



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 12:09 PM UTC

PDB ID : 9WMT / pdb_00009wmt
EMDB ID : EMD-66104
Title : Co-transcriptional histone H3K36 methylation complex containing RNA polymerase II elongation complex, Set2, and the upstream nucleosome. (temp115, type A)
Authors : Kujirai, T.; Ehara, H.; Ito, T.; Henmi, M.; Sekine, S.; Kurumizaka, H.
Deposited on : 2025-09-03
Resolution : 3.59 Å(reported)

This is a wwPDB EM Validation Summary 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:

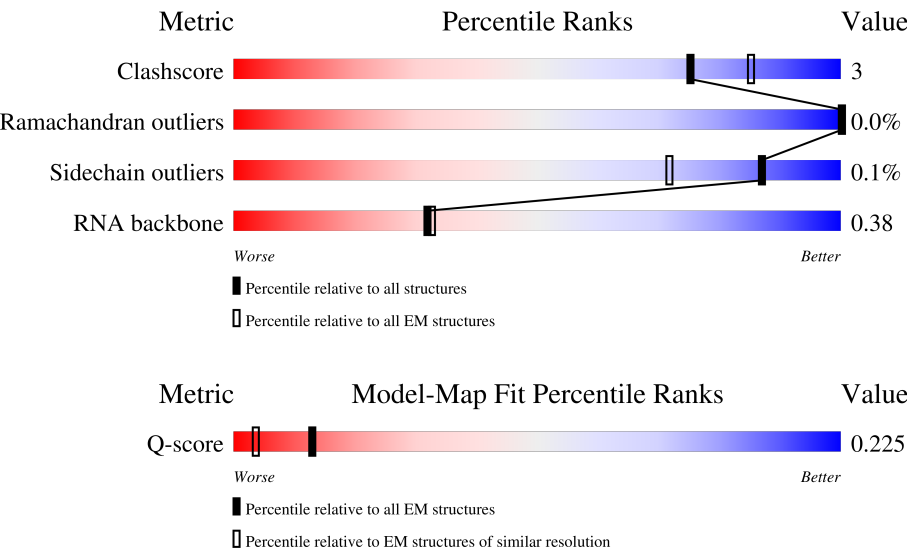
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.59 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	12565 (3.09 - 4.09)

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	76%5%19%
2	B	1227	88%7%5%
3	C	304	82%13%

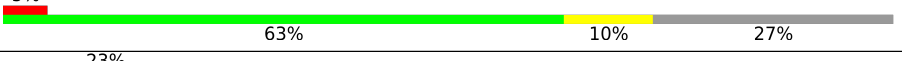
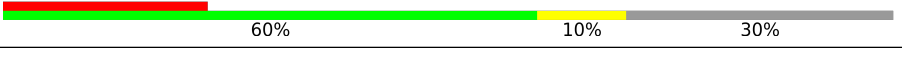
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Mol	Chain	Length	Quality of chain
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	M	113	
14	N	198	
15	P	20	
16	T	198	
17	V	108	
18	W	911	
19	m	1503	
20	n	417	
21	q	1084	
22	r	544	
23	s	725	
24	u	459	
25	v	396	
26	x	395	
27	a	139	
27	e	139	

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Mol	Chain	Length	Quality of chain
28	b	106	
28	f	106	
29	c	133	
29	g	133	
30	d	129	
30	h	129	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 78546 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	121	Total	C	N	O	P	0	0
			2482	1182	414	765	121		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	20	Total	C	N	O	P	0	0
			417	186	64	147	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	132	Total	C	N	O	P	0	0
			2710	1276	554	748	132		

- 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 Transcription elongation factor Spt6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	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 20 is a protein called Protein that interacts with Spt6p and copurifies with Spt5p and RNA polymerase II.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	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 21 is a protein called Component of the Paf1p complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	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
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 22 is a protein called RNAPII-associated chromatin remodeling Paf1 complex sub-

unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	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 23 is a protein called Histone-lysine N-methyltransferase, H3 lysine-36 specific.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	s	430	Total	C	N	O	S	0	0
			3415	2124	592	676	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 24 is a protein called Leo1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	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

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Chain	Residue	Modelled	Actual	Comment	Reference
u	-1	SER	-	expression tag	UNP C4R3K1
u	0	GLY	-	expression tag	UNP C4R3K1

- Molecule 25 is a protein called RNAP II-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	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 26 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
26	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 27 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	91	Total	C	N	O	S	0	0
			739	466	141	130	2		
27	e	104	Total	C	N	O	S	0	0
			841	530	163	145	3		

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 28 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
28	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
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805

- Molecule 29 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	c	106	Total	C	N	O	0	0
			819	517	160	142		
29	g	94	Total	C	N	O	0	0
			725	456	141	128		

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 30 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	94	Total	C	N	O	S	0	0
			732	459	131	139	3		
30	h	90	Total	C	N	O	S	0	0
			696	438	122	133	3		

There are 8 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
d	120	CYS	LYS	engineered mutation	UNP P06899
h	-3	GLY	-	expression tag	UNP P06899

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Chain	Residue	Modelled	Actual	Comment	Reference
h	-2	SER	-	expression tag	UNP P06899
h	-1	HIS	-	expression tag	UNP P06899
h	120	CYS	LYS	engineered mutation	UNP P06899

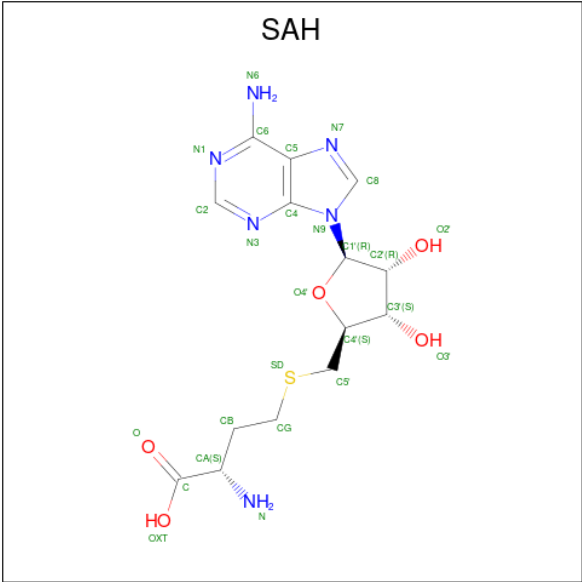
- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

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).

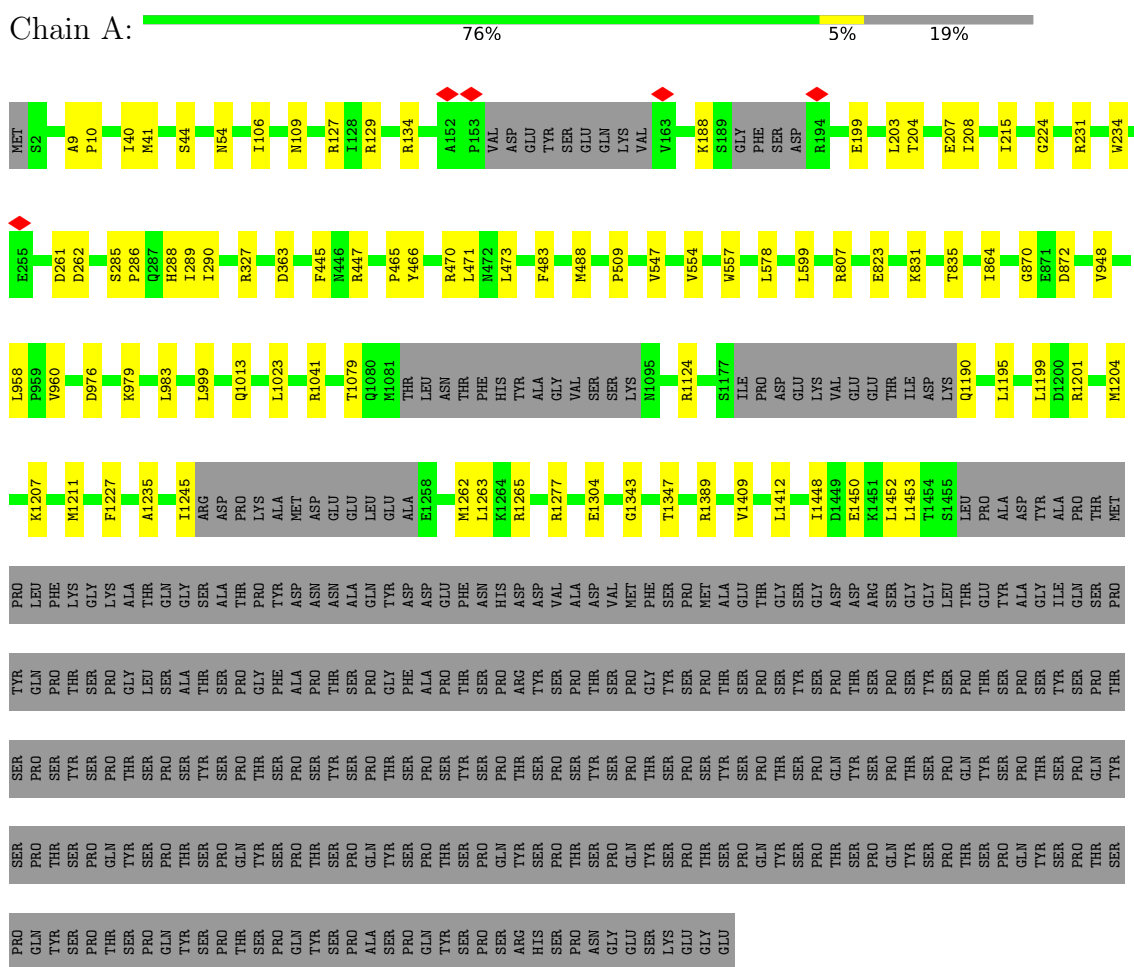


Mol	Chain	Residues	Atoms					AltConf
33	s	1	Total	C	N	O	S	0
			26	14	6	5	1	

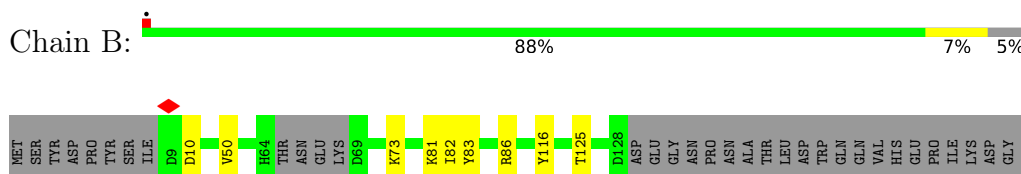
3 Residue-property plots

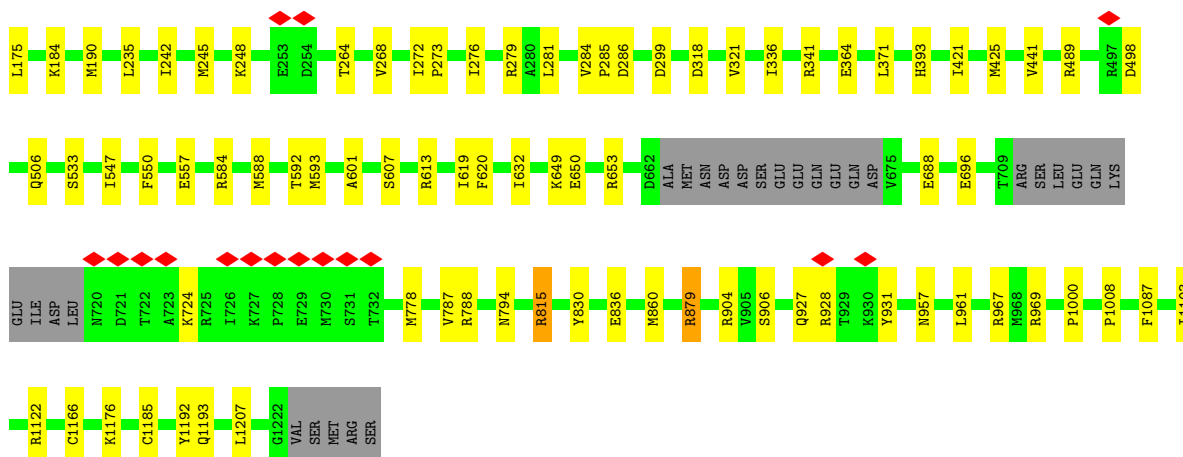
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: DNA-directed RNA polymerase subunit

