



Full wwPDB EM Validation Report ⓘ

Dec 29, 2024 – 08:55 PM EST

PDB ID : 7XN7
EMDB ID : EMD-33313
Title : RNA polymerase II elongation complex containing Spt4/5, Elf1, Spt6, Spn1 and Paf1C
Authors : Ehara, H.; Kujirai, T.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on : 2022-04-28
Resolution : 3.10 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

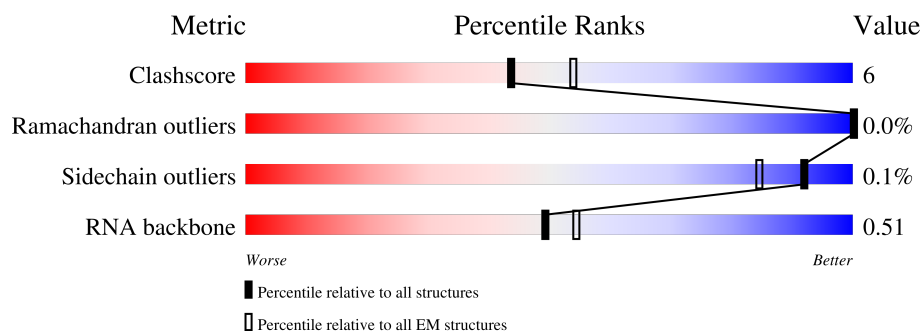
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.








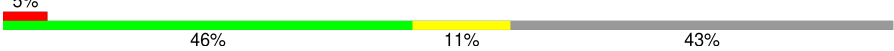

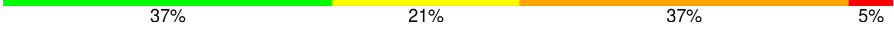






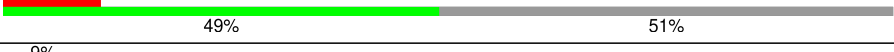



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

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

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Mol	Chain	Length	Quality of chain
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	M	113	
14	N	198	
15	P	19	
16	T	198	
17	V	108	
18	W	911	
19	m	1503	
20	n	417	
21	q	1084	
22	r	544	
23	u	459	
24	v	396	
25	x	395	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 66076 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

- Molecule 7 is a protein called RNA polymerase II subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1325	858	214	248	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1053	671	169	209	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			554	355	97	96	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 13 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	64	Total	C	N	O	S	0	0
			505	318	82	99	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP C4QZ45
M	-1	PRO	-	expression tag	UNP C4QZ45
M	0	GLY	-	expression tag	UNP C4QZ45

- Molecule 14 is a DNA chain called DNA (198-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	42	Total	C	N	O	P	0	0
			854	408	144	260	42		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	53	Total	C	N	O	P	0	0
			1090	515	217	305	53		

- 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	VAL	conflict	UNP C4R0E6

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	533	Total	C	N	O	S	0	0
			4232	2666	752	812	2		

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	-39	MET	-	initiating methionine	UNP C4R6B2
q	-38	LYS	-	expression tag	UNP C4R6B2
q	-37	ASP	-	expression tag	UNP C4R6B2
q	-36	HIS	-	expression tag	UNP C4R6B2
q	-35	LEU	-	expression tag	UNP C4R6B2
q	-34	ILE	-	expression tag	UNP C4R6B2
q	-33	HIS	-	expression tag	UNP C4R6B2
q	-32	ASN	-	expression tag	UNP C4R6B2
q	-31	HIS	-	expression tag	UNP C4R6B2
q	-30	HIS	-	expression tag	UNP C4R6B2
q	-29	LYS	-	expression tag	UNP C4R6B2
q	-28	HIS	-	expression tag	UNP C4R6B2
q	-27	GLU	-	expression tag	UNP C4R6B2
q	-26	HIS	-	expression tag	UNP C4R6B2
q	-25	ALA	-	expression tag	UNP C4R6B2
q	-24	HIS	-	expression tag	UNP C4R6B2
q	-23	ALA	-	expression tag	UNP C4R6B2
q	-22	GLU	-	expression tag	UNP C4R6B2
q	-21	HIS	-	expression tag	UNP C4R6B2
q	-20	ASP	-	expression tag	UNP C4R6B2
q	-19	TYR	-	expression tag	UNP C4R6B2
q	-18	LYS	-	expression tag	UNP C4R6B2
q	-17	ASP	-	expression tag	UNP C4R6B2
q	-16	ASP	-	expression tag	UNP C4R6B2
q	-15	ASP	-	expression tag	UNP C4R6B2
q	-14	ASP	-	expression tag	UNP C4R6B2
q	-13	LYS	-	expression tag	UNP C4R6B2
q	-12	GLU	-	expression tag	UNP C4R6B2
q	-11	HIS	-	expression tag	UNP C4R6B2
q	-10	LEU	-	expression tag	UNP C4R6B2
q	-9	TYR	-	expression tag	UNP C4R6B2
q	-8	PHE	-	expression tag	UNP C4R6B2
q	-7	GLN	-	expression tag	UNP C4R6B2
q	-6	GLY	-	expression tag	UNP C4R6B2
q	-5	SER	-	expression tag	UNP C4R6B2
q	-4	SER	-	expression tag	UNP C4R6B2
q	-3	GLY	-	expression tag	UNP C4R6B2
q	-2	SER	-	expression tag	UNP C4R6B2
q	-1	SER	-	expression tag	UNP C4R6B2
q	0	GLY	-	expression tag	UNP C4R6B2

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

unit.

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

There are 30 discrepancies between the modelled and reference sequences:

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

- Molecule 23 is a protein called Leo1.

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

There are 30 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

- Molecule 25 is a protein called Constituent of Paf1 complex with RNA polymerase II, Paf1p, Hpr1p, Ctr9, Leo1, Rtf1 and Ccr4p.

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

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	-29	MET	-	initiating methionine	UNP C4R1E6
x	-28	LYS	-	expression tag	UNP C4R1E6
x	-27	ASP	-	expression tag	UNP C4R1E6
x	-26	HIS	-	expression tag	UNP C4R1E6
x	-25	LEU	-	expression tag	UNP C4R1E6
x	-24	ILE	-	expression tag	UNP C4R1E6
x	-23	HIS	-	expression tag	UNP C4R1E6
x	-22	ASN	-	expression tag	UNP C4R1E6
x	-21	HIS	-	expression tag	UNP C4R1E6
x	-20	HIS	-	expression tag	UNP C4R1E6
x	-19	LYS	-	expression tag	UNP C4R1E6
x	-18	HIS	-	expression tag	UNP C4R1E6
x	-17	GLU	-	expression tag	UNP C4R1E6
x	-16	HIS	-	expression tag	UNP C4R1E6
x	-15	ALA	-	expression tag	UNP C4R1E6
x	-14	HIS	-	expression tag	UNP C4R1E6
x	-13	ALA	-	expression tag	UNP C4R1E6
x	-12	GLU	-	expression tag	UNP C4R1E6
x	-11	HIS	-	expression tag	UNP C4R1E6
x	-10	LEU	-	expression tag	UNP C4R1E6
x	-9	TYR	-	expression tag	UNP C4R1E6
x	-8	PHE	-	expression tag	UNP C4R1E6
x	-7	GLN	-	expression tag	UNP C4R1E6
x	-6	GLY	-	expression tag	UNP C4R1E6
x	-5	SER	-	expression tag	UNP C4R1E6
x	-4	SER	-	expression tag	UNP C4R1E6
x	-3	GLY	-	expression tag	UNP C4R1E6
x	-2	SER	-	expression tag	UNP C4R1E6
x	-1	SER	-	expression tag	UNP C4R1E6

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

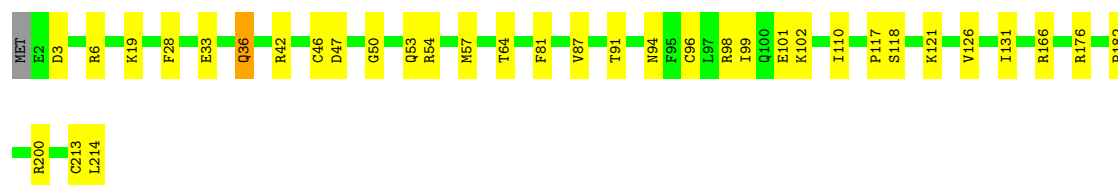
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

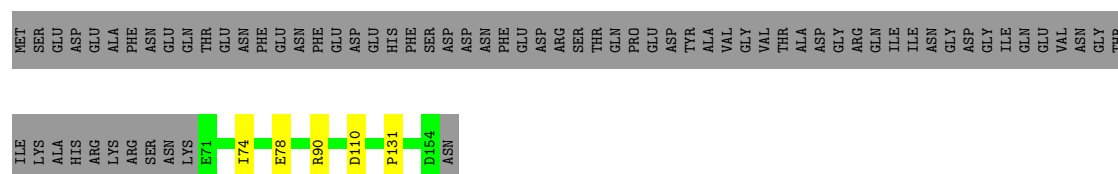
Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total 1	Mg 1	0

Chain E:  83% 16%




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

Chain F:  51% 46%




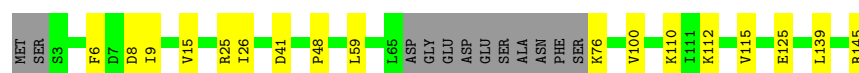
- Molecule 7: RNA polymerase II subunit

Chain G:  82% 18%




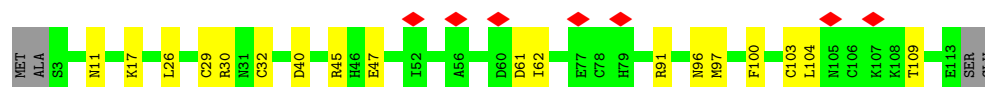
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  80% 12% 8%




- Molecule 9: DNA-directed RNA polymerase subunit

Chain I:  6% 81% 16%



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

Chain J:  82% 11% 7%



- Molecule 11: RNA polymerase II subunit B12.5

#1	I11	N29	L42	R47	D55	V56	T57	Y61	K62	V63	E64	H65	F68	Q76	T77	E78	K84	R89	A90	C91	L101	D102	H103	E107	N113	PHE	SER	LEU	ASN	ASP
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- Chain L:  56% 7% 38%

MET	SER	ARG	GLU	GLY	PHE	VAL	ALA	PRO	PRO	SER	GLY	THR	ASP	LEU	ALA	ALA	ALA	ALA	SER	SER	GLY	VAL	ALA	ALA	PRO	ASN	LYS	HIS	TYR	G28	V29	K30	Y31	T32	C33	G34		D70	A71	R72
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- Chain M: 

[illegible]

- Chain N: 6% 12% 79%

[illegible]

