



## Full wwPDB EM Validation Report ⓘ

Oct 4, 2022 – 02:44 AM JST

PDB ID : 7XSX  
EMDB ID : EMD-33436  
Title : RNA polymerase II elongation complex transcribing a nucleosome (EC49)  
Authors : Ehara, H.; Kujirai, T.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.  
Deposited on : 2022-05-15  
Resolution : 3.80 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](mailto: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>.

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

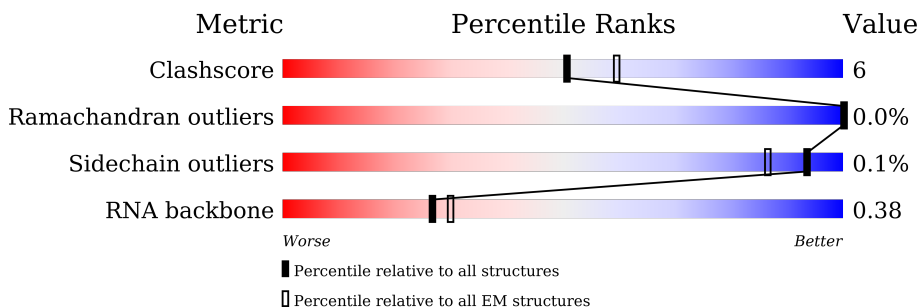
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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  $\geq 3$ , 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	70% 10% 19%
2	B	1227	80% 15% 5%
3	C	304	77% 9% 13%
4	D	186	6% 85% 8% 6%
5	E	214	84% 15%
6	F	155	50% 5% 46%
7	G	171	7% 83% 17%

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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	79% 17%
12	L	72	56% 7% 38%
13	M	113	5% 47% 10% 43%
14	N	198	18% 14% 31% 51%
15	P	19	21% 58% 21%
16	T	198	21% 19% 32% 45%
17	V	108	5% 73% 25%
18	W	911	11% 49% 10% 41%
19	m	1503	36% 79% 21%
20	n	417	33% 67%
21	q	1084	25% 86% 14%
22	r	544	19% 49% 51%
23	u	459	11% 45% 55%
24	v	396	34% 88% 12%
25	x	395	52% 48%
26	a	139	55% 45%
26	e	139	32% 67% 33%
27	b	106	7% 78% 22%
27	f	106	26% 74% 26%
28	c	133	65% 77% 23%
28	g	133	20% 52% 47%
29	d	129	43% 74% 26%

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Mol	Chain	Length	Quality of chain
29	h	129	
30	j	956	
31	k	531	

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 81134 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
			Total	C	N	O	S		
13	M	64	505	318	82	99	6	0	0

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
			Total	C	N	O	P		
14	N	97	2007	949	377	584	97	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	T	108	2202	1045	407	642	108	0	0

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

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

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
			Total	C	N	O	S		
18	W	533	4232	2666	752	812	2	0	0

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
			Total	C	N	O	S		
19	m	1187	9730	6162	1663	1877	28	0	0

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
			Total	C	N	O	S		
20	n	139	1115	716	193	202	4	0	0

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
			Total	C	N	O	S		
21	q	930	7552	4805	1283	1439	25	0	0



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
			Total	C	N	O	S		
22	r	266	2139	1342	374	412	11	0	0

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
			Total	C	N	O	S		
23	u	208	1707	1063	304	337	3	0	0

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
			Total	C	N	O	S		
24	v	349	2878	1835	510	528	5	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-2	GLY	-	expression tag	UNP C4R997

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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	
			Total	C	N	O			S
25	x	205	1682	1086	287	307	2	0	0

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
			Total	C	N	O	S		
26	a	76	615	390	115	108	2	0	0
26	e	93	757	477	146	132	2	0	0

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
			Total	C	N	O	S		
27	b	83	662	418	129	114	1	0	0
27	f	78	619	391	120	107	1	0	0

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	103	Total	C	N	O	0	0
			796	502	155	139		
28	g	70	Total	C	N	O	0	0
			544	342	109	93		

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	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
29	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

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	471	Total	C	N	O	S	0	0
			3832	2434	666	719	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
			Total	C	N	O	S		
31	k	429	3502	2215	613	664	10	0	0

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

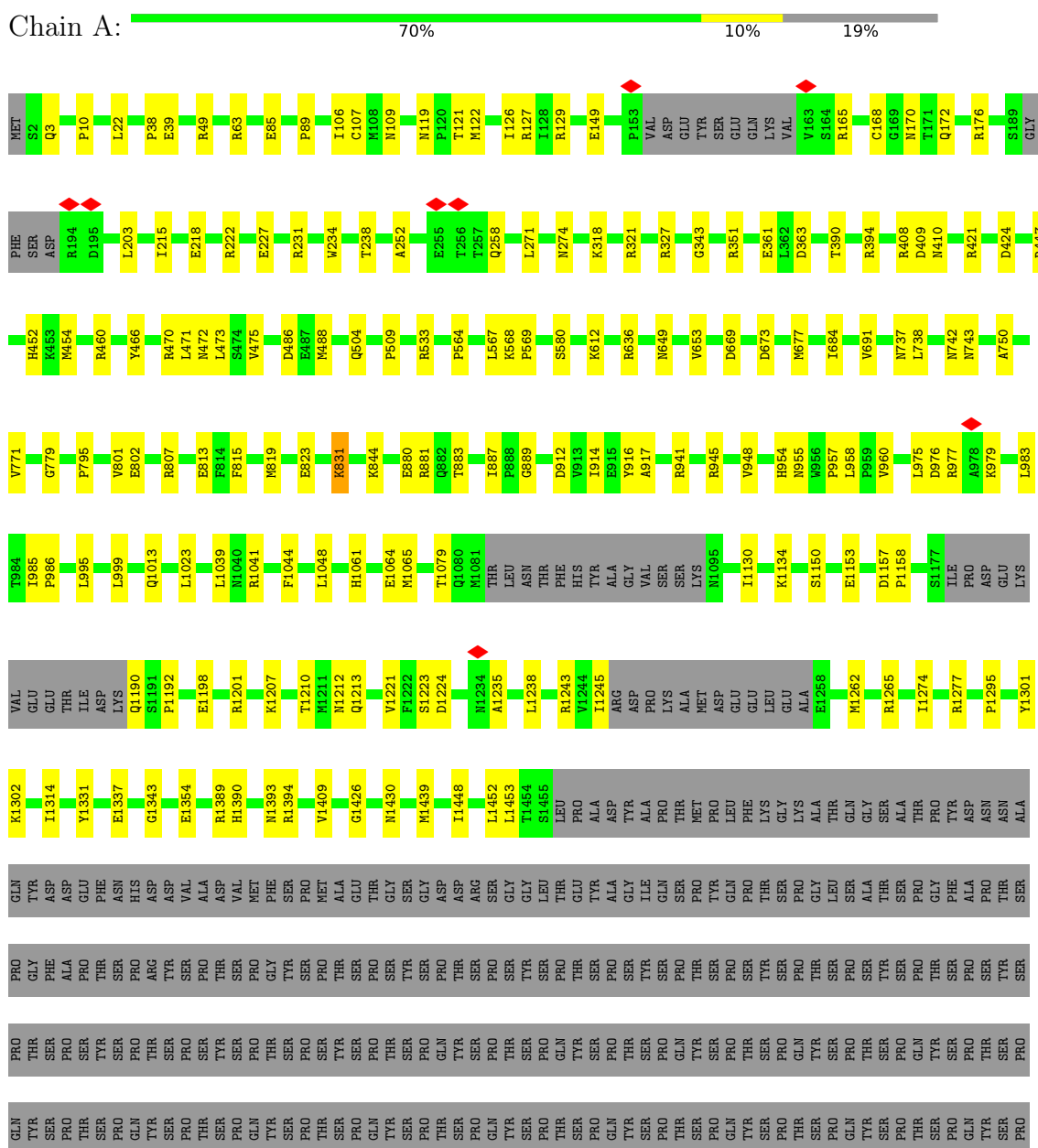
- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

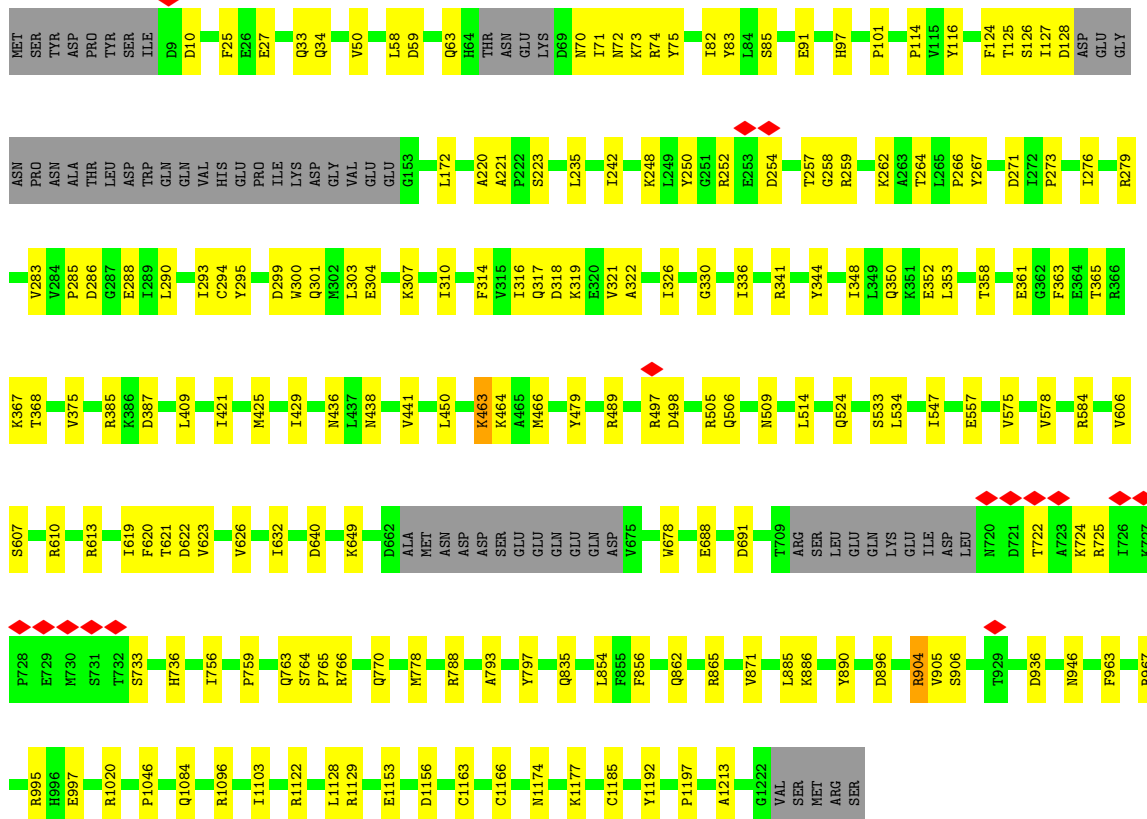




ALA  
SER  
PRO  
GLN  
TYR  
PRO  
SER  
PRO  
SER  
ARG  
HIS  
SER  
PRO  
ASN  
GLY  
GLU  
GLU  
GLY  
GLU

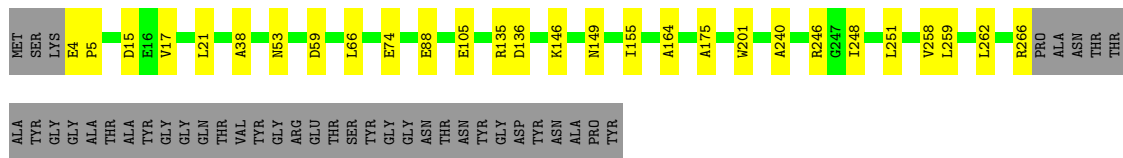
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



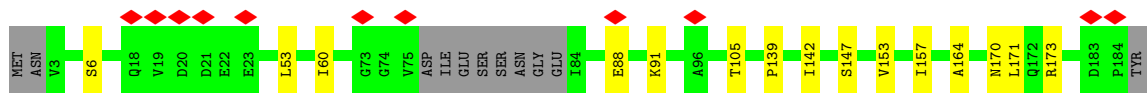
• Molecule 3: RNA polymerase II third largest subunit B44, part of central core

Chain C:

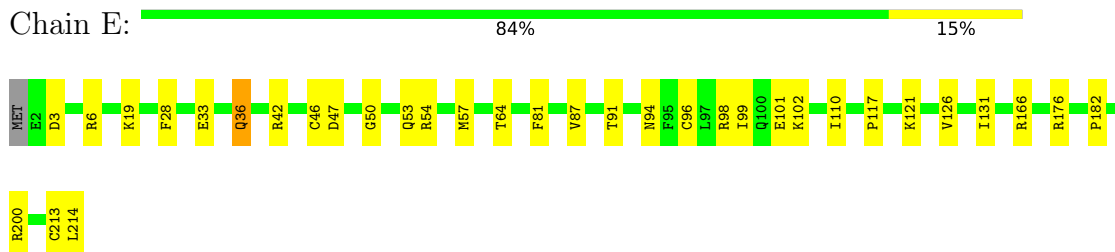


• Molecule 4: RNA polymerase II subunit B32

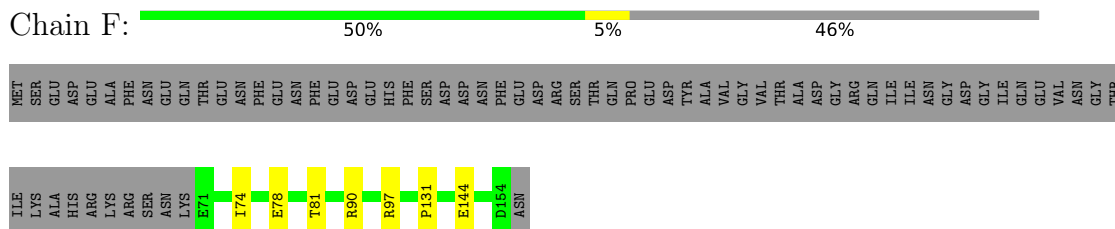
Chain D:



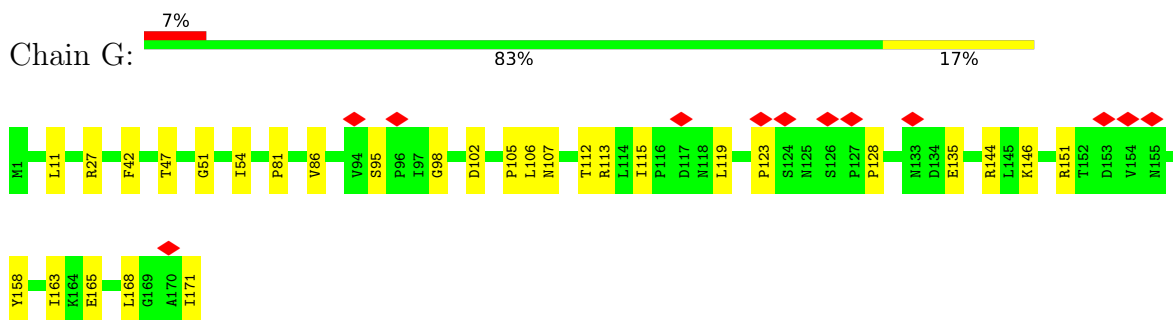
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



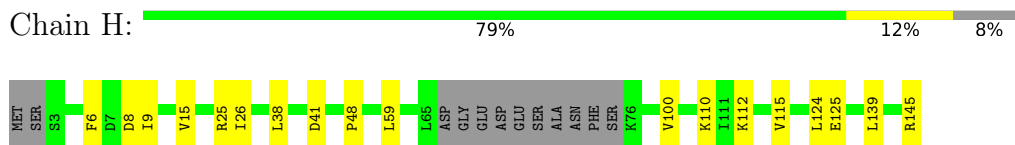
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III



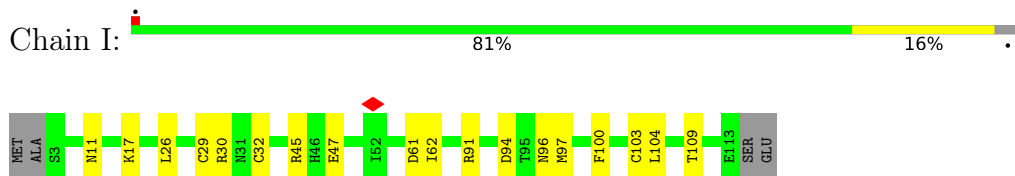
- Molecule 7: RNA polymerase II subunit



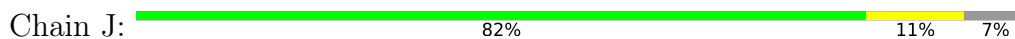
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase subunit

