



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 03:29 PM JST

PDB ID : 5XON
EMDB ID : EMD-6747
Title : RNA Polymerase II elongation complex bound with Spt4/5 and TFIIS
Authors : Ehara, H.; Yokoyama, T.; Shigematsu, H.; Shirouzu, M.; Sekine, S.
Deposited on : 2017-05-29
Resolution : 3.83 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

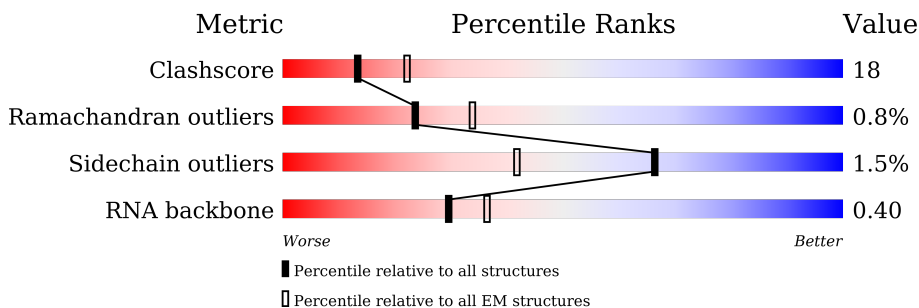
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.83 Å.

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







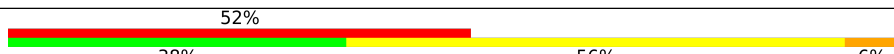


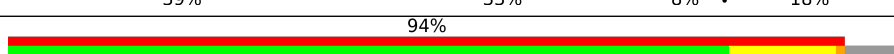

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

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

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Mol	Chain	Length	Quality of chain
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	P	30	
14	T	48	
15	N	48	
16	U	190	
17	V	108	
18	W	612	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 38369 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	1427	Total	C	N	O	S	0	0
			11239	7089	1958	2122	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1161	Total	C	N	O	S	0	0
			9261	5835	1636	1732	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	168	Total	C	N	O	S	0	0
			1314	812	237	263	2		

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1740	1094	312	324	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
			1324	858	214	247	5		

- Molecule 8 is a protein called RNA polymerase subunit ABC14.5, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	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		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	MET	-	see sequence details	UNP C4QY79
I	2	ALA	-	see sequence details	UNP C4QY79
I	3	SER	MET	see sequence details	UNP C4QY79
I	4	PHE	THR	see sequence details	UNP C4QY79
I	5	ARG	ASN	see sequence details	UNP C4QY79
I	6	PHE	VAL	see sequence details	UNP C4QY79
I	7	CYS	ASN	see sequence details	UNP C4QY79
I	8	LEU	SER	see sequence details	UNP C4QY79
I	9	GLU	LEU	see sequence details	UNP C4QY79
I	10	CYS	SER	see sequence details	UNP C4QY79

- 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	66	Total	C	N	O	S	0	0
			545	349	95	95	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, found in RNA polymerase complexes I, II, and III.

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

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	67	ILE	SER	see sequence details	UNP C4QWA8
L	68	GLN	LYS	see sequence details	UNP C4QWA8
L	70	ASP	LEU	see sequence details	UNP C4QWA8
L	71	ALA	THR	see sequence details	UNP C4QWA8
L	72	ARG	THR	see sequence details	UNP C4QWA8

- Molecule 13 is a RNA chain called RNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	16	Total	C	N	O	P	0	0
			338	151	55	116	16		

- Molecule 14 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	48	Total	C	N	O	P	0	0
			975	463	179	285	48		

- Molecule 15 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	43	Total	C	N	O	P	0	0
			889	422	163	261	43		

- Molecule 16 is a protein called General transcription elongation factor TFIIS.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	155	Total	C	N	O	S	0	0
			1239	774	223	232	10		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	96	GLY	-	expression tag	UNP C4R2R6
U	97	PRO	-	expression tag	UNP C4R2R6
U	98	GLY	-	expression tag	UNP C4R2R6
U	266	ALA	ASP	conflict	UNP C4R2R6
U	267	ALA	GLU	conflict	UNP C4R2R6

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	102	Total	C	N	O	S	0	0
			792	492	143	150	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	7	MET	-	expression tag	UNP C4R0E6

- Molecule 18 is a protein called Protein that forms a complex with Spt4p.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	329	Total	C	N	O	S	0	0
			2667	1698	483	485	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	204	GLY	-	expression tag	UNP C4R370
W	205	PRO	-	expression tag	UNP C4R370

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total	Zn	0
			2	2	
19	B	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
19	C	1	Total 1	Zn 1	0
19	I	2	Total 2	Zn 2	0
19	J	1	Total 1	Zn 1	0
19	L	1	Total 1	Zn 1	0
19	U	1	Total 1	Zn 1	0
19	V	1	Total 1	Zn 1	0

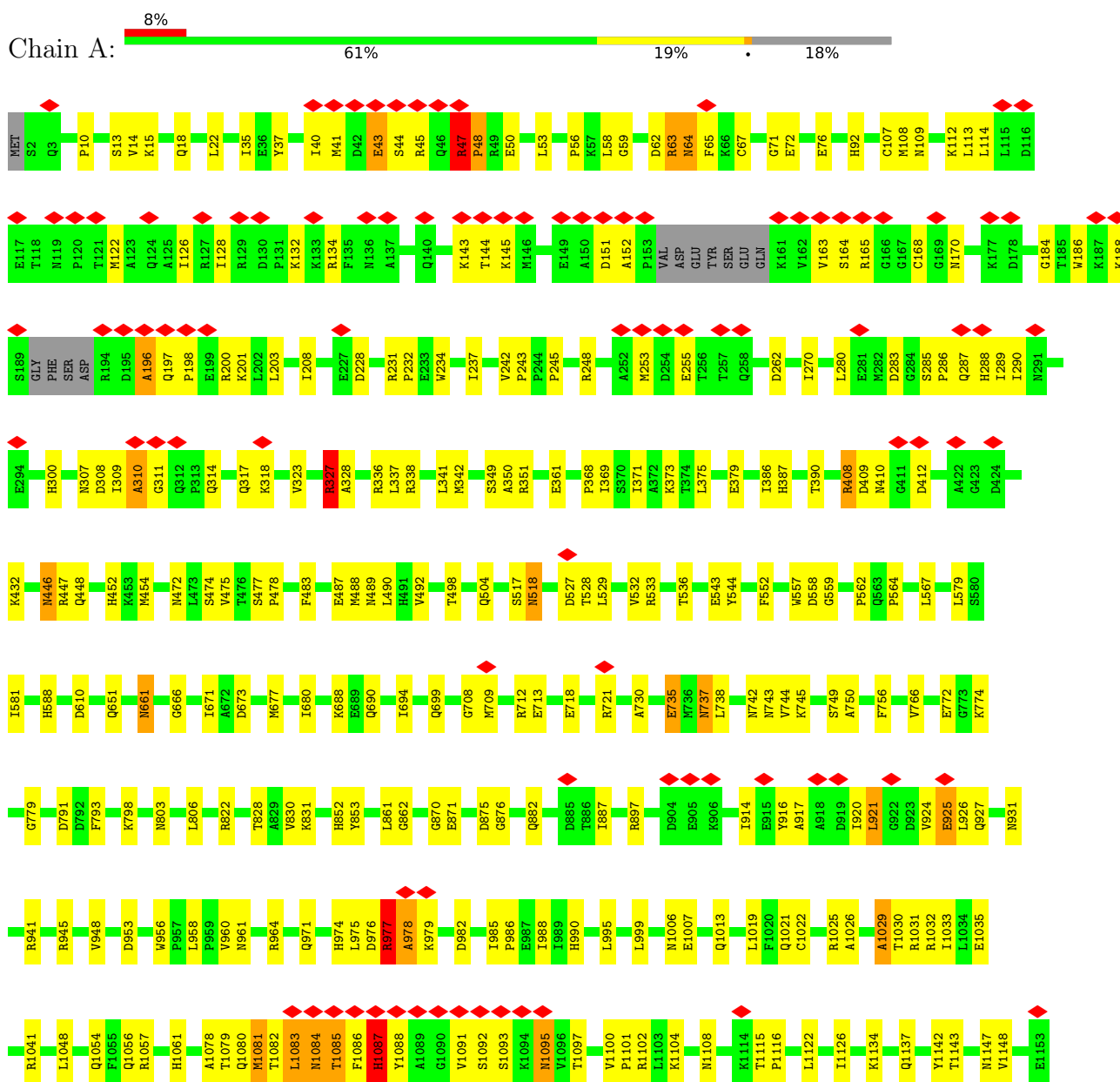
- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

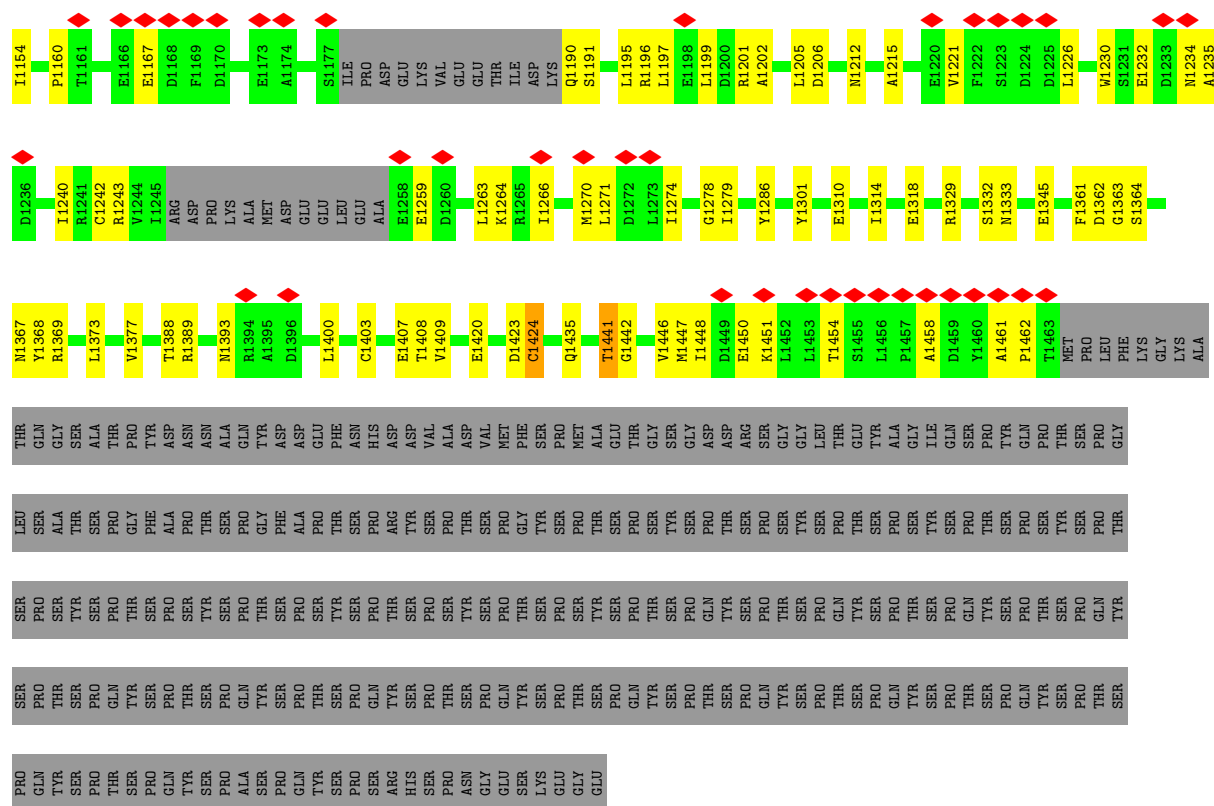
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total 1	Mg 1	0

3 Residue-property plots

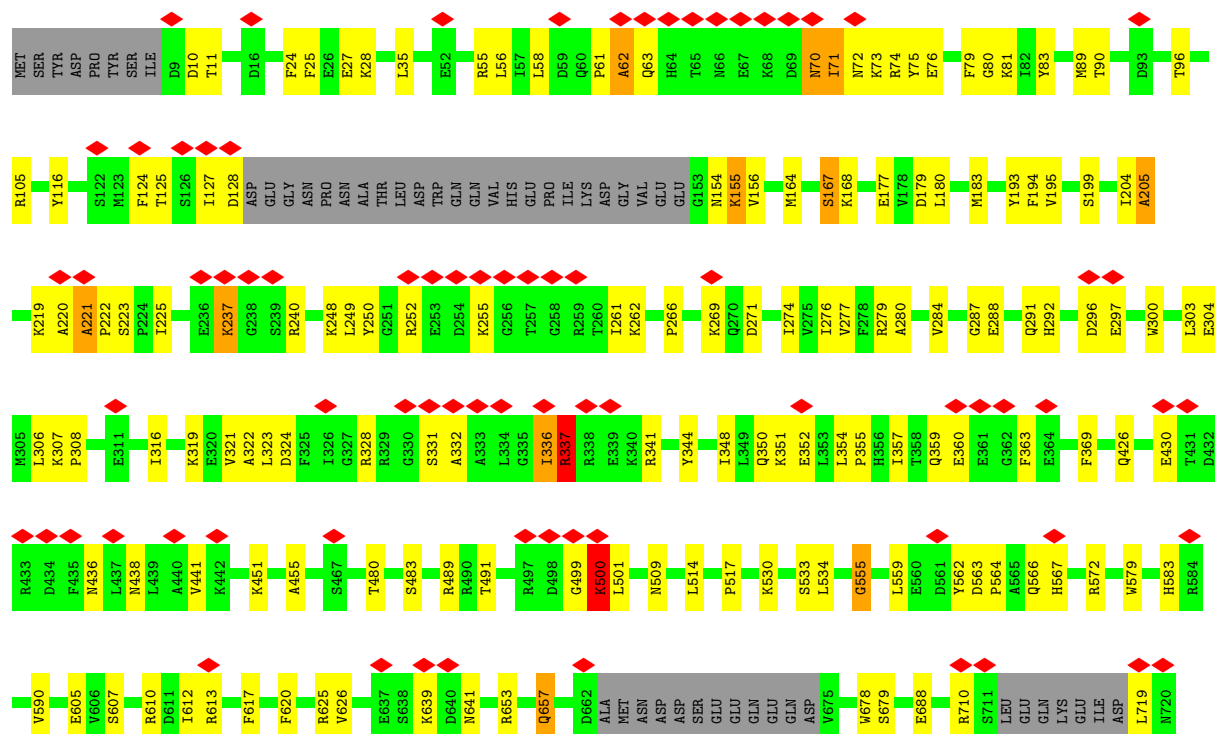
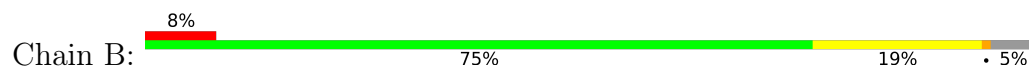
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

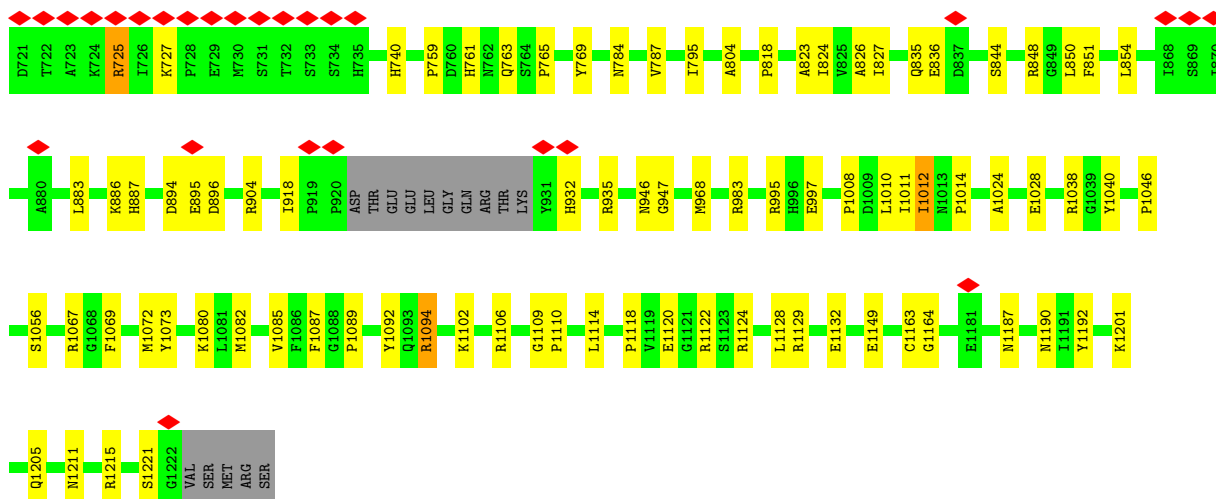
• Molecule 1: DNA-directed RNA polymerase subunit



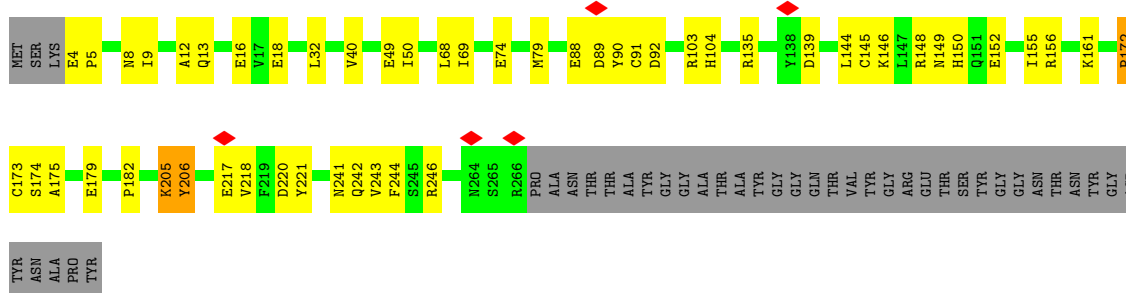


• Molecule 2: DNA-directed RNA polymerase subunit beta

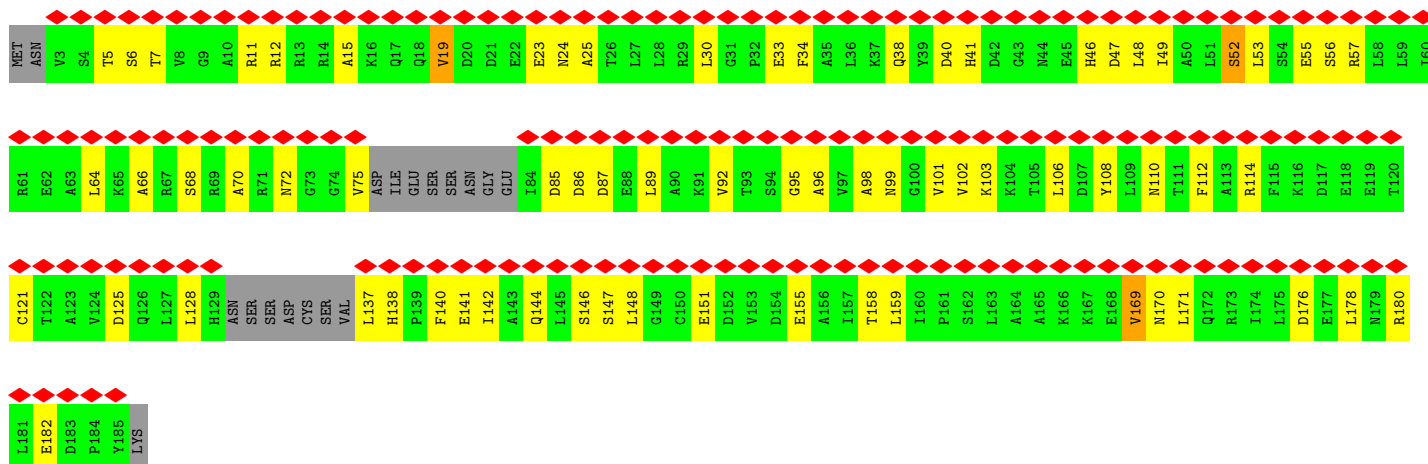
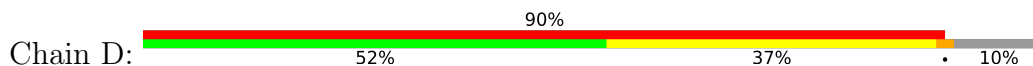




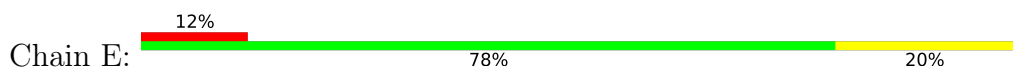
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core

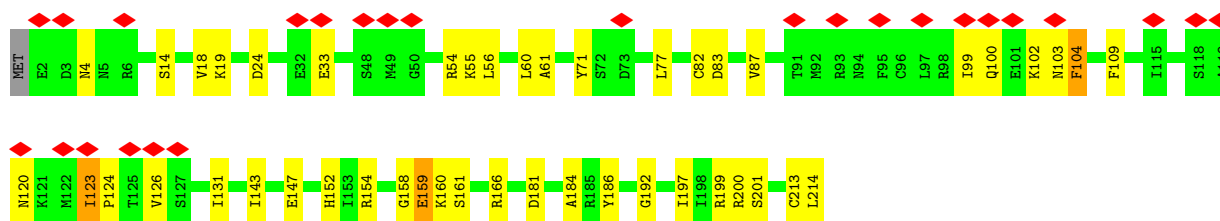


- Molecule 4: RNA polymerase II subunit B32



- Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III

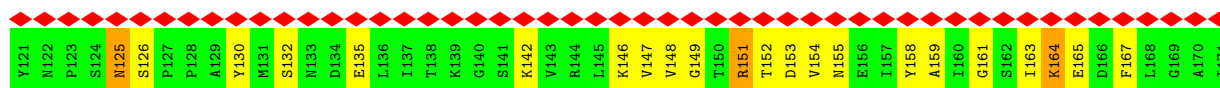
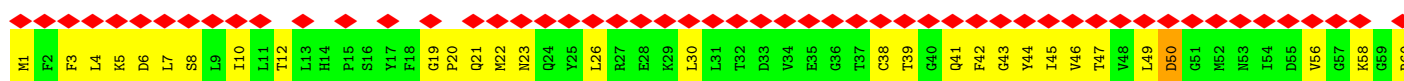




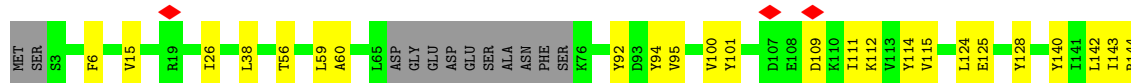
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III



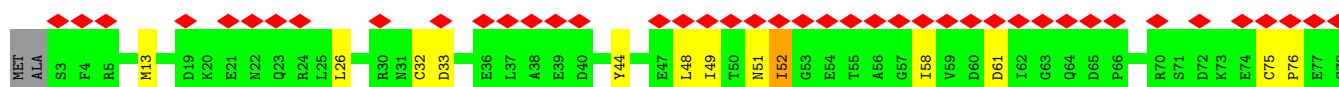
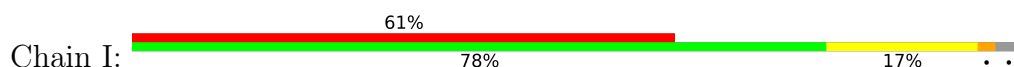
- Molecule 7: RNA polymerase II subunit

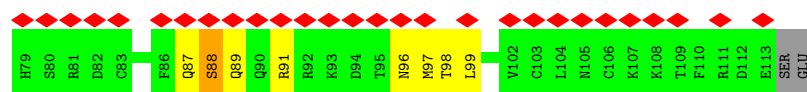


- Molecule 8: RNA polymerase subunit ABC14.5, common to RNA polymerases I, II, and III

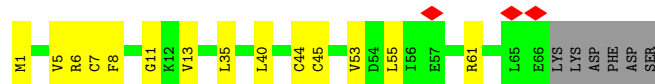


- Molecule 9: DNA-directed RNA polymerase subunit

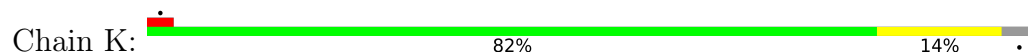




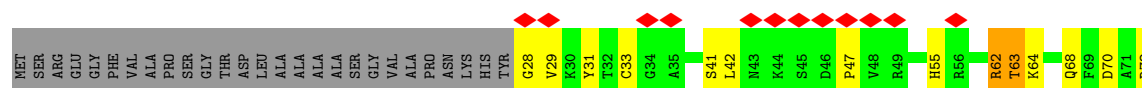
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