- Chain P:  37% 21% 37% 5%

- Chain T:  9% 14% 73%

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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	444232	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	0.127	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	356.16, 356.16, 356.16	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.484, 1.484, 1.484	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/11267	0.49	0/15222
2	B	0.33	0/9464	0.52	0/12763
3	C	0.33	0/2139	0.49	0/2895
4	D	0.23	0/1361	0.46	0/1837
5	E	0.30	0/1773	0.49	0/2385
6	F	0.33	0/687	0.50	0/931
7	G	0.28	0/1354	0.48	0/1837
8	H	0.33	0/1070	0.49	0/1444
9	I	0.24	0/934	0.50	0/1257
10	J	0.36	0/563	0.50	0/753
11	K	0.32	0/953	0.50	0/1291
12	L	0.32	0/365	0.56	0/484
13	M	0.24	0/513	0.41	0/693
14	N	0.96	6/952 (0.6%)	0.95	0/1464
15	P	1.17	5/449 (1.1%)	1.57	8/698 (1.1%)
16	T	1.06	13/1227 (1.1%)	0.98	0/1890
17	V	0.24	0/840	0.50	0/1140
18	W	0.24	0/4300	0.49	0/5812
19	m	0.24	0/9925	0.45	0/13424
20	n	0.23	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	0.25	0/1716	0.45	0/2310
All	All	0.34	24/67526 (0.0%)	0.52	8/91645 (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
15	P	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	10	G	C1'-N9	-6.75	1.37	1.46
15	P	6	G	C1'-N9	-6.44	1.37	1.46
16	T	34	DA	C1'-N9	-6.22	1.38	1.47
16	T	53	DA	C1'-N9	-6.03	1.38	1.47
14	N	-21	DG	C1'-N9	-5.90	1.39	1.47
16	T	32	DA	C1'-N9	-5.80	1.39	1.47
16	T	59	DA	C1'-N9	-5.70	1.39	1.47
16	T	47	DG	C1'-N9	-5.66	1.39	1.47
16	T	55	DA	C1'-N9	-5.63	1.39	1.47
16	T	52	DG	C1'-N9	-5.59	1.39	1.47
14	N	-22	DG	C1'-N9	-5.49	1.39	1.47
14	N	-10	DG	C1'-N9	-5.47	1.39	1.47
14	N	-19	DG	C1'-N9	-5.45	1.39	1.47
16	T	43	DA	C1'-N9	-5.44	1.39	1.47
15	P	-7	U	C1'-N1	5.33	1.56	1.48
16	T	50	DA	C1'-N9	-5.33	1.39	1.47
14	N	-14	DA	C1'-N9	-5.31	1.39	1.47
15	P	2	U	C1'-N1	5.25	1.56	1.48
14	N	-30	DA	C1'-N9	-5.24	1.40	1.47
16	T	48	DG	C1'-N9	-5.16	1.40	1.47
16	T	18	DC	C1'-N1	5.10	1.55	1.49
15	P	11	U	C1'-N1	5.09	1.56	1.48
16	T	41	DA	C1'-N9	-5.09	1.40	1.47
16	T	57	DA	C1'-N9	-5.07	1.40	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	-4	C	N3-C2-O2	-7.11	116.93	121.90
15	P	11	U	OP1-P-OP2	-6.44	109.93	119.60
15	P	-4	C	N1-C2-O2	6.32	122.69	118.90
15	P	-1	G	N3-C2-N2	-6.30	115.49	119.90
15	P	-3	U	N3-C2-O2	-6.09	117.94	122.20
15	P	-1	G	C2-N3-C4	5.90	114.85	111.90
15	P	-1	G	N3-C4-C5	-5.78	125.71	128.60
15	P	-1	G	C8-N9-C4	-5.46	104.22	106.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	P	-4	C	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	120	0
2	B	9284	0	9282	118	0
3	C	2098	0	2057	18	0
4	D	1349	0	1345	11	0
5	E	1741	0	1754	22	0
6	F	677	0	693	4	0
7	G	1325	0	1342	19	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	14	0
12	L	359	0	358	4	0
13	M	505	0	495	6	0
14	N	854	0	478	43	0
15	P	404	0	202	7	0
16	T	1090	0	590	36	0
17	V	824	0	795	17	0
18	W	4232	0	4278	57	0
19	m	9730	0	9588	0	0
20	n	1115	0	1186	0	0
21	q	7552	0	7545	0	0
22	r	2139	0	2155	0	0
23	u	1707	0	1676	0	0
24	v	2878	0	2873	0	0
25	x	1682	0	1731	0	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	C	1	0	0	0	0
26	I	2	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	M	1	0	0	0	0
26	V	1	0	0	0	0
27	A	1	0	0	0	0
All	All	66076	0	64947	463	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 (463) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-48:DC:H2''	14:N:-47:DC:C5	2.03	0.92
16:T:13:DT:H2''	16:T:14:DT:C7	1.99	0.92
16:T:13:DT:H2''	16:T:14:DT:H71	1.51	0.88
1:A:318:LYS:HE3	16:T:43:DA:C6	2.13	0.83
16:T:19:DC:H2'	16:T:20:DG:C8	2.17	0.80
14:N:-61:DT:C2'	14:N:-60:DT:H72	2.13	0.78
14:N:-45:DG:N2	16:T:45:DC:O2	2.16	0.77
14:N:-60:DT:H2'	14:N:-59:DT:H71	1.66	0.77
14:N:-61:DT:H2'	14:N:-60:DT:H72	1.66	0.76
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.26	0.75
14:N:-61:DT:H2'	14:N:-60:DT:C7	2.15	0.75
14:N:-48:DC:H2''	14:N:-47:DC:H5	1.52	0.74
14:N:-61:DT:C2'	14:N:-60:DT:C7	2.66	0.73
14:N:-54:DC:H2''	14:N:-53:DT:H72	1.71	0.72
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.70	0.72
1:A:807:ARG:NH1	2:B:724:LYS:O	2.23	0.71
14:N:-52:DC:O2	16:T:52:DG:N2	2.17	0.71
1:A:1207:LYS:O	1:A:1277:ARG:NH2	2.24	0.70
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
10:J:47:ARG:NH1	10:J:48:MET:SD	2.67	0.68
1:A:251:ILE:HD12	15:P:1:G:H21	1.58	0.67
14:N:-18:DG:H2'	14:N:-17:DT:C6	2.29	0.67
2:B:223:SER:O	2:B:252:ARG:NH2	2.27	0.67
1:A:107:CYS:SG	1:A:172:GLN:NE2	2.66	0.67
18:W:487:ILE:HD11	18:W:531:ARG:HB2	1.76	0.66
9:I:45:ARG:NH2	9:I:47:GLU:OE2	2.28	0.66
2:B:267:TYR:HB2	2:B:348:ILE:HD11	1.77	0.66
2:B:254:ASP:H	2:B:259:ARG:HH21	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ASP:OD1	1:A:737:ASN:ND2	2.29	0.65
18:W:342:GLU:HB3	18:W:351:ARG:HB3	1.79	0.65
16:T:19:DC:H2'	16:T:20:DG:H8	1.61	0.65
1:A:127:ARG:O	1:A:129:ARG:NH1	2.30	0.64
1:A:887:ILE:O	1:A:945:ARG:NH2	2.30	0.64
4:D:153:VAL:HG13	4:D:171:LEU:HD23	1.78	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:613:ARG:HH21	9:I:62:ILE:HD11	1.61	0.64
1:A:1158:PRO:HA	1:A:1192:PRO:HB3	1.80	0.63
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.24	0.63
1:A:361:GLU:OE1	1:A:460:ARG:NH2	2.29	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
17:V:89:ARG:NH1	17:V:109:ASP:OD2	2.31	0.63
1:A:1130:ILE:HG12	1:A:1134:LYS:HE2	1.81	0.63
11:K:57:THR:OG1	11:K:76:GLN:OE1	2.17	0.63
14:N:-56:DG:H2''	14:N:-55:DT:C6	2.33	0.63
16:T:50:DA:OP1	18:W:433:GLN:NE2	2.33	0.62
16:T:9:DG:H1'	16:T:10:DC:C5	2.34	0.62
18:W:351:ARG:HA	18:W:429:THR:HA	1.81	0.61
1:A:1201:ARG:NH2	1:A:1235:ALA:O	2.33	0.61
18:W:784:ASN:HB2	18:W:785:PRO:HD3	1.81	0.61
3:C:266:ARG:HD2	11:K:84:LYS:HZ3	1.66	0.61
1:A:39:GLU:OE2	1:A:49:ARG:NH1	2.34	0.61
1:A:466:TYR:HB2	1:A:470:ARG:NH2	2.16	0.61
5:E:47:ASP:OD2	5:E:53:GLN:NE2	2.19	0.60
1:A:22:LEU:HG	2:B:1213:ALA:HB2	1.83	0.60
16:T:9:DG:H2''	16:T:10:DC:H5	1.66	0.60
2:B:489:ARG:NH2	2:B:533:SER:O	2.35	0.60
15:P:-5:C:H1'	18:W:748:ARG:HD3	1.83	0.60
1:A:677:MET:HG3	2:B:722:THR:HB	1.84	0.60
18:W:527:THR:HA	18:W:530:LEU:HD12	1.84	0.60
1:A:1157:ASP:O	1:A:1243:ARG:NH2	2.29	0.59
2:B:294:CYS:SG	2:B:295:TYR:N	2.76	0.59
2:B:409:LEU:HD23	2:B:450:LEU:HD23	1.85	0.59
17:V:13:MET:N	17:V:49:CYS:O	2.26	0.59
2:B:235:LEU:HD23	2:B:242:ILE:HG13	1.83	0.59
14:N:-61:DT:N1	14:N:-60:DT:H72	2.18	0.59
17:V:57:LEU:HD11	17:V:81:LEU:HD22	1.84	0.59
1:A:227:GLU:OE1	1:A:231:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:ASP:HB3	2:B:649:LYS:HG3	1.84	0.59
7:G:27:ARG:NH1	7:G:54:ILE:O	2.36	0.59
8:H:48:PRO:O	8:H:145:ARG:NH1	2.36	0.59
1:A:149:GLU:HB2	1:A:165:ARG:HD3	1.84	0.58
17:V:9:GLU:HA	17:V:20:PRO:HA	1.84	0.58
1:A:1331:TYR:OH	1:A:1354:GLU:OE2	2.21	0.58
2:B:50:VAL:HG21	2:B:82:ILE:HD11	1.86	0.58
7:G:102:ASP:OD1	7:G:107:ASN:ND2	2.32	0.58
14:N:-56:DG:C2	16:T:57:DA:C2	2.92	0.58
1:A:85:GLU:O	1:A:274:ASN:ND2	2.33	0.58
18:W:327:ARG:NH1	18:W:335:GLY:O	2.36	0.58
2:B:63:GLN:NE2	2:B:70:ASN:OD1	2.35	0.58
5:E:101:GLU:HG3	5:E:102:LYS:HG2	1.86	0.57
7:G:86:VAL:HG22	7:G:146:LYS:HB2	1.86	0.57
1:A:568:LYS:HG2	1:A:569:PRO:HA	1.87	0.57
16:T:13:DT:H2''	16:T:14:DT:C5	2.39	0.57
18:W:392:ARG:NH1	18:W:398:GLU:OE1	2.36	0.57
18:W:352:LEU:HD11	18:W:435:LEU:HD11	1.87	0.57
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.37	0.57
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.85	0.57
18:W:665:ARG:HB2	18:W:708:ILE:HD11	1.87	0.57
14:N:-60:DT:C2'	14:N:-59:DT:H71	2.34	0.56
2:B:290:LEU:HD21	2:B:310:ILE:HD11	1.87	0.56
2:B:336:ILE:O	2:B:341:ARG:NH1	2.38	0.56
2:B:353:LEU:O	2:B:367:LYS:NZ	2.34	0.56
18:W:220:THR:N	18:W:223:ASP:OD2	2.33	0.56
5:E:28:PHE:HB2	5:E:64:THR:HG22	1.88	0.56
14:N:-11:DC:H2'	14:N:-10:DG:C8	2.40	0.56
17:V:15:CYS:HB3	17:V:32:CYS:SG	2.46	0.56
2:B:906:SER:OG	18:W:781:GLU:OE1	2.23	0.56
14:N:-20:DC:H2'	14:N:-19:DG:O4'	2.07	0.55
1:A:1452:LEU:HD23	6:F:131:PRO:HA	1.88	0.55
2:B:72:ASN:ND2	2:B:128:ASP:OD1	2.40	0.55
8:H:100:VAL:HG22	8:H:115:VAL:HG22	1.89	0.55
1:A:149:GLU:O	1:A:165:ARG:NH1	2.38	0.55
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.88	0.55
16:T:16:DA:H2''	16:T:17:DA:O4'	2.06	0.55
1:A:669:ASP:OD2	1:A:743:ASN:ND2	2.29	0.55
