Full wwPDB EM Validation Report ⓘ

Jun 26, 2024 – 02:41 PM JST

PDB ID	:	7XT7
EMDB ID	:	EMD-33441
Title	:	RNA polymerase II elongation complex transcribing a nucleosome (EC49B)
Authors	:	Ehara, H.; Kujirai, T.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on	:	2022-05-16
Resolution	:	4.20 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:

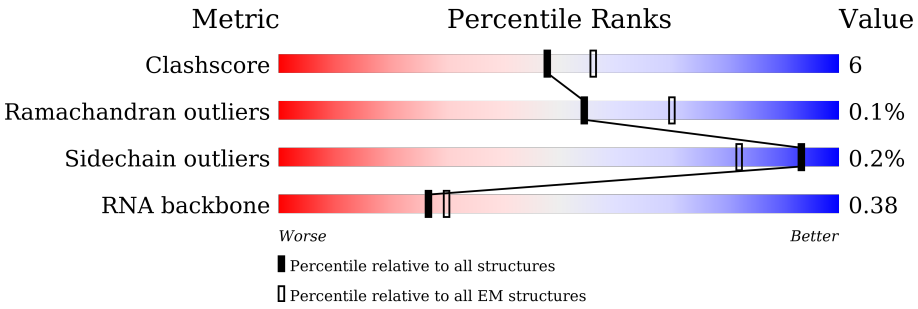
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 4.20 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)
Clashscore	158937	4297
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	71% 10% 19%
2	B	1227	80% 15% 5%
3	C	304	77% 9% 13%
4	D	186	10% 85% 8% 6%
5	E	214	84% 15%
6	F	155	49% 5% 46%
7	G	171	8% 84% 16%

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Mol	Chain	Length	Quality of chain
8	H	145	79% 12% 8%
9	I	115	81% 16%
10	J	72	82% 11% 7%
11	K	118	78% 18%
12	L	72	56% 7% 38%
13	M	113	6% 47% 10% 43%
14	N	198	30% 20% 30% 8% 42%
15	P	19	5% 21% 58% 21%
16	T	198	34% 20% 36% 8% 36%
17	V	108	6% 73% 25%
18	W	911	15% 49% 10% 41%
19	m	1503	45% 79% 21%
20	n	417	33% 67%
21	q	1084	30% 86% 14%
22	r	544	25% 49% 51%
23	u	459	18% 45% 55%
24	v	396	47% 88% 12%
25	x	395	8% 52% 48%
26	a	139	41% 66% 34%
26	e	139	42% 69% 30%
27	b	106	32% 76% 24%
27	f	106	31% 73% 26%
28	c	133	29% 72% 28%
28	g	133	46% 74% 26%
29	d	129	32% 71% 29%

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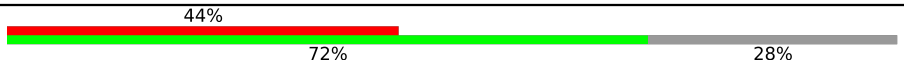
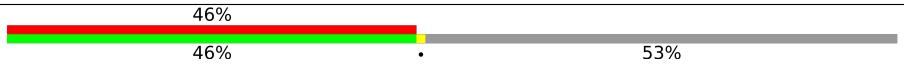
Mol	Chain	Length	Quality of chain
29	h	129	
30	j	1008	
31	k	531	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 82079 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	115	Total	C	N	O	P	0	0
			2377	1124	445	693	115		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	19	Total	C	N	O	P	0	0
			399	178	66	136	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	126	Total	C	N	O	P	0	0
			2570	1219	476	749	126		

- 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

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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

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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	92	Total	C	N	O	S	0	0
			746	471	142	131	2		
26	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 27 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	81	Total	C	N	O	S	0	0
			646	407	126	112	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	c	96	Total 743	C 466	N 146	O 131	0	0
28	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 29 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	92	Total 718	C 453	N 127	O 136	S 2	0	0
29	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 30 is a protein called FACT complex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	472	Total 3754	C 2382	N 658	O 701	S 13	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	-2	GLY	-	expression tag	UNP F2QPX0
j	-1	PRO	-	expression tag	UNP F2QPX0
j	0	GLY	-	expression tag	UNP F2QPX0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	k	429	Total	C	N	O	S	0	0
			3502	2215	613	664	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	Zn	0
			2	2	
32	B	1	Total	Zn	0
			1	1	
32	C	1	Total	Zn	0
			1	1	
32	I	2	Total	Zn	0
			2	2	
32	J	1	Total	Zn	0
			1	1	
32	L	1	Total	Zn	0
			1	1	
32	M	1	Total	Zn	0
			1	1	
32	V	1	Total	Zn	0
			1	1	

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

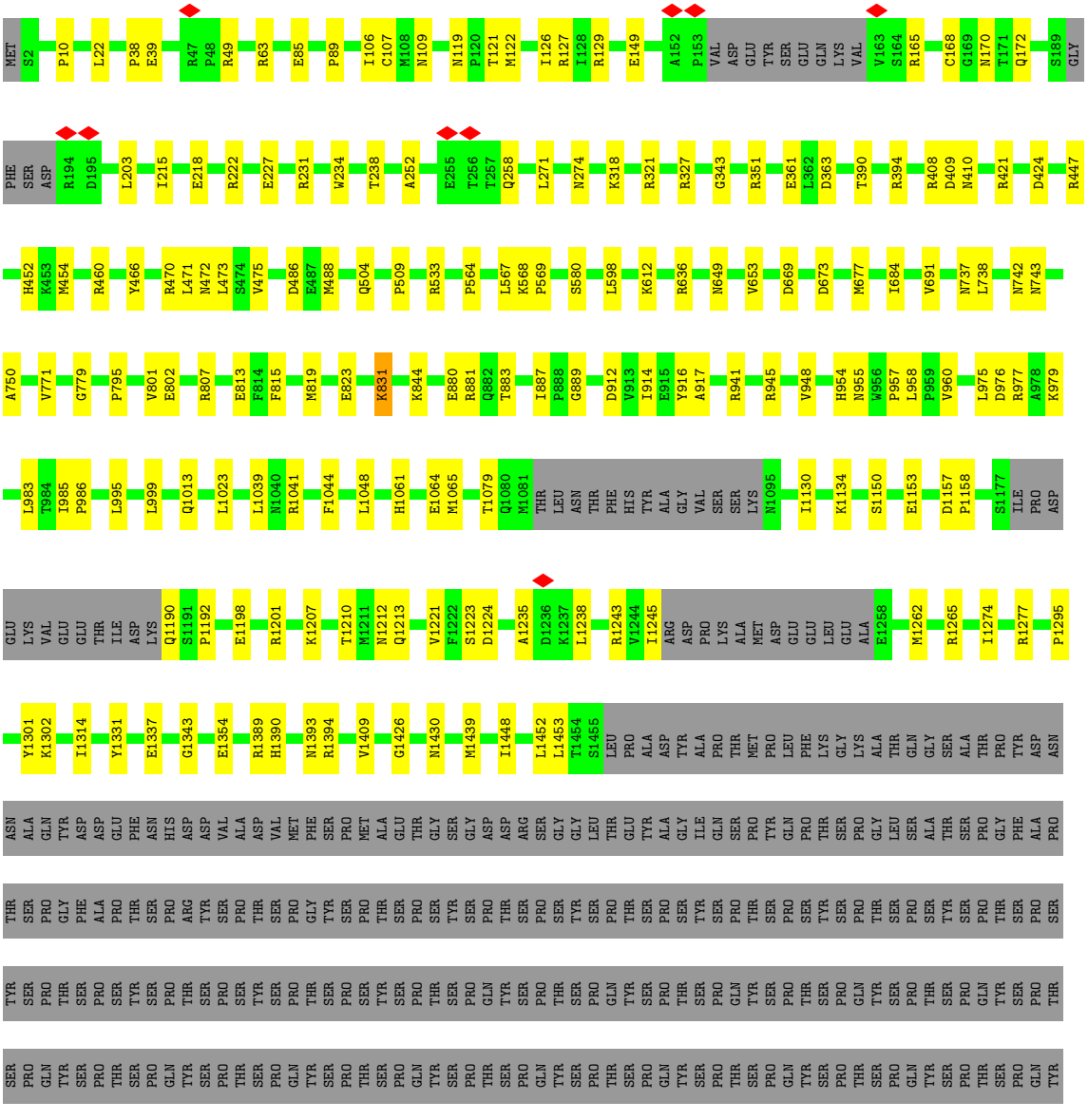
Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	Mg	0
			1	1	

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.

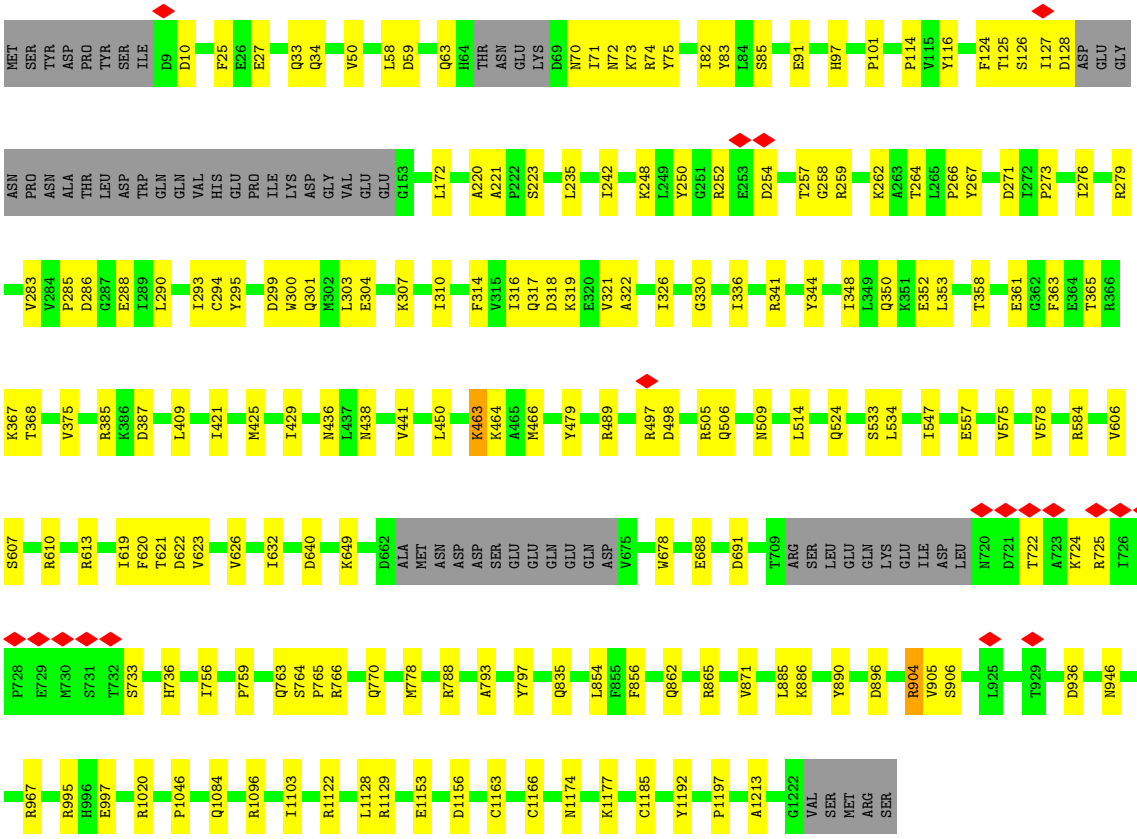
- Molecule 1: DNA-directed RNA polymerase subunit

Chain A:



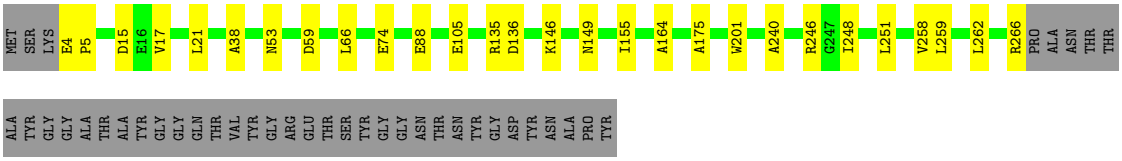
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



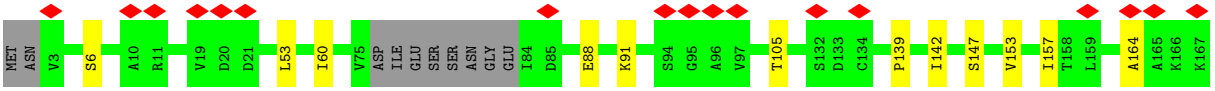
• Molecule 3: RNA polymerase II third largest subunit B44, part of central core

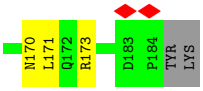
Chain C:



• Molecule 4: RNA polymerase II subunit B32

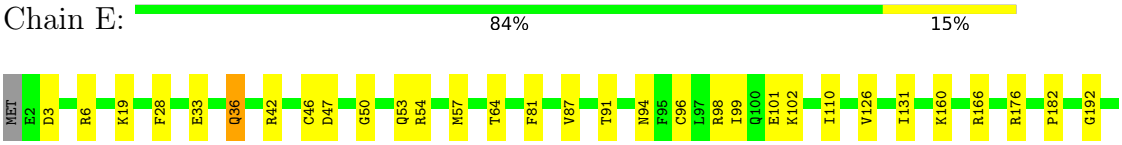
Chain D:





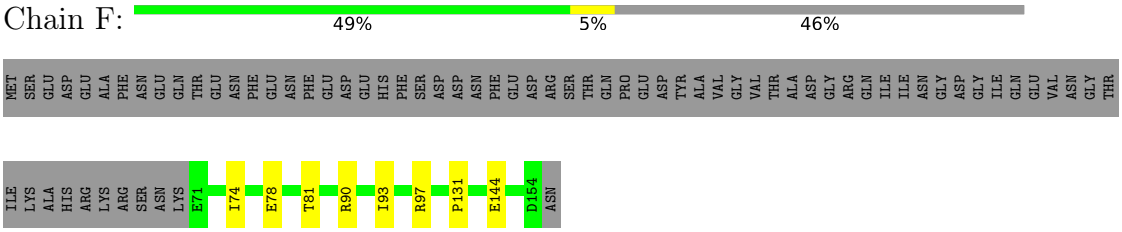
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



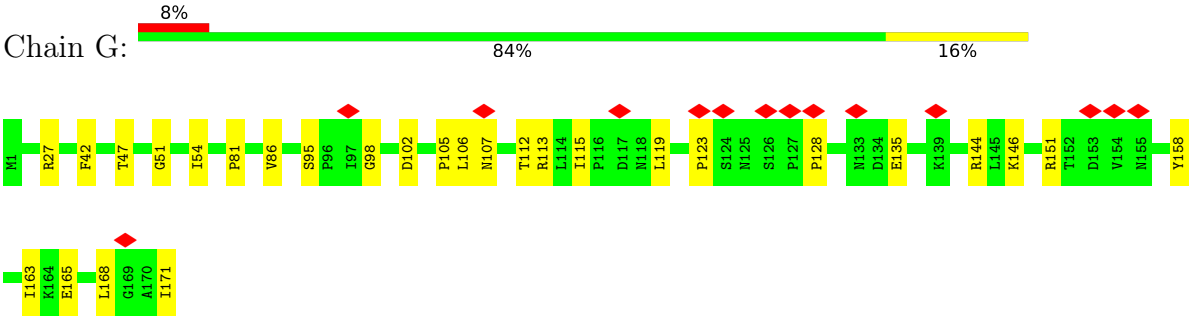
• Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

Chain F:



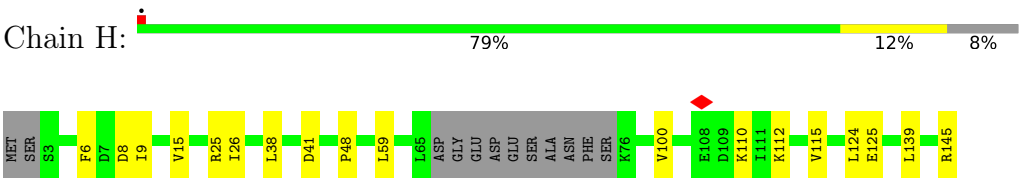
• Molecule 7: RNA polymerase II subunit

Chain G:



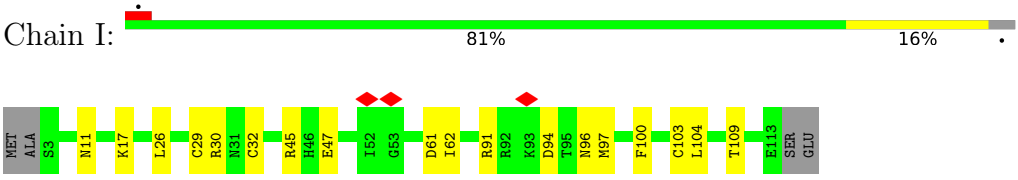
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



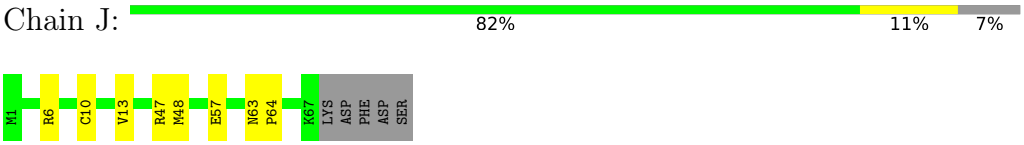
• Molecule 9: DNA-directed RNA polymerase subunit

Chain I:



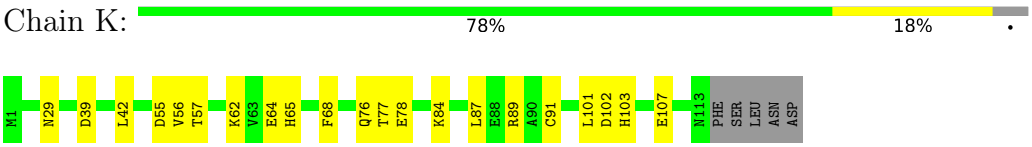
• Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J:



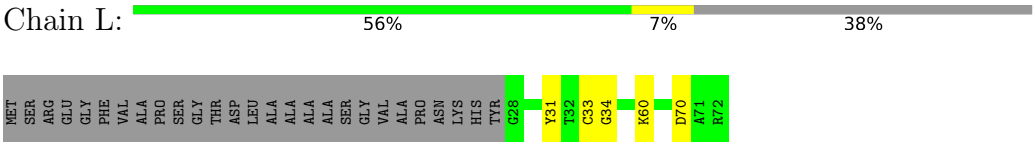
• Molecule 11: RNA polymerase II subunit B12.5

Chain K:



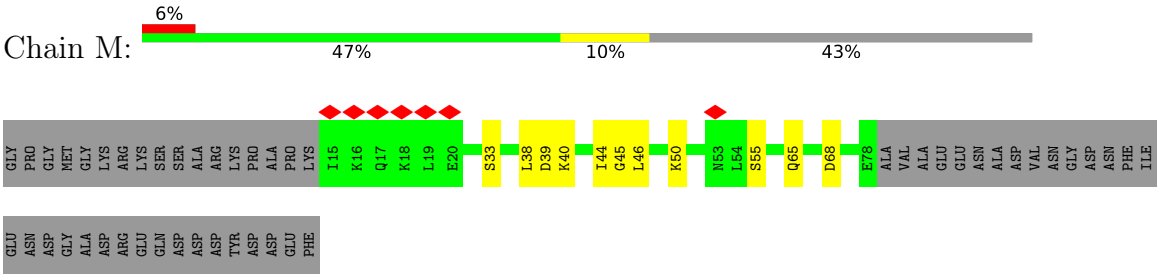
• Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L:



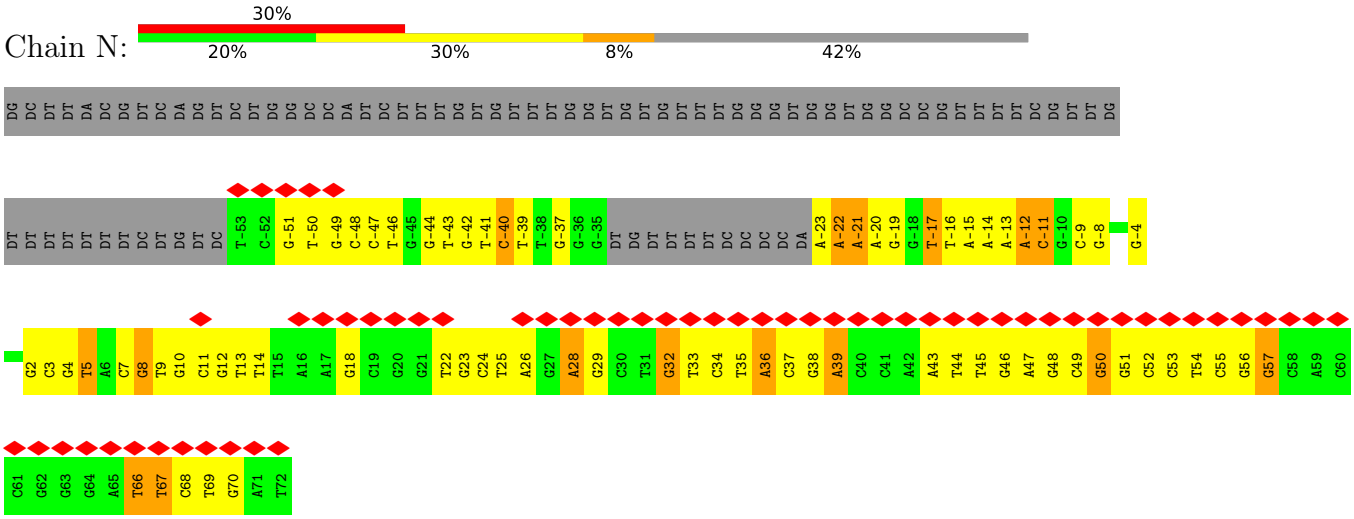
• Molecule 13: Transcription elongation factor 1 homolog