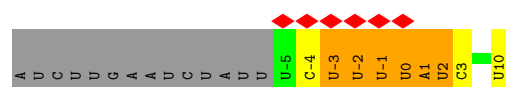
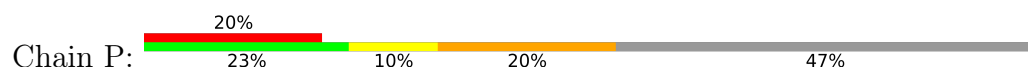
- Molecule 11: RNA polymerase II subunit B12.5



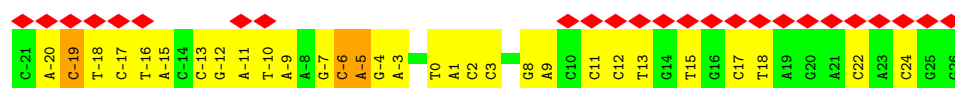
- Molecule 12: RNA polymerase subunit, found in RNA polymerase complexes I, II, and III



- Molecule 13: RNA (30-MER)



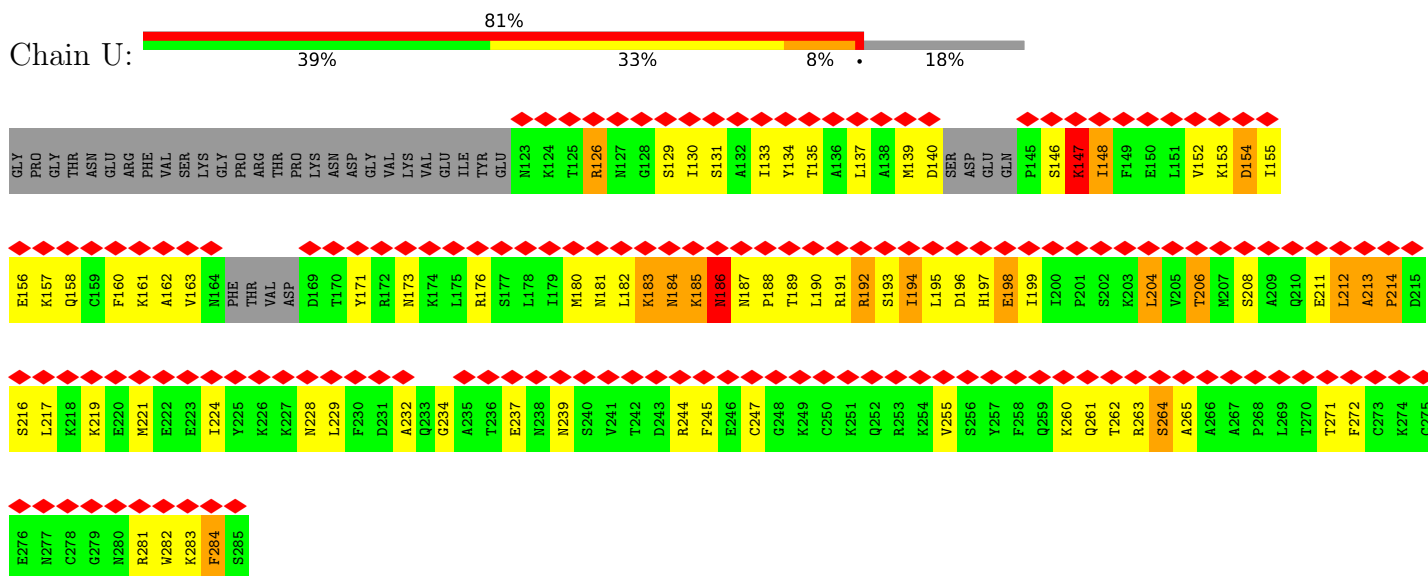
- Molecule 14: DNA (48-MER)



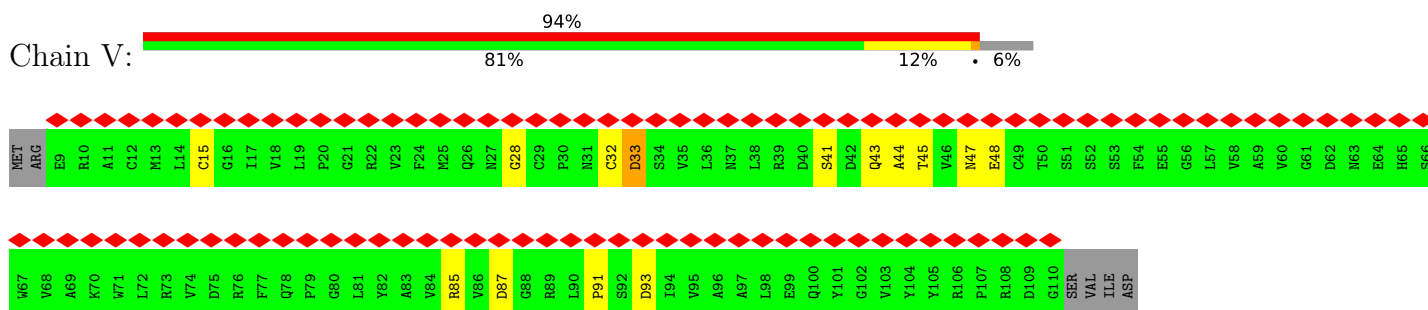
- Molecule 15: DNA (48-MER)



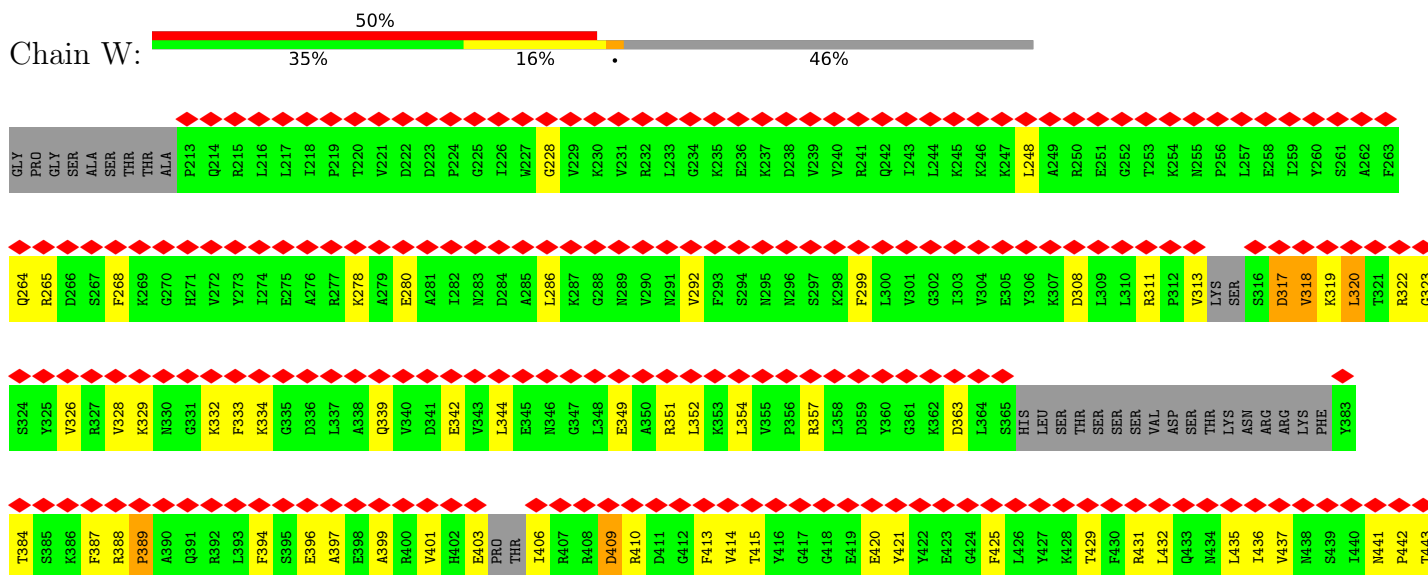
- Molecule 16: General transcription elongation factor TFIIS

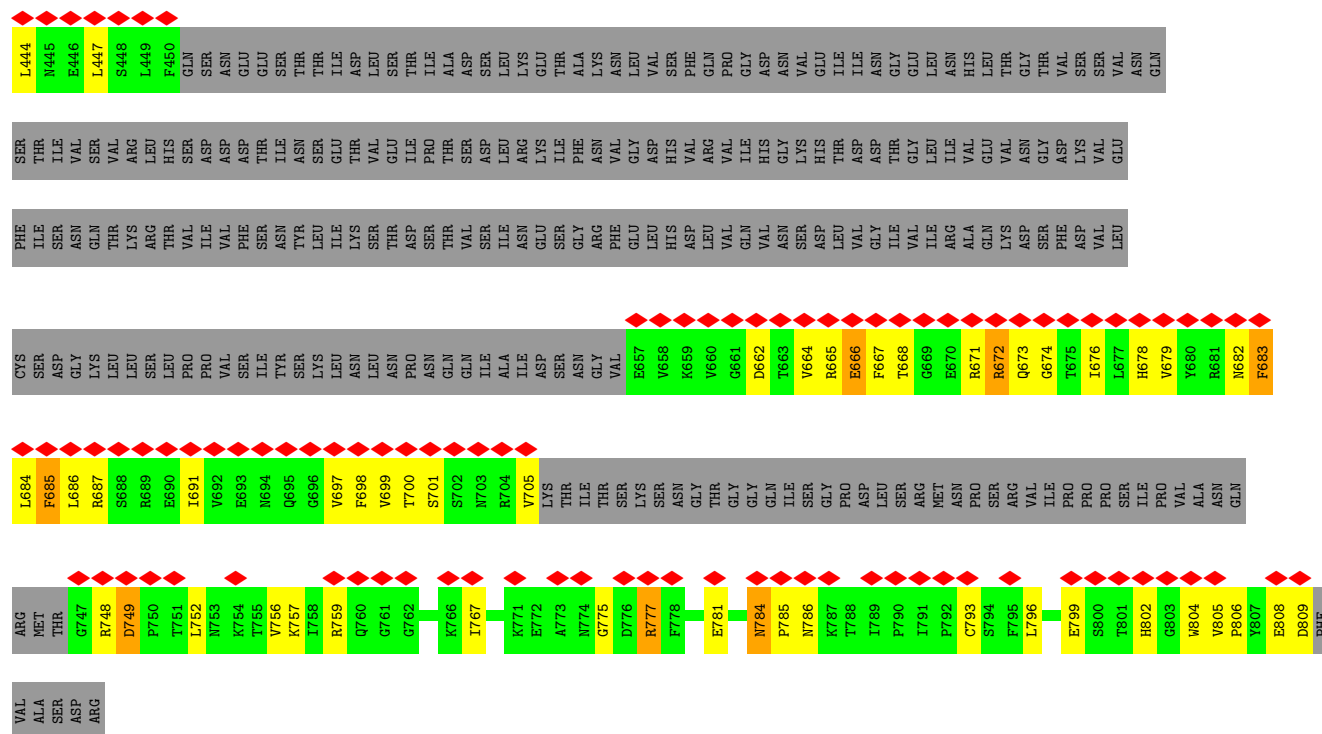


- Molecule 17: Transcription elongation factor SPT4



- Molecule 18: Protein that forms a complex with Spt4p





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	682749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.503	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0666	Depositor
Map size (\AA)	275.94, 275.94, 275.94	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.533, 1.533, 1.533	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/11449	0.69	42/15474 (0.3%)
2	B	0.26	0/9441	0.62	28/12732 (0.2%)
3	C	0.25	0/2139	0.50	2/2895 (0.1%)
4	D	0.31	0/1326	0.54	3/1788 (0.2%)
5	E	0.25	0/1772	0.56	1/2385 (0.0%)
6	F	0.24	0/687	0.52	1/931 (0.1%)
7	G	0.33	0/1353	0.60	4/1837 (0.2%)
8	H	0.25	0/1069	0.45	0/1444
9	I	0.22	0/934	0.40	0/1257
10	J	0.25	0/554	0.44	0/742
11	K	0.26	0/953	0.44	0/1291
12	L	0.25	0/365	0.70	2/484 (0.4%)
13	P	0.28	0/376	0.85	0/583
14	T	0.99	9/1092 (0.8%)	1.22	3/1680 (0.2%)
15	N	0.89	10/996 (1.0%)	1.21	6/1535 (0.4%)
16	U	0.29	0/1255	0.71	7/1677 (0.4%)
17	V	0.46	0/808	0.60	0/1097
18	W	0.40	0/2713	0.61	5/3646 (0.1%)
All	All	0.35	19/39282 (0.0%)	0.67	104/53478 (0.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	-6	DC	C3'-O3'	-6.37	1.35	1.44
15	N	2	DT	C1'-N1	6.00	1.57	1.49
15	N	-24	DC	C1'-N1	5.26	1.56	1.49
15	N	-19	DC	C1'-N1	5.24	1.56	1.49
15	N	-25	DC	C1'-N1	5.24	1.56	1.49
14	T	15	DT	C1'-N1	5.24	1.56	1.49
14	T	13	DT	C1'-N1	5.23	1.56	1.49
15	N	-22	DT	C1'-N1	5.23	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	22	DC	C1'-N1	5.21	1.56	1.49
14	T	24	DC	C1'-N1	5.19	1.56	1.49
14	T	12	DC	C1'-N1	5.19	1.55	1.49
15	N	-13	DC	C1'-N1	5.18	1.55	1.49
15	N	-15	DC	C1'-N1	5.16	1.55	1.49
15	N	-20	DT	C1'-N1	5.15	1.55	1.49
14	T	17	DC	C1'-N1	5.15	1.55	1.49
14	T	18	DT	C1'-N1	5.14	1.55	1.49
15	N	-18	DT	C1'-N1	5.14	1.55	1.49
14	T	11	DC	C1'-N1	5.11	1.55	1.49
15	N	-5	DT	C1'-N1	5.03	1.55	1.49

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ALA	CB-CA-C	16.63	135.04	110.10
2	B	221	ALA	N-CA-CB	-14.50	89.80	110.10
2	B	167	SER	CB-CA-C	14.38	137.42	110.10
1	A	47	ARG	C-N-CD	-13.03	91.93	120.60
1	A	861	LEU	CB-CA-C	-12.61	86.24	110.20
16	U	198	GLU	CB-CA-C	12.18	134.75	110.40
1	A	1368	TYR	N-CA-CB	-12.14	88.74	110.60
1	A	1367	ASN	CB-CA-C	-11.81	86.78	110.40
5	E	104	PHE	CB-CA-C	-11.77	86.86	110.40
1	A	328	ALA	N-CA-CB	-11.64	93.80	110.10
1	A	1029	ALA	CB-CA-C	-11.45	92.93	110.10
1	A	361	GLU	CB-CA-C	-11.20	88.01	110.40
1	A	978	ALA	N-CA-CB	-11.08	94.59	110.10
1	A	196	ALA	CB-CA-C	-10.87	93.80	110.10
1	A	310	ALA	N-CA-C	-10.73	82.03	111.00
1	A	925	GLU	CB-CA-C	10.60	131.60	110.40
1	A	58	LEU	N-CA-C	10.59	139.58	111.00
1	A	978	ALA	N-CA-C	10.46	139.24	111.00
2	B	168	LYS	N-CA-CB	-10.31	92.05	110.60
1	A	64	ASN	N-CA-CB	-10.17	92.29	110.60
2	B	337	ARG	N-CA-CB	-10.15	92.33	110.60
1	A	59	GLY	N-CA-C	-9.81	88.58	113.10
1	A	408	ARG	CB-CA-C	-9.79	90.82	110.40
2	B	80	GLY	N-CA-C	9.60	137.10	113.10
2	B	62	ALA	N-CA-CB	9.58	123.51	110.10
1	A	63	ARG	CB-CA-C	9.56	129.52	110.40
2	B	167	SER	N-CA-C	-9.50	85.35	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	926	LEU	N-CA-CB	-9.21	91.98	110.40
1	A	977	ARG	CB-CA-C	9.00	128.41	110.40
2	B	79	PHE	CB-CA-C	-8.95	92.50	110.40
2	B	887	HIS	N-CA-CB	-8.63	95.06	110.60
18	W	389	PRO	CA-N-CD	-8.53	99.56	111.50
2	B	886	LYS	CB-CA-C	-8.37	93.66	110.40
1	A	1030	THR	N-CA-C	8.21	133.16	111.00
2	B	237	LYS	N-CA-C	-8.13	89.05	111.00
2	B	657	GLN	CB-CA-C	-8.07	94.26	110.40
1	A	1368	TYR	N-CA-C	8.04	132.71	111.00
15	N	17	DA	O4'-C1'-N9	7.89	113.53	108.00
12	L	47	PRO	CB-CA-C	-7.85	92.38	112.00
2	B	81	LYS	N-CA-CB	7.83	124.70	110.60
15	N	16	DT	O4'-C1'-N1	-7.68	102.62	108.00
2	B	61	PRO	N-CA-C	7.67	132.04	112.10
14	T	-5	DA	O4'-C1'-N9	7.55	113.28	108.00
1	A	1030	THR	N-CA-CB	-7.54	95.97	110.30
2	B	220	ALA	N-CA-C	-7.53	90.67	111.00
2	B	205	ALA	CB-CA-C	7.50	121.36	110.10
2	B	221	ALA	N-CA-C	7.40	130.97	111.00
4	D	53	LEU	N-CA-C	7.38	130.94	111.00
2	B	887	HIS	N-CA-C	7.32	130.76	111.00
2	B	351	LYS	N-CA-C	7.27	130.62	111.00
4	D	19	VAL	CB-CA-C	-7.26	97.61	111.40
1	A	862	GLY	N-CA-C	7.24	131.20	113.10
7	G	50	ASP	N-CA-C	7.09	130.15	111.00
2	B	895	GLU	N-CA-C	7.01	129.92	111.00
16	U	199	ILE	N-CA-C	-6.92	92.32	111.00
16	U	214	PRO	CB-CA-C	-6.92	94.70	112.00
1	A	311	GLY	N-CA-C	6.87	130.28	113.10
1	A	1393	ASN	CB-CA-C	6.75	123.89	110.40
2	B	79	PHE	N-CA-C	6.72	129.15	111.00
1	A	921	LEU	N-CA-C	-6.70	92.91	111.00
1	A	197	GLN	N-CA-C	6.68	129.03	111.00
2	B	657	GLN	N-CA-C	6.43	128.36	111.00
16	U	183	LYS	CB-CA-C	-6.42	97.55	110.40
2	B	895	GLU	N-CA-CB	-6.40	99.08	110.60
14	T	-6	DC	O4'-C1'-N1	-6.37	103.54	108.00
2	B	1012	ILE	CB-CA-C	-6.29	99.02	111.60
12	L	63	THR	CB-CA-C	-6.27	94.67	111.60
6	F	140	ASP	CB-CA-C	-6.26	97.88	110.40
1	A	58	LEU	CB-CA-C	-6.26	98.31	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	GLU	CB-CA-C	-6.22	97.95	110.40
7	G	164	LYS	O-C-N	-6.18	112.81	122.70
1	A	338	ARG	CB-CA-C	6.08	122.57	110.40
1	A	64	ASN	N-CA-C	6.08	127.42	111.00
1	A	921	LEU	CB-CA-C	6.02	121.63	110.20
1	A	1441	THR	CB-CA-C	5.99	127.77	111.60
3	C	205	LYS	CB-CA-C	5.99	122.37	110.40
7	G	163	ILE	CB-CA-C	-5.97	99.66	111.60
2	B	220	ALA	CB-CA-C	-5.92	101.21	110.10
1	A	1442	GLY	N-CA-C	5.91	127.87	113.10
1	A	197	GLN	N-CA-CB	-5.90	99.98	110.60
3	C	206	TYR	N-CA-CB	-5.88	100.02	110.60
1	A	1029	ALA	N-CA-C	-5.86	95.19	111.00
14	T	-19	DC	O4'-C1'-N1	5.81	112.06	108.00
7	G	165	GLU	N-CA-CB	-5.76	100.22	110.60
15	N	16	DT	O4'-C4'-C3'	5.71	109.43	106.00
2	B	61	PRO	CB-CA-C	-5.62	97.95	112.00
16	U	199	ILE	N-CA-CB	5.53	123.53	110.80
4	D	52	SER	CB-CA-C	-5.52	99.61	110.10
15	N	16	DT	P-O3'-C3'	-5.48	113.13	119.70
1	A	977	ARG	C-N-CA	5.46	135.36	121.70
1	A	327	ARG	CB-CA-C	5.41	121.23	110.40
1	A	1424	CYS	CB-CA-C	-5.41	99.58	110.40
16	U	184	ASN	N-CA-C	-5.37	96.49	111.00
1	A	774	LYS	CB-CA-C	-5.32	99.77	110.40
2	B	894	ASP	N-CA-C	-5.30	96.69	111.00
18	W	317	ASP	CB-CG-OD2	5.25	123.03	118.30
18	W	409	ASP	CB-CG-OD2	5.23	123.01	118.30
18	W	363	ASP	CB-CG-OD2	5.22	123.00	118.30
16	U	154	ASP	CB-CG-OD2	5.21	122.98	118.30
18	W	662	ASP	CB-CG-OD2	5.20	122.98	118.30
15	N	16	DT	O4'-C1'-C2'	-5.12	101.81	105.90
2	B	205	ALA	N-CA-C	-5.10	97.23	111.00
15	N	16	DT	N3-C4-O4	5.04	122.92	119.90
1	A	544	TYR	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11239	0	11263	452	0
2	B	9261	0	9267	204	0
3	C	2098	0	2058	32	0
4	D	1314	0	1314	153	0
5	E	1740	0	1754	28	0
6	F	677	0	693	11	0
7	G	1324	0	1342	222	0
8	H	1052	0	1050	15	0
9	I	917	0	865	30	0
10	J	545	0	560	9	0
11	K	932	0	944	9	0
12	L	359	0	360	16	0
13	P	338	0	169	25	0
14	T	975	0	538	43	0
15	N	889	0	487	35	0
16	U	1239	0	1263	264	0
17	V	792	0	757	7	0
18	W	2667	0	2712	250	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
19	U	1	0	0	1	0
19	V	1	0	0	0	0
20	A	1	0	0	0	0
All	All	38369	0	37396	1359	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 18.

