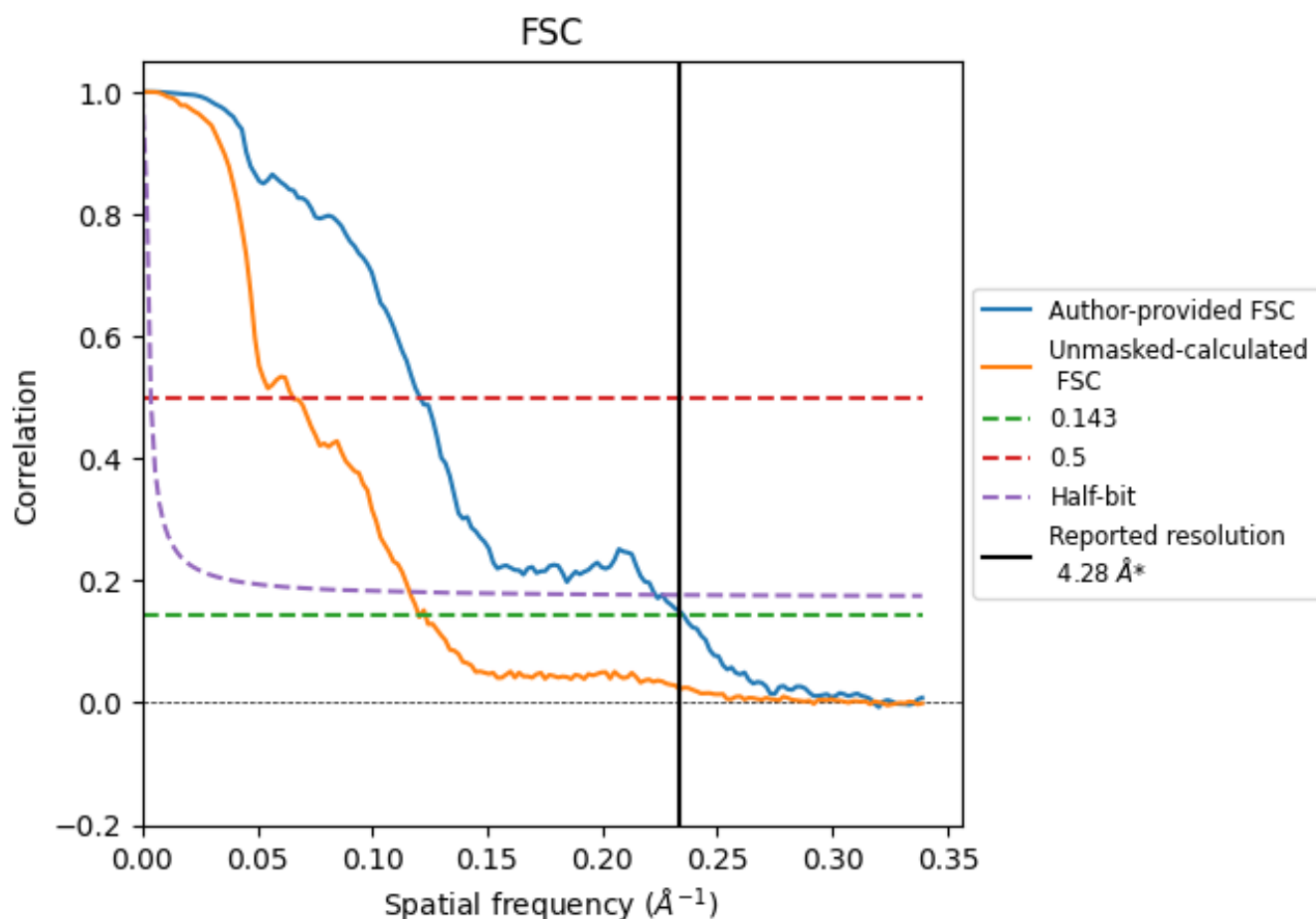


*Reported resolution corresponds to spatial frequency of 0.234 Å⁻¹

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 $0.234 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