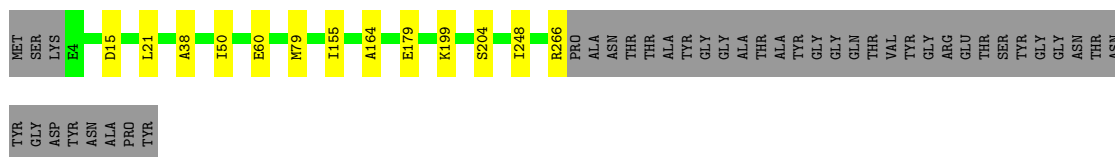
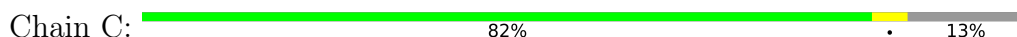


• Molecule 2: DNA-directed RNA polymerase subunit beta

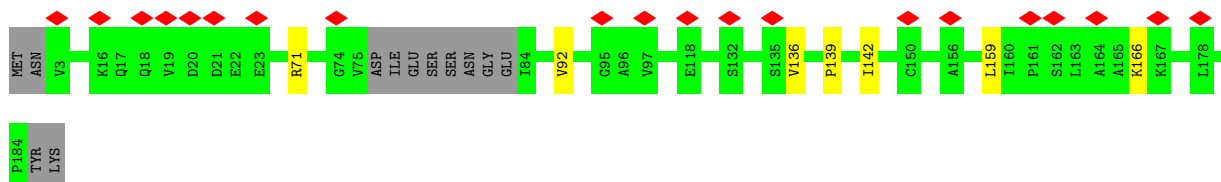




- Molecule 3: RNA polymerase II third largest subunit B44, part of central core



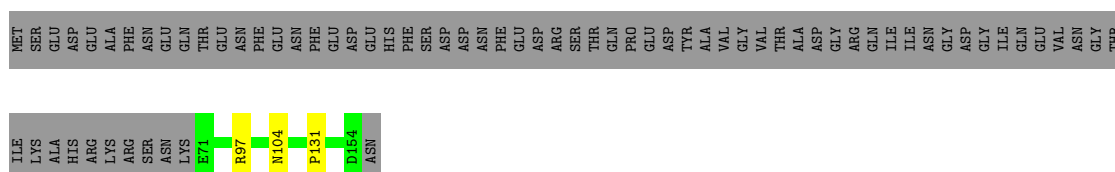
- Molecule 4: RNA polymerase II subunit B32



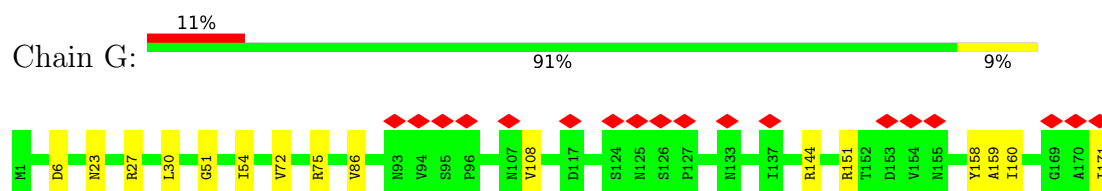
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



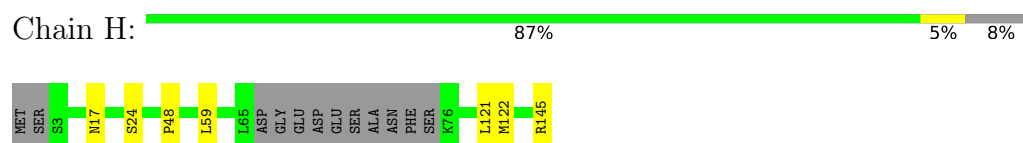
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III



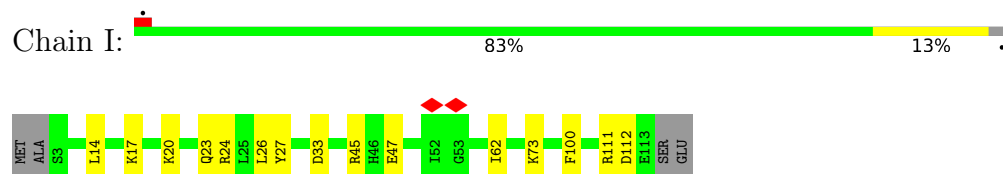
- Molecule 7: RNA polymerase II subunit



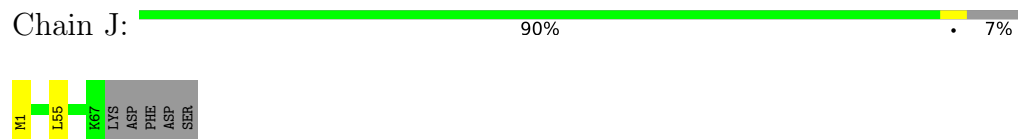
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



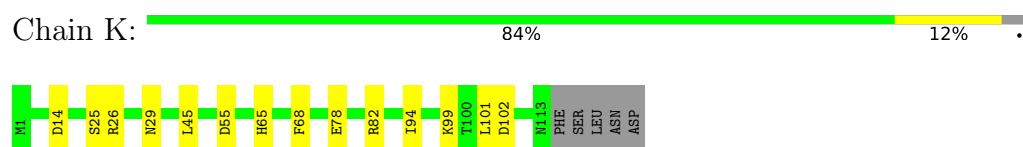
- Molecule 9: DNA-directed RNA polymerase subunit



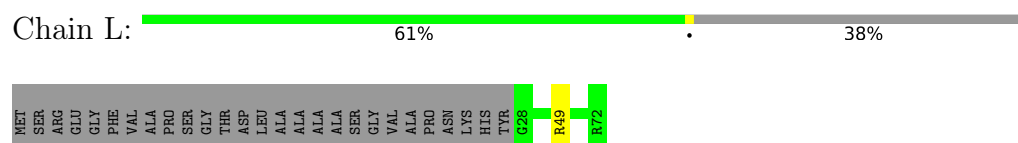
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



- Molecule 11: RNA polymerase II subunit B12.5



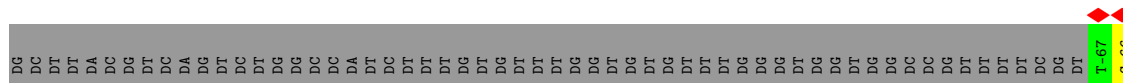
- Molecule 12: RNA polymerase subunit ABC10-alpha



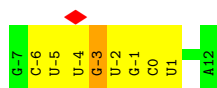
- Molecule 13: Transcription elongation factor 1 homolog



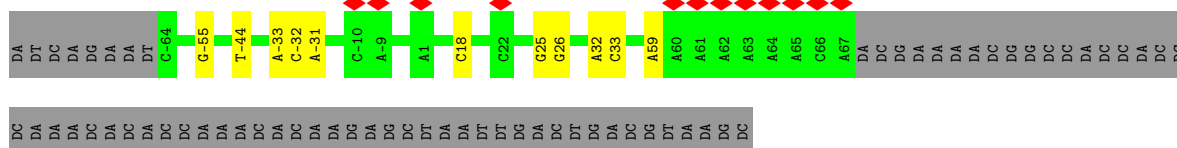
- Molecule 14: DNA (198-MER)



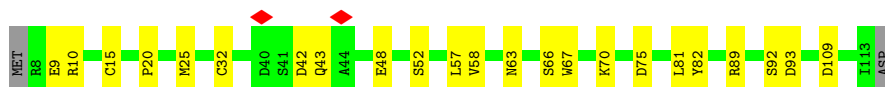
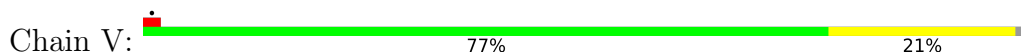
- Molecule 15: RNA (5'-R(P*GP*CP*UP*UP*GP*UP*GP*CP*UP*GP*UP*CP*UP*UP*CP*GP*UP*CP*CP*A)-3')



- Molecule 16: DNA (198-MER)

