Full wwPDB EM Validation Report ⓘ

Oct 4, 2022 – 02:34 AM JST

PDB ID	:	7XSE
EMDB ID	:	EMD-33424
Title	:	RNA polymerase II elongation complex transcribing a nucleosome (EC42)
Authors	:	Ehara, H.; Kujirai, T.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on	:	2022-05-13
Resolution	:	3.60 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:

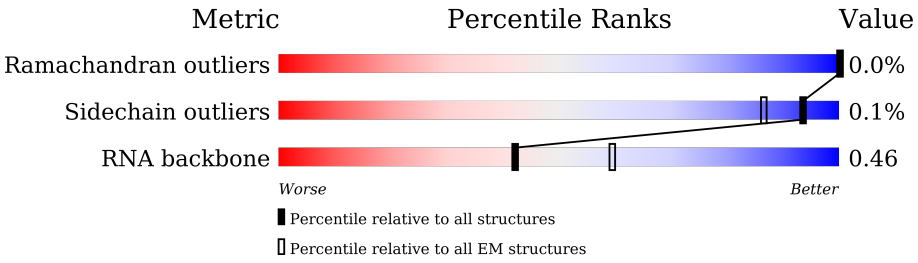
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.60 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	80% 19%
2	B	1227	95% 5%
3	C	304	87% 13%
4	D	186	94% 6%
5	E	214	99%
6	F	155	54% 46%
7	G	171	100%
8	H	145	92% 8%

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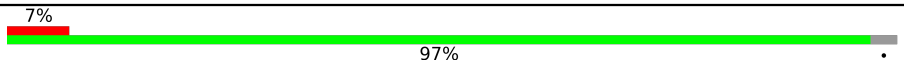
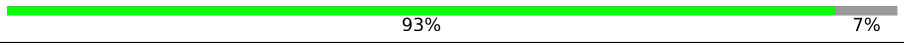
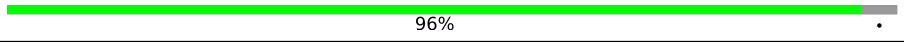
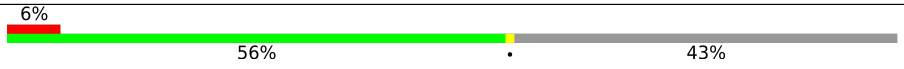
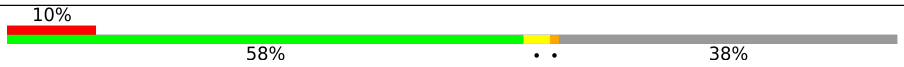
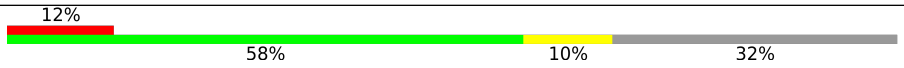
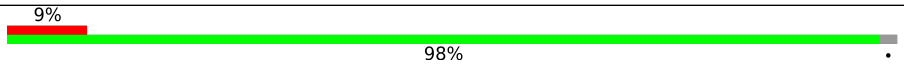
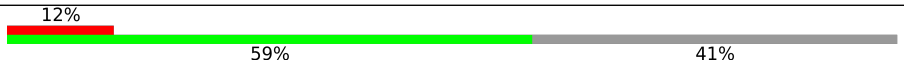
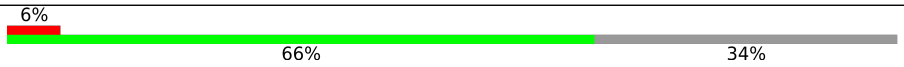
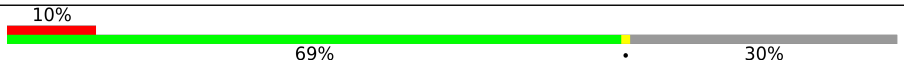
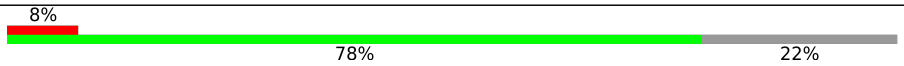
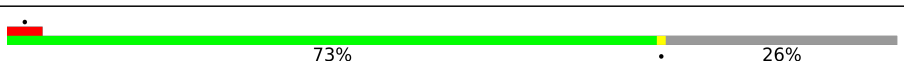
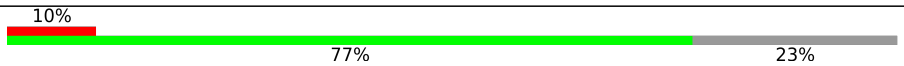
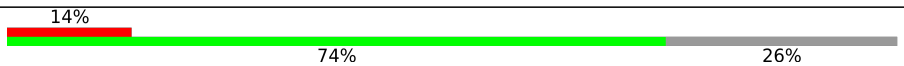
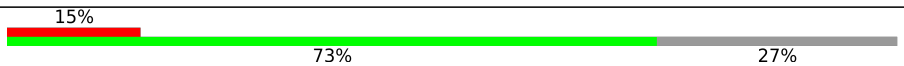
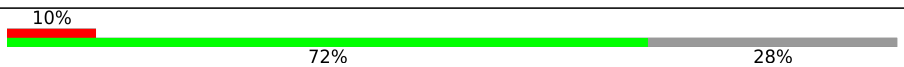
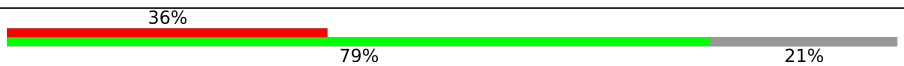
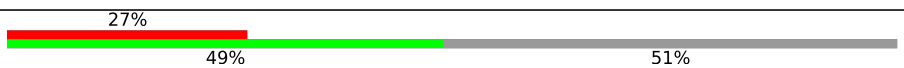
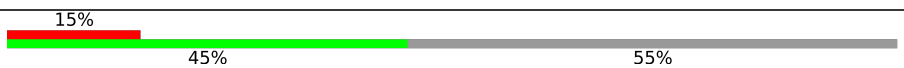
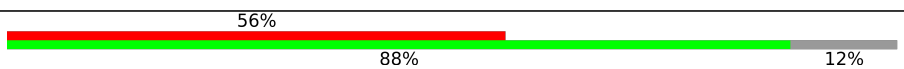
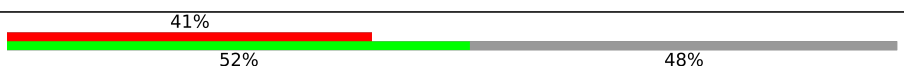
Mol	Chain	Length	Quality of chain
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	M	113	
14	N	198	
15	P	19	
16	T	198	
17	V	108	
18	W	911	
19	a	139	
19	e	139	
20	b	106	
20	f	106	
21	c	133	
21	g	133	
22	d	129	
22	h	129	
23	m	1503	
24	n	417	
25	q	1084	
26	r	544	
27	u	459	
28	v	396	
29	x	395	

2 Entry composition (i)

There are 31 unique types of molecules in this entry. The entry contains 75229 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
			Total	C	N	O	S		
1	A	1404	11064	6975	1930	2089	70	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1164	9284	5848	1639	1739	58	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	174	1349	828	244	274	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	213	1741	1094	312	325	10	0	0

- 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	123	Total	C	N	O	P	0	0
			2527	1198	458	748	123		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	19	Total	C	N	O	P	0	0
			404	179	65	141	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	134	Total	C	N	O	P	0	0
			2735	1296	519	787	133		

- 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	533	Total	C	N	O	S	0	0
			4232	2666	752	812	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	92	Total	C	N	O	S	0	0
			746	471	142	131	2		
19	e	97	Total	C	N	O	S	0	0
			795	501	155	137	2		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
20	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	c	103	Total 796	C 502	N 155	O 139	0	0
21	g	98	Total 757	C 475	N 149	O 133	0	0

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	m	1187	Total	C	N	O	S	0	0
			9730	6162	1663	1877	28		

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
q	-31	HIS	-	expression tag	UNP C4R6B2

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Chain	Residue	Modelled	Actual	Comment	Reference
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 subunit.

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 Leo1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 28 is a protein called RNAP II-associated protein.

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

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 29 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
29	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
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 30 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

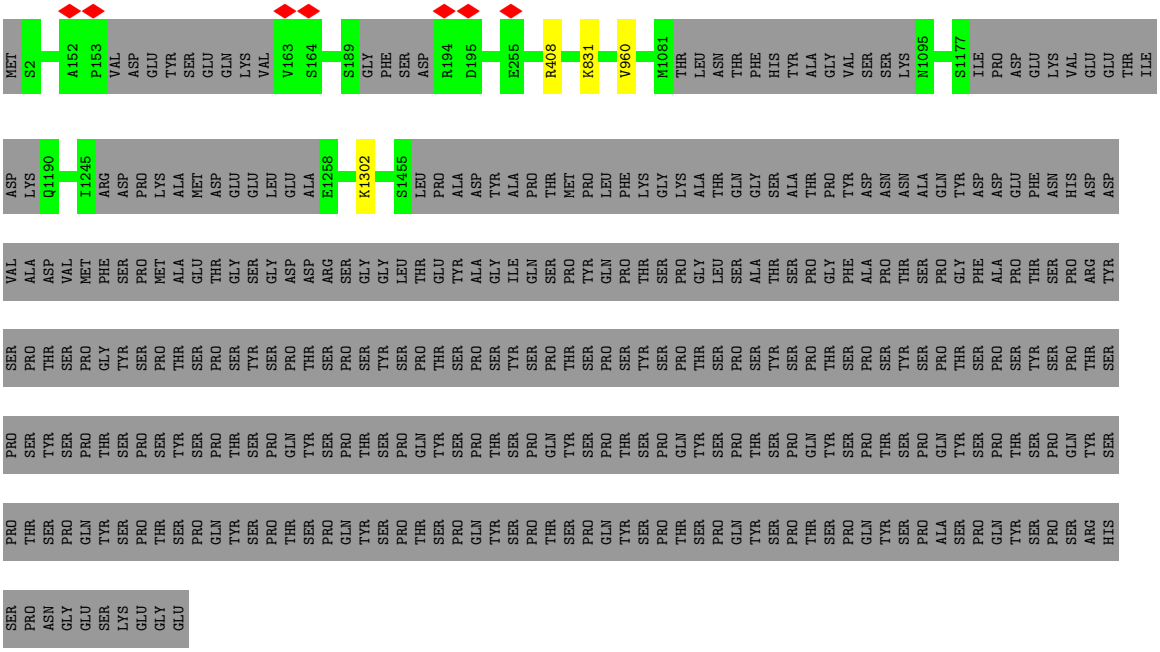
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total Mg 1 1	0

3 Residue-property plots (i)

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

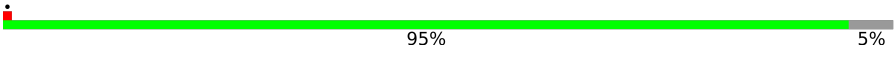
• Molecule 1: DNA-directed RNA polymerase subunit

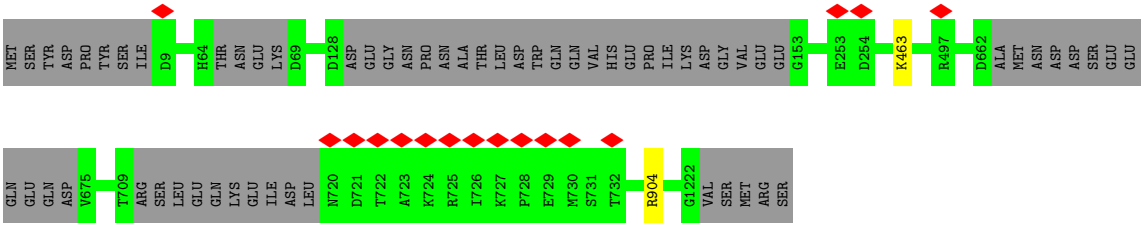
Chain A:



• Molecule 2: DNA-directed RNA polymerase subunit beta

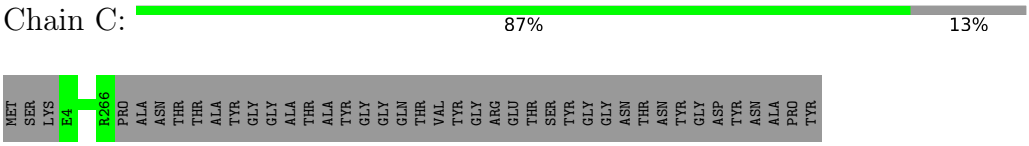
Chain B:





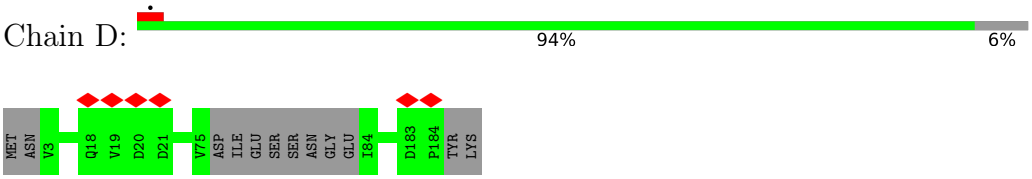
• Molecule 3: RNA polymerase II third largest subunit B44, part of central core

