



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:54 AM UTC

PDB ID : 8EYT / pdb_00008eyt
EMDB ID : EMD-28720
Title : 30S_delta_ksgA+KsgA complex
Authors : Sun, J.; Kinman, L.F.; Jahagirdar, D.; Ortega, J.; Davis, J.H.
Deposited on : 2022-10-28
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

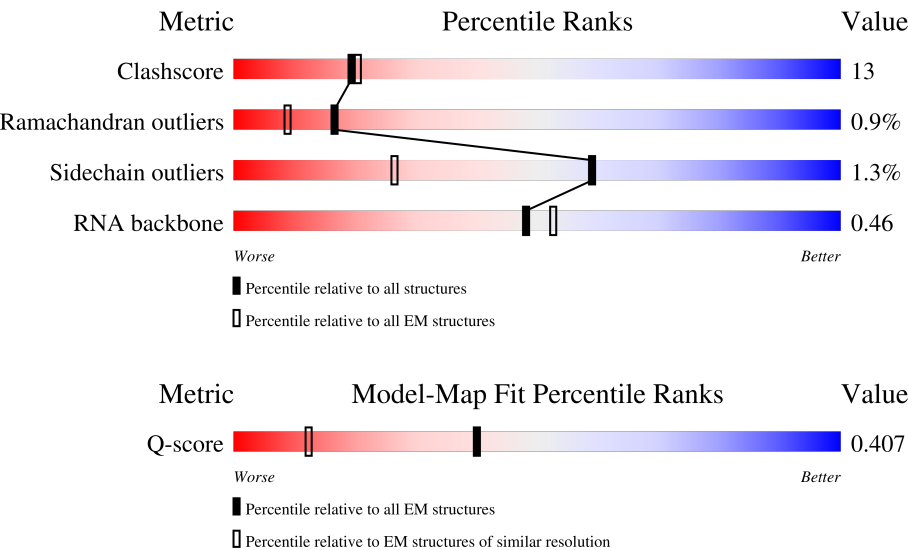
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

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



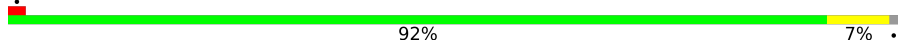
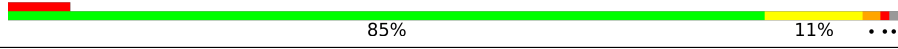
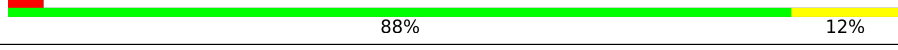
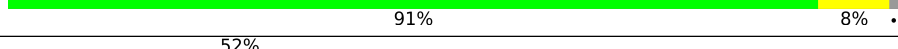
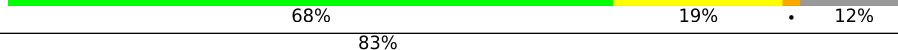
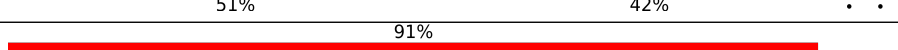
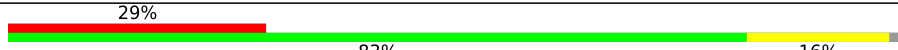
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	1415	7% 60% 29% 9%
2	B	241	90% 62% 29% 7%
3	D	206	6% 86% 13%

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Mol	Chain	Length	Quality of chain
4	E	167	
5	H	130	
6	L	124	
7	P	82	
8	Q	84	
9	T	87	
10	F	233	
11	G	179	
12	I	130	
13	J	103	
14	M	118	
15	N	101	
16	S	92	
17	O	135	
18	R	129	
19	U	89	
20	V	75	
21	W	254	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 50699 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1415	Total	C	N	O	P	0	0
			30367	13543	5577	9832	1415		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	A	deletion	GB 1776881223
A	?	-	G	deletion	GB 1776881223
A	?	-	A	deletion	GB 1776881223
A	?	-	U	deletion	GB 1776881223

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 5 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 6 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 7 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 8 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 9 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 14 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 15 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 16 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	81	Total	C	N	O	S	0	0
			651	416	124	109	2		

- Molecule 17 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 18 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 19 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	V	61	Total	C	N	O	0	0
			496	312	93	91		

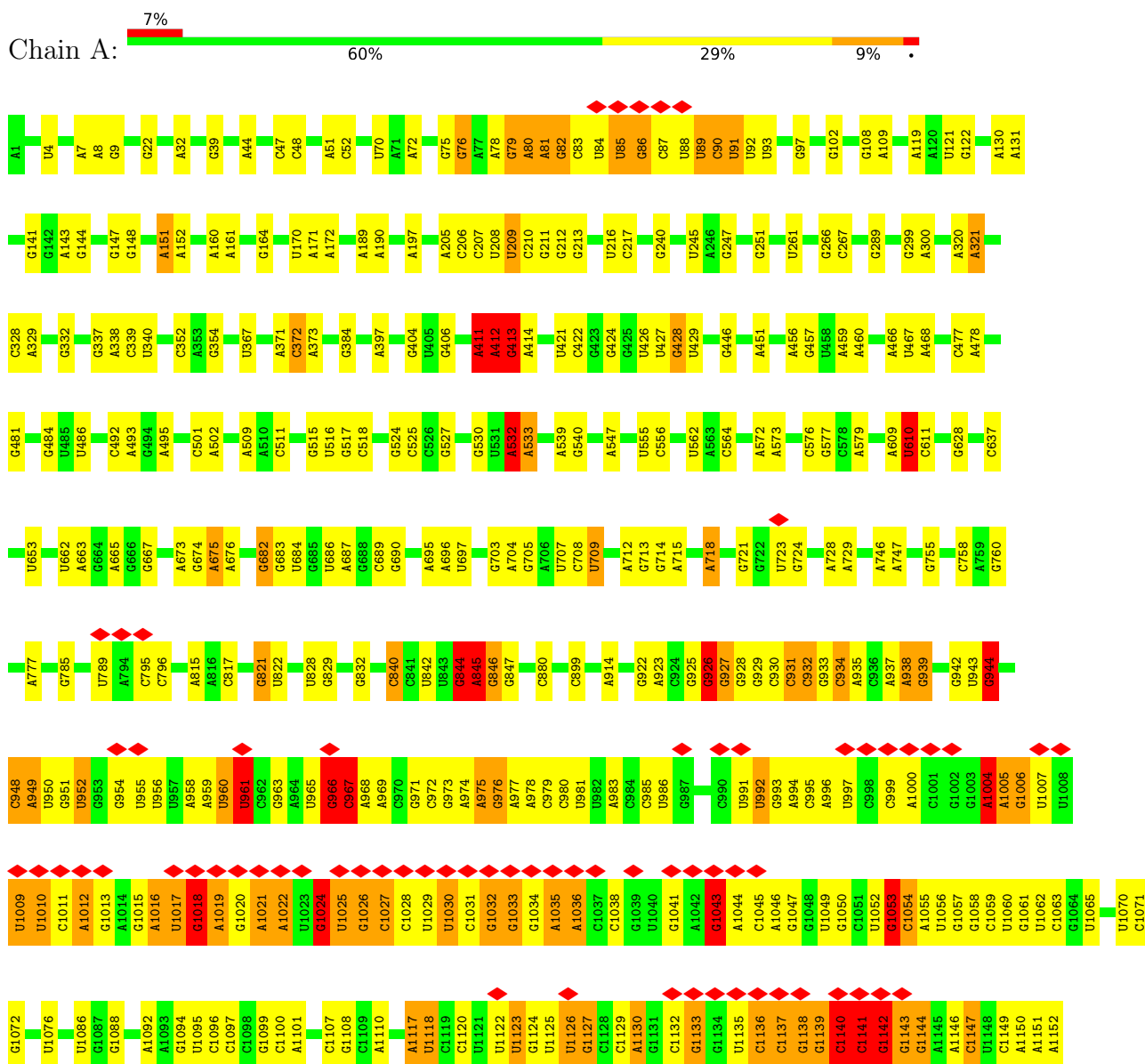
- Molecule 21 is a protein called Ribosomal RNA small subunit methyltransferase A.

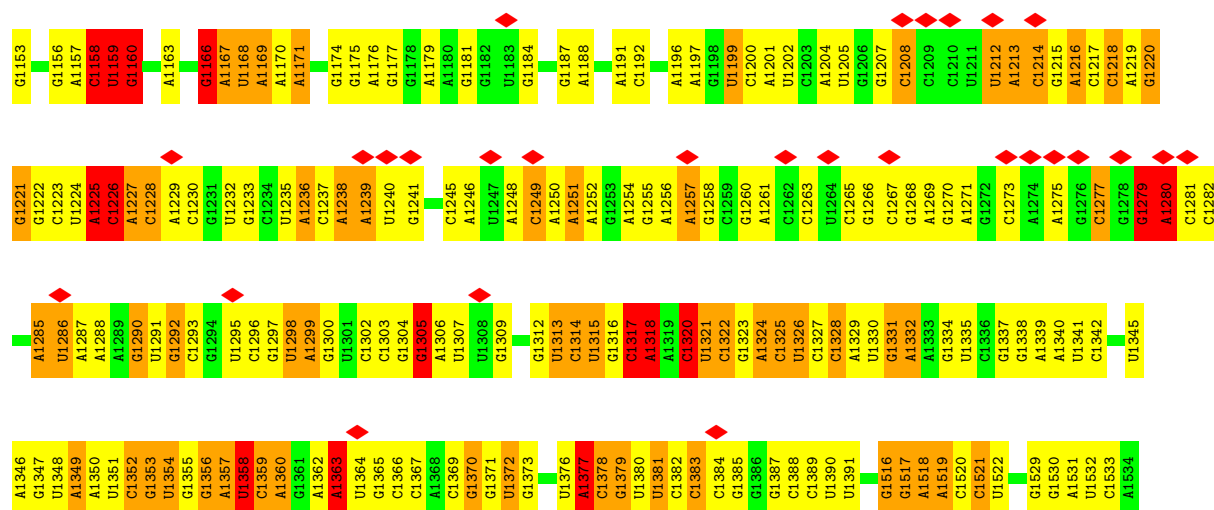
Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	254	Total	C	N	O	S	0	0
			1979	1263	340	363	13		

3 Residue-property plots

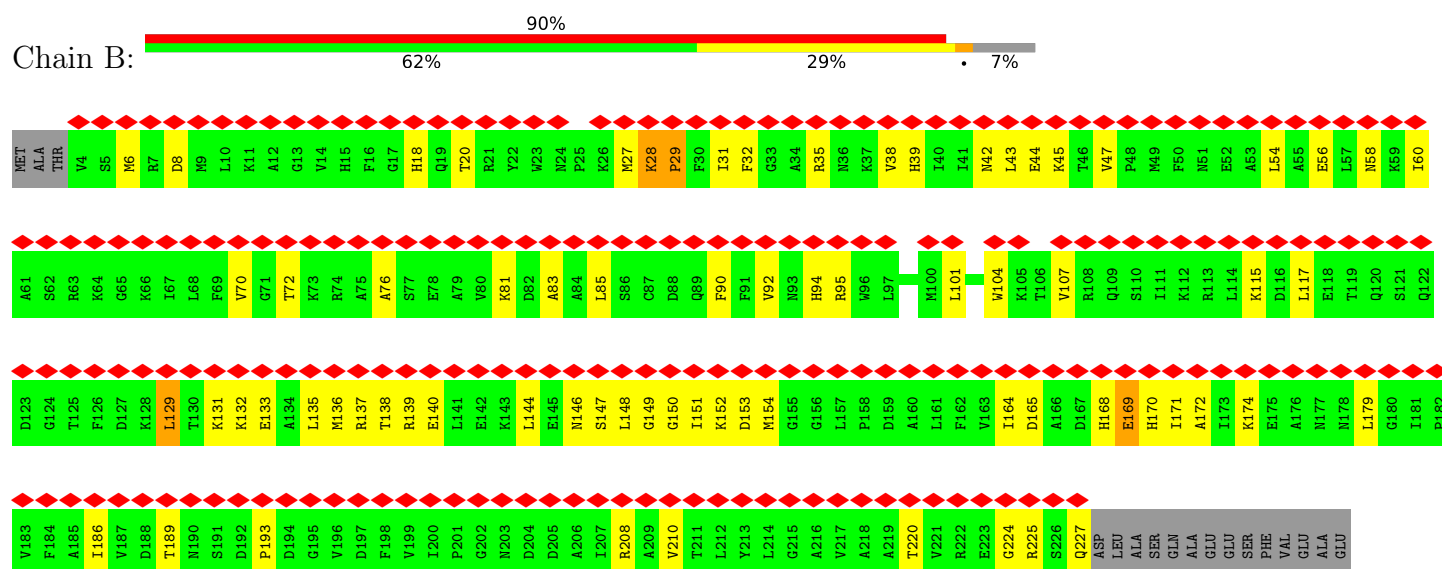
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

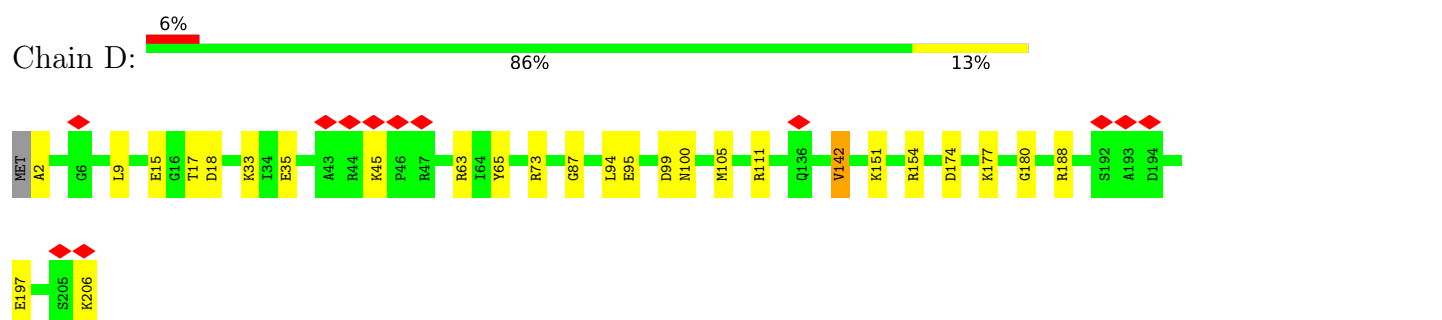




• Molecule 2: 30S ribosomal protein S2

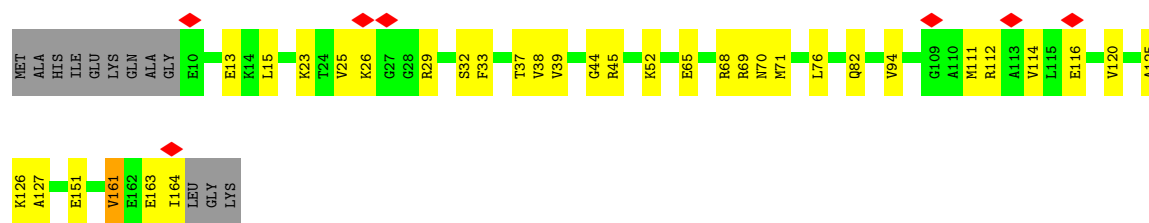


• Molecule 3: 30S ribosomal protein S4

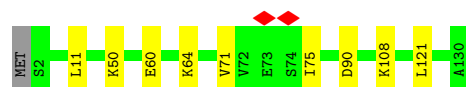
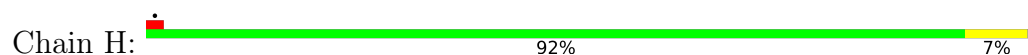


• Molecule 4: 30S ribosomal protein S5

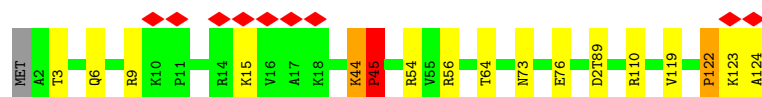
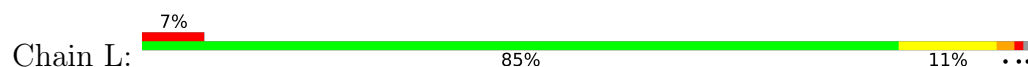




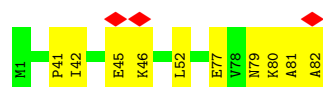
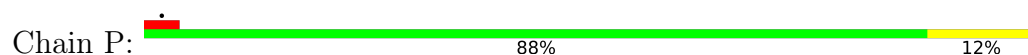
- Molecule 5: 30S ribosomal protein S8



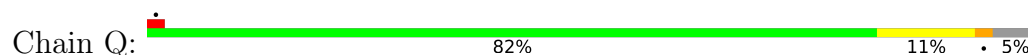
- Molecule 6: 30S ribosomal protein S12



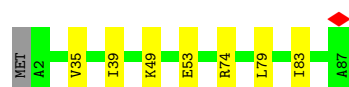
- Molecule 7: 30S ribosomal protein S16



- Molecule 8: 30S ribosomal protein S17



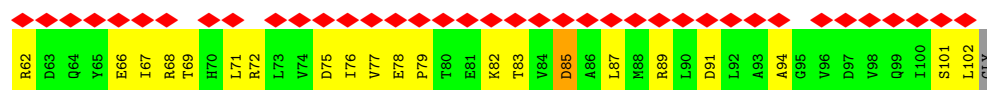
- Molecule 9: 30S ribosomal protein S20



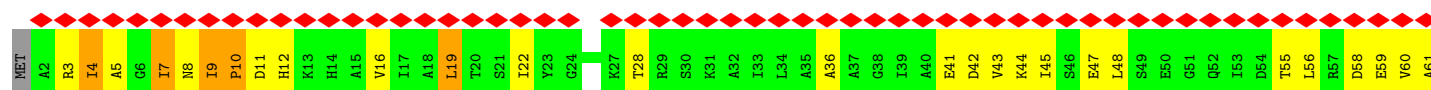
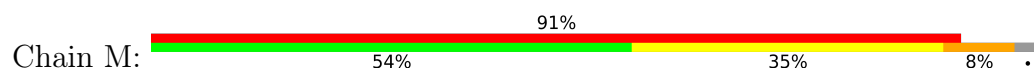
- Molecule 10: 30S ribosomal protein S3



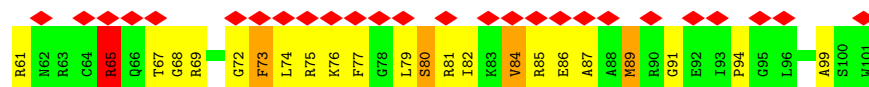
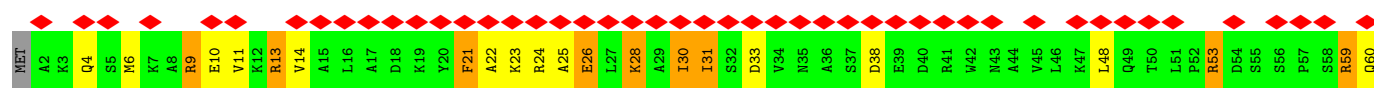




• Molecule 14: 30S ribosomal protein S13



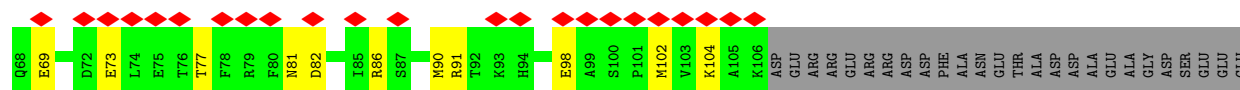
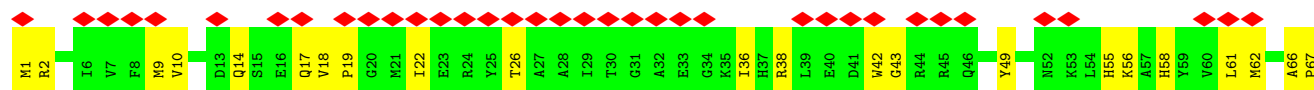
• Molecule 15: 30S ribosomal protein S14



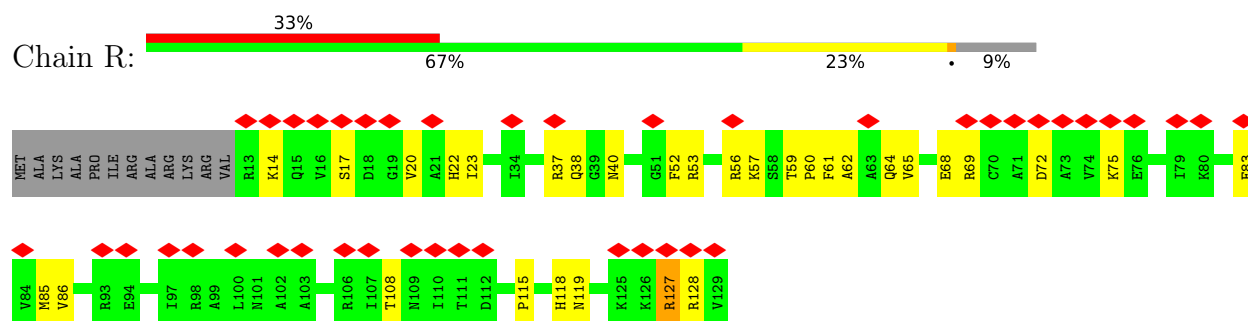
• Molecule 16: 30S ribosomal protein S19



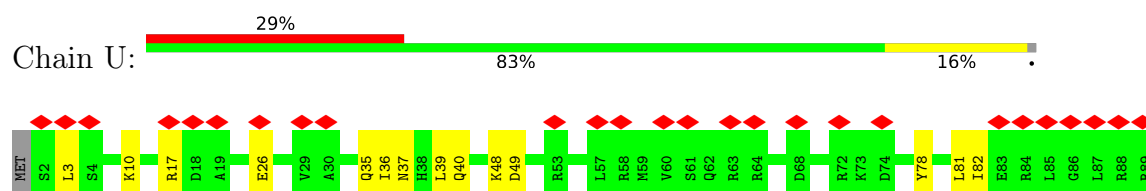
• Molecule 17: 30S ribosomal protein S6



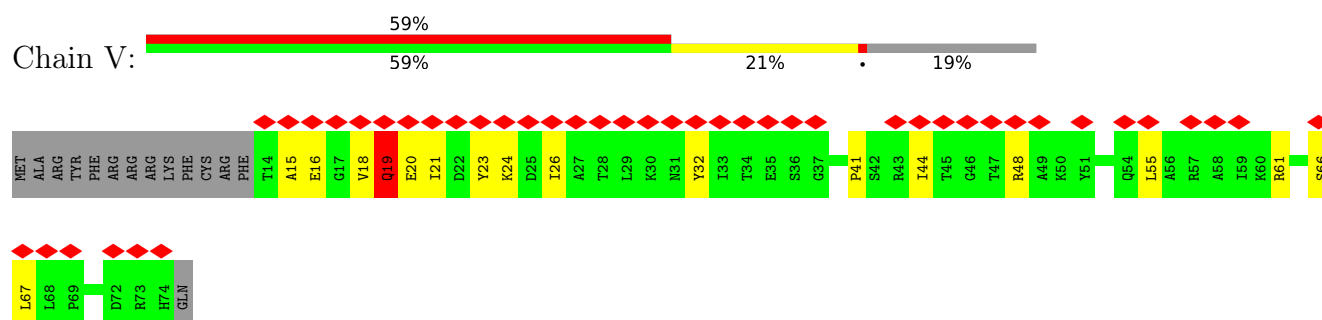
- Molecule 18: 30S ribosomal protein S11



- Molecule 19: 30S ribosomal protein S15



- Molecule 20: 30S ribosomal protein S18



- Molecule 21: Ribosomal RNA small subunit methyltransferase A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	231280	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	72	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	326.61002, 326.61002, 326.61002	wwPDB
Map dimensions	382, 382, 382	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D2T