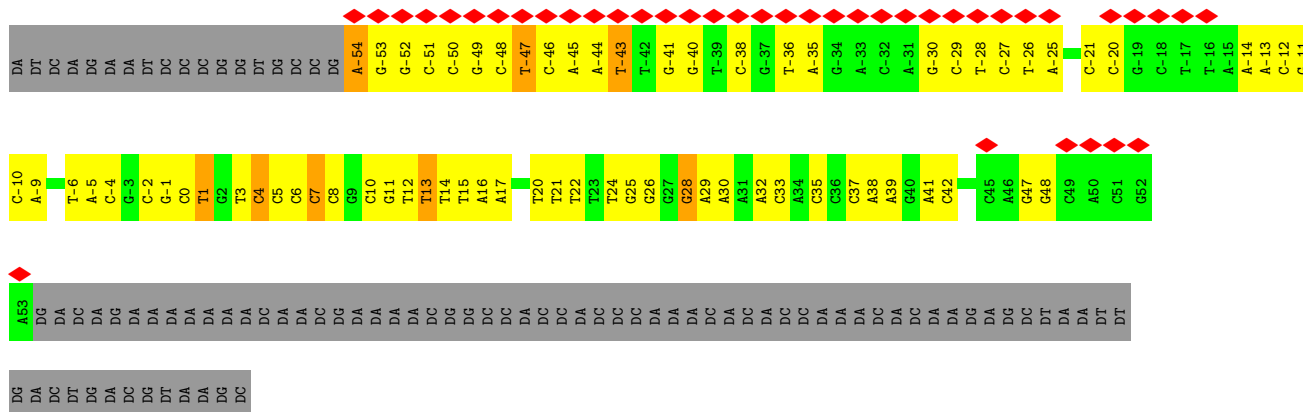


- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

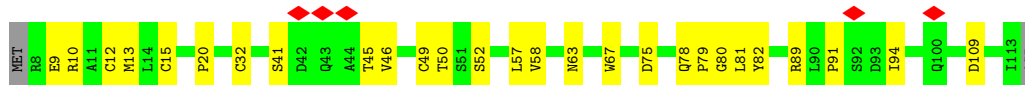
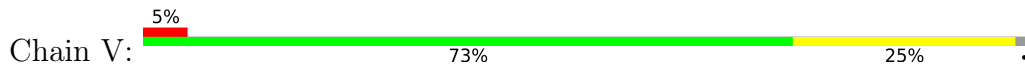




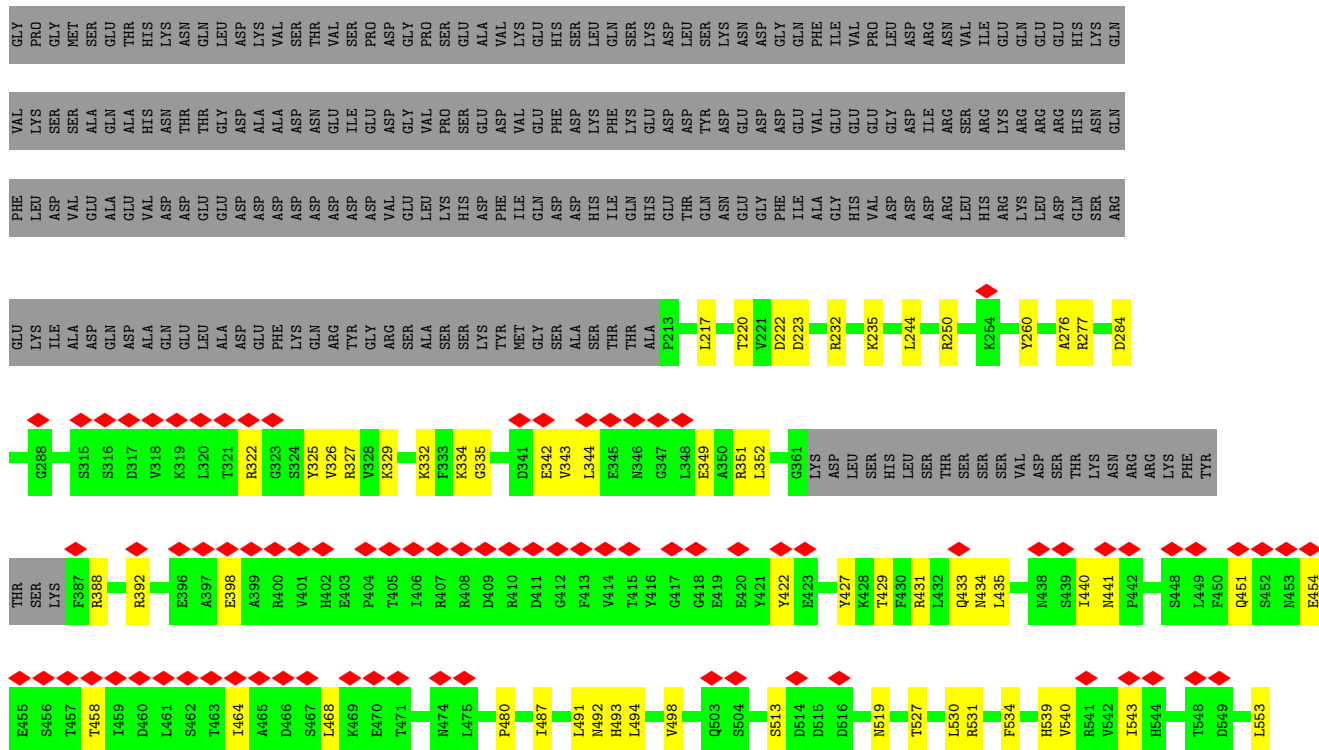
• Molecule 16: DNA (198-MER)



• Molecule 17: Transcription elongation factor SPT4



• Molecule 18: Transcription elongation factor SPT5





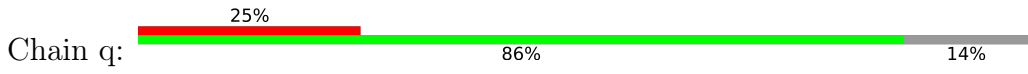
R939	E1038	E940	R941	S1063	L1054	A1055	D1064	I1065	E1066	D1067	I1068	D1069	A964	V965	R966	D1071	D1072	E1073	S1074	A1075	M1076	R1077	N1078	F1085	P1086	R1087	S1088	P1089	Q993	R994	I995	G996	S997	R998	L999	V1000	H1004	L1005	I1006	T1007	E1008	Q1009	L1010	T1011	I1025	V1026	F1027	D1028	P1029	D1030	V1031	E1032	H1034	F1035	Q1036						
G1037	E1038	M1039	S1063	L1054	A1055	D1064	I1065	E1066	D1067	I1068	D1069	A964	V965	R966	D1071	D1072	E1073	S1074	A1075	M1076	R1077	N1078	F1085	P1086	R1087	S1088	P1089	Q993	R994	I995	G996	S997	R998	L999	V1000	H1004	L1005	I1006	T1007	E1008	Q1009	L1010	T1011	I1025	V1026	F1027	D1028	P1029	D1030	V1031	E1032	H1034	F1035	Q1036							
M1241	Q1242	V1243	A1244	G1245	L1246	M1247	R1250	D1263	R1264	Q1265	E1266	E1267	I1268	D1269	K1270	Q1271	R1272	E1273	E1274	S1275	R1276	E1277	S1278	R1279	V1280	I1281	K1282	H1283	P1284	F1285	F1286	H1287	M1288	M1289	K1290	S1291	K1292	E1293	A1294	E1295	D1296	Y1297	L1298	A1299	A1300	R1301	P1302	V1303	G1304	D1305	V1306	V1307	I1308	P1309	S1311						
S1312	K1313	G1314	S1315	M1316	H1317	I1318	T1319	I1320	S1321	M1322	K1323	M1384	A1325	P1326	Q1327	I1328	L1329	Y1330	H1331	I1332	D1333	V1334	L1335	E1336	E1337	M1338	K1339	D1340	D1341	A1342	H1343	M1344	I1345	G1346	R1347	V1348	L1349	L1350	V1351	G1352	K1353	Y1354	R1355	Y1356	H1357	D1358	L1359	D1360	E1361	L1362	L1363	V1364	E1365	Y1366	V1367	M1368	N1369	A1371			
M1372	K1373	V1374	E1375	L1376	M1377	V1378	S1379	H1380	D1381	K1382	F1383	M1384	S1385	D1386	S1387	D1388	Y1390	V1391	K1392	E1393	M1394	L1395	E1396	R1397	Y1398	S1399	K1400	A1401	M1402	G1403	M1404	I1405	S1406	H1407	Y1408	I1409	F1410	T1411	F1412	M1413	R1414	K1415	A1416	G1417	G1418	W1419	F1420	F1421	L1422	L1423	F1424	K1425	L1426	N1427	P1428	T1429	S1430	E1431			
I1432	K1433	I1434	M1435	M1436	V1437	K1438	A1439	L1440	P1441	D1442	G1443	Y1444	L1445	L1446	A1447	M1448	N1449	V1450	Y1451	P1452	D1453	T1454	N1455	S1456	L1457	C1458	N1459	G1460	F1461	K1462	T1463	L1464	M1465	S1466	S1467	R1468	R1469	GLN	ILE	LYS	GLN	ARG	ARG	R1414	K1415	A1416	G1417	G1418	W1419	F1420	F1421	L1422	L1423	F1424	K1425	L1426	N1427	P1428	T1429	S1430	E1431
ASN	GLY	TYR	SER	VAL	ASP	ASP	ALA	PRO	ARG	TYR	ASN	LEU	LEU	LEU	PRO	GLU	THR	THR	GLN	GLU	THR	GLN	GLN	ALA	ALA	ALA	ALA	GLU	GLU	ASN	PRO	PRO	ASN	GLU	ALA	ALA	GLN	ASP	LEU	ASP	ASP	GLN	SER	ASP	GLN	GLU	LEU	LEU	ASN	ASN	SER	HIS	ALA	GLY	ALA	TYR	ASP	ASP			

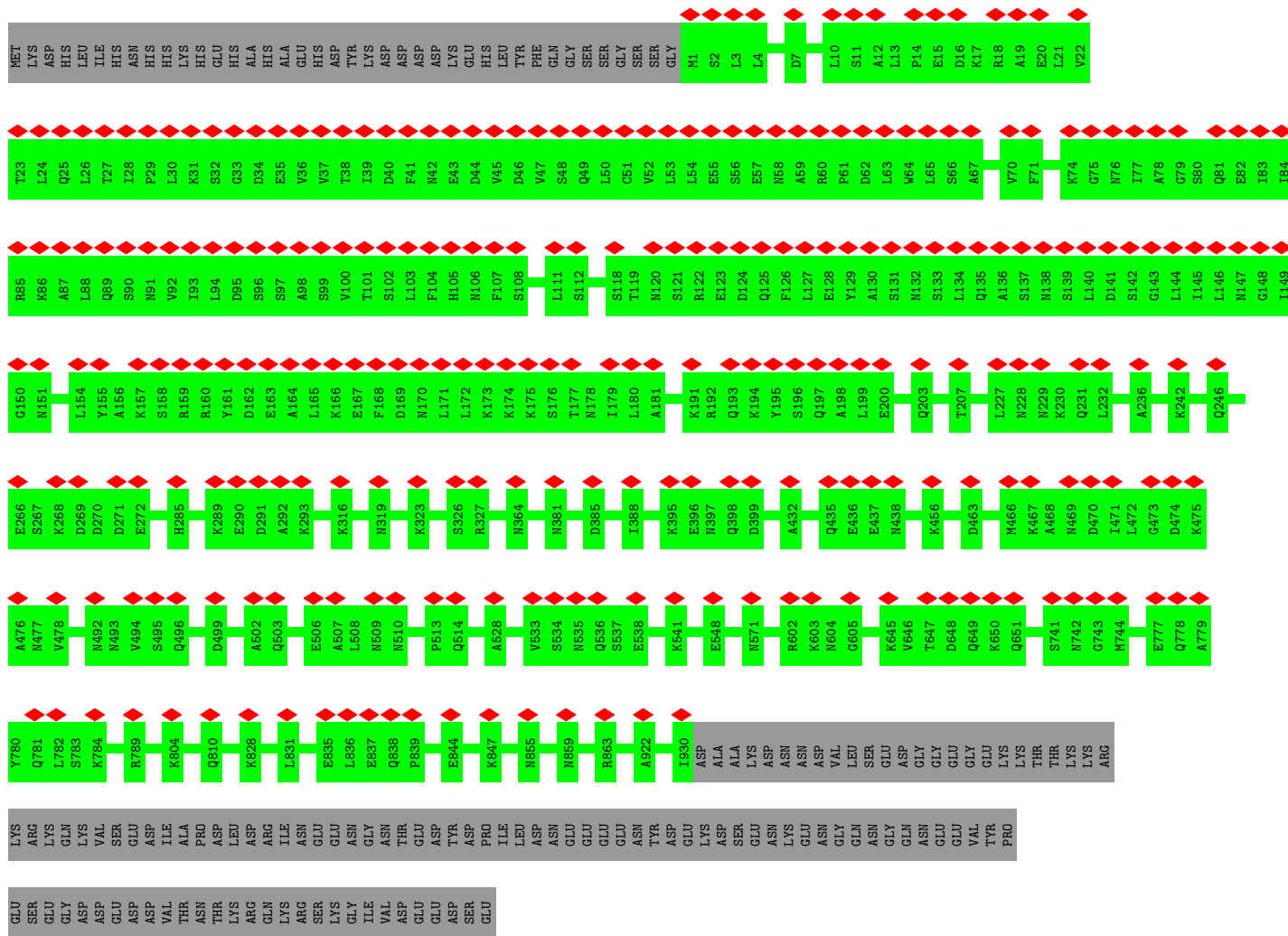
- Molecule 20: Protein that interacts with Spt6p and copurifies with Spt5p and RNA polymerase II



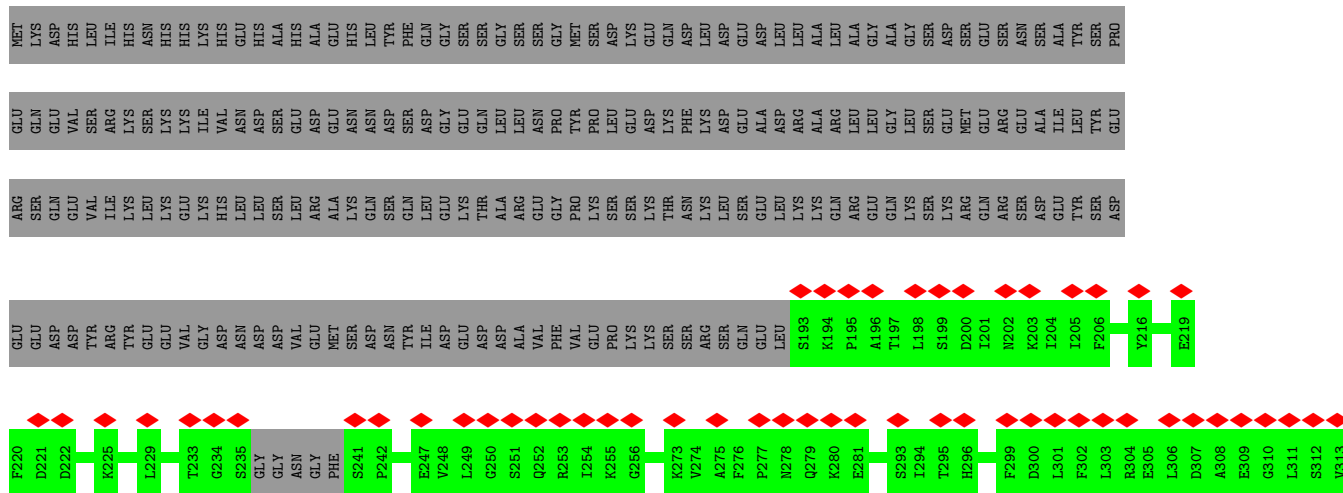
GLY	PRO	GLY	MET	SER	ASP	ASP	GLU	GLU	GLY	LYS	VAL	GLU	ASN	GLY	LYS	LEU	LEU	LEU	ASP	GLN	VAL	VAL	LEU	PRO	GLU	GLU	THR	THR	LYS	ASN	GLY	ASP	ASP	ALA	PRO	ASP	ASN	GLU	ASP	LEU	ASP	ASP	GLN	THR	GLY	GLY	VAL	GLN	VAL	THR	THR	THR	LEU	PRO	ASP	ASP	
ILE	SER	ASP	VAL	ASP	ASP	GLU	GLU	LYS	VAL	VAL	GLU	ALA	ASN	GLY	LYS	LEU	LEU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