16:T:9:DG:H2''	16:T:10:DC:C5	2.42	0.55
1:A:1210:THR:HB	1:A:1213:GLN:HG3	1.89	0.55
5:E:19:LYS:NZ	5:E:33:GLU:O	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-21:DG:N2	16:T:22:DC:O2	2.39	0.55
2:B:622:ASP:OD1	2:B:623:VAL:N	2.40	0.55
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.42	0.54
2:B:904:ARG:HH12	2:B:946:ASN:HB2	1.72	0.54
18:W:232:ARG:HH12	18:W:235:LYS:HE3	1.70	0.54
1:A:119:ASN:OD1	1:A:121:THR:OG1	2.23	0.54
14:N:-18:DG:H2'	14:N:-17:DT:H6	1.70	0.54
18:W:332:LYS:O	18:W:388:ARG:NH1	2.41	0.54
1:A:916:TYR:OH	1:A:983:LEU:O	2.19	0.54
14:N:-14:DA:C2	14:N:-13:DA:C2	2.96	0.54
7:G:151:ARG:HB3	7:G:158:TYR:HB2	1.89	0.54
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.89	0.54
11:K:29:ASN:ND2	11:K:78:GLU:O	2.41	0.54
18:W:325:TYR:OH	18:W:451:GLN:OE1	2.23	0.54
1:A:807:ARG:HD3	2:B:725:ARG:HA	1.89	0.54
1:A:218:GLU:OE1	1:A:222:ARG:NH1	2.41	0.54
11:K:103:HIS:NE2	11:K:107:GLU:OE2	2.40	0.54
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.89	0.54
7:G:144:ARG:HB2	7:G:171:ILE:HD13	1.90	0.54
4:D:6:SER:HB3	7:G:42:PHE:HZ	1.73	0.53
13:M:46:LEU:HD11	13:M:55:SER:HB3	1.91	0.53
17:V:10:ARG:HA	17:V:52:SER:HA	1.90	0.53
1:A:351:ARG:HB2	2:B:1128:LEU:HD21	1.91	0.53
2:B:91:GLU:OE2	2:B:97:HIS:NE2	2.29	0.53
1:A:533:ARG:HD3	1:A:750:ALA:HB2	1.91	0.53
18:W:451:GLN:NE2	18:W:454:GLU:OE1	2.41	0.53
18:W:513:SER:N	18:W:519:ASN:OD1	2.41	0.53
1:A:1426:GLY:O	1:A:1430:ASN:ND2	2.40	0.53
2:B:58:LEU:O	2:B:75:TYR:N	2.36	0.53
2:B:59:ASP:HB3	2:B:74:ARG:HG3	1.91	0.53
4:D:60:ILE:HG13	7:G:47:THR:HG21	1.91	0.53
14:N:-21:DG:N2	16:T:22:DC:C2	2.77	0.53
5:E:118:SER:OG	14:N:-16:DT:OP1	2.22	0.52
2:B:301:GLN:O	2:B:304:GLU:HG3	2.08	0.52
8:H:59:LEU:HD23	8:H:139:LEU:HD13	1.91	0.52
17:V:58:VAL:N	17:V:82:TYR:O	2.38	0.52
2:B:248:LYS:NZ	2:B:264:THR:OG1	2.42	0.52
16:T:16:DA:H2'	16:T:17:DA:C8	2.44	0.52
1:A:318:LYS:HE3	16:T:43:DA:N1	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.92	0.52
1:A:1153:GLU:OE2	9:I:45:ARG:NH1	2.40	0.52
2:B:74:ARG:HB2	2:B:124:PHE:HB2	1.92	0.52
5:E:81:PHE:HE1	5:E:110:ILE:HD13	1.74	0.52
2:B:904:ARG:NH1	2:B:905:VAL:O	2.43	0.51
13:M:38:LEU:HA	13:M:45:GLY:HA2	1.91	0.51
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.74	0.51
1:A:771:VAL:HG13	1:A:823:GLU:HG3	1.92	0.51
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.93	0.51
2:B:505:ARG:NH1	2:B:524:GLN:O	2.32	0.51
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.75	0.51
1:A:801:VAL:HG22	1:A:813:GLU:HB3	1.92	0.51
2:B:547:ILE:HG21	2:B:619:ILE:HG21	1.93	0.51
18:W:644:ASN:ND2	18:W:647:GLN:OE1	2.44	0.51
5:E:54:ARG:HA	5:E:57:MET:HE3	1.93	0.51
18:W:260:TYR:HD1	18:W:276:ALA:HA	1.75	0.51
18:W:326:VAL:HA	18:W:440:ILE:HD13	1.92	0.51
13:M:33:SER:HA	13:M:50:LYS:HE2	1.93	0.51
2:B:83:TYR:HB2	2:B:116:TYR:HB2	1.92	0.50
2:B:797:TYR:HE1	2:B:854:LEU:HD13	1.74	0.50
14:N:-61:DT:H2''	14:N:-60:DT:C7	2.41	0.50
18:W:563:GLU:HG2	18:W:574:ILE:HG12	1.92	0.50
9:I:17:LYS:N	9:I:26:LEU:O	2.39	0.50
16:T:18:DC:C2	16:T:19:DC:C5	3.00	0.50
1:A:1190:GLN:HA	1:A:1245:ILE:HA	1.94	0.50
5:E:87:VAL:HG23	5:E:91:THR:HB	1.92	0.50
14:N:-61:DT:H2'	14:N:-60:DT:H73	1.90	0.50
18:W:334:LYS:N	18:W:388:ARG:HH12	2.09	0.50
2:B:74:ARG:HH22	2:B:126:SER:HB3	1.77	0.49
2:B:607:SER:HB3	2:B:620:PHE:HB2	1.94	0.49
14:N:-18:DG:N2	14:N:-17:DT:C2	2.80	0.49
2:B:498:ASP:HB3	14:N:-31:DA:C4	2.47	0.49
16:T:20:DG:N2	16:T:21:DC:C2	2.81	0.49
17:V:63:ASN:HB3	17:V:75:ASP:HA	1.94	0.49
1:A:168:CYS:SG	1:A:170:ASN:ND2	2.85	0.49
2:B:300:TRP:HA	2:B:303:LEU:HD12	1.94	0.49
2:B:479:TYR:CZ	2:B:1096:ARG:HB3	2.48	0.49
4:D:105:THR:HG22	7:G:105:PRO:HD3	1.94	0.49
18:W:464:ILE:O	18:W:468:LEU:HG	2.12	0.49
18:W:590:ILE:O	18:W:593:SER:OG	2.26	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)
1:A:1223:SER:OG	1:A:1224:ASP:N	2.44	0.49
7:G:119:LEU:HD21	7:G:135:GLU:HB2	1.93	0.49
14:N:-51:DG:H2'	14:N:-50:DT:H71	1.95	0.49
18:W:222:ASP:O	18:W:277:ARG:NH2	2.30	0.49
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	1.94	0.49
5:E:81:PHE:CE1	5:E:110:ILE:HD13	2.48	0.49
7:G:112:THR:HA	7:G:115:ILE:HD12	1.95	0.49
1:A:673:ASP:OD1	1:A:673:ASP:N	2.44	0.49
18:W:634:PRO:HA	18:W:637:ILE:HD12	1.94	0.49
12:L:70:ASP:HB3	18:W:784:ASN:HB3	1.95	0.48
1:A:823:GLU:OE1	2:B:506:GLN:NE2	2.46	0.48
3:C:66:LEU:HD11	3:C:155:ILE:HD12	1.95	0.48
9:I:96:ASN:OD1	9:I:97:MET:N	2.46	0.48
1:A:738:LEU:HD13	1:A:742:ASN:HD22	1.77	0.48
2:B:318:ASP:HB3	2:B:321:VAL:HG22	1.94	0.48
2:B:610:ARG:NH2	9:I:61:ASP:OD2	2.46	0.48
2:B:314:PHE:O	2:B:317:GLN:NE2	2.46	0.48
3:C:105:GLU:N	3:C:105:GLU:OE1	2.46	0.48
14:N:-13:DA:C2	14:N:-12:DA:C4	3.01	0.48
2:B:365:THR:O	2:B:368:THR:OG1	2.29	0.48
1:A:253:MET:HG2	15:P:1:G:N2	2.29	0.48
1:A:977:ARG:HD2	1:A:979:LYS:HZ1	1.78	0.48
2:B:514:LEU:HD22	2:B:626:VAL:HG12	1.94	0.48
2:B:766:ARG:HH21	2:B:1020:ARG:HD3	1.77	0.48
9:I:29:CYS:CB	9:I:32:CYS:SG	2.99	0.48
15:P:1:G:H2'	15:P:2:U:O4'	2.12	0.48
18:W:666:GLU:HB2	18:W:671:ARG:HA	1.95	0.48
1:A:321:ARG:NH1	2:B:466:MET:SD	2.86	0.48
17:V:91:PRO:HD2	17:V:94:ILE:HB	1.95	0.48
18:W:599:HIS:HB3	18:W:677:LEU:HD21	1.96	0.48
9:I:103:CYS:SG	9:I:104:LEU:N	2.86	0.48
15:P:-5:C:C4	18:W:748:ARG:N	2.82	0.48
1:A:1150:SER:OG	1:A:1198:GLU:O	2.32	0.48
2:B:865:ARG:HD3	2:B:871:VAL:HG12	1.95	0.48
3:C:74:GLU:O	3:C:246:ARG:NH2	2.39	0.48
4:D:157:ILE:HG23	4:D:164:ALA:HB2	1.95	0.48
1:A:106:ILE:HD13	1:A:215:ILE:HD11	1.95	0.47
1:A:1150:SER:OG	1:A:1198:GLU:OE1	2.29	0.47
3:C:88:GLU:HG2	18:W:759:ARG:HD2	1.95	0.47
18:W:666:GLU:HA	18:W:705:VAL:HG12	1.96	0.47
2:B:788:ARG:O	2:B:967:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:THR:HA	5:E:94:ASN:ND2	2.29	0.47
5:E:213:CYS:SG	5:E:214:LEU:N	2.87	0.47
16:T:45:DC:H2'	16:T:46:DA:C8	2.49	0.47
18:W:603:GLN:HG3	18:W:609:VAL:HG22	1.95	0.47
1:A:486:ASP:OD1	15:P:10:G:O2'	2.20	0.47
2:B:303:LEU:O	2:B:307:LYS:HG2	2.15	0.47
1:A:912:ASP:OD1	1:A:912:ASP:N	2.44	0.47
2:B:80:GLY:N	2:B:118:ASP:O	2.42	0.47
1:A:472:ASN:O	1:A:475:VAL:HG22	2.14	0.47
1:A:580:SER:HB3	1:A:612:LYS:HA	1.97	0.47
1:A:983:LEU:HD13	1:A:1041:ARG:HA	1.96	0.47
2:B:421:ILE:HD11	2:B:441:VAL:HG12	1.97	0.47
2:B:896:ASP:OD2	12:L:31:TYR:OH	2.32	0.47
13:M:37:THR:O	13:M:46:LEU:N	2.29	0.47
14:N:-55:DT:H4'	14:N:-54:DC:H5'	1.97	0.47
2:B:101:PRO:HG2	2:B:172:LEU:HD11	1.96	0.47
11:K:62:LYS:HE3	11:K:64:GLU:OE2	2.15	0.47
17:V:41:SER:HB2	17:V:45:THR:HB	1.96	0.47
2:B:322:ALA:O	2:B:326:ILE:HG12	2.15	0.46
10:J:6:ARG:HD3	10:J:13:VAL:HG22	1.97	0.46
14:N:-19:DG:C2	14:N:-18:DG:C4	3.03	0.46
1:A:819:MET:O	1:A:823:GLU:HG2	2.14	0.46
1:A:1192:PRO:HA	1:A:1243:ARG:HH12	1.79	0.46
2:B:25:PHE:HZ	2:B:534:LEU:HG	1.81	0.46
2:B:273:PRO:HG2	2:B:276:ILE:HD12	1.97	0.46
3:C:4:GLU:HB3	3:C:5:PRO:HD3	1.96	0.46
18:W:260:TYR:CE1	18:W:277:ARG:HG3	2.49	0.46
1:A:363:ASP:HB3	1:A:509:PRO:HD3	1.97	0.46
3:C:17:VAL:HG12	3:C:240:ALA:HB1	1.96	0.46
5:E:98:ARG:NH1	5:E:102:LYS:HG3	2.31	0.46
7:G:123:PRO:HA	7:G:128:PRO:HB3	1.97	0.46
18:W:534:PHE:HB3	18:W:554:ILE:HD13	1.97	0.46
1:A:447:ARG:HB2	1:A:488:MET:HE3	1.98	0.46
5:E:96:CYS:SG	5:E:126:VAL:HG23	2.55	0.46
1:A:649:ASN:O	1:A:653:VAL:HG23	2.16	0.46
2:B:27:GLU:OE1	2:B:678:TRP:HB3	2.16	0.46
2:B:497:ARG:NH2	16:T:32:DA:OP2	2.48	0.46
4:D:139:PRO:HA	4:D:142:ILE:HD12	1.97	0.46
6:F:74:ILE:HG23	6:F:78:GLU:HG3	1.97	0.46
7:G:51:GLY:HA2	7:G:54:ILE:HD11	1.98	0.46
14:N:-56:DG:N1	16:T:57:DA:C2	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:O	1:A:231:ARG:NH2	2.46	0.46
16:T:40:DG:H1'	16:T:41:DA:H5''	1.98	0.46
18:W:451:GLN:HG3	18:W:458:THR:HA	1.98	0.46
1:A:409:ASP:OD1	1:A:410:ASN:N	2.49	0.46
2:B:318:ASP:OD1	2:B:319:LYS:N	2.48	0.46
16:T:14:DT:H2'	16:T:15:DT:C6	2.50	0.46
1:A:1065:MET:SD	1:A:1439:MET:HB2	2.56	0.46
1:A:1448:ILE:HD11	1:A:1453:LEU:HD11	1.97	0.46
14:N:-48:DC:C2'	14:N:-47:DC:C5	2.87	0.46
7:G:81:PRO:HG3	7:G:106:LEU:HD22	1.99	0.45
14:N:-18:DG:C2	14:N:-17:DT:C4	3.04	0.45
1:A:684:ILE:HG21	1:A:802:GLU:HG3	1.99	0.45
2:B:557:GLU:OE2	2:B:584:ARG:NH2	2.49	0.45
16:T:20:DG:C2	16:T:21:DC:C2	3.05	0.45
2:B:266:PRO:HG3	2:B:352:GLU:O	2.16	0.45
18:W:539:HIS:CE1	18:W:553:LEU:HD21	2.51	0.45
2:B:885:LEU:HD23	2:B:936:ASP:HB2	1.97	0.45
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.49	0.45