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	0.72	53/34002 (0.2%)	0.81	213/53040 (0.4%)
2	B	0.54	2/1784 (0.1%)	0.81	5/2403 (0.2%)
3	D	0.45	0/1665	0.52	1/2227 (0.0%)
4	E	0.49	1/1157 (0.1%)	0.54	0/1557
5	H	0.47	0/989	0.53	0/1326
6	L	0.50	0/960	1.28	3/1286 (0.2%)
7	P	0.59	0/659	0.53	0/884
8	Q	0.54	0/657	0.61	0/881
9	T	0.41	0/676	0.48	0/895
10	F	0.58	1/1651 (0.1%)	0.84	11/2225 (0.5%)
11	G	0.52	0/1195	0.95	6/1602 (0.4%)
12	I	1.74	23/1034 (2.2%)	1.55	20/1375 (1.5%)
13	J	0.83	0/805	1.06	3/1089 (0.3%)
14	M	5.72	5/892 (0.6%)	2.51	19/1193 (1.6%)
15	N	1.96	22/817 (2.7%)	1.52	18/1088 (1.7%)
16	S	1.34	3/667 (0.4%)	1.78	14/897 (1.6%)
17	O	0.32	0/881	0.55	0/1189
18	R	0.27	0/893	0.58	1/1205 (0.1%)
19	U	0.36	0/722	0.56	0/964
20	V	0.57	0/503	0.69	1/677 (0.1%)
21	W	2.94	4/2023 (0.2%)	1.56	18/2751 (0.7%)
All	All	1.18	114/54632 (0.2%)	0.93	333/80754 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	I	0	1
15	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	10	PRO	N-CD	164.86	3.78	1.47
21	W	183	PRO	N-CD	128.18	3.27	1.47
1	A	949	A	O3'-P	-18.26	1.33	1.61
16	S	5	LEU	CA-C	17.77	1.63	1.53
2	B	29	PRO	N-CA	16.76	1.69	1.47
21	W	182	THR	C-N	15.19	1.51	1.33
21	W	195	VAL	C-N	13.35	1.51	1.33
1	A	1320	C	O3'-P	-11.75	1.43	1.61
1	A	1214	C	O3'-P	11.22	1.77	1.61
1	A	1313	U	O3'-P	-9.63	1.46	1.61
1	A	1199	U	O3'-P	-9.15	1.47	1.61
1	A	1251	A	O3'-P	-9.12	1.47	1.61
1	A	1141	C	O3'-P	8.82	1.74	1.61
12	I	88	MET	C-O	-8.80	1.13	1.24
1	A	1363	A	O3'-P	8.62	1.74	1.61
1	A	973	G	O3'-P	-8.56	1.48	1.61
2	B	28	LYS	C-N	8.18	1.45	1.34
1	A	1356	G	O3'-P	-8.17	1.48	1.61
1	A	1307	U	O3'-P	-7.84	1.49	1.61
1	A	960	U	O3'-P	-7.80	1.49	1.61
21	W	184	PRO	C-N	7.33	1.50	1.33
1	A	1156	G	O3'-P	7.30	1.72	1.61
1	A	1160	G	O3'-P	-7.30	1.50	1.61
12	I	83	ILE	C-O	-7.29	1.15	1.24
12	I	19	VAL	C-O	-7.22	1.16	1.24
1	A	1357	A	O3'-P	-6.97	1.50	1.61
1	A	1321	U	O3'-P	-6.87	1.50	1.61
1	A	1371	G	O3'-P	-6.84	1.50	1.61
12	I	44	ALA	C-O	-6.83	1.16	1.24
1	A	967	C	O3'-P	-6.81	1.50	1.61
1	A	1279	G	O3'-P	6.67	1.71	1.61
15	N	84	VAL	C-O	-6.56	1.16	1.24
1	A	1232	U	O3'-P	-6.46	1.51	1.61
1	A	1056	U	O3'-P	-6.42	1.51	1.61
1	A	1118	U	O3'-P	-6.39	1.51	1.61
14	M	73	ILE	C-O	-6.38	1.16	1.24
12	I	29	VAL	C-O	-6.31	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	12	ARG	C-O	-6.27	1.16	1.24
12	I	85	ARG	C-O	-6.23	1.16	1.24
12	I	81	HIS	C-O	-6.22	1.16	1.24
15	N	87	ALA	C-O	-6.16	1.17	1.24
1	A	1369	C	O3'-P	-6.06	1.52	1.61
12	I	120	LYS	C-O	-6.04	1.17	1.23
1	A	960	U	C3'-O3'	6.03	1.52	1.43
12	I	30	ILE	C-O	-6.03	1.17	1.24
1	A	1372	U	O3'-P	6.03	1.70	1.61
15	N	10	GLU	C-O	-6.02	1.17	1.24
1	A	1326	U	O3'-P	-6.00	1.52	1.61
12	I	78	ALA	N-CA	-5.98	1.39	1.46
1	A	1012	A	O3'-P	-5.97	1.52	1.61
16	S	34	TRP	C-O	-5.96	1.15	1.24
1	A	1359	C	O3'-P	-5.95	1.52	1.61
12	I	16	ALA	C-O	-5.94	1.17	1.23
1	A	1249	C	O3'-P	-5.90	1.52	1.61
1	A	1318	A	O3'-P	-5.89	1.52	1.61
12	I	109	ARG	C-O	-5.85	1.16	1.24
1	A	1158	C	O3'-P	5.80	1.69	1.61
1	A	1024	G	O3'-P	5.78	1.69	1.61
1	A	532	A	O3'-P	-5.76	1.52	1.61
1	A	1303	C	O3'-P	-5.76	1.52	1.61
15	N	28	LYS	C-O	-5.75	1.17	1.24
12	I	8	GLY	C-O	-5.75	1.16	1.23
12	I	30	ILE	CA-C	-5.74	1.45	1.52
1	A	974	A	O3'-P	-5.74	1.52	1.61
14	M	106	ALA	C-O	-5.74	1.16	1.24
15	N	79	LEU	C-O	-5.73	1.16	1.23
12	I	86	ALA	C-O	-5.70	1.17	1.24
15	N	60	GLN	C-O	-5.68	1.17	1.23
14	M	11	ASP	CA-C	5.61	1.56	1.53
12	I	7	TYR	C-O	-5.59	1.17	1.23
1	A	1521	C	O3'-P	-5.58	1.52	1.61
1	A	1139	G	O3'-P	-5.56	1.52	1.61
1	A	1248	A	O3'-P	-5.56	1.52	1.61
1	A	1330	U	O3'-P	-5.53	1.52	1.61
15	N	26	GLU	C-O	-5.50	1.17	1.24
15	N	86	GLU	C-O	-5.49	1.17	1.24
1	A	942	G	O3'-P	-5.47	1.52	1.61
12	I	79	ILE	C-O	-5.47	1.17	1.24
15	N	4	GLN	C-O	-5.46	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1317	C	O3'-P	-5.44	1.52	1.61
1	A	1323	G	O3'-P	-5.44	1.52	1.61
1	A	950	U	P-OP2	-5.43	1.38	1.49
12	I	18	ARG	C-O	-5.41	1.17	1.24
1	A	1314	C	O3'-P	-5.37	1.53	1.61
4	E	23	LYS	C-O	-5.37	1.17	1.23
16	S	5	LEU	N-CA	5.36	1.49	1.46
1	A	1277	C	O3'-P	-5.35	1.53	1.61
15	N	13	ARG	C-O	-5.35	1.17	1.24
10	F	102	ASN	C-O	-5.33	1.17	1.23
15	N	53	ARG	CA-C	-5.31	1.45	1.52
1	A	413	G	O3'-P	-5.28	1.53	1.61
12	I	50	GLN	C-O	-5.27	1.19	1.24
15	N	25	ALA	C-O	-5.26	1.18	1.24
15	N	81	ARG	C-O	-5.23	1.18	1.24
15	N	9	ARG	C-O	-5.21	1.18	1.24
1	A	939	G	O3'-P	-5.20	1.53	1.61
15	N	89	MET	C-O	-5.20	1.18	1.24
1	A	1225	A	O3'-P	-5.20	1.53	1.61
1	A	1057	G	O3'-P	-5.19	1.53	1.61
1	A	1054	C	O3'-P	-5.18	1.53	1.61
15	N	85	ARG	C-O	-5.16	1.18	1.24
15	N	61	ARG	C-O	-5.15	1.18	1.24
12	I	22	LYS	C-O	-5.14	1.18	1.24
15	N	72	GLY	C-O	-5.14	1.17	1.24
1	A	1290	G	O3'-P	5.06	1.68	1.61
15	N	74	LEU	C-O	-5.05	1.18	1.24
12	I	110	GLN	C-O	-5.04	1.17	1.23
1	A	1370	G	O3'-P	-5.03	1.53	1.61
15	N	87	ALA	CA-C	-5.03	1.46	1.52
15	N	82	ILE	C-O	-5.02	1.18	1.24
14	M	87	ARG	C-O	-5.02	1.17	1.24
1	A	938	A	O3'-P	-5.01	1.53	1.61
12	I	118	LEU	C-O	-5.01	1.17	1.23
15	N	21	PHE	CA-C	-5.01	1.46	1.52

All (333) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	10	PRO	N-CD-CG	-61.68	10.69	103.20
21	W	183	PRO	N-CD-CG	-51.38	26.13	103.20
16	S	5	LEU	N-CA-C	35.58	137.95	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	44	LYS	CA-C-N	28.49	155.45	119.84
6	L	44	LYS	C-N-CA	28.49	155.45	119.84
14	M	10	PRO	CA-N-CD	-28.48	72.12	112.00
21	W	183	PRO	CA-N-CD	-19.96	84.05	112.00
1	A	1279	G	C1'-C2'-O2'	-18.96	79.96	108.40
2	B	28	LYS	CA-C-N	17.03	137.96	119.05
2	B	28	LYS	C-N-CA	17.03	137.96	119.05
14	M	11	ASP	N-CA-C	15.25	121.28	108.78
21	W	182	THR	CA-C-N	15.22	136.06	120.38
21	W	182	THR	C-N-CA	15.22	136.06	120.38
1	A	948	C	C2'-C3'-O3'	15.00	136.20	113.70
1	A	1004	A	C1'-C2'-O2'	-14.87	89.49	111.80
1	A	1024	G	P-O3'-C3'	-12.66	101.20	120.20
1	A	1126	U	C1'-C2'-O2'	-12.55	92.98	111.80
1	A	1279	G	C4'-C3'-O3'	-12.52	94.21	113.00
1	A	944	G	P-O3'-C3'	12.32	138.68	120.20
21	W	183	PRO	CB-CA-C	12.31	125.94	110.92
21	W	184	PRO	CA-C-N	12.01	134.85	119.84
21	W	184	PRO	C-N-CA	12.01	134.85	119.84
1	A	1049	U	C1'-C2'-O2'	-11.86	94.01	111.80
1	A	1359	C	C1'-C2'-O2'	-11.82	90.67	108.40
14	M	97	VAL	N-CA-C	11.81	122.65	110.72
1	A	952	U	C1'-C2'-O2'	-11.68	90.88	108.40
6	L	44	LYS	C-N-CD	-11.51	77.83	125.00
16	S	5	LEU	CA-C-O	11.51	124.61	117.94
1	A	1516	G	C4'-C3'-O3'	-11.47	92.19	109.40
1	A	1260	G	C1'-C2'-O2'	-11.10	91.75	108.40
10	F	108	LYS	CA-C-N	10.98	131.29	119.87
10	F	108	LYS	C-N-CA	10.98	131.29	119.87
12	I	103	PHE	N-CA-C	10.86	123.20	111.36
1	A	1366	C	C1'-C2'-O2'	-10.78	92.24	108.40
1	A	412	A	C1'-C2'-O2'	-10.73	92.31	108.40
21	W	182	THR	C-N-CD	-10.68	81.21	125.00
13	J	77	VAL	N-CA-C	10.53	121.36	110.62
21	W	195	VAL	CA-C-N	10.49	130.59	119.89
21	W	195	VAL	C-N-CA	10.49	130.59	119.89
1	A	1158	C	C4'-C3'-O3'	-10.44	97.34	113.00
1	A	1052	U	C1'-C2'-O2'	-10.32	92.92	108.40
1	A	1160	G	C4'-C3'-O3'	10.28	128.42	113.00
1	A	1297	G	C4'-C3'-O3'	10.28	124.82	109.40
1	A	1235	U	C1'-C2'-O2'	-10.25	93.03	108.40
1	A	1304	G	C4'-C3'-O3'	-10.23	97.66	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	958	A	C1'-C2'-O2'	-10.20	93.10	108.40
14	M	107	ARG	N-CA-C	10.04	123.26	111.71
1	A	1334	G	C1'-C2'-O2'	-9.85	93.62	108.40
1	A	1350	A	C1'-C2'-O2'	-9.81	93.69	108.40
1	A	1218	C	C1'-C2'-O2'	-9.62	93.97	108.40
12	I	104	VAL	N-CA-C	9.55	125.64	111.89
1	A	1127	G	C3'-C2'-O2'	9.49	124.93	110.70
1	A	1171	A	C1'-C2'-O2'	-9.30	94.44	108.40
10	F	132	ARG	CA-C-N	9.22	136.35	120.58
10	F	132	ARG	C-N-CA	9.22	136.35	120.58
1	A	973	G	C1'-C2'-O2'	-9.18	94.63	108.40
1	A	1370	G	C1'-C2'-O2'	-9.09	94.76	108.40
1	A	960	U	C3'-C2'-O2'	8.92	127.98	114.60
1	A	1270	G	C1'-C2'-O2'	-8.89	95.06	108.40
1	A	1325	C	C2'-C3'-O3'	8.87	127.00	113.70
1	A	1306	A	C1'-C2'-O2'	-8.80	95.19	108.40
1	A	1358	U	C4'-C3'-O3'	-8.80	99.80	113.00
1	A	1352	C	C1'-C2'-O2'	-8.60	95.51	108.40
1	A	960	U	N1-C1'-C2'	8.58	126.86	114.00
1	A	1141	C	C2'-C3'-O3'	8.57	122.36	109.50
15	N	23	LYS	N-CA-C	-8.55	92.60	110.80
1	A	1214	C	C1'-C2'-O2'	8.43	124.44	111.80
15	N	69	ARG	N-CA-C	8.39	120.22	109.65
1	A	1323	G	C1'-C2'-O2'	-8.35	95.88	108.40
1	A	1225	A	C1'-C2'-O2'	-8.34	99.29	111.80
1	A	1233	G	C1'-C2'-O2'	-8.32	95.92	108.40
1	A	1285	A	C1'-C2'-O2'	-8.29	99.37	111.80
1	A	1222	G	C3'-C2'-O2'	8.28	123.12	110.70
1	A	1147	C	C1'-C2'-O2'	-8.28	95.99	108.40
1	A	1016	A	C4'-C3'-O3'	8.18	125.27	113.00
10	F	101	ILE	N-CA-C	8.15	120.60	108.46
1	A	1228	C	C1'-C2'-O2'	-8.14	96.19	108.40
16	S	5	LEU	CA-C-N	8.11	134.49	121.18
16	S	5	LEU	C-N-CA	8.11	134.49	121.18
1	A	1248	A	P-O3'-C3'	7.96	132.15	120.20
1	A	844	G	N9-C1'-C2'	7.90	125.84	114.00
1	A	1159	U	C1'-C2'-O2'	-7.88	99.98	111.80
12	I	46	MET	N-CA-C	-7.87	102.79	111.36
13	J	94	ALA	N-CA-C	7.86	122.55	112.34
1	A	1214	C	C3'-C2'-O2'	-7.84	102.84	114.60
1	A	1341	U	C1'-C2'-O2'	-7.83	96.66	108.40
1	A	1016	A	C2'-C3'-O3'	-7.79	102.02	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1347	G	O4'-C1'-C2'	-7.71	98.09	105.80
16	S	4	SER	CA-C-N	7.71	131.37	123.04
16	S	4	SER	C-N-CA	7.71	131.37	123.04
1	A	413	G	C1'-C2'-O2'	-7.71	100.24	111.80
1	A	1377	A	P-O3'-C3'	7.68	131.71	120.20
1	A	1326	U	C1'-C2'-O2'	-7.66	96.92	108.40
2	B	29	PRO	CA-N-CD	-7.65	101.30	112.00
12	I	55	VAL	N-CA-C	7.62	119.45	112.29
1	A	1354	U	C1'-C2'-O2'	-7.60	97.00	108.40
1	A	943	U	C2'-C3'-O3'	7.57	125.06	113.70
1	A	1254	A	C1'-C2'-O2'	-7.56	97.06	108.40
1	A	1363	A	C2'-C3'-O3'	-7.55	98.17	109.50
1	A	1277	C	P-O3'-C3'	7.54	131.50	120.20
1	A	1204	A	C1'-C2'-O2'	-7.53	97.10	108.40
11	G	114	LYS	N-CA-C	7.48	119.07	111.07
1	A	1208	C	C4'-C3'-O3'	7.45	124.17	113.00
1	A	1241	G	C1'-C2'-O2'	-7.43	97.25	108.40
16	S	81	ARG	N-CA-C	7.43	119.45	111.36
16	S	5	LEU	N-CA-CB	-7.41	97.96	110.49
15	N	82	ILE	N-CA-C	7.41	118.20	110.72
1	A	1322	C	C1'-C2'-O2'	-7.40	100.70	111.80
1	A	411	A	C2'-C3'-O3'	-7.38	98.43	109.50
14	M	105	ASN	N-CA-C	7.35	121.82	112.86
1	A	1518	A	C1'-C2'-O2'	-7.29	100.86	111.80
1	A	1251	A	C1'-C2'-O2'	-7.24	97.54	108.40
1	A	1372	U	C3'-C2'-O2'	7.24	121.55	110.70
1	A	960	U	C2'-C3'-O3'	7.22	120.33	109.50
1	A	1160	G	O4'-C4'-C3'	-7.18	96.82	104.00
16	S	5	LEU	CB-CA-C	-7.16	106.75	117.07
1	A	1521	C	C1'-C2'-O2'	-7.16	97.66	108.40
1	A	1321	U	C1'-C2'-O2'	-7.13	97.70	108.40
12	I	104	VAL	CA-C-N	7.12	133.21	121.39
12	I	104	VAL	C-N-CA	7.12	133.21	121.39
11	G	33	ASP	N-CA-C	7.11	121.26	112.58
21	W	146	ASN	CB-CA-C	-7.07	99.06	110.79
16	S	79	THR	CB-CA-C	-7.04	97.54	109.72
1	A	926	G	C4'-C3'-O3'	7.03	119.94	109.40
1	A	1335	U	C4'-C3'-O3'	-7.02	102.47	113.00
1	A	1299	A	C1'-C2'-O2'	-7.00	101.30	111.80
1	A	1379	G	P-O3'-C3'	7.00	130.70	120.20
1	A	1279	G	C3'-C2'-O2'	-6.98	100.23	110.70
1	A	1268	G	C1'-C2'-O2'	-6.98	97.94	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1358	U	C1'-C2'-O2'	-6.96	97.95	108.40
1	A	974	A	C2'-C3'-O3'	6.95	119.93	109.50
1	A	1017	U	C4'-C3'-O3'	-6.92	102.61	113.00
1	A	1299	A	C4'-C3'-O3'	-6.92	99.02	109.40
12	I	98	LEU	O-C-N	6.92	129.56	122.09
1	A	1221	G	C1'-C2'-O2'	-6.91	98.04	108.40
1	A	1239	A	C4'-C3'-O3'	6.91	119.76	109.40
15	N	30	ILE	CB-CA-C	-6.91	102.82	112.14
1	A	1363	A	P-O3'-C3'	6.90	130.55	120.20
10	F	92	ALA	N-CA-C	6.89	118.79	111.28
1	A	1517	G	C4'-C3'-O3'	-6.89	99.07	109.40
1	A	1236	A	C3'-C2'-O2'	6.87	121.00	110.70
14	M	9	ILE	C-N-CD	6.85	153.09	125.00
1	A	1208	C	C1'-C2'-O2'	-6.84	98.14	108.40
12	I	56	ASP	N-CA-C	6.82	120.94	111.74
1	A	1250	A	C1'-C2'-O2'	-6.81	98.19	108.40
1	A	1221	G	C2'-C3'-O3'	-6.77	103.54	113.70
3	D	154	ARG	N-CA-C	6.75	118.72	111.36
1	A	1248	A	C4'-C3'-O3'	-6.73	102.91	113.00
1	A	1320	C	P-O3'-C3'	6.72	130.28	120.20
1	A	1304	G	C2'-C3'-O3'	6.71	123.77	113.70
1	A	1024	G	C4'-C3'-O3'	6.71	119.46	109.40
1	A	1349	A	C1'-C2'-O2'	-6.70	98.35	108.40
1	A	1327	C	C1'-C2'-O2'	-6.68	98.38	108.40
12	I	47	VAL	N-CA-C	6.68	117.43	110.62
15	N	73	PHE	N-CA-C	6.66	120.13	110.28
1	A	1222	G	C1'-C2'-O2'	-6.63	98.45	108.40
1	A	1357	A	C1'-C2'-O2'	-6.63	98.46	108.40
14	M	98	ARG	N-CA-C	6.63	120.06	112.57
1	A	1339	A	C1'-C2'-O2'	-6.62	98.47	108.40
12	I	97	GLU	N-CA-C	6.62	118.58	111.36
1	A	1057	G	C2'-C3'-O3'	-6.57	103.84	113.70
1	A	1279	G	N9-C1'-C2'	6.57	121.85	112.00
15	N	80	SER	CA-C-O	-6.56	114.47	121.88
12	I	129	LYS	N-CA-C	6.55	118.42	111.28
1	A	942	G	C3'-C2'-O2'	6.55	120.52	110.70
1	A	1232	U	C2'-C3'-O3'	-6.54	103.89	113.70
1	A	1141	C	C1'-C2'-O2'	6.54	121.60	111.80
16	S	8	GLY	CA-C-N	6.54	128.01	119.84
16	S	8	GLY	C-N-CA	6.54	128.01	119.84
1	A	1056	U	C2'-C3'-O3'	-6.53	103.91	113.70
14	M	11	ASP	CB-CA-C	-6.53	107.67	117.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	14	VAL	CB-CA-C	-6.49	103.27	112.22
12	I	7	TYR	N-CA-C	6.48	120.06	109.24
11	G	117	ALA	N-CA-C	-6.48	104.30	111.36
1	A	938	A	C1'-C2'-O2'	-6.44	98.74	108.40
1	A	1315	U	C4'-C3'-O3'	-6.44	103.34	113.00
14	M	113	ARG	N-CA-C	6.43	119.56	110.23
1	A	944	G	C2'-C3'-O3'	-6.43	104.06	113.70
1	A	1295	U	C1'-C2'-O2'	-6.43	98.76	108.40
1	A	1224	U	C4'-C3'-O3'	6.40	119.00	109.40
1	A	1318	A	C2'-C3'-O3'	-6.38	104.13	113.70
1	A	956	U	C2'-C3'-O3'	-6.38	104.13	113.70
1	A	1307	U	C2'-C3'-O3'	-6.38	104.13	113.70
1	A	1323	G	C3'-C2'-O2'	6.37	120.25	110.70
1	A	1018	G	O4'-C1'-C2'	-6.36	99.44	105.80
1	A	1249	C	C1'-C2'-O2'	-6.36	98.86	108.40
1	A	610	U	C4'-C3'-O3'	6.31	122.47	113.00
1	A	1342	C	C1'-C2'-O2'	-6.29	98.96	108.40
1	A	1359	C	C2'-C3'-O3'	6.29	123.13	113.70
1	A	1251	A	P-O3'-C3'	6.29	129.63	120.20
1	A	1205	U	C1'-C2'-O2'	-6.28	98.98	108.40
1	A	1226	C	C1'-C2'-O2'	-6.28	102.38	111.80
1	A	1327	C	C2'-C3'-O3'	-6.26	104.31	113.70
1	A	1372	U	C2'-C3'-O3'	6.24	123.06	113.70
1	A	954	G	C1'-C2'-O2'	-6.23	99.06	108.40
1	A	1325	C	C4'-C3'-O3'	-6.23	103.66	113.00
1	A	1330	U	C2'-C3'-O3'	-6.21	104.38	113.70
1	A	1334	G	C4'-C3'-O3'	-6.21	103.69	113.00
1	A	975	A	C4'-C3'-O3'	6.20	118.71	109.40
1	A	1166	G	N9-C1'-C2'	-6.18	102.73	112.00
10	F	106	VAL	CB-CA-C	-6.18	103.40	111.25
1	A	1372	U	C4'-C3'-O3'	-6.18	103.73	113.00
21	W	184	PRO	CB-CA-C	-6.17	103.40	110.92
1	A	844	G	C4'-C3'-O3'	6.16	118.63	109.40
1	A	952	U	C2'-C3'-O3'	-6.16	104.47	113.70
1	A	931	C	O4'-C4'-C3'	-6.15	97.85	104.00
1	A	1120	C	C2'-C3'-O3'	-6.10	104.54	113.70
15	N	67	THR	N-CA-C	6.07	122.71	113.61
1	A	1324	A	C1'-C2'-O2'	-6.01	99.39	108.40
12	I	78	ALA	N-CA-C	-5.99	104.75	111.28
1	A	1232	U	C1'-C2'-O2'	-5.98	99.44	108.40
1	A	1377	A	N9-C1'-C2'	-5.97	103.04	112.00
15	N	31	ILE	CB-CA-C	-5.94	102.64	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1142	G	C2'-C3'-O3'	-5.93	104.80	113.70
1	A	1377	A	C3'-C2'-O2'	5.89	119.53	110.70
1	A	961	U	C2'-C3'-O3'	-5.88	104.87	113.70
1	A	1142	G	C4'-C3'-O3'	5.88	121.82	113.00
1	A	973	G	P-O3'-C3'	5.87	129.00	120.20
1	A	1236	A	C1'-C2'-O2'	-5.86	99.61	108.40
1	A	1208	C	N1-C1'-C2'	-5.86	103.21	112.00
16	S	80	TYR	N-CA-C	5.86	116.98	107.32
1	A	1050	G	C2'-C3'-O3'	-5.85	104.92	113.70
1	A	960	U	C4'-C3'-C2'	-5.84	96.75	102.60
21	W	180	ALA	N-CA-C	-5.84	107.14	114.56
10	F	94	ILE	CB-CA-C	-5.84	104.41	112.24
1	A	1129	C	C2'-C3'-O3'	5.82	118.22	109.50
2	B	169	GLU	CB-CA-C	5.82	118.45	109.03
1	A	1017	U	C2'-C3'-O3'	5.80	122.41	113.70
14	M	11	ASP	CA-C-O	5.80	121.31	117.94
15	N	68	GLY	N-CA-C	5.79	123.82	114.90
1	A	1213	A	C3'-C2'-O2'	-5.79	105.91	114.60
1	A	1299	A	C2'-C3'-O3'	5.79	118.18	109.50
15	N	14	VAL	N-CA-C	5.79	116.56	110.72
1	A	1288	A	C1'-C2'-O2'	-5.73	99.81	108.40
10	F	100	GLN	CA-C-N	5.70	130.87	122.94
10	F	100	GLN	C-N-CA	5.70	130.87	122.94
1	A	951	G	C1'-C2'-O2'	-5.67	99.89	108.40
1	A	1220	G	C1'-C2'-O2'	-5.67	99.89	108.40
1	A	1322	C	O4'-C1'-C2'	-5.66	100.14	105.80
18	R	127	ARG	CB-CA-C	-5.66	99.17	110.42
1	A	1140	C	C1'-C2'-O2'	-5.59	100.01	108.40
1	A	968	A	C1'-C2'-O2'	-5.57	103.44	111.80
1	A	1159	U	P-O5'-C5'	5.57	129.26	120.90
1	A	845	A	C3'-C2'-O2'	5.56	119.04	110.70
1	A	1222	G	C2'-C3'-O3'	5.56	122.04	113.70
1	A	1273	C	C2'-C3'-O3'	-5.56	105.36	113.70
1	A	1313	U	P-O3'-C3'	5.55	128.53	120.20
1	A	1058	G	C1'-C2'-O2'	-5.54	100.09	108.40
1	A	1281	C	C1'-C2'-O2'	-5.52	103.52	111.80
1	A	411	A	C4'-C3'-O3'	-5.51	101.14	109.40
1	A	959	A	C3'-C2'-O2'	5.51	118.96	110.70
1	A	948	C	P-O3'-C3'	5.50	128.46	120.20
21	W	189	SER	O-C-N	-5.49	115.34	122.97
10	F	130	PHE	N-CA-C	5.49	119.08	112.38
1	A	1144	G	C4'-C3'-O3'	-5.47	104.80	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	972	C	C1'-C2'-O2'	-5.46	100.21	108.40
1	A	1013	G	C1'-C2'-O2'	-5.46	100.22	108.40
1	A	1332	A	C1'-C2'-O2'	-5.44	100.24	108.40
1	A	1012	A	P-O3'-C3'	-5.44	112.04	120.20
1	A	1359	C	N1-C1'-C2'	5.42	120.12	112.00
1	A	1236	A	C4'-C3'-O3'	-5.41	104.89	113.00
12	I	91	ASP	N-CA-C	5.41	119.87	112.68
1	A	1297	G	P-O3'-C3'	-5.41	112.09	120.20
1	A	1054	C	P-O5'-C5'	-5.39	112.81	120.90
1	A	1159	U	O5'-P-OP1	-5.39	91.83	108.00
15	N	59	ARG	N-CA-C	-5.39	106.21	112.89
1	A	1328	C	C1'-C2'-O2'	-5.38	100.33	108.40
15	N	65	ARG	N-CA-C	5.38	116.95	111.14
15	N	25	ALA	N-CA-C	5.38	117.14	111.28
1	A	1323	G	C2'-C3'-O3'	-5.37	105.64	113.70
14	M	86	TYR	N-CA-C	5.37	117.14	111.28
1	A	1224	U	C1'-C2'-O2'	-5.36	103.76	111.80
21	W	27	ASP	N-CA-C	-5.35	106.06	113.18
12	I	58	VAL	N-CA-C	5.34	116.07	110.62
1	A	1057	G	C1'-C2'-O2'	-5.32	100.42	108.40
1	A	1292	G	C4'-C3'-O3'	-5.32	105.02	113.00
14	M	61	ALA	N-CA-C	5.30	118.85	112.38
1	A	1043	G	C1'-C2'-O2'	-5.30	103.86	111.80
12	I	113	ARG	N-CA-C	5.30	116.92	110.41
21	W	183	PRO	N-CA-CB	-5.28	97.96	103.08
1	A	1018	G	O4'-C1'-N9	5.27	116.11	108.20
1	A	1348	U	C4'-C3'-O3'	-5.27	105.10	113.00
1	A	948	C	C1'-C2'-O2'	-5.27	100.50	108.40
1	A	966	G	C2'-C3'-O3'	5.27	121.60	113.70
12	I	10	GLY	CA-C-O	-5.25	117.00	121.57
1	A	963	G	C1'-C2'-O2'	-5.25	100.53	108.40
1	A	1052	U	C4'-C3'-O3'	-5.23	105.16	113.00
1	A	1280	A	C1'-C2'-O2'	-5.20	104.00	111.80
1	A	1059	C	C2'-C3'-O3'	-5.19	105.92	113.70
1	A	971	G	O4'-C1'-C2'	-5.19	100.61	105.80
15	N	11	VAL	CB-CA-C	-5.18	105.07	112.22
12	I	19	VAL	N-CA-C	5.18	115.37	108.11
1	A	1216	A	C1'-C2'-O2'	-5.18	100.63	108.40
1	A	1016	A	C1'-C2'-O2'	5.17	116.15	108.40
14	M	4	ILE	N-CA-C	5.17	120.09	109.34
1	A	1331	G	C2'-C3'-O3'	5.16	117.24	109.50
1	A	949	A	P-O3'-C3'	5.15	127.93	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	S	4	SER	N-CA-C	-5.15	105.67	112.94
12	I	98	LEU	CA-C-N	5.15	128.84	120.60
12	I	98	LEU	C-N-CA	5.15	128.84	120.60
1	A	1053	G	C1'-C2'-O2'	5.15	119.52	111.80
1	A	1156	G	C2'-C3'-O3'	-5.14	105.99	113.70
13	J	36	VAL	N-CA-C	5.14	115.31	108.11
15	N	75	ARG	N-CA-C	5.14	116.88	111.28
1	A	1130	A	C1'-C2'-O2'	-5.12	100.72	108.40
1	A	1142	G	C3'-C2'-O2'	5.12	118.38	110.70
1	A	1238	A	C1'-C2'-O2'	-5.12	100.72	108.40
11	G	73	VAL	CB-CA-C	-5.12	103.88	110.84
14	M	105	ASN	CB-CA-C	-5.12	103.02	111.36
21	W	115	PRO	CA-C-O	-5.12	114.94	120.92
15	N	73	PHE	N-CA-CB	-5.10	102.47	109.97
1	A	955	U	C2'-C3'-O3'	-5.09	106.06	113.70
11	G	32	VAL	CA-C-N	5.08	130.06	122.74
11	G	32	VAL	C-N-CA	5.08	130.06	122.74
1	A	960	U	O4'-C1'-C2'	-5.08	100.72	105.80
14	M	41	GLU	N-CA-C	5.08	116.81	111.28
1	A	1360	A	C1'-C2'-O2'	-5.07	100.80	108.40
14	M	19	LEU	N-CA-C	5.06	119.03	113.21
20	V	19	GLN	N-CA-C	-5.06	100.03	110.80
1	A	971	G	C3'-C2'-O2'	5.05	122.18	114.60
1	A	1237	C	C4'-C3'-O3'	-5.05	105.43	113.00
15	N	30	ILE	N-CA-C	5.05	115.77	110.62
1	A	1261	A	C2'-C3'-O3'	-5.04	106.13	113.70
14	M	16	VAL	N-CA-C	-5.04	98.86	109.34
1	A	1314	C	C4'-C3'-O3'	-5.04	105.44	113.00
1	A	1290	G	C2'-C3'-O3'	-5.04	106.15	113.70
1	A	1305	G	C4'-C3'-O3'	5.03	116.95	109.40
1	A	1376	U	C2'-C3'-O3'	-5.03	106.15	113.70
2	B	29	PRO	N-CA-C	-5.03	106.55	113.53
21	W	182	THR	CA-C-O	-5.03	115.22	120.70
1	A	1220	G	C2'-C3'-O3'	-5.02	106.16	113.70
14	M	43	VAL	N-CA-C	-5.02	100.52	107.80
1	A	971	G	P-O3'-C3'	-5.02	112.67	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	I	31	ASN	Mainchain