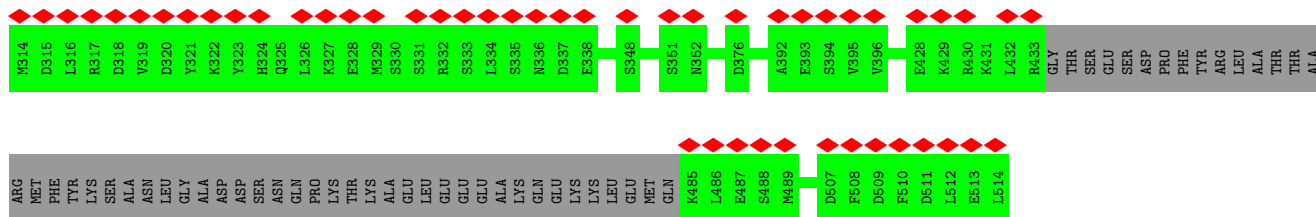
- Molecule 21: Component of the Paf1p complex





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

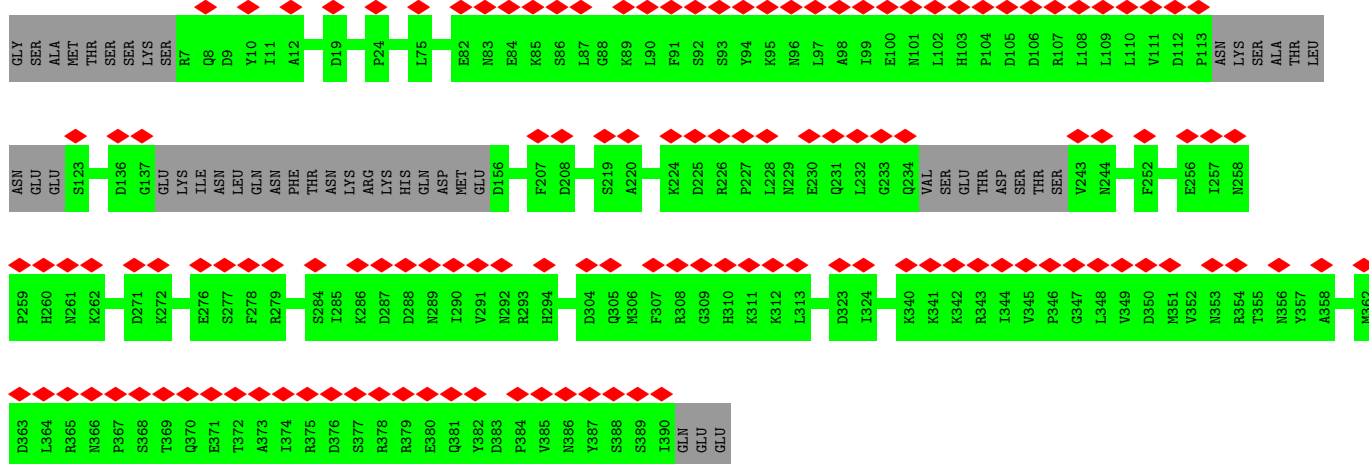
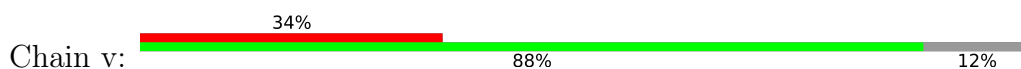




• Molecule 23: Leo1



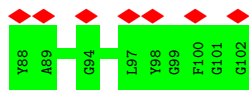
• Molecule 24: RNAP II-associated protein



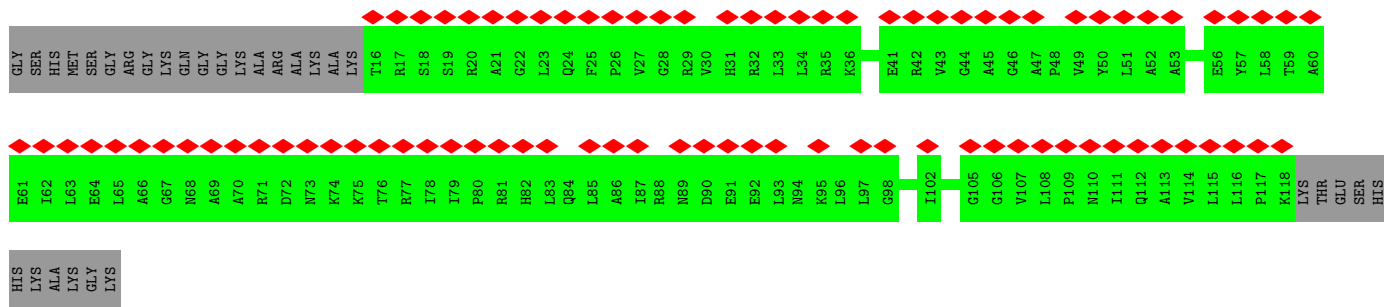
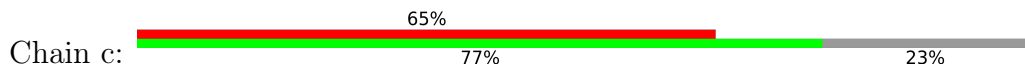
• Molecule 25: Constituent of Paf1 complex with RNA polymerase II, Paf1p, Hpr1p, Ctr9, Leo1, Rtf1 and Ccr4p



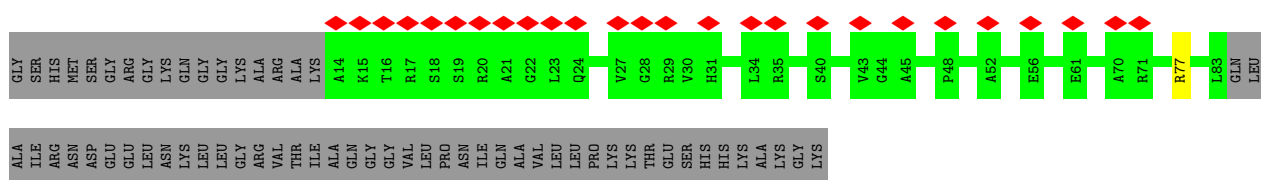




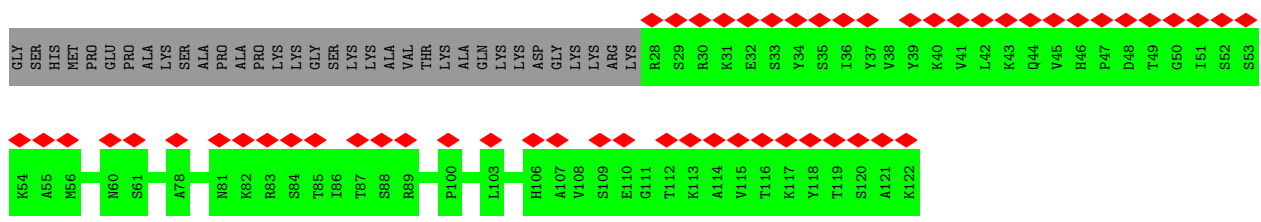
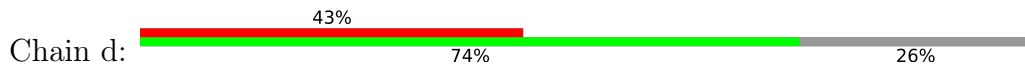
• Molecule 28: Histone H2A type 1-B/E



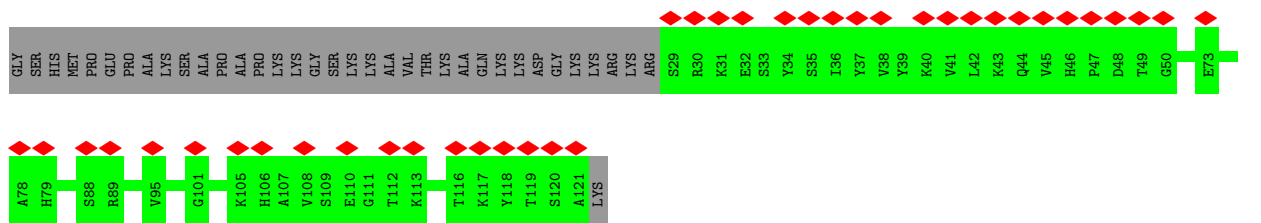
• Molecule 28: Histone H2A type 1-B/E



• Molecule 29: Histone H2B type 1-J

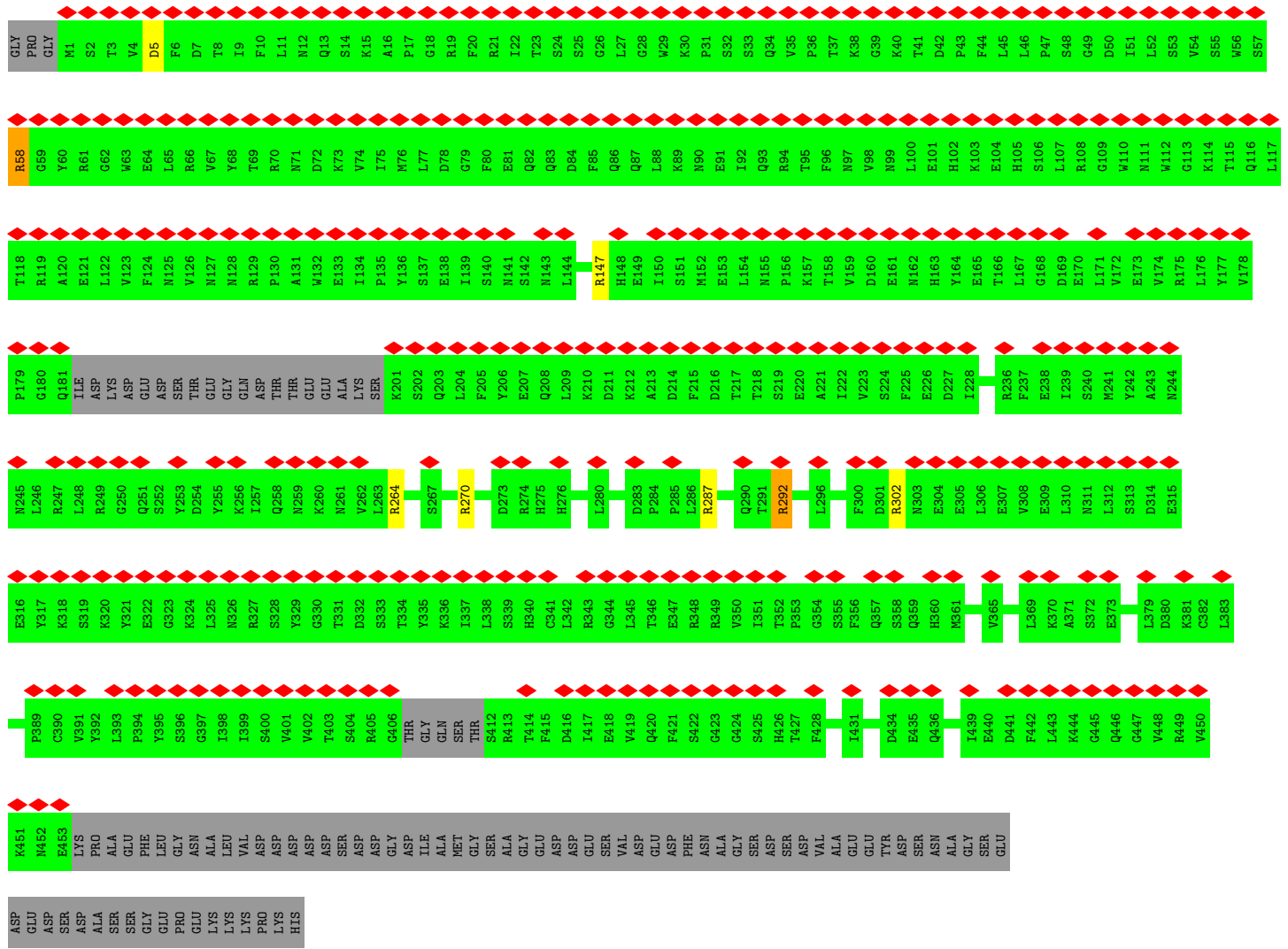
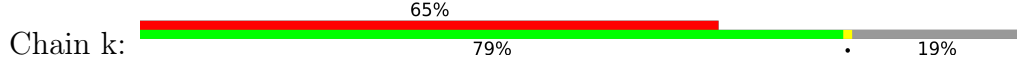


• Molecule 29: Histone H2B type 1-J





• Molecule 31: FACT complex subunit POB3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53755	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	0.123	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.013	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	1.484, 1.484, 1.484	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1/15222 (0.0%)
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	0.55	0/484
13	M	0.25	0/513	0.41	0/693
14	N	1.11	5/2253 (0.2%)	1.48	48/3478 (1.4%)
15	P	0.52	0/443	1.14	6/687 (0.9%)
16	T	1.09	5/2469 (0.2%)	1.38	37/3804 (1.0%)
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	0/622	0.53	0/834
26	e	0.33	0/766	0.58	0/1027
27	b	0.30	0/669	0.60	0/894
27	f	0.31	0/626	0.58	0/837
28	c	0.29	0/806	0.56	0/1089
28	g	0.34	0/552	0.60	1/743 (0.1%)
29	d	0.30	0/757	0.51	0/1015

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	0/3909	0.86	4/5264 (0.1%)
31	k	0.68	0/3579	0.89	8/4833 (0.2%)
All	All	0.42	10/83085 (0.0%)	0.63	105/113088 (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	6
16	T	0	10
30	j	0	1
31	k	0	2
All	All	0	19

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	-18	DG	C1'-N9	-6.21	1.38	1.47
14	N	-19	DG	C1'-N9	-5.96	1.39	1.47
14	N	-21	DA	C1'-N9	-5.89	1.39	1.47
16	T	28	DG	C1'-N9	-5.81	1.39	1.47
16	T	41	DA	C1'-N9	-5.73	1.39	1.47
14	N	-20	DA	C1'-N9	-5.69	1.39	1.47
16	T	48	DG	C1'-N9	-5.59	1.39	1.47
16	T	39	DA	C1'-N9	-5.45	1.39	1.47
14	N	-22	DA	C1'-N9	-5.19	1.40	1.47
16	T	47	DG	C1'-N9	-5.05	1.40	1.47

