



Full wwPDB EM Validation Report ⓘ

Jun 26, 2024 – 01:07 PM JST

PDB ID : 7XTI
EMDB ID : EMD-33450
Title : RNA polymerase II elongation complex transcribing a nucleosome (EC58hex)
Authors : Ehara, H.; Kujirai, T.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on : 2022-05-17
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

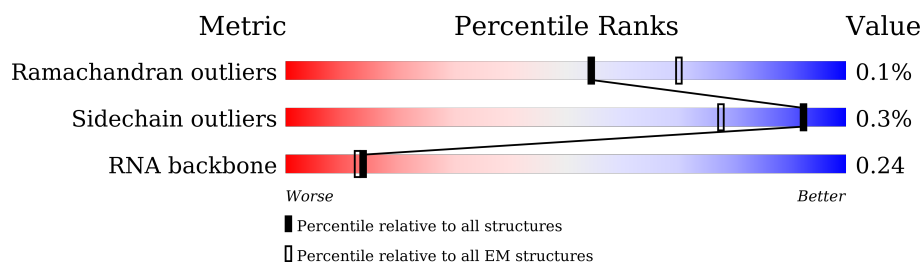
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance

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


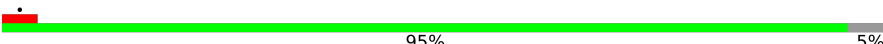



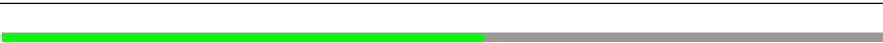

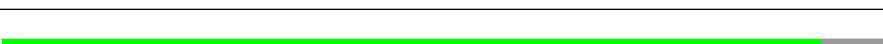
The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1743	
2	B	1227	
3	C	304	
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	

Continued on next page...

Continued from previous page...

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	m	1503	
20	n	417	
21	q	1084	
22	r	544	
23	u	459	
24	v	396	
25	x	395	
26	a	139	
26	e	139	
27	b	106	
27	f	106	
28	g	133	
29	h	129	
30	j	1008	
31	k	531	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 78660 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	74	Total	C	N	O	P	0	0
			1516	723	258	461	74		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	19	Total	C	N	O	P	0	0
			399	178	64	138	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	85	Total	C	N	O	P	0	0
			1744	824	346	489	85		

- 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 Transcription elongation factor Spt6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	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 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 Leo1.

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

There are 30 discrepancies between the modelled and reference sequences:

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

- Molecule 24 is a protein called RNAP II-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	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

Continued on next page...

Continued from previous page...

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

- Molecule 25 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
25	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
x	0	GLY	-	expression tag	UNP C4R1E6

- Molecule 26 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	75	Total	C	N	O	S	0	0
			606	385	114	105	2		
26	e	77	Total	C	N	O	S	0	0
			620	393	116	109	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 27 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
27	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 28 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	g	92	Total	C	N	O	0	0
			715	447	142	126		

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 29 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 30 is a protein called FACT complex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	471	Total	C	N	O	S	0	0
			3791	2403	663	712	13		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	-2	GLY	-	expression tag	UNP C4QYQ8
j	-1	PRO	-	expression tag	UNP C4QYQ8
j	0	GLY	-	expression tag	UNP C4QYQ8

- Molecule 31 is a protein called FACT complex subunit POB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	k	434	Total	C	N	O	S	0	0
			3535	2233	619	673	10		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	-2	GLY	-	expression tag	UNP F2QNN8
k	-1	PRO	-	expression tag	UNP F2QNN8
k	0	GLY	-	expression tag	UNP F2QNN8

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

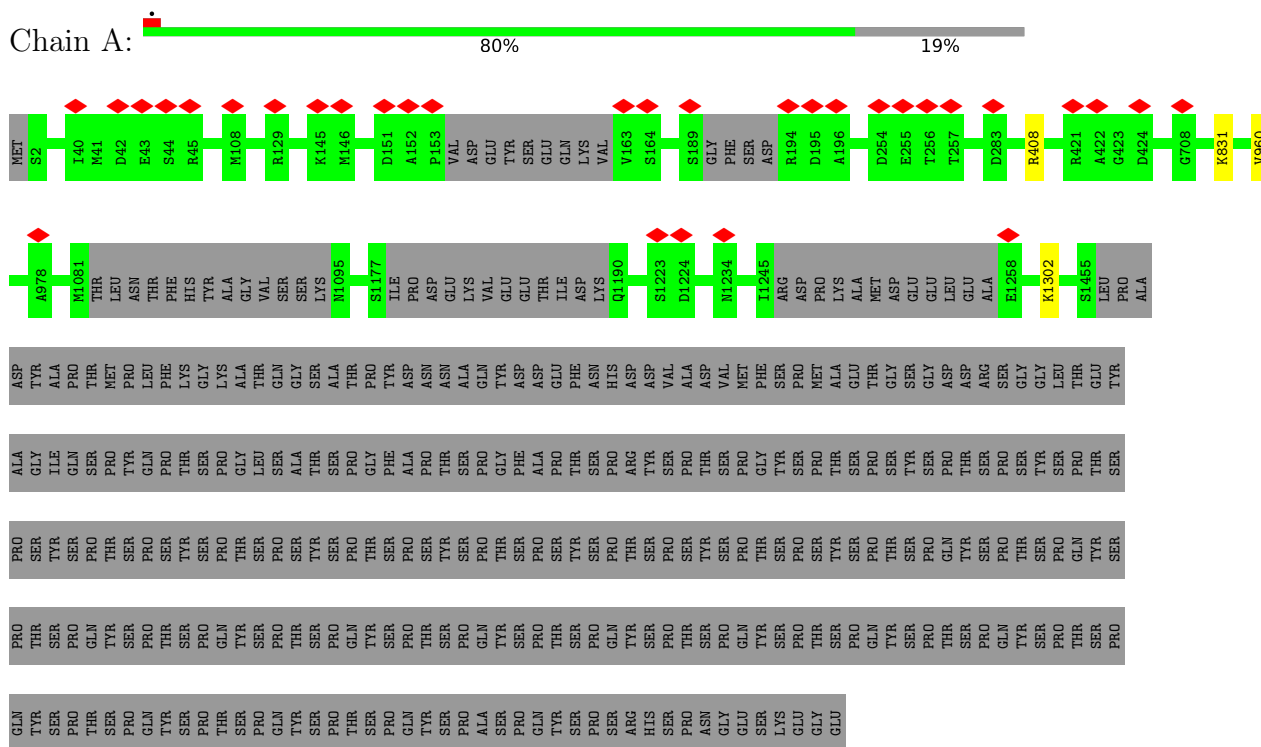
- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

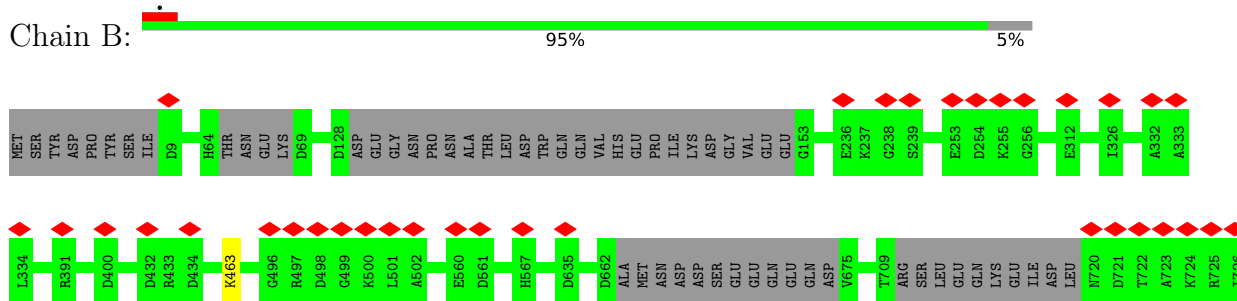
3 Residue-property plots

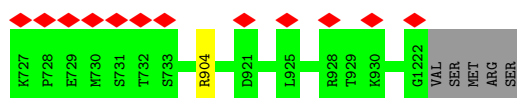
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

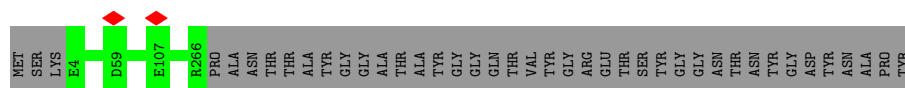
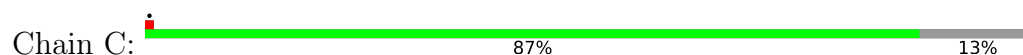


- Molecule 2: DNA-directed RNA polymerase subunit beta

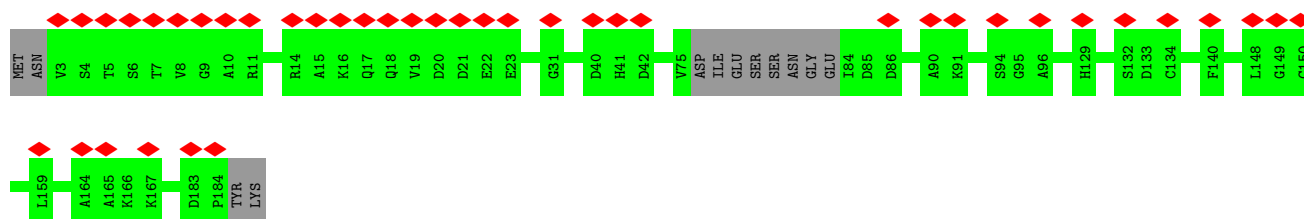




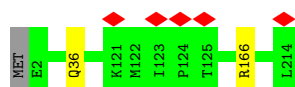
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core



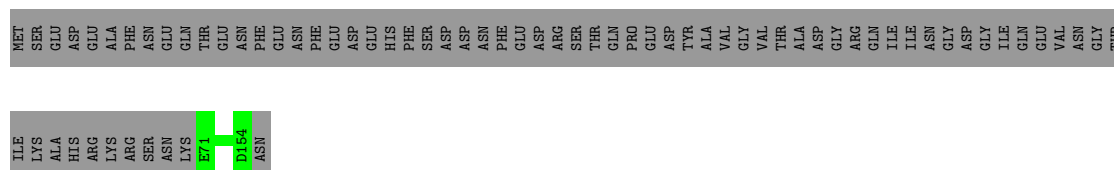
- Molecule 4: RNA polymerase II subunit B32



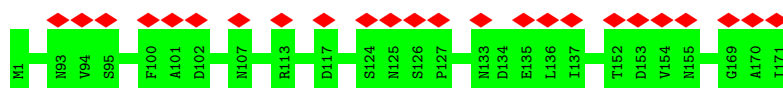
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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

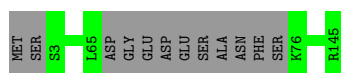


- Molecule 7: RNA polymerase II subunit

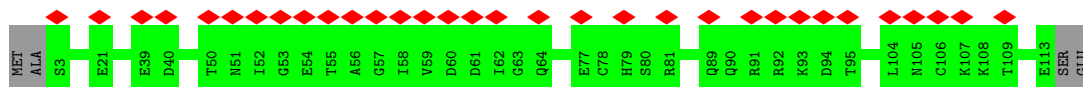


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

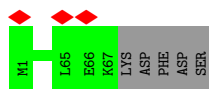
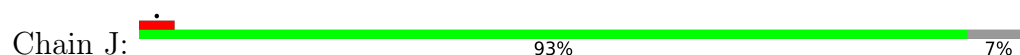




- Molecule 9: DNA-directed RNA polymerase subunit



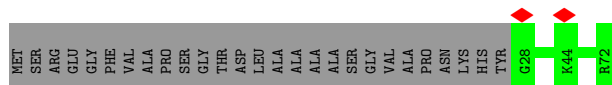
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



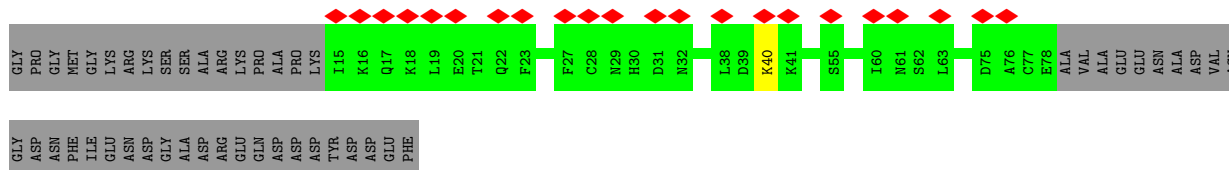
- Molecule 11: RNA polymerase II subunit B12.5



