



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:47 AM UTC

PDB ID : 7XTD / pdb_00007xtd
EMDB ID : EMD-33447
Title : RNA polymerase II elongation complex transcribing a nucleosome (EC58oct)
Authors : Ehara, H.; Kujirai, T.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on : 2022-05-16
Resolution : 3.90 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:

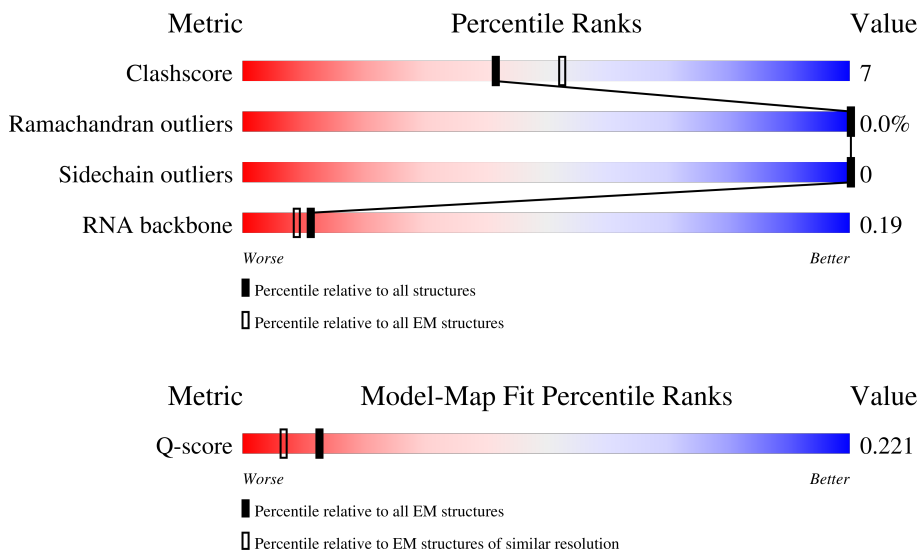
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	20% 84% 10% 6%
5	E	214	82% 17%
6	F	155	50% 5% 46%
7	G	171	15% 81% 19%
8	H	145	79% 13% 8%
9	I	115	30% 81% 16%
10	J	72	81% 12% 7%
11	K	118	77% 19%
12	L	72	6% 53% 10% 38%
13	M	113	23% 47% 10% 43%
14	N	198	34% 20% 36% 43%
15	P	19	21% 11% 32% 58%
16	T	198	36% 36% 26% 38%
17	V	108	37% 70% 28%
18	W	911	25% 48% 11% 41%
19	m	1503	37% 63% 16% 21%
20	n	417	13% 25% 8% 67%
21	q	1084	59% 71% 15% 14%
22	r	544	37% 40% 9% 51%
23	u	459	29% 39% 7% 55%
24	v	396	70% 70% 18% 12%
25	x	395	20% 46% 6% 48%
26	a	139	54% 45% 10% 45%
26	e	139	64% 57% 8% 35%
27	b	106	78% 67% 11% 22%

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Mol	Chain	Length	Quality of chain
27	f	106	<p>73%</p> <p>55% 19% 26%</p>
28	c	133	<p>77%</p> <p>63% 14% 23%</p>
28	g	133	<p>53%</p> <p>45% 8% 47%</p>
29	d	129	<p>73%</p> <p>62% 12% 26%</p>
29	h	129	<p>72%</p> <p>61% 11% 28%</p>
30	j	1008	<p>46%</p> <p>44% 54%</p>
31	k	531	<p>81%</p> <p>75% 6% 19%</p>

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 81668 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
10	J	67	554	355	97	96	6	0	0

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	112	2305	1099	389	705	112	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	P	19	399	178	64	138	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	T	123	2512	1189	497	703	123	0	0

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 40 discrepancies between the modelled and reference sequences:

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

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

unit.

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

There are 30 discrepancies between the modelled and reference sequences:

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

- Molecule 23 is a protein called Leo1.

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

There are 30 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 30 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	76	615	390	115	108	2	0	0
26	e	90	735	464	140	129	2	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 27 is a protein called Histone H4.

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	103	Total	C	N	O	0	0
			796	502	155	139		
28	g	70	Total	C	N	O	0	0
			544	342	109	93		

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
29	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 30 is a protein called FACT complex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	466	Total	C	N	O	S	0	0
			3780	2401	658	708	13		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	-2	GLY	-	expression tag	UNP C4QYQ8
j	-1	PRO	-	expression tag	UNP C4QYQ8
j	0	GLY	-	expression tag	UNP C4QYQ8

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

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

There are 3 discrepancies between the modelled and reference sequences:

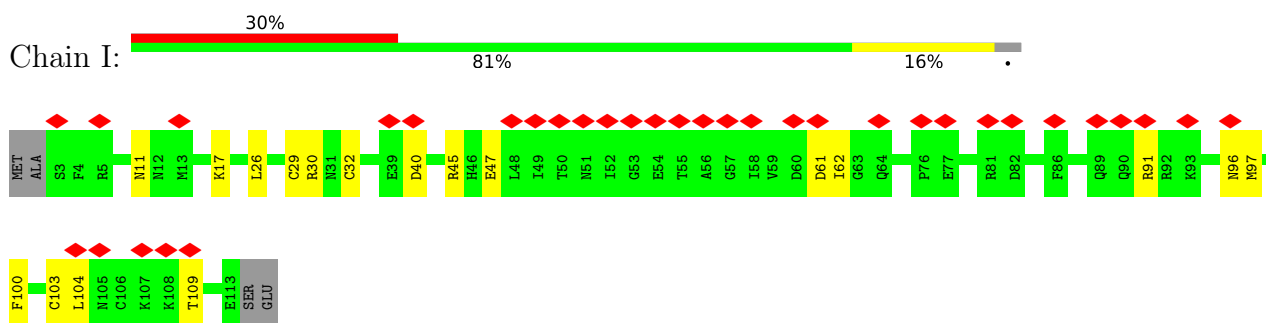
Chain	Residue	Modelled	Actual	Comment	Reference
k	-2	GLY	-	expression tag	UNP F2QNN8
k	-1	PRO	-	expression tag	UNP F2QNN8
k	0	GLY	-	expression tag	UNP F2QNN8

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

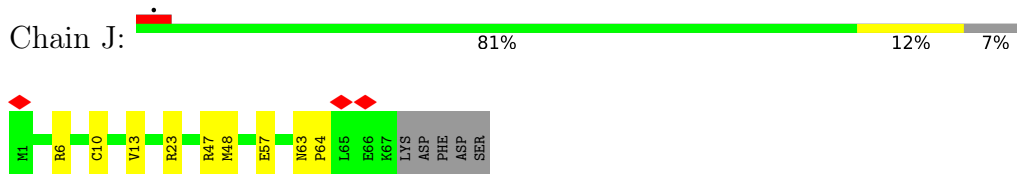
Mol	Chain	Residues	Atoms		AltConf
32	A	2	Total 2	Zn 2	0
32	B	1	Total 1	Zn 1	0
32	C	1	Total 1	Zn 1	0
32	I	2	Total 2	Zn 2	0
32	J	1	Total 1	Zn 1	0
32	L	1	Total 1	Zn 1	0
32	M	1	Total 1	Zn 1	0
32	V	1	Total 1	Zn 1	0

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

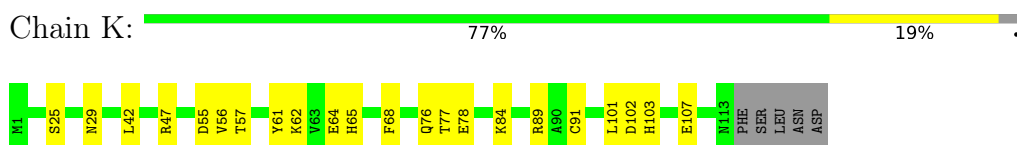
Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total 1	Mg 1	0



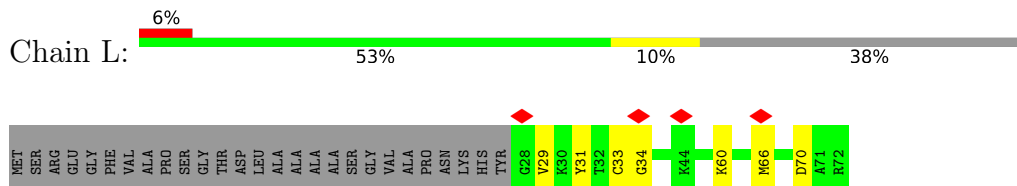
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



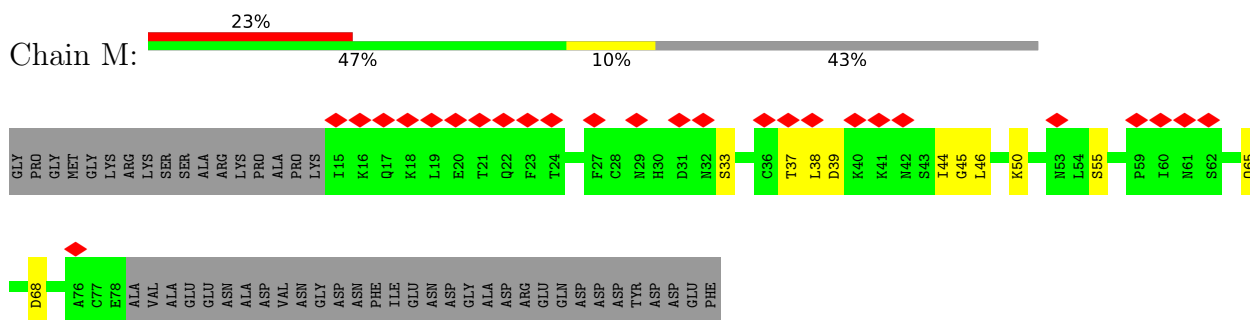
- Molecule 11: RNA polymerase II subunit B12.5



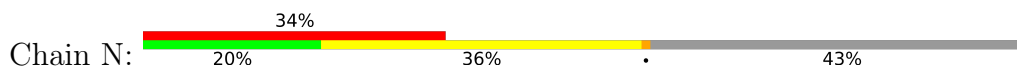
- Molecule 12: RNA polymerase subunit ABC10-alpha

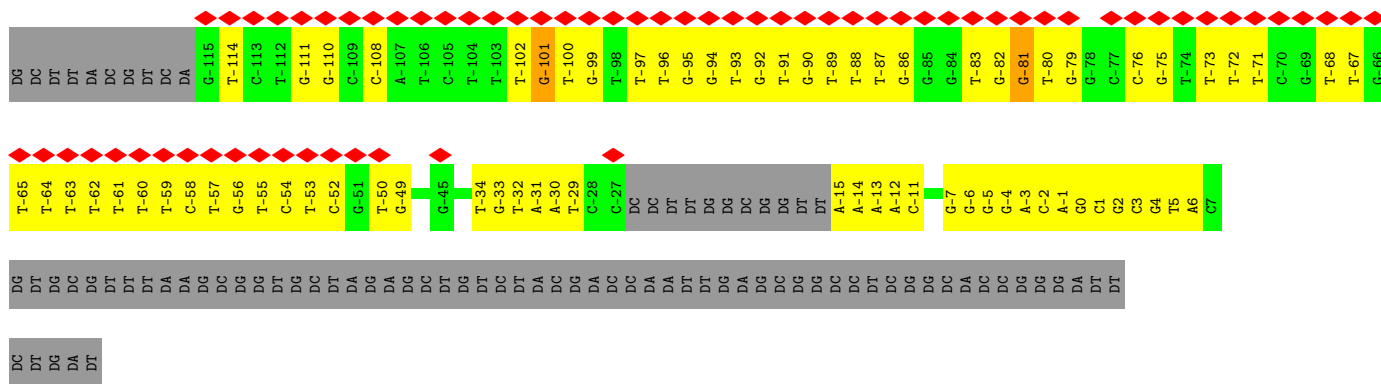


- Molecule 13: Transcription elongation factor 1 homolog

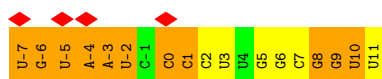


- Molecule 14: DNA (198-MER)

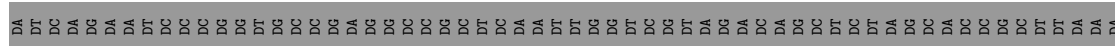




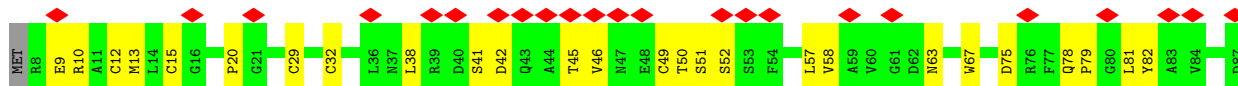
• Molecule 15: RNA (5'-R(P*UP*GP*UP*AP*AP*UP*CP*CP*CP*CP*UP*UP*GP*GP*CP*GP*GP*UP*U)-3')



• Molecule 16: DNA (198-MER)

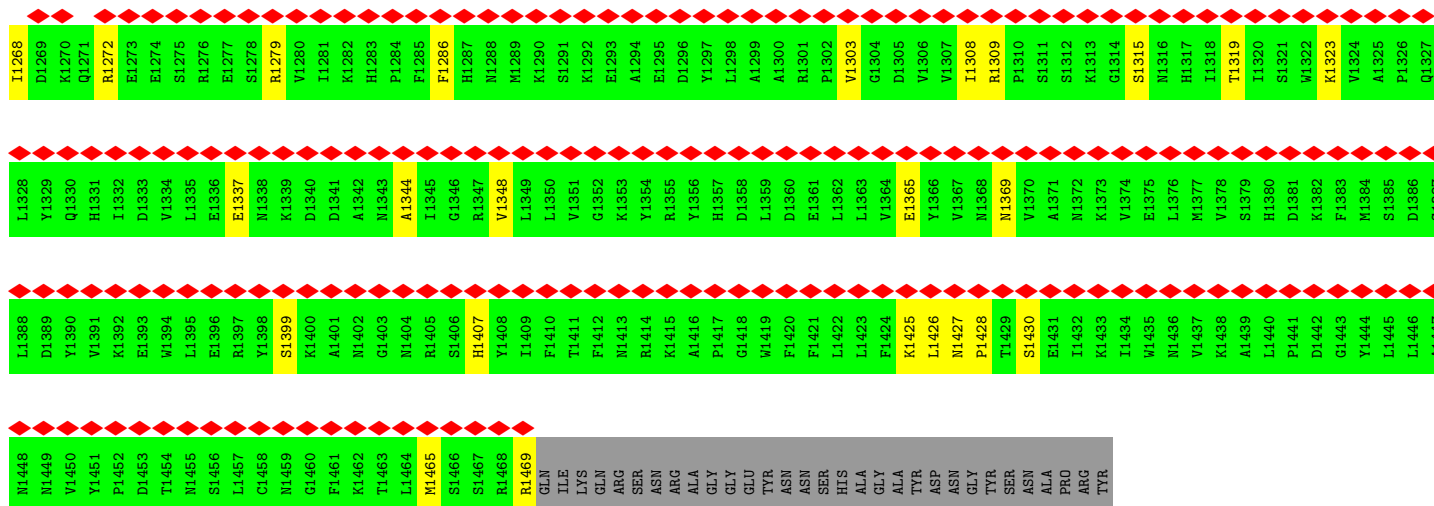


• Molecule 17: Transcription elongation factor SPT4

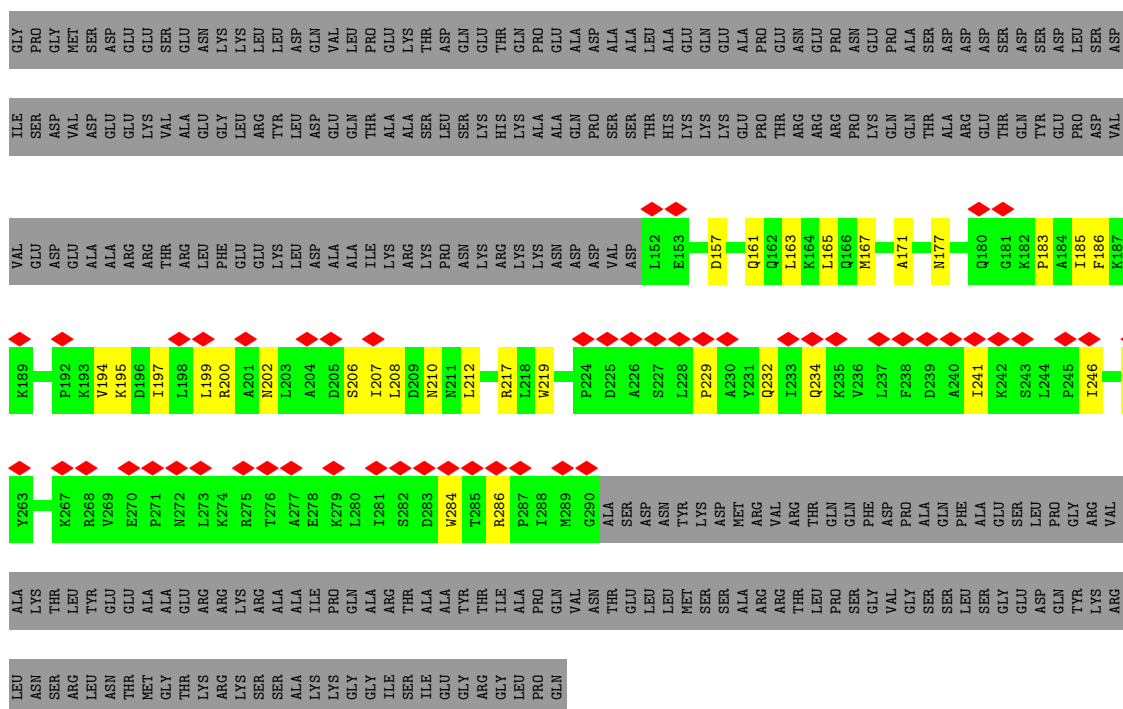


• Molecule 18: Transcription elongation factor SPT5

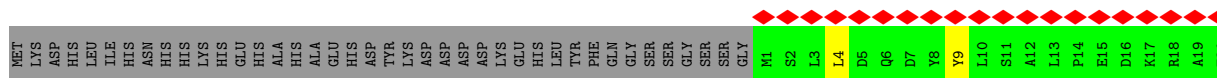




• Molecule 20: Protein that interacts with Spt6p and copurifies with Spt5p and RNA polymerase II



• Molecule 21: Component of the Paf1p complex

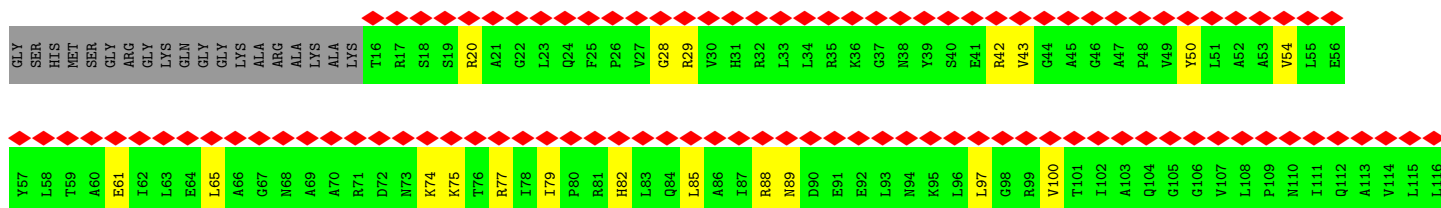
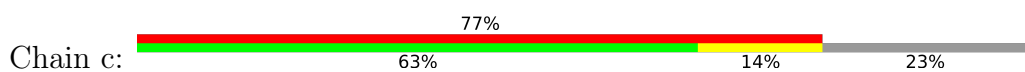




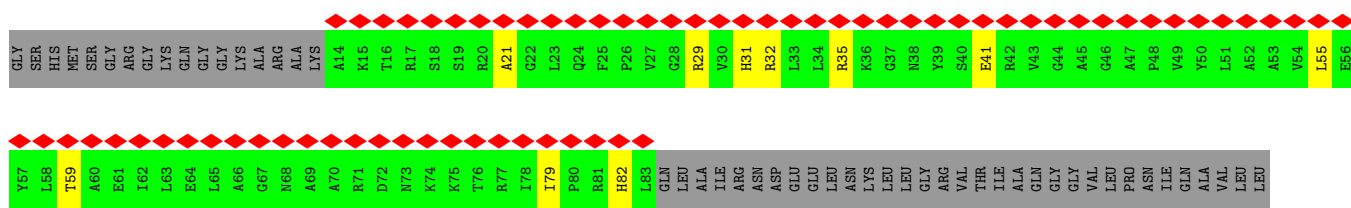
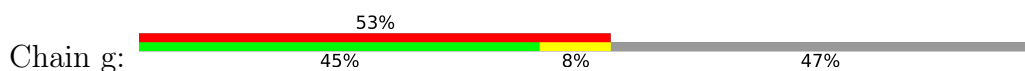
• Molecule 27: Histone H4