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	j	684	ARG	NE-CZ-NH1	9.45	125.03	120.30
30	j	836	ARG	NE-CZ-NH1	9.26	124.93	120.30
15	P	-4	C	C2-N1-C1'	8.54	128.20	118.80
15	P	-4	C	N1-C2-O2	8.39	123.94	118.90
14	N	-12	DA	N1-C6-N6	-8.28	113.63	118.60
14	N	-13	DA	N1-C6-N6	-8.26	113.64	118.60
14	N	-12	DA	C5-C6-N1	8.09	121.75	117.70
16	T	-54	DA	C5-C6-N1	7.89	121.65	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	10	DC	N3-C2-O2	-7.88	116.38	121.90
14	N	-14	DA	C5-C6-N1	7.79	121.60	117.70
14	N	47	DA	N1-C6-N6	-7.62	114.03	118.60
31	k	287	ARG	NE-CZ-NH2	-7.60	116.50	120.30
14	N	-3	DA	N1-C6-N6	-7.56	114.06	118.60
14	N	-4	DG	O4'-C1'-N9	7.55	113.28	108.00
14	N	-5	DG	O4'-C1'-N9	7.46	113.22	108.00
14	N	53	DC	N3-C2-O2	-7.46	116.68	121.90
14	N	-14	DA	N1-C6-N6	-7.40	114.16	118.60
14	N	-7	DG	O4'-C1'-N9	7.37	113.16	108.00
14	N	-15	DA	N1-C6-N6	-7.35	114.19	118.60
14	N	-15	DA	C5-C6-N1	7.33	121.37	117.70
16	T	6	DC	N3-C2-O2	-7.28	116.80	121.90
16	T	8	DC	N3-C2-O2	-7.19	116.87	121.90
14	N	-11	DC	N3-C2-O2	-7.14	116.90	121.90
31	k	287	ARG	NE-CZ-NH1	7.04	123.82	120.30
14	N	-1	DA	C4-C5-C6	-7.01	113.50	117.00
14	N	-1	DA	C5-C6-N1	7.01	121.20	117.70
14	N	-13	DA	C5-C6-N1	6.99	121.20	117.70
14	N	-9	DC	N3-C2-O2	-6.96	117.03	121.90
14	N	-12	DA	C4-C5-C6	-6.72	113.64	117.00
16	T	-45	DA	C4-C5-C6	-6.66	113.67	117.00
14	N	-13	DA	C4-C5-C6	-6.63	113.68	117.00
31	k	292	ARG	NE-CZ-NH1	6.61	123.61	120.30
16	T	-54	DA	N1-C6-N6	-6.60	114.64	118.60
14	N	54	DT	C6-C5-C7	-6.60	118.94	122.90
16	T	-48	DC	N3-C2-O2	-6.57	117.30	121.90
16	T	-50	DC	N3-C2-O2	-6.57	117.30	121.90
15	P	-4	C	N3-C2-O2	-6.55	117.32	121.90
1	A	176	ARG	NE-CZ-NH1	6.50	123.55	120.30
16	T	10	DC	N1-C2-O2	6.49	122.80	118.90
16	T	5	DC	N3-C2-O2	-6.49	117.36	121.90
16	T	4	DC	N3-C2-O2	-6.48	117.36	121.90
16	T	7	DC	N3-C2-O2	-6.47	117.37	121.90
15	P	11	A	OP1-P-OP2	-6.45	109.93	119.60
14	N	-3	DA	C4-C5-C6	-6.45	113.78	117.00
14	N	-15	DA	C4-C5-C6	-6.43	113.78	117.00
14	N	-3	DA	C5-C6-N1	6.34	120.87	117.70
16	T	15	DT	C6-C5-C7	-6.34	119.10	122.90
16	T	0	DC	N3-C2-O2	-6.20	117.56	121.90
14	N	52	DC	N3-C2-O2	-6.16	117.58	121.90
16	T	-45	DA	N1-C6-N6	-6.13	114.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	13	DT	C6-C5-C7	-6.10	119.24	122.90
14	N	-14	DA	C4-C5-C6	-6.01	114.00	117.00
14	N	53	DC	N3-C4-N4	-5.97	113.82	118.00
14	N	-1	DA	N1-C6-N6	-5.96	115.03	118.60
14	N	46	DG	N1-C6-O6	-5.95	116.33	119.90
14	N	54	DT	N3-C2-O2	-5.93	118.74	122.30
15	P	-4	C	C6-N1-C1'	-5.92	113.69	120.80
14	N	-8	DG	P-O3'-C3'	5.86	126.74	119.70
16	T	8	DC	N1-C2-O2	5.82	122.39	118.90
16	T	-43	DT	C6-C5-C7	-5.81	119.42	122.90
16	T	15	DT	P-O3'-C3'	5.80	126.66	119.70
14	N	-16	DT	C6-C5-C7	-5.80	119.42	122.90
16	T	12	DT	N3-C2-O2	-5.79	118.83	122.30
16	T	3	DT	C6-C5-C7	-5.79	119.43	122.90
14	N	47	DA	C4-C5-C6	-5.73	114.14	117.00
16	T	12	DT	C6-C5-C7	-5.68	119.49	122.90
14	N	-9	DC	N1-C2-O2	5.65	122.29	118.90
16	T	-54	DA	C4-C5-C6	-5.63	114.18	117.00
16	T	6	DC	N1-C2-O2	5.63	122.28	118.90
14	N	44	DT	C6-C5-C7	-5.61	119.54	122.90
31	k	302	ARG	NE-CZ-NH1	5.60	123.10	120.30
14	N	-8	DG	N1-C6-O6	-5.56	116.56	119.90
16	T	4	DC	O4'-C1'-N1	5.55	111.89	108.00
15	P	-4	C	C6-N1-C2	-5.54	118.08	120.30
31	k	270	ARG	NE-CZ-NH1	5.54	123.07	120.30
31	k	264	ARG	NE-CZ-NH1	5.54	123.07	120.30
16	T	1	DT	N3-C2-O2	-5.53	118.98	122.30
16	T	-47	DT	C6-C5-C7	-5.51	119.59	122.90
14	N	-9	DC	O4'-C4'-C3'	5.38	109.23	106.00
16	T	-51	DC	N3-C2-O2	-5.38	118.13	121.90
14	N	-16	DT	N3-C2-O2	-5.36	119.08	122.30
14	N	45	DT	C6-C5-C7	-5.36	119.69	122.90
31	k	58	ARG	NE-CZ-NH1	5.36	122.98	120.30
16	T	14	DT	C6-C5-C7	-5.32	119.71	122.90
14	N	47	DA	C5-C6-N1	5.31	120.36	117.70
14	N	-7	DG	N1-C6-O6	-5.29	116.72	119.90
30	j	817	ARG	NE-CZ-NH1	5.28	122.94	120.30
16	T	15	DT	N3-C2-O2	-5.26	119.15	122.30
14	N	-5	DG	N1-C6-O6	-5.18	116.79	119.90
16	T	-50	DC	N1-C2-O2	5.17	122.00	118.90
16	T	-45	DA	C5-C6-N1	5.16	120.28	117.70
14	N	-11	DC	N1-C2-O2	5.14	121.98	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	1	DT	C6-C5-C7	-5.14	119.82	122.90
14	N	-4	DG	N1-C6-O6	-5.12	116.83	119.90
30	j	616	ARG	NE-CZ-NH1	5.12	122.86	120.30
14	N	-2	DC	N3-C2-O2	-5.10	118.33	121.90
16	T	7	DC	N1-C2-O2	5.08	121.95	118.90
28	g	77	ARG	NE-CZ-NH1	5.08	122.84	120.30
14	N	-11	DC	O4'-C1'-N1	5.06	111.54	108.00
31	k	5	ASP	CB-CG-OD2	-5.05	113.75	118.30
16	T	3	DT	O4'-C1'-N1	5.05	111.54	108.00
16	T	11	DG	N1-C6-O6	-5.05	116.87	119.90
14	N	-13	DA	O4'-C1'-N9	5.04	111.53	108.00
14	N	-10	DG	N1-C6-O6	-5.04	116.87	119.90
16	T	14	DT	N3-C2-O2	-5.02	119.29	122.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	-10	DG	Sidechain
14	N	-12	DA	Sidechain
14	N	-5	DG	Sidechain
14	N	-6	DG	Sidechain
14	N	44	DT	Sidechain
14	N	46	DG	Sidechain
16	T	-46	DC	Sidechain
16	T	-47	DT	Sidechain
16	T	-49	DG	Sidechain
16	T	-52	DG	Sidechain
16	T	-53	DG	Sidechain
16	T	-54	DA	Sidechain
16	T	1	DT	Sidechain
16	T	13	DT	Sidechain
16	T	4	DC	Sidechain
16	T	7	DC	Sidechain
30	j	616	ARG	Sidechain
31	k	292	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	5	0
7	G	1325	0	1342	18	0
8	H	1053	0	1050	10	0
9	I	917	0	867	14	0
10	J	554	0	573	5	0
11	K	932	0	944	13	0
12	L	359	0	358	4	0
13	M	505	0	495	5	0
14	N	2007	0	1091	40	0
15	P	399	0	205	10	0
16	T	2202	0	1210	35	0
17	V	824	0	795	16	0
18	W	4232	0	4278	56	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	615	0	645	0	0
26	e	757	0	798	0	0
27	b	662	0	709	0	0
27	f	619	0	659	0	0
28	c	796	0	848	0	0
28	g	544	0	574	0	0
29	d	746	0	771	0	0
29	h	725	0	745	0	0
30	j	3832	0	3792	0	0
31	k	3502	0	3436	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	81134	0	79160	455	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 (455) 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)
16:T:-2:DC:H2''	16:T:-1:DG:C8	2.11	0.86
14:N:-22:DA:N6	14:N:-21:DA:C6	2.48	0.81
14:N:-48:DC:H2''	14:N:-47:DC:C6	2.20	0.77
14:N:-37:DG:N2	16:T:37:DC:O2	2.16	0.76
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:-22:DA:C6	14:N:-21:DA:C6	2.78	0.71
1:A:807:ARG:NH1	2:B:724:LYS:O	2.23	0.70
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:1262:MET:SD	1:A:1265:ARG:NH2	2.66	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	1.76	0.68
1:A:107:CYS:SG	1:A:172:GLN:NE2	2.66	0.68
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
9:I:45:ARG:NH2	9:I:47:GLU:OE2	2.29	0.66
16:T:25:DG:H2'	16:T:26:DG:C8	2.31	0.66
1:A:673:ASP:OD1	1:A:737:ASN:ND2	2.29	0.65
1:A:887:ILE:O	1:A:945:ARG:NH2	2.30	0.65
2:B:267:TYR:HB2	2:B:348:ILE:HD11	1.77	0.65
2:B:613:ARG:HH21	9:I:62:ILE:HD11	1.61	0.65
18:W:342:GLU:HB3	18:W:351:ARG:HB3	1.79	0.65
16:T:25:DG:H2'	16:T:26:DG:H8	1.62	0.65
1:A:127:ARG:O	1:A:129:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:285:PRO:HG2	2:B:288:GLU:HB2	1.80	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
16:T:42:DC:OP1	18:W:433:GLN:NE2	2.33	0.62
14:N:-22:DA:N6	14:N:-21:DA:N6	2.47	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
1:A:1130:ILE:HG12	1:A:1134:LYS:HE2	1.81	0.61
11:K:57:THR:OG1	11:K:76:GLN:OE1	2.17	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
16:T:-26:DT:H2''	16:T:-25:DA:C8	2.36	0.61
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
14:N:21:DG:H2''	14:N:22:DT:H5'	1.83	0.60
1:A:466:TYR:HB2	1:A:470:ARG:NH2	2.16	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	1.83	0.60
2:B:235:LEU:HD23	2:B:242:ILE:HG13	1.83	0.60
2:B:489:ARG:NH2	2:B:533:SER:O	2.35	0.60
14:N:-40:DC:H2''	14:N:-39:DT:H71	1.84	0.59
1:A:22:LEU:HG	2:B:1213:ALA:HB2	1.83	0.59
2:B:10:ASP:HB3	2:B:649:LYS:HG3	1.84	0.59
17:V:57:LEU:HD11	17:V:81:LEU:HD22	1.84	0.59
14:N:-22:DA:N1	14:N:-21:DA:C2	2.71	0.59
18:W:327:ARG:NH1	18:W:335:GLY:O	2.36	0.59
2:B:353:LEU:O	2:B:367:LYS:NZ	2.34	0.59
1:A:85:GLU:O	1:A:274:ASN:ND2	2.33	0.59
2:B:294:CYS:SG	2:B:295:TYR:N	2.76	0.59
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.24	0.59
1:A:1157:ASP:O	1:A:1243:ARG:NH2	2.29	0.59
2:B:409:LEU:HD23	2:B:450:LEU:HD23	1.85	0.58
2:B:63:GLN:NE2	2:B:70:ASN:OD1	2.35	0.58
7:G:27:ARG:NH1	7:G:54:ILE:O	2.36	0.58
2:B:50:VAL:HG21	2:B:82:ILE:HD11	1.86	0.58
17:V:9:GLU:HA	17:V:20:PRO:HA	1.84	0.58
16:T:-6:DT:H2''	16:T:-5:DA:N7	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:MET:HG3	2:B:722:THR:HB	1.84	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	0.57
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
2:B:91:GLU:OE2	2:B:97:HIS:NE2	2.29	0.57
7:G:86:VAL:HG22	7:G:146:LYS:HB2	1.86	0.57
1:A:63:ARG:NH2	15:P:0:G:OP1	2.37	0.57
18:W:392:ARG:NH1	18:W:398:GLU:OE1	2.36	0.57
17:V:13:MET:N	17:V:49:CYS:O	2.26	0.57
1:A:568:LYS:HG2	1:A:569:PRO:HA	1.87	0.57
14:N:5:DT:H2''	14:N:6:DA:N7	2.19	0.57
14:N:7:DC:H2''	14:N:8:DG:C8	2.40	0.57
2:B:290:LEU:HD21	2:B:310:ILE:HD11	1.87	0.56
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.37	0.56
2:B:336:ILE:O	2:B:341:ARG:NH1	2.38	0.56
18:W:232:ARG:HH12	18:W:235:LYS:HE3	1.71	0.56
1:A:486:ASP:OD1	15:P:10:C:O2'	2.20	0.56
17:V:58:VAL:N	17:V:82:TYR:O	2.38	0.56
8:H:48:PRO:O	8:H:145:ARG:NH1	2.36	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:-21:DC:H2''	16:T:-20:DC:H5'	1.88	0.56
1:A:1331:TYR:OH	1:A:1354:GLU:OE2	2.21	0.56
5:E:19:LYS:NZ	5:E:33:GLU:O	2.34	0.56
14:N:-22:DA:N6	14:N:-21:DA:N1	2.54	0.56
1:A:149:GLU:O	1:A:165:ARG:NH1	2.38	0.55
1:A:916:TYR:OH	1:A:983:LEU:O	2.19	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
14:N:-51:DG:H2''	14:N:-50:DT:C7	2.37	0.55
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.89	0.54
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.89	0.54
1:A:1210:THR:HB	1:A:1213:GLN:HG3	1.90	0.54
1:A:807:ARG:HD3	2:B:725:ARG:HA	1.89	0.54
7:G:102:ASP:OD1	7:G:107:ASN:ND2	2.32	0.54
17:V:10:ARG:HA	17:V:52:SER:HA	1.90	0.54
2:B:72:ASN:ND2	2:B:128:ASP:OD1	2.39	0.54
17:V:15:CYS:HB3	17:V:32:CYS:SG	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.41	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
3:C:266:ARG:HD2	11:K:84:LYS:HZ3	1.72	0.54
1:A:218:GLU:OE1	1:A:222:ARG:NH1	2.40	0.54
18:W:332:LYS:O	18:W:388:ARG:NH1	2.41	0.54
18:W:451:GLN:NE2	18:W:454:GLU:OE1	2.41	0.53
2:B:301:GLN:O	2:B:304:GLU:HG3	2.08	0.53
8:H:59:LEU:HD23	8:H:139:LEU:HD13	1.91	0.53
1:A:533:ARG:HD3	1:A:750:ALA:HB2	1.91	0.53
2:B:59:ASP:HB3	2:B:74:ARG:HG3	1.91	0.53
18:W:325:TYR:OH	18:W:451:GLN:OE1	2.23	0.53
1:A:351:ARG:HB2	2:B:1128:LEU:HD21	1.91	0.53
18:W:220:THR:N	18:W:223:ASP:OD2	2.33	0.53
14:N:37:DC:H2''	14:N:38:DG:C8	2.44	0.53
2:B:248:LYS:NZ	2:B:264:THR:OG1	2.42	0.53
5:E:81:PHE:HE1	5:E:110:ILE:HD13	1.74	0.53
9:I:17:LYS:N	9:I:26:LEU:O	2.39	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
15:P:6:U:H2'	15:P:7:C:C6	2.44	0.52
4:D:60:ILE:HG13	7:G:47:THR:HG21	1.90	0.52
2:B:906:SER:OG	18:W:781:GLU:OE1	2.24	0.52
4:D:6:SER:HB3	7:G:42:PHE:HZ	1.73	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
13:M:46:LEU:HD11	13:M:55:SER:HB3	1.90	0.52
2:B:904:ARG:NH1	2:B:905:VAL:O	2.43	0.52
14:N:-42:DG:C8	14:N:-41:DT:H71	2.45	0.52
5:E:47:ASP:OD2	5:E:53:GLN:NE2	2.19	0.52
16:T:-14:DA:H2''	16:T:-13:DA:C8	2.45	0.52
1:A:801:VAL:HG22	1:A:813:GLU:HB3	1.92	0.51
18:W:513:SER:N	18:W:519:ASN:OD1	2.41	0.51
2:B:83:TYR:HB2	2:B:116:TYR:HB2	1.92	0.51
14:N:-49:DG:H2''	14:N:-48:DC:C5	2.45	0.51
16:T:-12:DC:H2''	16:T:-11:DG:C8	2.45	0.51
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
18:W:563:GLU:HG2	18:W:574:ILE:HG12	1.93	0.51
1:A:771:VAL:HG13	1:A:823:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ARG:HB2	2:B:124:PHE:HB2	1.92	0.51
18:W:334:LYS:N	18:W:388:ARG:HH12	2.09	0.51
2:B:547:ILE:HG21	2:B:619:ILE:HG21	1.93	0.51
14:N:-40:DC:H2''	14:N:-39:DT:C7	2.40	0.51
16:T:-36:DT:H2''	16:T:-35:DA:N7	2.25	0.51
16:T:-10:DC:H2''	16:T:-9:DA:H8	1.75	0.51
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.92	0.51
16:T:-44:DA:H2''	16:T:-43:DT:O5'	2.10	0.51
2:B:622:ASP:OD1	2:B:623:VAL:N	2.40	0.51
13:M:38:LEU:HA	13:M:45:GLY:HA2	1.91	0.51
16:T:-2:DC:H2''	16:T:-1:DG:H8	1.71	0.51
1:A:1223:SER:OG	1:A:1224:ASP:N	2.44	0.51
5:E:87:VAL:HG23	5:E:91:THR:HB	1.91	0.51
7:G:119:LEU:HD21	7:G:135:GLU:HB2	1.93	0.50
18:W:644:ASN:ND2	18:W:647:GLN:OE1	2.44	0.50
18:W:222:ASP:O	18:W:277:ARG:NH2	2.30	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
1:A:1153:GLU:OE2	9:I:45:ARG:NH1	2.40	0.50
1:A:669:ASP:OD2	1:A:743:ASN:ND2	2.29	0.50
13:M:33:SER:HA	13:M:50:LYS:HE2	1.93	0.50
18:W:326:VAL:HA	18:W:440:ILE:HD13	1.92	0.50
18:W:464:ILE:O	18:W:468:LEU:HG	2.12	0.50
1:A:168:CYS:SG	1:A:170:ASN:ND2	2.85	0.50
4:D:105:THR:HG22	7:G:105:PRO:HD3	1.94	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	0.49
17:V:63:ASN:HB3	17:V:75:ASP:HA	1.94	0.49
1:A:1190:GLN:HA	1:A:1245:ILE:HA	1.94	0.49
2:B:514:LEU:HD22	2:B:626:VAL:HG12	1.94	0.49
1:A:738:LEU:HD13	1:A:742:ASN:HD22	1.77	0.49
9:I:29:CYS:CB	9:I:32:CYS:SG	2.99	0.49
