



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:59 AM UTC

PDB ID : 7XN7 / pdb_00007xn7
EMDB ID : EMD-33313
Title : RNA polymerase II elongation complex containing Spt4/5, Elf1, Spt6, Spn1 and Paf1C
Authors : Ehara, H.; Kujirai, T.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on : 2022-04-28
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

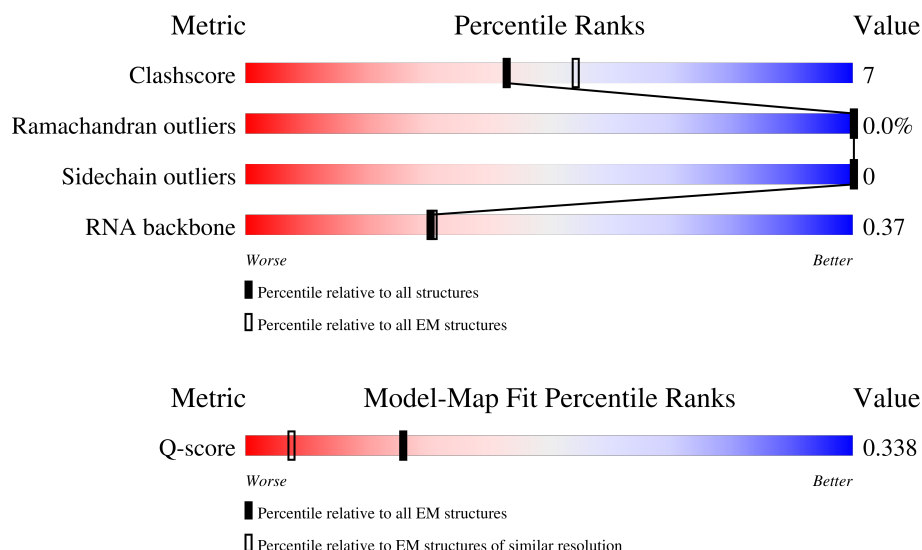
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.10 Å.

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



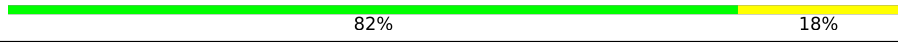
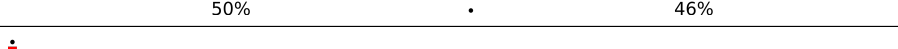
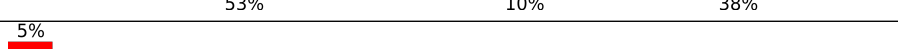
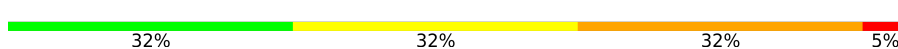
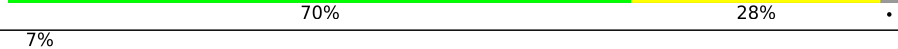
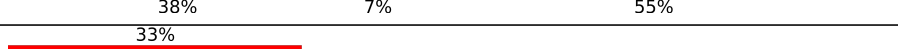
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

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

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

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	7	MET	VAL	conflict	UNP C4R0E6

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 40 discrepancies between the modelled and reference sequences:

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

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

unit.

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

There are 30 discrepancies between the modelled and reference sequences:

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

- Molecule 23 is a protein called Leo1.

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

There are 30 discrepancies between the modelled and reference sequences:

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 30 discrepancies between the modelled and reference sequences:

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

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

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

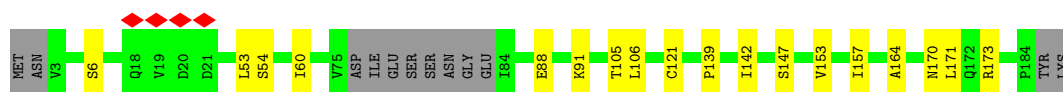
Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total 2	Zn 2	0
26	B	1	Total 1	Zn 1	0
26	C	1	Total 1	Zn 1	0
26	I	2	Total 2	Zn 2	0
26	J	1	Total 1	Zn 1	0
26	L	1	Total 1	Zn 1	0
26	M	1	Total 1	Zn 1	0
26	V	1	Total 1	Zn 1	0

- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

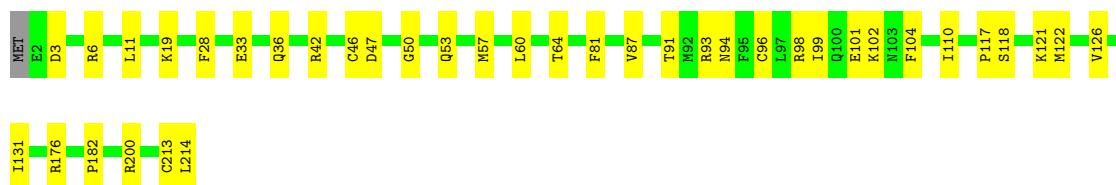
Response	Percentage
Yes, the U.S. is a democracy	78%
No, the U.S. is not a democracy	17%
Don't know	5%





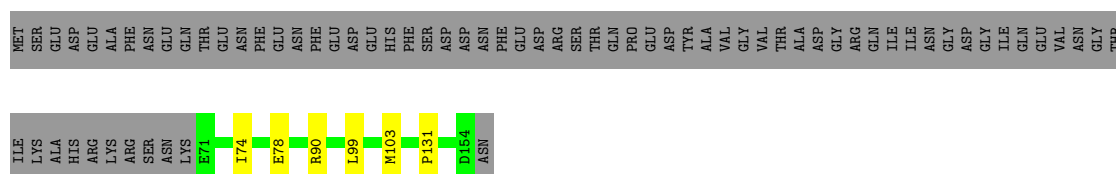
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 82% 18%



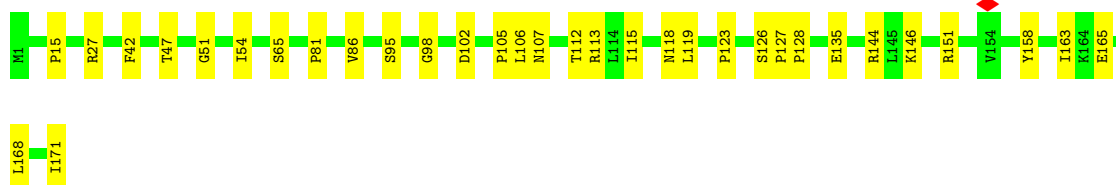
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

Chain F: 50% 46%



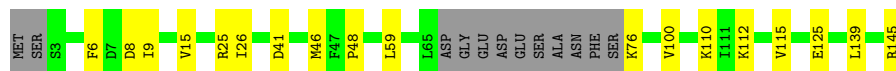
- Molecule 7: RNA polymerase II subunit

Chain G: 81% 19%



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

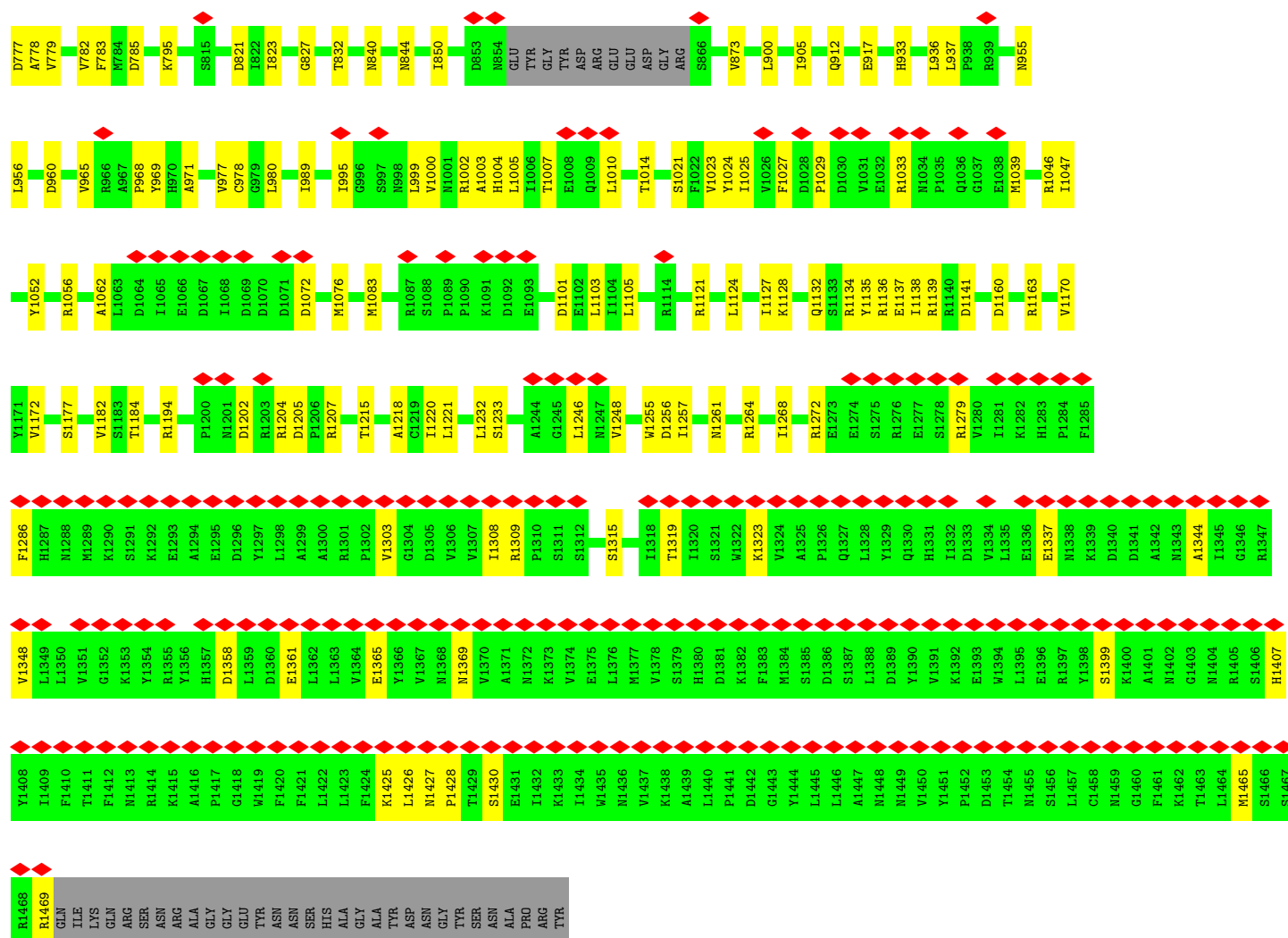
Chain H: 79% 12% 8%



- Molecule 9: DNA-directed RNA polymerase subunit

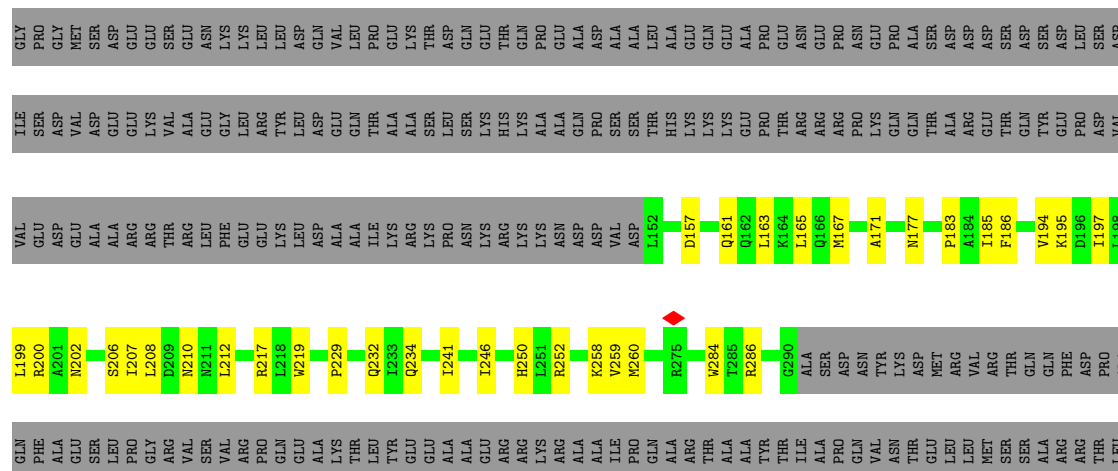
Chain I: 6% 81% 16%



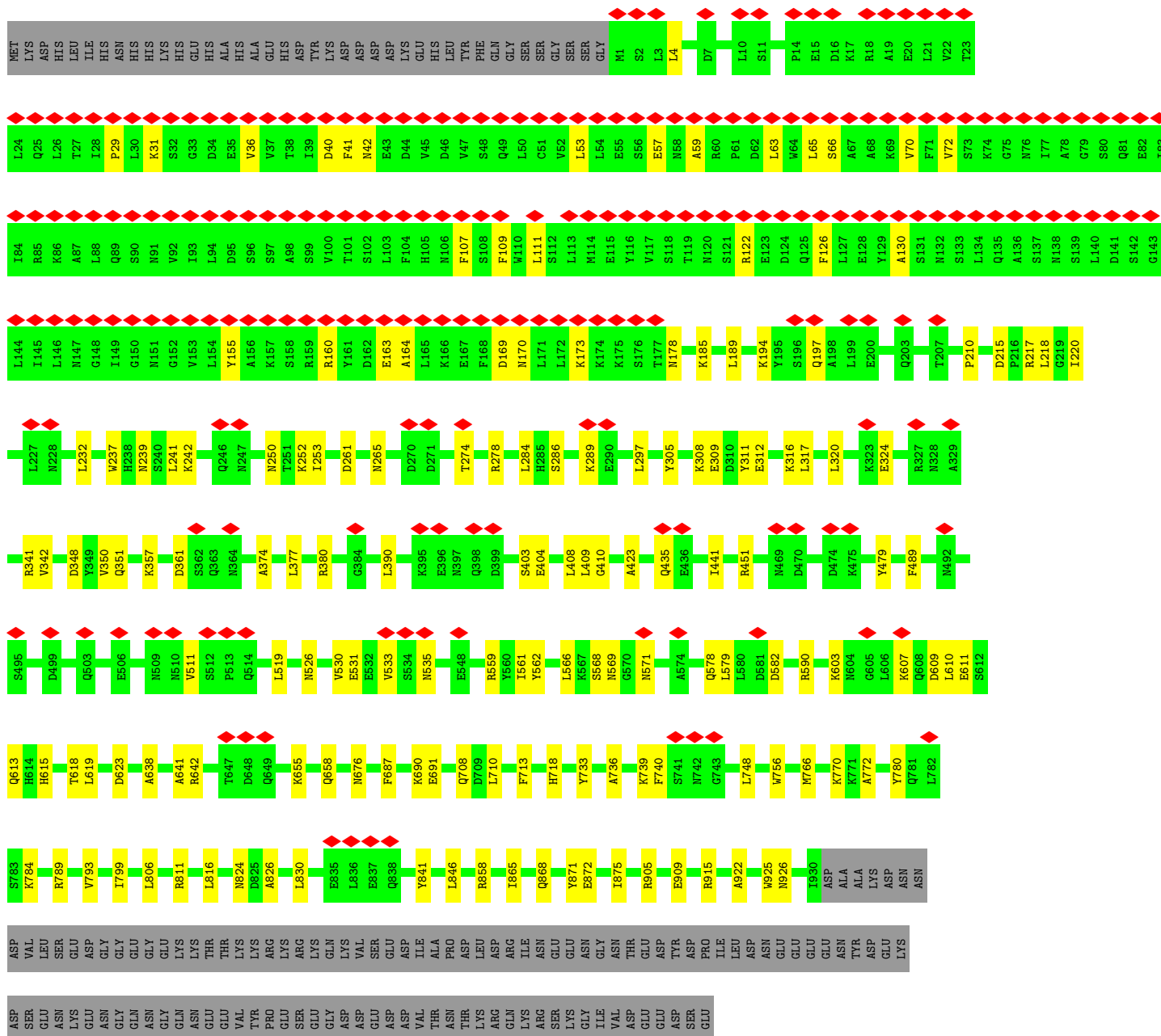


- Molecule 20: Protein that interacts with Spt6p and copurifies with Spt5p and RNA polymerase II

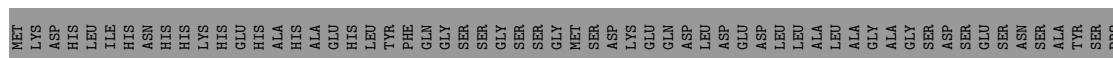
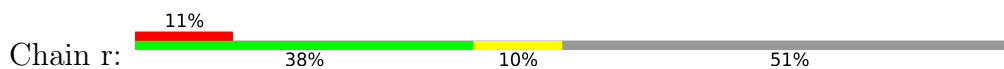
Chain n: 25% 8% 67%



