



Full wwPDB EM Validation Report ⓘ

Mar 18, 2026 – 01:00 AM UTC

PDB ID : 9WMW / pdb_00009wmw
EMDB ID : EMD-66107
Title : Co-transcriptional histone H3K36 methylation complex containing RNA polymerase II elongation complex, Set2, and the upstream nucleosome. (temp115, FACT-hexamer)
Authors : Kujirai, T.; Ehara, H.; Ito, T.; Henmi, M.; Sekine, S.; Kurumizaka, H.
Deposited on : 2025-09-03
Resolution : 3.62 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:

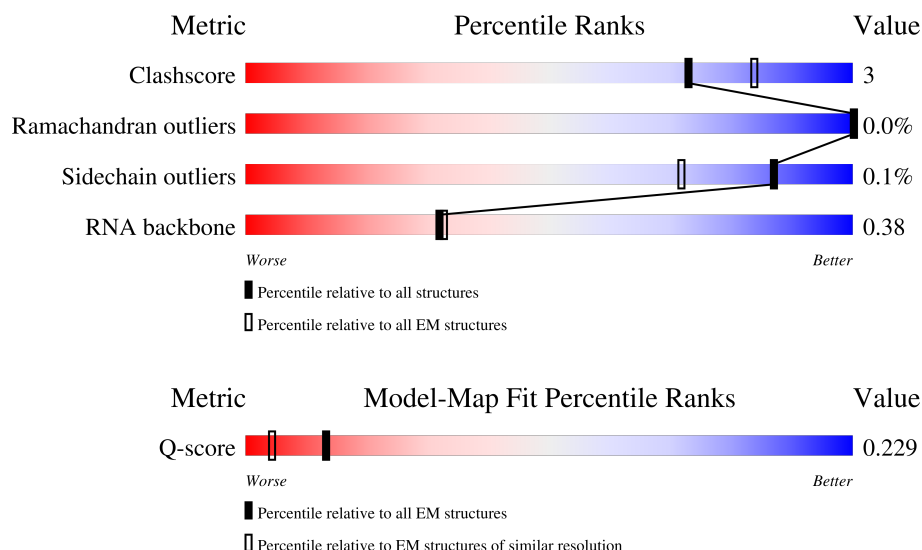
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.62 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11773 (3.12 - 4.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1743	
2	B	1227	
3	C	304	

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

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Mol	Chain	Length	Quality of chain
28	b	106	
28	f	106	
29	g	133	
30	h	129	
31	j	965	
32	k	531	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 78756 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1404	Total	C	N	O	S	0	0
			11064	6975	1930	2089	70		

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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	75	Total	C	N	O	P	0	0
			1548	732	276	465	75		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	86	Total	C	N	O	P	0	0
			1758	828	348	496	86		

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	7	MET	-	initiating methionine	UNP C4R0E6

- Molecule 18 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	535	Total	C	N	O	S	0	0
			4250	2680	754	814	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-2	GLY	-	expression tag	UNP C4R370
W	-1	PRO	-	expression tag	UNP C4R370
W	0	GLY	-	expression tag	UNP C4R370

- Molecule 19 is a protein called Transcription elongation factor Spt6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	m	1178	Total	C	N	O	S	0	0
			9653	6112	1648	1866	27		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	-2	GLY	-	expression tag	UNP C4R7H2
m	-1	PRO	-	expression tag	UNP C4R7H2
m	0	GLY	-	expression tag	UNP C4R7H2

- Molecule 20 is a protein called Protein that interacts with Spt6p and copurifies with Spt5p and RNA polymerase II.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	n	139	Total	C	N	O	S	0	0
			1115	716	193	202	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	-2	GLY	-	expression tag	UNP C4R7L8
n	-1	PRO	-	expression tag	UNP C4R7L8
n	0	GLY	-	expression tag	UNP C4R7L8

- Molecule 21 is a protein called Component of the Paf1p complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	930	Total	C	N	O	S	0	0
			7552	4805	1283	1439	25		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	-39	MET	-	initiating methionine	UNP C4R6B2
q	-38	LYS	-	expression tag	UNP C4R6B2

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Chain	Residue	Modelled	Actual	Comment	Reference
q	-37	ASP	-	expression tag	UNP C4R6B2
q	-36	HIS	-	expression tag	UNP C4R6B2
q	-35	LEU	-	expression tag	UNP C4R6B2
q	-34	ILE	-	expression tag	UNP C4R6B2
q	-33	HIS	-	expression tag	UNP C4R6B2
q	-32	ASN	-	expression tag	UNP C4R6B2
q	-31	HIS	-	expression tag	UNP C4R6B2
q	-30	HIS	-	expression tag	UNP C4R6B2
q	-29	LYS	-	expression tag	UNP C4R6B2
q	-28	HIS	-	expression tag	UNP C4R6B2
q	-27	GLU	-	expression tag	UNP C4R6B2
q	-26	HIS	-	expression tag	UNP C4R6B2
q	-25	ALA	-	expression tag	UNP C4R6B2
q	-24	HIS	-	expression tag	UNP C4R6B2
q	-23	ALA	-	expression tag	UNP C4R6B2
q	-22	GLU	-	expression tag	UNP C4R6B2
q	-21	HIS	-	expression tag	UNP C4R6B2
q	-20	ASP	-	expression tag	UNP C4R6B2
q	-19	TYR	-	expression tag	UNP C4R6B2
q	-18	LYS	-	expression tag	UNP C4R6B2
q	-17	ASP	-	expression tag	UNP C4R6B2
q	-16	ASP	-	expression tag	UNP C4R6B2
q	-15	ASP	-	expression tag	UNP C4R6B2
q	-14	ASP	-	expression tag	UNP C4R6B2
q	-13	LYS	-	expression tag	UNP C4R6B2
q	-12	GLU	-	expression tag	UNP C4R6B2
q	-11	HIS	-	expression tag	UNP C4R6B2
q	-10	LEU	-	expression tag	UNP C4R6B2
q	-9	TYR	-	expression tag	UNP C4R6B2
q	-8	PHE	-	expression tag	UNP C4R6B2
q	-7	GLN	-	expression tag	UNP C4R6B2
q	-6	GLY	-	expression tag	UNP C4R6B2
q	-5	SER	-	expression tag	UNP C4R6B2
q	-4	SER	-	expression tag	UNP C4R6B2
q	-3	GLY	-	expression tag	UNP C4R6B2
q	-2	SER	-	expression tag	UNP C4R6B2
q	-1	SER	-	expression tag	UNP C4R6B2
q	0	GLY	-	expression tag	UNP C4R6B2

- Molecule 22 is a protein called RNAPII-associated chromatin remodeling Paf1 complex sub-unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	266	Total	C	N	O	S	0	0
			2139	1342	374	412	11		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	-29	MET	-	initiating methionine	UNP F2QQ42
r	-28	LYS	-	expression tag	UNP F2QQ42
r	-27	ASP	-	expression tag	UNP F2QQ42
r	-26	HIS	-	expression tag	UNP F2QQ42
r	-25	LEU	-	expression tag	UNP F2QQ42
r	-24	ILE	-	expression tag	UNP F2QQ42
r	-23	HIS	-	expression tag	UNP F2QQ42
r	-22	ASN	-	expression tag	UNP F2QQ42
r	-21	HIS	-	expression tag	UNP F2QQ42
r	-20	HIS	-	expression tag	UNP F2QQ42
r	-19	LYS	-	expression tag	UNP F2QQ42
r	-18	HIS	-	expression tag	UNP F2QQ42
r	-17	GLU	-	expression tag	UNP F2QQ42
r	-16	HIS	-	expression tag	UNP F2QQ42
r	-15	ALA	-	expression tag	UNP F2QQ42
r	-14	HIS	-	expression tag	UNP F2QQ42
r	-13	ALA	-	expression tag	UNP F2QQ42
r	-12	GLU	-	expression tag	UNP F2QQ42
r	-11	HIS	-	expression tag	UNP F2QQ42
r	-10	LEU	-	expression tag	UNP F2QQ42
r	-9	TYR	-	expression tag	UNP F2QQ42
r	-8	PHE	-	expression tag	UNP F2QQ42
r	-7	GLN	-	expression tag	UNP F2QQ42
r	-6	GLY	-	expression tag	UNP F2QQ42
r	-5	SER	-	expression tag	UNP F2QQ42
r	-4	SER	-	expression tag	UNP F2QQ42
r	-3	GLY	-	expression tag	UNP F2QQ42
r	-2	SER	-	expression tag	UNP F2QQ42
r	-1	SER	-	expression tag	UNP F2QQ42
r	0	GLY	-	expression tag	UNP F2QQ42

- Molecule 23 is a protein called Histone-lysine N-methyltransferase, H3 lysine-36 specific.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	11	Total	C	N	O	0	0
			91	60	14	17		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	-2	GLY	-	expression tag	UNP C4QY01
s	-1	PRO	-	expression tag	UNP C4QY01
s	0	GLY	-	expression tag	UNP C4QY01

- Molecule 24 is a protein called Leo1.

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

There are 30 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-2	GLY	-	expression tag	UNP C4R997
v	-1	SER	-	expression tag	UNP C4R997
v	0	ALA	-	expression tag	UNP C4R997

- Molecule 26 is a protein called Constituent of Paf1 complex with RNA polymerase II, Paf1p, Hpr1p, Ctr9, Leo1, Rtf1 and Ccr4p.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	x	205	Total	C	N	O	S	0	0
			1682	1086	287	307	2		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	-29	MET	-	initiating methionine	UNP C4R1E6
x	-28	LYS	-	expression tag	UNP C4R1E6
x	-27	ASP	-	expression tag	UNP C4R1E6
x	-26	HIS	-	expression tag	UNP C4R1E6
x	-25	LEU	-	expression tag	UNP C4R1E6
x	-24	ILE	-	expression tag	UNP C4R1E6
x	-23	HIS	-	expression tag	UNP C4R1E6
x	-22	ASN	-	expression tag	UNP C4R1E6
x	-21	HIS	-	expression tag	UNP C4R1E6
x	-20	HIS	-	expression tag	UNP C4R1E6
x	-19	LYS	-	expression tag	UNP C4R1E6
x	-18	HIS	-	expression tag	UNP C4R1E6
x	-17	GLU	-	expression tag	UNP C4R1E6
x	-16	HIS	-	expression tag	UNP C4R1E6
x	-15	ALA	-	expression tag	UNP C4R1E6
x	-14	HIS	-	expression tag	UNP C4R1E6

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Chain	Residue	Modelled	Actual	Comment	Reference
x	-13	ALA	-	expression tag	UNP C4R1E6
x	-12	GLU	-	expression tag	UNP C4R1E6
x	-11	HIS	-	expression tag	UNP C4R1E6
x	-10	LEU	-	expression tag	UNP C4R1E6
x	-9	TYR	-	expression tag	UNP C4R1E6
x	-8	PHE	-	expression tag	UNP C4R1E6
x	-7	GLN	-	expression tag	UNP C4R1E6
x	-6	GLY	-	expression tag	UNP C4R1E6
x	-5	SER	-	expression tag	UNP C4R1E6
x	-4	SER	-	expression tag	UNP C4R1E6
x	-3	GLY	-	expression tag	UNP C4R1E6
x	-2	SER	-	expression tag	UNP C4R1E6
x	-1	SER	-	expression tag	UNP C4R1E6
x	0	GLY	-	expression tag	UNP C4R1E6

- Molecule 27 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	75	Total	C	N	O	S	0	0
			606	385	114	105	2		
27	e	77	Total	C	N	O	S	0	0
			620	393	116	109	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P84243
a	-2	SER	-	expression tag	UNP P84243
a	-1	HIS	-	expression tag	UNP P84243
a	36	MET	LYS	variant	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243
e	36	MET	LYS	variant	UNP P84243

- Molecule 28 is a protein called Histone H4.

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	93	Total	C	N	O	S	0	0
			722	453	129	137	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	-3	GLY	-	expression tag	UNP P06899
h	-2	SER	-	expression tag	UNP P06899
h	-1	HIS	-	expression tag	UNP P06899
h	120	CYS	LYS	engineered mutation	UNP P06899

- Molecule 31 is a protein called FACT complex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	471	Total	C	N	O	S	0	0
			3794	2406	663	712	13		

There are 27 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
j	939	UNK	-	expression tag	UNP C4QYQ8
j	940	UNK	-	expression tag	UNP C4QYQ8
j	941	UNK	-	expression tag	UNP C4QYQ8
j	942	UNK	-	expression tag	UNP C4QYQ8
j	943	UNK	-	expression tag	UNP C4QYQ8
j	944	UNK	-	expression tag	UNP C4QYQ8
j	945	UNK	-	expression tag	UNP C4QYQ8
j	946	UNK	-	expression tag	UNP C4QYQ8
j	947	UNK	-	expression tag	UNP C4QYQ8
j	948	UNK	-	expression tag	UNP C4QYQ8
j	949	UNK	-	expression tag	UNP C4QYQ8
j	950	UNK	-	expression tag	UNP C4QYQ8
j	951	UNK	-	expression tag	UNP C4QYQ8
j	952	UNK	-	expression tag	UNP C4QYQ8
j	953	UNK	-	expression tag	UNP C4QYQ8
j	954	UNK	-	expression tag	UNP C4QYQ8
j	955	UNK	-	expression tag	UNP C4QYQ8
j	956	UNK	-	expression tag	UNP C4QYQ8
j	957	UNK	-	expression tag	UNP C4QYQ8
j	958	UNK	-	expression tag	UNP C4QYQ8
j	959	UNK	-	expression tag	UNP C4QYQ8
j	960	UNK	-	expression tag	UNP C4QYQ8
j	961	UNK	-	expression tag	UNP C4QYQ8
j	962	UNK	-	expression tag	UNP C4QYQ8

- Molecule 32 is a protein called FACT complex subunit POB3.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

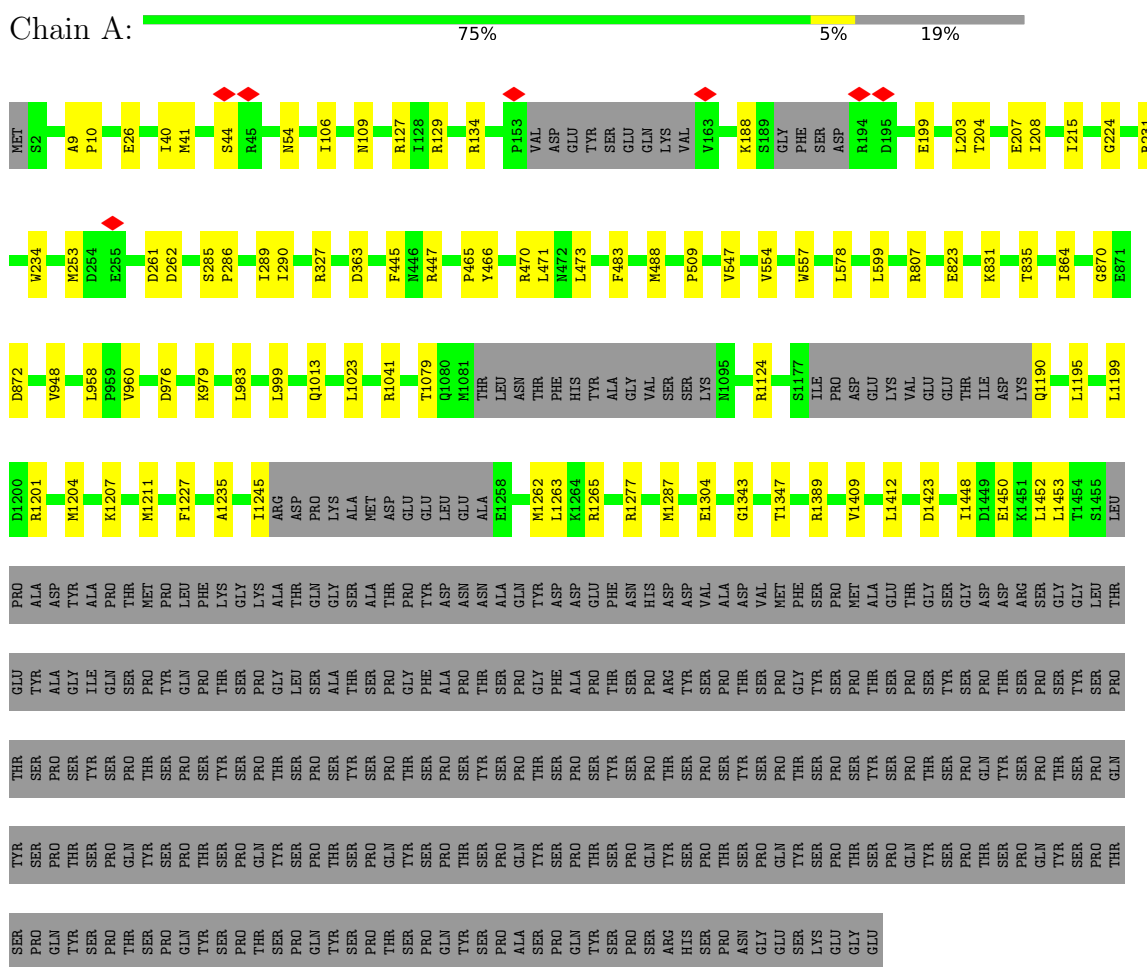
- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

