



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:55 PM UTC

PDB ID : 7XT7 / pdb_00007xt7
EMDB ID : EMD-33441
Title : RNA polymerase II elongation complex transcribing a nucleosome (EC49B)
Authors : Ehara, H.; Kujirai, T.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on : 2022-05-16
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

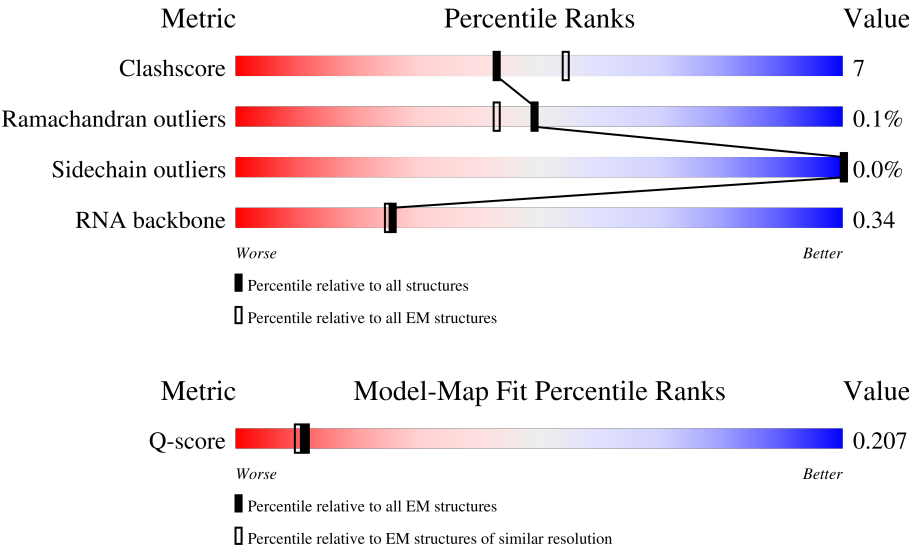
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	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	5410 (3.70 - 4.70)

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	19	
16	T	198	
17	V	108	
18	W	911	
19	m	1503	
20	n	417	
21	q	1084	
22	r	544	
23	u	459	
24	v	396	
25	x	395	
26	a	139	
26	e	139	
27	b	106	

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Mol	Chain	Length	Quality of chain
27	f	106	
28	c	133	
28	g	133	
29	d	129	
29	h	129	
30	j	1008	
31	k	531	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 82079 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
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	115	Total	C	N	O	P	0	0
			2377	1124	445	693	115		

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 40 discrepancies between the modelled and reference sequences:

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

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

unit.

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

There are 30 discrepancies between the modelled and reference sequences:

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

- Molecule 23 is a protein called Leo1.

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

There are 30 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 30 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	92	Total	C	N	O	S	0	0
			746	471	142	131	2		
26	e	97	Total	C	N	O	S	0	0
			795	501	155	137	2		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 27 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	81	Total	C	N	O	S	0	0
			646	407	126	112	1		
27	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 28 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	96	Total	C	N	O	0	0
			743	466	146	131		
28	g	98	Total	C	N	O	0	0
			757	475	149	133		

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	92	Total	C	N	O	S	0	0
			718	453	127	136	2		
29	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 30 is a protein called FACT complex subunit.

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	k	429	Total	C	N	O	S	0	0
			3502	2215	613	664	10		

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

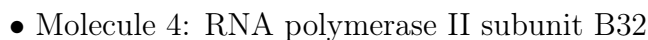
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

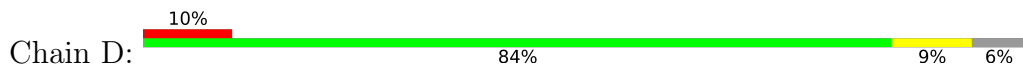
Chain B:

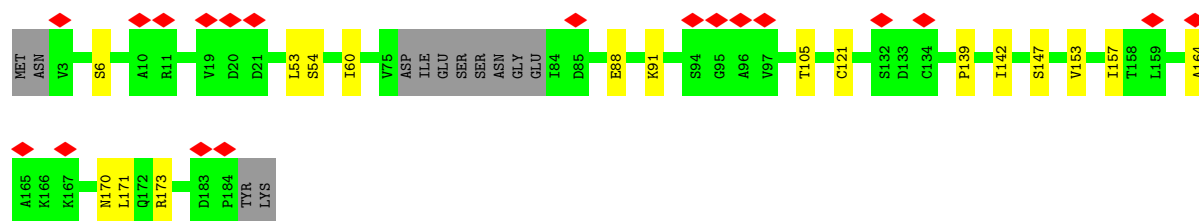


Chain C:



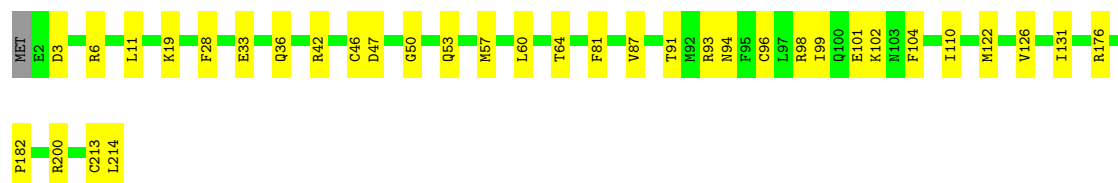
Chain D:





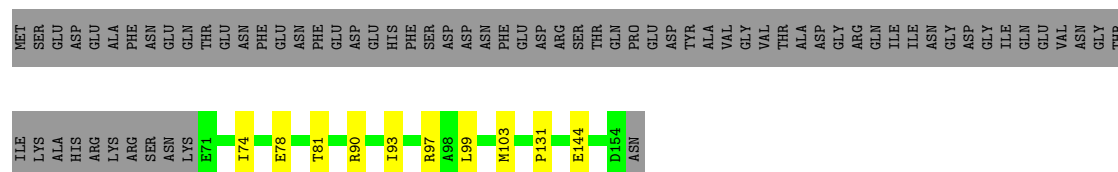
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 83% 16%



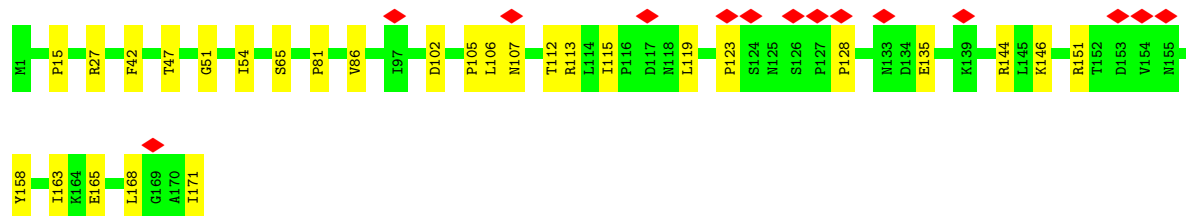
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

Chain F: 48% 6% 46%



- Molecule 7: RNA polymerase II subunit

Chain G: 8% 84% 16%



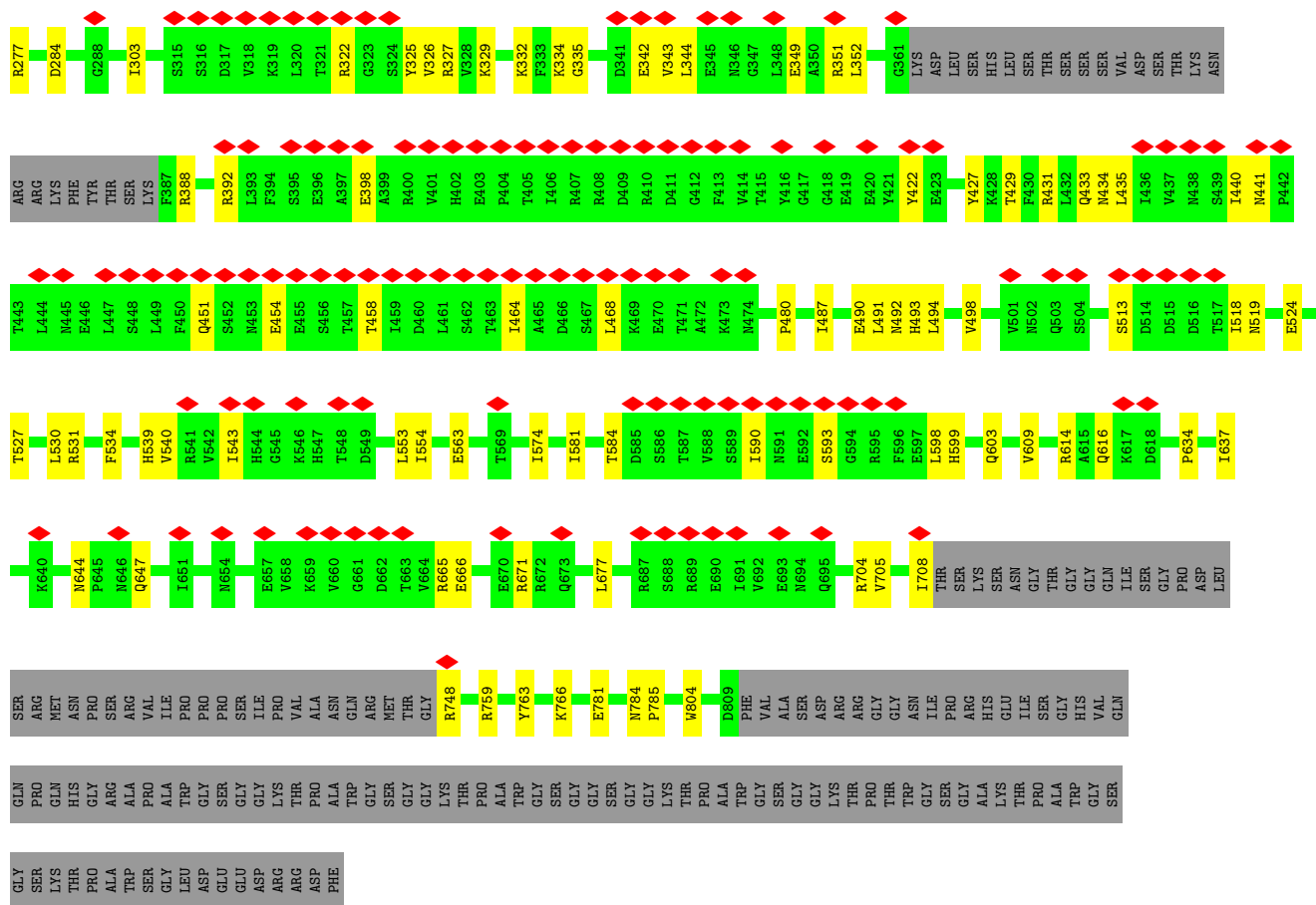
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 79% 13% 8%

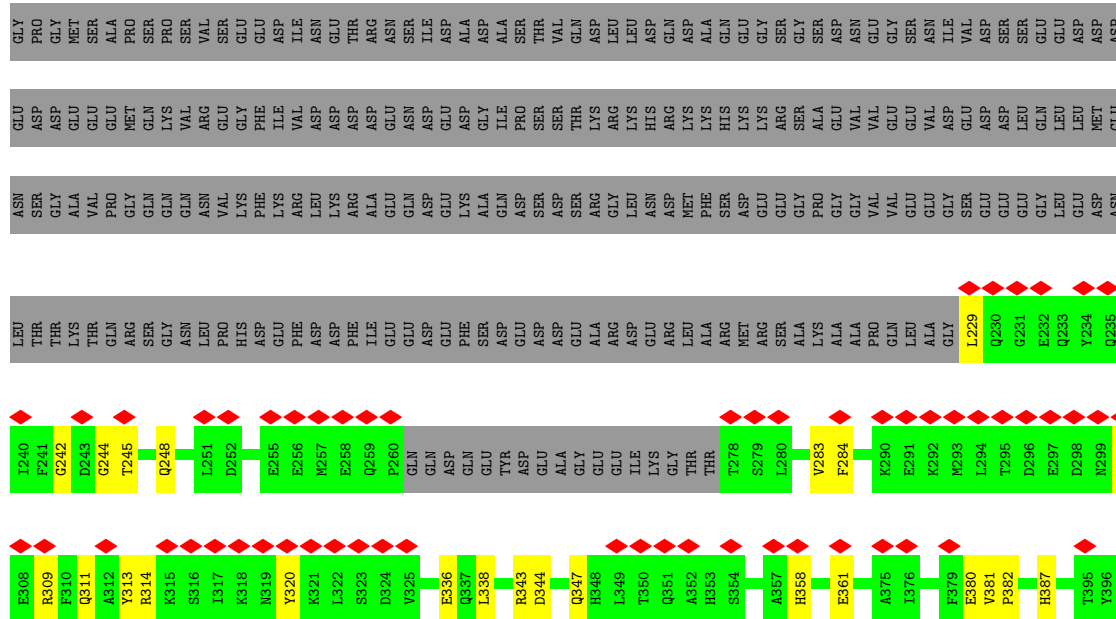


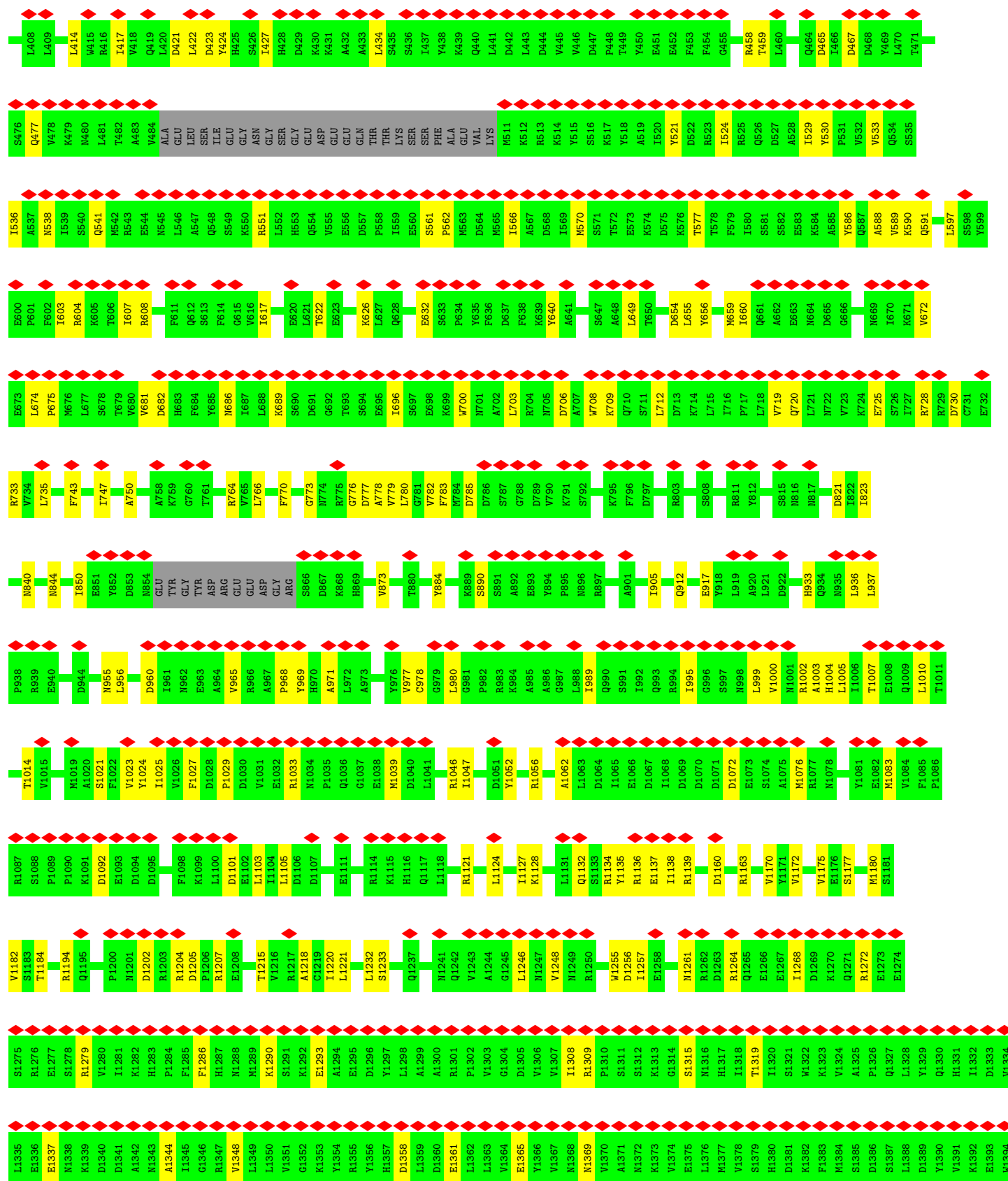
- Molecule 9: DNA-directed RNA polymerase subunit

Chain I: 80% 17% 3%

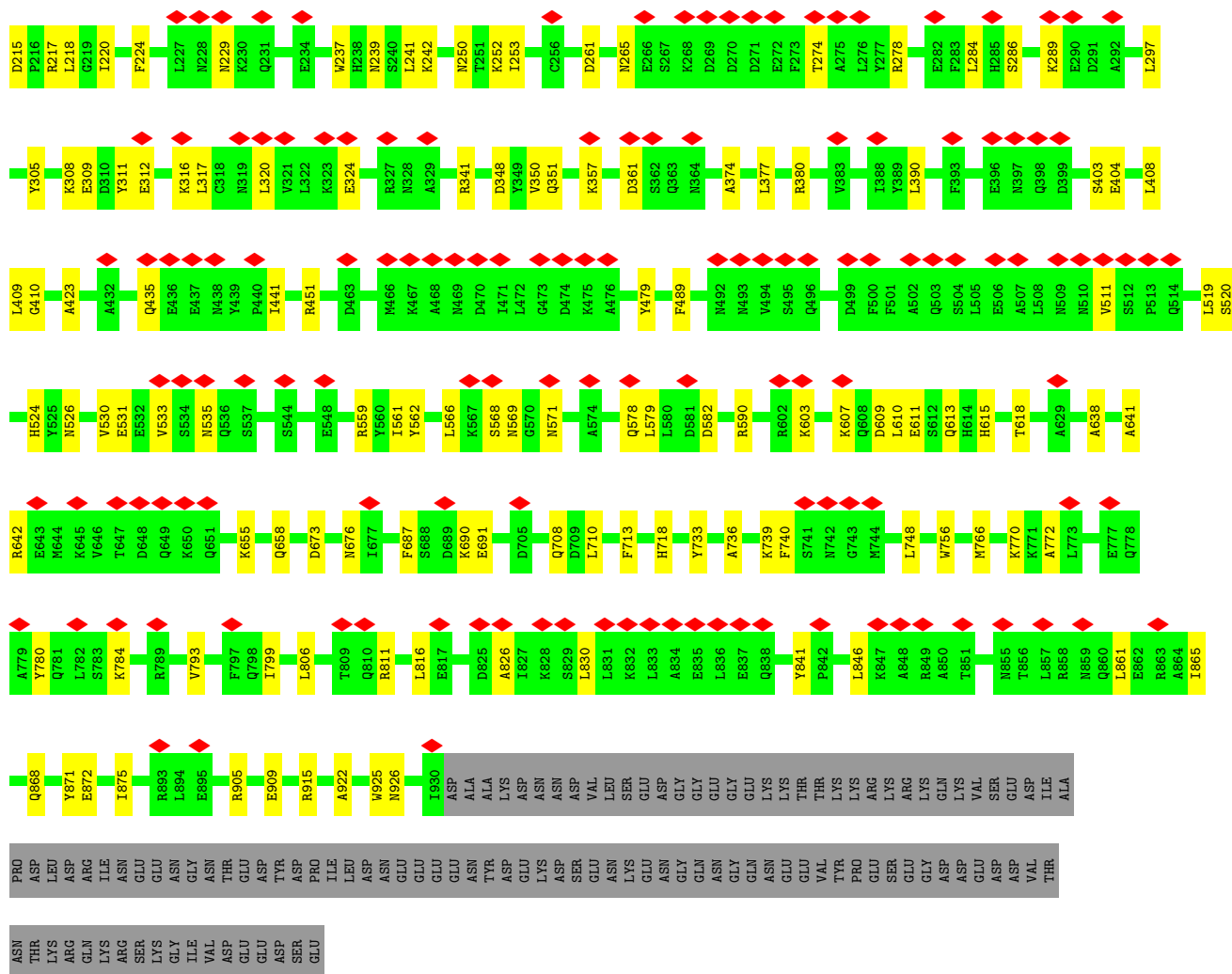


• Molecule 19: Transcription elongation factor Spt6

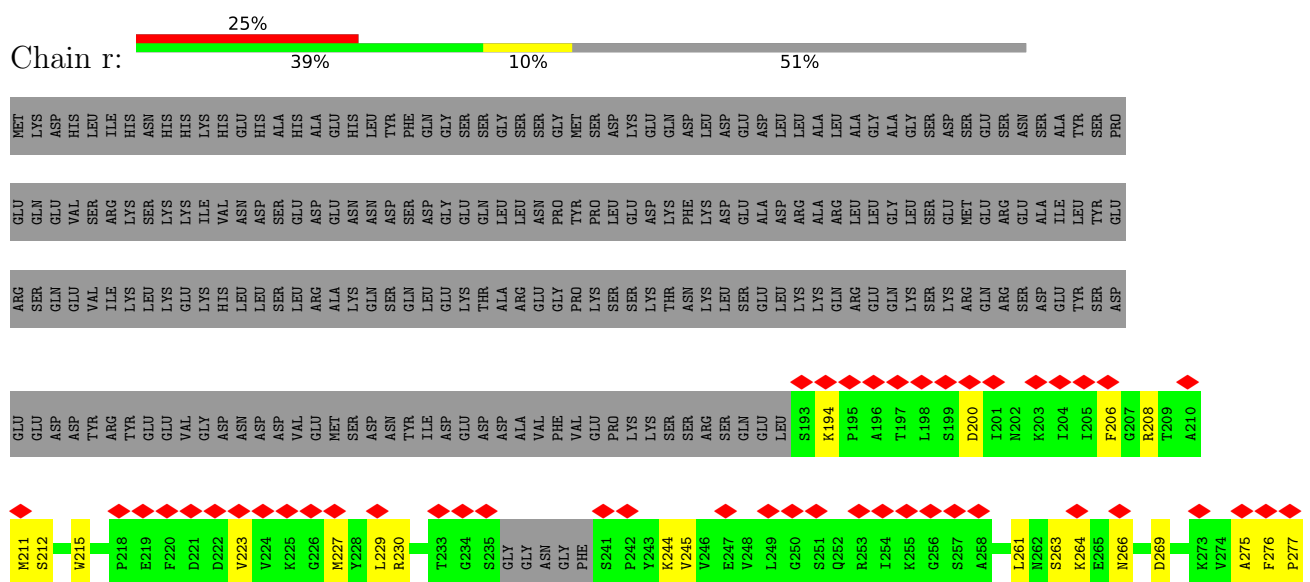


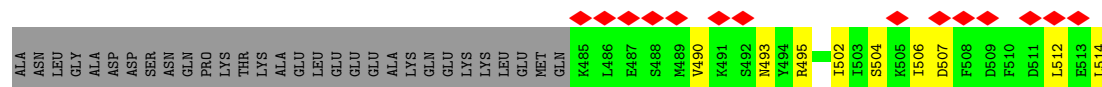
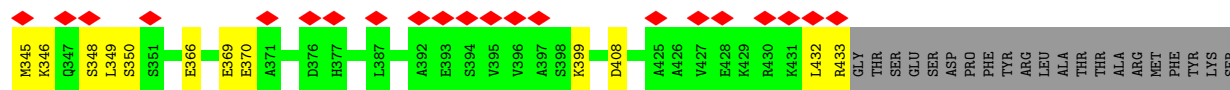
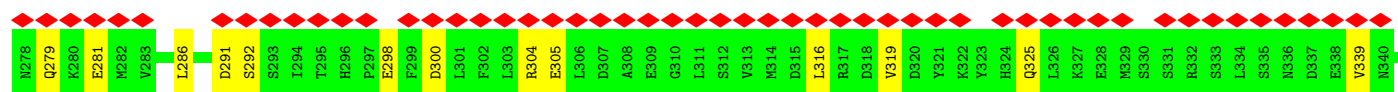