Chain C:



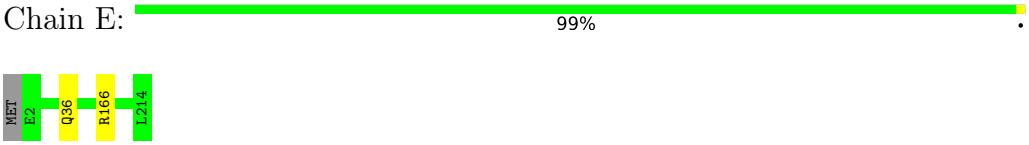
• Molecule 4: RNA polymerase II subunit B32

Chain D:



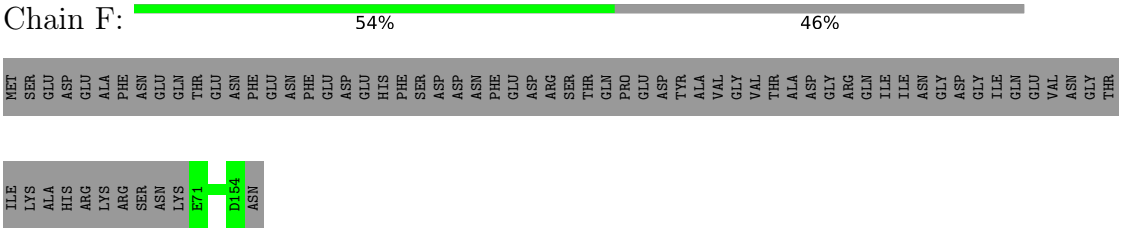
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



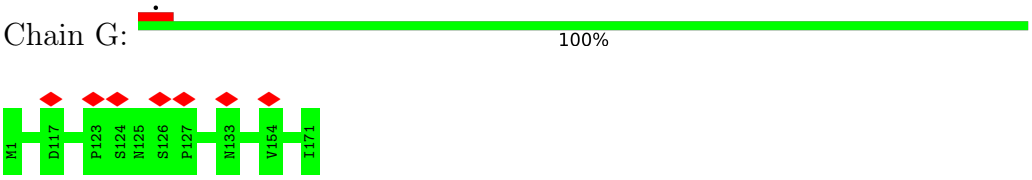
• Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

Chain F:



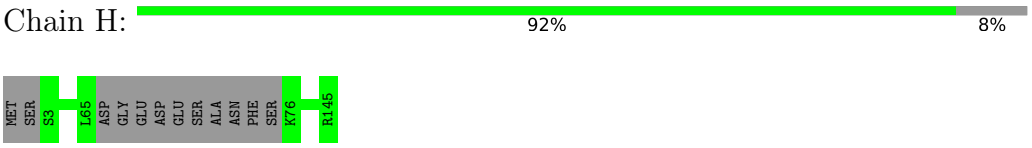
• Molecule 7: RNA polymerase II subunit

Chain G:



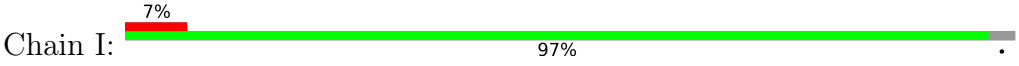
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

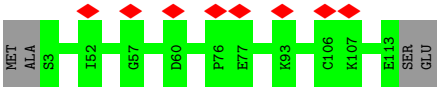
Chain H:



• Molecule 9: DNA-directed RNA polymerase subunit

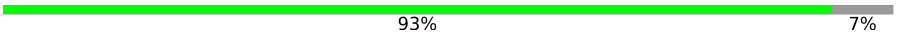
Chain I:





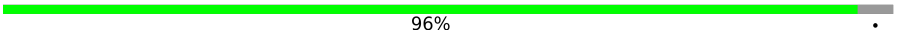
• Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J:



• Molecule 11: RNA polymerase II subunit B12.5

Chain K:

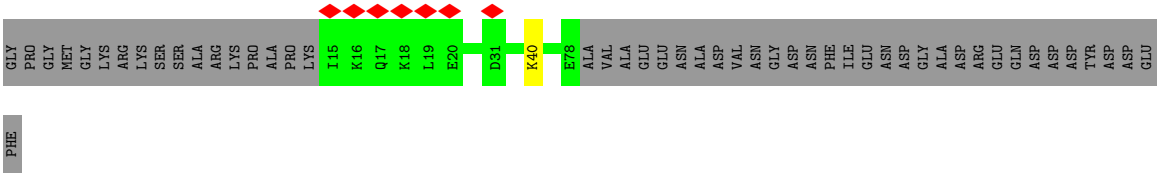


• Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L:

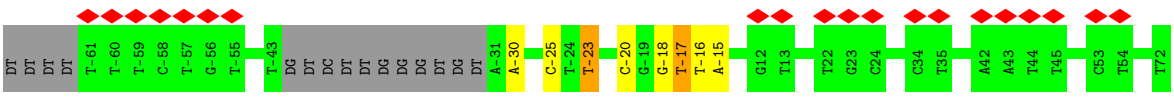
• Molecule 13: Transcription elongation factor 1 homolog

Chain M:



• Molecule 14: DNA (198-MER)

Chain N:

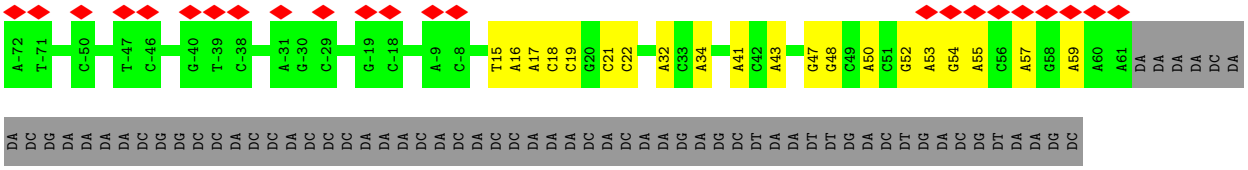


• Molecule 15: RNA (5'-R(P*UP*GP*CP*CP*UP*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*GP*UP*GP*U)-3')

Chain P:

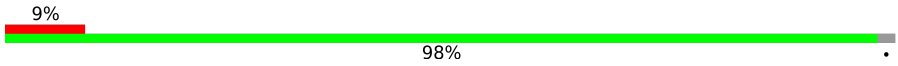
• Molecule 16: DNA (198-MER)

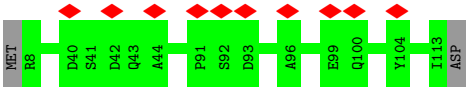
Chain T:



• Molecule 17: Transcription elongation factor SPT4

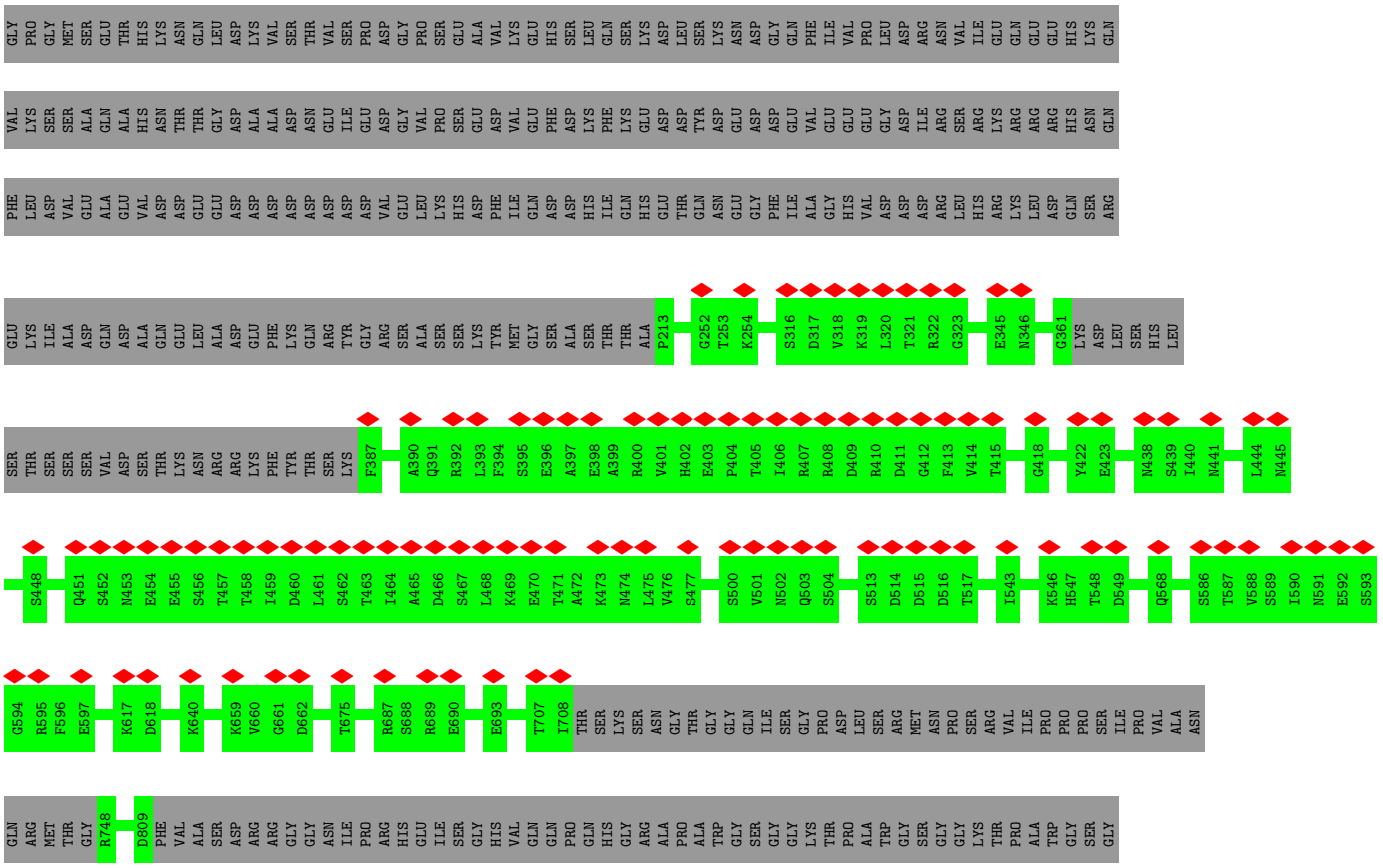
Chain V:





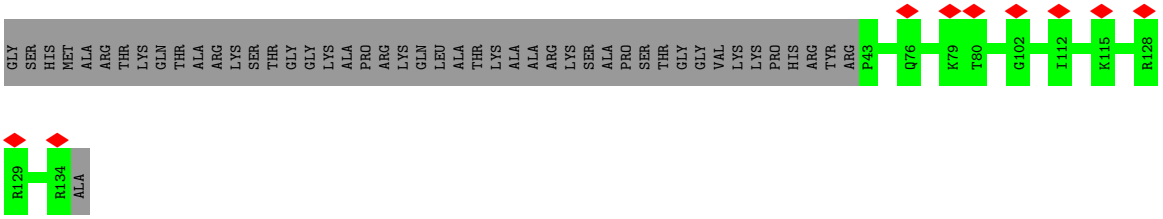
• Molecule 18: Transcription elongation factor SPT5

Chain W:



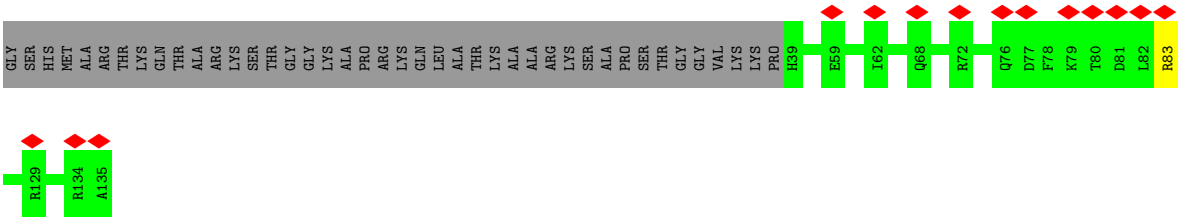
• Molecule 19: Histone H3.3

Chain a:



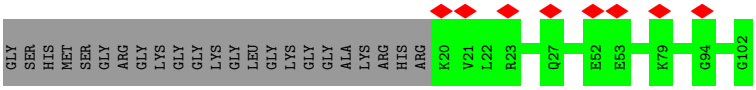
• Molecule 19: Histone H3.3

Chain e:



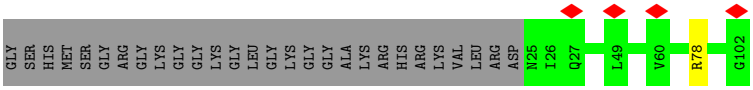
• Molecule 20: Histone H4

Chain b:



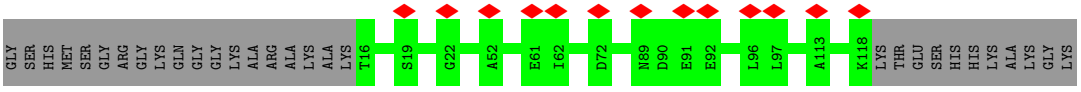
• Molecule 20: Histone H4

Chain f:



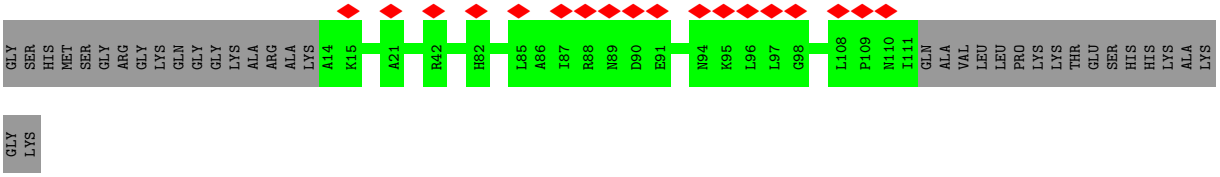
• Molecule 21: Histone H2A type 1-B/E

Chain c:



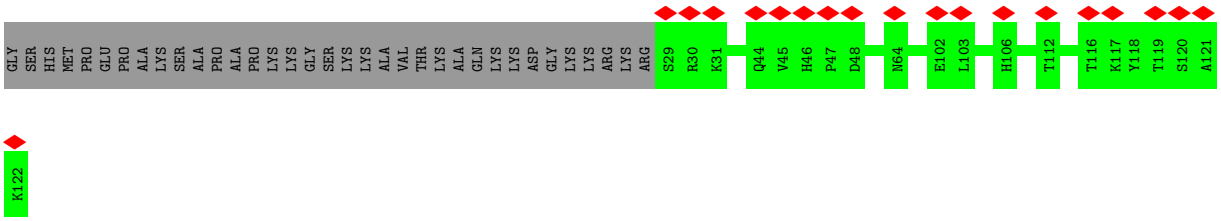
• Molecule 21: Histone H2A type 1-B/E

Chain g:



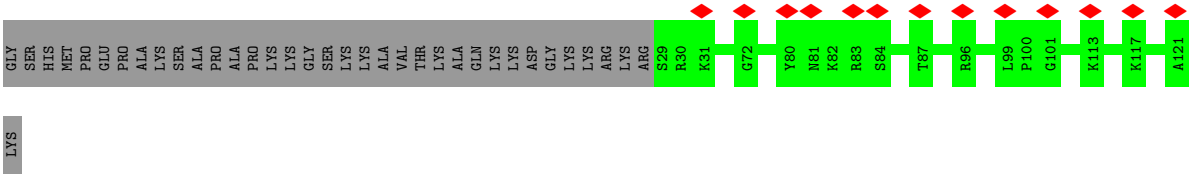
• Molecule 22: Histone H2B type 1-J

Chain d:



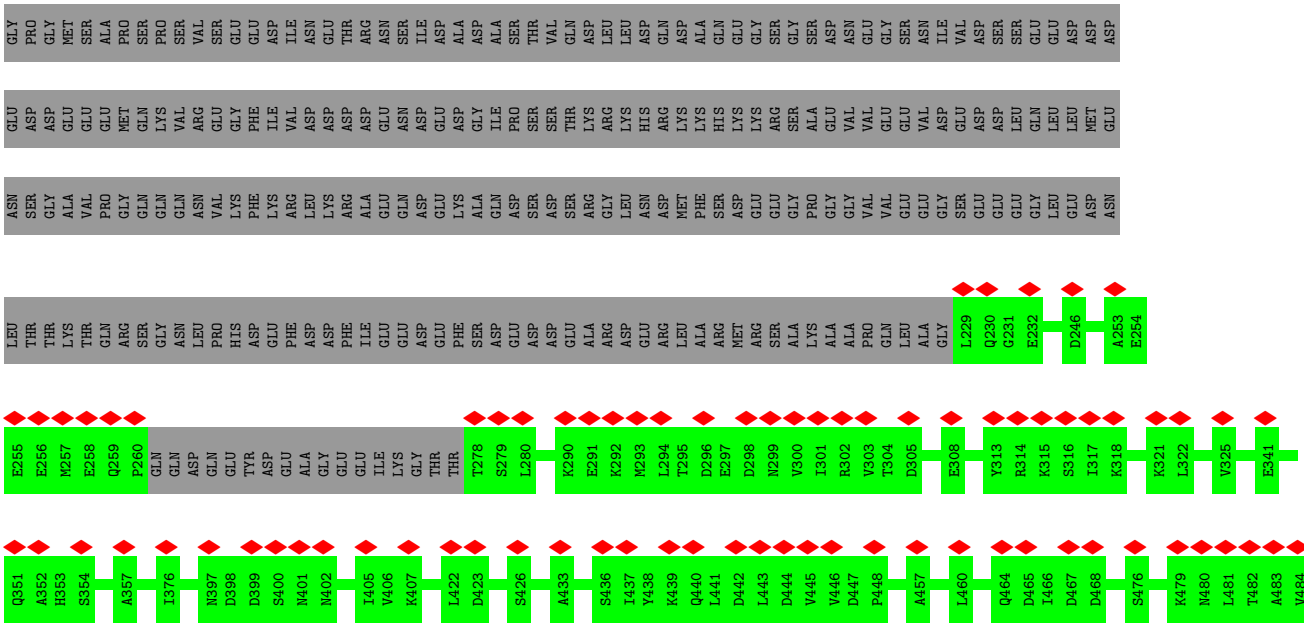
• Molecule 22: Histone H2B type 1-J

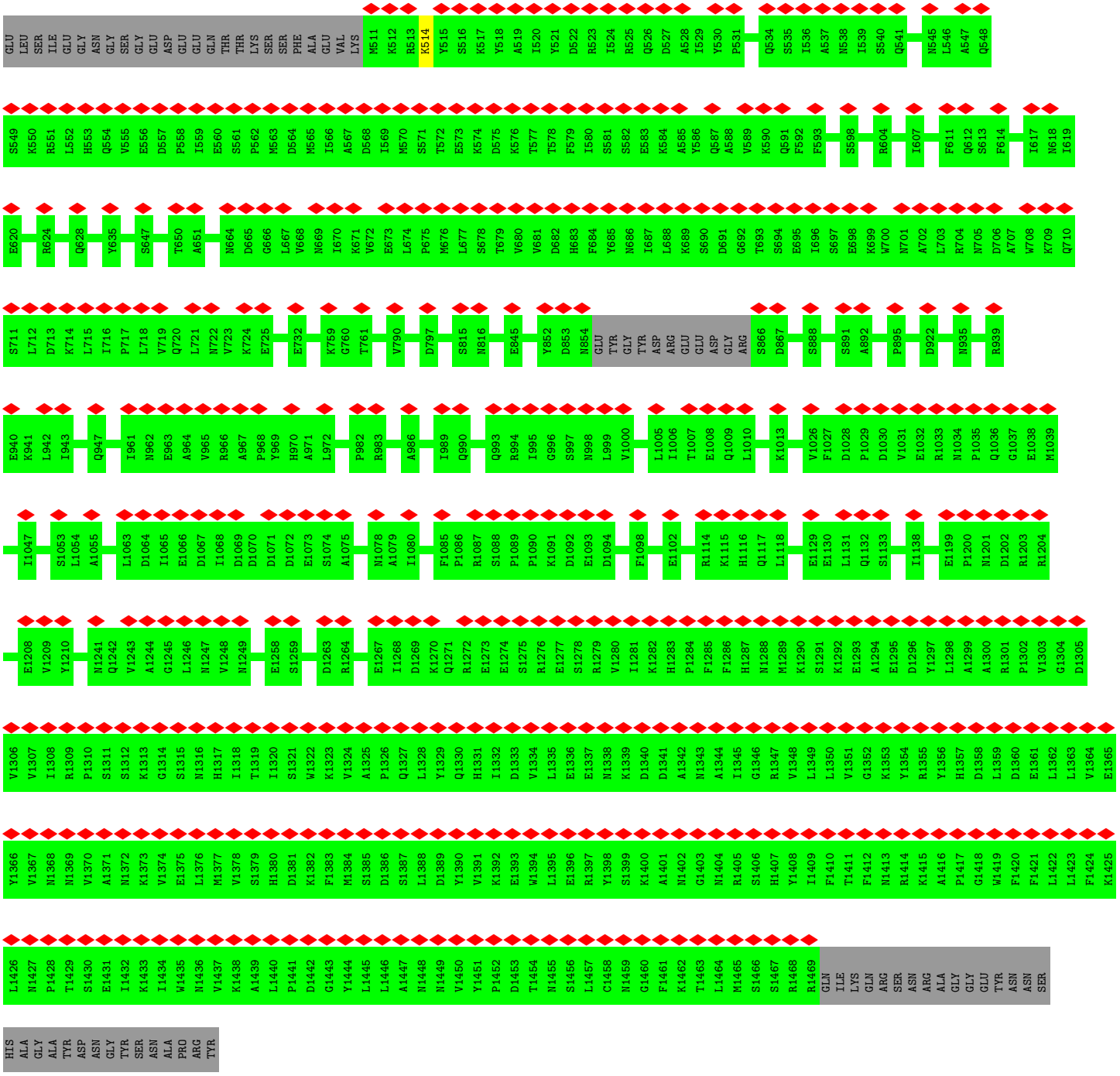
Chain h:



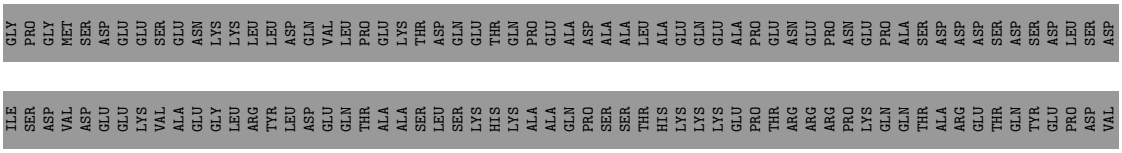
• Molecule 23: Transcription elongation factor Spt6

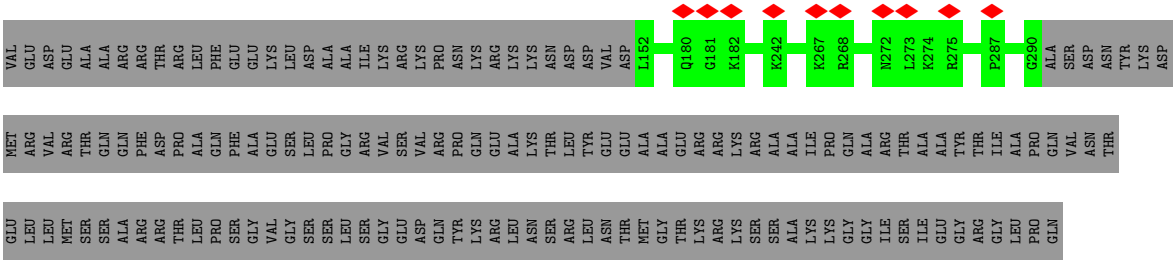
Chain m:





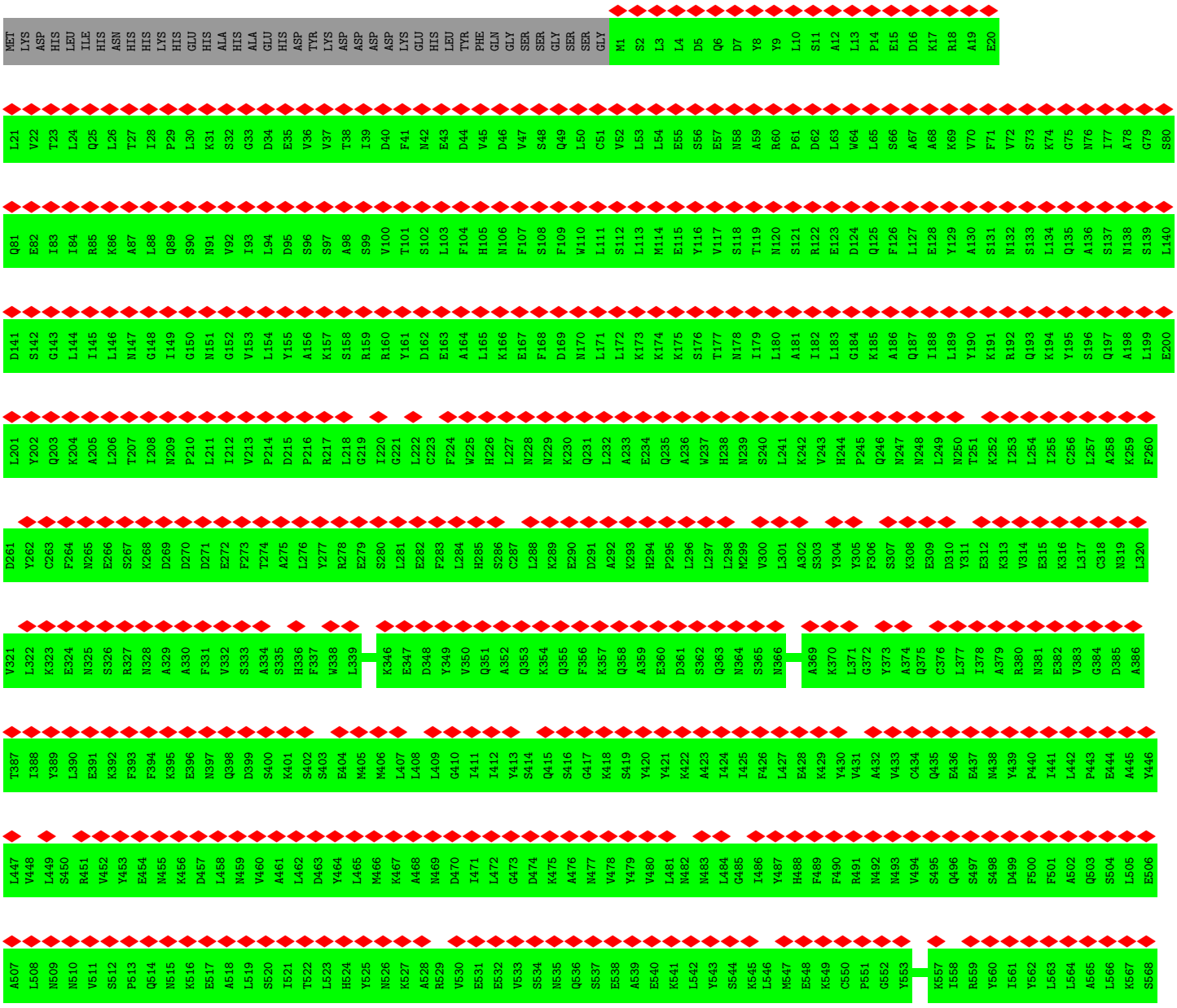
• Molecule 24: Protein that interacts with Spt6p and copurifies with Spt5p and RNA polymerase II

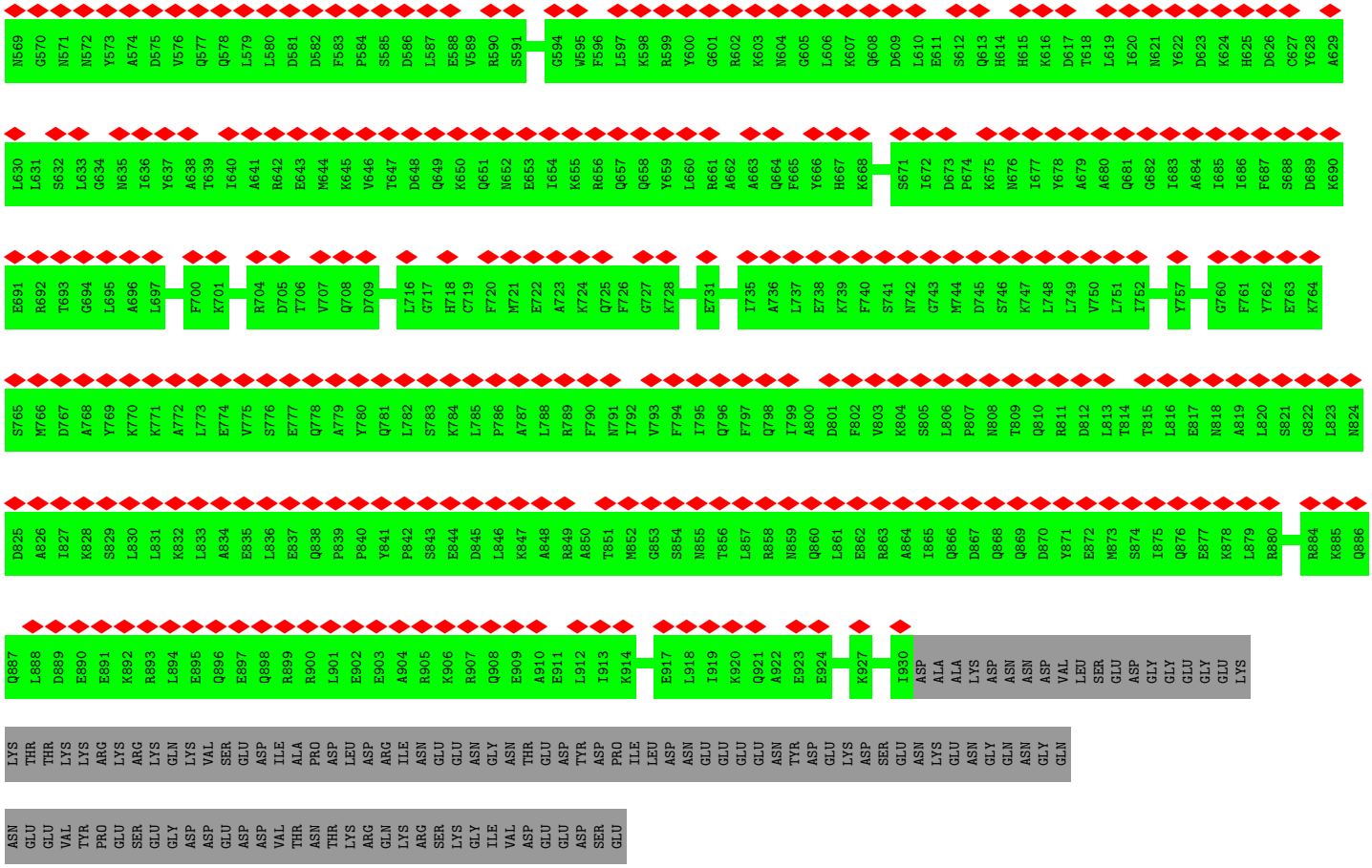




• Molecule 25: Component of the Paf1p complex

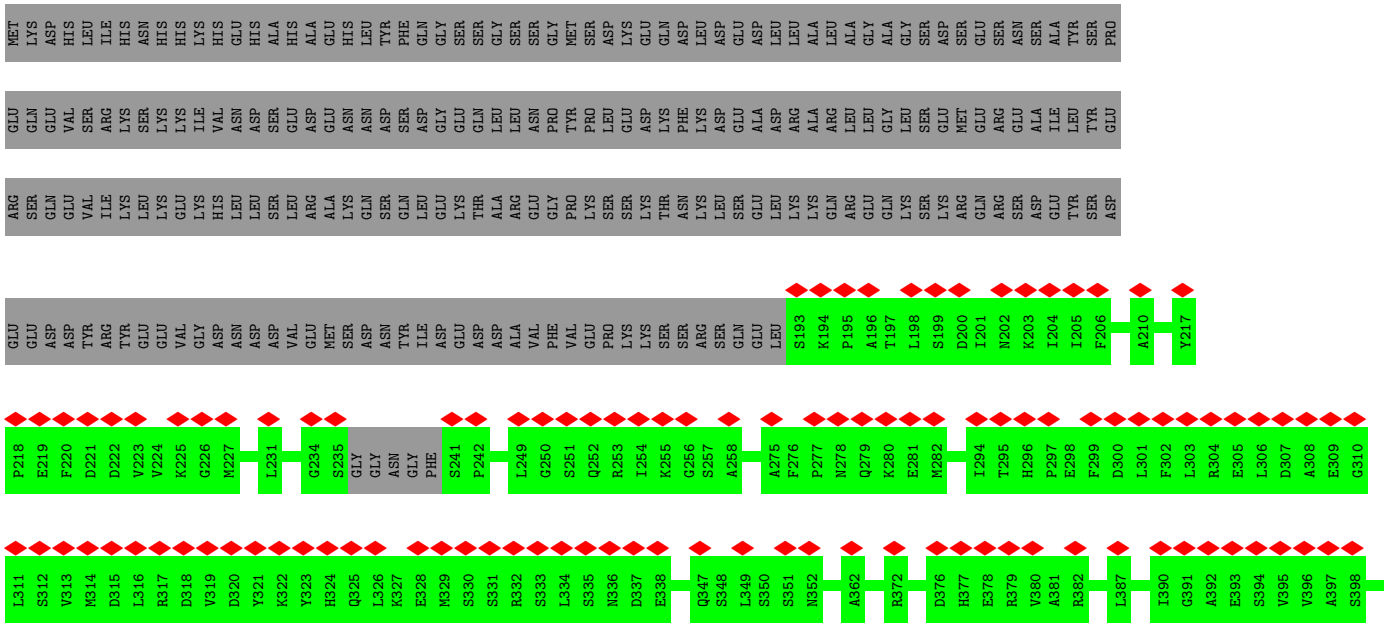
Chain q:

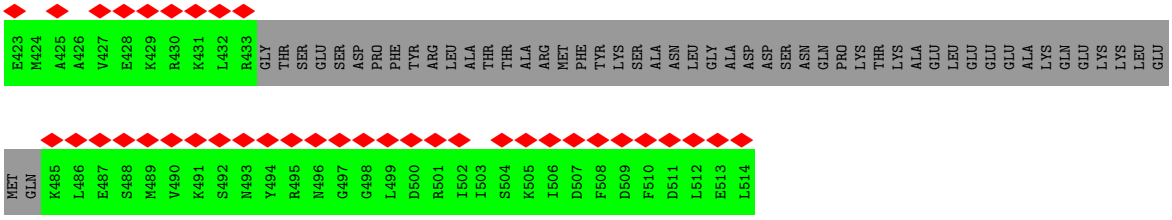




• Molecule 26: RNAPII-associated chromatin remodeling Paf1 complex subunit

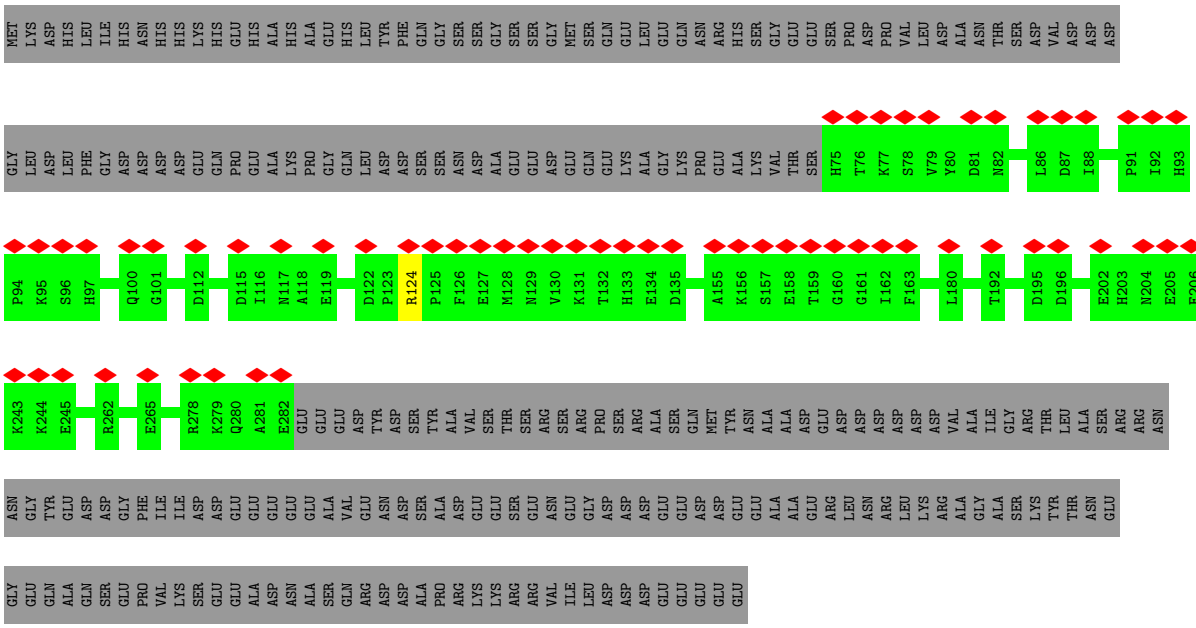
Chain r:





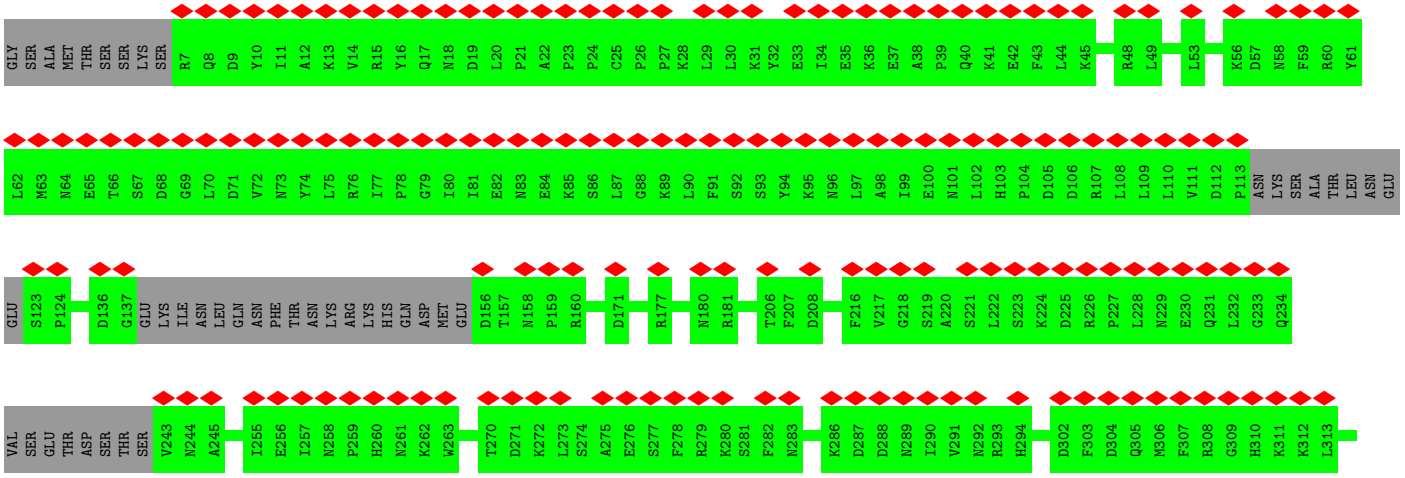
• Molecule 27: Leo1

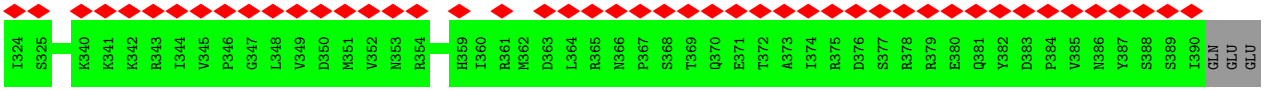
Chain u:



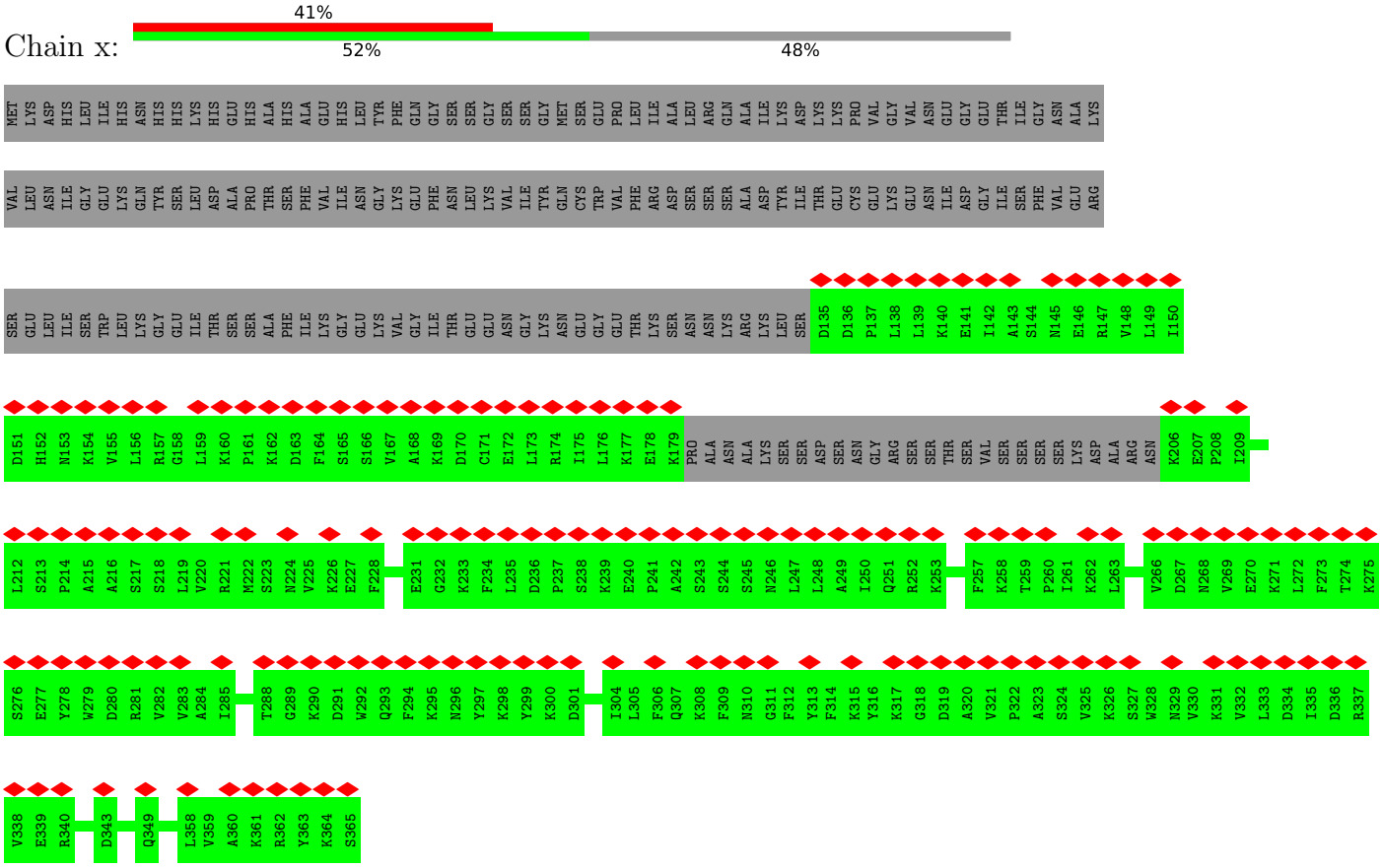
• Molecule 28: RNAP II-associated protein

Chain v:





• Molecule 29: Constituent of Paf1 complex with RNA polymerase II, Paf1p, Hpr1p, Ctr9, Leo1, Rtf1 and Ccr4p



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76913	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 ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.120	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	356.16, 356.16, 356.16	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.484, 1.484, 1.484	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/11267	0.49	0/15222
2	B	0.33	0/9464	0.52	0/12763
3	C	0.33	0/2139	0.49	0/2895
4	D	0.23	0/1361	0.46	0/1837
5	E	0.31	0/1773	0.50	0/2385
6	F	0.34	0/687	0.50	0/931
7	G	0.28	0/1354	0.48	0/1837
8	H	0.33	0/1070	0.49	0/1444
9	I	0.24	0/934	0.50	0/1257
10	J	0.36	0/563	0.51	0/753
11	K	0.32	0/953	0.50	0/1291
12	L	0.33	0/365	0.55	0/484
13	M	0.24	0/513	0.41	0/693
14	N	0.96	1/2831 (0.0%)	1.13	12/4368 (0.3%)
15	P	0.75	0/449	1.30	7/698 (1.0%)
16	T	1.00	13/3071 (0.4%)	1.16	19/4733 (0.4%)
17	V	0.24	0/840	0.50	0/1140
18	W	0.24	0/4300	0.49	0/5812
19	a	0.28	0/755	0.54	0/1012
19	e	0.35	0/806	0.64	1/1081 (0.1%)
20	b	0.30	0/669	0.59	0/894
20	f	0.38	0/626	0.68	1/837 (0.1%)
21	c	0.28	0/806	0.56	0/1089
21	g	0.27	0/766	0.54	0/1033
22	d	0.29	0/746	0.50	0/1001
22	h	0.32	0/736	0.52	0/990
23	m	0.24	0/9925	0.45	0/13424
24	n	0.26	0/1132	0.47	0/1526
25	q	0.24	0/7689	0.40	0/10368
26	r	0.24	0/2169	0.45	0/2901
27	u	0.24	0/1740	0.48	0/2347
28	v	0.25	0/2944	0.46	0/3973

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	x	0.25	0/1716	0.45	0/2310
All	All	0.39	14/77159 (0.0%)	0.58	40/105329 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	N	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	34	DA	C1'-N9	-6.24	1.38	1.47
16	T	53	DA	C1'-N9	-5.96	1.39	1.47
16	T	32	DA	C1'-N9	-5.80	1.39	1.47
16	T	59	DA	C1'-N9	-5.68	1.39	1.47
16	T	47	DG	C1'-N9	-5.67	1.39	1.47
16	T	55	DA	C1'-N9	-5.63	1.39	1.47
16	T	52	DG	C1'-N9	-5.51	1.39	1.47
16	T	43	DA	C1'-N9	-5.39	1.39	1.47
14	N	-30	DA	C1'-N9	-5.32	1.39	1.47
16	T	50	DA	C1'-N9	-5.30	1.39	1.47
16	T	48	DG	C1'-N9	-5.22	1.40	1.47
16	T	41	DA	C1'-N9	-5.07	1.40	1.47
16	T	57	DA	C1'-N9	-5.06	1.40	1.47
16	T	54	DG	C1'-N9	-5.05	1.40	1.47

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	T	16	DA	N1-C6-N6	-9.26	113.04	118.60
14	N	-15	DA	N1-C6-N6	-9.12	113.13	118.60
16	T	17	DA	N1-C6-N6	-8.96	113.22	118.60
15	P	10	G	OP1-P-O3'	8.58	124.07	105.20
16	T	21	DC	N3-C2-O2	-7.46	116.68	121.90
16	T	18	DC	N3-C2-O2	-7.29	116.80	121.90
15	P	11	U	OP1-P-OP2	-7.29	108.66	119.60
16	T	16	DA	O4'-C1'-N9	7.21	113.04	108.00
14	N	-20	DC	N3-C2-O2	-7.17	116.88	121.90
16	T	17	DA	C5-C6-N1	7.08	121.24	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	T	16	DA	C5-C6-N1	6.96	121.18	117.70
16	T	22	DC	N3-C2-O2	-6.95	117.04	121.90
16	T	18	DC	O4'-C1'-N1	6.82	112.78	108.00
16	T	19	DC	N3-C2-O2	-6.79	117.15	121.90
16	T	19	DC	O4'-C1'-N1	6.78	112.74	108.00
14	N	-15	DA	C5-C6-N1	6.73	121.06	117.70
16	T	16	DA	C4-C5-C6	-6.64	113.68	117.00
20	f	78	ARG	NE-CZ-NH1	6.55	123.58	120.30
19	e	83	ARG	NE-CZ-NH1	6.37	123.48	120.30
15	P	-1	G	N3-C2-N2	-6.34	115.46	119.90
14	N	-15	DA	C4-C5-C6	-6.29	113.86	117.00
14	N	-17	DT	P-O3'-C3'	6.16	127.09	119.70
14	N	-16	DT	N3-C2-O2	-6.13	118.62	122.30
16	T	15	DT	N3-C2-O2	-6.05	118.67	122.30
16	T	17	DA	C4-C5-C6	-6.00	114.00	117.00
16	T	21	DC	N1-C2-O2	5.95	122.47	118.90
14	N	-17	DT	N3-C2-O2	-5.90	118.76	122.30
15	P	-1	G	C2-N3-C4	5.83	114.82	111.90
14	N	-25	DC	P-O3'-C3'	5.77	126.62	119.70
15	P	-1	G	N3-C4-C5	-5.75	125.72	128.60
14	N	-17	DT	C6-C5-C7	-5.73	119.46	122.90
16	T	18	DC	N1-C2-O2	5.58	122.25	118.90
14	N	-16	DT	C6-C5-C7	-5.56	119.57	122.90
14	N	-20	DC	N1-C2-O2	5.51	122.21	118.90
15	P	-1	G	C8-N9-C4	-5.51	104.19	106.40
16	T	22	DC	N1-C2-O2	5.51	122.20	118.90
16	T	15	DT	C6-C5-C7	-5.50	119.60	122.90
14	N	-23	DT	O4'-C1'-N1	5.26	111.69	108.00
15	P	-1	G	N1-C6-O6	-5.09	116.84	119.90
16	T	19	DC	N1-C2-O2	5.09	121.95	118.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	-17	DT	Sidechain
14	N	-18	DG	Sidechain
14	N	-23	DT	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	51	83
2	B	1154/1227 (94%)	1119 (97%)	35 (3%)	0	100	100
3	C	261/304 (86%)	259 (99%)	2 (1%)	0	100	100
4	D	170/186 (91%)	166 (98%)	4 (2%)	0	100	100
5	E	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	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%)	106 (97%)	3 (3%)	0	100	100
10	J	65/72 (90%)	65 (100%)	0	0	100	100
11	K	111/118 (94%)	110 (99%)	1 (1%)	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%)	100 (96%)	4 (4%)	0	100	100
18	W	527/911 (58%)	508 (96%)	19 (4%)	0	100	100
19	a	90/139 (65%)	86 (96%)	4 (4%)	0	100	100
19	e	95/139 (68%)	95 (100%)	0	0	100	100
20	b	81/106 (76%)	78 (96%)	3 (4%)	0	100	100
20	f	76/106 (72%)	73 (96%)	3 (4%)	0	100	100
21	c	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
21	g	96/133 (72%)	93 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	d	92/129 (71%)	88 (96%)	4 (4%)	0	100	100
22	h	91/129 (70%)	90 (99%)	1 (1%)	0	100	100
23	m	1179/1503 (78%)	1157 (98%)	22 (2%)	0	100	100
24	n	137/417 (33%)	136 (99%)	1 (1%)	0	100	100
25	q	928/1084 (86%)	922 (99%)	6 (1%)	0	100	100
26	r	260/544 (48%)	254 (98%)	6 (2%)	0	100	100
27	u	206/459 (45%)	203 (98%)	3 (2%)	0	100	100
28	v	341/396 (86%)	327 (96%)	14 (4%)	0	100	100
29	x	201/395 (51%)	200 (100%)	1 (0%)	0	100	100
All	All	8563/11466 (75%)	8369 (98%)	193 (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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1219/1528 (80%)	1216 (100%)	3 (0%)	93	98
2	B	1018/1077 (94%)	1016 (100%)	2 (0%)	93	98
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%)	194 (99%)	2 (1%)	76	88
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	60 (98%)	1 (2%)	62	83
17	V	90/92 (98%)	90 (100%)	0	100	100
18	W	480/796 (60%)	480 (100%)	0	100	100
19	a	78/112 (70%)	78 (100%)	0	100	100
19	e	82/112 (73%)	82 (100%)	0	100	100
20	b	68/81 (84%)	68 (100%)	0	100	100
20	f	63/81 (78%)	63 (100%)	0	100	100
21	c	82/102 (80%)	82 (100%)	0	100	100
21	g	77/102 (76%)	77 (100%)	0	100	100
22	d	80/107 (75%)	80 (100%)	0	100	100
22	h	79/107 (74%)	79 (100%)	0	100	100
23	m	1087/1354 (80%)	1086 (100%)	1 (0%)	93	98
24	n	125/361 (35%)	125 (100%)	0	100	100
25	q	824/962 (86%)	824 (100%)	0	100	100
26	r	239/485 (49%)	239 (100%)	0	100	100
27	u	192/406 (47%)	191 (100%)	1 (0%)	88	95
28	v	325/369 (88%)	325 (100%)	0	100	100
29	x	190/354 (54%)	190 (100%)	0	100	100
All	All	7692/10063 (76%)	7682 (100%)	10 (0%)	93	98