All (1359) 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)
1:A:1363:GLY:CA	16:U:282:TRP:HA	1.30	1.62
7:G:100:PHE:HZ	18:W:698:PHE:CE1	1.21	1.54
7:G:100:PHE:CZ	18:W:698:PHE:CE1	1.94	1.53
16:U:133:ILE:HG21	16:U:155:ILE:CG2	1.38	1.49
1:A:1232:GLU:HG3	16:U:180:MET:CB	1.43	1.48
1:A:1232:GLU:CG	16:U:180:MET:CB	1.91	1.46
4:D:34:PHE:CE1	7:G:3:PHE:CD2	2.06	1.42
1:A:1232:GLU:CG	16:U:180:MET:HB3	1.45	1.41
4:D:34:PHE:CE1	7:G:3:PHE:CG	2.10	1.40
1:A:1080:GLN:C	16:U:262:THR:HG21	1.42	1.40
1:A:831:LYS:NZ	16:U:262:THR:HA	1.09	1.39
16:U:133:ILE:CG2	16:U:155:ILE:HG21	1.52	1.38
1:A:708:GLY:O	1:A:1093:SER:CB	1.68	1.38
1:A:1085:THR:HA	16:U:260:LYS:NZ	1.32	1.34
16:U:140:ASP:OD1	16:U:191:ARG:HB2	1.29	1.31
1:A:1450:GLU:OE2	7:G:58:LYS:HE2	1.10	1.27
2:B:336:ILE:O	2:B:341:ARG:HB2	1.14	1.27
4:D:24:ASN:HA	7:G:83:LYS:O	1.29	1.26
1:A:1080:GLN:C	16:U:262:THR:CG2	2.03	1.26
4:D:158:THR:HG21	7:G:167:PHE:CD2	1.71	1.25
2:B:70:ASN:O	2:B:127:ILE:HG22	1.18	1.24
7:G:100:PHE:CZ	18:W:698:PHE:CZ	2.24	1.24
7:G:100:PHE:CE1	18:W:698:PHE:CZ	2.24	1.24
1:A:831:LYS:NZ	16:U:262:THR:CA	1.99	1.23
4:D:33:GLU:OE1	7:G:42:PHE:CZ	1.92	1.23
18:W:333:PHE:CD1	18:W:354:LEU:HD21	1.73	1.22
18:W:409:ASP:HB2	18:W:413:PHE:CD2	1.73	1.22
13:P:3:C:O2	14:T:8:DG:N2	1.74	1.21
16:U:162:ALA:HB1	16:U:171:TYR:CD2	1.77	1.19
16:U:133:ILE:HD13	16:U:155:ILE:CG2	1.72	1.18
1:A:50:GLU:OE2	18:W:444:LEU:CD1	1.90	1.18
2:B:653:ARG:HD2	2:B:657:GLN:NE2	1.57	1.18
7:G:100:PHE:HZ	18:W:698:PHE:CD1	1.63	1.16
4:D:5:THR:O	7:G:7:LEU:HD22	1.46	1.16
4:D:25:ALA:HB3	7:G:85:GLU:HA	1.26	1.16
4:D:23:GLU:CD	7:G:82:PHE:CD1	2.19	1.15
1:A:831:LYS:HZ3	16:U:262:THR:CA	1.57	1.15
1:A:1080:GLN:CA	16:U:262:THR:CG2	2.24	1.15
2:B:307:LYS:NZ	9:I:13:MET:HE1	1.60	1.14
18:W:333:PHE:CG	18:W:354:LEU:HD21	1.80	1.14
4:D:34:PHE:CD1	7:G:3:PHE:CG	2.34	1.14
16:U:162:ALA:HB3	16:U:171:TYR:CE2	1.82	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:GLU:OE1	7:G:82:PHE:HA	1.42	1.14
16:U:162:ALA:HB3	16:U:171:TYR:HE2	1.04	1.13
1:A:1363:GLY:HA3	16:U:282:TRP:CA	1.77	1.13
2:B:70:ASN:O	2:B:127:ILE:CG2	1.97	1.13
16:U:162:ALA:CB	16:U:171:TYR:CE2	2.31	1.13
1:A:1363:GLY:CA	16:U:282:TRP:CA	2.26	1.13
1:A:1363:GLY:HA2	16:U:282:TRP:HA	1.24	1.13
18:W:676:ILE:HG12	18:W:686:LEU:HD21	1.22	1.13
1:A:1206:ASP:OD1	16:U:228:ASN:HB3	1.47	1.12
4:D:34:PHE:CD1	7:G:3:PHE:CD2	2.37	1.12
4:D:41:HIS:CE1	7:G:74:TYR:O	2.02	1.12
18:W:409:ASP:HB2	18:W:413:PHE:HD2	1.04	1.12
1:A:708:GLY:O	1:A:1093:SER:HB3	0.94	1.12
1:A:50:GLU:OE2	18:W:444:LEU:HD11	0.94	1.11
2:B:307:LYS:NZ	9:I:13:MET:CE	2.12	1.11
1:A:1085:THR:CA	16:U:260:LYS:NZ	2.14	1.11
18:W:684:LEU:HD12	18:W:699:VAL:HA	1.11	1.10
4:D:23:GLU:O	7:G:83:LYS:HB3	1.52	1.10
13:P:3:C:N3	14:T:8:DG:N1	1.96	1.10
1:A:1461:ALA:HA	7:G:20:PRO:HD2	1.20	1.10
4:D:7:THR:HG23	7:G:6:ASP:O	1.50	1.10
1:A:1080:GLN:HA	16:U:262:THR:HG22	1.20	1.09
1:A:1232:GLU:HG2	16:U:180:MET:HB3	1.32	1.09
1:A:1271:LEU:HD13	9:I:48:LEU:HD11	1.33	1.09
7:G:100:PHE:HE1	18:W:698:PHE:CE2	1.69	1.09
4:D:23:GLU:CG	7:G:82:PHE:HD1	1.66	1.08
15:N:15:DG:H2"	15:N:16:DT:H5"	1.31	1.08
18:W:684:LEU:CD1	18:W:699:VAL:HA	1.81	1.08
18:W:332:LYS:HD2	18:W:389:PRO:HD3	1.24	1.08
1:A:1080:GLN:HA	16:U:262:THR:CG2	1.82	1.08
4:D:34:PHE:CZ	7:G:3:PHE:CD2	2.41	1.08
16:U:130:ILE:HG23	16:U:134:TYR:CZ	1.87	1.08
1:A:47:ARG:HB3	1:A:48:PRO:HD2	1.28	1.07
1:A:1202:ALA:HA	16:U:224:ILE:CG2	1.82	1.07
1:A:1450:GLU:OE2	7:G:58:LYS:CE	2.00	1.07
1:A:1461:ALA:CA	7:G:20:PRO:HD2	1.83	1.07
1:A:1085:THR:CA	16:U:260:LYS:HZ3	1.64	1.07
1:A:1202:ALA:HA	16:U:224:ILE:HG21	1.10	1.07
18:W:664:VAL:HG21	18:W:686:LEU:CD1	1.84	1.07
16:U:216:SER:O	16:U:219:LYS:HG2	1.55	1.06
18:W:399:ALA:HB1	18:W:406:ILE:HD11	1.27	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:LEU:HD21	7:G:3:PHE:HE1	1.20	1.06
18:W:317:ASP:O	18:W:319:LYS:HG3	1.52	1.06
18:W:352:LEU:HD11	18:W:435:LEU:HD11	1.31	1.06
1:A:1232:GLU:HG3	16:U:180:MET:HB2	1.29	1.06
1:A:286:PRO:HG2	18:W:268:PHE:CE1	1.91	1.05
1:A:1232:GLU:CG	16:U:180:MET:HB2	1.78	1.05
15:N:-8:DA:H4'	15:N:-7:DA:OP1	1.51	1.05
7:G:100:PHE:CE1	18:W:698:PHE:CE2	2.44	1.05
16:U:187:ASN:HD21	16:U:214:PRO:HB3	1.11	1.05
1:A:1448:ILE:HB	7:G:61:ILE:CD1	1.86	1.05
12:L:62:ARG:HD3	12:L:63:THR:O	1.55	1.05
2:B:307:LYS:HZ3	9:I:13:MET:CE	1.71	1.04
1:A:831:LYS:HB3	1:A:1083:LEU:CD2	1.88	1.04
18:W:676:ILE:CG1	18:W:686:LEU:HD21	1.86	1.04
7:G:95:SER:HB3	18:W:682:ASN:HD22	1.21	1.04
16:U:185:LYS:O	16:U:187:ASN:N	1.91	1.04
1:A:1447:MET:HE1	7:G:60:ARG:HA	1.40	1.03
4:D:112:PHE:CE1	7:G:142:LYS:HD3	1.93	1.03
2:B:70:ASN:ND2	2:B:128:ASP:C	2.12	1.03
1:A:1234:ASN:ND2	16:U:213:ALA:O	1.90	1.03
16:U:130:ILE:CG2	16:U:134:TYR:CZ	2.42	1.03
15:N:13:DC:H2''	15:N:14:DG:O4'	1.59	1.02
18:W:320:LEU:HD22	18:W:432:LEU:CD1	1.88	1.02
18:W:664:VAL:HG11	18:W:676:ILE:HD11	1.37	1.02
1:A:1448:ILE:CB	7:G:61:ILE:HD11	1.90	1.02
2:B:653:ARG:HD2	2:B:657:GLN:CD	1.79	1.02
18:W:320:LEU:HD22	18:W:432:LEU:HD13	1.37	1.02
1:A:1361:PHE:CE1	16:U:281:ARG:NH1	2.27	1.02
4:D:41:HIS:NE2	7:G:74:TYR:O	1.91	1.02
16:U:130:ILE:CG2	16:U:134:TYR:CE1	2.43	1.02
2:B:336:ILE:O	2:B:341:ARG:CB	2.08	1.01
18:W:399:ALA:CB	18:W:406:ILE:HD11	1.90	1.01
18:W:664:VAL:CG2	18:W:686:LEU:CD1	2.38	1.01
14:T:-7:DG:H2''	14:T:-6:DC:H5''	1.36	1.01
1:A:1447:MET:CE	7:G:60:ARG:HG3	1.89	1.01
12:L:68:GLN:CD	18:W:767:ILE:HG12	1.80	1.01
16:U:196:ASP:OD1	16:U:197:HIS:N	1.94	1.01
16:U:162:ALA:CB	16:U:171:TYR:HE2	1.69	1.00
4:D:6:SER:HA	7:G:7:LEU:HD23	1.43	1.00
1:A:37:TYR:CE1	18:W:441:ASN:ND2	2.30	1.00
1:A:831:LYS:CB	1:A:1083:LEU:HD22	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:653:ARG:HD3	2:B:657:GLN:OE1	1.61	0.99
18:W:664:VAL:HG21	18:W:686:LEU:HD11	1.41	0.99
4:D:23:GLU:CD	7:G:82:PHE:HD1	1.60	0.98
15:N:-7:DA:H2"	15:N:-6:DA:N7	1.78	0.98
4:D:34:PHE:HE1	7:G:3:PHE:CB	1.76	0.98
2:B:71:ILE:HG12	2:B:73:LYS:HE3	1.41	0.98
1:A:1232:GLU:HG2	16:U:180:MET:CB	1.81	0.98
1:A:1448:ILE:HB	7:G:61:ILE:HD11	0.98	0.97
1:A:1447:MET:CE	7:G:60:ARG:HA	1.94	0.97
2:B:653:ARG:CD	2:B:657:GLN:NE2	2.26	0.97
4:D:34:PHE:CE1	7:G:3:PHE:CB	2.48	0.97
1:A:1137:GLN:NE2	16:U:232:ALA:HB1	1.78	0.97
18:W:396:GLU:OE2	18:W:414:VAL:HG23	1.64	0.97
2:B:904:ARG:HH21	18:W:786:ASN:HA	1.30	0.97
4:D:158:THR:CG2	7:G:167:PHE:CD2	2.48	0.96
16:U:162:ALA:HB1	16:U:171:TYR:HD2	1.23	0.96
18:W:664:VAL:CG2	18:W:686:LEU:HD13	1.95	0.96
1:A:1363:GLY:HA3	16:U:282:TRP:HA	1.00	0.96
1:A:186:TRP:O	1:A:198:PRO:HA	1.66	0.96
15:N:-7:DA:H2"	15:N:-6:DA:C8	2.00	0.96
4:D:40:ASP:HA	7:G:6:ASP:OD2	1.65	0.96
16:U:183:LYS:HG3	16:U:183:LYS:O	1.62	0.96
18:W:664:VAL:HG23	18:W:686:LEU:HD13	1.46	0.96
18:W:399:ALA:HB1	18:W:406:ILE:CD1	1.95	0.96
4:D:19:VAL:HG12	4:D:19:VAL:O	1.65	0.96
1:A:1080:GLN:O	16:U:262:THR:HG21	1.66	0.95
2:B:653:ARG:CD	2:B:657:GLN:CD	2.35	0.95
4:D:24:ASN:CA	7:G:83:LYS:O	2.15	0.95
1:A:253:MET:HG3	13:P:1:A:C2	2.01	0.95
1:A:1234:ASN:OD1	16:U:217:LEU:HD23	1.66	0.94
18:W:409:ASP:CB	18:W:413:PHE:CD2	2.50	0.94
1:A:253:MET:HG3	13:P:1:A:N1	1.80	0.94
1:A:1206:ASP:HB2	16:U:228:ASN:ND2	1.82	0.94
4:D:34:PHE:CD1	7:G:3:PHE:CD1	2.55	0.94
1:A:1134:LYS:HE3	16:U:229:LEU:HA	1.50	0.94
18:W:676:ILE:HG12	18:W:686:LEU:CD2	1.96	0.94
16:U:130:ILE:HA	16:U:155:ILE:HD12	1.50	0.94
18:W:409:ASP:CB	18:W:413:PHE:HD2	1.80	0.93
2:B:287:GLY:O	2:B:291:GLN:HB2	1.67	0.93
1:A:831:LYS:HZ1	16:U:262:THR:HA	1.24	0.93
1:A:1447:MET:SD	7:G:60:ARG:HA	2.08	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ASN:O	2:B:125:THR:HA	1.69	0.93
4:D:6:SER:CA	7:G:7:LEU:HD23	1.98	0.92
18:W:684:LEU:HD12	18:W:699:VAL:CA	1.99	0.92
18:W:684:LEU:HD11	18:W:699:VAL:HG13	1.48	0.92
1:A:50:GLU:CD	18:W:444:LEU:HD11	1.90	0.92
1:A:47:ARG:HB3	1:A:48:PRO:CD	1.97	0.92
1:A:37:TYR:CZ	18:W:441:ASN:ND2	2.38	0.92
4:D:34:PHE:CG	7:G:3:PHE:CE2	2.58	0.91
1:A:1232:GLU:HG2	16:U:180:MET:CG	2.01	0.91
4:D:112:PHE:CZ	7:G:142:LYS:HD3	2.05	0.90
1:A:1080:GLN:CA	16:U:262:THR:HG22	1.95	0.90
1:A:713:GLU:OE2	1:A:1092:SER:OG	1.87	0.90
1:A:1100:VAL:HB	1:A:1101:PRO:HD3	1.51	0.90
1:A:1232:GLU:HG3	16:U:180:MET:HB3	1.02	0.90
14:T:-18:DT:H3	15:N:19:DA:H2	0.94	0.90
16:U:130:ILE:HG22	16:U:134:TYR:CE1	2.07	0.90
1:A:1361:PHE:CE1	16:U:281:ARG:CZ	2.55	0.90
1:A:831:LYS:HZ1	16:U:262:THR:CA	1.77	0.89
16:U:140:ASP:HB2	16:U:191:ARG:HD2	1.55	0.89
16:U:183:LYS:NZ	16:U:185:LYS:HE3	1.87	0.89
4:D:6:SER:CB	7:G:7:LEU:HD23	2.02	0.89
18:W:394:PHE:HE2	18:W:396:GLU:HG2	1.37	0.89
1:A:831:LYS:HE3	16:U:262:THR:O	1.71	0.89
14:T:-18:DT:N3	15:N:19:DA:C2	2.26	0.88
1:A:1446:VAL:O	7:G:61:ILE:HB	1.74	0.88
16:U:247:CYS:HG	19:U:301:ZN:ZN	0.64	0.88
1:A:1461:ALA:HA	7:G:20:PRO:CD	2.04	0.88
16:U:130:ILE:HA	16:U:155:ILE:CD1	2.03	0.88
1:A:1081:MET:N	16:U:262:THR:HG23	1.88	0.88
13:P:3:C:N4	14:T:8:DG:O6	2.06	0.87
4:D:48:LEU:HD21	7:G:3:PHE:CE1	2.07	0.87
14:T:-18:DT:H2''	14:T:-17:DC:H5'	1.55	0.87
1:A:831:LYS:CB	1:A:1083:LEU:CD2	2.48	0.87
17:V:85:ARG:NH1	17:V:87:ASP:OD1	2.07	0.87
18:W:684:LEU:CD1	18:W:699:VAL:HG22	2.04	0.87
16:U:133:ILE:HD13	16:U:155:ILE:HG22	1.56	0.87
1:A:1234:ASN:CG	16:U:213:ALA:O	2.12	0.87
2:B:500:LYS:HG2	2:B:501:LEU:H	1.39	0.86
4:D:34:PHE:CD1	7:G:3:PHE:CE2	2.62	0.86
16:U:187:ASN:ND2	16:U:214:PRO:HB3	1.89	0.86
18:W:399:ALA:C	18:W:406:ILE:CD1	2.43	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:GLU:OE2	16:U:180:MET:HG3	1.76	0.86
1:A:1447:MET:HE3	7:G:60:ARG:HG3	1.57	0.86
18:W:666:GLU:OE1	18:W:671:ARG:HB2	1.76	0.86
14:T:-15:DA:N6	15:N:16:DT:O4	2.07	0.86
2:B:769:TYR:OH	16:U:265:ALA:CB	2.23	0.86
16:U:162:ALA:CB	16:U:171:TYR:CD2	2.53	0.86
2:B:337:ARG:O	2:B:341:ARG:HB3	1.76	0.86
18:W:320:LEU:CD2	18:W:432:LEU:HD13	2.04	0.86
1:A:1447:MET:HE1	7:G:60:ARG:HG3	1.56	0.86
2:B:769:TYR:OH	16:U:265:ALA:O	1.92	0.86
18:W:684:LEU:HG	18:W:699:VAL:HG22	1.58	0.86
16:U:140:ASP:OD1	16:U:191:ARG:CB	2.22	0.86
1:A:1271:LEU:CD1	9:I:48:LEU:HD11	2.06	0.85
2:B:769:TYR:OH	16:U:265:ALA:HB1	1.76	0.85
16:U:162:ALA:HB1	16:U:171:TYR:CE2	2.04	0.85
4:D:98:ALA:O	4:D:102:VAL:HB	1.77	0.85
4:D:158:THR:HG21	7:G:167:PHE:HD2	1.10	0.85
18:W:409:ASP:O	18:W:410:ARG:HG3	1.75	0.85
1:A:37:TYR:OH	18:W:441:ASN:ND2	2.10	0.85
18:W:667:PHE:HB3	18:W:701:SER:O	1.77	0.85
4:D:25:ALA:CB	7:G:85:GLU:HA	2.05	0.85
1:A:1206:ASP:OD1	16:U:228:ASN:CB	2.25	0.84
1:A:1264:LYS:HE2	9:I:44:TYR:CG	2.11	0.84
16:U:181:ASN:ND2	16:U:212:LEU:CD1	2.41	0.84
2:B:769:TYR:OH	16:U:265:ALA:C	2.16	0.84
18:W:333:PHE:CG	18:W:354:LEU:CD2	2.59	0.84
4:D:112:PHE:CZ	7:G:142:LYS:CD	2.60	0.84
16:U:184:ASN:O	16:U:185:LYS:O	1.94	0.84
1:A:1232:GLU:CD	16:U:180:MET:HB2	1.98	0.84
4:D:106:LEU:O	4:D:110:ASN:HB2	1.78	0.84
18:W:666:GLU:OE1	18:W:671:ARG:N	2.10	0.84
4:D:158:THR:CG2	7:G:167:PHE:HD2	1.85	0.84
16:U:185:LYS:HG2	16:U:191:ARG:NH2	1.91	0.84
1:A:1286:TYR:HD1	16:U:234:GLY:HA3	1.43	0.84
2:B:63:GLN:HE22	18:W:248:LEU:HB3	1.41	0.83
18:W:352:LEU:HD11	18:W:435:LEU:CD1	2.07	0.83
18:W:665:ARG:HA	18:W:673:GLN:HA	1.58	0.83
16:U:216:SER:O	16:U:219:LYS:CG	2.25	0.83
1:A:1447:MET:HE1	7:G:60:ARG:CA	2.08	0.83
1:A:40:ILE:HG22	1:A:41:MET:HE3	1.60	0.83
1:A:831:LYS:HB3	1:A:1083:LEU:HD23	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:189:THR:O	16:U:193:SER:N	2.12	0.83
1:A:735:GLU:OE1	16:U:244:ARG:NH1	2.11	0.83
4:D:48:LEU:HD11	7:G:3:PHE:CD1	2.14	0.83
18:W:329:LYS:HD2	18:W:436:ILE:HG13	1.60	0.83
4:D:23:GLU:CG	7:G:82:PHE:CD1	2.58	0.83
18:W:684:LEU:CG	18:W:699:VAL:HG22	2.09	0.82
16:U:133:ILE:HD13	16:U:155:ILE:HG21	1.62	0.82
18:W:676:ILE:CG1	18:W:686:LEU:CD2	2.55	0.82
16:U:185:LYS:HG2	16:U:191:ARG:HH22	1.43	0.82
4:D:23:GLU:HB3	7:G:82:PHE:HB3	1.61	0.82
4:D:25:ALA:HB3	7:G:85:GLU:CA	2.09	0.82
1:A:286:PRO:HG2	18:W:268:PHE:CZ	2.14	0.81
2:B:653:ARG:CD	2:B:657:GLN:OE1	2.28	0.81
15:N:14:DG:H4'	15:N:14:DG:OP1	1.78	0.81
2:B:769:TYR:HH	16:U:265:ALA:C	1.82	0.81
4:D:158:THR:HG21	7:G:167:PHE:CE2	2.15	0.81
2:B:73:LYS:HA	2:B:124:PHE:O	1.79	0.81
18:W:399:ALA:CB	18:W:406:ILE:CD1	2.55	0.81
4:D:23:GLU:HG2	7:G:82:PHE:HD1	1.44	0.81
1:A:1137:GLN:NE2	16:U:232:ALA:CB	2.43	0.81
7:G:95:SER:HB3	18:W:682:ASN:ND2	1.95	0.81
12:L:68:GLN:NE2	18:W:767:ILE:HD11	1.95	0.81
18:W:676:ILE:HA	18:W:686:LEU:HD23	1.62	0.80
1:A:831:LYS:CA	1:A:1083:LEU:CD2	2.59	0.80
1:A:1361:PHE:HE1	16:U:281:ARG:CZ	1.94	0.80
1:A:828:THR:OG1	16:U:261:GLN:CG	2.29	0.80
16:U:133:ILE:HD13	16:U:155:ILE:CB	2.11	0.80
18:W:357:ARG:HB3	18:W:389:PRO:HD2	1.64	0.80
1:A:286:PRO:CG	18:W:268:PHE:CZ	2.65	0.80
13:P:-1:U:O2'	13:P:0:U:OP1	2.00	0.80
1:A:1081:MET:N	16:U:262:THR:CG2	2.44	0.80
1:A:1461:ALA:N	7:G:20:PRO:HD2	1.95	0.80
8:H:56:THR:HB	8:H:144:ARG:HB3	1.64	0.80
1:A:828:THR:OG1	16:U:261:GLN:HG3	1.82	0.79
18:W:328:VAL:HA	18:W:435:LEU:HD23	1.64	0.79
18:W:357:ARG:C	18:W:389:PRO:HG2	2.02	0.79
18:W:399:ALA:C	18:W:406:ILE:HD11	2.02	0.79
1:A:772:GLU:HA	1:A:1086:PHE:CZ	2.17	0.79
1:A:831:LYS:HZ1	16:U:262:THR:HG23	1.47	0.79
2:B:74:ARG:HB2	2:B:124:PHE:HB2	1.64	0.79
1:A:1137:GLN:NE2	16:U:232:ALA:O	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:ARG:O	2:B:341:ARG:CB	2.31	0.79
1:A:1202:ALA:CA	16:U:224:ILE:HG21	2.04	0.78
1:A:1232:GLU:CG	16:U:180:MET:CG	2.58	0.78
4:D:49:ILE:HG21	7:G:4:LEU:HD12	1.65	0.78
16:U:140:ASP:CG	16:U:191:ARG:HB2	2.03	0.78
1:A:1462:PRO:HG3	7:G:19:GLY:H	1.47	0.78
18:W:394:PHE:CE2	18:W:396:GLU:HG2	2.18	0.78
1:A:1206:ASP:HB2	16:U:228:ASN:CG	2.04	0.78
1:A:831:LYS:CE	16:U:262:THR:HA	2.13	0.78
16:U:133:ILE:CG2	16:U:155:ILE:CG2	2.32	0.78
1:A:1085:THR:CA	16:U:260:LYS:HZ1	1.93	0.78
1:A:285:SER:HB2	1:A:290:ILE:HD11	1.65	0.78
4:D:34:PHE:CZ	7:G:3:PHE:HD2	2.02	0.78
14:T:-7:DG:C2'	14:T:-6:DC:H5''	2.14	0.78
1:A:831:LYS:HZ1	16:U:262:THR:CG2	1.96	0.78
14:T:-18:DT:N3	15:N:19:DA:H2	1.73	0.78
4:D:5:THR:O	7:G:7:LEU:CD2	2.30	0.77
12:L:68:GLN:OE1	18:W:767:ILE:HG12	1.84	0.77
18:W:664:VAL:CG2	18:W:686:LEU:HD11	2.08	0.77
4:D:19:VAL:O	4:D:19:VAL:CG1	2.32	0.77
18:W:679:VAL:HA	18:W:684:LEU:HD23	1.66	0.77
2:B:288:GLU:O	2:B:292:HIS:ND1	2.17	0.77
18:W:319:LYS:O	18:W:320:LEU:CB	2.33	0.77
1:A:41:MET:HA	1:A:41:MET:CE	2.15	0.76
4:D:34:PHE:HE1	7:G:3:PHE:HB2	1.50	0.76
16:U:176:ARG:O	16:U:180:MET:HG2	1.85	0.76
1:A:831:LYS:CE	16:U:262:THR:O	2.33	0.76
1:A:831:LYS:HA	1:A:1083:LEU:CD2	2.14	0.76
2:B:904:ARG:NH2	18:W:786:ASN:HA	2.00	0.76
2:B:70:ASN:ND2	2:B:128:ASP:O	2.19	0.76
2:B:55:ARG:HD2	2:B:76:GLU:OE2	1.85	0.76
4:D:34:PHE:CG	7:G:3:PHE:CZ	2.74	0.76
7:G:8:SER:HA	7:G:72:VAL:O	1.86	0.76
14:T:-20:DA:H2''	14:T:-19:DC:O5'	1.82	0.76
18:W:317:ASP:O	18:W:319:LYS:N	2.18	0.76
1:A:48:PRO:CG	1:A:56:PRO:HD3	2.14	0.76
1:A:1286:TYR:HD1	16:U:234:GLY:CA	1.99	0.76
7:G:100:PHE:CZ	18:W:698:PHE:CD1	2.52	0.76
18:W:674:GLY:CA	18:W:687:ARG:O	2.33	0.76
1:A:1085:THR:HA	16:U:260:LYS:HZ3	0.72	0.75
1:A:1364:SER:OG	16:U:283:LYS:HD3	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:16:DT:H2'	15:N:17:DA:C8	2.21	0.75
1:A:1154:ILE:HD12	9:I:44:TYR:HB3	1.68	0.75
5:E:158:GLY:O	5:E:161:SER:N	2.18	0.75
18:W:664:VAL:HG11	18:W:676:ILE:CD1	2.15	0.75
4:D:30:LEU:O	7:G:82:PHE:CE1	2.39	0.75
16:U:133:ILE:HG21	16:U:155:ILE:HG23	1.61	0.75
16:U:245:PHE:HB2	16:U:255:VAL:HG11	1.66	0.75
1:A:1080:GLN:CA	16:U:262:THR:HG21	1.99	0.74
5:E:102:LYS:O	5:E:103:ASN:OD1	2.04	0.74
1:A:831:LYS:CA	1:A:1083:LEU:HD22	2.16	0.74
1:A:1206:ASP:CB	16:U:228:ASN:ND2	2.51	0.74
2:B:83:TYR:HB2	2:B:116:TYR:HB2	1.70	0.74
7:G:132:SER:HB2	7:G:135:GLU:HB2	1.69	0.74
16:U:148:ILE:O	16:U:152:VAL:HG23	1.88	0.74
1:A:1202:ALA:CA	16:U:224:ILE:CG2	2.64	0.74
12:L:62:ARG:CD	12:L:63:THR:O	2.35	0.74
18:W:333:PHE:CD1	18:W:354:LEU:CD2	2.65	0.74
18:W:684:LEU:HD11	18:W:699:VAL:CG1	2.17	0.73
18:W:396:GLU:OE2	18:W:414:VAL:CG2	2.36	0.73
4:D:34:PHE:CE1	7:G:3:PHE:HB2	2.21	0.73
18:W:328:VAL:HG22	18:W:435:LEU:HD21	1.70	0.73
2:B:946:ASN:HB3	18:W:786:ASN:HB3	1.70	0.73
16:U:133:ILE:CB	16:U:155:ILE:HG21	2.18	0.73
8:H:112:LYS:HG2	8:H:125:GLU:HG2	1.70	0.73
16:U:133:ILE:CD1	16:U:155:ILE:CG2	2.61	0.73
1:A:1363:GLY:HA2	16:U:281:ARG:O	1.89	0.73
2:B:307:LYS:HZ1	9:I:13:MET:CE	2.01	0.73
15:N:-7:DA:C2'	15:N:-6:DA:N7	2.51	0.73
4:D:7:THR:HG21	7:G:6:ASP:HB2	1.70	0.72
1:A:1362:ASP:O	16:U:283:LYS:HD2	1.90	0.72
1:A:1447:MET:CE	7:G:60:ARG:CG	2.65	0.72
18:W:326:VAL:HG21	18:W:435:LEU:HD13	1.71	0.72
2:B:1221:SER:CB	4:D:12:ARG:HH12	2.02	0.72
12:L:68:GLN:CD	18:W:767:ILE:CG1	2.57	0.71
1:A:43:GLU:OE1	18:W:443:THR:HG21	1.90	0.71
15:N:14:DG:H2''	15:N:15:DG:H5'	1.71	0.71
2:B:58:LEU:HB2	2:B:75:TYR:HB2	1.73	0.71
1:A:699:GLN:O	9:I:98:THR:HG22	1.90	0.71
13:P:1:A:N7	13:P:2:U:C4	2.58	0.71
2:B:307:LYS:HZ2	9:I:13:MET:HE1	1.51	0.71
2:B:818:PRO:HG3	10:J:53:VAL:HG21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:684:LEU:HD11	18:W:699:VAL:HG22	1.71	0.71
1:A:310:ALA:CB	14:T:-4:DG:H5'	2.21	0.71
4:D:34:PHE:CD1	7:G:3:PHE:CE1	2.79	0.71
18:W:323:GLY:HA2	18:W:339:GLN:HE21	1.55	0.71
1:A:1232:GLU:CD	16:U:180:MET:CB	2.57	0.70
18:W:682:ASN:O	18:W:698:PHE:HD1	1.72	0.70
1:A:1232:GLU:HG2	16:U:180:MET:HG3	1.70	0.70
1:A:1447:MET:HE1	7:G:60:ARG:CG	2.20	0.70
18:W:666:GLU:OE1	18:W:671:ARG:CB	2.39	0.70
5:E:100:GLN:HE21	5:E:126:VAL:HA	1.57	0.70
1:A:974:HIS:O	1:A:977:ARG:NH1	2.24	0.70
4:D:6:SER:HB2	7:G:5:LYS:HE3	1.73	0.70
4:D:52:SER:O	4:D:56:SER:OG	2.05	0.70
16:U:189:THR:O	16:U:193:SER:CB	2.39	0.70
1:A:1232:GLU:OE2	16:U:180:MET:CG	2.39	0.70
2:B:489:ARG:NH2	2:B:533:SER:O	2.24	0.70
4:D:140:PHE:HE1	7:G:1:MET:SD	2.14	0.70
7:G:39:THR:O	7:G:43:GLY:N	2.24	0.70
4:D:23:GLU:HG2	7:G:82:PHE:CD1	2.26	0.70
18:W:320:LEU:HD22	18:W:432:LEU:HD11	1.74	0.70
16:U:184:ASN:O	16:U:185:LYS:C	2.30	0.70
1:A:1447:MET:CE	7:G:60:ARG:CA	2.69	0.69
7:G:91:VAL:HA	7:G:101:ALA:HA	1.73	0.69
18:W:674:GLY:HA2	18:W:687:ARG:O	1.92	0.69
1:A:184:GLY:O	1:A:200:ARG:HA	1.91	0.69
4:D:6:SER:HB3	7:G:7:LEU:CD2	2.22	0.69
2:B:1221:SER:HB3	4:D:12:ARG:HH22	1.57	0.69
3:C:88:GLU:OE2	18:W:759:ARG:NH1	2.26	0.69
3:C:90:TYR:OH	3:C:156:ARG:NH2	2.24	0.69
18:W:748:ARG:O	18:W:749:ASP:HB2	1.92	0.69
1:A:831:LYS:HZ1	16:U:262:THR:CB	2.04	0.69
1:A:1462:PRO:HD3	7:G:19:GLY:C	2.13	0.69
16:U:133:ILE:HD13	16:U:155:ILE:HB	1.74	0.69
1:A:1134:LYS:HG2	16:U:229:LEU:HD13	1.74	0.69
1:A:1226:LEU:HD11	1:A:1242:CYS:HB3	1.74	0.69
2:B:653:ARG:CD	2:B:657:GLN:HE22	2.05	0.69
3:C:49:GLU:HG2	12:L:68:GLN:HG2	1.73	0.69
16:U:140:ASP:HB2	16:U:191:ARG:CD	2.23	0.69
18:W:664:VAL:HG21	18:W:686:LEU:CD2	2.22	0.69
1:A:588:HIS:NE2	1:A:971:GLN:OE1	2.24	0.69
15:N:15:DG:H1'	15:N:16:DT:O4'	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:332:LYS:HG3	18:W:388:ARG:CB	2.22	0.69
18:W:357:ARG:HB3	18:W:389:PRO:CD	2.22	0.69
18:W:666:GLU:OE1	18:W:671:ARG:CA	2.41	0.69
16:U:137:LEU:HD11	16:U:182:LEU:HD13	1.75	0.69
16:U:173:ASN:OD1	16:U:176:ARG:NH1	2.26	0.69
18:W:684:LEU:CD1	18:W:699:VAL:CA	2.64	0.69
1:A:1450:GLU:CD	7:G:58:LYS:HE2	2.07	0.68
18:W:357:ARG:HB3	18:W:389:PRO:HG2	1.75	0.68
1:A:831:LYS:HA	1:A:1083:LEU:HD22	1.74	0.68
4:D:23:GLU:OE2	7:G:82:PHE:CD1	2.46	0.68
15:N:16:DT:H2'	15:N:17:DA:H8	1.55	0.68
3:C:90:TYR:HH	3:C:156:ARG:HH22	1.42	0.68
18:W:667:PHE:CB	18:W:701:SER:O	2.41	0.68
1:A:41:MET:HA	1:A:41:MET:HE2	1.74	0.68
18:W:357:ARG:O	18:W:389:PRO:HG2	1.94	0.68
2:B:1106:ARG:HE	2:B:1109:GLY:H	1.39	0.68
16:U:183:LYS:O	16:U:183:LYS:CG	2.34	0.68
18:W:318:VAL:HG12	18:W:318:VAL:O	1.94	0.68
1:A:48:PRO:HG2	1:A:56:PRO:HD3	1.75	0.67
4:D:34:PHE:CD2	7:G:3:PHE:CE2	2.82	0.67
4:D:112:PHE:CE1	7:G:142:LYS:CD	2.76	0.67
18:W:329:LYS:CD	18:W:436:ILE:HG13	2.24	0.67
1:A:1363:GLY:N	16:U:282:TRP:HA	2.06	0.67
1:A:1462:PRO:CD	7:G:21:GLN:H	2.07	0.67
4:D:112:PHE:HE1	7:G:142:LYS:HD3	1.56	0.67
4:D:41:HIS:HE2	7:G:74:TYR:C	1.98	0.67
5:E:19:LYS:NZ	5:E:33:GLU:O	2.26	0.67
16:U:130:ILE:HG23	16:U:134:TYR:CE2	2.30	0.67
2:B:324:ASP:OD2	2:B:328:ARG:NE	2.28	0.67
16:U:189:THR:O	16:U:193:SER:OG	2.13	0.67
18:W:399:ALA:CA	18:W:406:ILE:HD11	2.23	0.67
4:D:41:HIS:HE1	7:G:74:TYR:O	1.76	0.67
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.27	0.67
4:D:6:SER:HA	7:G:7:LEU:HA	1.77	0.67
4:D:34:PHE:CD1	7:G:3:PHE:CZ	2.83	0.67
18:W:352:LEU:CD1	18:W:435:LEU:HD11	2.19	0.66
1:A:1286:TYR:CD1	16:U:234:GLY:HA3	2.29	0.66
7:G:46:VAL:HG12	7:G:47:THR:HG23	1.78	0.66
18:W:329:LYS:HD2	18:W:436:ILE:CG1	2.25	0.66
1:A:1446:VAL:O	7:G:61:ILE:CB	2.42	0.66
7:G:97:ILE:O	7:G:97:ILE:HG22	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:183:LYS:HZ2	16:U:185:LYS:HE3	1.60	0.66
1:A:995:LEU:HD22	1:A:1048:LEU:HD22	1.76	0.66
1:A:132:LYS:NZ	1:A:1420:GLU:OE2	2.28	0.66
1:A:557:TRP:O	11:K:26:ARG:NH1	2.27	0.66
16:U:133:ILE:CD1	16:U:155:ILE:HB	2.25	0.66
1:A:1264:LYS:HE2	9:I:44:TYR:CD1	2.30	0.66
2:B:607:SER:HB2	2:B:620:PHE:HB2	1.77	0.66
4:D:34:PHE:HD1	7:G:3:PHE:CD1	2.10	0.66
18:W:409:ASP:O	18:W:410:ARG:CG	2.43	0.66
14:T:-13:DC:H2'	14:T:-12:DG:C8	2.31	0.66
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.28	0.66
5:E:181:ASP:O	5:E:184:ALA:N	2.24	0.66
16:U:133:ILE:HB	16:U:155:ILE:HD13	1.77	0.66
1:A:887:ILE:O	1:A:945:ARG:NH2	2.29	0.65
1:A:948:VAL:HA	5:E:200:ARG:HD2	1.78	0.65
2:B:70:ASN:O	2:B:127:ILE:CB	2.43	0.65
16:U:183:LYS:HZ1	16:U:185:LYS:HE3	1.60	0.65
1:A:831:LYS:HB3	1:A:1083:LEU:HB2	1.78	0.65
4:D:95:GLY:O	4:D:99:ASN:ND2	2.29	0.65
4:D:140:PHE:CE1	7:G:1:MET:SD	2.89	0.65
16:U:134:TYR:OH	16:U:152:VAL:HG22	1.96	0.65
18:W:664:VAL:HG23	18:W:686:LEU:CD1	2.14	0.65
1:A:1447:MET:SD	7:G:60:ARG:CA	2.83	0.65
16:U:133:ILE:HG21	16:U:155:ILE:HG21	0.67	0.65
16:U:194:ILE:O	16:U:198:GLU:OE2	2.15	0.65
1:A:1363:GLY:HA2	16:U:282:TRP:CA	2.07	0.65
16:U:133:ILE:CD1	16:U:155:ILE:HG21	2.25	0.65
2:B:63:GLN:NE2	18:W:248:LEU:HB3	2.09	0.65
2:B:352:GLU:O	2:B:355:PRO:HD3	1.97	0.65
13:P:-2:U:H6	13:P:-2:U:O5'	1.79	0.65
1:A:1205:LEU:HD21	16:U:221:MET:O	1.97	0.65
1:A:1085:THR:HA	16:U:260:LYS:CE	2.27	0.65
1:A:828:THR:OG1	16:U:261:GLN:HG2	1.97	0.64
16:U:156:GLU:O	16:U:160:PHE:HD2	1.79	0.64
18:W:332:LYS:HG3	18:W:388:ARG:HB3	1.78	0.64
1:A:48:PRO:HG3	1:A:56:PRO:HD3	1.79	0.64
14:T:1:DA:H2'	14:T:2:DC:H6	1.61	0.64
2:B:287:GLY:O	2:B:291:GLN:CB	2.44	0.64
2:B:688:GLU:OE2	2:B:740:HIS:NE2	2.19	0.64
3:C:91:CYS:SG	3:C:92:ASP:N	2.70	0.64
15:N:15:DG:H2''	15:N:16:DT:C5'	2.20	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:154:ASP:O	16:U:158:GLN:HG3	1.97	0.64
18:W:351:ARG:HG2	18:W:429:THR:HG22	1.77	0.64
18:W:409:ASP:CB	18:W:413:PHE:CE2	2.80	0.64
18:W:666:GLU:N	18:W:672:ARG:O	2.30	0.64
1:A:43:GLU:OE1	18:W:443:THR:CG2	2.45	0.64
1:A:1286:TYR:HB2	1:A:1310:GLU:O	1.97	0.64
5:E:61:ALA:HB3	5:E:77:LEU:HB3	1.80	0.64
1:A:1462:PRO:HD3	7:G:19:GLY:CA	2.28	0.64
18:W:664:VAL:CG1	18:W:676:ILE:HD11	2.21	0.64
1:A:828:THR:HG23	16:U:263:ARG:O	1.99	0.63
1:A:37:TYR:HE1	18:W:441:ASN:ND2	1.93	0.63
1:A:1234:ASN:HA	16:U:217:LEU:CD2	2.29	0.63
1:A:1447:MET:CE	7:G:60:ARG:CB	2.76	0.63
15:N:-11:DG:OP1	18:W:334:LYS:HE3	1.98	0.63
13:P:1:A:N7	13:P:2:U:C5	2.67	0.63
1:A:446:ASN:HD22	1:A:447:ARG:H	1.45	0.63
4:D:33:GLU:OE1	7:G:42:PHE:HZ	1.73	0.63
7:G:97:ILE:HG13	18:W:683:PHE:CD1	2.34	0.63
12:L:68:GLN:NE2	18:W:767:ILE:CD1	2.60	0.63
4:D:128:LEU:HD11	4:D:146:SER:HB2	1.80	0.63
1:A:1206:ASP:CA	16:U:228:ASN:ND2	2.61	0.63
14:T:1:DA:H2'	14:T:2:DC:C6	2.33	0.63
18:W:437:VAL:O	18:W:437:VAL:HG22	1.98	0.63
1:A:40:ILE:HG22	1:A:41:MET:CE	2.28	0.63
2:B:1187:ASN:HD21	2:B:1190:ASN:HB3	1.64	0.63
4:D:108:TYR:OH	7:G:88:ASP:HB2	1.99	0.63
14:T:-19:DC:H2'	14:T:-18:DT:C6	2.34	0.63
18:W:784:ASN:HB2	18:W:785:PRO:HD3	1.81	0.63
18:W:317:ASP:O	18:W:318:VAL:C	2.37	0.62
1:A:791:ASP:CG	9:I:87:GLN:HE21	2.02	0.62
7:G:158:TYR:CE1	18:W:700:THR:HG21	2.35	0.62
1:A:151:ASP:HA	1:A:164:SER:HA	1.81	0.62
1:A:982:ASP:O	1:A:1041:ARG:NH2	2.33	0.62
2:B:279:ARG:NH1	2:B:316:ILE:O	2.32	0.62
18:W:676:ILE:HA	18:W:686:LEU:CD2	2.29	0.62
3:C:74:GLU:O	3:C:246:ARG:NH2	2.32	0.62
15:N:-6:DA:OP2	15:N:-5:DT:H72	2.00	0.62
18:W:329:LYS:CG	18:W:436:ILE:HG13	2.29	0.62
1:A:1078:ALA:HA	1:A:1081:MET:HE3	1.82	0.62
1:A:1084:ASN:O	1:A:1086:PHE:N	2.31	0.62
2:B:316:ILE:HG21	2:B:322:ALA:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:672:ARG:HH12	18:W:691:ILE:HG13	1.63	0.62
1:A:113:LEU:O	1:A:165:ARG:NH2	2.33	0.62
1:A:1201:ARG:CZ	16:U:217:LEU:HD11	2.30	0.62
4:D:23:GLU:OE2	7:G:82:PHE:CE1	2.53	0.62
14:T:-5:DA:H5"	14:T:-5:DA:H8	1.63	0.62
1:A:1134:LYS:CE	16:U:229:LEU:HA	2.27	0.61
8:H:95:VAL:HG22	8:H:142:LEU:HG	1.82	0.61
1:A:53:LEU:O	1:A:248:ARG:NH2	2.32	0.61
4:D:112:PHE:HZ	7:G:142:LYS:CG	2.13	0.61
2:B:307:LYS:HZ1	9:I:13:MET:HE3	1.64	0.61
4:D:41:HIS:NE2	7:G:74:TYR:C	2.53	0.61
7:G:158:TYR:HB2	18:W:667:PHE:CE2	2.36	0.61
16:U:185:LYS:C	16:U:187:ASN:H	1.98	0.61
18:W:684:LEU:HD11	18:W:699:VAL:CB	2.30	0.61
1:A:610:ASP:OD1	1:A:971:GLN:NE2	2.32	0.61
2:B:71:ILE:HG12	2:B:73:LYS:CE	2.23	0.61
4:D:6:SER:HA	7:G:7:LEU:CD2	2.25	0.61
18:W:328:VAL:HG22	18:W:435:LEU:CD2	2.30	0.61
1:A:1079:THR:O	1:A:1079:THR:HG22	2.01	0.61
1:A:186:TRP:HZ3	1:A:201:LYS:HG2	1.64	0.61
1:A:1447:MET:HE3	7:G:60:ARG:CG	2.26	0.61
4:D:6:SER:CB	7:G:7:LEU:CD2	2.75	0.61
2:B:303:LEU:HD23	2:B:306:LEU:HD12	1.82	0.61
1:A:308:ASP:OD1	1:A:314:GLN:NE2	2.33	0.61
2:B:70:ASN:HD21	2:B:128:ASP:C	2.02	0.61
2:B:1038:ARG:HD2	2:B:1040:TYR:HE1	1.65	0.61
14:T:-20:DA:H61	15:N:21:DT:H3	1.47	0.61
2:B:1106:ARG:NH2	2:B:1110:PRO:O	2.32	0.61
1:A:286:PRO:HG3	18:W:268:PHE:CZ	2.36	0.60
1:A:708:GLY:O	1:A:1093:SER:OG	2.19	0.60
1:A:791:ASP:OD2	9:I:87:GLN:HG2	2.01	0.60
1:A:1423:ASP:O	1:A:1424:CYS:HB2	2.02	0.60
16:U:216:SER:C	16:U:219:LYS:HG2	2.21	0.60
1:A:114:LEU:HB3	1:A:145:LYS:HG2	1.82	0.60
2:B:262:LYS:HB3	2:B:271:ASP:HB3	1.83	0.60
2:B:291:GLN:NE2	2:B:563:ASP:OD1	2.34	0.60
4:D:23:GLU:HB2	7:G:83:LYS:H	1.65	0.60
1:A:255:GLU:HG2	2:B:935:ARG:HH12	1.67	0.60
1:A:307:ASN:ND2	1:A:323:VAL:O	2.34	0.60
3:C:217:GLU:HG2	3:C:218:VAL:O	2.02	0.60
16:U:135:THR:O	16:U:139:MET:HG2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:394:PHE:HE2	18:W:396:GLU:CG	2.14	0.60
1:A:708:GLY:C	1:A:1093:SER:CB	2.63	0.60
2:B:613:ARG:O	9:I:58:ILE:HD12	2.01	0.60
1:A:1083:LEU:HD12	1:A:1083:LEU:O	2.01	0.60
16:U:216:SER:CB	16:U:219:LYS:HE2	2.31	0.60
1:A:228:ASP:OD1	4:D:15:ALA:HB2	2.02	0.60
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.82	0.60
1:A:831:LYS:CA	1:A:1083:LEU:HD23	2.32	0.60
2:B:1129:ARG:HD3	14:T:2:DC:H5''	1.83	0.60
18:W:357:ARG:HB3	18:W:389:PRO:CG	2.31	0.60
4:D:34:PHE:HB3	7:G:3:PHE:CZ	2.37	0.60
7:G:158:TYR:CE1	18:W:700:THR:CG2	2.84	0.60
14:T:0:DT:C2	14:T:1:DA:C8	2.89	0.60
18:W:319:LYS:O	18:W:320:LEU:HB3	2.02	0.60
16:U:192:ARG:HD2	16:U:192:ARG:O	2.02	0.59
18:W:396:GLU:CD	18:W:414:VAL:CG2	2.70	0.59
1:A:286:PRO:CG	18:W:268:PHE:CE1	2.76	0.59
2:B:653:ARG:HD3	2:B:657:GLN:CD	2.10	0.59
4:D:66:ALA:O	4:D:70:ALA:HB2	2.01	0.59
16:U:129:SER:O	16:U:133:ILE:HG13	2.02	0.59
18:W:413:PHE:CE1	18:W:420:GLU:HB3	2.38	0.59
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	1.83	0.59
3:C:18:GLU:OE2	3:C:206:TYR:OH	2.15	0.59
4:D:121:CYS:O	4:D:125:ASP:HB2	2.02	0.59
7:G:100:PHE:HB3	7:G:107:ASN:HD21	1.67	0.59
11:K:29:ASN:ND2	11:K:78:GLU:O	2.35	0.59
16:U:131:SER:O	16:U:135:THR:HG23	2.01	0.59
17:V:44:ALA:O	17:V:48:GLU:HG2	2.01	0.59
4:D:96:ALA:HA	4:D:99:ASN:HD22	1.67	0.59
4:D:112:PHE:CZ	7:G:142:LYS:CE	2.86	0.59
7:G:4:LEU:HA	7:G:76:ALA:O	2.02	0.59
16:U:185:LYS:C	16:U:187:ASN:N	2.56	0.59
1:A:1462:PRO:HG3	7:G:19:GLY:N	2.16	0.59
5:E:213:CYS:SG	5:E:214:LEU:N	2.75	0.59
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.85	0.59
1:A:504:GLN:OE1	6:F:90:ARG:NH1	2.33	0.59
1:A:1462:PRO:HD2	7:G:21:GLN:H	1.67	0.59
1:A:1054:GLN:HG2	1:A:1057:ARG:HH21	1.67	0.59
13:P:2:U:H2'	13:P:3:C:C6	2.36	0.59
1:A:1363:GLY:HA3	16:U:282:TRP:C	2.23	0.59
14:T:-18:DT:H2'	14:T:-17:DC:C6	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:397:ALA:O	18:W:401:VAL:HG23	2.03	0.59
1:A:270:ILE:HG12	1:A:300:HIS:HB3	1.84	0.58
2:B:823:ALA:O	2:B:1089:PRO:HA	2.03	0.58
18:W:399:ALA:O	18:W:406:ILE:CD1	2.50	0.58
7:G:4:LEU:HD22	7:G:49:LEU:HD11	1.84	0.58
1:A:1462:PRO:HD3	7:G:19:GLY:HA3	1.85	0.58
2:B:276:ILE:O	2:B:280:ALA:HB2	2.04	0.58
16:U:208:SER:HB3	16:U:211:GLU:HB3	1.84	0.58
18:W:698:PHE:CE2	18:W:700:THR:HB	2.38	0.58
1:A:709:MET:CG	1:A:1091:VAL:HG13	2.32	0.58
2:B:451:LYS:O	2:B:455:ALA:HB2	2.03	0.58
4:D:7:THR:CG2	7:G:6:ASP:O	2.40	0.58
4:D:112:PHE:HZ	7:G:142:LYS:HG2	1.67	0.58
9:I:88:SER:O	9:I:89:GLN:NE2	2.37	0.58
16:U:160:PHE:HA	16:U:163:VAL:HG23	1.86	0.58
1:A:286:PRO:HG3	18:W:268:PHE:HZ	1.67	0.58
18:W:328:VAL:HA	18:W:435:LEU:CD2	2.33	0.58
18:W:684:LEU:HD11	18:W:699:VAL:CG2	2.32	0.58
16:U:126:ARG:O	16:U:130:ILE:HD12	2.03	0.58
16:U:160:PHE:O	16:U:163:VAL:HB	2.04	0.58
2:B:500:LYS:HG2	2:B:501:LEU:N	2.15	0.58
10:J:7:CYS:SG	10:J:8:PHE:N	2.77	0.58
18:W:389:PRO:HD2	18:W:389:PRO:O	2.04	0.58
1:A:1361:PHE:CZ	16:U:281:ARG:NH1	2.70	0.57
1:A:1446:VAL:O	7:G:61:ILE:CG1	2.51	0.57
4:D:33:GLU:HG3	7:G:41:GLN:O	2.04	0.57
4:D:112:PHE:CZ	7:G:142:LYS:HE3	2.39	0.57
1:A:128:ILE:O	1:A:134:ARG:NH2	2.37	0.57
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	1.84	0.57
18:W:394:PHE:CE2	18:W:396:GLU:CG	2.86	0.57
16:U:133:ILE:O	16:U:137:LEU:HB2	2.04	0.57
16:U:137:LEU:CD1	16:U:182:LEU:HD13	2.33	0.57
2:B:71:ILE:HG23	2:B:71:ILE:O	2.03	0.57
2:B:279:ARG:HG2	2:B:284:VAL:HA	1.85	0.57
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.20	0.57
1:A:47:ARG:CB	1:A:48:PRO:HD2	2.14	0.57
2:B:105:ARG:NH2	2:B:193:TYR:OH	2.37	0.57
1:A:22:LEU:HD12	2:B:1211:ASN:HA	1.87	0.57
1:A:35:ILE:HG13	1:A:242:VAL:HG21	1.87	0.57
1:A:446:ASN:HD22	1:A:447:ARG:N	2.02	0.57
2:B:590:VAL:HG12	2:B:617:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:-16:DT:H2"	14:T:-15:DA:C8	2.40	0.57
18:W:674:GLY:HA3	18:W:687:ARG:O	2.04	0.57
2:B:164:MET:HB2	2:B:194:PHE:HE1	1.70	0.57
1:A:369:ILE:HG22	1:A:373:LYS:HE2	1.86	0.57
1:A:1232:GLU:CG	16:U:180:MET:HG3	2.30	0.57
1:A:1235:ALA:HA	16:U:184:ASN:HD21	1.70	0.57
18:W:319:LYS:O	18:W:320:LEU:HB2	2.03	0.57
1:A:1286:TYR:CD1	16:U:234:GLY:CA	2.85	0.56
4:D:33:GLU:HB3	7:G:42:PHE:CE1	2.40	0.56
4:D:169:VAL:HG12	4:D:171:LEU:H	1.69	0.56
18:W:317:ASP:O	18:W:319:LYS:CG	2.42	0.56
1:A:977:ARG:HA	1:A:978:ALA:HB3	1.87	0.56
2:B:90:THR:HA	2:B:96:THR:HG22	1.87	0.56
7:G:97:ILE:CG1	18:W:683:PHE:CD1	2.88	0.56
1:A:745:LYS:O	1:A:749:SER:CB	2.54	0.56
1:A:738:LEU:HD22	1:A:742:ASN:HD22	1.71	0.56
1:A:1403:CYS:HB2	1:A:1408:THR:HG23	1.87	0.56
2:B:177:GLU:O	2:B:180:LEU:N	2.38	0.56
2:B:336:ILE:O	2:B:341:ARG:NE	2.39	0.56
4:D:86:ASP:OD2	4:D:110:ASN:ND2	2.36	0.56
4:D:138:HIS:HB3	4:D:141:GLU:HG2	1.87	0.56
2:B:55:ARG:CD	2:B:76:GLU:OE2	2.53	0.56
2:B:918:ILE:HD11	2:B:935:ARG:HB2	1.87	0.56
3:C:145:CYS:SG	3:C:146:LYS:N	2.79	0.56
18:W:664:VAL:HG21	18:W:686:LEU:HD21	1.87	0.56
1:A:483:PHE:HD2	2:B:836:GLU:HB2	1.70	0.56
18:W:332:LYS:HG3	18:W:388:ARG:HB2	1.86	0.56
7:G:12:THR:HA	7:G:68:ALA:O	2.06	0.56
16:U:194:ILE:HA	16:U:198:GLU:CD	2.26	0.56
1:A:168:CYS:SG	1:A:170:ASN:ND2	2.79	0.56