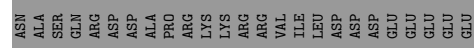
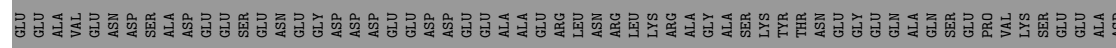
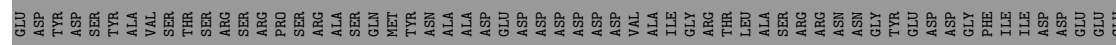
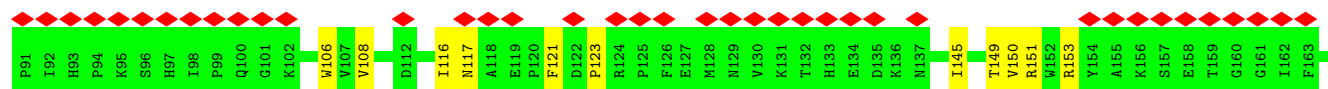
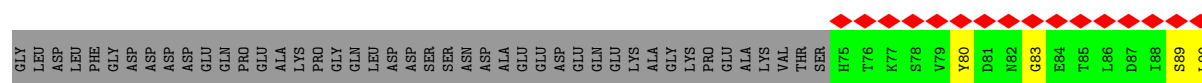
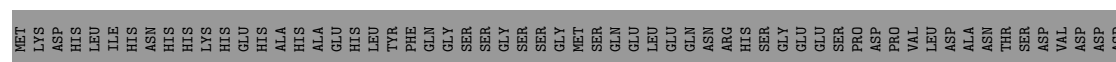
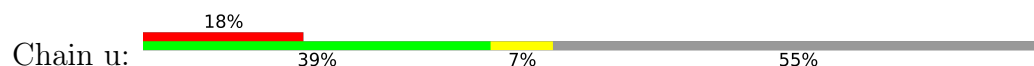


• Molecule 22: RNAPII-associated chromatin remodeling Paf1 complex subunit

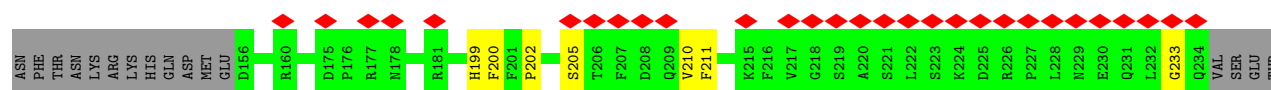
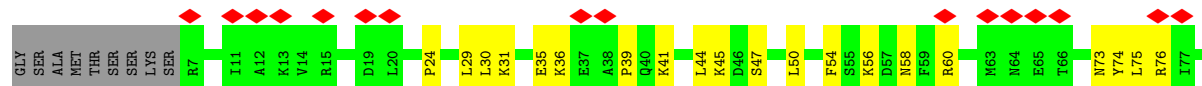


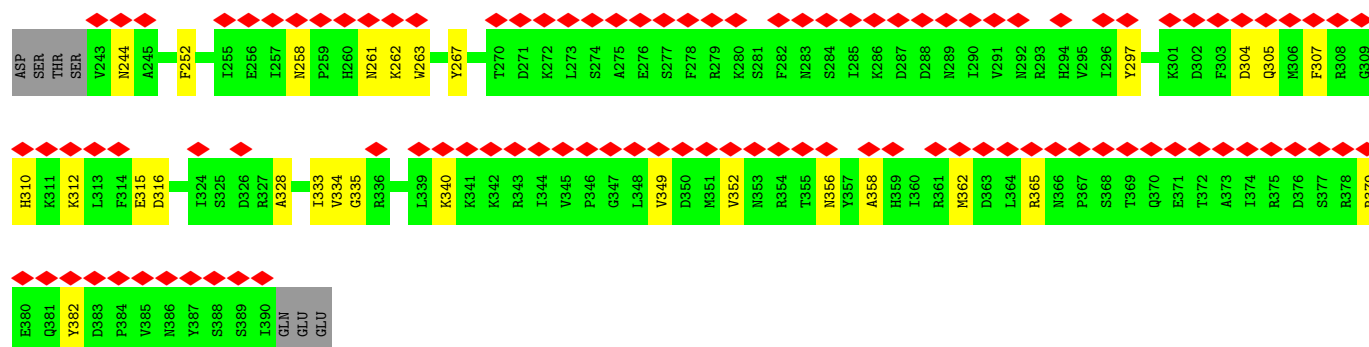


• Molecule 23: Leo1



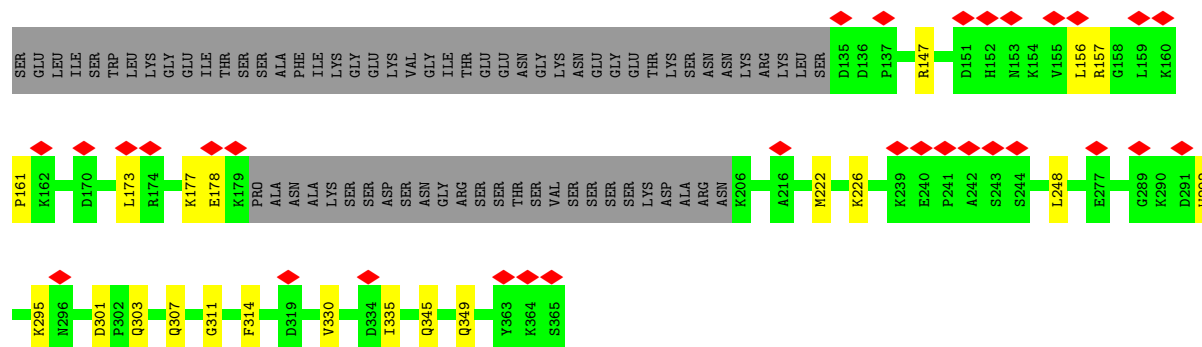
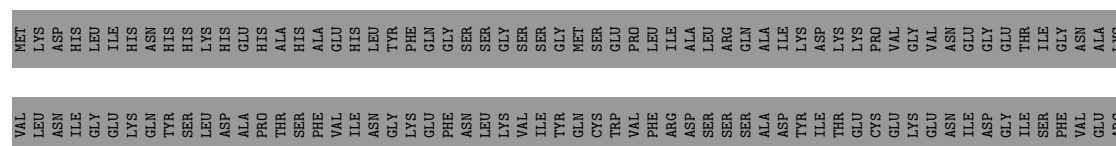
• Molecule 24: RNAP II-associated protein





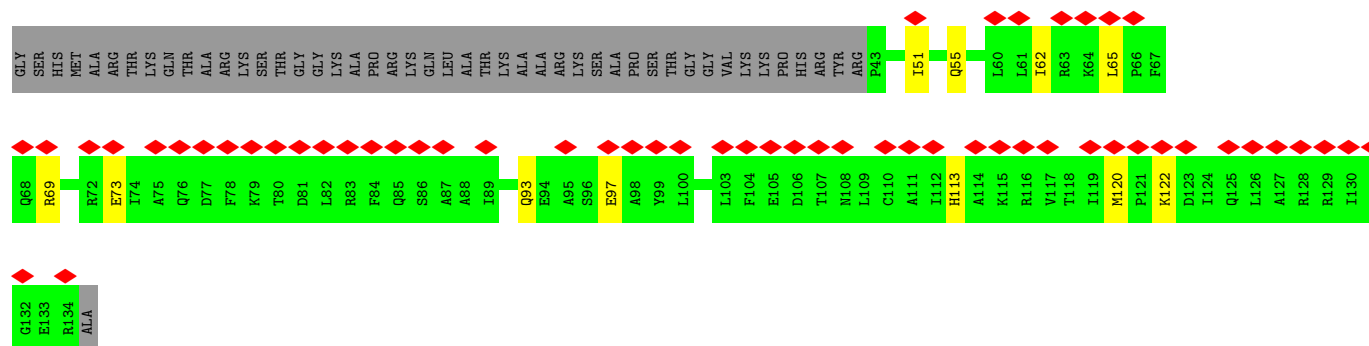
- Molecule 25: Constituent of Paf1 complex with RNA polymerase II, Paf1p, Hpr1p, Ctr9, Leo1, Rtf1 and Ccr4p

Chain x: 8% 47% 5% 48%



- Molecule 26: Histone H3.3

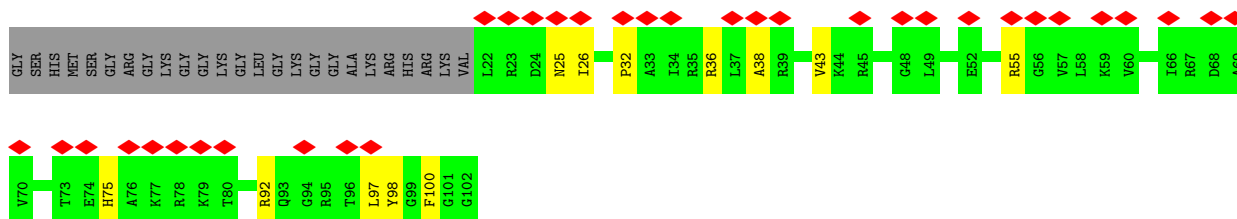
Chain a: 41% 58% 8% 34%



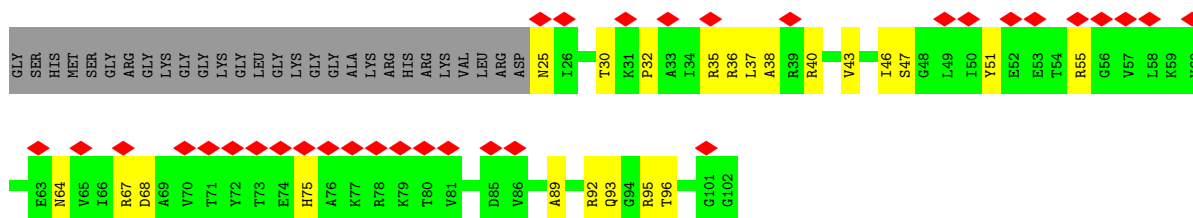
- Molecule 26: Histone H3.3

Chain e: 42% 60% 9% 30%

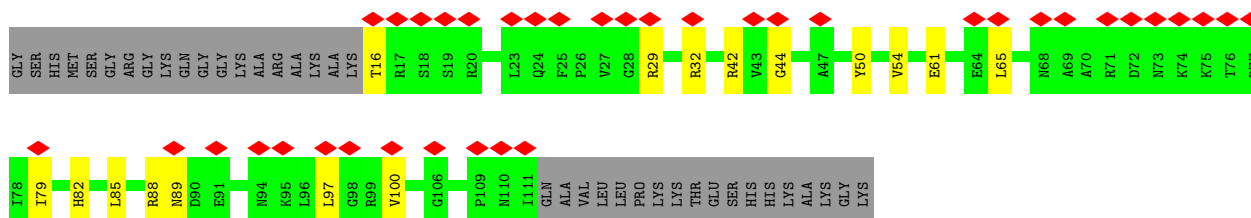
- Molecule 27: Histone H4



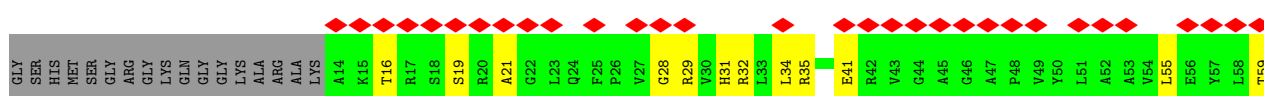
- Molecule 27: Histone H4

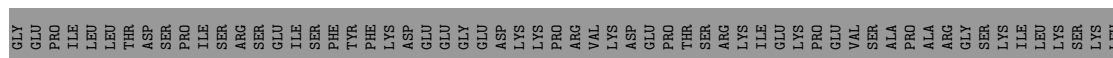


- Molecule 28: Histone H2A type 1-B/E



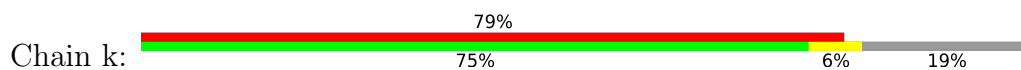
- Molecule 28: Histone H2A type 1-B/E





V959	S960	D961	E962	D963	P964	E965	D966	E967	D968	V969	S970	E971	E972	Y973	S974	A975	A976	E977	D978	GLY	SER	ASP	PHE	SER	GLU	GLU	ASP	ASP	SER	GLU	GLY	SER	ILE	ALA	E930	F931	F932	E933	N934	G935	G936	K877	D878	F879	S880	K881	P882	V883	V884	H885	L886	N887	T888	I889	P890	I891	E892	M893	L894	E895	P896	V897	K898
Q899	W900	L901	T902	D903	V904	I906	P907	Y908	S909	E910	G911	A912	V913	N914	L915	N916	N917	G918	T919	I920	M921	K922	T923	I924	Q925	A926	D927	P928	Y929	E930	F931	F932	E933	N934	G935	G936	W937	S938	F939	L940	G941	G942	G943	E944	S945	D946	D947	E948	E949	S950	E951	E952	E953	E954	S955	E956	F957	Q958					
C838	L839	L840	Q841	L842	L843	D844	T845	P846	F847	L848	W849	L852	E853	E854	L855	E856	V857	A858	H859	L860	E861	R862	V863	Q864	PHE	GLY	LEU	LYS	N869	F870	D871	L872	V873	F874	V875	P876	K877	D878	F879	S880	K881	P882	V883	V884	H885	L886	N887	T888	I889	P890	I891	E892	M893	L894	E895	P896	V897	K898					
E779	Q780	E781	Q782	E783	E784	R785	R786	R787	K788	A789	L790	L791	D792	K793	E794	F795	R796	R797	F798	A799	E800	E801	I802	S803	E804	A805	S806	N807	G808	L809	L810	D811	L812	E813	T814	P815	F816	R817	E818	L819	G820	F821	T822	G823	V824	P825	F826	R827	S828	S829	V830	L831	C832	L833	P834	T835	R836	D837					
L718	F719	F720	Q721	F722	C723	K724	E725	E726	L727	M728	V729	I730	I731	H732	C733	H734	L735	K736	I737	F738	L739	M740	I741	G742	K743	K744	K745	T746	F747	D748	V749	Q750	F751	Y752	R753	E754	V755	S756	D757	VAL	THR	VAL	ASP	GLU	THR	GLY	ASN	LYS	LYS	ARG	ARG	T77R	ARG	T77R	GLY	ASP	GLU	ASP	GLU				
Q658	A659	Q660	L661	V662	E663	F664	K665	G666	P667	P668	K669	K670	L671	E672	N673	V674	F675	V676	R677	P678	A679	P680	D681	S682	K683	R684	V685	T686	G687	T688	L689	F690	I691	H692	Q693	N694	G695	I696	R697	Y698	Q699	S700	P701	V702	A642	R703	S704	D705	H706	R707	V708	D709	I710	L711	F712	S713	N714	I715	K716	H717			
S598	V599	K600	K601	T602	E603	L604	P605	Y606	E607	D608	G609	D610	D611	K612	E613	F614	V615	R616	S617	L618	T619	F620	D621	S622	T623	N624	K625	E626	R627	M628	S629	E630	V631	F632	K633	A634	I635	T636	E637	L638	K639	K640	T641	A642	H643	K644	R645	D646	Q647	E648	R649	K650	T651	M652	E653	D654	V655	V656	A657				
I538	P539	Q540	K541	V542	K543	N544	L545	E546	I547	E548	D549	D550	P551	K552	A553	Q554	T555	I556	I557	L558	P559	I560	C561	G562	R563	P564	V565	P566	F567	H568	I569	N570	S571	K513	K572	K573	N574	G575	S576	K577	N578	E579	E580	G581	D582	Y583	M584	Y585	I586	R587	L588	N589	F590	N591	S592	P593	G594	M595	G596	S597			
ARG	ASN	GLU	THR	T482	N483	T484	E485	E486	E487	K488	E489	R490	L491	R492	K493	E494	I495	Q496	K497	Q498	L499	H500	E501	K502	I503	Q504	K505	E506	G507	L508	A509	R510	F511	N512	K513	S514	D515	A516	Q517	D518	G519	N520	E521	N522	H523	A524	V525	F526	K527	R528	Y529	E530	Y532	V533	R534	E535	S536	Q537					

• Molecule 31: FACT complex subunit POB3



GLY	PRO	GLY	M1	S2	T3	V4	D5	F6	D7	T8	I9	F10	L11	M12	Q13	S14	K15	A16	P17	G18	R19	F20	R21	I22	T23	S24	S25	G26	L27	G28	W29	K30	P31	S32	S33	Q34	V35	P36	T37	K38	G39	K40	T41	D42	P43	F44	L45	L46	P47	S48	G49	D50	I51	L52	S53	V54	S55	W56	S57
R58	G59	F60	R61	G62	W63	E64	L65	R66	V67	F68	T69	R70	M71	D72	K73	V74	I75	M76	L77	D78	G79	F80	E81	Q82	Q83	D84	F85	Q86	L87	L88	K89	N90	E91	I92	Q93	A94	T95	F96	N97	V98	N99	L100	E101	H102	K103	E104	H105	S106	L107	R108	G109	W110	M111	W112	G113	K114	T115	Q116	L117
T118	R119	A120	E121	L122	V123	F124	N125	V126	N127	N128	R129	P130	A131	W132	E133	I134	P135	Y136	S137	E138	I139	S140	F141	S142	N143	L144	L145	L146	L147	H148	E149	I150	S151	M152	E153	L154	N155	P156	K157	T158	V159	D160	E161	N162	H163	Y164	E165	T166	L167	G168	D169	E170	L171	V172	E173	V174	R175	L176	Y177
V178	P179	G180	Q181	ILE	ASP	LYS	ASP	GLU	SER	THR	GLY	GLN	ASP	THR	THR	GLU	ALA	LYS	SER	K201	S202	Q203	L204	F205	Y206	E207	Q208	L209	K210	D211	K212	A213	D214	F215	D216	T217	T218	S219	E220	A221	I222	V223	S224	F225	E226	D227	I228	L229	T232	P233	R234	G235	R236	F237	E238				

SER	I239	Q299	Q359	V419	SER
ALA	S240	F300	H360	Q420	ALA
GLU	M241	D301	M361	F421	GLY
ASP	Y242	R302	Q362	S422	ASP
GLU	A243	N303	P363	G423	GLU
SER	N244	E304	G364	G424	SER
VAL	N245	E305	V365	S425	VAL
ASP	L246	L306	N366	H426	ASP
GLU	R247	E307	C367	T427	GLU
ASP	L248	V308	S368	F428	ASP
PHE	R249	E309	L369	A429	PHE
ASN	G250	L310	K370	N430	ASN
ALA	Q251	N311	A371	I431	ALA
GLY	S252	L312	S372	M432	GLY
SER	Y253	S313	E373	K433	SER
ASP	D254	D314	G374	D434	ASP
ASP	Y255	E315	Q375	E435	VAL
VAL	K256	E316	I376	Q436	ALA
ALA	I257	Y317	Y377	Q437	ALA
GLU	Q258	K318	L378	K438	GLU
GLU	N259	L379	L379	P438	GLU
GLU	K260	S319	D380	I439	TYR
GLU	N261	K320	K381	E440	ASP
GLU	V262	Y321	C382	D441	SER
GLY	L263	E322	L383	F442	ASN
SER	R264	G323	F384	L443	ALA
GLU	I265	K324	F385	K444	GLY
GLU	F266	L325	F386	G445	SER
SER	S267	N326	A386	Q446	GLU
ALA	L268	R327	T387	G447	ASP
SER	P269	S328	K388	V448	ALA
SER	R270	Y329	P389	R449	SER
GLY	L271	G330	C390	V450	SER
GLU	D272	T331	V391	K451	GLY
PRO	D273	D332	Y392	N452	GLU
GLU	R274	S333	L393	E453	LYS
LYS	D275	T334	P394	LYS	LYS
LYS	H276	Y335	Y395	PRO	LYS
LYS	H277	K336	S396	ALA	LYS
LEU	L277	I337	G397	PHE	HIS
LEU	V278	L338	I398	LEU	
GLY	I279	S339	I399	GLY	
ASN	L280	H340	S400	ASN	
ALA	Q281	C341	V401	ALA	
LEU	V282	L342	V402	LEU	
VAL	D283	R343	T403	VAL	
ASP	P284	G344	S404	ASP	
ASP	P285	L345	R405	ASP	
ASP	L286	T346	G406	ASP	
SER	R287	E347	THR	SER	
ASP	Q288	R348	GLY	ASP	
GLY	G289	R349	GLN	GLY	
ASP	Q290	V350	SER	ASP	
ASP	T291	I351	THR	ASP	
GLY	R292	T352	S412	GLY	
ILE	Y293	P353	R413	ILE	
ALA	P294	G354	T414	ALA	
MET	F295	S355	F415	MET	
GLY	L296	F356	D416	GLY	
	V297	I417	I417		
	M298	Q357	E418		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28511	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.089	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size ($\text{\AA}$)	356.16, 356.16, 356.16	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.484, 1.484, 1.484	Depositor