- Molecule 12: RNA polymerase subunit ABC10-alpha

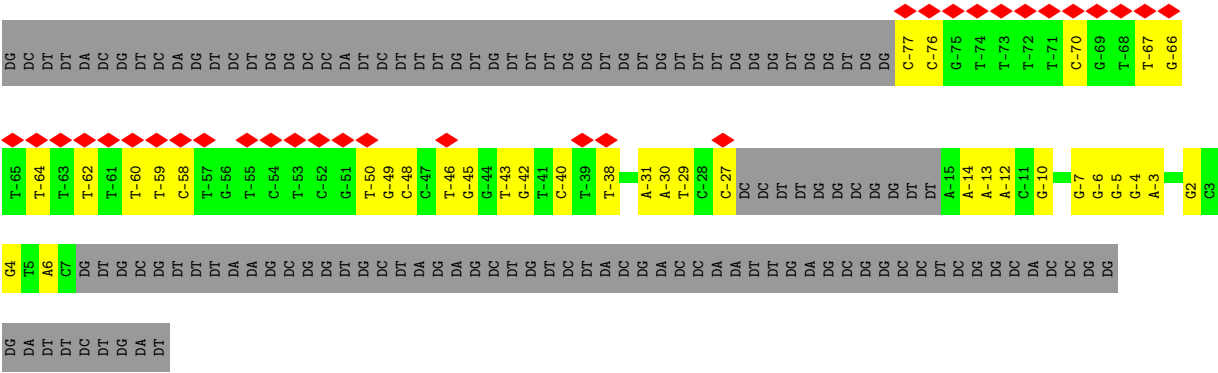


- Molecule 13: Transcription elongation factor 1 homolog

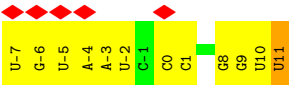


- Molecule 14: DNA (198-MER)

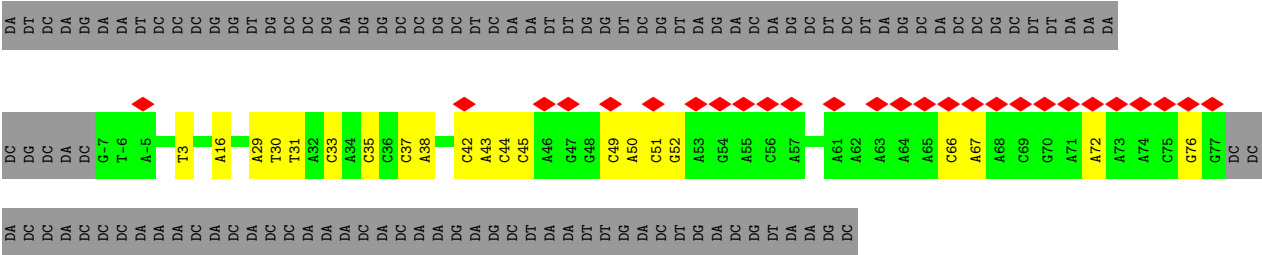
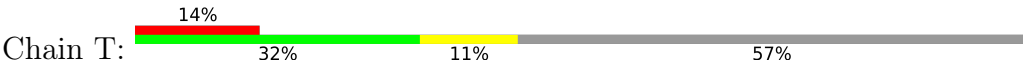




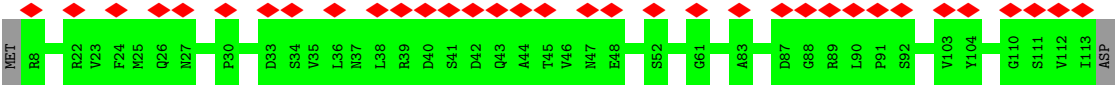
• Molecule 15: RNA (5'-R(P*UP*GP*UP*AP*AP*UP*CP*CP*CP*CP*UP*UP*GP*GP*CP*GP*GP*UP*U)-3')



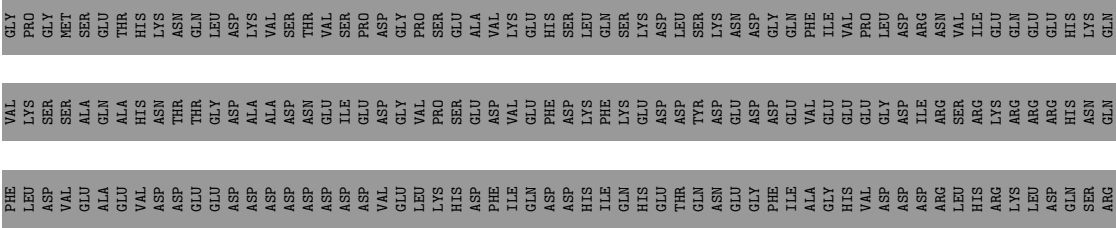
• Molecule 16: DNA (198-MER)

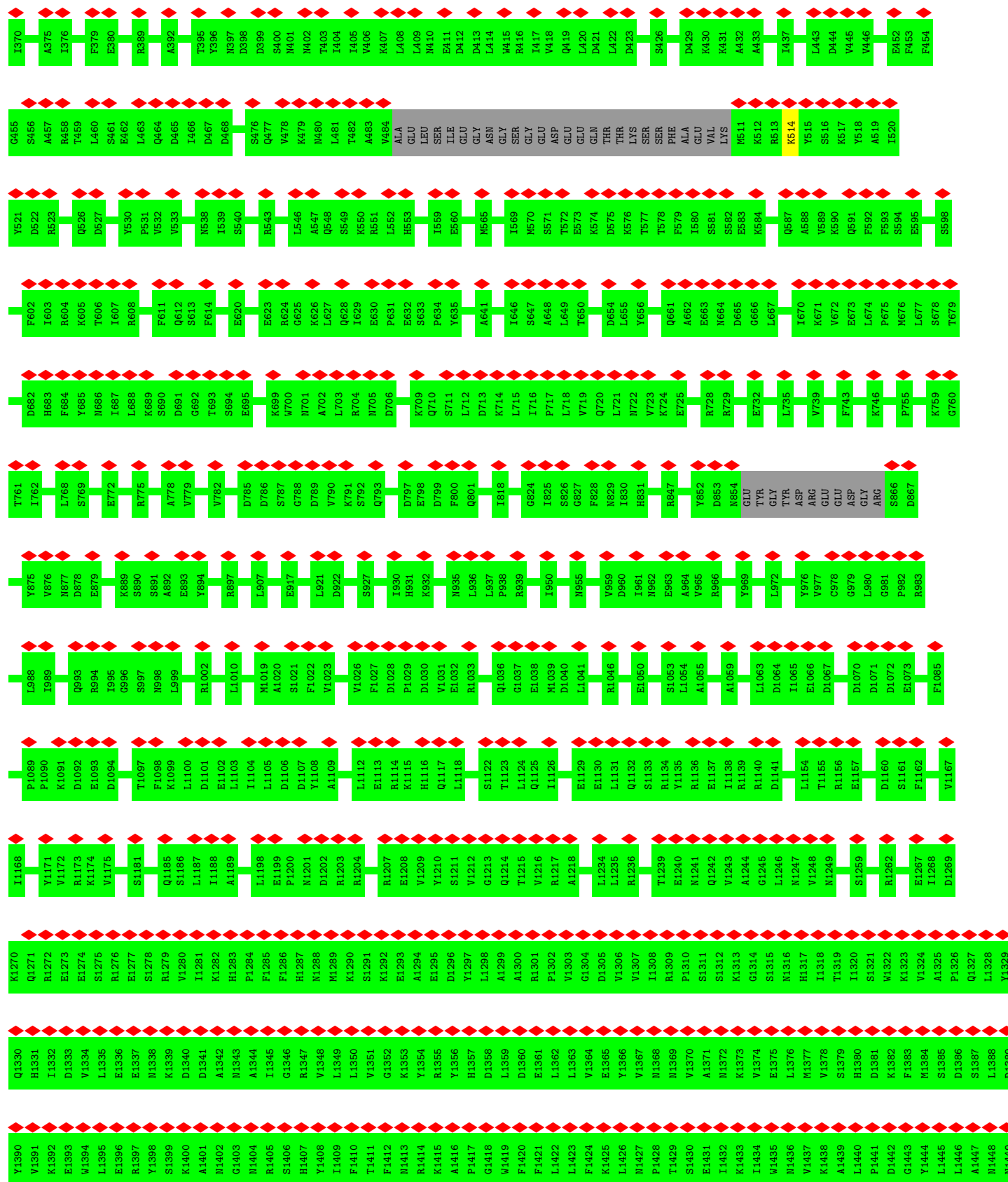


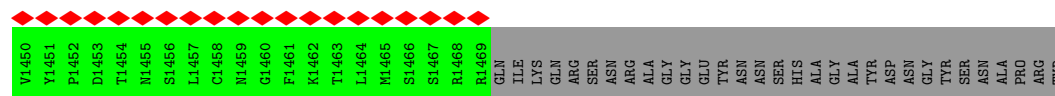
• Molecule 17: Transcription elongation factor SPT4



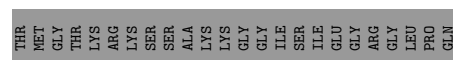
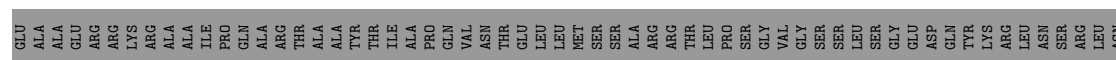
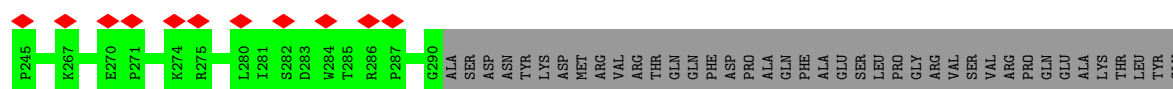
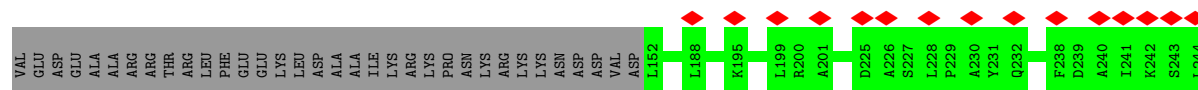
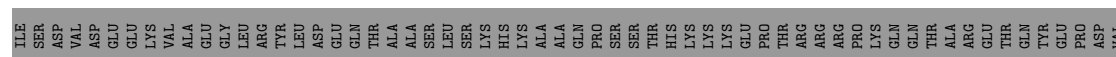
• Molecule 18: Transcription elongation factor SPT5



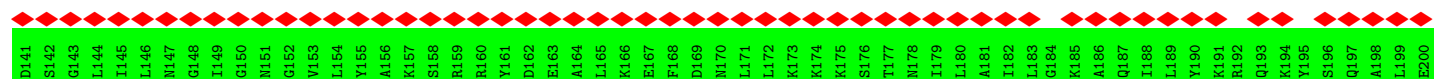
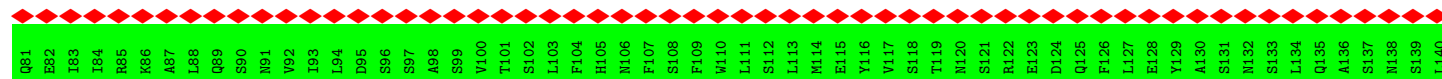
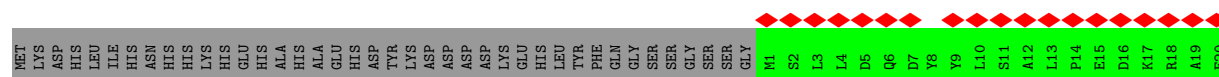
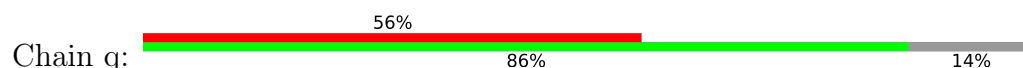