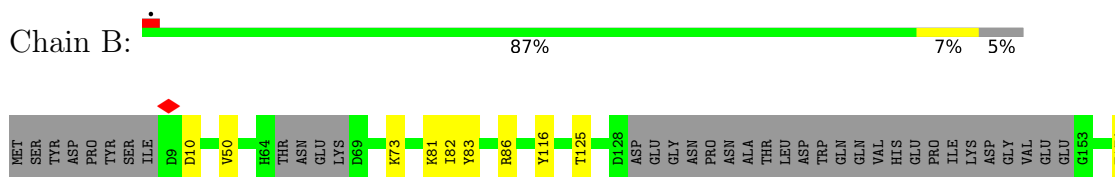
3 Residue-property plots

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

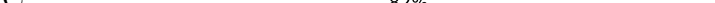
• Molecule 1: DNA-directed RNA polymerase subunit

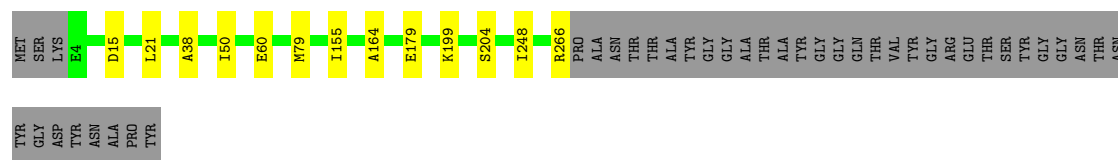


• Molecule 2: DNA-directed RNA polymerase subunit beta

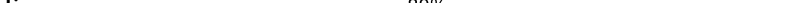


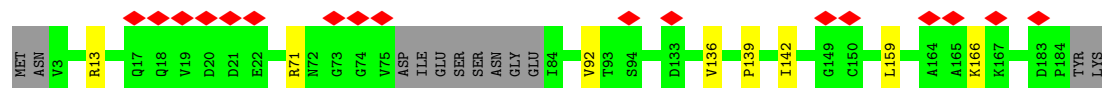
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core

Chain C:  82% 13%



- Molecule 4: RNA polymerase II subunit B32

Chain D:  9% 89% 6%

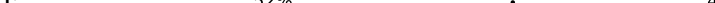


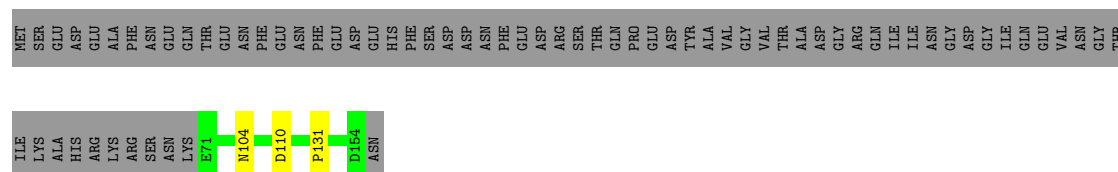
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:  92% 7%



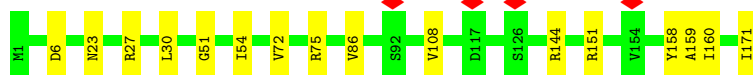
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:  52% 46%



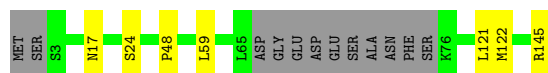
- Molecule 7: RNA polymerase II subunit

Chain G:  91% 9%



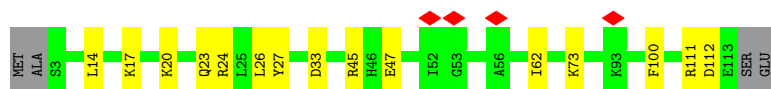
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  87% 5% 8%



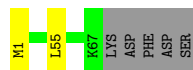
- Molecule 9: DNA-directed RNA polymerase subunit

Chain I:  83% 13% •



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

Chain J:  90% • 7%



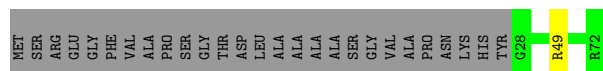
- Molecule 11: RNA polymerase II subunit B12.5

Chain K:  84% 12% •



- Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L:  61% • 38%

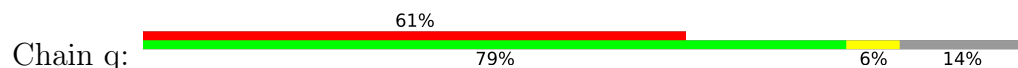


- Molecule 13: Transcription elongation factor 1 homolog

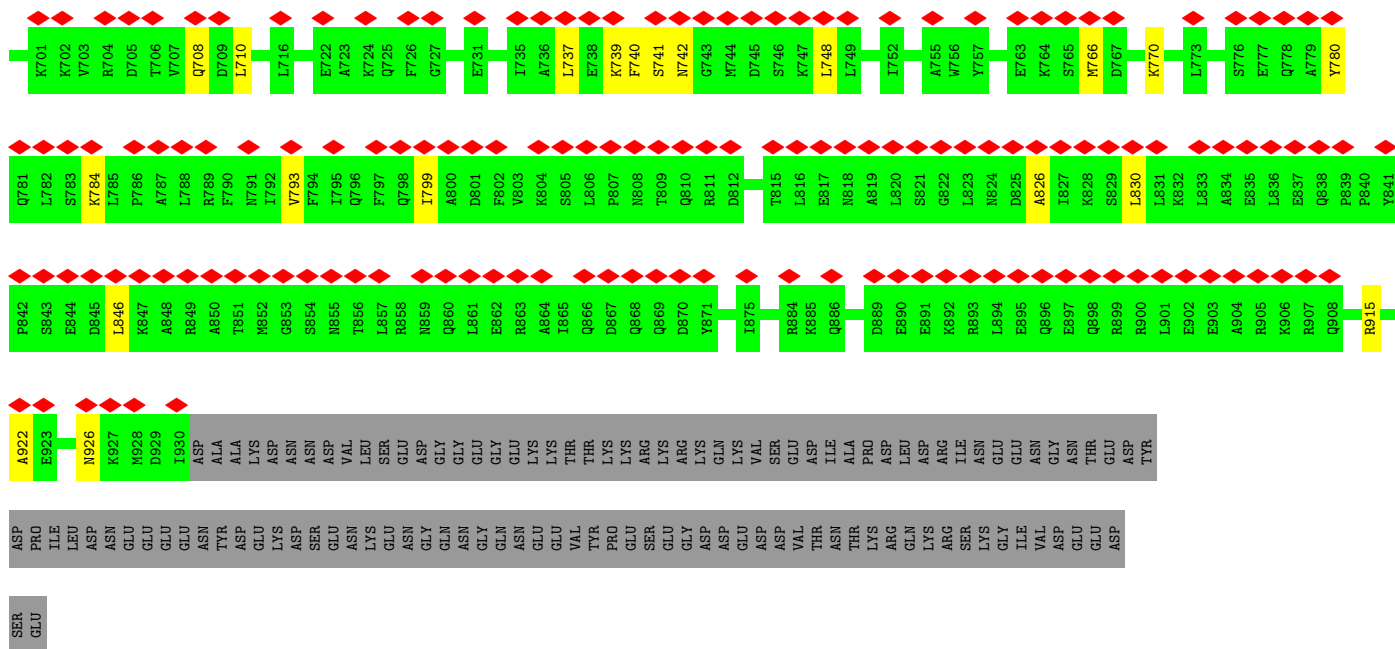
Chain M:  5% 51% 5% 43%



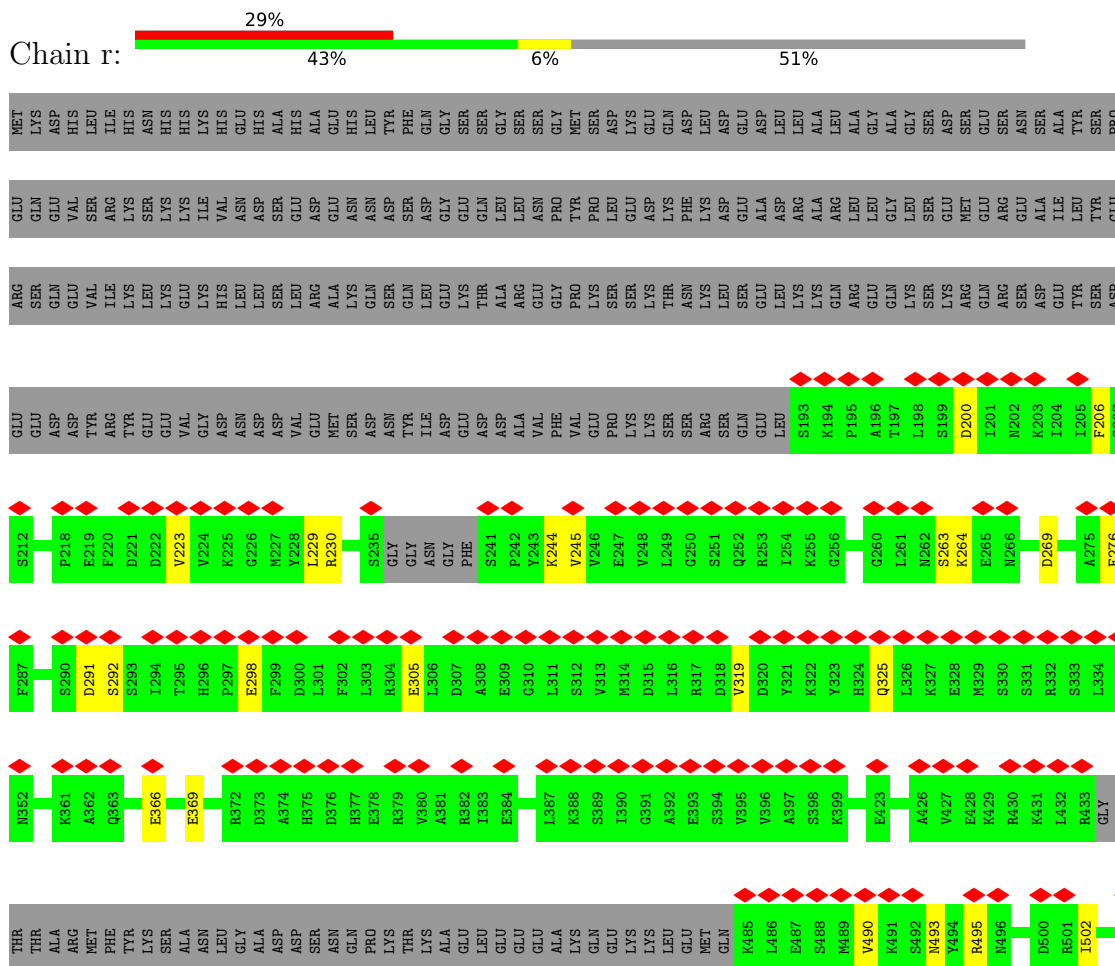
- Molecule 21: Component of the Paf1p complex



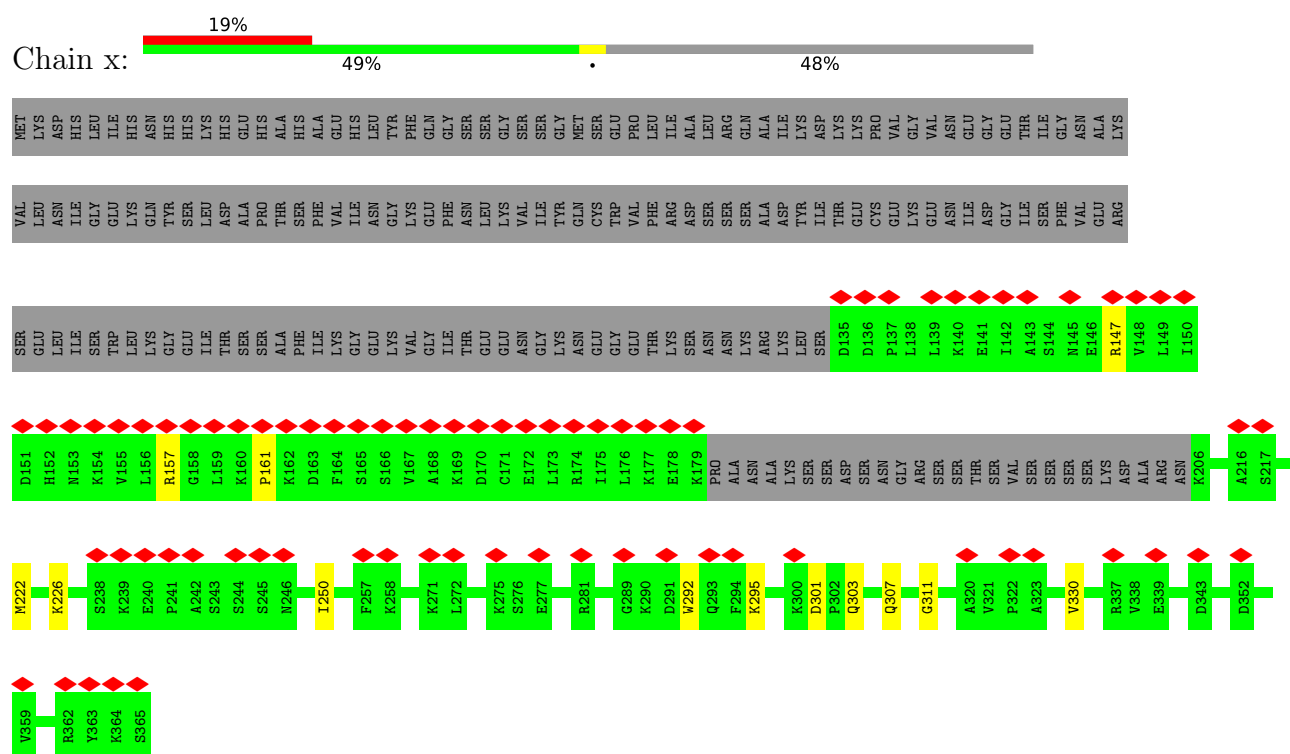
MET	LYS	ASP	HIS	LEU	ILE	HIS	ASN	HIS	HIS	LYS	HIS	GLU	HIS	ALA	ALA	GLU	HIS	ASP	ASP	TYR	LYS	ASP	ASP	ASP	ASP	GLU	LEU	LEU	PHE	GLN	GLY	SER	SER	GLY	SER	GLY	M1	S2	L3	L4	D5	Q6	D7	Y8	Y9	L10	S11	D62	L12	L13	P14	E15	D16	R18	A19	E20				
L21	V22	T23	L24	Q25	L26	T27	I28	P29	L30	K31	S32	G33	D34	E35	V36	V37	T38	I39	D40	F41	N42	E43	D44	V45	D46	V47	S48	Q49	L50	C51	V52	L53	L54	E55	S56	E57	N58	A59	R60	P61	D62	L63	M64	L65	S66	A67	A68	K69	V70	F71	V72	S73	K74	G75	N76	I77	A78	G79	S80	
Q81	E82	I84	I84	K86	A87	L88	Q89	S90	N91	V92	I93	L94	D95	S96	S97	A98	S99	V100	T101	S102	L103	F104	H105	N106	F107	S108	F109	W110	L111	S112	L113	M114	E115	Y116	V117	S118	T119	N120	S121	R122	E123	D124	Q125	F126	L127	K128	Y129	A130	S131	N132	S133	L134	Q135	A136	Q137	N138	S139	L140		
D141	S142	G143	I144	I145	L146	N147	Q148	I149	Q150	N151	Q152	V153	L154	Y155	A156	K157	S158	R159	R160	Y161	D162	E163	A164	L165	K166	E167	F168	D169	N170	L171	L172	K173	K174	K175	S176	T177	N178	I179	L180	A181	I182	L183	Q184	K185	A186	Q187	I188	L189	Y190	K191	R192	Q193	K194	Y195	S196	Q197	A198	E200		
L201	Y202	Q203	K204	A205	L206	T207	I208	N209	P210	L211	I212	V213	P214	D215	P216	R217	I220	C223	F224	W225	H226	L227	N228	N229	K230	Q231	L232	A233	E234	Q235	A236	W237	H238	N239	S240	L241	K242	V243	H244	P245	Q246	N247	N248	L249	N250	L253	L254	K323	L255	C256	K259	F260	D261	Y262	C263	F264				
N265	E266	S267	K268	D269	D270	D271	E272	F273	T274	A275	Y277	R278	E279	S280	L281	E282	F283	L284	H285	S286	C287	L288	K289	E290	D291	A292	K293	H294	P295	Q235	A236	W237	H238	N239	S240	L241	K242	V243	H244	P245	Q246	N247	N248	L249	N250	L253	L254	K323	L255	C256	K259	F260	D261	Y262	C263	F264				
N265	E266	S267	K268	D269	D270	D271	E272	F273	T274	A275	Y277	R278	E279	S280	L281	E282	F283	L284	H285	S286	C287	L288	K289	E290	D291	A292	K293	H294	P295	Q235	A236	W237	H238	N239	S240	L241	K242	V243	H244	P245	Q246	N247	N248	L249	N250	L253	L254	K323	L255	C256	K259	F260	D261	Y262	C263	F264				
S333	A334	S335	H336	F337	M338	L339	Y344	H345	K346	E347	D348	Y349	V350	K357	Q358	A359	E360	D361	S362	Q363	N364	S365	N366	T367	K370	A374	A379	R380	N381	E382	V383	G384	D385	A386	T387	I388	Y389	L390	E391	K392	F393	F394	K395	E396	N397	Q398	D399	S400	K401	S402	S403	M406								
L409	G410	I411	I412	I413	S414	Q415	S416	G417	Y421	I424	I425	E428	K429	Y430	V431	A432	V433	C434	Q435	E436	E437	M438	Y439	P440	I441	L442	P443	E444	A445	Y446	L447	R451	K456	D457	L458	M459	V460	A461	L462	D463	Y464	L465	M466	K467	A468	M469	D470	I471	L472	G473	D474	K475	A476	M477						
Y478	Y479	V480	L481	M482	M483	L484	G485	I486	Y487	H488	F489	F490	M492	M493	V494	S495	Q496	S497	S498	D499	F500	F501	A502	Q503	S504	L505	E506	L579	L580	D581	D582	N510	V511	S512	P513	Q514	N515	R599	R602	K603	M604	G605	L606	K607	Q608	D609	V530	E531	E532	V533	M669	S534	N535	Q536	S537	E538	A539	E540	K541	L542
Y543	S544	K545	L546	M547	E548	C550	P551	G552	R559	Y560	T561	Y562	L563	L564	A565	K567	S568	M569	G570	Y571	M572	A573	M574	Q503	S504	L505	E506	L579	L580	D581	D582	N510	V511	S512	P513	Q514	N515	R599	R602	K603	M604	G605	L606	K607	Q608	D609	V530	E531	E532	V533	M669	S534	N535	Q536	S537	E538	A539	E540	K541	L542
H625	D626	G627	G628	L631	M635	A638	A641	R642	E643	M644	M645	M646	T647	D648	M649	K650	M651	M652	M653	M654	K655	R656	Q657	M658	Y659	A663	M664	M665	M666	M667	M668	M669	L670	S671	L672	M676	L677	G681	G682	L683	A684	D689	M689	E691	R692	T693	G694	L695	A696	L697	E698									