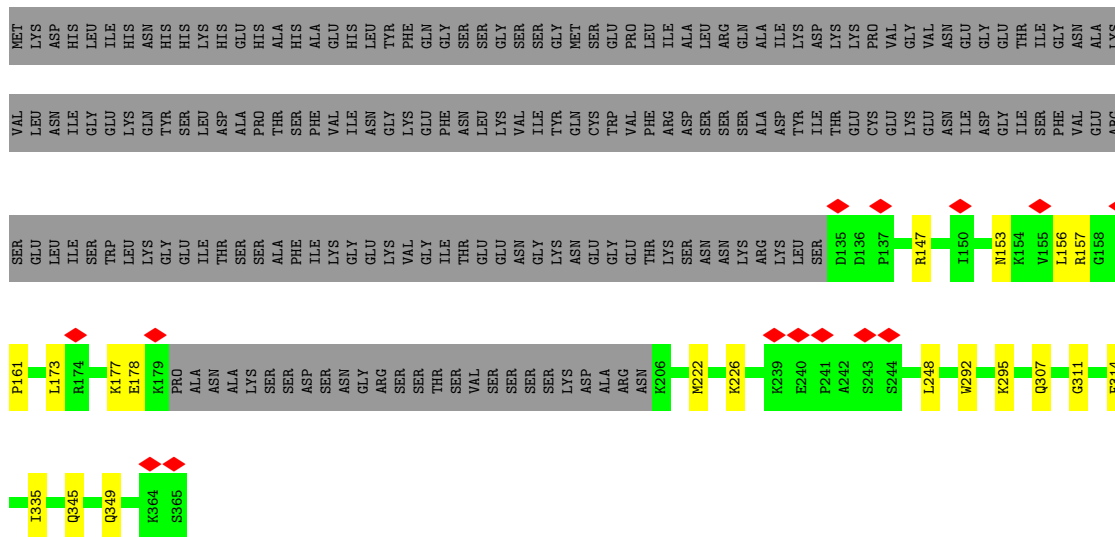
- Molecule 21: Component of the Paf1p complex



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







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	444232	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.127	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	356.16, 356.16, 356.16	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.484, 1.484, 1.484	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/11267	0.30	1/15222 (0.0%)
2	B	0.23	0/9464	0.29	0/12763
3	C	0.24	0/2139	0.30	0/2895
4	D	0.08	0/1361	0.24	0/1837
5	E	0.19	0/1773	0.27	0/2385
6	F	0.23	0/687	0.27	0/931
7	G	0.14	0/1354	0.27	0/1837
8	H	0.22	0/1070	0.28	0/1444
9	I	0.08	0/934	0.25	0/1257
10	J	0.25	0/563	0.27	0/753
11	K	0.23	0/953	0.29	0/1291
12	L	0.19	0/365	0.26	0/484
13	M	0.08	0/513	0.25	0/693
14	N	0.47	0/952	0.57	0/1464
15	P	0.93	7/449 (1.6%)	0.76	1/698 (0.1%)
16	T	0.52	0/1227	0.49	0/1890
17	V	0.08	0/840	0.21	0/1140
18	W	0.10	0/4300	0.26	0/5812
19	m	0.09	0/9925	0.25	0/13424
20	n	0.08	0/1132	0.22	0/1526
21	q	0.09	0/7689	0.21	0/10368
22	r	0.09	0/2169	0.24	0/2901
23	u	0.09	0/1740	0.22	0/2347
24	v	0.09	0/2944	0.23	0/3973
25	x	0.12	0/1716	0.25	0/2310
All	All	0.20	7/67526 (0.0%)	0.28	2/91645 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	P	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	10	G	C1'-N9	-7.03	1.37	1.48
15	P	6	G	C1'-N9	-6.74	1.37	1.48
15	P	-7	U	C1'-N1	6.20	1.56	1.47
15	P	-5	C	C1'-N1	5.46	1.55	1.47
15	P	2	U	C1'-N1	5.45	1.56	1.48
15	P	11	U	C1'-N1	5.29	1.56	1.48
15	P	9	U	C1'-N1	5.07	1.56	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1001	VAL	N-CA-C	-5.71	107.25	112.96
15	P	-3	U	O4'-C4'-C3'	5.12	109.12	104.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	P	-4	C	Sidechain