4:D:170:ASN:HB3	4:D:173:ARG:HG2	1.97	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
3:C:15:ASP:OD1	3:C:15:ASP:N	2.47	0.45
14:N:-30:DA:H61	16:T:30:DT:H3	1.65	0.45
2:B:463:LYS:NZ	2:B:464:LYS:HE2	2.31	0.45
16:T:11:DG:H1'	16:T:12:DT:H5'	1.98	0.45
18:W:344:LEU:HD12	18:W:349:GLU:HB2	1.99	0.45
1:A:532:VAL:O	1:A:536:THR:OG1	2.30	0.45
2:B:220:ALA:O	2:B:252:ARG:NH2	2.47	0.45
3:C:21:LEU:HD22	11:K:101:LEU:HD11	1.98	0.45
8:H:110:LYS:HE2	8:H:112:LYS:HE3	1.99	0.45
18:W:491:LEU:HB3	18:W:494:LEU:HD12	1.98	0.45
1:A:564:PRO:HG2	1:A:567:LEU:HD23	1.98	0.45
1:A:1061:HIS:O	1:A:1064:GLU:HG2	2.17	0.45
2:B:27:GLU:OE2	2:B:679:SER:OG	2.35	0.45
2:B:74:ARG:NH1	2:B:126:SER:OG	2.40	0.45
5:E:46:CYS:HB3	5:E:50:GLY:HA2	1.99	0.44
5:E:117:PRO:O	5:E:121:LYS:HG2	2.17	0.44
1:A:975:LEU:HD13	1:A:1039:LEU:HA	1.99	0.44
2:B:387:ASP:H	9:I:91:ARG:NH2	2.14	0.44
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.49	0.44
14:N:-21:DG:H2''	14:N:-20:DC:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:78:GLN:OE1	17:V:79:PRO:HD2	2.16	0.44
1:A:343:GLY:O	2:B:1129:ARG:NH1	2.45	0.44
1:A:880:GLU:O	1:A:957:PRO:HA	2.18	0.44
1:A:889:GLY:O	1:A:941:ARG:NH2	2.51	0.44
3:C:258:VAL:HG21	11:K:42:LEU:HD21	2.00	0.44
1:A:452:HIS:CE1	1:A:454:MET:HB2	2.52	0.44
4:D:54:SER:OG	4:D:121:CYS:SG	2.61	0.44
14:N:-61:DT:C2'	14:N:-60:DT:H73	2.42	0.44
1:A:779:GLY:HA3	2:B:509:ASN:HB2	1.99	0.43
1:A:1390:HIS:O	1:A:1394:ARG:HD3	2.17	0.43
8:H:25:ARG:HD3	8:H:41:ASP:OD1	2.18	0.43
14:N:-16:DT:H1'	14:N:-15:DA:H5'	1.99	0.43
2:B:640:ASP:OD1	2:B:640:ASP:N	2.50	0.43
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.00	0.43
17:V:67:TRP:NE1	18:W:217:LEU:O	2.51	0.43
18:W:250:ARG:NH2	18:W:284:ASP:OD2	2.50	0.43
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	1.99	0.43
14:N:-56:DG:N2	16:T:57:DA:N3	2.67	0.43
1:A:976:ASP:O	1:A:979:LYS:NZ	2.48	0.43
10:J:63:ASN:OD1	10:J:64:PRO:HD2	2.18	0.43
18:W:322:ARG:NE	18:W:343:VAL:H	2.17	0.43
18:W:763:TYR:HB3	18:W:766:LYS:HD3	2.00	0.43
1:A:329:ARG:NH1	2:B:1206:GLU:OE2	2.45	0.43
1:A:948:VAL:O	5:E:200:ARG:NH1	2.48	0.43
5:E:99:ILE:HG13	5:E:131:ILE:HD11	2.00	0.43
9:I:100:PHE:HB3	9:I:109:THR:HG23	1.99	0.43
13:M:65:GLN:N	13:M:68:ASP:OD2	2.44	0.43
18:W:444:LEU:HD23	18:W:444:LEU:HA	1.90	0.43
1:A:1098:LEU:HD23	1:A:1098:LEU:HA	1.89	0.43
2:B:221:ALA:O	2:B:223:SER:N	2.46	0.43
7:G:118:ASN:OD1	7:G:118:ASN:N	2.51	0.43
1:A:1389:ARG:O	1:A:1393:ASN:HB2	2.18	0.43
2:B:358:THR:HG1	2:B:363:PHE:HD2	1.67	0.43
2:B:721:ASP:OD2	2:B:724:LYS:N	2.41	0.43
2:B:1156:ASP:O	2:B:1197:PRO:HA	2.19	0.43
17:V:46:VAL:O	17:V:50:THR:N	2.44	0.43
1:A:266:LYS:HD2	1:A:266:LYS:HA	1.88	0.43
2:B:257:THR:OG1	2:B:258:GLY:N	2.50	0.43
4:D:88:GLU:HA	4:D:91:LYS:HE3	2.00	0.43
7:G:115:ILE:HG23	7:G:163:ILE:HD11	2.01	0.43
14:N:-56:DG:N2	16:T:57:DA:C2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ALA:HA	1:A:258:GLN:HA	2.00	0.43
1:A:473:LEU:HD21	2:B:835:GLN:HB2	2.00	0.43
1:A:815:PHE:O	1:A:819:MET:HG3	2.19	0.43
9:I:40:ASP:OD1	9:I:40:ASP:N	2.44	0.43
1:A:38:PRO:HA	1:A:271:LEU:HD23	2.01	0.42
2:B:763:GLN:HG2	2:B:765:PRO:HD2	2.01	0.42
8:H:8:ASP:OD1	8:H:9:ILE:N	2.48	0.42
9:I:29:CYS:HB3	9:I:32:CYS:SG	2.59	0.42
17:V:12:CYS:HA	17:V:50:THR:HA	2.01	0.42
1:A:421:ARG:HB3	1:A:424:ASP:HB2	2.01	0.42
2:B:85:SER:OG	2:B:114:PRO:HD2	2.20	0.42
2:B:237:LYS:HA	2:B:237:LYS:HD3	1.91	0.42
2:B:691:ASP:OD1	2:B:691:ASP:N	2.41	0.42
2:B:764:SER:OG	2:B:765:PRO:HD3	2.19	0.42
1:A:1221:VAL:HG21	1:A:1274:ILE:HD12	2.00	0.42
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.51	0.42
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.90	0.42
1:A:1201:ARG:HA	1:A:1238:LEU:HD12	2.01	0.42
2:B:250:TYR:HE2	2:B:262:LYS:HB2	1.82	0.42
2:B:557:GLU:HA	2:B:558:PRO:HD3	1.90	0.42
14:N:-48:DC:H2''	14:N:-47:DC:C6	2.50	0.42
17:V:42:ASP:OD1	17:V:42:ASP:N	2.53	0.42
1:A:504:GLN:OE1	6:F:90:ARG:NH1	2.38	0.42
2:B:330:GLY:HA3	2:B:344:TYR:HE2	1.84	0.42
16:T:9:DG:C1'	16:T:10:DC:C5	3.01	0.42
1:A:914:ILE:HG13	1:A:917:ALA:HB2	2.01	0.42
2:B:733:SER:HB3	2:B:736:HIS:CE1	2.54	0.42
5:E:176:ARG:HD3	5:E:214:LEU:HD11	2.02	0.42
18:W:543:ILE:HD11	18:W:581:ILE:HG13	2.01	0.42
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.91	0.42
6:F:110:ASP:N	6:F:110:ASP:OD1	2.53	0.42
7:G:165:GLU:H	7:G:168:LEU:HD12	1.85	0.42
18:W:349:GLU:HA	18:W:431:ARG:HA	2.02	0.42
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.91	0.42
1:A:691:VAL:HG11	1:A:795:PRO:HG3	2.02	0.42
2:B:283:VAL:HG13	2:B:283:VAL:O	2.18	0.42
2:B:293:ILE:HD13	2:B:375:VAL:HG11	2.02	0.42
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.85	0.42
4:D:106:LEU:HD23	4:D:106:LEU:HA	1.89	0.42
5:E:42:ARG:HG3	5:E:46:CYS:SG	2.60	0.42
9:I:29:CYS:SG	9:I:30:ARG:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:539:HIS:HB2	18:W:584:THR:HA	2.02	0.42
18:W:422:TYR:HB3	18:W:427:TYR:CE1	2.55	0.42
1:A:390:THR:O	1:A:394:ARG:HG2	2.20	0.41
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.88	0.41
1:A:1041:ARG:O	1:A:1044:PHE:N	2.50	0.41
2:B:279:ARG:NH1	2:B:316:ILE:O	2.52	0.41
2:B:479:TYR:CE2	2:B:778:MET:HG2	2.55	0.41
2:B:606:VAL:HG22	2:B:621:THR:HG22	2.02	0.41
16:T:37:DC:H2'	16:T:38:DA:C8	2.56	0.41
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.02	0.41
2:B:1153:GLU:OE1	2:B:1153:GLU:N	2.53	0.41
2:B:1174:ASN:OD1	2:B:1177:LYS:HB2	2.21	0.41
1:A:883:THR:HA	1:A:954:HIS:O	2.20	0.41
1:A:1343:GLY:HA2	5:E:182:PRO:HD2	2.01	0.41
2:B:33:GLN:HG2	2:B:34:GLN:N	2.36	0.41
3:C:135:ARG:NE	3:C:136:ASP:OD2	2.50	0.41
1:A:231:ARG:HB3	1:A:234:TRP:CD2	2.56	0.41
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.02	0.41
5:E:3:ASP:HA	5:E:6:ARG:HG2	2.01	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:2:U:H3	16:T:41:DA:H61	1.68	0.41
18:W:329:LYS:HB2	18:W:434:ASN:HA	2.02	0.41
1:A:152:ALA:HA	1:A:153:PRO:HD3	1.90	0.41
1:A:985:ILE:N	1:A:986:PRO:HD2	2.36	0.41
1:A:1210:THR:HG22	1:A:1212:ASN:H	1.86	0.41
1:A:1314:ILE:HB	1:A:1337:GLU:OE1	2.21	0.41
2:B:575:VAL:O	2:B:578:VAL:HG22	2.20	0.41
3:C:248:ILE:HG21	11:K:102:ASP:HB2	2.01	0.41
11:K:55:ASP:OD2	11:K:89:ARG:NH2	2.54	0.41
18:W:598:LEU:HD12	18:W:599:HIS:H	1.86	0.41
2:B:262:LYS:HB3	2:B:271:ASP:HB3	2.01	0.41
1:A:908:SER:OG	1:A:909:ILE:N	2.54	0.41
2:B:71:ILE:HG12	2:B:127:ILE:HG22	2.02	0.41
5:E:36:GLN:HE21	5:E:36:GLN:HB3	1.69	0.41
11:K:47:ARG:HD3	11:K:61:TYR:HD1	1.86	0.41
12:L:29:VAL:HG23	12:L:31:TYR:CE2	2.56	0.41
14:N:-28:DC:H2'	14:N:-27:DC:C6	2.56	0.41
16:T:24:DA:H2''	16:T:25:DG:H8	1.86	0.41
18:W:480:PRO:HA	18:W:498:VAL:HG12	2.02	0.41
18:W:540:VAL:HG11	18:W:554:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:614:ARG:NH2	18:W:616:GLN:HE21	2.19	0.41
1:A:636:ARG:HG3	1:A:880:GLU:OE2	2.21	0.41
1:A:664:SER:OG	1:A:665:ILE:N	2.55	0.41
4:D:53:LEU:HD13	4:D:147:SER:HB3	2.02	0.41
11:K:11:ILE:HD13	11:K:11:ILE:HA	1.89	0.41
1:A:473:LEU:CD2	2:B:835:GLN:HB2	2.50	0.40
7:G:126:SER:HA	7:G:127:PRO:HA	1.94	0.40
14:N:-54:DC:H2''	14:N:-53:DT:C7	2.47	0.40
18:W:492:ASN:OD1	18:W:493:HIS:N	2.54	0.40
1:A:493:PRO:HG3	1:A:502:LEU:HD12	2.04	0.40
2:B:425:MET:O	2:B:429:ILE:HG13	2.21	0.40
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.55	0.40
16:T:23:DA:H1'	16:T:24:DA:H5'	2.04	0.40
1:A:498:THR:CG2	2:B:1146:PHE:HD1	2.34	0.40
1:A:1295:PRO:HD3	1:A:1301:TYR:CE1	2.55	0.40
2:B:285:PRO:HB2	9:I:11:ASN:HD22	1.86	0.40
3:C:259:LEU:HD13	11:K:91:CYS:HB2	2.03	0.40
8:H:76:LYS:HE3	8:H:76:LYS:HB3	1.93	0.40
7:G:95:SER:OG	7:G:98:GLY:O	2.22	0.40
12:L:33:CYS:SG	12:L:34:GLY:N	2.95	0.40
14:N:-22:DG:N2	16:T:23:DA:C2	2.90	0.40
17:V:29:CYS:HB2	17:V:38:LEU:HD12	2.03	0.40
2:B:875:GLU:OE2	2:B:915:THR:OG1	2.26	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%)	1354 (97%)	37 (3%)	1 (0%)	48	79
2	B	1154/1227 (94%)	1118 (97%)	36 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	261/304 (86%)	259 (99%)	2 (1%)	0	100	100
4	D	170/186 (91%)	166 (98%)	4 (2%)	0	100	100
5	E	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	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%)	1157 (98%)	22 (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
All	All	7841/10452 (75%)	7666 (98%)	174 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	960	VAL