2:B:58:LEU:O	2:B:75:TYR:N	2.36	0.49
2:B:74:ARG:HH22	2:B:126:SER:HB3	1.77	0.49
14:N:-51:DG:H2'	14:N:-50:DT:H72	1.93	0.49
18:W:590:ILE:O	18:W:593:SER:OG	2.26	0.49
1:A:119:ASN:OD1	1:A:121:THR:OG1	2.23	0.49
14:N:5:DT:H2''	14:N:6:DA:C8	2.47	0.49
1:A:122:MET:O	1:A:126:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:610:ARG:NH2	9:I:61:ASP:OD2	2.46	0.49
1:A:321:ARG:NH1	2:B:466:MET:SD	2.86	0.49
9:I:103:CYS:SG	9:I:104:LEU:N	2.86	0.49
2:B:318:ASP:HB3	2:B:321:VAL:HG22	1.94	0.49
14:N:-45:DG:H2''	14:N:-44:DG:H5'	1.95	0.49
2:B:479:TYR:CZ	2:B:1096:ARG:HB3	2.48	0.49
5:E:81:PHE:CE1	5:E:110:ILE:HD13	2.48	0.49
14:N:39:DA:H2''	14:N:40:DC:H5'	1.95	0.49
2:B:766:ARG:HH21	2:B:1020:ARG:HD3	1.78	0.48
16:T:-10:DC:H2''	16:T:-9:DA:C8	2.48	0.48
1:A:1150:SER:OG	1:A:1198:GLU:O	2.32	0.48
3:C:66:LEU:HD11	3:C:155:ILE:HD12	1.95	0.48
18:W:666:GLU:HB2	18:W:671:ARG:HA	1.95	0.48
2:B:300:TRP:HA	2:B:303:LEU:HD12	1.94	0.48
1:A:343:GLY:O	2:B:1129:ARG:NH1	2.45	0.48
3:C:88:GLU:HG2	18:W:759:ARG:HD2	1.95	0.48
7:G:112:THR:HA	7:G:115:ILE:HD12	1.95	0.48
9:I:96:ASN:OD1	9:I:97:MET:N	2.46	0.48
1:A:819:MET:O	1:A:823:GLU:HG2	2.14	0.48
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	1.94	0.48
15:P:-2:G:N2	15:P:-1:G:N7	2.61	0.48
4:D:157:ILE:HG23	4:D:164:ALA:HB2	1.95	0.48
5:E:54:ARG:HA	5:E:57:MET:HE3	1.95	0.48
7:G:95:SER:OG	7:G:98:GLY:O	2.22	0.48
18:W:603:GLN:HG3	18:W:609:VAL:HG22	1.95	0.48
5:E:213:CYS:SG	5:E:214:LEU:N	2.87	0.48
12:L:70:ASP:HB3	18:W:784:ASN:HB3	1.95	0.48
1:A:472:ASN:O	1:A:475:VAL:HG22	2.14	0.48
1:A:673:ASP:OD1	1:A:673:ASP:N	2.44	0.48
1:A:823:GLU:OE1	2:B:506:GLN:NE2	2.46	0.48
2:B:314:PHE:O	2:B:317:GLN:NE2	2.46	0.48
16:T:37:DC:H2''	16:T:38:DA:C8	2.49	0.48
1:A:106:ILE:HD13	1:A:215:ILE:HD11	1.95	0.47
5:E:91:THR:HA	5:E:94:ASN:ND2	2.29	0.47
16:T:-38:DC:H5'	16:T:-38:DC:C6	2.49	0.47
1:A:504:GLN:OE1	6:F:90:ARG:NH1	2.38	0.47
3:C:17:VAL:HG12	3:C:240:ALA:HB1	1.97	0.47
3:C:105:GLU:N	3:C:105:GLU:OE1	2.46	0.47
18:W:260:TYR:CE1	18:W:277:ARG:HG3	2.49	0.47
1:A:1426:GLY:O	1:A:1430:ASN:ND2	2.40	0.47
15:P:-5:C:H1'	18:W:748:ARG:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:LEU:O	2:B:307:LYS:HG2	2.15	0.47
13:M:65:GLN:N	13:M:68:ASP:OD2	2.44	0.47
1:A:363:ASP:HB3	1:A:509:PRO:HD3	1.97	0.47
1:A:983:LEU:HD13	1:A:1041:ARG:HA	1.97	0.47
3:C:4:GLU:HB3	3:C:5:PRO:HD3	1.96	0.47
18:W:599:HIS:HB3	18:W:677:LEU:HD21	1.96	0.47
2:B:101:PRO:HG2	2:B:172:LEU:HD11	1.97	0.47
2:B:365:THR:O	2:B:368:THR:OG1	2.29	0.47
2:B:896:ASP:OD2	12:L:31:TYR:OH	2.32	0.47
17:V:41:SER:HB2	17:V:45:THR:HB	1.96	0.47
4:D:139:PRO:HA	4:D:142:ILE:HD12	1.97	0.47
11:K:62:LYS:HE3	11:K:64:GLU:OE2	2.15	0.47
17:V:91:PRO:HD2	17:V:94:ILE:HB	1.95	0.47
2:B:865:ARG:HD3	2:B:871:VAL:HG12	1.95	0.47
7:G:123:PRO:HA	7:G:128:PRO:HB3	1.97	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:220:ALA:O	2:B:252:ARG:NH2	2.47	0.47
2:B:788:ARG:O	2:B:967:ARG:NH1	2.47	0.47
2:B:885:LEU:HD23	2:B:936:ASP:HB2	1.97	0.47
1:A:649:ASN:O	1:A:653:VAL:HG23	2.16	0.46
10:J:6:ARG:HD3	10:J:13:VAL:HG22	1.97	0.46
2:B:421:ILE:HD11	2:B:441:VAL:HG12	1.97	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
15:P:-6:A:H2'	15:P:-5:C:O4'	2.15	0.46
18:W:534:PHE:HB3	18:W:554:ILE:HD13	1.97	0.46
1:A:215:ILE:O	1:A:231:ARG:NH2	2.46	0.46
2:B:497:ARG:NH2	16:T:24:DT:OP2	2.49	0.46
5:E:96:CYS:SG	5:E:126:VAL:HG23	2.56	0.46
16:T:-41:DG:C6	16:T:-40:DG:C6	3.04	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
1:A:564:PRO:HG2	1:A:567:LEU:HD23	1.98	0.46
2:B:463:LYS:NZ	2:B:464:LYS:HE2	2.31	0.46
2:B:505:ARG:NH1	2:B:524:GLN:O	2.32	0.46
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.49	0.46
2:B:25:PHE:HZ	2:B:534:LEU:HG	1.80	0.46
2:B:266:PRO:HG3	2:B:352:GLU:O	2.16	0.46
3:C:21:LEU:HD22	11:K:101:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:51:GLY:HA2	7:G:54:ILE:HD11	1.98	0.46
1:A:1065:MET:SD	1:A:1439:MET:HB2	2.56	0.46
2:B:557:GLU:OE2	2:B:584:ARG:NH2	2.49	0.46
6:F:74:ILE:HG23	6:F:78:GLU:HG3	1.97	0.46
4:D:170:ASN:HB3	4:D:173:ARG:HG2	1.97	0.46
5:E:117:PRO:O	5:E:121:LYS:HG2	2.17	0.46
1:A:409:ASP:OD1	1:A:410:ASN:N	2.49	0.45
2:B:27:GLU:OE1	2:B:678:TRP:HB3	2.16	0.45
2:B:318:ASP:OD1	2:B:319:LYS:N	2.48	0.45
15:P:2:G:H1	16:T:33:DC:H42	1.63	0.45
1:A:1061:HIS:O	1:A:1064:GLU:HG2	2.17	0.45
18:W:539:HIS:CE1	18:W:553:LEU:HD21	2.51	0.45
1:A:684:ILE:HG21	1:A:802:GLU:HG3	1.99	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:322:ALA:O	2:B:326:ILE:HG12	2.15	0.45
1:A:1390:HIS:O	1:A:1394:ARG:HD3	2.17	0.45
5:E:46:CYS:HB3	5:E:50:GLY:HA2	1.99	0.45
8:H:110:LYS:HE2	8:H:112:LYS:HE3	1.99	0.45
16:T:32:DA:H1'	16:T:33:DC:H5''	1.98	0.45
14:N:-22:DA:C6	14:N:-21:DA:N1	2.85	0.45
2:B:250:TYR:HE2	2:B:262:LYS:HB2	1.82	0.45
14:N:-44:DG:H2''	14:N:-43:DT:H71	1.99	0.45
17:V:46:VAL:O	17:V:50:THR:N	2.43	0.45
7:G:113:ARG:NH1	18:W:563:GLU:OE1	2.49	0.45
2:B:436:ASN:C	2:B:438:ASN:H	2.20	0.45
18:W:451:GLN:HG3	18:W:458:THR:HA	1.98	0.45
2:B:387:ASP:H	9:I:91:ARG:NH2	2.14	0.44
7:G:81:PRO:HG3	7:G:106:LEU:HD22	1.99	0.44
16:T:-29:DC:H2''	16:T:-28:DT:H71	1.99	0.44
2:B:640:ASP:OD1	2:B:640:ASP:N	2.50	0.44
14:N:28:DA:H2''	14:N:29:DG:C8	2.53	0.44
1:A:452:HIS:CE1	1:A:454:MET:HB2	2.52	0.44
1:A:880:GLU:O	1:A:957:PRO:HA	2.18	0.44
18:W:763:TYR:HB3	18:W:766:LYS:HD3	2.00	0.44
1:A:779:GLY:HA3	2:B:509:ASN:HB2	1.99	0.44
1:A:1041:ARG:O	1:A:1044:PHE:N	2.50	0.44
9:I:100:PHE:HB3	9:I:109:THR:HG23	1.99	0.44
2:B:221:ALA:O	2:B:223:SER:N	2.46	0.44
3:C:258:VAL:HG21	11:K:42:LEU:HD21	2.00	0.44
17:V:78:GLN:OE1	17:V:79:PRO:HD2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ARG:HB2	1:A:488:MET:HE3	1.98	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
2:B:254:ASP:H	2:B:259:ARG:NH2	2.13	0.44
1:A:948:VAL:O	5:E:200:ARG:NH1	2.48	0.44
2:B:886:LYS:HG2	2:B:890:TYR:OH	2.18	0.44
3:C:15:ASP:OD1	3:C:15:ASP:N	2.47	0.44
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.00	0.44
14:N:-22:DA:H61	16:T:22:DT:H3	1.65	0.44
2:B:691:ASP:OD1	2:B:691:ASP:N	2.41	0.44
4:D:88:GLU:HA	4:D:91:LYS:HE3	2.00	0.44
5:E:99:ILE:HG13	5:E:131:ILE:HD11	2.00	0.43
10:J:63:ASN:OD1	10:J:64:PRO:HD2	2.18	0.43
14:N:-47:DC:H2''	14:N:-46:DT:C5	2.53	0.43
2:B:257:THR:OG1	2:B:258:GLY:N	2.50	0.43
17:V:67:TRP:NE1	18:W:217:LEU:O	2.51	0.43
1:A:889:GLY:O	1:A:941:ARG:NH2	2.51	0.43
1:A:1389:ARG:O	1:A:1393:ASN:HB2	2.18	0.43
2:B:733:SER:HB3	2:B:736:HIS:CE1	2.54	0.43
8:H:25:ARG:HD3	8:H:41:ASP:OD1	2.18	0.43
14:N:1:DC:H2''	14:N:2:DG:C8	2.54	0.43
14:N:3:DC:H2''	14:N:4:DG:C8	2.53	0.43
18:W:344:LEU:HD12	18:W:349:GLU:HB2	1.99	0.43
2:B:330:GLY:HA3	2:B:344:TYR:HE2	1.84	0.43
7:G:115:ILE:HG23	7:G:163:ILE:HD11	2.01	0.43
18:W:250:ARG:NH2	18:W:284:ASP:OD2	2.50	0.43
1:A:38:PRO:HA	1:A:271:LEU:HD23	2.01	0.43
1:A:1343:GLY:HA2	5:E:182:PRO:HD2	2.00	0.43
16:T:-38:DC:H5'	16:T:-38:DC:H6	1.84	0.43
1:A:318:LYS:HE3	16:T:35:DC:N3	2.34	0.43
1:A:844:LYS:HD2	1:A:844:LYS:HA	1.79	0.43
1:A:252:ALA:HA	1:A:258:GLN:HA	2.00	0.43
1:A:815:PHE:O	1:A:819:MET:HG3	2.19	0.43
2:B:283:VAL:HG13	2:B:283:VAL:O	2.18	0.43
3:C:248:ILE:HG21	11:K:102:ASP:HB2	2.01	0.43
18:W:322:ARG:NE	18:W:343:VAL:H	2.17	0.43
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.90	0.43
2:B:262:LYS:HB3	2:B:271:ASP:HB3	2.01	0.43
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
18:W:543:ILE:HD11	18:W:581:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:LEU:HD23	7:G:11:LEU:HA	1.94	0.42
12:L:60:LYS:HB3	12:L:60:LYS:HE3	1.87	0.42
14:N:33:DT:H2"	14:N:34:DC:C6	2.53	0.42
17:V:12:CYS:HA	17:V:50:THR:HA	2.01	0.42
5:E:42:ARG:HG3	5:E:46:CYS:SG	2.59	0.42
1:A:1221:VAL:HG21	1:A:1274:ILE:HD12	2.01	0.42
2:B:279:ARG:NH1	2:B:316:ILE:O	2.52	0.42
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.02	0.42
6:F:81:THR:OG1	6:F:144:GLU:OE1	2.35	0.42
14:N:-43:DT:H71	14:N:-43:DT:OP2	2.20	0.42
14:N:11:DC:H2"	14:N:12:DG:C8	2.55	0.42
2:B:299:ASP:OD2	2:B:385:ARG:NH1	2.30	0.42
5:E:176:ARG:HD3	5:E:214:LEU:HD11	2.02	0.42
16:T:-5:DA:H2"	16:T:-4:DC:C5	2.54	0.42
1:A:421:ARG:HB3	1:A:424:ASP:HB2	2.01	0.42
2:B:479:TYR:CE2	2:B:778:MET:HG2	2.55	0.42
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.02	0.42
2:B:1156:ASP:O	2:B:1197:PRO:HA	2.19	0.42
18:W:539:HIS:HB2	18:W:584:THR:HA	2.02	0.42
1:A:1201:ARG:HA	1:A:1238:LEU:HD12	2.01	0.42
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.51	0.42
2:B:606:VAL:HG22	2:B:621:THR:HG22	2.02	0.42
3:C:74:GLU:O	3:C:246:ARG:NH2	2.39	0.42
9:I:29:CYS:SG	9:I:30:ARG:N	2.92	0.42
2:B:85:SER:OG	2:B:114:PRO:HD2	2.19	0.42
7:G:165:GLU:H	7:G:168:LEU:HD12	1.85	0.42
18:W:329:LYS:HB2	18:W:434:ASN:HA	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
1:A:976:ASP:O	1:A:979:LYS:NZ	2.48	0.41
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.78	0.41
14:N:-21:DA:H61	16:T:21:DT:H3	1.68	0.41
15:P:8:C:C2	16:T:28:DG:C2	3.08	0.41
17:V:80:GLY:HA2	18:W:244:LEU:HD21	2.02	0.41
5:E:36:GLN:HE21	5:E:36:GLN:HB3	1.69	0.41
18:W:422:TYR:HB3	18:W:427:TYR:CE1	2.55	0.41
8:H:6:PHE:HB3	8:H:59:LEU:HB2	2.03	0.41
13:M:39:ASP:HB3	13:M:44:ILE:HG13	2.03	0.41
15:P:-5:C:C6	18:W:748:ARG:HB2	2.55	0.41
18:W:349:GLU:HA	18:W:431:ARG:HA	2.02	0.41
1:A:1210:THR:HG22	1:A:1212:ASN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:GLN:HG2	2:B:34:GLN:N	2.36	0.41
2:B:1153:GLU:OE1	2:B:1153:GLU:N	2.53	0.41
1:A:473:LEU:CD2	2:B:835:GLN:HB2	2.50	0.41
1:A:914:ILE:HG13	1:A:917:ALA:HB2	2.01	0.41
2:B:293:ILE:HD13	2:B:375:VAL:HG11	2.02	0.41
2:B:764:SER:OG	2:B:765:PRO:HD3	2.19	0.41
14:N:31:DT:H2''	14:N:32:DG:C8	2.55	0.41
2:B:358:THR:HG1	2:B:363:PHE:HD2	1.67	0.41
9:I:94:ASP:OD1	9:I:94:ASP:N	2.49	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:763:GLN:HG2	2:B:765:PRO:HD2	2.01	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
18:W:614:ARG:NH2	18:W:616:GLN:HE21	2.19	0.41
1:A:109:ASN:HB2	1:A:168:CYS:SG	2.61	0.41
2:B:575:VAL:O	2:B:578:VAL:HG22	2.20	0.41
9:I:29:CYS:HB3	9:I:32:CYS:SG	2.59	0.41
1:A:3:GLN:OE1	1:A:3:GLN:N	2.46	0.41
1:A:471:LEU:HD23	1:A:475:VAL:HG23	2.03	0.41
1:A:1295:PRO:HD3	1:A:1301:TYR:CE1	2.56	0.41
1:A:1314:ILE:HB	1:A:1337:GLU:OE1	2.21	0.41
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.79	0.41
3:C:259:LEU:HD13	11:K:91:CYS:HB2	2.03	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
14:N:20:DG:C2	14:N:21:DG:C4	3.09	0.41
14:N:36:DA:H2''	14:N:37:DC:C6	2.55	0.41
15:P:-1:G:H2'	15:P:0:G:H8	1.86	0.41
16:T:16:DA:H2''	16:T:17:DA:H8	1.86	0.41
18:W:540:VAL:HG11	18:W:554:ILE:HD11	2.02	0.41
2:B:71:ILE:HG12	2:B:127:ILE:HG22	2.02	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
8:H:8:ASP:OD1	8:H:9:ILE:N	2.48	0.41
16:T:-30:DG:H2''	16:T:-29:DC:OP2	2.21	0.41
1:A:636:ARG:HG3	1:A:880:GLU:OE2	2.21	0.40
1:A:945:ARG:HG3	1:A:1301:TYR:OH	2.21	0.40
8:H:38:LEU:HD13	8:H:124:LEU:HD13	2.03	0.40
18:W:492:ASN:OD1	18:W:493:HIS:N	2.54	0.40
1:A:883:THR:HA	1:A:954:HIS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ILE:N	1:A:986:PRO:HD2	2.36	0.40
2:B:632:ILE:HD11	2:B:688:GLU:HB3	2.03	0.40
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.55	0.40
14:N:-22:DA:N6	16:T:22:DT:H3	2.20	0.40
14:N:21:DG:H2'	14:N:22:DT:C6	2.56	0.40
16:T:-27:DC:H2''	16:T:-26:DT:H71	2.03	0.40
16:T:-14:DA:H2''	16:T:-13:DA:H8	1.84	0.40
1:A:390:THR:O	1:A:394:ARG:HG2	2.21	0.40
2:B:1174:ASN:OD1	2:B:1177:LYS:HB2	2.21	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
1:A:995:LEU:HD22	1:A:1048:LEU:HD22	2.03	0.40
1:A:1150:SER:OG	1:A:1198:GLU:OE1	2.29	0.40
3:C:251:LEU:HD12	3:C:251:LEU:HA	1.92	0.40
14:N:18:DG:H2''	14:N:19:DC:C6	2.57	0.40
16:T:20:DT:C6	16:T:21:DT:H73	2.56	0.40
1:A:231:ARG:HB3	1:A:234:TRP:CD2	2.56	0.40
3:C:135:ARG:NE	3:C:136:ASP:OD2	2.50	0.40
12:L:33:CYS:SG	12:L:34:GLY:N	2.95	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%)	1353 (97%)	38 (3%)	1 (0%)	51 83
2	B	1154/1227 (94%)	1118 (97%)	36 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	106 (97%)	3 (3%)	0	100	100
10	J	65/72 (90%)	65 (100%)	0	0	100	100
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
12	L	43/72 (60%)	41 (95%)	2 (5%)	0	100	100
13	M	62/113 (55%)	62 (100%)	0	0	100	100
17	V	104/108 (96%)	100 (96%)	4 (4%)	0	100	100
18	W	527/911 (58%)	508 (96%)	19 (4%)	0	100	100
19	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	74/139 (53%)	70 (95%)	4 (5%)	0	100	100
26	e	91/139 (66%)	90 (99%)	1 (1%)	0	100	100
27	b	81/106 (76%)	78 (96%)	3 (4%)	0	100	100
27	f	76/106 (72%)	73 (96%)	3 (4%)	0	100	100
28	c	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
28	g	68/133 (51%)	66 (97%)	2 (3%)	0	100	100
29	d	93/129 (72%)	89 (96%)	4 (4%)	0	100	100
29	h	91/129 (70%)	90 (99%)	1 (1%)	0	100	100
30	j	467/956 (49%)	454 (97%)	12 (3%)	1 (0%)	47	79
31	k	423/531 (80%)	410 (97%)	12 (3%)	1 (0%)	47	79
All	All	9406/12953 (73%)	9187 (98%)	216 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	960	VAL

