



Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 10:30 am GMT

PDB ID : 5LMN
EMDB ID : EMD-4073
Title : Structure of bacterial 30S-IF1-IF3-mRNA translation pre-initiation complex (state-1A)
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on : 2016-08-01
Resolution : 3.55 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

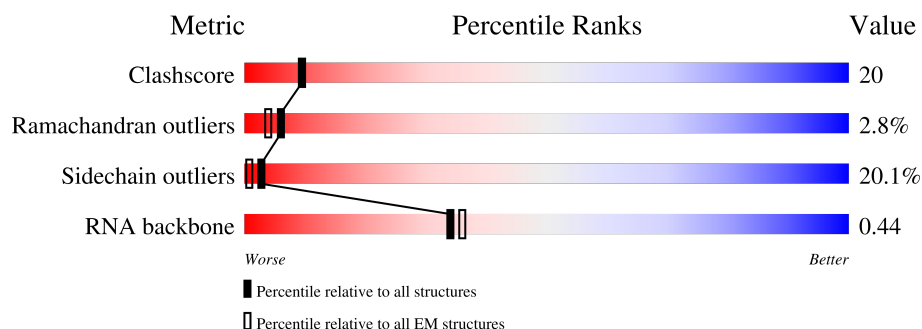
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.55 Å.

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





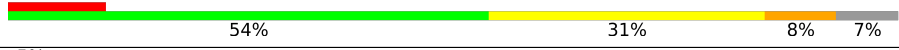

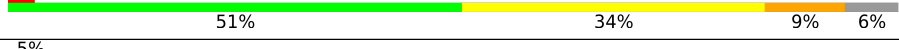


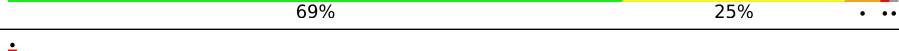
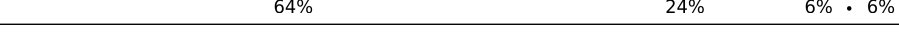
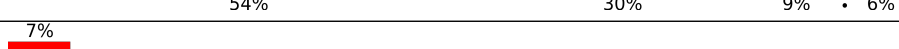


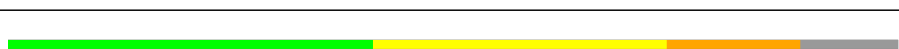

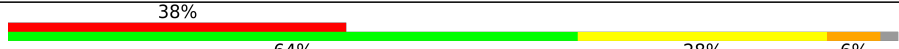


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	

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Mol	Chain	Length	Quality of chain
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	W	72	
23	X	171	
24	Y	42	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 54149 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1514	Total	C	N	O	P	0	0
			32527	14481	6019	10515	1512		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	127	Total	C	N	O	0	0
			999	633	193	173		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			792	498	156	137	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	120	Total	C	N	O	S	0	0
			892	554	169	166	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	117	Total	C	N	O	S	0	0
			933	577	192	162	2		

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0
			823	528	151	142	2		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	73	Total	C	N	O	0	0
			598	381	118	99		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	80	Total	C	N	O	S	0	0
			647	414	119	112	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	71	Total	C	N	O	S	0	0
			570	362	103	103	2		

- Molecule 23 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	168	Total	C	N	O	S	0	0
			1356	853	249	245	9		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	20	Total	C	N	O	P	0	0
			439	196	89	134	20		

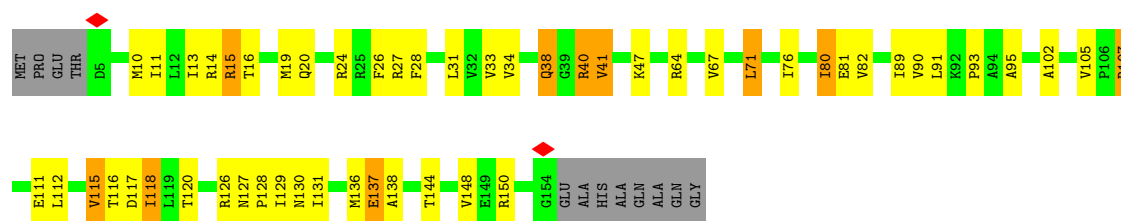
- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
25	A	126	Total	Mg	0
			126	126	
25	N	1	Total	Mg	0
			1	1	

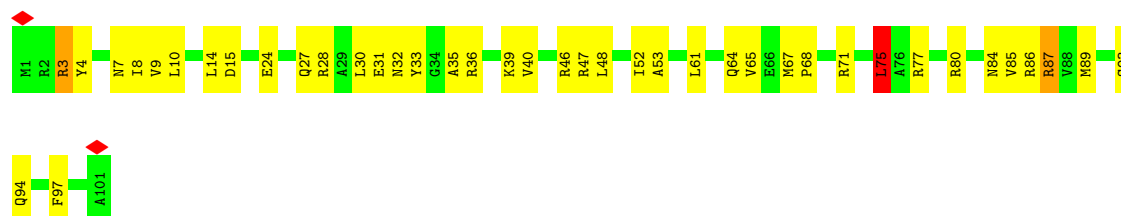
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	D	1	Total	Zn	0
			1	1	
26	N	1	Total	Zn	0
			1	1	

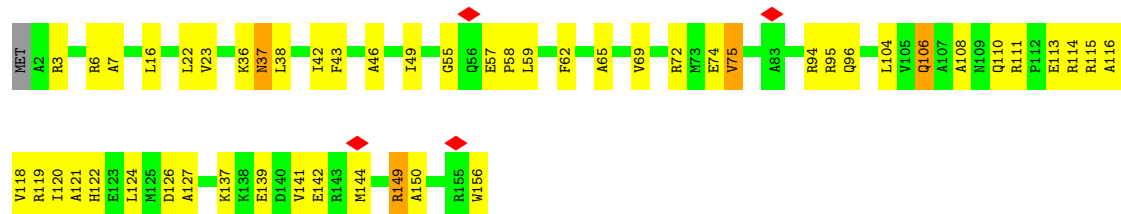




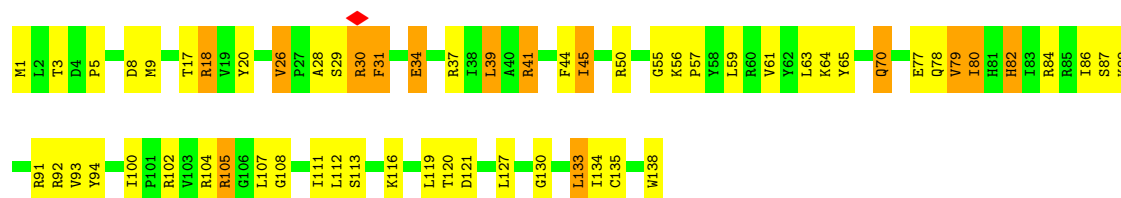
• Molecule 6: 30S ribosomal protein S6



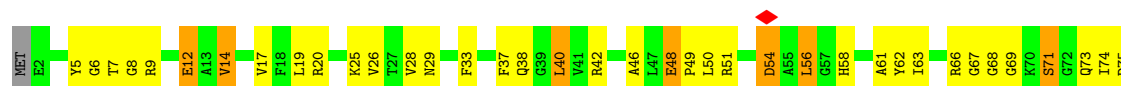
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

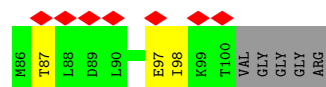
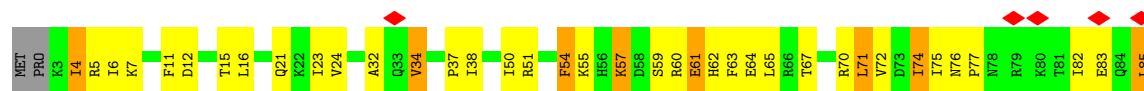