5.3.2 Protein sidechains ⓘ

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%)	92	96
2	B	1018/1077 (94%)	1016 (100%)	2 (0%)	92	96
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	149/160 (93%)	149 (100%)	0	100	100
5	E	196/197 (100%)	194 (99%)	2 (1%)	73	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%)	58	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%)	92	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%)	86	92
24	v	325/369 (88%)	325 (100%)	0	100	100
25	x	190/354 (54%)	190 (100%)	0	100	100
All	All	7083/9259 (76%)	7073 (100%)	10 (0%)	92	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

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Mol	Chain	Res	Type
19	m	514	LYS
23	u	124	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
8	H	44	ASN
9	I	11	ASN
18	W	433	GLN
18	W	644	ASN
19	m	955	ASN
20	n	232	GLN
21	q	147	ASN
25	x	296	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	19/19 (100%)	7 (36%)	3 (15%)

All (7) RNA backbone outliers are listed below:

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

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	-7	U
15	P	-3	U
15	P	-2	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

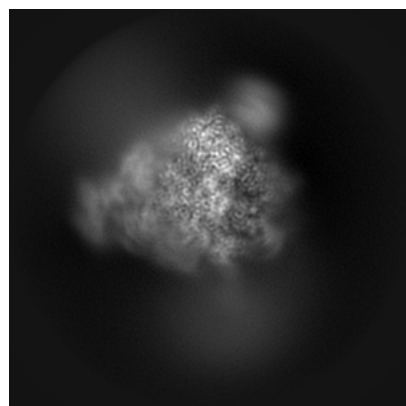
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33313. These allow visual inspection of the internal detail of the map and identification of artifacts.

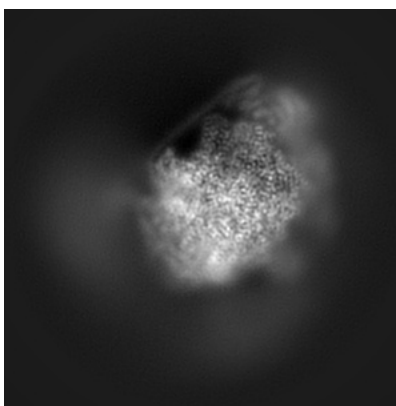
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

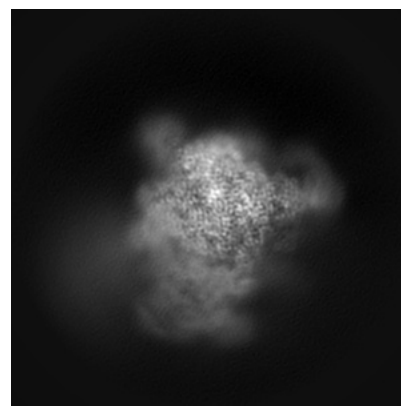
6.1.1 Primary map



X

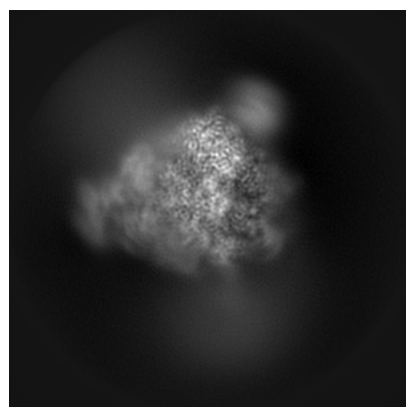


Y

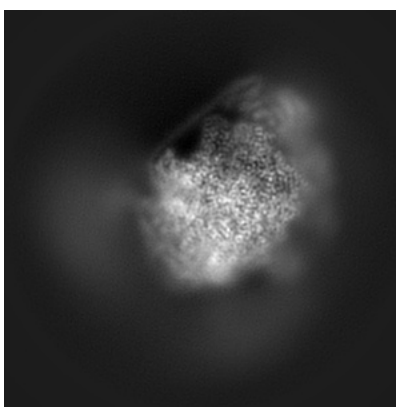


Z

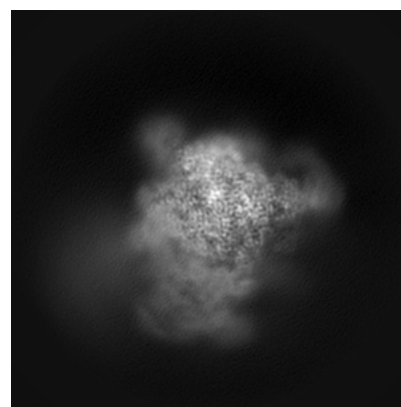
6.1.2 Raw map



X



Y

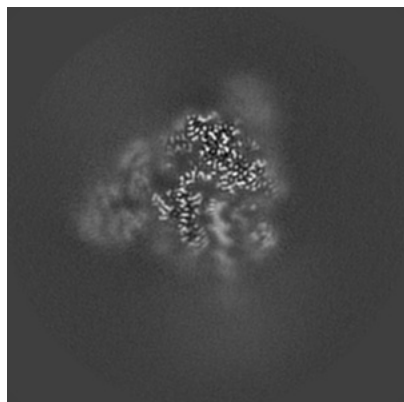


Z

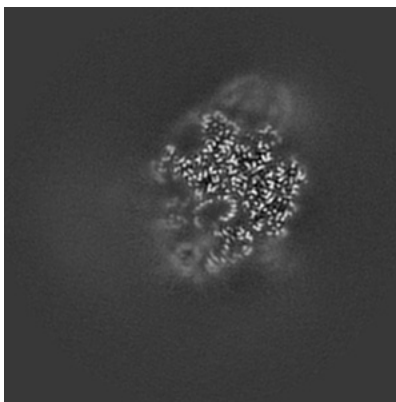
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

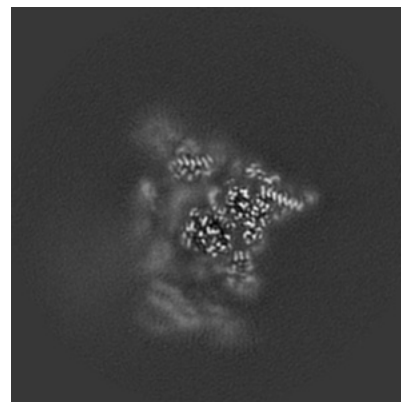
6.2.1 Primary map



X Index: 120

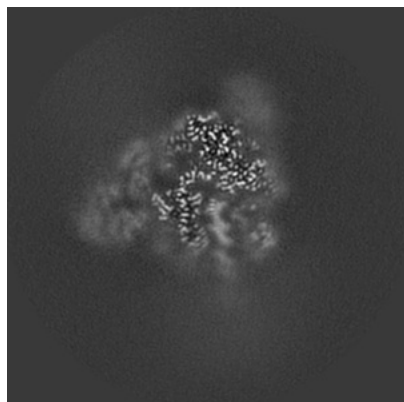


Y Index: 120

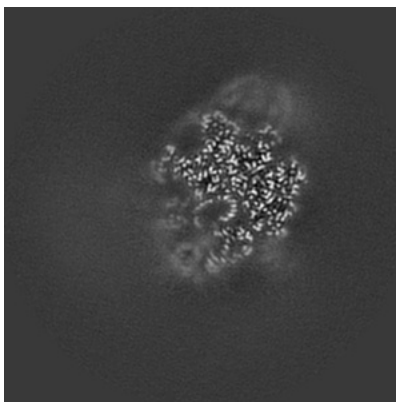


Z Index: 120

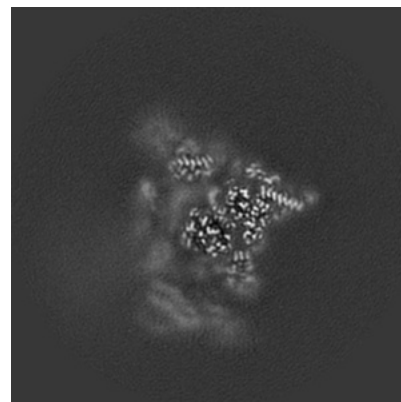
6.2.2 Raw map



X Index: 120



Y Index: 120

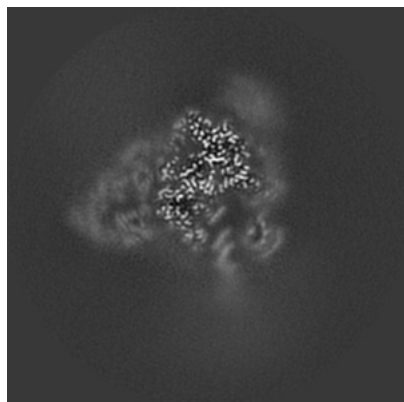


Z Index: 120

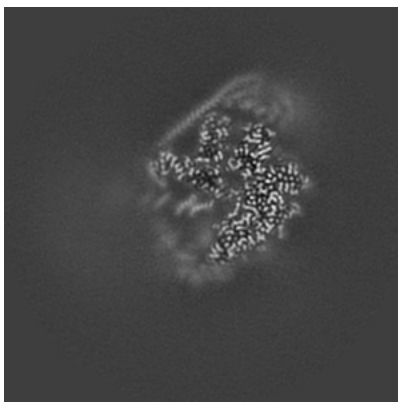
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