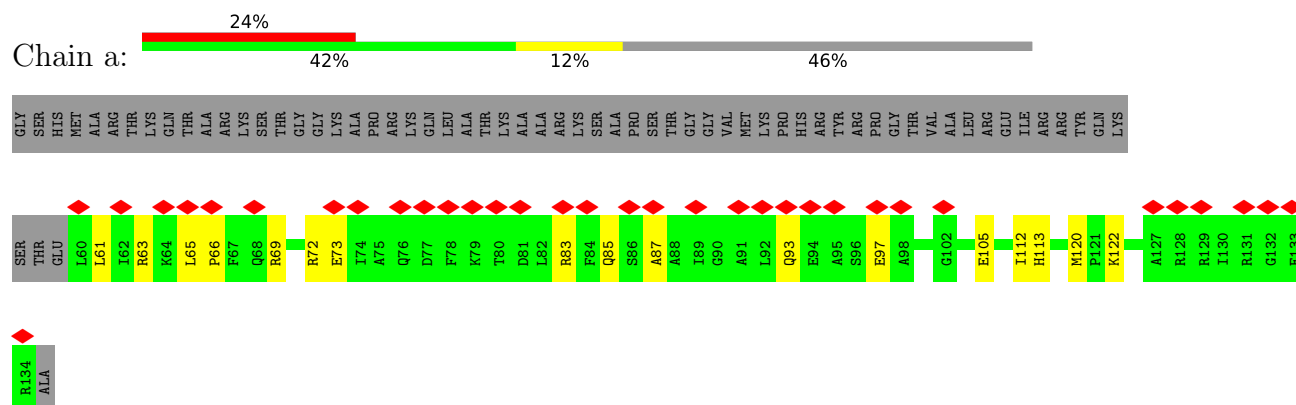
• Molecule 22: RNAPII-associated chromatin remodeling Paf1 complex subunit



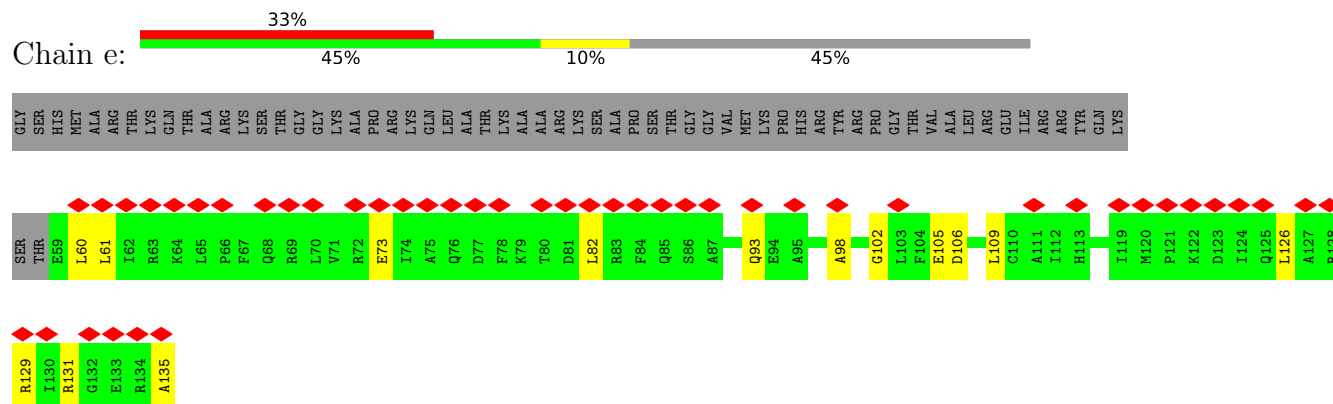




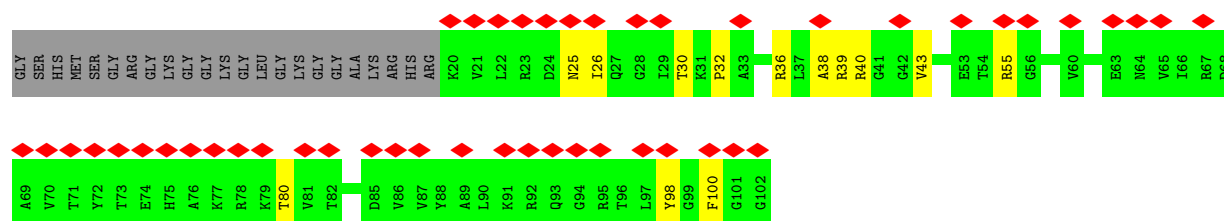
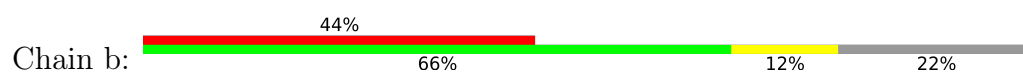
• Molecule 27: Histone H3.3



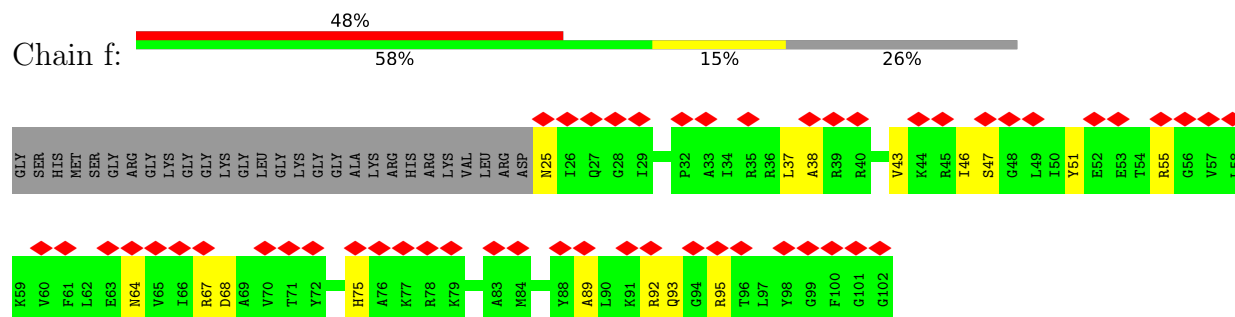
• Molecule 27: Histone H3.3



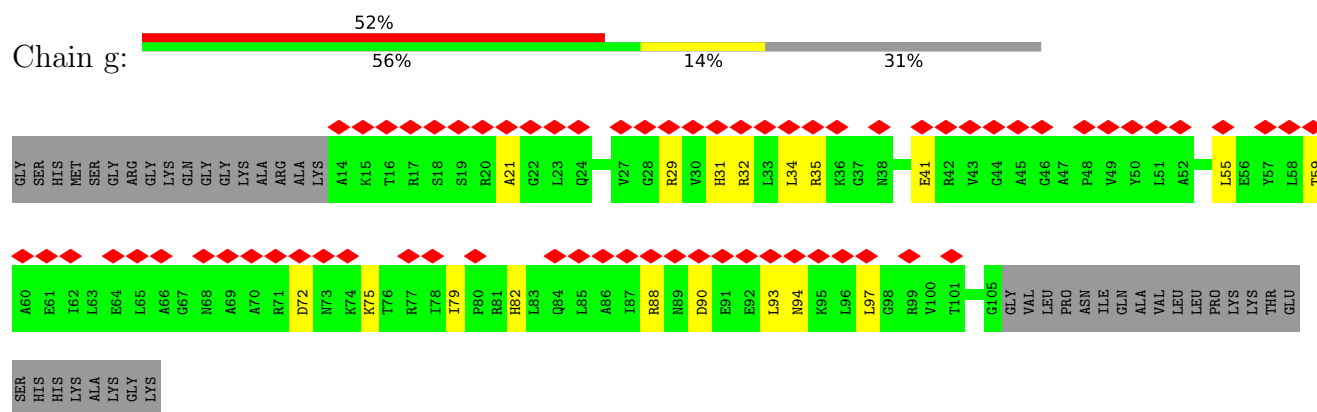
• Molecule 28: Histone H4



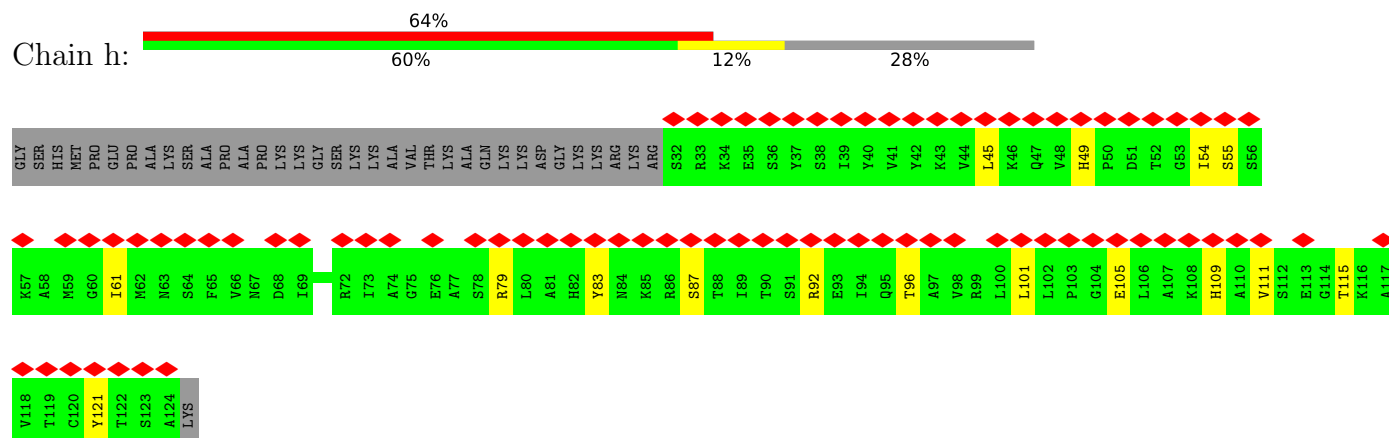
- Molecule 28: Histone H4



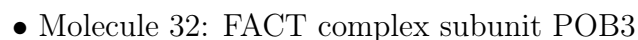
- Molecule 29: Histone H2A type 1-B/E

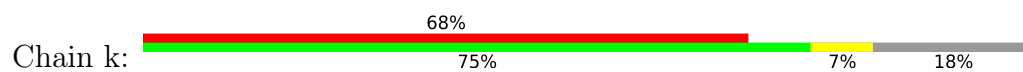


- Molecule 30: Histone H2B type 1-J



- Molecule 31: FACT complex subunit





ASP	VAL	ALA	ALA	GLU	GLU	TYR	ASP	SER	ASN	ALA	ALA	GLY	SER	GLU	GLU	ASP	GLU	GLU	ASP	VAL	PRO	GLU	GLU	GLY	LYS	LYS	LYS	ASN	GLY	ALA	LEU	VAL	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29821	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.147	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.016	Depositor
Map size ($\text{\AA}$)	398.25, 398.25, 398.25	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.475, 1.475, 1.475	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.21	0/11267	0.43	0/15222
2	B	0.21	0/9464	0.43	0/12763
3	C	0.21	0/2139	0.41	0/2895
4	D	0.15	0/1361	0.33	0/1837
5	E	0.20	0/1773	0.44	0/2385
6	F	0.20	0/687	0.38	0/931
7	G	0.15	0/1354	0.33	0/1837
8	H	0.21	0/1070	0.38	0/1444
9	I	0.12	0/934	0.28	0/1257
10	J	0.20	0/563	0.41	0/753
11	K	0.21	0/953	0.41	0/1291
12	L	0.20	0/365	0.45	0/484
13	M	0.17	0/513	0.37	0/693
14	N	0.51	0/1732	0.92	0/2674
15	P	0.26	0/462	0.60	0/716
16	T	0.51	0/1977	0.80	0/3044
17	V	0.15	0/840	0.33	0/1140
18	W	0.18	0/4319	0.43	1/5838 (0.0%)
19	m	0.18	0/9847	0.38	0/13321
20	n	0.18	0/1132	0.38	0/1526
21	q	0.17	0/7689	0.34	0/10368
22	r	0.17	0/2169	0.35	0/2901
23	s	0.12	0/92	0.29	0/122
24	u	0.15	0/1740	0.31	0/2347
25	v	0.16	0/2944	0.33	0/3973
26	x	0.15	0/1716	0.31	0/2310
27	a	0.47	0/613	0.64	0/822
27	e	0.25	0/627	0.43	0/841
28	b	0.43	0/669	0.64	0/894
28	f	0.29	0/626	0.46	0/837
29	g	0.21	0/723	0.36	0/973
30	h	0.31	0/733	0.39	0/987

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	j	0.84	0/3748	1.16	0/5044
32	k	0.80	0/3613	1.12	0/4881
All	All	0.33	0/80454	0.54	1/109351 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	N	0	3
16	T	0	1
31	j	0	1
32	k	0	1
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	W	435	LEU	N-CA-C	5.14	117.20	109.23