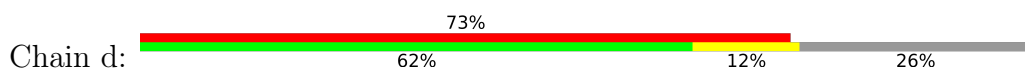
• Molecule 28: Histone H2A type 1-B/E

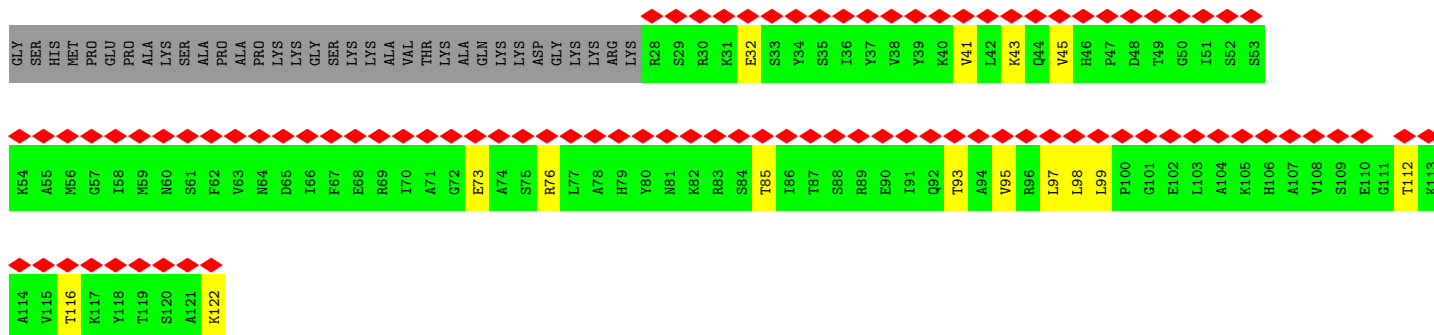


• Molecule 28: Histone H2A type 1-B/E

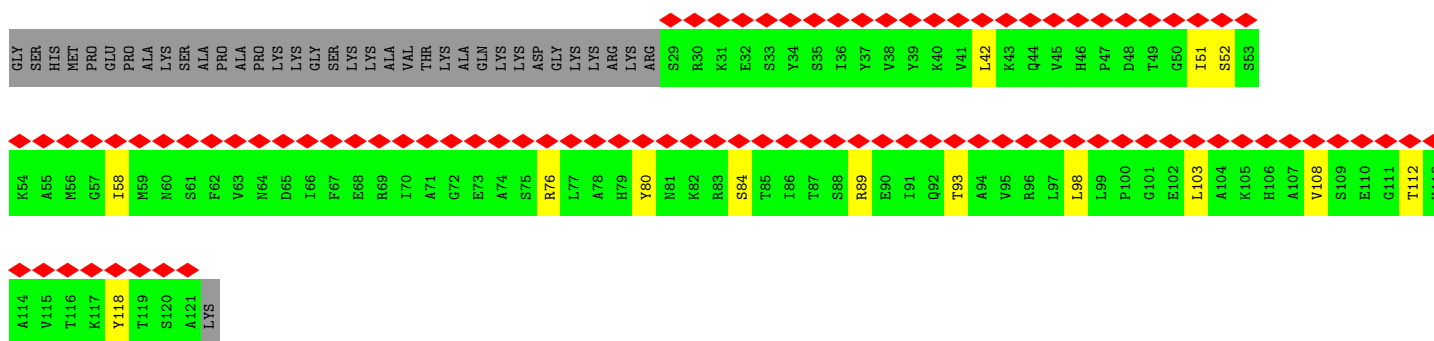


• Molecule 29: Histone H2B type 1-J

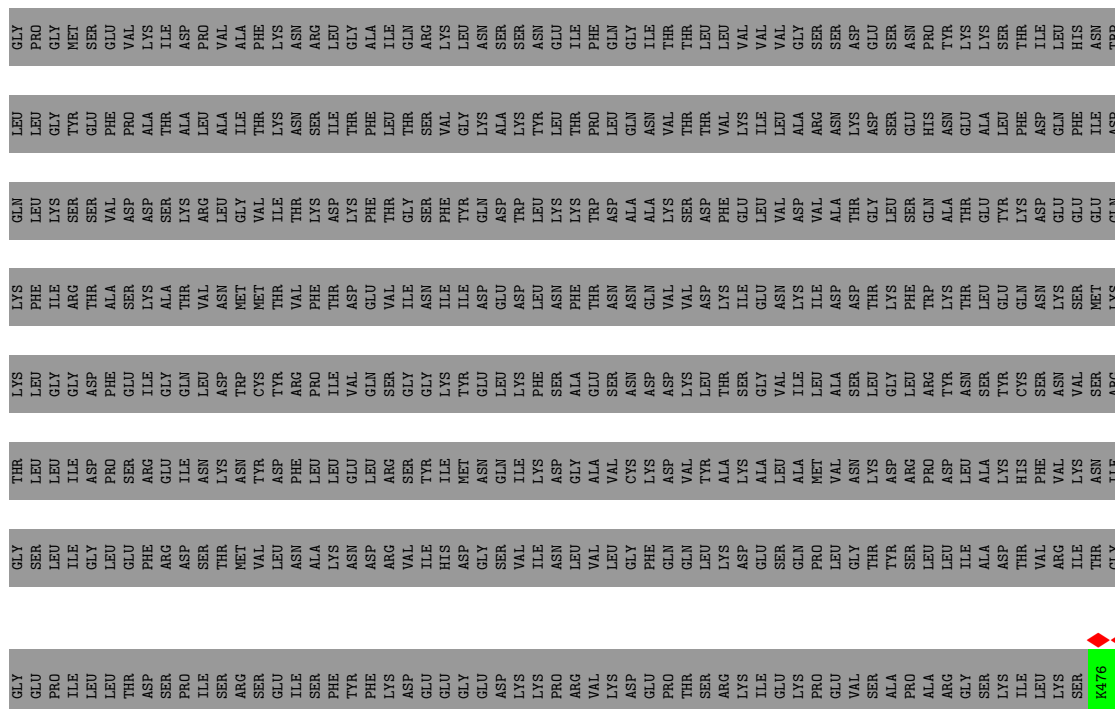




• Molecule 29: Histone H2B type 1-J



• Molecule 30: FACT complex subunit



E238	I239	S240	M241	Y242	A243	N244	N245	L246	R247	L248	R249	G250	Q251	S252	Y253	D254	Y255	K256	I257	Q258	N259	K260	N261	V262	L263	R264	I265	F266	S267	L268	P269	R270	L271	D272	D273	R274	H275	H276	L277	V278	I279	L280	Q281	V282	D283	P284	P285	L286	R287	Q288	G289	Q290	T291	R292	Y293	F294	F295	L296	V297
M298	Q299	F300	D301	R302	N303	E304	E305	L306	E307	V308	E309	L310	N311	L312	S313	D314	E315	E316	Y317	K318	S319	K320	Y321	E322	G323	K324	L325	N326	R327	S328	Y329	G330	T331	D332	S333	T334	Y335	K336	I337	L338	S339	H340	C341	L342	R343	G344	L345	T346	E347	R348	R349	V350	I351	T352	P353	G354	S355	F356	Q357
S358	Q359	H360	M361	Q362	P363	G364	V365	N366	C367	S368	L369	K370	A371	S372	E373	G374	Q375	I376	Y377	L378	L379	D380	K381	C382	L383	F384	F385	A386	T387	K388	P389	C390	V391	Y392	L393	P394	Y395	S396	G397	I398	I399	S400	V401	V402	T403	S404	R405	G406	THR	GLY	GLN	SER	THR	S412	R413	T414	F415	D416	I417
E418	V419	Q420	F421	S422	G423	G424	S425	H426	T427	F428	A429	M430	I431	M432	K433	D434	E435	Q436	K437	P438	I439	E440	D441	F442	L443	K444	G445	Q446	G447	V448	R449	V450	K451	M452	E453	LYS	PRO	ALA	GLU	PHE	LEU	GLY	ASN	ALA	LEU	VAL	ASP	ASP	ASP	ASP	SER	ASP	ASP	GLY	GLN	ASP	ILE	ALA	MET
GLY	SER	ALA	GLY	ASP	ASP	GLU	VAL	ASP	ASP	PHE	ASN	ALA	GLY	SER	ASP	ASP	VAL	ALA	GLU	TYR	ASP	SER	ASN	ALA	SER	GLU	ASP	GLU	ASP	ASP	ASP	ASP	LYS	LYS	LYS	LYS	PRO	PRO	GLU	LEU	GLY	ASN	ALA	LEU	VAL	ASP	ASP	ASP	SER	ASP	GLY	ASP	ILE	ALA	MET				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38828	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	0.096	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.009	Depositor
Map size (\AA)	356.16, 356.16, 356.16	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.484, 1.484, 1.484	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.22	0/11267	0.31	1/15222 (0.0%)
2	B	0.25	0/9464	0.32	0/12763
3	C	0.25	0/2139	0.30	0/2895
4	D	0.10	0/1361	0.24	0/1837
5	E	0.20	0/1773	0.27	0/2385
6	F	0.24	0/687	0.28	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	0.38	0/365	0.53	0/484
13	M	0.11	0/513	0.25	0/693
14	N	0.56	0/2575	0.82	1/3978 (0.0%)
15	P	0.41	0/443	0.69	1/687 (0.1%)
16	T	0.53	0/2827	0.73	0/4352
17	V	0.10	0/840	0.21	0/1140
18	W	0.12	0/4300	0.27	0/5812
19	m	0.11	0/9925	0.25	0/13424
20	n	0.10	0/1132	0.23	0/1526
21	q	0.11	0/7689	0.21	0/10368
22	r	0.25	0/2169	0.46	0/2901
23	u	0.29	0/1740	0.44	0/2347
24	v	0.11	0/2944	0.24	0/3973
25	x	0.13	0/1716	0.25	0/2310
26	a	0.22	0/622	0.38	0/834
26	e	0.30	0/743	0.50	0/996
27	b	0.22	0/669	0.46	0/894
27	f	0.32	0/626	0.47	0/837
28	c	0.23	0/806	0.40	0/1089
28	g	0.34	0/552	0.46	0/743
29	d	0.23	0/757	0.35	0/1015

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	h	0.21	0/736	0.35	0/990
30	j	0.80	0/3855	1.15	0/5191
31	k	0.77	0/3579	1.12	0/4833
All	All	0.33	0/83688	0.49	3/114032 (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	5
16	T	0	2
30	j	0	1
31	k	0	2
All	All	0	10