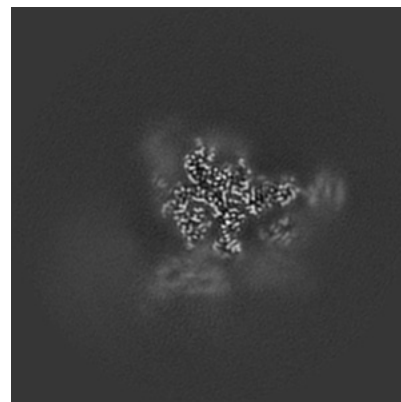
6.3.1 Primary map



X Index: 125

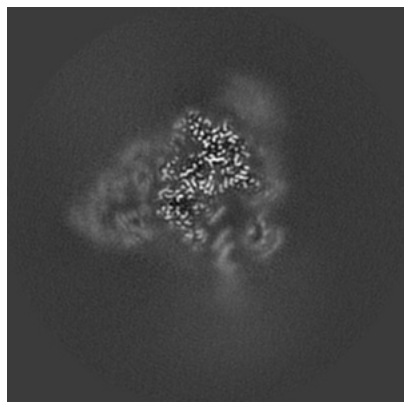


Y Index: 124

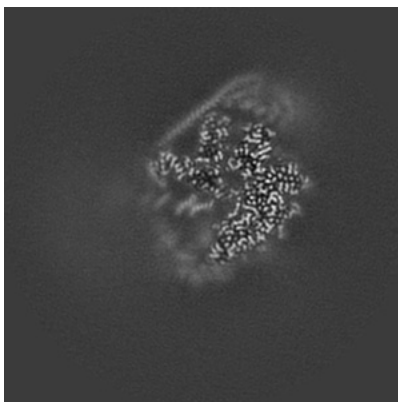


Z Index: 146

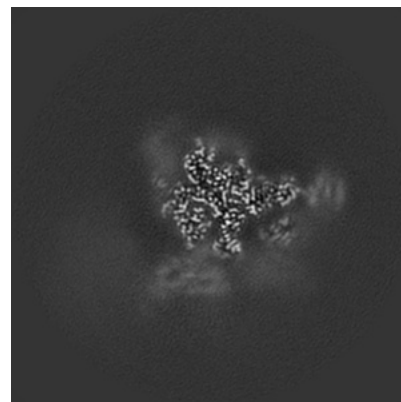
6.3.2 Raw map



X Index: 125



Y Index: 124

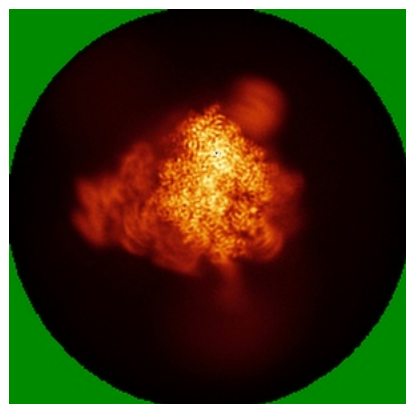


Z Index: 146

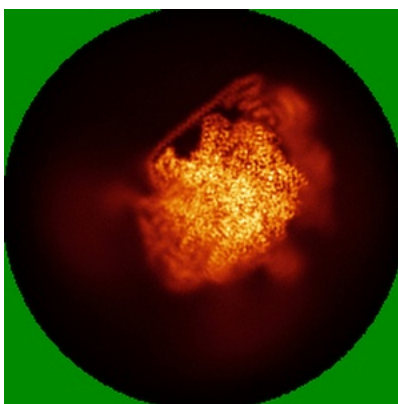
The images above show the largest variance slices of the map in three orthogonal directions.

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

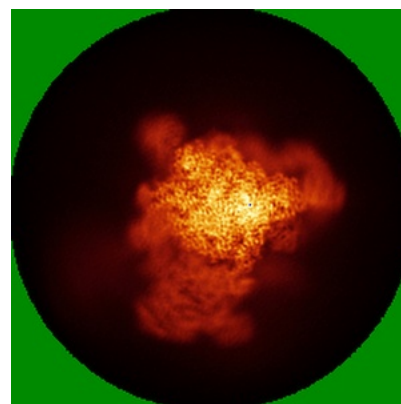
6.4.1 Primary map



X

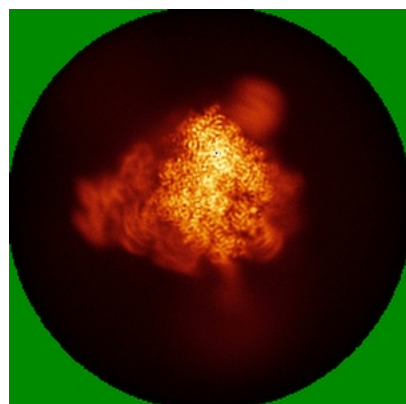


Y

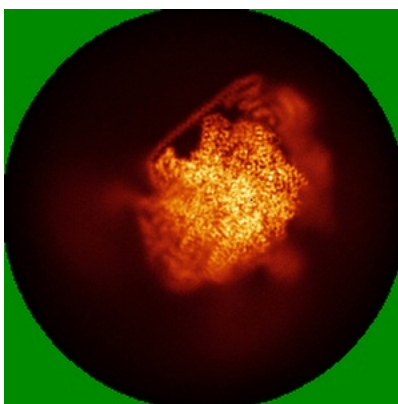


Z

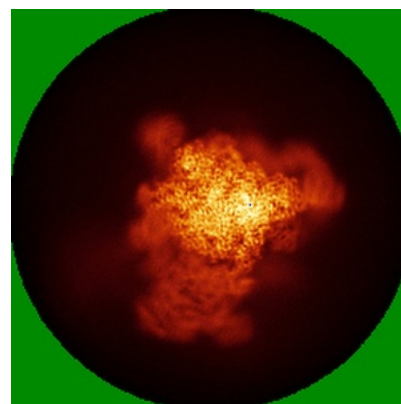
6.4.2 Raw map



X



Y

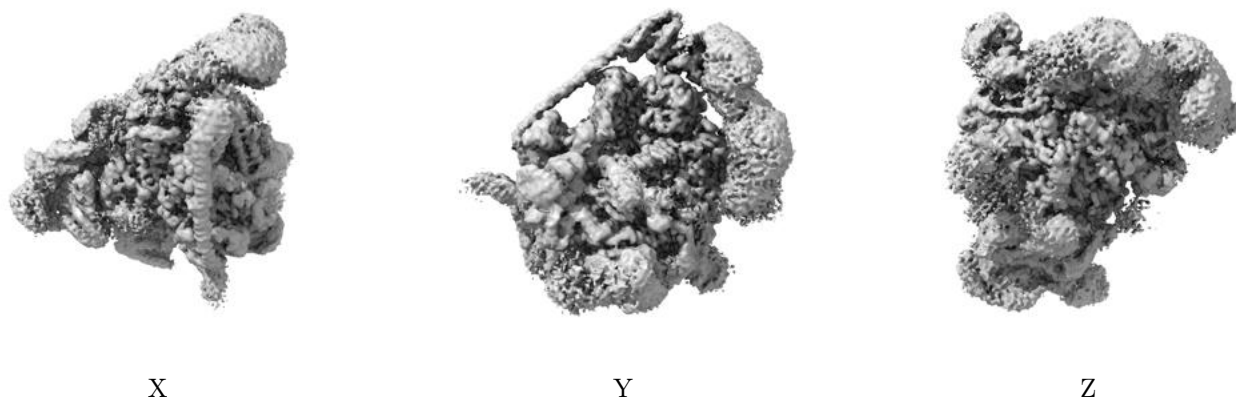


Z

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.

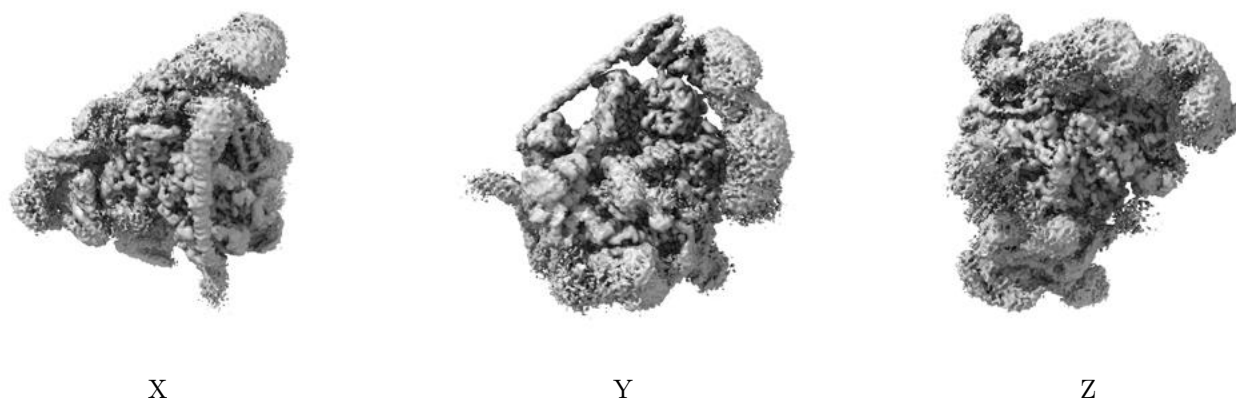
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