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Mol	Chain	Res	Type	Group
15	N	80	SER	Mainchain

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	30367	0	15283	407	0
2	B	1753	0	1780	91	0
3	D	1643	0	1707	22	0
4	E	1144	0	1185	21	0
5	H	979	0	1031	6	0
6	L	957	0	1017	13	0
7	P	649	0	666	16	0
8	Q	648	0	691	10	0
9	T	670	0	719	4	0
10	F	1624	0	1696	36	0
11	G	1181	0	1238	82	0
12	I	1022	0	1070	37	0
13	J	795	0	836	47	0
14	M	883	0	941	58	0
15	N	805	0	844	25	0
16	S	651	0	675	34	0
17	O	862	0	864	46	0
18	R	877	0	887	41	0
19	U	714	0	734	13	0
20	V	496	0	516	32	0
21	W	1979	0	1989	153	0
All	All	50699	0	36369	1082	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 13.

All (1082) 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:79:G:N2	1:A:91:U:C2	1.67	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:PRO:N	2:B:29:PRO:CA	1.69	1.47
2:B:72:THR:OG1	2:B:168:HIS:CE1	1.69	1.46
14:M:4:ILE:CD1	14:M:10:PRO:HD3	1.52	1.36
14:M:3:ARG:NH1	14:M:9:ILE:HD11	1.43	1.34
17:O:42:TRP:CZ3	17:O:102:MET:HE1	1.63	1.32
17:O:42:TRP:CE2	17:O:102:MET:CE	2.15	1.30
21:W:43:GLU:CD	21:W:111:PHE:CE1	2.10	1.30
14:M:4:ILE:HD12	14:M:10:PRO:CD	1.62	1.28
17:O:42:TRP:CH2	17:O:102:MET:HE1	1.67	1.28
17:O:42:TRP:CD2	17:O:102:MET:CE	2.20	1.22
1:A:1277:C:O2'	1:A:1279:G:H8	0.91	1.22
2:B:129:LEU:HD11	2:B:132:LYS:N	1.54	1.20
14:M:3:ARG:HH11	14:M:9:ILE:CD1	1.53	1.19
1:A:1004:A:H61	1:A:1026:G:C5'	1.54	1.19
17:O:42:TRP:CD2	17:O:102:MET:HE3	1.75	1.19
1:A:1166:G:O6	1:A:1168:U:H5''	1.43	1.17
2:B:72:THR:OG1	2:B:168:HIS:ND1	1.77	1.16
13:J:31:ARG:HD2	13:J:31:ARG:O	1.41	1.16
1:A:1004:A:N6	1:A:1026:G:H5'	1.58	1.16
1:A:992:U:O4	1:A:1043:G:H2'	1.46	1.15
17:O:42:TRP:CE2	17:O:102:MET:HE2	1.82	1.14
21:W:43:GLU:OE2	21:W:111:PHE:CE1	2.00	1.14
12:I:112:GLU:OE2	12:I:115:LYS:NZ	1.80	1.14
13:J:102:LEU:O	13:J:102:LEU:HD12	1.49	1.13
1:A:79:G:N2	1:A:91:U:O2	1.80	1.13
20:V:15:ALA:HB2	20:V:32:TYR:OH	1.49	1.13
11:G:31:MET:HE2	11:G:36:LYS:HG3	1.17	1.12
1:A:79:G:N2	1:A:91:U:N3	1.98	1.12
1:A:413:G:O2'	1:A:428:G:N2	1.82	1.11
11:G:28:ASN:OD1	11:G:36:LYS:NZ	1.84	1.09
17:O:42:TRP:CE3	17:O:102:MET:HE1	1.88	1.09
17:O:42:TRP:CZ2	17:O:102:MET:CE	2.35	1.09
21:W:173:VAL:HB	21:W:191:VAL:HG12	1.21	1.09
1:A:1380:U:C5	11:G:3:ARG:HG3	1.86	1.09
1:A:1133:G:H8	1:A:1133:G:H5''	1.13	1.08
1:A:1004:A:N6	1:A:1026:G:C5'	2.15	1.08
1:A:1004:A:H61	1:A:1026:G:H5'	1.04	1.07
10:F:130:PHE:CD2	10:F:157:LEU:HB3	1.89	1.07
1:A:684:U:O2'	18:R:40:ASN:HB3	1.55	1.07
17:O:42:TRP:CE3	17:O:102:MET:CE	2.42	1.03
7:P:80:LYS:HD2	7:P:80:LYS:C	1.84	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:C:O2'	2:B:131:LYS:HE2	1.60	1.02
2:B:129:LEU:HD11	2:B:132:LYS:H	1.04	1.02
13:J:91:ASP:OD1	13:J:91:ASP:O	1.79	1.01
21:W:17:GLN:HE22	21:W:19:PHE:HD2	1.09	1.01
1:A:1377:A:C2	11:G:7:ILE:HD12	1.95	1.01
11:G:50:LEU:HD21	11:G:124:LEU:HD12	1.41	1.00
2:B:129:LEU:HD12	2:B:132:LYS:HB3	1.44	1.00
2:B:72:THR:HG1	2:B:168:HIS:CE1	1.75	1.00
1:A:1377:A:N6	11:G:7:ILE:CG2	2.25	0.99
21:W:182:THR:C	21:W:183:PRO:HG3	1.67	0.99
2:B:129:LEU:CD1	2:B:132:LYS:HB3	1.93	0.99
1:A:922:G:H1	1:A:1533:C:H5	1.10	0.99
11:G:37:SER:OG	12:I:41:ARG:HD3	1.63	0.98
20:V:15:ALA:HB2	20:V:32:TYR:CZ	1.98	0.98
15:N:26:GLU:O	15:N:30:ILE:HG12	1.64	0.98
21:W:93:MET:SD	21:W:118:ILE:HD11	2.03	0.97
17:O:42:TRP:CZ2	17:O:102:MET:HE1	1.95	0.97
2:B:72:THR:CB	2:B:168:HIS:CE1	2.48	0.97
1:A:937:A:C2	1:A:1379:G:C6	2.52	0.97
1:A:1010:U:H5''	1:A:1010:U:H6	1.27	0.97
10:F:31:ASP:OD1	15:N:65:ARG:NH2	1.98	0.96
16:S:19:VAL:HG21	16:S:44:MET:HE2	1.46	0.96
1:A:1305:G:H21	1:A:1332:A:H2	1.04	0.96
1:A:1380:U:H5	11:G:3:ARG:HA	1.28	0.95
1:A:1377:A:C6	11:G:7:ILE:CG2	2.49	0.95
1:A:1377:A:N6	11:G:7:ILE:HG22	1.82	0.95
17:O:42:TRP:CZ2	17:O:102:MET:HE2	1.98	0.95
21:W:43:GLU:OE2	21:W:111:PHE:HE1	1.47	0.95
21:W:43:GLU:OE1	21:W:111:PHE:CD1	2.20	0.94
18:R:20:VAL:CG2	18:R:37:ARG:HH22	1.79	0.94
21:W:171:ILE:O	21:W:193:ARG:N	2.00	0.94
1:A:1277:C:O2'	1:A:1279:G:C8	1.77	0.94
1:A:981:U:H5''	15:N:6:MET:HE1	1.49	0.94
1:A:994:A:H61	1:A:1047:G:H1'	1.33	0.94
2:B:129:LEU:CD1	2:B:132:LYS:N	2.30	0.93
1:A:1133:G:H5''	1:A:1133:G:C8	2.03	0.93
21:W:195:VAL:O	21:W:195:VAL:CG2	2.11	0.93
1:A:1377:A:C6	11:G:7:ILE:HG21	2.04	0.93
14:M:3:ARG:HH11	14:M:9:ILE:HD11	0.96	0.92
13:J:102:LEU:O	13:J:102:LEU:CD1	2.18	0.92
1:A:927:G:C6	1:A:1391:U:C2	2.59	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:C:N4	1:A:1046:A:N3	2.19	0.91
1:A:79:G:C2	1:A:91:U:N3	2.38	0.90
1:A:532:A:N7	10:F:193:TYR:OH	2.04	0.90
14:M:47:GLU:HG3	14:M:47:GLU:O	1.71	0.90
19:U:36:ILE:O	19:U:40:GLN:NE2	2.05	0.90
1:A:1305:G:N2	1:A:1332:A:H2	1.68	0.89
11:G:27:VAL:HG13	11:G:40:GLU:HA	1.53	0.88
1:A:1380:U:C5	11:G:3:ARG:HA	2.08	0.88
21:W:195:VAL:O	21:W:195:VAL:HG23	1.73	0.88
1:A:1009:U:H5''	1:A:1009:U:H6	1.39	0.87
14:M:65:VAL:O	14:M:68:ASP:OD1	1.92	0.87
1:A:937:A:N1	1:A:1379:G:O6	2.08	0.87
1:A:1380:U:C4	11:G:3:ARG:HG3	2.09	0.86
1:A:1377:A:C2	11:G:7:ILE:CD1	2.59	0.86
17:O:42:TRP:CH2	17:O:102:MET:CE	2.52	0.86
17:O:42:TRP:CZ3	17:O:102:MET:CE	2.55	0.86
21:W:173:VAL:N	21:W:191:VAL:O	2.08	0.86
21:W:18:ASN:OD1	21:W:18:ASN:O	1.96	0.84
14:M:56:LEU:O	14:M:60:VAL:HG23	1.77	0.84
1:A:1166:G:C6	1:A:1168:U:H5''	2.12	0.84
2:B:72:THR:CB	2:B:168:HIS:HE1	1.90	0.84
2:B:129:LEU:CD1	2:B:132:LYS:H	1.86	0.83
17:O:18:VAL:HG23	17:O:19:PRO:HD3	1.60	0.83
21:W:40:ALA:HB3	21:W:108:LEU:HD13	1.60	0.83
21:W:173:VAL:CB	21:W:191:VAL:HG12	2.08	0.83
2:B:129:LEU:HD11	2:B:132:LYS:CA	2.08	0.83
11:G:50:LEU:HD21	11:G:124:LEU:CD1	2.09	0.83
21:W:40:ALA:HB3	21:W:108:LEU:CD1	2.09	0.83
1:A:532:A:N3	1:A:532:A:H2'	1.93	0.82
14:M:36:ALA:HB3	14:M:59:GLU:OE2	1.79	0.82
7:P:80:LYS:C	7:P:80:LYS:CD	2.52	0.82
21:W:226:ARG:HD2	21:W:226:ARG:O	1.79	0.82
3:D:197:GLU:OE1	3:D:197:GLU:N	2.09	0.82
11:G:31:MET:CE	11:G:36:LYS:HG3	2.07	0.82
1:A:1377:A:N1	11:G:7:ILE:HG21	1.95	0.81
14:M:95:LEU:HB3	14:M:96:PRO:CD	2.10	0.81
11:G:30:LEU:HD23	11:G:30:LEU:O	1.80	0.81
13:J:4:GLN:HG2	13:J:79:PRO:HG2	1.60	0.81
2:B:72:THR:OG1	2:B:168:HIS:HE1	1.63	0.81
21:W:76:GLN:HE22	21:W:87:ILE:HD12	1.46	0.81
1:A:1076:U:OP1	2:B:174:LYS:NZ	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:68:ASP:OD2	21:W:71:LEU:HD23	1.81	0.80
1:A:937:A:C2	1:A:1379:G:O6	2.33	0.80
21:W:40:ALA:CB	21:W:108:LEU:CD1	2.59	0.79
1:A:1021:A:N3	1:A:1021:A:H5''	1.98	0.79
1:A:994:A:N9	1:A:1216:A:H4'	1.98	0.79
21:W:43:GLU:CD	21:W:111:PHE:CZ	2.60	0.79
13:J:56:HIS:HD2	13:J:57:VAL:HG13	1.46	0.79
1:A:1377:A:C8	1:A:1377:A:H3'	2.17	0.79
21:W:17:GLN:NE2	21:W:19:PHE:HD2	1.80	0.79
2:B:129:LEU:HD13	2:B:133:GLU:OE1	1.82	0.79
10:F:130:PHE:CE2	10:F:157:LEU:HB3	2.18	0.78
1:A:933:G:N7	11:G:3:ARG:NH1	2.32	0.78
1:A:1377:A:N6	11:G:7:ILE:HG21	1.92	0.78
11:G:108:ALA:HB1	11:G:119:ARG:O	1.84	0.78
14:M:36:ALA:CB	14:M:59:GLU:OE2	2.33	0.77
20:V:19:GLN:OE1	20:V:20:GLU:HG2	1.85	0.77
20:V:15:ALA:CB	20:V:32:TYR:OH	2.31	0.77
1:A:979:C:O2	15:N:59:ARG:HD2	1.84	0.77
2:B:129:LEU:CD1	2:B:133:GLU:H	1.98	0.77
21:W:71:LEU:O	21:W:75:LEU:HB2	1.85	0.77
13:J:82:LYS:HA	13:J:85:ASP:OD1	1.85	0.77
11:G:27:VAL:HG22	11:G:43:VAL:HG21	1.64	0.77
14:M:100:GLN:OE1	14:M:100:GLN:N	2.17	0.77
1:A:845:A:N3	20:V:48:ARG:NH2	2.31	0.77
1:A:992:U:C2	1:A:1043:G:N7	2.53	0.77
20:V:16:GLU:O	20:V:16:GLU:HG3	1.83	0.77
14:M:56:LEU:HA	14:M:59:GLU:HB2	1.66	0.76
17:O:42:TRP:CE3	17:O:102:MET:HE3	2.17	0.76
21:W:141:GLN:HG2	21:W:143:GLU:OE1	1.84	0.76
21:W:40:ALA:CB	21:W:108:LEU:HD12	2.14	0.76
17:O:90:MET:HE1	20:V:61:ARG:HH11	1.50	0.76
21:W:157:TYR:O	21:W:221:ARG:NH2	2.18	0.76
17:O:1:MET:N	17:O:66:ALA:O	2.19	0.76
1:A:992:U:C4	1:A:1043:G:C8	2.74	0.76
13:J:91:ASP:OD1	13:J:91:ASP:C	2.28	0.76
7:P:79:ASN:O	7:P:82:ALA:OXT	2.04	0.76
10:F:86:LYS:O	10:F:90:VAL:HG12	1.85	0.75
12:I:129:LYS:O	12:I:130:ARG:OXT	2.05	0.75
12:I:118:LEU:HB3	12:I:123:ARG:O	1.86	0.75
14:M:3:ARG:NH1	14:M:9:ILE:CD1	2.25	0.75
18:R:65:VAL:HG12	18:R:69:ARG:HH12	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:19:GLN:HA	20:V:19:GLN:NE2	2.00	0.75
21:W:174:LEU:O	21:W:191:VAL:N	2.19	0.74
1:A:532:A:N6	10:F:193:TYR:CZ	2.52	0.74
21:W:169:ASN:O	21:W:194:LEU:HA	1.87	0.74
1:A:1017:U:H5''	1:A:1017:U:O2	1.88	0.74
2:B:133:GLU:HA	2:B:137:ARG:HB2	1.69	0.74
17:O:38:ARG:NH1	17:O:98:GLU:O	2.19	0.74
1:A:1009:U:H5''	1:A:1009:U:C6	2.22	0.73
21:W:43:GLU:OE1	21:W:111:PHE:CE1	2.36	0.73
1:A:1010:U:H6	1:A:1010:U:C5'	2.02	0.73
21:W:148:LEU:HB3	21:W:170:VAL:HG11	1.69	0.73
1:A:1137:C:H4'	1:A:1138:G:H5''	1.69	0.73
7:P:80:LYS:HD2	7:P:80:LYS:O	1.87	0.73
1:A:79:G:N1	1:A:91:U:N3	2.37	0.73
1:A:1298:U:O4	11:G:114:LYS:HB2	1.88	0.73
21:W:143:GLU:OE1	21:W:143:GLU:N	2.18	0.73
17:O:10:VAL:HG12	17:O:58:HIS:HB3	1.71	0.73
1:A:1004:A:N1	1:A:1026:G:O4'	2.22	0.73
1:A:151:A:H2	1:A:170:U:H3	1.36	0.73
1:A:1227:A:OP2	14:M:110:LYS:HE2	1.88	0.73
1:A:82:G:N2	1:A:88:U:H1'	2.04	0.72
21:W:43:GLU:CD	21:W:111:PHE:CD1	2.66	0.72
1:A:845:A:C2	20:V:48:ARG:NH2	2.55	0.72
14:M:4:ILE:HD12	14:M:10:PRO:HD3	0.78	0.72
1:A:1158:C:O2'	2:B:131:LYS:CE	2.37	0.72
1:A:994:A:H61	1:A:1047:G:C1'	2.03	0.72
11:G:13:LEU:HB3	11:G:14:PRO:HD2	1.72	0.72
1:A:927:G:C6	1:A:1391:U:O2	2.42	0.71
10:F:130:PHE:CE1	10:F:157:LEU:HD13	2.24	0.71
14:M:59:GLU:HA	14:M:62:LYS:NZ	2.05	0.71
1:A:1166:G:C8	1:A:1166:G:H3'	2.25	0.71
1:A:1169:A:H2'	1:A:1170:A:C8	2.26	0.71
1:A:927:G:N1	1:A:1391:U:O2	2.24	0.71
2:B:169:GLU:O	2:B:171:ILE:N	2.23	0.71
21:W:133:ILE:HD12	21:W:133:ILE:N	2.05	0.71
14:M:4:ILE:CD1	14:M:10:PRO:CD	2.41	0.71
21:W:40:ALA:HB1	21:W:108:LEU:HD12	1.71	0.70
16:S:6:LYS:HD2	16:S:6:LYS:C	2.15	0.70
21:W:43:GLU:HG3	21:W:111:PHE:CZ	2.27	0.70
1:A:995:C:C2	1:A:1047:G:H5'	2.26	0.70
1:A:938:A:H4'	11:G:95:ARG:NH2	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:G:H3'	1:A:944:G:C8	2.27	0.70
21:W:172:PRO:HA	21:W:192:VAL:HA	1.74	0.70
8:Q:4:LYS:HZ2	8:Q:4:LYS:HB2	1.55	0.70
14:M:101:ARG:HG3	14:M:101:ARG:O	1.92	0.70
1:A:1004:A:N6	1:A:1026:G:H5''	2.06	0.69
14:M:45:ILE:HA	14:M:48:LEU:CD1	2.22	0.69
16:S:36:ARG:NH2	16:S:75:ALA:O	2.24	0.69
1:A:1166:G:O6	1:A:1168:U:C5'	2.33	0.69
16:S:70:LYS:HB2	16:S:73:GLU:HG3	1.75	0.69
21:W:133:ILE:HD12	21:W:133:ILE:H	1.57	0.69
2:B:129:LEU:CD1	2:B:132:LYS:CB	2.69	0.69
4:E:151:GLU:N	4:E:151:GLU:OE1	2.23	0.69
13:J:89:ARG:O	13:J:89:ARG:HG3	1.92	0.69
1:A:1010:U:H5''	1:A:1010:U:C6	2.18	0.69
1:A:1026:G:N3	1:A:1026:G:H2'	2.05	0.69
20:V:15:ALA:O	20:V:21:ILE:HD11	1.92	0.69
20:V:21:ILE:HD13	20:V:55:LEU:HD12	1.75	0.69
1:A:995:C:N3	1:A:1046:A:H2'	2.07	0.69
1:A:1320:C:H41	16:S:37:ARG:HB3	1.56	0.68
14:M:4:ILE:CG1	14:M:10:PRO:HD3	2.22	0.68
1:A:1380:U:C4	11:G:3:ARG:CG	2.76	0.68
1:A:926:G:H4'	1:A:927:G:H5'	1.75	0.68
14:M:42:ASP:OD1	14:M:42:ASP:N	2.26	0.68
2:B:133:GLU:O	2:B:138:THR:N	2.26	0.68
21:W:168:CYS:SG	21:W:194:LEU:HB3	2.34	0.68
2:B:132:LYS:HA	2:B:136:MET:HE2	1.76	0.68
16:S:6:LYS:HD2	16:S:6:LYS:O	1.94	0.67
1:A:1004:A:H61	1:A:1026:G:C4'	2.05	0.67
11:G:73:VAL:HG21	11:G:145:ALA:HB2	1.75	0.67
17:O:17:GLN:OE1	17:O:17:GLN:N	2.27	0.67
21:W:108:LEU:N	21:W:108:LEU:HD22	2.09	0.67
1:A:1009:U:OP1	15:N:24:ARG:NH1	2.26	0.67
17:O:9:MET:HE2	17:O:86:ARG:HB3	1.77	0.67
21:W:28:SER:HB2	21:W:174:LEU:HD22	1.74	0.67
2:B:72:THR:HB	2:B:168:HIS:HE1	1.58	0.67
11:G:15:ASP:HB3	11:G:24:ALA:HB2	1.77	0.67
1:A:927:G:N1	1:A:1391:U:C2	2.62	0.67
1:A:991:U:C5	1:A:1212:U:H1'	2.29	0.67
11:G:92:ARG:HB3	11:G:93:PRO:HD2	1.77	0.67
1:A:1123:U:H2'	1:A:1124:G:H5''	1.75	0.66
2:B:137:ARG:HA	2:B:140:GLU:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:U:H5''	15:N:6:MET:CE	2.22	0.66
2:B:31:ILE:HD11	2:B:39:HIS:CD2	2.31	0.66
18:R:38:GLN:OE1	18:R:38:GLN:N	2.26	0.66
10:F:130:PHE:CE2	10:F:157:LEU:CB	2.78	0.66
1:A:994:A:C8	1:A:1216:A:H4'	2.30	0.66
4:E:164:ILE:C	4:E:164:ILE:HD12	2.21	0.66
21:W:76:GLN:NE2	21:W:87:ILE:HD12	2.09	0.66
1:A:840:C:C2	1:A:847:G:N2	2.63	0.66
1:A:846:G:OP1	1:A:846:G:H3'	1.95	0.66
1:A:995:C:N3	1:A:1046:A:C2'	2.58	0.66
11:G:31:MET:HE2	11:G:36:LYS:CG	2.11	0.66
1:A:978:A:C6	1:A:1318:A:C6	2.83	0.66
2:B:72:THR:HB	2:B:168:HIS:CE1	2.30	0.66
3:D:100:ASN:OD1	3:D:111:ARG:NH1	2.29	0.66
13:J:29:ALA:HB1	13:J:76:ILE:HD13	1.78	0.66
17:O:1:MET:H2	17:O:66:ALA:C	2.04	0.66
1:A:1024:G:N3	1:A:1024:G:O2'	2.22	0.65
2:B:44:GLU:N	2:B:44:GLU:OE1	2.28	0.65
14:M:8:ASN:HD21	14:M:66:GLU:CD	2.04	0.65
13:J:4:GLN:O	13:J:79:PRO:CD	2.44	0.65
17:O:1:MET:N	17:O:66:ALA:C	2.55	0.65
1:A:411:A:H4'	1:A:412:A:H5'	1.79	0.65
1:A:938:A:H4'	11:G:95:ARG:HH22	1.62	0.65
1:A:1016:A:O2'	1:A:1217:C:O2'	2.15	0.65
1:A:1522:U:H5''	18:R:128:ARG:HH22	1.60	0.65
7:P:77:GLU:O	7:P:81:ALA:HB3	1.95	0.65
10:F:81:GLY:HA2	10:F:84:VAL:HG22	1.77	0.65
13:J:31:ARG:HD2	13:J:31:ARG:C	2.17	0.65
14:M:45:ILE:HA	14:M:48:LEU:HD13	1.78	0.65
21:W:173:VAL:HB	21:W:191:VAL:CG1	2.13	0.65
2:B:129:LEU:HD11	2:B:133:GLU:N	2.12	0.65
11:G:73:VAL:HG21	11:G:145:ALA:CB	2.26	0.65
2:B:129:LEU:HD13	2:B:133:GLU:H	1.61	0.65
2:B:151:ILE:HA	2:B:154:MET:HG2	1.77	0.64
20:V:26:ILE:HD11	20:V:67:LEU:HD23	1.78	0.64
13:J:31:ARG:C	13:J:31:ARG:HH11	2.04	0.64
1:A:1372:U:OP1	12:I:73:SER:HB2	1.97	0.64
15:N:24:ARG:HB3	15:N:28:LYS:HZ3	1.63	0.64
18:R:20:VAL:HG22	18:R:83:GLU:OE2	1.98	0.64
11:G:118:LEU:C	11:G:120:LEU:H	2.05	0.64
14:M:113:ARG:HG2	14:M:113:ARG:HH11	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:107:PRO:HB2	21:W:134:ALA:HB2	1.80	0.64
1:A:992:U:O4	1:A:1043:G:C2'	2.37	0.64
2:B:32:PHE:HB2	2:B:42:ASN:HB2	1.78	0.64
17:O:104:LYS:HB2	17:O:104:LYS:NZ	2.13	0.64
2:B:129:LEU:HD12	2:B:132:LYS:CB	2.25	0.64
11:G:27:VAL:CG1	11:G:40:GLU:HA	2.25	0.64
21:W:41:MET:HB3	21:W:43:GLU:OE2	1.98	0.64
1:A:1021:A:H2'	1:A:1022:A:H5'	1.80	0.64
12:I:35:LEU:HD13	12:I:35:LEU:O	1.98	0.64
4:E:13:GLU:HG2	4:E:39:VAL:HG12	1.80	0.63
1:A:995:C:O2	1:A:1047:G:H5'	1.98	0.63
1:A:1381:U:H2'	1:A:1381:U:O2	1.97	0.63
21:W:59:LEU:C	21:W:61:GLN:H	2.04	0.63
1:A:1099:G:O5'	2:B:95:ARG:NH2	2.31	0.63
21:W:108:LEU:HD23	21:W:132:ALA:O	1.99	0.63
7:P:80:LYS:HD2	7:P:81:ALA:N	2.13	0.63
1:A:1027:C:N3	1:A:1035:A:N1	2.47	0.63
4:E:112:ARG:O	4:E:116:GLU:HG3	1.99	0.62
8:Q:4:LYS:HB2	8:Q:4:LYS:NZ	2.14	0.62
17:O:14:GLN:N	17:O:14:GLN:OE1	2.32	0.62
1:A:76:G:H1	1:A:93:U:H3	1.47	0.62
1:A:994:A:C4	1:A:1216:A:H4'	2.34	0.62
18:R:64:GLN:O	18:R:68:GLU:HG3	1.98	0.62
4:E:76:LEU:HD21	4:E:120:VAL:HG22	1.80	0.62
20:V:18:VAL:HG22	20:V:18:VAL:O	1.98	0.62
21:W:43:GLU:CG	21:W:111:PHE:CZ	2.83	0.62
13:J:4:GLN:O	13:J:79:PRO:HD3	2.00	0.62
14:M:90:ARG:HB2	14:M:97:VAL:HG22	1.82	0.62
16:S:4:SER:C	16:S:5:LEU:HD23	2.23	0.62
16:S:5:LEU:HD23	16:S:5:LEU:N	1.99	0.62
12:I:129:LYS:O	12:I:129:LYS:HD2	2.00	0.62
21:W:78:HIS:CD2	21:W:79:PRO:HD2	2.35	0.62
1:A:673:A:H2'	1:A:674:G:C8	2.35	0.61
16:S:3:ARG:HG2	16:S:3:ARG:HH11	1.65	0.61
1:A:1028:C:H2'	1:A:1029:U:C6	2.35	0.61
1:A:1099:G:H3'	2:B:95:ARG:HH12	1.65	0.61
2:B:169:GLU:C	2:B:171:ILE:H	2.09	0.61
14:M:68:ASP:OD1	14:M:68:ASP:N	2.32	0.61
1:A:676:A:H5''	18:R:115:PRO:HB3	1.83	0.61
12:I:35:LEU:HD13	12:I:35:LEU:C	2.25	0.61
21:W:58:ARG:HG3	21:W:58:ARG:HH11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1166:G:C8	1:A:1166:G:C3'	2.84	0.61
1:A:1377:A:C8	1:A:1377:A:C3'	2.84	0.61
14:M:58:ASP:OD1	14:M:58:ASP:O	2.18	0.61
18:R:20:VAL:HG21	18:R:37:ARG:HH22	1.63	0.61
21:W:42:VAL:HB	21:W:110:VAL:HG12	1.83	0.60
3:D:45:LYS:HE2	3:D:45:LYS:HA	1.83	0.60
1:A:952:U:O4	14:M:103:LYS:HE2	2.00	0.60
1:A:992:U:C2	1:A:1043:G:C5	2.88	0.60
2:B:31:ILE:HD11	2:B:39:HIS:CG	2.37	0.60
10:F:111:LEU:HD22	10:F:146:ALA:HB2	1.84	0.60
1:A:1009:U:C6	1:A:1009:U:C5'	2.85	0.60
2:B:28:LYS:O	2:B:31:ILE:HG22	2.01	0.60
17:O:90:MET:HE1	20:V:61:ARG:NH1	2.15	0.60
1:A:79:G:N1	1:A:91:U:C4	2.69	0.60
1:A:696:A:H2'	1:A:697:U:C6	2.37	0.60
13:J:32:THR:HG22	13:J:32:THR:O	2.01	0.60
1:A:1298:U:C4	11:G:114:LYS:HB2	2.37	0.60
8:Q:4:LYS:O	8:Q:4:LYS:HG3	2.00	0.60
12:I:25:ASN:O	12:I:62:ASP:HB3	2.02	0.60
1:A:1305:G:N2	1:A:1332:A:C2	2.55	0.60
2:B:225:ARG:HG2	2:B:225:ARG:HH11	1.67	0.60
1:A:944:G:C8	1:A:944:G:C3'	2.85	0.59
20:V:21:ILE:HD13	20:V:55:LEU:CD1	2.32	0.59
1:A:995:C:N3	1:A:1046:A:O2'	2.28	0.59
1:A:1377:A:N1	11:G:7:ILE:HD13	2.17	0.59
1:A:1158:C:C5	1:A:1160:G:H1'	2.37	0.59