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	-81	DG	C2'-C3'-O3'	-6.90	101.15	111.50
1	A	1001	VAL	N-CA-C	-5.67	107.29	112.96
15	P	10	U	OP1-P-O3'	5.51	124.55	108.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	-101	DG	Sidechain
14	N	-102	DT	Sidechain
14	N	-108	DC	Sidechain
14	N	-111	DG	Sidechain
14	N	-114	DT	Sidechain
16	T	103	DA	Sidechain
16	T	112	DT	Sidechain
30	j	616	ARG	Sidechain
31	k	292	ARG	Sidechain
31	k	58	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11064	0	11090	123	0
2	B	9284	0	9282	142	0
3	C	2098	0	2057	23	0
4	D	1349	0	1345	11	0
5	E	1741	0	1754	25	0
6	F	677	0	693	7	0
7	G	1325	0	1342	21	0
8	H	1053	0	1050	12	0
9	I	917	0	867	16	0
10	J	554	0	573	6	0
11	K	932	0	944	14	0
12	L	359	0	358	6	0
13	M	505	0	495	6	0
14	N	2305	0	1277	100	0
15	P	399	0	203	29	0
16	T	2512	0	1366	68	0
17	V	824	0	795	18	0
18	W	4232	0	4278	66	0
19	m	9730	0	9588	145	0
20	n	1115	0	1186	25	0
21	q	7552	0	7545	110	0
22	r	2139	0	2155	37	0
23	u	1707	0	1676	26	0
24	v	2878	0	2873	58	0
25	x	1682	0	1731	16	0
26	a	615	0	645	15	0
26	e	735	0	775	9	0
27	b	662	0	709	13	0
27	f	619	0	659	21	0
28	c	796	0	848	17	0
28	g	544	0	574	8	0
29	d	746	0	771	11	0
29	h	725	0	745	12	0
30	j	3780	0	3751	26	0
31	k	3502	0	3436	24	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	C	1	0	0	0	0
32	I	2	0	0	0	0
32	J	1	0	0	0	0
32	L	1	0	0	0	0
32	M	1	0	0	0	0
32	V	1	0	0	0	0
33	A	1	0	0	0	0
All	All	81668	0	79436	1076	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 (1076) 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:-72:DT:H2''	14:N:-71:DT:H71	1.42	0.98
14:N:-92:DG:H2''	14:N:-91:DT:H71	1.49	0.92
14:N:-53:DT:H2''	14:N:-52:DC:C5	2.05	0.92
16:T:2:DG:H2'	16:T:3:DT:H71	1.52	0.91
16:T:3:DT:H2'	16:T:4:DC:C6	2.07	0.90
30:j:587:ARG:HH12	31:k:287:ARG:CD	1.86	0.89
31:k:286:LEU:HD12	31:k:296:LEU:HD21	1.54	0.89
16:T:-3:DG:H2''	16:T:-2:DC:C5	2.13	0.83
27:f:49:LEU:HD21	30:j:727:LEU:HG	1.61	0.83
14:N:-14:DA:N6	14:N:-13:DA:C6	2.48	0.82
14:N:-61:DT:H2'	14:N:-60:DT:H72	1.61	0.82
16:T:20:DG:H2''	16:T:21:DC:H5'	1.61	0.81
14:N:-1:DA:C2	14:N:0:DG:C4	2.68	0.81
15:P:5:G:H2'	15:P:6:G:C8	2.14	0.81
14:N:-95:DG:N2	14:N:-94:DG:N2	2.28	0.81
15:P:5:G:H2'	15:P:6:G:H8	1.44	0.80
21:q:793:VAL:HG11	21:q:830:LEU:HG	1.64	0.80
14:N:-61:DT:C2'	14:N:-60:DT:H72	2.11	0.79
16:T:85:DC:H4'	28:c:42:ARG:HD3	1.64	0.79
14:N:-94:DG:H2''	14:N:-93:DT:C7	2.13	0.78
27:f:49:LEU:HD21	30:j:727:LEU:CG	2.14	0.77
14:N:-92:DG:H2''	14:N:-91:DT:C7	2.14	0.77
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.26	0.76
14:N:-95:DG:C2	14:N:-94:DG:C2	2.75	0.74
21:q:390:LEU:HB3	21:q:409:LEU:HD21	1.70	0.74
16:T:6:DC:H2''	16:T:7:DC:C5	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:6:G:H2'	15:P:7:C:C6	2.24	0.73
15:P:6:G:H2'	15:P:7:C:H6	1.52	0.73
30:j:587:ARG:HH12	31:k:287:ARG:HD3	1.52	0.72
2:B:792:MET:HE2	2:B:857:ARG:HH22	1.54	0.72
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.70	0.72
14:N:-14:DA:C6	14:N:-13:DA:C6	2.78	0.72
18:W:524:GLU:O	20:n:232:GLN:NE2	2.23	0.72
1:A:807:ARG:NH1	2:B:724:LYS:O	2.23	0.71
14:N:-91:DT:H3'	28:c:28:GLY:HA3	1.71	0.71
26:a:105:GLU:OE2	30:j:867:LEU:HD22	1.90	0.71
14:N:-94:DG:H2''	14:N:-93:DT:H71	1.71	0.71
1:A:1207:LYS:O	1:A:1277:ARG:NH2	2.24	0.70
5:E:60:LEU:O	21:q:915:ARG:NH1	2.23	0.70
15:P:1:C:H42	16:T:26:DG:H1	1.38	0.70
30:j:587:ARG:HH12	31:k:287:ARG:HD2	1.55	0.69
1:A:1262:MET:SD	1:A:1265:ARG:NH2	2.66	0.69
2:B:550:PHE:HB3	2:B:593:MET:HE1	1.75	0.69
2:B:879:ARG:HH21	15:P:-3:A:H4'	1.57	0.69
8:H:112:LYS:HG2	8:H:125:GLU:HG3	1.73	0.69
21:q:578:GLN:NE2	21:q:582:ASP:OD1	2.26	0.69
1:A:831:LYS:NZ	1:A:1079:THR:O	2.25	0.69
14:N:-30:DA:H2''	14:N:-29:DT:H72	1.74	0.69
19:m:382:PRO:HG2	19:m:955:ASN:HD22	1.58	0.69
14:N:-7:DG:C6	14:N:-6:DG:C6	2.80	0.68
18:W:303:ILE:HB	20:n:286:ARG:HH22	1.58	0.68
19:m:1160:ASP:O	19:m:1163:ARG:NH1	2.26	0.68
21:q:922:ALA:O	21:q:926:ASN:ND2	2.26	0.68
16:T:68:DA:H2''	16:T:69:DC:H5'	1.76	0.68
14:N:-76:DC:H2''	14:N:-75:DG:C8	2.29	0.68
21:q:531:GLU:O	21:q:535:ASN:N	2.26	0.68
31:k:146:GLY:HA2	31:k:252:SER:O	1.94	0.68
2:B:223:SER:O	2:B:252:ARG:NH2	2.27	0.68
22:r:230:ARG:NH1	22:r:292:SER:OG	2.27	0.68
10:J:47:ARG:NH1	10:J:48:MET:SD	2.68	0.67
1:A:107:CYS:SG	1:A:172:GLN:NE2	2.66	0.67
1:A:447:ARG:HB2	1:A:488:MET:HE3	1.77	0.67
18:W:487:ILE:HD11	18:W:531:ARG:HB2	1.76	0.67
21:q:169:ASP:OD1	21:q:185:LYS:NZ	2.28	0.67
21:q:59:ALA:HB1	21:q:63:LEU:HD12	1.77	0.67
19:m:380:GLU:HG3	19:m:382:PRO:HD2	1.77	0.66
19:m:682:ASP:O	19:m:686:ASN:ND2	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	2.28	0.66
14:N:-62:DT:H2'	14:N:-61:DT:H72	1.77	0.66
2:B:267:TYR:HB2	2:B:348:ILE:HD11	1.77	0.66
22:r:490:VAL:HG22	22:r:495:ARG:HE	1.60	0.66
1:A:673:ASP:OD1	1:A:737:ASN:ND2	2.29	0.65
2:B:254:ASP:H	2:B:259:ARG:HH21	1.44	0.65
14:N:-61:DT:C2'	14:N:-60:DT:C7	2.74	0.65
18:W:342:GLU:HB3	18:W:351:ARG:HB3	1.79	0.65
14:N:-59:DT:H2''	14:N:-58:DC:C5	2.32	0.65
1:A:127:ARG:O	1:A:129:ARG:NH1	2.30	0.65
25:x:292:TRP:HA	25:x:295:LYS:HE2	1.79	0.65
19:m:617:ILE:HG13	19:m:649:LEU:HD11	1.78	0.64
27:f:68:ASP:OD2	27:f:93:GLN:NE2	2.30	0.64
14:N:-72:DT:H2''	14:N:-71:DT:C7	2.25	0.64
20:n:260:MET:HG3	20:n:284:TRP:HZ3	1.63	0.64
25:x:157:ARG:HB3	25:x:161:PRO:HB3	1.78	0.64
1:A:887:ILE:O	1:A:945:ARG:NH2	2.30	0.64
2:B:613:ARG:HH21	9:I:62:ILE:HD11	1.61	0.64
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.24	0.64
2:B:285:PRO:HG2	2:B:288:GLU:HB2	1.80	0.64
3:C:266:ARG:HD2	11:K:84:LYS:HZ1	1.63	0.64
18:W:327:ARG:NH2	18:W:441:ASN:O	2.31	0.64
27:b:26:ILE:HG13	27:b:55:ARG:HD3	1.80	0.64
30:j:587:ARG:NH1	31:k:287:ARG:CD	2.60	0.64
4:D:153:VAL:HG13	4:D:171:LEU:HD23	1.78	0.64
1:A:361:GLU:OE1	1:A:460:ARG:NH2	2.29	0.64
21:q:31:LYS:HB2	21:q:57:GLU:HA	1.78	0.64
21:q:780:TYR:O	21:q:784:LYS:N	2.31	0.63
14:N:-34:DT:H2''	14:N:-33:DG:C8	2.33	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:1158:PRO:HA	1:A:1192:PRO:HB3	1.80	0.63
16:T:20:DG:H2'	16:T:21:DC:C6	2.34	0.63
3:C:107:GLU:O	3:C:107:GLU:HG2	1.99	0.63
1:A:881:ARG:HH21	1:A:955:ASN:HB3	1.64	0.63
27:f:49:LEU:CD2	30:j:727:LEU:HD11	2.29	0.63
1:A:1130:ILE:HG12	1:A:1134:LYS:HE2	1.81	0.63
11:K:57:THR:OG1	11:K:76:GLN:OE1	2.17	0.63
17:V:89:ARG:NH1	17:V:109:ASP:OD2	2.31	0.63
21:q:155:TYR:HA	21:q:160:ARG:HD3	1.80	0.63
19:m:343:ARG:NH1	19:m:347:GLN:OE1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:408:ASP:OD1	24:v:133:TYR:N	2.32	0.62
16:T:3:DT:H2'	16:T:4:DC:H6	1.60	0.62
19:m:551:ARG:NH2	19:m:689:LYS:O	2.31	0.62
21:q:65:LEU:HD13	24:v:81:ILE:HG12	1.81	0.62
21:q:590:ARG:NH1	21:q:618:THR:OG1	2.31	0.62
26:a:109:LEU:HD21	30:j:888:THR:HG21	1.80	0.62
16:T:6:DC:H2''	16:T:7:DC:H5	1.63	0.62
19:m:607:ILE:HG22	19:m:719:VAL:HG11	1.82	0.62
19:m:1101:ASP:OD1	19:m:1132:GLN:NE2	2.32	0.62
21:q:210:PRO:O	21:q:217:ARG:NH2	2.25	0.62
16:T:-7:DG:H2''	16:T:-6:DT:H71	1.81	0.61
18:W:351:ARG:HA	18:W:429:THR:HA	1.81	0.61
21:q:348:ASP:HB3	21:q:351:GLN:HB3	1.83	0.61
26:a:69:ARG:HB3	27:b:25:ASN:HD22	1.65	0.61
14:N:-101:DG:H4'	28:c:77:ARG:NH1	2.15	0.61
14:N:-14:DA:N6	14:N:-13:DA:N6	2.47	0.61
1:A:1201:ARG:NH2	1:A:1235:ALA:O	2.33	0.61
16:T:93:DA:H2''	16:T:94:DC:C5	2.35	0.61
18:W:784:ASN:HB2	18:W:785:PRO:HD3	1.81	0.61
5:E:47:ASP:OD2	5:E:53:GLN:NE2	2.19	0.61
14:N:0:DG:C2	14:N:1:DC:C2	2.87	0.61
19:m:434:LEU:HD11	19:m:467:ASP:HB2	1.81	0.61
21:q:708:GLN:OE1	21:q:739:LYS:NZ	2.34	0.61
23:u:145:ILE:O	23:u:149:THR:OG1	2.17	0.61
5:E:19:LYS:NZ	5:E:33:GLU:O	2.34	0.61
1:A:39:GLU:OE2	1:A:49:ARG:NH1	2.34	0.61
23:u:80:TYR:CZ	24:v:356:ASN:HB2	2.36	0.61
1:A:466:TYR:HB2	1:A:470:ARG:NH2	2.16	0.61
16:T:18:DC:C2'	16:T:19:DC:H5'	2.30	0.61
19:m:358:HIS:HB3	19:m:361:GLU:HB2	1.82	0.61
23:u:108:VAL:HG22	23:u:219:VAL:HB	1.83	0.61
23:u:199:LEU:HD11	24:v:211:PHE:HB3	1.81	0.61
27:f:49:LEU:HD21	30:j:727:LEU:CD1	2.30	0.60
19:m:421:ASP:OD1	19:m:422:LEU:N	2.34	0.60
1:A:22:LEU:HG	2:B:1213:ALA:HB2	1.83	0.60
14:N:-55:DT:H2''	14:N:-54:DC:C6	2.37	0.60
1:A:1157:ASP:O	1:A:1243:ARG:NH2	2.29	0.60
19:m:1221:LEU:HD11	19:m:1233:SER:HB2	1.82	0.60
2:B:489:ARG:NH2	2:B:533:SER:O	2.35	0.60
19:m:730:ASP:OD1	19:m:733:ARG:NH2	2.34	0.60
19:m:570:MET:HA	19:m:577:THR:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:785:ASP:O	19:m:912:GLN:NE2	2.35	0.60
18:W:527:THR:HA	18:W:530:LEU:HD12	1.84	0.60
2:B:235:LEU:HD23	2:B:242:ILE:HG13	1.83	0.59
2:B:294:CYS:SG	2:B:295:TYR:N	2.75	0.59
17:V:13:MET:N	17:V:49:CYS:O	2.26	0.59
20:n:217:ARG:HG3	20:n:259:VAL:HG21	1.84	0.59
1:A:677:MET:HG3	2:B:722:THR:HB	1.84	0.59
17:V:57:LEU:HD11	17:V:81:LEU:HD22	1.84	0.59
2:B:926:GLY:O	19:m:778:ALA:N	2.31	0.59
14:N:-14:DA:N1	14:N:-13:DA:C2	2.71	0.59
16:T:22:DC:H1'	16:T:23:DA:H5'	1.84	0.59
1:A:227:GLU:OE1	1:A:231:ARG:NH1	2.36	0.59
2:B:10:ASP:HB3	2:B:649:LYS:HG3	1.84	0.59
2:B:409:LEU:HD23	2:B:450:LEU:HD23	1.85	0.59
16:T:24:DA:H1'	16:T:25:DG:H5''	1.84	0.59
19:m:458:ARG:HG3	19:m:459:THR:HG23	1.83	0.59
26:a:69:ARG:HB3	27:b:25:ASN:ND2	2.18	0.59
30:j:587:ARG:NH1	31:k:287:ARG:HD3	2.18	0.59
7:G:102:ASP:OD1	7:G:107:ASN:ND2	2.31	0.59
7:G:27:ARG:NH1	7:G:54:ILE:O	2.36	0.59
8:H:48:PRO:O	8:H:145:ARG:NH1	2.36	0.59
16:T:18:DC:H2''	16:T:19:DC:H5'	1.85	0.59
19:m:1425:LYS:NZ	19:m:1430:SER:O	2.30	0.59
24:v:29:LEU:N	25:x:147:ARG:O	2.35	0.59
19:m:672:VAL:O	19:m:720:GLN:NE2	2.34	0.59
21:q:72:VAL:HG21	24:v:75:LEU:HD13	1.85	0.59
19:m:424:TYR:HA	19:m:427:ILE:HG12	1.84	0.59
21:q:253:ILE:HG12	21:q:297:LEU:HD21	1.84	0.59
17:V:9:GLU:HA	17:V:20:PRO:HA	1.84	0.58
22:r:194:LYS:HB2	22:r:316:LEU:HD12	1.84	0.58
14:N:0:DG:N2	14:N:1:DC:C2	2.71	0.58
21:q:690:LYS:NZ	25:x:178:GLU:OE1	2.36	0.58
23:u:191:THR:HG22	23:u:219:VAL:HG22	1.86	0.58
1:A:149:GLU:HB2	1:A:165:ARG:HD3	1.84	0.58
14:N:-56:DG:H2'	14:N:-55:DT:H71	1.84	0.58
16:T:25:DG:H2''	16:T:26:DG:H5''	1.84	0.58
21:q:806:LEU:O	21:q:811:ARG:NH1	2.36	0.58
2:B:50:VAL:HG21	2:B:82:ILE:HD11	1.86	0.58
24:v:312:LYS:HB3	24:v:315:GLU:HG2	1.84	0.58
2:B:63:GLN:NE2	2:B:70:ASN:OD1	2.35	0.58
21:q:766:MET:HG3	21:q:770:LYS:HE3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:1170:VAL:O	19:m:1215:THR:OG1	2.19	0.58
24:v:267:TYR:HB3	24:v:297:TYR:HB3	1.85	0.58
19:m:309:ARG:HH21	19:m:978:CYS:HA	1.69	0.58
2:B:928:ARG:NH2	19:m:777:ASP:O	2.36	0.58
14:N:-2:DC:H2'	14:N:-1:DA:C8	2.39	0.58
24:v:56:LYS:O	24:v:60:ARG:NH2	2.37	0.57
18:W:327:ARG:NH1	18:W:335:GLY:O	2.36	0.57
19:m:1177:SER:O	19:m:1194:ARG:NH1	2.37	0.57
14:N:-76:DC:H2''	14:N:-75:DG:H8	1.69	0.57
31:k:103:LYS:HE2	31:k:130:PRO:HG3	1.86	0.57
18:W:392:ARG:NH1	18:W:398:GLU:OE1	2.36	0.57
19:m:245:THR:HA	19:m:248:GLN:HB2	1.86	0.57
1:A:85:GLU:O	1:A:274:ASN:ND2	2.33	0.57
1:A:568:LYS:HG2	1:A:569:PRO:HA	1.87	0.57
14:N:-95:DG:N2	14:N:-94:DG:C2	2.72	0.57
14:N:-61:DT:C6	14:N:-60:DT:H72	2.39	0.57
17:V:58:VAL:N	17:V:82:TYR:O	2.38	0.57
5:E:101:GLU:HG3	5:E:102:LYS:HG2	1.86	0.57
23:u:121:PHE:HB3	23:u:153:ARG:HB3	1.85	0.57
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.37	0.57
7:G:86:VAL:HG22	7:G:146:LYS:HB2	1.86	0.57
18:W:352:LEU:HD11	18:W:435:LEU:HD11	1.87	0.57
15:P:-4:A:N3	15:P:-4:A:H2'	2.19	0.57
18:W:665:ARG:HB2	18:W:708:ILE:HD11	1.87	0.57
14:N:-61:DT:H2''	14:N:-60:DT:C7	2.35	0.56
14:N:-60:DT:H5''	27:b:30:THR:HG21	1.85	0.56
30:j:609:GLY:HA3	30:j:612:LYS:HD2	1.86	0.56
16:T:0:DC:H2'	16:T:1:DT:C6	2.40	0.56
19:m:529:ILE:HD11	19:m:566:ILE:HG12	1.87	0.56
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.85	0.56
14:N:-2:DC:H2'	14:N:-1:DA:H8	1.70	0.56
22:r:200:ASP:HB3	22:r:319:VAL:HG11	1.87	0.56
31:k:141:ASN:ND2	31:k:256:LYS:HD3	2.20	0.56
16:T:25:DG:H5'	16:T:25:DG:H8	1.71	0.56
23:u:209:LEU:HB2	24:v:252:PHE:HB2	1.87	0.56
26:e:54:TYR:O	27:f:40:ARG:NE	2.37	0.56
2:B:290:LEU:HD21	2:B:310:ILE:HD11	1.87	0.56
5:E:28:PHE:HB2	5:E:64:THR:HG22	1.88	0.56
6:F:103:MET:HE3	7:G:15:PRO:HG2	1.87	0.56
16:T:20:DG:H2''	16:T:21:DC:C5'	2.33	0.56
29:d:112:THR:O	29:d:116:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:k:108:ARG:CZ	31:k:127:ASN:HD22	2.19	0.56
2:B:336:ILE:O	2:B:341:ARG:NH1	2.38	0.56
2:B:906:SER:OG	18:W:781:GLU:OE1	2.23	0.56
15:P:1:C:N4	16:T:26:DG:H1	2.04	0.56
16:T:17:DA:H2'	16:T:18:DC:C6	2.40	0.56
18:W:220:THR:N	18:W:223:ASP:OD2	2.32	0.55
2:B:72:ASN:ND2	2:B:128:ASP:OD1	2.39	0.55
14:N:-4:DG:H2'	14:N:-3:DA:O4'	2.07	0.55
17:V:15:CYS:HB3	17:V:32:CYS:SG	2.46	0.55
1:A:1452:LEU:HD23	6:F:131:PRO:HA	1.89	0.55
14:N:-14:DA:N6	14:N:-13:DA:N1	2.54	0.55
16:T:-7:DG:H1'	16:T:-6:DT:C6	2.42	0.55
20:n:163:LEU:HD11	20:n:194:VAL:HG22	1.88	0.55
14:N:-94:DG:H2''	14:N:-93:DT:C5	2.42	0.55
16:T:0:DC:H2''	16:T:1:DT:O4'	2.06	0.55
16:T:25:DG:H2''	16:T:26:DG:C5'	2.37	0.55
8:H:100:VAL:HG22	8:H:115:VAL:HG22	1.89	0.55
14:N:-90:DG:C8	14:N:-89:DT:H72	2.42	0.55
2:B:622:ASP:OD1	2:B:623:VAL:N	2.40	0.55
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.88	0.55
18:W:232:ARG:HH12	18:W:235:LYS:HE3	1.70	0.55
1:A:569:PRO:HD2	8:H:46:MET:HE2	1.89	0.55
27:b:92:ARG:NH2	29:d:97:LEU:O	2.40	0.55
1:A:149:GLU:O	1:A:165:ARG:NH1	2.38	0.55
1:A:669:ASP:OD2	1:A:743:ASN:ND2	2.29	0.55
21:q:155:TYR:HB3	21:q:160:ARG:HB2	1.89	0.55
21:q:569:ASN:O	21:q:603:LYS:NZ	2.40	0.55
24:v:316:ASP:HB2	24:v:333:ILE:HB	1.88	0.55
1:A:1210:THR:HB	1:A:1213:GLN:HG3	1.90	0.54
21:q:239:ASN:HA	21:q:242:LYS:HD2	1.89	0.54
2:B:904:ARG:HH12	2:B:946:ASN:HB2	1.72	0.54
14:N:4:DG:C2	16:T:-3:DG:C2	2.95	0.54
19:m:465:ASP:OD1	19:m:604:ARG:NH1	2.40	0.54
19:m:956:LEU:O	19:m:1046:ARG:NH2	2.38	0.54
22:r:223:VAL:HG22	22:r:325:GLN:HG2	1.88	0.54
23:u:89:SER:HB3	24:v:365:ARG:HE	1.72	0.54
14:N:-5:DG:N2	16:T:6:DC:O2	2.39	0.54
2:B:58:LEU:O	2:B:75:TYR:N	2.36	0.54
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.42	0.54
7:G:151:ARG:HB3	7:G:158:TYR:HB2	1.89	0.54
19:m:300:VAL:O	19:m:304:THR:OG1	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:54:DG:H4'	27:b:45:ARG:CZ	2.37	0.54
19:m:917:GLU:OE2	19:m:969:TYR:OH	2.24	0.54
21:q:766:MET:HE1	21:q:799:ILE:HG23	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
18:W:325:TYR:OH	18:W:451:GLN:OE1	2.23	0.54
19:m:956:LEU:HD11	19:m:1138:ILE:HG21	1.89	0.54
21:q:41:PHE:CG	21:q:70:VAL:HG11	2.42	0.54
24:v:258:ASN:OD1	24:v:261:ASN:N	2.40	0.54
18:W:332:LYS:O	18:W:388:ARG:NH1	2.41	0.54
19:m:533:VAL:HG22	19:m:589:VAL:HG13	1.90	0.54
21:q:218:LEU:HA	21:q:237:TRP:HE1	1.73	0.54
23:u:80:TYR:OH	24:v:352:VAL:O	2.22	0.54
1:A:218:GLU:OE1	1:A:222:ARG:NH1	2.41	0.54
7:G:144:ARG:HB2	7:G:171:ILE:HD13	1.90	0.54
16:T:106:DG:OP1	28:c:75:LYS:HE3	2.07	0.54
19:m:236:GLU:OE2	20:n:252:ARG:NH2	2.41	0.54
24:v:54:PHE:O	24:v:58:ASN:N	2.33	0.54
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.89	0.54
1:A:807:ARG:HD3	2:B:725:ARG:HA	1.89	0.53
2:B:91:GLU:OE2	2:B:97:HIS:NE2	2.29	0.53
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.89	0.53
4:D:6:SER:HB3	7:G:42:PHE:HZ	1.73	0.53
2:B:245:MET:HE1	2:B:371:LEU:HD11	1.91	0.53
14:N:-82:DG:H2''	14:N:-81:DG:OP2	2.07	0.53
1:A:351:ARG:HB2	2:B:1128:LEU:HD21	1.91	0.53
2:B:936:ASP:OD1	2:B:938:SER:OG	2.26	0.53
19:m:1205:ASP:OD2	19:m:1207:ARG:NH2	2.40	0.53
21:q:641:ALA:HB1	21:q:655:LYS:HG3	1.89	0.53
13:M:46:LEU:HD11	13:M:55:SER:HB3	1.90	0.53
24:v:74:TYR:HE1	24:v:87:LEU:HD12	1.73	0.53
30:j:728:MET:HE3	30:j:752:TYR:CD2	2.44	0.53
1:A:533:ARG:HD3	1:A:750:ALA:HB2	1.91	0.53
19:m:1024:TYR:CG	19:m:1135:TYR:HE2	2.26	0.53
1:A:1426:GLY:O	1:A:1430:ASN:ND2	2.40	0.53
14:N:-59:DT:H2''	14:N:-58:DC:C6	2.43	0.53
27:b:92:ARG:HH12	29:d:98:LEU:HD23	1.73	0.53
2:B:248:LYS:NZ	2:B:264:THR:OG1	2.41	0.53
17:V:10:ARG:HA	17:V:52:SER:HA	1.90	0.53
18:W:451:GLN:NE2	18:W:454:GLU:OE1	2.42	0.53
21:q:170:ASN:HA	21:q:173:LYS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:v:262:LYS:HD3	24:v:305:GLN:HE21	1.74	0.53
5:E:118:SER:OG	14:N:0:DG:OP1	2.22	0.53
18:W:513:SER:N	18:W:519:ASN:OD1	2.41	0.53
19:m:1047:ILE:HG12	19:m:1127:ILE:HG12	1.90	0.53
2:B:301:GLN:O	2:B:304:GLU:HG3	2.08	0.53
20:n:229:PRO:O	20:n:234:GLN:NE2	2.37	0.53
21:q:309:GLU:OE1	21:q:311:TYR:OH	2.20	0.53
2:B:592:THR:HG23	23:u:226:PHE:CE1	2.44	0.52
10:J:23:ARG:NH2	22:r:399:LYS:HZ1	2.07	0.52
14:N:-5:DG:N2	16:T:6:DC:C2	2.77	0.52
28:c:79:ILE:HG12	28:c:82:HIS:CE1	2.44	0.52
4:D:60:ILE:HG13	7:G:47:THR:HG21	1.91	0.52
21:q:317:LEU:HD23	22:r:514:LEU:HD12	1.91	0.52
2:B:59:ASP:HB3	2:B:74:ARG:HG3	1.91	0.52
8:H:59:LEU:HD23	8:H:139:LEU:HD13	1.91	0.52
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.49	0.52
16:T:20:DG:H2'	16:T:21:DC:H6	1.74	0.52
19:m:1121:ARG:HA	19:m:1124:LEU:HD12	1.91	0.52
1:A:119:ASN:OD1	1:A:121:THR:OG1	2.23	0.52
13:M:38:LEU:HA	13:M:45:GLY:HA2	1.91	0.52
17:V:10:ARG:HG2	17:V:52:SER:HB3	1.92	0.52
5:E:81:PHE:HE1	5:E:110:ILE:HD13	1.74	0.52
15:P:7:C:H2'	15:P:8:G:O4'	2.09	0.52
19:m:338:LEU:HD11	19:m:417:ILE:HD11	1.91	0.52
21:q:404:GLU:OE1	21:q:404:GLU:N	2.42	0.52
26:e:48:LEU:O	26:e:52:ARG:HG3	2.09	0.52
24:v:210:VAL:HG13	24:v:334:VAL:HG21	1.92	0.52
19:m:465:ASP:OD2	19:m:608:ARG:NH2	2.43	0.52
21:q:451:ARG:NH1	24:v:35:GLU:OE1	2.42	0.52
1:A:1153:GLU:OE2	9:I:45:ARG:NH1	2.40	0.52
16:T:85:DC:C2	16:T:86:DC:C4	2.98	0.52
19:m:995:ILE:HD12	19:m:1010:LEU:HD21	1.91	0.52
19:m:1062:ALA:HB3	19:m:1083:MET:HE1	1.92	0.52
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.93	0.51
1:A:977:ARG:HD2	1:A:979:LYS:HZ1	1.75	0.51
2:B:74:ARG:HB2	2:B:124:PHE:HB2	1.92	0.51
2:B:904:ARG:NH1	2:B:905:VAL:O	2.43	0.51
14:N:-30:DA:H2''	14:N:-29:DT:C7	2.41	0.51
14:N:5:DT:H2'	14:N:6:DA:C8	2.45	0.51
15:P:7:C:C2	15:P:8:G:C8	2.98	0.51