5 Model quality

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	0.23	0/11267	0.31	1/15222 (0.0%)
2	B	0.24	0/9464	0.30	0/12763
3	C	0.25	0/2139	0.30	0/2895
4	D	0.11	0/1361	0.24	0/1837
5	E	0.22	0/1773	0.32	0/2385
6	F	0.24	0/687	0.26	0/931
7	G	0.15	0/1354	0.28	0/1837
8	H	0.23	0/1070	0.28	0/1444
9	I	0.10	0/934	0.25	0/1257
10	J	0.25	0/563	0.28	0/753
11	K	0.24	0/953	0.29	0/1291
12	L	0.20	0/365	0.27	0/484
13	M	0.10	0/513	0.25	0/693
14	N	0.54	0/2668	0.73	0/4119
15	P	0.33	0/443	0.52	0/687
16	T	0.60	2/2882 (0.1%)	0.73	0/4441
17	V	0.10	0/840	0.21	0/1140
18	W	0.11	0/4300	0.26	0/5812
19	m	0.11	0/9925	0.25	0/13424
20	n	0.10	0/1132	0.23	0/1526
21	q	0.10	0/7689	0.21	0/10368
22	r	0.11	0/2169	0.24	0/2901
23	u	0.11	0/1740	0.23	0/2347
24	v	0.11	0/2944	0.24	0/3973
25	x	0.13	0/1716	0.25	0/2310
26	a	0.20	0/755	0.35	0/1012
26	e	0.31	0/806	0.43	0/1081
27	b	0.22	0/653	0.45	0/873
27	f	0.25	0/626	0.42	0/837
28	c	0.20	0/752	0.37	0/1015
28	g	0.18	0/766	0.36	0/1033
29	d	0.20	0/729	0.34	0/979

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	h	0.19	0/736	0.32	0/990
30	j	0.81	0/3827	1.15	1/5159 (0.0%)
31	k	0.77	0/3579	1.12	0/4833
All	All	0.32	2/84120 (0.0%)	0.47	2/114652 (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	4
16	T	0	4
27	f	0	1
30	j	0	1
31	k	0	1
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	-33	DA	C1'-N9	-5.09	1.36	1.46
16	T	-53	DG	C1'-N9	-5.02	1.36	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	j	964	PRO	N-CA-CB	7.28	110.90	103.25
1	A	1001	VAL	N-CA-C	-5.79	107.17	112.96

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	-11	DC	Sidechain
14	N	-12	DA	Sidechain
14	N	-17	DT	Sidechain
14	N	-9	DC	Sidechain
16	T	11	DG	Sidechain
16	T	13	DT	Sidechain
16	T	14	DT	Sidechain

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Mol	Chain	Res	Type	Group
16	T	15	DT	Sidechain
27	f	36	ARG	Sidechain
30	j	616	ARG	Sidechain
31	k	58	ARG	Sidechain

5.2 Too-close contacts

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	118	0
2	B	9284	0	9282	137	0
3	C	2098	0	2057	24	0
4	D	1349	0	1345	11	0
5	E	1741	0	1754	24	0
6	F	677	0	693	9	0
7	G	1325	0	1342	18	0
8	H	1053	0	1050	11	0
9	I	917	0	867	17	0
10	J	554	0	573	6	0
11	K	932	0	944	15	0
12	L	359	0	358	6	0
13	M	505	0	495	5	0
14	N	2377	0	1293	96	0
15	P	399	0	205	10	0
16	T	2570	0	1411	73	0
17	V	824	0	795	17	0
18	W	4232	0	4278	68	0
19	m	9730	0	9588	144	0
20	n	1115	0	1186	25	0
21	q	7552	0	7545	108	0
22	r	2139	0	2155	41	0
23	u	1707	0	1676	26	0
24	v	2878	0	2873	57	0
25	x	1682	0	1731	16	0
26	a	746	0	786	9	0
26	e	795	0	832	12	0
27	b	646	0	687	11	0
27	f	619	0	659	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	c	743	0	784	13	0
28	g	757	0	802	14	0
29	d	718	0	740	12	0
29	h	725	0	745	13	0
30	j	3754	0	3654	22	0
31	k	3502	0	3436	26	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	I	2	0	0	0	0
32	J	1	0	0	0	0
32	L	1	0	0	0	0
32	M	1	0	0	0	0
32	V	1	0	0	0	0
33	A	1	0	0	0	0
All	All	82079	0	79711	1049	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 7.