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	-21	DG	Sidechain
14	N	-6	DG	Sidechain
14	N	14	DT	Sidechain
16	T	-2	DC	Sidechain
31	j	616	ARG	Sidechain
32	k	58	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11064	0	11090	61	0
2	B	9284	0	9282	61	0
3	C	2098	0	2057	10	0
4	D	1349	0	1345	5	0
5	E	1741	0	1754	11	0
6	F	677	0	693	3	0
7	G	1325	0	1342	10	0
8	H	1053	0	1050	4	0
9	I	917	0	864	10	0
10	J	554	0	573	1	0
11	K	932	0	944	11	0
12	L	359	0	358	1	0
13	M	505	0	495	3	0
14	N	1548	0	848	13	0
15	P	417	0	213	1	0
16	T	1758	0	953	13	0
17	V	824	0	795	11	0
18	W	4250	0	4296	55	0
19	m	9653	0	9500	64	0
20	n	1115	0	1186	16	0
21	q	7552	0	7545	43	0
22	r	2139	0	2155	18	0
23	s	91	0	98	2	0
24	u	1707	0	1676	23	0
25	v	2878	0	2873	26	0
26	x	1682	0	1731	8	0
27	a	606	0	639	20	0
27	e	620	0	650	13	0
28	b	662	0	709	14	0
28	f	619	0	659	12	0
29	g	715	0	755	13	0
30	h	722	0	737	13	0
31	j	3794	0	3700	34	0
32	k	3535	0	3467	32	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	C	1	0	0	0	0
33	I	2	0	0	0	0
33	J	1	0	0	0	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	V	1	0	0	0	0
34	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	78756	0	77032	508	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (508) 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)
32:k:374:GLY:HA2	32:k:387:THR:HG21	1.71	0.72
1:A:445:PHE:CE2	1:A:471:LEU:HD21	2.24	0.72
31:j:919:THR:HG23	31:j:920:ILE:N	2.07	0.70
18:W:461:LEU:HD13	19:m:278:THR:HA	1.74	0.70
29:g:88:ARG:NH2	29:g:97:LEU:O	2.24	0.70
32:k:386:ALA:O	32:k:387:THR:HG23	1.93	0.69
32:k:374:GLY:CA	32:k:387:THR:HG21	2.23	0.69
18:W:218:ILE:CD1	20:n:289:MET:HE1	2.22	0.68
18:W:444:LEU:HG	19:m:284:PHE:CE1	2.28	0.68
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.35	0.67
1:A:445:PHE:HE2	1:A:471:LEU:HD21	1.60	0.67
18:W:444:LEU:HD12	19:m:284:PHE:CD2	2.30	0.67
1:A:483:PHE:CD2	2:B:836:GLU:HB2	2.29	0.67
32:k:227:ASP:OD1	32:k:236:ARG:HG2	1.97	0.65
18:W:487:ILE:HD11	18:W:531:ARG:HB2	1.79	0.65
19:m:337:GLN:HG2	19:m:458:ARG:HH22	1.62	0.65
27:a:122:LYS:HD2	32:k:373:GLU:OE1	1.97	0.64
28:f:68:ASP:OD2	28:f:93:GLN:NE2	2.30	0.64
28:b:26:ILE:HG13	28:b:55:ARG:HD3	1.80	0.64
16:T:-1:DG:OP2	31:j:919:THR:HB	1.96	0.64
18:W:352:LEU:HD11	18:W:435:LEU:HD11	1.79	0.64
1:A:285:SER:HB2	1:A:290:ILE:HD11	1.80	0.63
28:b:39:ARG:HD2	31:j:913:VAL:HG13	1.80	0.63
19:m:473:ASN:HA	19:m:525:ARG:HH22	1.64	0.62
19:m:331:ARG:HH21	19:m:368:LYS:HB3	1.65	0.62
3:C:266:ARG:HH12	11:K:82:ARG:HH22	1.48	0.62
1:A:1211:MET:SD	1:A:1211:MET:N	2.73	0.61
18:W:444:LEU:HB2	19:m:284:PHE:CE2	2.35	0.61
27:a:69:ARG:HB3	28:b:25:ASN:HD22	1.65	0.61
1:A:831:LYS:NZ	1:A:1079:THR:O	2.34	0.60
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.34	0.60
31:j:824:VAL:HG23	31:j:888:THR:HG22	1.83	0.60
9:I:33:ASP:OD1	24:u:75:HIS:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:112:ILE:HG21	31:j:888:THR:HB	1.83	0.60
2:B:969:ARG:NH1	3:C:60:GLU:OE1	2.35	0.59
21:q:793:VAL:HG11	21:q:830:LEU:HG	1.83	0.59
21:q:922:ALA:O	21:q:926:ASN:ND2	2.35	0.59
14:N:5:DT:H2"	14:N:6:DT:C5	2.36	0.59
17:V:15:CYS:HB3	17:V:32:CYS:SG	2.42	0.59
16:T:-1:DG:OP1	31:j:919:THR:HA	2.03	0.59
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.85	0.59
1:A:1262:MET:SD	1:A:1265:ARG:NH2	2.76	0.59
27:a:69:ARG:HB3	28:b:25:ASN:ND2	2.18	0.59
2:B:778:MET:HE3	2:B:794:ASN:HB3	1.84	0.58
17:V:57:LEU:HD11	17:V:81:LEU:HD22	1.85	0.58
18:W:327:ARG:HB3	18:W:436:ILE:HD12	1.84	0.58
21:q:169:ASP:OD1	21:q:185:LYS:NZ	2.35	0.58
21:q:253:ILE:HG12	21:q:297:LEU:HD21	1.84	0.58
16:T:-1:DG:OP2	31:j:919:THR:CB	2.52	0.58
20:n:206:SER:O	20:n:210:ASN:ND2	2.35	0.58
28:b:30:THR:C	28:b:32:PRO:HD2	2.28	0.58
31:j:919:THR:CG2	31:j:920:ILE:N	2.67	0.58
2:B:1176:LYS:HD2	18:W:598:LEU:HD23	1.86	0.58
7:G:27:ARG:NH1	7:G:54:ILE:O	2.36	0.58
19:m:672:VAL:O	19:m:720:GLN:NE2	2.37	0.58
2:B:436:ASN:ND2	24:u:264:LEU:HD22	2.19	0.58
8:H:48:PRO:O	8:H:145:ARG:NH1	2.37	0.57
32:k:103:LYS:HE2	32:k:130:PRO:HG3	1.86	0.57
31:j:655:VAL:HG11	31:j:740:MET:HG3	1.86	0.57
31:j:609:GLY:HA3	31:j:612:LYS:HD2	1.86	0.57
4:D:71:ARG:HE	4:D:92:VAL:HG13	1.70	0.57
22:r:269:ASP:HB3	22:r:349:LEU:HD21	1.85	0.57
2:B:815:ARG:HD2	25:v:135:SER:HB3	1.86	0.57
18:W:616:GLN:OE1	18:W:619:SER:OG	2.23	0.57
31:j:916:ASN:O	31:j:919:THR:HG22	2.04	0.57
2:B:436:ASN:HD22	24:u:264:LEU:HD22	1.69	0.57
10:J:1:MET:HA	10:J:55:LEU:HB2	1.86	0.57
18:W:218:ILE:HG13	20:n:289:MET:HE1	1.86	0.57
2:B:489:ARG:NH2	2:B:533:SER:O	2.37	0.56
18:W:444:LEU:HG	19:m:284:PHE:CZ	2.39	0.56
25:v:233:GLY:O	25:v:244:ASN:ND2	2.38	0.56
2:B:190:MET:SD	2:B:190:MET:N	2.77	0.56
32:k:386:ALA:O	32:k:387:THR:CG2	2.54	0.56
1:A:127:ARG:O	1:A:129:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:VAL:HG21	2:B:82:ILE:HD11	1.86	0.56
13:M:49:CYS:SG	13:M:52:CYS:HB2	2.45	0.56
14:N:-5:DG:N2	14:N:-4:DG:N2	2.53	0.56
19:m:1261:ASN:OD1	19:m:1264:ARG:NH2	2.39	0.56
2:B:879:ARG:HG3	15:P:-3:G:H8	1.70	0.56
8:H:59:LEU:HD21	8:H:122:MET:HE1	1.87	0.56
21:q:531:GLU:O	21:q:535:ASN:N	2.37	0.56
32:k:7:ASP:O	32:k:8:THR:OG1	2.24	0.56
1:A:1207:LYS:O	1:A:1277:ARG:NH2	2.39	0.56
9:I:73:LYS:NZ	9:I:112:ASP:OD2	2.39	0.56
25:v:267:TYR:HB3	25:v:297:TYR:HB3	1.87	0.56
32:k:108:ARG:CZ	32:k:127:ASN:HD22	2.19	0.56
24:u:121:PHE:HB3	24:u:153:ARG:HB3	1.86	0.56
16:T:-7:DG:C2	16:T:-6:DA:C2	2.94	0.55
1:A:473:LEU:HD23	2:B:836:GLU:HG3	1.88	0.55
1:A:1201:ARG:NH2	1:A:1235:ALA:O	2.39	0.55
2:B:421:ILE:HD11	2:B:441:VAL:HG22	1.89	0.55
21:q:569:ASN:O	21:q:603:LYS:NZ	2.36	0.55
21:q:793:VAL:HG13	21:q:826:ALA:HB1	1.87	0.55
22:r:200:ASP:HB3	22:r:319:VAL:HG11	1.88	0.55
5:E:126:VAL:HG11	5:E:131:ILE:HG12	1.88	0.55
9:I:20:LYS:O	9:I:23:GLN:NE2	2.39	0.55
22:r:490:VAL:HG22	22:r:495:ARG:HE	1.72	0.55
3:C:248:ILE:HG21	11:K:102:ASP:HB2	1.88	0.55
14:N:-14:DT:H2"	14:N:-13:DT:H72	1.89	0.55
19:m:1056:ARG:HB3	19:m:1076:MET:HB3	1.88	0.54
31:j:583:TYR:HB3	31:j:621:ARG:HB2	1.88	0.54
2:B:281:LEU:HD12	2:B:364:GLU:HB2	1.88	0.54
2:B:927:GLN:HB2	2:B:931:TYR:HB3	1.89	0.54
18:W:524:GLU:O	20:n:232:GLN:NE2	2.40	0.54
24:u:209:LEU:HB2	25:v:252:PHE:HB2	1.88	0.54
4:D:159:LEU:HD22	7:G:86:VAL:HG11	1.90	0.54
21:q:157:LYS:NZ	25:v:71:ASP:OD1	2.40	0.54
24:u:272:TYR:O	24:u:276:ARG:HG2	2.08	0.54
19:m:607:ILE:HG22	19:m:719:VAL:HG11	1.89	0.54
9:I:100:PHE:HE1	9:I:111:ARG:HE	1.56	0.54
26:x:292:TRP:HA	26:x:295:LYS:HE2	1.89	0.54
21:q:155:TYR:HB2	21:q:164:ALA:HB2	1.90	0.53
2:B:557:GLU:OE2	2:B:584:ARG:NH1	2.40	0.53
13:M:33:SER:HA	13:M:50:LYS:HE2	1.90	0.53
17:V:89:ARG:NH1	17:V:109:ASP:OD2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:327:ARG:NH1	18:W:335:GLY:O	2.38	0.53
24:u:199:LEU:HD11	25:v:211:PHE:HB3	1.91	0.53
27:e:109:LEU:HD22	32:k:430:ASN:CG	2.33	0.53
14:N:5:DT:H72	31:j:598:SER:HA	1.89	0.53
30:h:105:GLU:HG3	30:h:109:HIS:CD2	2.44	0.53
19:m:1083:MET:HE1	19:m:1131:LEU:HD23	1.91	0.53
1:A:40:ILE:HG23	1:A:54:ASN:HD22	1.72	0.52
2:B:235:LEU:HD23	2:B:242:ILE:HG13	1.91	0.52
2:B:393:HIS:NE2	2:B:696:GLU:OE2	2.42	0.52
2:B:906:SER:OG	18:W:781:GLU:OE1	2.27	0.52
9:I:45:ARG:NH2	9:I:47:GLU:OE2	2.42	0.52
19:m:532:VAL:HG22	19:m:565:MET:HE2	1.91	0.52
24:u:145:ILE:O	24:u:149:THR:OG1	2.21	0.52
1:A:976:ASP:O	1:A:979:LYS:NZ	2.42	0.52
7:G:6:ASP:OD1	7:G:75:ARG:NH1	2.43	0.52
9:I:14:LEU:HB3	9:I:27:TYR:HB3	1.92	0.52
19:m:236:GLU:OE2	20:n:252:ARG:NH2	2.43	0.52
21:q:59:ALA:HB1	21:q:63:LEU:HD12	1.91	0.52
18:W:232:ARG:HH12	18:W:235:LYS:HE3	1.73	0.52
19:m:1426:LEU:HD13	19:m:1469:ARG:HH21	1.74	0.52
14:N:12:DG:C2	16:T:-11:DG:C2	2.97	0.52
19:m:725:GLU:OE2	19:m:728:ARG:NH2	2.36	0.52
21:q:766:MET:HG3	21:q:770:LYS:HE3	1.92	0.52
26:x:157:ARG:HB3	26:x:161:PRO:HB3	1.91	0.52
32:k:385:PHE:CZ	32:k:387:THR:OG1	2.62	0.52
21:q:215:ASP:OD1	21:q:217:ARG:NH1	2.43	0.52
21:q:578:GLN:NE2	21:q:582:ASP:OD1	2.44	0.52
27:a:112:ILE:HD13	31:j:888:THR:HB	1.90	0.52
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.38	0.51
1:A:1423:ASP:OD1	1:A:1423:ASP:N	2.41	0.51
21:q:830:LEU:HD22	21:q:846:LEU:HB3	1.91	0.51
5:E:60:LEU:O	21:q:915:ARG:NH1	2.39	0.51
21:q:357:LYS:NZ	21:q:361:ASP:OD1	2.43	0.51
21:q:451:ARG:NH1	25:v:35:GLU:OE1	2.43	0.51
21:q:239:ASN:HA	21:q:242:LYS:HD2	1.92	0.51
19:m:1033:ARG:HH12	19:m:1087:ARG:HH12	1.58	0.51
2:B:10:ASP:HB3	2:B:649:LYS:HG3	1.93	0.51
11:K:25:SER:O	26:x:307:GLN:NE2	2.41	0.51
24:u:114:LEU:HD11	24:u:150:VAL:HG23	1.92	0.51
29:g:55:LEU:O	29:g:59:THR:HG23	2.11	0.51
1:A:1124:ARG:NH2	1:A:1304:GLU:OE2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:229:VAL:HG21	18:W:286:LEU:HD11	1.92	0.51
19:m:1200:PRO:O	19:m:1203:ARG:NH1	2.43	0.51
1:A:447:ARG:HB2	1:A:488:MET:HE3	1.93	0.50
28:f:89:ALA:O	28:f:93:GLN:HG2	2.11	0.50
19:m:1002:ARG:HH11	19:m:1052:TYR:HH	1.58	0.50
1:A:1195:LEU:HB2	1:A:1263:LEU:HD21	1.93	0.50
18:W:218:ILE:CG1	20:n:289:MET:HE1	2.41	0.50
20:n:207:ILE:HG23	20:n:212:LEU:HB3	1.92	0.50
26:x:226:LYS:HG3	26:x:250:ILE:HG22	1.93	0.50
18:W:356:PRO:HG2	18:W:394:PHE:HB2	1.92	0.50
18:W:666:GLU:HG2	18:W:705:VAL:HG12	1.92	0.50
20:n:260:MET:HG3	20:n:284:TRP:HZ3	1.77	0.50
21:q:250:ASN:HA	21:q:253:ILE:HD12	1.93	0.50
28:b:98:TYR:HB3	30:h:61:ILE:HG23	1.94	0.50
1:A:286:PRO:HG2	1:A:289:ILE:HD12	1.93	0.50
19:m:1191:ASN:OD1	19:m:1193:GLN:NE2	2.42	0.50
19:m:1255:TRP:NE1	19:m:1260:GLU:OE1	2.42	0.50
27:a:61:LEU:HD22	28:b:36:ARG:HD2	1.92	0.50
18:W:666:GLU:HA	18:W:705:VAL:HA	1.94	0.50
27:e:129:ARG:HH11	27:e:129:ARG:HG2	1.77	0.50
2:B:245:MET:HE1	2:B:371:LEU:HD21	1.93	0.49
17:V:9:GLU:HA	17:V:20:PRO:HA	1.94	0.49
18:W:328:VAL:HA	18:W:435:LEU:HD23	1.94	0.49
1:A:1190:GLN:HA	1:A:1245:ILE:HA	1.95	0.49
18:W:704:ARG:NH1	19:m:632:GLU:OE2	2.46	0.49
20:n:163:LEU:HD11	20:n:194:VAL:HG22	1.94	0.49
20:n:216:VAL:HG13	20:n:237:LEU:HD13	1.94	0.49
24:u:191:THR:HG22	24:u:219:VAL:HG22	1.95	0.49
27:a:63:ARG:HB3	27:a:66:PRO:HD2	1.95	0.49
27:a:122:LYS:HB2	32:k:373:GLU:OE1	2.11	0.49
1:A:9:ALA:O	2:B:1193:GLN:NE2	2.44	0.49
14:N:-5:DG:N2	14:N:-4:DG:C2	2.80	0.49
18:W:327:ARG:NH2	18:W:441:ASN:O	2.46	0.49
18:W:351:ARG:HA	18:W:429:THR:HA	1.94	0.49
26:x:311:GLY:HA3	26:x:330:VAL:HG12	1.95	0.49
28:f:75:HIS:O	30:h:92:ARG:NH1	2.45	0.49
18:W:640:LYS:NZ	18:W:641:LEU:O	2.46	0.49
19:m:1041:LEU:HD11	19:m:1081:TYR:HD2	1.77	0.49
17:V:10:ARG:HA	17:V:52:SER:HA	1.95	0.49
19:m:1425:LYS:HE3	19:m:1428:PRO:HA	1.94	0.49
32:k:108:ARG:NH2	32:k:127:ASN:HD22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:ILE:O	2:B:341:ARG:NH1	2.46	0.49
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.95	0.49
14:N:-2:DC:OP1	28:b:32:PRO:HD3	2.12	0.49
21:q:31:LYS:HB2	21:q:57:GLU:HA	1.94	0.49
25:v:210:VAL:HG13	25:v:334:VAL:HG21	1.95	0.49
2:B:248:LYS:NZ	2:B:264:THR:OG1	2.46	0.48
18:W:317:ASP:O	18:W:318:VAL:C	2.55	0.48
32:k:239:ILE:CG2	32:k:246:LEU:HD11	2.43	0.48
2:B:613:ARG:HH21	9:I:62:ILE:HD11	1.76	0.48
21:q:479:TYR:HD1	25:v:30:LEU:HB3	1.78	0.48
21:q:390:LEU:HB3	21:q:409:LEU:HD21	1.96	0.48
2:B:601:ALA:HA	24:u:239:SER:HB3	1.95	0.48
27:e:61:LEU:HD12	28:f:37:LEU:HD23	1.95	0.48
1:A:106:ILE:HD13	1:A:215:ILE:HD11	1.96	0.48
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.46	0.48
19:m:1172:VAL:HA	19:m:1182:VAL:HG12	1.93	0.48
27:a:105:GLU:HB3	31:j:868:LYS:HD2	1.94	0.48
30:h:45:LEU:HD22	30:h:54:ILE:HG13	1.96	0.48
2:B:268:VAL:HG11	2:B:272:ILE:HD11	1.95	0.48
11:K:14:ASP:N	11:K:14:ASP:OD1	2.47	0.48
18:W:465:ALA:HA	18:W:468:LEU:HD12	1.95	0.48
29:g:79:ILE:HG12	29:g:82:HIS:CE1	2.48	0.48
31:j:869:ASN:ND2	31:j:888:THR:OG1	2.45	0.48
19:m:998:ASN:HD22	19:m:999:LEU:N	2.12	0.48
28:f:93:GLN:HB2	28:f:95:ARG:HG2	1.95	0.48
1:A:363:ASP:OD1	1:A:363:ASP:N	2.45	0.48
19:m:1269:ASP:OD1	19:m:1272:ARG:NH1	2.46	0.48
24:u:173:TRP:NE1	24:u:179:SER:OG	2.37	0.48
1:A:599:LEU:O	8:H:121:LEU:HD12	2.13	0.47
19:m:882:ARG:HH22	19:m:1156:ARG:HH21	1.62	0.47
24:u:80:TYR:CZ	25:v:356:ASN:HB2	2.49	0.47
29:g:29:ARG:HG3	29:g:32:ARG:HH21	1.79	0.47
1:A:204:THR:OG1	1:A:207:GLU:OE1	2.31	0.47
21:q:65:LEU:HD13	25:v:81:ILE:HG12	1.95	0.47
21:q:559:ARG:NH2	25:v:24:PRO:O	2.47	0.47
22:r:223:VAL:HG22	22:r:325:GLN:HG2	1.95	0.47
31:j:549:ILE:HD11	31:j:631:VAL:HG13	1.95	0.47
1:A:1199:LEU:HD13	1:A:1204:MET:HG3	1.96	0.47
18:W:494:LEU:HD21	20:n:183:PRO:HG3	1.96	0.47
21:q:72:VAL:HG21	25:v:75:LEU:HD13	1.97	0.47
2:B:550:PHE:HB3	2:B:593:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:g:29:ARG:HG3	29:g:32:ARG:NH2	2.29	0.47
29:g:41:GLU:HB2	30:h:87:SER:HB2	1.95	0.47
1:A:1227:PHE:HB2	1:A:1245:ILE:HD11	1.97	0.47
5:E:49:MET:SD	5:E:49:MET:N	2.76	0.47
22:r:493:ASN:HB2	22:r:502:ILE:HD11	1.96	0.47
24:u:108:VAL:HG22	24:u:219:VAL:HB	1.96	0.47
27:e:106:ASP:OD2	27:e:131:ARG:NH2	2.42	0.47
30:h:92:ARG:O	30:h:96:THR:HG23	2.15	0.47
19:m:780:LEU:HD12	19:m:900:LEU:HB3	1.97	0.47
27:a:93:GLN:O	27:a:97:GLU:HG3	2.15	0.47
31:j:644:LYS:HE2	31:j:648:GLU:OE2	2.15	0.47
32:k:374:GLY:HA3	32:k:387:THR:HG21	1.96	0.47
1:A:1450:GLU:OE2	7:G:23:ASN:ND2	2.47	0.47
21:q:708:GLN:OE1	21:q:739:LYS:NZ	2.48	0.47
17:V:78:GLN:O	17:V:82:TYR:OH	2.23	0.46
31:j:919:THR:CG2	31:j:920:ILE:H	2.28	0.46
19:m:1279:ARG:NH1	19:m:1315:SER:O	2.48	0.46
25:v:263:TRP:HE1	25:v:356:ASN:HD21	1.61	0.46
18:W:326:VAL:HA	18:W:440:ILE:HD13	1.97	0.46
11:K:29:ASN:ND2	11:K:78:GLU:O	2.49	0.46
19:m:625:GLY:O	19:m:629:ILE:HG12	2.14	0.46
27:a:113:HIS:CG	27:e:126:LEU:HD22	2.51	0.46
1:A:261:ASP:OD1	1:A:262:ASP:N	2.48	0.46
6:F:110:ASP:OD1	6:F:110:ASP:N	2.37	0.46
29:g:90:ASP:HB3	29:g:93:LEU:HB2	1.98	0.46
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.80	0.46
1:A:215:ILE:O	1:A:231:ARG:NH2	2.47	0.46
1:A:870:GLY:C	1:A:872:ASP:H	2.24	0.46
1:A:1452:LEU:HD22	6:F:131:PRO:HB3	1.98	0.46
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.98	0.46
22:r:211:MET:HB3	22:r:286:LEU:HD23	1.97	0.46
24:u:97:HIS:NE2	25:v:203:ASP:OD2	2.47	0.46
7:G:160:ILE:HD12	18:W:553:LEU:HD12	1.97	0.46
27:e:73:GLU:OE1	28:f:25:ASN:HB2	2.16	0.46
1:A:807:ARG:NH1	2:B:724:LYS:O	2.43	0.45
5:E:34:MET:HE2	5:E:34:MET:HB2	1.80	0.45
7:G:151:ARG:HB3	7:G:158:TYR:HB2	1.98	0.45
17:V:58:VAL:N	17:V:82:TYR:O	2.45	0.45
17:V:66:SER:HB2	18:W:260:TYR:HB3	1.98	0.45
21:q:210:PRO:O	21:q:217:ARG:NH2	2.39	0.45
28:b:38:ALA:HB1	28:b:43:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:385:PHE:CE2	32:k:387:THR:OG1	2.69	0.45
16:T:7:DC:OP2	27:a:63:ARG:HB2	2.16	0.45
18:W:215:ARG:NH2	19:m:234:TYR:CE1	2.85	0.45
22:r:276:PHE:HB2	22:r:279:GLN:HB2	1.98	0.45
1:A:864:ILE:HD12	5:E:169:LEU:HD11	1.99	0.45
2:B:86:ARG:NH2	22:r:369:GLU:OE1	2.50	0.45
19:m:1104:ILE:HD12	23:s:456:PRO:HB2	1.98	0.45
19:m:1425:LYS:NZ	19:m:1430:SER:O	2.41	0.45
28:f:75:HIS:HD2	30:h:96:THR:HG21	1.81	0.45
32:k:386:ALA:C	32:k:387:THR:HG23	2.41	0.45
11:K:99:LYS:HE2	11:K:99:LYS:HB2	1.73	0.45
13:M:46:LEU:HD11	13:M:55:SER:HB3	1.99	0.45
18:W:215:ARG:NH1	19:m:234:TYR:CE1	2.84	0.45
18:W:546:LYS:NZ	19:m:291:GLU:OE1	2.48	0.45
19:m:984:LYS:HE2	19:m:1015:VAL:HG21	1.99	0.45
21:q:189:LEU:HD22	21:q:194:LYS:HD2	1.98	0.45
28:f:92:ARG:NH2	30:h:101:LEU:HD13	2.32	0.45
12:L:49:ARG:HD3	22:r:339:VAL:HG11	1.98	0.45
19:m:1002:ARG:NH1	19:m:1052:TYR:OH	2.43	0.45
18:W:638:TYR:CZ	19:m:882:ARG:HG3	2.52	0.45
18:W:527:THR:HA	18:W:530:LEU:HD12	1.99	0.45
21:q:320:LEU:HD13	22:r:514:LEU:HD11	1.99	0.45
25:v:258:ASN:OD1	25:v:261:ASN:N	2.44	0.45
32:k:286:LEU:HD23	32:k:286:LEU:HA	1.84	0.45
3:C:15:ASP:OD1	3:C:15:ASP:N	2.44	0.45
19:m:527:ASP:OD1	19:m:528:ALA:N	2.47	0.45
28:f:64:ASN:HA	28:f:67:ARG:NH1	2.32	0.45
1:A:835:THR:HG21	1:A:1079:THR:HA	1.99	0.45
18:W:444:LEU:HD12	19:m:284:PHE:CG	2.52	0.45
31:j:503:ILE:CD1	31:j:907:PRO:HG3	2.47	0.45
1:A:948:VAL:O	5:E:200:ARG:NH1	2.50	0.44
18:W:751:THR:HG23	18:W:798:ILE:HG12	1.99	0.44
21:q:737:LEU:O	21:q:742:ASN:N	2.47	0.44
32:k:10:PHE:HB2	32:k:78:ASP:OD1	2.16	0.44
2:B:498:ASP:HB3	14:N:42:DA:C4	2.53	0.44
14:N:56:DG:C2	16:T:-55:DG:C2	3.05	0.44
19:m:992:ILE:HG22	19:m:997:SER:HA	1.99	0.44
27:a:83:ARG:HB2	28:b:80:THR:HG23	1.98	0.44
1:A:466:TYR:HB2	1:A:470:ARG:NH2	2.32	0.44
5:E:21:MET:HE2	5:E:186:TYR:HA	2.00	0.44
5:E:89:ILE:HD13	5:E:118:SER:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:628:LYS:HE3	19:m:661:GLN:HE22	1.82	0.44
22:r:366:GLU:HG2	24:u:252:VAL:HG22	1.99	0.44
1:A:231:ARG:HB3	1:A:234:TRP:CD2	2.53	0.44
1:A:599:LEU:HD12	1:A:599:LEU:HA	1.73	0.44
4:D:139:PRO:HA	4:D:142:ILE:HD12	1.99	0.44
19:m:1062:ALA:HB2	19:m:1103:LEU:HD11	1.99	0.44
28:b:40:ARG:O	31:j:867:LEU:HD21	2.17	0.44
2:B:588:MET:HE3	2:B:588:MET:HB3	1.88	0.44
16:T:17:DA:H5''	27:a:85:GLN:HG2	1.99	0.44
31:j:738:PRO:CG	31:j:745:LYS:HE2	2.48	0.44
1:A:41:MET:HG2	1:A:44:SER:HA	1.98	0.44
2:B:273:PRO:HG2	2:B:276:ILE:HD12	2.00	0.44
19:m:712:LEU:HA	19:m:715:LEU:HB2	1.98	0.44
24:u:90:LEU:HB2	25:v:362:MET:HE1	1.99	0.44
31:j:554:GLN:HA	31:j:638:LEU:HD21	1.99	0.44
32:k:210:LYS:HA	32:k:215:PHE:HD2	1.82	0.44
1:A:134:ARG:HH21	1:A:224:GLY:HA2	1.82	0.44
2:B:284:VAL:N	2:B:285:PRO:HD2	2.32	0.44
4:D:136:VAL:O	4:D:166:LYS:NZ	2.50	0.44
19:m:1064:ASP:OD1	23:s:457:LYS:NZ	2.46	0.44
19:m:1365:GLU:O	19:m:1369:ASN:ND2	2.49	0.44
21:q:568:SER:O	21:q:571:ASN:ND2	2.50	0.44
25:v:312:LYS:HB3	25:v:315:GLU:HG2	1.99	0.44
31:j:622:SER:CB	31:j:628:MET:HE2	2.48	0.44
1:A:1343:GLY:O	1:A:1347:THR:OG1	2.29	0.44
3:C:179:GLU:OE2	3:C:204:SER:OG	2.36	0.44
17:V:67:TRP:NE1	18:W:217:LEU:O	2.51	0.44
25:v:262:LYS:HD3	25:v:305:GLN:HE21	1.81	0.44
18:W:534:PHE:HB3	18:W:554:ILE:HD13	2.00	0.43
19:m:770:PHE:HB3	19:m:779:VAL:HG22	2.00	0.43
21:q:641:ALA:HB1	21:q:655:LYS:HG3	2.00	0.43
25:v:34:ILE:O	25:v:40:GLN:NE2	2.38	0.43
29:g:72:ASP:OD1	31:j:486:GLU:OE2	2.36	0.43
31:j:824:VAL:HG23	31:j:888:THR:CG2	2.49	0.43
1:A:1389:ARG:NH2	16:T:-44:DT:O2	2.50	0.43
19:m:1426:LEU:HD21	19:m:1465:MET:HE2	1.99	0.43
2:B:650:GLU:OE1	2:B:653:ARG:NH2	2.49	0.43
27:e:60:LEU:HD22	27:e:93:GLN:HG2	2.00	0.43
1:A:465:PRO:O	1:A:470:ARG:NH2	2.51	0.43
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	2.01	0.43
2:B:547:ILE:HG21	2:B:619:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:17:ASN:OD1	8:H:24:SER:OG	2.31	0.43
21:q:520:SER:O	21:q:524:HIS:ND1	2.48	0.43
21:q:617:ASP:OD1	21:q:621:ASN:ND2	2.51	0.43
22:r:230:ARG:NH1	22:r:292:SER:OG	2.44	0.43
22:r:245:VAL:HG23	22:r:298:GLU:HG2	2.01	0.43
27:a:87:ALA:HB1	28:b:100:PHE:CD1	2.54	0.43
31:j:865:PHE:O	31:j:866:GLY:C	2.61	0.43
7:G:144:ARG:HB2	7:G:171:ILE:HD13	1.99	0.43
18:W:472:ALA:O	18:W:476:VAL:HG23	2.18	0.43
9:I:23:GLN:O	9:I:24:ARG:NE	2.51	0.43
17:V:59:ALA:HB1	18:W:244:LEU:HD13	2.01	0.43
18:W:508:SER:HA	18:W:524:GLU:HA	1.99	0.43
19:m:242:GLY:HA3	20:n:258:LYS:HG2	2.00	0.43
19:m:1205:ASP:OD1	19:m:1207:ARG:NE	2.48	0.43
25:v:104:PRO:HA	25:v:107:ARG:HD3	2.00	0.43
26:x:222:MET:HE3	26:x:222:MET:HB3	1.84	0.43
29:g:88:ARG:NE	29:g:94:ASN:OD1	2.46	0.43
30:h:111:VAL:O	30:h:115:THR:HG23	2.19	0.43
31:j:869:ASN:OD1	31:j:890:PRO:HA	2.18	0.43
1:A:188:LYS:HE3	1:A:199:GLU:HB2	2.01	0.43
14:N:-12:DT:OP1	27:a:72:ARG:NH2	2.52	0.43
28:b:32:PRO:O	28:b:36:ARG:HG3	2.18	0.43
32:k:223:VAL:HG23	32:k:308:VAL:HG11	2.01	0.43
1:A:1448:ILE:HD11	1:A:1453:LEU:HD11	2.01	0.43
30:h:54:ILE:HG22	30:h:55:SER:O	2.18	0.43
1:A:1287:MET:HE3	1:A:1287:MET:HB2	1.96	0.43
11:K:55:ASP:OD1	11:K:55:ASP:N	2.41	0.43
27:a:65:LEU:HG	27:a:69:ARG:NH1	2.34	0.43
27:e:135:ALA:HB3	31:j:892:GLU:OE2	2.19	0.43
29:g:31:HIS:CD2	29:g:35:ARG:HH12	2.37	0.43
1:A:547:VAL:HG22	1:A:578:LEU:HD21	2.01	0.42
18:W:344:LEU:HD12	18:W:349:GLU:HB2	2.01	0.42
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	2.01	0.42
2:B:788:ARG:O	2:B:967:ARG:NH1	2.52	0.42
7:G:30:LEU:HD22	7:G:72:VAL:HG11	2.00	0.42
18:W:315:SER:O	18:W:316:SER:C	2.61	0.42
24:u:200:VAL:HA	24:u:211:THR:HA	2.01	0.42
26:x:301:ASP:OD1	26:x:303:GLN:NE2	2.53	0.42
19:m:545:ASN:ND2	19:m:553:HIS:O	2.53	0.42
21:q:155:TYR:HB3	21:q:160:ARG:HB2	2.02	0.42
22:r:277:PRO:HB2	22:r:305:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:u:208:ILE:HG22	25:v:253:LYS:HG3	2.00	0.42
2:B:860:MET:HE3	2:B:860:MET:HB3	1.84	0.42
18:W:752:LEU:HD23	18:W:770:VAL:HG12	2.00	0.42
20:n:217:ARG:HG3	20:n:259:VAL:HG21	2.02	0.42
30:h:79:ARG:HG2	30:h:83:TYR:CE2	2.54	0.42
2:B:83:TYR:HB2	2:B:116:TYR:HB2	2.01	0.42
2:B:928:ARG:NH2	19:m:775:ARG:O	2.52	0.42
1:A:983:LEU:HD13	1:A:1041:ARG:HA	2.01	0.42
9:I:62:ILE:HD12	9:I:62:ILE:HA	1.93	0.42
19:m:1325:ALA:HB3	19:m:1328:LEU:HB3	2.02	0.42
21:q:162:ASP:OD1	21:q:192:ARG:NH2	2.51	0.42
2:B:81:LYS:NZ	24:u:247:TYR:O	2.43	0.42
2:B:299:ASP:OD1	2:B:299:ASP:N	2.52	0.42
18:W:334:LYS:HB3	18:W:388:ARG:HH12	1.84	0.42
19:m:992:ILE:HA	19:m:995:ILE:HG12	2.02	0.42
21:q:766:MET:HE1	21:q:799:ILE:HG23	2.02	0.42
27:e:82:LEU:HD23	27:e:82:LEU:HA	1.78	0.42
27:e:109:LEU:CD2	32:k:430:ASN:OD1	2.68	0.42
2:B:607:SER:HB2	2:B:620:PHE:HB2	2.02	0.42
17:V:63:ASN:HB3	17:V:75:ASP:HA	2.01	0.42
28:f:51:TYR:O	28:f:55:ARG:HG3	2.20	0.42
1:A:203:LEU:HB3	1:A:208:ILE:HD11	2.01	0.42
2:B:632:ILE:HD11	2:B:688:GLU:HB3	2.01	0.42
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.55	0.42
3:C:79:MET:HE2	3:C:79:MET:HB3	1.87	0.42
18:W:336:ASP:OD2	18:W:357:ARG:NE	2.47	0.42
18:W:461:LEU:HD12	19:m:278:THR:HG23	2.01	0.42
19:m:380:GLU:HB3	19:m:978:CYS:SG	2.60	0.42
27:a:73:GLU:OE1	28:b:25:ASN:HB2	2.20	0.42
28:f:46:ILE:HG22	28:f:47:SER:O	2.20	0.42
21:q:9:TYR:OH	25:v:106:ASP:OD2	2.28	0.41
21:q:737:LEU:HD12	21:q:741:SER:HB2	2.01	0.41
21:q:41:PHE:CG	21:q:70:VAL:HG11	2.54	0.41
22:r:244:LYS:NZ	22:r:305:GLU:OE2	2.46	0.41
29:g:21:ALA:HB2	30:h:121:TYR:HB2	2.02	0.41
29:g:31:HIS:CE1	29:g:35:ARG:HH12	2.37	0.41
31:j:593:PRO:HG2	32:k:177:TYR:CE2	2.56	0.41
1:A:253:MET:SD	16:T:-31:DA:H2''	2.60	0.41
5:E:81:PHE:HE1	5:E:110:ILE:HD13	1.84	0.41
14:N:4:DG:H4'	31:j:601:LYS:HE2	2.03	0.41
21:q:780:TYR:O	21:q:784:LYS:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:u:268:GLU:HA	24:u:271:ARG:HG2	2.03	0.41
1:A:1412:LEU:HD13	2:B:1207:LEU:HD21	2.02	0.41
2:B:957:ASN:OD1	2:B:961:LEU:N	2.53	0.41
7:G:108:VAL:HG22	7:G:159:ALA:HB3	2.02	0.41
16:T:-6:DA:H5''	32:k:235:GLY:HA2	2.02	0.41
18:W:551:THR:HG21	18:W:586:SER:HA	2.03	0.41
22:r:263:SER:OG	22:r:264:LYS:N	2.53	0.41
2:B:592:THR:HA	24:u:226:PHE:HZ	1.86	0.41
21:q:710:LEU:HD13	21:q:740:PHE:HB2	2.01	0.41
28:f:38:ALA:HB1	28:f:43:VAL:HB	2.02	0.41
30:h:45:LEU:O	30:h:49:HIS:N	2.34	0.41
1:A:363:ASP:HB3	1:A:509:PRO:HD3	2.02	0.41
1:A:823:GLU:OE2	2:B:506:GLN:NE2	2.53	0.41
5:E:27:TYR:HA	5:E:63:PRO:HA	2.03	0.41
9:I:17:LYS:N	9:I:26:LEU:O	2.50	0.41
18:W:648:GLN:NE2	18:W:679:VAL:H	2.18	0.41
27:e:98:ALA:HA	32:k:410:SER:HB2	2.02	0.41
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.86	0.41
27:a:65:LEU:HB3	27:a:66:PRO:HD3	2.03	0.41
31:j:604:LEU:HD23	31:j:604:LEU:HA	1.88	0.41
32:k:258:GLN:OE1	32:k:260:LYS:HE2	2.20	0.41
2:B:318:ASP:HB3	2:B:321:VAL:HG22	2.02	0.41
3:C:50:ILE:HG12	3:C:155:ILE:HG22	2.03	0.41
14:N:-13:DT:H2'	14:N:-12:DT:H71	2.03	0.41
14:N:8:DG:C2	16:T:-7:DG:N2	2.88	0.41
19:m:449:THR:HG21	19:m:543:ARG:HD2	2.03	0.41
19:m:1001:ASN:OD1	19:m:1002:ARG:N	2.54	0.41
21:q:710:LEU:HD11	21:q:748:LEU:HD11	2.03	0.41
22:r:206:PHE:H	22:r:229:LEU:HD21	1.84	0.41
22:r:208:ARG:N	22:r:291:ASP:OD1	2.52	0.41
25:v:29:LEU:N	26:x:147:ARG:O	2.52	0.41
32:k:388:LYS:HA	32:k:389:PRO:HA	1.83	0.41
2:B:174:THR:O	2:B:175:LEU:C	2.64	0.41
24:u:89:SER:HB3	25:v:365:ARG:HE	1.86	0.41
6:F:104:ASN:HD22	6:F:104:ASN:HA	1.70	0.40
18:W:250:ARG:NH2	18:W:284:ASP:OD2	2.53	0.40
32:k:37:THR:O	32:k:38:LYS:C	2.64	0.40
32:k:269:PRO:HB3	32:k:302:ARG:HH21	1.85	0.40
1:A:557:TRP:O	11:K:26:ARG:NH1	2.54	0.40
2:B:184:LYS:HB3	2:B:787:VAL:HG21	2.03	0.40
2:B:479:TYR:CE2	2:B:778:MET:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:63:PRO:HB3	5:E:74:LEU:HD23	2.03	0.40
19:m:295:THR:OG1	19:m:298:ASP:OD2	2.37	0.40
27:a:120:MET:HE2	27:a:122:LYS:HE2	2.03	0.40
27:e:102:GLY:HA2	27:e:105:GLU:OE1	2.22	0.40
27:e:109:LEU:HD22	32:k:430:ASN:OD1	2.21	0.40
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.86	0.40
3:C:21:LEU:HD22	11:K:101:LEU:HD11	2.03	0.40
7:G:51:GLY:HA2	7:G:54:ILE:HD11	2.03	0.40
16:T:5:DC:H2''	16:T:6:DC:C5	2.56	0.40
19:m:1286:PHE:HA	19:m:1308:ILE:HB	2.03	0.40
31:j:614:PHE:CE2	32:k:112:TRP:HB3	2.56	0.40
32:k:10:PHE:CD2	32:k:61:ARG:NH1	2.89	0.40
1:A:109:ASN:HD21	20:n:199:LEU:HB3	1.85	0.40
2:B:1072:MET:HG3	2:B:1085:VAL:HB	2.04	0.40
18:W:524:GLU:HB2	20:n:232:GLN:HE22	1.87	0.40
19:m:243:ASP:OD1	19:m:243:ASP:N	2.55	0.40
31:j:917:TRP:O	31:j:921:MET:HG2	2.22	0.40
1:A:26:GLU:OE2	4:D:13:ARG:NH1	2.54	0.40
1:A:554:VAL:HB	1:A:557:TRP:HB2	2.04	0.40
2:B:815:ARG:NH1	25:v:132:GLN:O	2.54	0.40
3:C:199:LYS:HB3	3:C:199:LYS:HE2	1.80	0.40
19:m:965:VAL:HG21	19:m:992:ILE:HG21	2.03	0.40
20:n:241:ILE:HG23	20:n:246:ILE:HD12	2.03	0.40
29:g:34:LEU:HD23	29:g:34:LEU:HA	1.92	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%)	1357 (98%)	34 (2%)	1 (0%)	48 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1154/1227 (94%)	1127 (98%)	27 (2%)	0	100	100
3	C	261/304 (86%)	259 (99%)	2 (1%)	0	100	100
4	D	170/186 (91%)	168 (99%)	2 (1%)	0	100	100
5	E	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
6	F	82/155 (53%)	79 (96%)	3 (4%)	0	100	100
7	G	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
8	H	129/145 (89%)	125 (97%)	4 (3%)	0	100	100
9	I	109/115 (95%)	105 (96%)	4 (4%)	0	100	100
10	J	65/72 (90%)	65 (100%)	0	0	100	100
11	K	111/118 (94%)	109 (98%)	2 (2%)	0	100	100
12	L	43/72 (60%)	41 (95%)	2 (5%)	0	100	100
13	M	62/113 (55%)	61 (98%)	1 (2%)	0	100	100
17	V	104/108 (96%)	102 (98%)	2 (2%)	0	100	100
18	W	529/911 (58%)	506 (96%)	23 (4%)	0	100	100
19	m	1170/1503 (78%)	1152 (98%)	18 (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	s	9/725 (1%)	9 (100%)	0	0	100	100
24	u	206/459 (45%)	206 (100%)	0	0	100	100
25	v	341/396 (86%)	330 (97%)	11 (3%)	0	100	100
26	x	201/395 (51%)	200 (100%)	1 (0%)	0	100	100
27	a	73/139 (52%)	67 (92%)	6 (8%)	0	100	100
27	e	75/139 (54%)	73 (97%)	2 (3%)	0	100	100
28	b	81/106 (76%)	77 (95%)	4 (5%)	0	100	100
28	f	76/106 (72%)	73 (96%)	3 (4%)	0	100	100
29	g	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
30	h	91/129 (70%)	89 (98%)	2 (2%)	0	100	100
31	j	444/965 (46%)	428 (96%)	14 (3%)	2 (0%)	24	55
32	k	430/531 (81%)	409 (95%)	21 (5%)	0	100	100
All	All	9203/13425 (69%)	8989 (98%)	211 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	960	VAL
31	j	544	ASN
31	j	866	GLY