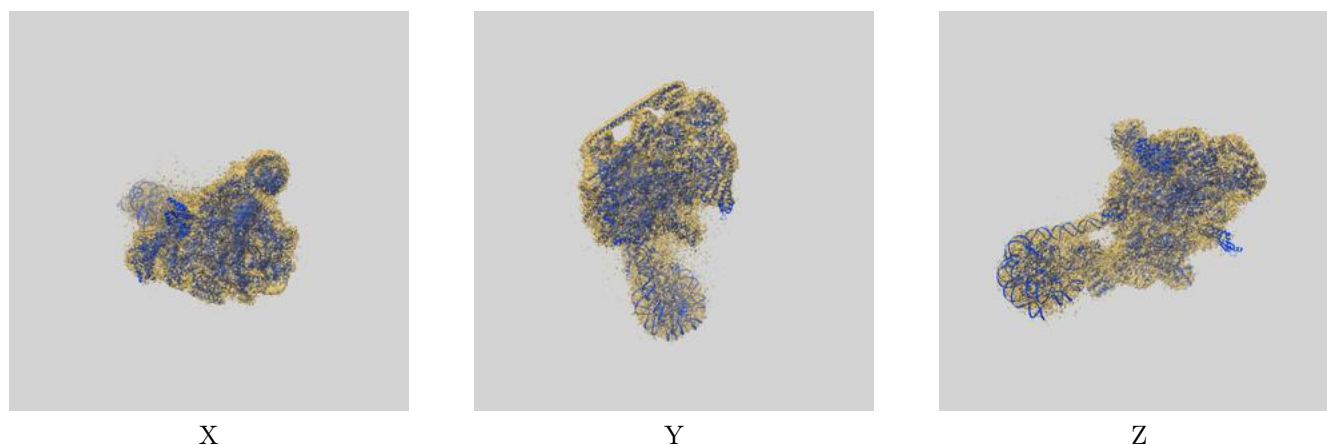
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.28	-	-
Author-provided FSC curve	4.25	8.29	4.48
Unmasked-calculated*	8.31	15.27	8.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.31 differs from the reported value 4.28 by more than 10 %

9 Map-model fit [i](#)

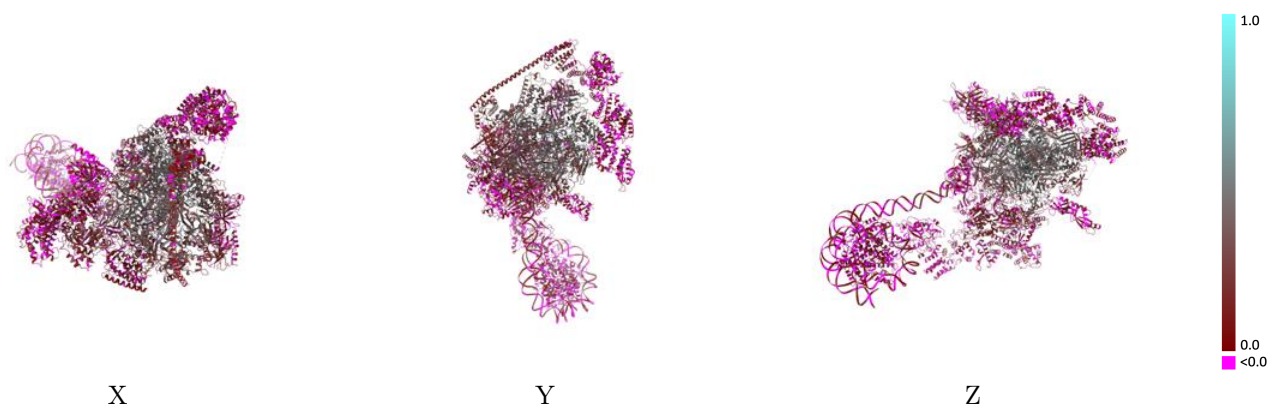
This section contains information regarding the fit between EMDB map EMD-66105 and PDB model 9WMU. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



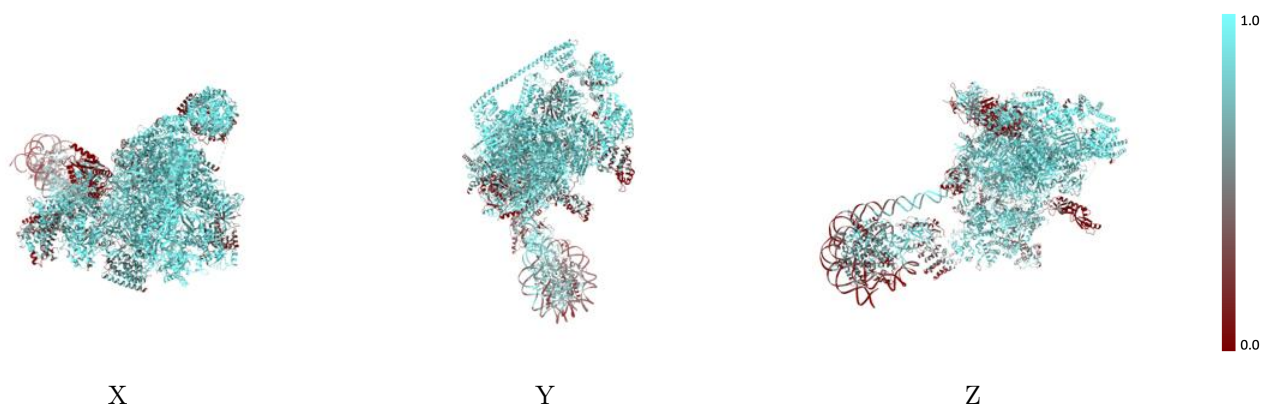
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