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:875:GLU:OE2	2:B:915:THR:OG1	2.26	0.51
16:T:6:DC:C2'	16:T:7:DC:C5	2.93	0.51
19:m:1056:ARG:HB3	19:m:1076:MET:HB3	1.91	0.51
18:W:590:ILE:O	18:W:593:SER:OG	2.26	0.51
21:q:871:TYR:CZ	21:q:875:ILE:HD11	2.45	0.51
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.74	0.51
24:v:233:GLY:O	24:v:244:ASN:ND2	2.44	0.51
1:A:801:VAL:HG22	1:A:813:GLU:HB3	1.92	0.51
2:B:86:ARG:NH1	22:r:369:GLU:OE2	2.44	0.51
28:c:85:LEU:O	28:c:89:ASN:HB2	2.11	0.51
27:f:89:ALA:O	27:f:93:GLN:HG2	2.10	0.51
1:A:771:VAL:HG13	1:A:823:GLU:HG3	1.92	0.51
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.75	0.51
18:W:326:VAL:HA	18:W:440:ILE:HD13	1.92	0.51
21:q:250:ASN:HA	21:q:253:ILE:HD12	1.91	0.51
21:q:286:SER:HA	21:q:289:LYS:HD2	1.92	0.51
5:E:87:VAL:HG23	5:E:91:THR:HB	1.91	0.51
13:M:33:SER:HA	13:M:50:LYS:HE2	1.93	0.51
18:W:260:TYR:HD1	18:W:276:ALA:HA	1.75	0.51
18:W:644:ASN:ND2	18:W:647:GLN:OE1	2.44	0.51
2:B:505:ARG:NH1	2:B:524:GLN:O	2.32	0.51
14:N:-83:DT:H2''	14:N:-82:DG:N7	2.26	0.51
14:N:-68:DT:H2''	14:N:-67:DT:H5'	1.92	0.51
29:d:41:VAL:O	29:d:45:VAL:HG22	2.10	0.51
2:B:547:ILE:HG21	2:B:619:ILE:HG21	1.93	0.51
2:B:797:TYR:HE1	2:B:854:LEU:HD13	1.74	0.51
1:A:1331:TYR:OH	1:A:1354:GLU:OE2	2.21	0.51
5:E:28:PHE:HE2	21:q:915:ARG:HB2	1.75	0.51
19:m:1172:VAL:HA	19:m:1182:VAL:HG12	1.93	0.51
22:r:244:LYS:NZ	22:r:305:GLU:OE2	2.37	0.51
1:A:1150:SER:OG	1:A:1198:GLU:OE1	2.29	0.50
14:N:-61:DT:H2'	14:N:-60:DT:C7	2.37	0.50
21:q:718:HIS:ND1	21:q:733:TYR:OH	2.38	0.50
24:v:104:PRO:HA	24:v:107:ARG:HD3	1.92	0.50
2:B:556:MET:HE3	2:B:581:GLY:HA3	1.93	0.50
14:N:-110:DG:OP2	28:c:74:LYS:NZ	2.44	0.50
14:N:-100:DT:H5'	28:c:77:ARG:NH2	2.26	0.50
18:W:563:GLU:HG2	18:W:574:ILE:HG12	1.92	0.50
1:A:1190:GLN:HA	1:A:1245:ILE:HA	1.93	0.50
2:B:83:TYR:HB2	2:B:116:TYR:HB2	1.92	0.50
2:B:436:ASN:C	2:B:438:ASN:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-81:DG:OP2	14:N:-81:DG:H2'	2.10	0.50
14:N:-7:DG:C6	14:N:-6:DG:N1	2.79	0.50
19:m:1046:ARG:HG3	19:m:1135:TYR:HE1	1.75	0.50
21:q:274:THR:HG23	22:r:506:ILE:HG12	1.93	0.50
20:n:206:SER:O	20:n:210:ASN:ND2	2.44	0.50
21:q:189:LEU:HD22	21:q:194:LYS:HD2	1.94	0.50
22:r:261:LEU:HB3	22:r:266:ASN:HB3	1.93	0.50
28:g:55:LEU:O	28:g:59:THR:HG23	2.11	0.50
19:m:244:GLY:O	19:m:248:GLN:N	2.44	0.50
19:m:840:ASN:O	19:m:844:ASN:ND2	2.44	0.50
21:q:109:PHE:CD1	21:q:130:ALA:HB1	2.46	0.50
21:q:408:LEU:HD13	24:v:44:LEU:HD22	1.92	0.50
21:q:676:ASN:HA	25:x:156:LEU:HD12	1.93	0.50
26:a:105:GLU:OE2	30:j:867:LEU:CD2	2.59	0.50
2:B:607:SER:HB3	2:B:620:PHE:HB2	1.94	0.50
19:m:933:HIS:HB3	19:m:936:LEU:HD12	1.94	0.50
21:q:568:SER:O	21:q:571:ASN:ND2	2.45	0.50
17:V:63:ASN:HB3	17:V:75:ASP:HA	1.94	0.50
19:m:562:PRO:HG3	19:m:700:TRP:CE3	2.47	0.50
24:v:263:TRP:HE1	24:v:356:ASN:HD21	1.59	0.50
27:f:49:LEU:HD21	30:j:727:LEU:HD11	1.93	0.50
1:A:168:CYS:SG	1:A:170:ASN:ND2	2.84	0.50
14:N:-62:DT:C2'	14:N:-61:DT:H72	2.40	0.50
19:m:766:LEU:HD13	19:m:783:PHE:HB2	1.93	0.50
19:m:1257:ILE:HG22	19:m:1261:ASN:HD21	1.77	0.50
22:r:208:ARG:N	22:r:291:ASP:OD1	2.44	0.50
22:r:276:PHE:HB2	22:r:279:GLN:HB2	1.92	0.50
1:A:916:TYR:OH	1:A:983:LEU:O	2.19	0.49
18:W:334:LYS:N	18:W:388:ARG:HH12	2.09	0.49
18:W:494:LEU:HD21	20:n:183:PRO:HG3	1.92	0.49
19:m:1027:PHE:HB3	19:m:1134:ARG:HH12	1.76	0.49
23:u:170:ILE:HD11	24:v:200:PHE:HD1	1.76	0.49
2:B:74:ARG:HH22	2:B:126:SER:HB3	1.77	0.49
9:I:17:LYS:N	9:I:26:LEU:O	2.39	0.49
15:P:5:G:C2	15:P:6:G:C5	3.00	0.49
16:T:25:DG:H5'	16:T:25:DG:C8	2.47	0.49
19:m:343:ARG:NH2	19:m:344:ASP:OD1	2.45	0.49
21:q:160:ARG:NH2	21:q:163:GLU:OE1	2.44	0.49
2:B:479:TYR:CZ	2:B:1096:ARG:HB3	2.48	0.49
2:B:498:ASP:HB3	14:N:-15:DA:C4	2.47	0.49
7:G:119:LEU:HD21	7:G:135:GLU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-88:DT:C6	14:N:-87:DT:H72	2.47	0.49
16:T:84:DC:H2''	16:T:85:DC:C6	2.47	0.49
16:T:92:DC:H2''	16:T:93:DA:C8	2.47	0.49
19:m:242:GLY:HA3	20:n:258:LYS:HG2	1.94	0.49
19:m:725:GLU:OE2	19:m:728:ARG:NH2	2.45	0.49
27:f:75:HIS:O	29:h:89:ARG:NH1	2.45	0.49
2:B:300:TRP:HA	2:B:303:LEU:HD12	1.94	0.49
1:A:1223:SER:OG	1:A:1224:ASP:N	2.44	0.49
4:D:105:THR:HG22	7:G:105:PRO:HD3	1.94	0.49
14:N:-97:DT:H2'	14:N:-96:DT:H71	1.93	0.49
14:N:-57:DT:H2''	14:N:-56:DG:H8	1.77	0.49
21:q:305:TYR:CZ	22:r:512:LEU:HD11	2.48	0.49
30:j:586:ILE:HD12	30:j:628:MET:SD	2.52	0.49
2:B:887:HIS:HB2	15:P:-3:A:C2	2.46	0.49
14:N:2:DG:N2	14:N:3:DC:O2	2.46	0.49
19:m:655:LEU:HG	19:m:659:MET:HE3	1.95	0.49
19:m:1170:VAL:HG12	19:m:1184:THR:HG22	1.95	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:928:ARG:NH1	19:m:776:GLY:H	2.11	0.49
7:G:112:THR:HA	7:G:115:ILE:HD12	1.95	0.49
5:E:81:PHE:CE1	5:E:110:ILE:HD13	2.48	0.49
9:I:96:ASN:OD1	9:I:97:MET:N	2.46	0.49
16:T:74:DA:H2''	16:T:75:DC:C5	2.48	0.49
18:W:464:ILE:O	18:W:468:LEU:HG	2.12	0.49
19:m:823:ILE:HB	19:m:873:VAL:HG22	1.95	0.49
21:q:816:LEU:HD13	21:q:865:ILE:HA	1.95	0.49
28:g:41:GLU:HB2	29:h:84:SER:HB2	1.95	0.49
31:k:108:ARG:NH2	31:k:127:ASN:HD22	2.11	0.49
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	1.94	0.48
12:L:70:ASP:HB3	18:W:784:ASN:HB3	1.95	0.48
14:N:-7:DG:N1	14:N:-6:DG:C2	2.81	0.48
15:P:0:C:O2'	15:P:1:C:OP2	2.27	0.48
19:m:1202:ASP:OD2	19:m:1204:ARG:NE	2.44	0.48
2:B:610:ARG:NH2	9:I:61:ASP:OD2	2.46	0.48
18:W:222:ASP:O	18:W:277:ARG:NH2	2.30	0.48
19:m:770:PHE:HB3	19:m:779:VAL:HG22	1.95	0.48
27:f:93:GLN:HB2	27:f:95:ARG:HG2	1.96	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
18:W:634:PRO:HA	18:W:637:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:n:207:ILE:HG23	20:n:212:LEU:HB3	1.94	0.48
23:u:202:GLU:HB3	24:v:210:VAL:HB	1.96	0.48
31:k:239:ILE:CG2	31:k:246:LEU:HD11	2.43	0.48
1:A:673:ASP:OD1	1:A:673:ASP:N	2.44	0.48
1:A:738:LEU:HD13	1:A:742:ASN:HD22	1.77	0.48
2:B:318:ASP:HB3	2:B:321:VAL:HG22	1.94	0.48
3:C:66:LEU:HD11	3:C:155:ILE:HD12	1.95	0.48
3:C:105:GLU:N	3:C:105:GLU:OE1	2.46	0.48
22:r:493:ASN:HB2	22:r:502:ILE:HD11	1.95	0.48
29:d:95:VAL:HG13	29:d:99:LEU:HD12	1.94	0.48
2:B:314:PHE:O	2:B:317:GLN:NE2	2.46	0.48
14:N:-93:DT:H4'	14:N:-92:DG:OP1	2.12	0.48
24:v:36:LYS:HB2	24:v:39:PRO:HD2	1.95	0.48
1:A:63:ARG:NH2	15:P:0:C:OP1	2.47	0.48
1:A:418:TYR:HE2	15:P:-2:U:O4	1.96	0.48
2:B:514:LEU:HD22	2:B:626:VAL:HG12	1.94	0.48
19:m:1365:GLU:O	19:m:1369:ASN:ND2	2.46	0.48
27:f:27:GLN:HB3	30:j:781:GLU:OE1	2.14	0.48
14:N:-62:DT:H2''	14:N:-61:DT:C6	2.49	0.48
15:P:1:C:N3	16:T:26:DG:N2	2.44	0.48
19:m:681:VAL:HG13	19:m:708:TRP:HE1	1.79	0.48
21:q:185:LYS:O	21:q:189:LEU:HG	2.14	0.48
21:q:607:LYS:HB2	21:q:610:LEU:HB2	1.96	0.48
1:A:321:ARG:NH1	2:B:466:MET:SD	2.86	0.48
17:V:91:PRO:HD2	17:V:94:ILE:HB	1.95	0.48
18:W:666:GLU:HB2	18:W:671:ARG:HA	1.95	0.48
19:m:1062:ALA:HA	19:m:1103:LEU:HD21	1.96	0.48
21:q:261:ASP:O	21:q:265:ASN:ND2	2.36	0.48
21:q:312:GLU:O	21:q:316:LYS:HG3	2.14	0.48
21:q:320:LEU:O	21:q:324:GLU:HG2	2.14	0.48
2:B:365:THR:O	2:B:368:THR:OG1	2.29	0.48
16:T:105:DA:H3'	28:c:75:LYS:HE3	1.95	0.48
18:W:603:GLN:HG3	18:W:609:VAL:HG22	1.95	0.48
20:n:163:LEU:HD22	20:n:197:ILE:HD13	1.96	0.48
24:v:304:ASP:OD2	24:v:340:LYS:NZ	2.45	0.48
26:e:61:LEU:HD12	27:f:37:LEU:HD23	1.95	0.48
5:E:91:THR:HA	5:E:94:ASN:ND2	2.28	0.48
14:N:-93:DT:H2''	14:N:-92:DG:C8	2.48	0.48
19:m:977:VAL:HB	19:m:980:LEU:HD12	1.94	0.48
29:h:89:ARG:O	29:h:93:THR:HG23	2.14	0.48
2:B:766:ARG:HH21	2:B:1020:ARG:HD3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:788:ARG:O	2:B:967:ARG:NH1	2.47	0.47
9:I:103:CYS:SG	9:I:104:LEU:N	2.86	0.47
18:W:599:HIS:HB3	18:W:677:LEU:HD21	1.96	0.47
19:m:1279:ARG:NH1	19:m:1315:SER:O	2.47	0.47
23:u:204:ASN:OD1	23:u:205:GLU:N	2.47	0.47
25:x:311:GLY:HA3	25:x:330:VAL:HG12	1.96	0.47
27:b:98:TYR:HB3	29:h:58:ILE:HG23	1.95	0.47
1:A:106:ILE:HD13	1:A:215:ILE:HD11	1.95	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
4:D:157:ILE:HG23	4:D:164:ALA:HB2	1.95	0.47
18:W:666:GLU:HA	18:W:705:VAL:HG12	1.96	0.47
19:m:1425:LYS:HE3	19:m:1428:PRO:HA	1.96	0.47
19:m:1003:ALA:O	19:m:1007:THR:HG23	2.14	0.47
19:m:1427:ASN:OD1	19:m:1430:SER:N	2.47	0.47
22:r:263:SER:OG	22:r:264:LYS:N	2.47	0.47
24:v:89:LYS:O	24:v:93:SER:N	2.46	0.47
30:j:593:PRO:HG2	31:k:177:TYR:CE2	2.48	0.47
9:I:29:CYS:CB	9:I:32:CYS:SG	2.99	0.47
21:q:710:LEU:HD11	21:q:748:LEU:HD11	1.96	0.47
24:v:199:HIS:O	24:v:328:ALA:N	2.47	0.47
3:C:88:GLU:HG2	18:W:759:ARG:HD2	1.95	0.47
5:E:93:ARG:HA	5:E:122:MET:HE1	1.97	0.47
21:q:4:LEU:HB2	24:v:103:HIS:CE1	2.49	0.47
22:r:366:GLU:O	22:r:369:GLU:HG2	2.15	0.47
2:B:896:ASP:OD2	12:L:31:TYR:OH	2.32	0.47
3:C:74:GLU:O	3:C:246:ARG:NH2	2.39	0.47
28:c:88:ARG:NH1	28:c:97:LEU:O	2.31	0.47
1:A:580:SER:HB3	1:A:612:LYS:HA	1.97	0.47
1:A:948:VAL:O	5:E:200:ARG:NH1	2.48	0.47
1:A:976:ASP:O	1:A:979:LYS:NZ	2.48	0.47
1:A:983:LEU:HD13	1:A:1041:ARG:HA	1.96	0.47
2:B:421:ILE:HD11	2:B:441:VAL:HG12	1.97	0.47
5:E:213:CYS:SG	5:E:214:LEU:N	2.87	0.47
13:M:37:THR:O	13:M:46:LEU:N	2.29	0.47
19:m:965:VAL:HG22	19:m:989:ILE:HG13	1.95	0.47
22:r:408:ASP:OD2	24:v:134:VAL:HG23	2.14	0.47
23:u:90:LEU:HB2	24:v:362:MET:HE1	1.96	0.47
15:P:-5:U:H1'	18:W:748:ARG:HD3	1.96	0.47
19:m:381:VAL:HG13	19:m:414:LEU:HD22	1.97	0.47
22:r:206:PHE:HB2	22:r:227:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:MET:O	1:A:823:GLU:HG2	2.14	0.47
3:C:4:GLU:HB3	3:C:5:PRO:HD3	1.96	0.47
17:V:41:SER:HB2	17:V:45:THR:HB	1.96	0.47
19:m:1337:GLU:HB2	19:m:1348:VAL:HB	1.95	0.47
21:q:155:TYR:HB2	21:q:164:ALA:HB2	1.96	0.47
1:A:472:ASN:O	1:A:475:VAL:HG22	2.14	0.47
1:A:1192:PRO:HA	1:A:1243:ARG:HH12	1.79	0.47
14:N:-86:DG:C2	16:T:87:DA:C2	3.03	0.47
14:N:-71:DT:H4'	26:a:83:ARG:HD3	1.97	0.47
21:q:4:LEU:HD22	24:v:105:ASP:HB2	1.97	0.47
1:A:912:ASP:OD1	1:A:912:ASP:N	2.44	0.46
2:B:101:PRO:HG2	2:B:172:LEU:HD11	1.96	0.46
2:B:322:ALA:O	2:B:326:ILE:HG12	2.15	0.46
7:G:123:PRO:HA	7:G:128:PRO:HB3	1.97	0.46
16:T:1:DT:C2	16:T:2:DG:C8	3.03	0.46
19:m:622:THR:O	19:m:626:LYS:N	2.41	0.46
19:m:1072:ASP:O	19:m:1076:MET:HG2	2.15	0.46
30:j:644:LYS:HE2	30:j:648:GLU:OE2	2.15	0.46
14:N:-56:DG:C2'	14:N:-55:DT:H71	2.46	0.46
15:P:1:C:H2'	15:P:2:C:O4'	2.15	0.46
18:W:260:TYR:CE1	18:W:277:ARG:HG3	2.49	0.46
18:W:704:ARG:NH1	19:m:632:GLU:OE2	2.43	0.46
19:m:1426:LEU:HD13	19:m:1469:ARG:HH21	1.80	0.46
21:q:710:LEU:HD13	21:q:740:PHE:HB2	1.98	0.46
24:v:310:HIS:NE2	24:v:316:ASP:OD2	2.48	0.46
1:A:363:ASP:HB3	1:A:509:PRO:HD3	1.97	0.46
2:B:25:PHE:HZ	2:B:534:LEU:HG	1.81	0.46
2:B:879:ARG:NH2	15:P:-3:A:H4'	2.27	0.46
6:F:74:ILE:HG23	6:F:78:GLU:HG3	1.97	0.46
7:G:51:GLY:HA2	7:G:54:ILE:HD11	1.98	0.46
10:J:6:ARG:HD3	10:J:13:VAL:HG22	1.97	0.46
11:K:62:LYS:HE3	11:K:64:GLU:OE2	2.15	0.46
19:m:380:GLU:HG2	19:m:978:CYS:HB2	1.97	0.46
21:q:374:ALA:HA	21:q:377:LEU:HD12	1.96	0.46
27:b:75:HIS:CD2	29:d:93:THR:HG21	2.49	0.46
1:A:215:ILE:O	1:A:231:ARG:NH2	2.45	0.46
2:B:273:PRO:HG2	2:B:276:ILE:HD12	1.98	0.46
2:B:497:ARG:NH2	16:T:16:DA:OP2	2.48	0.46
3:C:17:VAL:HG12	3:C:240:ALA:HB1	1.96	0.46
4:D:139:PRO:HA	4:D:142:ILE:HD12	1.96	0.46
5:E:98:ARG:NH1	5:E:102:LYS:HG3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:v:73:ASN:HB3	24:v:76:ARG:HE	1.79	0.46
25:x:173:LEU:HA	25:x:177:LYS:HD2	1.98	0.46
26:a:113:HIS:CG	26:e:126:LEU:HD22	2.51	0.46
2:B:27:GLU:OE1	2:B:678:TRP:HB3	2.16	0.46
5:E:96:CYS:SG	5:E:126:VAL:HG23	2.55	0.46
14:N:-3:DA:C2	14:N:-2:DC:C2	3.03	0.46
20:n:208:LEU:HD13	20:n:250:HIS:CE1	2.50	0.46
21:q:215:ASP:OD1	21:q:217:ARG:NH1	2.47	0.46
28:g:29:ARG:HG3	28:g:32:ARG:NH2	2.30	0.46
28:g:29:ARG:HG3	28:g:32:ARG:HH21	1.79	0.46
16:T:67:DA:C2	16:T:68:DA:C4	3.04	0.46
18:W:534:PHE:HB3	18:W:554:ILE:HD13	1.97	0.46
19:m:1426:LEU:HD21	19:m:1465:MET:HE2	1.96	0.46
24:v:349:VAL:HA	24:v:352:VAL:HB	1.98	0.46
26:a:93:GLN:O	26:a:97:GLU:HG3	2.15	0.46
1:A:649:ASN:O	1:A:653:VAL:HG23	2.16	0.46
14:N:2:DG:C2	14:N:3:DC:C2	3.03	0.46
19:m:306:LEU:HD13	19:m:314:ARG:HH21	1.80	0.46
27:b:38:ALA:HB1	27:b:43:VAL:HB	1.98	0.46
31:k:141:ASN:HD21	31:k:256:LYS:HD3	1.80	0.46
1:A:1448:ILE:HD11	1:A:1453:LEU:HD11	1.97	0.46
14:N:-61:DT:H4'	26:a:63:ARG:NH1	2.30	0.46
16:T:54:DG:H2''	16:T:55:DA:C8	2.51	0.46
23:u:170:ILE:HD11	24:v:200:PHE:CD1	2.50	0.46
26:e:73:GLU:OE1	27:f:25:ASN:HB2	2.16	0.46
27:f:75:HIS:HD2	29:h:93:THR:HG21	1.81	0.46
1:A:409:ASP:OD1	1:A:410:ASN:N	2.49	0.46
18:W:451:GLN:HG3	18:W:458:THR:HA	1.98	0.46
23:u:173:TRP:NE1	23:u:179:SER:OG	2.36	0.46
2:B:885:LEU:HD23	2:B:936:ASP:HB2	1.97	0.46
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.49	0.46
21:q:320:LEU:HD13	22:r:514:LEU:HD11	1.97	0.46
28:c:42:ARG:O	29:d:85:THR:HA	2.16	0.46
1:A:543:GLU:OE2	1:A:570:LYS:NZ	2.43	0.45
1:A:1065:MET:SD	1:A:1439:MET:HB2	2.56	0.45
2:B:557:GLU:OE2	2:B:584:ARG:NH2	2.48	0.45
4:D:170:ASN:HB3	4:D:173:ARG:HG2	1.97	0.45
7:G:81:PRO:HG3	7:G:106:LEU:HD22	1.99	0.45
16:T:51:DC:H2''	16:T:52:DG:C8	2.51	0.45
19:m:561:SER:HA	19:m:696:ILE:HG23	1.97	0.45
1:A:684:ILE:HG21	1:A:802:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:PRO:HG3	2:B:352:GLU:O	2.16	0.45
2:B:318:ASP:OD1	2:B:319:LYS:N	2.48	0.45
2:B:778:MET:HE2	2:B:1094:ARG:HD3	1.98	0.45
16:T:86:DC:OP1	28:c:43:VAL:N	2.38	0.45
21:q:107:PHE:O	21:q:111:LEU:HG	2.16	0.45
21:q:241:LEU:HD11	21:q:252:LYS:HG2	1.98	0.45
2:B:353:LEU:O	2:B:367:LYS:NZ	2.34	0.45
18:W:539:HIS:CE1	18:W:553:LEU:HD21	2.51	0.45
19:m:1218:ALA:HB1	19:m:1232:LEU:HB3	1.99	0.45
21:q:489:PHE:HE1	21:q:533:VAL:HG21	1.80	0.45
26:e:54:TYR:HB3	27:f:40:ARG:HB2	1.98	0.45
2:B:463:LYS:NZ	2:B:464:LYS:HE2	2.31	0.45
16:T:-7:DG:H1'	16:T:-6:DT:C5	2.52	0.45
19:m:654:ASP:OD2	19:m:933:HIS:NE2	2.50	0.45
19:m:1105:LEU:HD11	19:m:1128:LYS:HE2	1.98	0.45
26:a:62:ILE:O	26:a:93:GLN:NE2	2.48	0.45
3:C:21:LEU:HD22	11:K:101:LEU:HD11	1.98	0.45
16:T:67:DA:C6	16:T:68:DA:C6	3.04	0.45
19:m:521:TYR:HA	19:m:524:ILE:HD12	1.97	0.45
21:q:403:SER:OG	24:v:56:LYS:NZ	2.49	0.45
2:B:220:ALA:O	2:B:252:ARG:NH2	2.47	0.45
7:G:113:ARG:NH1	18:W:563:GLU:OE1	2.49	0.45
14:N:-14:DA:H61	16:T:14:DT:H3	1.65	0.45
21:q:479:TYR:HD1	24:v:30:LEU:HB3	1.82	0.45
23:u:106:TRP:CD1	23:u:217:LYS:HB2	2.52	0.45
18:W:344:LEU:HD12	18:W:349:GLU:HB2	1.99	0.45
19:m:475:SER:OG	19:m:522:ASP:OD1	2.29	0.45
19:m:1286:PHE:HA	19:m:1308:ILE:HB	1.99	0.45
21:q:155:TYR:O	21:q:160:ARG:N	2.42	0.45
31:k:10:PHE:HB2	31:k:78:ASP:OD1	2.16	0.45
2:B:27:GLU:OE2	2:B:679:SER:OG	2.35	0.45
2:B:1050:LEU:HD12	24:v:127:PHE:CG	2.51	0.45
18:W:491:LEU:HB3	18:W:494:LEU:HD12	1.98	0.45
19:m:1220:ILE:HA	19:m:1232:LEU:HD23	1.98	0.45
21:q:489:PHE:CE1	21:q:533:VAL:HG21	2.51	0.45
21:q:713:PHE:HB3	21:q:736:ALA:HB2	1.98	0.45
3:C:15:ASP:OD1	3:C:15:ASP:N	2.47	0.45
21:q:905:ARG:NE	21:q:909:GLU:OE2	2.30	0.45
1:A:975:LEU:HD13	1:A:1039:LEU:HA	1.99	0.45
4:D:54:SER:OG	4:D:121:CYS:SG	2.61	0.45
5:E:117:PRO:O	5:E:121:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:110:LYS:HE2	8:H:112:LYS:HE3	1.99	0.45
19:m:1029:PRO:O	19:m:1033:ARG:NH1	2.50	0.45
24:v:29:LEU:HB2	25:x:147:ARG:HB3	1.98	0.45
2:B:387:ASP:H	9:I:91:ARG:NH2	2.14	0.44
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.79	0.44
14:N:-81:DG:H2''	14:N:-80:DT:H72	1.99	0.44
15:P:-7:U:P	19:m:1173:ARG:HH12	2.39	0.44
19:m:999:LEU:HD23	19:m:1025:ILE:HD11	1.99	0.44
14:N:-73:DT:H2''	14:N:-72:DT:OP2	2.17	0.44
14:N:-14:DA:C6	14:N:-13:DA:N1	2.85	0.44
22:r:300:ASP:O	22:r:304:ARG:HG2	2.17	0.44
27:f:92:ARG:NH2	29:h:98:LEU:HD13	2.32	0.44
1:A:1061:HIS:O	1:A:1064:GLU:HG2	2.17	0.44
2:B:74:ARG:NH1	2:B:126:SER:OG	2.40	0.44
2:B:892:LYS:NZ	2:B:909:ASP:OD2	2.45	0.44
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.49	0.44
5:E:46:CYS:HB3	5:E:50:GLY:HA2	1.99	0.44
16:T:85:DC:H2''	16:T:86:DC:C5	2.52	0.44
19:m:336:GLU:OE1	19:m:458:ARG:NH2	2.50	0.44
30:j:622:SER:CB	30:j:628:MET:HE2	2.48	0.44
14:N:-7:DG:C2	14:N:-6:DG:C2	3.04	0.44
14:N:-5:DG:H2''	14:N:-4:DG:O4'	2.17	0.44
15:P:-2:U:H2'	15:P:-2:U:O2	2.17	0.44
17:V:78:GLN:OE1	17:V:79:PRO:HD2	2.16	0.44
19:m:735:LEU:HB3	19:m:937:LEU:HD21	1.99	0.44
19:m:782:VAL:HG11	19:m:905:ILE:HG13	1.99	0.44
19:m:1279:ARG:NH2	19:m:1344:ALA:O	2.51	0.44
21:q:357:LYS:NZ	21:q:361:ASP:OD1	2.50	0.44
23:u:116:ILE:HD13	23:u:150:VAL:HB	1.99	0.44
30:j:738:PRO:CG	30:j:745:LYS:HE2	2.48	0.44
1:A:564:PRO:HG2	1:A:567:LEU:HD23	1.98	0.44
18:W:216:LEU:HD22	19:m:229:LEU:HG	1.98	0.44
1:A:343:GLY:O	2:B:1129:ARG:NH1	2.45	0.44
1:A:452:HIS:CE1	1:A:454:MET:HB2	2.52	0.44
1:A:1098:LEU:HD23	1:A:1098:LEU:HA	1.89	0.44
3:C:258:VAL:HG21	11:K:42:LEU:HD21	2.00	0.44
15:P:-4:A:C2	18:W:748:ARG:HG2	2.52	0.44
16:T:-2:DC:H2'	16:T:-1:DG:C8	2.52	0.44
20:n:200:ARG:HG2	20:n:202:ASN:OD1	2.18	0.44
21:q:178:ASN:HA	24:v:91:PHE:CE2	2.52	0.44
21:q:641:ALA:HB2	21:q:658:GLN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:GLU:O	1:A:957:PRO:HA	2.18	0.44
1:A:889:GLY:O	1:A:941:ARG:NH2	2.51	0.44
3:C:79:MET:HE1	3:C:96:VAL:HG23	2.00	0.44
13:M:65:GLN:N	13:M:68:ASP:OD2	2.44	0.44
14:N:-50:DT:H2''	14:N:-49:DG:C8	2.53	0.44
19:m:640:TYR:HB3	19:m:1256:ASP:HB3	2.00	0.44
19:m:1039:MET:SD	19:m:1039:MET:N	2.90	0.44
22:r:277:PRO:HB2	22:r:305:GLU:HB3	2.00	0.44
25:x:314:PHE:HD2	25:x:335:ILE:HD11	1.82	0.44
30:j:503:ILE:CD1	30:j:907:PRO:HG3	2.47	0.44
1:A:701:ASN:CG	9:I:96:ASN:HD21	2.26	0.44
14:N:-95:DG:C2	14:N:-94:DG:N2	2.83	0.44
18:W:250:ARG:NH2	18:W:284:ASP:OD2	2.50	0.44
21:q:435:GLN:HG3	21:q:441:ILE:HD11	1.98	0.44
21:q:561:ILE:HD12	21:q:579:LEU:HD22	1.99	0.44
2:B:221:ALA:O	2:B:223:SER:N	2.46	0.44
2:B:640:ASP:OD1	2:B:640:ASP:N	2.51	0.44
16:T:6:DC:H2''	16:T:7:DC:C6	2.52	0.44