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%)	1219 (100%)	0	100	100
2	B	1018/1077 (94%)	1014 (100%)	4 (0%)	84	79
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	149/160 (93%)	149 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	61/66 (92%)	61 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	38 (100%)	0	100	100
13	M	61/99 (62%)	61 (100%)	0	100	100
17	V	90/92 (98%)	90 (100%)	0	100	100
18	W	482/796 (61%)	482 (100%)	0	100	100
19	m	1079/1354 (80%)	1078 (100%)	1 (0%)	88	87
20	n	125/361 (35%)	125 (100%)	0	100	100
21	q	824/962 (86%)	824 (100%)	0	100	100
22	r	239/485 (49%)	239 (100%)	0	100	100
23	s	11/649 (2%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	u	192/406 (47%)	192 (100%)	0	100	100
25	v	325/369 (88%)	325 (100%)	0	100	100
26	x	190/354 (54%)	190 (100%)	0	100	100
27	a	63/112 (56%)	63 (100%)	0	100	100
27	e	64/112 (57%)	64 (100%)	0	100	100
28	b	68/81 (84%)	68 (100%)	0	100	100
28	f	63/81 (78%)	63 (100%)	0	100	100
29	g	72/102 (71%)	71 (99%)	1 (1%)	59	68
30	h	79/107 (74%)	79 (100%)	0	100	100
31	j	412/852 (48%)	408 (99%)	4 (1%)	68	72
32	k	396/474 (84%)	395 (100%)	1 (0%)	86	81
All	All	8305/11829 (70%)	8294 (100%)	11 (0%)	87	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	425	MET
2	B	815	ARG
2	B	879	ARG
2	B	904	ARG
19	m	770	PHE
29	g	75	LYS
31	j	740	MET
31	j	865	PHE
31	j	867	LEU
31	j	888	THR
32	k	388	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	276	ASN
1	A	278	GLN
1	A	288	HIS
1	A	291	ASN
1	A	387	HIS