All (1049) 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:34:DC:C6	14:N:35:DT:H72	1.93	1.03
14:N:-49:DG:H2''	14:N:-48:DC:C5	2.00	0.97
14:N:24:DC:C2'	14:N:25:DT:H71	2.00	0.92
14:N:33:DT:H2''	14:N:34:DC:C5	2.08	0.89
16:T:-21:DC:H2''	16:T:-20:DC:C5	2.11	0.86
14:N:-51:DG:H2''	14:N:-50:DT:H71	1.57	0.86
14:N:57:DG:N2	16:T:-56:DC:C2	2.45	0.85
31:k:116:GLN:NE2	31:k:125:ASN:HD22	1.75	0.85
16:T:-51:DC:H2''	16:T:-50:DC:C5	2.12	0.85
16:T:-33:DA:H2''	16:T:-32:DC:C5	2.14	0.81
14:N:-22:DA:N6	14:N:-21:DA:C6	2.48	0.81
14:N:24:DC:H2''	14:N:25:DT:H71	1.63	0.81
14:N:66:DT:C6	14:N:67:DT:H72	2.16	0.81
14:N:24:DC:H2'	14:N:25:DT:H71	1.63	0.80
31:k:116:GLN:CD	31:k:125:ASN:ND2	2.40	0.80
14:N:-51:DG:C2'	14:N:-50:DT:H71	2.14	0.78
21:q:793:VAL:HG11	21:q:830:LEU:HG	1.64	0.78
14:N:10:DG:H2''	14:N:11:DC:C5	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-37:DG:N2	16:T:37:DC:O2	2.16	0.76
16:T:-51:DC:H2''	16:T:-50:DC:H5	1.47	0.75
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.26	0.75
31:k:116:GLN:CD	31:k:125:ASN:HD22	1.95	0.74
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.70	0.74
14:N:4:DG:N2	16:T:-3:DG:C4	2.56	0.74
21:q:390:LEU:HB3	21:q:409:LEU:HD21	1.70	0.73
14:N:33:DT:H2''	14:N:34:DC:H5	1.54	0.72
18:W:524:GLU:O	20:n:232:GLN:NE2	2.23	0.71
14:N:-22:DA:C6	14:N:-21:DA:C6	2.79	0.71
2:B:792:MET:HE2	2:B:857:ARG:HH22	1.54	0.70
1:A:807:ARG:NH1	2:B:724:LYS:O	2.23	0.70
30:j:515:ASP:HA	30:j:519:GLY:HA3	1.72	0.70
14:N:24:DC:C2'	14:N:25:DT:C7	2.69	0.70
28:g:88:ARG:NH2	28:g:97:LEU:O	2.24	0.69
14:N:-49:DG:H2''	14:N:-48:DC:H5	1.52	0.69
1:A:1262:MET:SD	1:A:1265:ARG:NH2	2.65	0.69
1:A:1207:LYS:O	1:A:1277:ARG:NH2	2.24	0.69
8:H:112:LYS:HG2	8:H:125:GLU:HG3	1.73	0.69
19:m:1160:ASP:O	19:m:1163:ARG:NH1	2.26	0.69
2:B:550:PHE:HB3	2:B:593:MET:HE1	1.75	0.69
1:A:831:LYS:NZ	1:A:1079:THR:O	2.25	0.69
5:E:60:LEU:O	21:q:915:ARG:NH1	2.23	0.69
18:W:487:ILE:HD11	18:W:531:ARG:HB2	1.75	0.69
21:q:531:GLU:O	21:q:535:ASN:N	2.26	0.69
18:W:303:ILE:HB	20:n:286:ARG:HH22	1.58	0.68
21:q:922:ALA:O	21:q:926:ASN:ND2	2.26	0.68
1:A:107:CYS:SG	1:A:172:GLN:NE2	2.66	0.68
28:g:28:GLY:HA3	30:j:974:SER:CB	2.22	0.68
16:T:-37:DG:C8	16:T:-36:DT:H72	2.28	0.68
21:q:578:GLN:NE2	21:q:582:ASP:OD1	2.26	0.67
14:N:-44:DG:H2''	14:N:-43:DT:H72	1.76	0.67
21:q:59:ALA:HB1	21:q:63:LEU:HD12	1.77	0.67
22:r:490:VAL:HG22	22:r:495:ARG:HE	1.60	0.67
14:N:36:DA:C2	16:T:-35:DA:C2	2.83	0.67
14:N:24:DC:H2'	14:N:25:DT:C7	2.24	0.67
10:J:47:ARG:NH1	10:J:48:MET:SD	2.67	0.67
22:r:230:ARG:NH1	22:r:292:SER:OG	2.27	0.66
2:B:223:SER:O	2:B:252:ARG:NH2	2.27	0.66
14:N:-40:DC:H2''	14:N:-39:DT:H71	1.77	0.66
21:q:169:ASP:OD1	21:q:185:LYS:NZ	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:45:ARG:NH2	9:I:47:GLU:OE2	2.29	0.66
19:m:617:ILE:HG13	19:m:649:LEU:HD11	1.78	0.66
16:T:-29:DC:H2''	16:T:-28:DT:H72	1.78	0.66
19:m:380:GLU:HG3	19:m:382:PRO:HD2	1.77	0.65
1:A:673:ASP:OD1	1:A:737:ASN:ND2	2.29	0.65
19:m:382:PRO:HG2	19:m:955:ASN:HD22	1.58	0.65
18:W:342:GLU:HB3	18:W:351:ARG:HB3	1.79	0.65
1:A:887:ILE:O	1:A:945:ARG:NH2	2.29	0.65
2:B:613:ARG:HH21	9:I:62:ILE:HD11	1.61	0.65
19:m:682:ASP:O	19:m:686:ASN:ND2	2.28	0.65
16:T:-40:DG:C8	16:T:-39:DT:H71	2.32	0.65
2:B:267:TYR:HB2	2:B:348:ILE:HD11	1.77	0.65
14:N:-48:DC:H2''	14:N:-47:DC:C6	2.32	0.65
1:A:447:ARG:HB2	1:A:488:MET:HE3	1.77	0.65
3:C:266:ARG:HD2	11:K:84:LYS:HZ1	1.61	0.65
27:f:68:ASP:OD2	27:f:93:GLN:NE2	2.30	0.65
1:A:127:ARG:O	1:A:129:ARG:NH1	2.30	0.64
27:b:26:ILE:HG13	27:b:55:ARG:HD3	1.80	0.64
30:j:621:ARG:CZ	31:k:156:PRO:HB2	2.27	0.64
4:D:54:SER:HG	4:D:121:CYS:HG	1.44	0.64
16:T:-18:DC:H4'	31:k:234:ARG:NH1	2.13	0.64
20:n:260:MET:HG3	20:n:284:TRP:HZ3	1.63	0.64
25:x:292:TRP:HA	25:x:295:LYS:HE2	1.79	0.64
21:q:31:LYS:HB2	21:q:57:GLU:HA	1.79	0.64
17:V:89:ARG:NH1	17:V:109:ASP:OD2	2.31	0.64
16:T:-60:DG:H5''	28:c:16:THR:HA	1.80	0.64
18:W:327:ARG:NH2	18:W:441:ASN:O	2.30	0.64
14:N:24:DC:H2''	14:N:25:DT:C7	2.28	0.64
19:m:343:ARG:NH1	19:m:347:GLN:OE1	2.31	0.64
25:x:157:ARG:HB3	25:x:161:PRO:HB3	1.78	0.64
2:B:285:PRO:HG2	2:B:288:GLU:HB2	1.80	0.64
16:T:-43:DT:H2''	16:T:-42:DT:C6	2.33	0.64
19:m:551:ARG:NH2	19:m:689:LYS:O	2.31	0.64
22:r:269:ASP:HB3	22:r:349:LEU:HD21	1.80	0.63
2:B:254:ASP:H	2:B:259:ARG:HH21	1.44	0.63
4:D:153:VAL:HG13	4:D:171:LEU:HD23	1.78	0.63
21:q:793:VAL:HG13	21:q:826:ALA:HB1	1.79	0.63
1:A:466:TYR:HB2	1:A:470:ARG:HH22	1.63	0.63
1:A:881:ARG:HH21	1:A:955:ASN:HB3	1.64	0.63
14:N:24:DC:H2''	14:N:25:DT:C6	2.33	0.63
21:q:590:ARG:NH1	21:q:618:THR:OG1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:-40:DG:C8	16:T:-39:DT:C7	2.82	0.62
21:q:780:TYR:O	21:q:784:LYS:N	2.31	0.62
16:T:42:DC:OP1	18:W:433:GLN:NE2	2.33	0.62
19:m:434:LEU:HD11	19:m:467:ASP:HB2	1.81	0.62
19:m:1101:ASP:OD1	19:m:1132:GLN:NE2	2.33	0.62
23:u:199:LEU:HD11	24:v:211:PHE:HB3	1.81	0.62
31:k:116:GLN:NE2	31:k:125:ASN:ND2	2.47	0.62
21:q:155:TYR:HA	21:q:160:ARG:HD3	1.80	0.62
1:A:1158:PRO:HA	1:A:1192:PRO:HB3	1.80	0.62
18:W:351:ARG:HA	18:W:429:THR:HA	1.81	0.62
21:q:65:LEU:HD13	24:v:81:ILE:HG12	1.81	0.62
14:N:-22:DA:N6	14:N:-21:DA:N6	2.47	0.62
11:K:57:THR:OG1	11:K:76:GLN:OE1	2.17	0.61
19:m:358:HIS:HB3	19:m:361:GLU:HB2	1.82	0.61
1:A:1130:ILE:HG12	1:A:1134:LYS:HE2	1.81	0.61
19:m:1221:LEU:HD11	19:m:1233:SER:HB2	1.81	0.61
23:u:80:TYR:CZ	24:v:356:ASN:HB2	2.36	0.61
1:A:361:GLU:OE1	1:A:460:ARG:NH2	2.29	0.61
1:A:1201:ARG:NH2	1:A:1235:ALA:O	2.33	0.61
19:m:730:ASP:OD1	19:m:733:ARG:NH2	2.34	0.61
21:q:348:ASP:HB3	21:q:351:GLN:HB3	1.82	0.61
14:N:11:DC:H2''	14:N:12:DG:C8	2.36	0.60
21:q:210:PRO:O	21:q:217:ARG:NH2	2.25	0.60
26:a:69:ARG:HB3	27:b:25:ASN:HD22	1.65	0.60
1:A:39:GLU:OE2	1:A:49:ARG:NH1	2.34	0.60
18:W:784:ASN:HB2	18:W:785:PRO:HD3	1.81	0.60
19:m:672:VAL:O	19:m:720:GLN:NE2	2.34	0.60
21:q:708:GLN:OE1	21:q:739:LYS:NZ	2.34	0.60
23:u:108:VAL:HG22	23:u:219:VAL:HB	1.83	0.60
19:m:421:ASP:OD1	19:m:422:LEU:N	2.34	0.60
18:W:527:THR:HA	18:W:530:LEU:HD12	1.84	0.60
19:m:424:TYR:HA	19:m:427:ILE:HG12	1.83	0.60
21:q:253:ILE:HG12	21:q:297:LEU:HD21	1.84	0.60
1:A:149:GLU:HB2	1:A:165:ARG:HD3	1.84	0.60
19:m:458:ARG:HG3	19:m:459:THR:HG23	1.83	0.60
19:m:607:ILE:HG22	19:m:719:VAL:HG11	1.82	0.60
22:r:408:ASP:OD1	24:v:133:TYR:N	2.32	0.60
1:A:466:TYR:HB2	1:A:470:ARG:NH2	2.16	0.60
2:B:235:LEU:HD23	2:B:242:ILE:HG13	1.83	0.60
14:N:38:DG:H2''	14:N:39:DA:H5'	1.83	0.60
2:B:489:ARG:NH2	2:B:533:SER:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HG	2:B:1213:ALA:HB2	1.83	0.59
17:V:57:LEU:HD11	17:V:81:LEU:HD22	1.84	0.59
2:B:10:ASP:HB3	2:B:649:LYS:HG3	1.84	0.59
24:v:312:LYS:HB3	24:v:315:GLU:HG2	1.85	0.59
14:N:43:DA:H1'	14:N:44:DT:H5'	1.84	0.59
20:n:217:ARG:HG3	20:n:259:VAL:HG21	1.84	0.59
16:T:-21:DC:H2''	16:T:-20:DC:H5	1.67	0.59
18:W:327:ARG:NH1	18:W:335:GLY:O	2.36	0.59
14:N:-22:DA:N1	14:N:-21:DA:C2	2.71	0.59
1:A:85:GLU:O	1:A:274:ASN:ND2	2.33	0.59
16:T:-23:DC:H2''	16:T:-22:DA:N7	2.18	0.59
19:m:785:ASP:O	19:m:912:GLN:NE2	2.35	0.59
26:a:69:ARG:HB3	27:b:25:ASN:ND2	2.18	0.59
2:B:409:LEU:HD23	2:B:450:LEU:HD23	1.85	0.59
14:N:54:DT:H2''	14:N:55:DC:C6	2.38	0.59
21:q:72:VAL:HG21	24:v:75:LEU:HD13	1.85	0.59
24:v:29:LEU:N	25:x:147:ARG:O	2.35	0.59
7:G:27:ARG:NH1	7:G:54:ILE:O	2.36	0.59
2:B:63:GLN:NE2	2:B:70:ASN:OD1	2.35	0.58
2:B:294:CYS:SG	2:B:295:TYR:N	2.76	0.58
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.24	0.58
14:N:69:DT:H2''	14:N:70:DG:H8	1.68	0.58
1:A:1157:ASP:O	1:A:1243:ARG:NH2	2.29	0.58
17:V:9:GLU:HA	17:V:20:PRO:HA	1.84	0.58
14:N:8:DG:C2	16:T:-7:DG:C2	2.92	0.58
2:B:50:VAL:HG21	2:B:82:ILE:HD11	1.86	0.58
21:q:806:LEU:O	21:q:811:ARG:NH1	2.36	0.58
1:A:677:MET:HG3	2:B:722:THR:HB	1.84	0.58
19:m:570:MET:HA	19:m:577:THR:HG21	1.84	0.58
21:q:766:MET:HG3	21:q:770:LYS:HE3	1.86	0.58
23:u:191:THR:HG22	23:u:219:VAL:HG22	1.85	0.58
2:B:91:GLU:OE2	2:B:97:HIS:NE2	2.29	0.58
24:v:267:TYR:HB3	24:v:297:TYR:HB3	1.85	0.58
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.85	0.58
14:N:34:DC:C6	14:N:35:DT:C7	2.80	0.58
21:q:690:LYS:NZ	25:x:178:GLU:OE1	2.36	0.58
1:A:227:GLU:OE1	1:A:231:ARG:NH1	2.36	0.58
22:r:194:LYS:HB2	22:r:316:LEU:HD12	1.84	0.58
7:G:86:VAL:HG22	7:G:146:LYS:HB2	1.86	0.57
23:u:145:ILE:O	23:u:149:THR:OG1	2.17	0.57
1:A:63:ARG:NH2	15:P:0:G:OP1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:53:DC:H2"	14:N:54:DT:H71	1.86	0.57
18:W:392:ARG:NH1	18:W:398:GLU:OE1	2.36	0.57
24:v:56:LYS:O	24:v:60:ARG:NH2	2.37	0.57
5:E:101:GLU:HG3	5:E:102:LYS:HG2	1.86	0.57
18:W:665:ARG:HB2	18:W:708:ILE:HD11	1.86	0.57
17:V:13:MET:N	17:V:49:CYS:O	2.26	0.57
2:B:928:ARG:NH2	19:m:777:ASP:O	2.36	0.57
14:N:-40:DC:H2"	14:N:-39:DT:C7	2.33	0.57
23:u:121:PHE:HB3	23:u:153:ARG:HB3	1.85	0.57
29:d:112:THR:O	29:d:116:THR:HG23	2.05	0.57
1:A:568:LYS:HG2	1:A:569:PRO:HA	1.87	0.57
14:N:22:DT:H2"	14:N:23:DG:N7	2.19	0.57
19:m:245:THR:HA	19:m:248:GLN:HB2	1.86	0.57
30:j:587:ARG:HH12	31:k:289:GLY:CA	2.18	0.57
2:B:290:LEU:HD21	2:B:310:ILE:HD11	1.87	0.56
19:m:300:VAL:O	19:m:304:THR:OG1	2.20	0.56
14:N:24:DC:H2"	14:N:25:DT:C5	2.40	0.56
22:r:200:ASP:HB3	22:r:319:VAL:HG11	1.87	0.56
30:j:587:ARG:HH12	31:k:289:GLY:HA2	1.70	0.56
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.37	0.56
14:N:4:DG:N2	16:T:-3:DG:N3	2.53	0.56
18:W:232:ARG:HH12	18:W:235:LYS:HE3	1.70	0.56
30:j:609:GLY:HA3	30:j:612:LYS:HD2	1.86	0.56
31:k:103:LYS:HE2	31:k:130:PRO:HG3	1.86	0.56
2:B:336:ILE:O	2:B:341:ARG:NH1	2.38	0.56
6:F:103:MET:HE3	7:G:15:PRO:HG2	1.87	0.56
8:H:48:PRO:O	8:H:145:ARG:NH1	2.36	0.56
17:V:58:VAL:N	17:V:82:TYR:O	2.38	0.56
19:m:309:ARG:HH21	19:m:978:CYS:HA	1.69	0.56
14:N:5:DT:OP1	27:f:30:THR:CG2	2.54	0.56
18:W:352:LEU:HD11	18:W:435:LEU:HD11	1.87	0.56
24:v:316:ASP:HB2	24:v:333:ILE:HB	1.88	0.56
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.88	0.56
19:m:1177:SER:O	19:m:1194:ARG:NH1	2.37	0.56
5:E:28:PHE:HB2	5:E:64:THR:HG22	1.88	0.56
23:u:209:LEU:HB2	24:v:252:PHE:HB2	1.87	0.56
16:T:-38:DC:H2"	16:T:-37:DG:H5'	1.88	0.56
20:n:163:LEU:HD11	20:n:194:VAL:HG22	1.88	0.56
31:k:108:ARG:CZ	31:k:127:ASN:HD22	2.19	0.56
1:A:149:GLU:O	1:A:165:ARG:NH1	2.38	0.55
14:N:-22:DA:N6	14:N:-21:DA:N1	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1331:TYR:OH	1:A:1354:GLU:OE2	2.21	0.55
14:N:4:DG:N2	16:T:-3:DG:C2	2.74	0.55
5:E:19:LYS:NZ	5:E:33:GLU:O	2.34	0.55
1:A:916:TYR:OH	1:A:983:LEU:O	2.19	0.55
7:G:102:ASP:OD1	7:G:107:ASN:ND2	2.31	0.55
7:G:151:ARG:HB3	7:G:158:TYR:HB2	1.89	0.55
20:n:229:PRO:O	20:n:234:GLN:NE2	2.37	0.55
19:m:529:ILE:HD11	19:m:566:ILE:HG12	1.87	0.55
21:q:569:ASN:O	21:q:603:LYS:NZ	2.40	0.55
27:b:92:ARG:NH2	29:d:97:LEU:O	2.40	0.55
19:m:956:LEU:O	19:m:1046:ARG:NH2	2.39	0.55
1:A:1452:LEU:HD23	6:F:131:PRO:HA	1.89	0.55
2:B:926:GLY:O	19:m:778:ALA:N	2.31	0.55
19:m:956:LEU:HD11	19:m:1138:ILE:HG21	1.88	0.55
19:m:1205:ASP:OD2	19:m:1207:ARG:NH2	2.40	0.55
21:q:239:ASN:HA	21:q:242:LYS:HD2	1.89	0.55
23:u:89:SER:HB3	24:v:365:ARG:HE	1.72	0.55
24:v:54:PHE:O	24:v:58:ASN:N	2.34	0.55
26:e:54:TYR:O	27:f:40:ARG:NE	2.37	0.55
2:B:904:ARG:HH12	2:B:946:ASN:HB2	1.72	0.55
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.89	0.55
16:T:-29:DC:C2'	16:T:-28:DT:H72	2.36	0.55
14:N:36:DA:C5	14:N:37:DC:C4	2.96	0.54
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.89	0.54
17:V:15:CYS:HB3	17:V:32:CYS:SG	2.46	0.54
19:m:465:ASP:OD1	19:m:604:ARG:NH1	2.40	0.54
1:A:807:ARG:HD3	2:B:725:ARG:HA	1.89	0.54
1:A:1210:THR:HB	1:A:1213:GLN:HG3	1.90	0.54
17:V:10:ARG:HA	17:V:52:SER:HA	1.90	0.54
21:q:641:ALA:HB1	21:q:655:LYS:HG3	1.89	0.54
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.42	0.54
22:r:223:VAL:HG22	22:r:325:GLN:HG2	1.88	0.54
2:B:72:ASN:ND2	2:B:128:ASP:OD1	2.39	0.54
14:N:33:DT:C2'	14:N:34:DC:C5	2.87	0.54
19:m:533:VAL:HG22	19:m:589:VAL:HG13	1.90	0.54
21:q:41:PHE:CG	21:q:70:VAL:HG11	2.42	0.54
1:A:569:PRO:HD2	8:H:46:MET:HE2	1.89	0.54
8:H:100:VAL:HG22	8:H:115:VAL:HG22	1.89	0.54
11:K:29:ASN:ND2	11:K:78:GLU:O	2.41	0.54
11:K:103:HIS:NE2	11:K:107:GLU:OE2	2.40	0.54
14:N:8:DG:H2'	14:N:9:DT:H71	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:v:74:TYR:HE1	24:v:87:LEU:HD12	1.73	0.54
1:A:218:GLU:OE1	1:A:222:ARG:NH1	2.41	0.54
16:T:-51:DC:C2'	16:T:-50:DC:C5	2.88	0.54
23:u:80:TYR:OH	24:v:352:VAL:O	2.22	0.54
14:N:44:DT:H2''	14:N:45:DT:C6	2.42	0.54
18:W:325:TYR:OH	18:W:451:GLN:OE1	2.23	0.54
2:B:301:GLN:O	2:B:304:GLU:HG3	2.08	0.54
18:W:332:LYS:O	18:W:388:ARG:NH1	2.41	0.54
30:j:652:MET:C	30:j:654:ASP:H	2.15	0.54
19:m:1024:TYR:CG	19:m:1135:TYR:HE2	2.26	0.53
27:b:92:ARG:HH12	29:d:98:LEU:HD23	1.74	0.53
8:H:59:LEU:HD23	8:H:139:LEU:HD13	1.91	0.53
18:W:451:GLN:NE2	18:W:454:GLU:OE1	2.42	0.53
1:A:533:ARG:HD3	1:A:750:ALA:HB2	1.91	0.53
21:q:766:MET:HE1	21:q:799:ILE:HG23	1.90	0.53
2:B:592:THR:HG23	23:u:226:PHE:CE1	2.44	0.53
2:B:59:ASP:HB3	2:B:74:ARG:HG3	1.91	0.53
28:c:79:ILE:HG12	28:c:82:HIS:CE1	2.44	0.53
1:A:351:ARG:HB2	2:B:1128:LEU:HD21	1.91	0.53
2:B:245:MET:HE1	2:B:371:LEU:HD11	1.91	0.53
14:N:8:DG:H2'	14:N:9:DT:C7	2.38	0.53
21:q:170:ASN:HA	21:q:173:LYS:HD2	1.91	0.53
5:E:81:PHE:HE1	5:E:110:ILE:HD13	1.74	0.53
19:m:236:GLU:OE2	20:n:252:ARG:NH2	2.41	0.53
21:q:155:TYR:HB3	21:q:160:ARG:HB2	1.89	0.53
2:B:248:LYS:NZ	2:B:264:THR:OG1	2.42	0.53
14:N:34:DC:C5	14:N:35:DT:H72	2.43	0.53
30:j:728:MET:HE3	30:j:752:TYR:CD2	2.44	0.53
4:D:6:SER:HB3	7:G:42:PHE:HZ	1.73	0.53
5:E:47:ASP:OD2	5:E:53:GLN:NE2	2.19	0.53
16:T:-31:DA:H2''	16:T:-30:DG:C8	2.44	0.53
18:W:220:THR:N	18:W:223:ASP:OD2	2.33	0.53
21:q:317:LEU:HD23	22:r:514:LEU:HD12	1.91	0.53
2:B:875:GLU:OE2	2:B:915:THR:OG1	2.26	0.52
21:q:408:LEU:HD13	24:v:44:LEU:HD22	1.92	0.52
2:B:797:TYR:HE1	2:B:854:LEU:HD13	1.74	0.52
7:G:144:ARG:HB2	7:G:171:ILE:HD13	1.90	0.52
9:I:104:LEU:O	9:I:107:LYS:NZ	2.39	0.52
16:T:-29:DC:H2''	16:T:-28:DT:C7	2.39	0.52
21:q:451:ARG:NH1	24:v:35:GLU:OE1	2.42	0.52
13:M:46:LEU:HD11	13:M:55:SER:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:14:DT:H3'	26:e:116:ARG:HD3	1.90	0.52
21:q:218:LEU:HA	21:q:237:TRP:HE1	1.73	0.52
29:h:102:GLU:HG3	29:h:106:HIS:CD2	2.44	0.52
9:I:17:LYS:N	9:I:26:LEU:O	2.39	0.52
14:N:52:DC:H2''	14:N:53:DC:C5	2.44	0.52
15:P:6:U:H2'	15:P:7:C:C6	2.44	0.52
16:T:-53:DG:H2''	16:T:-52:DG:N7	2.25	0.52
16:T:-18:DC:C4'	31:k:234:ARG:NH1	2.73	0.52
17:V:10:ARG:HG2	17:V:52:SER:HB3	1.92	0.52
19:m:1056:ARG:HB3	19:m:1076:MET:HB3	1.91	0.52
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.49	0.52
4:D:60:ILE:HG13	7:G:47:THR:HG21	1.90	0.52
14:N:-42:DG:C8	14:N:-41:DT:H71	2.45	0.52
30:j:938:SER:O	30:j:939:PHE:C	2.52	0.52
19:m:1425:LYS:NZ	19:m:1430:SER:O	2.30	0.52
24:v:262:LYS:HD3	24:v:305:GLN:HE21	1.73	0.52
26:e:48:LEU:O	26:e:52:ARG:HG3	2.09	0.52
2:B:904:ARG:NH1	2:B:905:VAL:O	2.43	0.52
29:d:41:VAL:O	29:d:45:VAL:HG22	2.10	0.52
10:J:23:ARG:NH2	22:r:399:LYS:HZ1	2.07	0.52
16:T:-37:DG:C2'	16:T:-36:DT:H72	2.39	0.52
1:A:801:VAL:HG22	1:A:813:GLU:HB3	1.92	0.52
19:m:1047:ILE:HG12	19:m:1127:ILE:HG12	1.91	0.52
27:f:89:ALA:O	27:f:93:GLN:HG2	2.10	0.52
18:W:513:SER:N	18:W:519:ASN:OD1	2.41	0.52
19:m:1121:ARG:HA	19:m:1124:LEU:HD12	1.91	0.52
19:m:1170:VAL:O	19:m:1215:THR:OG1	2.19	0.52
22:r:276:PHE:HB2	22:r:279:GLN:HB2	1.91	0.52
24:v:104:PRO:HA	24:v:107:ARG:HD3	1.92	0.52
24:v:258:ASN:OD1	24:v:261:ASN:N	2.40	0.52
2:B:353:LEU:O	2:B:367:LYS:NZ	2.34	0.51
18:W:260:TYR:HD1	18:W:276:ALA:HA	1.75	0.51
19:m:465:ASP:OD2	19:m:608:ARG:NH2	2.43	0.51
1:A:543:GLU:OE2	1:A:570:LYS:NZ	2.43	0.51
21:q:250:ASN:HA	21:q:253:ILE:HD12	1.91	0.51
21:q:871:TYR:CZ	21:q:875:ILE:HD11	2.45	0.51
30:j:542:VAL:HG11	30:j:557:ILE:HG21	1.92	0.51
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.74	0.51
2:B:83:TYR:HB2	2:B:116:TYR:HB2	1.92	0.51
14:N:-44:DG:OP2	23:u:273:ARG:NH2	2.41	0.51
16:T:-8:DC:H5'	26:e:43:PRO:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:308:LYS:NZ	22:r:504:SER:O	2.38	0.51
2:B:74:ARG:HB2	2:B:124:PHE:HB2	1.92	0.51
2:B:547:ILE:HG21	2:B:619:ILE:HG21	1.93	0.51
18:W:334:LYS:N	18:W:388:ARG:HH12	2.09	0.51
24:v:263:TRP:HE1	24:v:356:ASN:HD21	1.59	0.51
1:A:771:VAL:HG13	1:A:823:GLU:HG3	1.92	0.51
18:W:563:GLU:HG2	18:W:574:ILE:HG12	1.93	0.51
14:N:-49:DG:C2'	14:N:-48:DC:C5	2.86	0.51
21:q:274:THR:HG23	22:r:506:ILE:HG12	1.93	0.51
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.92	0.51
18:W:494:LEU:HD21	20:n:183:PRO:HG3	1.92	0.51
19:m:1046:ARG:HG3	19:m:1135:TYR:HE1	1.76	0.51
21:q:676:ASN:HA	25:x:156:LEU:HD12	1.93	0.51
24:v:210:VAL:HG13	24:v:334:VAL:HG21	1.92	0.51
28:g:55:LEU:O	28:g:59:THR:HG23	2.11	0.51
13:M:38:LEU:HA	13:M:45:GLY:HA2	1.91	0.51
23:u:170:ILE:HD11	24:v:200:PHE:HD1	1.76	0.51
30:j:935:GLY:HA3	30:j:940:LEU:HD11	1.93	0.51
19:m:995:ILE:HD12	19:m:1010:LEU:HD21	1.92	0.51
19:m:1172:VAL:HA	19:m:1182:VAL:HG12	1.93	0.51
24:v:233:GLY:O	24:v:244:ASN:ND2	2.44	0.51
2:B:86:ARG:NH1	22:r:369:GLU:OE2	2.44	0.51
7:G:119:LEU:HD21	7:G:135:GLU:HB2	1.93	0.51
18:W:644:ASN:ND2	18:W:647:GLN:OE1	2.44	0.51
26:e:129:ARG:HH11	26:e:129:ARG:HG2	1.76	0.51
1:A:1223:SER:OG	1:A:1224:ASP:N	2.44	0.50
2:B:622:ASP:OD1	2:B:623:VAL:N	2.40	0.50
20:n:206:SER:O	20:n:210:ASN:ND2	2.44	0.50
21:q:286:SER:HA	21:q:289:LYS:HD2	1.92	0.50
1:A:669:ASP:OD2	1:A:743:ASN:ND2	2.29	0.50
14:N:50:DG:H2''	14:N:51:DG:C8	2.46	0.50
18:W:326:VAL:HA	18:W:440:ILE:HD13	1.92	0.50
19:m:1261:ASN:OD1	19:m:1264:ARG:NH2	2.39	0.50
5:E:28:PHE:HE2	21:q:915:ARG:HB2	1.75	0.50
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.75	0.50
19:m:766:LEU:HD13	19:m:783:PHE:HB2	1.94	0.50
19:m:1062:ALA:HB3	19:m:1083:MET:HE1	1.92	0.50
1:A:977:ARG:HD2	1:A:979:LYS:HZ1	1.76	0.50
1:A:1153:GLU:OE2	9:I:45:ARG:NH1	2.40	0.50
5:E:87:VAL:HG23	5:E:91:THR:HB	1.92	0.50
16:T:-48:DC:C2'	16:T:-47:DT:H71	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:1027:PHE:HB3	19:m:1134:ARG:HH12	1.76	0.50
21:q:404:GLU:OE1	21:q:404:GLU:N	2.42	0.50
1:A:168:CYS:SG	1:A:170:ASN:ND2	2.85	0.50
18:W:464:ILE:O	18:W:468:LEU:HG	2.12	0.50
21:q:568:SER:O	21:q:571:ASN:ND2	2.45	0.50
27:f:75:HIS:O	29:h:89:ARG:NH1	2.45	0.50
16:T:-11:DG:H2"	16:T:-10:DC:C5	2.47	0.50
19:m:338:LEU:HD11	19:m:417:ILE:HD11	1.91	0.50
4:D:105:THR:HG22	7:G:105:PRO:HD3	1.94	0.50
13:M:33:SER:HA	13:M:50:LYS:HE2	1.93	0.50
18:W:634:PRO:HA	18:W:637:ILE:HD12	1.94	0.50
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.92	0.50
2:B:607:SER:HB3	2:B:620:PHE:HB2	1.94	0.50
21:q:160:ARG:NH2	21:q:163:GLU:OE1	2.44	0.50
21:q:189:LEU:HD22	21:q:194:LYS:HD2	1.94	0.50
28:c:85:LEU:O	28:c:89:ASN:HB2	2.11	0.50
2:B:498:ASP:HB3	14:N:-23:DA:C4	2.47	0.50
18:W:222:ASP:O	18:W:277:ARG:NH2	2.30	0.50
21:q:109:PHE:CD1	21:q:130:ALA:HB1	2.46	0.50
2:B:514:LEU:HD22	2:B:626:VAL:HG12	1.94	0.49
17:V:63:ASN:HB3	17:V:75:ASP:HA	1.94	0.49
19:m:840:ASN:O	19:m:844:ASN:ND2	2.44	0.49
22:r:261:LEU:HB3	22:r:266:ASN:HB3	1.94	0.49
1:A:119:ASN:OD1	1:A:121:THR:OG1	2.23	0.49
18:W:590:ILE:O	18:W:593:SER:OG	2.26	0.49
1:A:1190:GLN:HA	1:A:1245:ILE:HA	1.94	0.49
2:B:928:ARG:NH1	19:m:776:GLY:H	2.10	0.49
19:m:244:GLY:O	19:m:248:GLN:N	2.44	0.49
30:j:586:ILE:HD12	30:j:628:MET:SD	2.52	0.49
2:B:74:ARG:HH22	2:B:126:SER:HB3	1.77	0.49
14:N:22:DT:H2"	14:N:23:DG:C8	2.47	0.49
16:T:-63:DC:H2"	16:T:-62:DC:C5	2.46	0.49
19:m:562:PRO:HG3	19:m:700:TRP:CE3	2.47	0.49
1:A:738:LEU:HD13	1:A:742:ASN:HD22	1.77	0.49
19:m:917:GLU:OE2	19:m:969:TYR:OH	2.24	0.49
19:m:977:VAL:HB	19:m:980:LEU:HD12	1.94	0.49
26:e:61:LEU:HD12	27:f:37:LEU:HD23	1.95	0.49
2:B:436:ASN:C	2:B:438:ASN:H	2.20	0.49
2:B:610:ARG:NH2	9:I:61:ASP:OD2	2.46	0.49
9:I:29:CYS:CB	9:I:32:CYS:SG	2.99	0.49
14:N:5:DT:OP2	27:f:32:PRO:CD	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:NH1	2:B:466:MET:SD	2.86	0.49
2:B:318:ASP:HB3	2:B:321:VAL:HG22	1.94	0.49
9:I:103:CYS:SG	9:I:104:LEU:N	2.86	0.49
28:g:79:ILE:HG12	28:g:82:HIS:CE1	2.48	0.49
1:A:122:MET:O	1:A:126:ILE:HG12	2.13	0.49
2:B:479:TYR:CZ	2:B:1096:ARG:HB3	2.48	0.49
2:B:556:MET:HE3	2:B:581:GLY:HA3	1.93	0.49
16:T:-40:DG:N7	16:T:-39:DT:H73	2.28	0.49
19:m:655:LEU:HG	19:m:659:MET:HE3	1.95	0.49
21:q:718:HIS:ND1	21:q:733:TYR:OH	2.38	0.49
5:E:81:PHE:CE1	5:E:110:ILE:HD13	2.48	0.49
14:N:4:DG:C2'	14:N:5:DT:H72	2.43	0.49
19:m:242:GLY:HA3	20:n:258:LYS:HG2	1.94	0.49
19:m:1257:ILE:HG22	19:m:1261:ASN:HD21	1.77	0.49
19:m:1337:GLU:HB2	19:m:1348:VAL:HB	1.95	0.49
31:k:239:ILE:CG2	31:k:246:LEU:HD11	2.43	0.49
2:B:766:ARG:HH21	2:B:1020:ARG:HD3	1.78	0.49
18:W:704:ARG:NH1	19:m:632:GLU:OE2	2.43	0.49
19:m:343:ARG:NH2	19:m:344:ASP:OD1	2.45	0.49
19:m:770:PHE:HB3	19:m:779:VAL:HG22	1.95	0.49
1:A:1150:SER:OG	1:A:1198:GLU:O	2.32	0.48
20:n:207:ILE:HG23	20:n:212:LEU:HB3	1.94	0.48
24:v:36:LYS:HB2	24:v:39:PRO:HD2	1.95	0.48
28:c:88:ARG:NH1	28:c:97:LEU:O	2.31	0.48
2:B:58:LEU:O	2:B:75:TYR:N	2.36	0.48
3:C:66:LEU:HD11	3:C:155:ILE:HD12	1.95	0.48
4:D:157:ILE:HG23	4:D:164:ALA:HB2	1.95	0.48
14:N:55:DC:H4'	28:c:42:ARG:HD3	1.94	0.48
19:m:1170:VAL:HG12	19:m:1184:THR:HG22	1.95	0.48
21:q:816:LEU:HD13	21:q:865:ILE:HA	1.95	0.48
22:r:208:ARG:N	22:r:291:ASP:OD1	2.44	0.48
27:b:98:TYR:HB3	29:h:58:ILE:HG23	1.94	0.48
1:A:343:GLY:O	2:B:1129:ARG:NH1	2.45	0.48
7:G:112:THR:HA	7:G:115:ILE:HD12	1.95	0.48
18:W:666:GLU:HB2	18:W:671:ARG:HA	1.95	0.48
19:m:725:GLU:OE2	19:m:728:ARG:NH2	2.45	0.48
19:m:1365:GLU:O	19:m:1369:ASN:ND2	2.46	0.48
31:k:108:ARG:NH2	31:k:127:ASN:HD22	2.11	0.48
9:I:96:ASN:OD1	9:I:97:MET:N	2.46	0.48
16:T:-13:DA:H2''	16:T:-12:DC:C5	2.48	0.48
19:m:933:HIS:HB3	19:m:936:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:305:TYR:CZ	22:r:512:LEU:HD11	2.48	0.48
1:A:819:MET:O	1:A:823:GLU:HG2	2.14	0.48
2:B:300:TRP:HA	2:B:303:LEU:HD12	1.94	0.48
3:C:88:GLU:HG2	18:W:759:ARG:HD2	1.95	0.48
19:m:1062:ALA:HA	19:m:1103:LEU:HD21	1.96	0.48
20:n:163:LEU:HD22	20:n:197:ILE:HD13	1.96	0.48
21:q:320:LEU:O	21:q:324:GLU:HG2	2.14	0.48
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	1.94	0.48
5:E:213:CYS:SG	5:E:214:LEU:N	2.87	0.48
14:N:56:DG:H2''	14:N:57:DG:H5'	1.95	0.48
14:N:56:DG:C6	14:N:57:DG:C6	3.02	0.48
15:P:-2:G:N2	15:P:-1:G:N7	2.61	0.48
19:m:823:ILE:HB	19:m:873:VAL:HG22	1.95	0.48
24:v:89:LYS:O	24:v:93:SER:N	2.46	0.48
29:d:95:VAL:HG13	29:d:99:LEU:HD12	1.95	0.48
12:L:70:ASP:HB3	18:W:784:ASN:HB3	1.95	0.48
14:N:46:DG:C2	16:T:-45:DA:C2	3.02	0.48
18:W:603:GLN:HG3	18:W:609:VAL:HG22	1.95	0.48
19:m:1279:ARG:NH1	19:m:1315:SER:O	2.47	0.48
28:g:41:GLU:HB2	29:h:84:SER:HB2	1.95	0.48
1:A:472:ASN:O	1:A:475:VAL:HG22	2.14	0.48
19:m:1425:LYS:HE3	19:m:1428:PRO:HA	1.96	0.48
22:r:493:ASN:HB2	22:r:502:ILE:HD11	1.95	0.48
23:u:173:TRP:NE1	23:u:179:SER:OG	2.36	0.48
23:u:202:GLU:HB3	24:v:210:VAL:HB	1.96	0.48
24:v:304:ASP:OD2	24:v:340:LYS:NZ	2.45	0.48
25:x:311:GLY:HA3	25:x:330:VAL:HG12	1.96	0.48
1:A:1426:GLY:O	1:A:1430:ASN:ND2	2.40	0.48
2:B:314:PHE:O	2:B:317:GLN:NE2	2.46	0.48
14:N:-51:DG:H2''	14:N:-50:DT:C7	2.37	0.48
21:q:185:LYS:O	21:q:189:LEU:HG	2.14	0.48
21:q:309:GLU:OE1	21:q:311:TYR:OH	2.20	0.48
23:u:204:ASN:OD1	23:u:205:GLU:N	2.47	0.48
24:v:73:ASN:HB3	24:v:76:ARG:HE	1.79	0.48
29:h:42:LEU:HD22	29:h:51:ILE:HG13	1.95	0.48
1:A:823:GLU:OE1	2:B:506:GLN:NE2	2.46	0.48
5:E:93:ARG:HA	5:E:122:MET:HE1	1.96	0.48
1:A:486:ASP:OD1	15:P:10:C:O2'	2.20	0.47
3:C:105:GLU:N	3:C:105:GLU:OE1	2.46	0.47
13:M:65:GLN:N	13:M:68:ASP:OD2	2.44	0.47
16:T:37:DC:H2''	16:T:38:DA:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:1003:ALA:O	19:m:1007:THR:HG23	2.14	0.47
21:q:710:LEU:HD11	21:q:748:LEU:HD11	1.96	0.47
1:A:106:ILE:HD13	1:A:215:ILE:HD11	1.95	0.47
3:C:17:VAL:HG12	3:C:240:ALA:HB1	1.97	0.47
18:W:260:TYR:CE1	18:W:277:ARG:HG3	2.49	0.47
19:m:1202:ASP:OD2	19:m:1204:ARG:NE	2.44	0.47
21:q:312:GLU:O	21:q:316:LYS:HG3	2.14	0.47
22:r:366:GLU:O	22:r:369:GLU:HG2	2.14	0.47
1:A:673:ASP:OD1	1:A:673:ASP:N	2.44	0.47
2:B:365:THR:O	2:B:368:THR:OG1	2.28	0.47
2:B:896:ASP:OD2	12:L:31:TYR:OH	2.32	0.47
5:E:91:THR:HA	5:E:94:ASN:ND2	2.29	0.47
21:q:607:LYS:HB2	21:q:610:LEU:HB2	1.96	0.47
27:b:75:HIS:CD2	29:d:93:THR:HG21	2.49	0.47
27:f:93:GLN:HB2	27:f:95:ARG:HG2	1.95	0.47
2:B:101:PRO:HG2	2:B:172:LEU:HD11	1.96	0.47
3:C:4:GLU:HB3	3:C:5:PRO:HD3	1.96	0.47
4:D:139:PRO:HA	4:D:142:ILE:HD12	1.96	0.47
18:W:599:HIS:HB3	18:W:677:LEU:HD21	1.96	0.47
19:m:381:VAL:HG13	19:m:414:LEU:HD22	1.97	0.47
30:j:644:LYS:HE2	30:j:648:GLU:OE2	2.15	0.47
1:A:363:ASP:HB3	1:A:509:PRO:HD3	1.97	0.47
2:B:303:LEU:O	2:B:307:LYS:HG2	2.15	0.47
2:B:865:ARG:HD3	2:B:871:VAL:HG12	1.95	0.47
14:N:66:DT:H2'	14:N:67:DT:H72	1.96	0.47
15:P:-5:C:H1'	18:W:748:ARG:HD3	1.96	0.47
19:m:1427:ASN:OD1	19:m:1430:SER:N	2.47	0.47
26:a:62:ILE:O	26:a:93:GLN:NE2	2.48	0.47
28:g:29:ARG:HG3	28:g:32:ARG:HH21	1.79	0.47
1:A:983:LEU:HD13	1:A:1041:ARG:HA	1.97	0.47
14:N:13:DT:H2''	14:N:14:DT:H71	1.96	0.47
17:V:91:PRO:HD2	17:V:94:ILE:HB	1.95	0.47