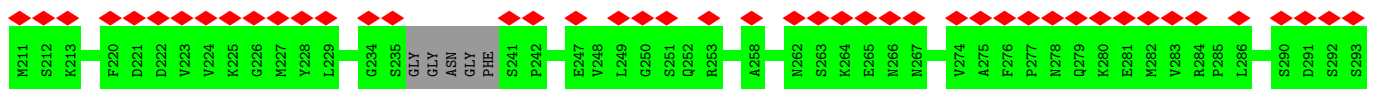
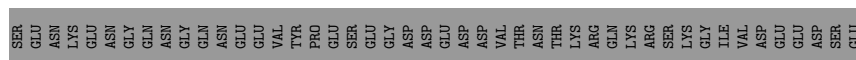


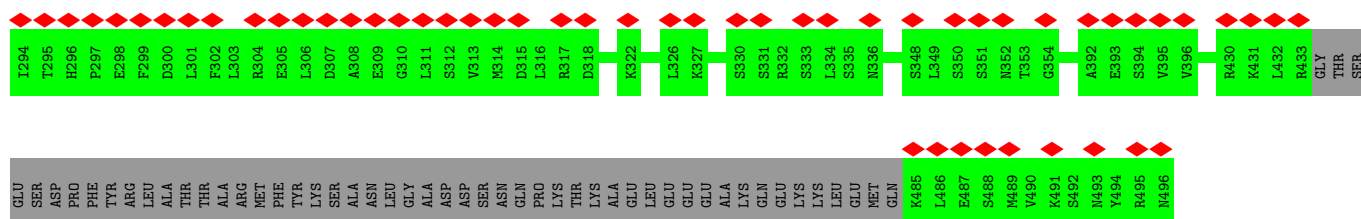
- Molecule 20: Protein that interacts with Spt6p and copurifies with Spt5p and RNA polymerase II



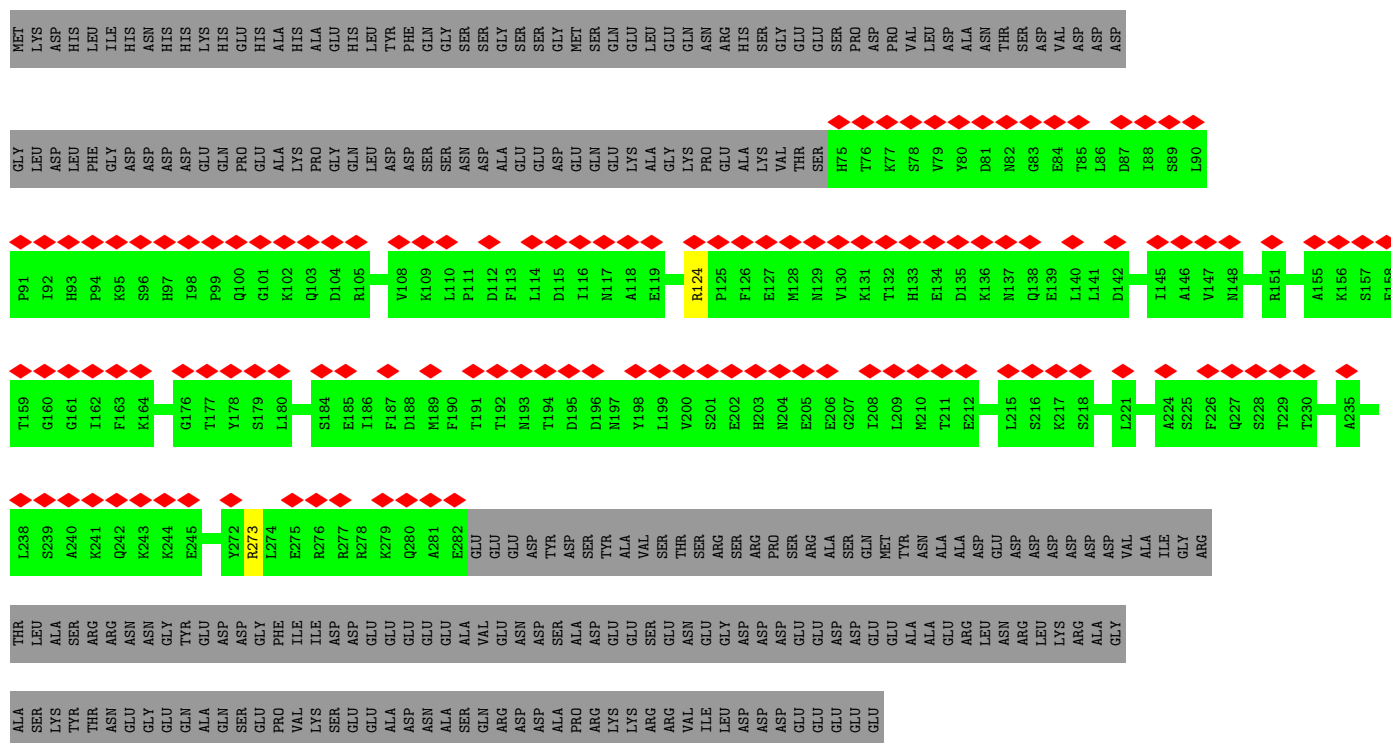
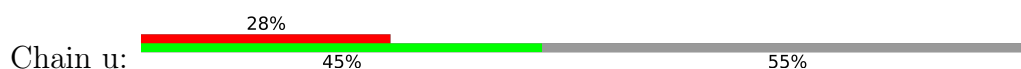
- Molecule 21: Component of the Paf1p complex



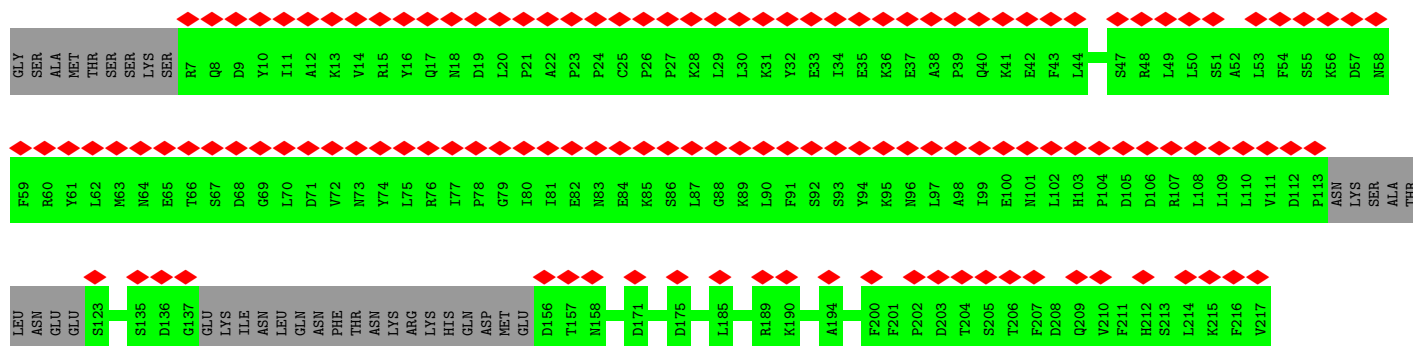
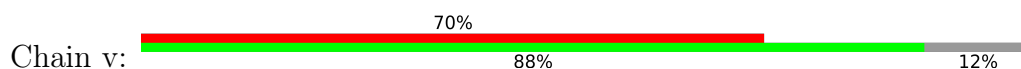


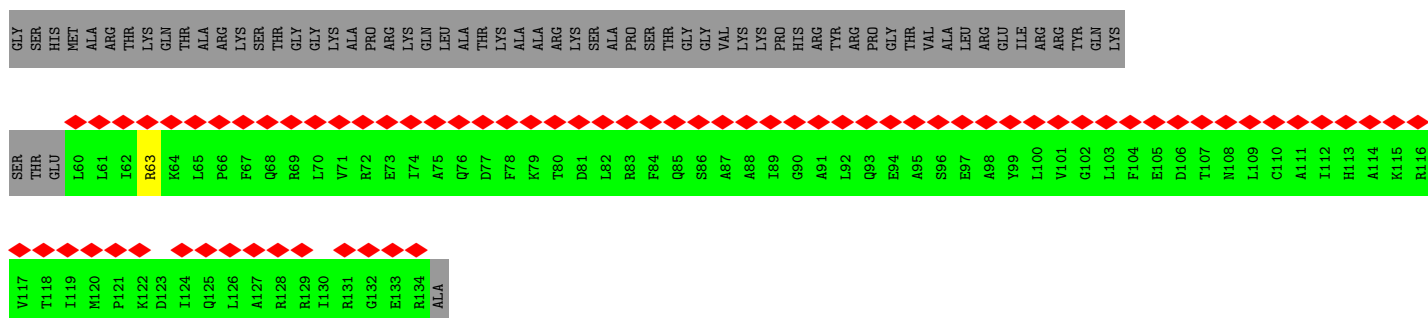
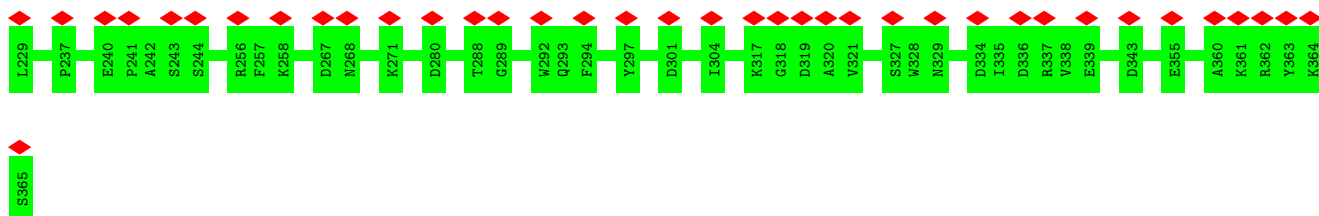


• Molecule 23: Leo1



• Molecule 24: RNAP II-associated protein





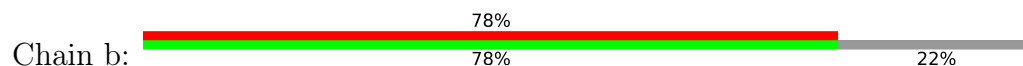


GLY SER HIS MET ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY LYS ALA PRO ARG LYS GLN LEU THR ALA LYS ARG LYS SER ALA PRO THR GLY VAL LYS LYS PRO HIS ARG TTR ARG PRO GLY THR VAL ALA ARG GLU ILE ARG TTR ARG LYS

SER THR E59 L60 L61 I62 R63 R64 K64 L65 P66 F67 Q68 R69 L70 L71 V71 R72 E73 I74 A75 Q76 D77 F78 K79 T80 D81 L82 R83 F84 Q85 S86 A87 A88 I89 G90 A91 L92 Q93 E94 A95 S96 E97 A98 Y99 L100 V101 G102 L103 F104 E105 D106 T107 N108 L109 C110 A111 I112 H113 K115 R116

V117 T118 I119 M120 P121 K122 D123 I124 Q125 L126 A127 R128 R129 I130 R131 G132 E133 R134 A135

• Molecule 27: Histone H4



GLY SER HIS MET SER GLY ARG GLY LYS GLY LYS LYS LEU GLY LYS GLY ALA LYS ARG K20 V21 L22 R23 D24 N25 I26 Q27 G28 I29 T30 K31 P32 A33 I34 R35 R36 L37 A38 R39 R40 G41 G42 V43 K44 R45 I46 S47 G48 L49 I50 Y51 E52 E53 T54 R55 G56

V57 L58 K59 V60 F61 L62 E63 M64 V65 I66 R67 D68 A69 V70 T71 Y72 T73 E74 H75 A76 K77 R78 K79 T80 V81 T82 A83 M84 D85 V86 V87 Y88 A89 L90 K91 Q92 Q93 R94 R95 T96 L97 Y98 G99 F100 G101 G102

• Molecule 27: Histone H4



GLY SER HIS MET SER GLY ARG GLY LYS GLY LYS LYS LEU GLY LYS GLY ALA LYS ARG ASP N25 I26 Q27 G28 I29 T30 K31 P32 A33 I34 R35 R36 L37 A38 R39 R40 G41 G42 V43 K44 R45 I46 S47 G48 L49 I50 Y51 E52 E53 T54 R55 G56

V57 L58 K59 V60 F61 L62 E63 M64 V65 I66 R67 D68 A69 V70 T71 Y72 T73 E74 H75 A76 K77 R78 K79 T80 V81 T82 A83 M84 D85 V86 V87 Y88 A89 L90 K91 Q92 Q93 R94 R95 T96 L97 Y98 G99 F100 G101 G102