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	ARG
1	A	831	LYS
1	A	1302	LYS
2	B	463	LYS
2	B	904	ARG
5	E	36	GLN
5	E	166	ARG
13	M	40	LYS
23	m	514	LYS

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Mol	Chain	Res	Type
27	u	124	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
8	H	44	ASN
9	I	11	ASN
18	W	433	GLN
18	W	644	ASN
20	b	25	ASN
20	f	25	ASN
23	m	955	ASN
24	n	232	GLN
25	q	147	ASN
28	v	305	GLN
29	x	296	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	19/19 (100%)	8 (42%)	2 (10%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	-6	G
15	P	-5	C
15	P	-4	C
15	P	-3	U
15	P	-2	G
15	P	-1	G
15	P	1	G
15	P	11	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	-7	U
15	P	-2	G

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

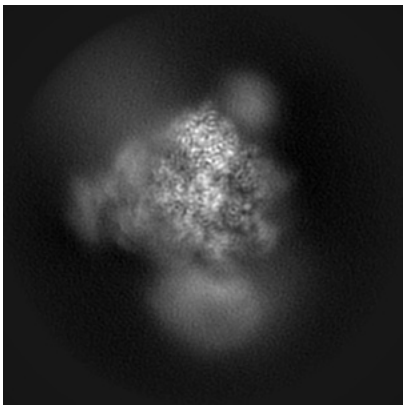
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33424. These allow visual inspection of the internal detail of the map and identification of artifacts.

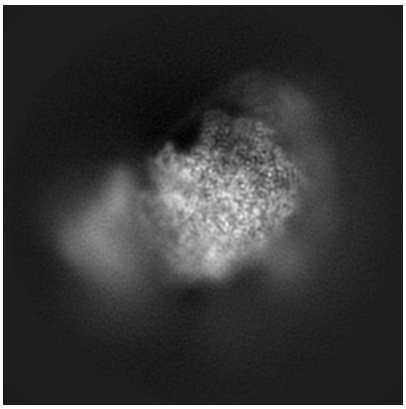
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

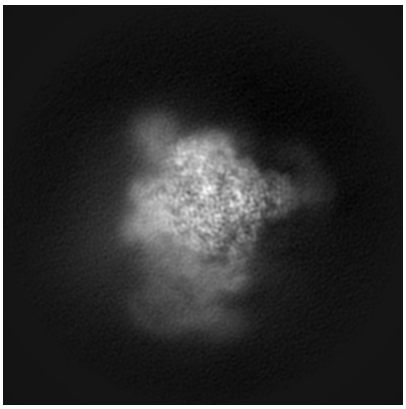
6.1.1 Primary map



X

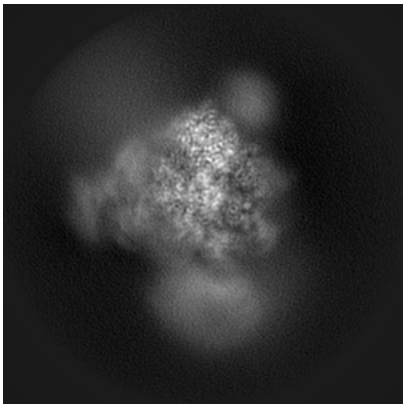


Y

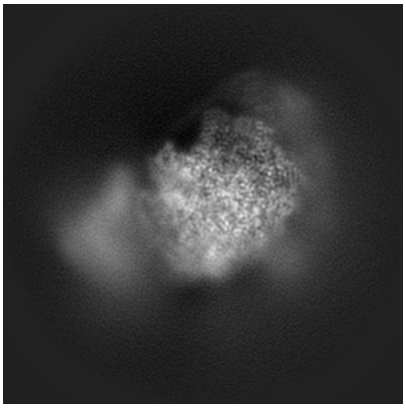


Z

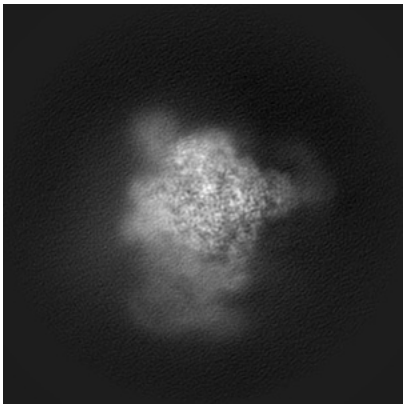
6.1.2 Raw map



X



Y

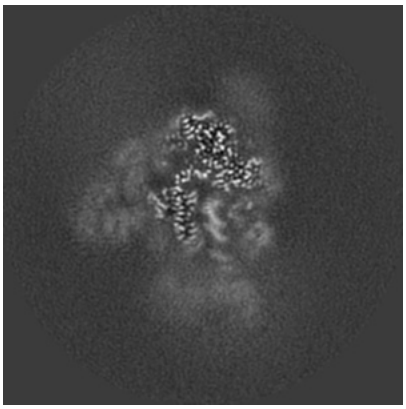


Z

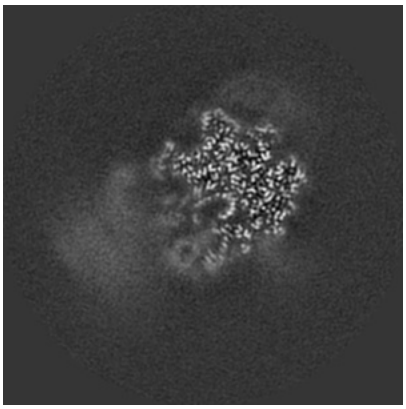
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

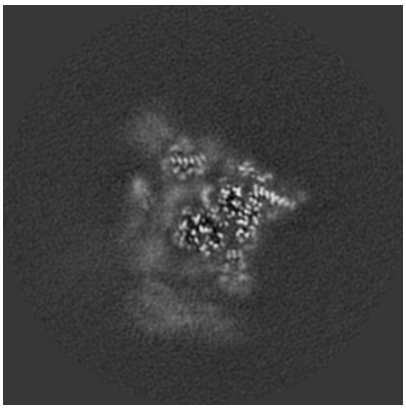
6.2.1 Primary map



X Index: 120

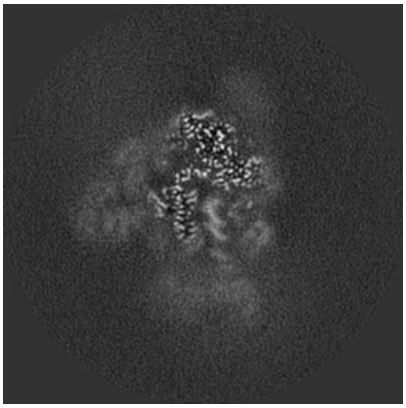


Y Index: 120

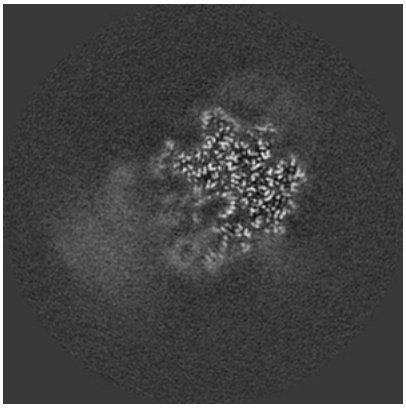


Z Index: 120

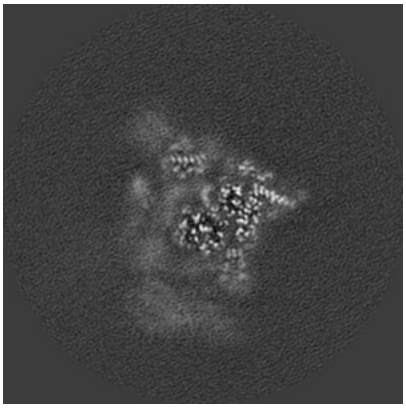
6.2.2 Raw map



X Index: 120



Y Index: 120

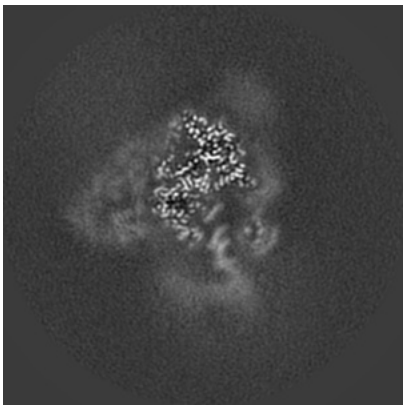


Z Index: 120

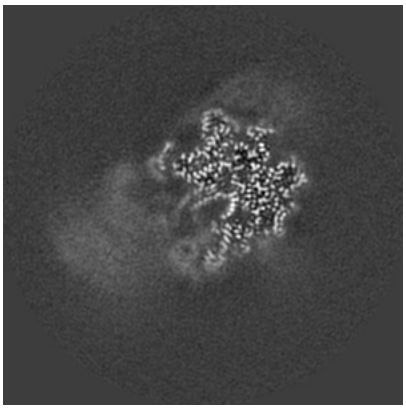
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

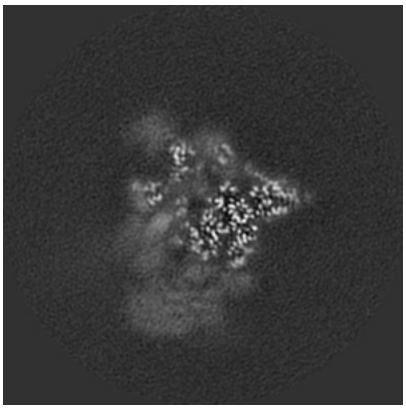
6.3.1 Primary map



X Index: 125

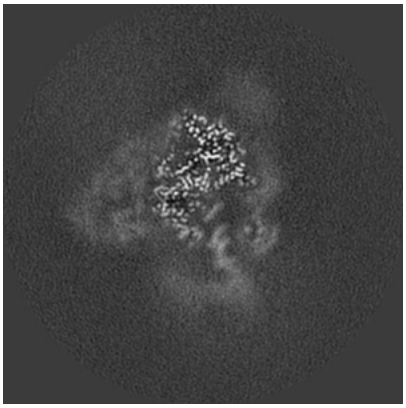


Y Index: 121

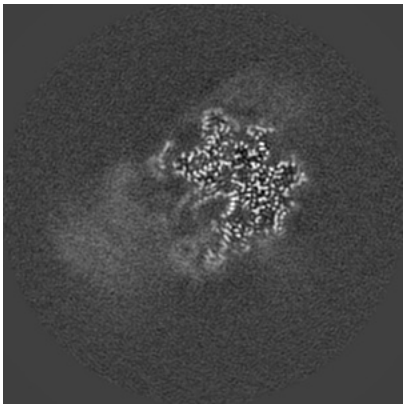


Z Index: 125

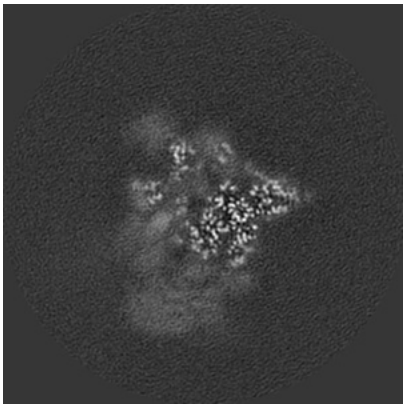
6.3.2 Raw map



X Index: 125



Y Index: 121



Z Index: 125

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

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.