Chain M:



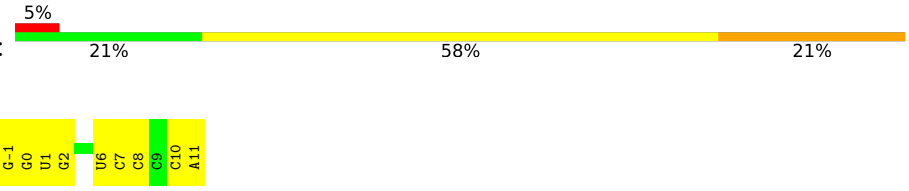
• Molecule 14: DNA (198-MER)

Chain N:



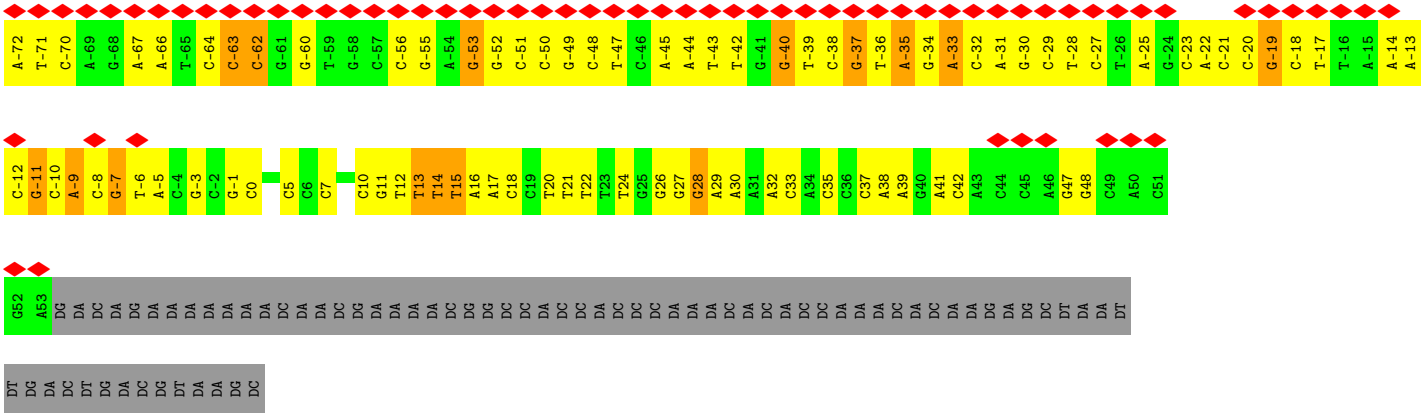
• Molecule 15: RNA (5'-R(P*GP*AP*CP*CP*CP*GP*GP*GP*UP*GP*UP*CP*UP*UP*CP*CP*CP*CP*A)-3')

Chain P:



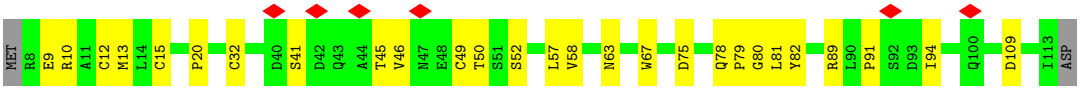
• Molecule 16: DNA (198-MER)

Chain T:



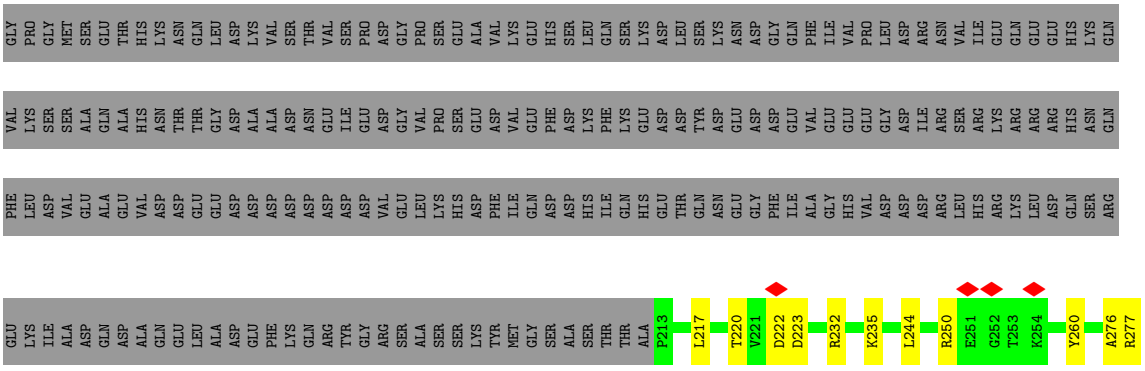
• Molecule 17: Transcription elongation factor SPT4

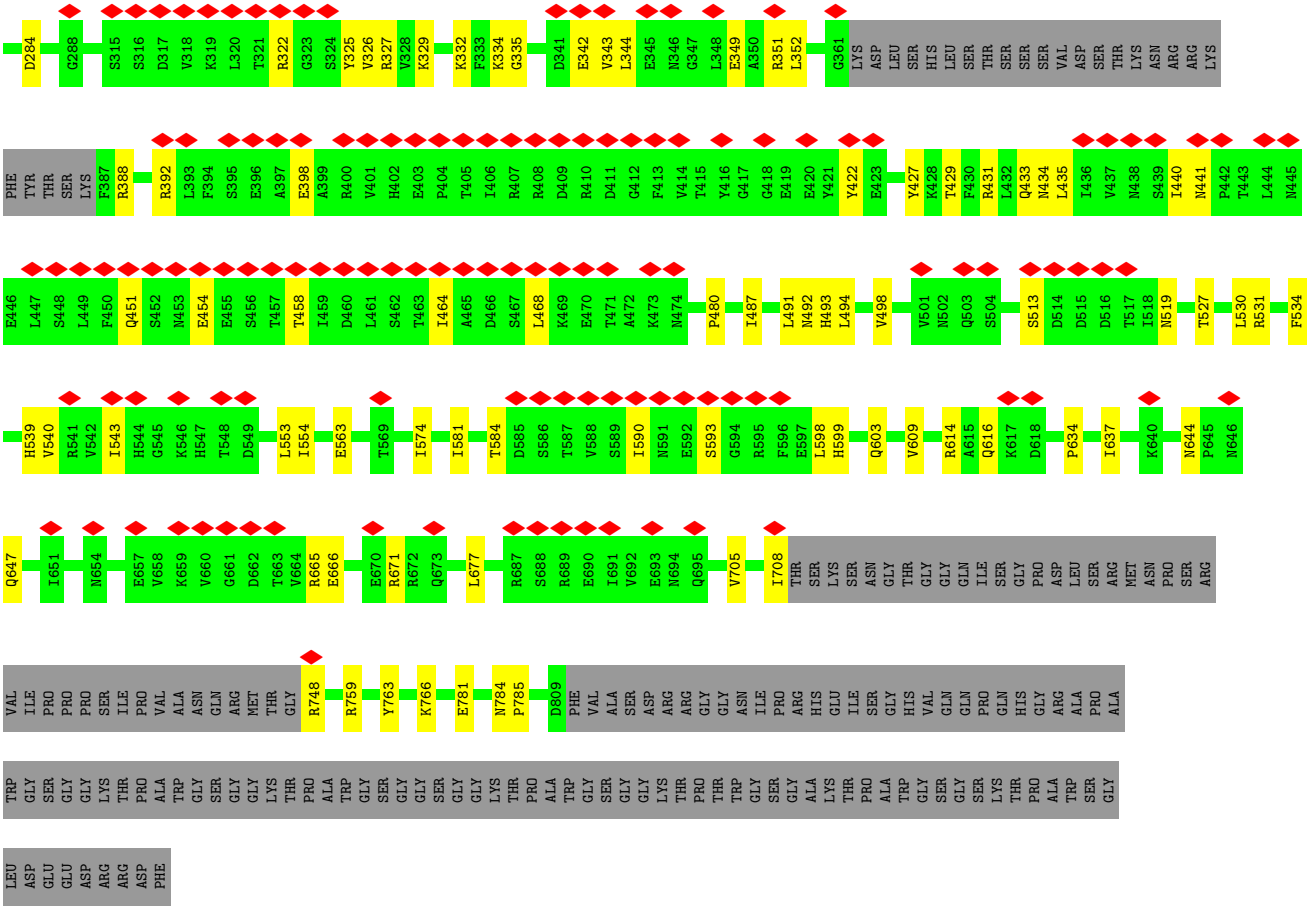
Chain V:



• Molecule 18: Transcription elongation factor SPT5

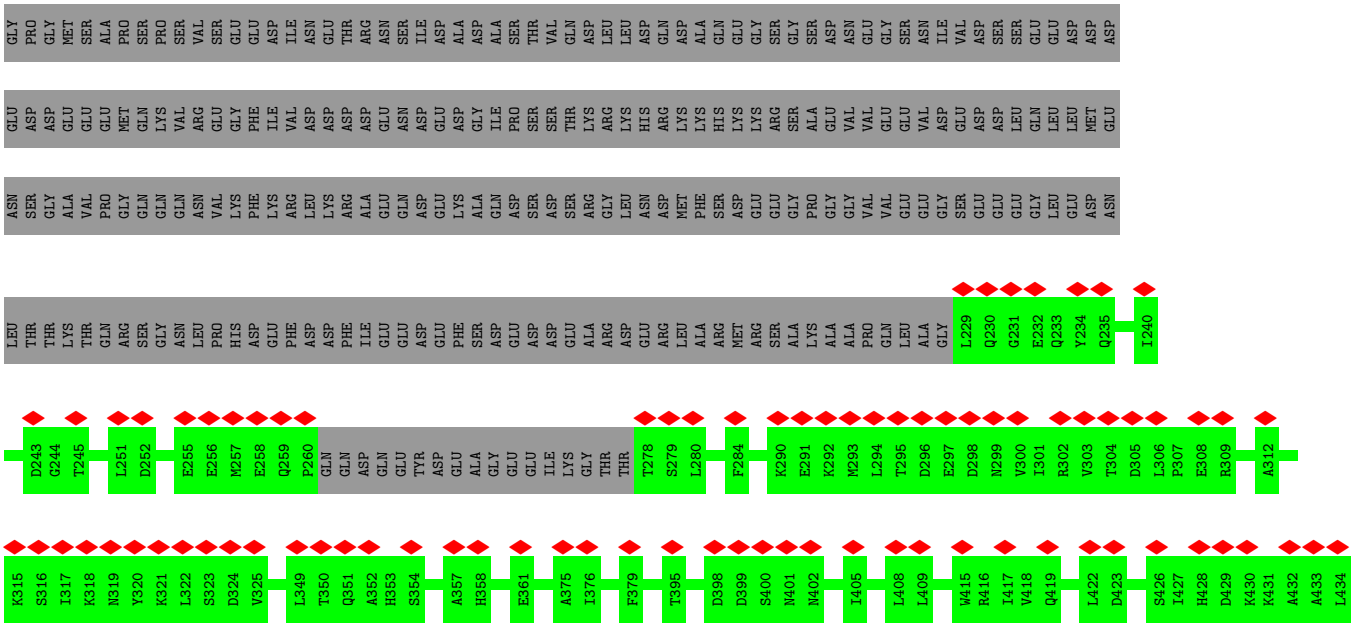
Chain W:

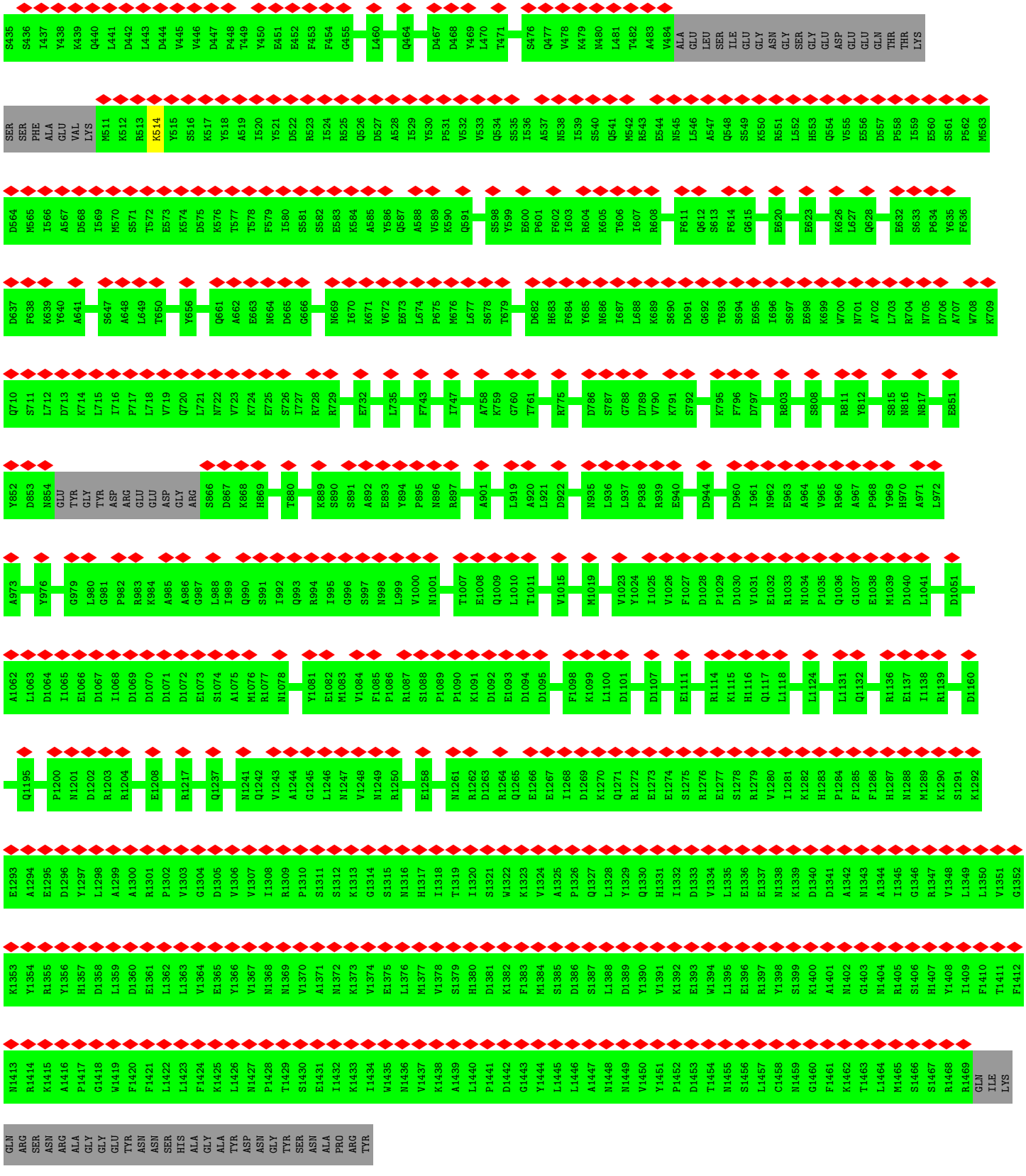




• Molecule 19: Transcription elongation factor Spt6

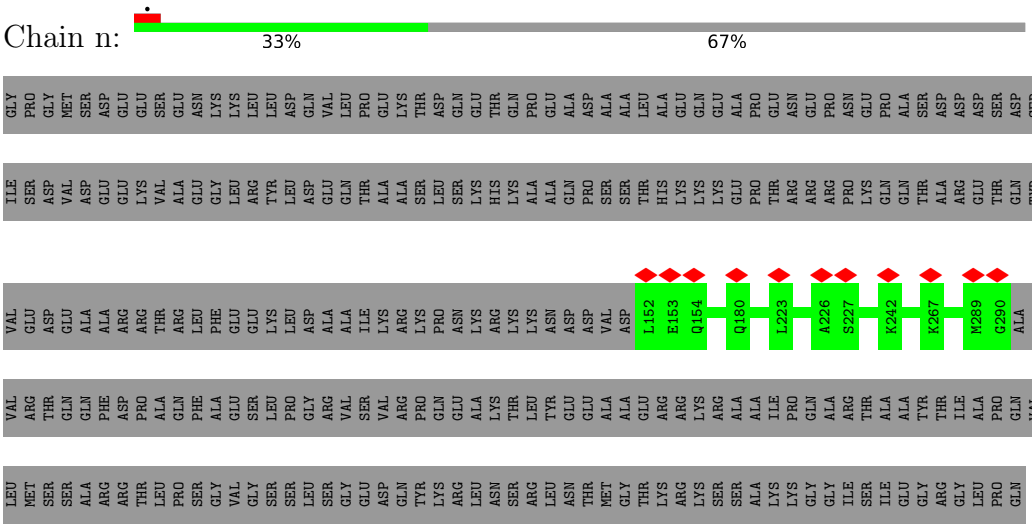
Chain m:





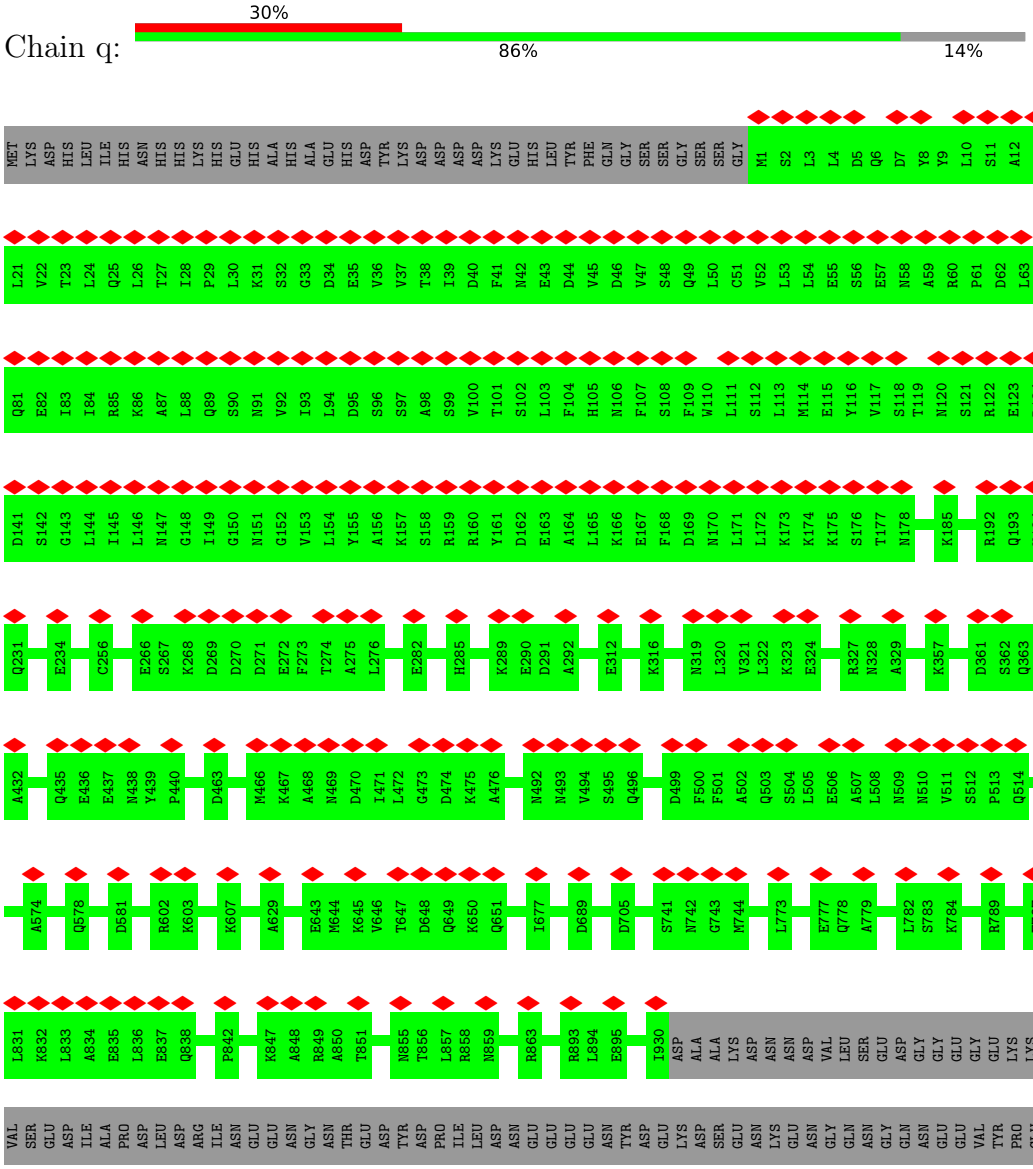
• Molecule 20: Protein that interacts with Spt6p and copurifies with Spt5p and RNA polymerase II

Chain n:

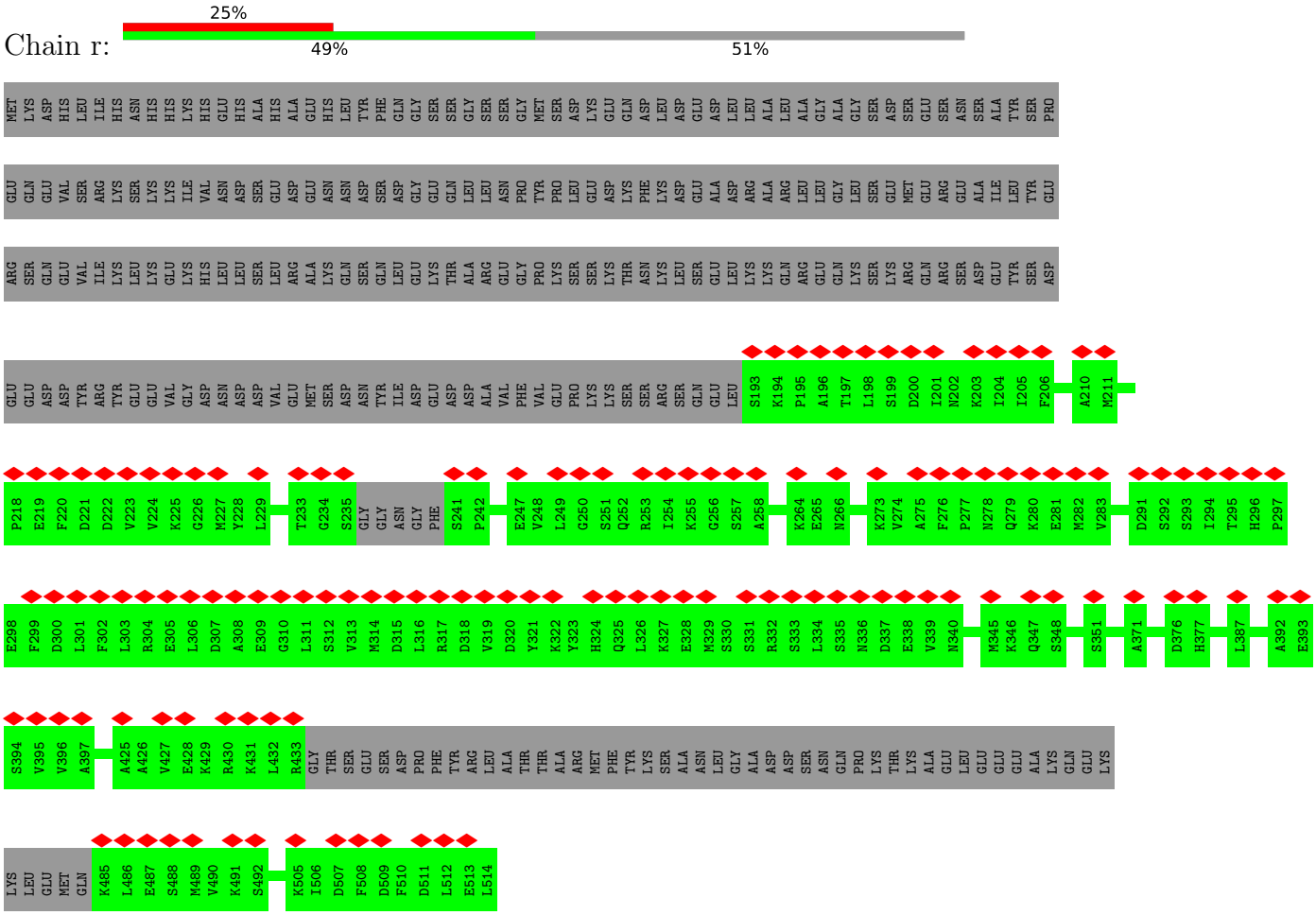


• Molecule 21: Component of the Paf1p complex

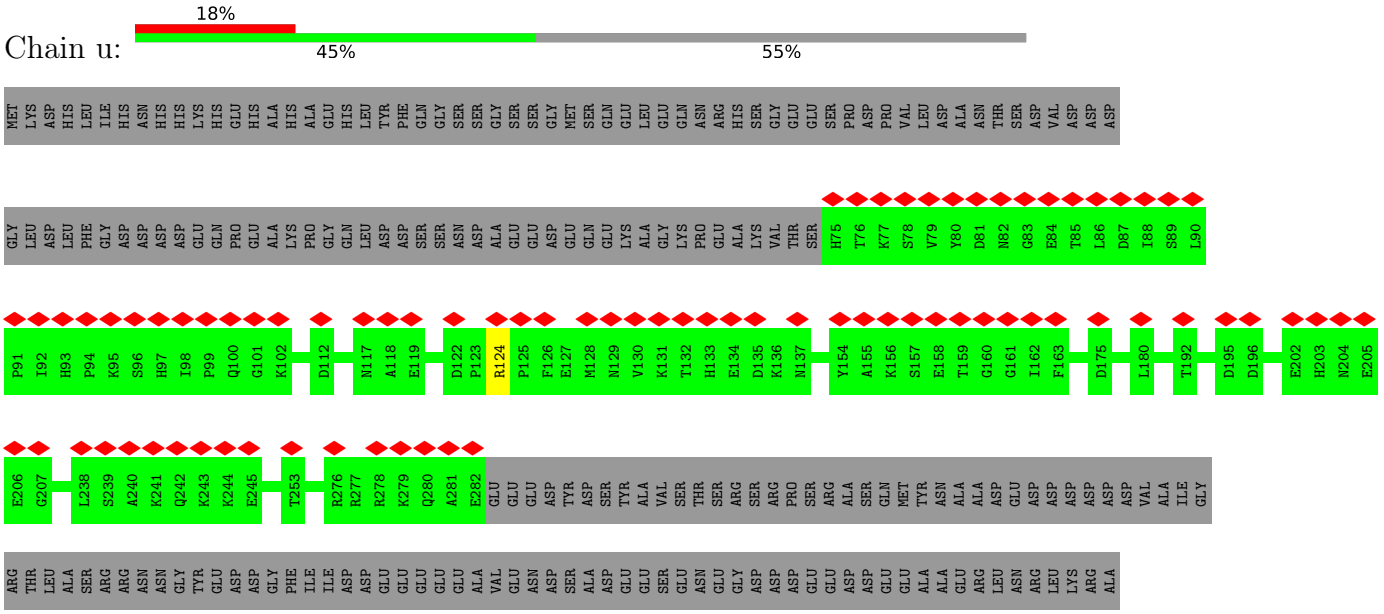
Chain q:



• Molecule 22: RNAPII-associated chromatin remodeling Paf1 complex subunit

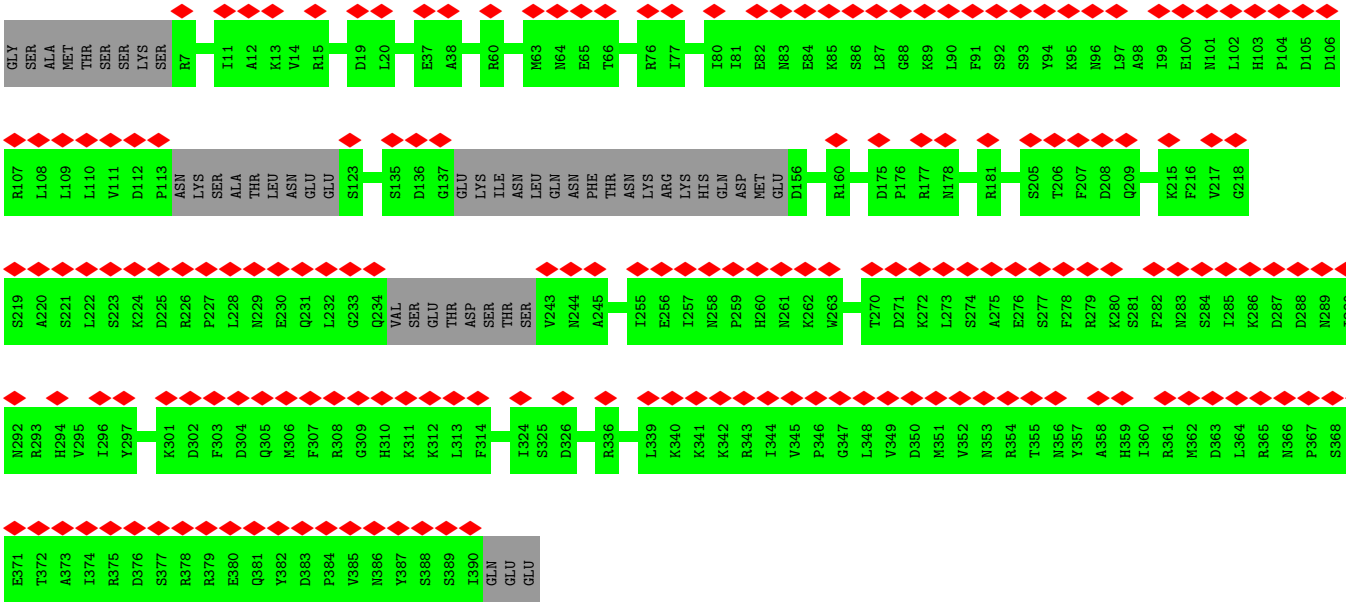


• Molecule 23: Leo1



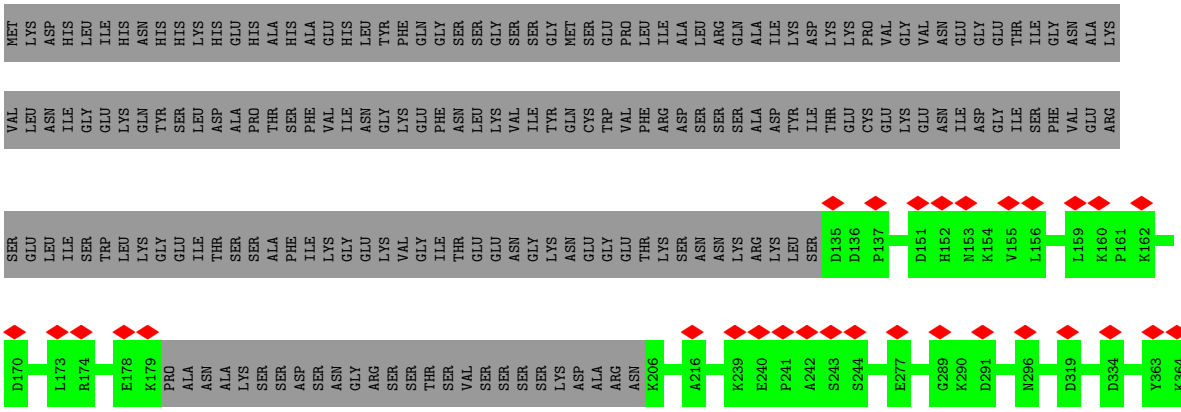
• Molecule 24: RNAP II-associated protein

Chain v:



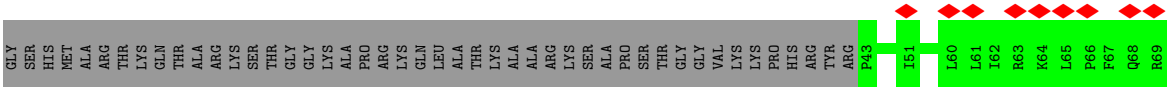
• Molecule 25: Constituent of Paf1 complex with RNA polymerase II, Paf1p, Hpr1p, Ctr9, Leo1, Rtf1 and Ccr4p

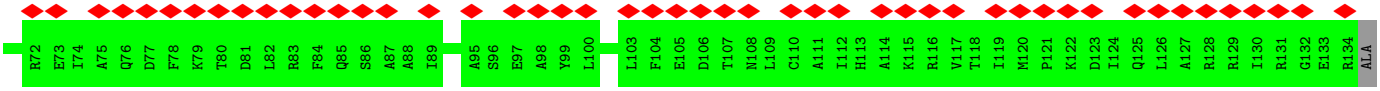
Chain x:



• Molecule 26: Histone H3.3

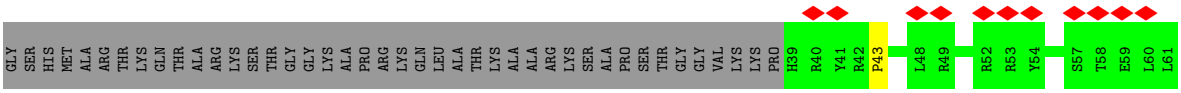
Chain a:

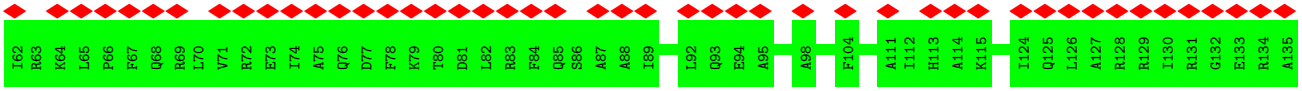




• Molecule 26: Histone H3.3

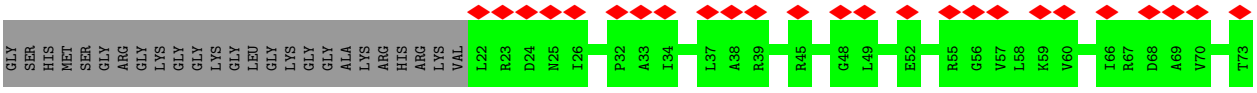
Chain e:

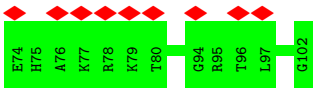




• Molecule 27: Histone H4

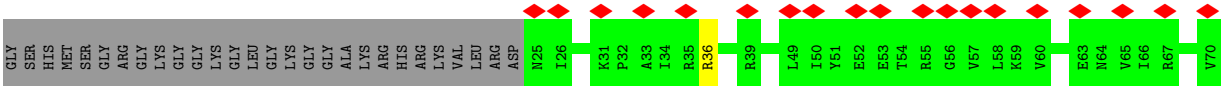
Chain b:

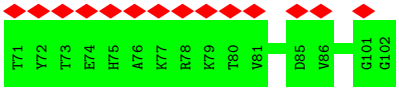




• Molecule 27: Histone H4

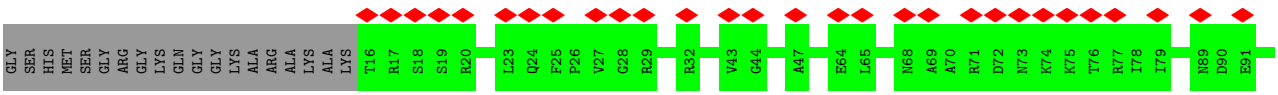
Chain f:

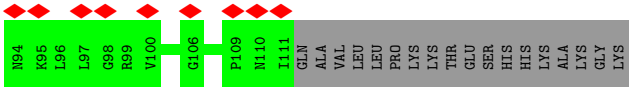




• Molecule 28: Histone H2A type 1-B/E

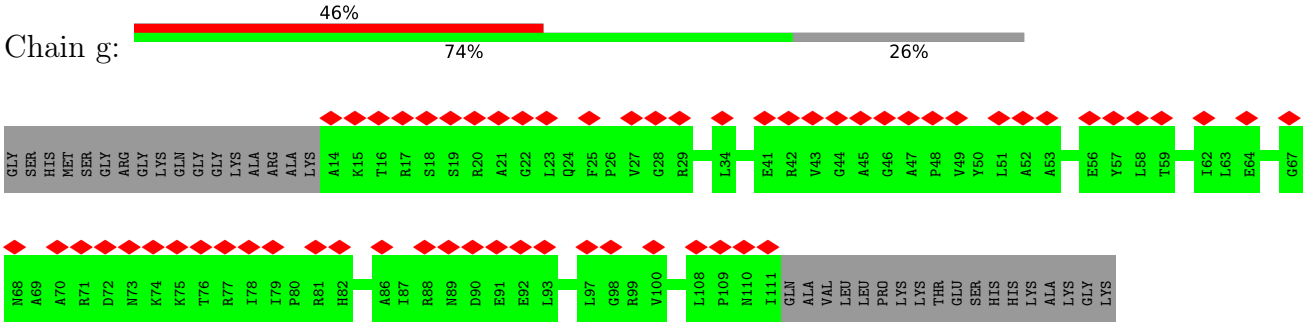
Chain c:





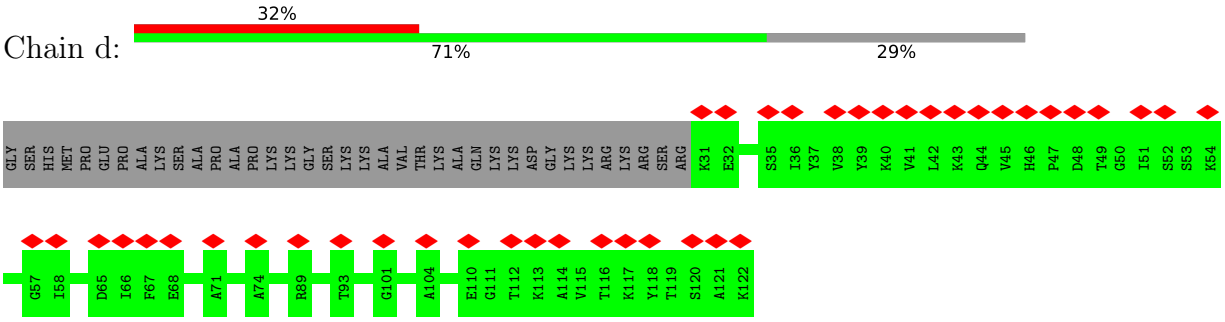
• Molecule 28: Histone H2A type 1-B/E

Chain g:



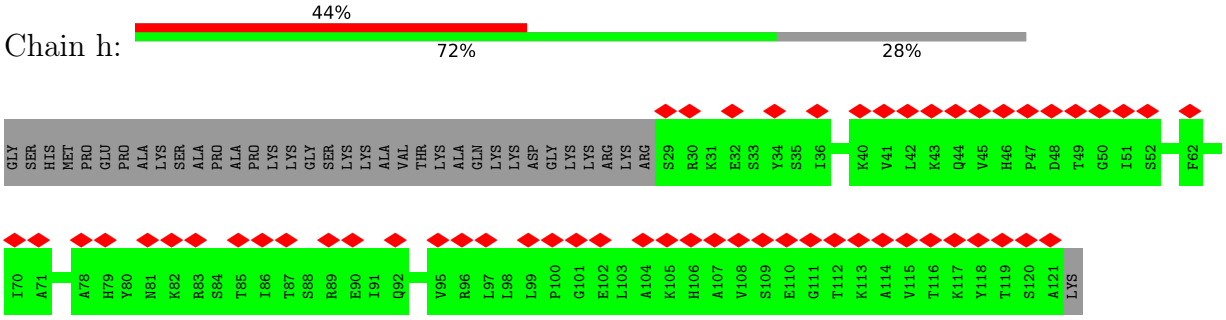
• Molecule 29: Histone H2B type 1-J

Chain d:



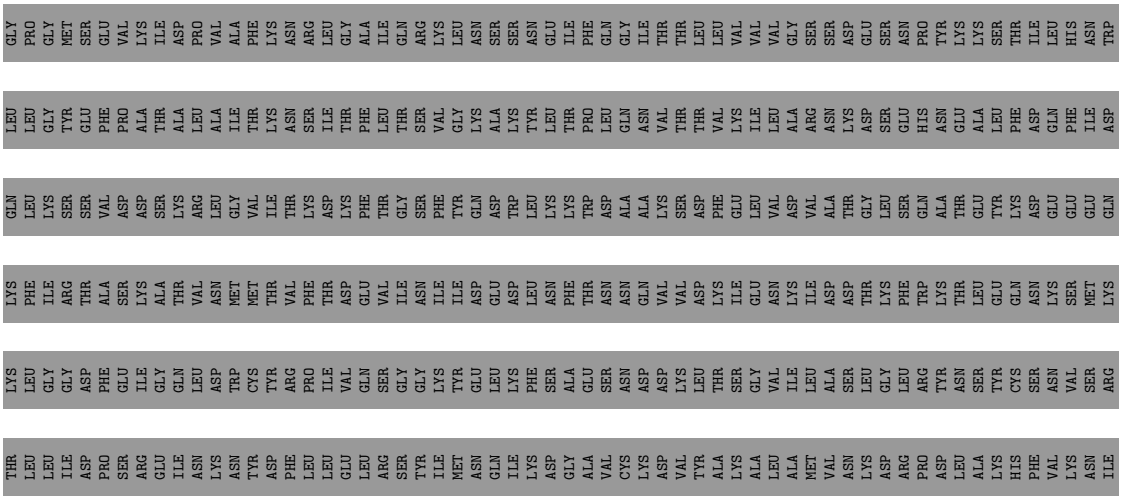
• Molecule 29: Histone H2B type 1-J

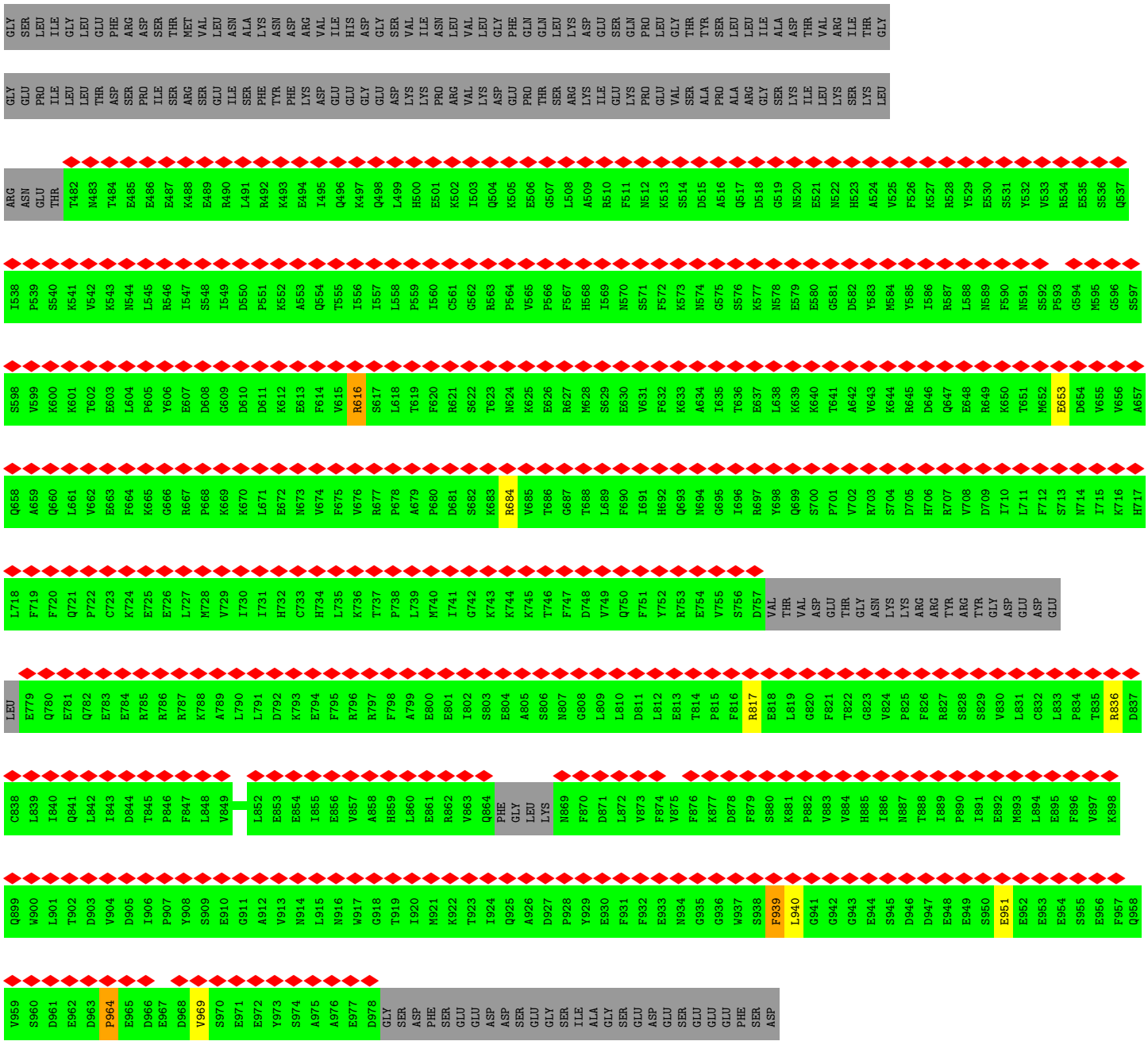
Chain h:



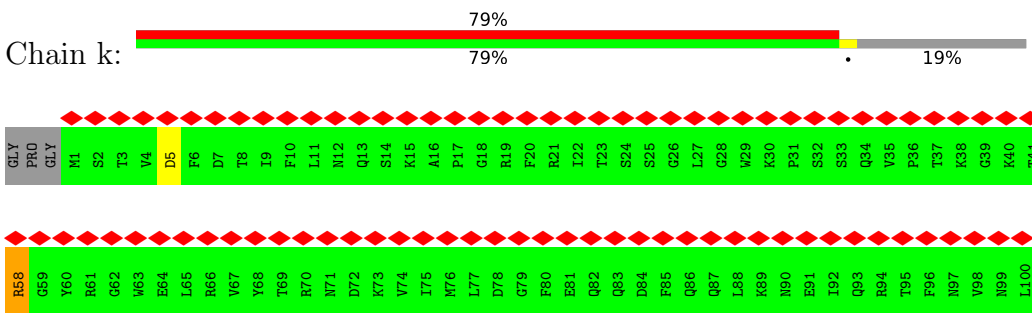
• Molecule 30: FACT complex subunit

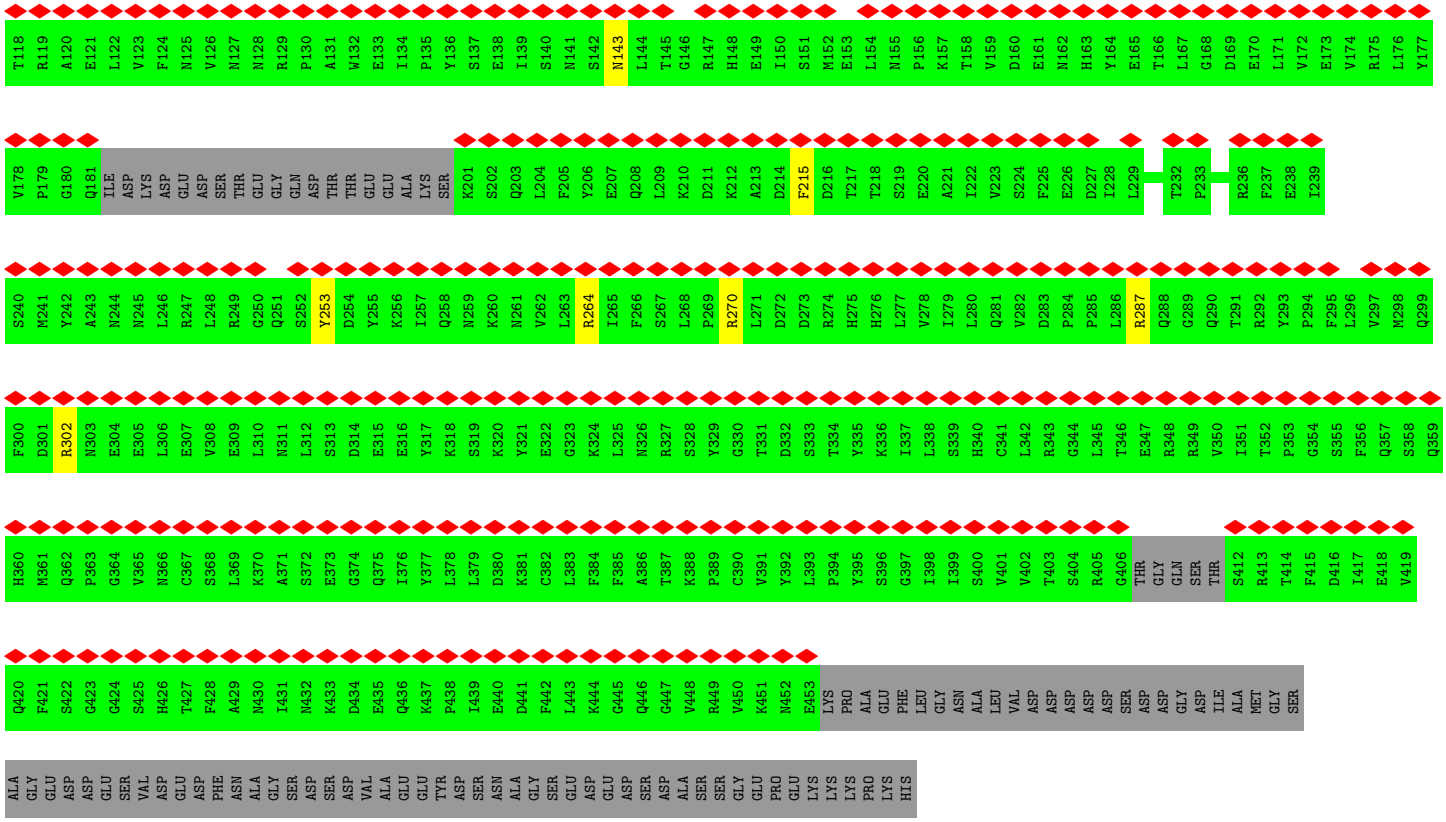
Chain j:





• Molecule 31: FACT complex subunit POB3




T118 R119 A120 E121 L122 V123 F124 N125 V126 N127 N128 R129 P130 A131 W132 E133 I134 P135 Y136 S137 E138 I139 S140 N141 S142 N143 L144 T145 G146 R147 H148 E149 I150 S151 M152 E153 L154 N155 P156 K157 T158 V159 D160 E161 N162 H163 Y164 E165 T166 L167 G168 D169 E170 L171 V172 E173 V174 R175 L176 Y177
V178 P179 G180 Q181 ILE ASP LYS ASP GLU ASP SER THR GLU GLY GLN ASP THR THR GLU GLU ALA LYS SER K201 S202 Q203 L204 F205 Y206 E207 Q208 L209 K210 D211 K212 A213 D214 F215 D216 T217 T218 S219 E220 A221 I222 V223 S224 F225 E226 D227 I228 L229 T232 P233 R236 F237 E238 I239
S240 M241 Y242 A243 N244 N245 L246 R247 L248 R249 G250 Q251 S252 Y253 D254 Y255 K256 I257 Q258 N259 K260 N261 V262 L263 R264 I265 F266 S267 L268 P269 R270 L271 D272 D273 R274 H275 H276 L277 V278 I279 L280 Q281 V282 D283 P284 P285 L286 R287 Q288 G289 Q290 T291 R292 Y293 P294 F295 L296 V297 M298 Q299
F300 D301 R302 N303 E304 E305 L306 E307 V308 E309 L310 N311 L312 S313 D314 E315 E316 I317 K318 S319 K320 Y321 E322 G323 K324 L325 N326 R327 S328 Y329 G330 T331 D332 S333 T334 Y335 K336 I337 L338 S339 H340 C341 L342 R343 G344 L345 T346 E347 R348 R349 V350 I351 T352 P353 G354 S355 F356 Q357 S358 Q359
H360 M361 Q362 P363 G364 V365 N366 C367 S368 L369 K370 A371 S372 E373 G374 Q375 I376 Y377 L378 L379 D380 K381 C382 L383 F384 F385 A386 T387 K388 P389 C390 V391 Y392 L393 P394 Y395 S396 G397 I398 I399 S400 V401 V402 T403 S404 R405 G406 THR GLY GLN SER THR S412 R413 T414 F415 D416 I417 E418 V419
Q420 F421 S422 G423 G424 S425 H426 T427 F428 A429 N430 I431 N432 K433 D434 E435 Q436 K437 P438 I439 E440 D441 F442 L443 K444 G445 Q446 G447 V448 R449 V450 K451 N452 E453 LYS PRO ALA GLU PHE LEU GLY ASN ALA LEU VAL ASP ASP ASP ASP SER ASP ASP GLY ASP ILE ALA MET GLY SER
ALA GLY GLU ASP ASP GLU SER VAL ASP GLU ASP PHE ASN ALA GLY SER ASP SER ASP VAL ALA GLU GLU TYR ASP SER ASN ALA GLY SER GLU ASP GLU ASP SER ASP ALA SER SER GLY GLU PRO GLU LYS LYS LYS PRO LYS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28511	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	0.089	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	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	0.32	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	0.31	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	0.34	0/1070	0.49	0/1444
9	I	0.25	0/934	0.50	0/1257
10	J	0.36	0/563	0.50	0/753
11	K	0.32	0/953	0.50	0/1291
12	L	0.33	0/365	0.56	0/484
13	M	0.25	0/513	0.41	0/693
14	N	1.10	20/2668 (0.7%)	1.22	21/4119 (0.5%)
15	P	0.52	0/443	1.14	6/687 (0.9%)
16	T	1.19	29/2882 (1.0%)	1.23	21/4441 (0.5%)
17	V	0.24	0/840	0.50	0/1140
18	W	0.25	0/4300	0.49	0/5812
19	m	0.24	0/9925	0.45	0/13424
20	n	0.24	0/1132	0.42	0/1526
21	q	0.24	0/7689	0.40	0/10368
22	r	0.24	0/2169	0.45	0/2901
23	u	0.24	0/1740	0.48	0/2347
24	v	0.25	0/2944	0.47	0/3973
25	x	0.26	0/1716	0.45	0/2310
26	a	0.29	0/755	0.55	0/1012
26	e	0.33	0/806	0.58	0/1081
27	b	0.30	0/653	0.59	0/873
27	f	0.33	0/626	0.57	0/837
28	c	0.28	0/752	0.56	0/1015
28	g	0.27	0/766	0.54	0/1033
29	d	0.29	0/729	0.49	0/979

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	h	0.27	0/736	0.47	0/990
30	j	0.69	0/3827	0.85	5/5159 (0.1%)
31	k	0.69	0/3579	0.87	5/4833 (0.1%)
All	All	0.44	49/84120 (0.1%)	0.61	58/114652 (0.1%)

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	4
16	T	0	4
27	f	0	1
30	j	0	1
31	k	0	1
All	All	0	11

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	-33	DA	C1'-N9	-7.85	1.36	1.47
14	N	68	DC	C1'-N1	7.78	1.59	1.49
16	T	-53	DG	C1'-N9	-7.74	1.36	1.47
14	N	50	DG	C1'-N9	-7.68	1.36	1.47
16	T	-37	DG	C1'-N9	-7.53	1.36	1.47
16	T	-34	DG	C1'-N9	-7.49	1.36	1.47
16	T	-44	DA	C1'-N9	-7.42	1.36	1.47
14	N	32	DG	C1'-N9	-7.34	1.36	1.47
16	T	-11	DG	C1'-N9	-7.25	1.37	1.47
14	N	39	DA	C1'-N9	-7.25	1.37	1.47
14	N	28	DA	C1'-N9	-7.06	1.37	1.47
16	T	-19	DG	C1'-N9	-7.03	1.37	1.47
14	N	26	DA	C1'-N9	-6.97	1.37	1.47
16	T	-49	DG	C1'-N9	-6.91	1.37	1.47
16	T	27	DG	C1'-N9	-6.82	1.37	1.47
14	N	18	DG	C1'-N9	-6.77	1.37	1.47
14	N	57	DG	C1'-N9	-6.72	1.37	1.47
16	T	0	DC	C1'-N1	6.68	1.57	1.49
16	T	26	DG	C1'-N9	-6.56	1.38	1.47
16	T	-70	DC	C1'-N1	6.55	1.57	1.49
14	N	47	DA	C1'-N9	-6.54	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	3	DC	C1'-N1	6.46	1.57	1.49
16	T	-35	DA	C1'-N9	-6.45	1.38	1.47
16	T	-55	DG	C1'-N9	-6.37	1.38	1.47
16	T	-62	DC	C1'-N1	6.13	1.57	1.49
16	T	-25	DA	C1'-N9	-6.12	1.38	1.47
14	N	67	DT	C1'-N1	6.06	1.57	1.49
14	N	-19	DG	C1'-N9	-5.98	1.38	1.47
14	N	-21	DA	C1'-N9	-5.90	1.39	1.47
14	N	7	DC	C1'-N1	5.89	1.56	1.49
16	T	-8	DC	C1'-N1	5.85	1.56	1.49
16	T	-40	DG	C1'-N9	-5.84	1.39	1.47
16	T	28	DG	C1'-N9	-5.82	1.39	1.47
16	T	-7	DG	C1'-N9	-5.77	1.39	1.47
14	N	36	DA	C1'-N9	-5.77	1.39	1.47
16	T	-6	DT	C1'-N1	5.76	1.56	1.49
16	T	41	DA	C1'-N9	-5.67	1.39	1.47
14	N	-20	DA	C1'-N9	-5.66	1.39	1.47
16	T	-14	DA	C1'-N9	-5.64	1.39	1.47
16	T	-60	DG	C1'-N9	-5.52	1.39	1.47
16	T	48	DG	C1'-N9	-5.47	1.39	1.47
14	N	5	DT	C1'-N1	5.41	1.56	1.49
16	T	39	DA	C1'-N9	-5.38	1.39	1.47
14	N	-40	DC	C1'-N1	5.30	1.56	1.49
16	T	-9	DA	C1'-N9	-5.27	1.39	1.47
14	N	8	DG	C1'-N9	-5.25	1.40	1.47
14	N	-22	DA	C1'-N9	-5.16	1.40	1.47
16	T	47	DG	C1'-N9	-5.10	1.40	1.47
16	T	-5	DA	C1'-N9	-5.10	1.40	1.47