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Mol	Chain	Res	Type
1	A	661	ASN
1	A	690	GLN
1	A	1056	GLN
1	A	1080	GLN
2	B	157	HIS
2	B	477	ASN
2	B	492	ASN
2	B	524	GLN
2	B	549	ASN
2	B	996	HIS
2	B	1074	ASN
2	B	1179	GLN
3	C	8	ASN
3	C	25	ASN
4	D	46	HIS
4	D	130	ASN
4	D	170	ASN
5	E	53	GLN
5	E	162	GLN
6	F	104	ASN
6	F	119	GLN
6	F	127	GLN
7	G	122	ASN
8	H	43	ASN
9	I	23	GLN
11	K	113	ASN
12	L	55	HIS
13	M	65	GLN
18	W	283	ASN
18	W	402	HIS
18	W	558	ASN
18	W	786	ASN
19	m	428	HIS
19	m	553	HIS
19	m	661	GLN
19	m	819	ASN
19	m	869	HIS
19	m	886	HIS
19	m	899	GLN
19	m	998	ASN
19	m	1191	ASN
19	m	1193	GLN

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Mol	Chain	Res	Type
19	m	1242	GLN
19	m	1288	ASN
19	m	1338	ASN
19	m	1436	ASN
20	n	156	GLN
20	n	232	GLN
21	q	58	ASN
21	q	132	ASN
21	q	147	ASN
21	q	187	GLN
21	q	319	ASN
21	q	397	ASN
21	q	398	GLN
21	q	503	GLN
21	q	526	ASN
21	q	615	HIS
21	q	625	HIS
22	r	279	GLN
22	r	493	ASN
24	u	103	GLN
24	u	138	GLN
24	u	172	GLN
24	u	261	GLN
25	v	64	ASN
25	v	199	HIS
25	v	283	ASN
25	v	305	GLN
25	v	381	GLN
26	x	246	ASN
26	x	251	GLN
28	b	25	ASN
27	e	85	GLN
29	g	38	ASN
31	j	523	HIS
31	j	578	ASN
31	j	841	GLN
31	j	869	ASN
31	j	916	ASN
32	k	93	GLN
32	k	127	ASN
32	k	148	HIS
32	k	362	GLN

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Mol	Chain	Res	Type
32	k	420	GLN

5.3.3 RNA ⓘ

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

All (8) RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

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 oligosaccharides 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.

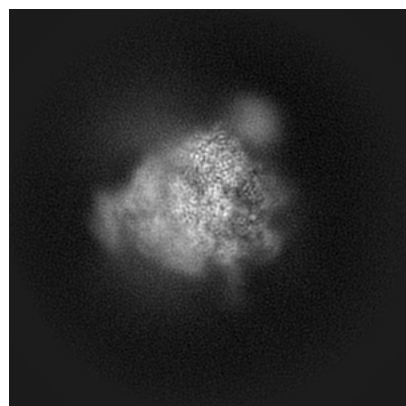
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66107. These allow visual inspection of the internal detail of the map and identification of artifacts.

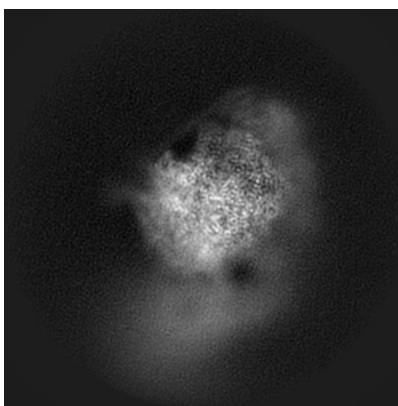
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

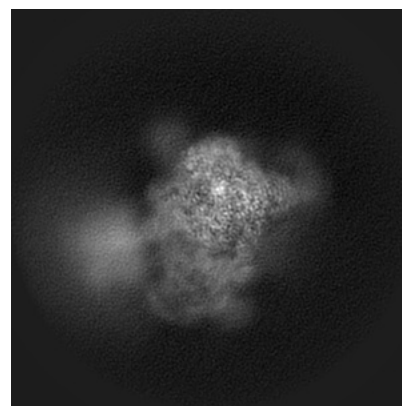
6.1.1 Primary map



X

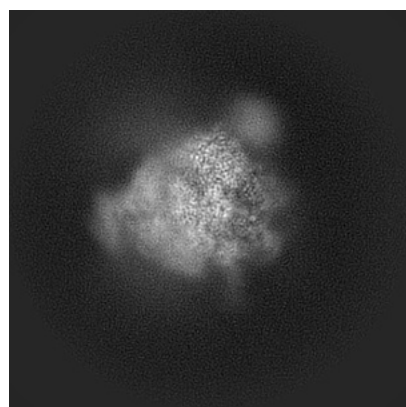


Y

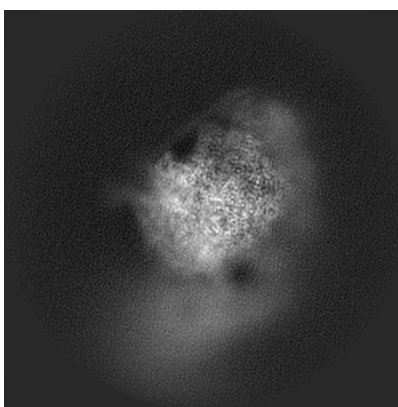


Z

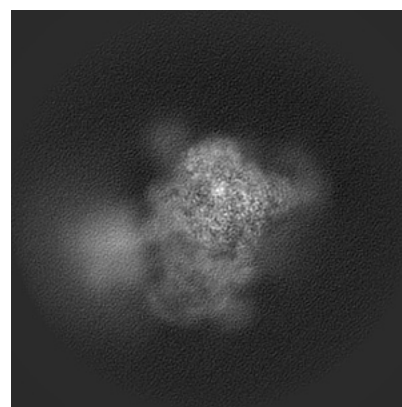
6.1.2 Raw map



X



Y

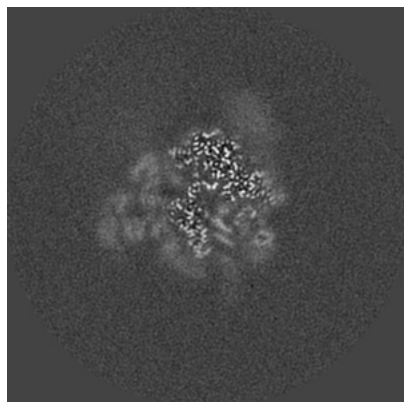


Z

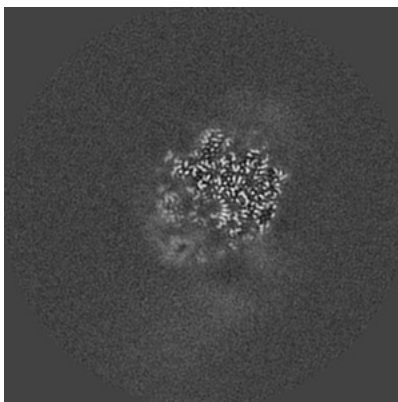
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