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Mol	Chain	Res	Type
30	j	543	LYS
31	k	147	ARG

### 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	97
2	B	1018/1077 (94%)	1016 (100%)	2 (0%)	93	97
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%)	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	94
24	v	325/369 (88%)	325 (100%)	0	100	100
25	x	190/354 (54%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	a	64/112 (57%)	64 (100%)	0	100	100
26	e	79/112 (70%)	79 (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	c	82/102 (80%)	82 (100%)	0	100	100
28	g	54/102 (53%)	54 (100%)	0	100	100
29	d	81/107 (76%)	81 (100%)	0	100	100
29	h	79/107 (74%)	79 (100%)	0	100	100
30	j	422/864 (49%)	422 (100%)	0	100	100
31	k	392/474 (83%)	392 (100%)	0	100	100
All	All	8467/11401 (74%)	8457 (100%)	10 (0%)	93	97

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

Mol	Chain	Res	Type
1	A	408	ARG
1	A	831	LYS
1	A	1302	LYS
2	B	463	LYS
2	B	904	ARG
5	E	36	GLN
5	E	166	ARG
13	M	40	LYS
19	m	514	LYS
23	u	124	ARG

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

Mol	Chain	Res	Type
8	H	44	ASN
9	I	11	ASN
18	W	433	GLN
19	m	955	ASN
20	n	232	GLN
27	b	25	ASN
28	c	73	ASN
30	j	750	GLN

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Mol	Chain	Res	Type
31	k	125	ASN
31	k	127	ASN
31	k	141	ASN

### 5.3.3 RNA [i](#)

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 [i](#)

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

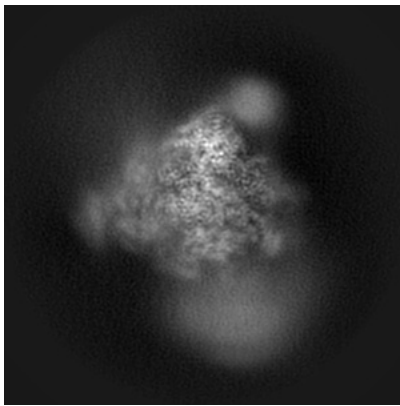
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33436. These allow visual inspection of the internal detail of the map and identification of artifacts.

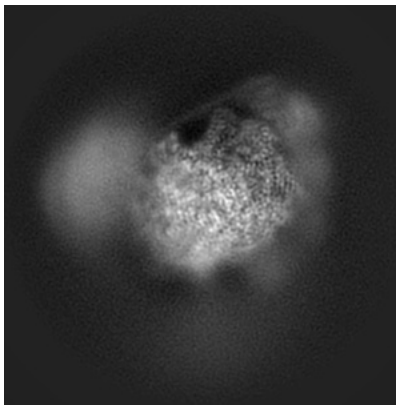
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

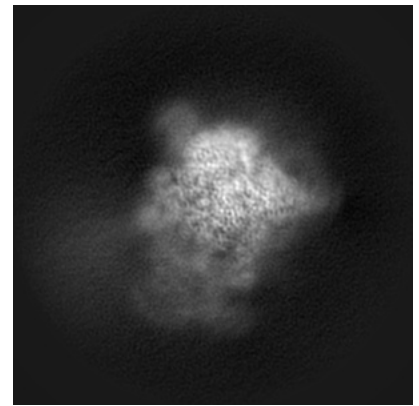
#### 6.1.1 Primary map



X

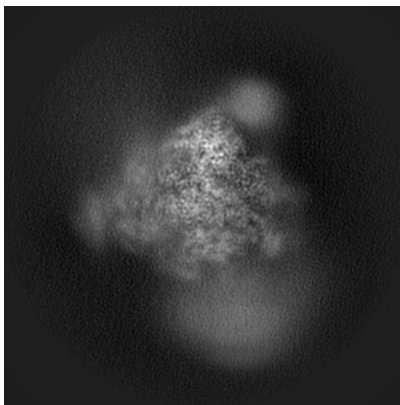


Y

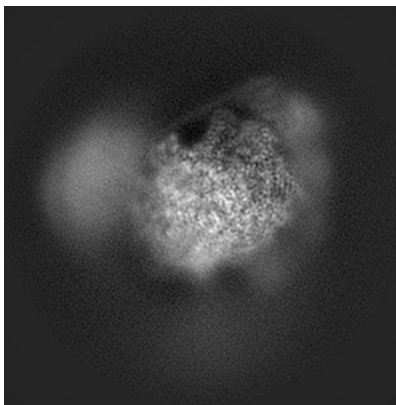


Z

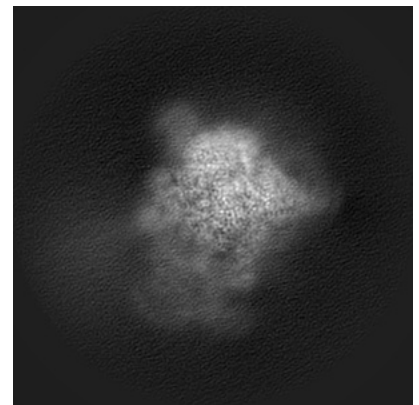
#### 6.1.2 Raw map



X



Y

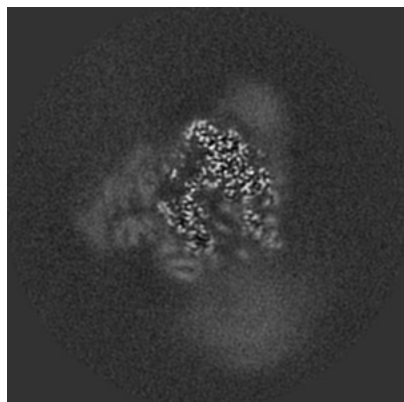


Z

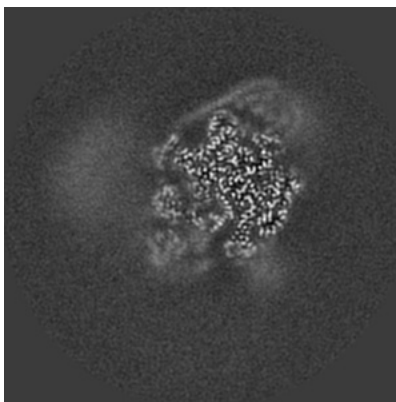
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

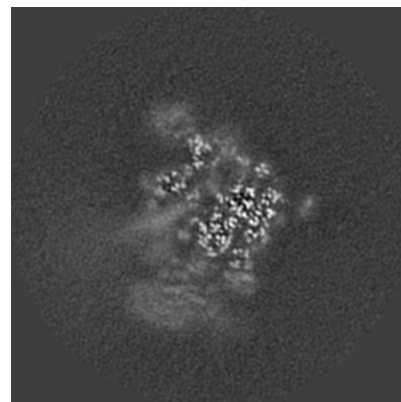
### 6.2.1 Primary map



X Index: 120

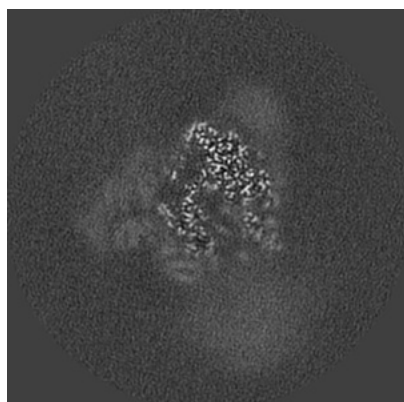


Y Index: 120

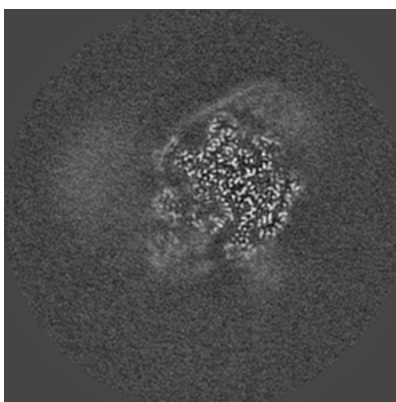


Z Index: 120

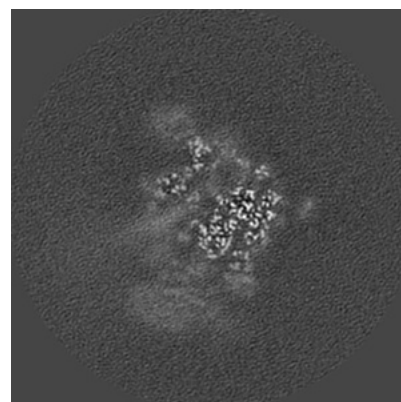
### 6.2.2 Raw map



X Index: 120



Y Index: 120

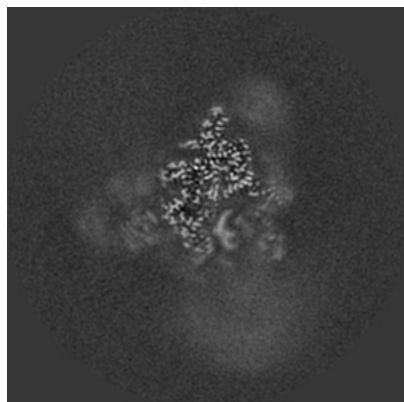


Z Index: 120

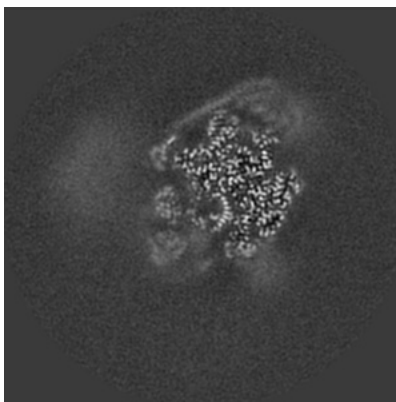
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