• Molecule 9: 30S ribosomal protein S9

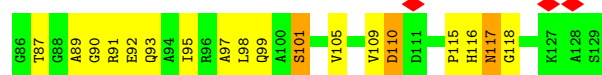




- Molecule 10: 30S ribosomal protein S10



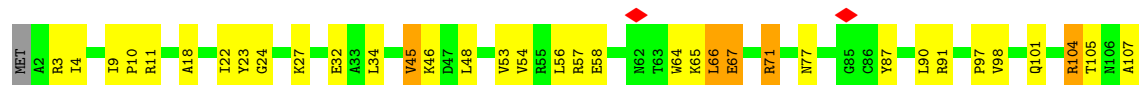
- Molecule 11: 30S ribosomal protein S11



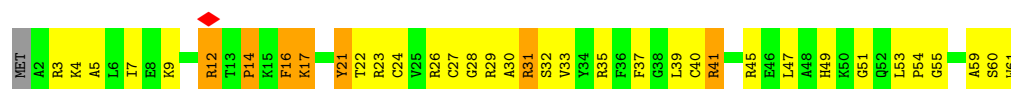
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



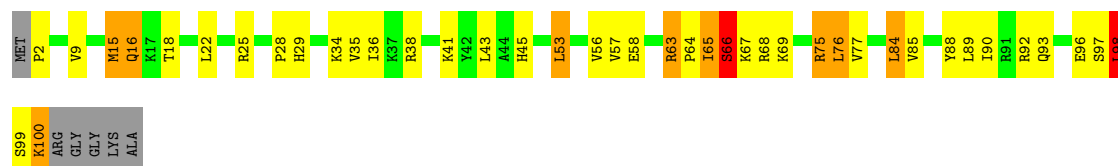
- Molecule 15: 30S ribosomal protein S15



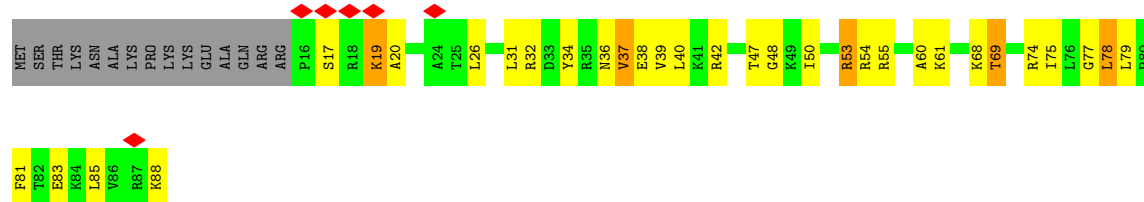
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

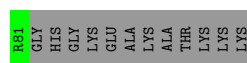


- Molecule 18: 30S ribosomal protein S18

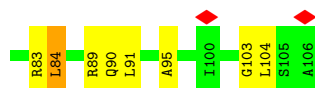


- Molecule 19: 30S ribosomal protein S19





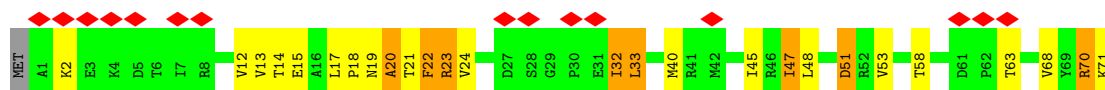
- Molecule 20: 30S ribosomal protein S20



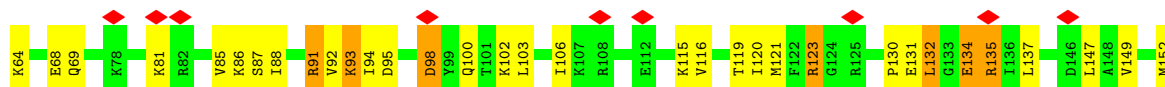
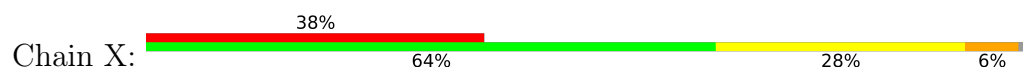
- Molecule 21: 30S ribosomal protein Thx



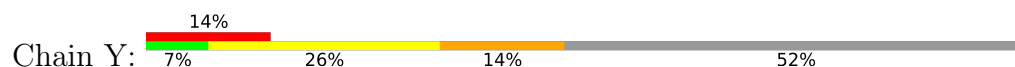
- Molecule 22: Translation initiation factor IF-1



- Molecule 23: Translation initiation factor IF-3



- Molecule 24: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86892	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.928	Depositor
Minimum map value	-0.364	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.09	Depositor
Map size (\AA)	348.4, 348.4, 348.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.38	5/36403 (0.0%)	0.76	22/56800 (0.0%)
2	B	0.43	0/1935	0.77	2/2609 (0.1%)
3	C	0.45	0/1636	0.79	0/2205
4	D	0.45	0/1733	0.84	1/2318 (0.0%)
5	E	0.50	0/1162	0.86	0/1564
6	F	0.42	0/856	0.81	1/1154 (0.1%)
7	G	0.43	0/1276	0.79	0/1709
8	H	0.47	0/1136	0.89	2/1527 (0.1%)
9	I	0.43	0/1018	0.73	0/1368
10	J	0.44	0/805	0.73	0/1082
11	K	0.43	0/907	0.71	0/1223
12	L	0.47	0/986	0.86	0/1320
13	M	0.43	0/943	0.76	0/1265
14	N	0.43	0/501	0.82	0/664
15	O	0.46	0/745	0.90	1/992 (0.1%)
16	P	0.55	0/716	0.85	1/963 (0.1%)
17	Q	0.46	0/836	0.82	0/1117
18	R	0.44	0/604	0.83	0/801
19	S	0.41	0/661	0.70	0/890
20	T	0.46	0/765	0.90	0/1007
21	V	0.47	0/212	0.79	0/277
22	W	0.44	0/580	0.76	0/782
23	X	0.42	0/1375	0.77	0/1844
24	Y	0.33	0/494	0.79	0/770
All	All	0.41	5/58285 (0.0%)	0.78	30/86251 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
8	H	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1459	C	O3'-P	-8.53	1.50	1.61
1	A	1458	G	O3'-P	7.51	1.70	1.61
1	A	999	C	O3'-P	-5.64	1.54	1.61
1	A	559	A	O3'-P	5.30	1.67	1.61
1	A	79	G	O3'-P	-5.17	1.54	1.61

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	G	O3'-P-O5'	-26.72	53.24	104.00
1	A	93	G	OP1-P-O3'	-22.17	56.43	105.20
1	A	93	G	P-O3'-C3'	-10.18	107.49	119.70
1	A	93	G	OP2-P-O3'	8.72	124.37	105.20
1	A	266	G	C2'-C3'-O3'	8.44	128.07	109.50
1	A	1001	A	C4'-C3'-O3'	-8.17	92.25	109.40
1	A	1498	U	C2'-C3'-O3'	7.46	125.91	109.50
1	A	1301	U	C2'-C3'-O3'	7.32	125.60	109.50
1	A	288	A	C2'-C3'-O3'	7.04	125.00	109.50
1	A	509	A	C4'-C3'-O3'	6.87	126.74	113.00
6	F	75	LEU	CA-CB-CG	6.83	131.02	115.30
1	A	792	A	C2'-C3'-O3'	6.59	124.25	113.70
1	A	115	G	C2'-C3'-O3'	6.50	124.11	113.70
2	B	221	LEU	CA-CB-CG	6.45	130.13	115.30
4	D	12	CYS	CA-CB-SG	6.23	125.21	114.00
1	A	815	A	C4'-C3'-O3'	-6.19	96.39	109.40
1	A	77	G	C2'-C3'-O3'	5.80	122.98	113.70
15	O	65	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	91	C	N1-C1'-C2'	-5.60	105.84	112.00
2	B	187	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	181	G	C2'-C3'-O3'	5.47	122.45	113.70
1	A	1101	A	C2'-C3'-O3'	5.44	122.40	113.70
1	A	484	G	C2'-C3'-O3'	5.43	122.39	113.70
1	A	428	G	C2'-C3'-O3'	5.39	122.32	113.70
8	H	133	LEU	CB-CG-CD1	-5.39	101.84	111.00
16	P	73	LEU	CA-CB-CG	-5.28	103.16	115.30
8	H	55	GLY	N-CA-C	5.26	126.26	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	C	C2'-C3'-O3'	5.14	121.93	113.70
1	A	77	G	N9-C1'-C2'	-5.10	106.39	112.00
1	A	1145	C	C2'-C3'-O3'	5.07	121.81	113.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1458	G	Sidechain
8	H	3	THR	Peptide