5.2 Too-close contacts [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	125	0
2	B	9284	0	9282	135	0
3	C	2098	0	2057	21	0
4	D	1349	0	1345	11	0
5	E	1741	0	1754	26	0
6	F	677	0	693	6	0
7	G	1325	0	1342	21	0
8	H	1053	0	1050	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	917	0	867	15	0
10	J	554	0	573	6	0
11	K	932	0	944	15	0
12	L	359	0	358	6	0
13	M	505	0	495	6	0
14	N	854	0	478	44	0
15	P	404	0	202	7	0
16	T	1090	0	590	36	0
17	V	824	0	795	18	0
18	W	4232	0	4278	67	0
19	m	9730	0	9588	145	0
20	n	1115	0	1186	25	0
21	q	7552	0	7545	109	0
22	r	2139	0	2155	42	0
23	u	1707	0	1676	27	0
24	v	2878	0	2873	58	0
25	x	1682	0	1731	15	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	C	1	0	0	0	0
26	I	2	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	M	1	0	0	0	0
26	V	1	0	0	0	0
27	A	1	0	0	0	0
All	All	66076	0	64947	862	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 (862) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-48:DC:H2''	14:N:-47:DC:C5	2.03	0.92
16:T:13:DT:H2''	16:T:14:DT:C7	1.99	0.92
16:T:13:DT:H2''	16:T:14:DT:H71	1.51	0.88
1:A:318:LYS:HE3	16:T:43:DA:C6	2.13	0.83
16:T:19:DC:H2'	16:T:20:DG:C8	2.17	0.80
21:q:793:VAL:HG11	21:q:830:LEU:HG	1.64	0.79
14:N:-61:DT:C2'	14:N:-60:DT:H72	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-45:DG:N2	16:T:45:DC:O2	2.16	0.77
14:N:-60:DT:H2'	14:N:-59:DT:H71	1.66	0.77
14:N:-61:DT:H2'	14:N:-60:DT:H72	1.66	0.76
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.26	0.75
14:N:-61:DT:H2'	14:N:-60:DT:C7	2.15	0.75
14:N:-48:DC:H2''	14:N:-47:DC:H5	1.52	0.74
21:q:390:LEU:HB3	21:q:409:LEU:HD21	1.70	0.74
14:N:-61:DT:C2'	14:N:-60:DT:C7	2.66	0.73
2:B:792:MET:HE2	2:B:857:ARG:HH22	1.54	0.73
14:N:-54:DC:H2''	14:N:-53:DT:H72	1.71	0.72
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.70	0.72
1:A:807:ARG:NH1	2:B:724:LYS:O	2.23	0.71
18:W:524:GLU:O	20:n:232:GLN:NE2	2.23	0.71
14:N:-52:DC:O2	16:T:52:DG:N2	2.17	0.71
1:A:1207:LYS:O	1:A:1277:ARG:NH2	2.24	0.70
5:E:60:LEU:O	21:q:915:ARG:NH1	2.23	0.70
8:H:112:LYS:HG2	8:H:125:GLU:HG3	1.73	0.69
1:A:1262:MET:SD	1:A:1265:ARG:NH2	2.66	0.69
2:B:550:PHE:HB3	2:B:593:MET:HE1	1.75	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
18:W:303:ILE:HB	20:n:286:ARG:HH22	1.58	0.68
19:m:382:PRO:HG2	19:m:955:ASN:HD22	1.58	0.68
21:q:531:GLU:O	21:q:535:ASN:N	2.26	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
10:J:47:ARG:NH1	10:J:48:MET:SD	2.67	0.68
1:A:251:ILE:HD12	15:P:1:G:H21	1.58	0.67
14:N:-52:DC:OP2	23:u:277:ARG:NH2	2.26	0.67
14:N:-18:DG:H2'	14:N:-17:DT:C6	2.29	0.67
2:B:223:SER:O	2:B:252:ARG:NH2	2.27	0.67
1:A:447:ARG:HB2	1:A:488:MET:HE3	1.77	0.67
1:A:107:CYS:SG	1:A:172:GLN:NE2	2.66	0.67
19:m:682:ASP:O	19:m:686:ASN:ND2	2.28	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
18:W:487:ILE:HD11	18:W:531:ARG:HB2	1.76	0.66
19:m:380:GLU:HG3	19:m:382:PRO:HD2	1.77	0.66
9:I:45:ARG:NH2	9:I:47:GLU:OE2	2.28	0.66
22:r:230:ARG:NH1	22:r:292:SER:OG	2.28	0.66
3:C:266:ARG:HD2	11:K:84:LYS:HZ3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:490:VAL:HG22	22:r:495:ARG:HE	1.60	0.66
2:B:267:TYR:HB2	2:B:348:ILE:HD11	1.77	0.66
2:B:254:ASP:H	2:B:259:ARG:HH21	1.44	0.66
1:A:673:ASP:OD1	1:A:737:ASN:ND2	2.29	0.65
18:W:342:GLU:HB3	18:W:351:ARG:HB3	1.79	0.65
19:m:617:ILE:HG13	19:m:649:LEU:HD11	1.78	0.65
25:x:292:TRP:HA	25:x:295:LYS:HE2	1.79	0.65
16:T:19:DC:H2'	16:T:20:DG:H8	1.61	0.65
25:x:157:ARG:HB3	25:x:161:PRO:HB3	1.78	0.65
1:A:127:ARG:O	1:A:129:ARG:NH1	2.30	0.64
1:A:887:ILE:O	1:A:945:ARG:NH2	2.30	0.64
20:n:260:MET:HG3	20:n:284:TRP:HZ3	1.63	0.64
4:D:153:VAL:HG13	4:D:171:LEU:HD23	1.78	0.64
18:W:327:ARG:NH2	18:W:441:ASN:O	2.30	0.64
21:q:31:LYS:HB2	21:q:57:GLU:HA	1.78	0.64
2:B:285:PRO:HG2	2:B:288:GLU:HB2	1.80	0.64
2:B:613:ARG:HH21	9:I:62:ILE:HD11	1.61	0.64
21:q:780:TYR:O	21:q:784:LYS:N	2.31	0.64
1:A:1158:PRO:HA	1:A:1192:PRO:HB3	1.80	0.63
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.24	0.63
1:A:361:GLU:OE1	1:A:460:ARG:NH2	2.29	0.63
21:q:793:VAL:HG13	21:q:826:ALA:HB1	1.79	0.63
1:A:466:TYR:HB2	1:A:470:ARG:HH22	1.63	0.63
1:A:881:ARG:HH21	1:A:955:ASN:HB3	1.64	0.63
17:V:89:ARG:NH1	17:V:109:ASP:OD2	2.31	0.63
22:r:269:ASP:HB3	22:r:349:LEU:HD21	1.80	0.63
1:A:1130:ILE:HG12	1:A:1134:LYS:HE2	1.81	0.63
11:K:57:THR:OG1	11:K:76:GLN:OE1	2.17	0.63
14:N:-56:DG:H2''	14:N:-55:DT:C6	2.33	0.63
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
16:T:50:DA:OP1	18:W:433:GLN:NE2	2.33	0.62
19:m:551:ARG:NH2	19:m:689:LYS:O	2.31	0.62
22:r:408:ASP:OD1	24:v:133:TYR:N	2.32	0.62
16:T:9:DG:H1'	16:T:10:DC:C5	2.34	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
21:q:210:PRO:O	21:q:217:ARG:NH2	2.25	0.62
19:m:607:ILE:HG22	19:m:719:VAL:HG11	1.82	0.61
18:W:351:ARG:HA	18:W:429:THR:HA	1.81	0.61
19:m:1101:ASP:OD1	19:m:1132:GLN:NE2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:348:ASP:HB3	21:q:351:GLN:HB3	1.83	0.61
19:m:434:LEU:HD11	19:m:467:ASP:HB2	1.81	0.61
1:A:1201:ARG:NH2	1:A:1235:ALA:O	2.33	0.61
18:W:784:ASN:HB2	18:W:785:PRO:HD3	1.81	0.61
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
1:A:39:GLU:OE2	1:A:49:ARG:NH1	2.34	0.61
5:E:19:LYS:NZ	5:E:33:GLU:O	2.34	0.61
19:m:358:HIS:HB3	19:m:361:GLU:HB2	1.82	0.61
1:A:466:TYR:HB2	1:A:470:ARG:NH2	2.16	0.61
23:u:80:TYR:CZ	24:v:356:ASN:HB2	2.36	0.60
23:u:199:LEU:HD11	24:v:211:PHE:HB3	1.81	0.60
5:E:47:ASP:OD2	5:E:53:GLN:NE2	2.19	0.60
23:u:108:VAL:HG22	23:u:219:VAL:HB	1.83	0.60
1:A:22:LEU:HG	2:B:1213:ALA:HB2	1.83	0.60
19:m:1221:LEU:HD11	19:m:1233:SER:HB2	1.82	0.60
19:m:421:ASP:OD1	19:m:422:LEU:N	2.34	0.60
16:T:9:DG:H2''	16:T:10:DC:H5	1.66	0.60
2:B:489:ARG:NH2	2:B:533:SER:O	2.35	0.60
19:m:570:MET:HA	19:m:577:THR:HG21	1.84	0.60
15:P:-5:C:H1'	18:W:748:ARG:HD3	1.83	0.60
1:A:677:MET:HG3	2:B:722:THR:HB	1.84	0.60
18:W:527:THR:HA	18:W:530:LEU:HD12	1.84	0.60
19:m:730:ASP:OD1	19:m:733:ARG:NH2	2.34	0.60
2:B:926:GLY:O	19:m:778:ALA:N	2.31	0.59
1:A:1157:ASP:O	1:A:1243:ARG:NH2	2.29	0.59
2:B:294:CYS:SG	2:B:295:TYR:N	2.76	0.59
19:m:785:ASP:O	19:m:912:GLN:NE2	2.35	0.59
20:n:217:ARG:HG3	20:n:259:VAL:HG21	1.84	0.59
2:B:409:LEU:HD23	2:B:450:LEU:HD23	1.85	0.59
17:V:13:MET:N	17:V:49:CYS:O	2.26	0.59
2:B:235:LEU:HD23	2:B:242:ILE:HG13	1.83	0.59
14:N:-61:DT:N1	14:N:-60:DT:H72	2.18	0.59
17:V:57:LEU:HD11	17:V:81:LEU:HD22	1.84	0.59
1:A:227:GLU:OE1	1:A:231:ARG:NH1	2.36	0.59
2:B:10:ASP:HB3	2:B:649:LYS:HG3	1.84	0.59
7:G:27:ARG:NH1	7:G:54:ILE:O	2.36	0.59
19:m:458:ARG:HG3	19:m:459:THR:HG23	1.83	0.59
19:m:672:VAL:O	19:m:720:GLN:NE2	2.34	0.59
8:H:48:PRO:O	8:H:145:ARG:NH1	2.36	0.59
19:m:424:TYR:HA	19:m:427:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:u:191:THR:HG22	23:u:219:VAL:HG22	1.85	0.59
24:v:29:LEU:N	25:x:147:ARG:O	2.35	0.59
1:A:149:GLU:HB2	1:A:165:ARG:HD3	1.84	0.58
19:m:1425:LYS:NZ	19:m:1430:SER:O	2.30	0.58
21:q:72:VAL:HG21	24:v:75:LEU:HD13	1.85	0.58
21:q:253:ILE:HG12	21:q:297:LEU:HD21	1.84	0.58
21:q:690:LYS:NZ	25:x:178:GLU:OE1	2.36	0.58
22:r:194:LYS:HB2	22:r:316:LEU:HD12	1.84	0.58
17:V:9:GLU:HA	17:V:20:PRO:HA	1.84	0.58
21:q:806:LEU:O	21:q:811:ARG:NH1	2.36	0.58
24:v:312:LYS:HB3	24:v:315:GLU:HG2	1.85	0.58
2:B:50:VAL:HG21	2:B:82:ILE:HD11	1.86	0.58
7:G:102:ASP:OD1	7:G:107:ASN:ND2	2.32	0.58
14:N:-56:DG:C2	16:T:57:DA:C2	2.92	0.58
1:A:85:GLU:O	1:A:274:ASN:ND2	2.33	0.58
18:W:327:ARG:NH1	18:W:335:GLY:O	2.36	0.58
21:q:766:MET:HG3	21:q:770:LYS:HE3	1.86	0.58
2:B:63:GLN:NE2	2:B:70:ASN:OD1	2.35	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	0.57
24:v:56:LYS:O	24:v:60:ARG:NH2	2.37	0.57
24:v:267:TYR:HB3	24:v:297:TYR:HB3	1.85	0.57
5:E:101:GLU:HG3	5:E:102:LYS:HG2	1.86	0.57
7:G:86:VAL:HG22	7:G:146:LYS:HB2	1.86	0.57
19:m:1177:SER:O	19:m:1194:ARG:NH1	2.37	0.57
1:A:568:LYS:HG2	1:A:569:PRO:HA	1.87	0.57
16:T:13:DT:H2''	16:T:14:DT:C5	2.39	0.57
19:m:245:THR:HA	19:m:248:GLN:HB2	1.86	0.57
23:u:121:PHE:HB3	23:u:153:ARG:HB3	1.85	0.57
18:W:392:ARG:NH1	18:W:398:GLU:OE1	2.36	0.57
18:W:352:LEU:HD11	18:W:435:LEU:HD11	1.87	0.57
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.37	0.57
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.85	0.57
18:W:665:ARG:HB2	18:W:708:ILE:HD11	1.87	0.57
19:m:529:ILE:HD11	19:m:566:ILE:HG12	1.87	0.56
14:N:-60:DT:C2'	14:N:-59:DT:H71	2.34	0.56
6:F:103:MET:HE3	7:G:15:PRO:HG2	1.87	0.56
23:u:209:LEU:HB2	24:v:252:PHE:HB2	1.87	0.56
2:B:290:LEU:HD21	2:B:310:ILE:HD11	1.87	0.56
2:B:336:ILE:O	2:B:341:ARG:NH1	2.38	0.56
18:W:220:THR:N	18:W:223:ASP:OD2	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:28:PHE:HB2	5:E:64:THR:HG22	1.88	0.56
14:N:-11:DC:H2'	14:N:-10:DG:C8	2.40	0.56
17:V:15:CYS:HB3	17:V:32:CYS:SG	2.46	0.56
2:B:906:SER:OG	18:W:781:GLU:OE1	2.23	0.56
14:N:-20:DC:H2'	14:N:-19:DG:O4'	2.07	0.55
1:A:1452:LEU:HD23	6:F:131:PRO:HA	1.88	0.55
2:B:72:ASN:ND2	2:B:128:ASP:OD1	2.40	0.55
8:H:100:VAL:HG22	8:H:115:VAL:HG22	1.89	0.55
19:m:300:VAL:O	19:m:304:THR:OG1	2.20	0.55
1:A:149:GLU:O	1:A:165:ARG:NH1	2.38	0.55
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.88	0.55
16:T:16:DA:H2''	16:T:17:DA:O4'	2.06	0.55
20:n:163:LEU:HD11	20:n:194:VAL:HG22	1.88	0.55
22:r:223:VAL:HG22	22:r:325:GLN:HG2	1.88	0.55
1:A:669:ASP:OD2	1:A:743:ASN:ND2	2.29	0.55
16:T:9:DG:H2''	16:T:10:DC:C5	2.42	0.55
24:v:316:ASP:HB2	24:v:333:ILE:HB	1.88	0.55
1:A:1210:THR:HB	1:A:1213:GLN:HG3	1.89	0.55
14:N:-21:DG:N2	16:T:22:DC:O2	2.39	0.55
22:r:200:ASP:HB3	22:r:319:VAL:HG11	1.87	0.55
1:A:569:PRO:HD2	8:H:46:MET:HE2	1.89	0.55
2:B:622:ASP:OD1	2:B:623:VAL:N	2.40	0.55
19:m:956:LEU:O	19:m:1046:ARG:NH2	2.38	0.55
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.42	0.54
21:q:155:TYR:HB3	21:q:160:ARG:HB2	1.89	0.54
21:q:569:ASN:O	21:q:603:LYS:NZ	2.40	0.54
23:u:89:SER:HB3	24:v:365:ARG:HE	1.72	0.54
2:B:904:ARG:HH12	2:B:946:ASN:HB2	1.72	0.54
18:W:232:ARG:HH12	18:W:235:LYS:HE3	1.70	0.54
19:m:465:ASP:OD1	19:m:604:ARG:NH1	2.40	0.54
19:m:956:LEU:HD11	19:m:1138:ILE:HG21	1.88	0.54
24:v:54:PHE:O	24:v:58:ASN:N	2.33	0.54
24:v:258:ASN:OD1	24:v:261:ASN:N	2.40	0.54
21:q:41:PHE:CG	21:q:70:VAL:HG11	2.42	0.54
1:A:119:ASN:OD1	1:A:121:THR:OG1	2.23	0.54
21:q:239:ASN:HA	21:q:242:LYS:HD2	1.89	0.54
21:q:766:MET:HE1	21:q:799:ILE:HG23	1.90	0.54
14:N:-18:DG:H2'	14:N:-17:DT:H6	1.70	0.54
18:W:332:LYS:O	18:W:388:ARG:NH1	2.41	0.54
1:A:916:TYR:OH	1:A:983:LEU:O	2.19	0.54
14:N:-14:DA:C2	14:N:-13:DA:C2	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:151:ARG:HB3	7:G:158:TYR:HB2	1.89	0.54
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.89	0.54
11:K:29:ASN:ND2	11:K:78:GLU:O	2.41	0.54
18:W:325:TYR:OH	18:W:451:GLN:OE1	2.23	0.54
21:q:218:LEU:HA	21:q:237:TRP:HE1	1.73	0.54
1:A:807:ARG:HD3	2:B:725:ARG:HA	1.89	0.54
19:m:533:VAL:HG22	19:m:589:VAL:HG13	1.90	0.54
1:A:218:GLU:OE1	1:A:222:ARG:NH1	2.41	0.54
11:K:103:HIS:NE2	11:K:107:GLU:OE2	2.40	0.54
19:m:236:GLU:OE2	20:n:252:ARG:NH2	2.41	0.54
19:m:917:GLU:OE2	19:m:969:TYR:OH	2.24	0.54
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.89	0.54
7:G:144:ARG:HB2	7:G:171:ILE:HD13	1.90	0.54
2:B:245:MET:HE1	2:B:371:LEU:HD11	1.91	0.53
4:D:6:SER:HB3	7:G:42:PHE:HZ	1.73	0.53
19:m:1205:ASP:OD2	19:m:1207:ARG:NH2	2.40	0.53
13:M:46:LEU:HD11	13:M:55:SER:HB3	1.91	0.53
17:V:10:ARG:HA	17:V:52:SER:HA	1.90	0.53
1:A:351:ARG:HB2	2:B:1128:LEU:HD21	1.91	0.53
2:B:91:GLU:OE2	2:B:97:HIS:NE2	2.29	0.53
20:n:229:PRO:O	20:n:234:GLN:NE2	2.37	0.53
21:q:641:ALA:HB1	21:q:655:LYS:HG3	1.89	0.53
23:u:80:TYR:OH	24:v:352:VAL:O	2.22	0.53
1:A:533:ARG:HD3	1:A:750:ALA:HB2	1.91	0.53
18:W:451:GLN:NE2	18:W:454:GLU:OE1	2.41	0.53
18:W:513:SER:N	18:W:519:ASN:OD1	2.41	0.53
1:A:1426:GLY:O	1:A:1430:ASN:ND2	2.40	0.53
2:B:936:ASP:OD1	2:B:938:SER:OG	2.26	0.53
19:m:1024:TYR:CG	19:m:1135:TYR:HE2	2.26	0.53
21:q:170:ASN:HA	21:q:173:LYS:HD2	1.91	0.53
2:B:58:LEU:O	2:B:75:TYR:N	2.36	0.53
21:q:309:GLU:OE1	21:q:311:TYR:OH	2.20	0.53
24:v:74:TYR:HE1	24:v:87:LEU:HD12	1.73	0.53
2:B:59:ASP:HB3	2:B:74:ARG:HG3	1.91	0.53
2:B:592:THR:HG23	23:u:226:PHE:CE1	2.44	0.53
4:D:60:ILE:HG13	7:G:47:THR:HG21	1.91	0.53
14:N:-21:DG:N2	16:T:22:DC:C2	2.77	0.53
5:E:118:SER:OG	14:N:-16:DT:OP1	2.22	0.52
19:m:1047:ILE:HG12	19:m:1127:ILE:HG12	1.90	0.52
21:q:317:LEU:HD23	22:r:514:LEU:HD12	1.91	0.52
2:B:301:GLN:O	2:B:304:GLU:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:59:LEU:HD23	8:H:139:LEU:HD13	1.91	0.52
17:V:58:VAL:N	17:V:82:TYR:O	2.38	0.52
24:v:262:LYS:HD3	24:v:305:GLN:HE21	1.74	0.52
2:B:248:LYS:NZ	2:B:264:THR:OG1	2.42	0.52
16:T:16:DA:H2'	16:T:17:DA:C8	2.44	0.52
19:m:1121:ARG:HA	19:m:1124:LEU:HD12	1.91	0.52
21:q:451:ARG:NH1	24:v:35:GLU:OE1	2.42	0.52
1:A:318:LYS:HE3	16:T:43:DA:N1	2.24	0.52
17:V:10:ARG:HG2	17:V:52:SER:HB3	1.92	0.52
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.49	0.52
10:J:23:ARG:NH2	22:r:399:LYS:HZ1	2.07	0.52
19:m:465:ASP:OD2	19:m:608:ARG:NH2	2.43	0.52
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.92	0.52
19:m:1062:ALA:HB3	19:m:1083:MET:HE1	1.92	0.52
24:v:210:VAL:HG13	24:v:334:VAL:HG21	1.92	0.52
1:A:1153:GLU:OE2	9:I:45:ARG:NH1	2.40	0.52
19:m:338:LEU:HD11	19:m:417:ILE:HD11	1.91	0.52
19:m:1056:ARG:HB3	19:m:1076:MET:HB3	1.91	0.52
2:B:74:ARG:HB2	2:B:124:PHE:HB2	1.92	0.52
5:E:81:PHE:HE1	5:E:110:ILE:HD13	1.74	0.52
21:q:404:GLU:OE1	21:q:404:GLU:N	2.42	0.52
2:B:904:ARG:NH1	2:B:905:VAL:O	2.43	0.51
13:M:38:LEU:HA	13:M:45:GLY:HA2	1.91	0.51
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.74	0.51
1:A:771:VAL:HG13	1:A:823:GLU:HG3	1.92	0.51
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.93	0.51
2:B:875:GLU:OE2	2:B:915:THR:OG1	2.26	0.51
21:q:250:ASN:HA	21:q:253:ILE:HD12	1.91	0.51
21:q:871:TYR:CZ	21:q:875:ILE:HD11	2.45	0.51
24:v:233:GLY:O	24:v:244:ASN:ND2	2.44	0.51
2:B:505:ARG:NH1	2:B:524:GLN:O	2.32	0.51
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.75	0.51
19:m:995:ILE:HD12	19:m:1010:LEU:HD21	1.92	0.51
2:B:86:ARG:NH1	22:r:369:GLU:OE2	2.44	0.51
21:q:286:SER:HA	21:q:289:LYS:HD2	1.92	0.51
1:A:801:VAL:HG22	1:A:813:GLU:HB3	1.92	0.51