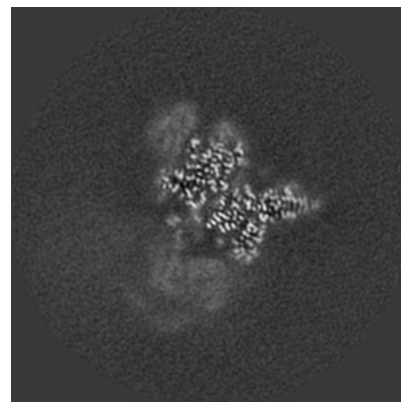
### 6.3.1 Primary map



X Index: 127

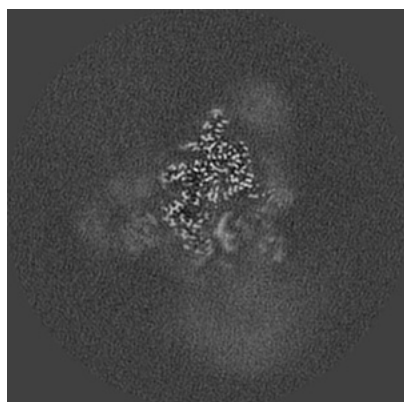


Y Index: 121

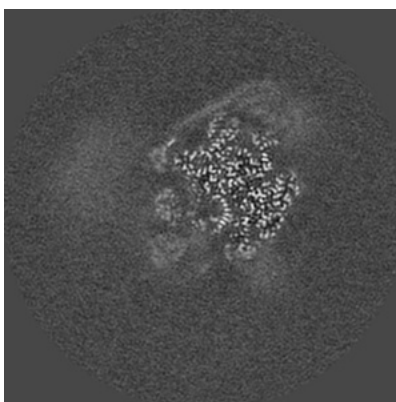


Z Index: 129

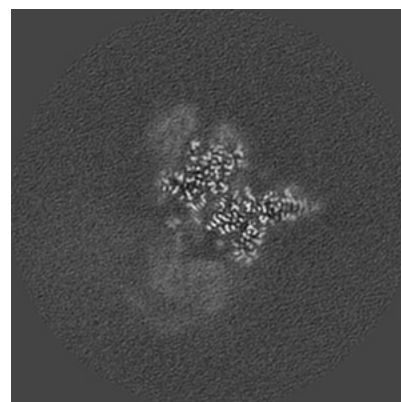
### 6.3.2 Raw map



X Index: 127



Y Index: 121

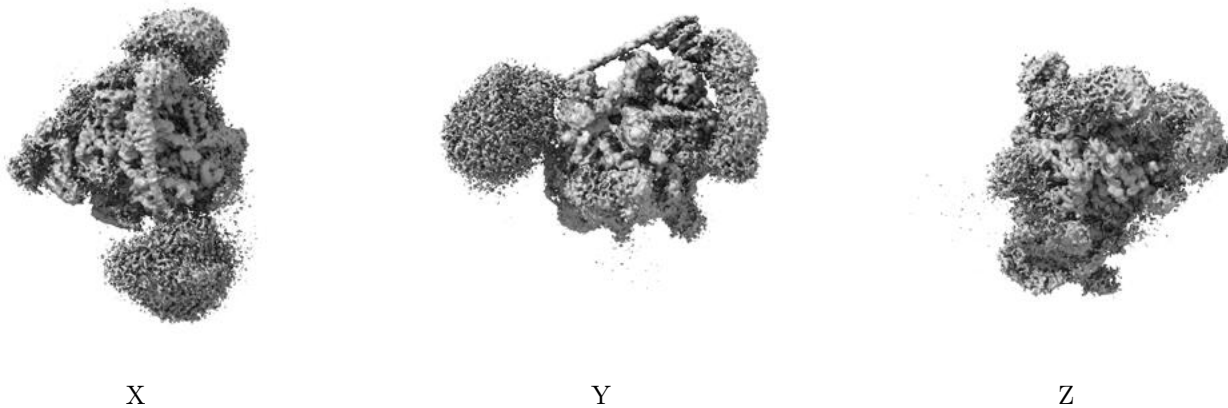


Z Index: 129

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

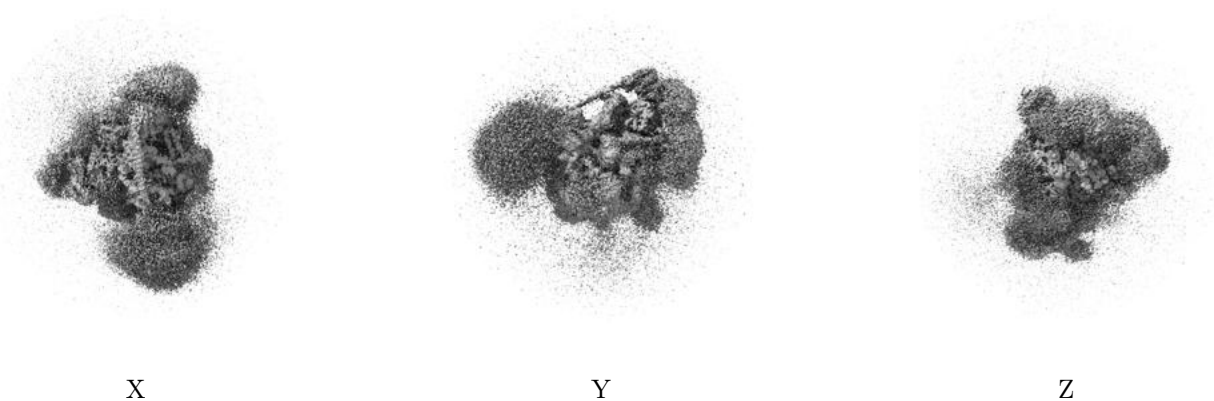
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

## 6.5 Mask visualisation [i](#)

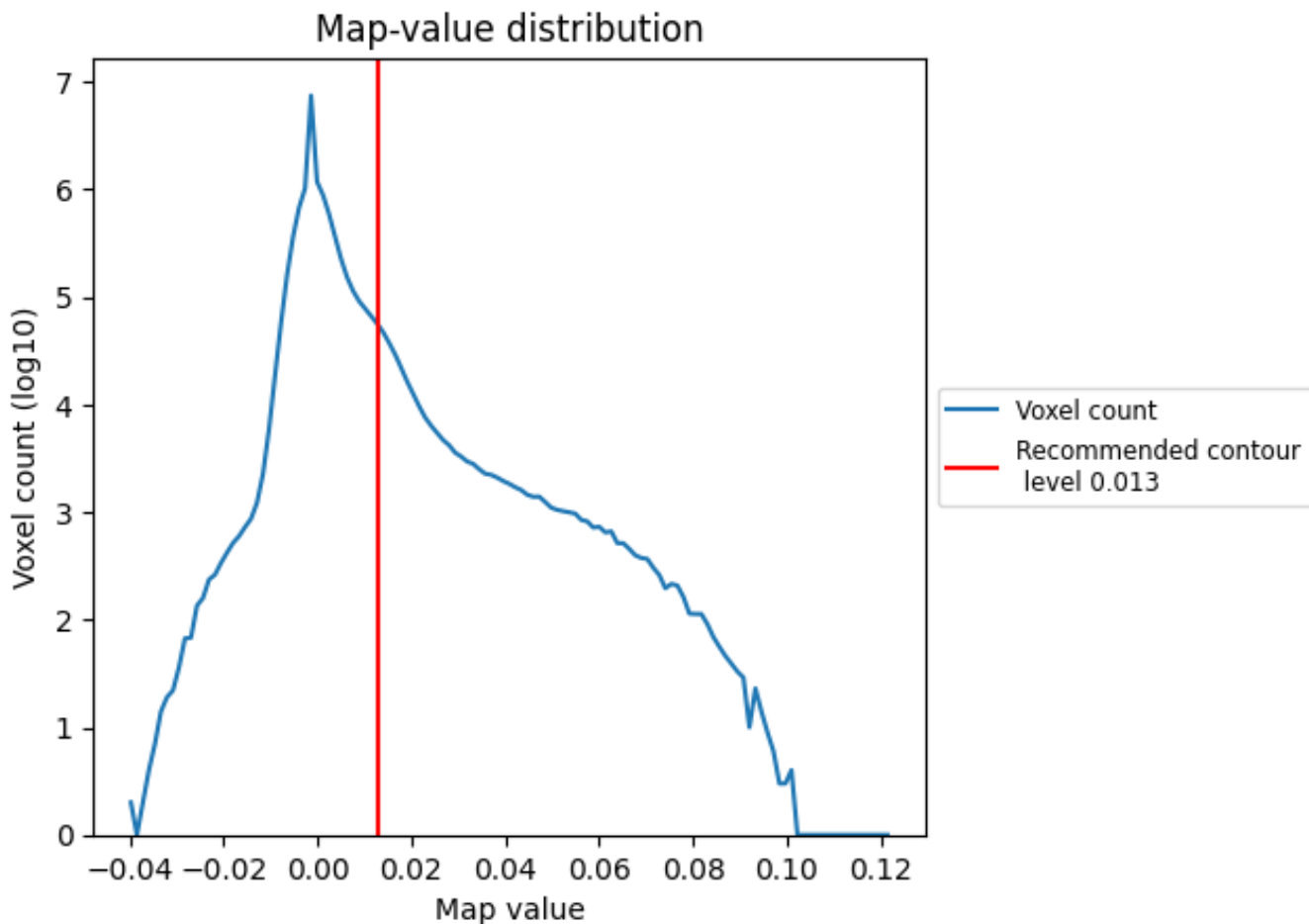
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

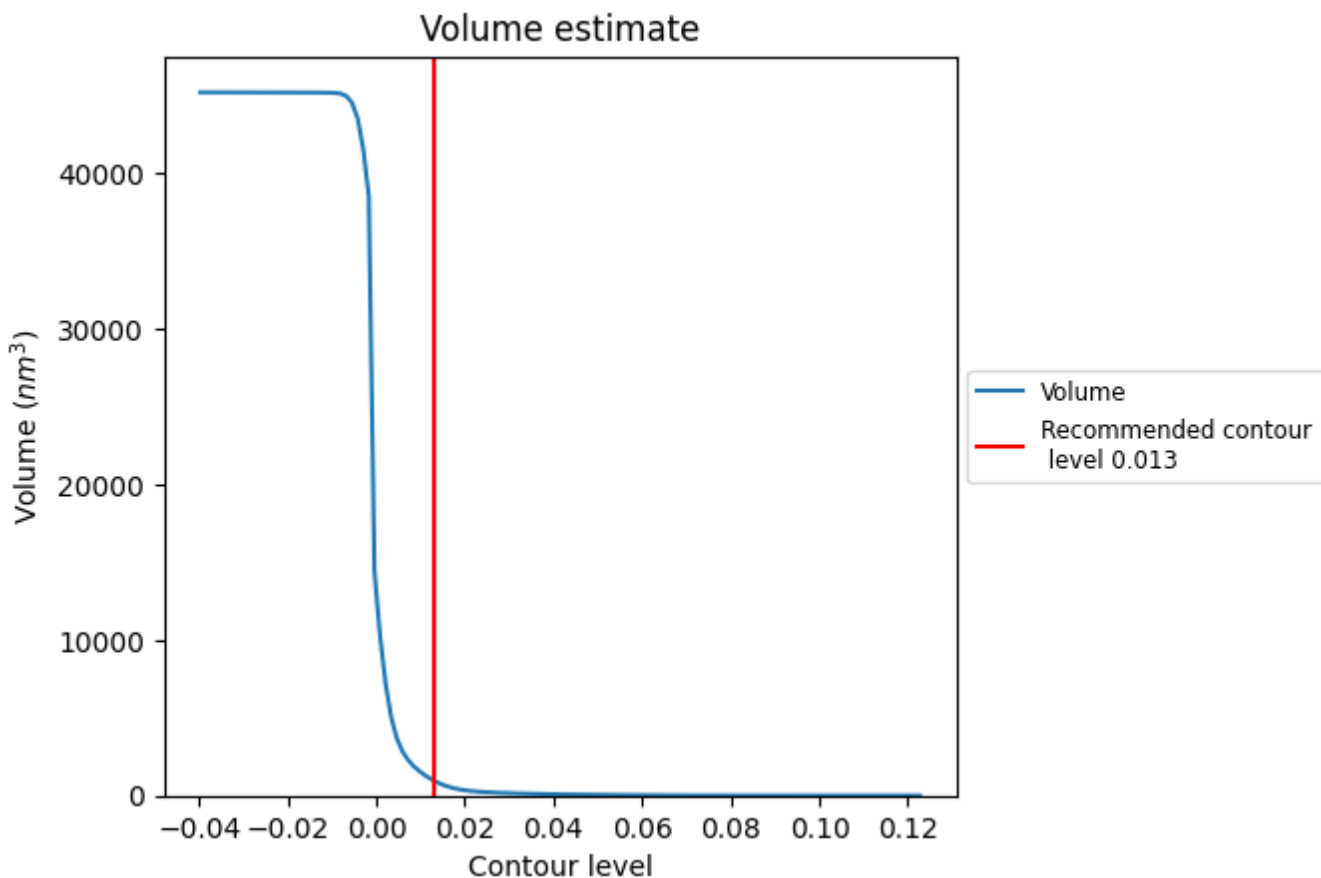
This section contains the results of statistical analysis of the map.