2:B:129:LEU:HD11	2:B:133:GLU:H	1.65	0.59
8:Q:83:VAL:O	8:Q:83:VAL:HG23	2.01	0.59
12:I:75:GLN:O	12:I:79:ILE:HG13	2.01	0.59
1:A:927:G:O6	1:A:1391:U:N3	2.35	0.59
1:A:682:G:H8	1:A:682:G:H5''	1.67	0.59
1:A:1130:A:OP1	12:I:18:ARG:NH2	2.32	0.59
1:A:686:U:C6	1:A:703:G:N2	2.71	0.59
1:A:1286:U:H2'	1:A:1286:U:O2	2.03	0.59
2:B:225:ARG:HG2	2:B:225:ARG:NH1	2.18	0.59
20:V:21:ILE:CD1	20:V:55:LEU:CD1	2.81	0.59
21:W:93:MET:SD	21:W:118:ILE:CD1	2.86	0.59
21:W:195:VAL:O	21:W:195:VAL:HG22	1.98	0.59
1:A:1027:C:C2	1:A:1035:A:C2	2.92	0.58
1:A:1118:U:H5'	12:I:106:ARG:HG3	1.84	0.58
11:G:61:ALA:HA	11:G:64:VAL:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:31:ARG:O	13:J:31:ARG:CD	2.34	0.58
11:G:46:ALA:CB	11:G:120:LEU:HD23	2.33	0.58
11:G:47:LEU:C	11:G:47:LEU:HD23	2.28	0.58
19:U:36:ILE:C	19:U:40:GLN:HE22	2.12	0.58
1:A:1358:U:H5	1:A:1363:A:H62	1.51	0.58
9:T:39:ILE:HD11	9:T:83:ILE:HG13	1.86	0.58
20:V:19:GLN:HA	20:V:19:GLN:HE21	1.66	0.58
21:W:71:LEU:O	21:W:75:LEU:CB	2.52	0.58
1:A:1004:A:H62	1:A:1027:C:H5	1.51	0.57
10:F:87:LEU:O	10:F:90:VAL:HG13	2.04	0.57
21:W:19:PHE:CE1	21:W:182:THR:HG21	2.39	0.57
1:A:1071:C:H2'	1:A:1072:G:H8	1.67	0.57
2:B:76:ALA:HB2	2:B:210:VAL:HG11	1.86	0.57
21:W:232:LEU:HB2	21:W:233:PHE:HD1	1.70	0.57
1:A:1133:G:N2	1:A:1142:G:C4	2.72	0.57
1:A:928:G:N2	1:A:1390:U:C2	2.72	0.57
7:P:45:GLU:OE1	7:P:45:GLU:N	2.22	0.57
16:S:50:ALA:HB1	16:S:57:HIS:HB3	1.85	0.57
1:A:80:A:O5'	1:A:80:A:H8	1.88	0.57
1:A:966:G:H2'	1:A:967:C:C5	2.39	0.57
2:B:169:GLU:C	2:B:169:GLU:OE2	2.48	0.57
11:G:73:VAL:HG13	11:G:73:VAL:O	2.03	0.57
14:M:8:ASN:ND2	14:M:66:GLU:CD	2.62	0.57
17:O:73:GLU:O	17:O:77:THR:HG23	2.05	0.57
1:A:1099:G:H3'	2:B:95:ARG:NH1	2.19	0.57
21:W:119:SER:O	21:W:123:MET:SD	2.63	0.57
21:W:139:MET:HA	21:W:190:ALA:O	2.05	0.57
1:A:1118:U:H1'	1:A:1179:A:C4	2.40	0.57
1:A:1277:C:C2'	1:A:1279:G:C8	2.84	0.57
17:O:22:ILE:O	17:O:26:THR:OG1	2.21	0.57
20:V:41:PRO:HG2	20:V:44:ILE:HD12	1.86	0.57
1:A:1022:A:O5'	1:A:1022:A:H8	1.88	0.56
6:L:122:PRO:C	6:L:124:ALA:H	2.13	0.56
9:T:35:VAL:HG11	9:T:79:LEU:HD13	1.86	0.56
13:J:35:GLN:HA	13:J:35:GLN:OE1	2.05	0.56
14:M:95:LEU:HB3	14:M:96:PRO:HD2	1.87	0.56
1:A:1010:U:C5'	1:A:1010:U:C6	2.84	0.56
13:J:46:LYS:HA	13:J:67:ILE:O	2.05	0.56
16:S:3:ARG:HH11	16:S:3:ARG:CG	2.18	0.56
21:W:18:ASN:ND2	21:W:185:PRO:HG3	2.20	0.56
1:A:1004:A:N6	1:A:1027:C:H5	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:19:ASN:OD1	10:F:54:ARG:NE	2.36	0.56
1:A:1356:G:H2'	1:A:1357:A:C8	2.41	0.56
7:P:46:LYS:H	7:P:46:LYS:HD2	1.71	0.56
13:J:24:GLU:O	13:J:28:THR:HG23	2.05	0.56
1:A:459:A:H2'	1:A:460:A:H8	1.71	0.56
1:A:426:U:OP1	3:D:33:LYS:NZ	2.28	0.56
1:A:1017:U:C2'	1:A:1018:G:H5'	2.36	0.56
11:G:30:LEU:HD23	11:G:30:LEU:C	2.31	0.56
1:A:952:U:C4	14:M:103:LYS:HE2	2.41	0.55
1:A:1027:C:O2	1:A:1035:A:C2	2.59	0.55
13:J:29:ALA:HB1	13:J:76:ILE:CD1	2.36	0.55
21:W:100:LEU:HA	21:W:103:LYS:HG3	1.88	0.55
1:A:459:A:H2'	1:A:460:A:C8	2.41	0.55
1:A:492:C:H2'	1:A:493:A:C8	2.41	0.55
1:A:78:A:O5'	1:A:78:A:H8	1.89	0.55
1:A:1291:U:OP1	11:G:37:SER:HB3	2.06	0.55
21:W:147:ARG:HG3	21:W:156:ALA:O	2.06	0.55
1:A:1019:A:H4'	1:A:1019:A:OP1	2.05	0.55
4:E:65:GLU:OE1	4:E:68:ARG:NH1	2.38	0.55
10:F:129:MET:HE3	10:F:129:MET:HA	1.88	0.55
13:J:4:GLN:HG2	13:J:4:GLN:O	2.05	0.55
17:O:42:TRP:CE2	17:O:102:MET:HE1	2.12	0.55
21:W:33:ILE:CG2	21:W:109:ARG:NH2	2.68	0.55
1:A:82:G:H22	1:A:88:U:H1'	1.70	0.55
1:A:1221:G:H4'	16:S:77:THR:HG21	1.89	0.55
21:W:59:LEU:O	21:W:61:GLN:N	2.39	0.55
4:E:161:VAL:HG12	4:E:161:VAL:O	2.04	0.55
17:O:43:GLY:C	17:O:58:HIS:HD2	2.14	0.55
2:B:42:ASN:HD21	2:B:44:GLU:HB2	1.71	0.55
1:A:1030:U:H2'	1:A:1032:G:O6	2.07	0.55
1:A:1377:A:N1	11:G:7:ILE:CD1	2.69	0.55
12:I:123:ARG:NH1	12:I:124:ARG:O	2.39	0.55
1:A:1167:A:H2'	1:A:1169:A:N7	2.20	0.55
1:A:1117:A:H4'	12:I:106:ARG:NH1	2.22	0.55
5:H:90:ASP:OD1	5:H:90:ASP:N	2.31	0.55
7:P:41:PRO:HG2	7:P:42:ILE:HG12	1.89	0.55
1:A:1157:A:C4	1:A:1181:G:N1	2.75	0.54
12:I:129:LYS:C	12:I:130:ARG:OXT	2.50	0.54
1:A:927:G:O6	1:A:1391:U:C2	2.60	0.54
20:V:20:GLU:HA	20:V:20:GLU:OE1	2.07	0.54
21:W:136:MET:HE1	21:W:196:PRO:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:G:HO2'	1:A:428:G:H21	1.50	0.54
2:B:20:THR:HG22	2:B:39:HIS:CE1	2.43	0.54
12:I:22:LYS:HG2	12:I:62:ASP:OD1	2.08	0.54
1:A:147:G:H2'	1:A:148:G:C8	2.43	0.54
1:A:261:U:OP2	9:T:74:ARG:NH2	2.40	0.54
1:A:714:G:H2'	1:A:715:A:C8	2.43	0.54
21:W:42:VAL:HB	21:W:110:VAL:CG1	2.37	0.54
1:A:1100:C:OP2	2:B:95:ARG:NH1	2.41	0.54
1:A:1309:G:OP1	14:M:91:HIS:NE2	2.28	0.54
11:G:37:SER:HG	12:I:41:ARG:HD3	1.69	0.54
1:A:1071:C:H2'	1:A:1072:G:C8	2.42	0.54
1:A:1088:G:H21	1:A:1167:A:H62	1.55	0.54
13:J:29:ALA:CB	13:J:76:ILE:HD11	2.38	0.54
1:A:1187:G:H2'	1:A:1188:A:C8	2.42	0.54
21:W:130:THR:HG23	21:W:131:ASP:H	1.72	0.54
1:A:927:G:O5'	1:A:927:G:H8	1.90	0.54
21:W:81:LEU:HD11	21:W:85:LEU:HD11	1.90	0.54
1:A:1004:A:C2'	1:A:1004:A:N3	2.71	0.54
12:I:29:VAL:O	12:I:29:VAL:HG12	2.08	0.54
14:M:4:ILE:HG21	14:M:60:VAL:HG21	1.89	0.53
21:W:80:PHE:O	21:W:84:LYS:NZ	2.41	0.53
1:A:846:G:H2'	1:A:847:G:C8	2.44	0.53
1:A:1118:U:C5'	12:I:106:ARG:HG3	2.38	0.53
1:A:1380:U:C5	11:G:3:ARG:CG	2.77	0.53
20:V:23:TYR:CD1	20:V:23:TYR:C	2.85	0.53
21:W:33:ILE:CG2	21:W:109:ARG:HH21	2.21	0.53
21:W:139:MET:HB2	21:W:191:VAL:HG22	1.90	0.53
1:A:515:G:H2'	1:A:516:U:C6	2.43	0.53
1:A:980:C:O2'	15:N:13:ARG:NH1	2.42	0.53
1:A:992:U:C5	1:A:1043:G:C8	2.96	0.53
21:W:71:LEU:N	21:W:71:LEU:CD2	2.71	0.53
1:A:996:A:H2'	1:A:997:U:C6	2.44	0.53
2:B:29:PRO:N	2:B:29:PRO:C	2.59	0.53
3:D:188:ARG:HD2	3:D:188:ARG:O	2.08	0.53
10:F:30:ALA:CB	15:N:77:PHE:O	2.57	0.53
17:O:2:ARG:HG2	17:O:91:ARG:NH1	2.23	0.53
1:A:1227:A:H3'	1:A:1227:A:H8	1.74	0.53
11:G:12:ILE:HD13	11:G:25:LYS:HG2	1.89	0.53
13:J:31:ARG:C	13:J:31:ARG:NH1	2.66	0.53
21:W:109:ARG:HD2	21:W:135:ASP:OD1	2.08	0.53
21:W:182:THR:O	21:W:183:PRO:HG3	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:U:O2	1:A:1280:A:H2'	2.09	0.53
1:A:1007:U:H3'	1:A:1007:U:H6	1.74	0.53
14:M:3:ARG:HH11	14:M:9:ILE:CG1	2.20	0.53
16:S:31:LEU:HD13	16:S:49:ILE:HG12	1.90	0.53
21:W:98:GLY:O	21:W:101:ALA:HB3	2.09	0.53
10:F:130:PHE:CD1	10:F:130:PHE:C	2.87	0.53
14:M:59:GLU:HA	14:M:62:LYS:HZ1	1.74	0.53
19:U:26:GLU:HG3	19:U:81:LEU:HD22	1.89	0.53
21:W:71:LEU:N	21:W:71:LEU:HD22	2.24	0.53
2:B:90:PHE:HA	2:B:150:GLY:HA3	1.91	0.52
15:N:48:LEU:O	15:N:48:LEU:HG	2.08	0.52
21:W:64:VAL:CG1	21:W:87:ILE:HG12	2.40	0.52
18:R:14:LYS:HE3	18:R:14:LYS:HA	1.90	0.52
17:O:42:TRP:CG	17:O:102:MET:HE3	2.38	0.52
1:A:718:A:H5'	18:R:119:ASN:OD1	2.08	0.52
2:B:28:LYS:N	2:B:29:PRO:CD	2.73	0.52
14:M:59:GLU:C	14:M:62:LYS:HZ3	2.16	0.52
21:W:21:ASN:HD22	21:W:182:THR:CG2	2.22	0.52
1:A:961:U:P	1:A:961:U:H6	2.33	0.52
1:A:976:G:H2'	1:A:1362:A:N1	2.24	0.52
1:A:994:A:N1	1:A:1047:G:O2'	2.38	0.52
1:A:1017:U:H2'	1:A:1018:G:H5'	1.91	0.52
2:B:58:ASN:ND2	2:B:220:THR:OG1	2.42	0.52
11:G:126:ASP:O	11:G:129:GLU:N	2.34	0.52
17:O:18:VAL:HG21	17:O:58:HIS:CE1	2.45	0.52
1:A:682:G:H1	1:A:708:C:H42	1.58	0.52
2:B:208:ARG:H	2:B:208:ARG:HD3	1.75	0.52
18:R:72:ASP:O	18:R:75:LYS:NZ	2.31	0.52
1:A:978:A:C5	1:A:1318:A:C6	2.98	0.52
1:A:1382:C:H2'	1:A:1383:C:C6	2.45	0.52
11:G:23:LEU:O	11:G:27:VAL:HG23	2.10	0.52
1:A:108:G:H5'	1:A:109:A:H5''	1.91	0.52
1:A:1227:A:H3'	1:A:1227:A:C8	2.44	0.52
21:W:18:ASN:HD21	21:W:185:PRO:HG3	1.75	0.52
21:W:58:ARG:HG3	21:W:58:ARG:NH1	2.25	0.52
1:A:686:U:C5	1:A:703:G:C2	2.98	0.52
1:A:1036:A:H8	1:A:1036:A:OP2	1.92	0.52
1:A:1158:C:C6	1:A:1160:G:H1'	2.45	0.52
12:I:43:THR:O	12:I:43:THR:HG22	2.10	0.52
1:A:1143:G:H2'	1:A:1144:G:H8	1.74	0.52
1:A:1223:C:P	16:S:78:ARG:HH12	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:65:ARG:O	8:Q:67:LEU:HD22	2.10	0.52
1:A:746:A:H2'	1:A:747:A:C8	2.45	0.51
18:R:20:VAL:CG1	18:R:22:HIS:CE1	2.93	0.51
1:A:76:G:O5'	1:A:76:G:H8	1.93	0.51
1:A:337:G:H2'	1:A:338:A:C8	2.46	0.51
2:B:92:VAL:HG12	2:B:147:SER:O	2.10	0.51
12:I:92:GLU:HA	12:I:92:GLU:OE1	2.10	0.51
21:W:149:VAL:HG11	21:W:172:PRO:HG3	1.91	0.51
10:F:11:ARG:NH2	10:F:177:THR:O	2.44	0.51
15:N:31:ILE:O	15:N:31:ILE:HG22	2.11	0.51
21:W:42:VAL:CB	21:W:110:VAL:HG12	2.40	0.51
21:W:92:ALA:HA	21:W:95:PHE:CE2	2.45	0.51
2:B:8:ASP:OD1	2:B:8:ASP:N	2.42	0.51
11:G:28:ASN:O	11:G:31:MET:HB3	2.11	0.51
1:A:1009:U:H2'	1:A:1010:U:C6	2.46	0.51
2:B:115:LYS:NZ	2:B:153:ASP:OD1	2.31	0.51
13:J:29:ALA:CB	13:J:76:ILE:CD1	2.89	0.51
13:J:35:GLN:HG2	13:J:78:GLU:OE2	2.11	0.51
21:W:38:GLY:O	21:W:106:GLN:NE2	2.43	0.51
4:E:163:GLU:OE1	4:E:163:GLU:HA	2.10	0.51
1:A:684:U:H1'	18:R:40:ASN:HA	1.91	0.51
1:A:1015:G:H2'	1:A:1016:A:C8	2.46	0.51
1:A:1345:U:OP1	12:I:122:ARG:NH1	2.42	0.51
1:A:1377:A:H61	11:G:7:ILE:HG21	1.68	0.51
1:A:1519:A:C4	21:W:116:TYR:CE2	2.98	0.51
15:N:21:PHE:CD1	15:N:21:PHE:C	2.89	0.51
1:A:899:C:O2	21:W:248:ARG:NH2	2.44	0.51
4:E:25:VAL:HG12	4:E:26:LYS:H	1.76	0.51
1:A:1223:C:P	16:S:78:ARG:NH1	2.84	0.51
1:A:682:G:H8	1:A:682:G:C5'	2.24	0.50
1:A:1004:A:C6	1:A:1026:G:H5''	2.46	0.50
10:F:24:ALA:HB1	10:F:28:GLU:HG2	1.92	0.50
1:A:932:C:OP2	1:A:932:C:H6	1.93	0.50
1:A:1315:U:O2'	1:A:1360:A:O2'	2.29	0.50
16:S:3:ARG:HD3	16:S:3:ARG:N	2.27	0.50
21:W:33:ILE:HG23	21:W:109:ARG:NH2	2.26	0.50
1:A:90:C:O2'	1:A:91:U:P	2.69	0.50
1:A:1313:U:H2'	1:A:1314:C:C6	2.46	0.50
2:B:169:GLU:C	2:B:171:ILE:N	2.65	0.50
18:R:20:VAL:HG12	18:R:22:HIS:CE1	2.46	0.50
21:W:42:VAL:HA	21:W:63:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:154:SER:OG	21:W:155:LYS:N	2.44	0.50
6:L:56:ARG:HH11	6:L:56:ARG:HG3	1.77	0.50
21:W:40:ALA:CB	21:W:108:LEU:HD13	2.30	0.50
11:G:15:ASP:CG	11:G:20:SER:O	2.54	0.50
11:G:27:VAL:HG22	11:G:43:VAL:CG2	2.40	0.50
11:G:50:LEU:HD23	11:G:121:ALA:HA	1.93	0.50
21:W:236:GLU:OE1	21:W:236:GLU:N	2.37	0.50
1:A:1377:A:C2	11:G:7:ILE:HD13	2.43	0.50
1:A:8:A:N6	3:D:206:LYS:HB3	2.26	0.50
1:A:1157:A:N3	1:A:1181:G:C2	2.80	0.50
1:A:1387:G:H2'	1:A:1388:C:H6	1.77	0.50
2:B:164:ILE:HD13	2:B:186:ILE:HD12	1.94	0.50
21:W:33:ILE:HG22	21:W:109:ARG:NH2	2.27	0.50
1:A:996:A:H2'	1:A:997:U:H6	1.77	0.49
1:A:1133:G:C8	1:A:1133:G:C5'	2.87	0.49
3:D:95:GLU:OE2	3:D:100:ASN:ND2	2.35	0.49
10:F:114:LYS:HD3	10:F:185:ASN:OD1	2.12	0.49
16:S:19:VAL:CG2	16:S:44:MET:HE2	2.30	0.49
18:R:22:HIS:NE2	18:R:85:MET:SD	2.85	0.49
1:A:610:U:H2'	1:A:611:C:C6	2.47	0.49
1:A:713:G:H2'	1:A:714:G:C8	2.47	0.49
4:E:15:LEU:HD23	4:E:37:THR:HG22	1.93	0.49
1:A:675:A:H1'	18:R:118:HIS:CD2	2.47	0.49
1:A:1133:G:H8	1:A:1133:G:C5'	2.04	0.49
1:A:1133:G:N2	1:A:1142:G:N3	2.60	0.49
17:O:90:MET:CE	20:V:61:ARG:HH11	2.22	0.49
20:V:21:ILE:CD1	20:V:55:LEU:HD12	2.39	0.49
21:W:141:GLN:HE21	21:W:143:GLU:CD	2.20	0.49
1:A:1257:A:H2'	1:A:1257:A:O5'	2.12	0.49
1:A:1367:C:H5''	12:I:116:VAL:HG22	1.95	0.49
2:B:135:LEU:O	2:B:139:ARG:HG3	2.12	0.49
2:B:169:GLU:OE1	2:B:172:ALA:HB3	2.11	0.49
16:S:3:ARG:CG	16:S:3:ARG:NH1	2.72	0.49
21:W:41:MET:HA	21:W:109:ARG:O	2.12	0.49
2:B:129:LEU:CD1	2:B:132:LYS:CA	2.80	0.49
6:L:54:ARG:HD2	6:L:64:THR:HG22	1.95	0.49
10:F:20:SER:HB2	15:N:94:PRO:HG3	1.94	0.49
17:O:81:ASN:OD1	17:O:82:ASP:N	2.45	0.49
1:A:1218:C:H2'	1:A:1219:A:C8	2.48	0.49
11:G:118:LEU:C	11:G:120:LEU:N	2.70	0.49
13:J:4:GLN:HG2	13:J:79:PRO:CG	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:232:LEU:HB2	21:W:233:PHE:CD1	2.48	0.49
1:A:209:U:O2'	1:A:211:G:N7	2.38	0.49
1:A:1226:C:N4	14:M:103:LYS:HG3	2.26	0.49
10:F:70:THR:O	10:F:105:GLU:HA	2.12	0.49
14:M:36:ALA:HB1	14:M:59:GLU:OE2	2.08	0.49
15:N:22:ALA:HA	15:N:26:GLU:HB2	1.95	0.49
1:A:994:A:N1	1:A:1047:G:H4'	2.26	0.49
11:G:31:MET:HE1	11:G:36:LYS:HE2	1.93	0.49
21:W:119:SER:HA	21:W:122:LEU:CD1	2.42	0.49
1:A:1387:G:H2'	1:A:1388:C:C6	2.48	0.49
11:G:138:ARG:O	11:G:141:VAL:HG12	2.13	0.49
1:A:102:G:HO2'	1:A:151:A:H8	1.57	0.49
11:G:32:VAL:HG13	11:G:32:VAL:O	2.12	0.49
16:S:63:THR:H	16:S:66:MET:HG3	1.77	0.49
1:A:952:U:C5	14:M:103:LYS:HE2	2.48	0.48
1:A:1176:A:H2'	1:A:1177:G:C8	2.47	0.48
21:W:21:ASN:HD22	21:W:182:THR:HG23	1.78	0.48
21:W:226:ARG:HD2	21:W:226:ARG:C	2.37	0.48
1:A:171:A:H2'	1:A:172:A:C8	2.48	0.48
1:A:89:U:H2'	1:A:90:C:C6	2.48	0.48
1:A:1378:C:H5'	1:A:1378:C:C6	2.48	0.48
16:S:30:PRO:HA	16:S:48:THR:O	2.14	0.48
1:A:1166:G:C6	1:A:1168:U:C5'	2.91	0.48
1:A:1388:C:H2'	1:A:1389:C:H6	1.78	0.48
3:D:99:ASP:OD1	3:D:100:ASN:N	2.45	0.48
5:H:64:LYS:HG2	5:H:71:VAL:HG11	1.94	0.48
8:Q:68:SER:OG	8:Q:69:LYS:N	2.38	0.48
16:S:3:ARG:N	16:S:3:ARG:CD	2.71	0.48
21:W:108:LEU:N	21:W:108:LEU:CD2	2.75	0.48
21:W:133:ILE:N	21:W:133:ILE:CD1	2.73	0.48
1:A:1377:A:H61	11:G:7:ILE:CG2	2.17	0.48
2:B:18:HIS:HB2	2:B:189:THR:OG1	2.14	0.48
21:W:59:LEU:C	21:W:61:GLN:N	2.71	0.48
21:W:115:PRO:HD2	21:W:118:ILE:CG2	2.42	0.48
1:A:91:U:O2'	1:A:92:U:O4'	2.31	0.48
1:A:846:G:H8	1:A:846:G:OP2	1.97	0.48
1:A:1175:G:H2'	1:A:1176:A:H8	1.79	0.48
4:E:38:VAL:HG11	4:E:114:VAL:HG22	1.96	0.48
4:E:164:ILE:C	4:E:164:ILE:CD1	2.86	0.48
12:I:83:ILE:O	12:I:83:ILE:HG22	2.14	0.48
1:A:1143:G:H2'	1:A:1144:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1314:C:H2'	1:A:1315:U:C6	2.49	0.48
14:M:5:ALA:O	14:M:8:ASN:HB2	2.13	0.48
20:V:24:LYS:HB2	20:V:24:LYS:HE2	1.64	0.48
13:J:46:LYS:HB3	13:J:68:ARG:HG2	1.95	0.48
21:W:27:ASP:O	21:W:30:VAL:HG12	2.13	0.48
1:A:1004:A:C6	1:A:1026:G:C5'	2.95	0.48
1:A:1378:C:H5'	1:A:1378:C:H6	1.79	0.48
1:A:927:G:C6	1:A:1391:U:N3	2.82	0.48
1:A:1100:C:C6	2:B:95:ARG:NH1	2.82	0.48
1:A:1223:C:OP1	16:S:78:ARG:NH1	2.47	0.48
1:A:707:U:H6	1:A:707:U:O5'	1.97	0.47
1:A:1246:A:C2	1:A:1292:G:C2	3.02	0.47
2:B:94:HIS:ND1	2:B:146:ASN:HB3	2.29	0.47
1:A:299:G:H2'	1:A:300:A:C8	2.49	0.47
21:W:104:MET:HE2	21:W:104:MET:HB3	1.70	0.47
1:A:999:C:H2'	1:A:1000:A:H8	1.79	0.47
1:A:1166:G:C4	1:A:1168:U:OP2	2.68	0.47
1:A:1317:C:H5''	1:A:1317:C:H6	1.78	0.47
14:M:12:HIS:CG	14:M:12:HIS:O	2.67	0.47
14:M:90:ARG:NH1	14:M:95:LEU:HD13	2.28	0.47
18:R:53:ARG:NH1	18:R:57:LYS:HE2	2.29	0.47
1:A:610:U:H2'	1:A:611:C:H6	1.79	0.47
1:A:686:U:C5	1:A:703:G:N2	2.82	0.47
2:B:151:ILE:HG13	2:B:154:MET:SD	2.55	0.47
1:A:81:A:N6	1:A:85:U:C5	2.83	0.47
1:A:1191:A:OP1	10:F:4:LYS:NZ	2.34	0.47
19:U:3:LEU:N	19:U:35:GLN:HE22	2.13	0.47
1:A:938:A:O5'	1:A:938:A:H8	1.97	0.47
1:A:981:U:OP1	15:N:9:ARG:NH1	2.47	0.47
1:A:1027:C:N3	1:A:1035:A:C6	2.82	0.47
2:B:6:MET:HE3	2:B:6:MET:HB2	1.84	0.47
6:L:76:GLU:OE1	6:L:76:GLU:HA	2.15	0.47
10:F:130:PHE:CZ	10:F:157:LEU:HD13	2.48	0.47
14:M:45:ILE:O	14:M:45:ILE:HG22	2.15	0.47
2:B:27:MET:HE1	2:B:193:PRO:HG3	1.97	0.47
10:F:70:THR:HG21	10:F:76:VAL:HG21	1.96	0.47
14:M:4:ILE:CG2	14:M:60:VAL:HG21	2.44	0.47
18:R:127:ARG:NH1	18:R:127:ARG:HG2	2.28	0.47
21:W:21:ASN:OD1	21:W:22:ASP:N	2.47	0.47
1:A:662:U:H2'	1:A:663:A:C8	2.50	0.47
21:W:159:ARG:HD2	21:W:215:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:A:H2'	1:A:696:A:C8	2.48	0.47
1:A:1271:A:O5'	1:A:1271:A:H8	1.98	0.47
10:F:186:THR:HG22	10:F:199:LYS:HG2	1.97	0.47
14:M:3:ARG:NH1	14:M:9:ILE:CG1	2.78	0.47
14:M:44:LYS:O	14:M:48:LEU:HD12	2.15	0.47
21:W:62:LEU:HG	21:W:85:LEU:HB3	1.97	0.47
21:W:174:LEU:HB3	21:W:191:VAL:HB	1.97	0.47
1:A:1004:A:N6	1:A:1027:C:C5	2.83	0.46
1:A:1024:G:N3	1:A:1024:G:C2'	2.77	0.46
3:D:105:MET:SD	3:D:180:GLY:HA3	2.55	0.46
8:Q:10:GLY:HA3	8:Q:25:ILE:HD13	1.97	0.46
17:O:90:MET:HB3	17:O:90:MET:HE2	1.70	0.46
21:W:225:ILE:HA	21:W:228:SER:HB3	1.96	0.46
1:A:1377:A:C6	11:G:7:ILE:CB	2.97	0.46
1:A:1377:A:C6	11:G:7:ILE:HB	2.50	0.46
2:B:129:LEU:HD11	2:B:132:LYS:C	2.39	0.46
14:M:59:GLU:CA	14:M:62:LYS:NZ	2.78	0.46
1:A:704:A:C4	1:A:705:G:C8	3.04	0.46
4:E:94:VAL:CG1	4:E:111:MET:HE3	2.44	0.46
21:W:135:ASP:HA	21:W:195:VAL:HA	1.98	0.46
13:J:10:LEU:O	13:J:71:LEU:HA	2.15	0.46
1:A:967:C:O5'	1:A:967:C:H6	1.99	0.46
7:P:80:LYS:HD2	7:P:81:ALA:HA	1.97	0.46
12:I:72:ILE:HD12	12:I:72:ILE:H	1.80	0.46
13:J:52:LEU:HD23	13:J:62:ARG:HD3	1.97	0.46
17:O:26:THR:HG23	17:O:36:ILE:CD1	2.45	0.46
21:W:56:GLY:O	21:W:58:ARG:HG2	2.15	0.46
1:A:371:A:H2'	1:A:372:C:O4'	2.14	0.46
1:A:1227:A:C8	1:A:1227:A:C3'	2.98	0.46
2:B:117:LEU:HD11	2:B:133:GLU:HG2	1.98	0.46
3:D:35:GLU:N	3:D:35:GLU:OE1	2.48	0.46
16:S:11:ILE:HD11	16:S:44:MET:HE1	1.98	0.46
16:S:80:TYR:CD2	16:S:80:TYR:O	2.69	0.46
21:W:48:LEU:HD12	21:W:48:LEU:H	1.80	0.46
1:A:939:G:H5'	11:G:102:ARG:CZ	2.46	0.46