18:W:763:TYR:HB3	18:W:766:LYS:HD3	2.00	0.44
19:m:536:ILE:HG12	19:m:700:TRP:CZ3	2.53	0.44
19:m:538:ASN:HB3	19:m:541:GLN:HB2	2.00	0.44
19:m:590:LYS:HD2	19:m:706:ASP:HB2	1.99	0.44
19:m:603:ILE:HD13	19:m:708:TRP:HZ3	1.83	0.44
19:m:968:PRO:HA	19:m:971:ALA:HB3	1.99	0.44
21:q:868:GLN:O	21:q:872:GLU:HG2	2.17	0.44
25:x:222:MET:HE3	25:x:222:MET:HB3	1.84	0.44
26:e:60:LEU:HD22	26:e:93:GLN:HG2	2.00	0.44
1:A:636:ARG:HH12	1:A:878:GLN:CD	2.25	0.43
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	1.99	0.43
8:H:25:ARG:HD3	8:H:41:ASP:OD1	2.18	0.43
15:P:-6:G:H2'	15:P:-5:U:O4'	2.18	0.43
18:W:518:ILE:HD13	20:n:185:ILE:HD13	2.00	0.43
19:m:685:TYR:O	19:m:689:LYS:N	2.41	0.43
21:q:217:ARG:HA	21:q:220:ILE:HD12	2.00	0.43
28:c:100:VAL:HG12	27:f:96:THR:HB	2.00	0.43
29:d:43:LYS:HA	29:d:43:LYS:HD3	1.70	0.43
27:f:64:ASN:HA	27:f:67:ARG:NH1	2.32	0.43
29:h:51:ILE:HG22	29:h:52:SER:O	2.18	0.43
1:A:1390:HIS:O	1:A:1394:ARG:HD3	2.17	0.43
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.00	0.43
14:N:-63:DT:H2''	14:N:-62:DT:C7	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:8:G:H2'	15:P:8:G:N3	2.33	0.43
19:m:477:GLN:OE1	19:m:477:GLN:N	2.42	0.43
21:q:526:ASN:O	21:q:530:VAL:HG23	2.18	0.43
22:r:206:PHE:H	22:r:229:LEU:HD21	1.83	0.43
23:u:117:ASN:HB3	23:u:151:ARG:HG2	2.00	0.43
28:c:50:TYR:O	28:c:54:VAL:HG23	2.18	0.43
1:A:779:GLY:HA3	2:B:509:ASN:HB2	1.99	0.43
5:E:99:ILE:HG13	5:E:131:ILE:HD11	1.99	0.43
10:J:63:ASN:OD1	10:J:64:PRO:HD2	2.18	0.43
14:N:-82:DG:H2''	14:N:-81:DG:H8	1.84	0.43
16:T:75:DC:H2''	16:T:76:DG:C8	2.52	0.43
17:V:67:TRP:NE1	18:W:217:LEU:O	2.51	0.43
19:m:305:ASP:OD1	19:m:1014:THR:OG1	2.33	0.43
19:m:817:ASN:OD1	19:m:819:ASN:ND2	2.42	0.43
20:n:167:MET:HE3	20:n:219:TRP:CD2	2.53	0.43
21:q:261:ASP:HB2	24:v:58:ASN:ND2	2.34	0.43
21:q:559:ARG:NH2	24:v:24:PRO:O	2.51	0.43
27:b:32:PRO:O	27:b:36:ARG:HG3	2.18	0.43
1:A:100:LYS:NZ	1:A:104:GLU:OE2	2.49	0.43
1:A:329:ARG:NH1	2:B:1206:GLU:OE2	2.45	0.43
5:E:104:PHE:HZ	21:q:925:TRP:HZ3	1.66	0.43
14:N:0:DG:H1'	14:N:1:DC:H5'	1.99	0.43
16:T:-3:DG:H2''	16:T:-2:DC:H5	1.78	0.43
16:T:60:DA:C2	16:T:61:DA:C2	3.06	0.43
17:V:46:VAL:O	17:V:50:THR:N	2.44	0.43
18:W:322:ARG:NE	18:W:343:VAL:H	2.17	0.43
19:m:306:LEU:O	19:m:311:GLN:NE2	2.51	0.43
19:m:955:ASN:HD21	19:m:978:CYS:HB3	1.83	0.43
2:B:721:ASP:OD2	2:B:724:LYS:N	2.41	0.43
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.28	0.43
5:E:11:LEU:HD21	5:E:57:MET:HE1	2.00	0.43
7:G:118:ASN:OD1	7:G:118:ASN:N	2.51	0.43
14:N:-80:DT:H2''	14:N:-79:DG:H5'	2.01	0.43
14:N:-65:DT:H1'	14:N:-64:DT:H5'	2.00	0.43
21:q:284:LEU:HD11	21:q:297:LEU:HD22	2.01	0.43
24:v:31:LYS:HA	25:x:147:ARG:HH12	1.82	0.43
2:B:776:GLN:NE2	15:P:9:G:OP1	2.49	0.43
18:W:490:GLU:CD	20:n:229:PRO:HA	2.43	0.43
19:m:1005:LEU:HA	19:m:1010:LEU:HD12	2.01	0.43
19:m:1309:ARG:NH2	19:m:1319:THR:HG21	2.34	0.43
21:q:308:LYS:NZ	22:r:504:SER:O	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:u:83:GLY:HA2	24:v:358:ALA:HB3	2.01	0.43
30:j:593:PRO:HG2	31:k:177:TYR:HE2	1.83	0.43
2:B:257:THR:OG1	2:B:258:GLY:N	2.50	0.43
3:C:107:GLU:O	3:C:107:GLU:CG	2.66	0.43
14:N:-57:DT:H2''	14:N:-56:DG:C8	2.53	0.43
18:W:468:LEU:HD11	19:m:283:VAL:HG13	2.01	0.43
20:n:157:ASP:HA	20:n:210:ASN:HD21	1.83	0.43
21:q:511:VAL:HG11	21:q:519:LEU:HD12	2.01	0.43
1:A:1389:ARG:O	1:A:1393:ASN:HB2	2.18	0.43
2:B:1156:ASP:O	2:B:1197:PRO:HA	2.19	0.43
14:N:-82:DG:H2''	14:N:-81:DG:C8	2.54	0.43
14:N:2:DG:N3	14:N:3:DC:C2	2.87	0.43
19:m:1002:ARG:HH11	19:m:1052:TYR:HH	1.65	0.43
30:j:730:ILE:HG21	30:j:750:GLN:HE21	1.83	0.43
31:k:223:VAL:HG23	31:k:308:VAL:HG11	2.00	0.43
2:B:250:TYR:HE2	2:B:262:LYS:HB2	1.82	0.43
2:B:763:GLN:HG2	2:B:765:PRO:HD2	2.01	0.43
6:F:103:MET:HE1	7:G:65:SER:O	2.19	0.43
7:G:115:ILE:HG23	7:G:163:ILE:HD11	2.01	0.43
8:H:8:ASP:OD1	8:H:9:ILE:N	2.48	0.43
21:q:9:TYR:OH	24:v:106:ASP:OD2	2.20	0.43
21:q:40:ASP:CG	21:q:42:ASN:HD22	2.26	0.43
21:q:122:ARG:HB2	21:q:126:PHE:CE2	2.54	0.43
21:q:841:TYR:HB2	21:q:846:LEU:HD21	2.01	0.43
28:g:31:HIS:CD2	28:g:35:ARG:HH12	2.37	0.43
4:D:88:GLU:HA	4:D:91:LYS:HE3	2.00	0.43
9:I:40:ASP:OD1	9:I:40:ASP:N	2.44	0.43
9:I:100:PHE:HB3	9:I:109:THR:HG23	1.99	0.43
14:N:-61:DT:H2''	14:N:-60:DT:C6	2.53	0.43
24:v:311:LYS:HE2	24:v:311:LYS:HB2	1.90	0.43
25:x:226:LYS:HB2	25:x:248:LEU:HD21	2.00	0.43
1:A:421:ARG:HB3	1:A:424:ASP:HB2	2.01	0.42
1:A:815:PHE:O	1:A:819:MET:HG3	2.19	0.42
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.51	0.42
2:B:691:ASP:OD1	2:B:691:ASP:N	2.41	0.42
2:B:764:SER:OG	2:B:765:PRO:HD3	2.19	0.42
17:V:12:CYS:HA	17:V:50:THR:HA	2.01	0.42
19:m:1399:SER:HA	19:m:1407:HIS:CE1	2.54	0.42
21:q:53:LEU:O	21:q:57:GLU:HG2	2.19	0.42
21:q:267:SER:O	22:r:494:TYR:OH	2.34	0.42
21:q:611:GLU:HG2	21:q:615:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:g:31:HIS:CE1	28:g:35:ARG:HH12	2.37	0.42
1:A:38:PRO:HA	1:A:271:LEU:HD23	2.01	0.42
1:A:473:LEU:HD21	2:B:835:GLN:HB2	2.00	0.42
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.88	0.42
2:B:1133:MET:HE2	16:T:17:DA:H4'	2.01	0.42
9:I:29:CYS:HB3	9:I:32:CYS:SG	2.59	0.42
15:P:2:C:H2'	15:P:3:U:C6	2.54	0.42
19:m:773:GLY:N	19:m:777:ASP:OD2	2.52	0.42
21:q:102:SER:OG	21:q:137:SER:OG	2.30	0.42
24:v:41:LYS:HB3	24:v:45:LYS:HE3	2.01	0.42
24:v:202:PRO:HG2	24:v:382:TYR:OH	2.19	0.42
1:A:252:ALA:HA	1:A:258:GLN:HA	2.00	0.42
1:A:1221:VAL:HG21	1:A:1274:ILE:HD12	2.01	0.42
2:B:85:SER:OG	2:B:114:PRO:HD2	2.20	0.42
2:B:237:LYS:HA	2:B:237:LYS:HD3	1.90	0.42
2:B:733:SER:HB3	2:B:736:HIS:CE1	2.54	0.42
20:n:195:LYS:HE3	20:n:199:LEU:HD11	2.00	0.42
21:q:189:LEU:HB3	21:q:194:LYS:HB2	2.01	0.42
24:v:307:PHE:HE1	24:v:335:GLY:HA3	1.83	0.42
2:B:330:GLY:HA3	2:B:344:TYR:HE2	1.84	0.42
2:B:592:THR:HG23	23:u:226:PHE:CZ	2.54	0.42
14:N:-33:DG:H2''	14:N:-32:DT:H72	2.02	0.42
20:n:208:LEU:HD22	20:n:250:HIS:CD2	2.54	0.42
21:q:830:LEU:HD22	21:q:846:LEU:HB3	2.02	0.42
22:r:245:VAL:HG23	22:r:298:GLU:HG2	2.01	0.42
22:r:370:GLU:HG3	23:u:251:VAL:HA	2.01	0.42
29:h:76:ARG:HG2	29:h:80:TYR:CE2	2.54	0.42
1:A:914:ILE:HG13	1:A:917:ALA:HB2	2.01	0.42
1:A:1201:ARG:HA	1:A:1238:LEU:HD12	2.01	0.42
19:m:1261:ASN:OD1	19:m:1264:ARG:NH2	2.39	0.42
26:a:65:LEU:HG	26:a:69:ARG:NH1	2.34	0.42
31:k:269:PRO:HB3	31:k:302:ARG:HH21	1.85	0.42
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.90	0.42
1:A:266:LYS:HD2	1:A:266:LYS:HA	1.88	0.42
1:A:1041:ARG:O	1:A:1044:PHE:N	2.50	0.42
2:B:283:VAL:HG13	2:B:283:VAL:O	2.18	0.42
4:D:106:LEU:HD23	4:D:106:LEU:HA	1.89	0.42
5:E:42:ARG:HG3	5:E:46:CYS:SG	2.60	0.42
5:E:176:ARG:HD3	5:E:214:LEU:HD11	2.02	0.42
18:W:539:HIS:HB2	18:W:584:THR:HA	2.02	0.42
19:m:750:ALA:HB2	19:m:1139:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:x:345:GLN:O	25:x:349:GLN:HG3	2.20	0.42
12:L:60:LYS:HB3	12:L:60:LYS:HE3	1.86	0.42
14:N:2:DG:C2	14:N:3:DC:O2	2.72	0.42
18:W:543:ILE:HD11	18:W:581:ILE:HG13	2.01	0.42
19:m:743:PHE:O	19:m:747:ILE:HG12	2.20	0.42
20:n:161:GLN:O	20:n:165:LEU:HG	2.19	0.42
21:q:638:ALA:HB1	21:q:642:ARG:HH22	1.84	0.42
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.91	0.42
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.91	0.42
2:B:293:ILE:HD13	2:B:375:VAL:HG11	2.02	0.42
15:P:-4:A:H61	18:W:752:LEU:HD12	1.85	0.42
16:T:6:DC:C2	16:T:7:DC:C4	3.07	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
27:f:38:ALA:HB1	27:f:43:VAL:HB	2.02	0.42
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.85	0.42
14:N:-68:DT:C5	14:N:-67:DT:H73	2.55	0.42
19:m:708:TRP:CZ2	19:m:712:LEU:HD21	2.55	0.42
21:q:29:PRO:HA	21:q:36:VAL:HG12	2.02	0.42
1:A:152:ALA:HA	1:A:153:PRO:HD3	1.90	0.42
1:A:504:GLN:OE1	6:F:90:ARG:NH1	2.38	0.42
1:A:1218:ILE:HG12	1:A:1270:MET:HE1	2.02	0.42
2:B:279:ARG:NH1	2:B:316:ILE:O	2.53	0.42
14:N:-33:DG:H2''	14:N:-32:DT:OP2	2.19	0.42
18:W:349:GLU:HA	18:W:431:ARG:HA	2.02	0.42
19:m:1255:TRP:HD1	19:m:1257:ILE:HG12	1.85	0.42
22:r:208:ARG:HA	22:r:211:MET:HE3	2.02	0.42
22:r:275:ALA:HB2	22:r:281:GLU:HA	2.02	0.42
29:h:108:VAL:O	29:h:112:THR:HG23	2.19	0.42
2:B:606:VAL:HG22	2:B:621:THR:HG22	2.02	0.41
7:G:165:GLU:H	7:G:168:LEU:HD12	1.85	0.41
14:N:-33:DG:H2''	14:N:-32:DT:C7	2.50	0.41
14:N:4:DG:N2	16:T:-3:DG:C4	2.88	0.41
19:m:709:LYS:HA	19:m:712:LEU:HD12	2.02	0.41
19:m:821:ASP:HA	19:m:850:ILE:HD13	2.01	0.41
19:m:960:ASP:HB2	19:m:1024:TYR:CZ	2.54	0.41
19:m:1246:LEU:HB3	19:m:1248:VAL:HG23	2.01	0.41
22:r:211:MET:HB3	22:r:286:LEU:HD23	2.02	0.41
31:k:157:LYS:HD3	31:k:166:THR:HG21	2.02	0.41
31:k:258:GLN:OE1	31:k:260:LYS:HE2	2.20	0.41
1:A:390:THR:O	1:A:394:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:VAL:HG11	1:A:795:PRO:HG3	2.02	0.41
2:B:479:TYR:CE2	2:B:778:MET:HG2	2.55	0.41
2:B:557:GLU:HA	2:B:558:PRO:HD3	1.90	0.41
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.02	0.41
2:B:837:ASP:CG	2:B:1020:ARG:HH22	2.28	0.41
3:C:36:MET:HE3	3:C:176:ILE:HD13	2.01	0.41
17:V:13:MET:HE2	17:V:51:SER:HB2	2.01	0.41
18:W:422:TYR:HB3	18:W:427:TYR:CE1	2.55	0.41
19:m:656:TYR:CE2	19:m:660:ILE:HD11	2.54	0.41
21:q:562:TYR:CZ	21:q:566:LEU:HD11	2.55	0.41
29:d:73:GLU:OE2	29:d:76:ARG:NH1	2.48	0.41
2:B:1174:ASN:OD1	2:B:1177:LYS:HB2	2.20	0.41
9:I:29:CYS:SG	9:I:30:ARG:N	2.92	0.41
19:m:313:TYR:HB3	19:m:422:LEU:HD11	2.02	0.41
19:m:597:LEU:HD13	19:m:708:TRP:HE3	1.84	0.41
19:m:674:LEU:HD12	19:m:675:PRO:HD2	2.02	0.41
20:n:171:ALA:HB2	20:n:219:TRP:CD1	2.55	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
26:e:106:ASP:OD2	26:e:131:ARG:NH2	2.42	0.41
27:f:51:TYR:O	27:f:55:ARG:HG3	2.20	0.41
1:A:1210:THR:HG22	1:A:1212:ASN:H	1.86	0.41
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.02	0.41
2:B:1153:GLU:OE1	2:B:1153:GLU:N	2.53	0.41
19:m:397:ASN:HB3	19:m:401:ASN:HA	2.02	0.41
19:m:423:ASP:O	19:m:427:ILE:HG23	2.21	0.41
21:q:66:SER:O	21:q:70:VAL:HG23	2.20	0.41
21:q:189:LEU:HD13	21:q:197:GLN:HB2	2.02	0.41
1:A:1343:GLY:HA2	5:E:182:PRO:HD2	2.01	0.41
3:C:135:ARG:NE	3:C:136:ASP:OD2	2.50	0.41
11:K:25:SER:O	25:x:307:GLN:NE2	2.53	0.41
14:N:-60:DT:O2	16:T:61:DA:H2	2.04	0.41
15:P:-6:G:C5	15:P:-5:U:C4	3.08	0.41
21:q:278:ARG:NH2	22:r:507:ASP:O	2.53	0.41
27:f:46:ILE:HG22	27:f:47:SER:O	2.20	0.41
30:j:730:ILE:CG2	30:j:750:GLN:HE21	2.34	0.41
31:k:257:ILE:HD11	31:k:286:LEU:HD11	2.01	0.41
1:A:231:ARG:HB3	1:A:234:TRP:CD2	2.56	0.41
1:A:985:ILE:N	1:A:986:PRO:HD2	2.36	0.41
2:B:262:LYS:HB3	2:B:271:ASP:HB3	2.01	0.41
6:F:110:ASP:OD1	6:F:110:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:6:PHE:HB3	8:H:59:LEU:HB2	2.02	0.41
16:T:-6:DT:H2''	16:T:-5:DA:C8	2.55	0.41
18:W:598:LEU:HD12	18:W:599:HIS:H	1.85	0.41
19:m:586:TYR:CE2	19:m:703:LEU:HD12	2.56	0.41
19:m:1136:ARG:HD2	19:m:1137:GLU:O	2.21	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
31:k:37:THR:O	31:k:38:LYS:C	2.64	0.41
1:A:883:THR:HA	1:A:954:HIS:O	2.21	0.41
1:A:1314:ILE:HB	1:A:1337:GLU:OE1	2.21	0.41
2:B:575:VAL:O	2:B:578:VAL:HG22	2.20	0.41
6:F:99:LEU:HG	6:F:103:MET:HE2	2.02	0.41
14:N:-12:DA:H2'	14:N:-11:DC:C6	2.56	0.41
18:W:540:VAL:HG11	18:W:554:ILE:HD11	2.01	0.41
19:m:314:ARG:HD3	19:m:320:TYR:CE1	2.56	0.41
20:n:177:ASN:HD21	20:n:186:PHE:HE2	1.67	0.41
21:q:350:VAL:HA	21:q:380:ARG:NH1	2.36	0.41
21:q:410:GLY:HA2	21:q:423:ALA:HA	2.03	0.41
21:q:756:TRP:HB3	21:q:772:ALA:HB2	2.03	0.41
23:u:121:PHE:CE2	23:u:123:PRO:HG3	2.56	0.41
11:K:55:ASP:OD2	11:K:89:ARG:NH2	2.54	0.41
16:T:25:DG:H2''	16:T:26:DG:O5'	2.20	0.41
18:W:329:LYS:HB2	18:W:434:ASN:HA	2.02	0.41
28:g:21:ALA:HB2	29:h:118:TYR:HB2	2.02	0.41
1:A:636:ARG:HG3	1:A:880:GLU:OE2	2.21	0.41
1:A:908:SER:OG	1:A:909:ILE:N	2.54	0.41
2:B:86:ARG:HD3	2:B:86:ARG:HA	1.89	0.41
5:E:3:ASP:HA	5:E:6:ARG:HG2	2.01	0.41
8:H:76:LYS:HE3	8:H:76:LYS:HB3	1.93	0.41
11:K:47:ARG:HD3	11:K:61:TYR:HD1	1.86	0.41
13:M:39:ASP:HB3	13:M:44:ILE:HG13	2.03	0.41
14:N:4:DG:C8	14:N:5:DT:H72	2.56	0.41
15:P:9:G:O2'	15:P:10:U:H5'	2.21	0.41
16:T:8:DC:H2''	16:T:9:DG:H8	1.86	0.41
16:T:67:DA:C2	16:T:68:DA:N3	2.89	0.41
16:T:67:DA:N1	16:T:68:DA:C2	2.89	0.41
18:W:480:PRO:HA	18:W:498:VAL:HG12	2.02	0.41
19:m:283:VAL:HG12	19:m:284:PHE:CD1	2.56	0.41
21:q:824:ASN:CG	21:q:858:ARG:HH21	2.29	0.41
25:x:153:ASN:OD1	25:x:153:ASN:N	2.54	0.41
26:e:82:LEU:HA	26:e:82:LEU:HD23	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:h:103:LEU:HD23	29:h:103:LEU:HA	1.88	0.41
31:k:10:PHE:CD2	31:k:61:ARG:NH1	2.89	0.41
1:A:473:LEU:CD2	2:B:835:GLN:HB2	2.50	0.41
2:B:33:GLN:HG2	2:B:34:GLN:N	2.35	0.41
2:B:71:ILE:HG12	2:B:127:ILE:HG22	2.02	0.41
3:C:135:ARG:HE	3:C:136:ASP:CG	2.28	0.41
3:C:248:ILE:HG21	11:K:102:ASP:HB2	2.01	0.41
12:L:29:VAL:HG23	12:L:31:TYR:CE2	2.56	0.41
16:T:64:DA:OP1	26:a:69:ARG:NH2	2.52	0.41
19:m:1141:ASP:OD1	19:m:1141:ASP:N	2.51	0.41
28:c:20:ARG:HD3	29:d:122:LYS:O	2.21	0.41
28:c:29:ARG:NH1	29:d:32:GLU:HB3	2.36	0.41
1:A:664:SER:OG	1:A:665:ILE:N	2.55	0.40
3:C:259:LEU:HD13	11:K:91:CYS:HB2	2.03	0.40
9:I:62:ILE:HD12	9:I:62:ILE:HA	1.93	0.40
17:V:42:ASP:N	17:V:42:ASP:OD1	2.53	0.40
18:W:492:ASN:OD1	18:W:493:HIS:N	2.54	0.40
18:W:614:ARG:NH2	18:W:616:GLN:HE21	2.19	0.40
19:m:588:ALA:HA	19:m:591:GLN:HG2	2.04	0.40
19:m:900:LEU:HD12	19:m:900:LEU:HA	1.95	0.40
20:n:241:ILE:HG23	20:n:246:ILE:HD12	2.04	0.40
21:q:341:ARG:NH2	24:v:50:LEU:HB2	2.36	0.40
21:q:687:PHE:O	21:q:691:GLU:N	2.54	0.40
26:a:120:MET:HE2	26:a:122:LYS:HE2	2.03	0.40
2:B:807:GLN:OE1	24:v:129:ARG:NH1	2.51	0.40
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.55	0.40
14:N:-99:DG:C2	16:T:100:DA:C2	3.10	0.40
19:m:827:GLY:HA3	19:m:832:THR:OG1	2.21	0.40
19:m:1303:VAL:HA	19:m:1323:LYS:HD3	2.03	0.40
21:q:619:LEU:HA	21:q:623:ASP:O	2.22	0.40
22:r:261:LEU:HD12	22:r:287:PHE:HB3	2.04	0.40
22:r:316:LEU:HD23	22:r:316:LEU:HA	1.83	0.40
26:a:118:THR:HA	27:b:45:ARG:O	2.21	0.40
1:A:493:PRO:HG3	1:A:502:LEU:HD12	2.04	0.40
1:A:498:THR:CG2	2:B:1146:PHE:HD1	2.34	0.40
1:A:1295:PRO:HD3	1:A:1301:TYR:CE1	2.55	0.40
2:B:439:LEU:HD11	23:u:264:LEU:HB3	2.03	0.40
4:D:53:LEU:HD13	4:D:147:SER:HB3	2.02	0.40
12:L:66:MET:HE1	18:W:804:TRP:HZ2	1.86	0.40
14:N:-32:DT:H2''	14:N:-31:DA:O5'	2.22	0.40
14:N:-1:DA:C2	14:N:0:DG:C5	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:421:ASP:OD1	19:m:421:ASP:C	2.64	0.40
21:q:609:ASP:O	21:q:613:GLN:HG3	2.20	0.40
25:x:301:ASP:OD1	25:x:303:GLN:NE2	2.54	0.40
30:j:614:PHE:CE2	31:k:112:TRP:HB3	2.56	0.40
1:A:1150:SER:OG	1:A:1198:GLU:O	2.32	0.40
2:B:285:PRO:HB2	9:I:11:ASN:HD22	1.86	0.40
17:V:29:CYS:HB2	17:V:38:LEU:HD12	2.03	0.40
19:m:474:TYR:HB3	19:m:477:GLN:HB2	2.04	0.40
19:m:606:THR:HG21	19:m:684:PHE:HZ	1.87	0.40
19:m:1002:ARG:NH2	19:m:1023:VAL:O	2.47	0.40
19:m:1268:ILE:O	19:m:1272:ARG:HG3	2.21	0.40
23:u:142:ASP:HA	23:u:145:ILE:HG22	2.04	0.40
1:A:599:LEU:HD13	8:H:123:CYS:HB2	2.04	0.40
2:B:86:ARG:NH2	22:r:369:GLU:OE1	2.54	0.40
2:B:1152:MET:HE3	2:B:1152:MET:HB3	1.91	0.40
7:G:31:LEU:HD23	7:G:31:LEU:HA	1.95	0.40
7:G:126:SER:HA	7:G:127:PRO:HA	1.94	0.40
12:L:33:CYS:SG	12:L:34:GLY:N	2.95	0.40
16:T:7:DC:H1'	16:T:8:DC:H5'	2.04	0.40
18:W:524:GLU:HB2	20:n:232:GLN:HE22	1.86	0.40
21:q:341:ARG:NH2	24:v:47:SER:O	2.54	0.40
21:q:789:ARG:O	21:q:793:VAL:HG23	2.21	0.40
22:r:432:LEU:HD11	22:r:433:ARG:NH1	2.36	0.40
24:v:205:SER:O	24:v:379:ARG:NH2	2.49	0.40
24:v:262:LYS:HD3	24:v:305:GLN:NE2	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1392/1743 (80%)	1354 (97%)	37 (3%)	1 (0%)	48 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1154/1227 (94%)	1117 (97%)	37 (3%)	0	100	100
3	C	261/304 (86%)	259 (99%)	2 (1%)	0	100	100
4	D	170/186 (91%)	166 (98%)	4 (2%)	0	100	100
5	E	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	166 (98%)	3 (2%)	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%)	506 (96%)	21 (4%)	0	100	100
19	m	1179/1503 (78%)	1157 (98%)	22 (2%)	0	100	100
20	n	137/417 (33%)	136 (99%)	1 (1%)	0	100	100
21	q	928/1084 (86%)	922 (99%)	6 (1%)	0	100	100
22	r	260/544 (48%)	254 (98%)	6 (2%)	0	100	100
23	u	206/459 (45%)	204 (99%)	2 (1%)	0	100	100
24	v	341/396 (86%)	327 (96%)	14 (4%)	0	100	100
25	x	201/395 (51%)	200 (100%)	1 (0%)	0	100	100
26	a	74/139 (53%)	70 (95%)	4 (5%)	0	100	100
26	e	88/139 (63%)	87 (99%)	1 (1%)	0	100	100
27	b	81/106 (76%)	78 (96%)	3 (4%)	0	100	100
27	f	76/106 (72%)	73 (96%)	3 (4%)	0	100	100
28	c	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
28	g	68/133 (51%)	66 (97%)	2 (3%)	0	100	100
29	d	93/129 (72%)	89 (96%)	4 (4%)	0	100	100
29	h	91/129 (70%)	90 (99%)	1 (1%)	0	100	100
30	j	462/1008 (46%)	449 (97%)	12 (3%)	1 (0%)	43	74
31	k	423/531 (80%)	411 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9398/13005 (72%)	9176 (98%)	220 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	960	VAL
30	j	543	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1219/1528 (80%)	1219 (100%)	0	100	100
2	B	1018/1077 (94%)	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	64/112 (57%)	64 (100%)	0	100	100
26	e	77/112 (69%)	77 (100%)	0	100	100
27	b	68/81 (84%)	68 (100%)	0	100	100
27	f	63/81 (78%)	63 (100%)	0	100	100
28	c	82/102 (80%)	82 (100%)	0	100	100
28	g	54/102 (53%)	54 (100%)	0	100	100
29	d	81/107 (76%)	81 (100%)	0	100	100
29	h	79/107 (74%)	79 (100%)	0	100	100
30	j	417/910 (46%)	417 (100%)	0	100	100
31	k	392/474 (83%)	392 (100%)	0	100	100
All	All	8460/11447 (74%)	8460 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) 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	436	HIS
1	A	491	HIS
1	A	737	ASN
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	458	ASN