1:A:1451:LYS:O	1:A:1454:THR:OG1	2.20	0.56
18:W:666:GLU:CD	18:W:671:ARG:HB2	2.26	0.56
1:A:350:ALA:O	1:A:489:ASN:HA	2.07	0.55
1:A:974:HIS:O	1:A:976:ASP:N	2.38	0.55
7:G:97:ILE:HG13	18:W:683:PHE:CG	2.41	0.55
16:U:181:ASN:ND2	16:U:212:LEU:HD11	2.19	0.55
1:A:1137:GLN:NE2	16:U:232:ALA:C	2.59	0.55
18:W:683:PHE:N	18:W:683:PHE:CD2	2.73	0.55
1:A:15:LYS:O	1:A:1424:CYS:HB2	2.06	0.55
1:A:1100:VAL:HB	1:A:1101:PRO:CD	2.30	0.55
1:A:1202:ALA:CB	16:U:224:ILE:HG23	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:-17:DC:H2''	14:T:-16:DT:OP1	2.06	0.55
16:U:183:LYS:NZ	16:U:185:LYS:CE	2.63	0.55
16:U:190:LEU:O	16:U:194:ILE:HB	2.07	0.55
1:A:337:LEU:HD23	1:A:341:LEU:HD12	1.88	0.55
16:U:134:TYR:CZ	16:U:152:VAL:HG22	2.41	0.55
1:A:47:ARG:CB	1:A:48:PRO:CD	2.61	0.55
2:B:904:ARG:HH21	18:W:786:ASN:CA	2.09	0.55
16:U:216:SER:OG	16:U:219:LYS:HE2	2.06	0.55
18:W:409:ASP:HB2	18:W:413:PHE:CE2	2.35	0.55
1:A:1271:LEU:HD13	9:I:48:LEU:CD1	2.23	0.55
18:W:344:LEU:CD1	18:W:349:GLU:HB2	2.35	0.55
1:A:317:GLN:HG3	1:A:318:LYS:H	1.71	0.55
1:A:1447:MET:HE1	7:G:60:ARG:CB	2.36	0.55
18:W:396:GLU:CD	18:W:414:VAL:HG21	2.27	0.55
18:W:748:ARG:O	18:W:749:ASP:CB	2.54	0.55
1:A:828:THR:CG2	16:U:264:SER:HA	2.36	0.54
1:A:831:LYS:CB	1:A:1083:LEU:HD23	2.26	0.54
1:A:1389:ARG:NH1	1:A:1407:GLU:OE2	2.40	0.54
4:D:33:GLU:OE1	7:G:42:PHE:CE1	2.58	0.54
1:A:41:MET:CE	1:A:41:MET:CA	2.86	0.54
7:G:125:ASN:HD22	7:G:126:SER:H	1.55	0.54
14:T:-6:DC:C2'	14:T:-5:DA:C8	2.91	0.54
1:A:941:ARG:HH21	1:A:945:ARG:HH22	1.55	0.54
2:B:223:SER:O	2:B:252:ARG:NH2	2.36	0.54
3:C:79:MET:O	3:C:161:LYS:NZ	2.34	0.54
18:W:684:LEU:CD1	18:W:699:VAL:CG2	2.80	0.54
1:A:243:PRO:O	1:A:248:ARG:NH1	2.41	0.54
1:A:1361:PHE:O	16:U:281:ARG:HD3	2.07	0.54
1:A:831:LYS:HB3	1:A:1083:LEU:CB	2.38	0.54
1:A:1362:ASP:HB2	16:U:272:PHE:CD1	2.43	0.54
1:A:1462:PRO:HD3	7:G:21:GLN:H	1.71	0.54
1:A:379:GLU:O	1:A:432:LYS:HA	2.07	0.54
16:U:147:LYS:H	16:U:147:LYS:HD2	1.72	0.54
1:A:286:PRO:HG2	18:W:268:PHE:HE1	1.67	0.54
4:D:112:PHE:HZ	7:G:142:LYS:CD	2.20	0.54
18:W:352:LEU:HD11	18:W:435:LEU:HD21	1.90	0.54
1:A:564:PRO:HG2	1:A:567:LEU:HD23	1.89	0.54
1:A:661:ASN:ND2	2:B:1082:MET:HB3	2.23	0.54
1:A:941:ARG:HH21	1:A:945:ARG:NH2	2.05	0.54
2:B:804:ALA:HB3	2:B:983:ARG:HH22	1.72	0.54
2:B:1010:LEU:HD22	2:B:1092:TYR:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:71:TYR:OH	5:E:154:ARG:O	2.23	0.54
8:H:38:LEU:HD13	8:H:124:LEU:HD13	1.90	0.54
4:D:99:ASN:O	4:D:103:LYS:HB2	2.07	0.54
6:F:140:ASP:OD1	6:F:141:GLY:N	2.41	0.54
16:U:140:ASP:CB	16:U:191:ARG:HB2	2.37	0.54
16:U:214:PRO:HD2	16:U:217:LEU:HB3	1.90	0.54
18:W:676:ILE:HG13	18:W:686:LEU:HD21	1.80	0.54
1:A:1148:VAL:HG23	1:A:1199:LEU:HD22	1.90	0.54
2:B:27:GLU:OE1	2:B:678:TRP:HB3	2.07	0.54
7:G:151:ARG:HG2	18:W:667:PHE:O	2.08	0.54
1:A:1078:ALA:HA	1:A:1081:MET:CE	2.38	0.53
4:D:34:PHE:CE2	7:G:3:PHE:CD2	2.96	0.53
13:P:-1:U:H2'	13:P:-1:U:O2	2.07	0.53
1:A:1363:GLY:HA3	16:U:283:LYS:N	2.24	0.53
11:K:14:ASP:OD1	11:K:15:ASP:N	2.42	0.53
15:N:-8:DA:C4'	15:N:-7:DA:OP1	2.39	0.53
4:D:34:PHE:CB	7:G:3:PHE:CZ	2.91	0.53
4:D:87:ASP:OD1	4:D:103:LYS:HG3	2.09	0.53
7:G:95:SER:O	7:G:130:TYR:OH	2.26	0.53
1:A:109:ASN:HD22	1:A:170:ASN:ND2	2.06	0.53
13:P:-3:U:H3'	13:P:-2:U:C5	2.44	0.53
18:W:665:ARG:HB2	18:W:705:VAL:HG11	1.90	0.53
1:A:351:ARG:HB2	2:B:1128:LEU:HD11	1.89	0.53
6:F:107:VAL:HB	6:F:111:ILE:HD11	1.91	0.53
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.89	0.53
8:H:60:ALA:O	8:H:140:TYR:HB2	2.09	0.53
2:B:195:VAL:HA	2:B:199:SER:O	2.09	0.53
1:A:1056:GLN:HB3	6:F:84:TYR:HE2	1.74	0.53
1:A:852:HIS:HB3	6:F:139:PRO:HG3	1.91	0.53
4:D:23:GLU:O	7:G:83:LYS:CB	2.41	0.53
18:W:409:ASP:OD2	18:W:415:THR:OG1	2.21	0.53
18:W:682:ASN:O	18:W:698:PHE:CD1	2.59	0.53
16:U:183:LYS:HZ2	16:U:185:LYS:CE	2.22	0.53
1:A:109:ASN:HD22	1:A:170:ASN:HD21	1.57	0.53
2:B:300:TRP:HA	2:B:303:LEU:HB2	1.91	0.53
16:U:216:SER:CA	16:U:219:LYS:HE2	2.39	0.53
17:V:43:GLN:NE2	17:V:47:ASN:OD1	2.39	0.53
1:A:1137:GLN:HE21	16:U:232:ALA:HB1	1.68	0.52
2:B:946:ASN:CB	18:W:786:ASN:HB3	2.36	0.52
18:W:664:VAL:CG1	18:W:676:ILE:CD1	2.85	0.52
2:B:354:LEU:HB3	2:B:357:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:100:VAL:HG22	8:H:115:VAL:HG22	1.92	0.52
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.92	0.52
2:B:451:LYS:O	2:B:455:ALA:CB	2.57	0.52
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.36	0.52
4:D:6:SER:CA	7:G:7:LEU:CD2	2.81	0.52
1:A:1088:TYR:OH	16:U:237:GLU:CG	2.58	0.52
1:A:1232:GLU:OE2	16:U:176:ARG:O	2.28	0.52
1:A:680:ILE:HG23	1:A:730:ALA:HB1	1.90	0.52
15:N:15:DG:H1'	15:N:16:DT:C4'	2.39	0.52
1:A:1160:PRO:HB3	1:A:1190:GLN:HE21	1.75	0.52
2:B:827:ILE:HG22	2:B:1014:PRO:HG3	1.92	0.52
4:D:49:ILE:HG21	7:G:4:LEU:CD1	2.38	0.52
14:T:-15:DA:H8	14:T:-15:DA:OP2	1.92	0.52
17:V:41:SER:HB2	17:V:45:THR:HB	1.91	0.52
18:W:672:ARG:NH1	18:W:691:ILE:HG13	2.24	0.52
2:B:563:ASP:HB3	2:B:566:GLN:HB3	1.91	0.52
2:B:883:LEU:HB3	2:B:932:HIS:CE1	2.45	0.52
4:D:137:LEU:HB3	4:D:142:ILE:HD11	1.91	0.52
1:A:1206:ASP:CB	16:U:228:ASN:CG	2.76	0.52
3:C:148:ARG:NH1	10:J:61:ARG:HA	2.25	0.52
4:D:48:LEU:HD11	7:G:3:PHE:CE1	2.45	0.52
4:D:176:ASP:O	4:D:180:ARG:HB2	2.09	0.52
2:B:332:ALA:HB2	2:B:344:TYR:CZ	2.45	0.52
2:B:369:PHE:HB3	2:B:579:TRP:HZ3	1.74	0.52
2:B:826:ALA:O	2:B:1011:ILE:HA	2.10	0.52
1:A:10:PRO:HG2	2:B:1192:TYR:CD1	2.46	0.51
1:A:803:ASN:ND2	2:B:725:ARG:HB2	2.25	0.51
2:B:72:ASN:O	2:B:125:THR:CA	2.53	0.51
4:D:23:GLU:HB3	7:G:82:PHE:CB	2.34	0.51
5:E:126:VAL:HG11	5:E:131:ILE:HG12	1.92	0.51
18:W:332:LYS:CG	18:W:388:ARG:HB2	2.39	0.51
1:A:447:ARG:HB2	1:A:488:MET:HE3	1.91	0.51
1:A:699:GLN:CD	9:I:99:LEU:HD11	2.30	0.51
1:A:713:GLU:CD	1:A:1092:SER:OG	2.49	0.51
1:A:1362:ASP:O	16:U:283:LYS:CD	2.58	0.51
7:G:89:ALA:HB2	7:G:103:VAL:HG22	1.92	0.51
7:G:97:ILE:CG1	18:W:683:PHE:CG	2.93	0.51
16:U:181:ASN:HD22	16:U:212:LEU:HD13	1.75	0.51
16:U:176:ARG:O	16:U:180:MET:CG	2.58	0.51
1:A:349:SER:HB2	2:B:1128:LEU:HD12	1.93	0.51
1:A:1104:LYS:O	1:A:1108:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1373:LEU:O	1:A:1377:VAL:HG23	2.11	0.51
1:A:1197:LEU:HD11	1:A:1240:ILE:HD12	1.92	0.51
14:T:-16:DT:H2''	14:T:-15:DA:N7	2.26	0.51
16:U:130:ILE:HG22	16:U:134:TYR:CD1	2.45	0.51
1:A:1085:THR:C	16:U:260:LYS:HZ1	2.13	0.51
16:U:271:THR:HB	16:U:284:PHE:HB2	1.93	0.51
5:E:158:GLY:O	5:E:160:LYS:N	2.44	0.51
13:P:1:A:C5	13:P:2:U:C4	2.99	0.51
1:A:831:LYS:NZ	16:U:262:THR:CB	2.68	0.51
2:B:156:VAL:HG11	2:B:441:VAL:HG21	1.93	0.51
2:B:500:LYS:CG	2:B:501:LEU:H	2.15	0.51
7:G:153:ASP:O	7:G:155:ASN:N	2.42	0.51
12:L:68:GLN:NE2	18:W:767:ILE:CG1	2.73	0.51
1:A:671:ILE:HG12	1:A:806:LEU:HD21	1.93	0.51
4:D:34:PHE:HE2	7:G:80:LYS:HB3	1.74	0.51
4:D:112:PHE:CZ	7:G:142:LYS:CG	2.92	0.51
13:P:-2:U:OP2	13:P:-2:U:H5	1.94	0.51
18:W:805:VAL:HG12	18:W:808:GLU:HG2	1.93	0.51
7:G:49:LEU:N	7:G:75:ARG:O	2.33	0.51
7:G:149:GLY:O	7:G:159:ALA:HA	2.11	0.51
18:W:349:GLU:HG2	18:W:431:ARG:HA	1.92	0.51
18:W:679:VAL:HG13	18:W:684:LEU:HD21	1.92	0.51
1:A:871:GLU:OE1	5:E:201:SER:OG	2.21	0.50
4:D:148:LEU:HD13	4:D:159:LEU:HD13	1.93	0.50
18:W:805:VAL:CG1	18:W:808:GLU:HG2	2.41	0.50
1:A:1361:PHE:O	16:U:281:ARG:HB3	2.10	0.50
2:B:336:ILE:O	2:B:337:ARG:O	2.29	0.50
6:F:92:ARG:HH22	7:G:63:PRO:HG3	1.76	0.50
16:U:181:ASN:HD22	16:U:212:LEU:CD1	2.22	0.50
16:U:186:ASN:OD1	16:U:187:ASN:OD1	2.28	0.50
3:C:9:ILE:HG21	3:C:12:ALA:HB2	1.94	0.50
4:D:66:ALA:O	4:D:70:ALA:CB	2.58	0.50
7:G:1:MET:N	7:G:80:LYS:O	2.35	0.50
1:A:1458:ALA:HA	7:G:20:PRO:HG3	1.92	0.50
2:B:10:ASP:OD1	2:B:11:THR:N	2.43	0.50
8:H:111:ILE:HD12	8:H:128:TYR:HA	1.92	0.50
13:P:1:A:C8	13:P:2:U:C5	3.00	0.50
1:A:336:ARG:HH22	2:B:1114:LEU:HD21	1.76	0.50
1:A:1232:GLU:CD	16:U:180:MET:HG3	2.32	0.50
3:C:88:GLU:HG2	18:W:759:ARG:HD2	1.94	0.50
14:T:-6:DC:H2'	14:T:-5:DA:C8	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:286:LEU:HD22	18:W:292:VAL:HG21	1.93	0.50
18:W:676:ILE:HG13	18:W:686:LEU:CD2	2.37	0.50
1:A:114:LEU:HD13	1:A:145:LYS:HB3	1.93	0.50
1:A:1448:ILE:N	7:G:61:ILE:HG12	2.26	0.50
2:B:225:ILE:HD13	2:B:248:LYS:HD3	1.93	0.50
2:B:337:ARG:O	2:B:341:ARG:HB2	2.09	0.50
16:U:153:LYS:O	16:U:157:LYS:HG3	2.12	0.50
18:W:678:HIS:HB2	18:W:685:PHE:HB2	1.93	0.50
2:B:70:ASN:ND2	2:B:128:ASP:CA	2.74	0.50
7:G:125:ASN:HD22	7:G:126:SER:N	2.09	0.50
1:A:122:MET:O	1:A:126:ILE:HG12	2.11	0.50
1:A:830:VAL:HG12	1:A:1083:LEU:HD21	1.92	0.50
1:A:920:ILE:O	1:A:921:LEU:C	2.49	0.50
1:A:958:LEU:HD21	1:A:1019:LEU:HD23	1.92	0.50
1:A:977:ARG:HG3	1:A:979:LYS:HB2	1.94	0.50
2:B:307:LYS:HB3	2:B:308:PRO:HD3	1.94	0.50
2:B:563:ASP:O	2:B:567:HIS:N	2.44	0.50
16:U:160:PHE:HA	16:U:163:VAL:CG2	2.40	0.50
16:U:181:ASN:ND2	16:U:212:LEU:HD13	2.24	0.50
16:U:187:ASN:HD21	16:U:214:PRO:CB	2.03	0.50
2:B:56:LEU:O	2:B:76:GLU:HA	2.12	0.49
2:B:328:ARG:HA	2:B:341:ARG:HD3	1.94	0.49
5:E:160:LYS:NZ	5:E:192:GLY:O	2.42	0.49
16:U:134:TYR:CE2	16:U:152:VAL:HG22	2.46	0.49
1:A:528:THR:HG21	1:A:651:GLN:HG2	1.94	0.49
1:A:712:ARG:HH12	9:I:91:ARG:HD2	1.77	0.49
1:A:1230:TRP:HZ2	16:U:176:ARG:NH1	2.10	0.49
3:C:241:ASN:OD1	3:C:242:GLN:N	2.44	0.49
5:E:99:ILE:HG13	5:E:131:ILE:HD11	1.94	0.49
1:A:1085:THR:O	16:U:260:LYS:CE	2.60	0.49
3:C:40:VAL:HB	3:C:172:PRO:HG3	1.94	0.49
12:L:68:GLN:NE2	18:W:767:ILE:HG12	2.27	0.49
18:W:357:ARG:CB	18:W:389:PRO:HG2	2.42	0.49
1:A:694:ILE:HD13	1:A:718:GLU:HG3	1.95	0.49
1:A:1279:ILE:HD12	1:A:1318:GLU:HB3	1.94	0.49
2:B:896:ASP:OD2	12:L:31:TYR:OH	2.31	0.49
1:A:791:ASP:OD1	9:I:87:GLN:NE2	2.36	0.49
4:D:6:SER:HB2	7:G:5:LYS:CE	2.41	0.49
1:A:112:LYS:HB3	1:A:165:ARG:HH22	1.77	0.49
1:A:245:PRO:HA	1:A:248:ARG:HG2	1.95	0.49
1:A:673:ASP:OD2	1:A:737:ASN:OD1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:LYS:HB2	1:A:1083:LEU:HD22	1.91	0.49
1:A:1264:LYS:HE2	9:I:44:TYR:CB	2.43	0.49
2:B:76:GLU:OE1	2:B:124:PHE:HE2	1.95	0.49
2:B:250:TYR:HE2	2:B:262:LYS:HB2	1.78	0.49
1:A:92:HIS:CD2	1:A:237:ILE:HD11	2.48	0.49
5:E:102:LYS:HB2	5:E:104:PHE:CE2	2.47	0.49
16:U:194:ILE:O	16:U:194:ILE:HD13	2.12	0.49
18:W:775:GLY:O	18:W:777:ARG:N	2.42	0.49
1:A:673:ASP:O	1:A:677:MET:HG2	2.12	0.49
1:A:1202:ALA:HB1	16:U:224:ILE:HG23	1.95	0.49
16:U:216:SER:HA	16:U:219:LYS:HE2	1.94	0.49
18:W:403:GLU:O	18:W:403:GLU:HG3	2.12	0.49
18:W:684:LEU:CD1	18:W:699:VAL:CB	2.91	0.49
1:A:472:ASN:O	1:A:475:VAL:HG22	2.13	0.49
3:C:50:ILE:HA	3:C:155:ILE:HG22	1.93	0.49
18:W:399:ALA:O	18:W:406:ILE:HD12	2.13	0.49
18:W:409:ASP:OD2	18:W:413:PHE:CE2	2.66	0.49
18:W:678:HIS:HD2	18:W:685:PHE:HD2	1.60	0.49
1:A:953:ASP:O	1:A:956:TRP:NE1	2.46	0.48
1:A:1088:TYR:OH	16:U:237:GLU:HG3	2.13	0.48
1:A:350:ALA:HB3	1:A:490:LEU:HB3	1.95	0.48
1:A:745:LYS:O	1:A:749:SER:HB2	2.14	0.48
3:C:32:LEU:HD21	3:C:244:PHE:CE1	2.48	0.48
7:G:96:PRO:HD2	18:W:683:PHE:CE2	2.47	0.48
15:N:17:DA:C2	15:N:18:DG:C4	3.00	0.48
1:A:742:ASN:O	1:A:744:VAL:N	2.46	0.48
2:B:266:PRO:CG	2:B:352:GLU:HB3	2.43	0.48
4:D:112:PHE:CZ	7:G:142:LYS:HG2	2.46	0.48
7:G:38:CYS:HB2	7:G:44:TYR:CE1	2.48	0.48
12:L:70:ASP:C	12:L:72:ARG:H	2.16	0.48
1:A:310:ALA:HB1	14:T:-4:DG:H5'	1.94	0.48
1:A:742:ASN:O	1:A:745:LYS:N	2.38	0.48
1:A:1085:THR:CB	16:U:260:LYS:NZ	2.77	0.48
2:B:555:GLY:O	2:B:583:HIS:CD2	2.66	0.48
2:B:1163:CYS:SG	2:B:1164:GLY:N	2.86	0.48
7:G:100:PHE:HE1	18:W:698:PHE:CD2	2.23	0.48
18:W:399:ALA:O	18:W:406:ILE:HD11	2.14	0.48
1:A:253:MET:HA	13:P:1:A:C2	2.49	0.48
1:A:1142:TYR:HA	1:A:1278:GLY:HA3	1.95	0.48
2:B:653:ARG:O	2:B:657:GLN:HG3	2.14	0.48
8:H:94:TYR:HD2	8:H:143:ILE:HD12	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1362:ASP:HB2	16:U:272:PHE:CE1	2.47	0.48
3:C:69:ILE:HD11	3:C:144:LEU:HD21	1.95	0.48
7:G:42:PHE:HA	7:G:80:LYS:HD2	1.95	0.48
14:T:8:DG:H2''	14:T:9:DA:C8	2.48	0.48
15:N:16:DT:H2''	15:N:17:DA:C5'	2.44	0.48
16:U:188:PRO:O	16:U:192:ARG:CB	2.62	0.48
14:T:2:DC:H2'	14:T:3:DC:H6	1.78	0.48
18:W:308:ASP:HA	18:W:311:ARG:HG3	1.96	0.48
18:W:678:HIS:HD2	18:W:685:PHE:CD2	2.31	0.48
1:A:286:PRO:O	1:A:288:HIS:N	2.47	0.48
3:C:135:ARG:NH2	3:C:139:ASP:OD1	2.46	0.48
4:D:41:HIS:CE1	7:G:74:TYR:N	2.81	0.48
14:T:-18:DT:H2'	14:T:-17:DC:C5	2.48	0.48
14:T:-5:DA:H5''	14:T:-5:DA:C8	2.45	0.48
1:A:327:ARG:HG2	1:A:1409:VAL:HG21	1.95	0.48
2:B:291:GLN:O	2:B:564:PRO:HG3	2.14	0.48
14:T:-4:DG:H2''	14:T:-3:DA:C8	2.49	0.48
2:B:319:LYS:HE2	2:B:323:LEU:HD11	1.96	0.48
2:B:610:ARG:NE	2:B:612:ILE:HG12	2.29	0.48
4:D:49:ILE:CG2	7:G:4:LEU:HD12	2.40	0.48
10:J:1:MET:HA	10:J:55:LEU:HB2	1.95	0.48
17:V:91:PRO:HB2	17:V:93:ASP:OD1	2.14	0.48
1:A:924:VAL:O	1:A:925:GLU:C	2.52	0.47
1:A:985:ILE:HA	1:A:988:ILE:HD12	1.96	0.47
1:A:1202:ALA:HA	16:U:224:ILE:HG23	1.89	0.47
1:A:1400:LEU:HA	1:A:1403:CYS:SG	2.53	0.47
3:C:174:SER:OG	3:C:175:ALA:N	2.47	0.47
7:G:148:VAL:HG22	7:G:161:GLY:HA2	1.95	0.47
16:U:157:LYS:O	16:U:161:LYS:HB2	2.14	0.47
1:A:699:GLN:NE2	9:I:99:LEU:HD21	2.29	0.47
2:B:25:PHE:HZ	2:B:534:LEU:HG	1.79	0.47
2:B:70:ASN:CG	2:B:128:ASP:N	2.67	0.47
4:D:38:GLN:HE21	7:G:5:LYS:HZ2	1.61	0.47
16:U:214:PRO:HD2	16:U:217:LEU:CB	2.44	0.47
18:W:384:THR:OG1	18:W:387:PHE:HD2	1.97	0.47
5:E:60:LEU:HD12	5:E:77:LEU:O	2.14	0.47
7:G:158:TYR:HB2	18:W:667:PHE:HE2	1.76	0.47
7:G:3:PHE:O	7:G:77:VAL:HA	2.14	0.47
18:W:437:VAL:O	18:W:437:VAL:CG2	2.61	0.47
5:E:54:ARG:HB2	5:E:83:ASP:OD1	2.14	0.47
18:W:413:PHE:HE1	18:W:420:GLU:HB3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:678:HIS:HB2	18:W:685:PHE:CB	2.45	0.47
1:A:487:GLU:OE2	2:B:1102:LYS:HD3	2.15	0.47
1:A:1137:GLN:HE22	16:U:232:ALA:C	2.18	0.47
1:A:1362:ASP:O	16:U:283:LYS:CG	2.63	0.47
4:D:64:LEU:HB3	4:D:89:LEU:HG	1.95	0.47
13:P:1:A:N6	13:P:2:U:N3	2.63	0.47
1:A:342:MET:HB3	2:B:1132:GLU:HG2	1.97	0.47
1:A:558:ASP:OD1	1:A:559:GLY:N	2.46	0.47
2:B:514:LEU:HD22	2:B:626:VAL:HG12	1.97	0.47
2:B:1072:MET:SD	2:B:1085:VAL:HB	2.55	0.47
4:D:23:GLU:OE1	7:G:82:PHE:CD1	2.65	0.47
7:G:97:ILE:O	7:G:97:ILE:CG2	2.63	0.47
12:L:29:VAL:O	12:L:41:SER:HA	2.14	0.47
18:W:396:GLU:CD	18:W:414:VAL:HG23	2.30	0.47
18:W:684:LEU:N	18:W:697:VAL:O	2.47	0.47
1:A:831:LYS:HB3	1:A:1083:LEU:HD22	1.62	0.47
1:A:1061:HIS:ND1	6:F:87:LYS:HE3	2.30	0.47
2:B:179:ASP:O	2:B:183:MET:HG2	2.15	0.47
8:H:144:ARG:HG3	8:H:145:ARG:HG2	1.97	0.47
1:A:1097:THR:HG22	1:A:1102:ARG:HB2	1.96	0.47
2:B:219:LYS:HA	2:B:219:LYS:HD3	1.69	0.47
4:D:85:ASP:OD1	4:D:86:ASP:N	2.48	0.47
5:E:158:GLY:O	5:E:159:GLU:C	2.52	0.47
1:A:831:LYS:HZ3	16:U:262:THR:HA	0.64	0.46
1:A:914:ILE:HG13	1:A:917:ALA:HB2	1.96	0.46
1:A:1205:LEU:HD23	16:U:224:ILE:HB	1.97	0.46
7:G:22:MET:O	7:G:26:LEU:HG	2.15	0.46
14:T:-10:DT:H2'	14:T:-9:DA:C8	2.50	0.46
16:U:206:THR:HG22	16:U:208:SER:HB2	1.97	0.46
1:A:793:PHE:CD1	1:A:798:LYS:HD2	2.51	0.46
11:K:65:HIS:HE1	11:K:67:LEU:HD12	1.79	0.46
15:N:15:DG:C2'	15:N:16:DT:H5''	2.23	0.46
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.96	0.46
1:A:474:SER:OG	1:A:651:GLN:NE2	2.47	0.46
2:B:559:LEU:O	2:B:562:TYR:N	2.45	0.46
4:D:25:ALA:CB	7:G:85:GLU:CA	2.83	0.46
10:J:6:ARG:HD3	10:J:13:VAL:HG22	1.96	0.46
1:A:766:VAL:HG23	1:A:803:ASN:O	2.15	0.46
1:A:1234:ASN:ND2	16:U:212:LEU:O	2.48	0.46
2:B:336:ILE:HD12	2:B:336:ILE:H	1.80	0.46
15:N:5:DC:H2''	15:N:6:DT:H5'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:413:PHE:HZ	18:W:420:GLU:CD	2.17	0.46
2:B:480:THR:HG23	2:B:483:SER:H	1.80	0.46
3:C:68:LEU:O	10:J:5:VAL:HG11	2.15	0.46
1:A:735:GLU:CB	1:A:756:PHE:HE1	2.28	0.46
2:B:300:TRP:O	2:B:304:GLU:HB2	2.15	0.46
1:A:92:HIS:HD2	1:A:237:ILE:HD11	1.80	0.46
1:A:408:ARG:HD3	1:A:412:ASP:HB2	1.97	0.46
1:A:666:GLY:HA3	2:B:1069:PHE:CZ	2.51	0.46
1:A:1202:ALA:CA	16:U:224:ILE:HG23	2.45	0.46
3:C:149:ASN:OD1	3:C:150:HIS:CD2	2.68	0.46
4:D:7:THR:CG2	7:G:6:ASP:HB2	2.44	0.46
1:A:452:HIS:CE1	1:A:454:MET:HB2	2.50	0.46
1:A:745:LYS:O	1:A:749:SER:HB3	2.16	0.46
2:B:725:ARG:HD3	2:B:727:LYS:HE3	1.97	0.46
5:E:82:CYS:SG	5:E:83:ASP:N	2.89	0.46
15:N:13:DC:H2''	15:N:14:DG:C8	2.50	0.46
1:A:152:ALA:N	1:A:163:VAL:O	2.45	0.46
13:P:-3:U:H3'	13:P:-2:U:C6	2.50	0.46
14:T:-20:DA:C8	14:T:-19:DC:C5	3.04	0.46
1:A:280:LEU:HD13	1:A:289:ILE:HG22	1.98	0.46
2:B:491:THR:OG1	2:B:530:LYS:HB2	2.16	0.46
1:A:985:ILE:N	1:A:986:PRO:HD2	2.31	0.45
1:A:1022:CYS:O	1:A:1026:ALA:HB2	2.15	0.45
7:G:5:LYS:HE2	7:G:42:PHE:CZ	2.51	0.45
12:L:28:GLY:HA3	12:L:42:LEU:O	2.16	0.45
16:U:188:PRO:O	16:U:192:ARG:N	2.38	0.45
18:W:388:ARG:HB2	18:W:389:PRO:CD	2.46	0.45
18:W:664:VAL:CG2	18:W:686:LEU:CD2	2.93	0.45
1:A:1085:THR:C	16:U:260:LYS:NZ	2.69	0.45
1:A:977:ARG:HB2	1:A:978:ALA:HB3	1.96	0.45
2:B:332:ALA:HB2	2:B:344:TYR:CE2	2.51	0.45
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.50	0.45
4:D:176:ASP:O	4:D:180:ARG:CB	2.64	0.45
16:U:146:SER:C	16:U:148:ILE:H	2.19	0.45
18:W:322:ARG:HD3	18:W:342:GLU:HA	1.99	0.45
18:W:352:LEU:CD1	18:W:435:LEU:HD21	2.46	0.45
18:W:672:ARG:HH12	18:W:691:ILE:CG1	2.29	0.45
1:A:1100:VAL:CB	1:A:1101:PRO:HD3	2.34	0.45
2:B:499:GLY:C	2:B:500:LYS:HD2	2.36	0.45
4:D:55:GLU:HG2	4:D:121:CYS:SG	2.57	0.45
15:N:-6:DA:OP2	15:N:-5:DT:C7	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:146:SER:O	16:U:148:ILE:HG22	2.17	0.45
1:A:203:LEU:HB3	1:A:208:ILE:HD11	1.99	0.45
1:A:386:ILE:O	1:A:390:THR:HG23	2.17	0.45
1:A:1232:GLU:CD	16:U:180:MET:CG	2.83	0.45
2:B:1120:GLU:O	2:B:1124:ARG:NH2	2.33	0.45
4:D:72:ASN:HB3	4:D:75:VAL:HB	1.98	0.45
13:P:3:C:N3	14:T:8:DG:C2	2.81	0.45
1:A:309:ILE:C	1:A:310:ALA:O	2.40	0.45
1:A:713:GLU:OE2	1:A:1092:SER:CB	2.64	0.45
1:A:1082:THR:CB	16:U:260:LYS:HZ3	2.30	0.45
1:A:1085:THR:O	16:U:260:LYS:NZ	2.50	0.45
1:A:1388:THR:OG1	1:A:1389:ARG:N	2.49	0.45
1:A:1462:PRO:HD2	7:G:21:GLN:N	2.31	0.45
2:B:252:ARG:HB3	2:B:255:LYS:HB3	1.99	0.45
4:D:30:LEU:O	7:G:82:PHE:CZ	2.70	0.45
9:I:51:ASN:HB3	9:I:52:ILE:H	1.58	0.45
15:N:4:DT:H2'	15:N:5:DC:C6	2.51	0.45
1:A:67:CYS:O	1:A:71:GLY:N	2.45	0.45
1:A:661:ASN:HD21	2:B:1082:MET:HB3	1.80	0.45
1:A:1191:SER:OG	1:A:1259:GLU:OE1	2.21	0.45
1:A:1195:LEU:HB2	1:A:1263:LEU:HD11	1.98	0.45
2:B:555:GLY:O	2:B:583:HIS:HD2	2.00	0.45
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.81	0.45
3:C:173:CYS:SG	3:C:243:VAL:HG11	2.57	0.45
4:D:6:SER:HB3	7:G:7:LEU:HD21	1.98	0.45
7:G:56:VAL:HG12	7:G:72:VAL:HG22	1.99	0.45
7:G:98:GLY:HA3	7:G:110:VAL:O	2.17	0.45
16:U:133:ILE:CD1	16:U:155:ILE:CB	2.84	0.45
4:D:57:ARG:HD2	4:D:110:ASN:HA	1.99	0.45
5:E:24:ASP:OD2	5:E:186:TYR:OH	2.28	0.45
1:A:231:ARG:HB3	1:A:234:TRP:CD2	2.52	0.44
1:A:387:HIS:O	1:A:390:THR:OG1	2.24	0.44
1:A:1206:ASP:HA	16:U:228:ASN:ND2	2.32	0.44
1:A:1264:LYS:CE	9:I:44:TYR:CD1	2.99	0.44
2:B:269:LYS:HE2	2:B:331:SER:HA	1.98	0.44
2:B:276:ILE:O	2:B:280:ALA:CB	2.64	0.44
2:B:795:ILE:HB	2:B:854:LEU:HB2	1.99	0.44
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.52	0.44
13:P:-2:U:C5	13:P:-2:U:OP2	2.70	0.44
15:N:-6:DA:C8	15:N:-6:DA:O5'	2.71	0.44
16:U:183:LYS:C	16:U:185:LYS:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:MET:HE3	1:A:41:MET:N	2.32	0.44
1:A:699:GLN:NE2	9:I:99:LEU:HD11	2.32	0.44
2:B:154:ASN:OD1	2:B:155:LYS:N	2.45	0.44
2:B:947:GLY:HA3	2:B:968:MET:SD	2.57	0.44
16:U:182:LEU:O	16:U:191:ARG:HD3	2.17	0.44
18:W:409:ASP:OD2	18:W:413:PHE:HE2	2.00	0.44
18:W:664:VAL:HG21	18:W:686:LEU:CG	2.45	0.44
1:A:1116:PRO:HB3	1:A:1314:ILE:HG23	1.99	0.44
1:A:1441:THR:HG23	6:F:88:TYR:HD1	1.82	0.44
2:B:436:ASN:O	2:B:438:ASN:N	2.39	0.44
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	2.00	0.44
4:D:23:GLU:OE1	7:G:82:PHE:CA	2.36	0.44
8:H:92:TYR:CD1	8:H:144:ARG:HB2	2.52	0.44
17:V:28:GLY:HA3	17:V:33:ASP:CG	2.38	0.44
1:A:875:ASP:CG	1:A:876:GLY:H	2.21	0.44
4:D:68:SER:HB2	4:D:92:VAL:HG21	1.99	0.44
7:G:116:PRO:HA	7:G:164:LYS:HD3	1.98	0.44
15:N:20:DG:H2''	15:N:21:DT:H5''	1.99	0.44
1:A:64:ASN:OD1	1:A:65:PHE:N	2.51	0.44
1:A:772:GLU:HA	1:A:1086:PHE:CE2	2.53	0.44
1:A:882:GLN:NE2	1:A:961:ASN:HA	2.33	0.44
7:G:151:ARG:HG3	18:W:667:PHE:CD1	2.40	0.44
1:A:375:LEU:HD13	1:A:492:VAL:HG21	1.99	0.44
1:A:1345:GLU:OE1	5:E:199:ARG:HD3	2.17	0.44
1:A:62:ASP:OD1	1:A:63:ARG:N	2.47	0.44
4:D:169:VAL:HG12	4:D:170:ASN:N	2.31	0.44
7:G:95:SER:HB3	18:W:682:ASN:CB	2.48	0.44
7:G:151:ARG:HG2	18:W:668:THR:HG23	2.00	0.44
8:H:109:ASP:OD1	8:H:128:TYR:N	2.50	0.44
1:A:735:GLU:HG3	1:A:756:PHE:CE1	2.52	0.44
1:A:1226:LEU:HD12	1:A:1243:ARG:O	2.18	0.44
1:A:1446:VAL:O	7:G:61:ILE:HG12	2.18	0.44
1:A:1447:MET:HB2	6:F:133:VAL:HB	2.00	0.44
12:L:63:THR:OG1	12:L:64:LYS:N	2.49	0.44
1:A:107:CYS:SG	1:A:108:MET:N	2.91	0.44
1:A:231:ARG:HH11	1:A:232:PRO:HD2	1.83	0.43
1:A:248:ARG:HG3	1:A:248:ARG:O	2.18	0.43
1:A:1205:LEU:HD22	16:U:221:MET:HA	2.00	0.43
2:B:237:LYS:HD3	2:B:237:LYS:HA	1.90	0.43
2:B:344:TYR:CE2	2:B:348:ILE:HD11	2.53	0.43
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:151:GLU:N	4:D:155:GLU:OE1	2.46	0.43
7:G:85:GLU:HG2	7:G:87:VAL:HG13	2.00	0.43
14:T:-6:DC:H2''	14:T:-5:DA:C8	2.53	0.43
16:U:189:THR:O	16:U:193:SER:CA	2.66	0.43
16:U:284:PHE:HD2	16:U:284:PHE:HA	1.72	0.43
1:A:533:ARG:HD3	1:A:750:ALA:HA	2.00	0.43
1:A:536:THR:HG21	1:A:579:LEU:HD22	2.00	0.43
1:A:986:PRO:O	1:A:990:HIS:HB2	2.19	0.43
1:A:1212:ASN:O	1:A:1215:ALA:N	2.50	0.43
2:B:35:LEU:HD22	2:B:167:SER:HB3	1.99	0.43
2:B:426:GLN:O	2:B:430:GLU:HG3	2.18	0.43
2:B:1221:SER:HB2	4:D:12:ARG:HH12	1.82	0.43
16:U:156:GLU:O	16:U:160:PHE:CD2	2.64	0.43
18:W:442:PRO:HB2	18:W:447:LEU:CD1	2.48	0.43
1:A:253:MET:CG	13:P:1:A:C2	2.89	0.43
1:A:735:GLU:HG3	1:A:756:PHE:CD1	2.54	0.43
1:A:779:GLY:HA3	2:B:509:ASN:HB2	2.00	0.43
1:A:1095:ASN:O	1:A:1115:THR:HG21	2.18	0.43
1:A:1329:ARG:HG2	5:E:147:GLU:OE2	2.17	0.43
4:D:52:SER:O	4:D:56:SER:CB	2.66	0.43
4:D:158:THR:CG2	7:G:167:PHE:CE2	2.94	0.43
12:L:33:CYS:SG	12:L:55:HIS:HB3	2.59	0.43
13:P:-1:U:C5	13:P:-1:U:OP2	2.71	0.43
15:N:-6:DA:O5'	15:N:-6:DA:H8	2.01	0.43
18:W:333:PHE:CD2	18:W:354:LEU:CD2	3.00	0.43
1:A:143:LYS:HG3	1:A:144:THR:HG23	2.00	0.43
1:A:1122:LEU:HD13	1:A:1126:ILE:HG22	2.00	0.43
3:C:4:GLU:HB3	3:C:5:PRO:HD3	2.00	0.43
7:G:50:ASP:OD1	7:G:50:ASP:C	2.56	0.43
18:W:344:LEU:HD12	18:W:349:GLU:HB2	2.00	0.43
1:A:337:LEU:HD12	1:A:1408:THR:HG21	2.01	0.43
1:A:897:ARG:HD3	1:A:1032:ARG:HD2	2.01	0.43
1:A:961:ASN:HD22	1:A:964:ARG:CZ	2.32	0.43
1:A:1061:HIS:CE1	6:F:87:LYS:HE3	2.53	0.43
1:A:1143:THR:HG23	1:A:1147:ASN:HB2	1.99	0.43
2:B:204:ILE:O	2:B:205:ALA:C	2.56	0.43
3:C:103:ARG:HH21	3:C:152:GLU:CD	2.21	0.43
13:P:-2:U:H6	13:P:-2:U:C5'	2.31	0.43
18:W:265:ARG:HD2	18:W:265:ARG:HA	1.71	0.43
1:A:527:ASP:HB2	2:B:835:GLN:NE2	2.34	0.43
4:D:34:PHE:CE2	7:G:80:LYS:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:152:THR:HG22	7:G:154:VAL:H	1.83	0.43
9:I:87:GLN:O	9:I:88:SER:HB2	2.18	0.43
1:A:50:GLU:OE1	18:W:444:LEU:HD21	2.19	0.43
1:A:368:PRO:HD2	1:A:371:ILE:HD12	2.01	0.43
2:B:249:LEU:HD13	2:B:261:ILE:HG12	2.00	0.43
3:C:13:GLN:HE21	3:C:16:GLU:HG2	1.84	0.43
10:J:7:CYS:HB3	10:J:11:GLY:H	1.84	0.43
14:T:0:DT:C2	14:T:1:DA:N7	2.87	0.43
1:A:317:GLN:HG3	1:A:318:LYS:N	2.33	0.43
1:A:1332:SER:OG	1:A:1333:ASN:N	2.51	0.43
2:B:769:TYR:OH	16:U:265:ALA:CA	2.66	0.43
4:D:114:ARG:NH2	4:D:178:LEU:HB3	2.33	0.43
7:G:84:GLY:N	7:G:147:VAL:O	2.45	0.43
9:I:96:ASN:OD1	9:I:97:MET:N	2.52	0.43
18:W:344:LEU:HD11	18:W:349:GLU:HB2	2.01	0.43
1:A:961:ASN:HD22	1:A:964:ARG:NH2	2.17	0.43
4:D:30:LEU:C	7:G:82:PHE:CE1	2.92	0.43
1:A:409:ASP:OD1	1:A:410:ASN:N	2.52	0.43
2:B:605:GLU:O	2:B:625:ARG:NH2	2.31	0.43
4:D:101:VAL:HG13	7:G:105:PRO:HA	2.00	0.43
5:E:143:ILE:H	5:E:143:ILE:HG13	1.66	0.43
1:A:37:TYR:HE1	18:W:441:ASN:HD21	1.51	0.42
1:A:529:LEU:O	1:A:532:VAL:HG12	2.18	0.42
7:G:10:ILE:HA	7:G:70:PHE:O	2.19	0.42
17:V:15:CYS:HB3	17:V:32:CYS:SG	2.59	0.42
1:A:831:LYS:N	1:A:1083:LEU:HD23	2.35	0.42
2:B:1106:ARG:NH1	2:B:1118:PRO:HB3	2.34	0.42
7:G:45:ILE:HG23	7:G:78:VAL:HG12	2.00	0.42
18:W:421:TYR:HA	18:W:425:PHE:O	2.19	0.42
1:A:13:SER:HB2	1:A:1435:GLN:NE2	2.34	0.42
1:A:1100:VAL:CB	1:A:1101:PRO:CD	2.95	0.42
5:E:123:ILE:HB	5:E:124:PRO:HD3	2.01	0.42
8:H:101:TYR:CZ	8:H:114:TYR:HB3	2.55	0.42
14:T:2:DC:H2'	14:T:3:DC:C6	2.54	0.42
16:U:129:SER:O	16:U:133:ILE:CG1	2.66	0.42
18:W:388:ARG:HB2	18:W:389:PRO:HD3	2.01	0.42
1:A:1031:ARG:O	1:A:1035:GLU:HB2	2.18	0.42
4:D:33:GLU:OE1	7:G:42:PHE:CE2	2.63	0.42
7:G:79:TRP:CZ3	7:G:81:PRO:HD3	2.54	0.42
18:W:749:ASP:HB3	18:W:752:LEU:HD11	2.01	0.42
1:A:562:PRO:HG3	1:A:581:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:572:ARG:HB3	2:B:579:TRP:HE1	1.84	0.42
6:F:92:ARG:NH2	7:G:63:PRO:HB3	2.34	0.42
18:W:799:GLU:HB3	18:W:804:TRP:CZ3	2.55	0.42
1:A:1080:GLN:OE1	16:U:283:LYS:HE2	2.20	0.42
2:B:296:ASP:OD1	2:B:297:GLU:N	2.52	0.42
2:B:1073:TYR:HE2	3:C:179:GLU:HA	1.84	0.42
3:C:104:HIS:HD2	3:C:149:ASN:HA	1.85	0.42
7:G:112:THR:HA	7:G:115:ILE:HD12	2.01	0.42
9:I:75:CYS:HA	9:I:76:PRO:HD3	1.93	0.42
10:J:44:CYS:SG	10:J:45:CYS:N	2.93	0.42
18:W:278:LYS:HD2	18:W:280:GLU:OE2	2.20	0.42
18:W:332:LYS:HE3	18:W:357:ARG:HB2	2.01	0.42
1:A:72:GLU:HB3	1:A:76:GLU:HB2	2.02	0.42
1:A:1361:PHE:O	16:U:281:ARG:CB	2.68	0.42
4:D:23:GLU:CB	7:G:83:LYS:H	2.31	0.42
7:G:97:ILE:HG13	18:W:683:PHE:CB	2.50	0.42
18:W:352:LEU:HD21	18:W:435:LEU:CD1	2.50	0.42
18:W:676:ILE:CA	18:W:686:LEU:CD2	2.97	0.42
2:B:639:LYS:HG3	2:B:641:ASN:H	1.85	0.42
3:C:89:ASP:OD1	18:W:757:LYS:HD3	2.20	0.42
5:E:55:LYS:HG3	5:E:56:LEU:HD12	2.01	0.42
11:K:63:VAL:HG22	11:K:71:PHE:HB3	2.02	0.42
15:N:16:DT:C2'	15:N:17:DA:C8	2.96	0.42
16:U:161:LYS:HD3	16:U:204:LEU:HG	2.02	0.42
2:B:127:ILE:HG13	2:B:127:ILE:O	2.20	0.42
2:B:710:ARG:NH1	2:B:719:LEU:HG	2.35	0.42
4:D:144:GLN:HA	4:D:147:SER:HB2	2.02	0.42
5:E:87:VAL:HG11	5:E:109:PHE:HE2	1.83	0.42
2:B:24:PHE:CE1	2:B:28:LYS:HD2	2.55	0.42
4:D:41:HIS:HE1	7:G:7:LEU:O	2.03	0.42
4:D:178:LEU:O	4:D:182:GLU:HB2	2.20	0.42
18:W:672:ARG:HH22	18:W:691:ILE:HD11	1.85	0.42
1:A:1082:THR:CB	16:U:260:LYS:NZ	2.82	0.41
1:A:1202:ALA:HA	16:U:224:ILE:HD13	2.02	0.41
2:B:784:ASN:HB2	2:B:787:VAL:HG22	2.02	0.41
2:B:844:SER:HB3	2:B:848:ARG:NH1	2.35	0.41
4:D:46:HIS:CD2	4:D:47:ASP:H	2.37	0.41
9:I:32:CYS:HB3	9:I:33:ASP:H	1.73	0.41
14:T:-12:DG:N2	15:N:14:DG:N3	2.68	0.41
1:A:552:PHE:CE1	11:K:74:ARG:HB2	2.55	0.41
1:A:1266:ILE:O	1:A:1270:MET:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:352:LEU:HD11	18:W:435:LEU:CD2	2.49	0.41
1:A:408:ARG:HB3	1:A:409:ASP:H	1.74	0.41
1:A:1006:ASN:OD1	1:A:1007:GLU:N	2.51	0.41
7:G:23:ASN:HA	7:G:26:LEU:HD12	2.02	0.41
7:G:100:PHE:CE1	18:W:698:PHE:CD2	3.02	0.41
16:U:133:ILE:CG1	16:U:155:ILE:HG21	2.49	0.41
18:W:806:PRO:O	18:W:808:GLU:N	2.45	0.41
1:A:1134:LYS:HD3	16:U:229:LEU:HD12	2.02	0.41
2:B:221:ALA:HB3	2:B:222:PRO:HD3	2.02	0.41
4:D:34:PHE:HD2	7:G:82:PHE:HZ	1.69	0.41
4:D:38:GLN:HE21	7:G:5:LYS:NZ	2.18	0.41
8:H:6:PHE:HB3	8:H:59:LEU:HB2	2.01	0.41
1:A:188:LYS:HB2	1:A:196:ALA:HB3	2.02	0.41
1:A:1201:ARG:NE	16:U:217:LEU:HD11	2.36	0.41
1:A:1221:VAL:HG21	1:A:1274:ILE:HD12	2.03	0.41
2:B:89:MET:O	2:B:96:THR:HA	2.20	0.41
2:B:274:ILE:O	2:B:277:VAL:HG22	2.21	0.41
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	2.02	0.41
3:C:220:ASP:OD1	3:C:221:TYR:N	2.50	0.41
14:T:-20:DA:N1	15:N:22:DG:N2	2.68	0.41
14:T:-12:DG:H3'	14:T:-11:DA:C8	2.55	0.41
18:W:756:VAL:HG11	18:W:796:LEU:HD22	2.02	0.41
1:A:517:SER:O	1:A:518:ASN:CG	2.59	0.41
1:A:945:ARG:HG3	1:A:1301:TYR:OH	2.20	0.41
1:A:1082:THR:HB	16:U:260:LYS:HZ3	1.86	0.41
1:A:1206:ASP:OD1	16:U:228:ASN:CG	2.59	0.41
1:A:1286:TYR:CD1	16:U:234:GLY:HA2	2.54	0.41
2:B:850:LEU:HG	2:B:851:PHE:CD2	2.55	0.41
4:D:141:GLU:HA	4:D:144:GLN:HB2	2.01	0.41
16:U:213:ALA:HA	16:U:214:PRO:HA	1.80	0.41
1:A:448:GLN:HE22	1:A:489:ASN:HD22	1.68	0.41
1:A:870:GLY:HA3	1:A:1369:ARG:NH1	2.35	0.41
1:A:1167:GLU:OE1	1:A:1196:ARG:NH2	2.53	0.41
2:B:904:ARG:NH1	18:W:781:GLU:CG	2.83	0.41
2:B:1056:SER:OG	2:B:1067:ARG:NH1	2.53	0.41
2:B:266:PRO:HG2	2:B:352:GLU:HB3	2.03	0.41
4:D:24:ASN:OD1	7:G:84:GLY:HA3	2.21	0.41
7:G:97:ILE:HG12	18:W:683:PHE:CD1	2.56	0.41
18:W:749:ASP:HB3	18:W:752:LEU:CD1	2.51	0.41
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.85	0.41
1:A:14:VAL:H	1:A:1435:GLN:HE22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:LYS:CB	1:A:1083:LEU:HB2	2.48	0.41
1:A:1021:GLN:HB3	1:A:1025:ARG:NH1	2.36	0.41
1:A:1206:ASP:HA	16:U:228:ASN:HD22	1.86	0.41
2:B:350:GLN:NE2	2:B:359:GLN:O	2.54	0.41
10:J:35:LEU:HD22	10:J:40:LEU:HD12	2.02	0.41
11:K:103:HIS:NE2	11:K:107:GLU:OE2	2.54	0.41
13:P:-3:U:O2	13:P:-3:U:H2'	2.19	0.41
18:W:399:ALA:CB	18:W:406:ILE:HD13	2.44	0.41
2:B:307:LYS:HZ3	9:I:13:MET:HE1	1.39	0.41
2:B:826:ALA:HB3	2:B:1011:ILE:HG12	2.03	0.41
4:D:106:LEU:O	4:D:110:ASN:CB	2.58	0.41
13:P:1:A:C6	13:P:2:U:N3	2.89	0.41
14:T:-20:DA:N1	15:N:21:DT:O2	2.53	0.41
16:U:146:SER:O	16:U:148:ILE:N	2.54	0.41
18:W:322:ARG:CD	18:W:342:GLU:HA	2.51	0.41
18:W:322:ARG:CD	18:W:342:GLU:HG3	2.51	0.41
1:A:262:ASP:OD1	1:A:317:GLN:NE2	2.45	0.40
1:A:822:ARG:NH2	2:B:517:PRO:O	2.54	0.40
1:A:927:GLN:HG3	1:A:931:ASN:HD21	1.86	0.40
1:A:1134:LYS:CD	16:U:229:LEU:HD12	2.52	0.40
1:A:1458:ALA:HA	7:G:20:PRO:CG	2.51	0.40
2:B:27:GLU:OE2	2:B:679:SER:OG	2.39	0.40
2:B:844:SER:HB3	2:B:848:ARG:HH12	1.86	0.40
3:C:13:GLN:HE21	3:C:16:GLU:CG	2.33	0.40
4:D:34:PHE:CE2	7:G:3:PHE:CE2	3.09	0.40
5:E:152:HIS:CD2	5:E:197:ILE:HG12	2.57	0.40
11:K:53:TYR:HA	11:K:54:PRO:HD3	1.95	0.40
3:C:32:LEU:HD21	3:C:244:PHE:HE1	1.85	0.40
7:G:86:VAL:HA	7:G:146:LYS:HA	2.02	0.40
16:U:146:SER:C	16:U:148:ILE:N	2.74	0.40
16:U:186:ASN:OD1	16:U:187:ASN:CG	2.60	0.40
18:W:228:GLY:HA3	18:W:299:PHE:CZ	2.55	0.40
18:W:409:ASP:C	18:W:410:ARG:HG3	2.37	0.40
1:A:498:THR:HG21	2:B:1149:GLU:OE1	2.21	0.40
2:B:360:GLU:HG3	2:B:363:PHE:CD2	2.56	0.40
5:E:14:SER:O	5:E:18:VAL:HG23	2.21	0.40
16:U:194:ILE:HA	16:U:198:GLU:OE1	2.19	0.40
18:W:389:PRO:CD	18:W:389:PRO:O	2.68	0.40
18:W:664:VAL:O	18:W:673:GLN:HA	2.21	0.40
18:W:684:LEU:HD11	18:W:699:VAL:CA	2.49	0.40
1:A:1029:ALA:O	1:A:1033:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1087:HIS:O	1:A:1088:TYR:HB2	2.22	0.40
2:B:71:ILE:O	2:B:71:ILE:CG2	2.69	0.40
1:A:477:SER:H	1:A:478:PRO:HD2	1.86	0.40
8:H:94:TYR:HB3	8:H:143:ILE:HB	2.03	0.40
18:W:667:PHE:CD2	18:W:668:THR:HG23	2.56	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	1417/1743 (81%)	1235 (87%)	169 (12%)	13 (1%)	17	53
2	B	1151/1227 (94%)	987 (86%)	159 (14%)	5 (0%)	34	70
3	C	261/304 (86%)	231 (88%)	27 (10%)	3 (1%)	14	50
4	D	162/186 (87%)	141 (87%)	20 (12%)	1 (1%)	25	62
5	E	211/214 (99%)	190 (90%)	19 (9%)	2 (1%)	17	53
6	F	82/155 (53%)	70 (85%)	12 (15%)	0	100	100
7	G	169/171 (99%)	150 (89%)	19 (11%)	0	100	100
8	H	129/145 (89%)	111 (86%)	18 (14%)	0	100	100
9	I	109/115 (95%)	93 (85%)	14 (13%)	2 (2%)	8	40
10	J	64/72 (89%)	62 (97%)	2 (3%)	0	100	100
11	K	111/118 (94%)	99 (89%)	12 (11%)	0	100	100
12	L	43/72 (60%)	37 (86%)	6 (14%)	0	100	100
16	U	149/190 (78%)	120 (80%)	24 (16%)	5 (3%)	3	30
17	V	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
18	W	317/612 (52%)	288 (91%)	26 (8%)	3 (1%)	17	53
All	All	4475/5432 (82%)	3911 (87%)	530 (12%)	34 (1%)	24	56