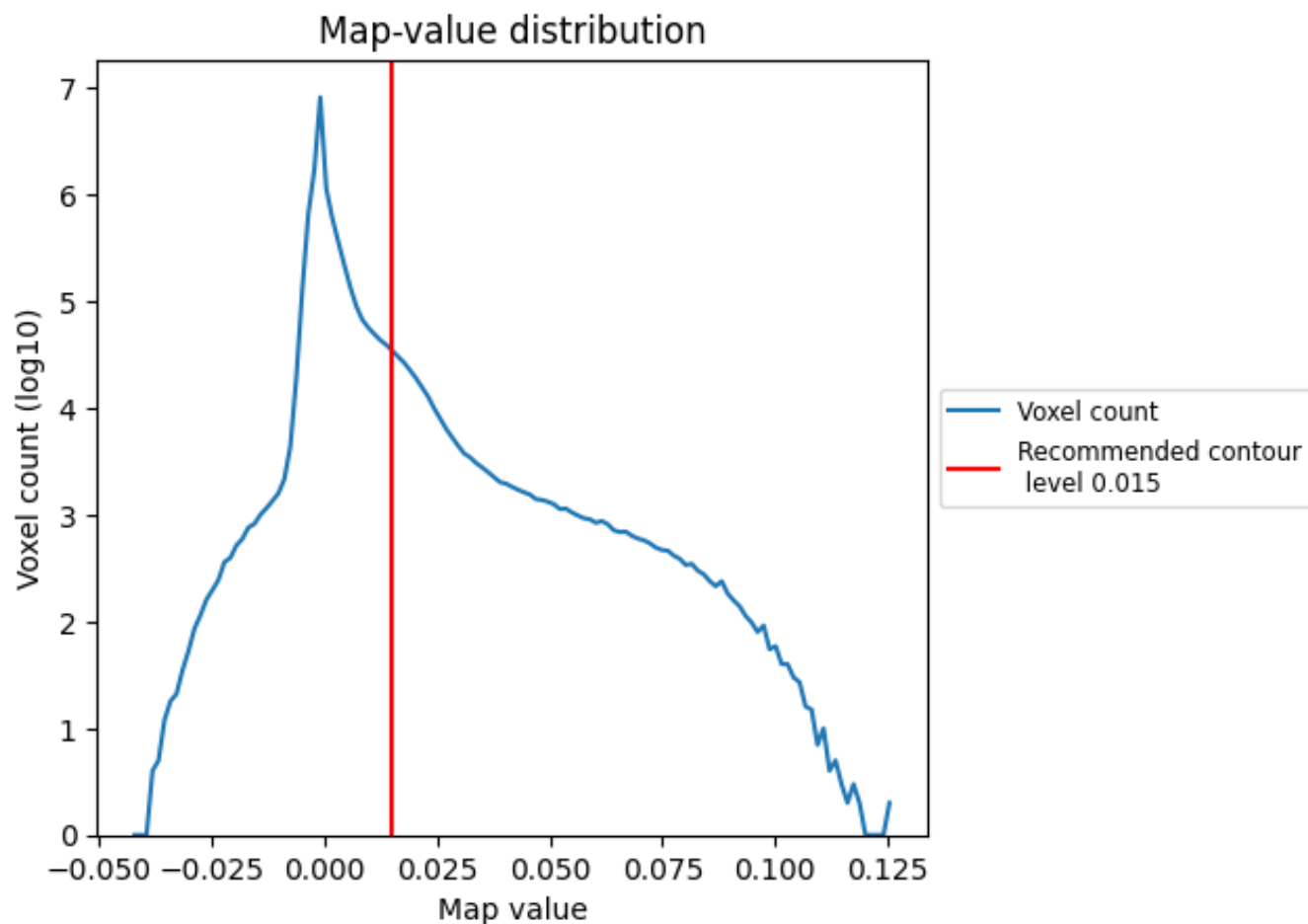
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

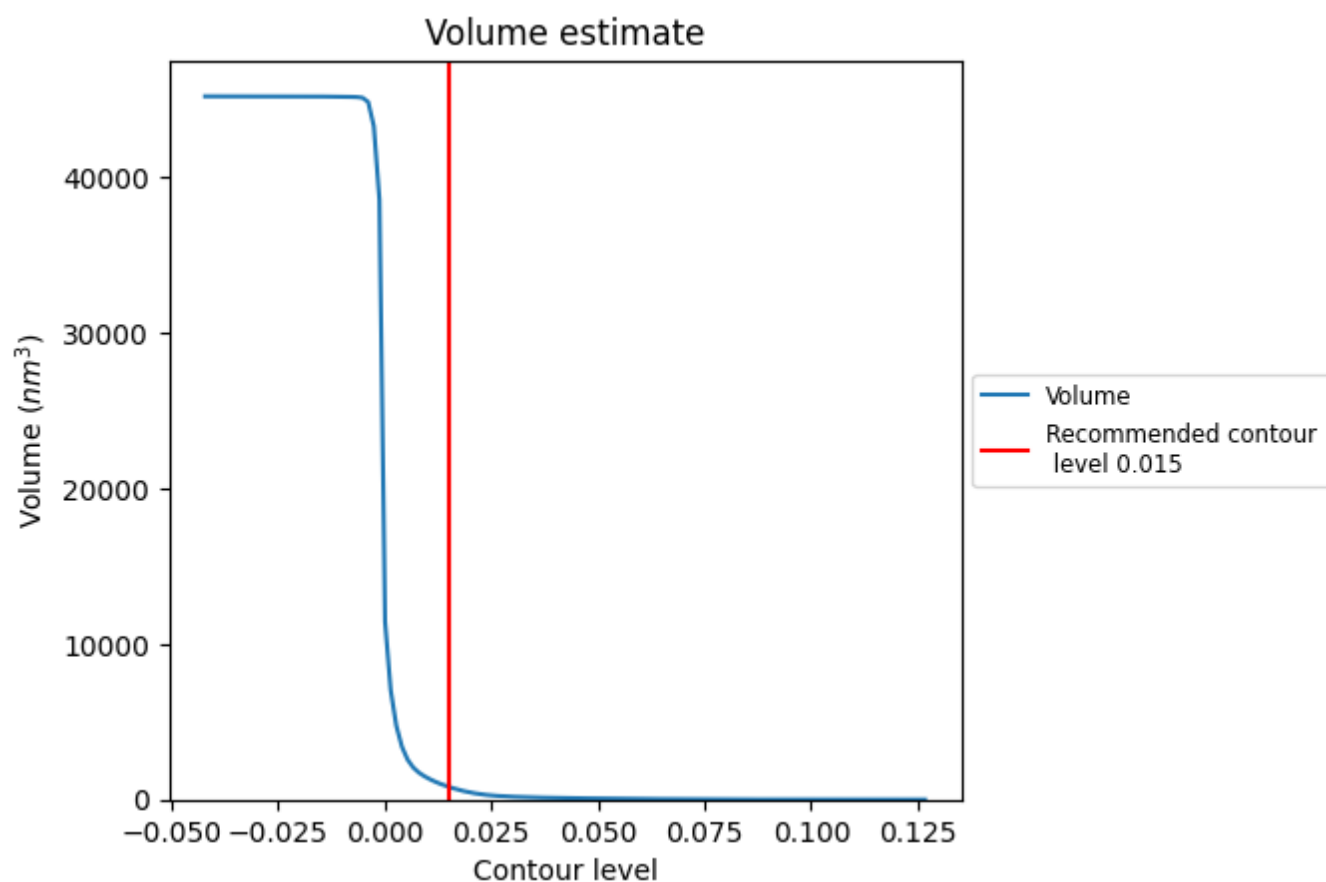
This section contains the results of statistical analysis of the map.

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.

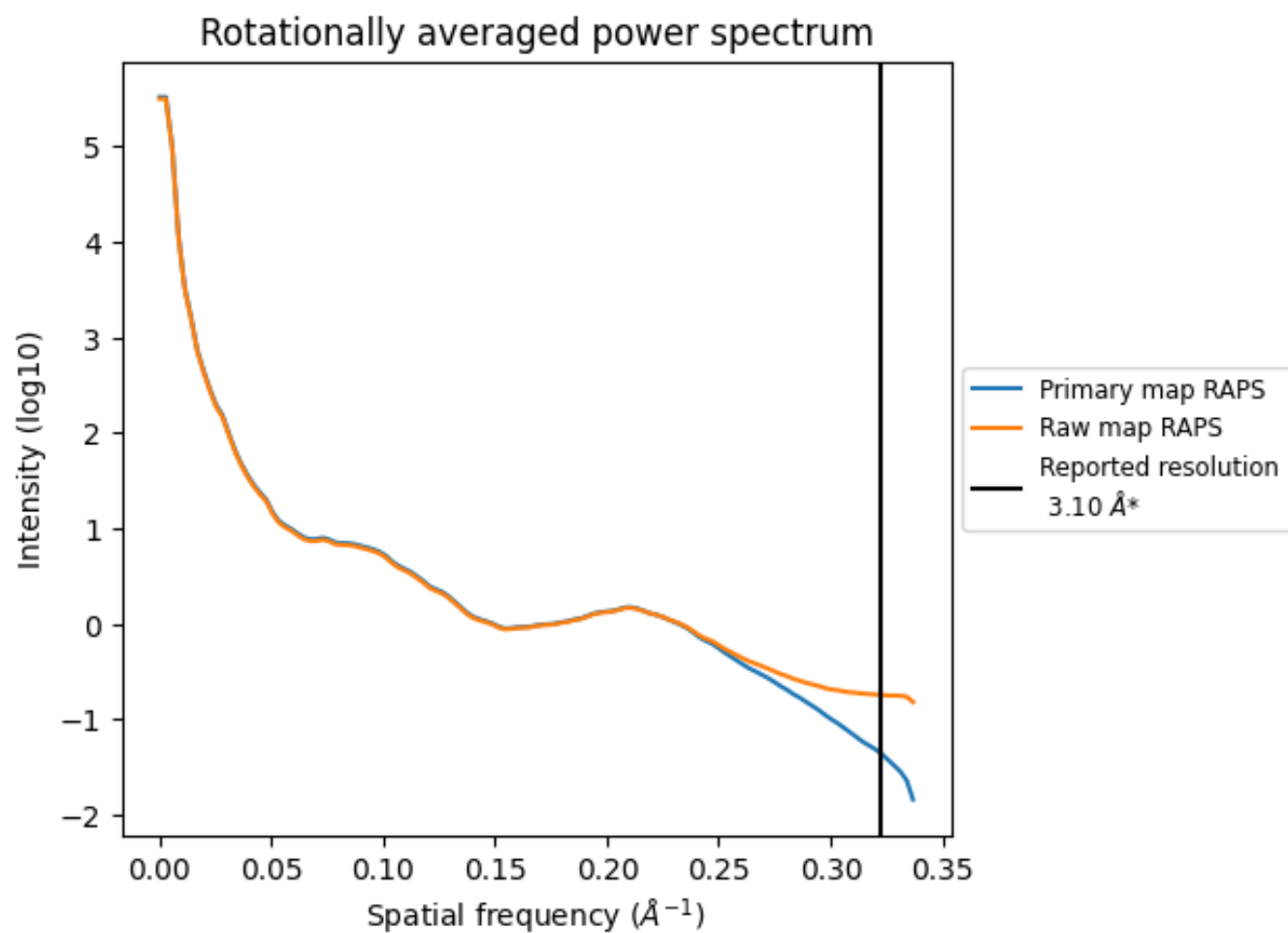
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 824 nm³; this corresponds to an approximate mass of 744 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 ⓘ