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Mol	Chain	Res	Type
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	38	GLN
4	D	130	ASN
4	D	170	ASN
5	E	31	GLN
5	E	36	GLN
7	G	24	GLN
10	J	52	HIS
12	L	55	HIS
13	M	32	ASN
18	W	242	GLN
18	W	539	HIS
18	W	644	ASN
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	132	ASN
21	q	147	ASN
21	q	187	GLN
21	q	353	GLN
21	q	397	ASN
21	q	398	GLN
21	q	438	ASN
21	q	615	HIS
21	q	658	GLN
21	q	715	ASN
21	q	781	GLN
22	r	232	ASN

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Mol	Chain	Res	Type
22	r	493	ASN
23	u	138	GLN
24	v	229	ASN
24	v	283	ASN
24	v	381	GLN
25	x	251	GLN
27	b	25	ASN
27	b	75	HIS
28	c	73	ASN
28	c	110	ASN
29	d	64	ASN
29	d	92	GLN
26	e	85	GLN
30	j	578	ASN
30	j	750	GLN
30	j	841	GLN
30	j	864	GLN
30	j	887	ASN
30	j	916	ASN
31	k	93	GLN
31	k	127	ASN
31	k	143	ASN
31	k	148	HIS
31	k	362	GLN
31	k	420	GLN
31	k	446	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	19/19 (100%)	10 (52%)	1 (5%)