2:B:547:ILE:HG21	2:B:619:ILE:HG21	1.93	0.51
18:W:590:ILE:O	18:W:593:SER:OG	2.26	0.51
22:r:244:LYS:NZ	22:r:305:GLU:OE2	2.37	0.51
1:A:1331:TYR:OH	1:A:1354:GLU:OE2	2.21	0.51
18:W:644:ASN:ND2	18:W:647:GLN:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:v:104:PRO:HA	24:v:107:ARG:HD3	1.92	0.51
18:W:260:TYR:HD1	18:W:276:ALA:HA	1.75	0.51
18:W:326:VAL:HA	18:W:440:ILE:HD13	1.92	0.51
19:m:1172:VAL:HA	19:m:1182:VAL:HG12	1.93	0.51
5:E:28:PHE:HE2	21:q:915:ARG:HB2	1.75	0.51
13:M:33:SER:HA	13:M:50:LYS:HE2	1.93	0.51
21:q:274:THR:HG23	22:r:506:ILE:HG12	1.93	0.51
2:B:83:TYR:HB2	2:B:116:TYR:HB2	1.92	0.50
2:B:556:MET:HE3	2:B:581:GLY:HA3	1.93	0.50
2:B:797:TYR:HE1	2:B:854:LEU:HD13	1.74	0.50
22:r:261:LEU:HB3	22:r:266:ASN:HB3	1.93	0.50
22:r:276:PHE:HB2	22:r:279:GLN:HB2	1.91	0.50
14:N:-61:DT:H2''	14:N:-60:DT:C7	2.41	0.50
18:W:563:GLU:HG2	18:W:574:ILE:HG12	1.92	0.50
9:I:17:LYS:N	9:I:26:LEU:O	2.39	0.50
19:m:244:GLY:O	19:m:248:GLN:N	2.44	0.50
19:m:1046:ARG:HG3	19:m:1135:TYR:HE1	1.75	0.50
21:q:408:LEU:HD13	24:v:44:LEU:HD22	1.92	0.50
1:A:1150:SER:OG	1:A:1198:GLU:OE1	2.29	0.50
16:T:18:DC:C2	16:T:19:DC:C5	3.00	0.50
1:A:1190:GLN:HA	1:A:1245:ILE:HA	1.94	0.50
5:E:87:VAL:HG23	5:E:91:THR:HB	1.92	0.50
20:n:206:SER:O	20:n:210:ASN:ND2	2.44	0.50
14:N:-61:DT:H2'	14:N:-60:DT:H73	1.90	0.50
18:W:334:LYS:N	18:W:388:ARG:HH12	2.09	0.50
2:B:436:ASN:C	2:B:438:ASN:H	2.20	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
21:q:676:ASN:HA	25:x:156:LEU:HD12	1.93	0.50
21:q:189:LEU:HD22	21:q:194:LYS:HD2	1.94	0.50
21:q:718:HIS:ND1	21:q:733:TYR:OH	2.38	0.50
18:W:494:LEU:HD21	20:n:183:PRO:HG3	1.92	0.50
24:v:263:TRP:HE1	24:v:356:ASN:HD21	1.59	0.50
2:B:74:ARG:HH22	2:B:126:SER:HB3	1.77	0.49
2:B:607:SER:HB3	2:B:620:PHE:HB2	1.94	0.49
14:N:-18:DG:N2	14:N:-17:DT:C2	2.80	0.49
19:m:562:PRO:HG3	19:m:700:TRP:CE3	2.47	0.49
19:m:766:LEU:HD13	19:m:783:PHE:HB2	1.94	0.49
19:m:840:ASN:O	19:m:844:ASN:ND2	2.44	0.49
19:m:343:ARG:NH2	19:m:344:ASP:OD1	2.45	0.49
21:q:109:PHE:CD1	21:q:130:ALA:HB1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:160:ARG:NH2	21:q:163:GLU:OE1	2.44	0.49
2:B:498:ASP:HB3	14:N:-31:DA:C4	2.47	0.49
16:T:20:DG:N2	16:T:21:DC:C2	2.81	0.49
17:V:63:ASN:HB3	17:V:75:ASP:HA	1.94	0.49
19:m:1257:ILE:HG22	19:m:1261:ASN:HD21	1.77	0.49
1:A:168:CYS:SG	1:A:170:ASN:ND2	2.85	0.49
19:m:242:GLY:HA3	20:n:258:LYS:HG2	1.94	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:300:TRP:HA	2:B:303:LEU:HD12	1.94	0.49
2:B:479:TYR:CZ	2:B:1096:ARG:HB3	2.48	0.49
4:D:105:THR:HG22	7:G:105:PRO:HD3	1.94	0.49
18:W:464:ILE:O	18:W:468:LEU:HG	2.12	0.49
19:m:725:GLU:OE2	19:m:728:ARG:NH2	2.45	0.49
1:A:122:MET:O	1:A:126:ILE:HG12	2.13	0.49
1:A:1223:SER:OG	1:A:1224:ASP:N	2.44	0.49
7:G:119:LEU:HD21	7:G:135:GLU:HB2	1.93	0.49
14:N:-51:DG:H2'	14:N:-50:DT:H71	1.95	0.49
18:W:222:ASP:O	18:W:277:ARG:NH2	2.30	0.49
21:q:305:TYR:CZ	22:r:512:LEU:HD11	2.48	0.49
19:m:655:LEU:HG	19:m:659:MET:HE3	1.95	0.49
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	1.94	0.49
2:B:928:ARG:NH1	19:m:776:GLY:H	2.11	0.49
5:E:81:PHE:CE1	5:E:110:ILE:HD13	2.48	0.49
7:G:112:THR:HA	7:G:115:ILE:HD12	1.95	0.49
19:m:1170:VAL:HG12	19:m:1184:THR:HG22	1.95	0.49
21:q:816:LEU:HD13	21:q:865:ILE:HA	1.95	0.49
1:A:673:ASP:OD1	1:A:673:ASP:N	2.44	0.49
18:W:634:PRO:HA	18:W:637:ILE:HD12	1.94	0.49
12:L:70:ASP:HB3	18:W:784:ASN:HB3	1.95	0.48
20:n:207:ILE:HG23	20:n:212:LEU:HB3	1.94	0.48
1:A:823:GLU:OE1	2:B:506:GLN:NE2	2.46	0.48
3:C:66:LEU:HD11	3:C:155:ILE:HD12	1.95	0.48
9:I:96:ASN:OD1	9:I:97:MET:N	2.46	0.48
19:m:770:PHE:HB3	19:m:779:VAL:HG22	1.95	0.48
19:m:823:ILE:HB	19:m:873:VAL:HG22	1.95	0.48
1:A:738:LEU:HD13	1:A:742:ASN:HD22	1.77	0.48
2:B:318:ASP:HB3	2:B:321:VAL:HG22	1.94	0.48
2:B:610:ARG:NH2	9:I:61:ASP:OD2	2.46	0.48
2:B:314:PHE:O	2:B:317:GLN:NE2	2.46	0.48
3:C:105:GLU:N	3:C:105:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-13:DA:C2	14:N:-12:DA:C4	3.01	0.48
23:u:202:GLU:HB3	24:v:210:VAL:HB	1.96	0.48
24:v:36:LYS:HB2	24:v:39:PRO:HD2	1.95	0.48
2:B:365:THR:O	2:B:368:THR:OG1	2.29	0.48
19:m:1202:ASP:OD2	19:m:1204:ARG:NE	2.44	0.48
1:A:253:MET:HG2	15:P:1:G:N2	2.29	0.48
1:A:977:ARG:HD2	1:A:979:LYS:HZ1	1.78	0.48
2:B:514:LEU:HD22	2:B:626:VAL:HG12	1.94	0.48
19:m:1062:ALA:HA	19:m:1103:LEU:HD21	1.95	0.48
22:r:493:ASN:HB2	22:r:502:ILE:HD11	1.95	0.48
2:B:766:ARG:HH21	2:B:1020:ARG:HD3	1.77	0.48
9:I:29:CYS:CB	9:I:32:CYS:SG	2.99	0.48
15:P:1:G:H2'	15:P:2:U:O4'	2.12	0.48
18:W:666:GLU:HB2	18:W:671:ARG:HA	1.95	0.48
19:m:1365:GLU:O	19:m:1369:ASN:ND2	2.46	0.48
21:q:320:LEU:O	21:q:324:GLU:HG2	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:599:HIS:HB3	18:W:677:LEU:HD21	1.96	0.48
19:m:1425:LYS:HE3	19:m:1428:PRO:HA	1.96	0.48
22:r:206:PHE:HB2	22:r:227:MET:HE1	1.96	0.48
22:r:208:ARG:N	22:r:291:ASP:OD1	2.44	0.48
9:I:103:CYS:SG	9:I:104:LEU:N	2.86	0.48
15:P:-5:C:C4	18:W:748:ARG:N	2.82	0.48
19:m:681:VAL:HG13	19:m:708:TRP:HE1	1.79	0.48
20:n:163:LEU:HD22	20:n:197:ILE:HD13	1.96	0.48
21:q:185:LYS:O	21:q:189:LEU:HG	2.14	0.48
21:q:312:GLU:O	21:q:316:LYS:HG3	2.14	0.48
23:u:204:ASN:OD1	23:u:205:GLU:N	2.47	0.48
2:B:865:ARG:HD3	2:B:871:VAL:HG12	1.95	0.48
3:C:74:GLU:O	3:C:246:ARG:NH2	2.39	0.48
4:D:157:ILE:HG23	4:D:164:ALA:HB2	1.95	0.48
25:x:311:GLY:HA3	25:x:330:VAL:HG12	1.96	0.48
1:A:106:ILE:HD13	1:A:215:ILE:HD11	1.95	0.47
3:C:88:GLU:HG2	18:W:759:ARG:HD2	1.95	0.47
18:W:666:GLU:HA	18:W:705:VAL:HG12	1.96	0.47
19:m:1279:ARG:NH1	19:m:1315:SER:O	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
24:v:304:ASP:OD2	24:v:340:LYS:NZ	2.45	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
5:E:91:THR:HA	5:E:94:ASN:ND2	2.29	0.47
16:T:45:DC:H2''	16:T:46:DA:C8	2.49	0.47
18:W:603:GLN:HG3	18:W:609:VAL:HG22	1.95	0.47
24:v:199:HIS:O	24:v:328:ALA:N	2.47	0.47
1:A:486:ASP:OD1	15:P:10:G:O2'	2.20	0.47
2:B:303:LEU:O	2:B:307:LYS:HG2	2.15	0.47
5:E:93:ARG:HA	5:E:122:MET:HE1	1.96	0.47
19:m:1427:ASN:OD1	19:m:1430:SER:N	2.47	0.47
19:m:1003:ALA:O	19:m:1007:THR:HG23	2.14	0.47
1:A:912:ASP:OD1	1:A:912:ASP:N	2.44	0.47
2:B:80:GLY:N	2:B:118:ASP:O	2.42	0.47
19:m:965:VAL:HG22	19:m:989:ILE:HG13	1.96	0.47
19:m:977:VAL:HB	19:m:980:LEU:HD12	1.94	0.47
22:r:366:GLU:O	22:r:369:GLU:HG2	2.15	0.47
1:A:472:ASN:O	1:A:475:VAL:HG22	2.14	0.47
1:A:580:SER:HB3	1:A:612:LYS:HA	1.97	0.47
1:A:983:LEU:HD13	1:A:1041:ARG:HA	1.96	0.47
2:B:421:ILE:HD11	2:B:441:VAL:HG12	1.97	0.47
2:B:896:ASP:OD2	12:L:31:TYR:OH	2.32	0.47
13:M:37:THR:O	13:M:46:LEU:N	2.29	0.47
21:q:4:LEU:HB2	24:v:103:HIS:CE1	2.50	0.47
21:q:261:ASP:O	21:q:265:ASN:ND2	2.36	0.47
21:q:710:LEU:HD11	21:q:748:LEU:HD11	1.96	0.47
5:E:213:CYS:SG	5:E:214:LEU:N	2.87	0.47
19:m:381:VAL:HG13	19:m:414:LEU:HD22	1.97	0.47
23:u:90:LEU:HB2	24:v:362:MET:HE1	1.96	0.47
14:N:-55:DT:H4'	14:N:-54:DC:H5'	1.97	0.47
19:m:1337:GLU:HB2	19:m:1348:VAL:HB	1.95	0.47
24:v:310:HIS:NE2	24:v:316:ASP:OD2	2.48	0.47
2:B:101:PRO:HG2	2:B:172:LEU:HD11	1.96	0.47
11:K:62:LYS:HE3	11:K:64:GLU:OE2	2.15	0.47
17:V:41:SER:HB2	17:V:45:THR:HB	1.96	0.47
19:m:622:THR:O	19:m:626:LYS:N	2.41	0.47
19:m:1072:ASP:O	19:m:1076:MET:HG2	2.15	0.47
21:q:155:TYR:HB2	21:q:164:ALA:HB2	1.96	0.47
21:q:710:LEU:HD13	21:q:740:PHE:HB2	1.97	0.47
2:B:322:ALA:O	2:B:326:ILE:HG12	2.15	0.46
10:J:6:ARG:HD3	10:J:13:VAL:HG22	1.97	0.46
14:N:-19:DG:C2	14:N:-18:DG:C4	3.03	0.46
22:r:346:LYS:O	22:r:350:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:408:ASP:OD2	24:v:134:VAL:HG23	2.15	0.46
1:A:819:MET:O	1:A:823:GLU:HG2	2.14	0.46
1:A:1192:PRO:HA	1:A:1243:ARG:HH12	1.79	0.46
2:B:25:PHE:HZ	2:B:534:LEU:HG	1.81	0.46
2:B:273:PRO:HG2	2:B:276:ILE:HD12	1.97	0.46
3:C:4:GLU:HB3	3:C:5:PRO:HD3	1.96	0.46
18:W:260:TYR:CE1	18:W:277:ARG:HG3	2.49	0.46
21:q:4:LEU:HD22	24:v:105:ASP:HB2	1.96	0.46
21:q:374:ALA:HA	21:q:377:LEU:HD12	1.96	0.46
22:r:212:SER:HA	22:r:215:TRP:HD1	1.79	0.46
1:A:363:ASP:HB3	1:A:509:PRO:HD3	1.97	0.46
3:C:17:VAL:HG12	3:C:240:ALA:HB1	1.96	0.46
5:E:98:ARG:NH1	5:E:102:LYS:HG3	2.31	0.46
7:G:123:PRO:HA	7:G:128:PRO:HB3	1.97	0.46
18:W:534:PHE:HB3	18:W:554:ILE:HD13	1.97	0.46
25:x:173:LEU:HA	25:x:177:LYS:HD2	1.98	0.46
5:E:96:CYS:SG	5:E:126:VAL:HG23	2.55	0.46
18:W:704:ARG:NH1	19:m:632:GLU:OE2	2.43	0.46
19:m:306:LEU:HD13	19:m:314:ARG:HH21	1.80	0.46
19:m:380:GLU:HG2	19:m:978:CYS:HB2	1.97	0.46
19:m:1426:LEU:HD13	19:m:1469:ARG:HH21	1.80	0.46
24:v:73:ASN:HB3	24:v:76:ARG:HE	1.79	0.46
1:A:649:ASN:O	1:A:653:VAL:HG23	2.16	0.46
2:B:27:GLU:OE1	2:B:678:TRP:HB3	2.16	0.46
2:B:353:LEU:O	2:B:367:LYS:NZ	2.34	0.46
2:B:497:ARG:NH2	16:T:32:DA:OP2	2.48	0.46
4:D:139:PRO:HA	4:D:142:ILE:HD12	1.97	0.46
6:F:74:ILE:HG23	6:F:78:GLU:HG3	1.97	0.46
21:q:215:ASP:OD1	21:q:217:ARG:NH1	2.47	0.46
7:G:51:GLY:HA2	7:G:54:ILE:HD11	1.98	0.46
14:N:-56:DG:N1	16:T:57:DA:C2	2.83	0.46
19:m:1426:LEU:HD21	19:m:1465:MET:HE2	1.97	0.46
24:v:349:VAL:HA	24:v:352:VAL:HB	1.98	0.46
1:A:215:ILE:O	1:A:231:ARG:NH2	2.46	0.46
1:A:543:GLU:OE2	1:A:570:LYS:NZ	2.43	0.46
16:T:40:DG:H1'	16:T:41:DA:H5''	1.98	0.46
18:W:451:GLN:HG3	18:W:458:THR:HA	1.98	0.46
20:n:208:LEU:HD13	20:n:250:HIS:CE1	2.50	0.46
21:q:489:PHE:HE1	21:q:533:VAL:HG21	1.80	0.46
1:A:409:ASP:OD1	1:A:410:ASN:N	2.49	0.46
2:B:318:ASP:OD1	2:B:319:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:14:DT:H2'	16:T:15:DT:C6	2.50	0.46
1:A:1065:MET:SD	1:A:1439:MET:HB2	2.56	0.46
1:A:1448:ILE:HD11	1:A:1453:LEU:HD11	1.97	0.46
12:L:49:ARG:HG2	22:r:339:VAL:HG11	1.98	0.46
14:N:-48:DC:C2'	14:N:-47:DC:C5	2.87	0.46
7:G:81:PRO:HG3	7:G:106:LEU:HD22	1.99	0.45
14:N:-18:DG:C2	14:N:-17:DT:C4	3.04	0.45
19:m:561:SER:HA	19:m:696:ILE:HG23	1.97	0.45
19:m:1105:LEU:HD11	19:m:1128:LYS:HE2	1.98	0.45
23:u:170:ILE:HD11	24:v:200:PHE:CD1	2.50	0.45
1:A:684:ILE:HG21	1:A:802:GLU:HG3	1.99	0.45
2:B:557:GLU:OE2	2:B:584:ARG:NH2	2.49	0.45
16:T:20:DG:C2	16:T:21:DC:C2	3.05	0.45
19:m:654:ASP:OD2	19:m:933:HIS:NE2	2.50	0.45
21:q:241:LEU:HD11	21:q:252:LYS:HG2	1.98	0.45
21:q:320:LEU:HD13	22:r:514:LEU:HD11	1.97	0.45
2:B:266:PRO:HG3	2:B:352:GLU:O	2.16	0.45
2:B:778:MET:HE2	2:B:1094:ARG:HD3	1.98	0.45
18:W:539:HIS:CE1	18:W:553:LEU:HD21	2.51	0.45
19:m:1286:PHE:HA	19:m:1308:ILE:HB	1.98	0.45
2:B:885:LEU:HD23	2:B:936:ASP:HB2	1.97	0.45
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.49	0.45
4:D:170:ASN:HB3	4:D:173:ARG:HG2	1.97	0.45
7:G:113:ARG:NH1	18:W:563:GLU:OE1	2.49	0.45
19:m:1218:ALA:HB1	19:m:1232:LEU:HB3	1.99	0.45
21:q:713:PHE:HB3	21:q:736:ALA:HB2	1.97	0.45
3:C:15:ASP:OD1	3:C:15:ASP:N	2.47	0.45
21:q:479:TYR:HD1	24:v:30:LEU:HB3	1.81	0.45
23:u:106:TRP:CD1	23:u:217:LYS:HB2	2.52	0.45
14:N:-30:DA:H61	16:T:30:DT:H3	1.65	0.45
19:m:521:TYR:HA	19:m:524:ILE:HD12	1.97	0.45
19:m:1170:VAL:O	19:m:1215:THR:OG1	2.19	0.45
21:q:107:PHE:O	21:q:111:LEU:HG	2.17	0.45
21:q:403:SER:OG	24:v:56:LYS:NZ	2.49	0.45
22:r:221:ASP:OD1	22:r:251:SER:OG	2.33	0.45
23:u:173:TRP:NE1	23:u:179:SER:OG	2.36	0.45
2:B:463:LYS:NZ	2:B:464:LYS:HE2	2.31	0.45
16:T:11:DG:H1'	16:T:12:DT:H5'	1.98	0.45
18:W:344:LEU:HD12	18:W:349:GLU:HB2	1.99	0.45
21:q:489:PHE:CE1	21:q:533:VAL:HG21	2.51	0.45
2:B:220:ALA:O	2:B:252:ARG:NH2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:LEU:HD22	11:K:101:LEU:HD11	1.98	0.45
19:m:1220:ILE:HA	19:m:1232:LEU:HD23	1.98	0.45
8:H:110:LYS:HE2	8:H:112:LYS:HE3	1.99	0.45
18:W:491:LEU:HB3	18:W:494:LEU:HD12	1.98	0.45
21:q:155:TYR:O	21:q:160:ARG:N	2.43	0.45
24:v:29:LEU:HB2	25:x:147:ARG:HB3	1.98	0.45
1:A:564:PRO:HG2	1:A:567:LEU:HD23	1.98	0.45
1:A:1061:HIS:O	1:A:1064:GLU:HG2	2.17	0.45
2:B:74:ARG:NH1	2:B:126:SER:OG	2.40	0.45
5:E:46:CYS:HB3	5:E:50:GLY:HA2	1.99	0.44
5:E:117:PRO:O	5:E:121:LYS:HG2	2.17	0.44
1:A:975:LEU:HD13	1:A:1039:LEU:HA	1.99	0.44
2:B:387:ASP:H	9:I:91:ARG:NH2	2.14	0.44
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.49	0.44
2:B:1050:LEU:HD12	24:v:127:PHE:CG	2.52	0.44
19:m:999:LEU:HD23	19:m:1025:ILE:HD11	1.99	0.44
19:m:1029:PRO:O	19:m:1033:ARG:NH1	2.51	0.44
14:N:-21:DG:H2''	14:N:-20:DC:O4'	2.17	0.44
17:V:78:GLN:OE1	17:V:79:PRO:HD2	2.16	0.44
21:q:357:LYS:NZ	21:q:361:ASP:OD1	2.50	0.44
19:m:735:LEU:HB3	19:m:937:LEU:HD21	1.99	0.44
19:m:1279:ARG:NH2	19:m:1344:ALA:O	2.51	0.44
21:q:905:ARG:NE	21:q:909:GLU:OE2	2.30	0.44
22:r:316:LEU:HD23	22:r:316:LEU:HA	1.83	0.44
23:u:116:ILE:HD13	23:u:150:VAL:HB	1.99	0.44
25:x:314:PHE:HD1	25:x:335:ILE:HD11	1.82	0.44
1:A:343:GLY:O	2:B:1129:ARG:NH1	2.45	0.44
1:A:880:GLU:O	1:A:957:PRO:HA	2.18	0.44
1:A:889:GLY:O	1:A:941:ARG:NH2	2.51	0.44
3:C:258:VAL:HG21	11:K:42:LEU:HD21	2.00	0.44
19:m:336:GLU:OE1	19:m:458:ARG:NH2	2.50	0.44
19:m:782:VAL:HG11	19:m:905:ILE:HG13	1.99	0.44
21:q:641:ALA:HB2	21:q:658:GLN:HB2	1.99	0.44
22:r:300:ASP:O	22:r:304:ARG:HG2	2.17	0.44
1:A:636:ARG:HH12	1:A:878:GLN:CD	2.25	0.44
3:C:79:MET:HE1	3:C:96:VAL:HG23	2.00	0.44
19:m:640:TYR:HB3	19:m:1256:ASP:HB3	2.00	0.44
21:q:868:GLN:O	21:q:872:GLU:HG2	2.17	0.44
1:A:452:HIS:CE1	1:A:454:MET:HB2	2.52	0.44
19:m:536:ILE:HG12	19:m:700:TRP:CZ3	2.53	0.44
19:m:1039:MET:SD	19:m:1039:MET:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:435:GLN:HG3	21:q:441:ILE:HD11	1.98	0.44
4:D:54:SER:OG	4:D:121:CYS:SG	2.61	0.44
14:N:-61:DT:C2'	14:N:-60:DT:H73	2.42	0.44
18:W:216:LEU:HD22	19:m:229:LEU:HG	1.98	0.44
20:n:200:ARG:HG2	20:n:202:ASN:OD1	2.18	0.44
19:m:590:LYS:HD2	19:m:706:ASP:HB2	1.99	0.44
19:m:968:PRO:HA	19:m:971:ALA:HB3	1.98	0.44
21:q:178:ASN:HA	24:v:91:PHE:CE2	2.52	0.44
21:q:217:ARG:HA	21:q:220:ILE:HD12	2.00	0.44
21:q:561:ILE:HD12	21:q:579:LEU:HD22	1.98	0.44
1:A:701:ASN:CG	9:I:96:ASN:HD21	2.26	0.43
1:A:779:GLY:HA3	2:B:509:ASN:HB2	1.99	0.43
1:A:1390:HIS:O	1:A:1394:ARG:HD3	2.17	0.43
2:B:924:GLU:O	19:m:795:LYS:NZ	2.42	0.43
8:H:25:ARG:HD3	8:H:41:ASP:OD1	2.18	0.43
14:N:-16:DT:H1'	14:N:-15:DA:H5'	1.99	0.43
18:W:518:ILE:HD13	20:n:185:ILE:HD13	2.00	0.43
19:m:603:ILE:HD13	19:m:708:TRP:HZ3	1.82	0.43
21:q:559:ARG:NH2	24:v:24:PRO:O	2.51	0.43
23:u:117:ASN:HB3	23:u:151:ARG:HG2	2.00	0.43
24:v:311:LYS:HE2	24:v:311:LYS:HB2	1.90	0.43
2:B:640:ASP:OD1	2:B:640:ASP:N	2.50	0.43
11:K:56:VAL:HG22	11:K:77:THR:HG22	2.00	0.43