1:A:1062:U:H2'	1:A:1063:C:C6	2.51	0.46
2:B:70:VAL:HA	2:B:92:VAL:HG23	1.97	0.46
7:P:42:ILE:HG22	7:P:42:ILE:O	2.16	0.46
13:J:102:LEU:CD1	13:J:102:LEU:C	2.82	0.46
17:O:69:GLU:OE1	17:O:69:GLU:N	2.37	0.46
21:W:91:ASP:O	21:W:94:THR:OG1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:U:N3	1:A:1043:G:C8	2.83	0.46
1:A:1004:A:H3'	1:A:1024:G:N2	2.31	0.46
21:W:68:ASP:OD2	21:W:70:ASP:HB3	2.16	0.46
1:A:682:G:N2	1:A:709:U:C2	2.84	0.46
1:A:1099:G:P	2:B:95:ARG:NH2	2.88	0.46
1:A:1309:G:C6	1:A:1329:A:N1	2.84	0.46
1:A:926:G:H4'	1:A:927:G:C5'	2.45	0.46
1:A:1383:C:H2'	1:A:1384:C:C6	2.51	0.46
10:F:108:LYS:HA	10:F:109:PRO:HD2	1.63	0.46
13:J:7:ARG:HD3	13:J:75:ASP:OD1	2.16	0.46
21:W:136:MET:CE	21:W:196:PRO:HD3	2.46	0.46
21:W:137:HIS:CE1	21:W:193:ARG:HG3	2.50	0.46
1:A:539:A:H2'	1:A:540:G:C8	2.51	0.45
1:A:1137:C:C4'	1:A:1138:G:H5''	2.44	0.45
2:B:45:LYS:HA	2:B:45:LYS:HD3	1.78	0.45
10:F:130:PHE:CE2	10:F:157:LEU:HB2	2.52	0.45
13:J:26:VAL:O	13:J:30:LYS:HB3	2.16	0.45
14:M:62:LYS:HD3	14:M:62:LYS:N	2.30	0.45
19:U:17:ARG:HH11	19:U:17:ARG:HG3	1.80	0.45
19:U:78:TYR:O	19:U:82:ILE:HG23	2.16	0.45
1:A:939:G:H5'	11:G:102:ARG:NH1	2.31	0.45
1:A:1027:C:C2	1:A:1035:A:N1	2.84	0.45
5:H:11:LEU:HD22	5:H:75:ILE:HD11	1.98	0.45
6:L:44:LYS:HB3	6:L:45:PRO:HD3	1.62	0.45
21:W:66:GLU:OE2	21:W:67:LEU:N	2.49	0.45
1:A:1251:A:H2'	1:A:1252:A:C8	2.51	0.45
1:A:1321:U:H3'	1:A:1322:C:H2'	1.99	0.45
1:A:1388:C:H2'	1:A:1389:C:C6	2.52	0.45
3:D:65:TYR:OH	3:D:95:GLU:OE1	2.30	0.45
20:V:15:ALA:CA	20:V:32:TYR:OH	2.64	0.45
21:W:108:LEU:CD2	21:W:132:ALA:O	2.65	0.45
21:W:118:ILE:O	21:W:118:ILE:CG1	2.65	0.45
21:W:208:ARG:HB3	21:W:208:ARG:NH1	2.31	0.45
21:W:223:LYS:HG3	21:W:228:SER:HB2	1.98	0.45
1:A:1157:A:C5	1:A:1181:G:C6	3.04	0.45
1:A:1317:C:H5''	1:A:1317:C:C6	2.51	0.45
2:B:132:LYS:HD3	2:B:137:ARG:NH2	2.31	0.45
3:D:151:LYS:O	3:D:151:LYS:HG3	2.17	0.45
15:N:38:ASP:OD1	15:N:38:ASP:N	2.48	0.45
21:W:193:ARG:HE	21:W:195:VAL:CG1	2.29	0.45
21:W:205:LYS:HE2	21:W:265:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:G:OP2	2:B:95:ARG:NH2	2.43	0.45
1:A:1318:A:H5''	16:S:10:PHE:CE1	2.52	0.45
2:B:81:LYS:C	2:B:83:ALA:H	2.24	0.45
4:E:29:ARG:HG2	4:E:29:ARG:HH11	1.81	0.45
9:T:49:LYS:O	9:T:53:GLU:HG3	2.16	0.45
18:R:127:ARG:HG2	18:R:127:ARG:HH11	1.81	0.45
1:A:927:G:C2	1:A:1391:U:O2	2.70	0.45
2:B:101:LEU:HB3	2:B:179:LEU:HD12	1.97	0.45
2:B:133:GLU:CD	2:B:137:ARG:HH21	2.24	0.45
4:E:44:GLY:O	4:E:45:ARG:HG2	2.17	0.45
13:J:11:LYS:HG2	13:J:71:LEU:HG	1.98	0.45
21:W:115:PRO:C	21:W:117:ASN:N	2.73	0.45
20:V:23:TYR:CD1	20:V:23:TYR:O	2.70	0.45
1:A:842:U:O2	1:A:844:G:N2	2.50	0.45
1:A:1028:C:H2'	1:A:1029:U:H6	1.79	0.45
15:N:30:ILE:O	15:N:33:ASP:OD1	2.35	0.45
19:U:48:LYS:HB2	19:U:48:LYS:HE2	1.62	0.45
21:W:75:LEU:O	21:W:75:LEU:HD23	2.16	0.45
21:W:118:ILE:O	21:W:118:ILE:HG13	2.17	0.45
1:A:1007:U:H3'	1:A:1007:U:C6	2.50	0.45
1:A:1125:U:OP1	13:J:37:ARG:HD3	2.17	0.45
3:D:15:GLU:OE2	3:D:63:ARG:NH1	2.50	0.45
10:F:20:SER:CB	15:N:94:PRO:HG3	2.47	0.45
11:G:146:GLU:HA	11:G:149:LYS:HE2	1.99	0.45
18:R:69:ARG:HB2	18:R:69:ARG:CZ	2.47	0.45
1:A:212:G:H2'	1:A:213:G:C8	2.51	0.45
1:A:524:G:H2'	1:A:525:C:C6	2.52	0.45
1:A:999:C:H2'	1:A:1000:A:C8	2.52	0.45
1:A:1036:A:OP2	1:A:1036:A:C8	2.70	0.45
11:G:27:VAL:HG11	11:G:40:GLU:HB2	1.99	0.45
16:S:63:THR:HG22	16:S:64:ASP:N	2.32	0.45
18:R:37:ARG:CZ	18:R:37:ARG:HA	2.47	0.45
21:W:66:GLU:O	21:W:89:GLN:HA	2.17	0.45
6:L:122:PRO:O	6:L:124:ALA:N	2.50	0.44
12:I:27:LYS:HE2	12:I:27:LYS:HB3	1.33	0.44
11:G:146:GLU:N	11:G:146:GLU:OE1	2.49	0.44
12:I:97:GLU:O	12:I:97:GLU:HG3	2.16	0.44
20:V:21:ILE:O	20:V:21:ILE:HG22	2.16	0.44
21:W:131:ASP:C	21:W:133:ILE:H	2.25	0.44
21:W:233:PHE:CE2	21:W:260:MET:HB3	2.52	0.44
1:A:978:A:C6	1:A:1318:A:C5	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:233:PHE:CZ	21:W:260:MET:HB3	2.52	0.44
1:A:206:C:H2'	1:A:207:C:C6	2.52	0.44
1:A:320:A:H2'	1:A:321:A:O4'	2.18	0.44
1:A:684:U:C1'	18:R:40:ASN:HB3	2.47	0.44
1:A:1118:U:H1'	1:A:1179:A:C5	2.53	0.44
7:P:80:LYS:HD2	7:P:81:ALA:CA	2.47	0.44
15:N:28:LYS:HE2	15:N:28:LYS:HB2	1.71	0.44
21:W:135:ASP:HB2	21:W:195:VAL:HG12	1.99	0.44
1:A:160:A:H2'	1:A:161:A:C8	2.52	0.44
1:A:1004:A:H3'	1:A:1024:G:H22	1.82	0.44
3:D:174:ASP:OD2	3:D:177:LYS:HG2	2.17	0.44
7:P:77:GLU:O	7:P:81:ALA:CB	2.63	0.44
1:A:1187:G:H2'	1:A:1188:A:H8	1.83	0.44
2:B:144:LEU:HD13	2:B:148:LEU:HD12	2.00	0.44
7:P:80:LYS:CD	7:P:81:ALA:N	2.78	0.44
18:R:61:PHE:O	18:R:65:VAL:HG23	2.18	0.44
21:W:145:VAL:HG21	21:W:190:ALA:HB3	2.00	0.44
21:W:193:ARG:HE	21:W:195:VAL:HG11	1.81	0.44
1:A:477:C:H2'	1:A:478:A:C8	2.53	0.44
1:A:929:G:H2'	1:A:930:C:C6	2.51	0.44
1:A:1004:A:H61	1:A:1026:G:C3'	2.31	0.44
11:G:65:ALA:HB2	11:G:128:ALA:HB2	1.98	0.44
12:I:7:TYR:CD2	12:I:7:TYR:C	2.95	0.44
1:A:1004:A:C4	1:A:1026:G:N7	2.81	0.44
10:F:77:ILE:HA	10:F:84:VAL:CG1	2.48	0.44
16:S:5:LEU:HD23	16:S:5:LEU:HA	1.30	0.44
17:O:42:TRP:CZ2	17:O:61:LEU:HD12	2.53	0.44
1:A:1265:C:O2	1:A:1271:A:C2	2.70	0.44
14:M:3:ARG:NH2	14:M:7:ILE:HG22	2.33	0.44
14:M:59:GLU:HA	14:M:62:LYS:HZ3	1.79	0.44
1:A:90:C:HO2'	1:A:91:U:P	2.40	0.43
1:A:689:C:H2'	1:A:690:G:C8	2.53	0.43
11:G:60:GLU:OE2	11:G:64:VAL:HG13	2.18	0.43
17:O:18:VAL:HG21	17:O:58:HIS:HE1	1.82	0.43
1:A:89:U:H2'	1:A:90:C:C5	2.53	0.43
1:A:684:U:H1'	18:R:40:ASN:CB	2.48	0.43
1:A:1191:A:H2'	1:A:1192:C:C6	2.53	0.43
1:A:1225:A:N3	1:A:1225:A:C2'	2.81	0.43
6:L:3:THR:HB	6:L:6:GLN:HG3	2.00	0.43
8:Q:19:LYS:HD3	8:Q:49:GLU:OE1	2.18	0.43
21:W:118:ILE:O	21:W:118:ILE:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:C:H2'	1:A:208:U:C6	2.53	0.43
3:D:73:ARG:HE	3:D:73:ARG:HB3	1.47	0.43
3:D:142:VAL:HG22	3:D:142:VAL:O	2.17	0.43
13:J:35:GLN:HB2	13:J:78:GLU:OE2	2.18	0.43
13:J:66:GLU:HG2	15:N:99:ALA:HB2	1.99	0.43
21:W:173:VAL:CG1	21:W:191:VAL:CG1	2.96	0.43
1:A:91:U:H2'	1:A:92:U:H6	1.84	0.43
1:A:667:G:O2'	19:U:49:ASP:OD1	2.30	0.43
1:A:845:A:C2	20:V:48:ARG:NE	2.84	0.43
1:A:1026:G:N3	1:A:1026:G:C2'	2.80	0.43
1:A:1033:G:H2'	1:A:1034:G:C8	2.53	0.43
1:A:1053:G:N7	1:A:1199:U:H3'	2.34	0.43
1:A:1140:C:C2'	1:A:1141:C:H5'	2.48	0.43
1:A:1157:A:C2	1:A:1181:G:C4	3.07	0.43
1:A:1157:A:H1'	1:A:1181:G:N2	2.33	0.43
1:A:1166:G:C5	1:A:1168:U:OP2	2.72	0.43
1:A:1381:U:O2	1:A:1381:U:C2'	2.67	0.43
13:J:22:THR:O	13:J:26:VAL:HG12	2.18	0.43
14:M:3:ARG:HD3	14:M:9:ILE:HD13	2.00	0.43
18:R:20:VAL:HG11	18:R:22:HIS:CE1	2.53	0.43
18:R:52:PHE:CD2	18:R:62:ALA:HB2	2.54	0.43
1:A:532:A:N6	10:F:193:TYR:OH	2.46	0.43
1:A:1092:A:H5''	11:G:4:ARG:NH1	2.33	0.43
10:F:30:ALA:HB2	15:N:77:PHE:C	2.44	0.43
16:S:5:LEU:HB3	16:S:6:LYS:H	1.40	0.43
20:V:15:ALA:HB2	20:V:32:TYR:CE1	2.50	0.43
21:W:243:ILE:HG12	21:W:256:GLN:OE1	2.19	0.43
10:F:30:ALA:HB2	15:N:77:PHE:O	2.18	0.43
12:I:12:ARG:NH1	12:I:107:ASP:OD2	2.52	0.43
12:I:54:LEU:HD12	12:I:54:LEU:HA	1.59	0.43
21:W:140:LEU:O	21:W:190:ALA:N	2.50	0.43
1:A:87:C:H3'	1:A:88:U:H6	1.83	0.43
1:A:1152:A:OP1	13:J:72:ARG:NH2	2.52	0.43
2:B:35:ARG:O	2:B:38:VAL:HG12	2.18	0.43
11:G:31:MET:CE	11:G:36:LYS:HE2	2.49	0.43
18:R:23:ILE:HD11	18:R:86:VAL:HG22	1.99	0.43
18:R:53:ARG:HD3	18:R:53:ARG:HA	1.69	0.43
18:R:61:PHE:O	18:R:64:GLN:HG3	2.18	0.43
1:A:684:U:H1'	18:R:40:ASN:HB3	2.00	0.43
1:A:1328:C:H5''	14:M:28:THR:HG21	2.00	0.43
8:Q:6:ARG:HE	8:Q:6:ARG:HB3	1.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:142:HIS:O	11:G:146:GLU:OE1	2.37	0.43
20:V:66:SER:O	20:V:66:SER:OG	2.35	0.43
21:W:58:ARG:HH21	21:W:84:LYS:NZ	2.16	0.43
1:A:76:G:O5'	1:A:76:G:C8	2.70	0.43
1:A:91:U:H2'	1:A:92:U:C6	2.54	0.43
1:A:102:G:O2'	1:A:151:A:H8	2.02	0.43
1:A:728:A:H2'	1:A:729:A:C8	2.54	0.43
13:J:47:GLU:OE2	15:N:76:LYS:HE2	2.18	0.43
11:G:71:PRO:O	11:G:71:PRO:HG2	2.19	0.43
13:J:59:LYS:O	13:J:59:LYS:HG3	2.19	0.43
21:W:30:VAL:HG13	21:W:31:SER:N	2.34	0.43
1:A:1136:C:H3'	1:A:1137:C:C6	2.54	0.42
11:G:75:VAL:HG21	11:G:86:GLN:OE1	2.19	0.42
1:A:1317:C:H2'	1:A:1318:A:H5'	2.01	0.42
2:B:56:GLU:O	2:B:60:ILE:HG22	2.19	0.42
11:G:121:ALA:O	11:G:125:SER:N	2.39	0.42
18:R:56:ARG:O	18:R:59:THR:OG1	2.36	0.42
1:A:845:A:H5''	1:A:845:A:H8	1.85	0.42
1:A:994:A:C8	1:A:1216:A:C4'	3.00	0.42
1:A:1159:U:O5'	2:B:131:LYS:NZ	2.48	0.42
1:A:1298:U:C4	11:G:114:LYS:CB	3.01	0.42
15:N:89:MET:C	15:N:91:GLY:N	2.76	0.42
19:U:10:LYS:HE3	19:U:10:LYS:HB2	1.72	0.42
1:A:995:C:N3	1:A:1047:G:H5'	2.34	0.42
1:A:1138:G:C5	1:A:1140:C:H1'	2.54	0.42
5:H:108:LYS:HG3	5:H:121:LEU:HD11	2.00	0.42
10:F:155:GLY:O	10:F:196:ILE:HG12	2.18	0.42
1:A:555:U:H2'	1:A:556:C:C6	2.54	0.42
1:A:1096:C:H2'	1:A:1097:C:H6	1.85	0.42
1:A:1352:C:H2'	1:A:1353:G:C8	2.55	0.42
2:B:169:GLU:OE2	2:B:171:ILE:N	2.46	0.42
6:L:15:LYS:H	6:L:15:LYS:HG2	1.50	0.42
11:G:124:LEU:HD23	11:G:124:LEU:HA	1.89	0.42
21:W:118:ILE:O	21:W:122:LEU:HD11	2.19	0.42
1:A:189:A:H2'	1:A:190:A:C8	2.55	0.42
1:A:1060:U:H5''	13:J:53:ILE:HD12	2.02	0.42
1:A:1133:G:C2	1:A:1142:G:C2	3.08	0.42
14:M:19:LEU:HD23	14:M:19:LEU:N	2.33	0.42
19:U:37:ASN:HA	19:U:40:GLN:NE2	2.35	0.42
19:U:40:GLN:NE2	19:U:40:GLN:H	2.18	0.42
1:A:880:C:OP1	6:L:9:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:U:C6	1:A:1007:U:C3'	3.03	0.42
1:A:1060:U:H2'	1:A:1061:G:H8	1.84	0.42
1:A:1160:G:N3	1:A:1160:G:H2'	2.34	0.42
12:I:6:TYR:CD1	12:I:6:TYR:N	2.87	0.42
17:O:9:MET:HE2	17:O:86:ARG:HG2	2.01	0.42
1:A:501:C:H2'	1:A:502:A:C8	2.54	0.42
1:A:1382:C:H2'	1:A:1383:C:H6	1.85	0.42
4:E:52:LYS:HE2	4:E:52:LYS:HB3	1.77	0.42
18:R:20:VAL:HG23	18:R:37:ARG:HH22	1.77	0.42
21:W:115:PRO:O	21:W:118:ILE:N	2.50	0.42
21:W:197:HIS:HB2	21:W:200:MET:HE1	2.01	0.42
1:A:609:A:C2'	1:A:610:U:H5'	2.49	0.42
2:B:104:TRP:O	2:B:107:VAL:HG12	2.19	0.42
12:I:127:PHE:O	12:I:127:PHE:CG	2.68	0.42
20:V:15:ALA:CB	20:V:32:TYR:CZ	2.87	0.42
21:W:92:ALA:HA	21:W:95:PHE:HE2	1.85	0.42
1:A:985:C:H2'	1:A:986:U:C6	2.55	0.42
10:F:40:ARG:HG2	10:F:55:ILE:HD12	2.01	0.42
21:W:68:ASP:OD2	21:W:71:LEU:CD2	2.63	0.42
1:A:82:G:C2	1:A:88:U:H1'	2.54	0.41
1:A:339:C:H2'	1:A:340:U:C6	2.55	0.41
1:A:934:C:C4	1:A:1345:U:C5	3.08	0.41
1:A:1107:C:C4	1:A:1108:G:C8	3.08	0.41
2:B:149:GLY:O	2:B:152:LYS:HD2	2.20	0.41
12:I:129:LYS:HD2	12:I:129:LYS:C	2.45	0.41
18:R:83:GLU:HB3	18:R:108:THR:OG1	2.20	0.41
21:W:25:VAL:HG23	21:W:26:ILE:H	1.85	0.41
21:W:139:MET:O	21:W:139:MET:SD	2.77	0.41
21:W:184:PRO:HA	21:W:185:PRO:HD3	1.83	0.41
1:A:1519:A:C2	21:W:18:ASN:OD1	2.73	0.41
13:J:27:GLU:N	13:J:27:GLU:CD	2.78	0.41
18:R:60:PRO:O	18:R:64:GLN:HG2	2.21	0.41
1:A:929:G:H2'	1:A:930:C:H6	1.85	0.41
1:A:1149:C:H2'	1:A:1150:A:C8	2.55	0.41
1:A:1269:A:N1	1:A:1312:G:O2'	2.38	0.41
4:E:69:ARG:O	4:E:71:MET:N	2.52	0.41
13:J:44:THR:HG23	13:J:69:THR:O	2.21	0.41
17:O:49:TYR:CE1	20:V:66:SER:HA	2.55	0.41
21:W:78:HIS:CD2	21:W:79:PRO:CD	3.04	0.41
1:A:216:U:H2'	1:A:217:C:C6	2.56	0.41
1:A:1022:A:O5'	1:A:1022:A:C8	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:94:LEU:HA	3:D:94:LEU:HD23	1.88	0.41
3:D:151:LYS:HB3	3:D:151:LYS:HZ2	1.84	0.41
6:L:110:ARG:HB2	6:L:119:VAL:HG21	2.03	0.41
16:S:13:LEU:O	16:S:13:LEU:HG	2.19	0.41
17:O:42:TRP:HZ2	17:O:61:LEU:HD12	1.84	0.41
1:A:1096:C:H2'	1:A:1097:C:C6	2.55	0.41
16:S:80:TYR:O	16:S:80:TYR:CG	2.72	0.41
19:U:39:LEU:HD23	19:U:39:LEU:HA	1.89	0.41
1:A:1257:A:O5'	1:A:1257:A:C2'	2.69	0.41
11:G:144:MET:HE2	11:G:144:MET:HB2	1.95	0.41
21:W:142:LYS:HD2	21:W:142:LYS:HA	1.76	0.41
1:A:937:A:C6	1:A:1379:G:O6	2.71	0.41
1:A:1047:G:C8	1:A:1047:G:H3'	2.56	0.41
1:A:1166:G:O5'	1:A:1166:G:H8	2.03	0.41
1:A:1207:G:H2'	1:A:1208:C:C6	2.55	0.41
1:A:1377:A:N1	11:G:7:ILE:CG2	2.71	0.41
3:D:9:LEU:HD23	3:D:9:LEU:HA	1.89	0.41
17:O:55:HIS:O	17:O:56:LYS:HB2	2.21	0.41
1:A:1228:C:H5''	1:A:1228:C:H6	1.85	0.41
2:B:224:GLY:O	2:B:227:GLN:HG2	2.21	0.41
4:E:82:GLN:HE21	4:E:82:GLN:HB3	1.66	0.41
13:J:31:ARG:C	13:J:31:ARG:CD	2.90	0.41
16:S:53:ASN:O	16:S:77:THR:HG22	2.21	0.41
19:U:3:LEU:H	19:U:35:GLN:HE22	1.68	0.41
1:A:427:U:OP2	1:A:428:G:O2'	2.29	0.41
1:A:1021:A:N3	1:A:1021:A:C5'	2.78	0.41
1:A:1027:C:OP2	1:A:1027:C:C6	2.74	0.41
1:A:1070:U:H2'	1:A:1071:C:H6	1.86	0.41
2:B:43:LEU:O	2:B:47:VAL:HG23	2.20	0.41
2:B:54:LEU:O	2:B:58:ASN:ND2	2.44	0.41
2:B:81:LYS:O	2:B:85:LEU:HD13	2.20	0.41
3:D:87:GLY:HA3	3:D:197:GLU:HG2	2.02	0.41
4:E:32:SER:OG	4:E:33:PHE:N	2.54	0.41
4:E:111:MET:HE1	4:E:125:ALA:HB1	2.02	0.41
5:H:60:GLU:OE1	5:H:60:GLU:C	2.64	0.41
6:L:54:ARG:CD	6:L:64:THR:HG22	2.50	0.41
7:P:52:LEU:HD23	7:P:52:LEU:HA	1.88	0.41
10:F:121:THR:O	10:F:125:GLU:HG3	2.20	0.41
11:G:13:LEU:HB3	11:G:14:PRO:CD	2.48	0.41
11:G:27:VAL:CG2	11:G:43:VAL:HG21	2.43	0.41
12:I:123:ARG:HD2	12:I:124:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:58:ASP:OD1	14:M:58:ASP:C	2.64	0.41
17:O:61:LEU:HD23	17:O:62:MET:N	2.35	0.41
18:R:20:VAL:HG23	18:R:37:ARG:HH12	1.84	0.41
1:A:517:G:N1	1:A:533:A:OP1	2.47	0.41
1:A:1005:A:H2'	1:A:1006:G:O4'	2.21	0.41
1:A:1032:G:C2	1:A:1033:G:H1'	2.56	0.41
12:I:92:GLU:O	12:I:92:GLU:CG	2.69	0.41
14:M:22:ILE:H	14:M:22:ILE:HG12	1.73	0.41
16:S:8:GLY:HA2	16:S:9:PRO:HD3	1.93	0.41
17:O:1:MET:H3	17:O:67:PRO:HA	1.85	0.41
18:R:83:GLU:OE1	18:R:83:GLU:N	2.54	0.41
1:A:1158:C:H3'	1:A:1158:C:O2	2.22	0.40
1:A:1158:C:O2	1:A:1158:C:C2'	2.68	0.40
4:E:126:LYS:HD3	4:E:127:ALA:H	1.85	0.40
6:L:56:ARG:HG3	6:L:56:ARG:NH1	2.36	0.40
7:P:80:LYS:CE	7:P:81:ALA:N	2.84	0.40
8:Q:4:LYS:NZ	8:Q:4:LYS:CB	2.77	0.40
12:I:45:ARG:HH11	12:I:45:ARG:HD2	1.75	0.40
14:M:113:ARG:HG2	14:M:113:ARG:NH1	2.32	0.40
15:N:73:PHE:CD1	15:N:73:PHE:C	2.99	0.40
1:A:79:G:C2	1:A:91:U:C2	2.73	0.40
1:A:404:G:N7	3:D:2:ALA:HB3	2.36	0.40
1:A:712:A:H2'	1:A:713:G:C8	2.56	0.40
2:B:148:LEU:HA	2:B:151:ILE:HG22	2.02	0.40
2:B:179:LEU:HD23	2:B:179:LEU:HA	1.88	0.40
3:D:17:THR:OG1	3:D:18:ASP:N	2.54	0.40
6:L:73:ASN:OD1	6:L:73:ASN:N	2.54	0.40
12:I:118:LEU:N	12:I:118:LEU:HD23	2.36	0.40
13:J:78:GLU:O	13:J:78:GLU:HG3	2.21	0.40
14:M:59:GLU:CA	14:M:62:LYS:HZ3	2.34	0.40
21:W:120:THR:HA	21:W:123:MET:HE1	2.03	0.40
21:W:184:PRO:HG2	21:W:184:PRO:O	2.21	0.40
1:A:86:G:O4'	1:A:87:C:H5	2.04	0.40
1:A:1005:A:N6	1:A:1025:U:OP1	2.55	0.40
1:A:1018:G:N3	1:A:1018:G:H2'	2.36	0.40
1:A:1138:G:N7	1:A:1140:C:H1'	2.36	0.40
1:A:1522:U:OP1	18:R:128:ARG:NH2	2.55	0.40
10:F:85:GLU:OE1	10:F:88:ARG:NH2	2.45	0.40
11:G:15:ASP:OD1	11:G:20:SER:N	2.55	0.40
13:J:31:ARG:NH1	13:J:32:THR:HA	2.37	0.40
20:V:23:TYR:O	20:V:23:TYR:HD1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:20:LEU:HD12	21:W:21:ASN:N	2.36	0.40
13:J:6:ILE:HG23	13:J:101:SER:O	2.20	0.40
18:R:17:SER:O	18:R:17:SER:OG	2.31	0.40
18:R:53:ARG:HH11	18:R:57:LYS:HE2	1.86	0.40
21:W:39:GLN:HB2	21:W:41:MET:HE1	2.04	0.40
21:W:93:MET:HB2	21:W:93:MET:HE3	1.80	0.40
1:A:339:C:H2'	1:A:340:U:H6	1.86	0.40
1:A:411:A:H4'	1:A:412:A:C5'	2.50	0.40
1:A:821:G:H2'	1:A:822:U:C6	2.57	0.40
2:B:144:LEU:HB3	2:B:148:LEU:HD12	2.04	0.40
5:H:50:LYS:HE3	5:H:50:LYS:HB3	1.82	0.40
10:F:184:TYR:HA	10:F:200:VAL:O	2.21	0.40
16:S:27:ASP:OD1	16:S:29:LYS:NZ	2.55	0.40
16:S:47:LEU:HD23	16:S:47:LEU:HA	1.89	0.40
18:R:69:ARG:HB2	18:R:69:ARG:NH1	2.37	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	
2	B	222/241 (92%)	202 (91%)	17 (8%)	3 (1%)	9	30
3	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
4	E	153/167 (92%)	147 (96%)	4 (3%)	2 (1%)	9	31
5	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
6	L	120/124 (97%)	114 (95%)	3 (2%)	3 (2%)	4	16
7	P	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
8	Q	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
9	T	84/87 (97%)	84 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	F	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
11	G	149/179 (83%)	131 (88%)	14 (9%)	4 (3%)	4	15
12	I	125/130 (96%)	117 (94%)	7 (6%)	1 (1%)	16	44
13	J	97/103 (94%)	95 (98%)	1 (1%)	1 (1%)	12	38
14	M	112/118 (95%)	98 (88%)	11 (10%)	3 (3%)	4	15
15	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
16	S	79/92 (86%)	74 (94%)	5 (6%)	0	100	100
17	O	104/135 (77%)	97 (93%)	7 (7%)	0	100	100
18	R	115/129 (89%)	108 (94%)	7 (6%)	0	100	100
19	U	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
20	V	59/75 (79%)	55 (93%)	3 (5%)	1 (2%)	7	25
21	W	252/254 (99%)	227 (90%)	19 (8%)	6 (2%)	4	17
All	All	2547/2759 (92%)	2392 (94%)	131 (5%)	24 (1%)	16	41