6.4.2 Raw map

X

Y

Z

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.

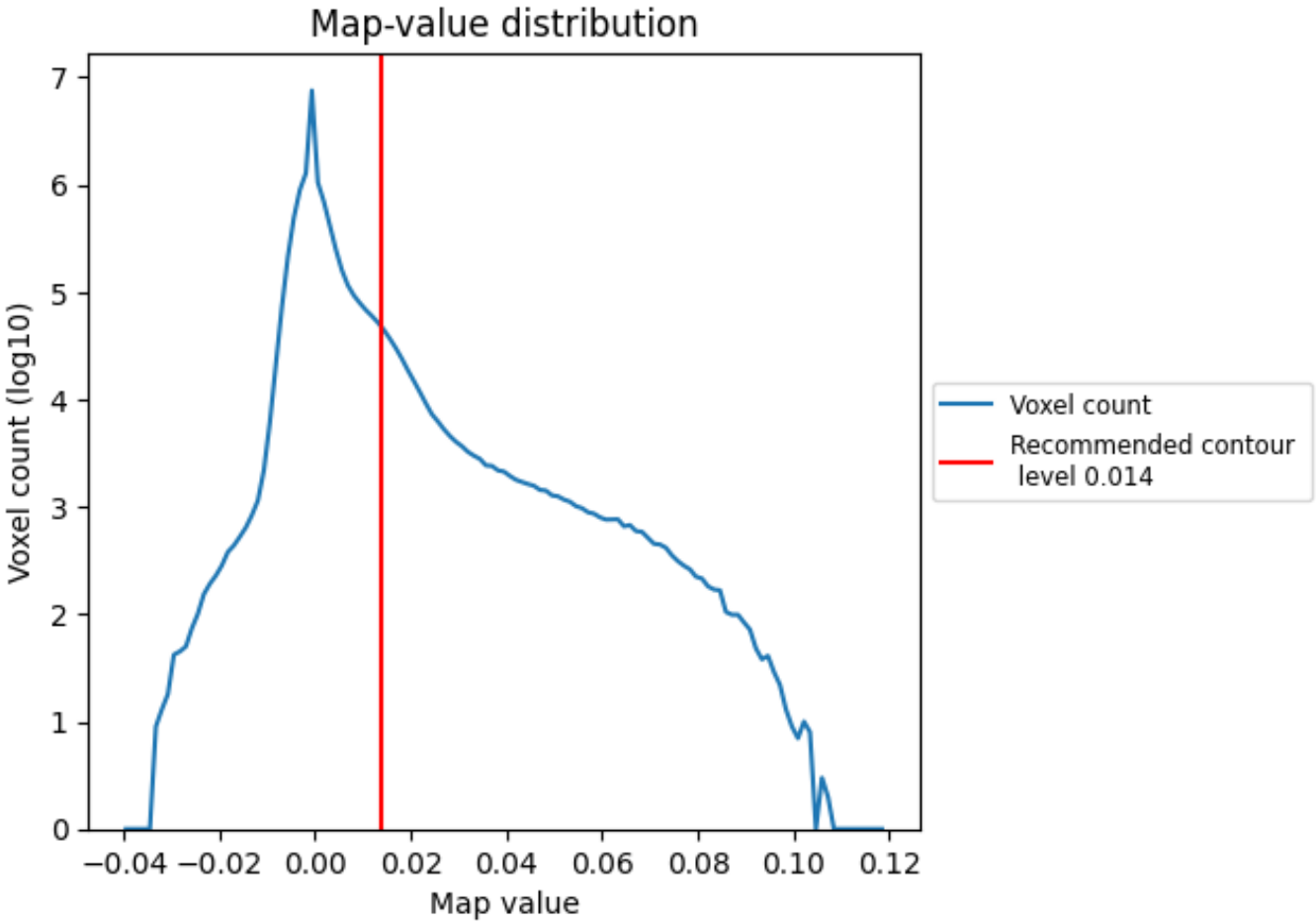
6.5 Mask visualisation (i)

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

7 Map analysis

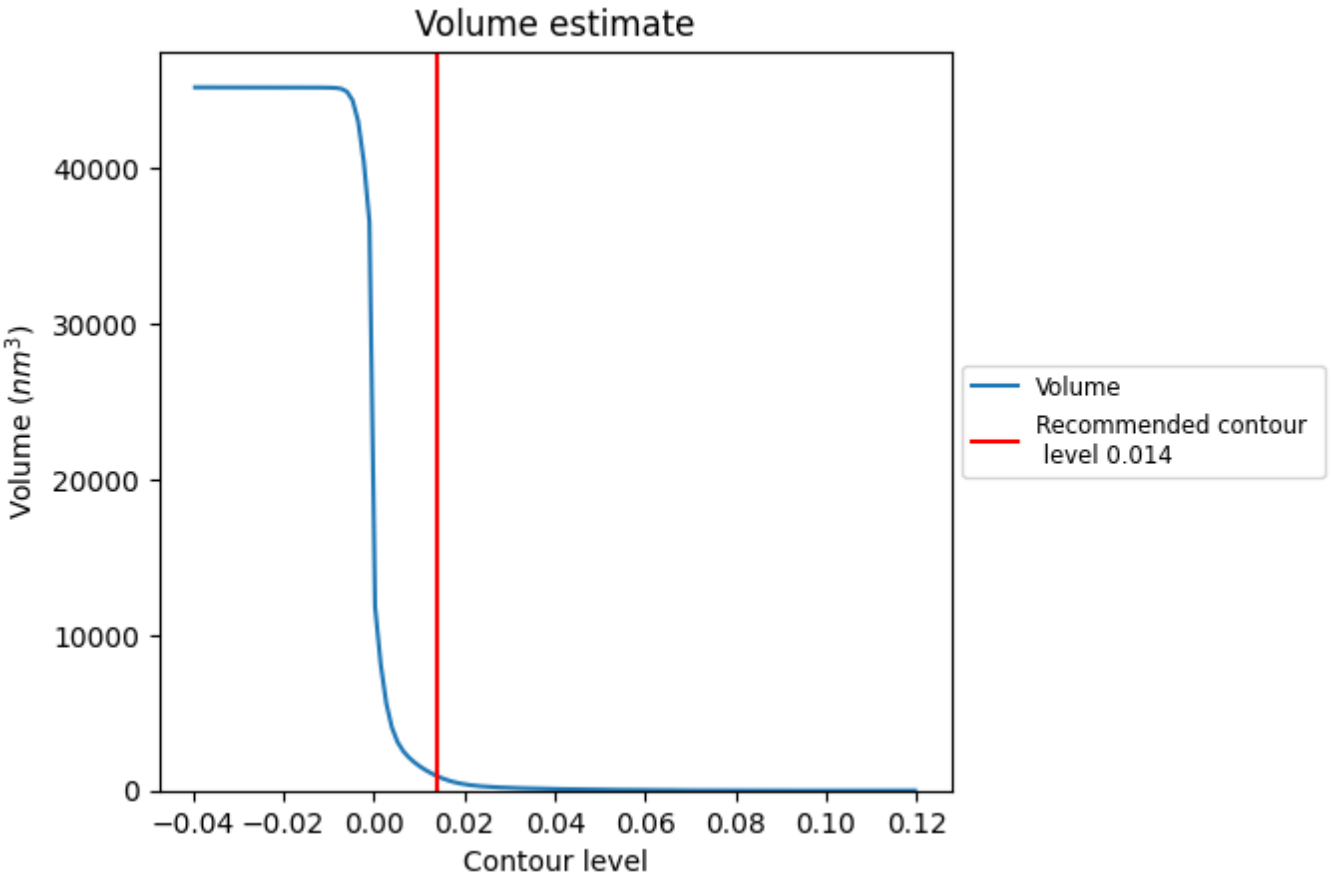
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

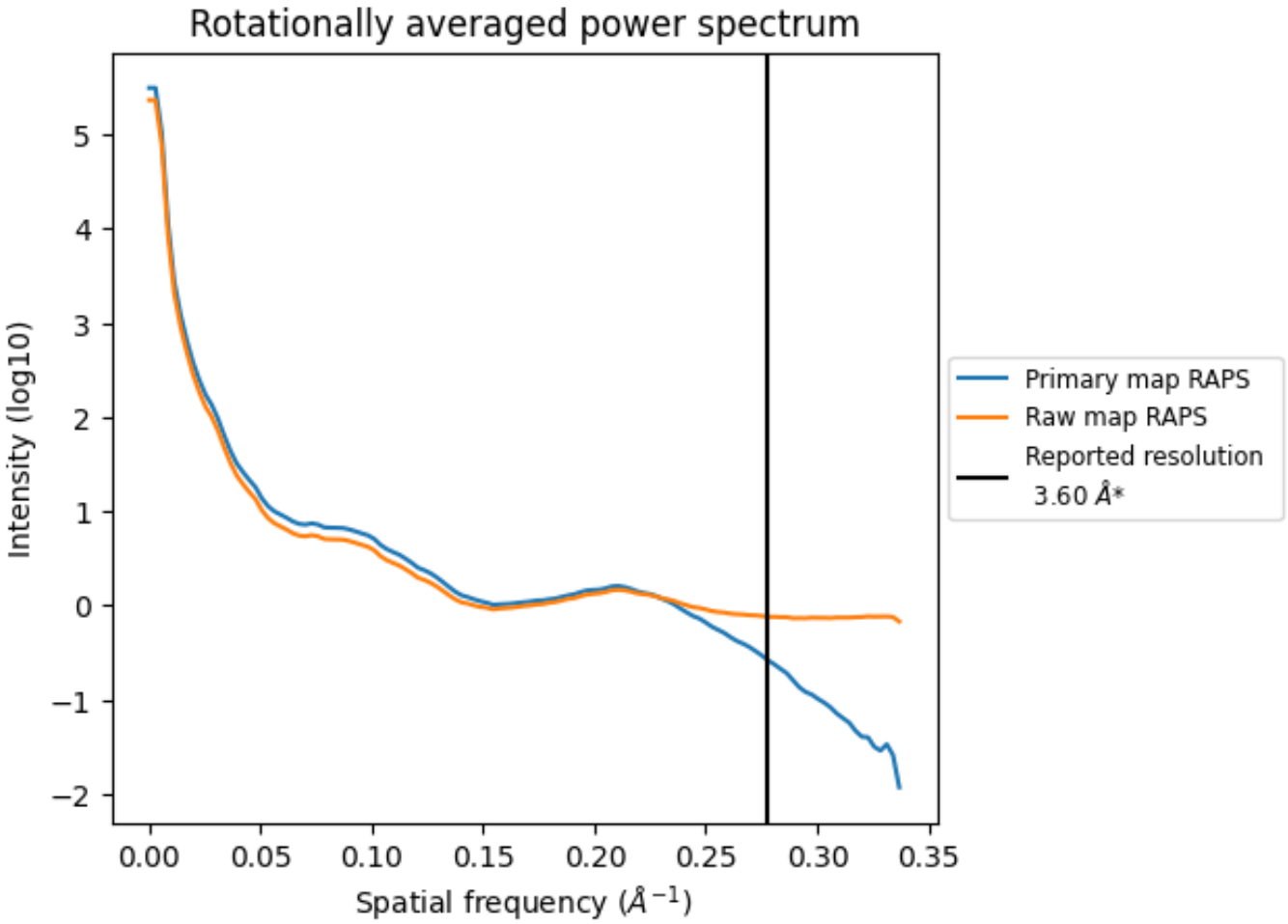
7.2 Volume estimate



The volume at the recommended contour level is 927 nm^3; this corresponds to an approximate mass of 837 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 (i)