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	48	PRO
1	A	743	ASN
1	A	1085	THR
2	B	62	ALA
2	B	337	ARG
4	D	169	VAL
16	U	185	LYS
16	U	186	ASN
18	W	318	VAL
18	W	320	LEU
1	A	975	LEU
9	I	88	SER
18	W	749	ASP
1	A	327	ARG
1	A	853	TYR
1	A	1084	ASN
1	A	1087	HIS
2	B	155	LYS
3	C	205	LYS
5	E	159	GLU
16	U	147	LYS
1	A	287	GLN
2	B	500	LYS
9	I	52	ILE
1	A	283	ASP
1	A	960	VAL
3	C	172	PRO
5	E	123	ILE
16	U	239	ASN
1	A	916	TYR
2	B	555	GLY
16	U	213	ALA
3	C	182	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1238/1528 (81%)	1222 (99%)	16 (1%)	69	82
2	B	1016/1077 (94%)	1008 (99%)	8 (1%)	81	89
3	C	236/264 (89%)	235 (100%)	1 (0%)	91	95
4	D	143/160 (89%)	142 (99%)	1 (1%)	84	91
5	E	196/197 (100%)	193 (98%)	3 (2%)	65	81
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	145 (98%)	3 (2%)	55	74
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	103 (97%)	3 (3%)	43	67
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	37 (97%)	1 (3%)	46	69
16	U	139/171 (81%)	127 (91%)	12 (9%)	10	39
17	V	86/92 (94%)	85 (99%)	1 (1%)	71	84
18	W	290/548 (53%)	279 (96%)	11 (4%)	33	60
All	All	3995/4792 (83%)	3935 (98%)	60 (2%)	66	81