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	32527	0	16428	1137	0
2	B	1900	0	1951	112	0
3	C	1612	0	1677	58	0
4	D	1703	0	1766	65	0
5	E	1146	0	1207	50	0
6	F	843	0	857	18	0
7	G	1257	0	1296	29	0
8	H	1116	0	1177	33	0
9	I	999	0	1015	79	0
10	J	792	0	829	37	0
11	K	892	0	913	38	0
12	L	970	0	1057	43	0
13	M	933	0	992	19	0
14	N	492	0	527	52	0
15	O	734	0	771	17	0
16	P	700	0	720	14	0
17	Q	823	0	891	29	0
18	R	598	0	670	34	0
19	S	647	0	673	27	0
20	T	763	0	861	31	0
21	V	208	0	221	11	0
22	W	570	0	599	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	X	1356	0	1401	40	0
24	Y	439	0	218	17	0
25	A	126	0	0	0	0
25	N	1	0	0	0	0
26	D	1	0	0	1	0
26	N	1	0	0	0	0
All	All	54149	0	38717	1807	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 20.

All (1807) 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:563:A:N6	1:A:884:U:H3	1.13	1.44
23:X:91:ARG:N	23:X:94:ILE:HD11	1.33	1.41
5:E:15:ARG:CG	5:E:28:PHE:CE1	2.06	1.38
23:X:91:ARG:H	23:X:94:ILE:CD1	1.39	1.35
1:A:89:C:C2'	1:A:90:U:H5'	1.57	1.32
11:K:91:ARG:NH1	18:R:88:LYS:NZ	1.73	1.32
1:A:1358:U:N3	1:A:1363(A):A:N6	1.80	1.29
1:A:1081:G:OP1	5:E:16:THR:HG23	1.32	1.29
9:I:12:GLU:O	9:I:68:GLY:N	1.62	1.29
11:K:91:ARG:NH1	18:R:88:LYS:HZ2	1.26	1.28
1:A:1371:G:OP1	9:I:12:GLU:HB2	1.10	1.26
1:A:1371:G:OP1	9:I:12:GLU:CB	1.85	1.25
1:A:961:U:N3	1:A:1201:A:N6	1.84	1.23
9:I:12:GLU:O	9:I:68:GLY:CA	1.84	1.23
2:B:28:PHE:O	2:B:30:ARG:N	1.69	1.22
5:E:15:ARG:NH2	5:E:26:PHE:CD1	2.06	1.22
1:A:961:U:H3	1:A:1201:A:N6	1.37	1.22
22:W:23:ARG:NE	22:W:33:LEU:CD2	2.02	1.22
1:A:93:G:H2'	1:A:96:U:O4'	1.06	1.20
22:W:22:PHE:CE2	22:W:47:ILE:HD12	1.77	1.18
7:G:37:ASN:ND2	9:I:40:LEU:O	1.77	1.17
1:A:93:G:H5''	1:A:96:U:OP2	1.44	1.17
1:A:93:G:C2'	1:A:96:U:O4'	1.92	1.17
5:E:15:ARG:HG3	5:E:28:PHE:CE1	1.75	1.16
5:E:15:ARG:HG2	5:E:28:PHE:CE1	1.76	1.11
5:E:15:ARG:HG3	5:E:28:PHE:HE1	0.96	1.11
1:A:1358:U:H3	1:A:1363(A):A:N6	1.38	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:23:ARG:HE	22:W:33:LEU:HD21	1.08	1.10
1:A:1219:U:H2'	1:A:1220:G:C8	1.88	1.09
1:A:793:U:H3'	1:A:794:A:H5''	1.27	1.08
9:I:12:GLU:HB3	9:I:68:GLY:HA2	1.17	1.08
1:A:1370:G:O3'	9:I:12:GLU:HG2	1.52	1.08
5:E:15:ARG:NH2	5:E:26:PHE:CE1	2.17	1.08
1:A:89:C:H2'	1:A:90:U:H5'	1.31	1.07
1:A:89:C:O2'	1:A:90:U:H5'	1.57	1.05
1:A:1080:A:H4'	5:E:16:THR:OG1	1.56	1.04
22:W:13:VAL:HA	22:W:24:VAL:HG22	1.37	1.04
5:E:15:ARG:HG2	5:E:28:PHE:CD1	1.91	1.04
1:A:829:G:O4'	2:B:26:PRO:HG2	1.58	1.03
22:W:23:ARG:NH2	22:W:33:LEU:HD23	1.72	1.03
22:W:23:ARG:HE	22:W:33:LEU:CD2	1.68	1.02
2:B:17:PHE:HD1	2:B:18:GLY:N	1.57	1.02
1:A:1081:G:P	5:E:16:THR:HG23	2.00	1.02
5:E:15:ARG:CG	5:E:28:PHE:HE1	1.54	1.02
10:J:38:ILE:HG23	10:J:71:LEU:O	1.60	1.01
22:W:21:THR:O	22:W:22:PHE:HD1	1.42	1.01
22:W:23:ARG:CZ	22:W:33:LEU:HD23	1.90	1.00
1:A:79:G:H2'	1:A:80:G:H8	1.24	1.00
1:A:664:G:H22	1:A:741:G:H1	1.08	1.00
1:A:1349:A:OP2	9:I:118:LYS:HD3	1.63	0.99
17:Q:63:ARG:HH11	17:Q:63:ARG:HG3	1.28	0.99
22:W:22:PHE:HE2	22:W:47:ILE:HD12	0.85	0.98
1:A:1371:G:P	9:I:12:GLU:HB2	2.04	0.98
2:B:24:TRP:CD1	2:B:40:HIS:CE1	2.53	0.96
1:A:80:G:H3'	1:A:81:U:H5''	1.46	0.96
1:A:1370:G:O3'	9:I:12:GLU:CG	2.13	0.96
2:B:21:ARG:HA	2:B:39:ILE:HA	1.47	0.96
4:D:29:PRO:O	4:D:35:ARG:HD3	1.64	0.96
19:S:72:GLY:O	19:S:75:ALA:N	1.99	0.96
7:G:37:ASN:ND2	9:I:40:LEU:HD12	1.81	0.96
1:A:1219:U:H2'	1:A:1220:G:H8	1.20	0.96
11:K:91:ARG:HH12	18:R:88:LYS:CE	1.78	0.95
22:W:32:ILE:HD13	22:W:32:ILE:H	1.32	0.95
12:L:53:ARG:HG2	12:L:53:ARG:HH11	1.29	0.94
1:A:1458:G:OP1	20:T:35:THR:OG1	1.87	0.93
10:J:38:ILE:CG2	10:J:71:LEU:O	2.16	0.92
1:A:981:U:H4'	14:N:21:TYR:HE2	1.31	0.92
7:G:37:ASN:HD21	9:I:40:LEU:HD12	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:U:H2'	1:A:223:U:C6	2.05	0.91
23:X:130:PRO:O	23:X:134:GLU:HB2	1.71	0.91
1:A:973:G:H3'	1:A:974:A:H5''	1.52	0.90
4:D:26:CYS:SG	26:D:300:ZN:ZN	1.59	0.90
9:I:12:GLU:O	9:I:68:GLY:HA3	1.69	0.90
1:A:93:G:H2'	1:A:96:U:C1'	2.01	0.90
1:A:1081:G:P	5:E:16:THR:CG2	2.59	0.90
1:A:426:G:OP1	4:D:36:ARG:NH2	2.04	0.90
22:W:23:ARG:NE	22:W:33:LEU:HD21	1.73	0.89