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	170	HIS
6	L	45	PRO
20	V	19	GLN
21	W	183	PRO
6	L	123	LYS
14	M	88	GLY
14	M	95	LEU
21	W	60	ASP
21	W	78	HIS
4	E	70	ASN
12	I	32	GLN
13	J	57	VAL
21	W	79	PRO
2	B	129	LEU
11	G	11	LYS
11	G	119	ARG
21	W	43	GLU
21	W	116	TYR
11	G	71	PRO
14	M	96	PRO
2	B	165	ASP

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Mol	Chain	Res	Type
11	G	13	LEU
6	L	122	PRO
4	E	161	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	186 (100%)	0	100	100
3	D	172/173 (99%)	171 (99%)	1 (1%)	78	92
4	E	118/126 (94%)	118 (100%)	0	100	100
5	H	104/105 (99%)	104 (100%)	0	100	100
6	L	102/103 (99%)	101 (99%)	1 (1%)	68	88
7	P	65/65 (100%)	65 (100%)	0	100	100
8	Q	74/78 (95%)	72 (97%)	2 (3%)	39	74
9	T	65/66 (98%)	65 (100%)	0	100	100
10	F	170/190 (90%)	168 (99%)	2 (1%)	63	87
11	G	124/147 (84%)	122 (98%)	2 (2%)	55	83
12	I	105/107 (98%)	100 (95%)	5 (5%)	23	56
13	J	87/90 (97%)	83 (95%)	4 (5%)	24	58
14	M	92/96 (96%)	89 (97%)	3 (3%)	33	69
15	N	83/84 (99%)	80 (96%)	3 (4%)	31	66
16	S	71/79 (90%)	68 (96%)	3 (4%)	26	61
17	O	92/116 (79%)	92 (100%)	0	100	100
18	R	90/99 (91%)	90 (100%)	0	100	100
19	U	76/77 (99%)	76 (100%)	0	100	100
20	V	52/65 (80%)	52 (100%)	0	100	100
21	W	217/217 (100%)	215 (99%)	2 (1%)	70	89
All	All	2145/2282 (94%)	2117 (99%)	28 (1%)	59	86