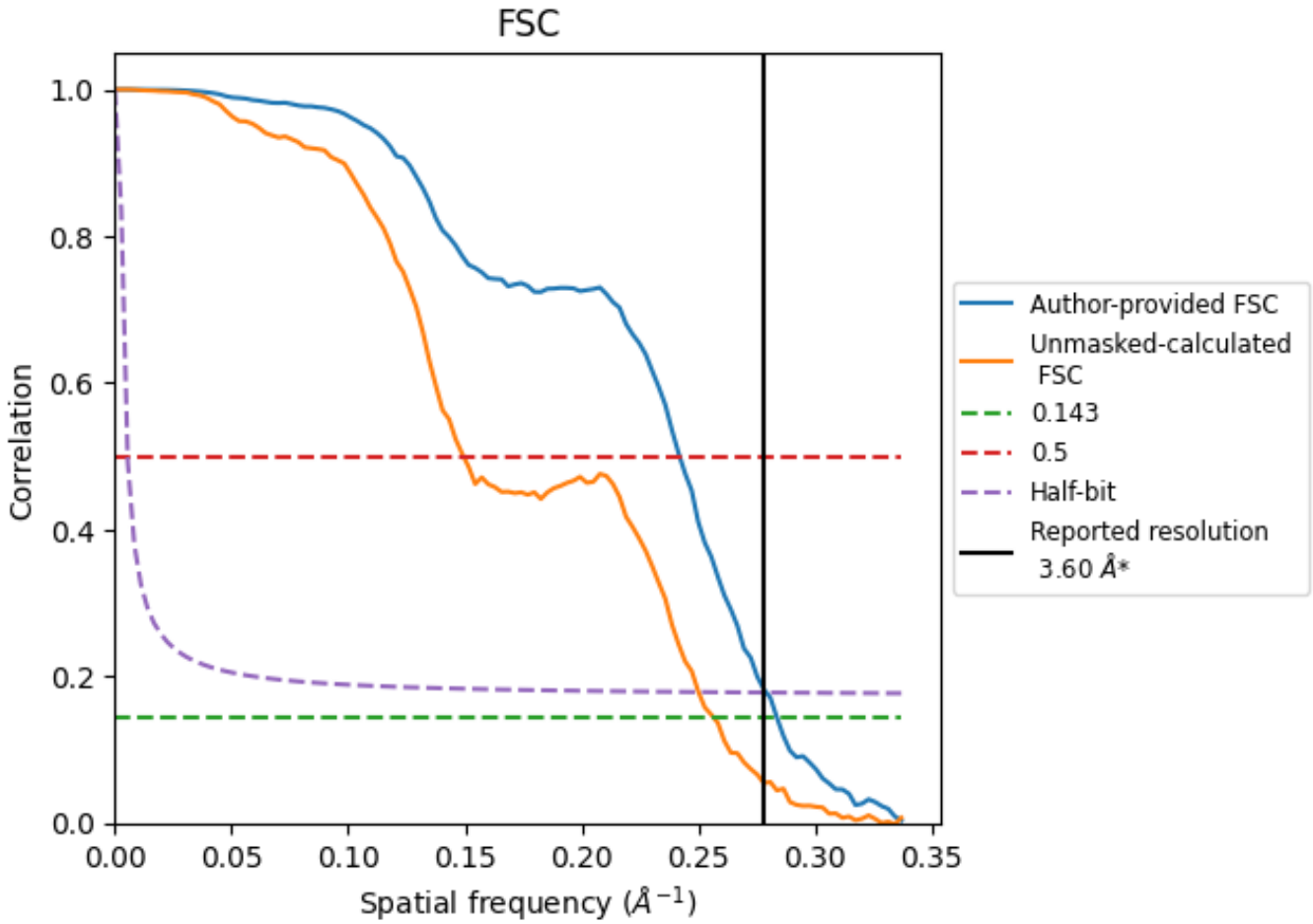


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

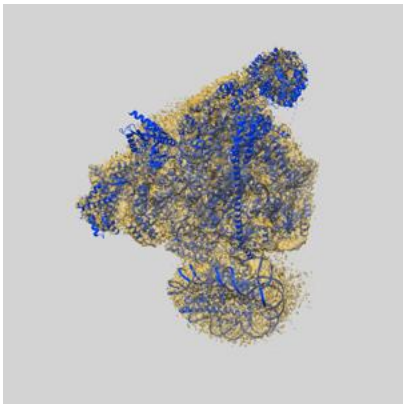
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.53	4.13	3.58
Unmasked-calculated*	3.90	6.70	4.00

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

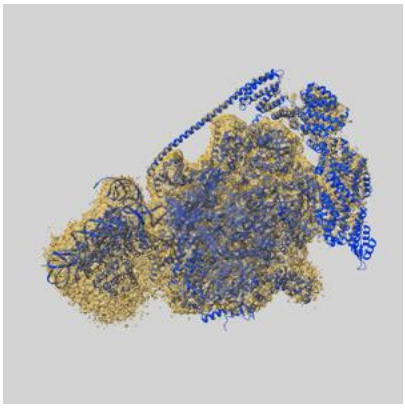
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33424 and PDB model 7XSE. Per-residue inclusion information can be found in section 3 on page 15.

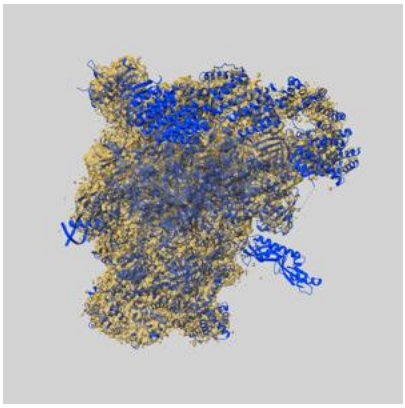
9.1 Map-model overlay



X



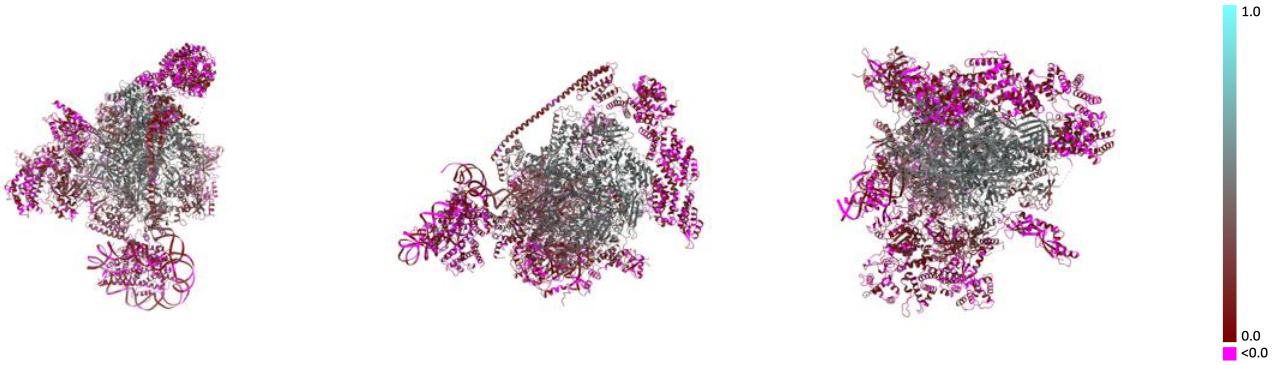
Y



Z

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.

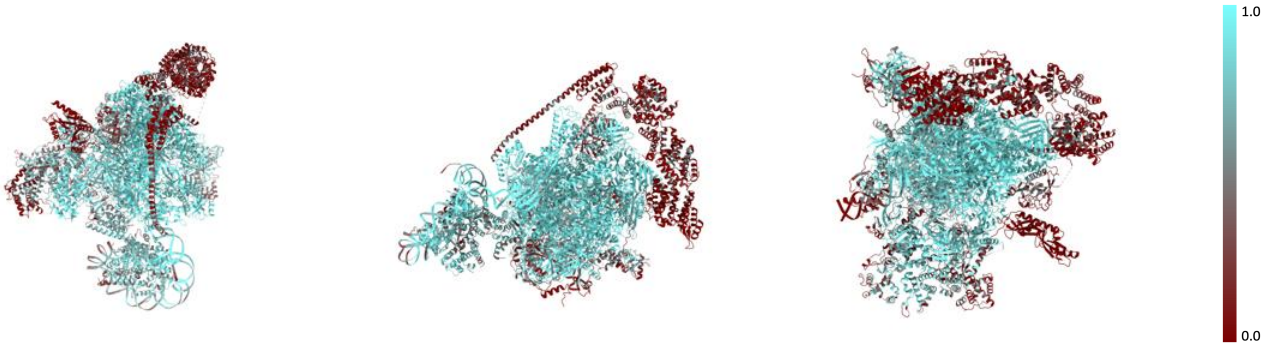
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

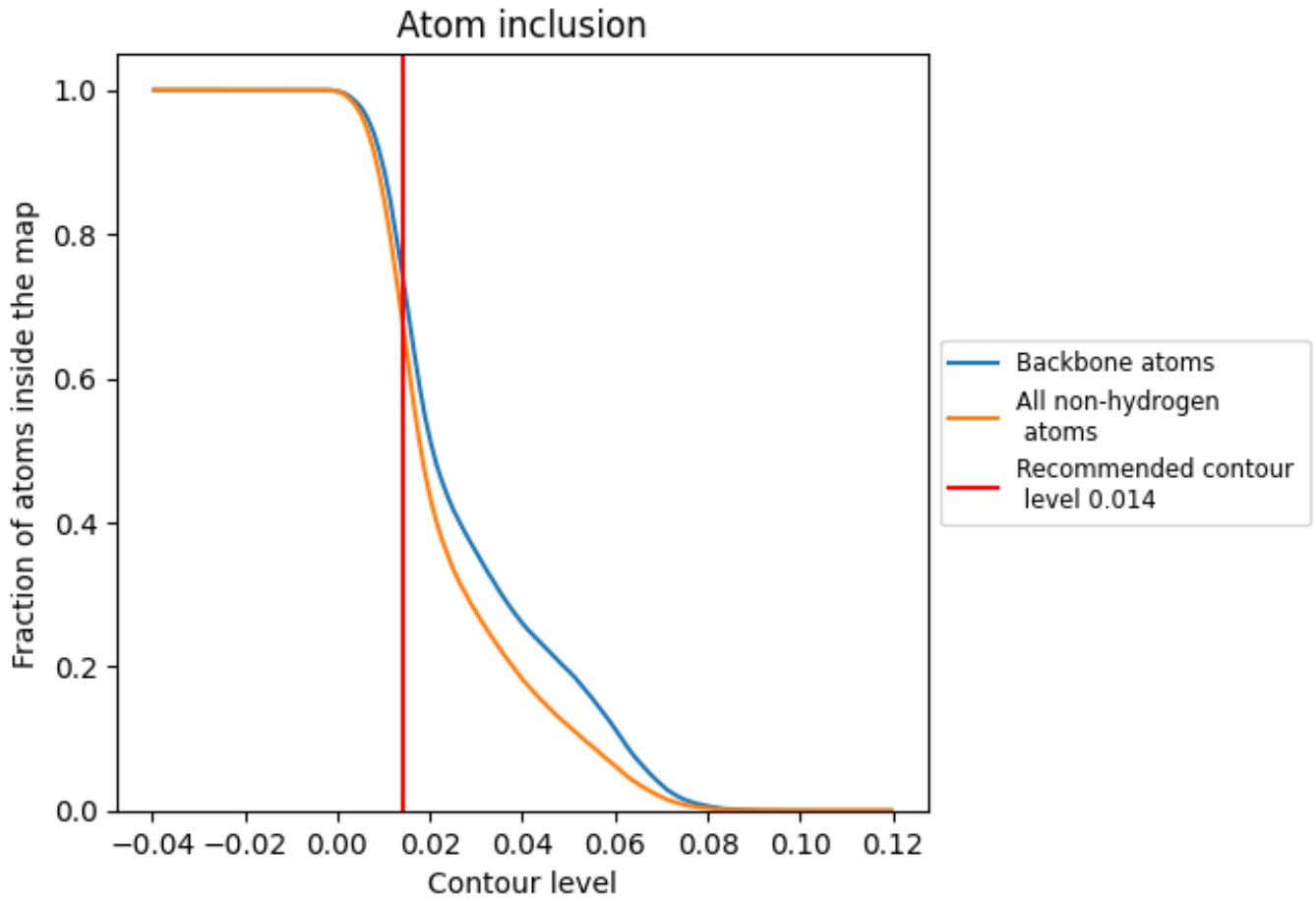
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 75% of all backbone atoms, 68% 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	0.6824	0.2380
A	0.9429	0.4470
B	0.9380	0.4540
C	0.9535	0.4810
D	0.8577	0.1860
E	0.9616	0.4200
F	0.9726	0.4860
G	0.8682	0.2860
H	0.9662	0.4760
I	0.8326	0.2790
J	0.9499	0.4800
K	0.9694	0.4810
L	0.9569	0.4190
M	0.7659	0.1840
N	0.7056	0.0780
P	0.9431	0.3110
T	0.7280	0.1290
V	0.8436	0.1010
W	0.6975	0.1730
a	0.7403	0.0460
b	0.7846	0.0500
c	0.7289	0.0080
d	0.7019	0.0360
e	0.7500	0.0180
f	0.8101	0.0840
g	0.7131	0.0030
h	0.7288	0.0330
m	0.4658	0.0730
n	0.7037	0.1690
q	0.1295	0.0660
r	0.3749	0.1360
u	0.5826	0.1740
v	0.3471	0.0980
x	0.2345	0.2380