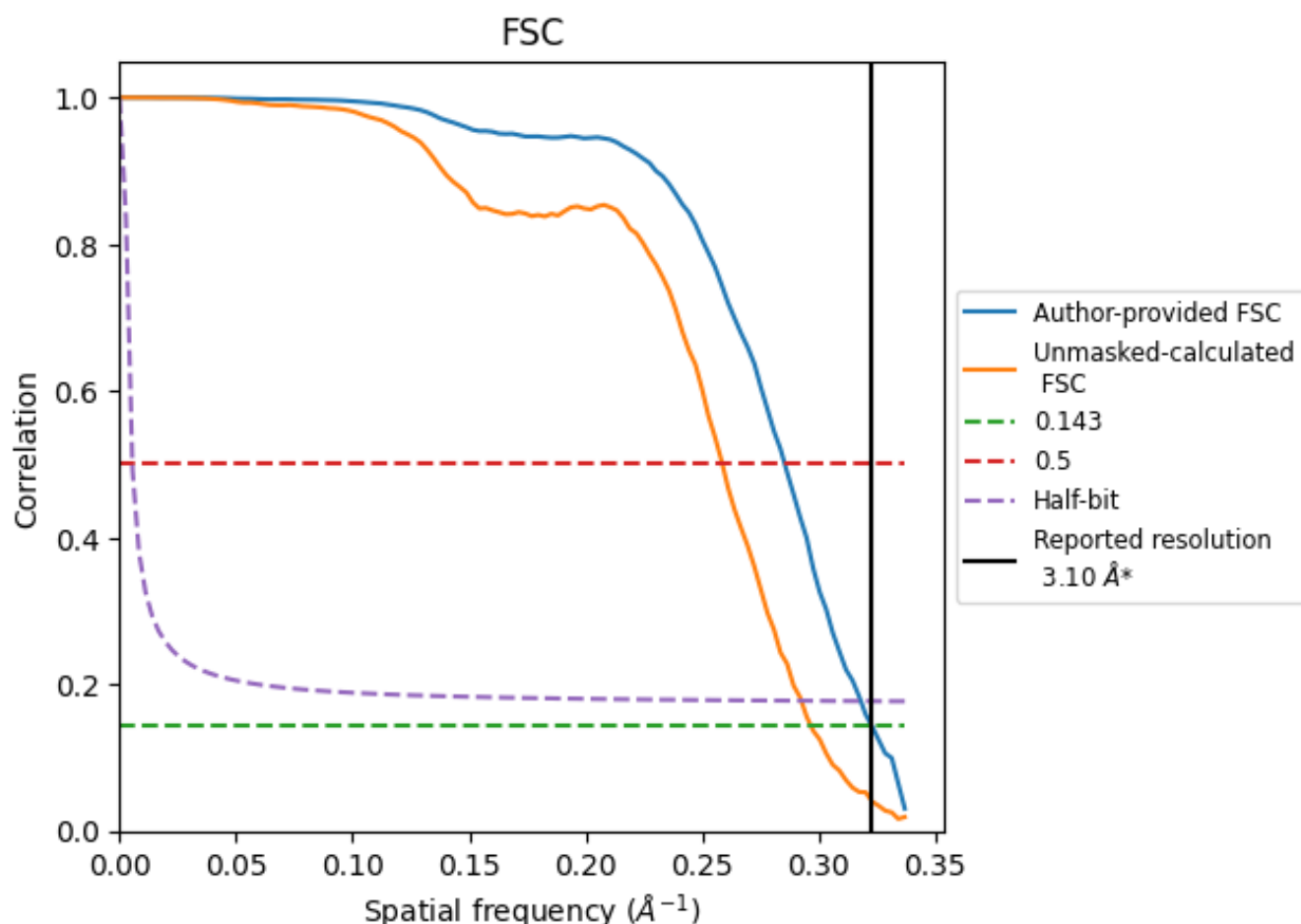


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

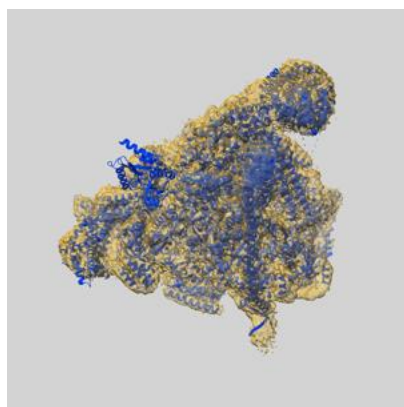
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.50	3.14
Unmasked-calculated*	3.37	3.87	3.42

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

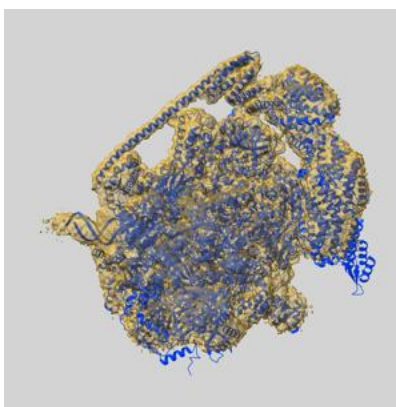
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33313 and PDB model 7XN7. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

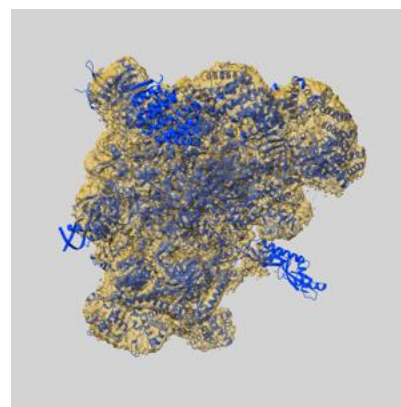
9.1 Map-model overlay [i](#)



X



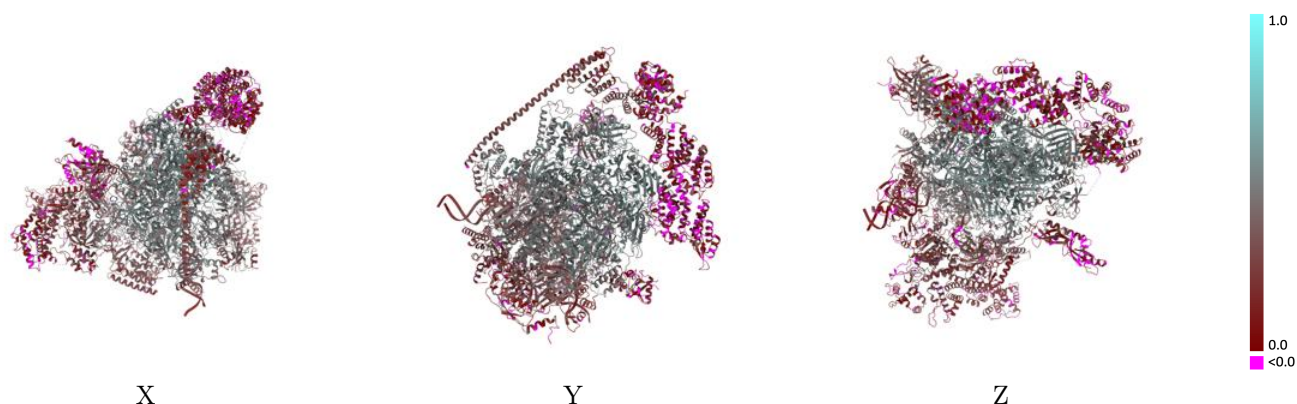
Y



Z

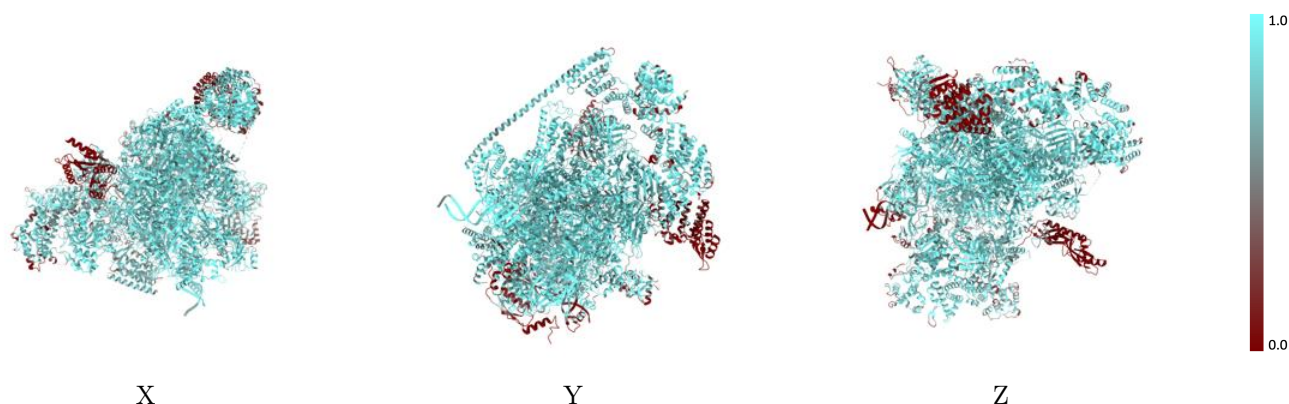
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



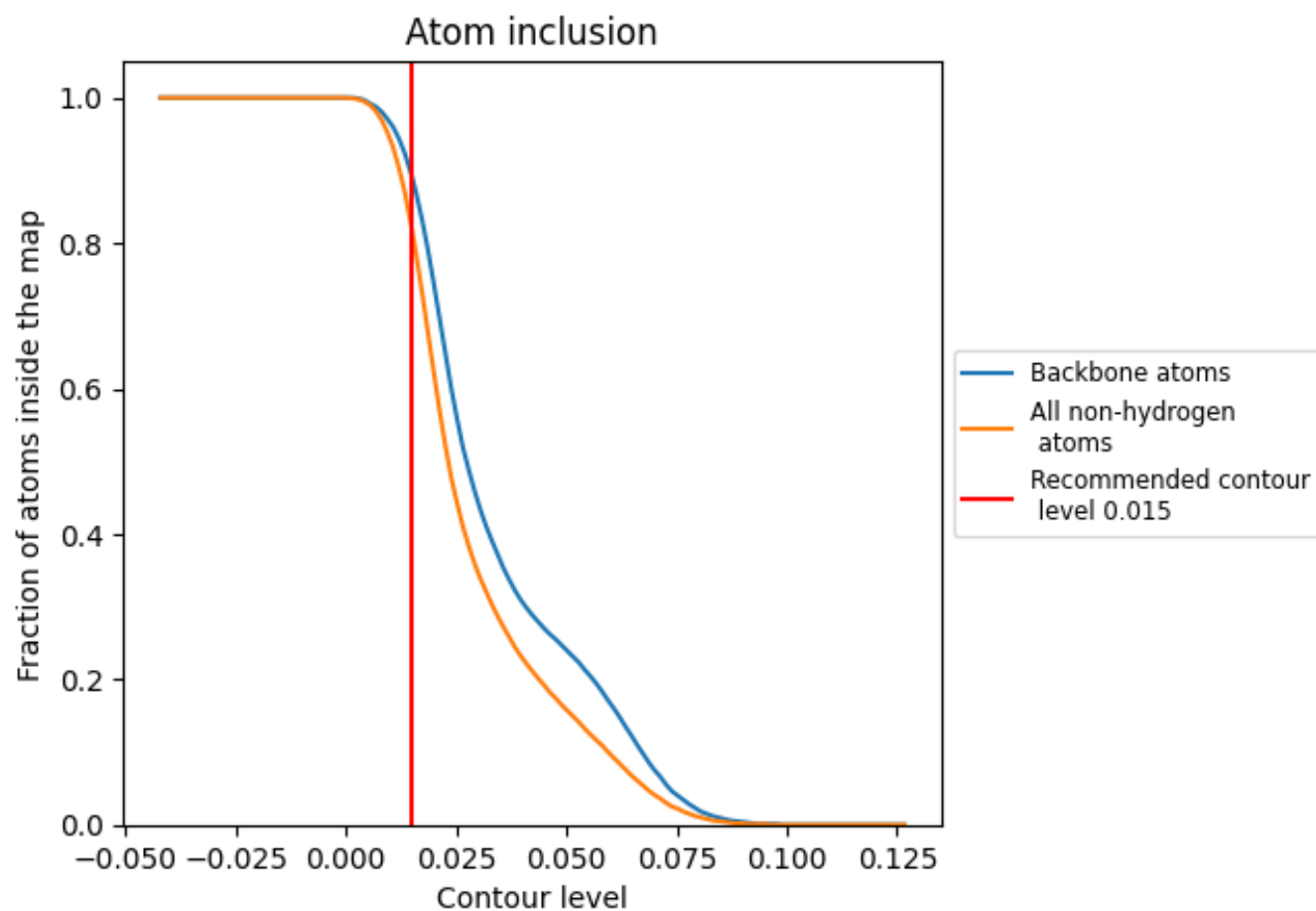
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.3380
A	 0.9470	 0.4890
B	 0.9460	 0.4960
C	 0.9470	 0.5170
D	 0.8800	 0.2810
E	 0.9620	 0.4750
F	 0.9740	 0.5280
G	 0.9110	 0.3780
H	 0.9480	 0.5050
I	 0.8610	 0.3750
J	 0.9560	 0.5230
K	 0.9630	 0.5200
L	 0.9630	 0.4870
M	 0.7880	 0.2360
N	 0.8000	 0.2410
P	 0.9410	 0.3480
T	 0.8140	 0.2970
V	 0.9060	 0.1830
W	 0.7800	 0.2680
m	 0.6700	 0.1780
n	 0.8020	 0.2350
q	 0.6820	 0.1390
r	 0.6800	 0.2310
u	 0.6610	 0.2960
v	 0.5700	 0.2150
x	 0.7940	 0.3550