22:r:263:SER:OG	22:r:264:LYS:N	2.47	0.47
1:A:504:GLN:OE1	6:F:90:ARG:NH1	2.38	0.47
7:G:123:PRO:HA	7:G:128:PRO:HB3	1.97	0.47
17:V:41:SER:HB2	17:V:45:THR:HB	1.96	0.47
19:m:1426:LEU:HD13	19:m:1469:ARG:HH21	1.80	0.47
21:q:374:ALA:HA	21:q:377:LEU:HD12	1.96	0.47
28:g:29:ARG:HG3	28:g:32:ARG:NH2	2.29	0.47
31:k:116:GLN:OE1	31:k:125:ASN:ND2	2.47	0.47
16:T:-51:DC:C2	16:T:-50:DC:C4	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:681:VAL:HG13	19:m:708:TRP:HE1	1.78	0.47
19:m:1426:LEU:HD21	19:m:1465:MET:HE2	1.97	0.47
22:r:206:PHE:HB2	22:r:227:MET:HE1	1.96	0.47
22:r:408:ASP:OD2	24:v:134:VAL:HG23	2.14	0.47
24:v:199:HIS:O	24:v:328:ALA:N	2.47	0.47
1:A:580:SER:HB3	1:A:612:LYS:HA	1.97	0.47
2:B:273:PRO:HG2	2:B:276:ILE:HD12	1.97	0.47
2:B:906:SER:OG	18:W:781:GLU:OE1	2.24	0.47
11:K:62:LYS:HE3	11:K:64:GLU:OE2	2.15	0.47
14:N:55:DC:H5''	28:c:44:GLY:HA2	1.97	0.47
23:u:170:ILE:HD11	24:v:200:PHE:CD1	2.50	0.47
26:a:93:GLN:O	26:a:97:GLU:HG3	2.15	0.47
2:B:788:ARG:O	2:B:967:ARG:NH1	2.47	0.47
10:J:6:ARG:HD3	10:J:13:VAL:HG22	1.97	0.47
19:m:306:LEU:HD13	19:m:314:ARG:HH21	1.80	0.47
19:m:965:VAL:HG22	19:m:989:ILE:HG13	1.96	0.47
22:r:212:SER:HA	22:r:215:TRP:HD1	1.79	0.47
29:h:89:ARG:O	29:h:93:THR:HG23	2.14	0.47
1:A:649:ASN:O	1:A:653:VAL:HG23	2.15	0.46
2:B:220:ALA:O	2:B:252:ARG:NH2	2.47	0.46
2:B:885:LEU:HD23	2:B:936:ASP:HB2	1.97	0.46
15:P:-6:A:H2'	15:P:-5:C:O4'	2.15	0.46
21:q:4:LEU:HB2	24:v:103:HIS:CE1	2.49	0.46
21:q:489:PHE:HE1	21:q:533:VAL:HG21	1.80	0.46
14:N:10:DG:N2	16:T:-9:DA:C2	2.84	0.46
18:W:491:LEU:HB3	18:W:494:LEU:HD12	1.98	0.46
18:W:666:GLU:HA	18:W:705:VAL:HG12	1.96	0.46
23:u:90:LEU:HB2	24:v:362:MET:HE1	1.96	0.46
14:N:66:DT:H2'	14:N:67:DT:C7	2.45	0.46
14:N:66:DT:C4	14:N:67:DT:O4	2.68	0.46
18:W:534:PHE:HB3	18:W:554:ILE:HD13	1.97	0.46
20:n:208:LEU:HD13	20:n:250:HIS:CE1	2.50	0.46
21:q:155:TYR:HB2	21:q:164:ALA:HB2	1.96	0.46
2:B:421:ILE:HD11	2:B:441:VAL:HG12	1.97	0.46
2:B:936:ASP:OD1	2:B:938:SER:OG	2.26	0.46
5:E:96:CYS:SG	5:E:126:VAL:HG23	2.56	0.46
26:a:113:HIS:CG	26:e:126:LEU:HD22	2.51	0.46
1:A:564:PRO:HG2	1:A:567:LEU:HD23	1.98	0.46
2:B:497:ARG:NH2	16:T:24:DT:OP2	2.49	0.46
19:m:1002:ARG:HH11	19:m:1052:TYR:HH	1.63	0.46
21:q:241:LEU:HD11	21:q:252:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:v:310:HIS:NE2	24:v:316:ASP:OD2	2.48	0.46
1:A:1192:PRO:HA	1:A:1243:ARG:HH12	1.79	0.46
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.49	0.46
5:E:98:ARG:NH1	5:E:102:LYS:HG3	2.31	0.46
19:m:380:GLU:HG2	19:m:978:CYS:HB2	1.97	0.46
22:r:345:MET:O	22:r:348:SER:OG	2.31	0.46
2:B:266:PRO:HG3	2:B:352:GLU:O	2.16	0.46
2:B:463:LYS:NZ	2:B:464:LYS:HE2	2.31	0.46
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.28	0.46
4:D:170:ASN:HB3	4:D:173:ARG:HG2	1.97	0.46
16:T:-9:DA:OP2	27:f:35:ARG:NH1	2.48	0.46
22:r:346:LYS:O	22:r:350:SER:N	2.48	0.46
1:A:215:ILE:O	1:A:231:ARG:NH2	2.46	0.46
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.49	0.46
6:F:74:ILE:HG23	6:F:78:GLU:HG3	1.97	0.46
12:L:49:ARG:HG2	22:r:339:VAL:HG11	1.98	0.46
21:q:713:PHE:HB3	21:q:736:ALA:HB2	1.97	0.46
26:e:73:GLU:OE1	27:f:25:ASN:HB2	2.16	0.46
1:A:1065:MET:SD	1:A:1439:MET:HB2	2.56	0.46
4:D:54:SER:OG	4:D:121:CYS:SG	2.61	0.46
7:G:51:GLY:HA2	7:G:54:ILE:HD11	1.98	0.46
14:N:-51:DG:H2'	14:N:-50:DT:H71	1.97	0.46
15:P:2:G:H1	16:T:33:DC:H42	1.63	0.46
16:T:-18:DC:C2'	16:T:-17:DT:H71	2.45	0.46
21:q:4:LEU:HD22	24:v:105:ASP:HB2	1.96	0.46
21:q:320:LEU:HD13	22:r:514:LEU:HD11	1.97	0.46
21:q:710:LEU:HD13	21:q:740:PHE:HB2	1.97	0.46
29:d:73:GLU:OE2	29:d:76:ARG:NH1	2.48	0.46
27:f:75:HIS:HD2	29:h:93:THR:HG21	1.80	0.46
28:g:90:ASP:HB3	28:g:93:LEU:HB2	1.98	0.46
1:A:409:ASP:OD1	1:A:410:ASN:N	2.49	0.46
2:B:25:PHE:HZ	2:B:534:LEU:HG	1.81	0.46
2:B:318:ASP:OD1	2:B:319:LYS:N	2.48	0.46
2:B:557:GLU:OE2	2:B:584:ARG:NH2	2.49	0.46
3:C:21:LEU:HD22	11:K:101:LEU:HD11	1.98	0.46
18:W:539:HIS:CE1	18:W:553:LEU:HD21	2.51	0.46
19:m:387:HIS:NE2	19:m:1021:SER:OG	2.42	0.46
31:k:175:ARG:HH22	31:k:289:GLY:HA2	1.81	0.46
19:m:561:SER:HA	19:m:696:ILE:HG23	1.97	0.45
21:q:561:ILE:HD12	21:q:579:LEU:HD22	1.99	0.45
22:r:300:ASP:O	22:r:304:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:h:42:LEU:O	29:h:46:HIS:N	2.35	0.45
1:A:684:ILE:HG21	1:A:802:GLU:HG3	1.99	0.45
1:A:1061:HIS:O	1:A:1064:GLU:HG2	2.17	0.45
2:B:322:ALA:O	2:B:326:ILE:HG12	2.15	0.45
8:H:110:LYS:HE2	8:H:112:LYS:HE3	1.99	0.45
18:W:216:LEU:HD22	19:m:229:LEU:HG	1.98	0.45
21:q:403:SER:OG	24:v:56:LYS:NZ	2.50	0.45
26:e:106:ASP:OD2	26:e:131:ARG:NH2	2.42	0.45
30:j:503:ILE:CD1	30:j:907:PRO:HG3	2.47	0.45
1:A:1390:HIS:O	1:A:1394:ARG:HD3	2.17	0.45
2:B:27:GLU:OE1	2:B:678:TRP:HB3	2.16	0.45
16:T:-72:DA:H1'	16:T:-71:DT:C6	2.51	0.45
16:T:32:DA:H1'	16:T:33:DC:H5''	1.98	0.45
19:m:1072:ASP:O	19:m:1076:MET:HG2	2.15	0.45
21:q:489:PHE:CE1	21:q:533:VAL:HG21	2.51	0.45
26:e:54:TYR:HB3	27:f:40:ARG:HB2	1.98	0.45
31:k:374:GLY:HA3	31:k:387:THR:OG1	2.17	0.45
1:A:912:ASP:OD1	1:A:912:ASP:N	2.44	0.45
19:m:1220:ILE:HA	19:m:1232:LEU:HD23	1.98	0.45
21:q:107:PHE:O	21:q:111:LEU:HG	2.17	0.45
27:f:92:ARG:NH2	29:h:98:LEU:HD13	2.31	0.45
1:A:1448:ILE:HD11	1:A:1453:LEU:HD11	1.97	0.45
2:B:505:ARG:NH1	2:B:524:GLN:O	2.32	0.45
19:m:477:GLN:OE1	19:m:477:GLN:N	2.42	0.45
19:m:1286:PHE:HA	19:m:1308:ILE:HB	1.98	0.45
31:k:10:PHE:HB2	31:k:78:ASP:OD1	2.16	0.45
14:N:-22:DA:C6	14:N:-21:DA:N1	2.85	0.45
25:x:173:LEU:HA	25:x:177:LYS:HD2	1.98	0.45
5:E:46:CYS:HB3	5:E:50:GLY:HA2	1.99	0.45
16:T:-21:DC:C2'	16:T:-20:DC:C5	2.92	0.45
17:V:46:VAL:O	17:V:50:THR:N	2.44	0.45
2:B:250:TYR:HE2	2:B:262:LYS:HB2	1.82	0.45
2:B:1176:LYS:HZ1	18:W:598:LEU:HB3	1.81	0.45
19:m:521:TYR:HA	19:m:524:ILE:HD12	1.97	0.45
21:q:479:TYR:HD1	24:v:30:LEU:HB3	1.82	0.45
24:v:349:VAL:HA	24:v:352:VAL:HB	1.98	0.45
7:G:113:ARG:NH1	18:W:563:GLU:OE1	2.49	0.45
14:N:-44:DG:C2'	14:N:-43:DT:H72	2.44	0.45
19:m:782:VAL:HG11	19:m:905:ILE:HG13	1.99	0.45
19:m:1218:ALA:HB1	19:m:1232:LEU:HB3	1.99	0.45
23:u:106:TRP:CD1	23:u:217:LYS:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:v:31:LYS:HA	25:x:147:ARG:HH12	1.82	0.45
2:B:387:ASP:H	9:I:91:ARG:NH2	2.14	0.45
2:B:886:LYS:HG2	2:B:890:TYR:OH	2.17	0.45
19:m:590:LYS:HD2	19:m:706:ASP:HB2	1.99	0.45
19:m:1039:MET:SD	19:m:1039:MET:N	2.90	0.45
21:q:641:ALA:HB2	21:q:658:GLN:HB2	1.99	0.45
28:c:42:ARG:O	29:d:85:THR:HA	2.16	0.45
16:T:-7:DG:H5'	26:e:40:ARG:HH11	1.82	0.44
18:W:451:GLN:HG3	18:W:458:THR:HA	1.98	0.44
19:m:1105:LEU:HD11	19:m:1128:LYS:HE2	1.98	0.44
19:m:1358:ASP:OD1	19:m:1361:GLU:N	2.33	0.44
24:v:29:LEU:HB2	25:x:147:ARG:HB3	1.98	0.44
2:B:640:ASP:OD1	2:B:640:ASP:N	2.50	0.44
2:B:778:MET:HE2	2:B:1094:ARG:HD3	1.99	0.44
3:C:79:MET:HE1	3:C:96:VAL:HG23	2.00	0.44
18:W:763:TYR:HB3	18:W:766:LYS:HD3	2.00	0.44
19:m:336:GLU:OE1	19:m:458:ARG:NH2	2.50	0.44
19:m:968:PRO:HA	19:m:971:ALA:HB3	1.99	0.44
21:q:178:ASN:HA	24:v:91:PHE:CE2	2.52	0.44
1:A:1041:ARG:O	1:A:1044:PHE:N	2.50	0.44
7:G:81:PRO:HG3	7:G:106:LEU:HD22	1.99	0.44
14:N:54:DT:H2''	14:N:55:DC:C5	2.52	0.44
19:m:640:TYR:HB3	19:m:1256:ASP:HB3	2.00	0.44
19:m:654:ASP:OD2	19:m:933:HIS:NE2	2.50	0.44
21:q:868:GLN:O	21:q:872:GLU:HG2	2.17	0.44
1:A:452:HIS:CE1	1:A:454:MET:HB2	2.52	0.44
3:C:258:VAL:HG21	11:K:42:LEU:HD21	2.00	0.44
14:N:12:DG:H2''	14:N:13:DT:C7	2.47	0.44
14:N:48:DG:H2''	14:N:49:DC:C6	2.53	0.44
23:u:117:ASN:HB3	23:u:151:ARG:HG2	2.00	0.44
1:A:779:GLY:HA3	2:B:509:ASN:HB2	1.99	0.44
1:A:880:GLU:O	1:A:957:PRO:HA	2.18	0.44
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	1.99	0.44
1:A:975:LEU:HD13	1:A:1039:LEU:HA	1.99	0.44
2:B:1050:LEU:HD12	24:v:127:PHE:CG	2.52	0.44
9:I:100:PHE:HB3	9:I:109:THR:HG23	1.99	0.44
14:N:-22:DA:H61	16:T:22:DT:H3	1.65	0.44
16:T:-31:DA:H2''	16:T:-30:DG:H8	1.82	0.44
21:q:40:ASP:CG	21:q:42:ASN:HD22	2.26	0.44
21:q:435:GLN:HG3	21:q:441:ILE:HD11	1.98	0.44
29:d:43:LYS:HA	29:d:43:LYS:HD3	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:j:738:PRO:CG	30:j:745:LYS:HE2	2.48	0.44
2:B:221:ALA:O	2:B:223:SER:N	2.46	0.44
17:V:78:GLN:OE1	17:V:79:PRO:HD2	2.16	0.44
19:m:603:ILE:HD13	19:m:708:TRP:HZ3	1.83	0.44
19:m:622:THR:O	19:m:626:LYS:N	2.41	0.44
24:v:307:PHE:HE1	24:v:335:GLY:HA3	1.83	0.44
25:x:314:PHE:HD2	25:x:335:ILE:HD11	1.82	0.44
27:b:38:ALA:HB1	27:b:43:VAL:HB	1.98	0.44
2:B:254:ASP:H	2:B:259:ARG:NH2	2.13	0.44
5:E:11:LEU:HD21	5:E:57:MET:HE1	2.00	0.44
5:E:99:ILE:HG13	5:E:131:ILE:HD11	2.00	0.44
14:N:8:DG:C6	16:T:-9:DA:N6	2.86	0.44
19:m:536:ILE:HG12	19:m:700:TRP:CZ3	2.53	0.44
4:D:88:GLU:HA	4:D:91:LYS:HE3	2.00	0.44
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.00	0.44
19:m:305:ASP:OD1	19:m:1014:THR:OG1	2.33	0.44
20:n:200:ARG:HG2	20:n:202:ASN:OD1	2.18	0.44
21:q:357:LYS:NZ	21:q:361:ASP:OD1	2.50	0.44
21:q:559:ARG:NH2	24:v:24:PRO:O	2.51	0.44
30:j:622:SER:CB	30:j:628:MET:HE2	2.48	0.44
2:B:257:THR:OG1	2:B:258:GLY:N	2.50	0.44
19:m:1029:PRO:O	19:m:1033:ARG:NH1	2.50	0.44
22:r:244:LYS:NZ	22:r:305:GLU:OE2	2.37	0.44
1:A:100:LYS:NZ	1:A:104:GLU:OE2	2.49	0.43
1:A:948:VAL:O	5:E:200:ARG:NH1	2.48	0.43
2:B:691:ASP:OD1	2:B:691:ASP:N	2.41	0.43
8:H:25:ARG:HD3	8:H:41:ASP:OD1	2.18	0.43
14:N:-47:DC:H2"	14:N:-46:DT:C5	2.53	0.43
14:N:8:DG:O6	16:T:-9:DA:N6	2.51	0.43
21:q:215:ASP:OD1	21:q:217:ARG:NH1	2.47	0.43
21:q:217:ARG:HA	21:q:220:ILE:HD12	2.00	0.43
28:c:50:TYR:O	28:c:54:VAL:HG23	2.18	0.43
26:e:60:LEU:HD22	26:e:93:GLN:HG2	2.00	0.43
27:f:64:ASN:HA	27:f:67:ARG:NH1	2.32	0.43
31:k:223:VAL:HG23	31:k:308:VAL:HG11	2.00	0.43
10:J:63:ASN:OD1	10:J:64:PRO:HD2	2.19	0.43
19:m:999:LEU:HD23	19:m:1025:ILE:HD11	1.99	0.43
3:C:15:ASP:OD1	3:C:15:ASP:N	2.47	0.43
19:m:955:ASN:HD21	19:m:978:CYS:HB3	1.83	0.43
19:m:1309:ARG:NH2	19:m:1319:THR:HG21	2.33	0.43
21:q:53:LEU:O	21:q:57:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:511:VAL:HG11	21:q:519:LEU:HD12	2.01	0.43
22:r:370:GLU:HG3	23:u:251:VAL:HA	2.01	0.43
28:g:16:THR:O	28:g:19:SER:OG	2.36	0.43
29:h:51:ILE:HG22	29:h:52:SER:O	2.18	0.43
1:A:1389:ARG:O	1:A:1393:ASN:HB2	2.18	0.43
7:G:115:ILE:HG23	7:G:163:ILE:HD11	2.01	0.43
16:T:-72:DA:H2''	16:T:-71:DT:H71	2.00	0.43
19:m:735:LEU:HB3	19:m:937:LEU:HD21	1.99	0.43
20:n:167:MET:HE3	20:n:219:TRP:CD2	2.53	0.43
24:v:41:LYS:HB3	24:v:45:LYS:HE3	2.00	0.43
30:j:543:LYS:HG3	31:k:61:ARG:HA	2.00	0.43
1:A:38:PRO:HA	1:A:271:LEU:HD23	2.01	0.43
2:B:733:SER:HB3	2:B:736:HIS:CE1	2.54	0.43
17:V:67:TRP:NE1	18:W:217:LEU:O	2.51	0.43
22:r:206:PHE:H	22:r:229:LEU:HD21	1.82	0.43
23:u:116:ILE:HD13	23:u:150:VAL:HB	1.99	0.43
27:b:32:PRO:O	27:b:36:ARG:HG3	2.18	0.43
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.90	0.43
1:A:889:GLY:O	1:A:941:ARG:NH2	2.51	0.43
2:B:330:GLY:HA3	2:B:344:TYR:HE2	1.84	0.43
16:T:-67:DA:C6	16:T:-66:DA:C6	3.06	0.43
18:W:250:ARG:NH2	18:W:284:ASP:OD2	2.50	0.43
18:W:344:LEU:HD12	18:W:349:GLU:HB2	1.99	0.43
20:n:195:LYS:HE3	20:n:199:LEU:HD11	2.01	0.43
21:q:611:GLU:HG2	21:q:615:HIS:CD2	2.54	0.43
23:u:83:GLY:HA2	24:v:358:ALA:HB3	2.01	0.43
25:x:226:LYS:HB2	25:x:248:LEU:HD21	2.00	0.43
1:A:636:ARG:HH12	1:A:878:GLN:CD	2.25	0.43
1:A:1343:GLY:HA2	5:E:182:PRO:HD2	2.01	0.43
2:B:283:VAL:HG13	2:B:283:VAL:O	2.18	0.43
14:N:5:DT:OP2	27:f:32:PRO:HD2	2.18	0.43
14:N:38:DG:C2	16:T:-37:DG:C2	3.06	0.43
21:q:261:ASP:HB2	24:v:58:ASN:ND2	2.34	0.43
25:x:222:MET:HE3	25:x:222:MET:HB3	1.84	0.43
28:c:100:VAL:HG12	27:f:96:THR:HB	2.00	0.43
28:g:31:HIS:CD2	28:g:35:ARG:HH12	2.37	0.43
1:A:318:LYS:HE3	16:T:35:DC:N3	2.34	0.43
3:C:248:ILE:HG21	11:K:102:ASP:HB2	2.01	0.43
14:N:-44:DG:H2''	14:N:-43:DT:OP2	2.19	0.43
14:N:2:DG:N2	16:T:-1:DG:H22	2.16	0.43
14:N:28:DA:H2''	14:N:29:DG:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:8:C:C2	16:T:28:DG:C2	3.07	0.43
19:m:960:ASP:HB2	19:m:1024:TYR:CZ	2.54	0.43
20:n:157:ASP:HA	20:n:210:ASN:HD21	1.83	0.43
21:q:122:ARG:HB2	21:q:126:PHE:CE2	2.54	0.43
1:A:252:ALA:HA	1:A:258:GLN:HA	2.00	0.43
2:B:262:LYS:HB3	2:B:271:ASP:HB3	2.01	0.43
18:W:322:ARG:NE	18:W:343:VAL:H	2.17	0.43
19:m:538:ASN:HB3	19:m:541:GLN:HB2	2.00	0.43
21:q:261:ASP:O	21:q:265:ASN:ND2	2.36	0.43
20:n:208:LEU:HD22	20:n:250:HIS:CD2	2.54	0.43
22:r:245:VAL:HG23	22:r:298:GLU:HG2	2.01	0.43
1:A:815:PHE:O	1:A:819:MET:HG3	2.19	0.42
2:B:592:THR:HG23	23:u:226:PHE:CZ	2.54	0.42
21:q:526:ASN:O	21:q:530:VAL:HG23	2.18	0.42
28:g:31:HIS:CE1	28:g:35:ARG:HH12	2.37	0.42
1:A:844:LYS:HD2	1:A:844:LYS:HA	1.79	0.42
3:C:36:MET:HE3	3:C:176:ILE:HD13	2.01	0.42
6:F:103:MET:HE1	7:G:65:SER:O	2.19	0.42
16:T:-9:DA:P	27:f:35:ARG:HH22	2.42	0.42
17:V:12:CYS:HA	17:V:50:THR:HA	2.01	0.42
18:W:543:ILE:HD11	18:W:581:ILE:HG13	2.01	0.42
1:A:473:LEU:HD21	2:B:835:GLN:HB2	2.00	0.42
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.85	0.42
5:E:104:PHE:HZ	21:q:925:TRP:HZ3	1.66	0.42
12:L:60:LYS:HB3	12:L:60:LYS:HE3	1.87	0.42
18:W:490:GLU:CD	20:n:229:PRO:HA	2.44	0.42
22:r:277:PRO:HB2	22:r:305:GLU:HB3	2.00	0.42
2:B:1156:ASP:O	2:B:1197:PRO:HA	2.19	0.42
16:T:-28:DT:C6	16:T:-27:DC:C5	3.07	0.42
16:T:-22:DA:H2''	16:T:-21:DC:C5	2.53	0.42
19:m:1399:SER:HA	19:m:1407:HIS:CE1	2.54	0.42
24:v:202:PRO:HG2	24:v:382:TYR:OH	2.19	0.42
2:B:279:ARG:NH1	2:B:316:ILE:O	2.52	0.42
2:B:299:ASP:OD2	2:B:385:ARG:NH1	2.30	0.42
2:B:479:TYR:CE2	2:B:778:MET:HG2	2.55	0.42
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.02	0.42
5:E:176:ARG:HD3	5:E:214:LEU:HD11	2.02	0.42
14:N:-44:DG:H2''	14:N:-43:DT:C7	2.48	0.42
18:W:468:LEU:HD11	19:m:283:VAL:HG13	2.01	0.42
18:W:518:ILE:HD13	20:n:185:ILE:HD13	2.00	0.42
19:m:708:TRP:CZ2	19:m:712:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:n:161:GLN:O	20:n:165:LEU:HG	2.19	0.42
28:g:34:LEU:HD23	28:g:34:LEU:HA	1.91	0.42
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.02	0.42
16:T:-51:DC:OP1	29:d:84:SER:N	2.46	0.42
17:V:13:MET:HE2	17:V:51:SER:HB2	2.01	0.42
19:m:750:ALA:HB2	19:m:1139:ARG:HB2	2.01	0.42
19:m:1246:LEU:HB3	19:m:1248:VAL:HG23	2.01	0.42
29:h:76:ARG:HG2	29:h:80:TYR:CE2	2.54	0.42
1:A:1201:ARG:HA	1:A:1238:LEU:HD12	2.01	0.42
1:A:1221:VAL:HG21	1:A:1274:ILE:HD12	2.00	0.42
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.51	0.42
2:B:837:ASP:CG	2:B:1020:ARG:HH22	2.28	0.42
5:E:42:ARG:HG3	5:E:46:CYS:SG	2.59	0.42
18:W:539:HIS:HB2	18:W:584:THR:HA	2.02	0.42
29:h:108:VAL:O	29:h:112:THR:HG23	2.19	0.42
30:j:595:MET:HE2	30:j:595:MET:HB3	1.98	0.42
31:k:286:LEU:HD23	31:k:286:LEU:HA	1.89	0.42
1:A:421:ARG:HB3	1:A:424:ASP:HB2	2.01	0.42
2:B:85:SER:OG	2:B:114:PRO:HD2	2.19	0.42
6:F:81:THR:OG1	6:F:144:GLU:OE1	2.35	0.42
19:m:955:ASN:ND2	19:m:978:CYS:HB3	2.35	0.42
19:m:1000:VAL:HB	19:m:1004:HIS:ND1	2.35	0.42
20:n:177:ASN:HD21	20:n:186:PHE:HE2	1.67	0.42
21:q:29:PRO:HA	21:q:36:VAL:HG12	2.02	0.42
21:q:830:LEU:HD22	21:q:846:LEU:HB3	2.02	0.42
29:d:103:LEU:HD12	29:d:103:LEU:HA	1.88	0.42
30:j:730:ILE:HG21	30:j:750:GLN:HE21	1.83	0.42
2:B:606:VAL:HG22	2:B:621:THR:HG22	2.02	0.42
2:B:807:GLN:OE1	24:v:129:ARG:NH1	2.51	0.42
6:F:99:LEU:HG	6:F:103:MET:HE2	2.02	0.42
7:G:165:GLU:H	7:G:168:LEU:HD12	1.85	0.42
14:N:-51:DG:C2'	14:N:-50:DT:C7	2.93	0.42
19:m:306:LEU:O	19:m:311:GLN:NE2	2.51	0.42
19:m:773:GLY:N	19:m:777:ASP:OD2	2.52	0.42
19:m:821:ASP:HA	19:m:850:ILE:HD13	2.01	0.42
19:m:1005:LEU:HA	19:m:1010:LEU:HD12	2.01	0.42
21:q:189:LEU:HB3	21:q:194:LYS:HB2	2.01	0.42
31:k:258:GLN:OE1	31:k:260:LYS:HE2	2.20	0.42
31:k:269:PRO:HB3	31:k:302:ARG:HH21	1.85	0.42
15:P:-5:C:C6	18:W:748:ARG:HB2	2.55	0.42
17:V:80:GLY:HA2	18:W:244:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:480:PRO:HA	18:W:498:VAL:HG12	2.02	0.42
19:m:597:LEU:HD13	19:m:708:TRP:HE3	1.84	0.42
21:q:9:TYR:OH	24:v:106:ASP:OD2	2.20	0.42
21:q:284:LEU:HD11	21:q:297:LEU:HD22	2.01	0.42
21:q:562:TYR:CZ	21:q:566:LEU:HD11	2.55	0.42
26:a:65:LEU:HG	26:a:69:ARG:NH1	2.34	0.42
31:k:388:LYS:HA	31:k:389:PRO:HA	1.80	0.42
1:A:691:VAL:HG11	1:A:795:PRO:HG3	2.02	0.41
2:B:892:LYS:NZ	2:B:909:ASP:OD2	2.45	0.41
9:I:29:CYS:SG	9:I:30:ARG:N	2.92	0.41
16:T:-37:DG:H2'	16:T:-36:DT:H72	2.02	0.41
19:m:656:TYR:CE2	19:m:660:ILE:HD11	2.54	0.41
21:q:673:ASP:OD1	25:x:157:ARG:NH2	2.46	0.41
21:q:841:TYR:HB2	21:q:846:LEU:HD21	2.01	0.41
25:x:345:GLN:O	25:x:349:GLN:HG3	2.20	0.41
30:j:652:MET:C	30:j:654:ASP:N	2.76	0.41
1:A:473:LEU:CD2	2:B:835:GLN:HB2	2.50	0.41
1:A:1210:THR:HG22	1:A:1212:ASN:H	1.86	0.41
2:B:764:SER:OG	2:B:765:PRO:HD3	2.19	0.41
2:B:1152:MET:HE3	2:B:1152:MET:HB3	1.91	0.41
14:N:-21:DA:H61	16:T:21:DT:H3	1.69	0.41
18:W:329:LYS:HB2	18:W:434:ASN:HA	2.02	0.41
19:m:423:ASP:O	19:m:427:ILE:HG23	2.21	0.41
21:q:189:LEU:HD13	21:q:197:GLN:HB2	2.02	0.41
22:r:208:ARG:HA	22:r:211:MET:HE3	2.02	0.41
22:r:408:ASP:OD2	24:v:133:TYR:HB2	2.20	0.41
26:a:73:GLU:OE1	27:b:25:ASN:HB2	2.20	0.41
2:B:33:GLN:HG2	2:B:34:GLN:N	2.36	0.41
2:B:763:GLN:HG2	2:B:765:PRO:HD2	2.01	0.41
8:H:6:PHE:HB3	8:H:59:LEU:HB2	2.03	0.41
11:K:25:SER:O	25:x:307:GLN:NE2	2.54	0.41
14:N:8:DG:N2	16:T:-7:DG:N3	2.69	0.41
18:W:422:TYR:HB3	18:W:427:TYR:CE1	2.55	0.41
20:n:171:ALA:HB2	20:n:219:TRP:CD1	2.55	0.41
21:q:638:ALA:HB1	21:q:642:ARG:HH22	1.84	0.41
1:A:1218:ILE:HG12	1:A:1270:MET:HE1	2.02	0.41
2:B:293:ILE:HD13	2:B:375:VAL:HG11	2.02	0.41
3:C:74:GLU:O	3:C:246:ARG:NH2	2.39	0.41
9:I:94:ASP:OD1	9:I:94:ASP:N	2.49	0.41
13:M:39:ASP:HB3	13:M:44:ILE:HG13	2.03	0.41
21:q:66:SER:O	21:q:70:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:135:ARG:HE	3:C:136:ASP:CG	2.28	0.41
5:E:36:GLN:HE21	5:E:36:GLN:HB3	1.69	0.41
14:N:66:DT:H2'	14:N:67:DT:C6	2.55	0.41
18:W:349:GLU:HA	18:W:431:ARG:HA	2.02	0.41
19:m:1002:ARG:NH2	19:m:1023:VAL:O	2.47	0.41
22:r:316:LEU:HD23	22:r:316:LEU:HA	1.83	0.41
22:r:432:LEU:HD12	22:r:433:ARG:HD2	2.02	0.41
23:u:168:SER:HB2	24:v:200:PHE:HB3	2.02	0.41
28:c:61:GLU:O	28:c:65:LEU:HG	2.20	0.41
27:f:46:ILE:HG22	27:f:47:SER:O	2.20	0.41
27:f:51:TYR:O	27:f:55:ARG:HG3	2.20	0.41
1:A:914:ILE:HG13	1:A:917:ALA:HB2	2.01	0.41
1:A:976:ASP:O	1:A:979:LYS:NZ	2.48	0.41
9:I:29:CYS:HB3	9:I:32:CYS:SG	2.59	0.41
16:T:29:DA:H2'	16:T:30:DA:C8	2.56	0.41
19:m:283:VAL:HG12	19:m:284:PHE:CD1	2.56	0.41
19:m:764:ARG:N	19:m:821:ASP:OD2	2.48	0.41
19:m:1255:TRP:HD1	19:m:1257:ILE:HG12	1.85	0.41
19:m:1279:ARG:NH2	19:m:1344:ALA:O	2.51	0.41
21:q:278:ARG:NH2	22:r:507:ASP:O	2.53	0.41
2:B:350:GLN:HE22	2:B:361:GLU:HG2	1.86	0.41
2:B:1153:GLU:OE1	2:B:1153:GLU:N	2.53	0.41
3:C:149:ASN:OD1	3:C:149:ASN:N	2.54	0.41
5:E:3:ASP:HA	5:E:6:ARG:HG2	2.01	0.41
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.78	0.41
8:H:8:ASP:OD1	8:H:9:ILE:N	2.48	0.41
15:P:-1:G:H2'	15:P:0:G:H8	1.86	0.41
16:T:-61:DG:OP1	28:c:32:ARG:NH1	2.52	0.41
18:W:614:ARG:NH2	18:W:616:GLN:HE21	2.19	0.41
19:m:1175:VAL:HA	19:m:1180:MET:HG3	2.03	0.41
21:q:350:VAL:HA	21:q:380:ARG:NH1	2.36	0.41
3:C:259:LEU:HD13	11:K:91:CYS:HB2	2.03	0.41
16:T:-72:DA:H2''	16:T:-71:DT:OP2	2.21	0.41
19:m:314:ARG:HD3	19:m:320:TYR:CE1	2.56	0.41
24:v:205:SER:O	24:v:379:ARG:NH2	2.49	0.41
25:x:301:ASP:OD1	25:x:303:GLN:NE2	2.54	0.41
30:j:587:ARG:HH12	31:k:289:GLY:C	2.28	0.41
1:A:109:ASN:HB2	1:A:168:CYS:SG	2.61	0.41
1:A:471:LEU:HD23	1:A:475:VAL:HG23	2.03	0.41
1:A:1150:SER:OG	1:A:1198:GLU:OE1	2.29	0.41
1:A:1314:ILE:HB	1:A:1337:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:PRO:HB2	9:I:11:ASN:HD22	1.86	0.41
2:B:425:MET:O	2:B:429:ILE:HG13	2.21	0.41
2:B:439:LEU:HD11	23:u:264:LEU:HB3	2.03	0.41
2:B:575:VAL:O	2:B:578:VAL:HG22	2.20	0.41
2:B:632:ILE:HD11	2:B:688:GLU:HB3	2.03	0.41
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.79	0.41
3:C:251:LEU:HD12	3:C:251:LEU:HA	1.92	0.41
4:D:53:LEU:HD13	4:D:147:SER:HB3	2.02	0.41
14:N:-42:DG:C8	14:N:-41:DT:C7	3.04	0.41
16:T:-40:DG:C8	16:T:-39:DT:H73	2.56	0.41
16:T:-18:DC:H2'	16:T:-17:DT:H71	2.02	0.41
18:W:540:VAL:HG11	18:W:554:ILE:HD11	2.01	0.41
19:m:313:TYR:HB3	19:m:422:LEU:HD11	2.03	0.41
19:m:674:LEU:HD12	19:m:675:PRO:HD2	2.02	0.41
19:m:743:PHE:O	19:m:747:ILE:HG12	2.20	0.41
19:m:780:LEU:HD12	19:m:780:LEU:HA	1.90	0.41
20:n:241:ILE:HG23	20:n:246:ILE:HD12	2.03	0.41
21:q:905:ARG:NE	21:q:909:GLU:OE2	2.30	0.41
23:u:121:PHE:CE2	23:u:123:PRO:HG3	2.56	0.41
28:c:29:ARG:NH1	29:d:32:GLU:HB3	2.36	0.41
27:f:38:ALA:HB1	27:f:43:VAL:HB	2.02	0.41
30:j:730:ILE:CG2	30:j:750:GLN:HE21	2.33	0.41
31:k:37:THR:O	31:k:38:LYS:C	2.64	0.41
1:A:883:THR:HA	1:A:954:HIS:O	2.20	0.41
1:A:945:ARG:HG3	1:A:1301:TYR:OH	2.21	0.41
2:B:71:ILE:HG12	2:B:127:ILE:HG22	2.02	0.41
8:H:38:LEU:HD13	8:H:124:LEU:HD13	2.03	0.41
11:K:39:ASP:OD1	11:K:39:ASP:N	2.54	0.41
14:N:-22:DA:N6	16:T:22:DT:H3	2.19	0.41
14:N:34:DC:C4	14:N:35:DT:C4	3.09	0.41
16:T:-19:DG:H2''	16:T:-18:DC:C5	2.56	0.41
21:q:341:ARG:NH2	24:v:47:SER:O	2.54	0.41
21:q:410:GLY:HA2	21:q:423:ALA:HA	2.03	0.41
26:a:51:ILE:O	26:a:55:GLN:HG3	2.20	0.41
28:g:88:ARG:NE	28:g:94:ASN:OD1	2.46	0.41
1:A:636:ARG:HG3	1:A:880:GLU:OE2	2.21	0.40
1:A:701:ASN:CG	9:I:96:ASN:HD21	2.26	0.40
1:A:985:ILE:N	1:A:986:PRO:HD2	2.36	0.40
1:A:1295:PRO:HD3	1:A:1301:TYR:CE1	2.56	0.40
2:B:86:ARG:NH2	22:r:369:GLU:OE1	2.54	0.40
18:W:492:ASN:OD1	18:W:493:HIS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:524:GLU:HB2	20:n:232:GLN:HE22	1.85	0.40
19:m:1092:ASP:OD1	19:m:1092:ASP:N	2.48	0.40
19:m:1136:ARG:HD2	19:m:1137:GLU:O	2.21	0.40
22:r:275:ALA:HB2	22:r:281:GLU:HA	2.01	0.40
22:r:432:LEU:HD11	22:r:433:ARG:NH1	2.36	0.40
27:b:97:LEU:HD21	27:b:100:PHE:CD2	2.56	0.40
1:A:390:THR:O	1:A:394:ARG:HG2	2.20	0.40
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.88	0.40
2:B:1174:ASN:OD1	2:B:1177:LYS:HB2	2.20	0.40
3:C:135:ARG:NE	3:C:136:ASP:OD2	2.50	0.40
6:F:93:ILE:HD13	6:F:93:ILE:HA	1.97	0.40
9:I:62:ILE:HD12	9:I:62:ILE:HA	1.93	0.40
19:m:586:TYR:CE2	19:m:703:LEU:HD12	2.56	0.40
19:m:709:LYS:HA	19:m:712:LEU:HD12	2.02	0.40
19:m:1268:ILE:O	19:m:1272:ARG:HG3	2.21	0.40
21:q:609:ASP:O	21:q:613:GLN:HG3	2.20	0.40
21:q:756:TRP:HB3	21:q:772:ALA:HB2	2.03	0.40
21:q:861:LEU:HD23	21:q:861:LEU:HA	1.95	0.40
28:g:21:ALA:HB2	29:h:118:TYR:HB2	2.02	0.40
1:A:995:LEU:HD22	1:A:1048:LEU:HD22	2.03	0.40
2:B:928:ARG:HH11	19:m:776:GLY:H	1.68	0.40
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.55	0.40
14:N:5:DT:OP1	27:f:30:THR:HG22	2.20	0.40
19:m:397:ASN:HB3	19:m:401:ASN:HA	2.02	0.40
19:m:524:ILE:O	19:m:530:TYR:HB2	2.22	0.40
19:m:588:ALA:HA	19:m:591:GLN:HG2	2.04	0.40
19:m:884:TYR:CE1	19:m:890:SER:HB3	2.56	0.40
21:q:341:ARG:NH2	24:v:50:LEU:HB2	2.36	0.40
24:v:136:ASP:N	24:v:136:ASP:OD1	2.54	0.40
26:a:120:MET:HE2	26:a:122:LYS:HE2	2.03	0.40
12:L:33:CYS:SG	12:L:34:GLY:N	2.95	0.40
14:N:12:DG:H2''	14:N:13:DT:C5	2.56	0.40
19:m:1290:LYS:H	19:m:1293:GLU:HB2	1.87	0.40
21:q:224:PHE:CD1	21:q:229:ASN:HB3	2.56	0.40
21:q:520:SER:O	21:q:524:HIS:ND1	2.52	0.40
28:c:88:ARG:HA	28:c:88:ARG:HD3	1.94	0.40
31:k:10:PHE:CD2	31:k:61:ARG:NH1	2.89	0.40
1:A:231:ARG:HB3	1:A:234:TRP:CD2	2.56	0.40
3:C:262:LEU:HD11	11:K:87:LEU:HD23	2.03	0.40
11:K:55:ASP:OD2	11:K:89:ARG:NH2	2.54	0.40
12:L:66:MET:HE1	18:W:804:TRP:HZ2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:32:DG:N1	16:T:-33:DA:C2	2.90	0.40
14:N:66:DT:H2'	14:N:67:DT:C5	2.57	0.40
16:T:20:DT:C6	16:T:21:DT:H73	2.56	0.40
18:W:598:LEU:HD12	18:W:599:HIS:H	1.86	0.40
21:q:687:PHE:O	21:q:691:GLU:N	2.54	0.40
22:r:211:MET:HB3	22:r:286:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1392/1743 (80%)	1355 (97%)	36 (3%)	1 (0%)	48	82
2	B	1154/1227 (94%)	1119 (97%)	35 (3%)	0	100	100
3	C	261/304 (86%)	259 (99%)	2 (1%)	0	100	100
4	D	170/186 (91%)	167 (98%)	3 (2%)	0	100	100
5	E	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	167 (99%)	2 (1%)	0	100	100
8	H	129/145 (89%)	125 (97%)	4 (3%)	0	100	100
9	I	109/115 (95%)	107 (98%)	2 (2%)	0	100	100
10	J	65/72 (90%)	65 (100%)	0	0	100	100
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
12	L	43/72 (60%)	41 (95%)	2 (5%)	0	100	100
13	M	62/113 (55%)	62 (100%)	0	0	100	100
17	V	104/108 (96%)	100 (96%)	4 (4%)	0	100	100
18	W	527/911 (58%)	508 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	m	1179/1503 (78%)	1158 (98%)	21 (2%)	0	100	100
20	n	137/417 (33%)	136 (99%)	1 (1%)	0	100	100
21	q	928/1084 (86%)	922 (99%)	6 (1%)	0	100	100
22	r	260/544 (48%)	254 (98%)	6 (2%)	0	100	100
23	u	206/459 (45%)	204 (99%)	2 (1%)	0	100	100
24	v	341/396 (86%)	327 (96%)	14 (4%)	0	100	100
25	x	201/395 (51%)	200 (100%)	1 (0%)	0	100	100
26	a	90/139 (65%)	86 (96%)	4 (4%)	0	100	100
26	e	95/139 (68%)	93 (98%)	1 (1%)	1 (1%)	11	45
27	b	79/106 (74%)	76 (96%)	3 (4%)	0	100	100
27	f	76/106 (72%)	73 (96%)	3 (4%)	0	100	100
28	c	94/133 (71%)	93 (99%)	1 (1%)	0	100	100
28	g	96/133 (72%)	93 (97%)	3 (3%)	0	100	100
29	d	90/129 (70%)	86 (96%)	4 (4%)	0	100	100
29	h	91/129 (70%)	90 (99%)	1 (1%)	0	100	100
30	j	466/1008 (46%)	433 (93%)	28 (6%)	5 (1%)	11	45
31	k	423/531 (80%)	404 (96%)	18 (4%)	1 (0%)	43	77
All	All	9441/13005 (73%)	9198 (97%)	235 (2%)	8 (0%)	49	82