17:V:67:TRP:NE1	18:W:217:LEU:O	2.51	0.43
18:W:250:ARG:NH2	18:W:284:ASP:OD2	2.50	0.43
19:m:305:ASP:OD1	19:m:1014:THR:OG1	2.34	0.43
19:m:538:ASN:HB3	19:m:541:GLN:HB2	2.00	0.43
19:m:685:TYR:O	19:m:689:LYS:N	2.41	0.43
21:q:526:ASN:O	21:q:530:VAL:HG23	2.18	0.43
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	1.99	0.43
5:E:104:PHE:HZ	21:q:925:TRP:HZ3	1.66	0.43
14:N:-56:DG:N2	16:T:57:DA:N3	2.67	0.43
19:m:955:ASN:HD21	19:m:978:CYS:HB3	1.83	0.43
20:n:167:MET:HE3	20:n:219:TRP:CD2	2.53	0.43
21:q:40:ASP:CG	21:q:42:ASN:HD22	2.26	0.43
23:u:83:GLY:HA2	24:v:358:ALA:HB3	2.01	0.43
1:A:100:LYS:NZ	1:A:104:GLU:OE2	2.49	0.43
1:A:976:ASP:O	1:A:979:LYS:NZ	2.48	0.43
10:J:63:ASN:OD1	10:J:64:PRO:HD2	2.18	0.43
18:W:322:ARG:NE	18:W:343:VAL:H	2.17	0.43
18:W:763:TYR:HB3	18:W:766:LYS:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:306:LEU:O	19:m:311:GLN:NE2	2.51	0.43
21:q:261:ASP:HB2	24:v:58:ASN:ND2	2.34	0.43
22:r:206:PHE:H	22:r:229:LEU:HD21	1.83	0.43
24:v:31:LYS:HA	25:x:147:ARG:HH12	1.82	0.43
1:A:329:ARG:NH1	2:B:1206:GLU:OE2	2.45	0.43
1:A:948:VAL:O	5:E:200:ARG:NH1	2.48	0.43
5:E:99:ILE:HG13	5:E:131:ILE:HD11	2.00	0.43
9:I:100:PHE:HB3	9:I:109:THR:HG23	1.99	0.43
13:M:65:GLN:N	13:M:68:ASP:OD2	2.44	0.43
18:W:444:LEU:HD23	18:W:444:LEU:HA	1.90	0.43
19:m:1309:ARG:NH2	19:m:1319:THR:HG21	2.34	0.43
21:q:511:VAL:HG11	21:q:519:LEU:HD12	2.01	0.43
25:x:226:LYS:HB2	25:x:248:LEU:HD21	2.00	0.43
1:A:1098:LEU:HD23	1:A:1098:LEU:HA	1.89	0.43
2:B:221:ALA:O	2:B:223:SER:N	2.46	0.43
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
19:m:1261:ASN:OD1	19:m:1264:ARG:NH2	2.39	0.43
19:m:1005:LEU:HA	19:m:1010:LEU:HD12	2.01	0.43
21:q:284:LEU:HD11	21:q:297:LEU:HD22	2.01	0.43
21:q:308:LYS:NZ	22:r:504:SER:O	2.38	0.43
22:r:345:MET:O	22:r:348:SER:OG	2.31	0.43
1:A:1389:ARG:O	1:A:1393:ASN:HB2	2.18	0.43
2:B:721:ASP:OD2	2:B:724:LYS:N	2.41	0.43
2:B:1156:ASP:O	2:B:1197:PRO:HA	2.19	0.43
6:F:103:MET:HE1	7:G:65:SER:O	2.19	0.43
17:V:46:VAL:O	17:V:50:THR:N	2.44	0.43
19:m:477:GLN:OE1	19:m:477:GLN:N	2.42	0.43
20:n:157:ASP:HA	20:n:210:ASN:HD21	1.83	0.43
22:r:245:VAL:HG23	22:r:298:GLU:HG2	2.01	0.43
22:r:277:PRO:HB2	22:r:305:GLU:HB3	2.00	0.43
1:A:266:LYS:HD2	1:A:266:LYS:HA	1.88	0.43
2:B:257:THR:OG1	2:B:258:GLY:N	2.50	0.43
4:D:88:GLU:HA	4:D:91:LYS:HE3	2.00	0.43
7:G:115:ILE:HG23	7:G:163:ILE:HD11	2.01	0.43
14:N:-56:DG:N2	16:T:57:DA:C2	2.87	0.43
18:W:468:LEU:HD11	19:m:283:VAL:HG13	2.01	0.43
18:W:490:GLU:CD	20:n:229:PRO:HA	2.44	0.43
19:m:1399:SER:HA	19:m:1407:HIS:CE1	2.54	0.43
1:A:252:ALA:HA	1:A:258:GLN:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LEU:HD21	2:B:835:GLN:HB2	2.00	0.43
1:A:815:PHE:O	1:A:819:MET:HG3	2.19	0.43
9:I:40:ASP:OD1	9:I:40:ASP:N	2.44	0.43
19:m:1002:ARG:HH11	19:m:1052:TYR:HH	1.66	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
24:v:202:PRO:HG2	24:v:382:TYR:OH	2.19	0.43
1:A:38:PRO:HA	1:A:271:LEU:HD23	2.01	0.42
2:B:763:GLN:HG2	2:B:765:PRO:HD2	2.01	0.42
8:H:8:ASP:OD1	8:H:9:ILE:N	2.48	0.42
9:I:29:CYS:HB3	9:I:32:CYS:SG	2.59	0.42
17:V:12:CYS:HA	17:V:50:THR:HA	2.01	0.42
20:n:208:LEU:HD22	20:n:250:HIS:CD2	2.54	0.42
1:A:421:ARG:HB3	1:A:424:ASP:HB2	2.01	0.42
2:B:85:SER:OG	2:B:114:PRO:HD2	2.20	0.42
2:B:237:LYS:HA	2:B:237:LYS:HD3	1.91	0.42
2:B:592:THR:HG23	23:u:226:PHE:CZ	2.54	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
21:q:53:LEU:O	21:q:57:GLU:HG2	2.18	0.42
24:v:41:LYS:HB3	24:v:45:LYS:HE3	2.01	0.42
24:v:307:PHE:HE1	24:v:335:GLY:HA3	1.83	0.42
25:x:222:MET:HE3	25:x:222:MET:HB3	1.84	0.42
1:A:1221:VAL:HG21	1:A:1274:ILE:HD12	2.00	0.42
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.51	0.42
19:m:750:ALA:HB2	19:m:1139:ARG:HB2	2.01	0.42
19:m:773:GLY:N	19:m:777:ASP:OD2	2.52	0.42
20:n:195:LYS:HE3	20:n:199:LEU:HD11	2.01	0.42
21:q:611:GLU:HG2	21:q:615:HIS:CD2	2.54	0.42
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.90	0.42
1:A:1201:ARG:HA	1:A:1238:LEU:HD12	2.01	0.42
2:B:250:TYR:HE2	2:B:262:LYS:HB2	1.82	0.42
2:B:557:GLU:HA	2:B:558:PRO:HD3	1.90	0.42
14:N:-48:DC:H2''	14:N:-47:DC:C6	2.50	0.42
17:V:42:ASP:OD1	17:V:42:ASP:N	2.53	0.42
21:q:189:LEU:HB3	21:q:194:LYS:HB2	2.01	0.42
1:A:504:GLN:OE1	6:F:90:ARG:NH1	2.38	0.42
2:B:330:GLY:HA3	2:B:344:TYR:HE2	1.84	0.42
16:T:9:DG:C1'	16:T:10:DC:C5	3.01	0.42
1:A:914:ILE:HG13	1:A:917:ALA:HB2	2.01	0.42
2:B:733:SER:HB3	2:B:736:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:176:ARG:HD3	5:E:214:LEU:HD11	2.02	0.42
21:q:638:ALA:HB1	21:q:642:ARG:HH22	1.84	0.42
18:W:543:ILE:HD11	18:W:581:ILE:HG13	2.01	0.42
21:q:830:LEU:HD22	21:q:846:LEU:HB3	2.02	0.42
22:r:208:ARG:HA	22:r:211:MET:HE3	2.02	0.42
22:r:370:GLU:HG3	23:u:251:VAL:HA	2.01	0.42
25:x:345:GLN:O	25:x:349:GLN:HG3	2.20	0.42
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.91	0.42
3:C:36:MET:HE3	3:C:176:ILE:HD13	2.01	0.42
7:G:165:GLU:H	7:G:168:LEU:HD12	1.85	0.42
18:W:349:GLU:HA	18:W:431:ARG:HA	2.02	0.42
19:m:743:PHE:O	19:m:747:ILE:HG12	2.20	0.42
19:m:960:ASP:HB2	19:m:1024:TYR:CZ	2.54	0.42
20:n:161:GLN:O	20:n:165:LEU:HG	2.19	0.42
22:r:275:ALA:HB2	22:r:281:GLU:HA	2.01	0.42
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.91	0.42
1:A:691:VAL:HG11	1:A:795:PRO:HG3	2.02	0.42
2:B:283:VAL:HG13	2:B:283:VAL:O	2.18	0.42
2:B:293:ILE:HD13	2:B:375:VAL:HG11	2.02	0.42
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.85	0.42
4:D:106:LEU:HD23	4:D:106:LEU:HA	1.89	0.42
5:E:42:ARG:HG3	5:E:46:CYS:SG	2.60	0.42
9:I:29:CYS:SG	9:I:30:ARG:N	2.92	0.42
17:V:13:MET:HE2	17:V:51:SER:HB2	2.01	0.42
18:W:539:HIS:HB2	18:W:584:THR:HA	2.02	0.42
19:m:955:ASN:ND2	19:m:978:CYS:HB3	2.35	0.42
19:m:1255:TRP:HD1	19:m:1257:ILE:HG12	1.85	0.42
21:q:29:PRO:HA	21:q:36:VAL:HG12	2.02	0.42
1:A:1218:ILE:HG12	1:A:1270:MET:HE1	2.02	0.42
18:W:422:TYR:HB3	18:W:427:TYR:CE1	2.55	0.42
19:m:656:TYR:CE2	19:m:660:ILE:HD11	2.54	0.42
19:m:708:TRP:CZ2	19:m:712:LEU:HD21	2.54	0.42
19:m:821:ASP:HA	19:m:850:ILE:HD13	2.01	0.42
1:A:390:THR:O	1:A:394:ARG:HG2	2.20	0.41
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.88	0.41
1:A:1041:ARG:O	1:A:1044:PHE:N	2.50	0.41
2:B:279:ARG:NH1	2:B:316:ILE:O	2.52	0.41
2:B:479:TYR:CE2	2:B:778:MET:HG2	2.55	0.41
19:m:709:LYS:HA	19:m:712:LEU:HD12	2.02	0.41
19:m:1000:VAL:HB	19:m:1004:HIS:ND1	2.35	0.41
2:B:606:VAL:HG22	2:B:621:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:837:ASP:CG	2:B:1020:ARG:HH22	2.28	0.41
19:m:597:LEU:HD13	19:m:708:TRP:HE3	1.84	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
24:v:352:VAL:O	24:v:355:THR:OG1	2.38	0.41
16:T:37:DC:H2'	16:T:38:DA:C8	2.56	0.41
19:m:423:ASP:O	19:m:427:ILE:HG23	2.20	0.41
19:m:674:LEU:HD12	19:m:675:PRO:HD2	2.02	0.41
19:m:1246:LEU:HB3	19:m:1248:VAL:HG23	2.01	0.41
21:q:189:LEU:HD13	21:q:197:GLN:HB2	2.02	0.41
21:q:562:TYR:CZ	21:q:566:LEU:HD11	2.55	0.41
22:r:211:MET:HB3	22:r:286:LEU:HD23	2.03	0.41
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.02	0.41
2:B:1153:GLU:OE1	2:B:1153:GLU:N	2.53	0.41
2:B:1174:ASN:OD1	2:B:1177:LYS:HB2	2.21	0.41
19:m:397:ASN:HB3	19:m:401:ASN:HA	2.02	0.41
19:m:586:TYR:CE2	19:m:703:LEU:HD12	2.56	0.41
1:A:883:THR:HA	1:A:954:HIS:O	2.20	0.41
1:A:1343:GLY:HA2	5:E:182:PRO:HD2	2.01	0.41
3:C:135:ARG:NE	3:C:136:ASP:OD2	2.50	0.41
6:F:99:LEU:HG	6:F:103:MET:HE2	2.02	0.41
11:K:25:SER:O	25:x:307:GLN:NE2	2.53	0.41
19:m:313:TYR:HB3	19:m:422:LEU:HD11	2.03	0.41
19:m:1136:ARG:HD2	19:m:1137:GLU:O	2.21	0.41
20:n:177:ASN:HD21	20:n:186:PHE:HE2	1.67	0.41
21:q:66:SER:O	21:q:70:VAL:HG23	2.20	0.41
23:u:168:SER:HB2	24:v:200:PHE:HB3	2.02	0.41
1:A:231:ARG:HB3	1:A:234:TRP:CD2	2.56	0.41
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.02	0.41
5:E:3:ASP:HA	5:E:6:ARG:HG2	2.01	0.41
8:H:6:PHE:HB3	8:H:59:LEU:HB2	2.03	0.41
13:M:39:ASP:HB3	13:M:44:ILE:HG13	2.03	0.41
15:P:2:U:H3	16:T:41:DA:H61	1.68	0.41
18:W:329:LYS:HB2	18:W:434:ASN:HA	2.02	0.41
19:m:1358:ASP:OD1	19:m:1361:GLU:N	2.33	0.41
23:u:121:PHE:CE2	23:u:123:PRO:HG3	2.56	0.41
1:A:152:ALA:HA	1:A:153:PRO:HD3	1.90	0.41
1:A:985:ILE:N	1:A:986:PRO:HD2	2.36	0.41
1:A:1210:THR:HG22	1:A:1212:ASN:H	1.86	0.41
1:A:1314:ILE:HB	1:A:1337:GLU:OE1	2.21	0.41
2:B:575:VAL:O	2:B:578:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:248:ILE:HG21	11:K:102:ASP:HB2	2.01	0.41
11:K:55:ASP:OD2	11:K:89:ARG:NH2	2.54	0.41
18:W:598:LEU:HD12	18:W:599:HIS:H	1.86	0.41
21:q:410:GLY:HA2	21:q:423:ALA:HA	2.03	0.41
21:q:824:ASN:CG	21:q:858:ARG:HH21	2.29	0.41
1:A:1150:SER:OG	1:A:1198:GLU:O	2.32	0.41
2:B:262:LYS:HB3	2:B:271:ASP:HB3	2.01	0.41
3:C:135:ARG:HE	3:C:136:ASP:CG	2.28	0.41
19:m:283:VAL:HG12	19:m:284:PHE:CD1	2.56	0.41
21:q:350:VAL:HA	21:q:380:ARG:NH1	2.36	0.41
1:A:908:SER:OG	1:A:909:ILE:N	2.54	0.41
2:B:71:ILE:HG12	2:B:127:ILE:HG22	2.02	0.41
5:E:36:GLN:HE21	5:E:36:GLN:HB3	1.69	0.41
11:K:47:ARG:HD3	11:K:61:TYR:HD1	1.86	0.41
12:L:29:VAL:HG23	12:L:31:TYR:CE2	2.56	0.41
14:N:-28:DC:H2'	14:N:-27:DC:C6	2.56	0.41
16:T:24:DA:H2''	16:T:25:DG:H8	1.86	0.41
18:W:480:PRO:HA	18:W:498:VAL:HG12	2.02	0.41
18:W:540:VAL:HG11	18:W:554:ILE:HD11	2.01	0.41
18:W:614:ARG:NH2	18:W:616:GLN:HE21	2.19	0.41
19:m:314:ARG:HD3	19:m:320:TYR:CE1	2.56	0.41
19:m:387:HIS:NE2	19:m:1021:SER:OG	2.43	0.41
21:q:278:ARG:NH2	22:r:507:ASP:O	2.53	0.41
21:q:756:TRP:HB3	21:q:772:ALA:HB2	2.03	0.41
25:x:153:ASN:OD1	25:x:153:ASN:N	2.54	0.41
1:A:636:ARG:HG3	1:A:880:GLU:OE2	2.21	0.41
1:A:664:SER:OG	1:A:665:ILE:N	2.55	0.41
2:B:439:LEU:HD11	23:u:264:LEU:HB3	2.03	0.41
4:D:53:LEU:HD13	4:D:147:SER:HB3	2.02	0.41
11:K:11:ILE:HD13	11:K:11:ILE:HA	1.89	0.41
19:m:588:ALA:HA	19:m:591:GLN:HG2	2.03	0.41
19:m:1002:ARG:NH2	19:m:1023:VAL:O	2.47	0.41
21:q:687:PHE:O	21:q:691:GLU:N	2.54	0.41
24:v:205:SER:O	24:v:379:ARG:NH2	2.49	0.41
1:A:473:LEU:CD2	2:B:835:GLN:HB2	2.50	0.40
2:B:807:GLN:OE1	24:v:129:ARG:NH1	2.51	0.40
7:G:126:SER:HA	7:G:127:PRO:HA	1.94	0.40
14:N:-54:DC:H2''	14:N:-53:DT:C7	2.47	0.40
18:W:492:ASN:OD1	18:W:493:HIS:N	2.54	0.40
20:n:241:ILE:HG23	20:n:246:ILE:HD12	2.04	0.40
1:A:493:PRO:HG3	1:A:502:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ARG:NH2	22:r:369:GLU:OE1	2.54	0.40
2:B:425:MET:O	2:B:429:ILE:HG13	2.21	0.40
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.55	0.40
12:L:66:MET:HE1	18:W:804:TRP:HZ2	1.86	0.40
16:T:23:DA:H1'	16:T:24:DA:H5'	2.04	0.40
18:W:524:GLU:HB2	20:n:232:GLN:HE22	1.85	0.40
21:q:232:LEU:HD23	21:q:232:LEU:HA	1.98	0.40
21:q:341:ARG:NH2	24:v:50:LEU:HB2	2.36	0.40
22:r:432:LEU:HD11	22:r:433:ARG:NH1	2.36	0.40
1:A:498:THR:CG2	2:B:1146:PHE:HD1	2.34	0.40
1:A:1295:PRO:HD3	1:A:1301:TYR:CE1	2.55	0.40
2:B:285:PRO:HB2	9:I:11:ASN:HD22	1.86	0.40
3:C:259:LEU:HD13	11:K:91:CYS:HB2	2.03	0.40
8:H:76:LYS:HE3	8:H:76:LYS:HB3	1.93	0.40
19:m:827:GLY:HA3	19:m:832:THR:OG1	2.21	0.40
19:m:1141:ASP:OD1	19:m:1141:ASP:N	2.52	0.40
19:m:1268:ILE:O	19:m:1272:ARG:HG3	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:432:LEU:HD12	22:r:433:ARG:HD2	2.02	0.40
2:B:33:GLN:HG2	2:B:34:GLN:N	2.36	0.40
7:G:95:SER:OG	7:G:98:GLY:O	2.22	0.40
12:L:33:CYS:SG	12:L:34:GLY:N	2.95	0.40
14:N:-22:DG:N2	16:T:23:DA:C2	2.90	0.40
17:V:29:CYS:HB2	17:V:38:LEU:HD12	2.03	0.40
19:m:421:ASP:OD1	19:m:421:ASP:C	2.64	0.40
19:m:474:TYR:HB3	19:m:477:GLN:HB2	2.04	0.40
21:q:341:ARG:NH2	24:v:47:SER:O	2.54	0.40
21:q:609:ASP:O	21:q:613:GLN:HG3	2.20	0.40
21:q:789:ARG:O	21:q:793:VAL:HG23	2.21	0.40
19:m:606:THR:HG21	19:m:684:PHE:HZ	1.87	0.40
19:m:900:LEU:HD12	19:m:900:LEU:HA	1.95	0.40
21:q:311:TYR:HB3	21:q:342:VAL:HG13	2.04	0.40
23:u:142:ASP:HA	23:u:145:ILE:HG22	2.04	0.40
24:v:262:LYS:HD3	24:v:305:GLN:NE2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	78
2	B	1154/1227 (94%)	1118 (97%)	36 (3%)	0	100	100
3	C	261/304 (86%)	259 (99%)	2 (1%)	0	100	100
4	D	170/186 (91%)	166 (98%)	4 (2%)	0	100	100
5	E	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	167 (99%)	2 (1%)	0	100	100
8	H	129/145 (89%)	125 (97%)	4 (3%)	0	100	100
9	I	109/115 (95%)	106 (97%)	3 (3%)	0	100	100
10	J	65/72 (90%)	65 (100%)	0	0	100	100
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
12	L	43/72 (60%)	41 (95%)	2 (5%)	0	100	100
13	M	62/113 (55%)	62 (100%)	0	0	100	100
17	V	104/108 (96%)	100 (96%)	4 (4%)	0	100	100
18	W	527/911 (58%)	508 (96%)	19 (4%)	0	100	100
19	m	1179/1503 (78%)	1157 (98%)	22 (2%)	0	100	100
20	n	137/417 (33%)	136 (99%)	1 (1%)	0	100	100
21	q	928/1084 (86%)	922 (99%)	6 (1%)	0	100	100
22	r	260/544 (48%)	254 (98%)	6 (2%)	0	100	100
23	u	206/459 (45%)	204 (99%)	2 (1%)	0	100	100
24	v	341/396 (86%)	327 (96%)	14 (4%)	0	100	100
25	x	201/395 (51%)	200 (100%)	1 (0%)	0	100	100
All	All	7841/10452 (75%)	7666 (98%)	174 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	960	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1219/1528 (80%)	1219 (100%)	0	100	100
2	B	1018/1077 (94%)	1018 (100%)	0	100	100
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	149/160 (93%)	149 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	61/66 (92%)	61 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	38 (100%)	0	100	100
13	M	61/99 (62%)	61 (100%)	0	100	100
17	V	90/92 (98%)	90 (100%)	0	100	100
18	W	480/796 (60%)	480 (100%)	0	100	100
19	m	1087/1354 (80%)	1087 (100%)	0	100	100
20	n	125/361 (35%)	125 (100%)	0	100	100
21	q	824/962 (86%)	824 (100%)	0	100	100
22	r	239/485 (49%)	239 (100%)	0	100	100
23	u	192/406 (47%)	192 (100%)	0	100	100
24	v	325/369 (88%)	325 (100%)	0	100	100
25	x	190/354 (54%)	190 (100%)	0	100	100
All	All	7083/9259 (76%)	7083 (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 (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	265	HIS
1	A	291	ASN
1	A	295	GLN
1	A	364	GLN
1	A	491	HIS
1	A	1056	GLN
2	B	215	GLN
2	B	317	GLN
2	B	350	GLN
2	B	388	GLN
2	B	438	ASN
2	B	458	ASN
2	B	736	HIS
2	B	1074	ASN
3	C	11	ASN
3	C	13	GLN
3	C	25	ASN
3	C	150	HIS
4	D	38	GLN
4	D	130	ASN
4	D	170	ASN
5	E	31	GLN
5	E	36	GLN
7	G	24	GLN
8	H	44	ASN
9	I	11	ASN
10	J	52	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	553	HIS
19	m	554	GLN
19	m	896	ASN
19	m	1116	HIS