• Molecule 28: Histone H2A type 1-B/E

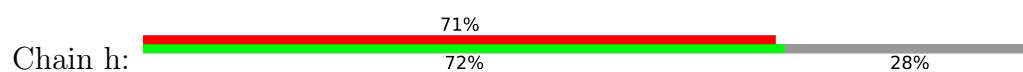


GLY SER HIS MET SER GLY ARG GLY LYS GLY LYS LYS ALA ARG ALA LYS A14 K15 T16 R17 S18 S19 R20 A21 G22 L23 Q24 F25 P26 V27 G28 R29 V30 H31 R32 L33 L34 R35 K36 G37 N38 Y39 S40 E41 R42 V43 G44 A45 A46 G47 P48 V49 Y50 L51 A52 A53 V54 L55 E56

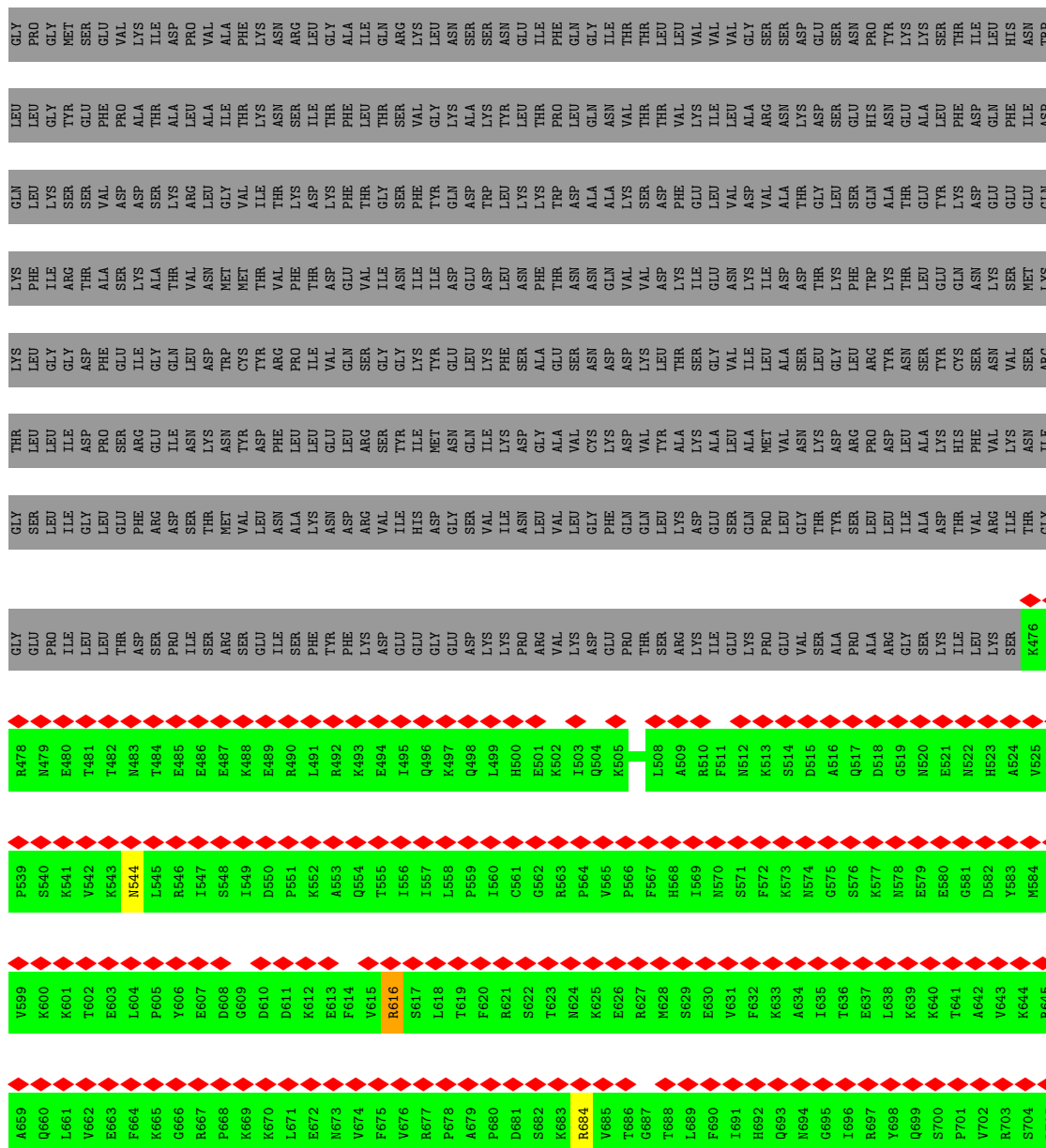
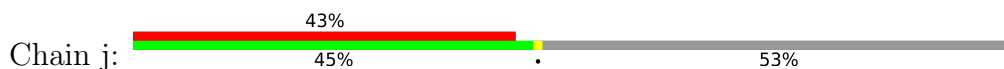
Y57 L58 T59 A60 E61 I62 L63 E64 L65 A66 G67 M68 A69 A70 R71 D72 N73 K74 K76 T76 R77 I78 I79 P80 R81 H82 L83 L85 A86 I87 R88 M89 D90 E91 E92 L93 N94 K95 L96 L97 G98 R99 V100 T101 I102 A103 G104 G105

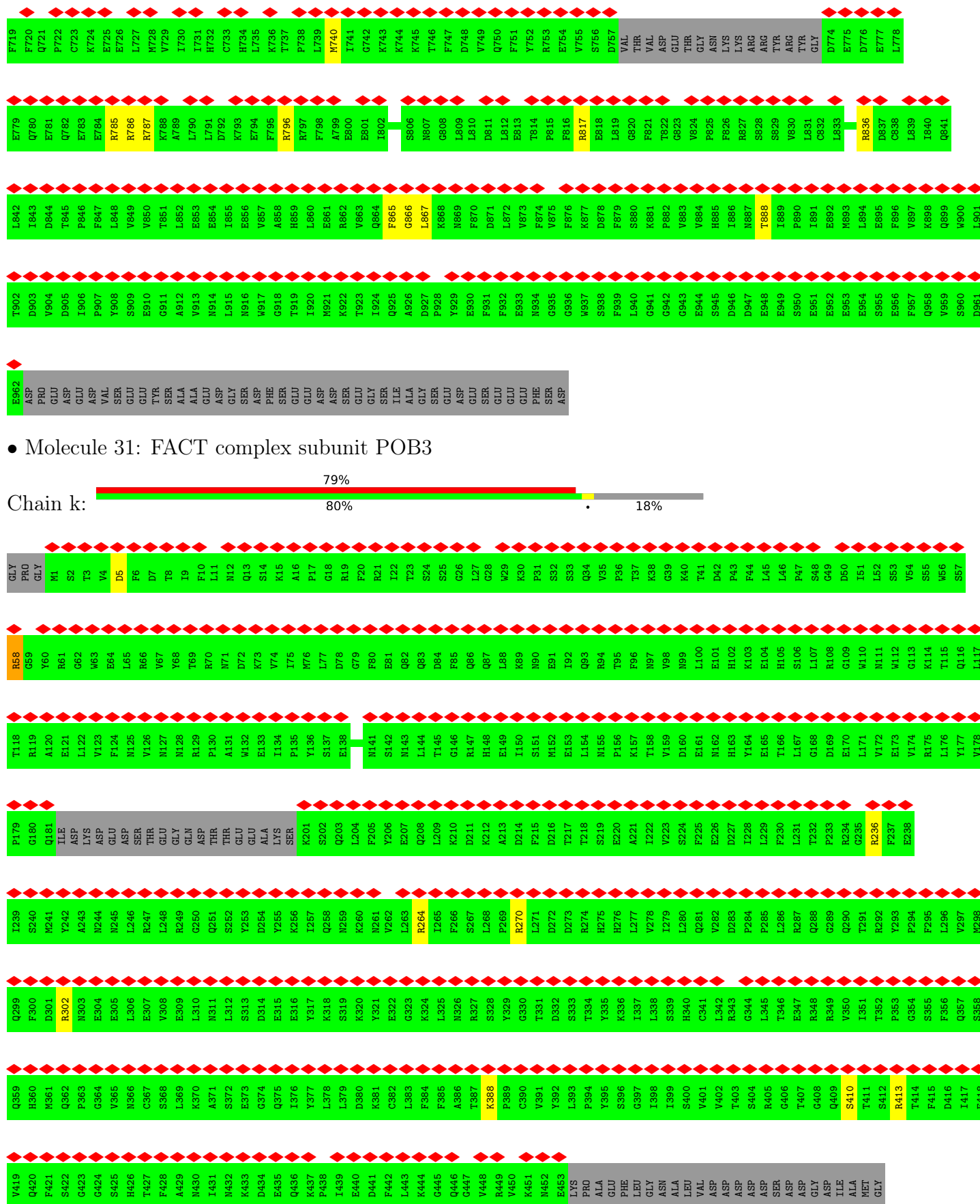
PRO LYS LYS THR GLU SER HIS HIS ALA LYS LYS

• Molecule 29: Histone H2B type 1-J



- Molecule 30: FACT complex subunit





SER	ALA	GLY	GLU	ASP	ASP	GLU	SER	VAL	ASP	GLU	ASP	PHE	ASN	ALA	GLY	SER	SER	SER	ASP	ASP	VAL	VAL	ALA	GLU	GLU	TYR	ASP	SER	ASN	ALA	GLY	SER	GLU	ASP	GLU	ASP	SER	ASP	ASP	ALA	SER	SER	GLY	GLU	PRO	GLU	LYS	LYS	LYS	PRO	LYS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29919	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 ($e^-/\text{\AA}^2$)	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	0.080	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.009	Depositor
Map size (\AA)	356.16, 356.16, 356.16	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	0.32	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	0.24	0/1361	0.46	0/1837
5	E	0.30	0/1773	0.49	0/2385
6	F	0.34	0/687	0.50	0/931
7	G	0.28	0/1354	0.48	0/1837
8	H	0.34	0/1070	0.49	0/1444
9	I	0.24	0/934	0.50	0/1257
10	J	0.36	0/563	0.50	0/753
11	K	0.32	0/953	0.51	0/1291
12	L	0.33	0/365	0.56	0/484
13	M	0.25	0/513	0.41	0/693
14	N	1.23	25/1693 (1.5%)	1.22	10/2611 (0.4%)
15	P	0.41	0/443	0.83	2/687 (0.3%)
16	T	1.18	14/1963 (0.7%)	1.18	9/3024 (0.3%)
17	V	0.25	0/840	0.50	0/1140
18	W	0.27	0/4300	0.53	2/5812 (0.0%)
19	m	0.24	0/9925	0.45	0/13424
20	n	0.24	0/1132	0.41	0/1526
21	q	0.24	0/7689	0.40	0/10368
22	r	0.24	0/2169	0.45	0/2901
23	u	0.28	0/1740	0.52	1/2347 (0.0%)
24	v	0.25	0/2944	0.47	0/3973
25	x	0.26	0/1716	0.45	0/2310
26	a	0.38	0/613	0.57	0/822
26	e	0.30	0/627	0.58	0/841
27	b	0.36	0/669	0.60	0/894
27	f	0.34	0/626	0.63	1/837 (0.1%)
28	g	0.28	0/723	0.54	0/973
29	h	0.33	0/736	0.48	0/990
30	j	0.68	0/3865	0.84	8/5206 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	k	0.69	0/3613	0.86	5/4881 (0.1%)
All	All	0.43	39/80469 (0.0%)	0.59	38/109359 (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
30	j	0	1
31	k	0	1
All	All	0	5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	-29	DT	C1'-N1	7.24	1.58	1.49
16	T	30	DT	C1'-N1	7.07	1.58	1.49
16	T	42	DC	C1'-N1	7.00	1.58	1.49
16	T	49	DC	C1'-N1	6.93	1.58	1.49
14	N	-27	DC	C1'-N1	6.87	1.58	1.49
16	T	37	DC	C1'-N1	6.83	1.58	1.49
14	N	-60	DT	C1'-N1	6.82	1.58	1.49
14	N	-48	DC	C1'-N1	6.78	1.58	1.49
16	T	51	DC	C1'-N1	6.76	1.58	1.49
14	N	-67	DT	C1'-N1	6.69	1.57	1.49
14	N	-46	DT	C1'-N1	6.68	1.57	1.49
14	N	-59	DT	C1'-N1	6.62	1.57	1.49
16	T	44	DC	C1'-N1	6.41	1.57	1.49
14	N	-64	DT	C1'-N1	6.37	1.57	1.49
16	T	35	DC	C1'-N1	6.37	1.57	1.49
14	N	-76	DC	C1'-N1	6.36	1.57	1.49
14	N	-70	DC	C1'-N1	6.34	1.57	1.49
16	T	45	DC	C1'-N1	6.34	1.57	1.49
14	N	-43	DT	C1'-N1	6.31	1.57	1.49
16	T	66	DC	C1'-N1	6.27	1.57	1.49
14	N	-10	DG	C1'-N9	-6.26	1.38	1.47
14	N	-7	DG	C1'-N9	-6.23	1.38	1.47
16	T	33	DC	C1'-N1	6.19	1.57	1.49
14	N	-50	DT	C1'-N1	6.13	1.57	1.49
14	N	-58	DC	C1'-N1	6.11	1.57	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	31	DT	C1'-N1	6.04	1.57	1.49
14	N	-5	DG	C1'-N9	-5.96	1.39	1.47
14	N	-13	DA	C1'-N9	-5.90	1.39	1.47
16	T	16	DA	C1'-N9	-5.83	1.39	1.47
14	N	-12	DA	C1'-N9	-5.67	1.39	1.47
14	N	2	DG	C1'-N9	-5.59	1.39	1.47
14	N	4	DG	C1'-N9	-5.56	1.39	1.47
14	N	-6	DG	C1'-N9	-5.54	1.39	1.47
14	N	6	DA	C1'-N9	-5.23	1.40	1.47
14	N	-14	DA	C1'-N9	-5.22	1.40	1.47
14	N	-3	DA	C1'-N9	-5.09	1.40	1.47
16	T	76	DG	C1'-N9	-5.07	1.40	1.47
16	T	3	DT	C1'-N1	5.06	1.55	1.49
14	N	-4	DG	C1'-N9	-5.04	1.40	1.47