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	j	684	ARG	NE-CZ-NH1	9.37	124.99	120.30
30	j	836	ARG	NE-CZ-NH1	9.30	124.95	120.30
15	P	-4	C	C2-N1-C1'	8.58	128.24	118.80
15	P	-4	C	N1-C2-O2	8.42	123.95	118.90
14	N	-14	DA	N1-C6-N6	-8.40	113.56	118.60
14	N	-15	DA	N1-C6-N6	-8.06	113.77	118.60
16	T	17	DA	N1-C6-N6	-7.97	113.82	118.60
14	N	-13	DA	C5-C6-N1	7.91	121.66	117.70
14	N	-12	DA	C5-C6-N1	7.78	121.59	117.70
16	T	16	DA	C5-C6-N1	7.38	121.39	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	-13	DA	N1-C6-N6	-7.34	114.20	118.60
16	T	17	DA	C5-C6-N1	7.13	121.26	117.70
14	N	-14	DA	C5-C6-N1	7.08	121.24	117.70
14	N	-14	DA	C4-C5-C6	-7.06	113.47	117.00
16	T	16	DA	N1-C6-N6	-7.03	114.38	118.60
14	N	-15	DA	C5-C6-N1	6.99	121.20	117.70
16	T	-7	DG	O4'-C1'-N9	6.96	112.87	108.00
14	N	-12	DA	N1-C6-N6	-6.86	114.49	118.60
14	N	-15	DA	C4-C5-C6	-6.73	113.64	117.00
15	P	-4	C	N3-C2-O2	-6.67	117.23	121.90
16	T	-64	DC	O4'-C1'-N1	6.67	112.67	108.00
16	T	7	DC	O4'-C1'-N1	6.48	112.53	108.00
15	P	11	A	OP1-P-OP2	-6.44	109.94	119.60
16	T	16	DA	C4-C5-C6	-6.42	113.79	117.00
30	j	964	PRO	N-CA-CB	6.33	110.90	103.30
16	T	10	DC	O4'-C1'-N1	6.31	112.41	108.00
14	N	-12	DA	C4-C5-C6	-6.28	113.86	117.00
14	N	66	DT	O4'-C1'-N1	6.18	112.33	108.00
16	T	18	DC	N3-C2-O2	-6.11	117.62	121.90
16	T	17	DA	C4-C5-C6	-6.02	113.99	117.00
14	N	-13	DA	C4-C5-C6	-6.00	114.00	117.00
15	P	-4	C	C6-N1-C1'	-5.97	113.64	120.80
14	N	-11	DC	O4'-C1'-N1	5.93	112.15	108.00
16	T	15	DT	C6-C5-C7	-5.88	119.37	122.90
16	T	13	DT	C6-C5-C7	-5.85	119.39	122.90
14	N	-17	DT	C6-C5-C7	-5.82	119.41	122.90
16	T	12	DT	N3-C2-O2	-5.80	118.82	122.30
31	k	264	ARG	NE-CZ-NH1	5.73	123.16	120.30
14	N	-16	DT	N3-C2-O2	-5.69	118.89	122.30
31	k	302	ARG	NE-CZ-NH1	5.67	123.14	120.30
14	N	-4	DG	O4'-C1'-N9	5.63	111.94	108.00
16	T	12	DT	C6-C5-C7	-5.59	119.54	122.90
15	P	-4	C	C6-N1-C2	-5.52	118.09	120.30
16	T	-60	DG	O4'-C1'-N9	5.50	111.85	108.00
16	T	-63	DC	O4'-C1'-N1	5.46	111.82	108.00
14	N	-16	DT	C6-C5-C7	-5.44	119.63	122.90
14	N	-17	DT	O4'-C1'-N1	5.39	111.78	108.00
16	T	5	DC	O4'-C1'-N1	5.39	111.77	108.00
31	k	270	ARG	NE-CZ-NH1	5.35	122.98	120.30
14	N	-8	DG	O4'-C1'-N9	5.34	111.74	108.00
16	T	14	DT	N3-C2-O2	-5.32	119.11	122.30
16	T	-62	DC	O4'-C1'-N1	5.31	111.72	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	k	58	ARG	NE-CZ-NH1	5.29	122.94	120.30
16	T	14	DT	C6-C5-C7	-5.25	119.75	122.90
14	N	8	DG	O4'-C1'-N9	5.19	111.63	108.00
30	j	817	ARG	NE-CZ-NH1	5.17	122.88	120.30
30	j	616	ARG	NE-CZ-NH1	5.12	122.86	120.30
31	k	5	ASP	CB-CG-OD2	-5.08	113.73	118.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	-11	DC	Sidechain
14	N	-12	DA	Sidechain
14	N	-17	DT	Sidechain
14	N	-9	DC	Sidechain
16	T	11	DG	Sidechain
16	T	13	DT	Sidechain
16	T	14	DT	Sidechain
16	T	15	DT	Sidechain
27	f	36	ARG	Sidechain
30	j	616	ARG	Sidechain
31	k	58	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11064	0	11090	112	0
2	B	9284	0	9282	115	0
3	C	2098	0	2057	21	0
4	D	1349	0	1345	9	0
5	E	1741	0	1754	21	0
6	F	677	0	693	6	0
7	G	1325	0	1342	17	0
8	H	1053	0	1050	10	0
9	I	917	0	867	15	0
10	J	554	0	573	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	932	0	944	14	0
12	L	359	0	358	4	0
13	M	505	0	495	5	0
14	N	2377	0	1293	87	0
15	P	399	0	205	10	0
16	T	2570	0	1411	62	0
17	V	824	0	795	16	0
18	W	4232	0	4278	57	0
19	m	9730	0	9588	0	0
20	n	1115	0	1186	0	0
21	q	7552	0	7545	0	0
22	r	2139	0	2155	0	0
23	u	1707	0	1676	0	0
24	v	2878	0	2873	0	0
25	x	1682	0	1731	0	0
26	a	746	0	786	0	0
26	e	795	0	832	0	0
27	b	646	0	687	0	0
27	f	619	0	659	0	0
28	c	743	0	784	0	0
28	g	757	0	802	0	0
29	d	718	0	740	0	0
29	h	725	0	745	0	0
30	j	3754	0	3654	0	0
31	k	3502	0	3436	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	I	2	0	0	0	0
32	J	1	0	0	0	0
32	L	1	0	0	0	0
32	M	1	0	0	0	0
32	V	1	0	0	0	0
33	A	1	0	0	0	0
All	All	82079	0	79711	518	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (518) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-49:DG:H2"	14:N:-48:DC:C5	2.00	0.97
14:N:24:DC:C2'	14:N:25:DT:H71	2.00	0.92
14:N:33:DT:H2"	14:N:34:DC:C5	2.08	0.89
16:T:-21:DC:H2"	16:T:-20:DC:C5	2.11	0.86
14:N:57:DG:N2	16:T:-56:DC:C2	2.45	0.85
16:T:-51:DC:H2"	16:T:-50:DC:C5	2.12	0.85
16:T:-33:DA:H2"	16:T:-32:DC:C5	2.14	0.81
14:N:-22:DA:N6	14:N:-21:DA:C6	2.48	0.81
14:N:24:DC:H2"	14:N:25:DT:H71	1.63	0.81
14:N:66:DT:C6	14:N:67:DT:H72	2.16	0.81
14:N:24:DC:H2'	14:N:25:DT:H71	1.63	0.80
14:N:10:DG:H2"	14:N:11:DC:C5	2.20	0.77
14:N:-37:DG:N2	16:T:37:DC:O2	2.16	0.76
16:T:-51:DC:H2"	16:T:-50:DC:H5	1.47	0.75
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.26	0.75
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.70	0.74
14:N:4:DG:N2	16:T:-3:DG:C4	2.56	0.74
14:N:33:DT:H2"	14:N:34:DC:H5	1.54	0.72
14:N:-22:DA:C6	14:N:-21:DA:C6	2.79	0.71
16:T:-29:DC:H2"	16:T:-28:DT:H71	1.73	0.70
1:A:807:ARG:NH1	2:B:724:LYS:O	2.23	0.70
14:N:24:DC:C2'	14:N:25:DT:C7	2.69	0.70
14:N:-49:DG:H2"	14:N:-48:DC:H5	1.52	0.69
14:N:34:DC:H2'	14:N:35:DT:H71	1.74	0.69
1:A:1262:MET:SD	1:A:1265:ARG:NH2	2.65	0.69
1:A:1207:LYS:O	1:A:1277:ARG:NH2	2.24	0.69
8:H:112:LYS:HG2	8:H:125:GLU:HG3	1.73	0.69
1:A:831:LYS:NZ	1:A:1079:THR:O	2.25	0.69
14:N:-51:DG:C2'	14:N:-50:DT:H72	2.23	0.69
18:W:487:ILE:HD11	18:W:531:ARG:HB2	1.75	0.69
1:A:107:CYS:SG	1:A:172:GLN:NE2	2.66	0.68
16:T:-37:DG:C8	16:T:-36:DT:H72	2.28	0.68
14:N:-44:DG:H2"	14:N:-43:DT:H72	1.76	0.67
14:N:36:DA:C2	16:T:-35:DA:C2	2.83	0.67
14:N:24:DC:H2'	14:N:25:DT:C7	2.24	0.67
10:J:47:ARG:NH1	10:J:48:MET:SD	2.67	0.67
2:B:223:SER:O	2:B:252:ARG:NH2	2.27	0.66
14:N:-40:DC:H2"	14:N:-39:DT:H71	1.77	0.66
9:I:45:ARG:NH2	9:I:47:GLU:OE2	2.29	0.66
1:A:673:ASP:OD1	1:A:737:ASN:ND2	2.29	0.65
18:W:342:GLU:HB3	18:W:351:ARG:HB3	1.79	0.65
1:A:887:ILE:O	1:A:945:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:613:ARG:HH21	9:I:62:ILE:HD11	1.61	0.65
16:T:-40:DG:C8	16:T:-39:DT:H71	2.32	0.65
2:B:267:TYR:HB2	2:B:348:ILE:HD11	1.77	0.65
14:N:-48:DC:H2"	14:N:-47:DC:C6	2.32	0.65
1:A:127:ARG:O	1:A:129:ARG:NH1	2.30	0.64
14:N:34:DC:C6	14:N:35:DT:C7	2.80	0.64
17:V:89:ARG:NH1	17:V:109:ASP:OD2	2.31	0.64
18:W:327:ARG:NH2	18:W:441:ASN:O	2.30	0.64
14:N:24:DC:H2"	14:N:25:DT:C7	2.28	0.64
2:B:285:PRO:HG2	2:B:288:GLU:HB2	1.80	0.64
16:T:-43:DT:H2"	16:T:-42:DT:C6	2.33	0.64
2:B:254:ASP:H	2:B:259:ARG:HH21	1.44	0.63
4:D:153:VAL:HG13	4:D:171:LEU:HD23	1.78	0.63
1:A:466:TYR:HB2	1:A:470:ARG:HH22	1.63	0.63
1:A:881:ARG:HH21	1:A:955:ASN:HB3	1.64	0.63
14:N:24:DC:H2"	14:N:25:DT:C6	2.33	0.63
16:T:-40:DG:C8	16:T:-39:DT:C7	2.82	0.62
16:T:42:DC:OP1	18:W:433:GLN:NE2	2.33	0.62
1:A:1158:PRO:HA	1:A:1192:PRO:HB3	1.80	0.62
18:W:351:ARG:HA	18:W:429:THR:HA	1.81	0.62
14:N:-22:DA:N6	14:N:-21:DA:N6	2.47	0.62
11:K:57:THR:OG1	11:K:76:GLN:OE1	2.17	0.61
1:A:1130:ILE:HG12	1:A:1134:LYS:HE2	1.81	0.61
1:A:361:GLU:OE1	1:A:460:ARG:NH2	2.29	0.61
1:A:1201:ARG:NH2	1:A:1235:ALA:O	2.33	0.61
14:N:11:DC:H2"	14:N:12:DG:C8	2.36	0.60
1:A:39:GLU:OE2	1:A:49:ARG:NH1	2.34	0.60
18:W:784:ASN:HB2	18:W:785:PRO:HD3	1.81	0.60
18:W:527:THR:HA	18:W:530:LEU:HD12	1.84	0.60
1:A:149:GLU:HB2	1:A:165:ARG:HD3	1.84	0.60
1:A:466:TYR:HB2	1:A:470:ARG:NH2	2.16	0.60
2:B:235:LEU:HD23	2:B:242:ILE:HG13	1.83	0.60
14:N:38:DG:H2"	14:N:39:DA:H5'	1.83	0.60
2:B:489:ARG:NH2	2:B:533:SER:O	2.35	0.59
1:A:22:LEU:HG	2:B:1213:ALA:HB2	1.83	0.59
17:V:57:LEU:HD11	17:V:81:LEU:HD22	1.84	0.59
2:B:10:ASP:HB3	2:B:649:LYS:HG3	1.84	0.59
2:B:353:LEU:O	2:B:367:LYS:NZ	2.34	0.59
14:N:43:DA:H1'	14:N:44:DT:H5'	1.84	0.59
16:T:-21:DC:H2"	16:T:-20:DC:H5	1.67	0.59
18:W:327:ARG:NH1	18:W:335:GLY:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-22:DA:N1	14:N:-21:DA:C2	2.71	0.59
1:A:85:GLU:O	1:A:274:ASN:ND2	2.33	0.59
16:T:-23:DC:H2"	16:T:-22:DA:N7	2.18	0.59
2:B:409:LEU:HD23	2:B:450:LEU:HD23	1.85	0.59
14:N:54:DT:H2"	14:N:55:DC:C6	2.38	0.59
7:G:27:ARG:NH1	7:G:54:ILE:O	2.36	0.59
2:B:63:GLN:NE2	2:B:70:ASN:OD1	2.35	0.58
2:B:294:CYS:SG	2:B:295:TYR:N	2.76	0.58
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.24	0.58
14:N:69:DT:H2"	14:N:70:DG:H8	1.68	0.58
1:A:1157:ASP:O	1:A:1243:ARG:NH2	2.29	0.58
17:V:9:GLU:HA	17:V:20:PRO:HA	1.84	0.58
14:N:8:DG:C2	16:T:-7:DG:C2	2.92	0.58
2:B:50:VAL:HG21	2:B:82:ILE:HD11	1.86	0.58
1:A:677:MET:HG3	2:B:722:THR:HB	1.84	0.58
2:B:91:GLU:OE2	2:B:97:HIS:NE2	2.29	0.58
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.85	0.58
1:A:227:GLU:OE1	1:A:231:ARG:NH1	2.36	0.58
7:G:86:VAL:HG22	7:G:146:LYS:HB2	1.86	0.57
1:A:63:ARG:NH2	15:P:0:G:OP1	2.36	0.57
14:N:53:DC:H2"	14:N:54:DT:H71	1.86	0.57
18:W:392:ARG:NH1	18:W:398:GLU:OE1	2.36	0.57
5:E:101:GLU:HG3	5:E:102:LYS:HG2	1.86	0.57
18:W:665:ARG:HB2	18:W:708:ILE:HD11	1.86	0.57
17:V:13:MET:N	17:V:49:CYS:O	2.26	0.57
14:N:-40:DC:H2"	14:N:-39:DT:C7	2.33	0.57
1:A:568:LYS:HG2	1:A:569:PRO:HA	1.87	0.57
14:N:22:DT:H2"	14:N:23:DG:N7	2.19	0.57
2:B:290:LEU:HD21	2:B:310:ILE:HD11	1.87	0.56
14:N:24:DC:H2"	14:N:25:DT:C5	2.40	0.56
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.37	0.56
14:N:4:DG:N2	16:T:-3:DG:N3	2.53	0.56
18:W:232:ARG:HH12	18:W:235:LYS:HE3	1.70	0.56
2:B:336:ILE:O	2:B:341:ARG:NH1	2.38	0.56
8:H:48:PRO:O	8:H:145:ARG:NH1	2.36	0.56
17:V:58:VAL:N	17:V:82:TYR:O	2.38	0.56
1:A:486:ASP:OD1	15:P:10:C:O2'	2.20	0.56
18:W:352:LEU:HD11	18:W:435:LEU:HD11	1.87	0.56
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.88	0.56
5:E:28:PHE:HB2	5:E:64:THR:HG22	1.88	0.56
16:T:-38:DC:H2"	16:T:-37:DG:H5'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLU:O	1:A:165:ARG:NH1	2.38	0.55
14:N:-22:DA:N6	14:N:-21:DA:N1	2.54	0.55
1:A:1331:TYR:OH	1:A:1354:GLU:OE2	2.21	0.55
14:N:4:DG:N2	16:T:-3:DG:C2	2.74	0.55
5:E:19:LYS:NZ	5:E:33:GLU:O	2.34	0.55
1:A:916:TYR:OH	1:A:983:LEU:O	2.19	0.55
7:G:102:ASP:OD1	7:G:107:ASN:ND2	2.31	0.55
7:G:151:ARG:HB3	7:G:158:TYR:HB2	1.89	0.55
1:A:1452:LEU:HD23	6:F:131:PRO:HA	1.89	0.55
2:B:904:ARG:HH12	2:B:946:ASN:HB2	1.72	0.55
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.89	0.55
14:N:-51:DG:H2"	14:N:-50:DT:C7	2.37	0.55
14:N:36:DA:C5	14:N:37:DC:C4	2.96	0.54
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.89	0.54
17:V:15:CYS:HB3	17:V:32:CYS:SG	2.46	0.54
1:A:807:ARG:HD3	2:B:725:ARG:HA	1.89	0.54
1:A:1210:THR:HB	1:A:1213:GLN:HG3	1.90	0.54
17:V:10:ARG:HA	17:V:52:SER:HA	1.90	0.54
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.42	0.54
2:B:72:ASN:ND2	2:B:128:ASP:OD1	2.39	0.54
14:N:33:DT:C2'	14:N:34:DC:C5	2.87	0.54
8:H:100:VAL:HG22	8:H:115:VAL:HG22	1.89	0.54
11:K:29:ASN:ND2	11:K:78:GLU:O	2.41	0.54
11:K:103:HIS:NE2	11:K:107:GLU:OE2	2.40	0.54
14:N:8:DG:H2'	14:N:9:DT:H71	1.89	0.54
1:A:218:GLU:OE1	1:A:222:ARG:NH1	2.41	0.54
14:N:34:DC:C5	14:N:35:DT:H73	2.42	0.54
16:T:-51:DC:C2'	16:T:-50:DC:C5	2.88	0.54
14:N:44:DT:H2"	14:N:45:DT:C6	2.42	0.54
18:W:325:TYR:OH	18:W:451:GLN:OE1	2.23	0.54
2:B:301:GLN:O	2:B:304:GLU:HG3	2.08	0.54
18:W:332:LYS:O	18:W:388:ARG:NH1	2.41	0.54
8:H:59:LEU:HD23	8:H:139:LEU:HD13	1.91	0.53
14:N:34:DC:C6	14:N:35:DT:H73	2.43	0.53
18:W:451:GLN:NE2	18:W:454:GLU:OE1	2.42	0.53
1:A:533:ARG:HD3	1:A:750:ALA:HB2	1.91	0.53
7:G:95:SER:OG	7:G:98:GLY:O	2.22	0.53
2:B:59:ASP:HB3	2:B:74:ARG:HG3	1.91	0.53
1:A:351:ARG:HB2	2:B:1128:LEU:HD21	1.91	0.53
14:N:8:DG:H2'	14:N:9:DT:C7	2.38	0.53
5:E:81:PHE:HE1	5:E:110:ILE:HD13	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:LYS:NZ	2:B:264:THR:OG1	2.42	0.53
4:D:6:SER:HB3	7:G:42:PHE:HZ	1.73	0.53
5:E:47:ASP:OD2	5:E:53:GLN:NE2	2.19	0.53
16:T:-31:DA:H2"	16:T:-30:DG:C8	2.44	0.53
18:W:220:THR:N	18:W:223:ASP:OD2	2.33	0.53
2:B:797:TYR:HE1	2:B:854:LEU:HD13	1.74	0.52
7:G:144:ARG:HB2	7:G:171:ILE:HD13	1.90	0.52
13:M:46:LEU:HD11	13:M:55:SER:HB3	1.90	0.52
9:I:17:LYS:N	9:I:26:LEU:O	2.39	0.52
14:N:52:DC:H2"	14:N:53:DC:C5	2.44	0.52
15:P:6:U:H2'	15:P:7:C:C6	2.44	0.52
16:T:-53:DG:H2"	16:T:-52:DG:N7	2.25	0.52
17:V:10:ARG:HG2	17:V:52:SER:HB3	1.92	0.52
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.49	0.52
4:D:60:ILE:HG13	7:G:47:THR:HG21	1.90	0.52
14:N:-42:DG:C8	14:N:-41:DT:H71	2.45	0.52
2:B:904:ARG:NH1	2:B:905:VAL:O	2.43	0.52
16:T:-37:DG:C2'	16:T:-36:DT:H72	2.39	0.52
1:A:801:VAL:HG22	1:A:813:GLU:HB3	1.92	0.52
18:W:513:SER:N	18:W:519:ASN:OD1	2.41	0.52
18:W:260:TYR:HD1	18:W:276:ALA:HA	1.75	0.51
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.74	0.51
2:B:83:TYR:HB2	2:B:116:TYR:HB2	1.92	0.51
2:B:74:ARG:HB2	2:B:124:PHE:HB2	1.92	0.51
2:B:547:ILE:HG21	2:B:619:ILE:HG21	1.93	0.51
18:W:334:LYS:N	18:W:388:ARG:HH12	2.09	0.51
1:A:771:VAL:HG13	1:A:823:GLU:HG3	1.92	0.51
18:W:563:GLU:HG2	18:W:574:ILE:HG12	1.93	0.51
14:N:-49:DG:C2'	14:N:-48:DC:C5	2.86	0.51
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.92	0.51
13:M:38:LEU:HA	13:M:45:GLY:HA2	1.91	0.51
7:G:119:LEU:HD21	7:G:135:GLU:HB2	1.93	0.51
18:W:644:ASN:ND2	18:W:647:GLN:OE1	2.44	0.51
1:A:1223:SER:OG	1:A:1224:ASP:N	2.44	0.50
2:B:622:ASP:OD1	2:B:623:VAL:N	2.40	0.50
3:C:266:ARG:HD2	11:K:84:LYS:HZ3	1.75	0.50
1:A:669:ASP:OD2	1:A:743:ASN:ND2	2.29	0.50
14:N:50:DG:H2"	14:N:51:DG:C8	2.46	0.50
18:W:326:VAL:HA	18:W:440:ILE:HD13	1.92	0.50
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.75	0.50
1:A:977:ARG:HD2	1:A:979:LYS:HZ1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1153:GLU:OE2	9:I:45:ARG:NH1	2.40	0.50
5:E:87:VAL:HG23	5:E:91:THR:HB	1.92	0.50
16:T:-48:DC:C2'	16:T:-47:DT:H71	2.41	0.50
1:A:168:CYS:SG	1:A:170:ASN:ND2	2.85	0.50
18:W:464:ILE:O	18:W:468:LEU:HG	2.12	0.50
16:T:-11:DG:H2"	16:T:-10:DC:C5	2.47	0.50
4:D:105:THR:HG22	7:G:105:PRO:HD3	1.94	0.50
13:M:33:SER:HA	13:M:50:LYS:HE2	1.93	0.50
18:W:634:PRO:HA	18:W:637:ILE:HD12	1.94	0.50
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.92	0.50
2:B:607:SER:HB3	2:B:620:PHE:HB2	1.94	0.50
2:B:498:ASP:HB3	14:N:-23:DA:C4	2.47	0.50
18:W:222:ASP:O	18:W:277:ARG:NH2	2.30	0.50
2:B:514:LEU:HD22	2:B:626:VAL:HG12	1.94	0.49
17:V:63:ASN:HB3	17:V:75:ASP:HA	1.94	0.49
1:A:119:ASN:OD1	1:A:121:THR:OG1	2.23	0.49
18:W:590:ILE:O	18:W:593:SER:OG	2.26	0.49
1:A:1190:GLN:HA	1:A:1245:ILE:HA	1.94	0.49
2:B:74:ARG:HH22	2:B:126:SER:HB3	1.77	0.49
14:N:22:DT:H2"	14:N:23:DG:C8	2.47	0.49
16:T:-63:DC:H2"	16:T:-62:DC:C5	2.46	0.49
1:A:738:LEU:HD13	1:A:742:ASN:HD22	1.77	0.49
14:N:-51:DG:H2'	14:N:-50:DT:H72	1.93	0.49
2:B:610:ARG:NH2	9:I:61:ASP:OD2	2.46	0.49
9:I:29:CYS:CB	9:I:32:CYS:SG	2.99	0.49
1:A:321:ARG:NH1	2:B:466:MET:SD	2.86	0.49
2:B:318:ASP:HB3	2:B:321:VAL:HG22	1.94	0.49
5:E:54:ARG:HA	5:E:57:MET:HE3	1.93	0.49
9:I:103:CYS:SG	9:I:104:LEU:N	2.86	0.49
16:T:-29:DC:H2"	16:T:-28:DT:C7	2.39	0.49
1:A:122:MET:O	1:A:126:ILE:HG12	2.13	0.49
2:B:479:TYR:CZ	2:B:1096:ARG:HB3	2.48	0.49
16:T:-40:DG:N7	16:T:-39:DT:H73	2.28	0.49
5:E:81:PHE:CE1	5:E:110:ILE:HD13	2.48	0.49
14:N:4:DG:C2'	14:N:5:DT:H72	2.43	0.49
2:B:766:ARG:HH21	2:B:1020:ARG:HD3	1.78	0.49
1:A:1150:SER:OG	1:A:1198:GLU:O	2.32	0.48
2:B:58:LEU:O	2:B:75:TYR:N	2.36	0.48
3:C:66:LEU:HD11	3:C:155:ILE:HD12	1.95	0.48
4:D:157:ILE:HG23	4:D:164:ALA:HB2	1.95	0.48
1:A:343:GLY:O	2:B:1129:ARG:NH1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:112:THR:HA	7:G:115:ILE:HD12	1.95	0.48
18:W:666:GLU:HB2	18:W:671:ARG:HA	1.95	0.48
9:I:96:ASN:OD1	9:I:97:MET:N	2.46	0.48
16:T:-13:DA:H2"	16:T:-12:DC:C5	2.48	0.48
1:A:819:MET:O	1:A:823:GLU:HG2	2.14	0.48
2:B:300:TRP:HA	2:B:303:LEU:HD12	1.94	0.48
3:C:88:GLU:HG2	18:W:759:ARG:HD2	1.95	0.48
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	1.94	0.48
5:E:213:CYS:SG	5:E:214:LEU:N	2.87	0.48
14:N:56:DG:H2"	14:N:57:DG:H5'	1.95	0.48
14:N:56:DG:C6	14:N:57:DG:C6	3.02	0.48
15:P:-2:G:N2	15:P:-1:G:N7	2.61	0.48
12:L:70:ASP:HB3	18:W:784:ASN:HB3	1.95	0.48
14:N:46:DG:C2	16:T:-45:DA:C2	3.02	0.48
18:W:603:GLN:HG3	18:W:609:VAL:HG22	1.95	0.48
1:A:472:ASN:O	1:A:475:VAL:HG22	2.14	0.48
1:A:1426:GLY:O	1:A:1430:ASN:ND2	2.40	0.48
2:B:314:PHE:O	2:B:317:GLN:NE2	2.46	0.48
1:A:823:GLU:OE1	2:B:506:GLN:NE2	2.46	0.48
3:C:105:GLU:N	3:C:105:GLU:OE1	2.46	0.47
13:M:65:GLN:N	13:M:68:ASP:OD2	2.44	0.47
16:T:37:DC:H2"	16:T:38:DA:C8	2.49	0.47
1:A:106:ILE:HD13	1:A:215:ILE:HD11	1.95	0.47
3:C:17:VAL:HG12	3:C:240:ALA:HB1	1.97	0.47
18:W:260:TYR:CE1	18:W:277:ARG:HG3	2.49	0.47
1:A:673:ASP:OD1	1:A:673:ASP:N	2.44	0.47
2:B:365:THR:O	2:B:368:THR:OG1	2.28	0.47
2:B:896:ASP:OD2	12:L:31:TYR:OH	2.32	0.47
5:E:91:THR:HA	5:E:94:ASN:ND2	2.29	0.47
2:B:101:PRO:HG2	2:B:172:LEU:HD11	1.96	0.47
3:C:4:GLU:HB3	3:C:5:PRO:HD3	1.96	0.47
4:D:139:PRO:HA	4:D:142:ILE:HD12	1.96	0.47
18:W:599:HIS:HB3	18:W:677:LEU:HD21	1.96	0.47
1:A:363:ASP:HB3	1:A:509:PRO:HD3	1.97	0.47
2:B:303:LEU:O	2:B:307:LYS:HG2	2.15	0.47
2:B:865:ARG:HD3	2:B:871:VAL:HG12	1.95	0.47
14:N:66:DT:H2'	14:N:67:DT:H72	1.96	0.47
15:P:-5:C:H1'	18:W:748:ARG:HD3	1.96	0.47
1:A:983:LEU:HD13	1:A:1041:ARG:HA	1.97	0.47
14:N:13:DT:H2"	14:N:14:DT:H71	1.96	0.47
17:V:91:PRO:HD2	17:V:94:ILE:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:GLN:OE1	6:F:90:ARG:NH1	2.38	0.47
7:G:123:PRO:HA	7:G:128:PRO:HB3	1.97	0.47
17:V:41:SER:HB2	17:V:45:THR:HB	1.96	0.47
16:T:-51:DC:C2	16:T:-50:DC:C4	3.03	0.47
1:A:580:SER:HB3	1:A:612:LYS:HA	1.97	0.47
2:B:273:PRO:HG2	2:B:276:ILE:HD12	1.97	0.47
2:B:906:SER:OG	18:W:781:GLU:OE1	2.24	0.47
11:K:62:LYS:HE3	11:K:64:GLU:OE2	2.15	0.47
2:B:788:ARG:O	2:B:967:ARG:NH1	2.47	0.47
10:J:6:ARG:HD3	10:J:13:VAL:HG22	1.97	0.47
1:A:649:ASN:O	1:A:653:VAL:HG23	2.15	0.46
2:B:220:ALA:O	2:B:252:ARG:NH2	2.47	0.46
2:B:885:LEU:HD23	2:B:936:ASP:HB2	1.97	0.46
15:P:-6:A:H2'	15:P:-5:C:O4'	2.15	0.46
14:N:10:DG:N2	16:T:-9:DA:C2	2.84	0.46
18:W:491:LEU:HB3	18:W:494:LEU:HD12	1.98	0.46
18:W:666:GLU:HA	18:W:705:VAL:HG12	1.96	0.46
14:N:66:DT:H2'	14:N:67:DT:C7	2.45	0.46
14:N:66:DT:C4	14:N:67:DT:O4	2.68	0.46
18:W:534:PHE:HB3	18:W:554:ILE:HD13	1.97	0.46
2:B:421:ILE:HD11	2:B:441:VAL:HG12	1.97	0.46
5:E:96:CYS:SG	5:E:126:VAL:HG23	2.56	0.46
1:A:564:PRO:HG2	1:A:567:LEU:HD23	1.98	0.46
2:B:497:ARG:NH2	16:T:24:DT:OP2	2.49	0.46
1:A:1192:PRO:HA	1:A:1243:ARG:HH12	1.79	0.46
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.49	0.46
5:E:98:ARG:NH1	5:E:102:LYS:HG3	2.31	0.46
2:B:266:PRO:HG3	2:B:352:GLU:O	2.16	0.46
2:B:463:LYS:NZ	2:B:464:LYS:HE2	2.31	0.46
4:D:170:ASN:HB3	4:D:173:ARG:HG2	1.97	0.46
1:A:215:ILE:O	1:A:231:ARG:NH2	2.46	0.46
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.49	0.46
6:F:74:ILE:HG23	6:F:78:GLU:HG3	1.97	0.46
1:A:1065:MET:SD	1:A:1439:MET:HB2	2.56	0.46
7:G:51:GLY:HA2	7:G:54:ILE:HD11	1.98	0.46
15:P:2:G:H1	16:T:33:DC:H42	1.63	0.46
16:T:-18:DC:C2'	16:T:-17:DT:H71	2.45	0.46
1:A:409:ASP:OD1	1:A:410:ASN:N	2.49	0.46
2:B:25:PHE:HZ	2:B:534:LEU:HG	1.81	0.46
2:B:318:ASP:OD1	2:B:319:LYS:N	2.48	0.46
2:B:557:GLU:OE2	2:B:584:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:LEU:HD22	11:K:101:LEU:HD11	1.98	0.46
18:W:539:HIS:CE1	18:W:553:LEU:HD21	2.51	0.46
1:A:684:ILE:HG21	1:A:802:GLU:HG3	1.99	0.45
1:A:1061:HIS:O	1:A:1064:GLU:HG2	2.17	0.45
2:B:322:ALA:O	2:B:326:ILE:HG12	2.15	0.45
8:H:110:LYS:HE2	8:H:112:LYS:HE3	1.99	0.45
1:A:1390:HIS:O	1:A:1394:ARG:HD3	2.17	0.45
2:B:27:GLU:OE1	2:B:678:TRP:HB3	2.16	0.45
16:T:-72:DA:H1'	16:T:-71:DT:C6	2.51	0.45
16:T:32:DA:H1'	16:T:33:DC:H5"	1.98	0.45
1:A:912:ASP:OD1	1:A:912:ASP:N	2.44	0.45
1:A:1448:ILE:HD11	1:A:1453:LEU:HD11	1.97	0.45
2:B:505:ARG:NH1	2:B:524:GLN:O	2.32	0.45
14:N:-22:DA:C6	14:N:-21:DA:N1	2.85	0.45
5:E:46:CYS:HB3	5:E:50:GLY:HA2	1.99	0.45
16:T:-21:DC:C2'	16:T:-20:DC:C5	2.92	0.45
17:V:46:VAL:O	17:V:50:THR:N	2.44	0.45
2:B:250:TYR:HE2	2:B:262:LYS:HB2	1.82	0.45
7:G:113:ARG:NH1	18:W:563:GLU:OE1	2.49	0.45
14:N:-44:DG:C2'	14:N:-43:DT:H72	2.44	0.45
2:B:387:ASP:H	9:I:91:ARG:NH2	2.14	0.45
2:B:886:LYS:HG2	2:B:890:TYR:OH	2.17	0.45
2:B:436:ASN:C	2:B:438:ASN:H	2.20	0.44
18:W:451:GLN:HG3	18:W:458:THR:HA	1.98	0.44
2:B:640:ASP:OD1	2:B:640:ASP:N	2.50	0.44
18:W:763:TYR:HB3	18:W:766:LYS:HD3	2.00	0.44
1:A:1041:ARG:O	1:A:1044:PHE:N	2.50	0.44
7:G:81:PRO:HG3	7:G:106:LEU:HD22	1.99	0.44
14:N:54:DT:H2"	14:N:55:DC:C5	2.52	0.44
1:A:452:HIS:CE1	1:A:454:MET:HB2	2.52	0.44
3:C:258:VAL:HG21	11:K:42:LEU:HD21	2.00	0.44
14:N:12:DG:H2"	14:N:13:DT:C7	2.47	0.44
14:N:48:DG:H2"	14:N:49:DC:C6	2.53	0.44
1:A:779:GLY:HA3	2:B:509:ASN:HB2	1.99	0.44
1:A:880:GLU:O	1:A:957:PRO:HA	2.18	0.44
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	1.99	0.44
1:A:975:LEU:HD13	1:A:1039:LEU:HA	1.99	0.44
9:I:100:PHE:HB3	9:I:109:THR:HG23	1.99	0.44
14:N:-22:DA:H61	16:T:22:DT:H3	1.65	0.44
16:T:-31:DA:H2"	16:T:-30:DG:H8	1.82	0.44
2:B:221:ALA:O	2:B:223:SER:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:78:GLN:OE1	17:V:79:PRO:HD2	2.16	0.44
1:A:447:ARG:HB2	1:A:488:MET:HE3	1.98	0.44
2:B:254:ASP:H	2:B:259:ARG:NH2	2.13	0.44
5:E:99:ILE:HG13	5:E:131:ILE:HD11	2.00	0.44
14:N:8:DG:C6	16:T:-9:DA:N6	2.86	0.44
4:D:88:GLU:HA	4:D:91:LYS:HE3	2.00	0.44
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.00	0.44
2:B:257:THR:OG1	2:B:258:GLY:N	2.50	0.44
1:A:948:VAL:O	5:E:200:ARG:NH1	2.48	0.43
2:B:691:ASP:OD1	2:B:691:ASP:N	2.41	0.43
8:H:25:ARG:HD3	8:H:41:ASP:OD1	2.18	0.43
14:N:-47:DC:H2"	14:N:-46:DT:C5	2.53	0.43
14:N:8:DG:O6	16:T:-9:DA:N6	2.51	0.43
10:J:63:ASN:OD1	10:J:64:PRO:HD2	2.19	0.43
3:C:15:ASP:OD1	3:C:15:ASP:N	2.47	0.43
1:A:1389:ARG:O	1:A:1393:ASN:HB2	2.18	0.43
7:G:115:ILE:HG23	7:G:163:ILE:HD11	2.01	0.43
1:A:38:PRO:HA	1:A:271:LEU:HD23	2.01	0.43
2:B:733:SER:HB3	2:B:736:HIS:CE1	2.54	0.43
17:V:67:TRP:NE1	18:W:217:LEU:O	2.51	0.43
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.90	0.43
1:A:889:GLY:O	1:A:941:ARG:NH2	2.51	0.43
2:B:330:GLY:HA3	2:B:344:TYR:HE2	1.84	0.43
16:T:-67:DA:C6	16:T:-66:DA:C6	3.06	0.43
18:W:250:ARG:NH2	18:W:284:ASP:OD2	2.50	0.43
18:W:344:LEU:HD12	18:W:349:GLU:HB2	1.99	0.43
1:A:1343:GLY:HA2	5:E:182:PRO:HD2	2.01	0.43
2:B:283:VAL:HG13	2:B:283:VAL:O	2.18	0.43
5:E:160:LYS:NZ	5:E:192:GLY:O	2.50	0.43
14:N:38:DG:C2	16:T:-37:DG:C2	3.06	0.43
1:A:318:LYS:HE3	16:T:35:DC:N3	2.34	0.43
3:C:248:ILE:HG21	11:K:102:ASP:HB2	2.01	0.43
14:N:-44:DG:H2"	14:N:-43:DT:OP2	2.19	0.43
14:N:2:DG:N2	16:T:-1:DG:H22	2.16	0.43
14:N:28:DA:H2"	14:N:29:DG:C8	2.54	0.43
15:P:8:C:C2	16:T:28:DG:C2	3.07	0.43
1:A:252:ALA:HA	1:A:258:GLN:HA	2.00	0.43
2:B:262:LYS:HB3	2:B:271:ASP:HB3	2.01	0.43
18:W:322:ARG:NE	18:W:343:VAL:H	2.17	0.43
1:A:815:PHE:O	1:A:819:MET:HG3	2.19	0.42
1:A:844:LYS:HD2	1:A:844:LYS:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:12:CYS:HA	17:V:50:THR:HA	2.01	0.42
18:W:543:ILE:HD11	18:W:581:ILE:HG13	2.01	0.42
1:A:473:LEU:HD21	2:B:835:GLN:HB2	2.00	0.42
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.85	0.42
12:L:60:LYS:HB3	12:L:60:LYS:HE3	1.87	0.42
2:B:1156:ASP:O	2:B:1197:PRO:HA	2.19	0.42
16:T:-28:DT:C6	16:T:-27:DC:C5	3.07	0.42
16:T:-22:DA:H2"	16:T:-21:DC:C5	2.53	0.42
2:B:279:ARG:NH1	2:B:316:ILE:O	2.52	0.42
2:B:299:ASP:OD2	2:B:385:ARG:NH1	2.30	0.42
2:B:479:TYR:CE2	2:B:778:MET:HG2	2.55	0.42
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.02	0.42
5:E:176:ARG:HD3	5:E:214:LEU:HD11	2.02	0.42
14:N:-44:DG:H2"	14:N:-43:DT:C7	2.48	0.42
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.02	0.42
1:A:1201:ARG:HA	1:A:1238:LEU:HD12	2.01	0.42
1:A:1221:VAL:HG21	1:A:1274:ILE:HD12	2.00	0.42
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.51	0.42
5:E:42:ARG:HG3	5:E:46:CYS:SG	2.59	0.42
18:W:539:HIS:HB2	18:W:584:THR:HA	2.02	0.42
1:A:421:ARG:HB3	1:A:424:ASP:HB2	2.01	0.42
2:B:85:SER:OG	2:B:114:PRO:HD2	2.19	0.42
6:F:81:THR:OG1	6:F:144:GLU:OE1	2.35	0.42
2:B:606:VAL:HG22	2:B:621:THR:HG22	2.02	0.42
7:G:165:GLU:H	7:G:168:LEU:HD12	1.85	0.42
15:P:-5:C:C6	18:W:748:ARG:HB2	2.55	0.42
17:V:80:GLY:HA2	18:W:244:LEU:HD21	2.02	0.42
18:W:480:PRO:HA	18:W:498:VAL:HG12	2.02	0.42
1:A:691:VAL:HG11	1:A:795:PRO:HG3	2.02	0.41
9:I:29:CYS:SG	9:I:30:ARG:N	2.92	0.41
16:T:-37:DG:H2'	16:T:-36:DT:H72	2.02	0.41
1:A:473:LEU:CD2	2:B:835:GLN:HB2	2.50	0.41
1:A:1210:THR:HG22	1:A:1212:ASN:H	1.86	0.41
2:B:764:SER:OG	2:B:765:PRO:HD3	2.19	0.41
14:N:-21:DA:H61	16:T:21:DT:H3	1.69	0.41
18:W:329:LYS:HB2	18:W:434:ASN:HA	2.02	0.41
2:B:33:GLN:HG2	2:B:34:GLN:N	2.36	0.41
2:B:763:GLN:HG2	2:B:765:PRO:HD2	2.01	0.41
8:H:6:PHE:HB3	8:H:59:LEU:HB2	2.03	0.41
14:N:8:DG:N2	16:T:-7:DG:N3	2.69	0.41
18:W:422:TYR:HB3	18:W:427:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:ILE:HD13	2:B:375:VAL:HG11	2.02	0.41
3:C:74:GLU:O	3:C:246:ARG:NH2	2.39	0.41
9:I:94:ASP:OD1	9:I:94:ASP:N	2.49	0.41
13:M:39:ASP:HB3	13:M:44:ILE:HG13	2.03	0.41
5:E:36:GLN:HE21	5:E:36:GLN:HB3	1.69	0.41
14:N:66:DT:H2'	14:N:67:DT:C6	2.55	0.41
18:W:349:GLU:HA	18:W:431:ARG:HA	2.02	0.41
1:A:914:ILE:HG13	1:A:917:ALA:HB2	2.01	0.41
1:A:976:ASP:O	1:A:979:LYS:NZ	2.48	0.41
9:I:29:CYS:HB3	9:I:32:CYS:SG	2.59	0.41
16:T:29:DA:H2'	16:T:30:DA:C8	2.56	0.41
2:B:350:GLN:HE22	2:B:361:GLU:HG2	1.86	0.41
2:B:1153:GLU:OE1	2:B:1153:GLU:N	2.53	0.41
3:C:149:ASN:OD1	3:C:149:ASN:N	2.54	0.41
5:E:3:ASP:HA	5:E:6:ARG:HG2	2.01	0.41
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.78	0.41
8:H:8:ASP:OD1	8:H:9:ILE:N	2.48	0.41
15:P:-1:G:H2'	15:P:0:G:H8	1.86	0.41
18:W:614:ARG:NH2	18:W:616:GLN:HE21	2.19	0.41
3:C:259:LEU:HD13	11:K:91:CYS:HB2	2.03	0.41
16:T:-72:DA:H2"	16:T:-71:DT:OP2	2.21	0.41
1:A:109:ASN:HB2	1:A:168:CYS:SG	2.61	0.41
1:A:471:LEU:HD23	1:A:475:VAL:HG23	2.03	0.41
1:A:1150:SER:OG	1:A:1198:GLU:OE1	2.29	0.41
1:A:1314:ILE:HB	1:A:1337:GLU:OE1	2.21	0.41
2:B:285:PRO:HB2	9:I:11:ASN:HD22	1.86	0.41
2:B:425:MET:O	2:B:429:ILE:HG13	2.21	0.41
2:B:575:VAL:O	2:B:578:VAL:HG22	2.20	0.41
2:B:632:ILE:HD11	2:B:688:GLU:HB3	2.03	0.41
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.79	0.41
3:C:251:LEU:HD12	3:C:251:LEU:HA	1.92	0.41
4:D:53:LEU:HD13	4:D:147:SER:HB3	2.02	0.41
14:N:-42:DG:C8	14:N:-41:DT:C7	3.04	0.41
16:T:-40:DG:C8	16:T:-39:DT:H73	2.56	0.41
16:T:-18:DC:H2'	16:T:-17:DT:H71	2.02	0.41
18:W:540:VAL:HG11	18:W:554:ILE:HD11	2.01	0.41
1:A:883:THR:HA	1:A:954:HIS:O	2.20	0.41
1:A:945:ARG:HG3	1:A:1301:TYR:OH	2.21	0.41
2:B:71:ILE:HG12	2:B:127:ILE:HG22	2.02	0.41
8:H:38:LEU:HD13	8:H:124:LEU:HD13	2.03	0.41
11:K:39:ASP:OD1	11:K:39:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-22:DA:N6	16:T:22:DT:H3	2.19	0.41
14:N:34:DC:C4	14:N:35:DT:C4	3.09	0.41
16:T:-19:DG:H2"	16:T:-18:DC:C5	2.56	0.41
1:A:636:ARG:HG3	1:A:880:GLU:OE2	2.21	0.40
1:A:985:ILE:N	1:A:986:PRO:HD2	2.36	0.40
1:A:1295:PRO:HD3	1:A:1301:TYR:CE1	2.56	0.40
18:W:492:ASN:OD1	18:W:493:HIS:N	2.54	0.40
1:A:390:THR:O	1:A:394:ARG:HG2	2.20	0.40
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.88	0.40
2:B:1174:ASN:OD1	2:B:1177:LYS:HB2	2.20	0.40
3:C:135:ARG:NE	3:C:136:ASP:OD2	2.50	0.40
6:F:93:ILE:HD13	6:F:93:ILE:HA	1.97	0.40
9:I:62:ILE:HD12	9:I:62:ILE:HA	1.93	0.40
1:A:995:LEU:HD22	1:A:1048:LEU:HD22	2.03	0.40
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.55	0.40
2:B:358:THR:HG1	2:B:363:PHE:HD2	1.68	0.40
12:L:33:CYS:SG	12:L:34:GLY:N	2.95	0.40
14:N:12:DG:H2"	14:N:13:DT:C5	2.56	0.40
1:A:231:ARG:HB3	1:A:234:TRP:CD2	2.56	0.40
3:C:262:LEU:HD11	11:K:87:LEU:HD23	2.03	0.40
11:K:55:ASP:OD2	11:K:89:ARG:NH2	2.54	0.40
14:N:32:DG:N1	16:T:-33:DA:C2	2.90	0.40
14:N:66:DT:H2'	14:N:67:DT:C5	2.57	0.40
16:T:20:DT:C6	16:T:21:DT:H73	2.56	0.40
18:W:598:LEU:HD12	18:W:599:HIS:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1392/1743 (80%)	1355 (97%)	36 (3%)	1 (0%)	51 85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	167 (98%)	3 (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%)	167 (99%)	2 (1%)	0	100	100
8	H	129/145 (89%)	125 (97%)	4 (3%)	0	100	100
9	I	109/115 (95%)	107 (98%)	2 (2%)	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	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	90/139 (65%)	86 (96%)	4 (4%)	0	100	100
26	e	95/139 (68%)	93 (98%)	1 (1%)	1 (1%)	14	52
27	b	79/106 (74%)	76 (96%)	3 (4%)	0	100	100
27	f	76/106 (72%)	73 (96%)	3 (4%)	0	100	100
28	c	94/133 (71%)	93 (99%)	1 (1%)	0	100	100
28	g	96/133 (72%)	93 (97%)	3 (3%)	0	100	100
29	d	90/129 (70%)	86 (96%)	4 (4%)	0	100	100
29	h	91/129 (70%)	90 (99%)	1 (1%)	0	100	100
30	j	466/1008 (46%)	433 (93%)	28 (6%)	5 (1%)	14	52
31	k	423/531 (80%)	404 (96%)	18 (4%)	1 (0%)	47	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9441/13005 (73%)	9198 (97%)	235 (2%)	8 (0%)	54 85