22:W:23:ARG:CZ	22:W:33:LEU:CD2	2.49	0.89
1:A:1350:A:N7	9:I:118:LYS:NZ	2.21	0.88
11:K:91:ARG:HH12	18:R:88:LYS:NZ	1.50	0.88
3:C:12:LEU:HD21	3:C:18:TRP:CD1	2.08	0.88
22:W:21:THR:C	22:W:22:PHE:CD1	2.47	0.88
1:A:981:U:H4'	14:N:21:TYR:CE2	2.09	0.88
2:B:17:PHE:HD1	2:B:18:GLY:H	0.93	0.88
1:A:1327:C:H5''	21:V:20:LYS:HB2	1.55	0.87
1:A:961:U:O4	1:A:1201:A:N1	2.08	0.87
3:C:12:LEU:HD11	14:N:51:GLY:CA	2.05	0.87
1:A:1128:C:H1'	1:A:1146:A:H61	1.40	0.87
22:W:22:PHE:HE2	22:W:47:ILE:CD1	1.81	0.87
4:D:34:GLU:OE1	4:D:34:GLU:N	2.08	0.86
1:A:1025:U:H2'	1:A:1026:G:C8	2.11	0.86
3:C:92:ALA:O	3:C:95:THR:O	1.93	0.86
20:T:15:ARG:HG2	20:T:15:ARG:HH11	1.39	0.86
1:A:1495:U:H5''	23:X:93:LYS:O	1.75	0.85
23:X:94:ILE:HG23	23:X:98:ASP:OD2	1.75	0.85
1:A:792:A:H4'	1:A:793:U:H5''	1.57	0.85
1:A:829:G:O4'	2:B:26:PRO:CG	2.24	0.85
9:I:12:GLU:HB3	9:I:68:GLY:CA	2.05	0.85
2:B:17:PHE:CD1	2:B:18:GLY:N	2.44	0.85
2:B:129:GLU:C	2:B:130:ARG:HD2	1.96	0.85
14:N:23:ARG:NH1	14:N:30:ALA:HB2	1.92	0.85
1:A:793:U:H3'	1:A:794:A:C5'	2.06	0.84
22:W:14:THR:HB	22:W:23:ARG:O	1.78	0.84
1:A:89:C:O2'	1:A:90:U:C5'	2.24	0.84
1:A:224:C:OP1	20:T:74:LYS:CE	2.26	0.84
1:A:1081:G:OP1	5:E:16:THR:CG2	2.24	0.84
1:A:1232:U:H5''	9:I:124:GLN:NE2	1.93	0.84
11:K:91:ARG:NH1	18:R:88:LYS:HZ1	1.71	0.84
2:B:129:GLU:O	2:B:130:ARG:HB2	1.75	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:A:H2'	1:A:947:G:C8	2.14	0.83
1:A:1314:C:OP2	19:S:6:LYS:HB3	1.76	0.83
18:R:53:ARG:HH21	18:R:60:ALA:HB2	1.42	0.83
1:A:1513:A:H2'	1:A:1514:C:C6	2.14	0.82
15:O:65:ARG:HH11	15:O:65:ARG:HG2	1.43	0.82
1:A:829:G:C4'	2:B:26:PRO:HG3	2.10	0.82
1:A:829:G:H4'	2:B:26:PRO:HG3	1.61	0.82
1:A:563:A:N1	1:A:884:U:O4	2.13	0.82
1:A:1218:C:H2'	1:A:1219:U:C6	2.15	0.82
1:A:1358:U:C2	1:A:1363(A):A:N6	2.48	0.82
2:B:28:PHE:O	2:B:30:ARG:HG3	1.80	0.81
22:W:21:THR:O	22:W:22:PHE:CD1	2.32	0.81
3:C:14:ILE:HD13	3:C:14:ILE:H	1.45	0.81
1:A:981:U:C4'	14:N:21:TYR:HE2	1.93	0.81
2:B:8:LYS:O	2:B:9:GLU:HB2	1.79	0.80
9:I:42:ARG:NH2	9:I:71:SER:CB	2.44	0.80
3:C:12:LEU:CD2	3:C:18:TRP:NE1	2.45	0.80
11:K:91:ARG:HH12	18:R:88:LYS:HZ2	1.07	0.80
1:A:1232:U:H5''	9:I:124:GLN:HE21	1.46	0.80
1:A:1152:A:OP1	10:J:70:ARG:NH2	2.14	0.79
3:C:64:VAL:HB	3:C:99:VAL:HG23	1.63	0.79
2:B:24:TRP:HB2	2:B:190:THR:OG1	1.81	0.79
1:A:814:A:O2'	1:A:815:A:H3'	1.82	0.79
1:A:79:G:H2'	1:A:80:G:C8	2.13	0.79
4:D:35:ARG:CB	4:D:35:ARG:HH11	1.95	0.79
4:D:35:ARG:HH11	4:D:35:ARG:HB3	1.47	0.79
9:I:42:ARG:HH21	9:I:71:SER:HB2	1.47	0.78
1:A:224:C:OP1	20:T:74:LYS:HE3	1.82	0.78
22:W:21:THR:C	22:W:22:PHE:HD1	1.87	0.78
1:A:961:U:H3	1:A:1201:A:H61	0.79	0.77
1:A:745:C:H2'	1:A:746:A:C8	2.19	0.77
1:A:674:G:H2'	1:A:675:A:H8	1.48	0.77
2:B:25:ASN:HD21	2:B:27:LYS:HB3	1.50	0.77
1:A:658:G:C2	1:A:749:C:N3	2.53	0.77
1:A:1287:A:H2'	1:A:1288:A:C8	2.20	0.77
2:B:16:HIS:NE2	2:B:214:ILE:HD11	1.99	0.77
1:A:972:C:O3'	10:J:57:LYS:HG3	1.83	0.77
5:E:40:ARG:HG2	5:E:40:ARG:HH11	1.50	0.77
23:X:88:ILE:HD13	23:X:106:ILE:HG12	1.65	0.77
11:K:91:ARG:NH1	18:R:88:LYS:CE	2.43	0.77
11:K:91:ARG:HH11	18:R:88:LYS:NZ	1.76	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:A:N6	1:A:884:U:N3	1.91	0.76
1:A:1391:U:H2'	1:A:1392:G:C8	2.20	0.76
1:A:1111:A:N1	3:C:177:THR:HG22	2.01	0.76
10:J:38:ILE:O	10:J:71:LEU:N	2.15	0.76
5:E:127:ASN:HB3	5:E:130:ASN:HB2	1.65	0.76
10:J:6:ILE:HD11	10:J:23:ILE:HG21	1.68	0.76
5:E:15:ARG:CG	5:E:28:PHE:CD1	2.59	0.75
11:K:91:ARG:HH11	18:R:88:LYS:HZ1	1.30	0.75
1:A:1151:A:O2'	1:A:1152:A:H8	1.68	0.75
1:A:1399:C:C2	1:A:1502:A:N6	2.54	0.75
1:A:370:C:C2	1:A:392:G:N2	2.54	0.75
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.20	0.75
3:C:30:ARG:NH1	14:N:35:ARG:O	2.20	0.75
9:I:117:HIS:HE1	9:I:123:PRO:HB3	1.49	0.75
11:K:91:ARG:HH12	18:R:88:LYS:HE3	1.50	0.75
1:A:89:C:C2	1:A:90:U:C6	2.74	0.75
1:A:253:U:H2'	1:A:254:G:C8	2.21	0.75
22:W:23:ARG:HH21	22:W:33:LEU:HD23	1.51	0.75
1:A:715:A:H2'	1:A:716:A:C8	2.21	0.74
3:C:8:ILE:HG23	3:C:16:ARG:HE	1.51	0.74
1:A:677:U:H3	1:A:713:G:H22	1.33	0.74
2:B:21:ARG:HD3	2:B:21:ARG:H	1.52	0.74
1:A:528:C:H3'	1:A:529:G:H5''	1.69	0.74