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	j	836	ARG	NE-CZ-NH1	9.37	124.99	120.30
15	P	10	U	OP1-P-O3'	8.82	124.60	105.20
18	W	431	ARG	NE-CZ-NH1	7.90	124.25	120.30
30	j	684	ARG	NE-CZ-NH1	7.64	124.12	120.30
16	T	43	DA	O4'-C1'-N9	7.49	113.24	108.00
16	T	31	DT	O4'-C1'-N1	7.28	113.09	108.00
14	N	-30	DA	O4'-C1'-N9	7.12	112.98	108.00
30	j	786	ARG	NE-CZ-NH1	7.06	123.83	120.30
14	N	-31	DA	O4'-C1'-N9	7.04	112.93	108.00
15	P	11	U	OP1-P-OP2	-7.04	109.04	119.60
14	N	-49	DG	O4'-C1'-N9	6.93	112.85	108.00
14	N	-38	DT	O4'-C1'-N1	6.86	112.80	108.00
14	N	-43	DT	O4'-C1'-N1	6.83	112.78	108.00
16	T	52	DG	O4'-C1'-N9	6.65	112.66	108.00
14	N	-45	DG	P-O3'-C3'	6.49	127.49	119.70
30	j	817	ARG	NE-CZ-NH1	6.43	123.52	120.30
18	W	410	ARG	NE-CZ-NH1	6.37	123.48	120.30
16	T	29	DA	O4'-C1'-N9	6.28	112.40	108.00
16	T	72	DA	O4'-C1'-N9	6.18	112.33	108.00
16	T	50	DA	O4'-C1'-N9	6.06	112.24	108.00
14	N	-27	DC	O4'-C1'-N1	6.05	112.23	108.00
23	u	273	ARG	NE-CZ-NH1	6.02	123.31	120.30
16	T	33	DC	O4'-C1'-N1	6.00	112.20	108.00
16	T	38	DA	O4'-C1'-N9	5.81	112.07	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	j	785	ARG	NE-CZ-NH1	5.71	123.15	120.30
27	f	45	ARG	NE-CZ-NH1	5.65	123.12	120.30
30	j	787	ARG	NE-CZ-NH1	5.63	123.12	120.30
14	N	-66	DG	O4'-C1'-N9	5.59	111.92	108.00
31	k	264	ARG	NE-CZ-NH1	5.57	123.08	120.30
31	k	302	ARG	NE-CZ-NH1	5.45	123.03	120.30
30	j	796	ARG	NE-CZ-NH1	5.44	123.02	120.30
14	N	-76	DC	O4'-C1'-N1	5.42	111.79	108.00
31	k	270	ARG	NE-CZ-NH1	5.41	123.01	120.30
31	k	58	ARG	NE-CZ-NH1	5.40	123.00	120.30
14	N	-40	DC	O4'-C1'-N1	5.27	111.69	108.00
30	j	616	ARG	NE-CZ-NH1	5.23	122.91	120.30
16	T	67	DA	O4'-C1'-N9	5.13	111.59	108.00
31	k	5	ASP	CB-CG-OD2	-5.04	113.77	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	-42	DG	Sidechain
14	N	-62	DT	Sidechain
14	N	-77	DC	Sidechain
30	j	616	ARG	Sidechain
31	k	58	ARG	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%)	1354 (97%)	37 (3%)	1 (0%)	51	84
2	B	1154/1227 (94%)	1117 (97%)	37 (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%)	504 (96%)	22 (4%)	1 (0%)	47	79
19	m	1179/1503 (78%)	1158 (98%)	21 (2%)	0	100	100
20	n	137/417 (33%)	136 (99%)	1 (1%)	0	100	100
21	q	928/1084 (86%)	922 (99%)	6 (1%)	0	100	100
22	r	260/544 (48%)	254 (98%)	6 (2%)	0	100	100
23	u	206/459 (45%)	204 (99%)	2 (1%)	0	100	100
24	v	341/396 (86%)	327 (96%)	14 (4%)	0	100	100
25	x	201/395 (51%)	200 (100%)	1 (0%)	0	100	100
26	a	73/139 (52%)	67 (92%)	6 (8%)	0	100	100
26	e	75/139 (54%)	73 (97%)	2 (3%)	0	100	100
27	b	81/106 (76%)	77 (95%)	4 (5%)	0	100	100
27	f	76/106 (72%)	73 (96%)	3 (4%)	0	100	100
28	g	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
29	h	91/129 (70%)	89 (98%)	2 (2%)	0	100	100
30	j	467/1008 (46%)	446 (96%)	19 (4%)	2 (0%)	34	71
31	k	430/531 (81%)	409 (95%)	20 (5%)	1 (0%)	47	79
All	All	9224/12743 (72%)	8982 (97%)	237 (3%)	5 (0%)	54	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	960	VAL
30	j	544	ASN
18	W	319	LYS
31	k	410	SER
30	j	866	GLY

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%)	1216 (100%)	3 (0%)	93	96
2	B	1018/1077 (94%)	1016 (100%)	2 (0%)	93	96
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	86
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	61/66 (92%)	61 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	38 (100%)	0	100	100
13	M	61/99 (62%)	60 (98%)	1 (2%)	62	79
17	V	90/92 (98%)	90 (100%)	0	100	100
18	W	480/796 (60%)	477 (99%)	3 (1%)	86	91
19	m	1087/1354 (80%)	1086 (100%)	1 (0%)	93	97
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	u	192/406 (47%)	191 (100%)	1 (0%)	88	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	v	325/369 (88%)	325 (100%)	0	100	100
25	x	190/354 (54%)	190 (100%)	0	100	100
26	a	63/112 (56%)	62 (98%)	1 (2%)	62	79
26	e	64/112 (57%)	64 (100%)	0	100	100
27	b	68/81 (84%)	68 (100%)	0	100	100
27	f	63/81 (78%)	63 (100%)	0	100	100
28	g	72/102 (71%)	71 (99%)	1 (1%)	67	81
29	h	79/107 (74%)	79 (100%)	0	100	100
30	j	412/910 (45%)	408 (99%)	4 (1%)	76	86
31	k	396/474 (84%)	393 (99%)	3 (1%)	81	89
All	All	8300/11238 (74%)	8278 (100%)	22 (0%)	92	95

All (22) 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
18	W	318	VAL
18	W	319	LYS
18	W	459	ILE
19	m	514	LYS
23	u	124	ARG
26	a	63	ARG
28	g	75	LYS
30	j	740	MET
30	j	865	PHE
30	j	867	LEU
30	j	888	THR
31	k	236	ARG
31	k	388	LYS
31	k	413	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	737	ASN
8	H	44	ASN
9	I	11	ASN
18	W	644	ASN
19	m	955	ASN
20	n	232	GLN
21	q	147	ASN
25	x	296	ASN
27	b	25	ASN
30	j	916	ASN
31	k	127	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	19/19 (100%)	10 (52%)	1 (5%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	-6	G
15	P	-5	U
15	P	-4	A
15	P	-3	A
15	P	-2	U
15	P	0	C
15	P	1	C
15	P	8	G
15	P	9	G
15	P	11	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	-7	U

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

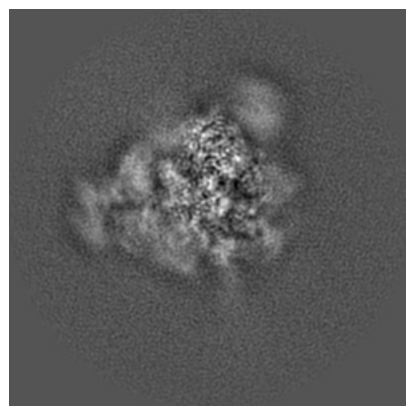
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33450. These allow visual inspection of the internal detail of the map and identification of artifacts.

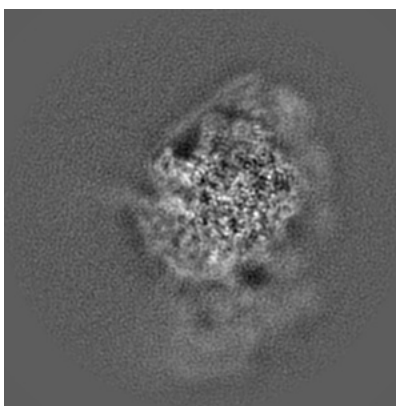
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

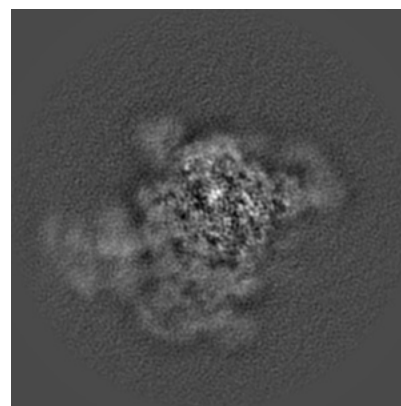
6.1.1 Primary map



X

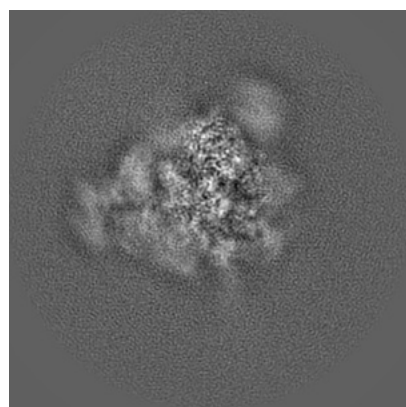


Y

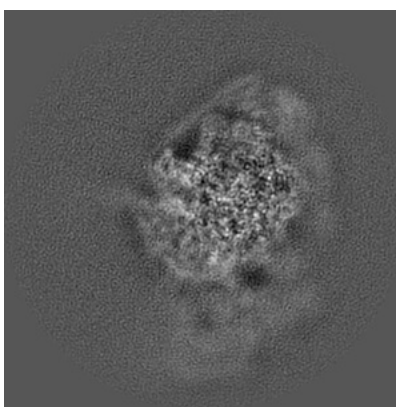


Z

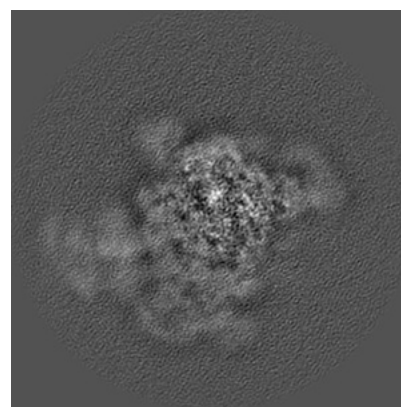
6.1.2 Raw map



X



Y

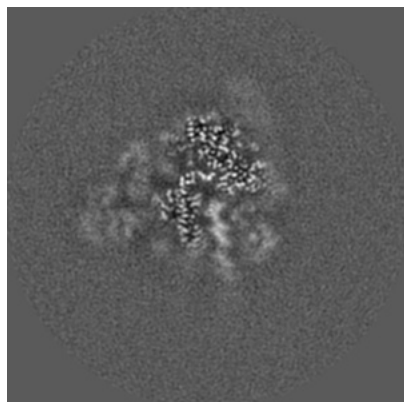


Z

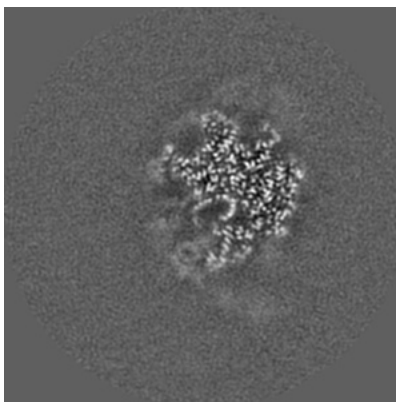
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