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Mol	Chain	Res	Type
19	m	1288	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	187	GLN
21	q	353	GLN
21	q	397	ASN
21	q	398	GLN
21	q	438	ASN
21	q	615	HIS
21	q	625	HIS
21	q	658	GLN
21	q	715	ASN
21	q	781	GLN
22	r	336	ASN
22	r	416	ASN
22	r	493	ASN
23	u	138	GLN
24	v	229	ASN
24	v	283	ASN
24	v	381	GLN
25	x	251	GLN
25	x	296	ASN

5.3.3 RNA ⓘ

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

All (7) RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
15	P	1	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	-7	U
15	P	-3	U
15	P	-2	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

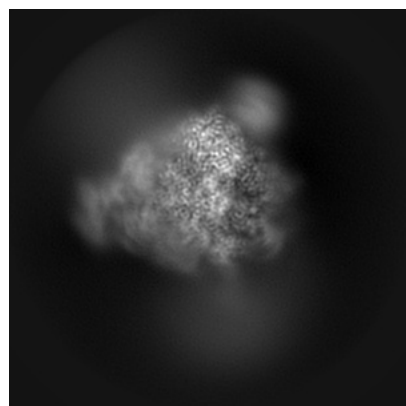
6 Map visualisation [i](#)

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

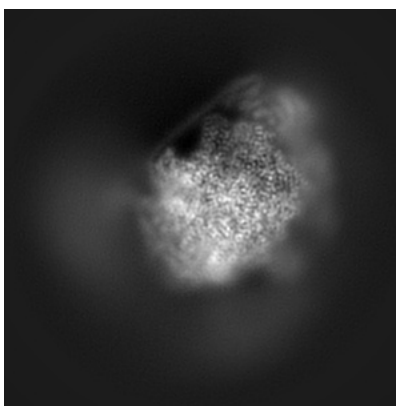
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

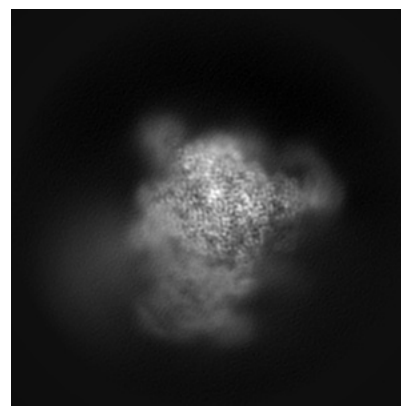
6.1.1 Primary map



X

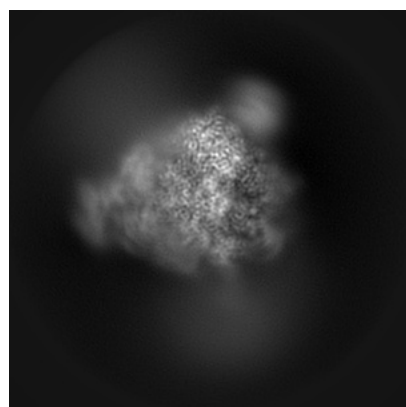


Y

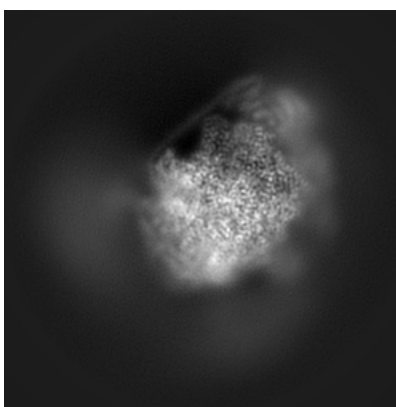


Z

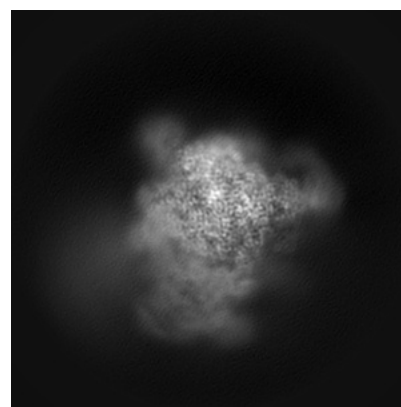
6.1.2 Raw map



X



Y

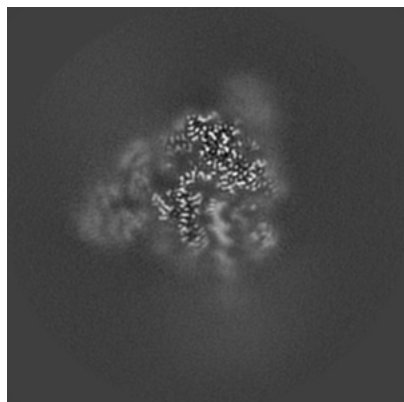


Z

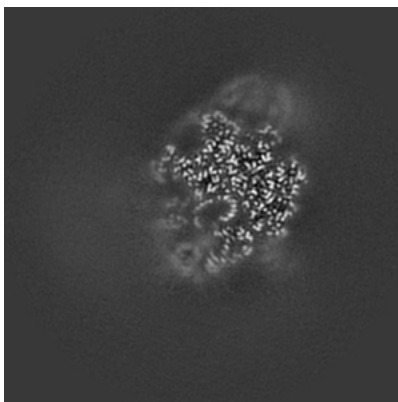
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

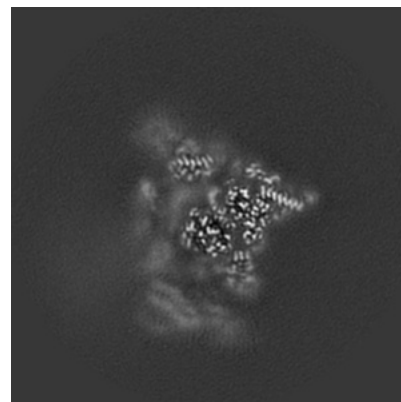
6.2.1 Primary map



X Index: 120

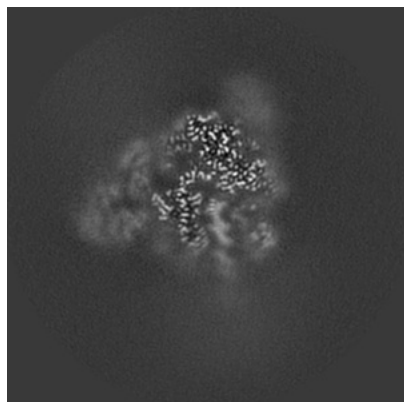


Y Index: 120

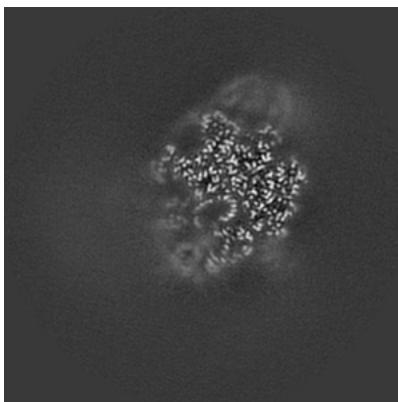


Z Index: 120

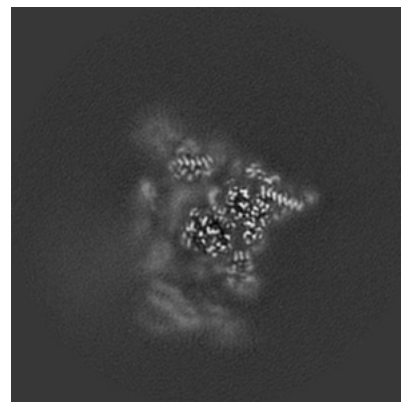
6.2.2 Raw map



X Index: 120



Y Index: 120

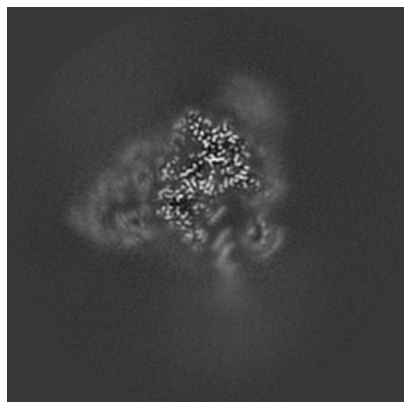


Z Index: 120

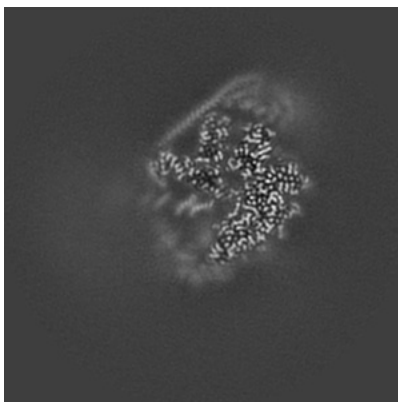
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