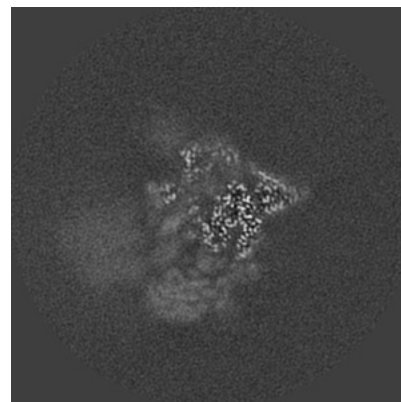
6.2.1 Primary map



X Index: 135

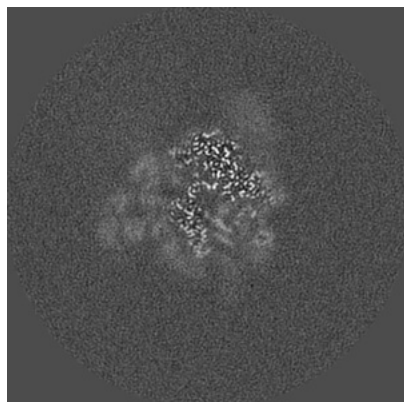


Y Index: 135

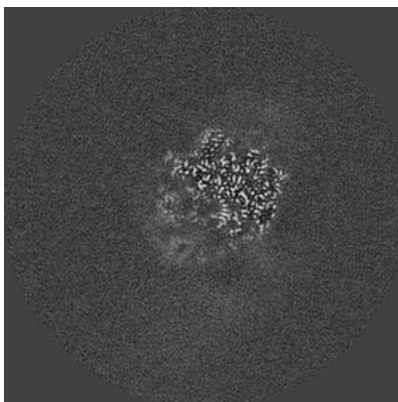


Z Index: 135

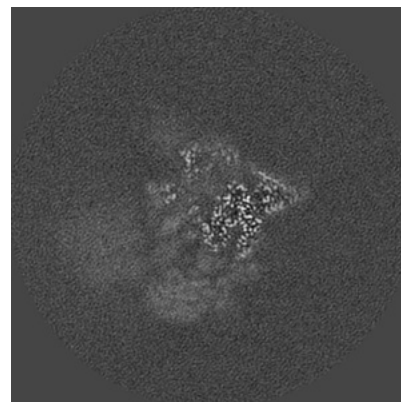
6.2.2 Raw map



X Index: 135



Y Index: 135

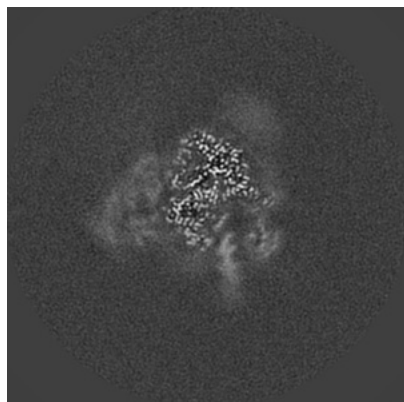


Z Index: 135

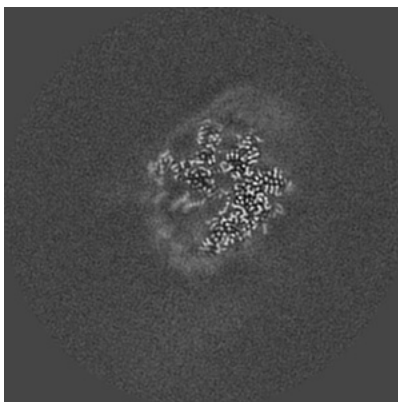
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

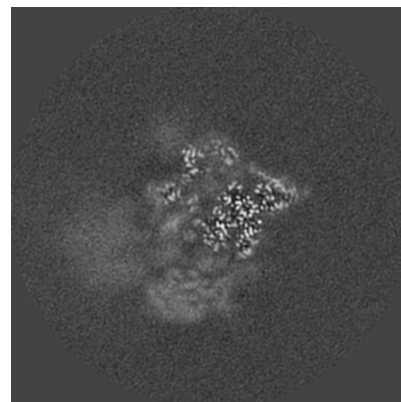
6.3.1 Primary map



X Index: 141

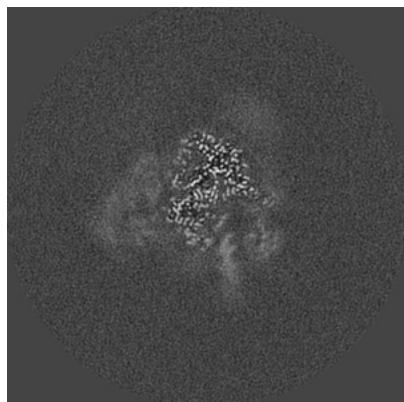


Y Index: 142

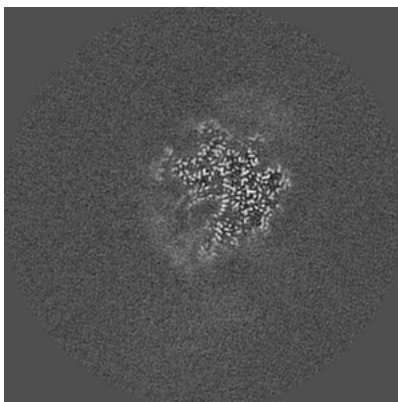


Z Index: 136

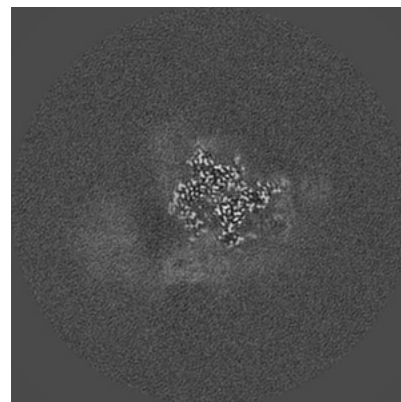
6.3.2 Raw map



X Index: 141



Y Index: 139

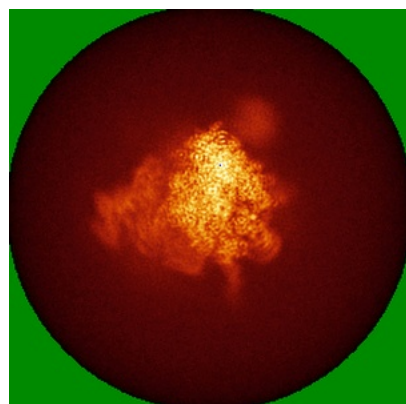


Z Index: 154

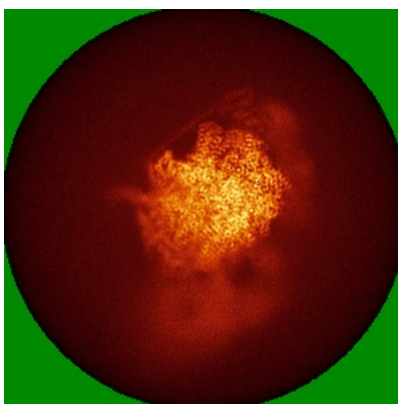
The images above show the largest variance slices of the map in three orthogonal directions.

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

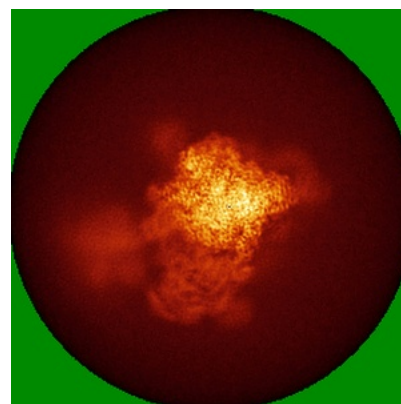
6.4.1 Primary map



X

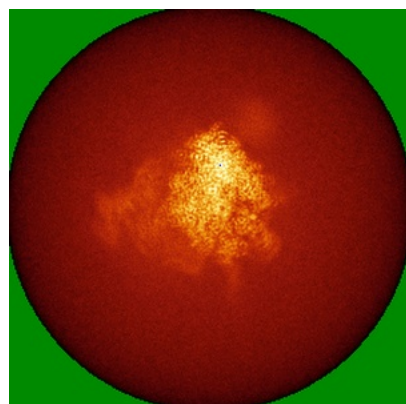


Y

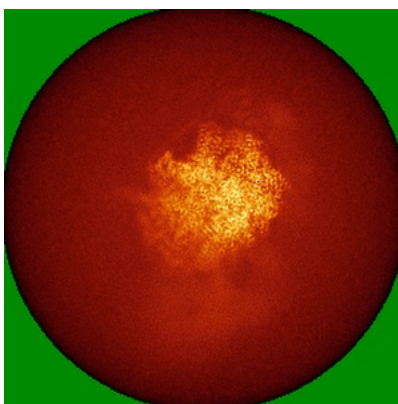


Z

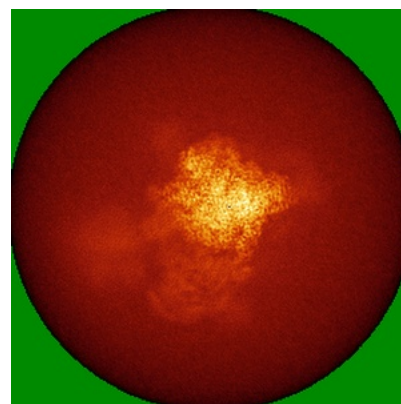
6.4.2 Raw map



X



Y



Z

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

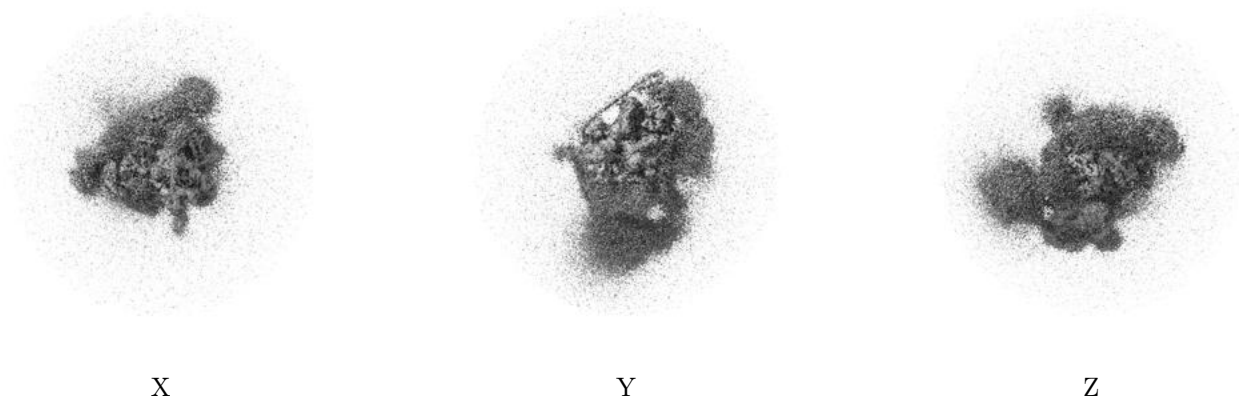
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

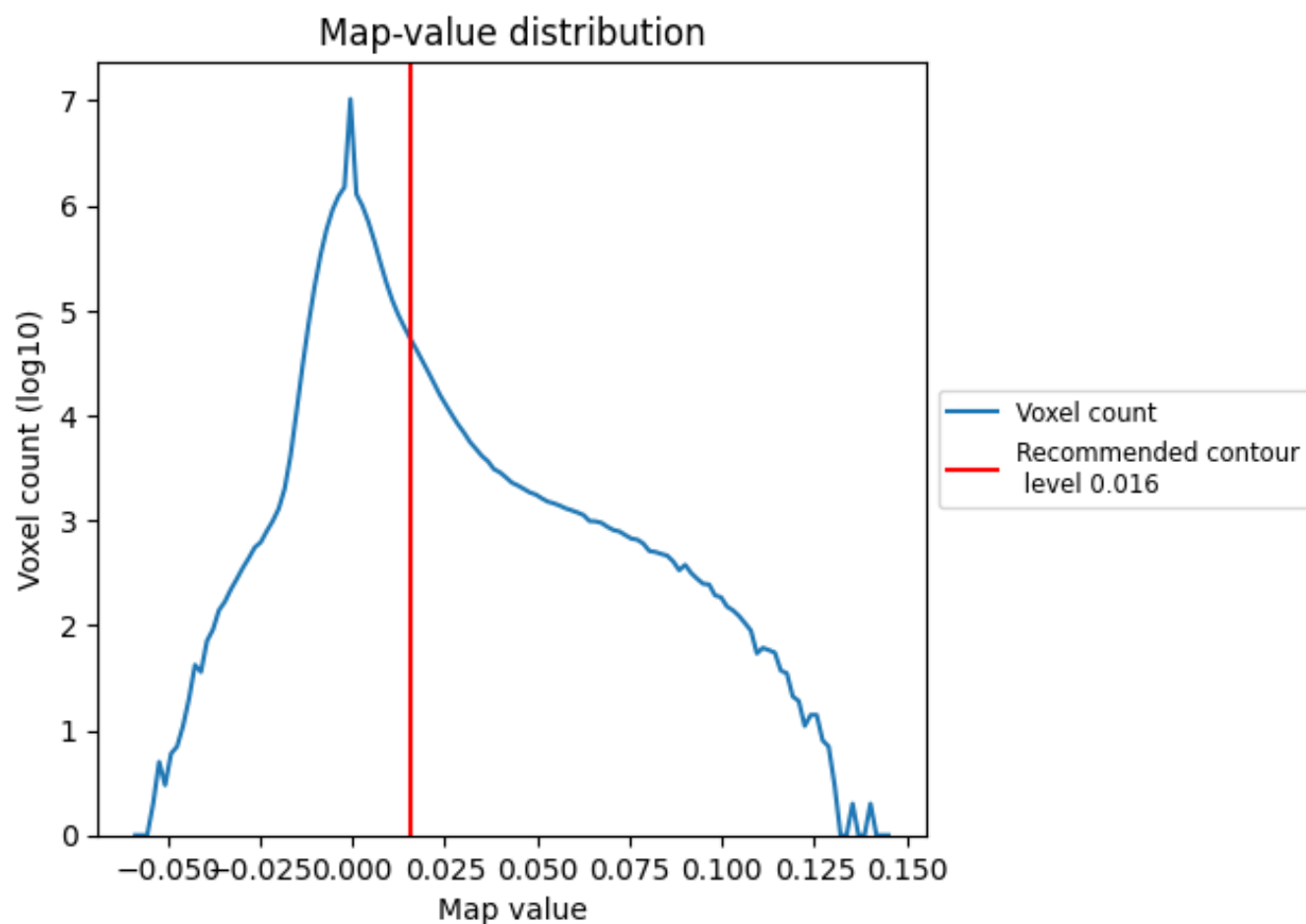
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

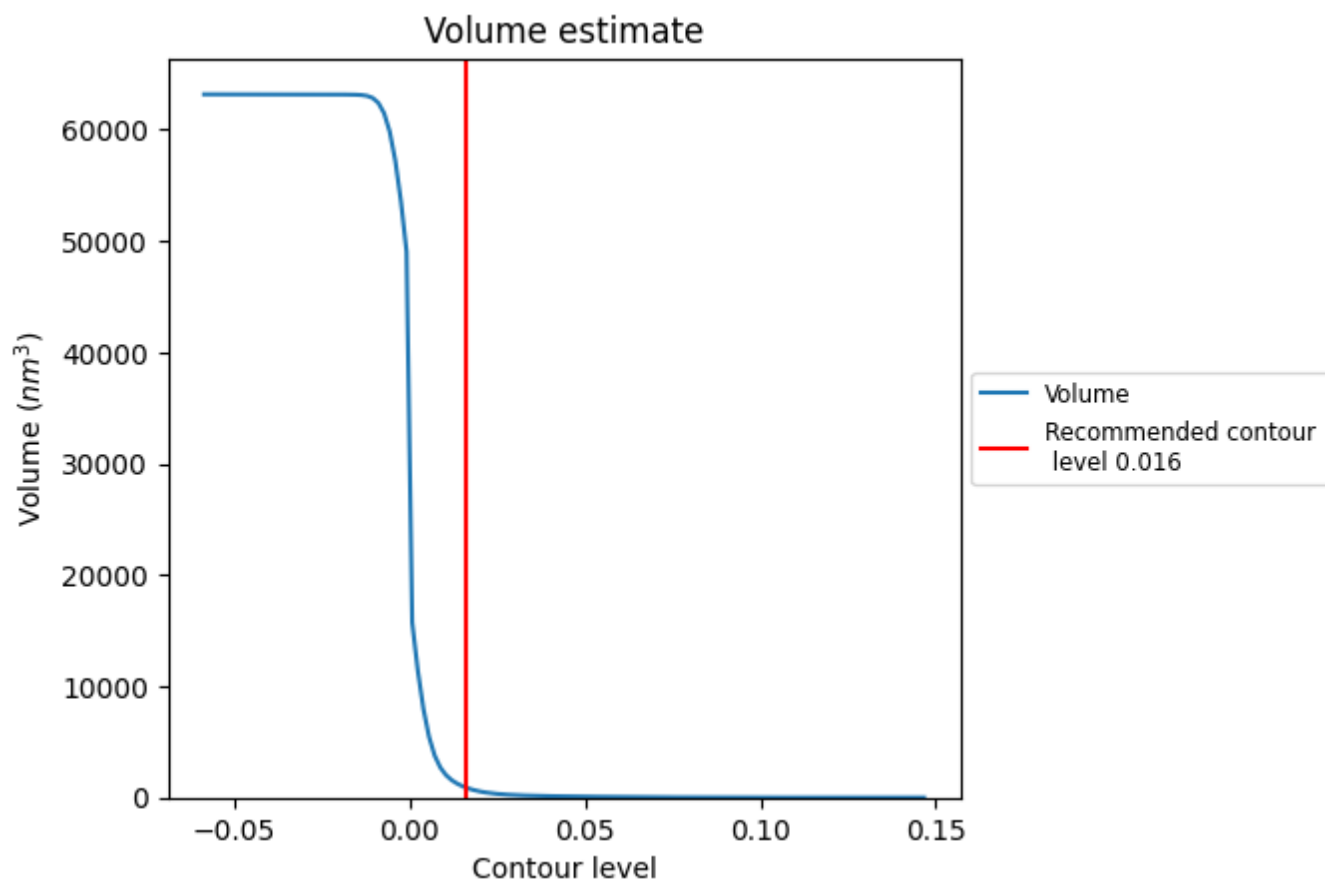
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