5:E:15:ARG:CD	5:E:28:PHE:CE1	2.70	0.74
1:A:1349:A:P	9:I:118:LYS:HD3	2.27	0.74
3:C:12:LEU:CD2	3:C:18:TRP:CD1	2.71	0.74
9:I:42:ARG:NH2	9:I:71:SER:HA	2.01	0.74
2:B:25:ASN:HD21	2:B:27:LYS:CB	2.01	0.74
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.70	0.74
1:A:568:G:N2	1:A:883:C:C2	2.56	0.74
3:C:14:ILE:HD13	3:C:14:ILE:N	2.02	0.73
2:B:28:PHE:C	2:B:30:ARG:H	1.92	0.73
1:A:1099:G:C6	1:A:1100:C:N3	2.57	0.73
7:G:75:VAL:HG21	7:G:144:MET:HB3	1.69	0.73
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.68	0.73
22:W:53:VAL:HG12	22:W:71:LYS:HA	1.69	0.73
1:A:1225:A:H2'	1:A:1226:C:C6	2.23	0.73
17:Q:98:LEU:HD23	17:Q:98:LEU:H	1.53	0.73
1:A:30:U:H3'	1:A:31:G:H5''	1.68	0.73
23:X:102:LYS:O	23:X:106:ILE:HG13	1.87	0.73
1:A:312:C:H2'	1:A:313:A:C8	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:40:LEU:O	9:I:40:LEU:HD12	1.88	0.72
1:A:765:G:C6	1:A:812:C:N3	2.57	0.72
1:A:1391:U:H2'	1:A:1392:G:H8	1.54	0.72
14:N:24:CYS:HB3	14:N:29:ARG:H	1.54	0.72
18:R:37:VAL:HG21	18:R:78:LEU:HB3	1.70	0.72
1:A:1080:A:C4'	5:E:16:THR:OG1	2.35	0.72
3:C:58:GLU:HB2	3:C:65:ALA:HB3	1.71	0.72
10:J:50:ILE:HD11	10:J:60:ARG:NH1	2.04	0.72
22:W:32:ILE:HB	22:W:63:THR:O	1.88	0.72
1:A:19:C:H2'	1:A:20:U:H6	1.54	0.72
1:A:73:G:H1	1:A:96:U:H3	1.38	0.72
1:A:559:A:H4'	1:A:560:U:O5'	1.88	0.72
11:K:62:GLN:HG2	11:K:97:ALA:HB2	1.71	0.72
1:A:222:U:H2'	1:A:223:U:H6	1.52	0.72
1:A:113:G:H1'	1:A:354:G:H5'	1.71	0.72
1:A:195:A:H4'	20:T:68:LYS:HD3	1.72	0.72
11:K:25:TYR:HE1	24:Y:29:G:H5''	1.53	0.72
14:N:23:ARG:HG3	14:N:30:ALA:HA	1.72	0.72
22:W:45:ILE:HD13	22:W:70:ARG:HB3	1.70	0.72
1:A:91:C:H3'	1:A:91:C:C6	2.25	0.71
1:A:1264:C:H2'	1:A:1265:G:H8	1.55	0.71
5:E:76:ILE:HD12	5:E:118:ILE:HG21	1.71	0.71
23:X:106:ILE:HG23	23:X:116:VAL:HG11	1.73	0.71
9:I:117:HIS:CE1	9:I:123:PRO:HB3	2.24	0.71
23:X:94:ILE:CG2	23:X:98:ASP:OD2	2.39	0.71
2:B:223:ILE:HG21	2:B:230:VAL:HB	1.73	0.71
1:A:1305:G:HO2'	1:A:1306:A:H8	1.37	0.71
1:A:1349:A:H5''	9:I:121:ARG:HB2	1.73	0.71
10:J:38:ILE:HG23	10:J:71:LEU:HB3	1.73	0.71
1:A:961:U:O2	1:A:983:A:H2'	1.90	0.70
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.73	0.70
1:A:486:U:H2'	1:A:487:A:H8	1.55	0.70
1:A:1281:U:H4'	1:A:1282:C:OP2	1.91	0.70
1:A:253:U:H2'	1:A:254:G:H8	1.56	0.70
1:A:501:C:H2'	1:A:502:G:H8	1.55	0.70
3:C:12:LEU:HD11	14:N:51:GLY:HA3	1.73	0.70
8:H:17:THR:HG21	8:H:80:ILE:HD13	1.72	0.70
1:A:89:C:H2'	1:A:90:U:C5'	2.15	0.70
9:I:116:LYS:HB3	9:I:122:ALA:HA	1.73	0.70
1:A:1192:C:H2'	1:A:1193:G:O4'	1.92	0.70
23:X:130:PRO:O	23:X:134:GLU:CB	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:C:H2'	1:A:399:G:H8	1.55	0.70
16:P:38:TYR:CE2	16:P:50:LYS:HB3	2.27	0.70
1:A:434:U:H2'	1:A:435:C:C6	2.26	0.69
19:S:72:GLY:O	19:S:74:PHE:N	2.25	0.69
1:A:38:G:H22	1:A:397:A:H5'	1.56	0.69
1:A:1244:C:H2'	1:A:1245:A:H8	1.57	0.69
3:C:28:GLN:OE1	3:C:28:GLN:N	2.24	0.69
9:I:42:ARG:HH21	9:I:71:SER:CB	2.03	0.69
1:A:528:C:H41	12:L:49:ASN:HD22	1.39	0.69
2:B:112:VAL:HG23	2:B:149:LEU:HD13	1.74	0.69
22:W:32:ILE:HD13	22:W:32:ILE:N	2.06	0.69
1:A:501:C:H2'	1:A:502:G:C8	2.28	0.69
3:C:131:ARG:HH11	3:C:131:ARG:HG2	1.57	0.69
10:J:61:GLU:OE1	14:N:49:HIS:CE1	2.45	0.69
12:L:53:ARG:HG2	12:L:53:ARG:NH1	2.05	0.69
23:X:94:ILE:HG23	23:X:98:ASP:CG	2.13	0.69
2:B:129:GLU:O	2:B:130:ARG:CB	2.41	0.69
10:J:61:GLU:OE1	14:N:49:HIS:NE2	2.26	0.69
14:N:9:LYS:HE3	14:N:21:TYR:O	1.92	0.69
3:C:7:PRO:CA	3:C:11:ARG:HH21	2.06	0.69
1:A:872:A:O2'	1:A:873:A:H3'	1.93	0.68
2:B:16:HIS:HE2	2:B:214:ILE:HD11	1.57	0.68
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.74	0.68
1:A:1373:G:H5''	7:G:36:LYS:HB2	1.76	0.68
9:I:42:ARG:NH2	9:I:71:SER:CA	2.56	0.68
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.75	0.68
1:A:678:U:H2'	1:A:679:C:C6	2.28	0.68
1:A:917:G:H2'	1:A:918:A:C8	2.29	0.68
1:A:924:C:H4'	1:A:1399:C:OP2	1.93	0.68
3:C:12:LEU:HD23	3:C:18:TRP:CE2	2.27	0.68
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.76	0.68
1:A:335:C:H2'	1:A:336:C:C6	2.29	0.68
1:A:961:U:C2	1:A:1201:A:N6	2.55	0.68
7:G:37:ASN:ND2	9:I:40:LEU:CD1	2.55	0.68
17:Q:63:ARG:HG3	17:Q:63:ARG:NH1	2.01	0.67