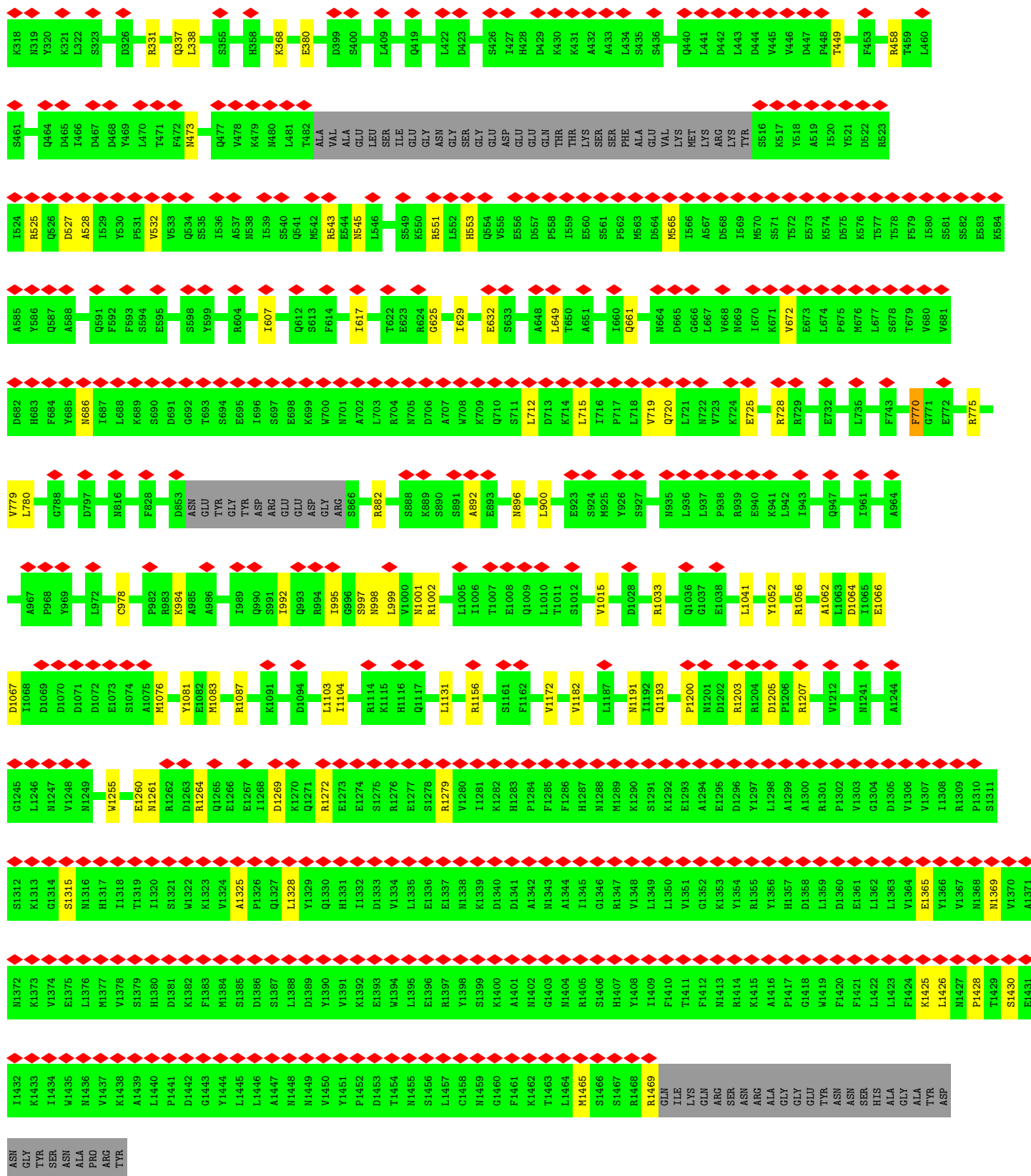


- Molecule 17: Transcription elongation factor SPT4



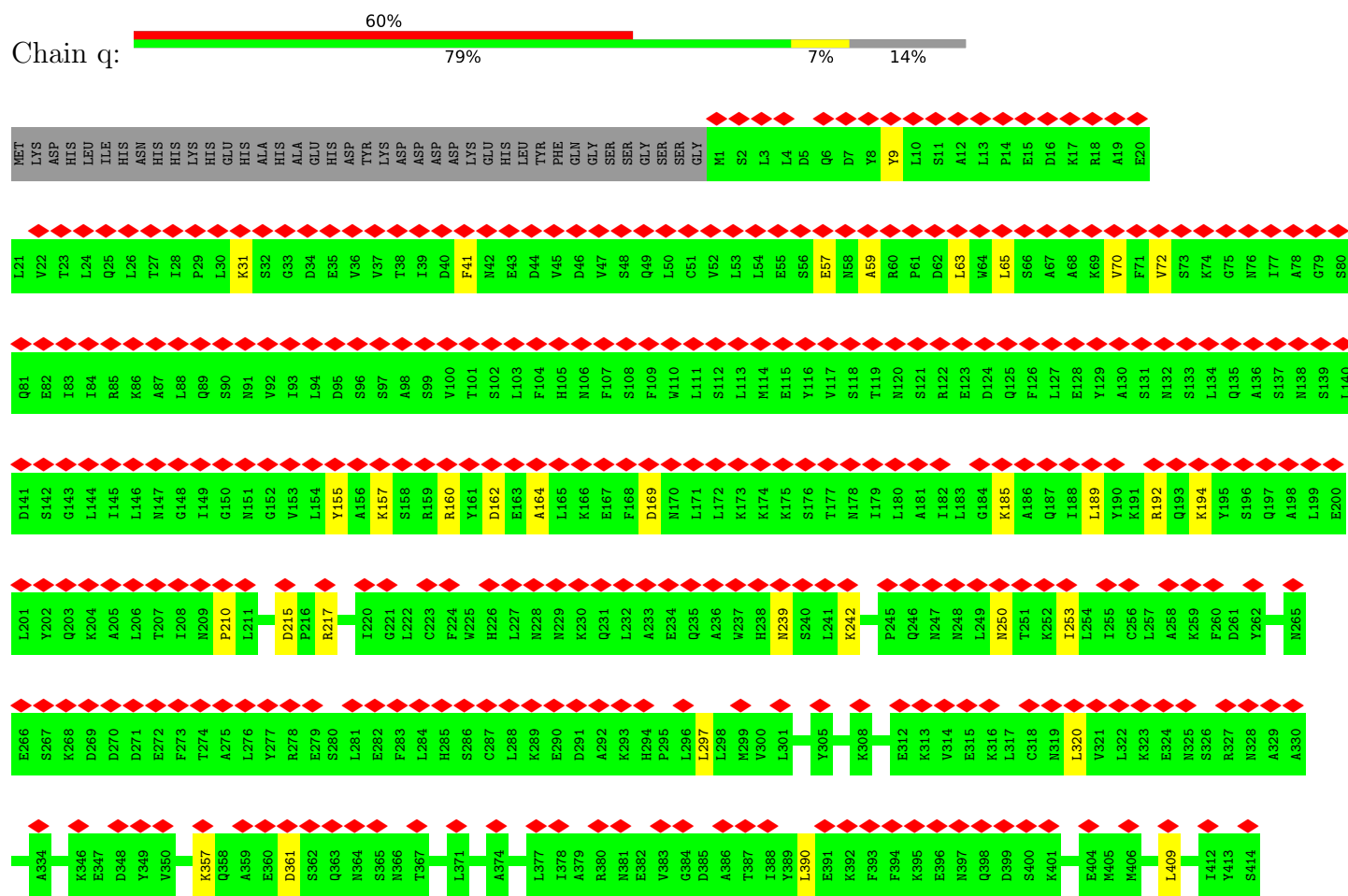
- Molecule 18: Transcription elongation factor SPT5

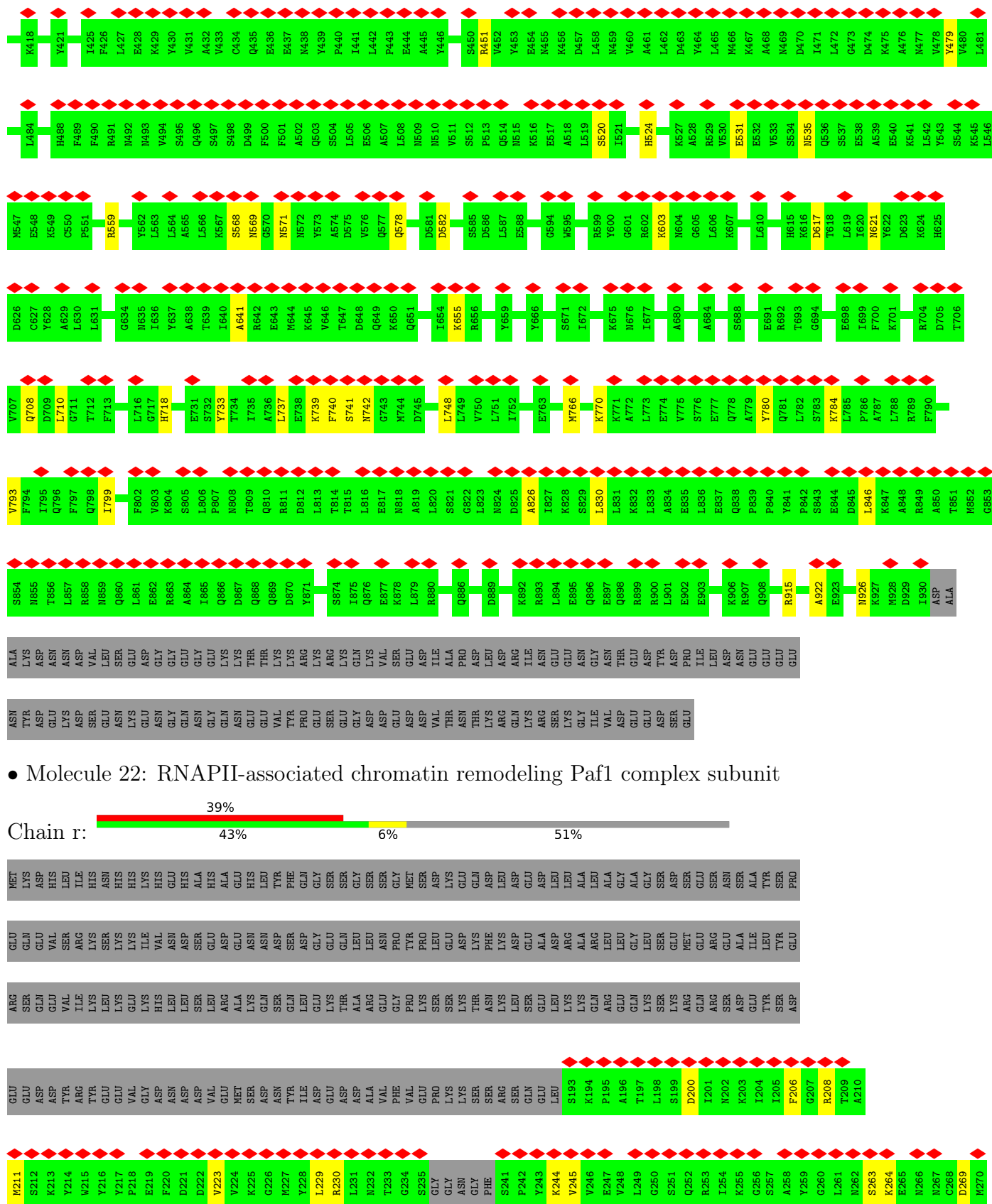




- Molecule 20: Protein that interacts with Spt6p and copurifies with Spt5p and RNA polymerase II

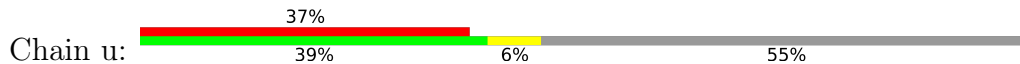
- Molecule 21: Component of the Paf1p complex





GLY	PRO	TYR	MET	GLU	LYS	LEU	ASP	LYS	TRP	LYS	ALA	LYS	HIS	GLU	LYS	LYS	ASP	ASN	LEU	LYS	ASP	LYS	ASP	LYS	VAL	ILE	GLN	LEU	SER	LYS	LYS	LYS	ASP	LYS	LYS	LYS	ASP	LYS	VAL	ILE	GLY	GLN	LYS	LYS	HIS	LYS	LYS	GLN	SER	GLY	GLU	LYS	LYS	ALA	LYS	LYS	LYS	GLU	SER	LEU	GLY	PRO	LYS	LYS	LYS	ASP	ASP	MET	ILE	ASN	VAL	PRO	GLU	THR	ALA
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- Molecule 24: Leo1



MET	LYS	ASP	HIS	HIS	LEU	ILE	HIS	ASN	HIS	HIS	LYS	HIS	GLU	HIS	ALA	HIS	ALA	GLU	HIS	LEU	PHE	THR	GLN	GLY	SER	SER	SER	SER	GLY	CYS	MET	SER	SER	GLN	GLU	LEU	GLU	GLN	ASN	ARG	ARG	SER	SER	GLY	GLU	GLU	PRO	PRO	VAL	LEU	ASP	ALA	ALA	ASN	THR	SER	ASP	VAL	ASP	ASP	ASP	ASP
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GLY	LEU	LEU	PHE	GLY	ASP	ASP	ASP	GLU	GLN	PRO	GLU	ALA	LYS	PRO	GLY	GLN	LEU	ASP	ASP	SER	SER	ASN	ASP	ALA	ALA	GLU	GLU	ASP	GLU	GLU	GLN	GLU	LYS	ALA	GLY	LYS	PRO	PRO	GLU	GLU	LYS	THR	VAL	SER	H75	T76	K77	V78	S79	Y90	D81	N82	G83	E84	T85	L86	D87	I88	S89	S90
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P91	I92	H93	P94	K95	S96	H97	I98	P99	Q100	G101	K102	D104	R105	W106	V107	V108	K109	L110	P111	D112	F113	L114	D115	I116	N117	A118	E119	P120	F121	D122	P123	R124	P125	F126	E127	M128	N129	V130	K131	T132	H133	E134	D135	K136	N137	Q138	E139	L140	L141	D142	K143	L144	I145	A146	V147	N148	V149	T150
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R151	R152	R153	R154	A155	K156	S157	E158	T159	G160	I161	L162	F163	K164		M167		T170	I171	Q172	W173	E174	D175	G176	T177	Y178	S179	L180	R181	W182	G183	S184	E185	I186	F187	D188	M189	F190	T191	T192	N193	T194	D195	D196	N197	Y198	L199	V200	S201	E202	H203	N204	E205	E206	G207	T208	L209	M210	T211	E212
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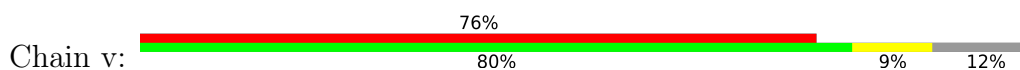
S213	T214	L215	S216	K217	S218	V219	K220	L221	F226	Q227	S228	T229	T230	H231	Q232	K233	L234	A235	K236	A237	L238	S239	A240	K241	Q242	K243	K244	E245	S246	Y247	V252	T253	R252	R263	L264	E265	E268	N269	E270	R271	Y272	T273	L274	E275	R276	R277	R278	K279	Q280	A281	E282	GLU	GLU	GLU	SP
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[illegible]