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	960	VAL
30	j	964	PRO
30	j	939	PHE
30	j	951	GLU
30	j	969	VAL
30	j	653	GLU
31	k	215	PHE
26	e	43	PRO

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 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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	V	90/92 (98%)	90 (100%)	0	100 100
18	W	480/796 (60%)	480 (100%)	0	100 100
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
24	v	325/369 (88%)	325 (100%)	0	100 100
25	x	190/354 (54%)	190 (100%)	0	100 100
26	a	78/112 (70%)	78 (100%)	0	100 100
26	e	82/112 (73%)	82 (100%)	0	100 100
27	b	66/81 (82%)	66 (100%)	0	100 100
27	f	63/81 (78%)	63 (100%)	0	100 100
28	c	76/102 (74%)	76 (100%)	0	100 100
28	g	77/102 (76%)	77 (100%)	0	100 100
29	d	78/107 (73%)	78 (100%)	0	100 100
29	h	79/107 (74%)	79 (100%)	0	100 100
30	j	400/910 (44%)	398 (100%)	2 (0%)	88 93
31	k	392/474 (83%)	389 (99%)	3 (1%)	81 89
All	All	8474/11447 (74%)	8459 (100%)	15 (0%)	93 96

All (15) 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
19	m	514	LYS
23	u	124	ARG
30	j	939	PHE

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Mol	Chain	Res	Type
30	j	940	LEU
31	k	143	ASN
31	k	253	TYR
31	k	287	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	737	ASN
8	H	44	ASN
9	I	11	ASN
18	W	433	GLN
19	m	955	ASN
20	n	232	GLN
25	x	296	ASN
27	b	25	ASN
28	c	73	ASN
30	j	750	GLN
31	k	125	ASN
31	k	127	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	19/19 (100%)	6 (31%)	1 (5%)

All (6) RNA backbone outliers are listed below:

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

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	-7	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.