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	142	VAL
6	L	45	PRO
8	Q	4	LYS
8	Q	83	VAL
10	F	90	VAL
10	F	101	ILE
11	G	42	ILE
11	G	76	LYS
12	I	15	SER
12	I	21	ILE
12	I	45	ARG
12	I	111	VAL
12	I	126	GLN
13	J	36	VAL
13	J	83	THR
13	J	85	ASP
13	J	87	LEU
14	M	7	ILE
14	M	55	THR
14	M	108	THR
15	N	53	ARG
15	N	65	ARG
15	N	84	VAL
16	S	4	SER
16	S	6	LYS
16	S	33	THR
21	W	133	ILE
21	W	149	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	168	HIS
2	B	170	HIS
2	B	190	ASN
3	D	116	GLN
4	E	82	GLN
9	T	3	ASN
9	T	20	HIS
9	T	61	GLN
11	G	142	HIS

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Mol	Chain	Res	Type
14	M	8	ASN
17	O	37	HIS
17	O	55	HIS
17	O	58	HIS
17	O	63	ASN
18	R	118	HIS
19	U	40	GLN
21	W	18	ASN
21	W	137	HIS
21	W	202	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1412/1415 (99%)	291 (20%)	43 (3%)

All (291) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	7	A
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	44	A
1	A	47	C
1	A	48	C
1	A	51	A
1	A	52	C
1	A	70	U
1	A	72	A
1	A	75	G
1	A	76	G
1	A	79	G
1	A	80	A
1	A	81	A
1	A	82	G
1	A	83	C
1	A	84	U
1	A	85	U

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Mol	Chain	Res	Type
1	A	86	G
1	A	89	U
1	A	90	C
1	A	91	U
1	A	97	G
1	A	119	A
1	A	121	U
1	A	122	G
1	A	130	A
1	A	131	A
1	A	141	G
1	A	143	A
1	A	144	G
1	A	151	A
1	A	152	A
1	A	164	G
1	A	197	A
1	A	205	A
1	A	209	U
1	A	210	C
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	397	A
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G

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Mol	Chain	Res	Type
1	A	414	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	446	G
1	A	451	A
1	A	456	A
1	A	457	G
1	A	466	A
1	A	467	U
1	A	468	A
1	A	481	G
1	A	484	G
1	A	486	U
1	A	495	A
1	A	509	A
1	A	511	C
1	A	518	C
1	A	527	G
1	A	530	G
1	A	532	A
1	A	533	A
1	A	547	A
1	A	562	U
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	610	U
1	A	628	G
1	A	637	C
1	A	653	U
1	A	665	A
1	A	675	A
1	A	682	G
1	A	683	G
1	A	687	A
1	A	709	U
1	A	718	A

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Mol	Chain	Res	Type
1	A	721	G
1	A	723	U
1	A	724	G
1	A	755	G
1	A	758	C
1	A	760	G
1	A	777	A
1	A	785	G
1	A	789	U
1	A	795	C
1	A	796	C
1	A	815	A
1	A	817	C
1	A	821	G
1	A	828	U
1	A	829	G
1	A	832	G
1	A	840	C
1	A	844	G
1	A	845	A
1	A	846	G
1	A	914	A
1	A	923	A
1	A	925	G
1	A	926	G
1	A	927	G
1	A	932	C
1	A	934	C
1	A	935	A
1	A	944	G
1	A	948	C
1	A	949	A
1	A	960	U
1	A	961	U
1	A	965	U
1	A	966	G
1	A	967	C
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	983	A

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Mol	Chain	Res	Type
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1006	G
1	A	1009	U
1	A	1010	U
1	A	1011	C
1	A	1012	A
1	A	1018	G
1	A	1019	A
1	A	1020	G
1	A	1021	A
1	A	1022	A
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1035	A
1	A	1036	A
1	A	1038	C
1	A	1041	G
1	A	1044	A
1	A	1045	C
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1110	A
1	A	1117	A
1	A	1122	U
1	A	1123	U
1	A	1127	G
1	A	1132	C
1	A	1133	G

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Mol	Chain	Res	Type
1	A	1136	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1142	G
1	A	1143	G
1	A	1146	A
1	A	1147	C
1	A	1151	A
1	A	1153	G
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1163	A
1	A	1166	G
1	A	1167	A
1	A	1168	U
1	A	1169	A
1	A	1171	A
1	A	1174	G
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1200	C
1	A	1201	A
1	A	1202	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1220	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1229	A
1	A	1230	C
1	A	1236	A
1	A	1238	A
1	A	1239	A
1	A	1240	U

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Mol	Chain	Res	Type
1	A	1245	C
1	A	1249	C
1	A	1255	G
1	A	1256	A
1	A	1257	A
1	A	1258	G
1	A	1263	C
1	A	1266	G
1	A	1267	C
1	A	1275	A
1	A	1279	G
1	A	1280	A
1	A	1282	C
1	A	1285	A
1	A	1286	U
1	A	1287	A
1	A	1290	G
1	A	1293	C
1	A	1296	C
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1316	G
1	A	1317	C
1	A	1318	A
1	A	1320	C
1	A	1324	A
1	A	1326	U
1	A	1331	G
1	A	1337	G
1	A	1338	G
1	A	1340	A
1	A	1346	A
1	A	1349	A
1	A	1351	U
1	A	1353	G
1	A	1354	U
1	A	1355	G
1	A	1358	U
1	A	1359	C
1	A	1363	A
1	A	1364	U

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Mol	Chain	Res	Type
1	A	1365	G
1	A	1370	G
1	A	1373	G
1	A	1377	A
1	A	1378	C
1	A	1381	U
1	A	1383	C
1	A	1385	G
1	A	1517	G
1	A	1518	A
1	A	1519	A
1	A	1520	C
1	A	1521	C
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	89	U
1	A	90	C
1	A	121	U
1	A	413	G
1	A	428	G
1	A	467	U
1	A	532	A
1	A	844	G
1	A	845	A
1	A	926	G
1	A	931	C
1	A	948	C
1	A	975	A
1	A	1009	U
1	A	1010	U
1	A	1024	G
1	A	1030	U
1	A	1031	C
1	A	1043	G
1	A	1054	C
1	A	1135	U

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Mol	Chain	Res	Type
1	A	1136	C
1	A	1141	C
1	A	1147	C
1	A	1159	U
1	A	1160	G
1	A	1168	U
1	A	1213	A
1	A	1214	C
1	A	1225	A
1	A	1239	A
1	A	1255	G
1	A	1257	A
1	A	1298	U
1	A	1299	A
1	A	1325	C
1	A	1337	G
1	A	1363	A
1	A	1364	U
1	A	1516	G
1	A	1517	G
1	A	1518	A
1	A	1519	A

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	D2T	L	89	6	8,9,10	1.90	2 (25%)	6,11,13	1.45	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	D2T	L	89	6	-	3/7/12/14	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	89	D2T	CB-CA	-4.05	1.53	1.54
6	L	89	D2T	CB1-SB	-2.04	1.75	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	89	D2T	CB-CA-N	2.16	113.47	109.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	89	D2T	CG-CB-SB-CB1
6	L	89	D2T	SB-CB-CG-OD1
6	L	89	D2T	SB-CB-CG-OD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1391:U	O3'	1507:A	P	18.51
1	A	789:U	O3'	794:A	P	6.85
1	A	1214:C	O3'	1215:G	P	1.78
1	A	949:A	O3'	950:U	P	1.33

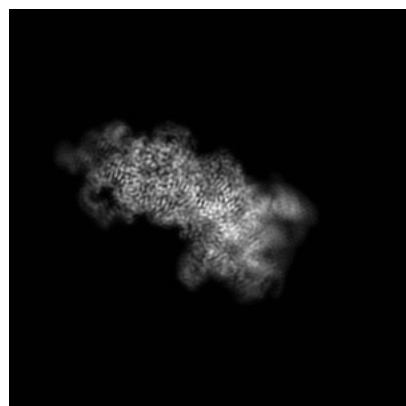
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28720. These allow visual inspection of the internal detail of the map and identification of artifacts.

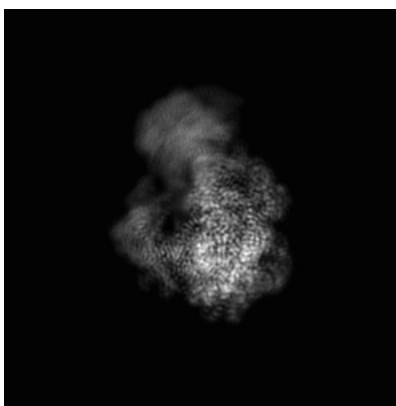
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

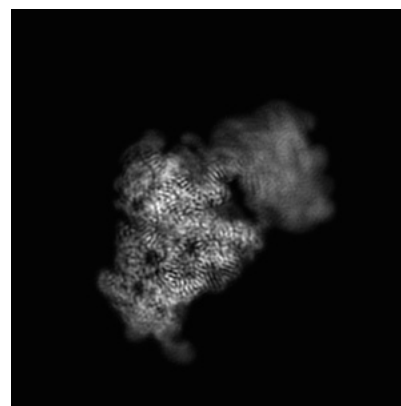
6.1.1 Primary map



X

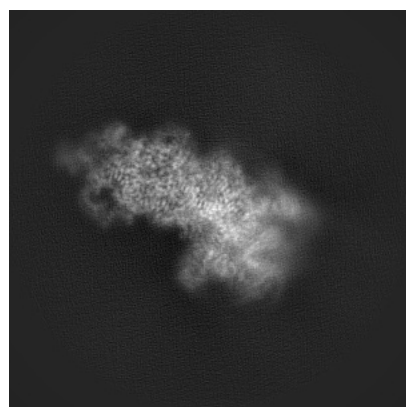


Y

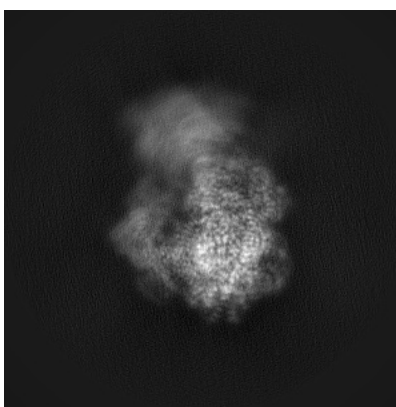


Z

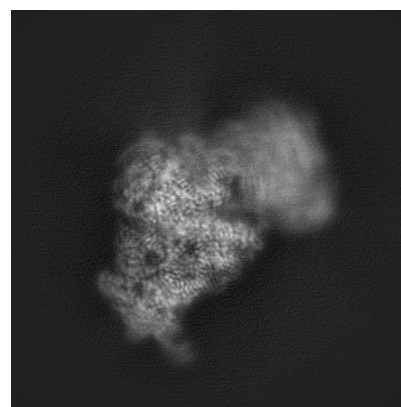
6.1.2 Raw map



X



Y

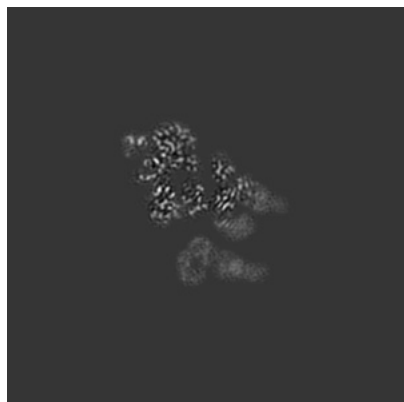


Z

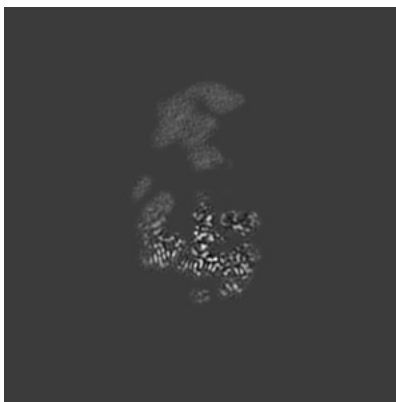
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

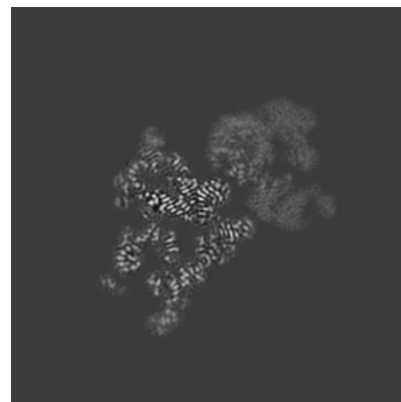
6.2.1 Primary map



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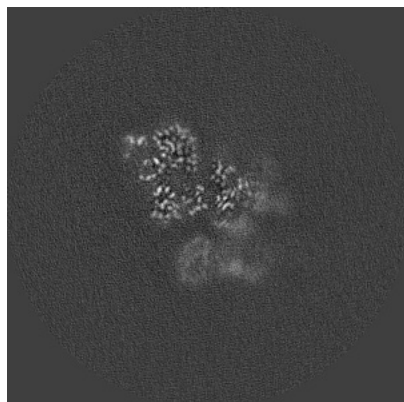


Y Index: 191

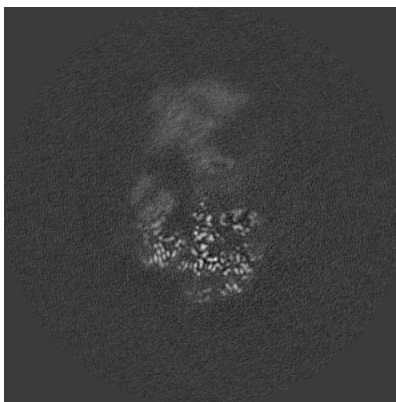


Z Index: 191

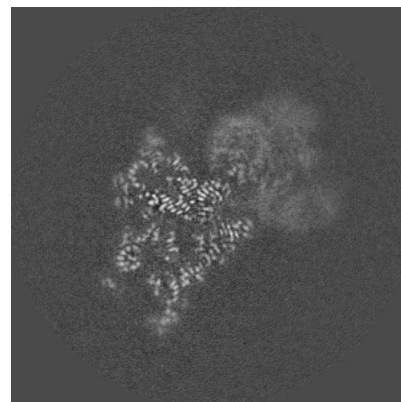
6.2.2 Raw map



X Index: 191



Y Index: 191

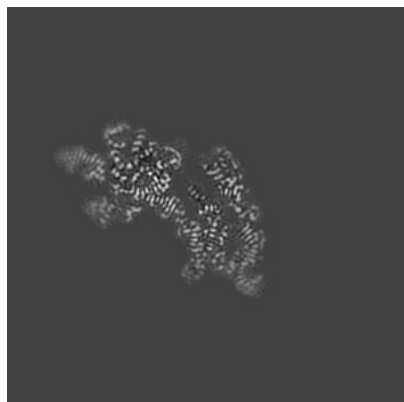


Z Index: 191

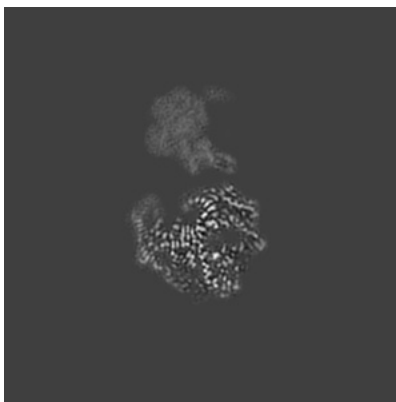
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

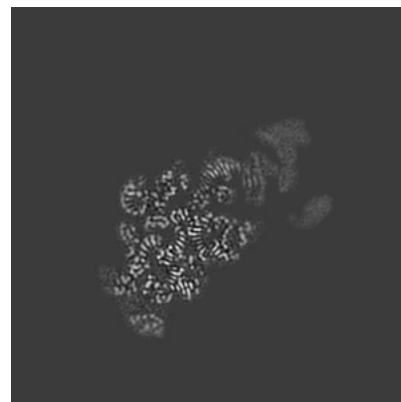
6.3.1 Primary map



X Index: 151

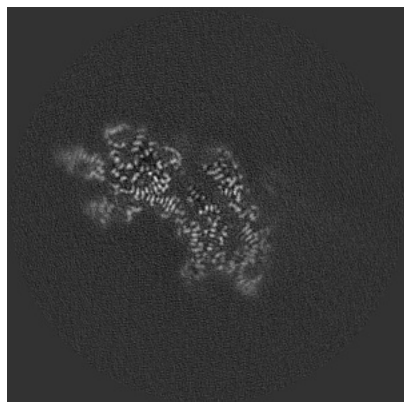


Y Index: 202

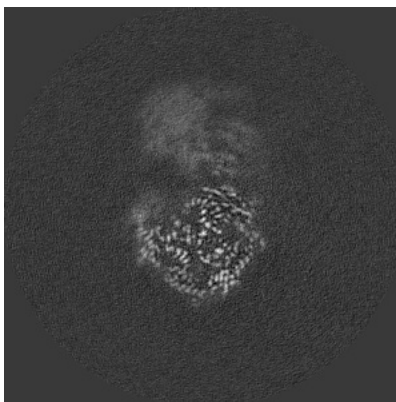


Z Index: 210

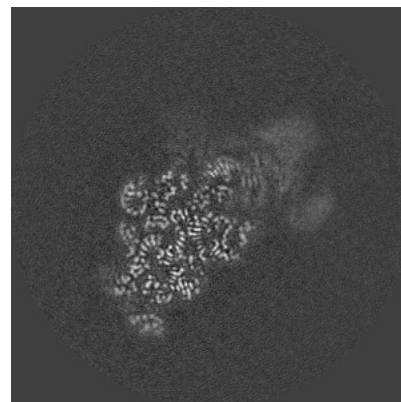
6.3.2 Raw map



X Index: 151



Y Index: 205

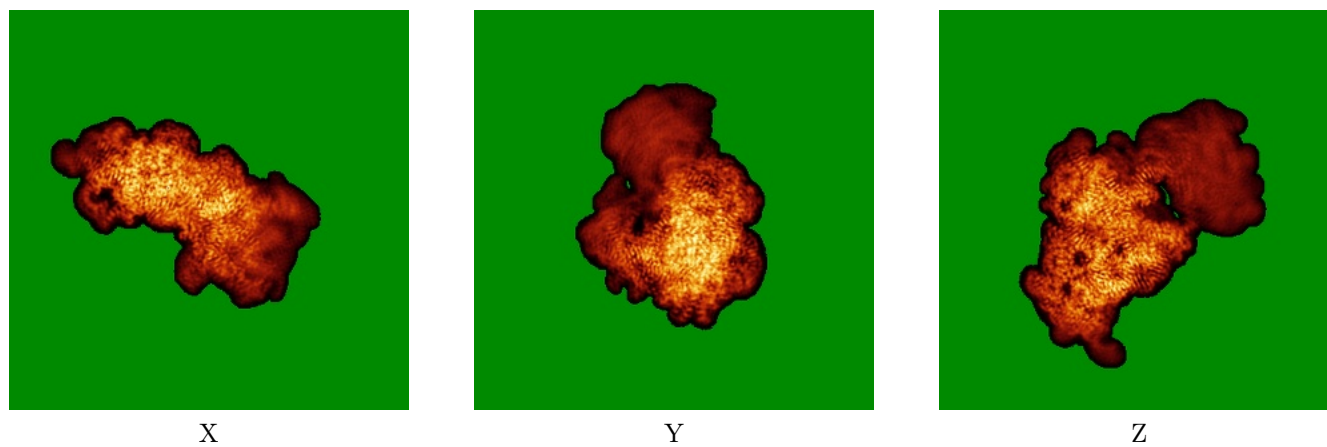


Z Index: 210

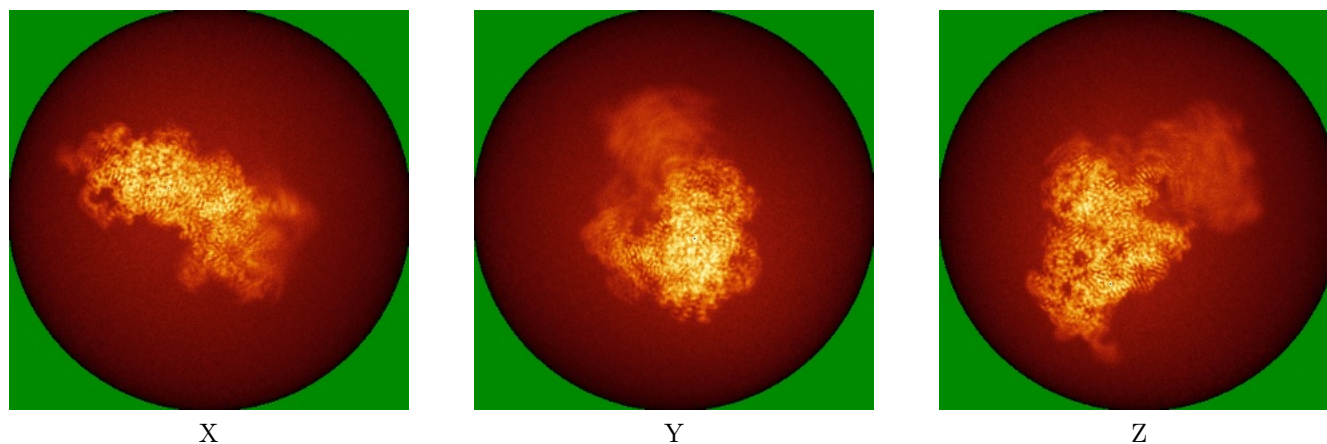
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