### 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.

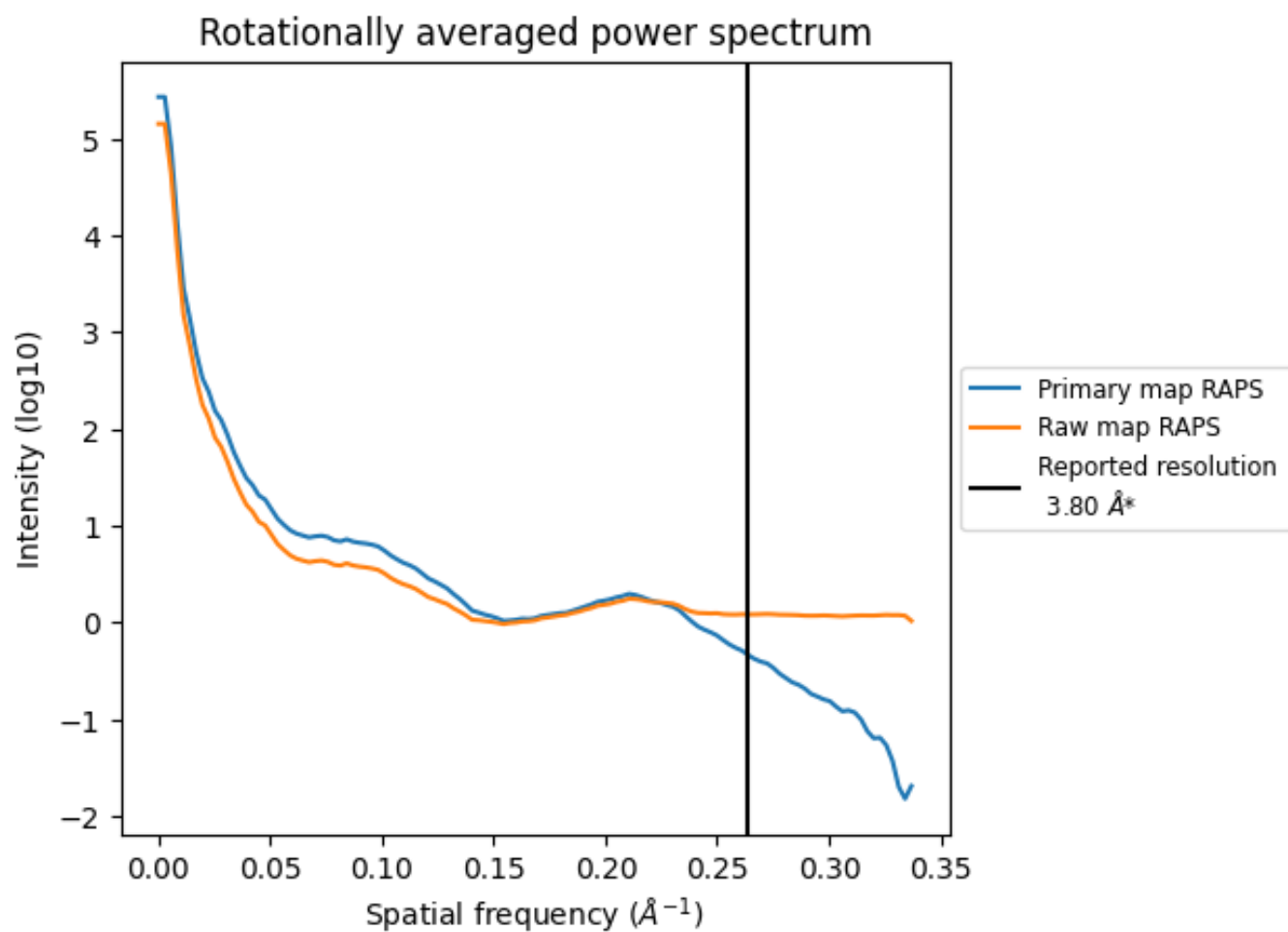
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 964 nm<sup>3</sup>; this corresponds to an approximate mass of 871 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

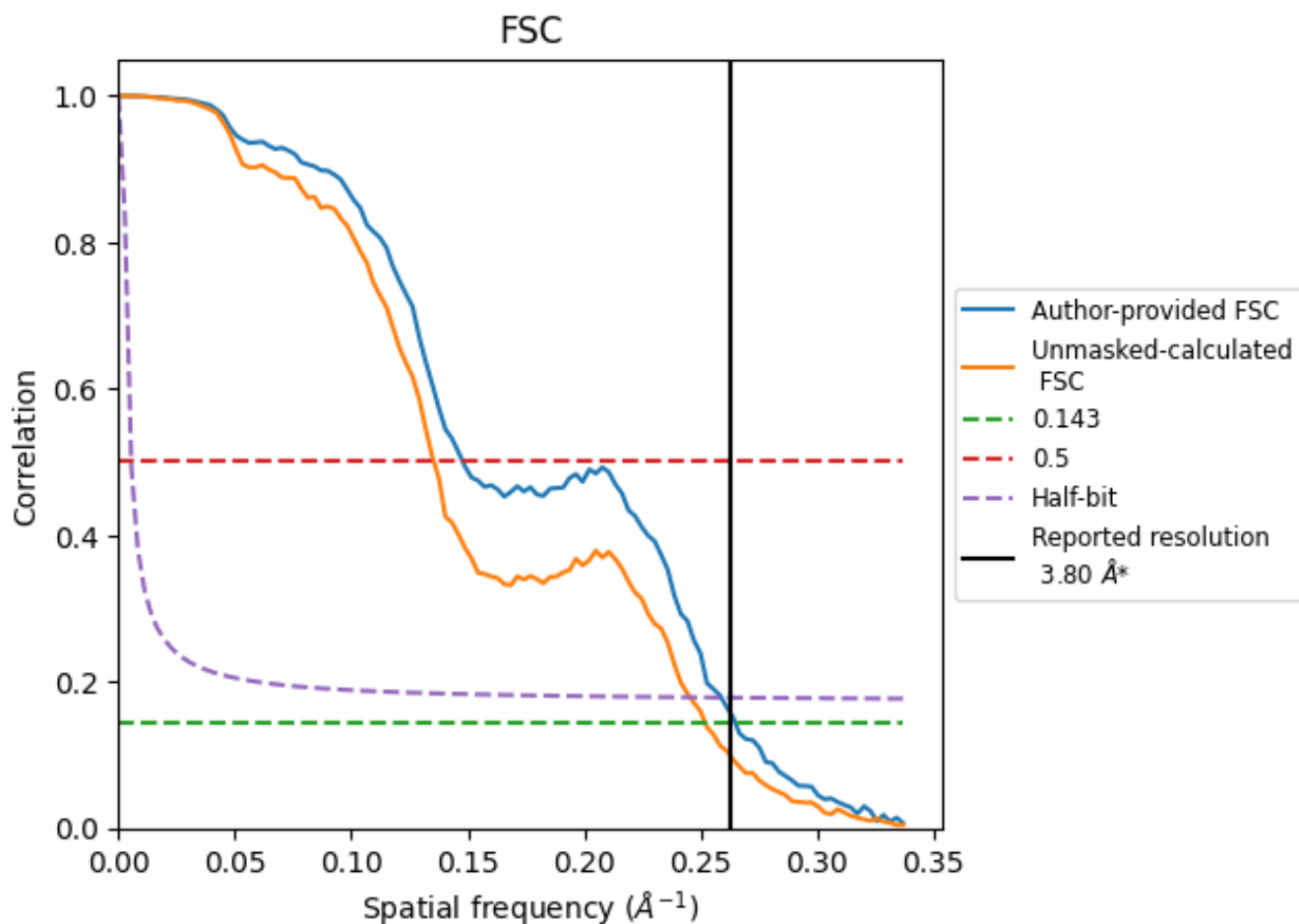


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

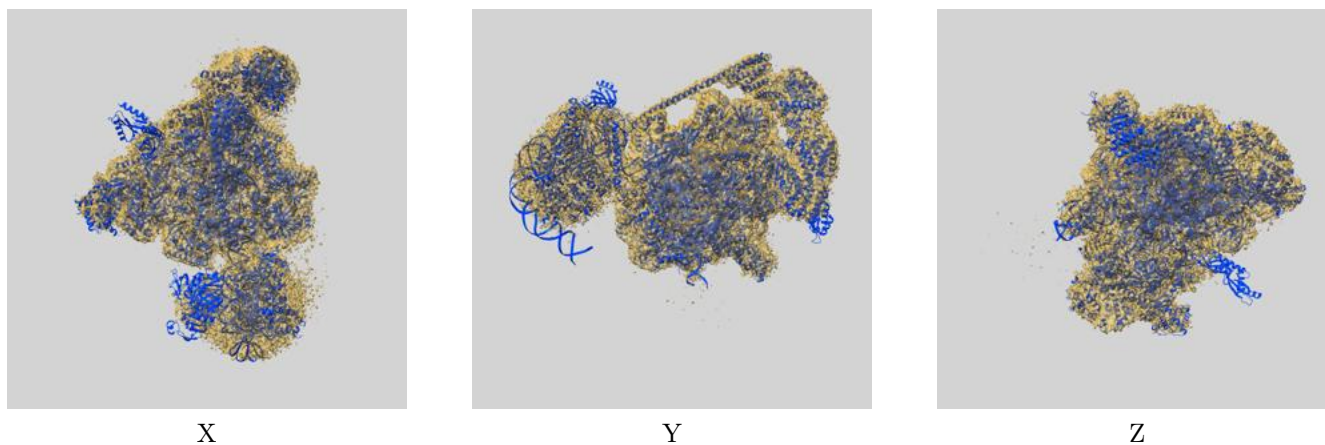
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	6.76	3.86
Unmasked-calculated*	3.97	7.39	4.07

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

## 9 Map-model fit [i](#)

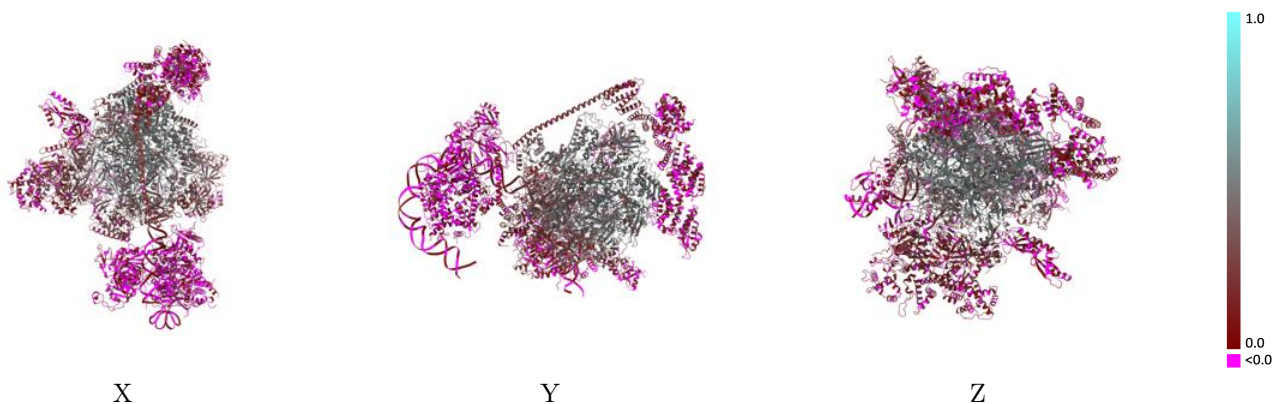
This section contains information regarding the fit between EMDB map EMD-33436 and PDB model 7XSX. Per-residue inclusion information can be found in section 3 on page 16.

### 9.1 Map-model overlay [i](#)



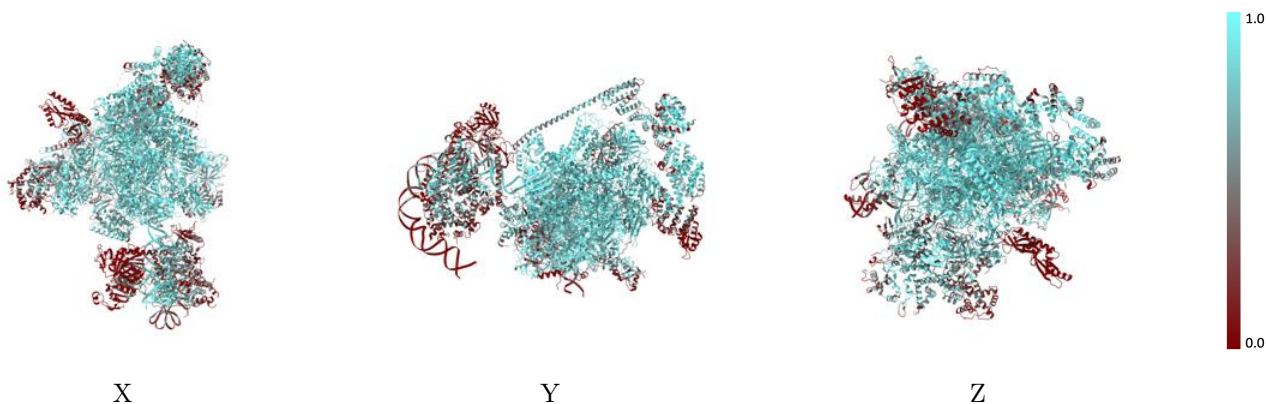
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



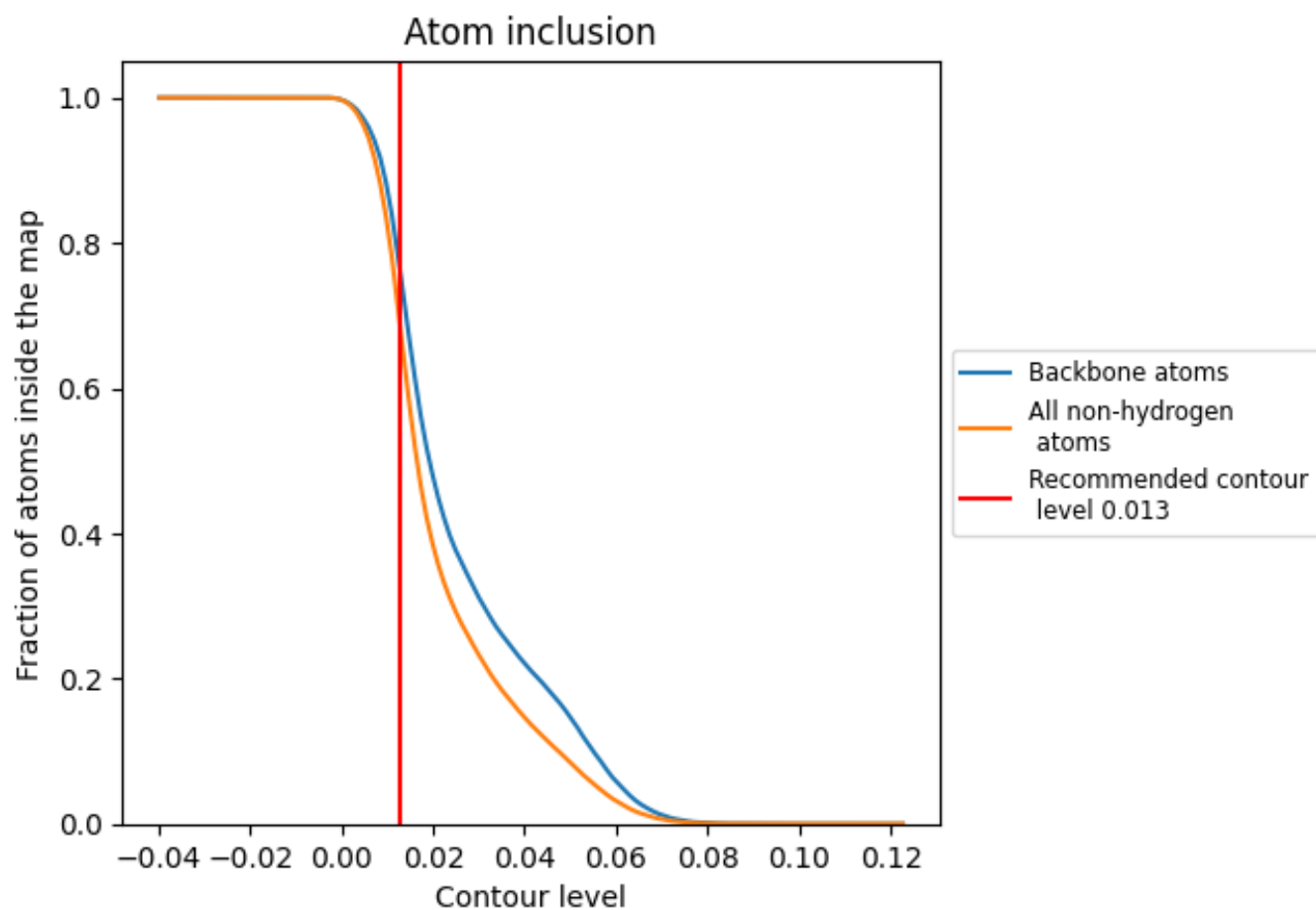
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

## 9.4 Atom inclusion [i](#)











































































At the recommended contour level, 75% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6775	 0.2270
A	 0.9290	 0.4470
B	 0.9290	 0.4580
C	 0.9355	 0.4740
D	 0.7979	 0.2140
E	 0.9398	 0.4140
F	 0.9498	 0.4830
G	 0.8360	 0.3030
H	 0.9304	 0.4650
I	 0.8817	 0.3190
J	 0.9369	 0.4820
K	 0.9563	 0.4750
L	 0.9454	 0.4350
M	 0.8115	 0.1650
N	 0.5556	 0.1000
P	 0.9023	 0.3150
T	 0.5690	 0.1130
V	 0.8736	 0.1210
W	 0.7045	 0.1890
a	 0.8339	 0.0090
b	 0.7830	 -0.0210
c	 0.2023	 -0.0010
d	 0.3741	 0.0070
e	 0.4691	 0.0300
f	 0.5429	 0.0060
g	 0.4914	 0.0030
h	 0.4760	 -0.0080
j	 0.3091	 -0.0020
k	 0.1774	 0.0110
m	 0.4585	 0.1050
n	 0.7894	 0.1970
q	 0.5974	 0.0820
r	 0.4876	 0.1320
u	 0.6084	 0.1870
v	 0.5302	 0.1150
x	 0.7218	 0.2700