All (8) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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%)	1018 (100%)	0	100	100
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	480/796 (60%)	480 (100%)	0	100	100
19	m	1087/1354 (80%)	1087 (100%)	0	100	100
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%)	192 (100%)	0	100	100
24	v	325/369 (88%)	325 (100%)	0	100	100
25	x	190/354 (54%)	190 (100%)	0	100	100
26	a	78/112 (70%)	78 (100%)	0	100	100
26	e	82/112 (73%)	82 (100%)	0	100	100
27	b	66/81 (82%)	66 (100%)	0	100	100
27	f	63/81 (78%)	63 (100%)	0	100	100
28	c	76/102 (74%)	76 (100%)	0	100	100
28	g	77/102 (76%)	77 (100%)	0	100	100
29	d	78/107 (73%)	78 (100%)	0	100	100
29	h	79/107 (74%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	j	400/910 (44%)	398 (100%)	2 (0%)	81	81
31	k	392/474 (83%)	390 (100%)	2 (0%)	81	81
All	All	8474/11447 (74%)	8470 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	j	939	PHE
30	j	940	LEU
31	k	143	ASN
31	k	253	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	265	HIS
1	A	291	ASN
1	A	295	GLN
1	A	364	GLN
1	A	491	HIS
1	A	737	ASN
1	A	1021	GLN
1	A	1056	GLN
2	B	157	HIS
2	B	215	GLN
2	B	317	GLN
2	B	350	GLN
2	B	388	GLN
2	B	438	ASN
2	B	736	HIS
2	B	1074	ASN
3	C	11	ASN
3	C	13	GLN
3	C	25	ASN
3	C	150	HIS
4	D	130	ASN
5	E	31	GLN
5	E	36	GLN
5	E	142	ASN