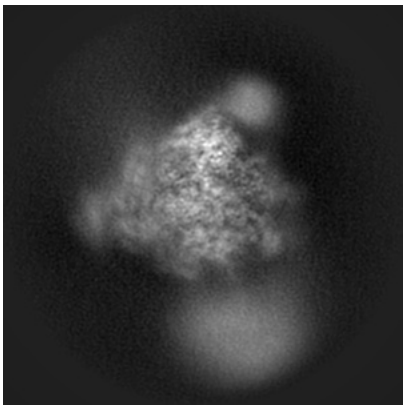
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33441. These allow visual inspection of the internal detail of the map and identification of artifacts.

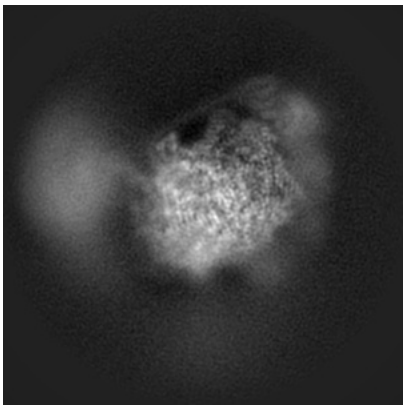
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

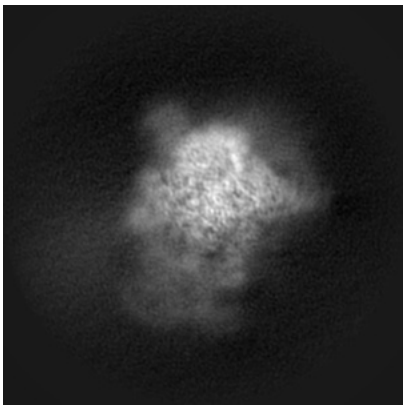
6.1.1 Primary map



X

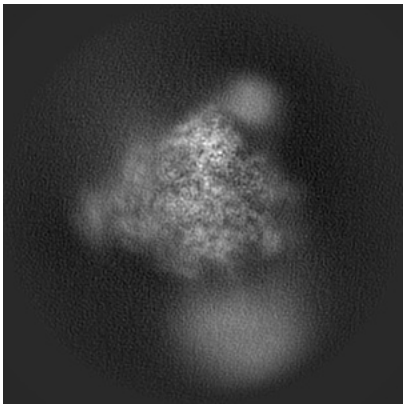


Y

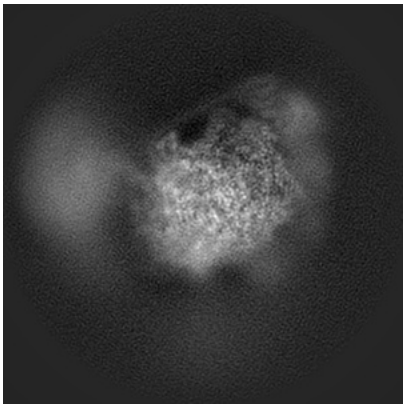


Z

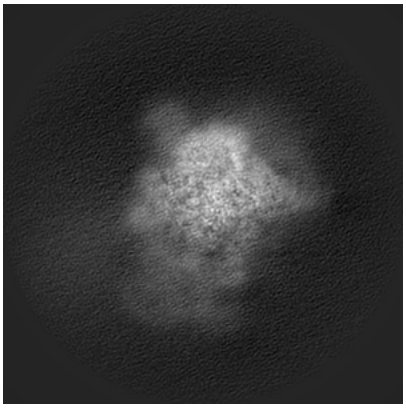
6.1.2 Raw map



X



Y

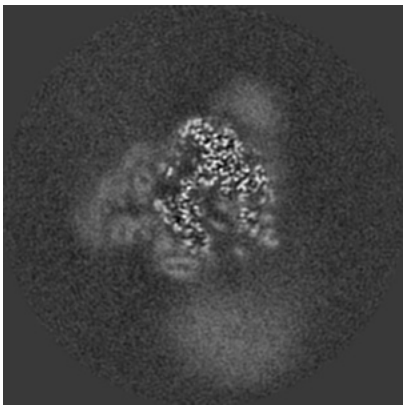


Z

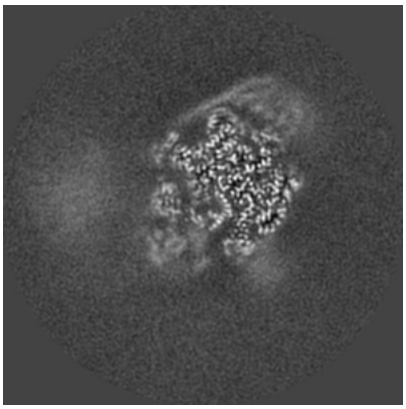
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

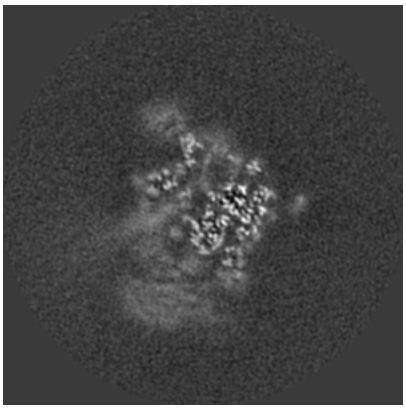
6.2.1 Primary map



X Index: 120

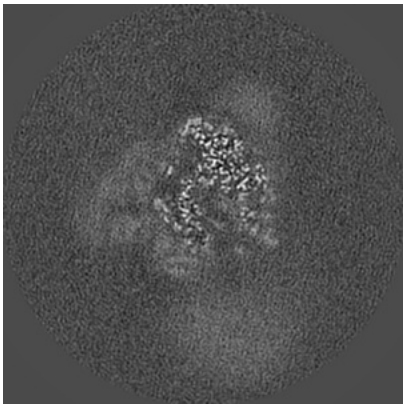


Y Index: 120

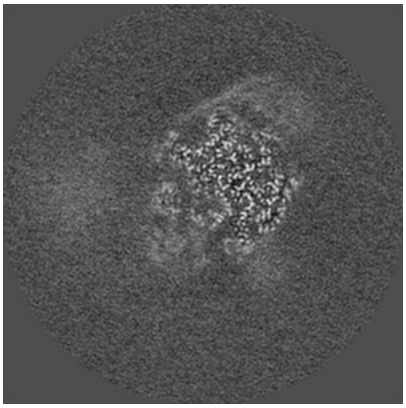


Z Index: 120

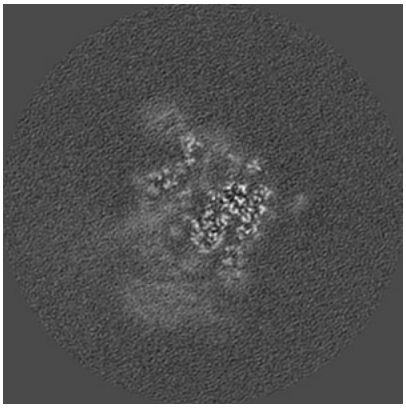
6.2.2 Raw map



X Index: 120



Y Index: 120

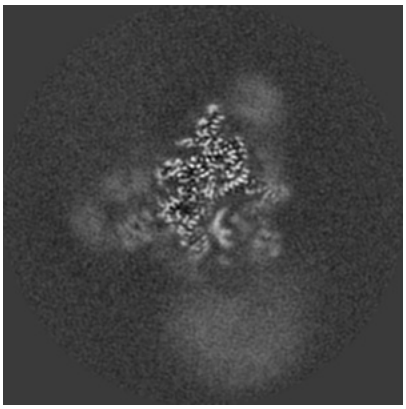


Z Index: 120

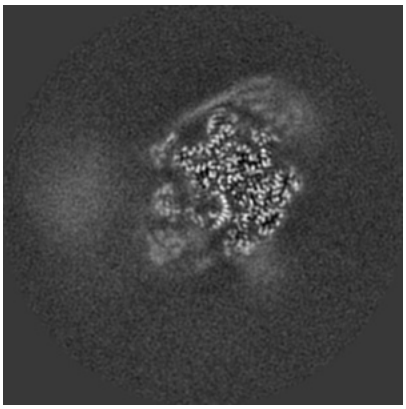
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

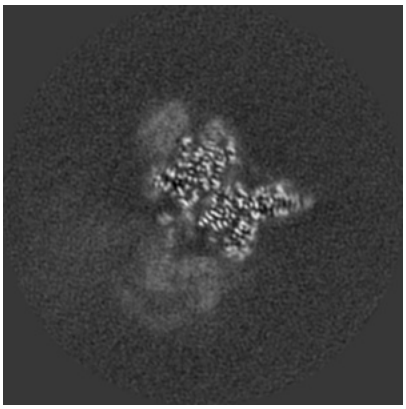
6.3.1 Primary map



X Index: 127

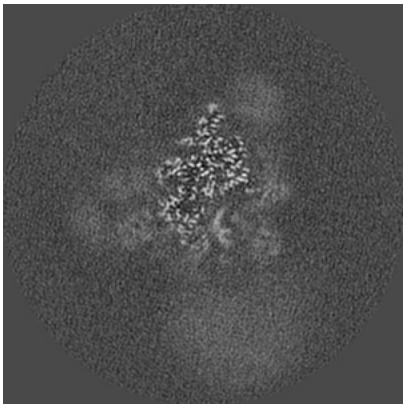


Y Index: 121

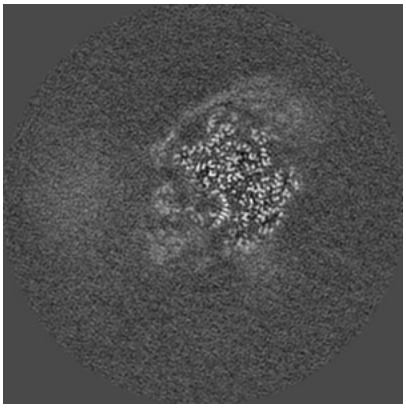


Z Index: 129

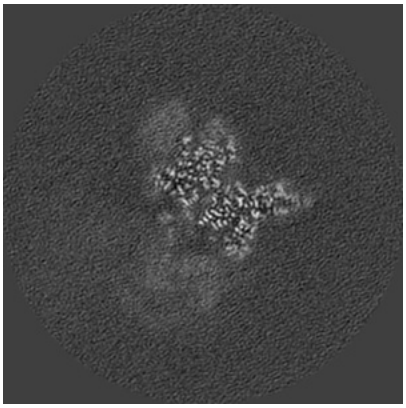
6.3.2 Raw map



X Index: 127



Y Index: 121

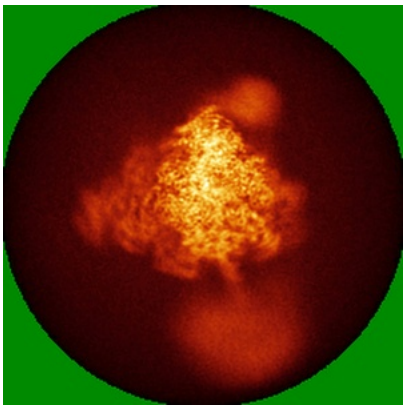


Z Index: 129

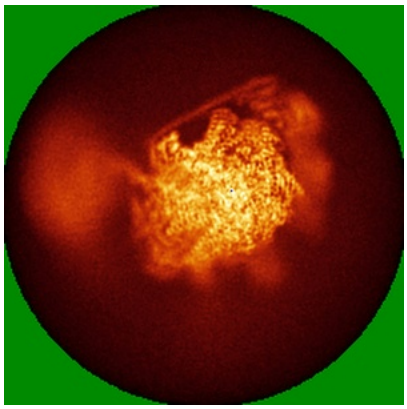
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

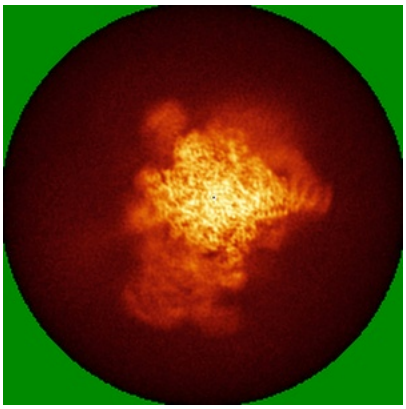
6.4.1 Primary map



X

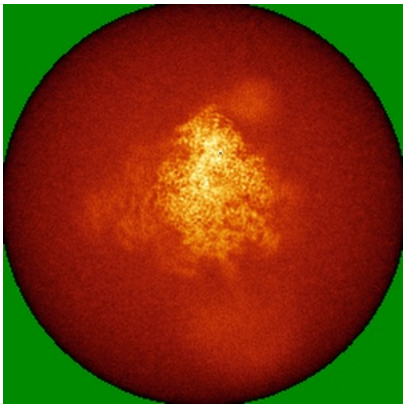


Y

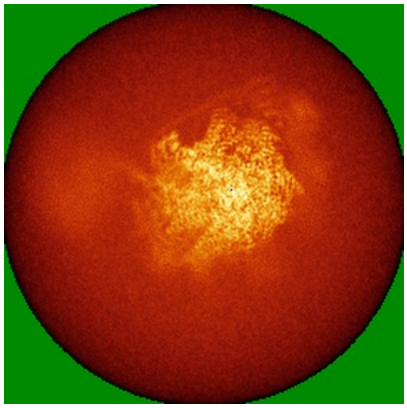


Z

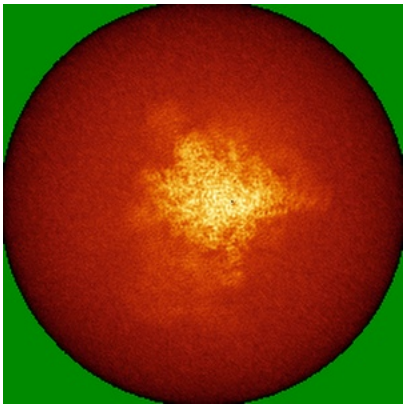
6.4.2 Raw map



X



Y

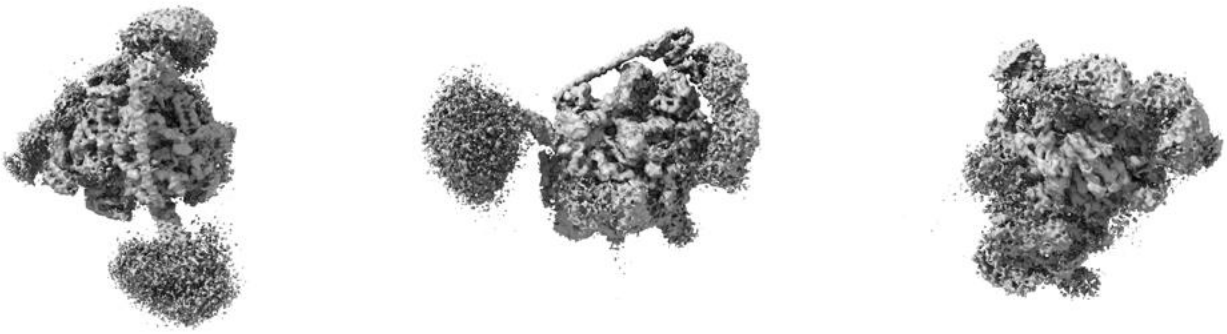


Z

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



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.

6.5.2 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.

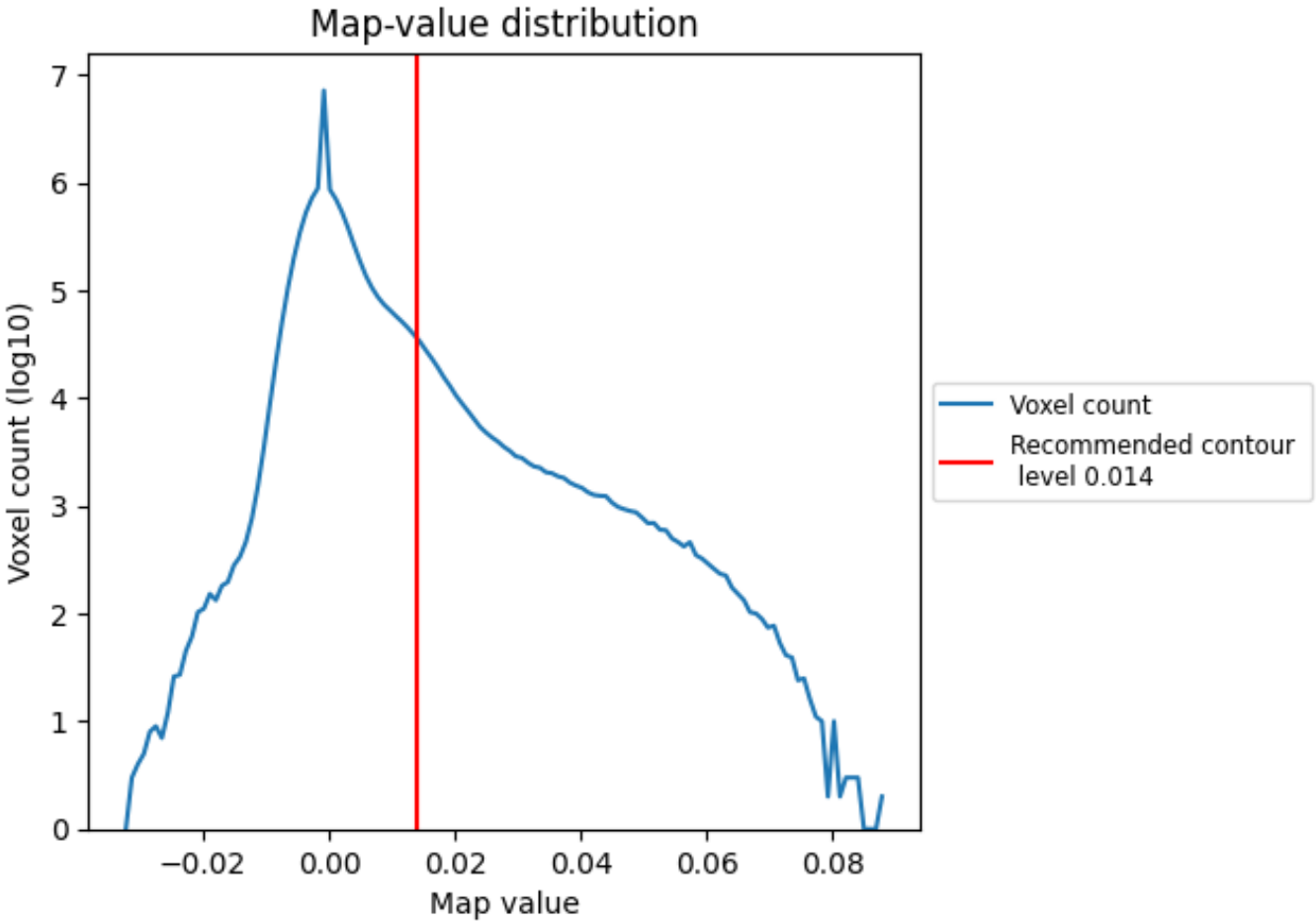
6.6 Mask visualisation (i)