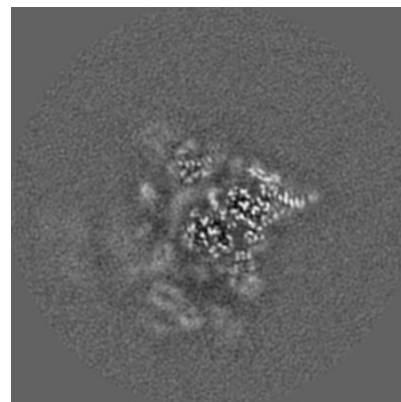
6.2.1 Primary map



X Index: 120

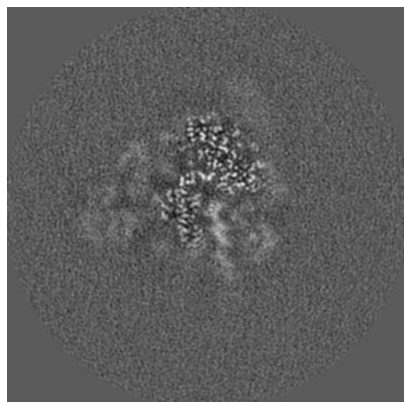


Y Index: 120

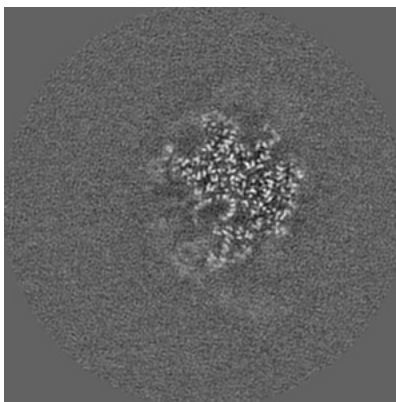


Z Index: 120

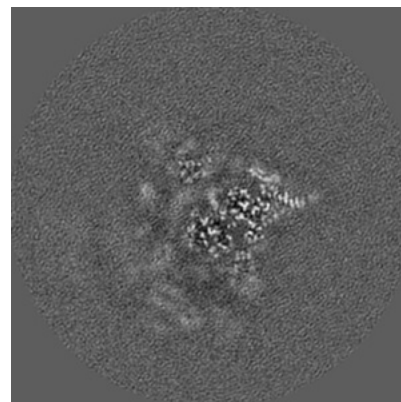
6.2.2 Raw map



X Index: 120



Y Index: 120

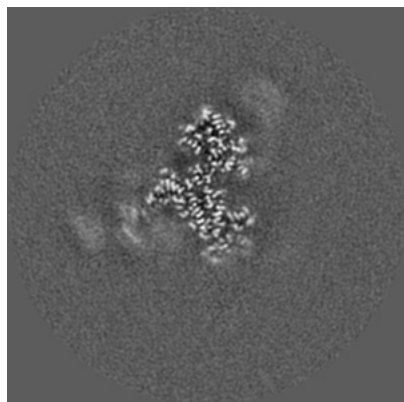


Z Index: 120

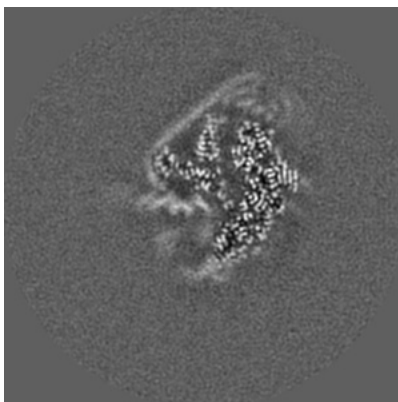
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

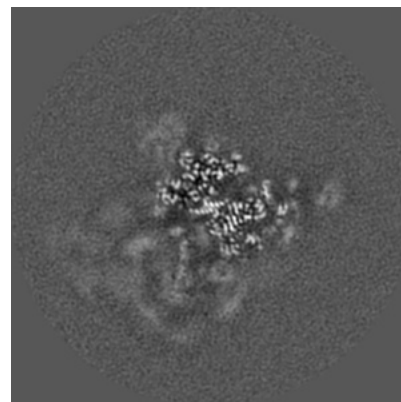
6.3.1 Primary map



X Index: 141

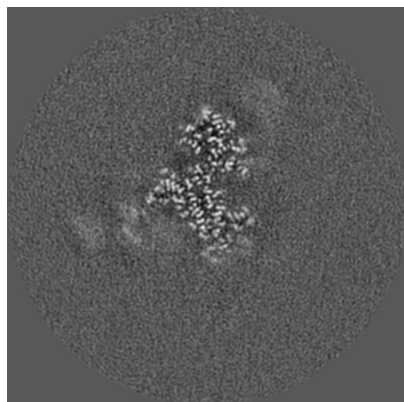


Y Index: 127

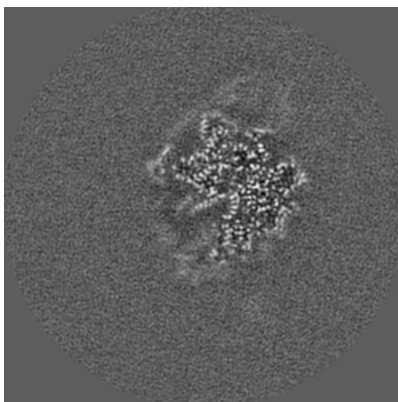


Z Index: 137

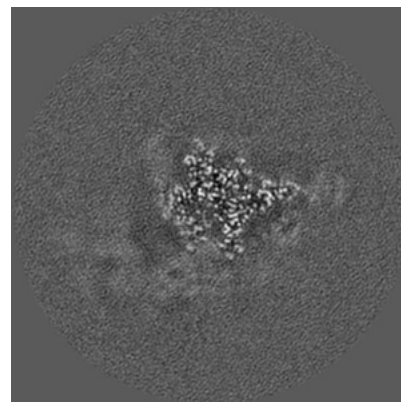
6.3.2 Raw map



X Index: 141



Y Index: 122

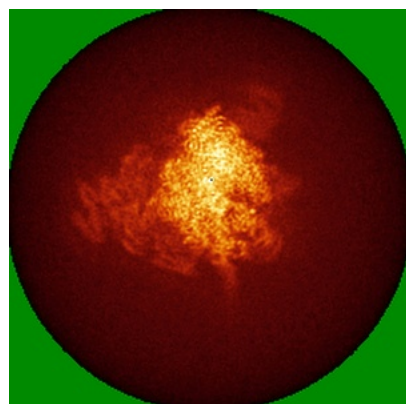


Z Index: 144

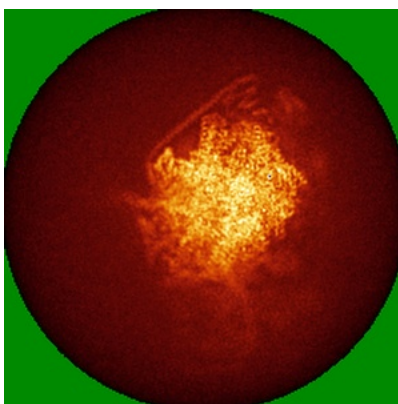
The images above show the largest variance slices of the map in three orthogonal directions.

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

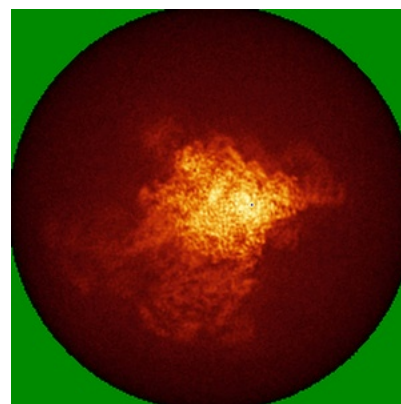
6.4.1 Primary map



X

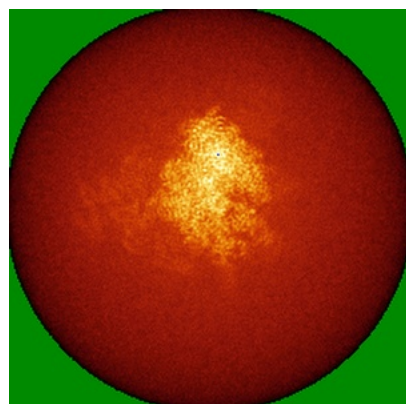


Y

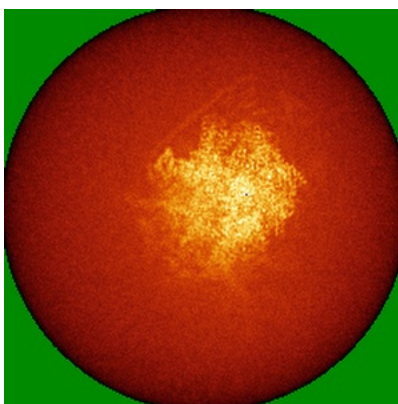


Z

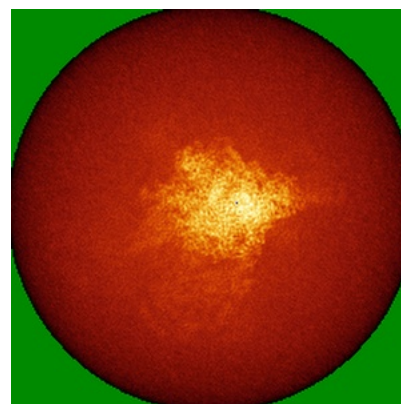
6.4.2 Raw map



X



Y

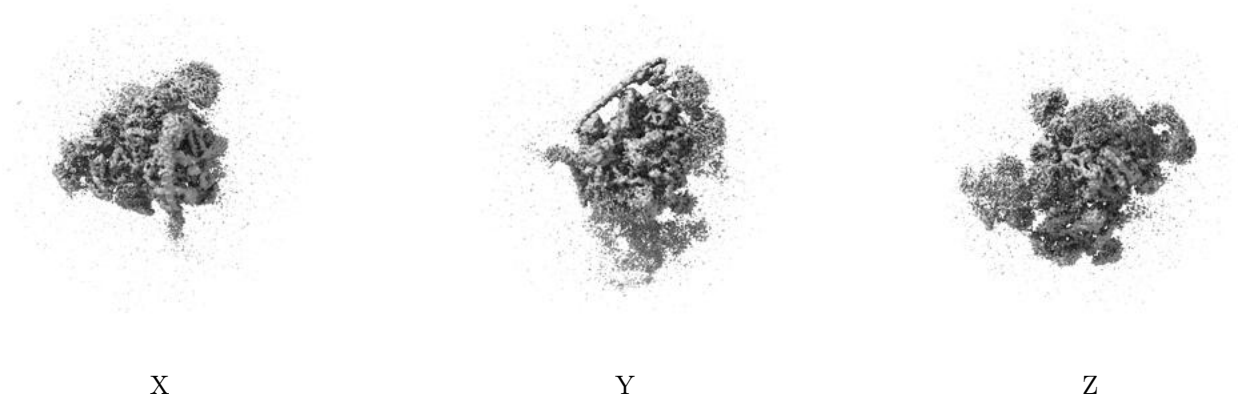


Z

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

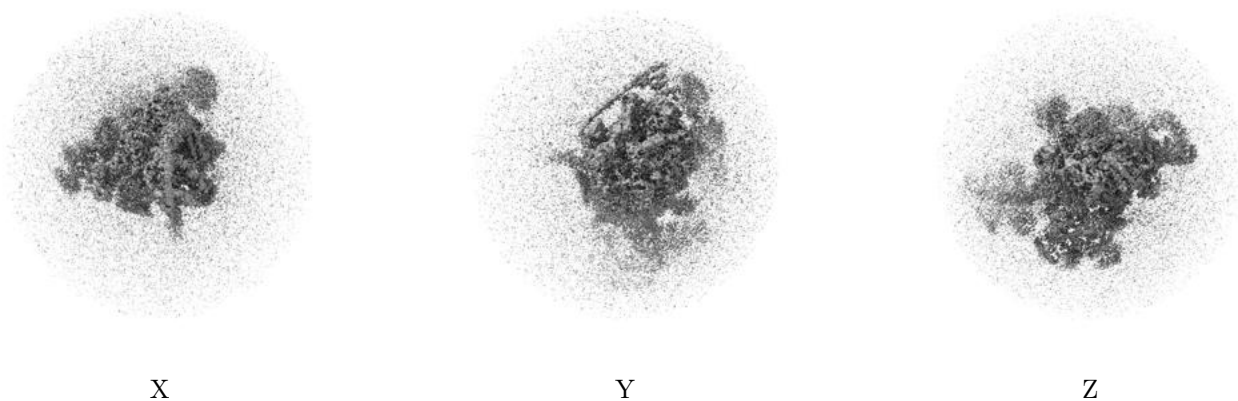
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