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Mol	Chain	Res	Type
8	H	44	ASN
9	I	11	ASN
10	J	52	HIS
13	M	32	ASN
18	W	242	GLN
18	W	283	ASN
18	W	547	HIS
19	m	299	ASN
19	m	402	ASN
19	m	428	HIS
19	m	896	ASN
19	m	1116	HIS
19	m	1288	ASN
19	m	1338	ASN
19	m	1407	HIS
20	n	156	GLN
20	n	177	ASN
20	n	232	GLN
21	q	105	HIS
21	q	187	GLN
21	q	319	ASN
21	q	397	ASN
21	q	398	GLN
21	q	438	ASN
21	q	615	HIS
21	q	625	HIS
21	q	658	GLN
21	q	781	GLN
22	r	336	ASN
22	r	416	ASN
22	r	493	ASN
23	u	138	GLN
24	v	229	ASN
24	v	283	ASN
24	v	381	GLN
25	x	251	GLN
26	a	55	GLN
26	a	76	GLN
27	b	25	ASN
27	b	75	HIS
29	d	64	ASN
29	d	92	GLN

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Mol	Chain	Res	Type
30	j	750	GLN
30	j	841	GLN
30	j	887	ASN
30	j	916	ASN
31	k	125	ASN
31	k	127	ASN
31	k	148	HIS
31	k	362	GLN
31	k	420	GLN

5.3.3 RNA ⓘ

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

All (6) RNA backbone outliers are listed below:

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

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	-7	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no 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.

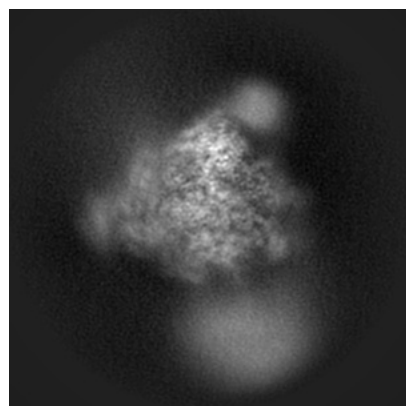
6 Map visualisation [i](#)

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

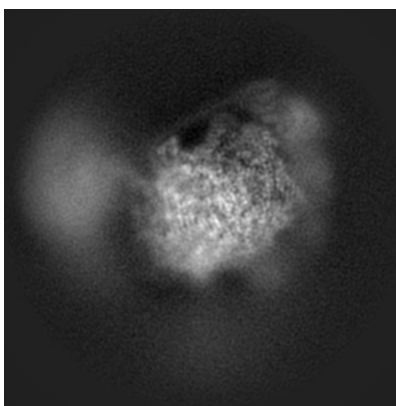
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

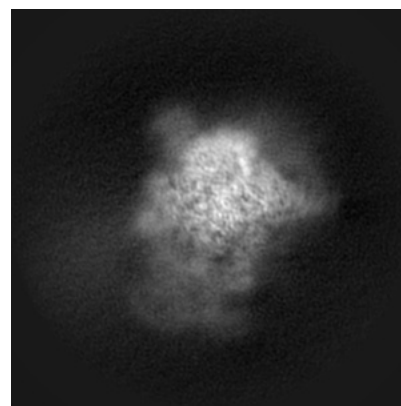
6.1.1 Primary map



X

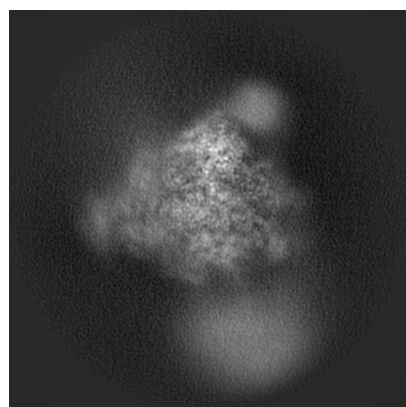


Y

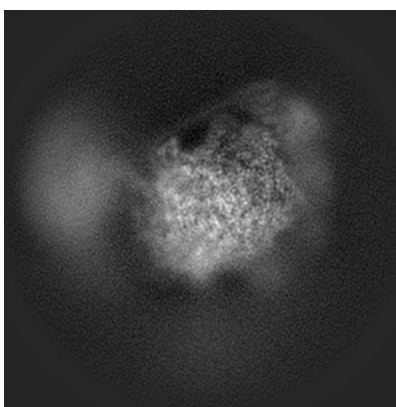


Z

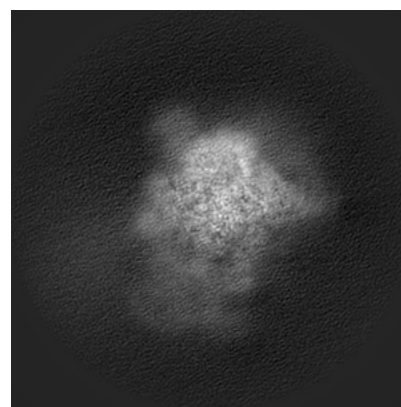
6.1.2 Raw map



X



Y

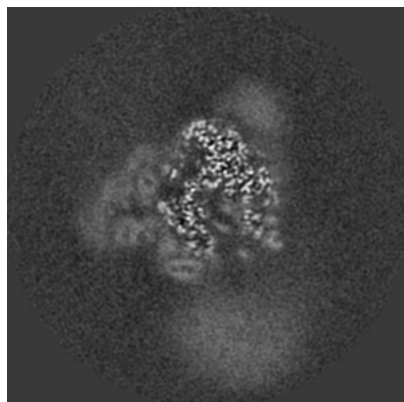


Z

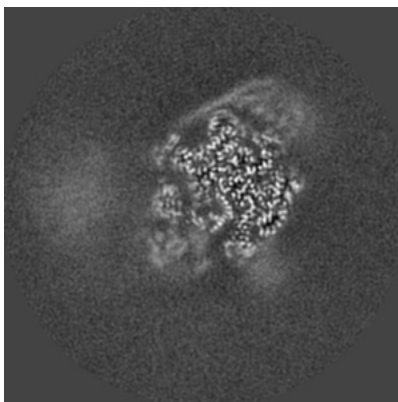
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

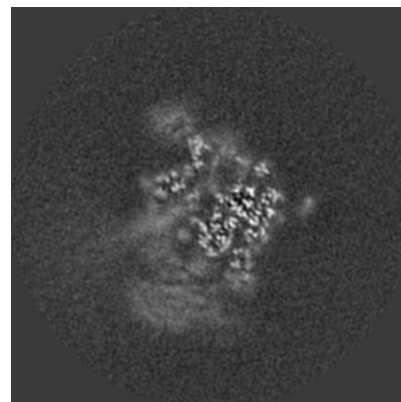
6.2.1 Primary map



X Index: 120

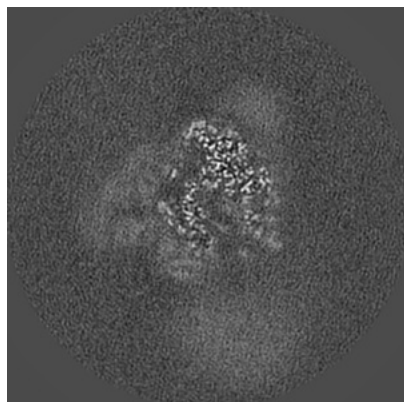


Y Index: 120

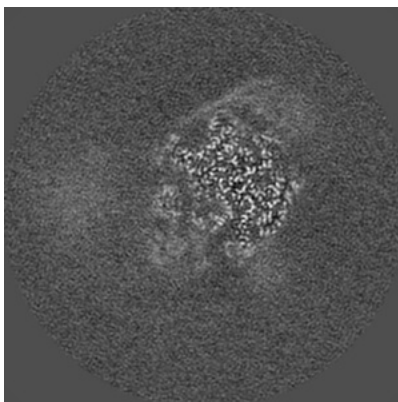


Z Index: 120

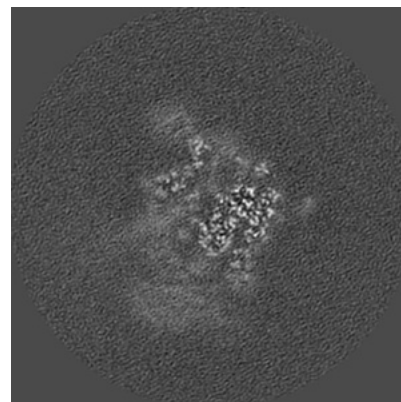
6.2.2 Raw map



X Index: 120



Y Index: 120

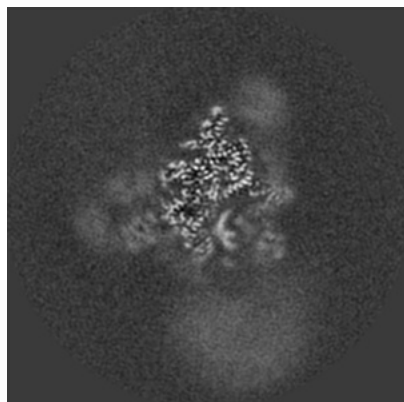


Z Index: 120

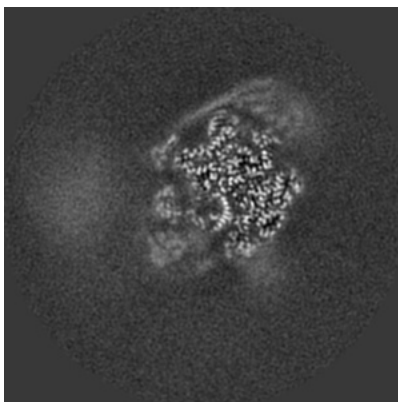
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

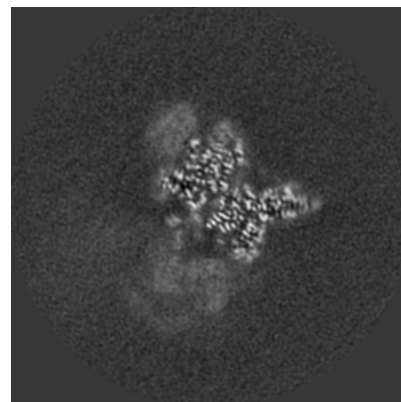
6.3.1 Primary map



X Index: 127

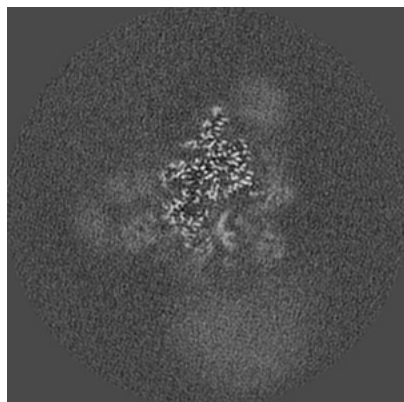


Y Index: 121

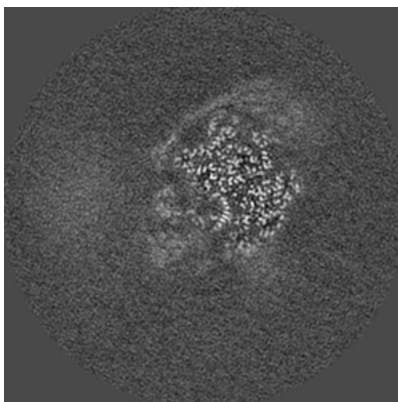


Z Index: 129

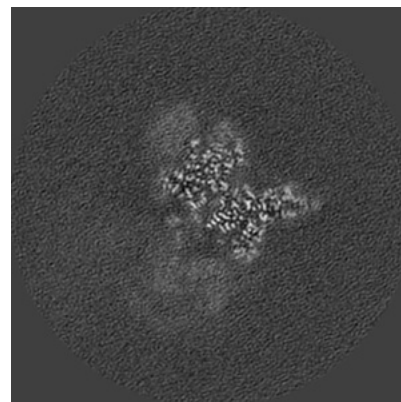
6.3.2 Raw map



X Index: 127



Y Index: 121

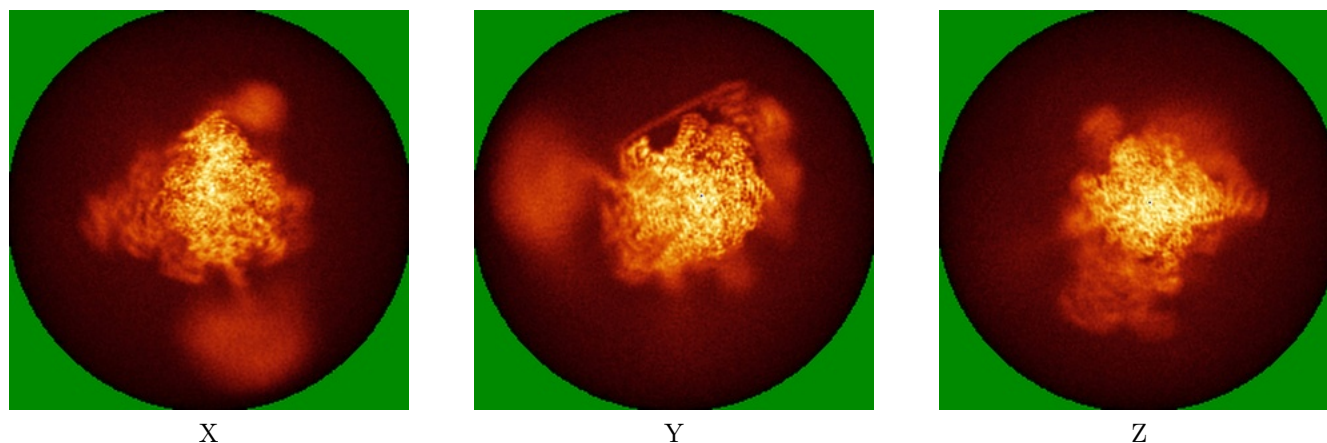


Z Index: 129

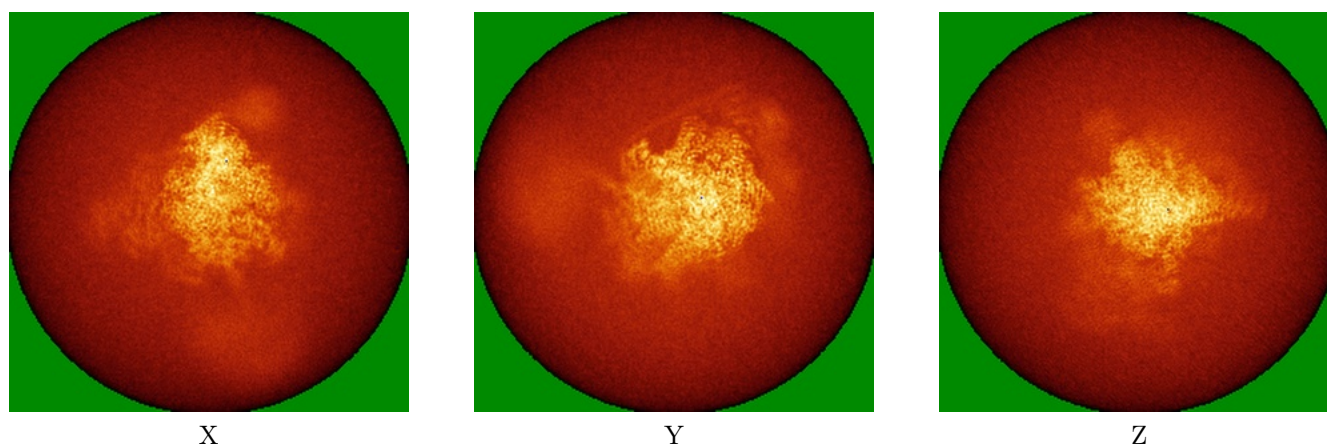
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

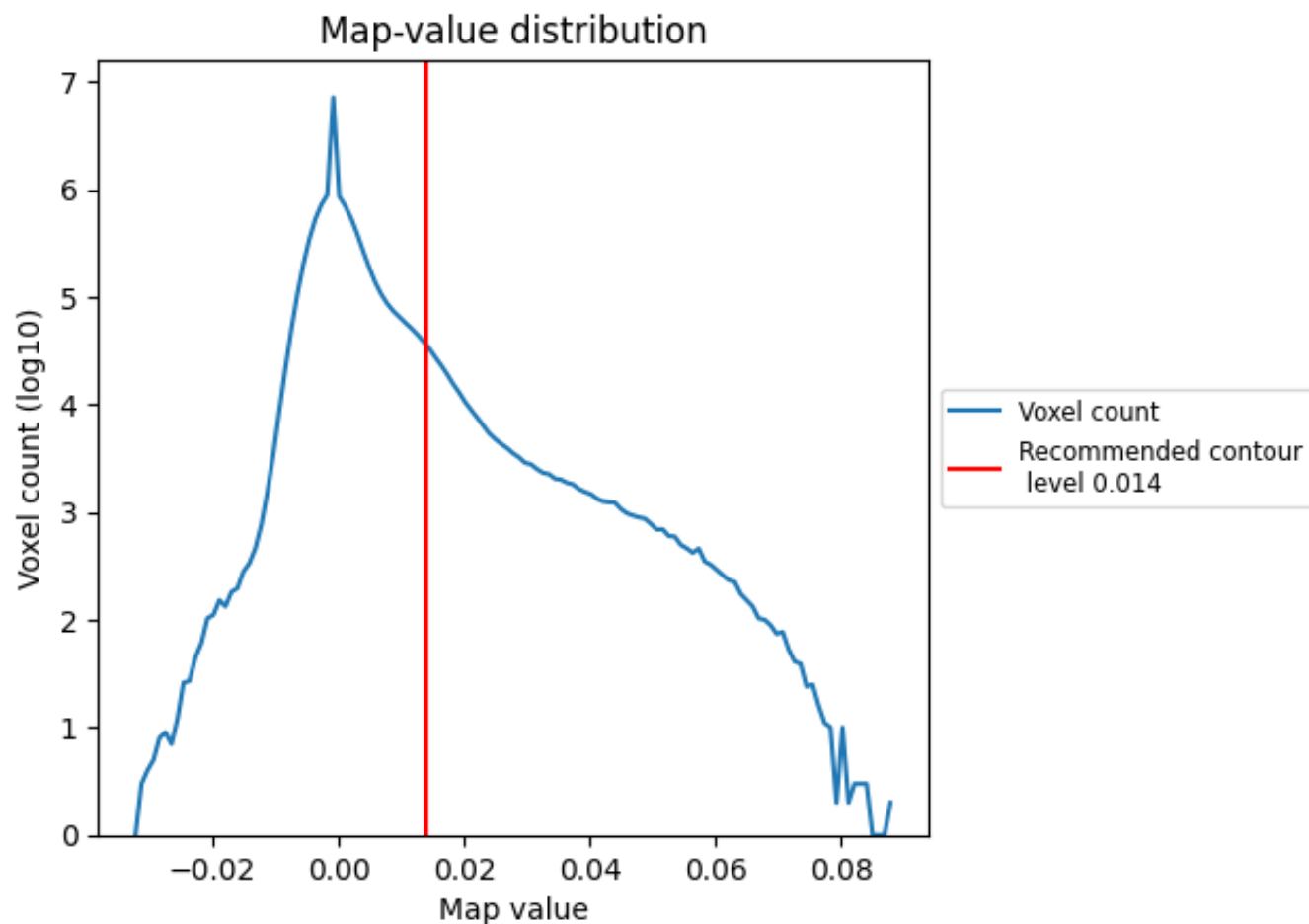
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