All (10) RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
15	P	1	C
15	P	8	G
15	P	9	G
15	P	11	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	-7	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

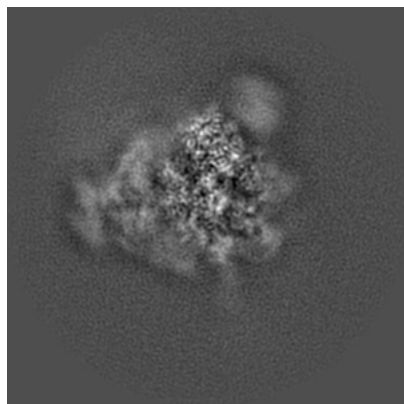
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33447. These allow visual inspection of the internal detail of the map and identification of artifacts.

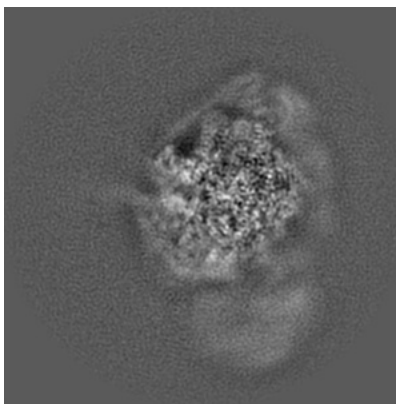
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

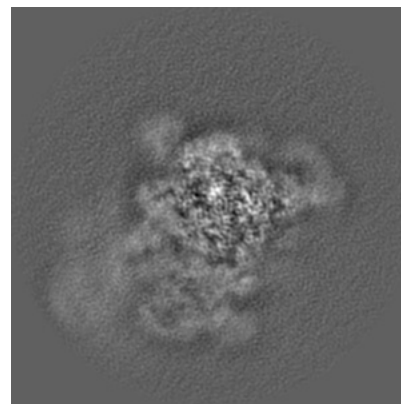
6.1.1 Primary map



X

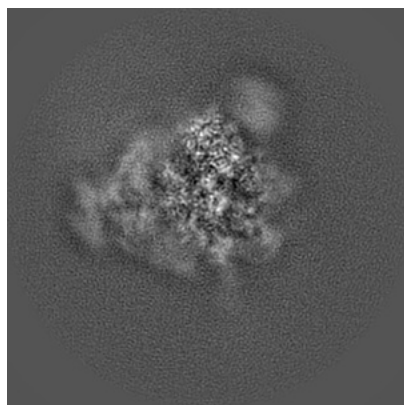


Y

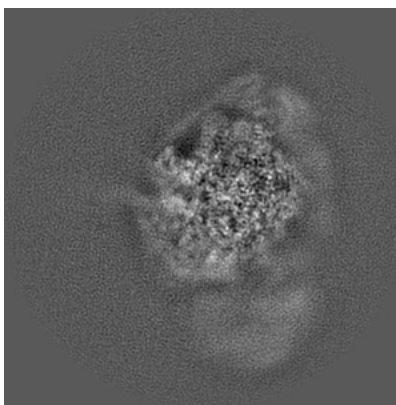


Z

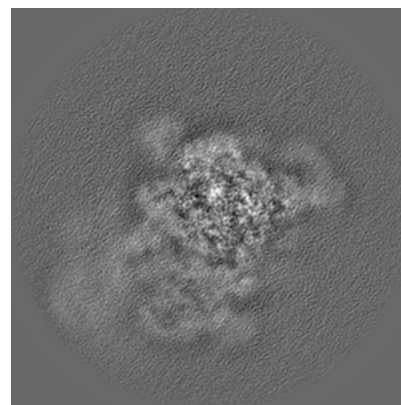
6.1.2 Raw map



X



Y

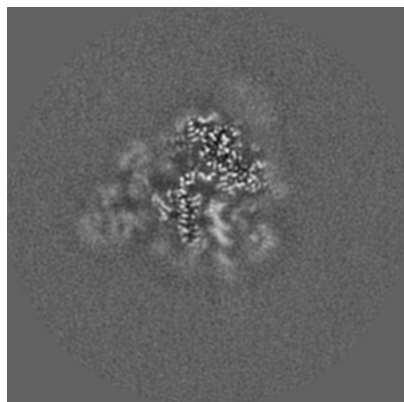


Z

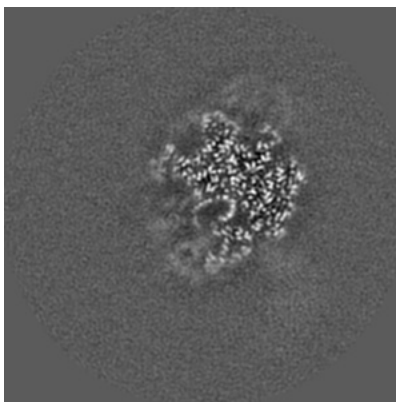
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

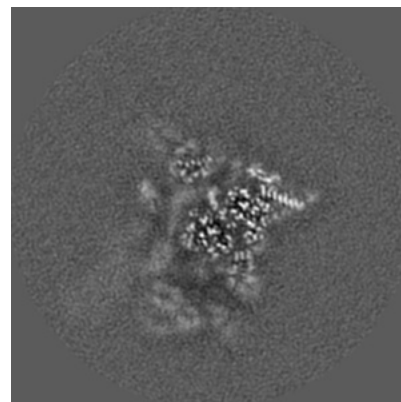
6.2.1 Primary map



X Index: 120

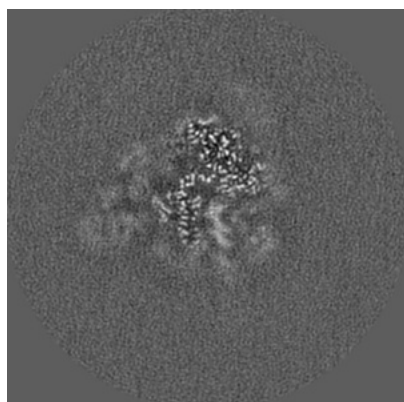


Y Index: 120

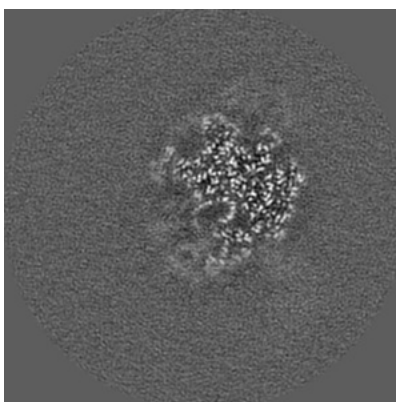


Z Index: 120

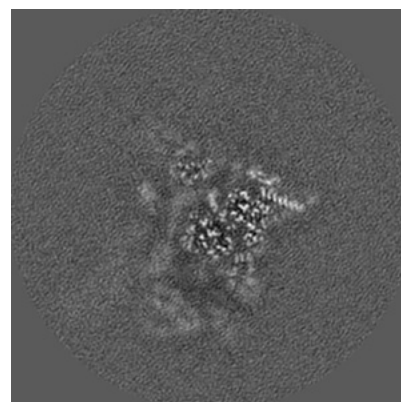
6.2.2 Raw map



X Index: 120



Y Index: 120

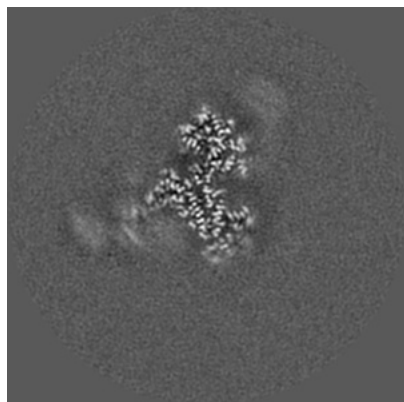


Z Index: 120

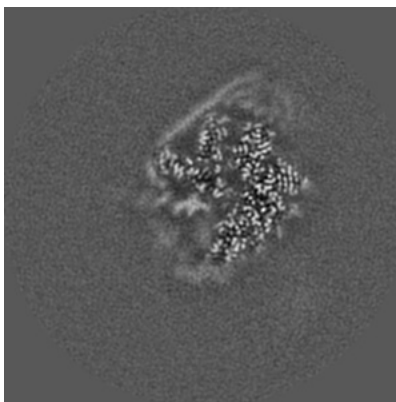
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

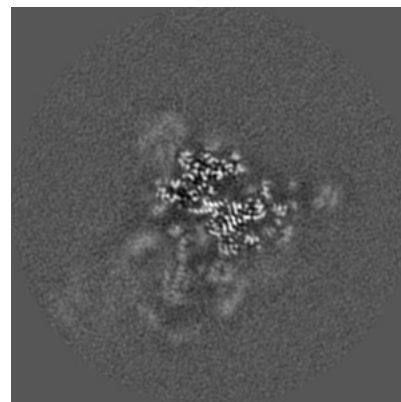
6.3.1 Primary map



X Index: 141

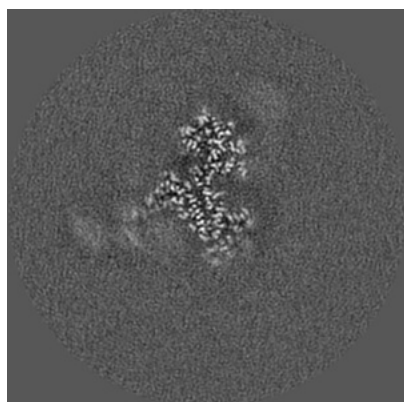


Y Index: 125

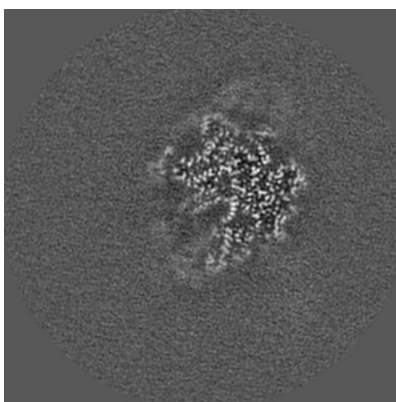


Z Index: 137

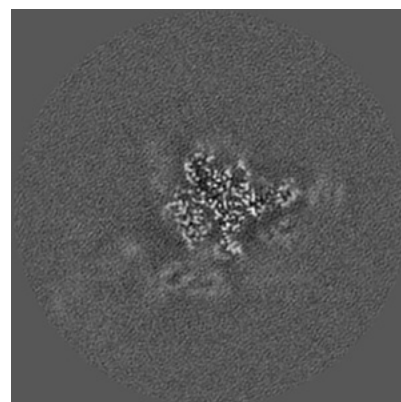
6.3.2 Raw map



X Index: 141



Y Index: 121

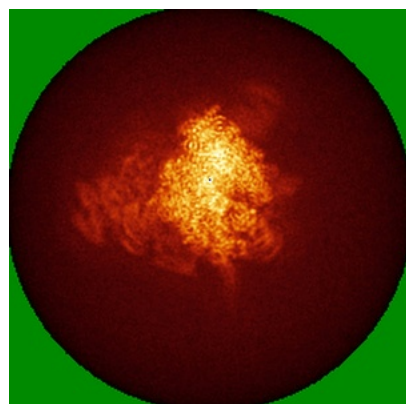


Z Index: 146

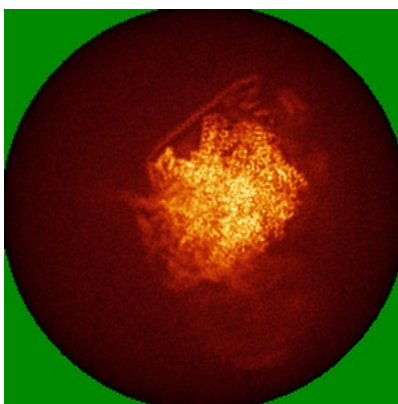
The images above show the largest variance slices of the map in three orthogonal directions.

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

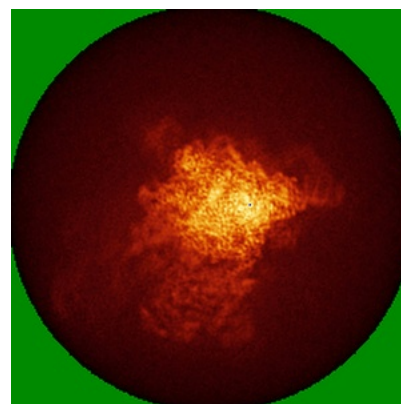
6.4.1 Primary map



X

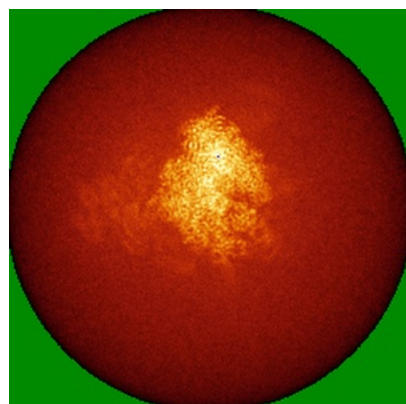


Y

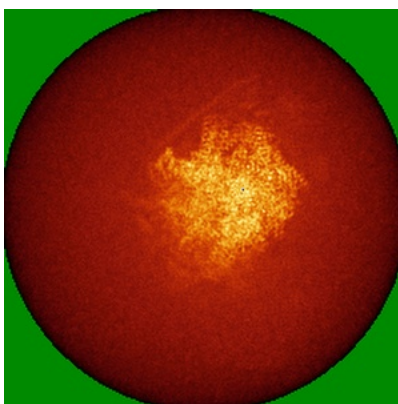


Z

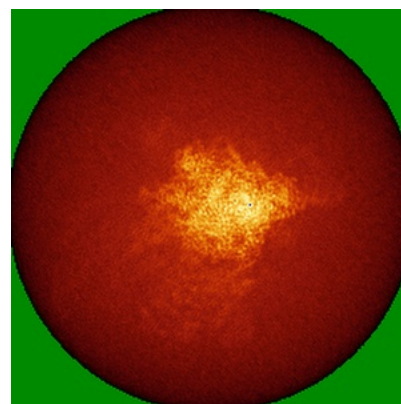
6.4.2 Raw map



X



Y

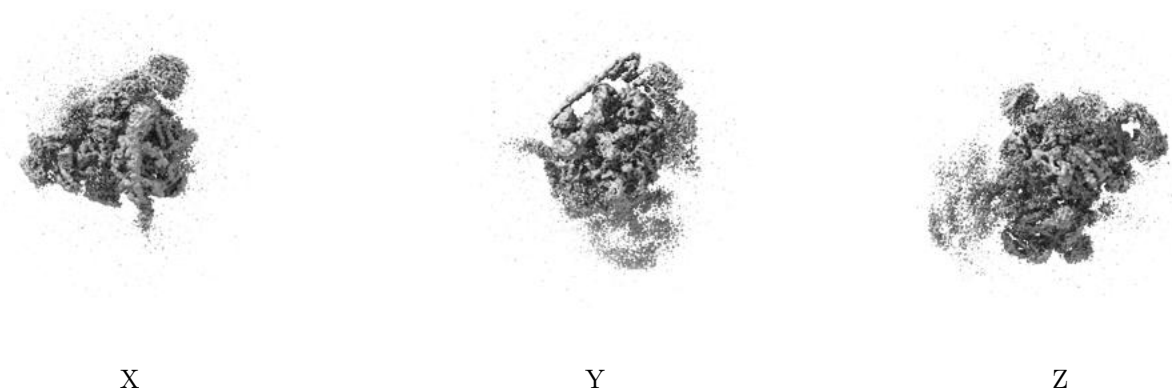


Z

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

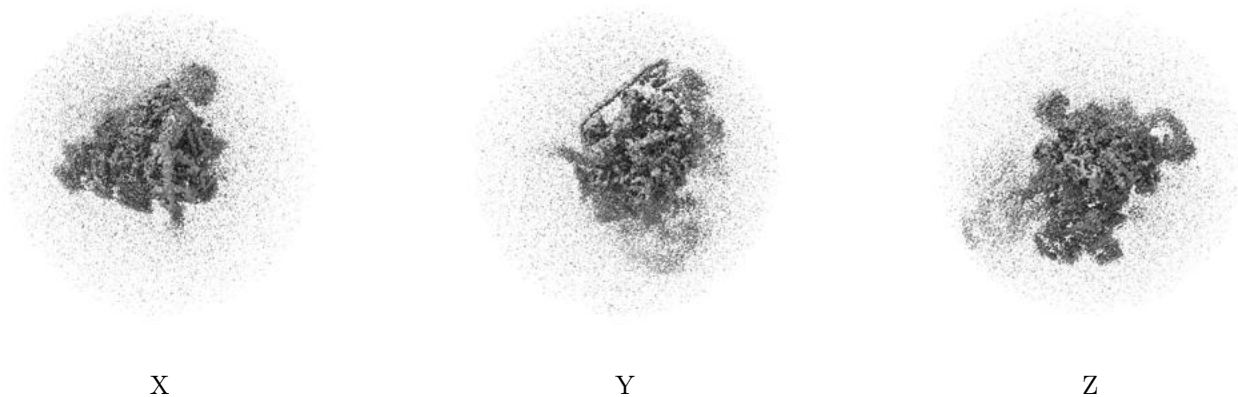
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

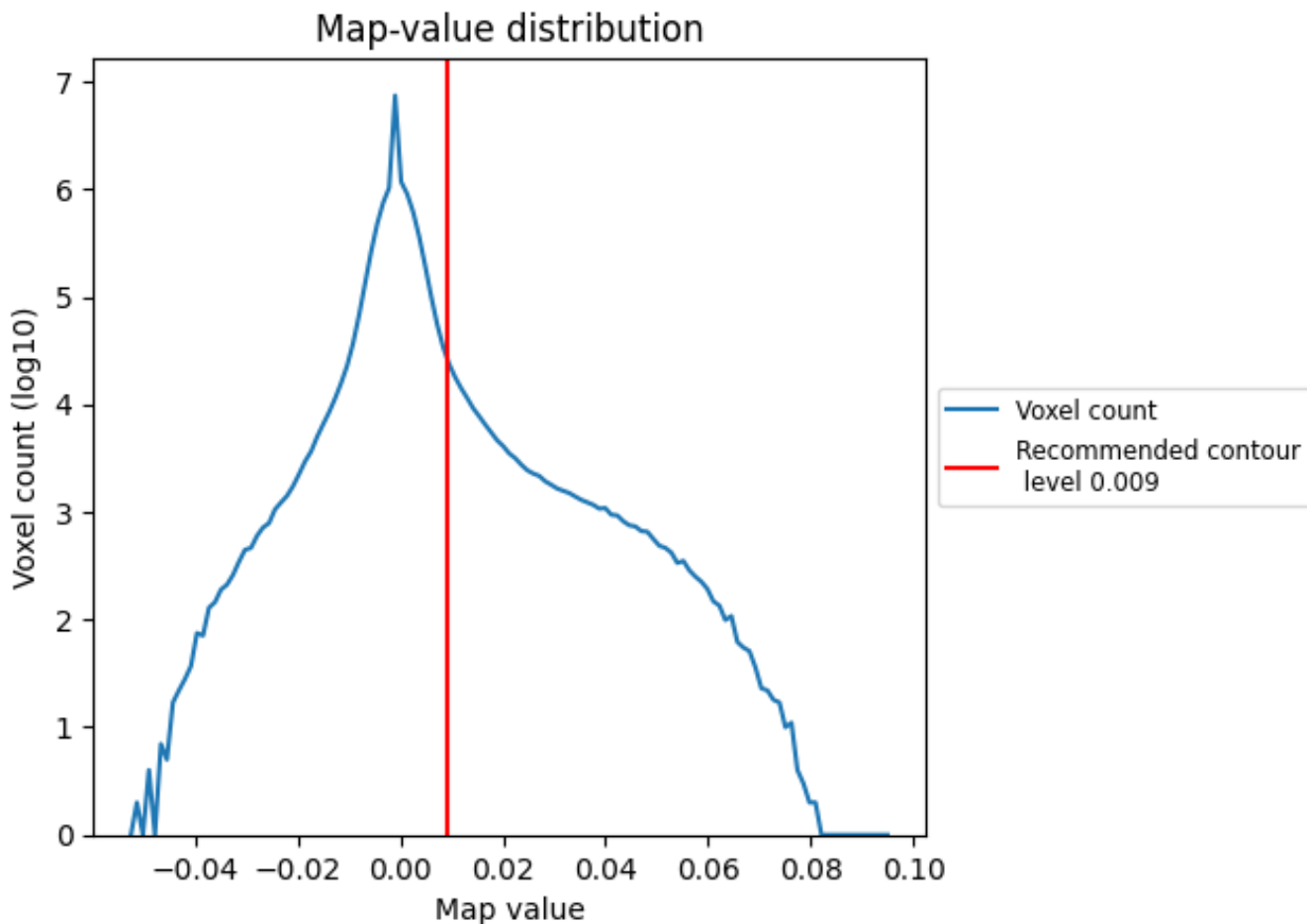
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