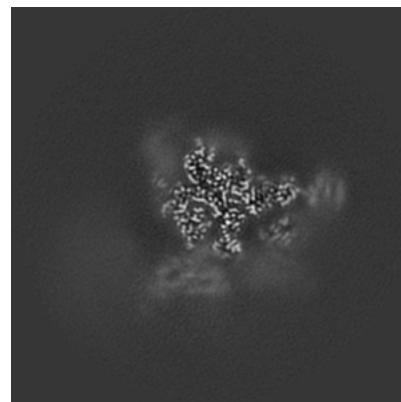
6.3.1 Primary map



X Index: 125

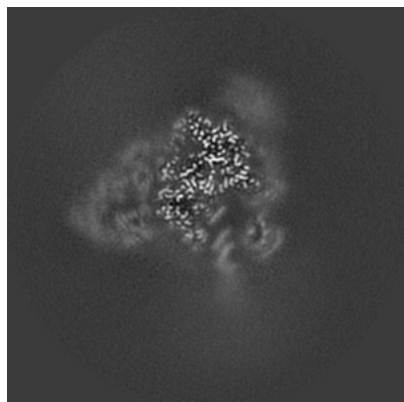


Y Index: 124

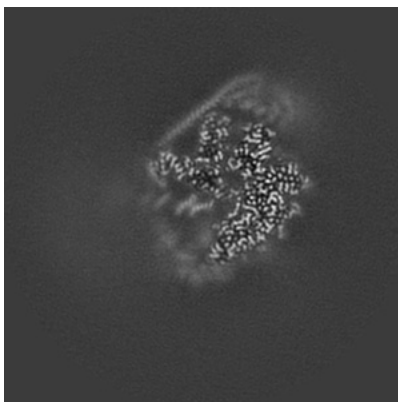


Z Index: 146

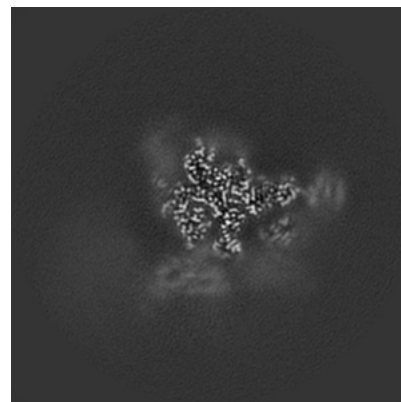
6.3.2 Raw map



X Index: 125



Y Index: 124

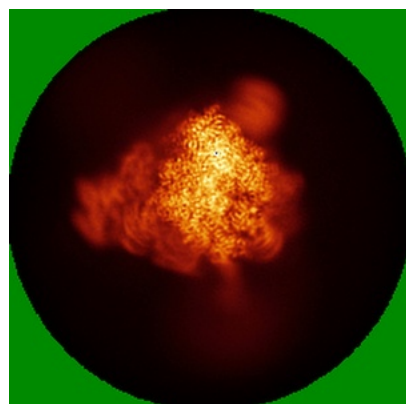


Z Index: 146

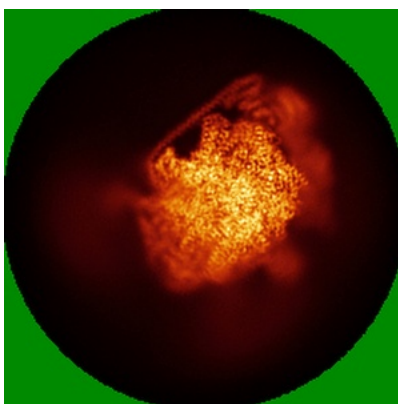
The images above show the largest variance slices of the map in three orthogonal directions.

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

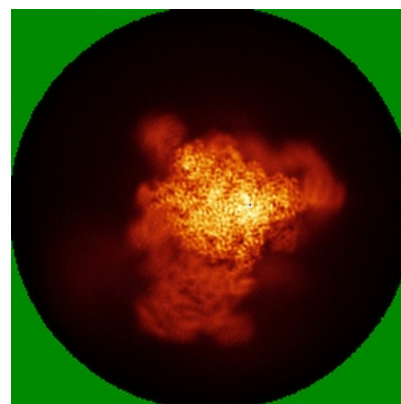
6.4.1 Primary map



X

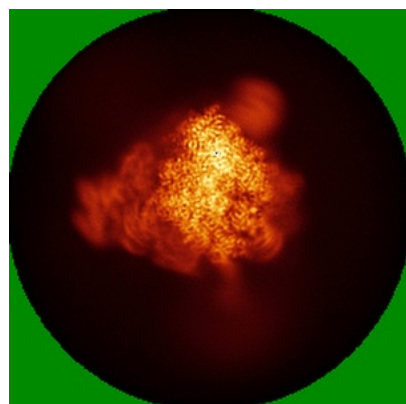


Y

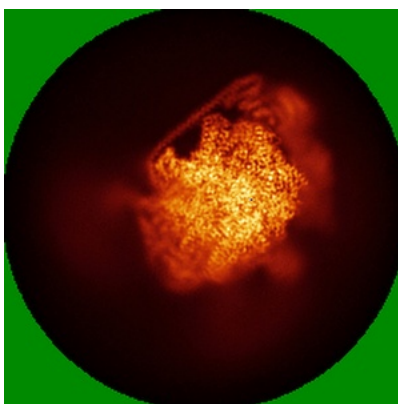


Z

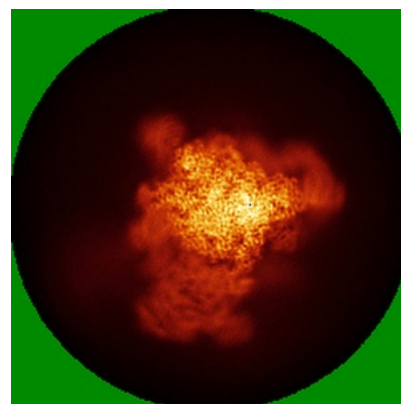
6.4.2 Raw map



X



Y

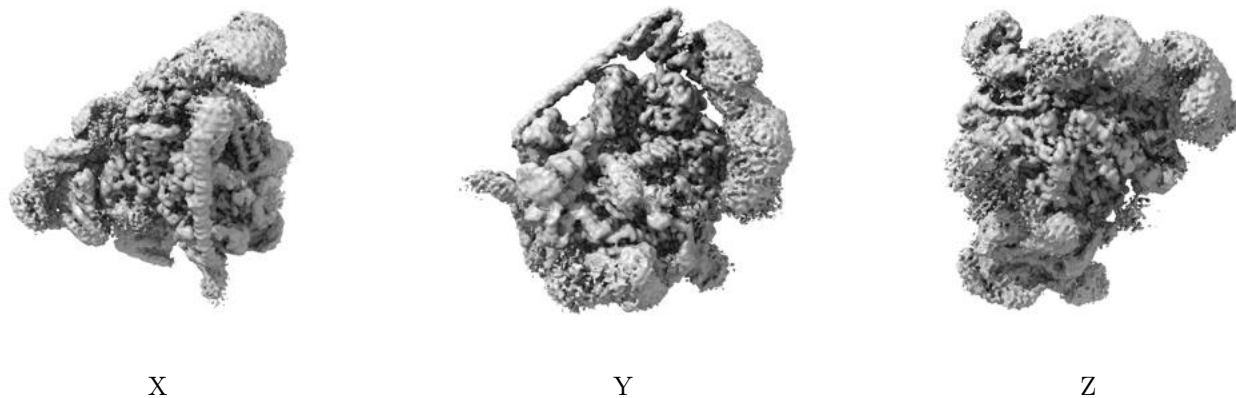


Z

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

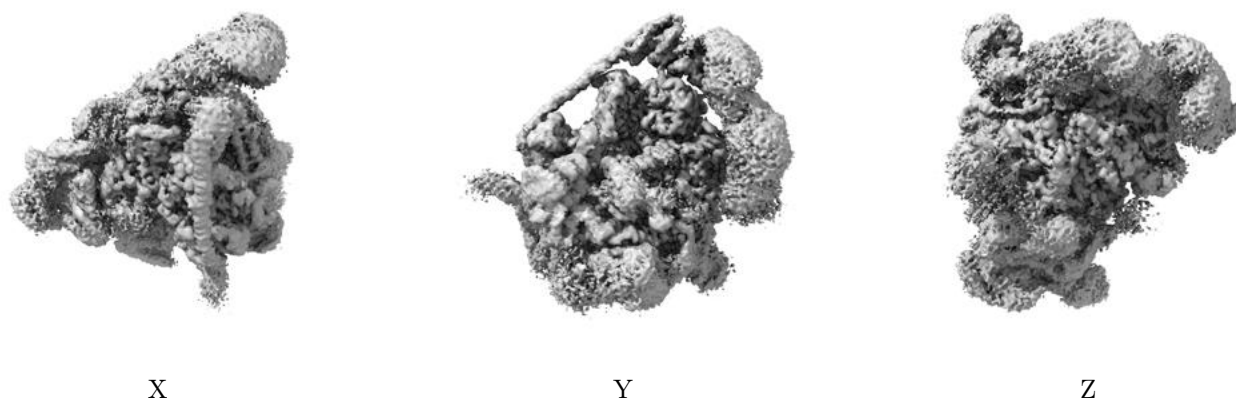
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

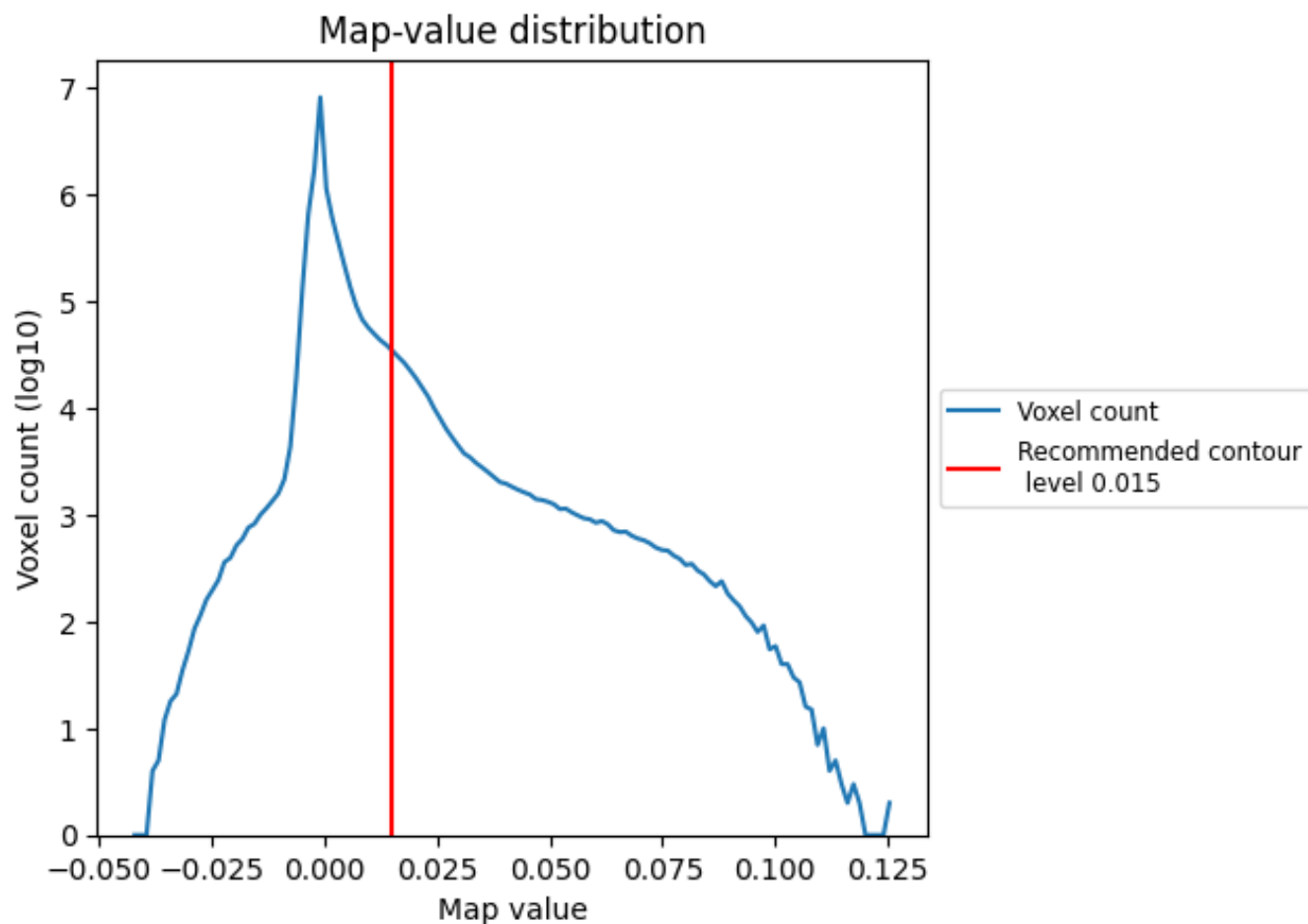
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

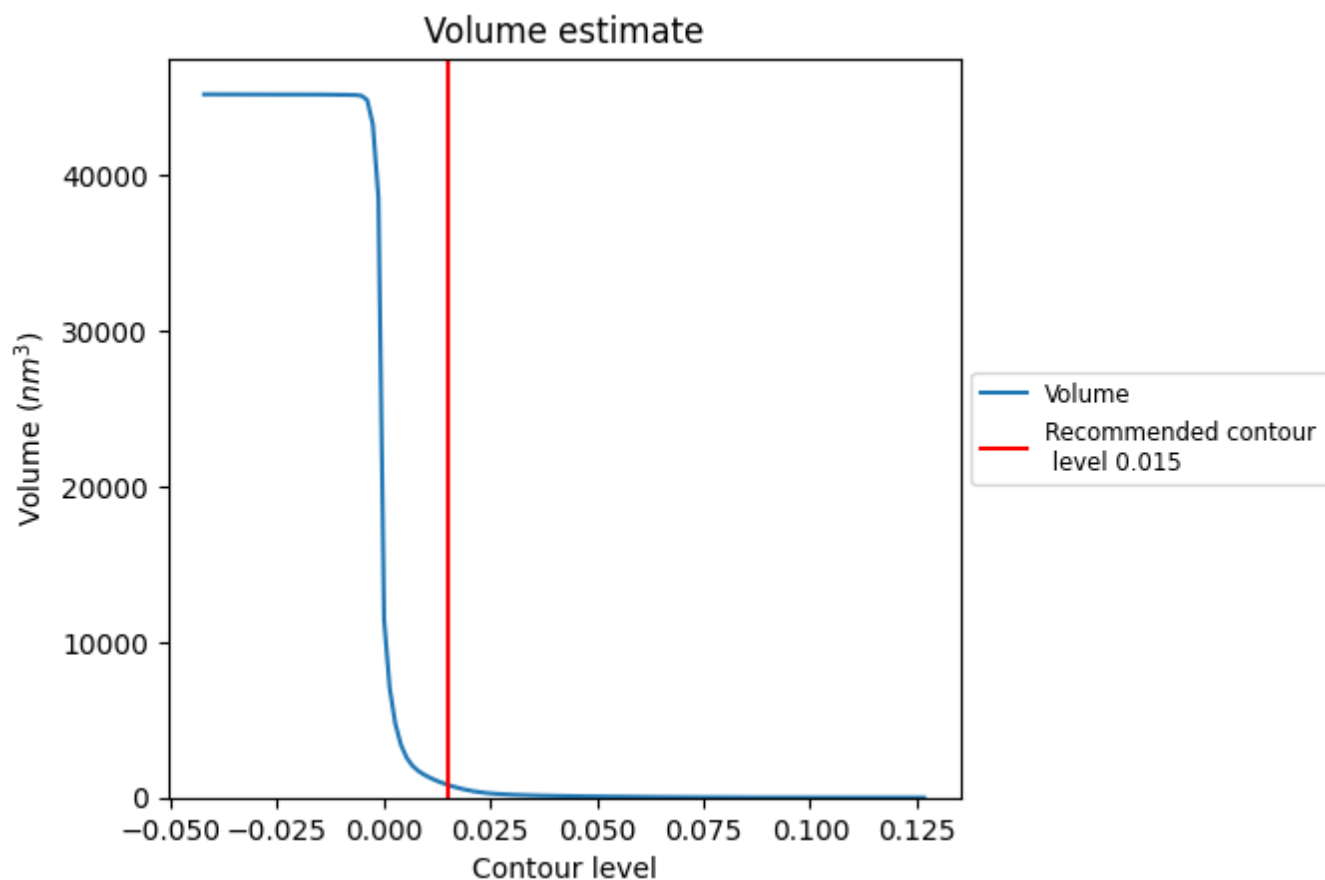
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