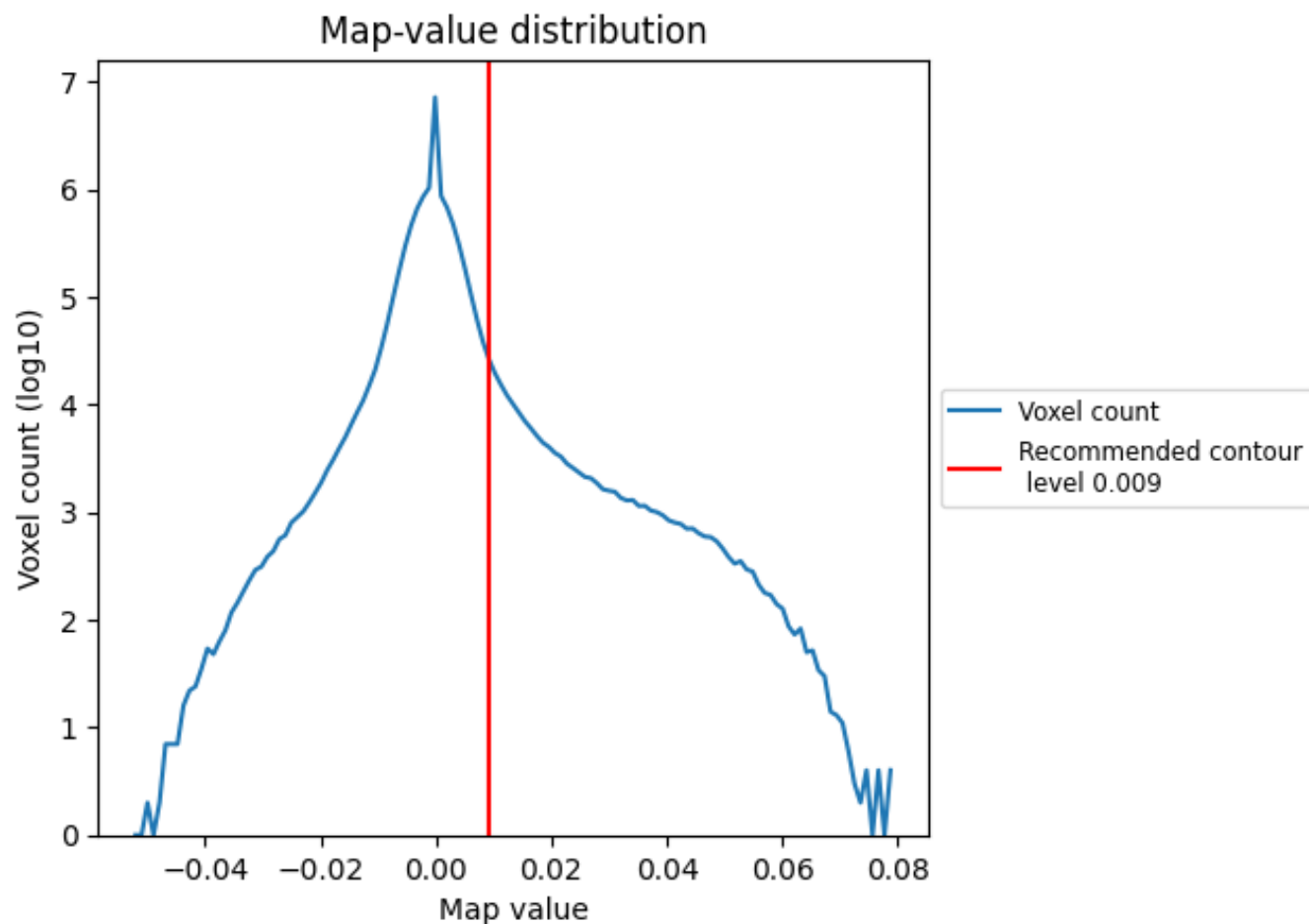
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

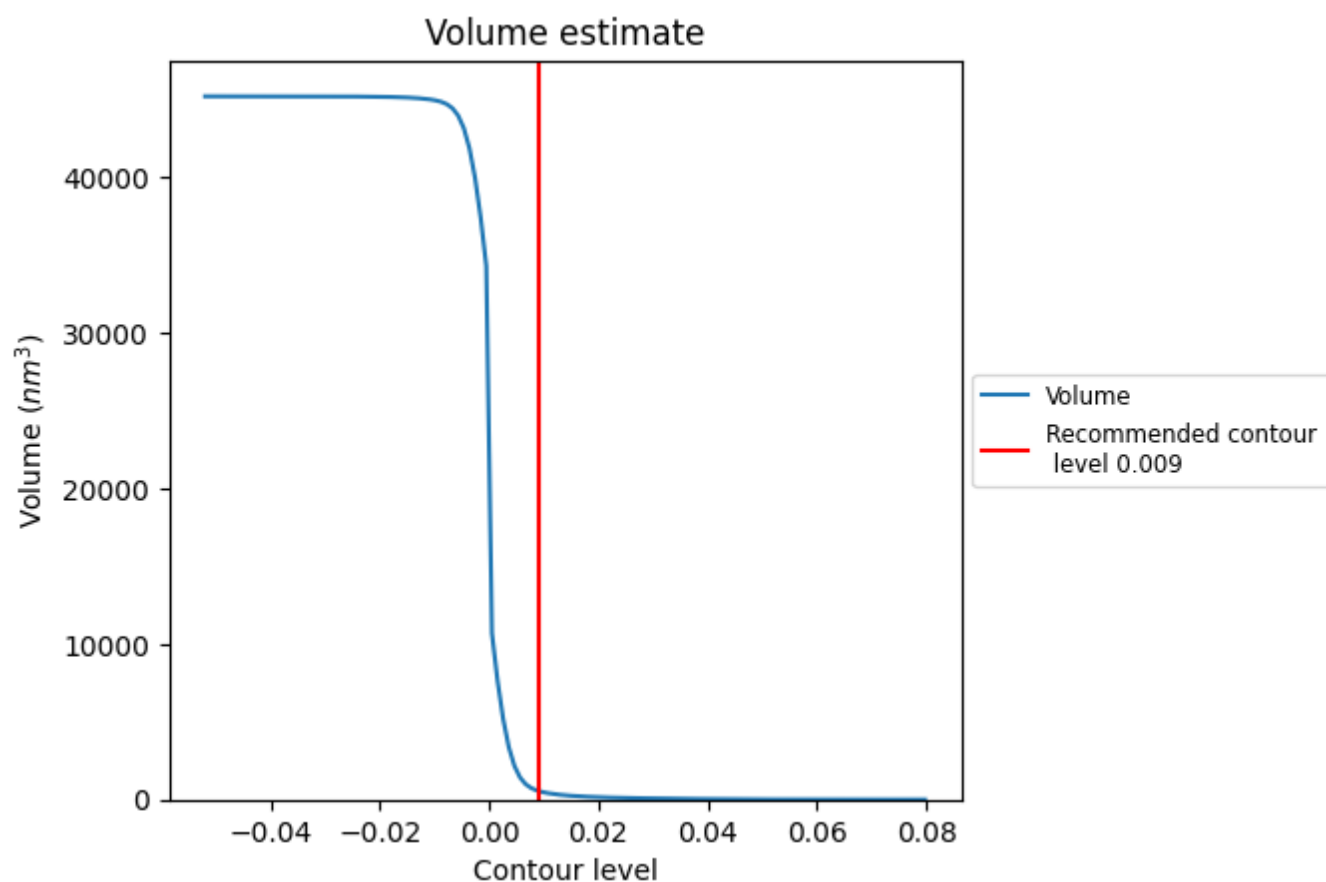
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

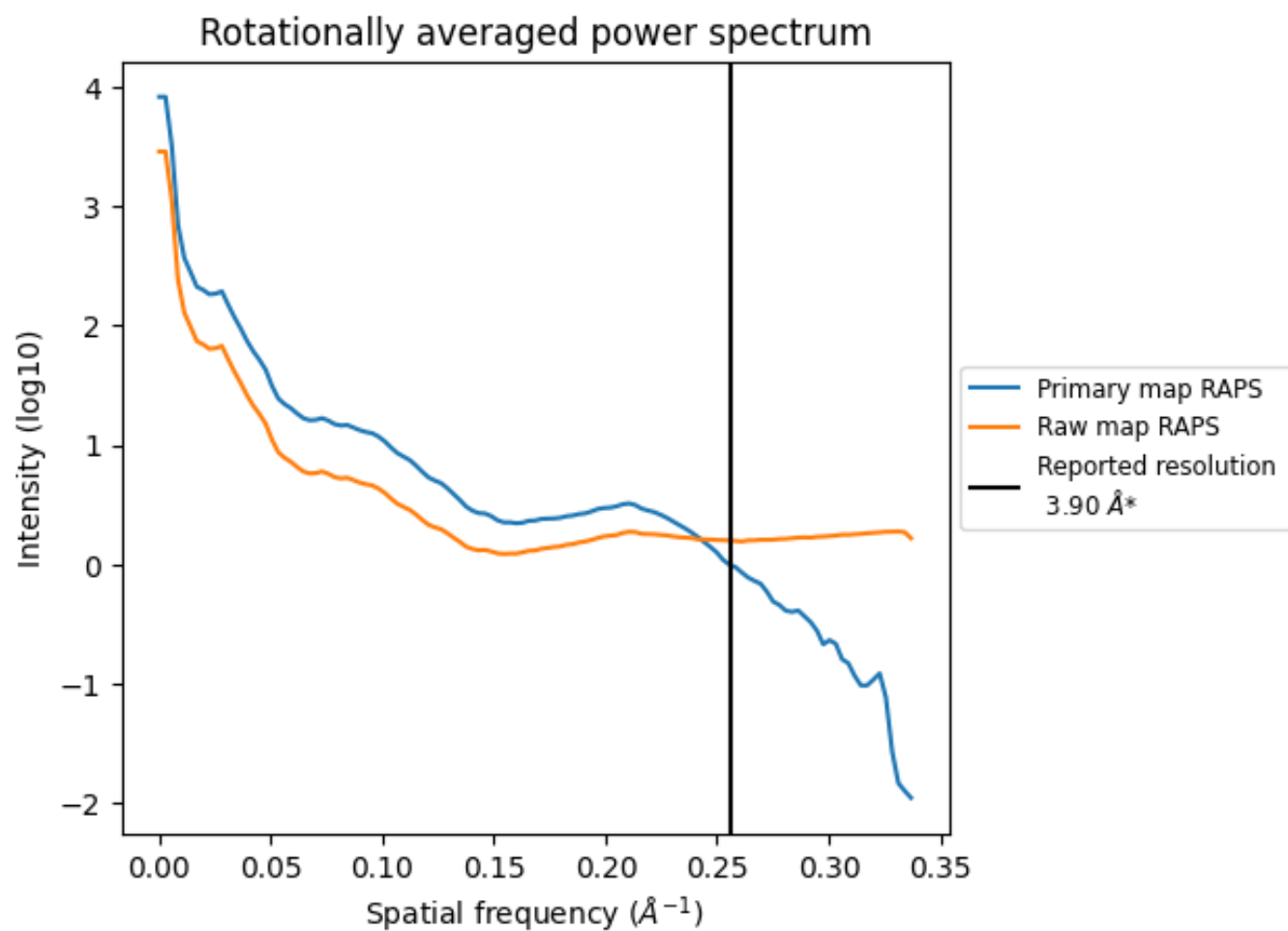
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 557 nm³; this corresponds to an approximate mass of 503 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 ⓘ