19:S:71:LEU:HD23	19:S:71:LEU:C	2.14	0.67
1:A:955:U:H2'	1:A:956:U:H6	1.59	0.67
3:C:7:PRO:HA	3:C:11:ARG:NH2	2.09	0.67
1:A:1127:G:N2	1:A:1145:C:C2	2.62	0.67
1:A:992:U:H4'	1:A:993:G:O5'	1.95	0.67
1:A:1347:G:C8	9:I:107:ARG:HB3	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:U:H4'	1:A:871:U:H5''	1.77	0.67
1:A:891:U:H2'	1:A:892:A:H8	1.60	0.67
1:A:1392:G:N2	1:A:1502:A:H8	1.93	0.67
1:A:227:G:N2	16:P:62:VAL:O	2.24	0.67
1:A:674:G:H2'	1:A:675:A:C8	2.29	0.66
1:A:618:C:H5''	1:A:619:U:H5''	1.76	0.66
1:A:1314:C:H2'	1:A:1315:U:C6	2.31	0.66
17:Q:65:ILE:O	17:Q:66:SER:HB2	1.95	0.66
1:A:946:A:H8	1:A:946:A:H5'	1.59	0.66
2:B:74:LYS:HD2	2:B:169:LYS:HD2	1.76	0.66
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.78	0.66
20:T:15:ARG:HG2	20:T:15:ARG:NH1	2.11	0.66
1:A:829:G:C4'	2:B:26:PRO:CG	2.73	0.66
21:V:3:LYS:O	21:V:11:GLY:HA2	1.95	0.66
1:A:312:C:H2'	1:A:313:A:H8	1.58	0.66
1:A:1249:C:H4'	9:I:73:GLN:HE22	1.61	0.66
1:A:636:U:H5'	17:Q:2:PRO:HG3	1.78	0.65
1:A:20:U:H2'	1:A:21:G:O4'	1.96	0.65
1:A:123:C:H5''	1:A:311:C:O2'	1.96	0.65
1:A:247:G:OP2	17:Q:100:LYS:HB2	1.96	0.65
1:A:1227:A:H1'	13:M:117:VAL:HB	1.77	0.65
5:E:33:VAL:HG13	5:E:112:LEU:HD22	1.78	0.65
6:F:48:LEU:HD22	6:F:52:ILE:HD12	1.78	0.65
7:G:49:ILE:HD13	7:G:118:VAL:HA	1.77	0.65
9:I:17:VAL:HG22	9:I:63:ILE:HG12	1.78	0.65
1:A:89:C:C3'	1:A:90:U:H5'	2.26	0.65
1:A:792:A:H4'	1:A:793:U:C5'	2.26	0.65
1:A:1349:A:OP1	9:I:118:LYS:HB3	1.96	0.65
2:B:15:VAL:O	2:B:204:ASN:OD1	2.14	0.65
22:W:40:MET:HA	22:W:45:ILE:HD12	1.78	0.65
1:A:575:G:H4'	1:A:576:G:H5''	1.78	0.65
1:A:1187:G:H21	14:N:60:SER:HB3	1.61	0.65
1:A:333:G:N2	1:A:334:C:C2	2.64	0.65
1:A:757:U:H2'	1:A:758:G:O4'	1.95	0.65
1:A:829:G:C1'	2:B:26:PRO:HG2	2.26	0.65
1:A:1196:U:H5'	1:A:1197:G:H5'	1.79	0.65
1:A:1371:G:P	9:I:12:GLU:CB	2.77	0.65
1:A:1126:U:O2	1:A:1126:U:H2'	1.96	0.65
9:I:42:ARG:HH22	9:I:71:SER:HA	1.60	0.65
16:P:20:VAL:HG23	16:P:35:LYS:HA	1.78	0.65
22:W:14:THR:CB	22:W:23:ARG:O	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:U:H3'	4:D:5:ILE:HD11	1.79	0.65
1:A:524:G:C6	1:A:525:C:N4	2.65	0.65
4:D:8:VAL:CG1	4:D:21:LEU:HB2	2.27	0.65
4:D:78:LEU:HG	4:D:96:LEU:HD23	1.79	0.65
1:A:570:G:C6	1:A:873:A:C2	2.86	0.64
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.80	0.64
1:A:765:G:N2	1:A:813:U:OP2	2.30	0.64
2:B:24:TRP:CD1	2:B:40:HIS:HE1	2.11	0.64
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.79	0.64
10:J:37:PRO:HA	10:J:72:VAL:CG2	2.27	0.64
1:A:827:U:O4	1:A:872:A:N1	2.30	0.64
1:A:877:C:OP1	8:H:88:LYS:HD3	1.97	0.64
1:A:148:G:H2'	1:A:149:A:C8	2.32	0.64
1:A:344:A:H4'	1:A:345:C:OP2	1.96	0.64
1:A:532:A:N6	3:C:193:TYR:HB3	2.12	0.64
1:A:617:G:N1	1:A:618:C:C4	2.65	0.64
1:A:676:A:H2'	1:A:677:U:C6	2.32	0.64
3:C:153:VAL:HG22	3:C:198:VAL:HG13	1.78	0.64
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.79	0.64
1:A:576:G:H3'	1:A:577:G:H5''	1.80	0.64
1:A:46:G:H2'	1:A:366:C:C5	2.32	0.64
1:A:658:G:C2	1:A:749:C:C2	2.86	0.64
1:A:93:G:C5'	1:A:96:U:OP2	2.36	0.63
1:A:1458:G:OP1	20:T:35:THR:CB	2.46	0.63
3:C:7:PRO:HA	3:C:11:ARG:HH21	1.63	0.63
1:A:61:G:H2'	1:A:62:U:O4'	1.98	0.63
1:A:1081:G:P	5:E:16:THR:HG21	2.36	0.63
3:C:124:ILE:HG21	3:C:196:LEU:HD22	1.79	0.63
4:D:170:VAL:HG22	4:D:171:GLY:H	1.64	0.63
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.80	0.63
12:L:32:PHE:HB3	12:L:84:LEU:HD11	1.81	0.63
1:A:56:U:H2'	1:A:57:G:C8	2.33	0.63
1:A:293:G:C4	1:A:305:G:N2	2.67	0.63
1:A:1049:U:H4'	1:A:1050:G:OP2	1.99	0.63
4:D:101:LEU:O	4:D:104:VAL:HG12	1.98	0.63
1:A:398:C:H2'	1:A:399:G:C8	2.33	0.63
1:A:296:U:H2'	1:A:297:G:C8	2.33	0.63
10:J:37:PRO:HA	10:J:72:VAL:HG23	1.79	0.63
11:K:115:PRO:HB2	11:K:118:GLY:H	1.63	0.63
1:A:651:C:H2'	1:A:652:U:C6	2.34	0.63
1:A:669:U:H2'	1:A:670:G:C8	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1358:U:O4	1:A:1363(A):A:N1	2.32	0.63
2:B:130:ARG:HA	2:B:130:ARG:HE	1.64	0.63
23:X:47:LEU:HD12	23:X:57:ALA:HB2	1.80	0.63
1:A:928:G:H1	1:A:1389:C:H42	1.45	0.63
2:B:24:TRP:NE1	2:B:40:HIS:CE1	2.66	0.63
12:L:54:LYS:HG2	12:L:75:HIS:HE1	1.64	0.63