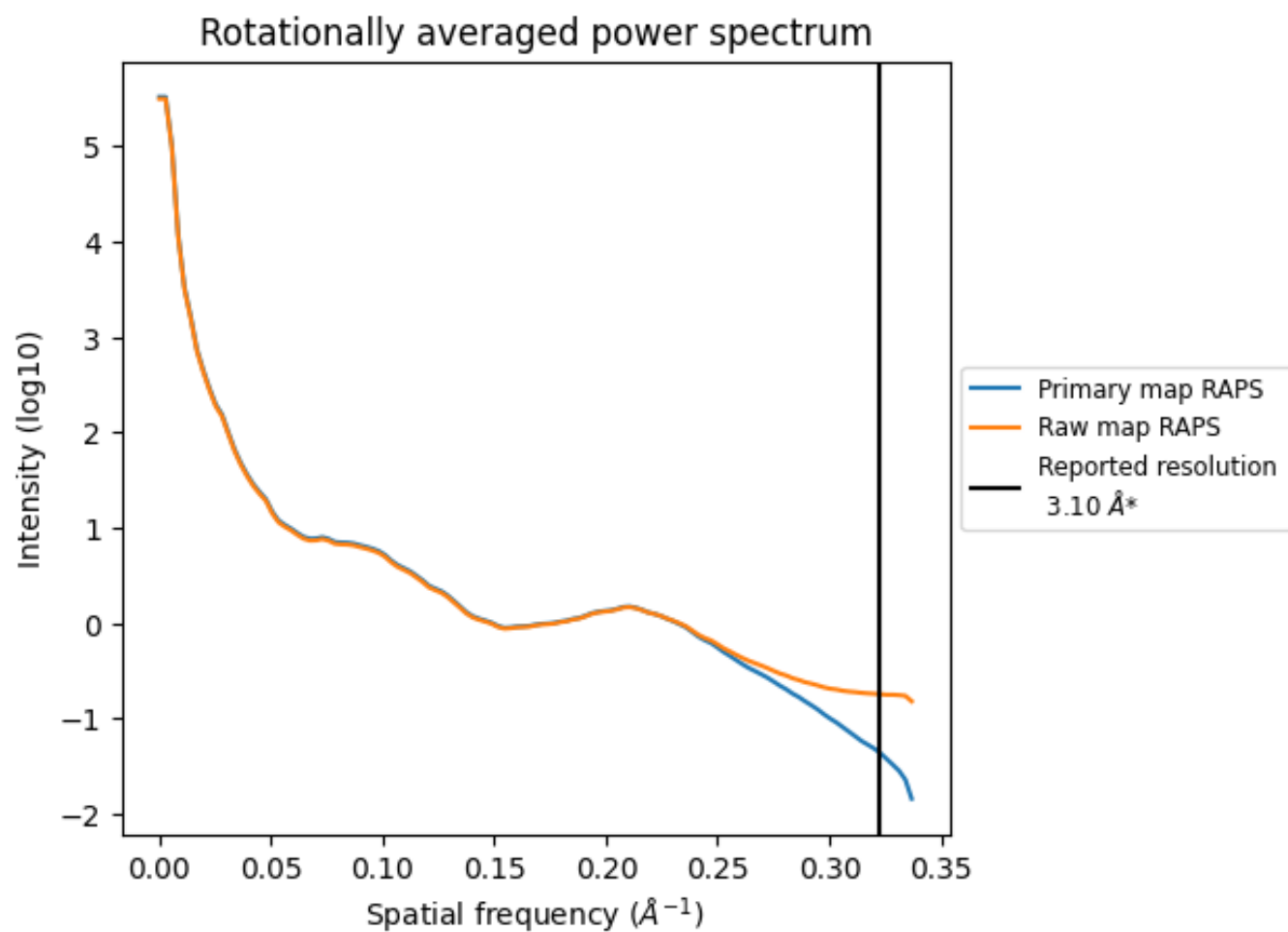
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 824 nm^3 ; this corresponds to an approximate mass of 744 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

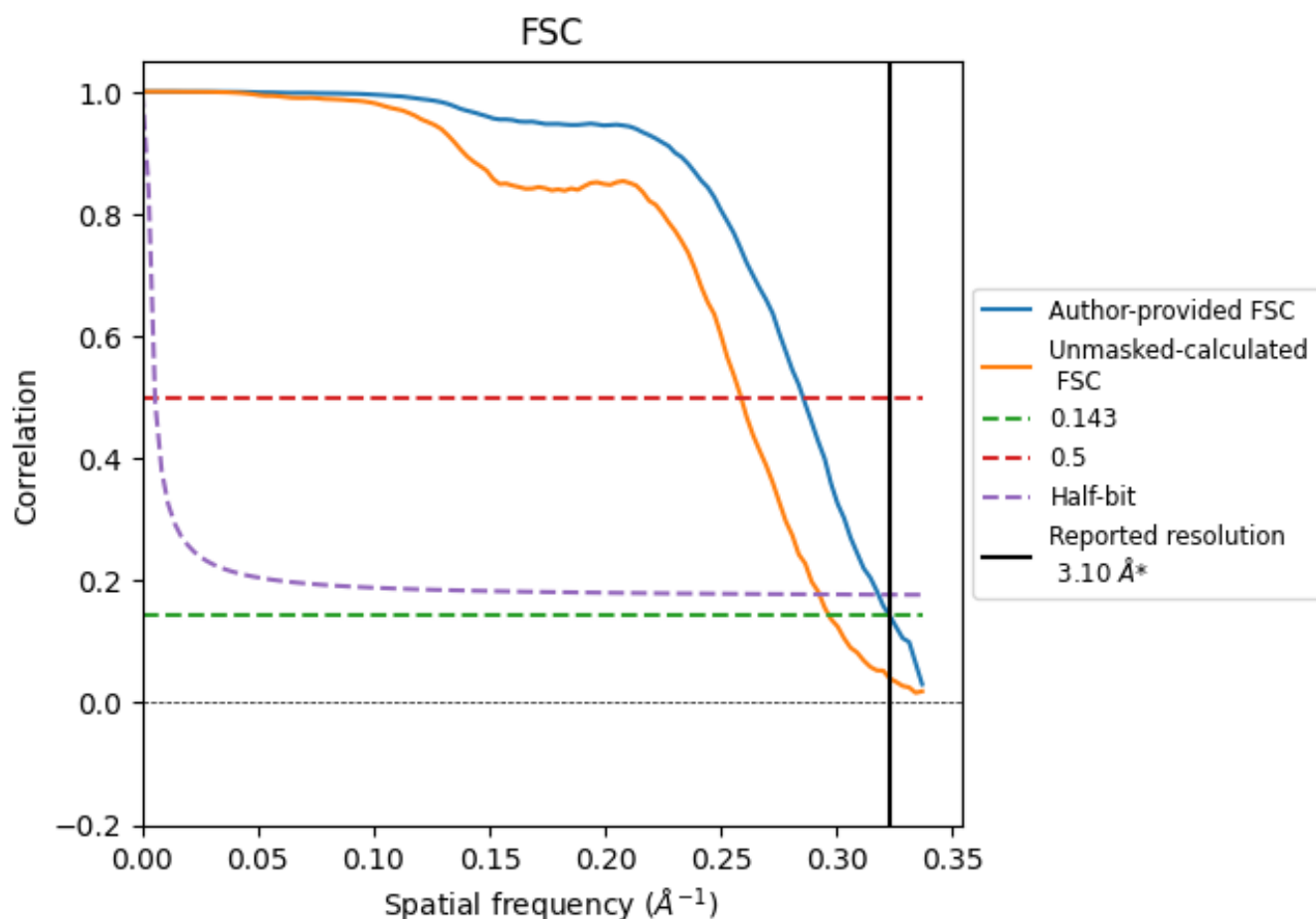


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

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

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

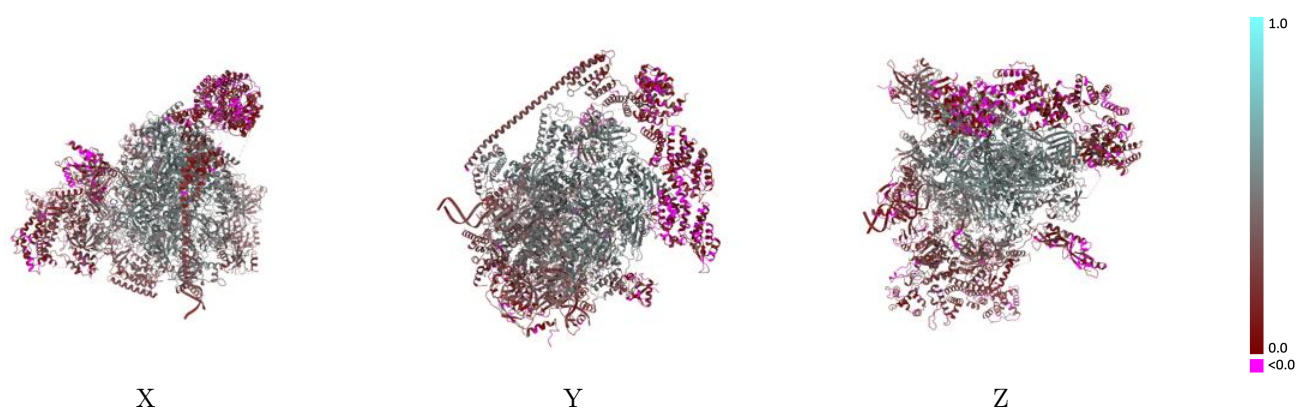
9 Map-model fit [i](#)

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

9.1 Map-model overlay [i](#)

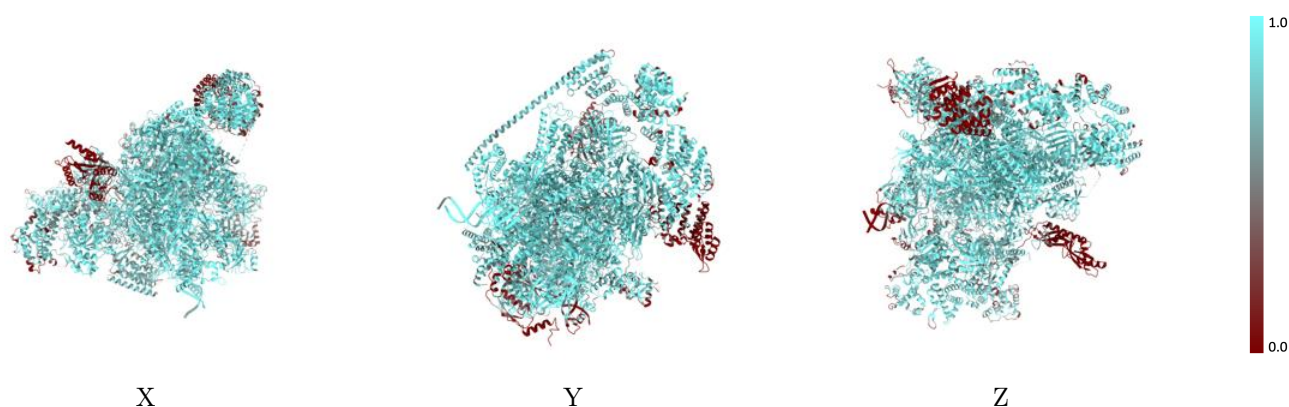
This section was not generated.

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



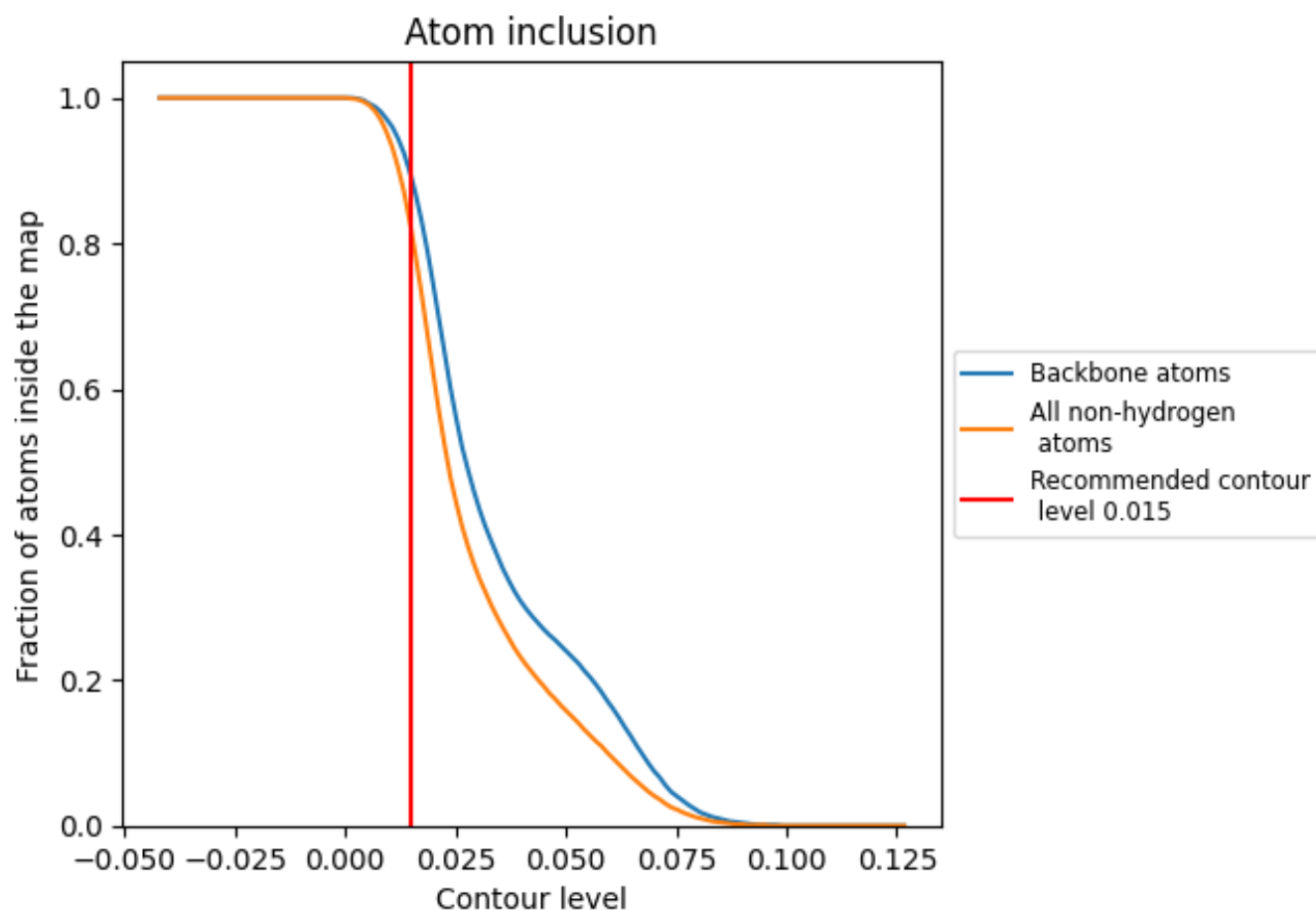
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

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