ALA	VAL	GLU	ASN	ASP	SER	ALA	ASP	GLU	GLU	SER	GLU	ASN	GLY	ASP	ASP	GLU	GLU	ALA	ALA	GLU	ARG	ASN	ARG	LEU	LYS	ARG	GLY	ALA	ALA	SER	LYS	TYR	THR	ASN	GLY	GLY	GLN	GLN	GLN	SER	PRO	GLU	VAL	LYS	SER	GLU	ALA	ASP	ASN	ALA
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SER	GLN	ARG	ASP	ASP	ALA	PRO	ARG	LYS	LYS	ARG	ARG	VAL	ILE	LEU	ASP	ASP	ASP	GLU	GLU	GLU	GLU	GLU
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- Molecule 25: RNAP II-associated protein

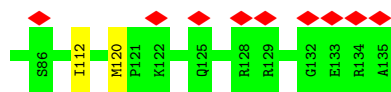


GLY	SER	ALA	MET	THR	SER	SER	LYS	SER	R7	Q8	D9	Y10	I11	A12	K13	V14	R15	Y16	Q17	N18	D19	L20	P21	A22	P23	P24	C25	P26	P27	K28	L29	L30	K31	Y32	E33	I34	E35	K36	E37	Q40	K41	E42	F43	L44	L49	L50	S51	K56	D57	R60	Y61	L62	M63	N64	F65
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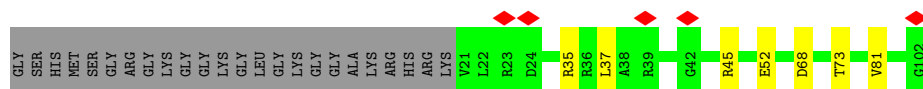
	G69	L70	D71	V72	H73	W74	L75	R76	I77	P78	G79	I80	I81	S82	N83	E84	K85	S86	L87	K88	K89	L90	F91	S92	S93	Y94	K95	N96	L97	A98	I99	E100	M101	L102	H103	P104	D105	D106	R107	L108	L109	L110	V111	D112	P113	ASN	LYS	SER	ALA	THR	LEU	ASN	GLU	S123	Q132	S135
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D136	G137	LYS	ILE	ASN	LEU	GLN	ASN	PHE	THR	ASN	LYS	ARG	LYS	HIS	GLN	ASP	MET	GLU	D156	T157	N158	P159	R160	S161	Q162	L163	H164	E167	F170	D171	E172	V173	I174	D175	P176	R177	N178	K179	N180	R181	L182	Q183	S184	L185	I186	H187	P188	R189	K190	K191	I192	K193	A194	V195	K196
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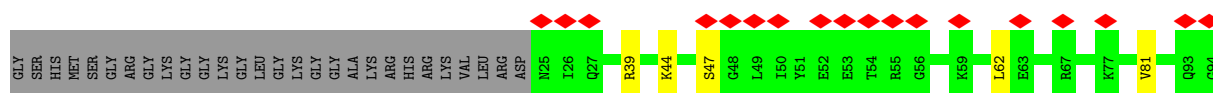
F200	F201	F202	D203	T204	S205	T206	F207	D208	D209	V210	F211	H212	S213	L214	K215	F216	V217	G218	S219	A220	S221	L222	S223	K224	D225	R226	P227	L228	N229	E230	Q231	L232	G233	Q234	VAL	SER	SER	GLU	THR	ASP	THR	SER	THR	SER	SER	V243	N244	A245	S246	L247	L248	T249	S250	L251	F252	K253	P254	I255	E256	I257	N258	P259
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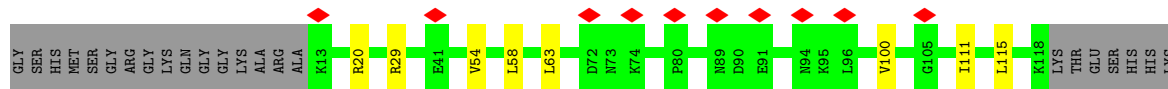
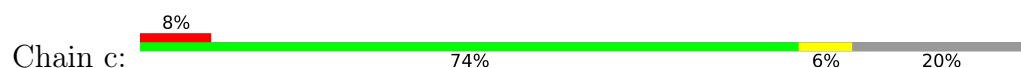
- Molecule 28: Histone H4



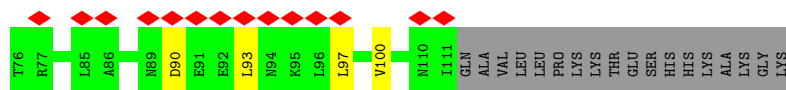
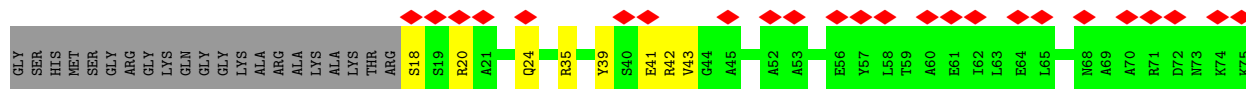
- Molecule 28: Histone H4



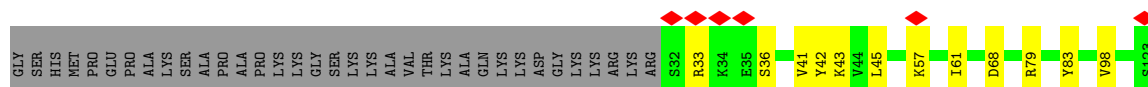
- Molecule 29: Histone H2A type 1-B/E



- Molecule 29: Histone H2A type 1-B/E

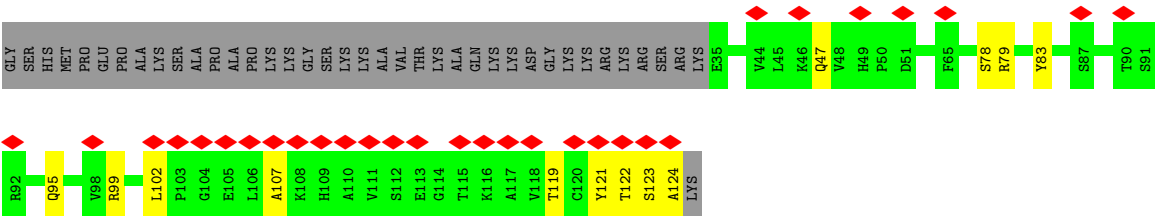


- Molecule 30: Histone H2B type 1-J





• Molecule 30: 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	35823	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 ($e^-/\text{\AA}^2$)	58	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	0.151	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	398.25, 398.25, 398.25	wwPDB
Map dimensions	270, 270, 270	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/11267	0.42	0/15222
2	B	0.20	0/9464	0.43	0/12763
3	C	0.20	0/2139	0.40	0/2895
4	D	0.14	0/1361	0.33	0/1837
5	E	0.19	0/1773	0.43	0/2385
6	F	0.18	0/687	0.37	0/931
7	G	0.14	0/1354	0.33	0/1837
8	H	0.20	0/1070	0.38	0/1444
9	I	0.11	0/934	0.28	0/1257
10	J	0.19	0/563	0.41	0/753
11	K	0.20	0/953	0.41	0/1291
12	L	0.20	0/365	0.45	0/484
13	M	0.15	0/513	0.37	0/693
14	N	0.29	0/2770	0.59	0/4278
15	P	0.25	0/462	0.59	0/716
16	T	0.27	0/3055	0.51	0/4706
17	V	0.16	0/840	0.44	0/1140
18	W	0.17	0/4319	0.41	0/5838
19	m	0.17	0/9847	0.38	0/13321
20	n	0.17	0/1132	0.38	0/1526
21	q	0.16	0/7689	0.33	0/10368
22	r	0.16	0/2169	0.34	0/2901
23	s	0.20	0/3469	0.49	0/4670
24	u	0.14	0/1740	0.31	0/2347
25	v	0.15	0/2944	0.33	0/3973
26	x	0.13	0/1716	0.30	0/2310
27	a	0.27	0/747	0.56	0/1001
27	e	0.28	0/853	0.55	0/1144
28	b	0.26	0/660	0.58	0/883
28	f	0.28	0/626	0.54	0/837
29	c	0.24	0/829	0.58	0/1118
29	g	0.23	0/734	0.52	0/991

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	d	0.25	0/743	0.57	0/998
30	h	0.27	0/707	0.62	0/954
All	All	0.20	0/80494	0.42	0/109812

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	58	0
3	C	2098	0	2057	10	0
4	D	1349	0	1345	4	0
5	E	1741	0	1754	11	0
6	F	677	0	693	3	0
7	G	1325	0	1342	10	0
8	H	1053	0	1050	4	0
9	I	917	0	864	10	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	2482	0	1378	12	0
15	P	417	0	213	1	0
16	T	2710	0	1459	10	0
17	V	824	0	795	22	0
18	W	4250	0	4296	69	0
19	m	9653	0	9500	68	0
20	n	1115	0	1186	20	0
21	q	7552	0	7545	44	0
22	r	2139	0	2155	18	0
23	s	3415	0	3351	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	u	1707	0	1676	20	0
25	v	2878	0	2873	26	0
26	x	1682	0	1731	8	0
27	a	739	0	778	5	0
27	e	841	0	883	10	0
28	b	653	0	696	6	0
28	f	619	0	659	7	0
29	c	819	0	879	10	0
29	g	725	0	764	14	0
30	d	732	0	750	11	0
30	h	696	0	706	9	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	0	0
All	All	78546	0	76139	473	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.