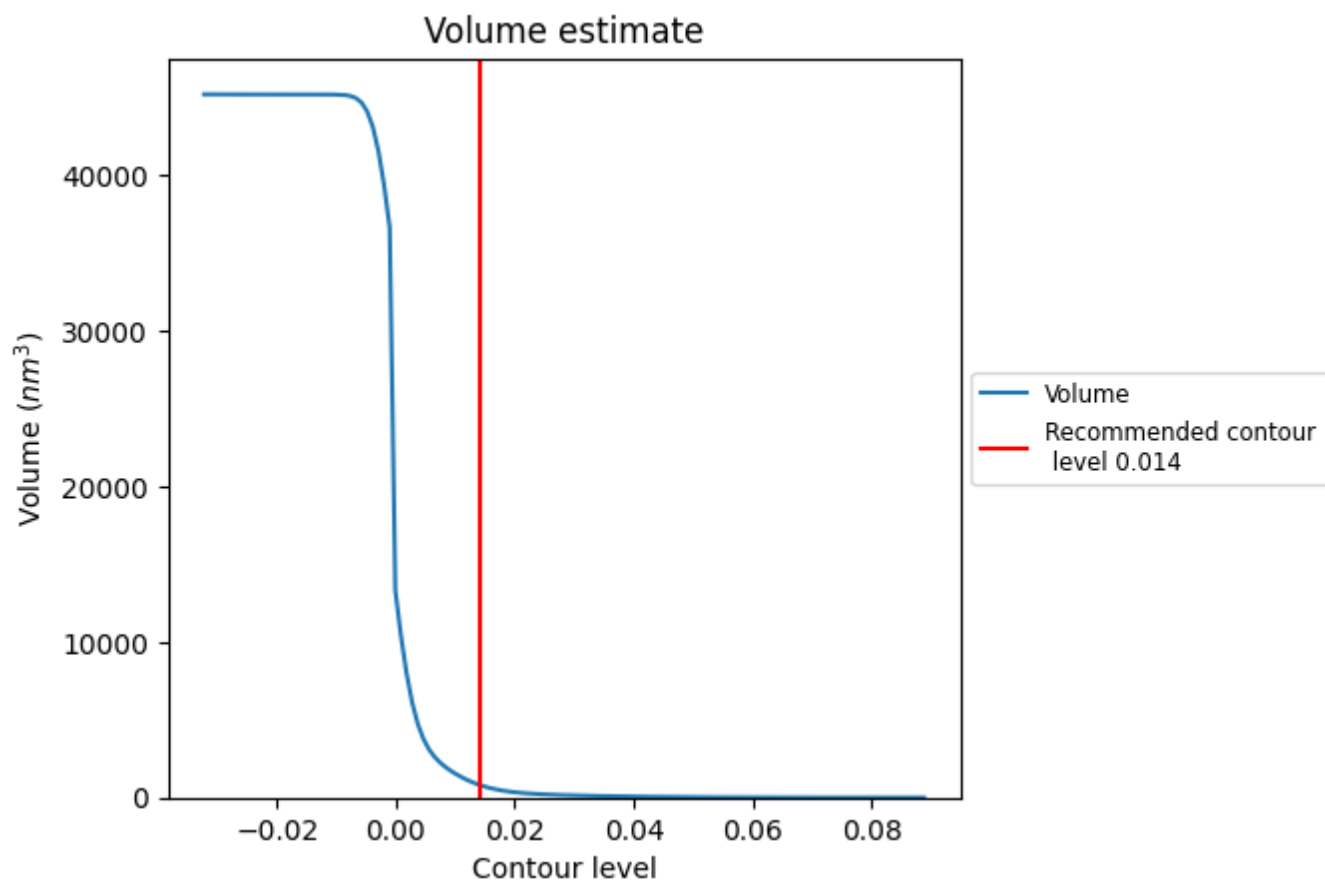
This section contains the results of statistical analysis of the map.

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.

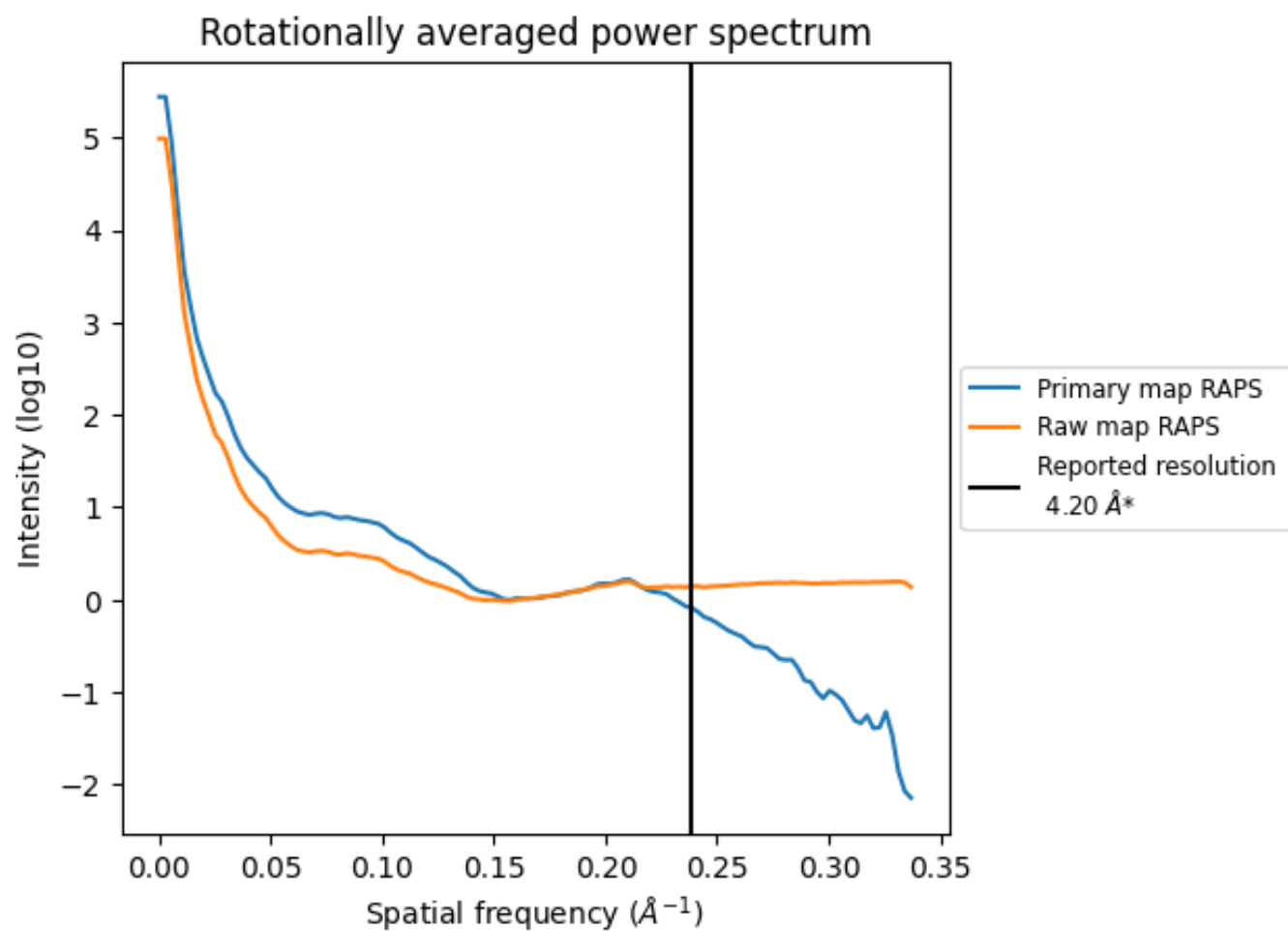
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 822 nm³; this corresponds to an approximate mass of 743 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

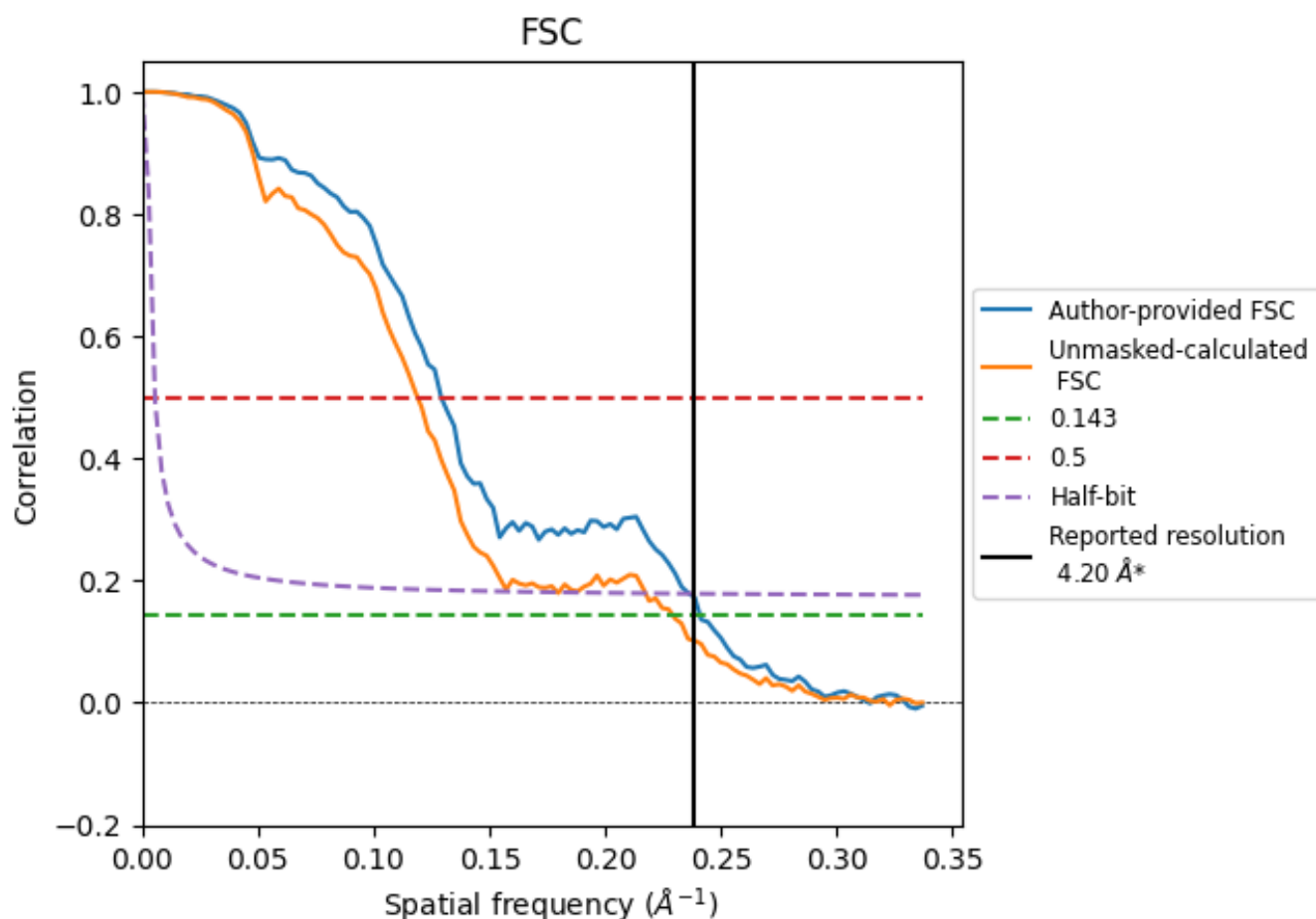


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

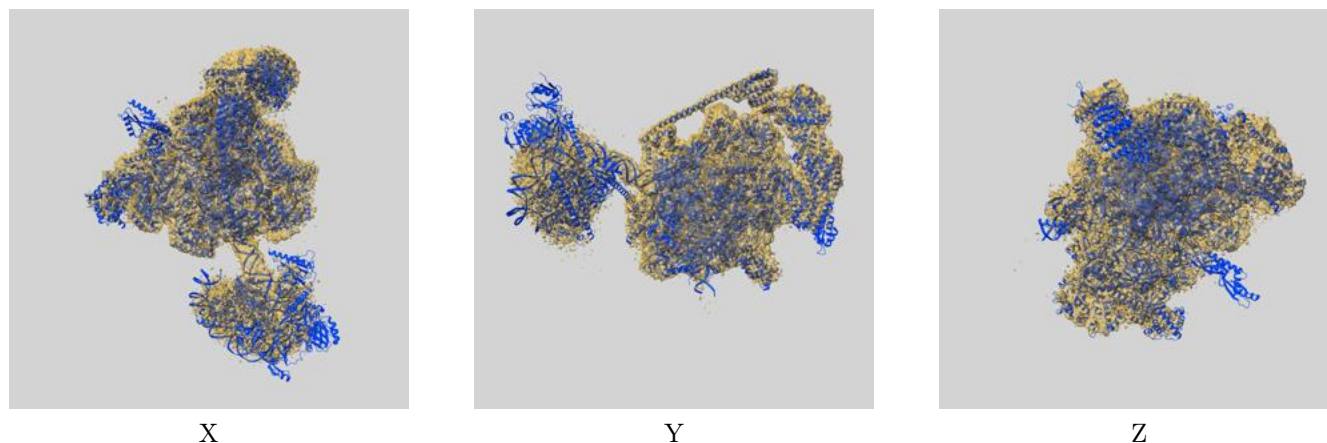
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.15	7.75	4.23
Unmasked-calculated*	4.36	8.40	5.57

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

9 Map-model fit [i](#)

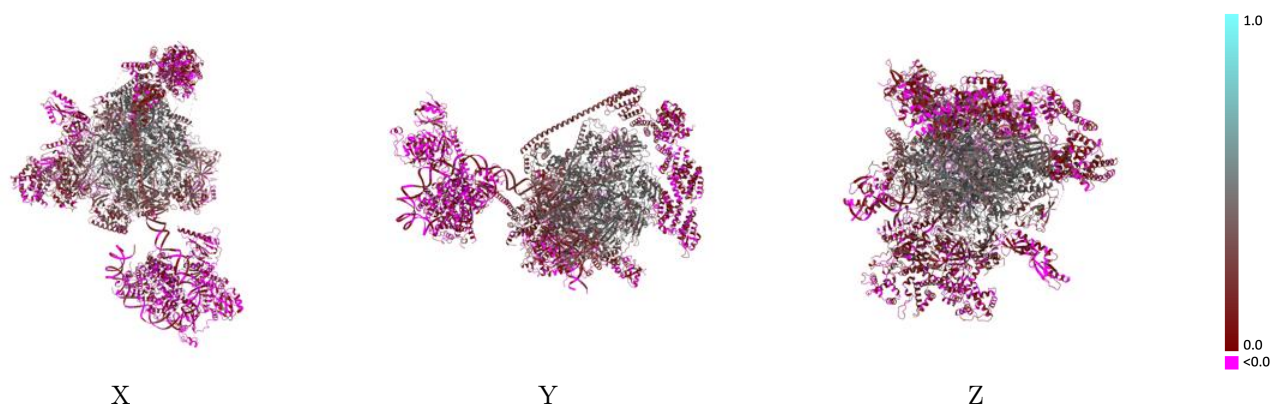
This section contains information regarding the fit between EMDB map EMD-33441 and PDB model 7XT7. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



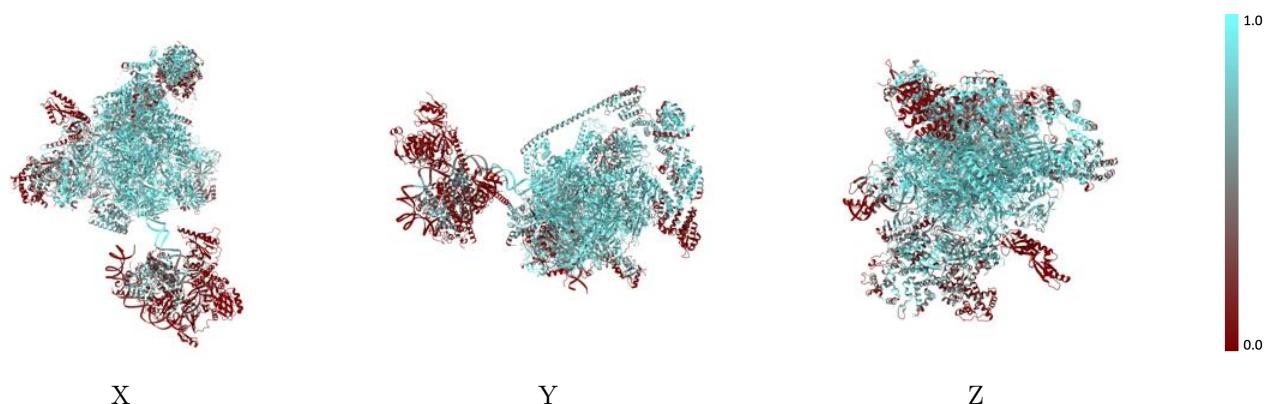
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



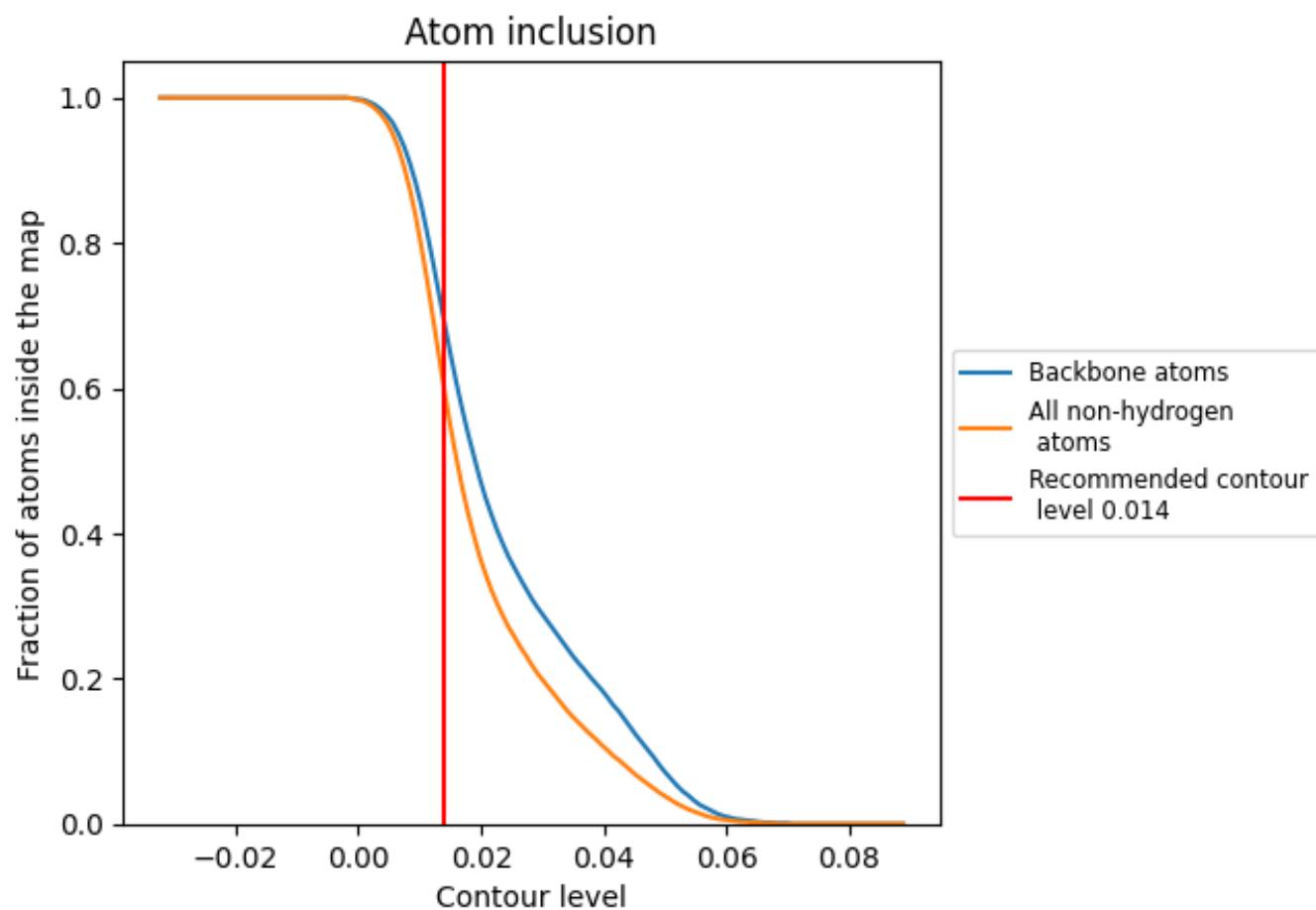
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

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