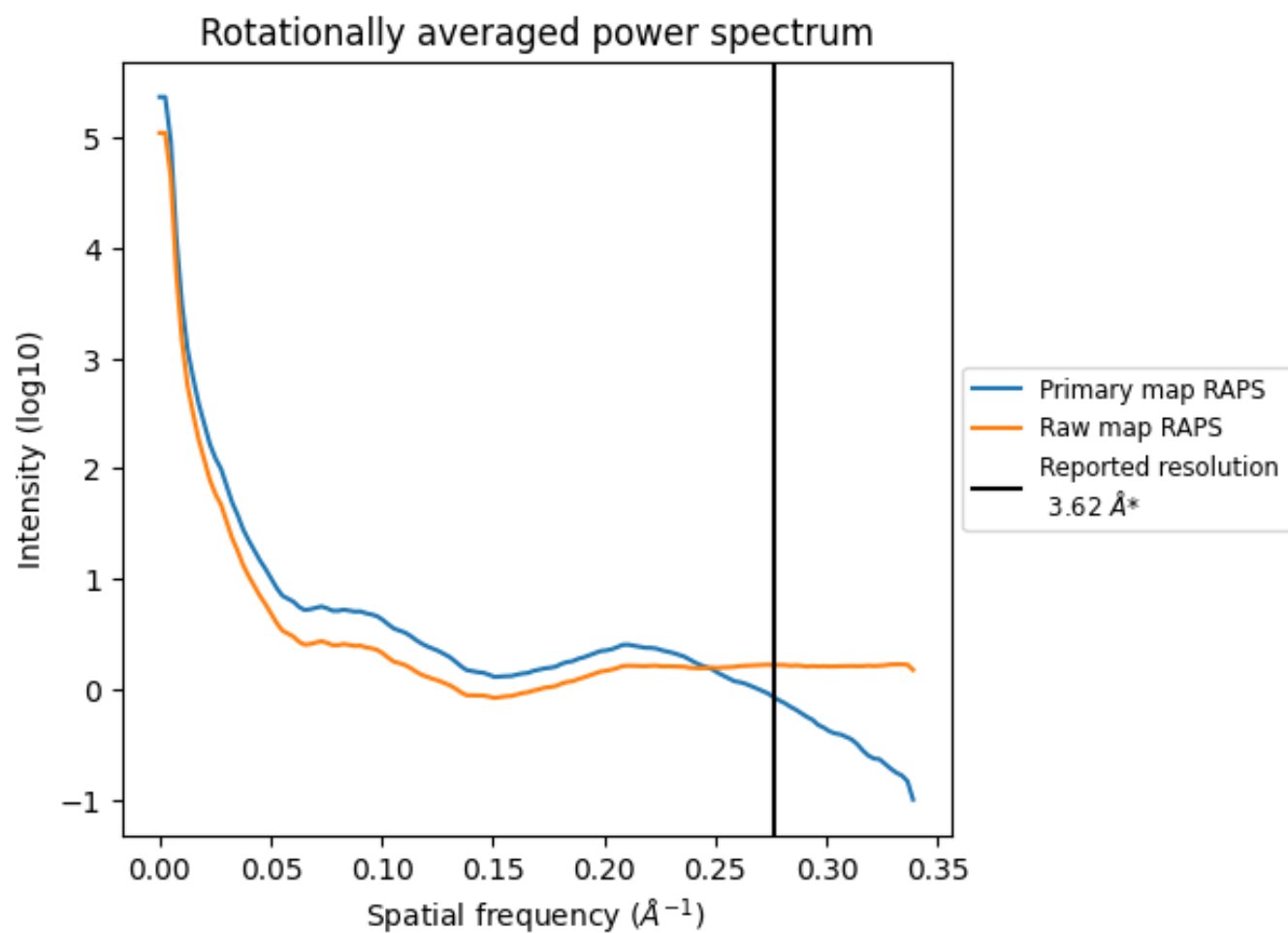
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 903 nm³; this corresponds to an approximate mass of 815 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

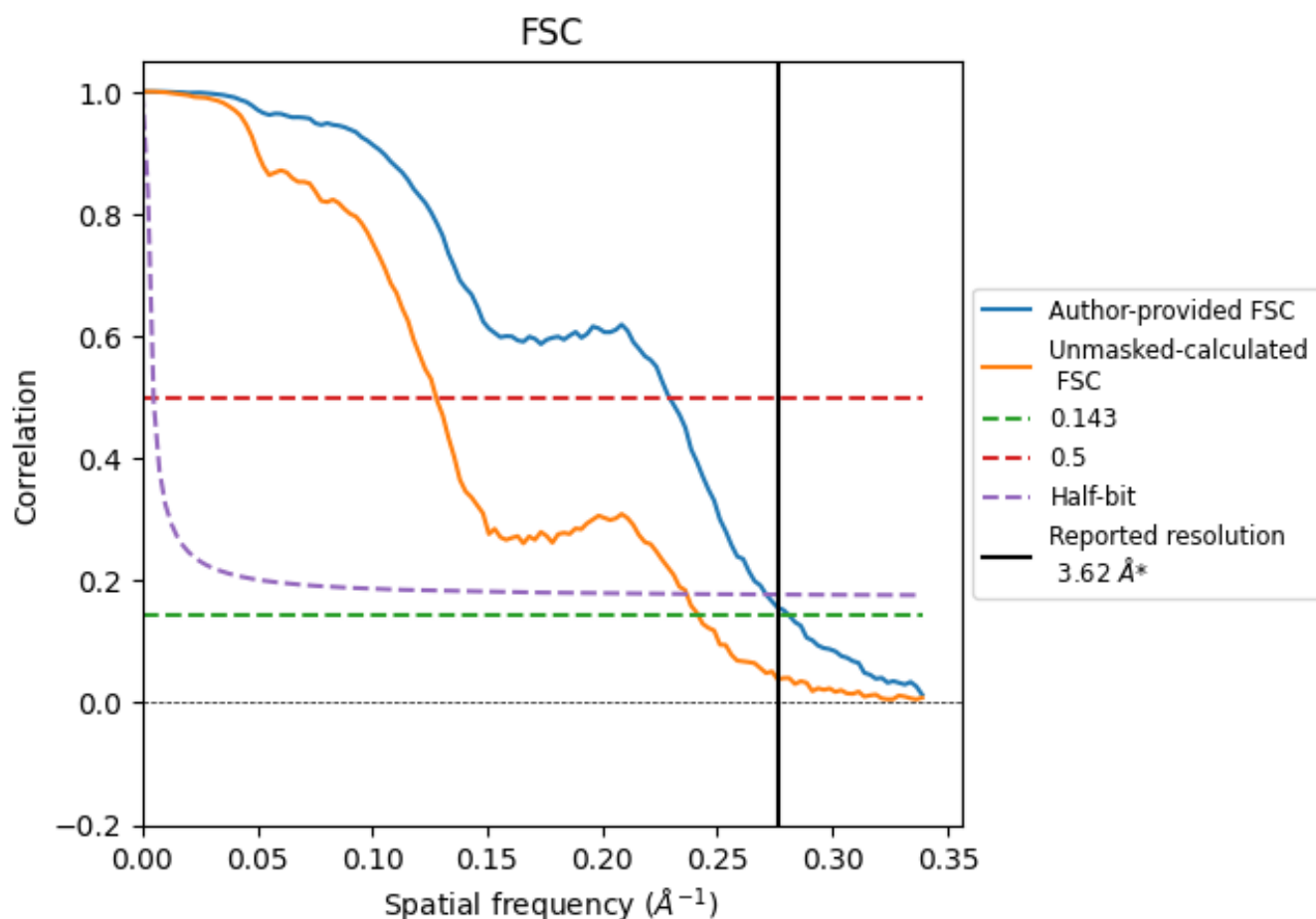


*Reported resolution corresponds to spatial frequency of 0.276 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.276 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

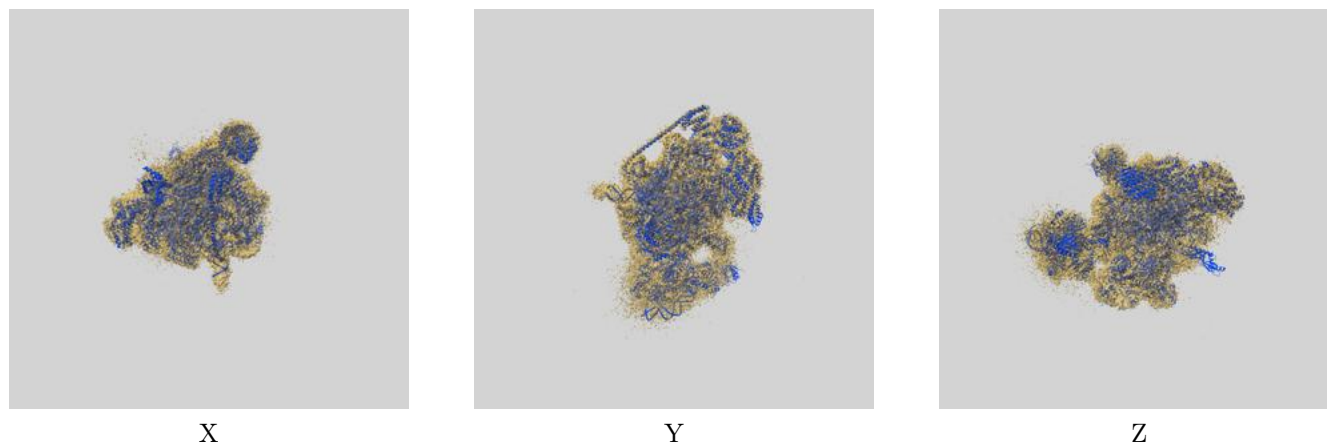
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	3.56	4.36	3.69
Unmasked-calculated*	4.14	7.83	4.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.62 by more than 10 %

9 Map-model fit [i](#)

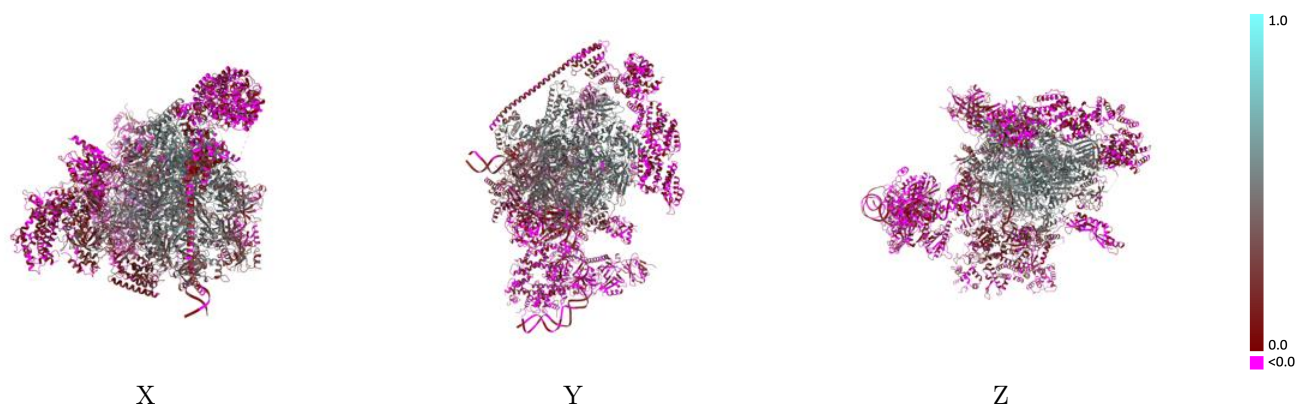
This section contains information regarding the fit between EMDB map EMD-66107 and PDB model 9WMW. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



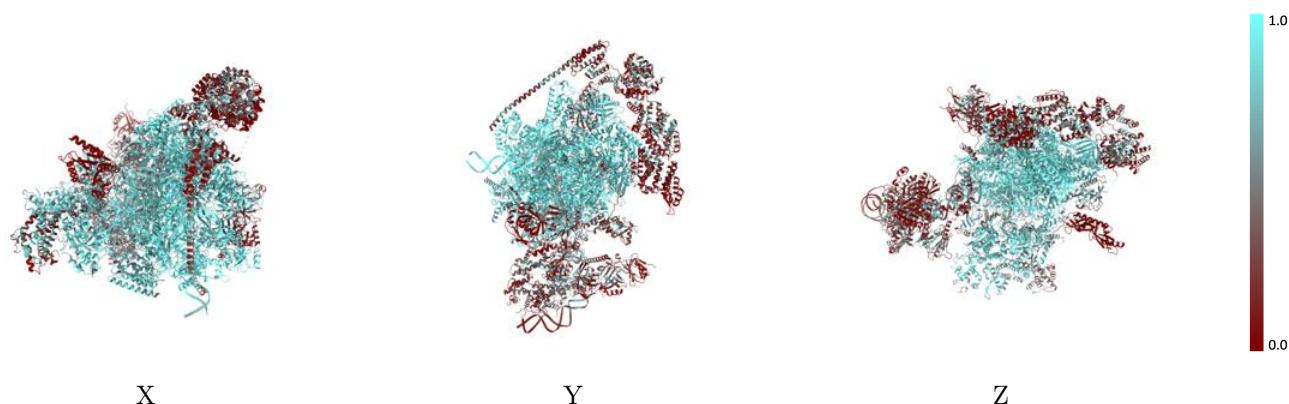
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



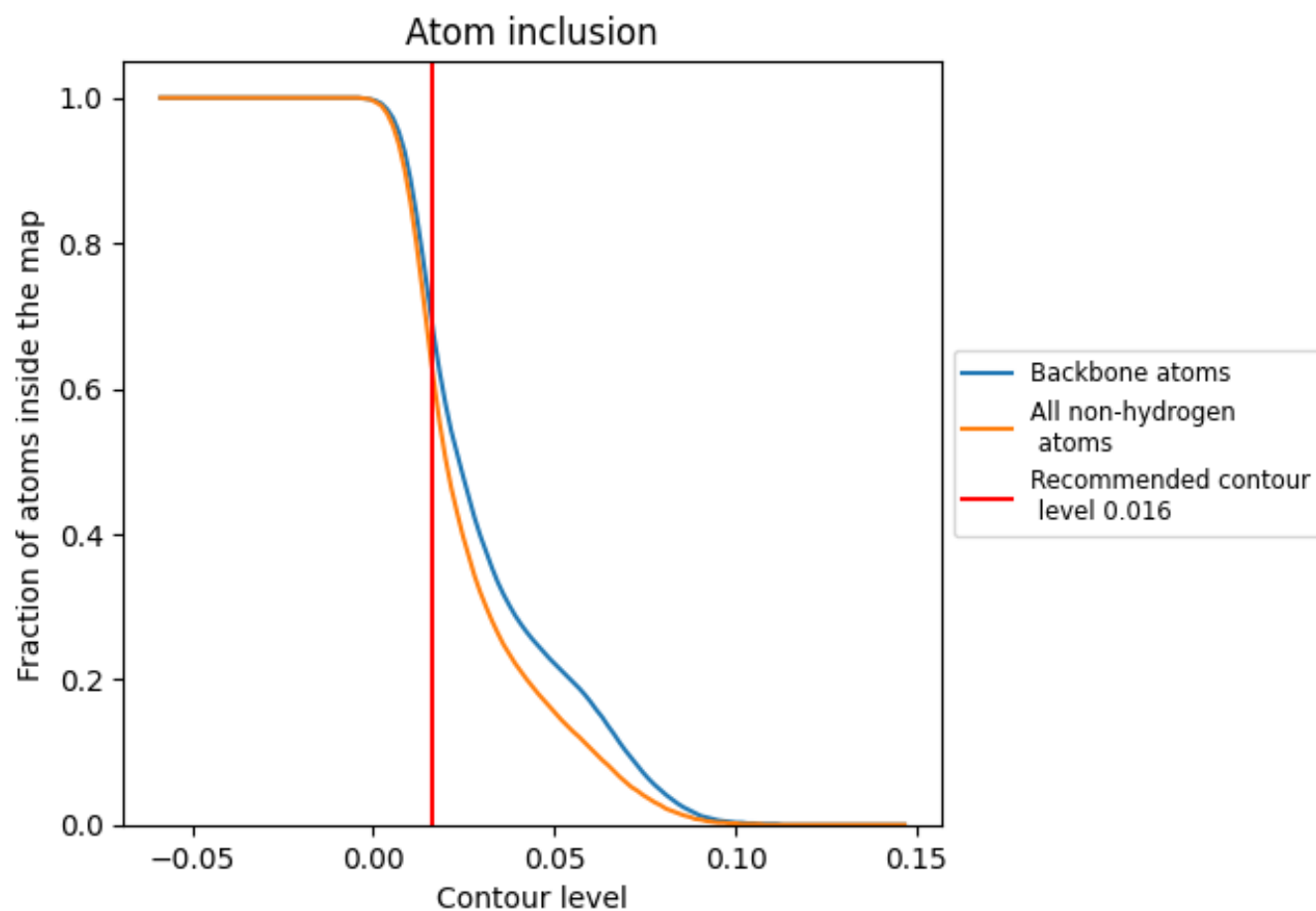
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 64% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6370	 0.2290
A	 0.9330	 0.4680
B	 0.9290	 0.4740
C	 0.9390	 0.5000
D	 0.7730	 0.2030
E	 0.9460	 0.4450
F	 0.9540	 0.5060
G	 0.8470	 0.3080
H	 0.9520	 0.4850
I	 0.8810	 0.3290
J	 0.9500	 0.5150
K	 0.9550	 0.5040
L	 0.9570	 0.4610
M	 0.7640	 0.1520
N	 0.6340	 0.1100
P	 0.8420	 0.3260
T	 0.6860	 0.1610
V	 0.8310	 0.1080
W	 0.7330	 0.1850
a	 0.4790	 0.0130
b	 0.3730	 0.0110
e	 0.3860	 0.0120
f	 0.3530	 0.0550
g	 0.2160	 0.0290
h	 0.1650	 -0.0500
j	 0.3280	 0.0050
k	 0.1830	 0.0000
m	 0.6060	 0.0810
n	 0.8170	 0.1630
q	 0.2720	 0.0400
r	 0.3490	 0.1160
s	 0.2780	 0.0340
u	 0.2470	 0.1020
v	 0.1900	 0.0570
x	 0.4610	 0.2300