The worst 5 of 473 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)
17:V:43:GLN:HB2	29:g:42:ARG:HD2	1.67	0.76
18:W:215:ARG:NH2	19:m:234:TYR:HE1	1.85	0.75
23:s:258:ILE:HG21	23:s:265:THR:HG21	1.68	0.74
18:W:304:VAL:HB	20:n:286:ARG:HH21	1.54	0.72
1:A:445:PHE:CE2	1:A:471:LEU:HD21	2.24	0.72

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	1392/1743 (80%)	1356 (97%)	35 (2%)	1 (0%)	48	79
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
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%)	61 (98%)	1 (2%)	0	100	100
17	V	104/108 (96%)	101 (97%)	3 (3%)	0	100	100
18	W	529/911 (58%)	503 (95%)	26 (5%)	0	100	100
19	m	1170/1503 (78%)	1152 (98%)	18 (2%)	0	100	100
20	n	137/417 (33%)	135 (98%)	2 (2%)	0	100	100
21	q	928/1084 (86%)	923 (100%)	5 (0%)	0	100	100
22	r	260/544 (48%)	254 (98%)	6 (2%)	0	100	100
23	s	428/725 (59%)	412 (96%)	16 (4%)	0	100	100
24	u	206/459 (45%)	206 (100%)	0	0	100	100
25	v	341/396 (86%)	330 (97%)	11 (3%)	0	100	100
26	x	201/395 (51%)	200 (100%)	1 (0%)	0	100	100
27	a	89/139 (64%)	89 (100%)	0	0	100	100
27	e	102/139 (73%)	100 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	b	80/106 (76%)	77 (96%)	3 (4%)	0	100	100
28	f	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
29	c	104/133 (78%)	101 (97%)	3 (3%)	0	100	100
29	g	92/133 (69%)	90 (98%)	2 (2%)	0	100	100
30	d	92/129 (71%)	91 (99%)	1 (1%)	0	100	100
30	h	88/129 (68%)	83 (94%)	5 (6%)	0	100	100
All	All	8985/12191 (74%)	8789 (98%)	195 (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	81
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	m	1079/1354 (80%)	1078 (100%)	1 (0%)	88	87
20	n	125/361 (35%)	125 (100%)	0	100	100
21	q	824/962 (86%)	824 (100%)	0	100	100
22	r	239/485 (49%)	239 (100%)	0	100	100
23	s	380/649 (59%)	380 (100%)	0	100	100
24	u	192/406 (47%)	192 (100%)	0	100	100
25	v	325/369 (88%)	325 (100%)	0	100	100
26	x	190/354 (54%)	190 (100%)	0	100	100
27	a	77/112 (69%)	77 (100%)	0	100	100
27	e	87/112 (78%)	87 (100%)	0	100	100
28	b	67/81 (83%)	67 (100%)	0	100	100
28	f	63/81 (78%)	63 (100%)	0	100	100
29	c	84/102 (82%)	84 (100%)	0	100	100
29	g	74/102 (72%)	74 (100%)	0	100	100
30	d	80/107 (75%)	80 (100%)	0	100	100
30	h	76/107 (71%)	76 (100%)	0	100	100
All	All	8065/10712 (75%)	8060 (100%)	5 (0%)	87	87

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
19	m	770	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
21	q	319	ASN

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Mol	Chain	Res	Type
24	u	93	HIS
21	q	398	GLN
22	r	493	ASN
24	u	261	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	19/20 (95%)	8 (42%)	0

5 of 8 RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	1.12	3 (11%)	36,40,40	2.11	10 (27%)

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	-	-	1/15/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	s	1904	SAH	C2-N3	2.67	1.38	1.33
33	s	1904	SAH	C2-N1	2.56	1.38	1.33
33	s	1904	SAH	OXT-C	-2.35	1.23	1.30

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	s	1904	SAH	N3-C2-N1	-5.56	120.16	128.58
33	s	1904	SAH	C5-C4-N3	-4.62	120.36	126.72
33	s	1904	SAH	N9-C8-N7	-3.89	108.41	113.94
33	s	1904	SAH	C5'-SD-CG	-3.56	91.70	102.26
33	s	1904	SAH	C2-N3-C4	3.46	120.27	111.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

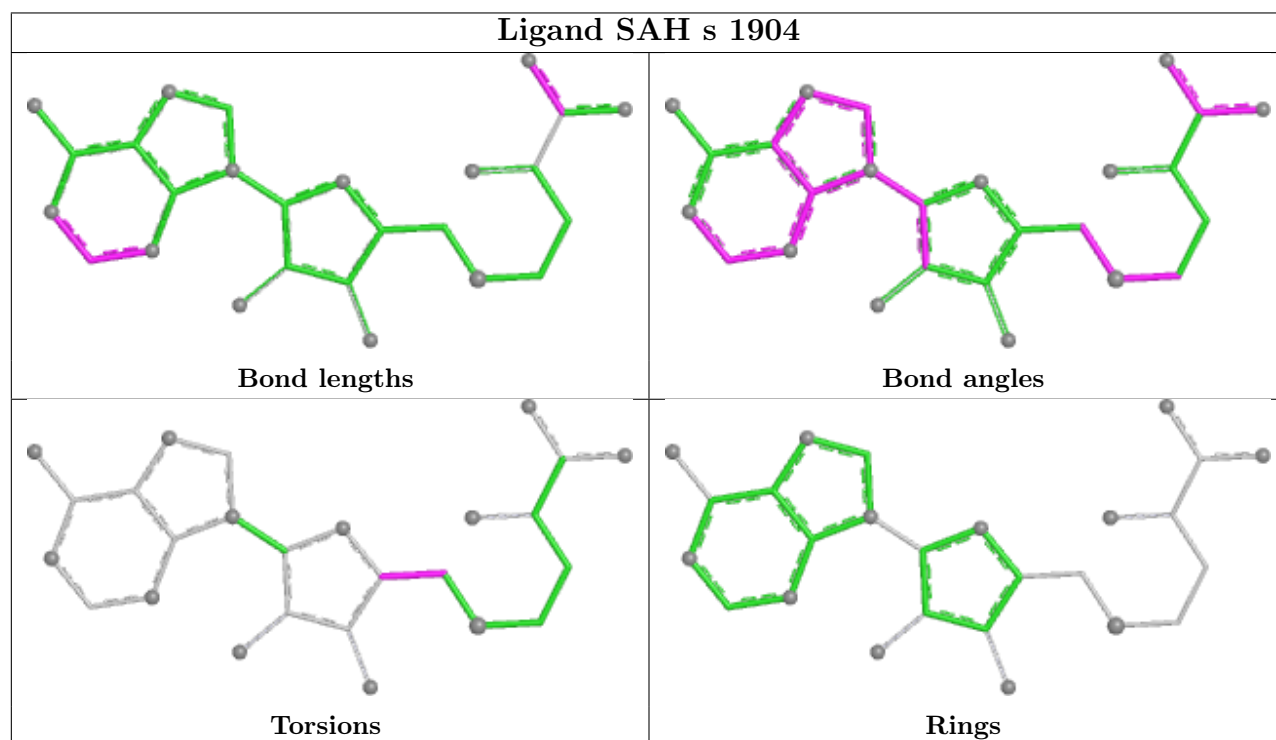
Mol	Chain	Res	Type	Atoms
33	s	1904	SAH	C3'-C4'-C5'-SD

There are no ring outliers.

No monomer is involved in short contacts.

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.

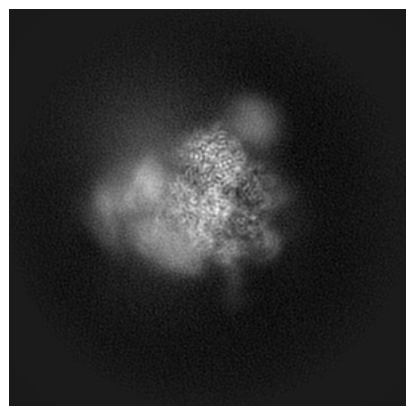
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66104. These allow visual inspection of the internal detail of the map and identification of artifacts.

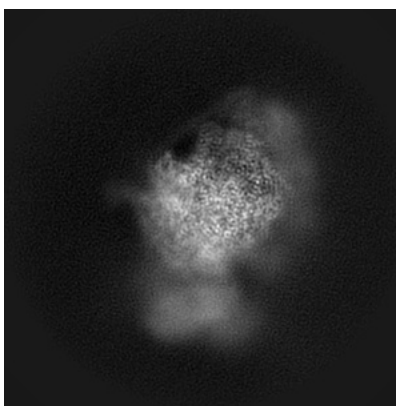
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

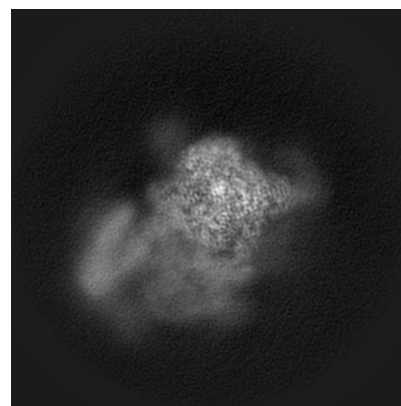
6.1.1 Primary map



X

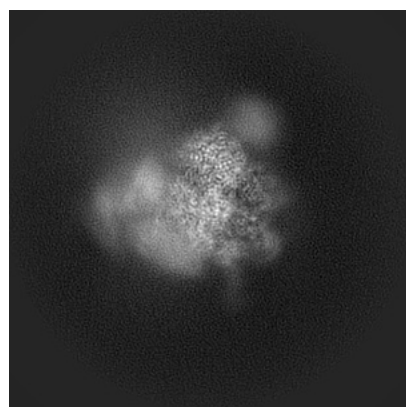


Y

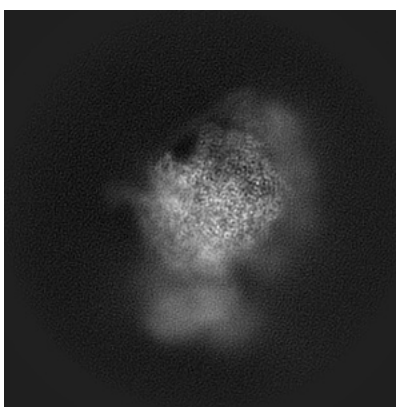


Z

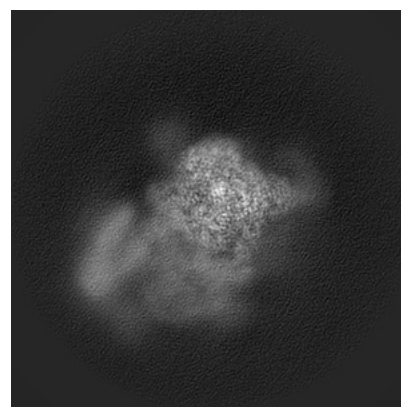
6.1.2 Raw map



X



Y

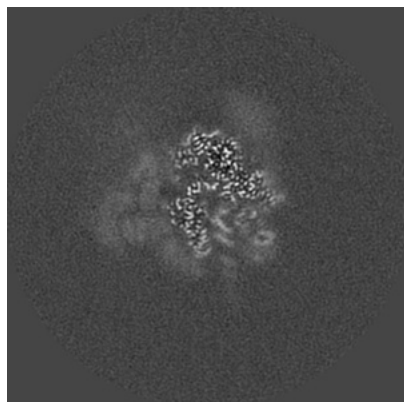


Z

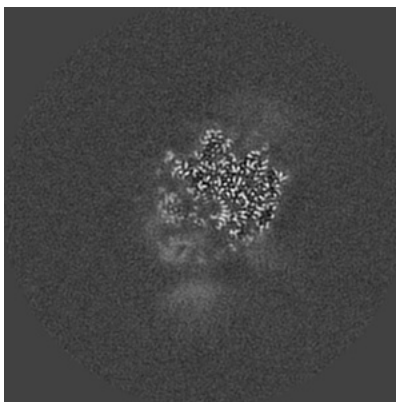
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