14:N:9:LYS:HG3	14:N:21:TYR:CD1	2.34	0.63
1:A:1278:U:H5''	1:A:1279:A:O4'	1.99	0.63
2:B:8:LYS:O	2:B:9:GLU:CB	2.47	0.63
4:D:162:LEU:HD12	4:D:178:VAL:HG23	1.79	0.63
1:A:10:A:H2'	1:A:11:G:H8	1.63	0.62
1:A:513:C:H2'	1:A:514:C:C6	2.35	0.62
1:A:1116:C:H2'	1:A:1117:G:H5''	1.82	0.62
2:B:187:LEU:HD13	2:B:205:ASP:HA	1.81	0.62
9:I:42:ARG:HH22	9:I:71:SER:CA	2.12	0.62
3:C:116:VAL:O	3:C:120:VAL:HG23	2.00	0.62
1:A:501:C:OP1	12:L:117:ARG:NH2	2.31	0.62
1:A:613:C:H2'	1:A:614:A:C8	2.35	0.62
1:A:1251:A:H2'	1:A:1252:A:O4'	1.99	0.62
9:I:116:LYS:HA	9:I:123:PRO:HD3	1.82	0.62
1:A:354:G:N2	1:A:355:C:C2	2.68	0.62
1:A:1001:A:OP2	1:A:1001:A:H8	1.81	0.62
1:A:1477:C:H2'	1:A:1478:C:C6	2.35	0.62
15:O:65:ARG:HH11	15:O:65:ARG:CG	2.12	0.62
1:A:56:U:H2'	1:A:57:G:H8	1.65	0.62
1:A:955:U:H1'	1:A:1227:A:N6	2.15	0.62
1:A:1015:A:H2'	1:A:1016:A:C8	2.35	0.62
1:A:1312:G:C2	1:A:1326:C:C2	2.88	0.62
1:A:89:C:H2'	1:A:90:U:H6	1.65	0.61
1:A:324:G:N2	1:A:326:G:H3'	2.14	0.61
2:B:61:LEU:HD23	2:B:161:ALA:HB2	1.82	0.61
1:A:528:C:H41	12:L:49:ASN:ND2	1.98	0.61
1:A:568:G:C2	1:A:883:C:N3	2.68	0.61
1:A:1394:A:H8	1:A:1394:A:OP1	1.83	0.61
4:D:70:ILE:HD11	4:D:97:LEU:HD21	1.81	0.61
17:Q:45:HIS:HB2	17:Q:65:ILE:HD13	1.81	0.61
18:R:53:ARG:HH21	18:R:60:ALA:CB	2.13	0.61
2:B:12:GLU:CD	2:B:12:GLU:H	1.98	0.61
1:A:1263:C:H2'	1:A:1264:C:C6	2.35	0.61
4:D:3:ARG:HA	4:D:3:ARG:CZ	2.30	0.61
16:P:39:TYR:CD1	16:P:73:LEU:HD21	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:C:H5''	20:T:75:ASN:HD22	1.66	0.61
1:A:322:C:H2'	1:A:323:U:H6	1.64	0.61
1:A:1521:G:H2'	1:A:1522:U:C6	2.34	0.61
1:A:80:G:H3'	1:A:81:U:C5'	2.26	0.61
1:A:891:U:H2'	1:A:892:A:C8	2.36	0.61
2:B:158:LEU:HD23	2:B:159:PRO:HD2	1.82	0.61
12:L:113:ARG:HH11	12:L:113:ARG:HB3	1.65	0.61
1:A:1323:G:H2'	1:A:1324:A:C8	2.36	0.61
1:A:1431:C:C2	1:A:1470:G:N2	2.69	0.61
1:A:1493:A:H4'	1:A:1494:G:OP1	2.01	0.61
1:A:728:A:H2'	1:A:729:A:C8	2.36	0.61
1:A:923:A:H2'	1:A:924:C:O4'	2.00	0.61
1:A:630:G:H2'	1:A:631:G:O4'	2.00	0.60
1:A:765:G:C2	1:A:812:C:O2	2.54	0.60
1:A:1371:G:OP1	9:I:12:GLU:HB3	1.92	0.60
2:B:25:ASN:ND2	2:B:27:LYS:HB3	2.15	0.60
19:S:49:ILE:CG2	19:S:71:LEU:HD11	2.31	0.60
1:A:321:A:H2'	1:A:322:C:C6	2.36	0.60
1:A:769:G:H4'	1:A:1513:A:H4'	1.83	0.60
1:A:1264:C:H2'	1:A:1265:G:C8	2.36	0.60
2:B:130:ARG:HE	2:B:130:ARG:CA	2.14	0.60
2:B:130:ARG:HB3	2:B:131:PRO:HD2	1.82	0.60
5:E:11:ILE:HG21	5:E:105:VAL:HG13	1.81	0.60
22:W:12:VAL:O	22:W:24:VAL:HG13	2.01	0.60
1:A:1081:G:OP2	5:E:16:THR:HG21	2.01	0.60
8:H:34:GLU:HG2	8:H:37:ARG:HH21	1.65	0.60
22:W:23:ARG:HH11	22:W:23:ARG:CG	2.14	0.60
1:A:404:U:H5'	4:D:122:ARG:HD2	1.82	0.60
20:T:44:ALA:HB1	20:T:91:LEU:HB2	1.83	0.60
1:A:235:C:O2'	1:A:236:G:H5'	2.01	0.60
1:A:446:G:N2	1:A:489:C:C2	2.70	0.60
10:J:38:ILE:HG22	10:J:71:LEU:O	1.98	0.60
1:A:518:C:H2'	1:A:530:G:C8	2.36	0.60
1:A:736:C:H2'	1:A:737:A:C8	2.37	0.60
9:I:113:LYS:NZ	9:I:119:ALA:O	2.28	0.60
18:R:53:ARG:NH2	18:R:60:ALA:HB2	2.13	0.60
23:X:115:LYS:HB3	23:X:164:LEU:HD21	1.83	0.60
3:C:96:GLY:C	3:C:97:LYS:HG2	2.23	0.60
1:A:1128:C:H1'	1:A:1146:A:N6	2.15	0.59
4:D:166:LYS:HG3	4:D:178:VAL:HG21	1.84	0.59
8:H:41:ARG:HB3	8:H:41:ARG:HH11	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:C:H2'	1:A:1438:G:H8	1.67	0.59
20:T:67:ALA:HB1	20:T:74:LYS:HG2	1.85	0.59
24:Y:27:G:H2'	24:Y:28:A:O4'	2.02	0.59
1:A:975:A:C8	1:A:975:A:H5'	2.37	0.59
1:A:1346:A:C8	1:A:1348:U:C2	2.91	0.59
1:A:1502:A:H2'	1:A:1504:G:C8	2.37	0.59
2:B:28:PHE:HA	2:B:194:PRO:HG3	1.83	0.59
1:A:524:G:H2'	1:A:525:C:C6	2.37	0.59
1:A:1542:U:H5'	18:R:19:LYS:HB3	1.84	0.59
1:A:91:C:C6	1:A:91:C:C3'	2.86	0.59
1:A:296:U:H2'	1:A:297:G:H8	1.67	0.59
1:A:588:G:N2	1:A:589:C:C2	2.69	0.59
1:A:1182:G:H4'	1:A:1183:A:H5''	1.85	0.59
2:B:28:PHE:C	2:B:30:ARG:N	2.49	0.59
23:X:94:ILE:HG23	23:X:98:ASP:OD1	2.01	0.59
1:A:392:G:H2'	1:A:393:A:H8	1.66	0.59
1:A:444:C:C2	1:A:491:G:N2	2.71	0.59
1:A:1000:U:C6	1:A:1000:U:H3'	2.38	0.59
1:A:1225:A:H2'	1:A:1226:C:C5	2.38	0.59
1:A:1536:C:H42	24:Y:29:G:H1	1.51	0.59
1:A:78:G:H8	1:A:78:G:OP2	1.86	0.59
1:A:328:C:H4'	1:A:329:A:C5'	2.33	0.59