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	44	SER
1	A	45	ARG
1	A	446	ASN
1	A	518	ASN
1	A	661	ASN
1	A	688	LYS
1	A	690	GLN
1	A	721	ARG
1	A	735	GLU
1	A	737	ASN
1	A	977	ARG
1	A	1081	MET
1	A	1083	LEU
1	A	1087	HIS
1	A	1095	ASN

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Mol	Chain	Res	Type
2	B	70	ASN
2	B	71	ILE
2	B	240	ARG
2	B	336	ILE
2	B	500	LYS
2	B	725	ARG
2	B	1094	ARG
2	B	1122	ARG
3	C	8	ASN
4	D	11	ARG
5	E	4	ASN
5	E	120	ASN
5	E	166	ARG
7	G	106	LEU
7	G	125	ASN
7	G	151	ARG
9	I	26	LEU
9	I	49	ILE
9	I	61	ASP
12	L	62	ARG
16	U	126	ARG
16	U	147	LYS
16	U	148	ILE
16	U	186	ASN
16	U	192	ARG
16	U	194	ILE
16	U	195	LEU
16	U	204	LEU
16	U	206	THR
16	U	212	LEU
16	U	264	SER
16	U	284	PHE
17	V	33	ASP
18	W	264	GLN
18	W	313	VAL
18	W	666	GLU
18	W	672	ARG
18	W	683	PHE
18	W	685	PHE
18	W	777	ARG
18	W	784	ASN
18	W	793	CYS