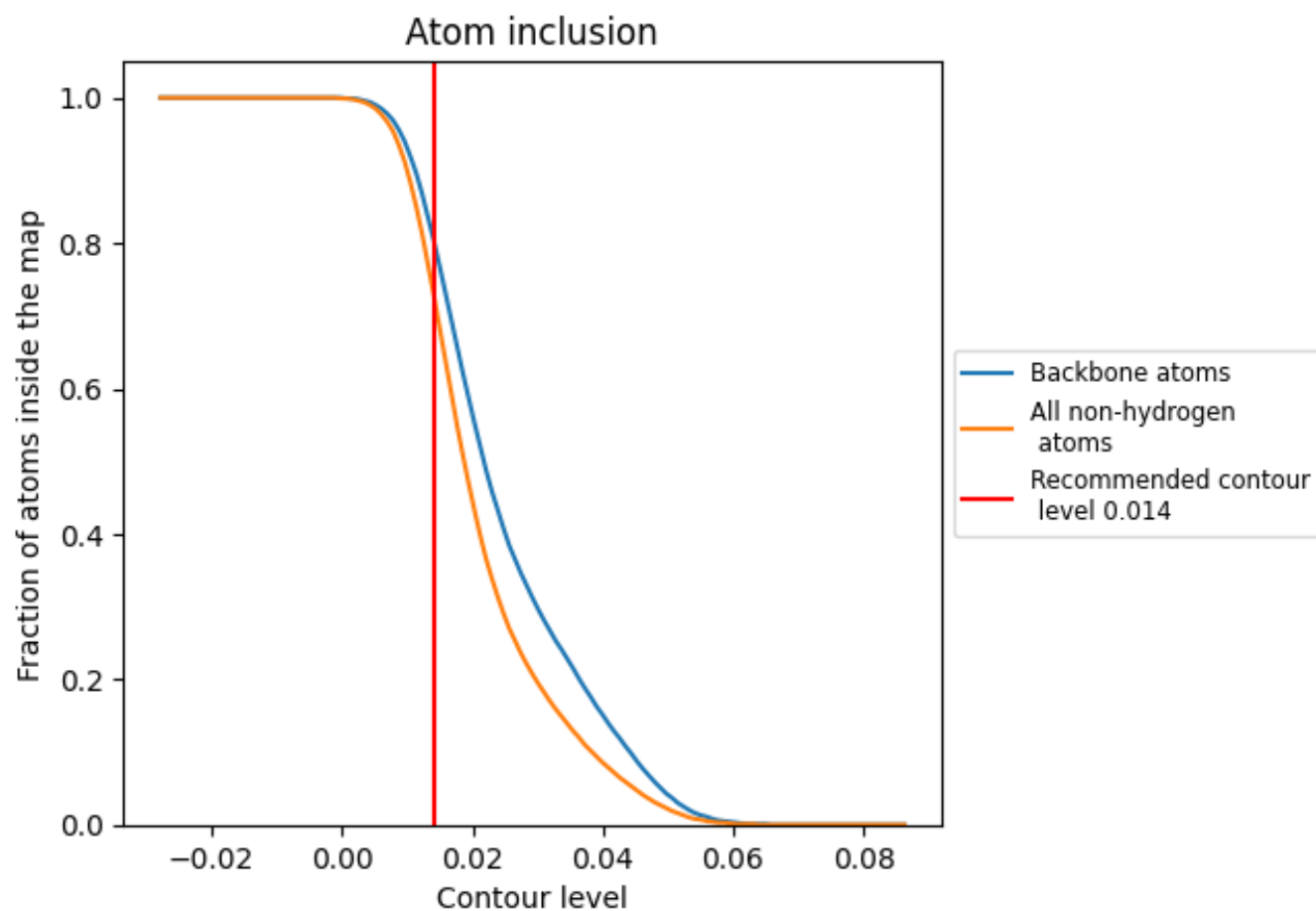
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7320	 0.1890
A	 0.9240	 0.3800
B	 0.9050	 0.3800
C	 0.9160	 0.4000
D	 0.8150	 0.1620
E	 0.9490	 0.3470
F	 0.9420	 0.4200
G	 0.8500	 0.2590
H	 0.9310	 0.3910
I	 0.8830	 0.2090
J	 0.9130	 0.3920
K	 0.9320	 0.4130
L	 0.9050	 0.3330
M	 0.8310	 0.1350
N	 0.5000	 0.0580
P	 0.8940	 0.2780
T	 0.5330	 0.0910
V	 0.8510	 0.0580
W	 0.7370	 0.1260
a	 0.7680	 0.0230
b	 0.7770	 0.0380
c	 0.4920	 0.0280
d	 0.5680	 0.0150
e	 0.3760	 0.0300
f	 0.4000	 -0.0160
g	 0.6670	 0.0170
h	 0.5320	 0.0240
m	 0.6350	 0.0860
n	 0.6740	 0.1170
q	 0.7460	 0.0730
r	 0.4490	 0.0880
s	 0.5110	 0.0240
u	 0.4790	 0.0960
v	 0.5030	 0.0580
x	 0.7500	 0.1980