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

7 Map analysis

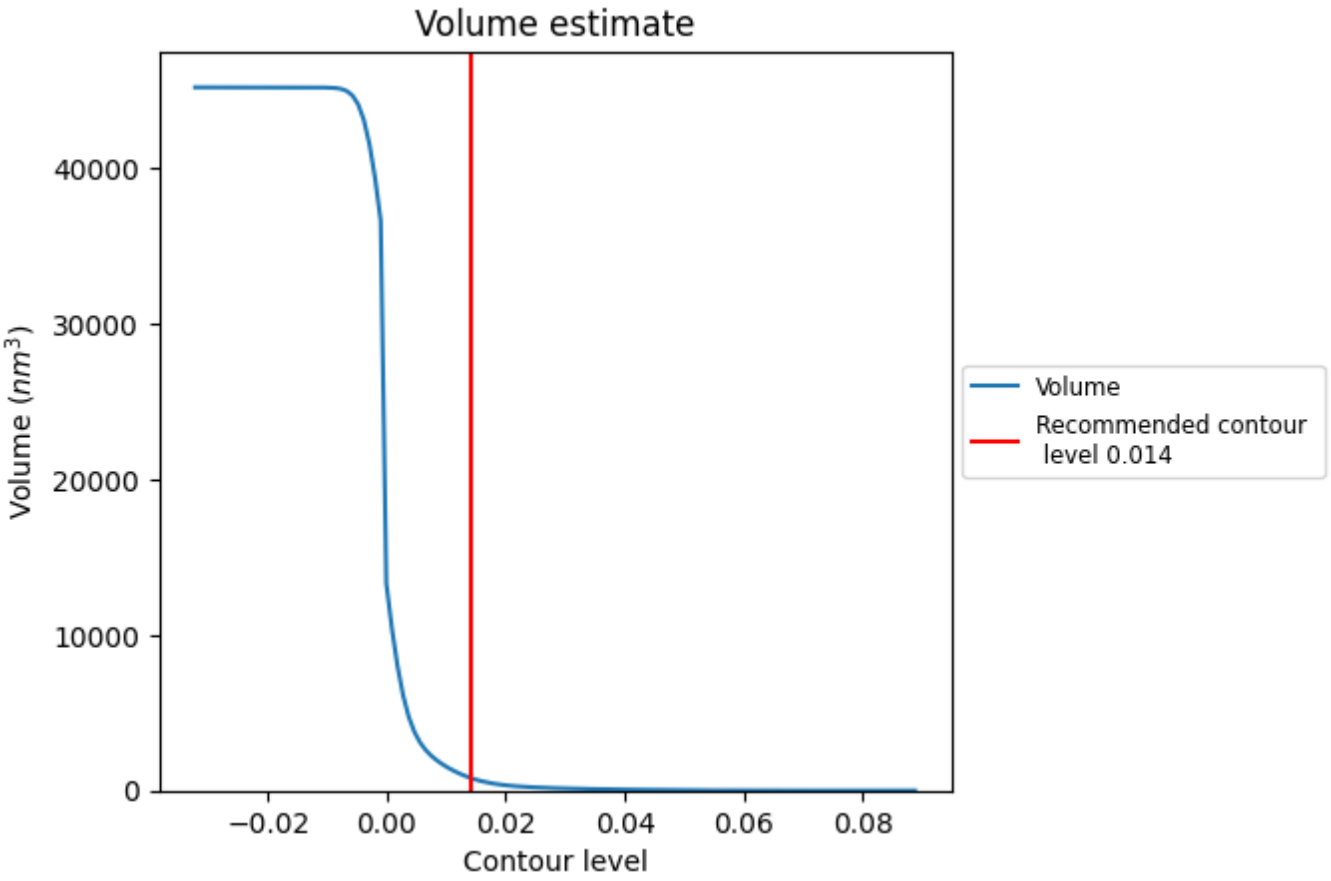
This section contains the results of statistical analysis of the map.

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.

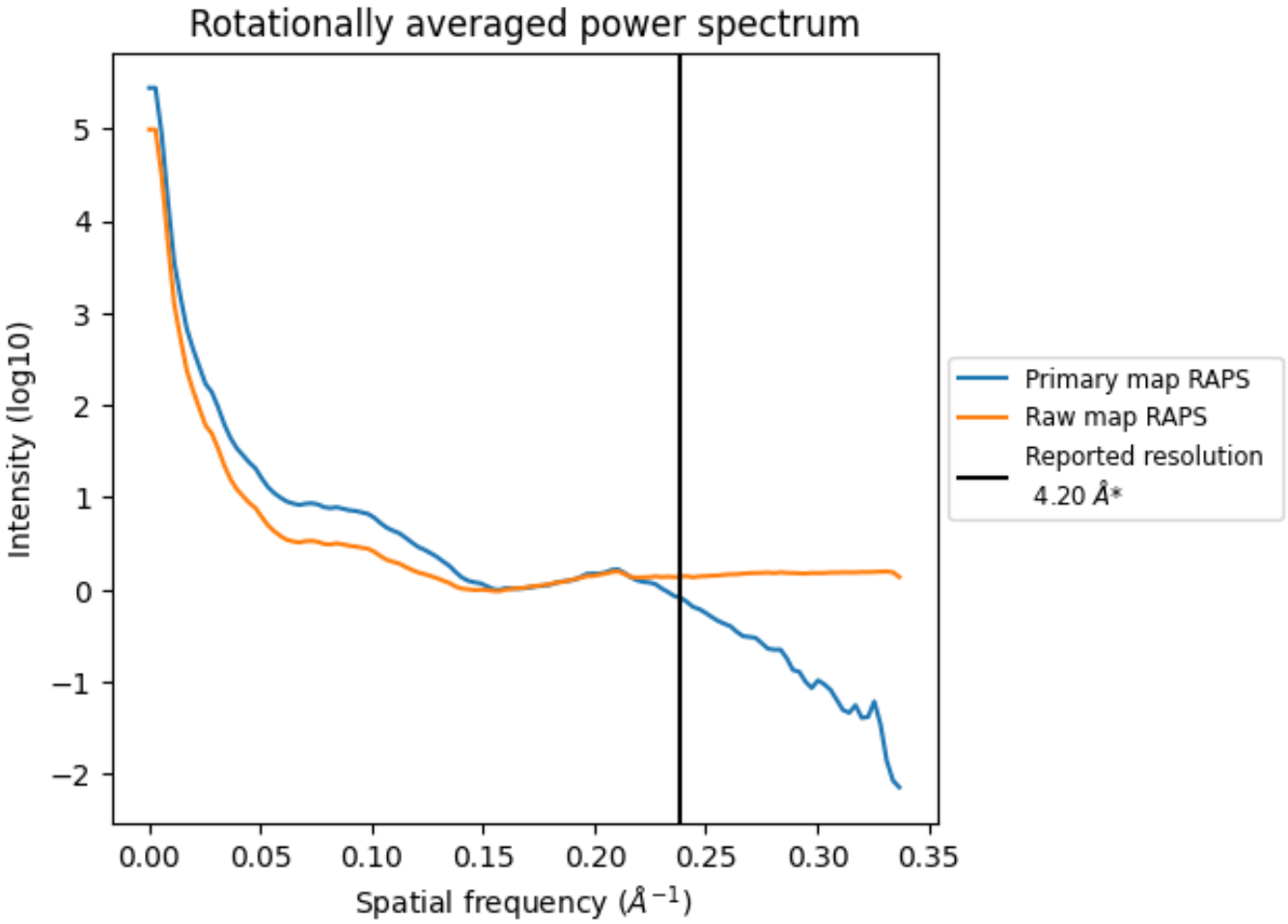
7.2 Volume estimate



The volume at the recommended contour level is 822 nm^3; this corresponds to an approximate mass of 743 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)

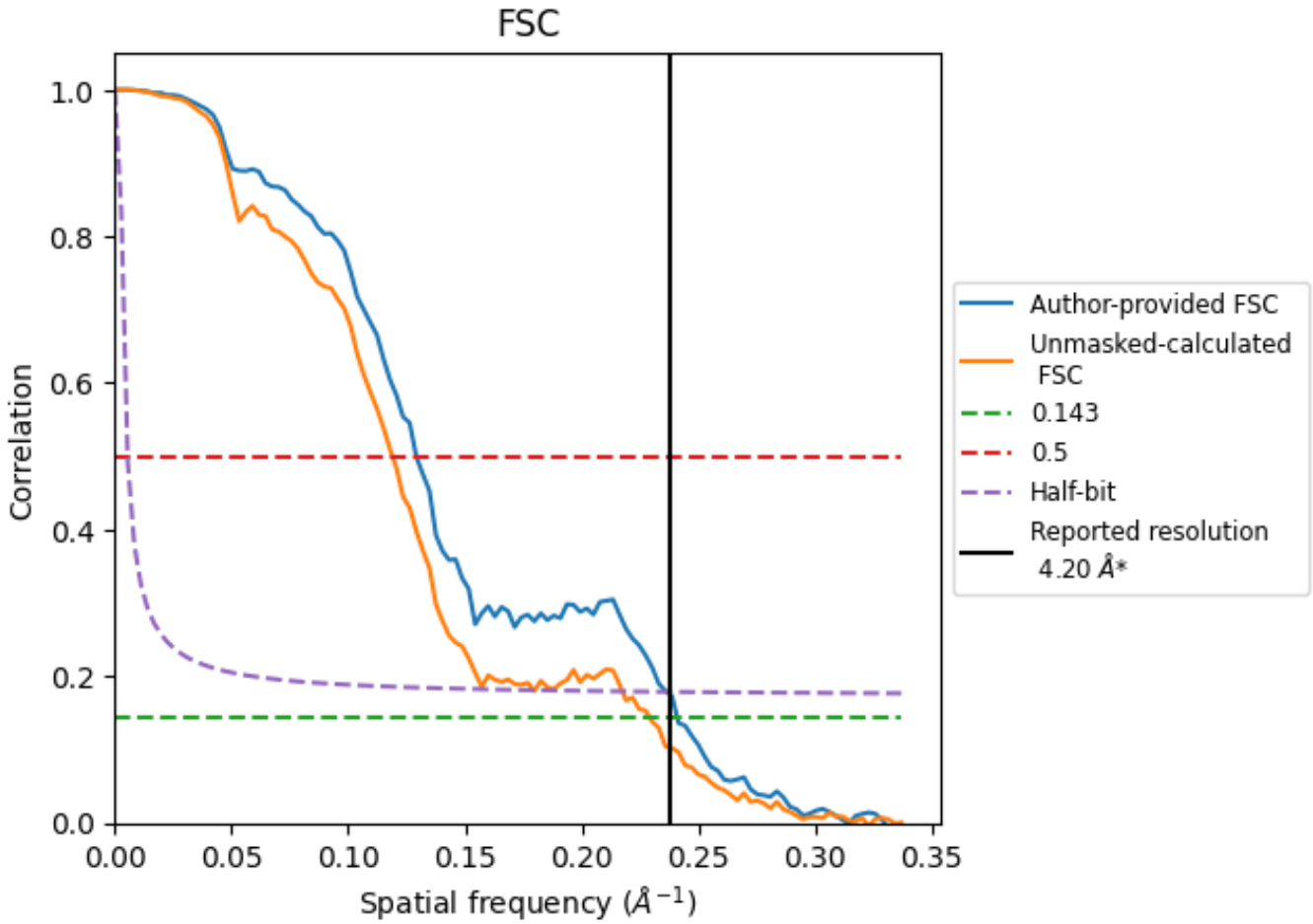


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

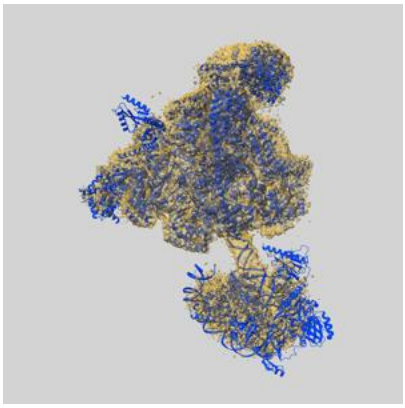
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.15	7.75	4.23
Unmasked-calculated*	4.36	8.40	5.57

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

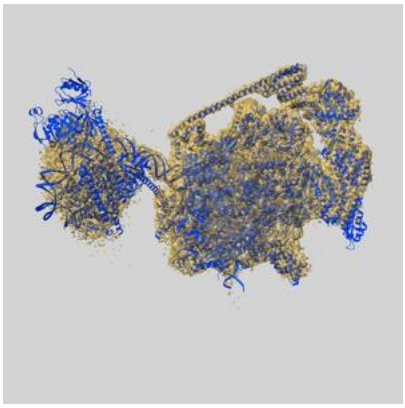
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33441 and PDB model 7XT7. Per-residue inclusion information can be found in section 3 on page 16.

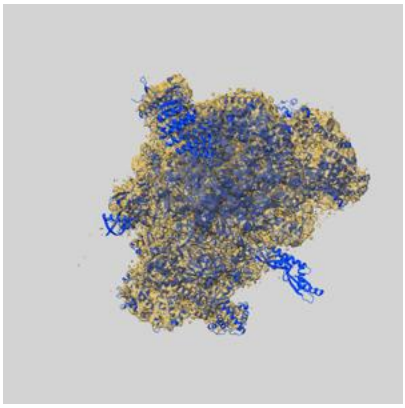
9.1 Map-model overlay



X



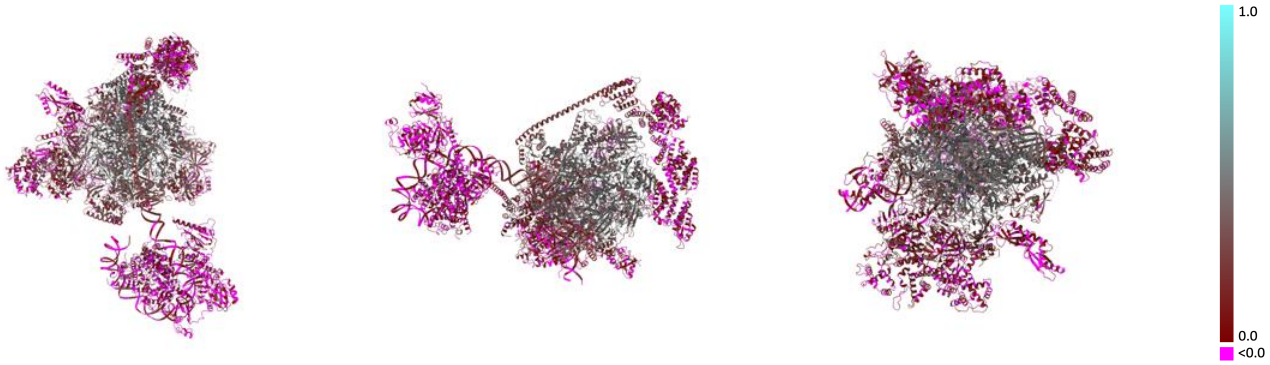
Y



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.

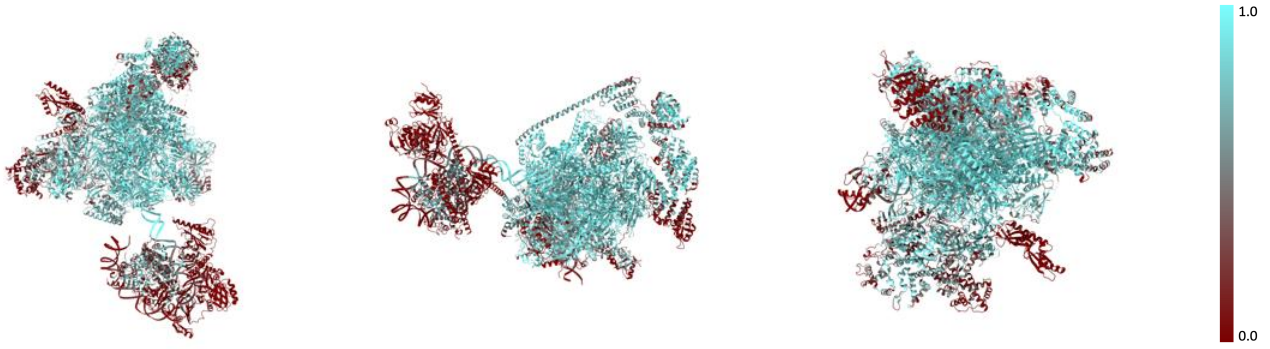
9.2 Q-score mapped to coordinate model (i)



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.

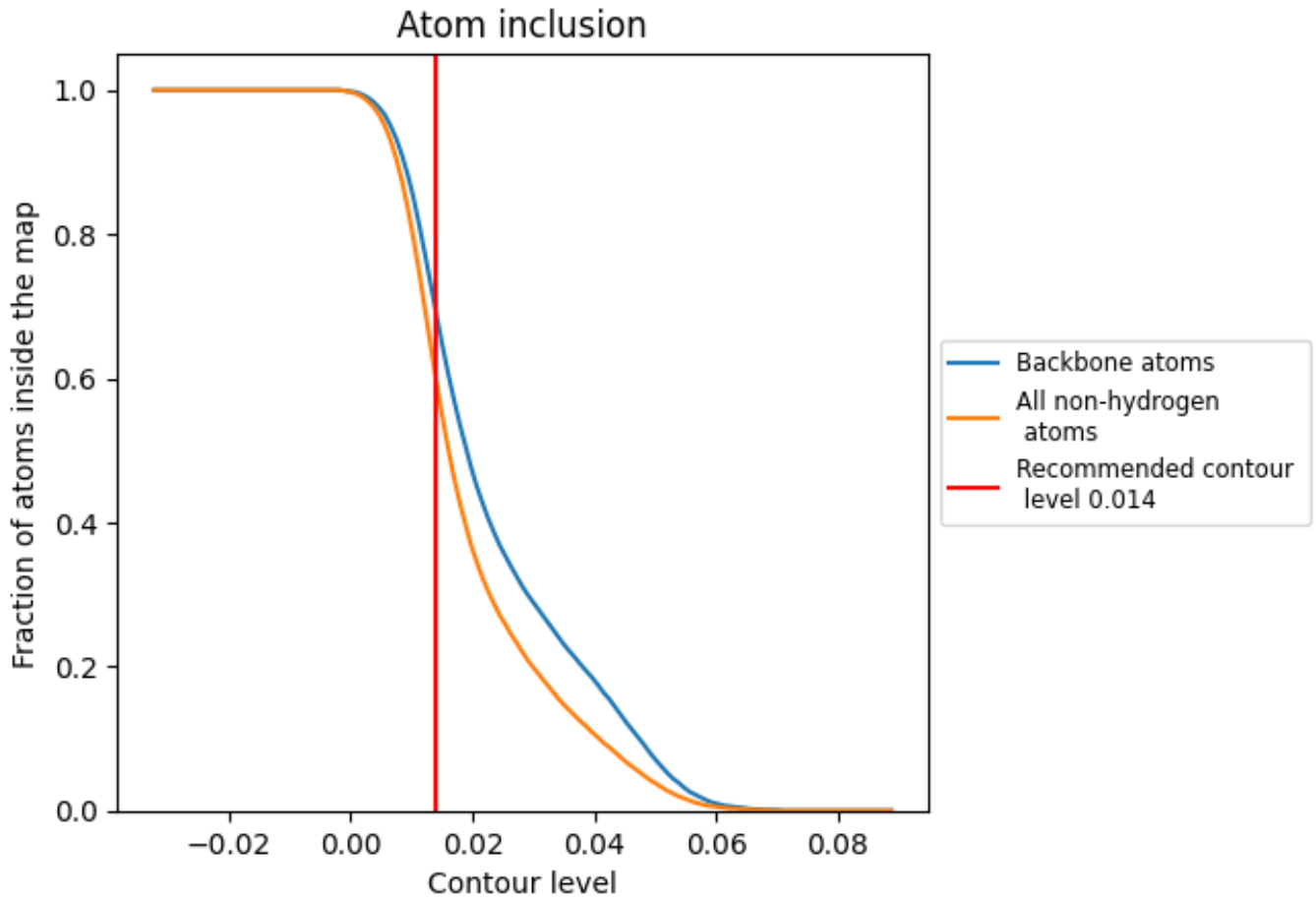
9.3 Atom inclusion mapped to coordinate model (i)



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, 69% of all backbone atoms, 60% 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	0.5990	0.2070
A	0.8990	0.4130
B	0.8980	0.4220
C	0.8980	0.4370
D	0.7310	0.1980
E	0.9270	0.3900
F	0.9270	0.4500
G	0.7920	0.2670
H	0.8790	0.4240
I	0.8240	0.2600
J	0.8960	0.4370
K	0.9210	0.4320
L	0.9190	0.4140
M	0.7540	0.1560
N	0.4210	0.0810
P	0.8670	0.2980
T	0.4280	0.1120
V	0.8420	0.1120
W	0.6310	0.1700
a	0.3400	-0.0220
b	0.5020	0.0350
c	0.4690	0.0370
d	0.4470	-0.0070
e	0.3510	0.0080
f	0.4760	0.0200
g	0.3510	0.0400
h	0.3260	0.0350
j	0.0400	0.0170
k	0.0300	0.0040
m	0.3720	0.0820
n	0.6930	0.1790
q	0.5490	0.0930
r	0.3990	0.1240
u	0.5080	0.1530
v	0.4210	0.0850
x	0.6520	0.2290