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Mol	Chain	Res	Type
18	W	802	HIS
18	W	809	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	170	ASN
1	A	214	HIS
1	A	359	ASN
1	A	446	ASN
1	A	448	GLN
1	A	489	ASN
1	A	661	ASN
1	A	699	GLN
1	A	768	GLN
1	A	787	HIS
1	A	927	GLN
1	A	931	ASN
1	A	961	ASN
1	A	968	ASN
1	A	1137	GLN
1	A	1190	GLN
1	A	1435	GLN
2	B	63	GLN
2	B	97	HIS
2	B	102	GLN
2	B	206	GLN
2	B	426	GLN
2	B	651	HIS
2	B	657	GLN
2	B	794	ASN
2	B	1093	GLN
3	C	8	ASN
3	C	13	GLN
3	C	150	HIS
4	D	17	GLN
4	D	38	GLN
4	D	46	HIS
4	D	99	ASN
5	E	4	ASN
5	E	100	GLN

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Mol	Chain	Res	Type
5	E	120	ASN
5	E	145	HIS
7	G	125	ASN
8	H	44	ASN
9	I	87	GLN
16	U	181	ASN
16	U	184	ASN
16	U	187	ASN
18	W	339	GLN
18	W	402	HIS
18	W	434	ASN
18	W	441	ASN
18	W	678	HIS
18	W	682	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	15/30 (50%)	7 (46%)	1 (6%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	-4	C
13	P	-3	U
13	P	-2	U
13	P	0	U
13	P	1	A
13	P	2	U
13	P	10	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	P	-1	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

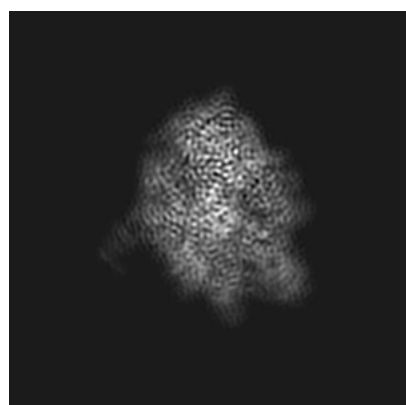
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6747. These allow visual inspection of the internal detail of the map and identification of artifacts.

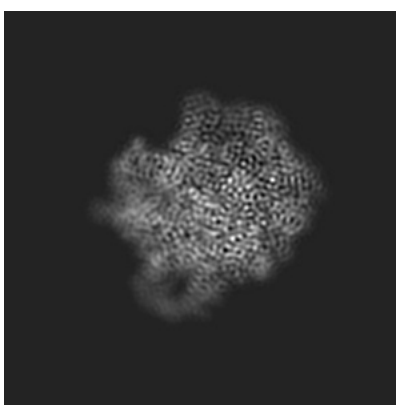
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

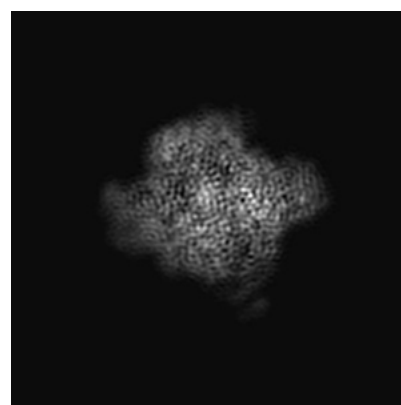
6.1.1 Primary map



X



Y

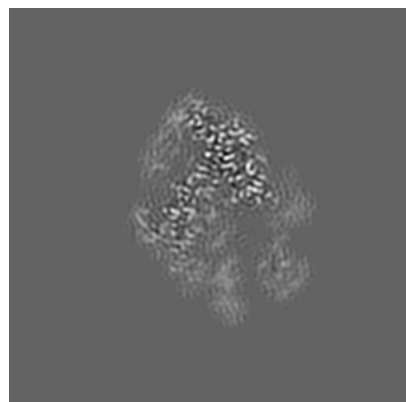


Z

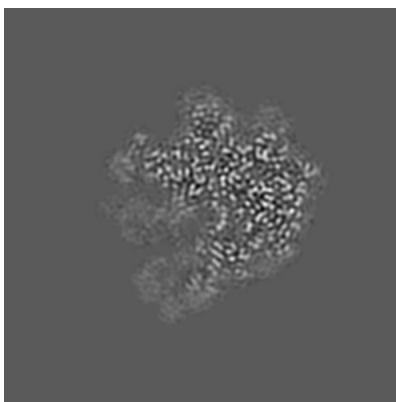
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

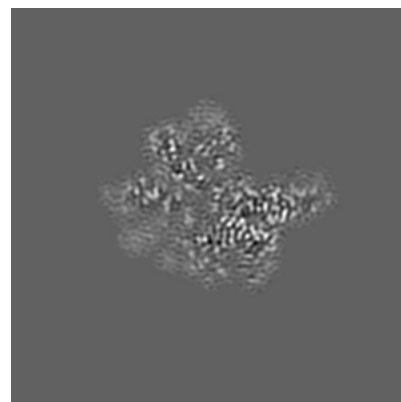
6.2.1 Primary map



X Index: 90



Y Index: 90



Z Index: 90

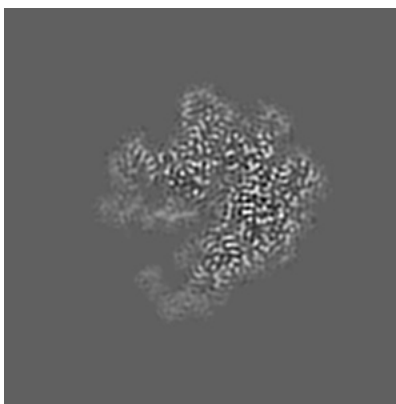
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

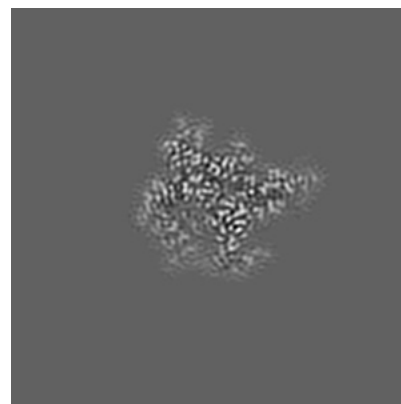
6.3.1 Primary map



X Index: 107



Y Index: 93



Z Index: 105

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0666. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