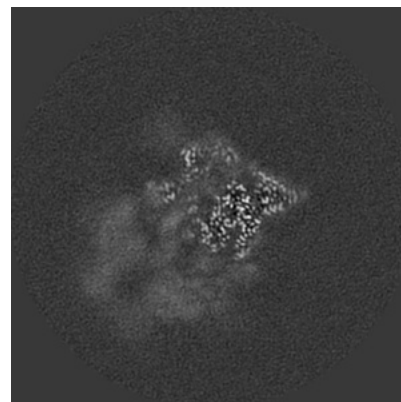
6.2.1 Primary map



X Index: 135

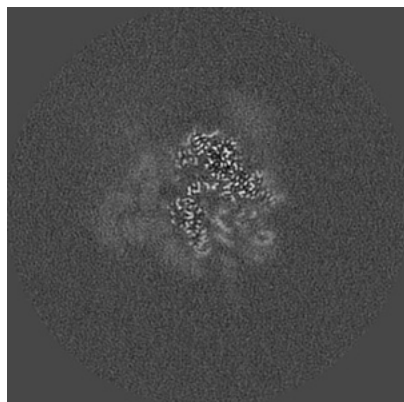


Y Index: 135

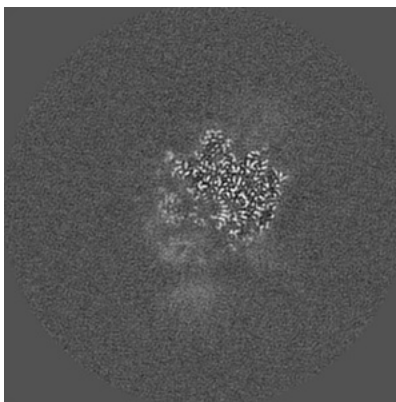


Z Index: 135

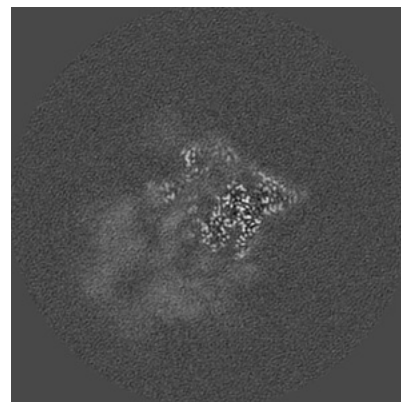
6.2.2 Raw map



X Index: 135



Y Index: 135

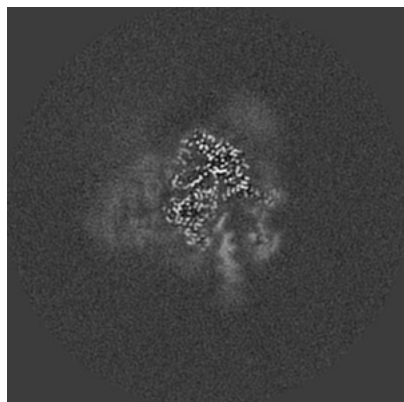


Z Index: 135

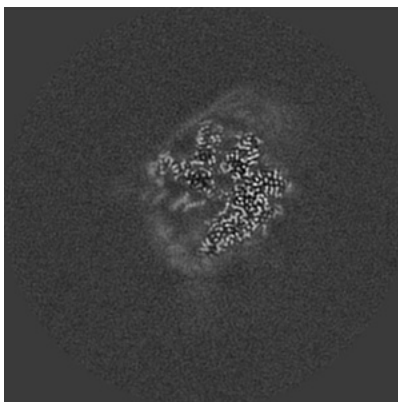
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

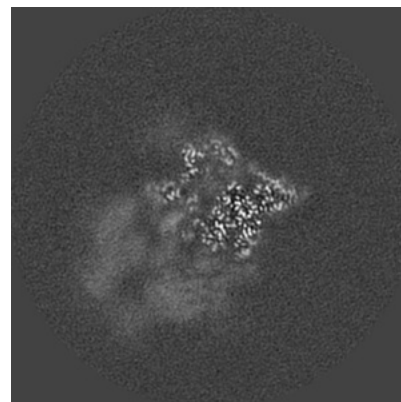
6.3.1 Primary map



X Index: 140

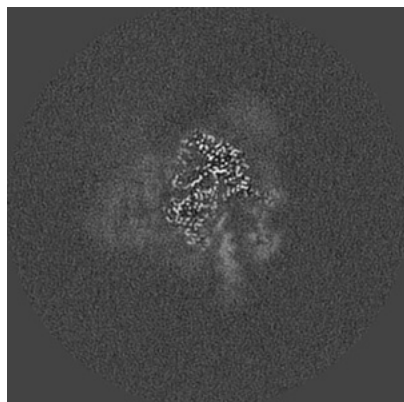


Y Index: 142

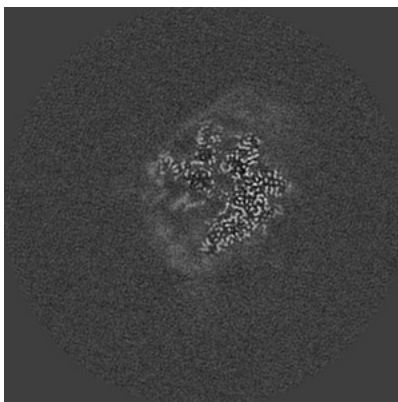


Z Index: 136

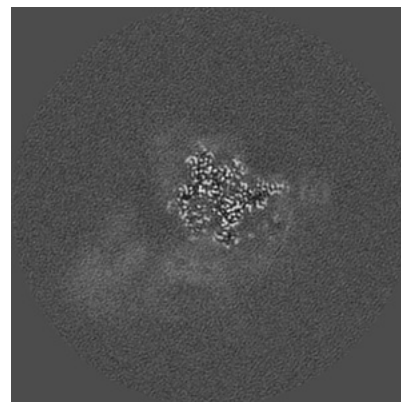
6.3.2 Raw map



X Index: 140



Y Index: 142

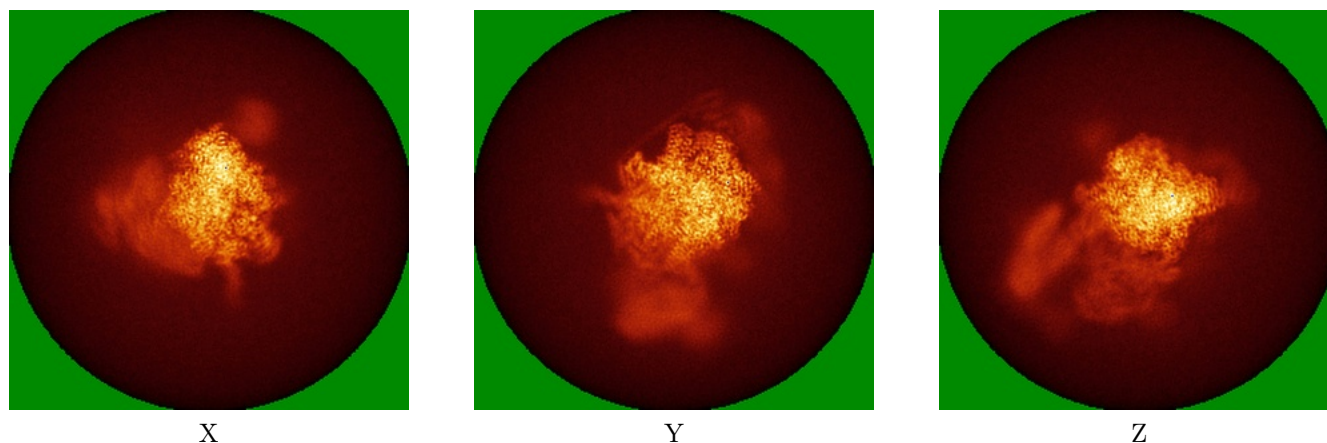


Z Index: 155

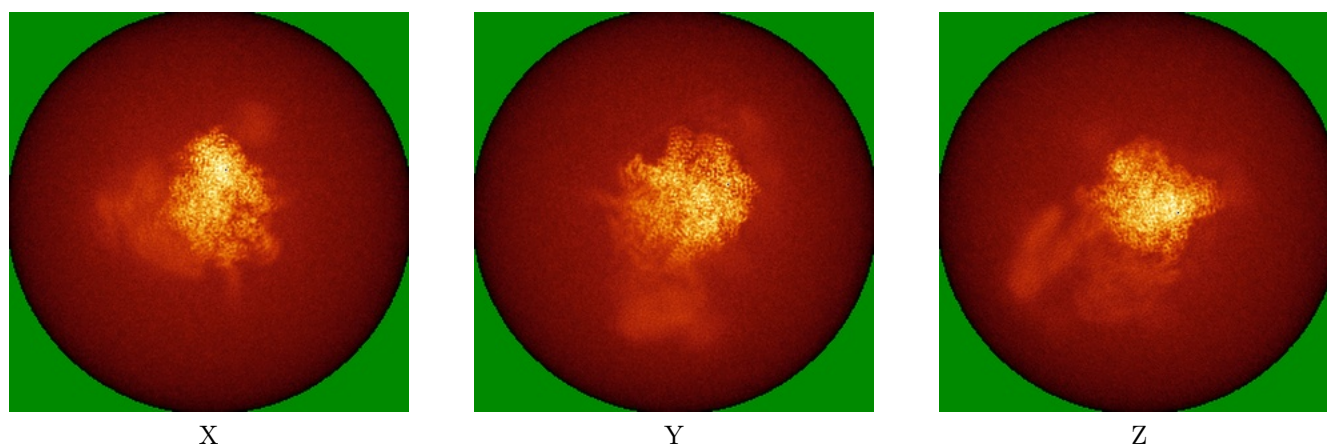
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

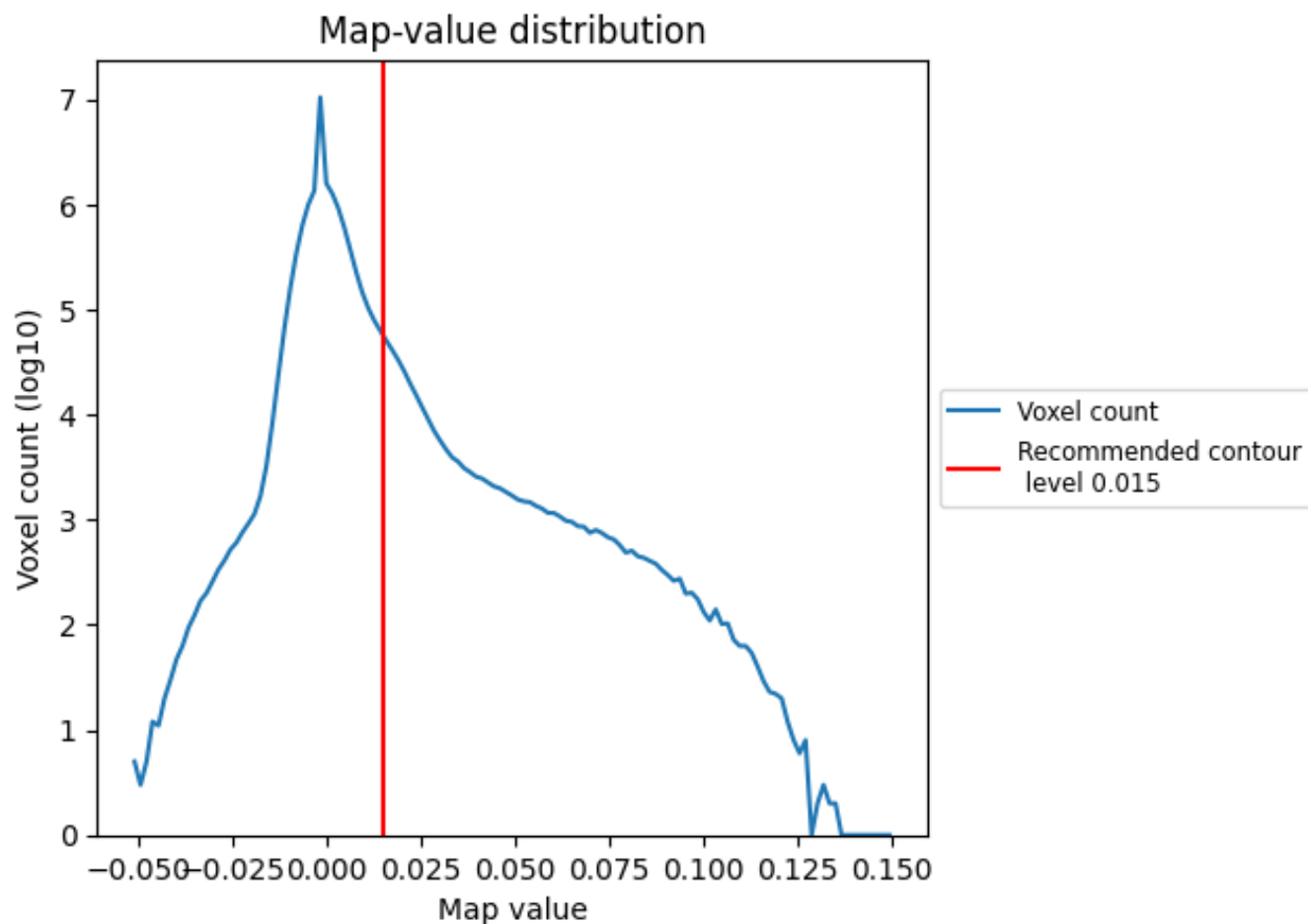
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