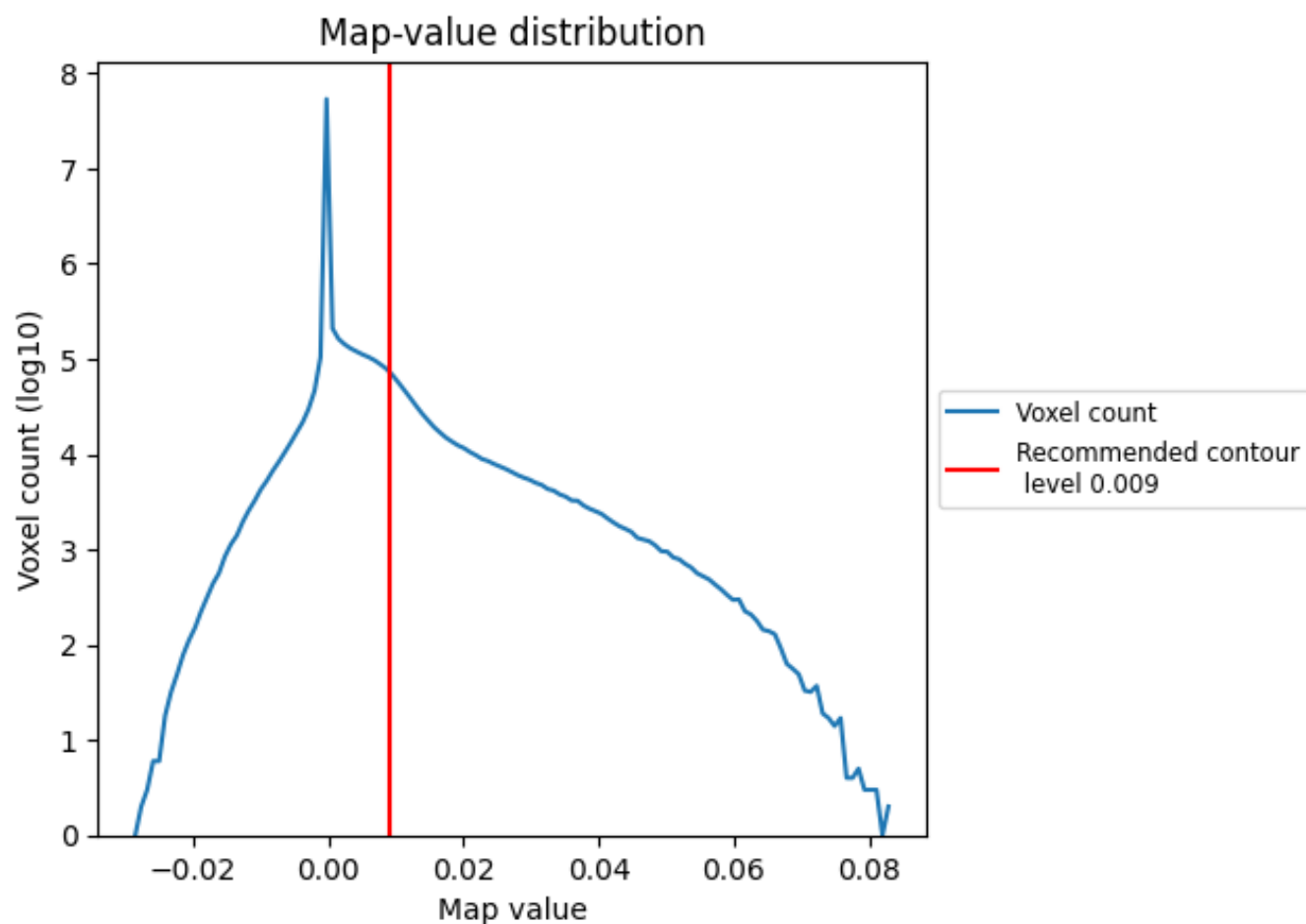
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

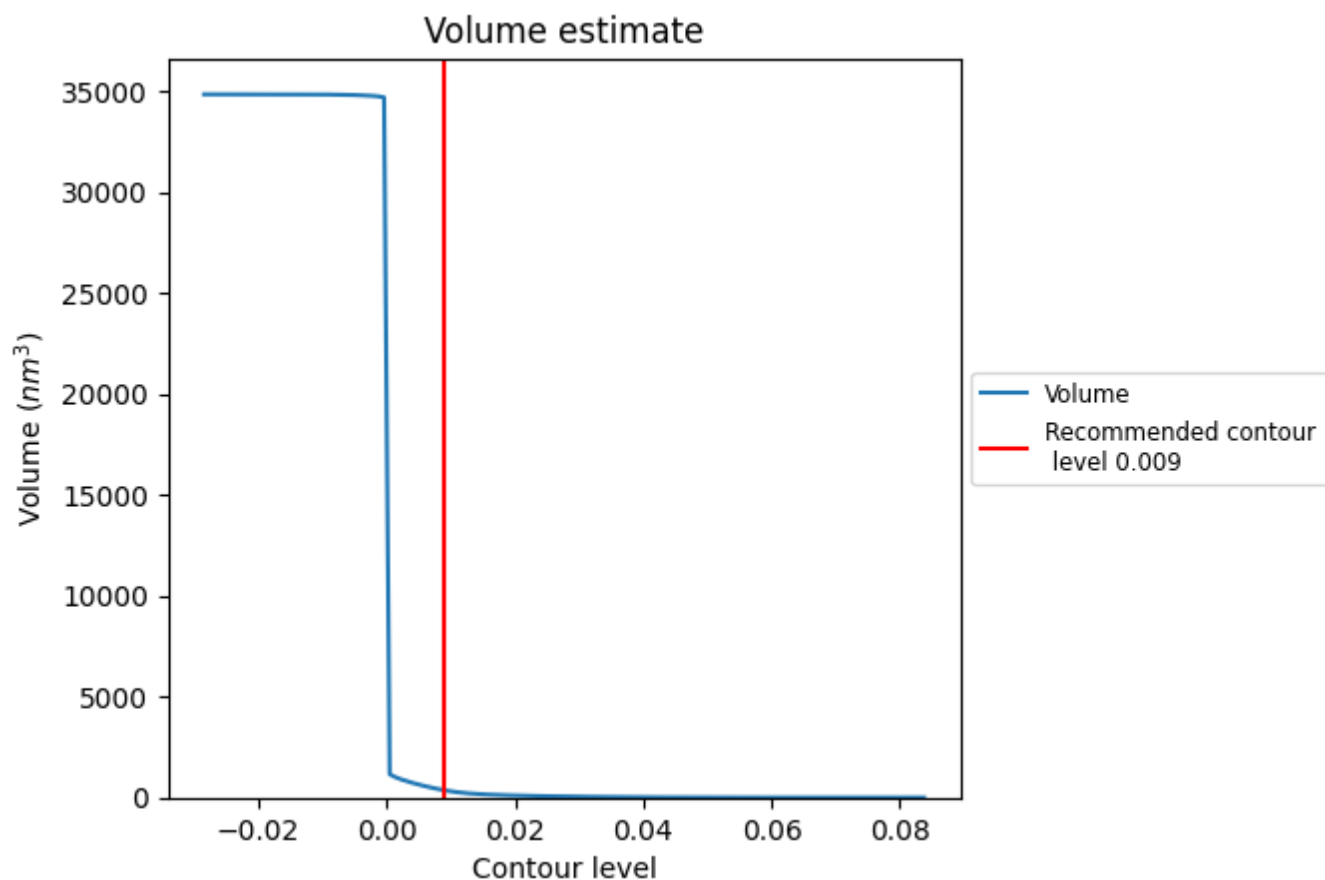
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

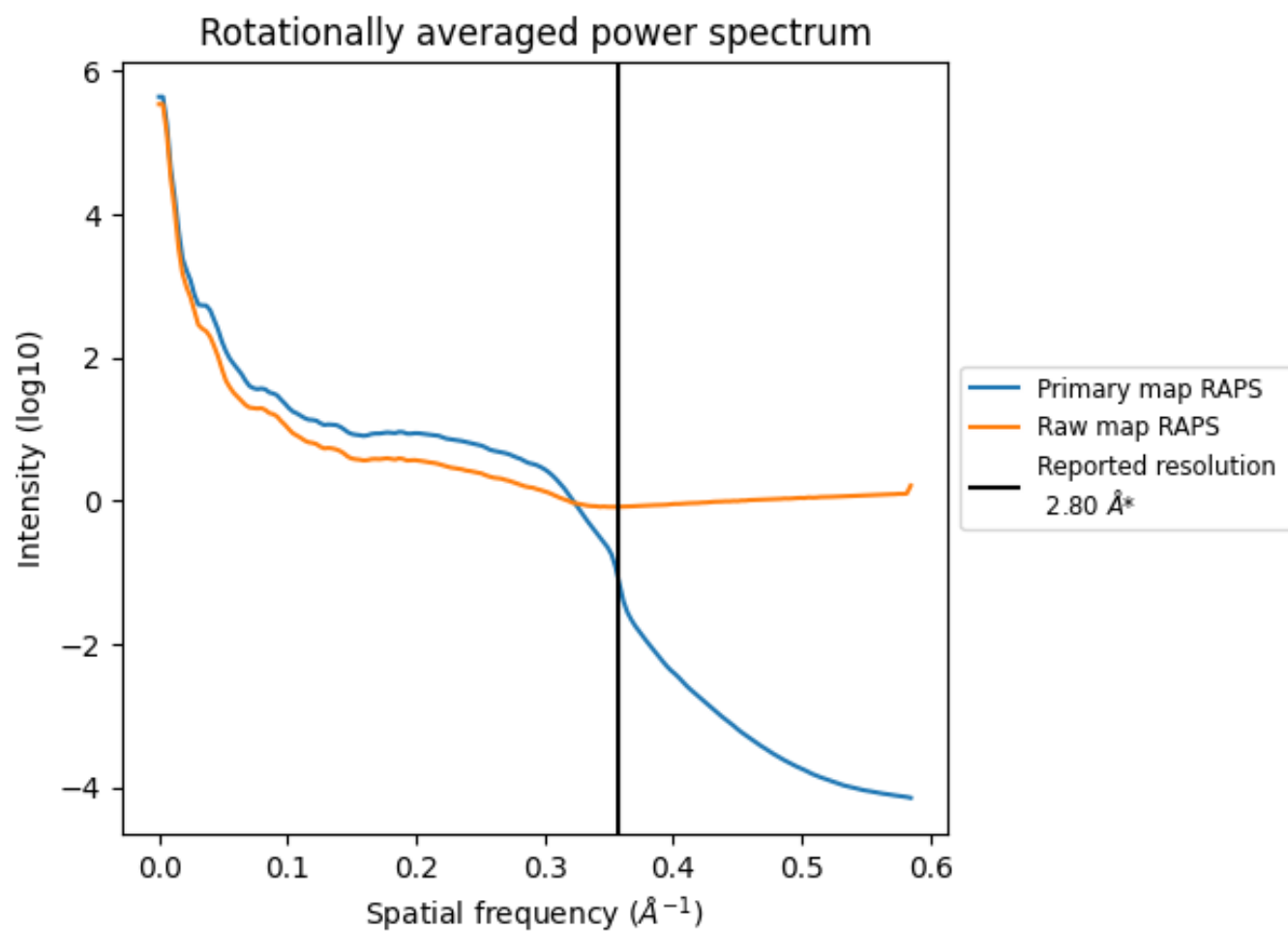
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 360 nm^3 ; this corresponds to an approximate mass of 326 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 ⓘ

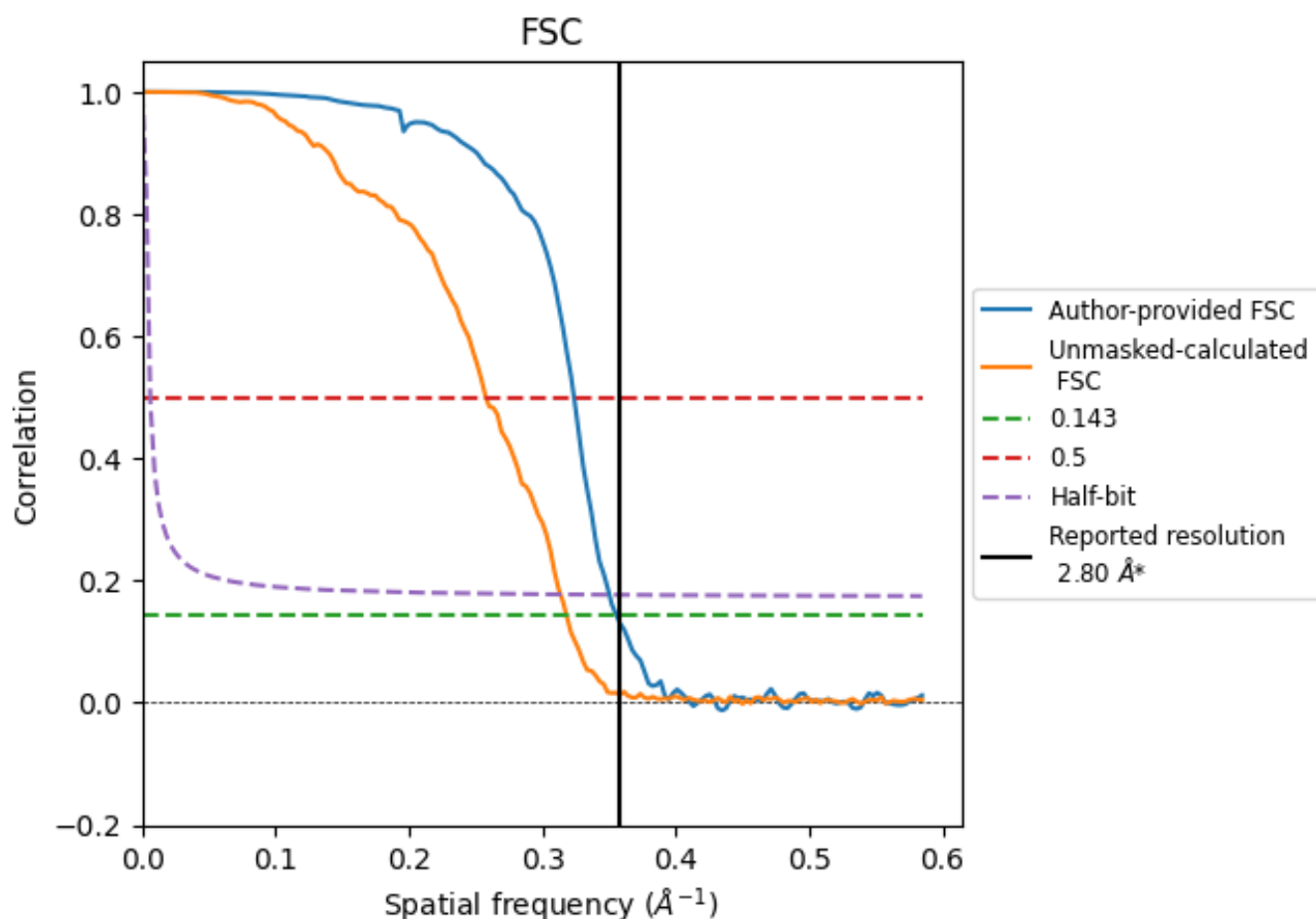


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

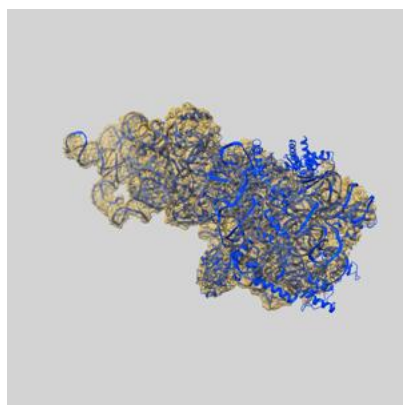
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.81	3.09	2.85
Unmasked-calculated*	3.14	3.88	3.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.14 differs from the reported value 2.8 by more than 10 %

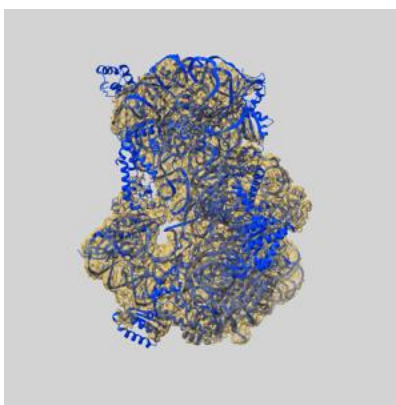
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28720 and PDB model 8EYT. Per-residue inclusion information can be found in section [3](#) on page [8](#).

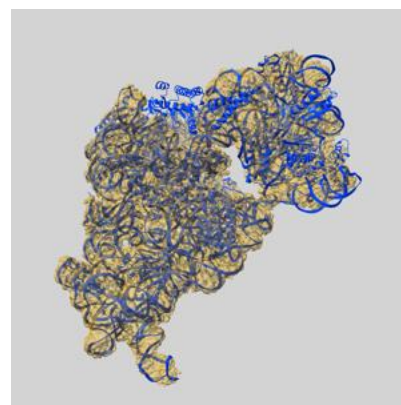
9.1 Map-model overlay [i](#)



X



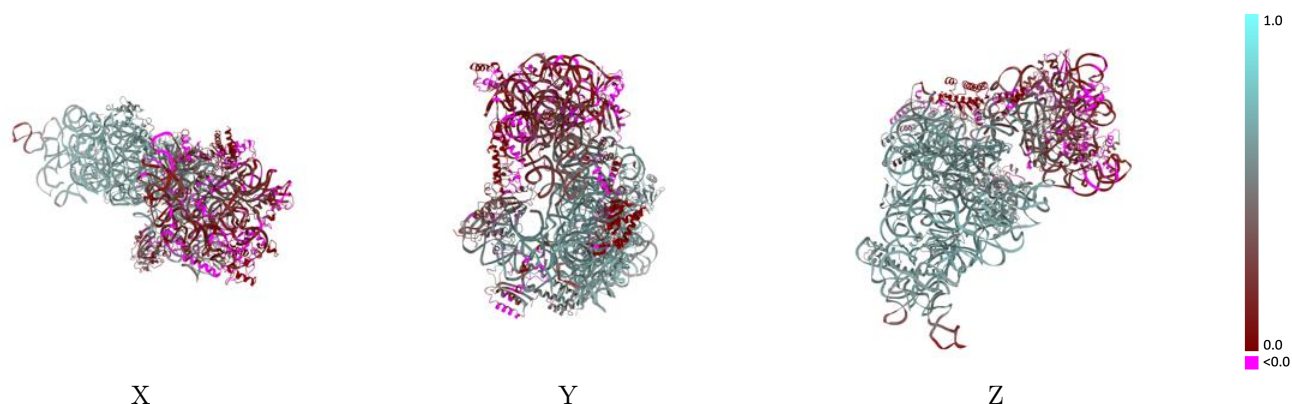
Y



Z

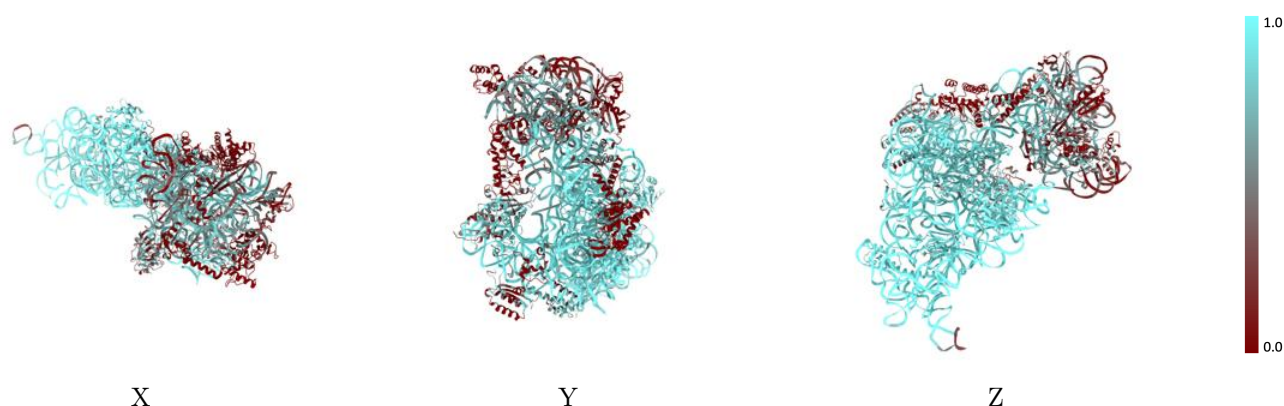
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



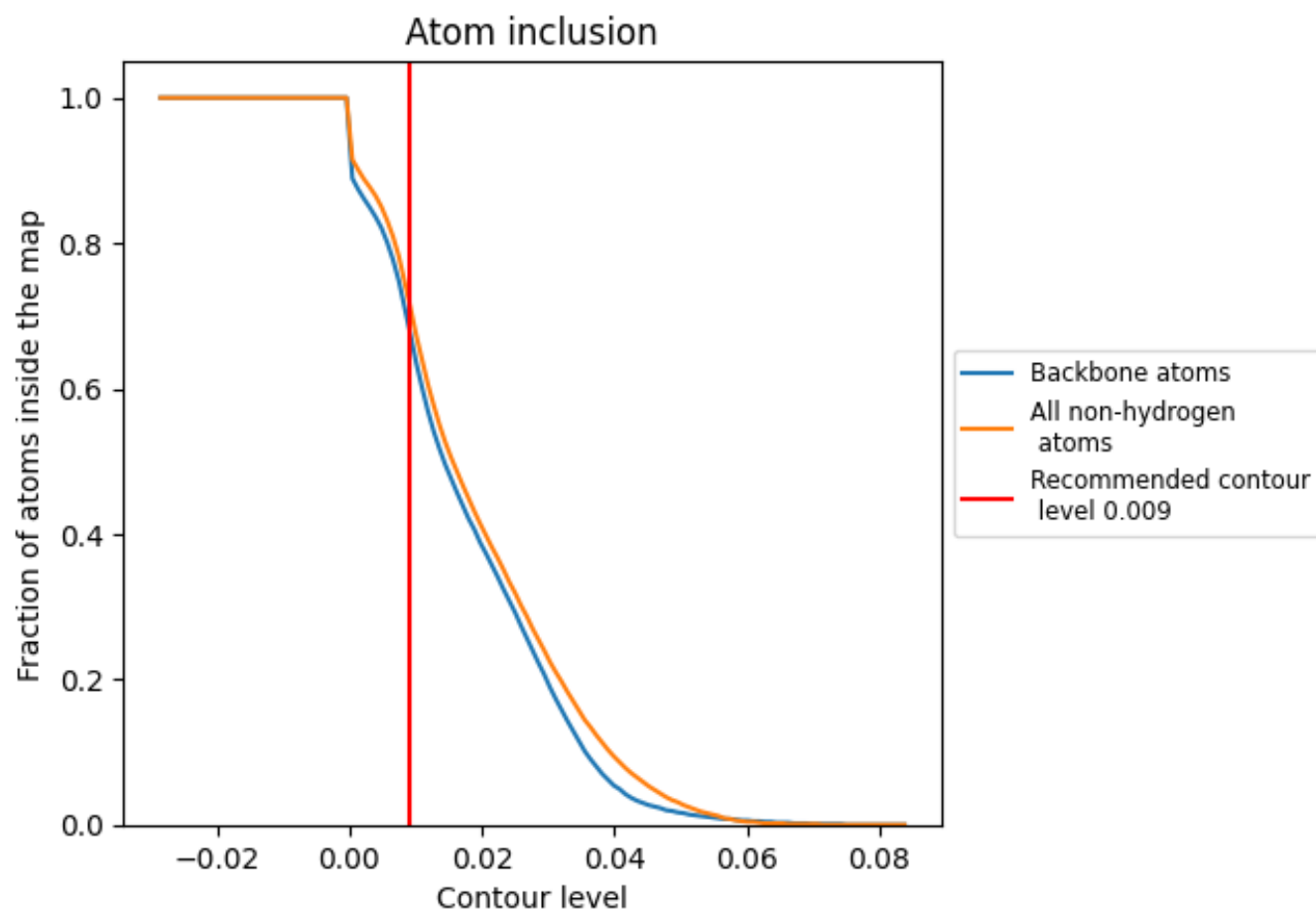
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7200	 0.4070
A	 0.8750	 0.4750
B	 0.0190	 0.0300
D	 0.8480	 0.5530
E	 0.8860	 0.5740
F	 0.3630	 0.2400
G	 0.0120	 -0.0260
H	 0.9100	 0.5970
I	 0.3430	 0.1710
J	 0.1470	 0.0580
L	 0.8620	 0.5630
M	 0.0850	 0.0010
N	 0.2690	 0.1090
O	 0.3760	 0.3060
P	 0.9140	 0.6030
Q	 0.9070	 0.5810
R	 0.5170	 0.3160
S	 0.2020	 0.0530
T	 0.9340	 0.5730
U	 0.6090	 0.4570
V	 0.2560	 0.1840
W	 0.5150	 0.3290