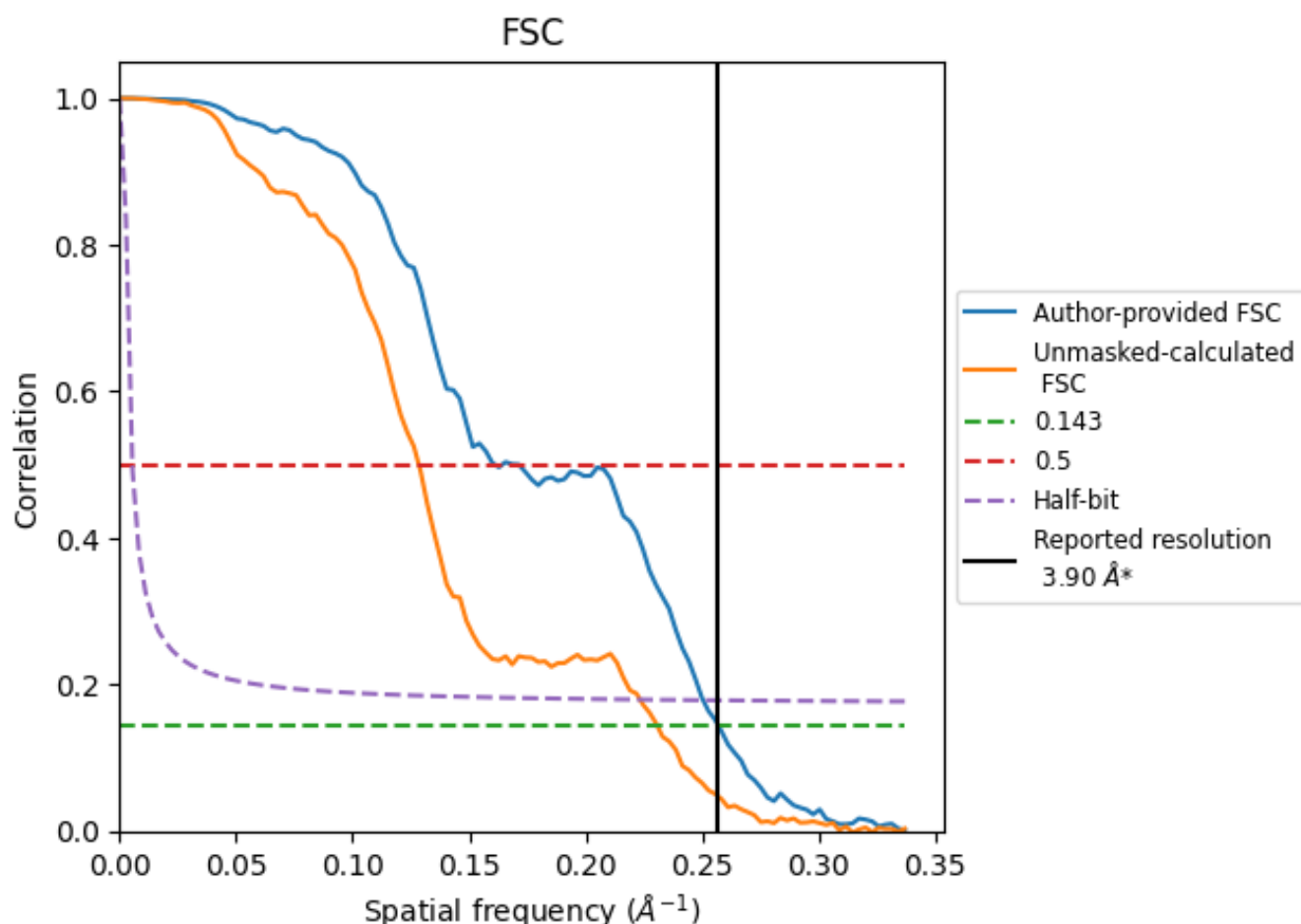


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.89	6.21	3.99
Unmasked-calculated*	4.33	7.79	4.48

*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 4.33 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

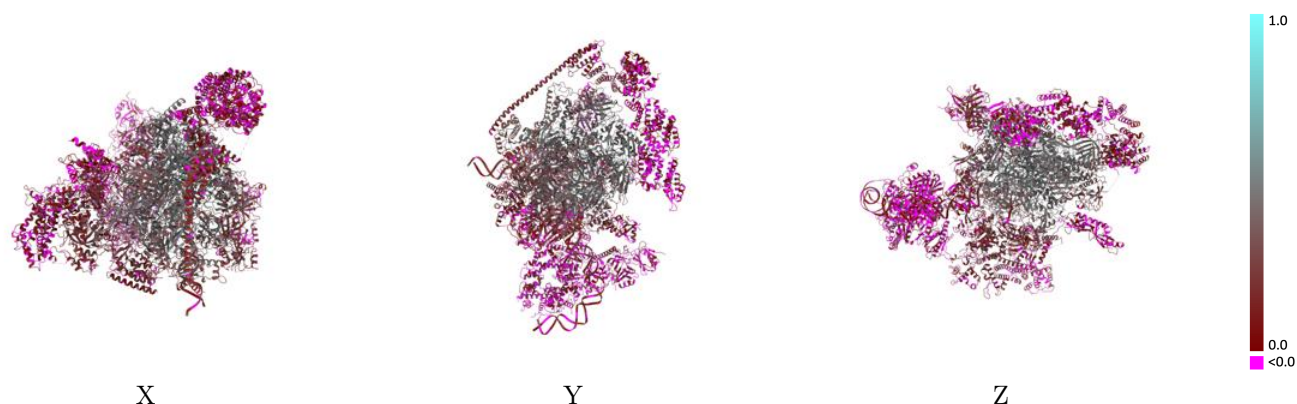
This section contains information regarding the fit between EMDB map EMD-33450 and PDB model 7XTI. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



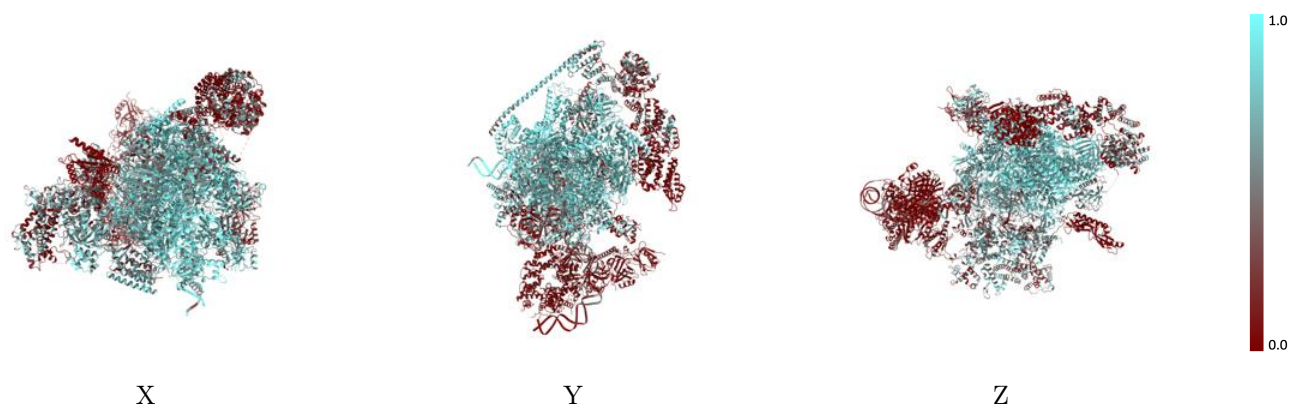
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



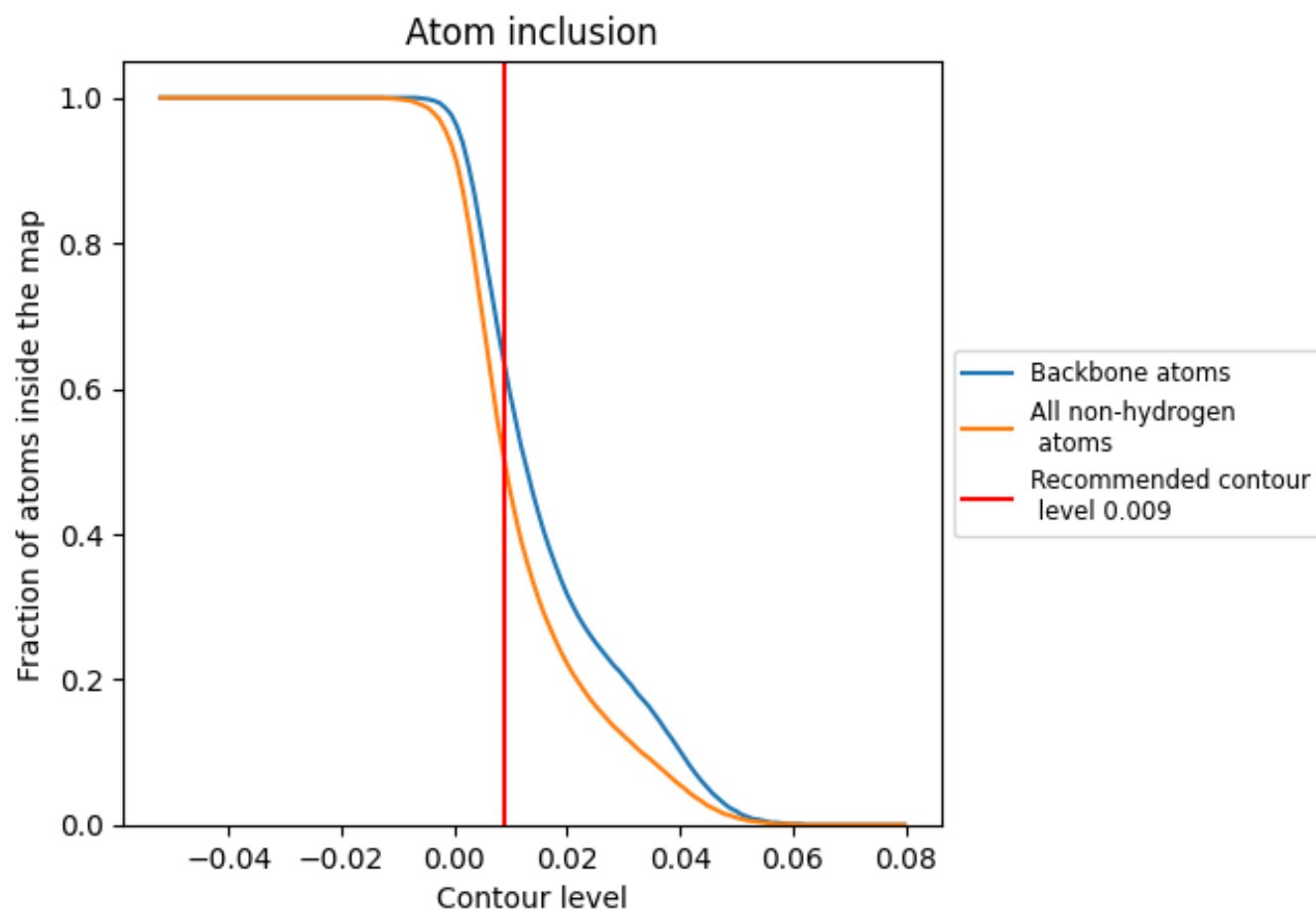
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 50% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4970	0.2230
A	0.8010	0.4150
B	0.7730	0.4240
C	0.8280	0.4490
D	0.5760	0.2200
E	0.8190	0.3930
F	0.8340	0.4540
G	0.6500	0.3110
H	0.8320	0.4370
I	0.5660	0.2580
J	0.8030	0.4390
K	0.8600	0.4490
L	0.7760	0.3940
M	0.4840	0.1560
N	0.5170	0.1350
P	0.7170	0.3150
T	0.5760	0.1810
V	0.5270	0.1470
W	0.4440	0.2020
a	0.0510	0.0260
b	0.0130	-0.0180
e	0.0620	0.0120
f	0.0540	0.0290
g	0.0200	-0.0390
h	0.0110	0.0110
j	0.0970	0.0240
k	0.0470	0.0070
m	0.3840	0.1050
n	0.5920	0.1790
q	0.3060	0.0760
r	0.3890	0.1540
u	0.3300	0.1560
v	0.2050	0.0880
x	0.4290	0.2490