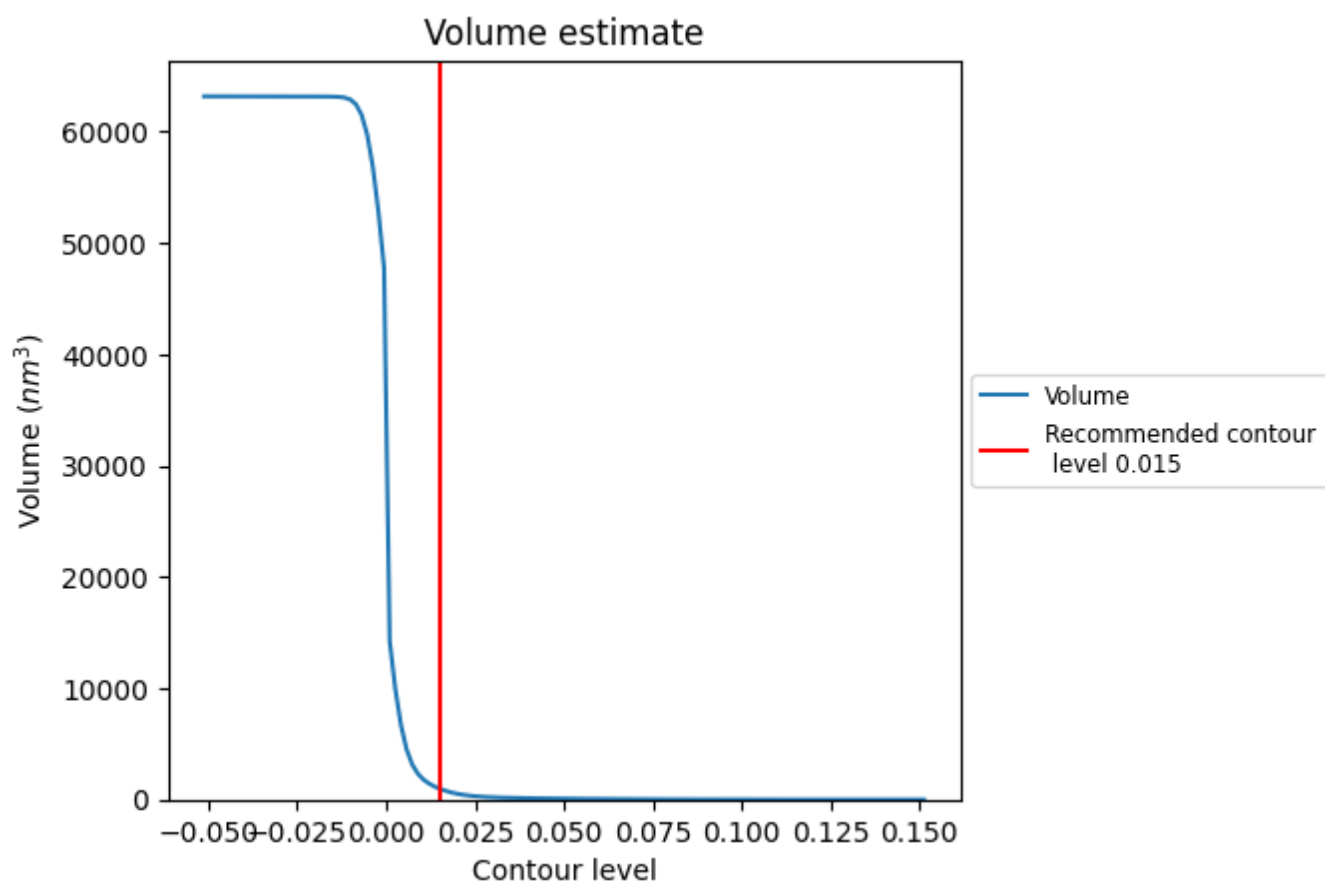
This section contains the results of statistical analysis of the map.

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.

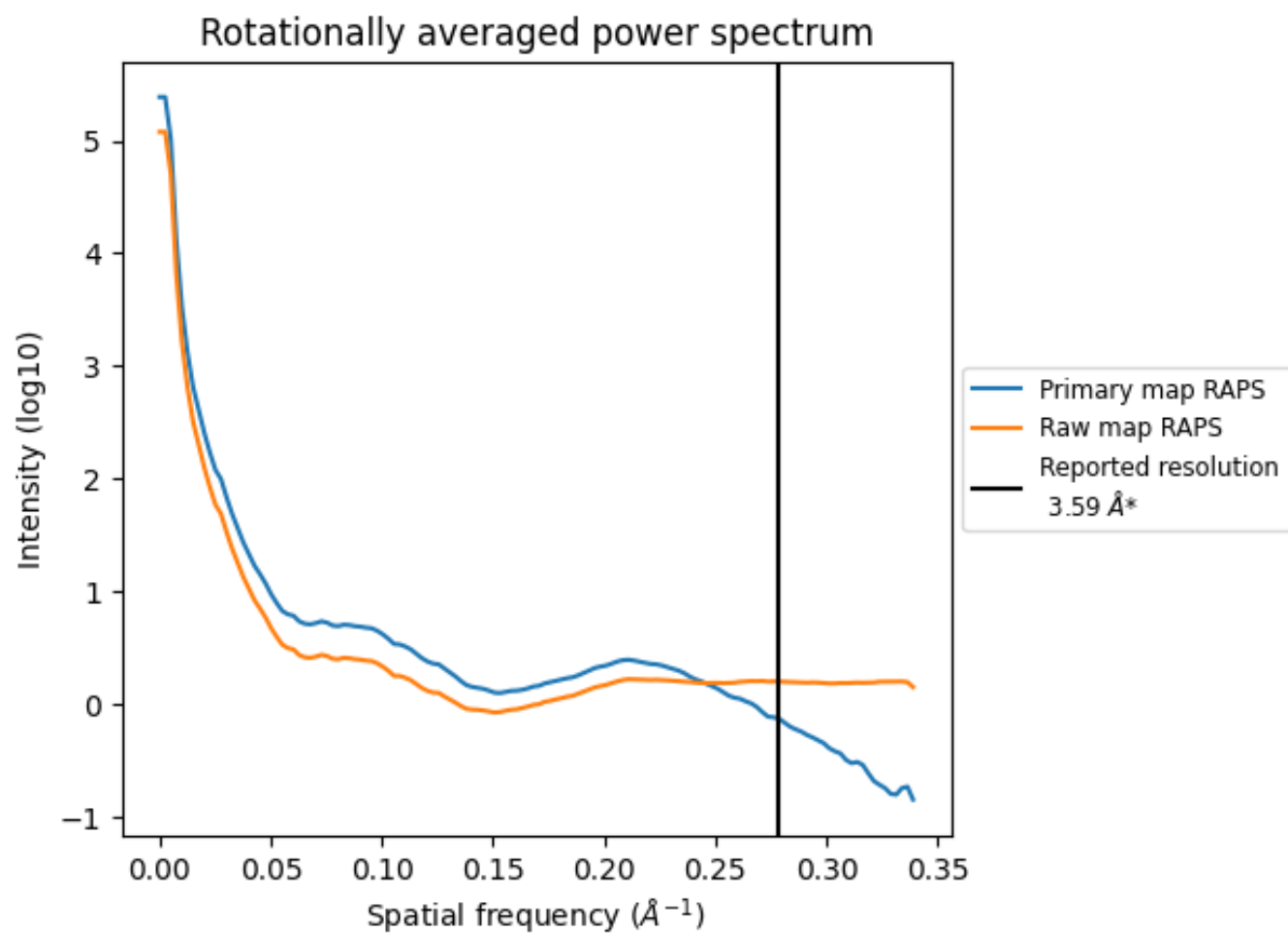
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 985 nm³; this corresponds to an approximate mass of 889 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 ⓘ

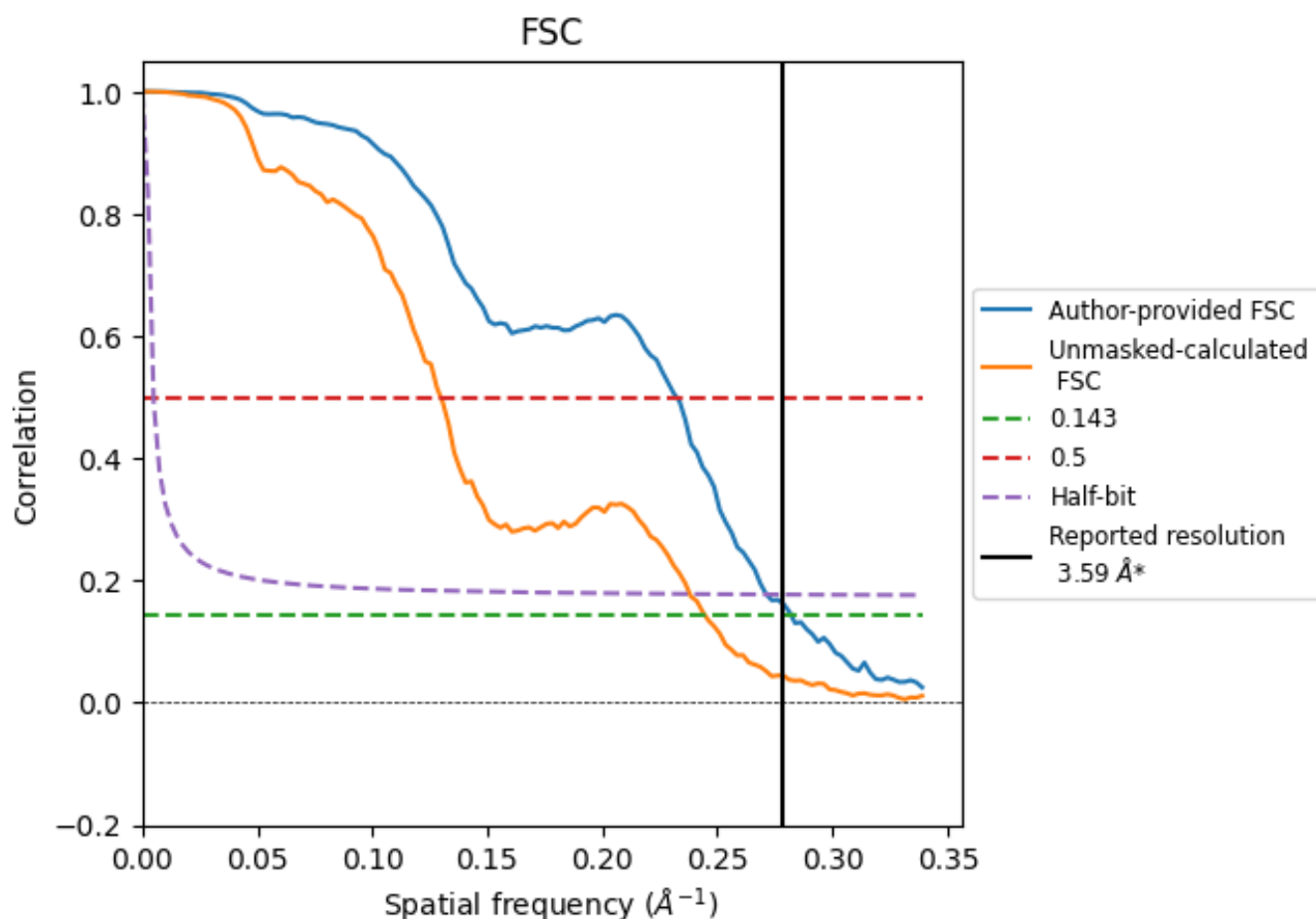


*Reported resolution corresponds to spatial frequency of 0.279 Å⁻¹

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 $0.279 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