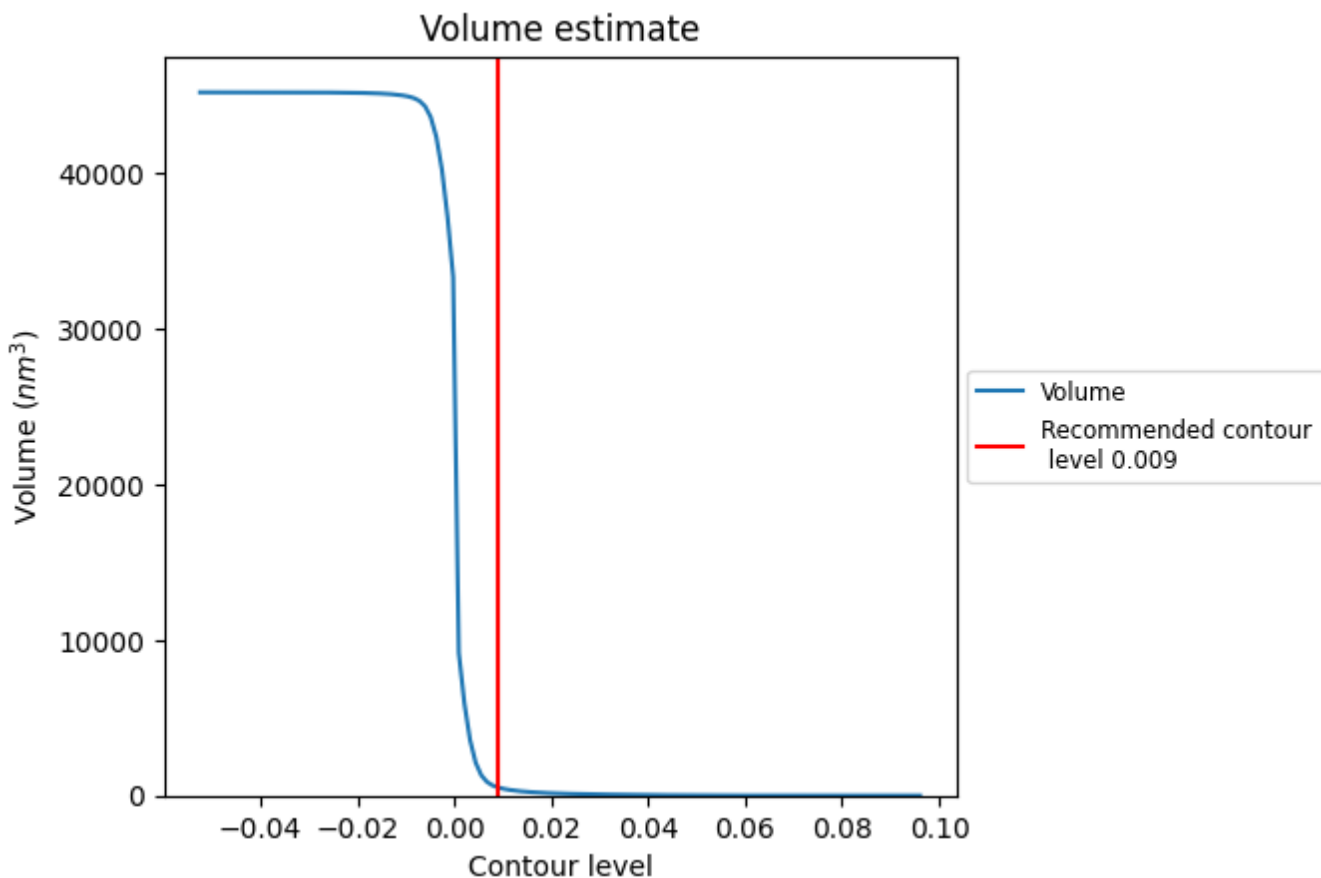
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

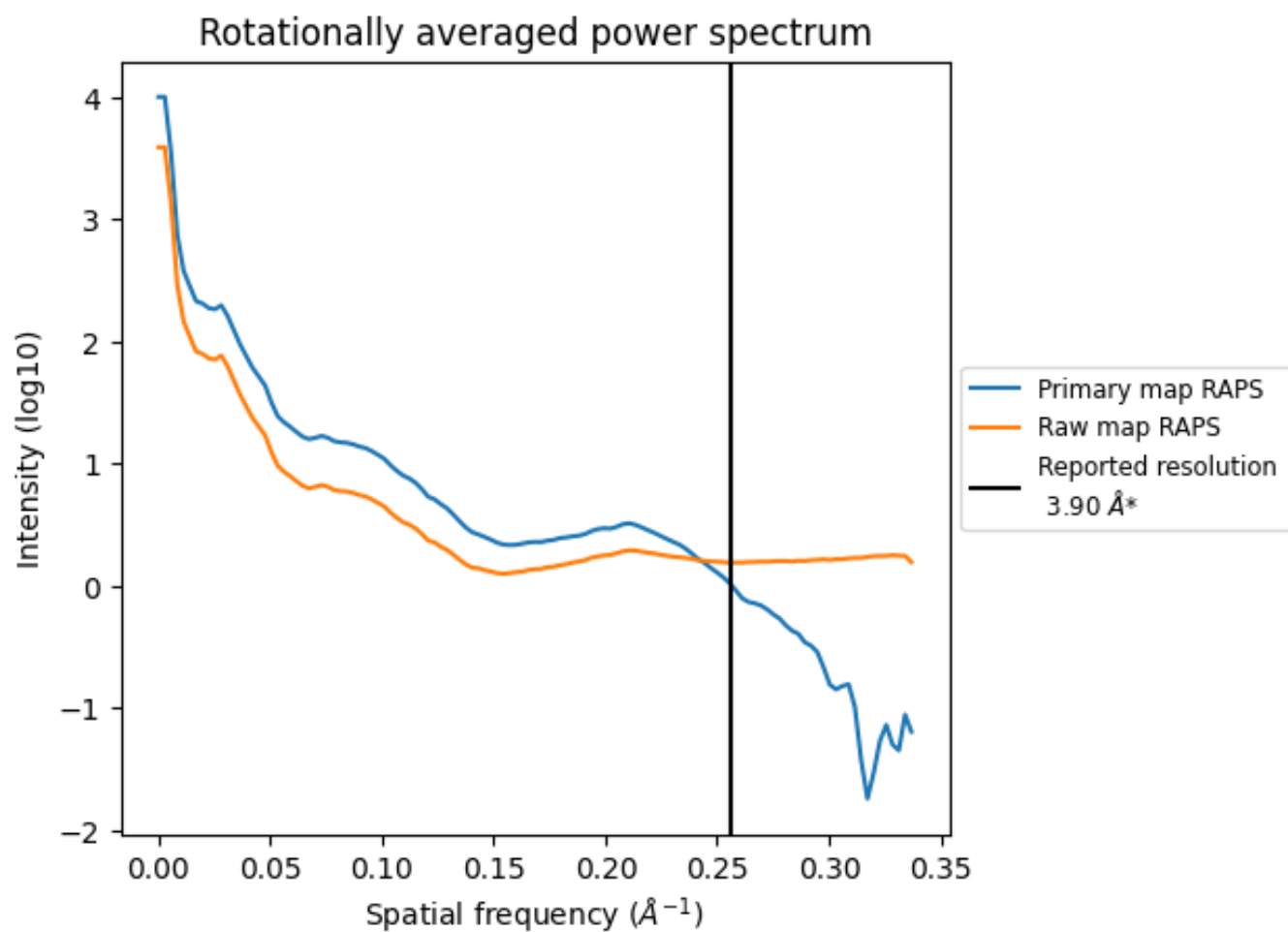
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 526 nm^3 ; this corresponds to an approximate mass of 475 kDa.

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

7.3 Rotationally averaged power spectrum i

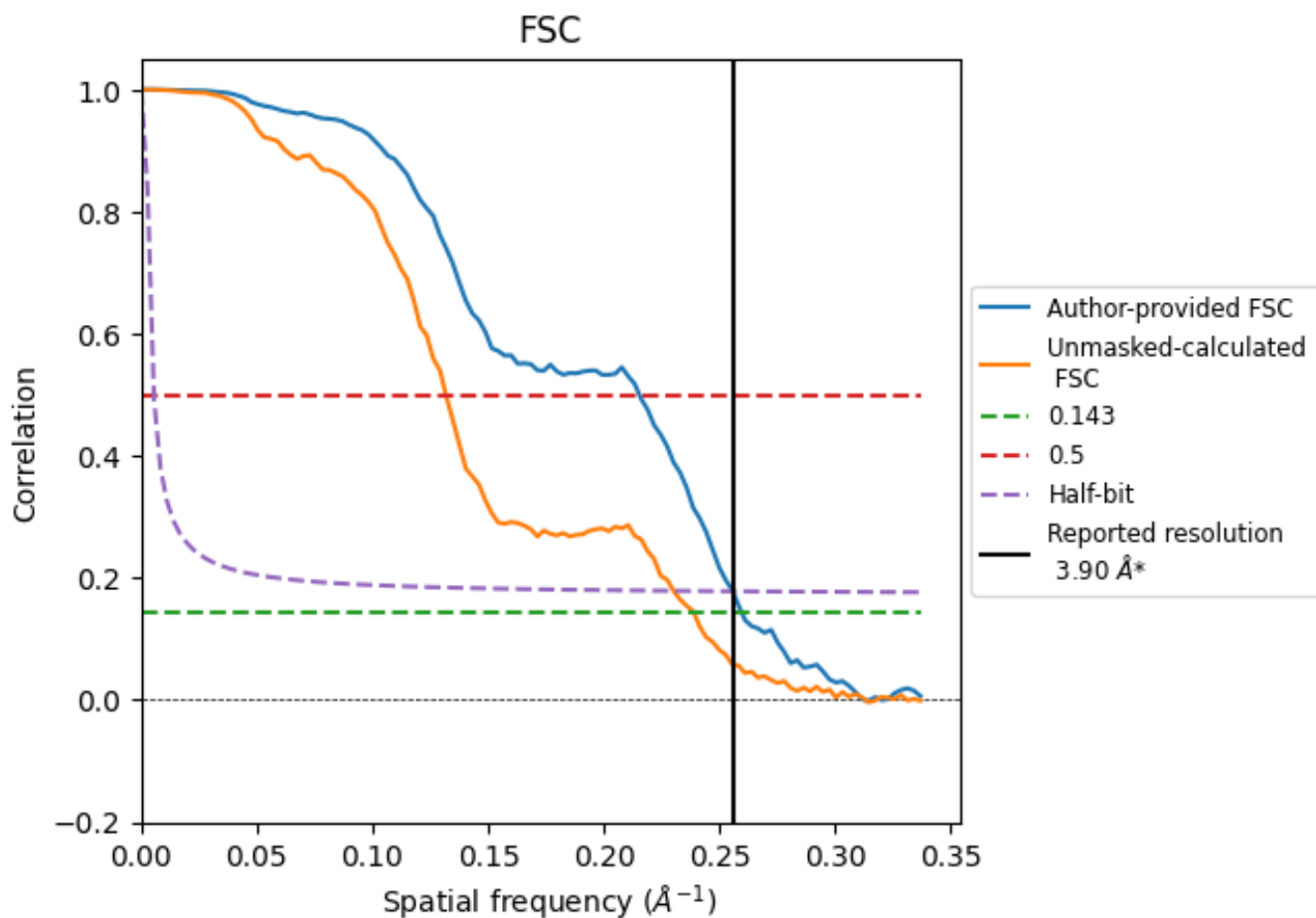


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

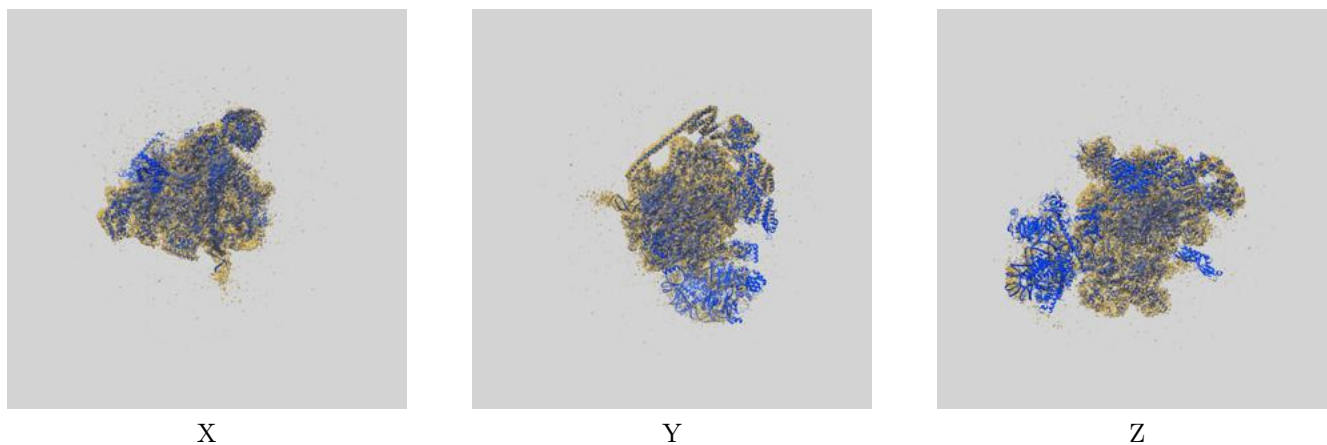
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.85	4.64	3.91
Unmasked-calculated*	4.19	7.59	4.34

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

9 Map-model fit [i](#)

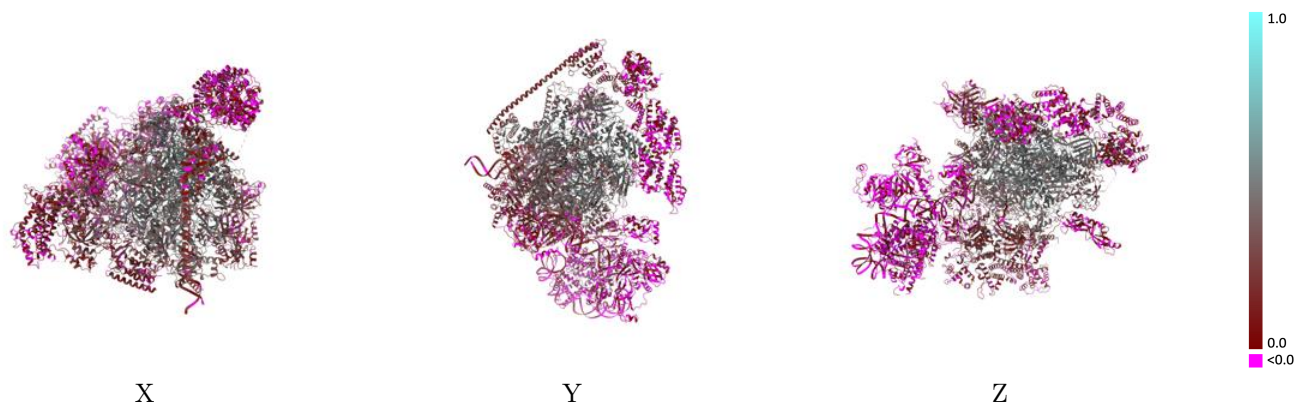
This section contains information regarding the fit between EMDB map EMD-33447 and PDB model 7XTD. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



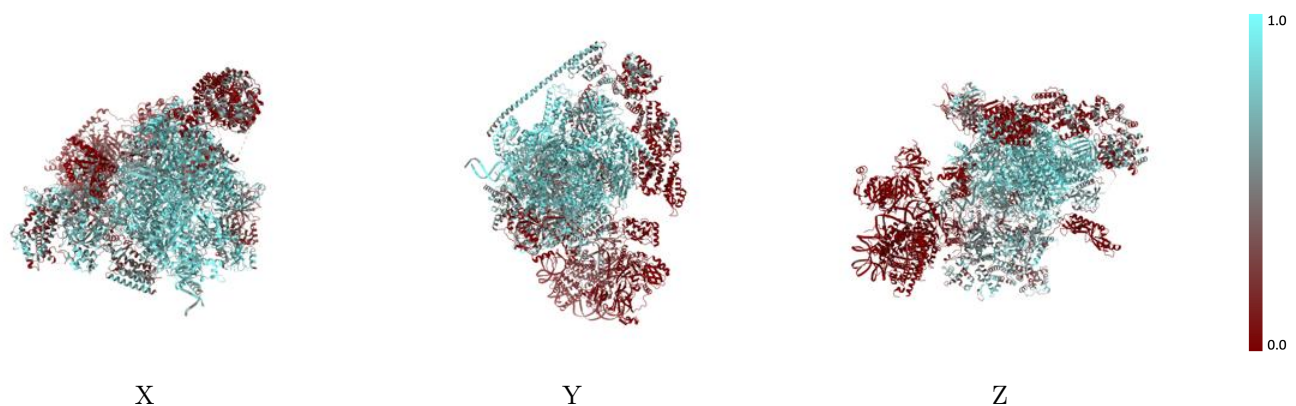
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



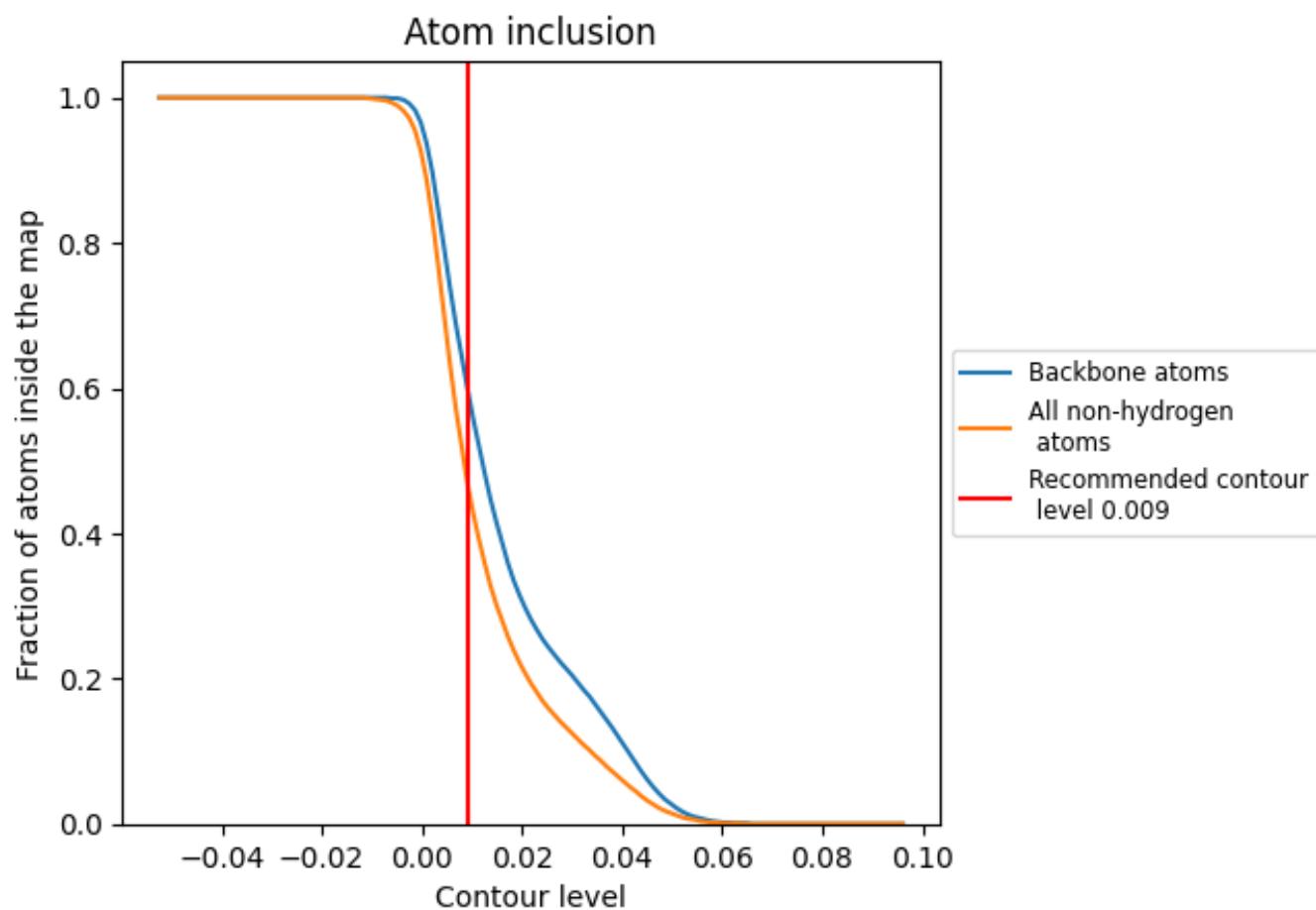
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 47% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4720	 0.2210
A	 0.8070	 0.4220
B	 0.7830	 0.4370
C	 0.8350	 0.4550
D	 0.5840	 0.2180
E	 0.8350	 0.4030
F	 0.8500	 0.4680
G	 0.6570	 0.3200
H	 0.8420	 0.4480
I	 0.5620	 0.2560
J	 0.8260	 0.4530
K	 0.8580	 0.4640
L	 0.7900	 0.4030
M	 0.4520	 0.1740
N	 0.3410	 0.0870
P	 0.7520	 0.3230
T	 0.3710	 0.1150
V	 0.5460	 0.1410
W	 0.4460	 0.2030
a	 0.0440	 0.0430
b	 0.0130	 0.0010
c	 0.0060	 0.0020
d	 0.0190	 0.0010
e	 0.0280	 0.0190
f	 0.0290	 -0.0230
g	 0.0040	 0.0030
h	 0.0040	 0.0010
j	 0.0480	 0.0270
k	 0.0060	 0.0010
m	 0.4210	 0.1310
n	 0.4850	 0.1470
q	 0.2850	 0.0790
r	 0.2050	 0.0950
u	 0.3130	 0.1560
v	 0.2020	 0.0990
x	 0.4440	 0.2670