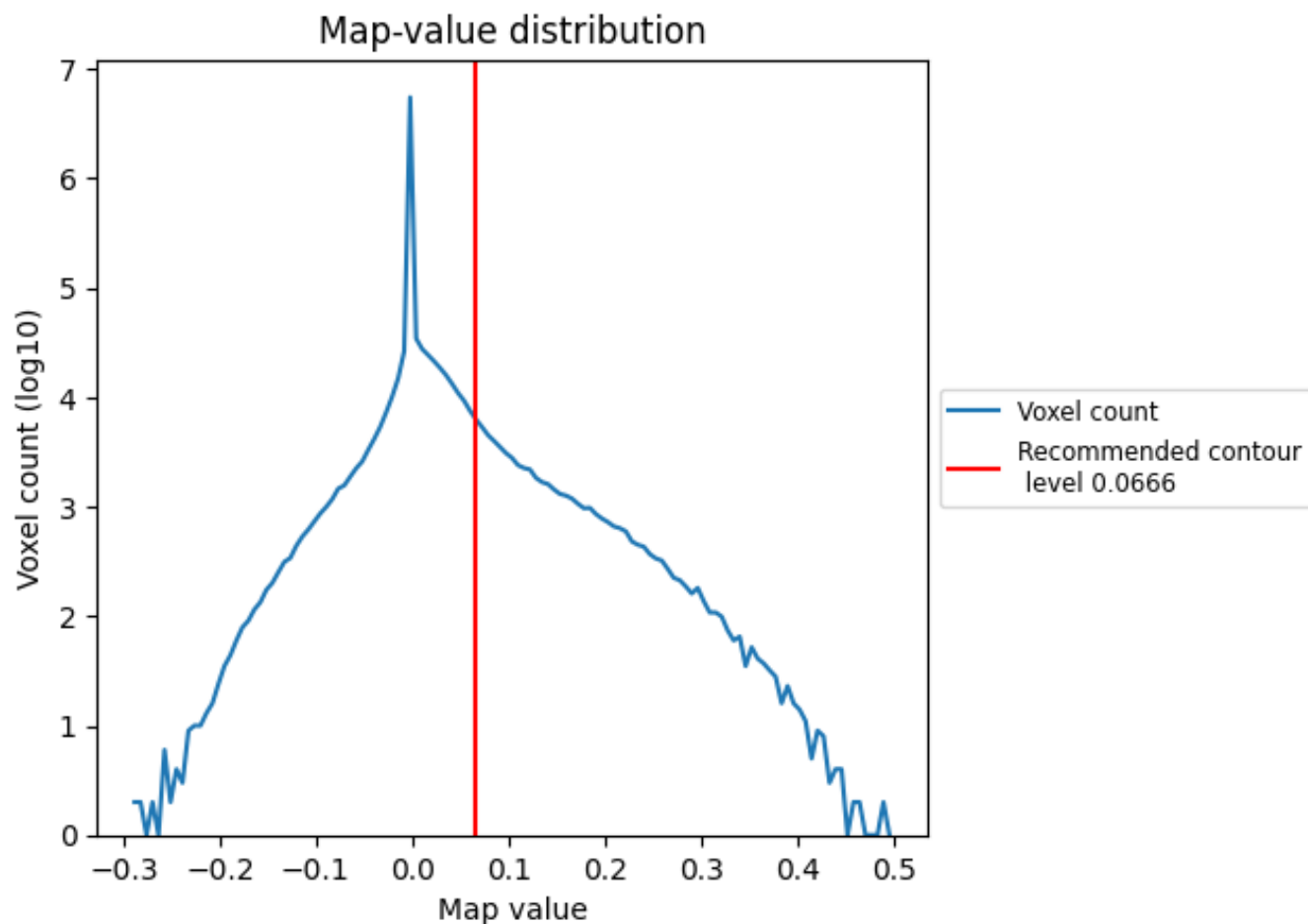
6.5 Mask visualisation

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

7 Map analysis [i](#)

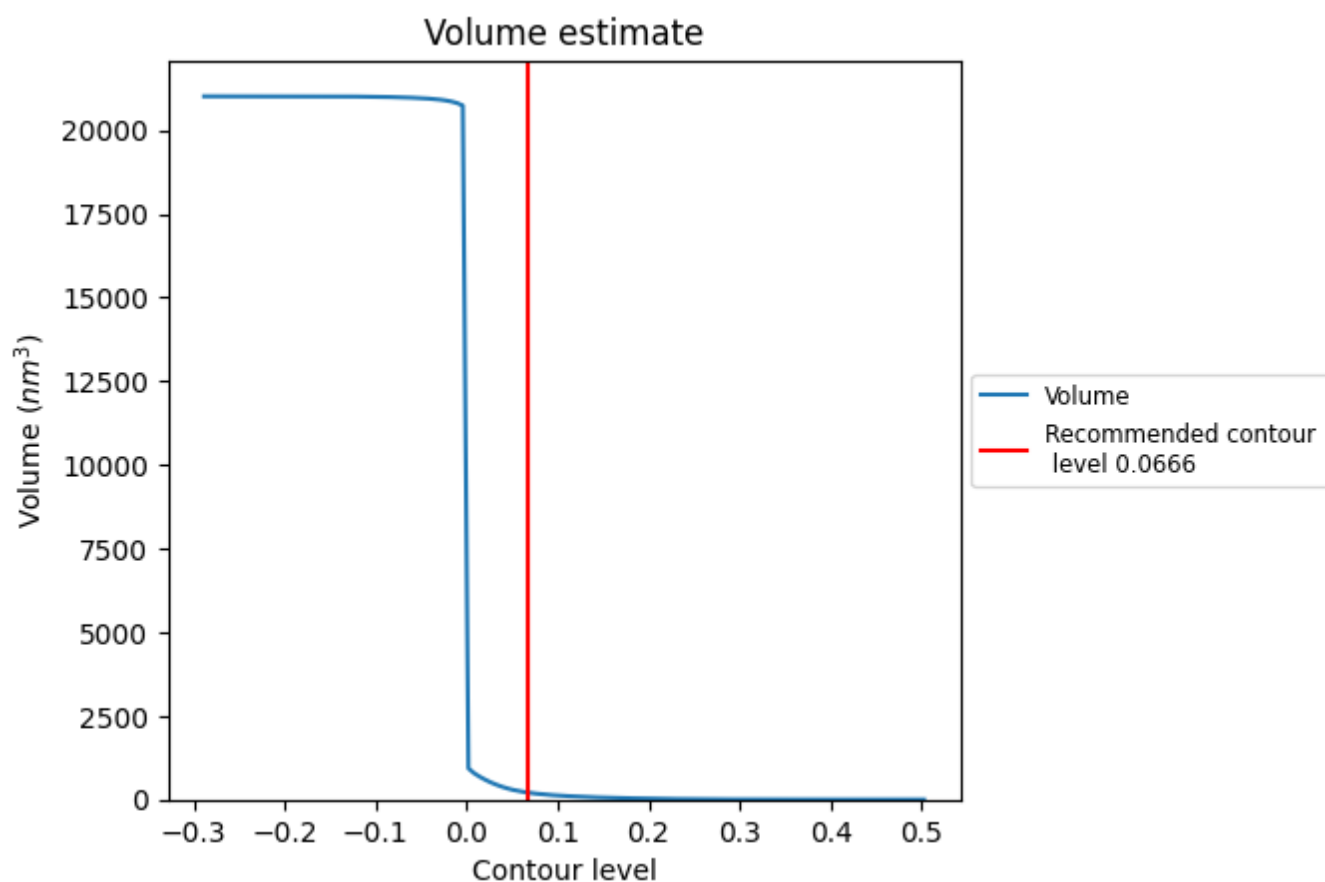
This section contains the results of statistical analysis of the map.

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.

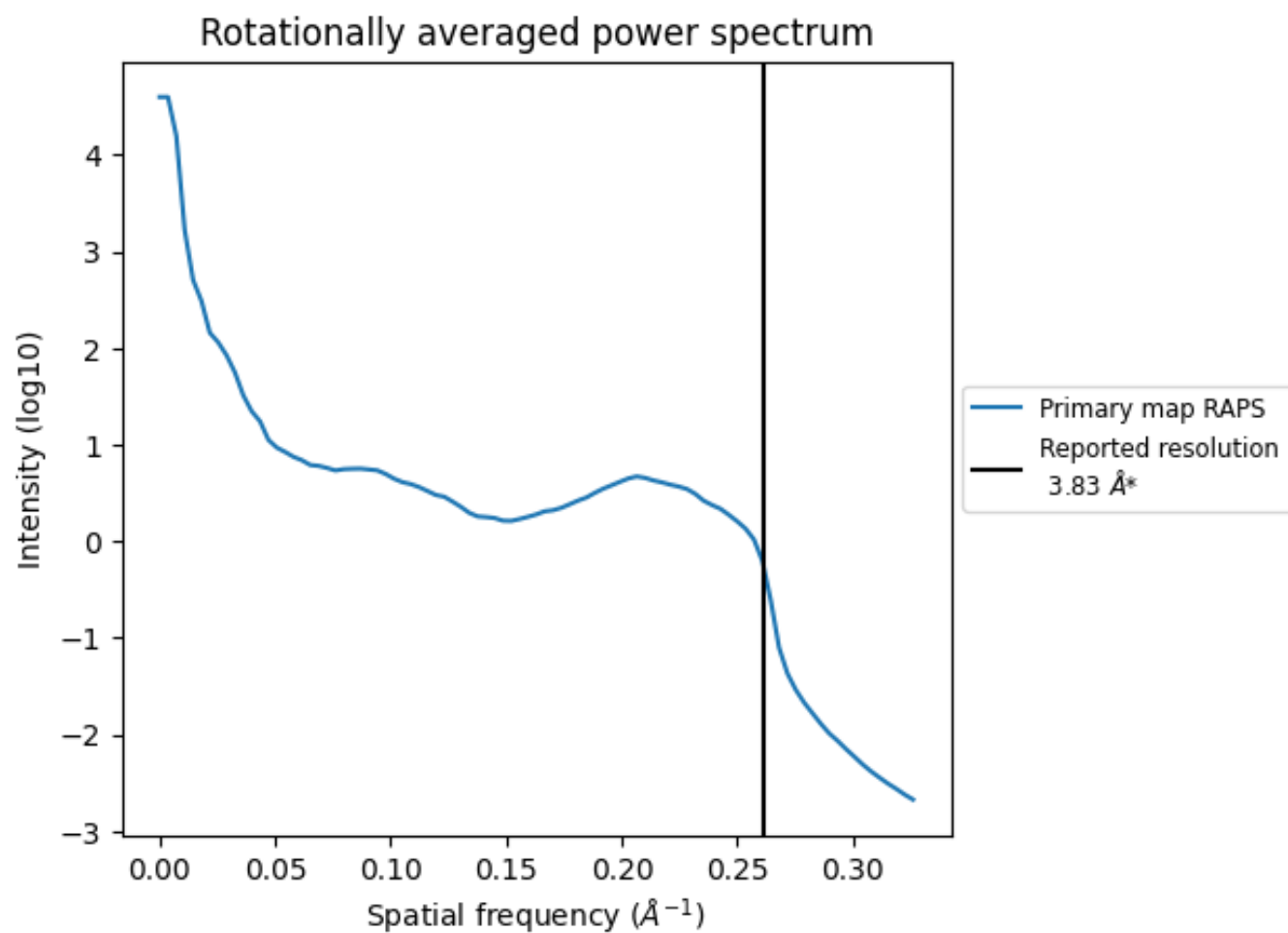
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm³; this corresponds to an approximate mass of 191 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

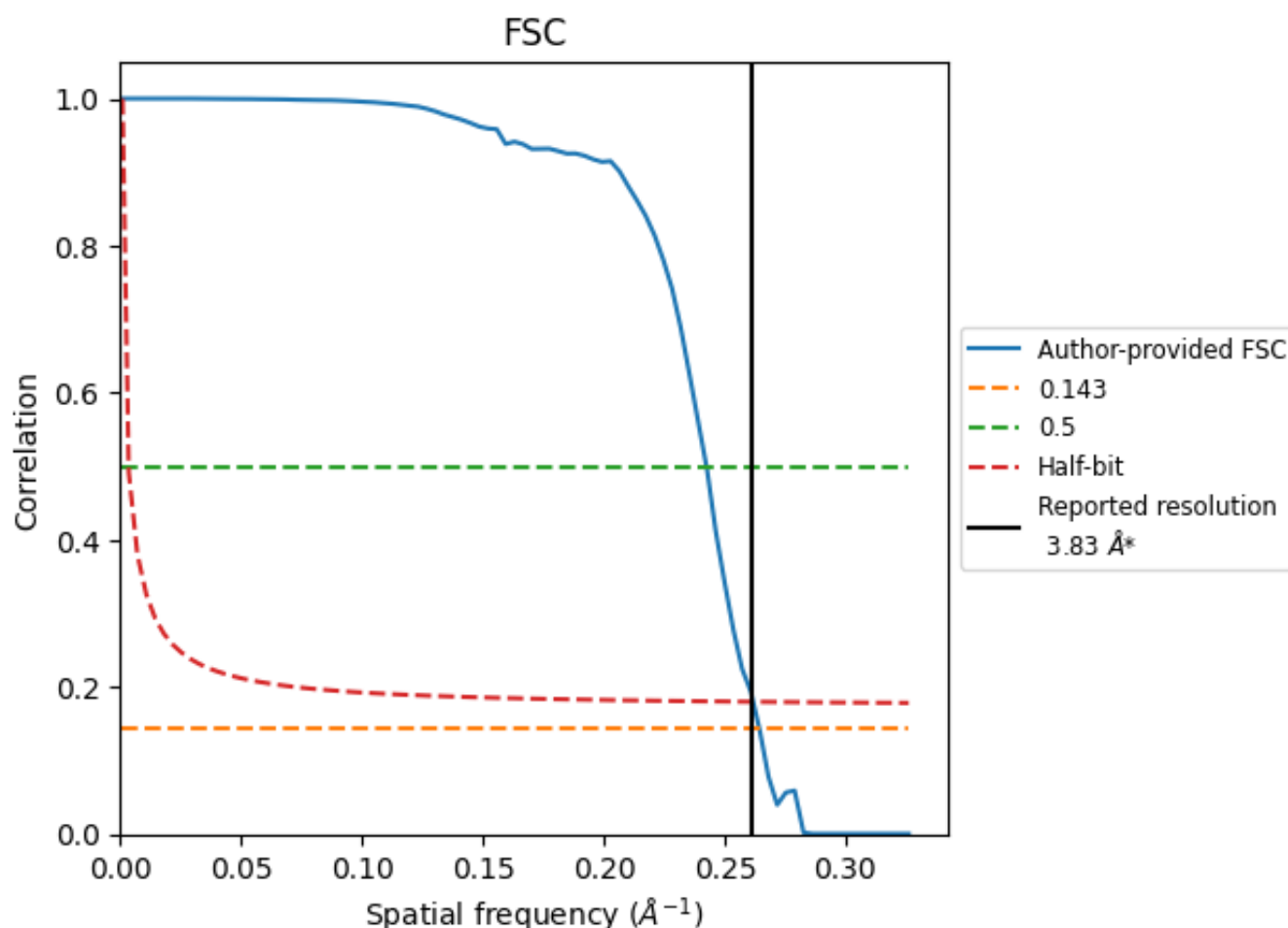


*Reported resolution corresponds to spatial frequency of 0.261 Å⁻¹

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 0.261 \AA^{-1}

8.2 Resolution estimates [i](#)

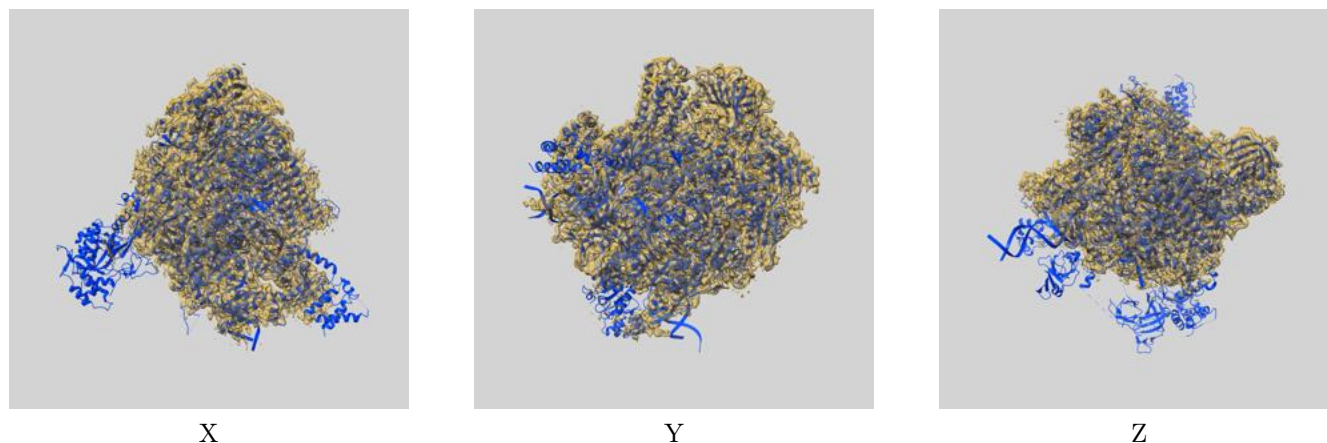
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.83	-	-
Author-provided FSC curve	3.78	4.12	3.82
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

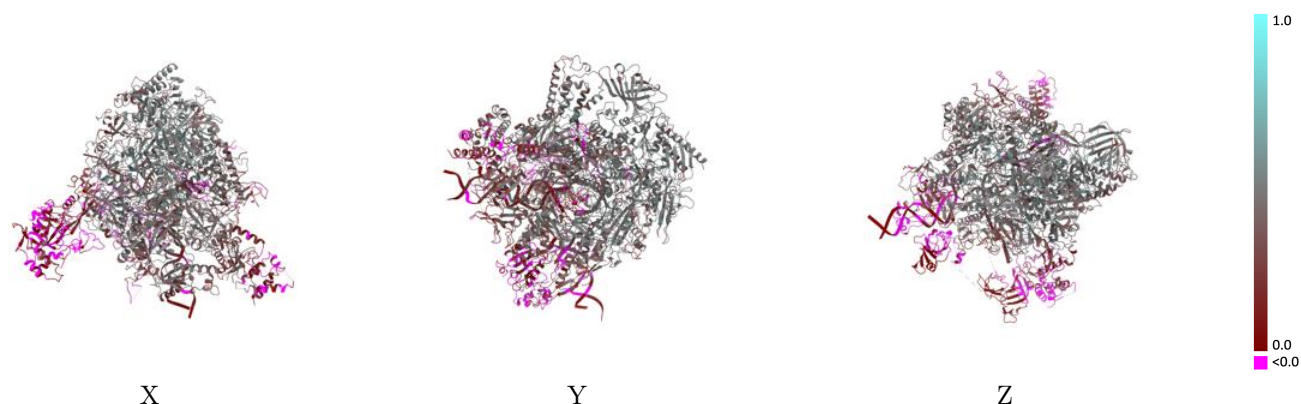
This section contains information regarding the fit between EMDB map EMD-6747 and PDB model 5XON. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



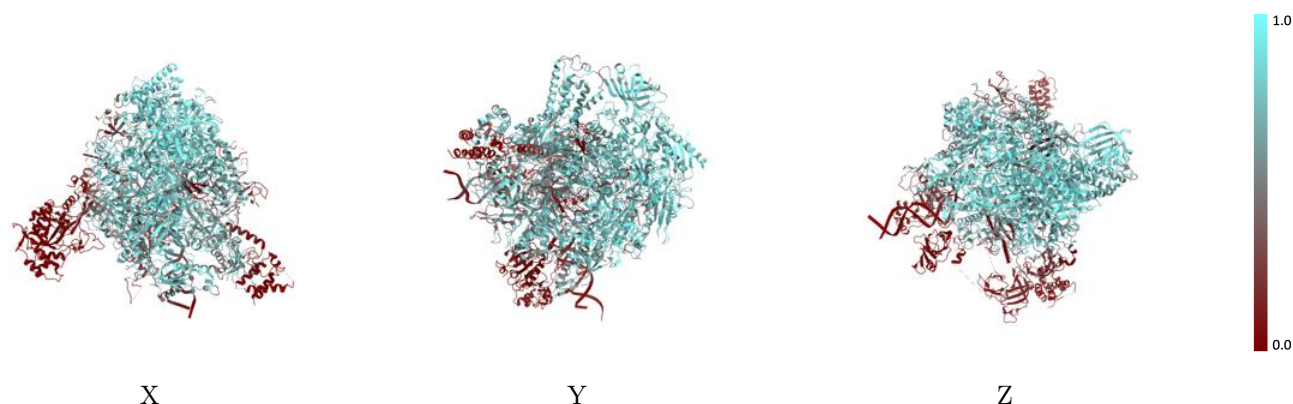
The images above show the 3D surface view of the map at the recommended contour level 0.0666 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



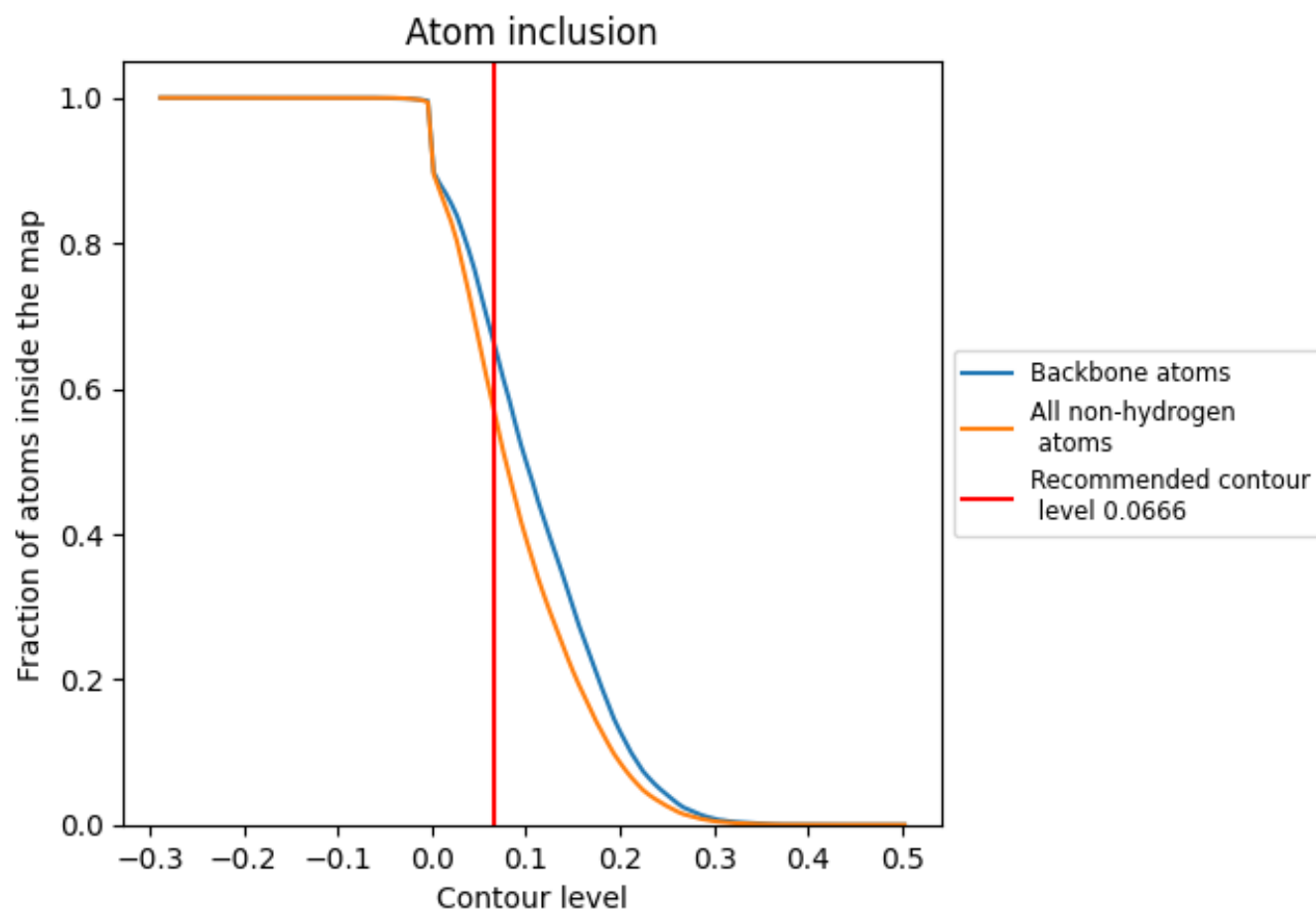
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0666).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 57% 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 (0.0666) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5680	 0.3360
A	 0.7109	 0.4260
B	 0.7301	 0.4330
C	 0.7911	 0.4560
D	 0.0016	 -0.0280
E	 0.7047	 0.4120
F	 0.7523	 0.4670
G	 0.0752	 0.0730
H	 0.7863	 0.4550
I	 0.3281	 0.1860
J	 0.8094	 0.4670
K	 0.7847	 0.4540
L	 0.6063	 0.3260
N	 0.2576	 0.0980
P	 0.5473	 0.3630
T	 0.3867	 0.1670
U	 0.0337	 0.0710
V	 0.0039	 0.0070
W	 0.0709	 0.0530