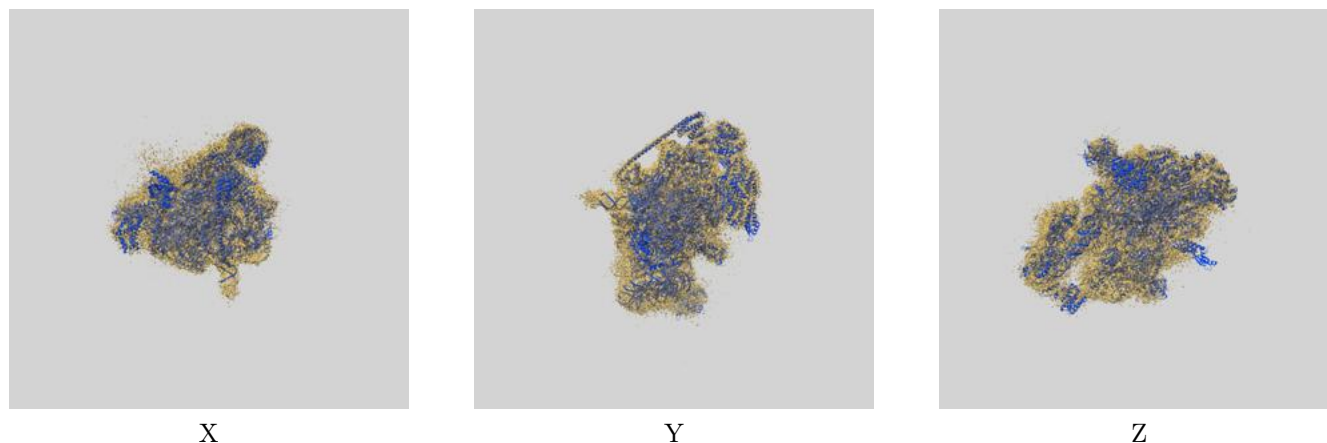
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.59	-	-
Author-provided FSC curve	3.55	4.31	3.68
Unmasked-calculated*	4.09	7.71	4.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.59 by more than 10 %

9 Map-model fit [i](#)

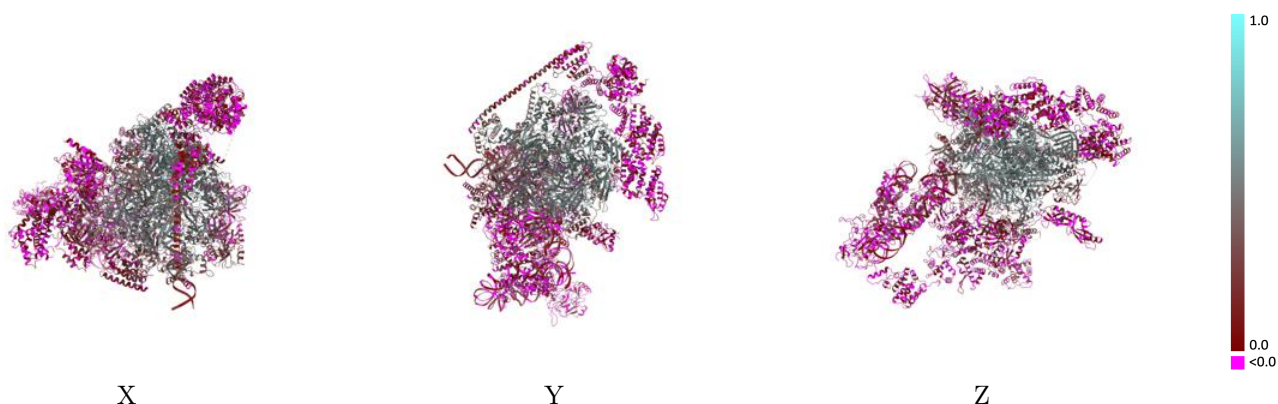
This section contains information regarding the fit between EMDB map EMD-66104 and PDB model 9WMT. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



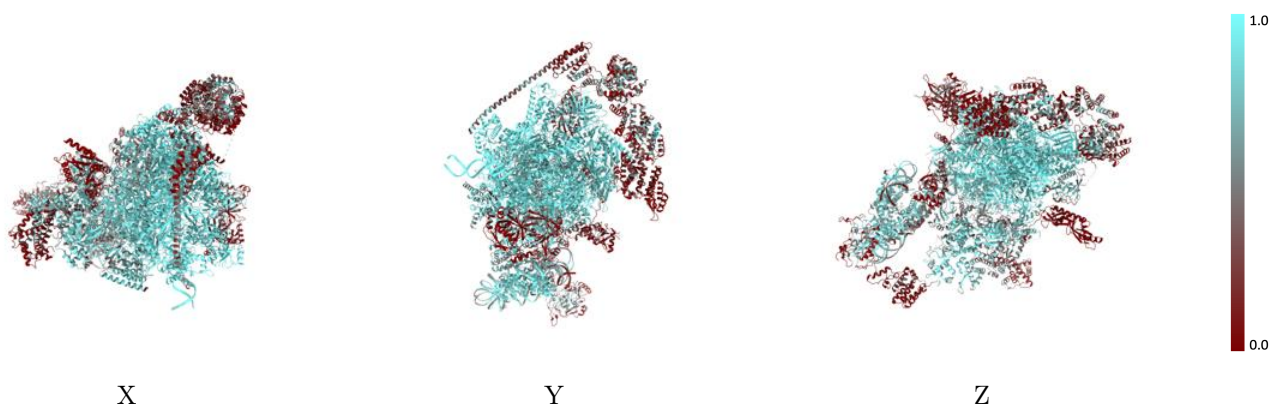
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



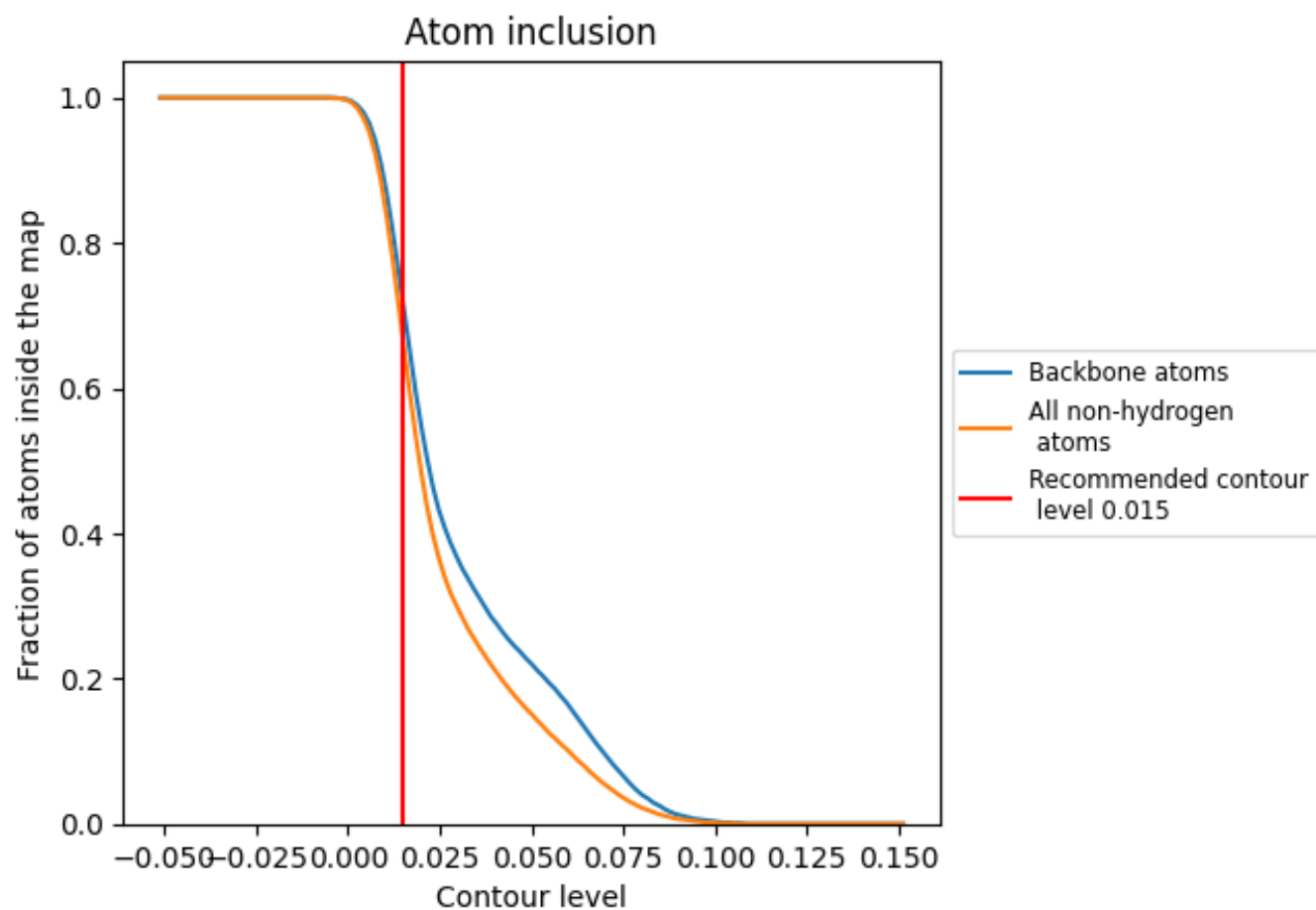
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 66% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6650	 0.2250
A	 0.9470	 0.4690
B	 0.9390	 0.4770
C	 0.9550	 0.5070
D	 0.7280	 0.1600
E	 0.9600	 0.4480
F	 0.9590	 0.5000
G	 0.7980	 0.2700
H	 0.9600	 0.4840
I	 0.9160	 0.3420
J	 0.9480	 0.5090
K	 0.9570	 0.5110
L	 0.9540	 0.4560
M	 0.8040	 0.1460
N	 0.7620	 0.0890
P	 0.8320	 0.2980
T	 0.7650	 0.1240
V	 0.8790	 0.1050
W	 0.6960	 0.1530
a	 0.8250	 0.0160
b	 0.8640	 0.0210
c	 0.7870	 0.0310
d	 0.7960	 0.0070
e	 0.6890	 0.0140
f	 0.6540	 0.0260
g	 0.4940	 0.0290
h	 0.5590	 0.0250
m	 0.4870	 0.0470
n	 0.7580	 0.1650
q	 0.2820	 0.0510
r	 0.2240	 0.1160
s	 0.2450	 0.0090
u	 0.1700	 0.0920
v	 0.1510	 0.0410
x	 0.4930	 0.2330