1:A:1082:G:H2'	1:A:1083:U:O4'	2.02	0.59
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.37	0.59
17:Q:85:VAL:HG12	17:Q:89:LEU:HD12	1.82	0.59
20:T:73:HIS:O	20:T:77:ALA:N	2.22	0.59
1:A:224:C:OP1	20:T:74:LYS:HE2	2.00	0.59
1:A:518:C:H5''	1:A:519:C:C6	2.38	0.59
7:G:37:ASN:CG	9:I:40:LEU:O	2.40	0.59
1:A:1372:U:H5''	9:I:71:SER:HB3	1.83	0.58
4:D:8:VAL:HG11	4:D:21:LEU:CB	2.32	0.58
11:K:99:GLN:HG2	11:K:105:VAL:HG21	1.85	0.58
1:A:216:G:C6	1:A:217:C:N4	2.72	0.58
1:A:688:G:H2'	1:A:689:C:O4'	2.02	0.58
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.85	0.58
1:A:658:G:N2	1:A:749:C:C2	2.71	0.58
1:A:916:G:H2'	1:A:917:G:H8	1.67	0.58
1:A:1507:A:H5''	1:A:1507:A:H8	1.69	0.58
18:R:34:TYR:HB3	18:R:69:THR:HG22	1.85	0.58
1:A:1065:U:H4'	1:A:1066:C:O5'	2.03	0.58
1:A:1443:G:C6	1:A:1444:C:N4	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:VAL:CG1	3:C:196:LEU:HD23	2.34	0.58
2:B:25:ASN:ND2	2:B:27:LYS:N	2.51	0.58
9:I:51:ARG:HG2	9:I:56:LEU:HD11	1.85	0.58
1:A:309:G:H2'	1:A:310:G:H8	1.67	0.58
1:A:645:C:H2'	1:A:646:U:O4'	2.04	0.58
1:A:664:G:N2	1:A:741:G:H1	1.89	0.58
1:A:715:A:H2'	1:A:716:A:H8	1.65	0.58
10:J:7:LYS:HB3	10:J:97:GLU:HB2	1.84	0.58
1:A:718:G:H5'	11:K:117:ASN:HB2	1.86	0.58
1:A:1305:G:H5'	21:V:4:GLY:C	2.24	0.58
1:A:446:G:C2	1:A:489:C:N3	2.72	0.58
1:A:1164:G:H1	1:A:1172:C:H42	1.51	0.58
12:L:36:VAL:HG22	12:L:82:VAL:HG23	1.86	0.58
1:A:1091:U:O2	1:A:1093:A:C8	2.57	0.58
1:A:1308:U:H2'	1:A:1309:G:C8	2.39	0.58
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.86	0.58
5:E:15:ARG:HD3	5:E:28:PHE:CE1	2.39	0.58
5:E:127:ASN:O	5:E:131:ILE:HB	2.04	0.58
9:I:5:TYR:CE2	9:I:7:THR:OG1	2.57	0.58
14:N:9:LYS:HG3	14:N:21:TYR:O	2.03	0.58
1:A:93:G:H5''	1:A:96:U:P	2.42	0.57
1:A:262:A:H5''	20:T:76:ALA:HB2	1.85	0.57
1:A:1161:C:H2'	1:A:1162:C:C6	2.39	0.57
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.86	0.57
3:C:39:ILE:HG23	3:C:91:LEU:HD11	1.86	0.57
1:A:474:G:H2'	1:A:475:G:C8	2.40	0.57
1:A:737:A:H2'	1:A:738:C:C6	2.39	0.57
1:A:977:A:H1'	1:A:982:U:O4	2.03	0.57
1:A:1217:C:N4	1:A:1218:C:N4	2.53	0.57
19:S:71:LEU:HD23	19:S:71:LEU:O	2.04	0.57
1:A:97:G:H2'	1:A:98:G:O4'	2.05	0.57
1:A:1119:C:H42	1:A:1154:G:H1	1.53	0.57
1:A:172:A:H2'	1:A:174:C:H5	1.69	0.57
1:A:794:A:H2'	1:A:795:C:C6	2.39	0.57
12:L:89:ARG:HA	12:L:97:ARG:HA	1.85	0.57
1:A:142:G:O2'	1:A:196:A:N1	2.37	0.57
1:A:828:A:H4'	1:A:828:A:OP1	2.03	0.57
1:A:1365:G:C6	1:A:1366:C:C4	2.93	0.57
1:A:1497:G:OP2	23:X:91:ARG:NH1	2.37	0.57
1:A:1536:C:N4	24:Y:29:G:H1	2.02	0.57
2:B:24:TRP:CG	2:B:40:HIS:CE1	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:23:ILE:HG23	10:J:85:LEU:HD22	1.86	0.57
14:N:21:TYR:HD1	14:N:21:TYR:H	1.53	0.57
1:A:624:C:H2'	1:A:625:G:H8	1.70	0.57
1:A:998:G:N2	1:A:999:C:C2	2.72	0.57
2:B:51:LEU:HA	2:B:201:ILE:HG12	1.87	0.57
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.85	0.57
14:N:9:LYS:CE	14:N:21:TYR:O	2.52	0.57
4:D:56:VAL:HG12	4:D:202:LEU:HD21	1.86	0.57
13:M:22:ILE:HG22	13:M:24:GLY:H	1.69	0.57
1:A:443:C:C2	1:A:492:G:C2	2.92	0.57
1:A:491:G:C4	1:A:492:G:C8	2.93	0.57
1:A:701:C:H4'	1:A:702:A:O5'	2.04	0.57
1:A:765:G:C5	1:A:812:C:N3	2.73	0.57
1:A:864:A:H2'	1:A:865:A:C8	2.39	0.57
1:A:981:U:C5'	14:N:21:TYR:HE2	2.17	0.57
1:A:1244:C:H2'	1:A:1245:A:C8	2.40	0.57
2:B:12:GLU:HG3	2:B:16:HIS:CB	2.34	0.57
10:J:32:ALA:HB2	10:J:76:ASN:HB2	1.87	0.57
1:A:1048:G:H1	1:A:1209:C:H42	1.53	0.56
1:A:1384:C:H2'	1:A:1385:G:C8	2.40	0.56
6:F:9:VAL:HB	6:F:87:ARG:HB3	1.87	0.56
1:A:988:G:N1	1:A:989:C:C2	2.73	0.56
11:K:91:ARG:CZ	18:R:88:LYS:HZ2	2.10	0.56
17:Q:28:PRO:HA	17:Q:35:VAL:HA	1.87	0.56
1:A:392:G:H2'	1:A:393:A:C8	2.40	0.56
1:A:428:G:H4'	1:A:429:U:O5'	2.05	0.56
1:A:751:U:C5	1:A:752:G:C5	2.93	0.56
1:A:939:G:H2'	1:A:940:C:C6	2.41	0.56
1:A:1232:U:P	9:I:124:GLN:HE22	2.28	0.56
1:A:1232:U:C5'	9:I:124:GLN:NE2	2.68	0.56
1:A:1488:G:H2'	1:A:1489:G:H8	1.70	0.56
1:A:1509:C:H2'	1:A:1510:U:O4'	2.06	0.56
4:D:64:LEU:HD12	4:D:203:VAL:HG21	1.87	0.56
9:I:19:LEU:HD12	9:I:84:ALA:HB3	1.88	0.56
22:W:23:ARG:HG3	22:W:23:ARG:NH1	2.20	0.56
1:A:291:C:O2	1:A:310:G:C2	2.59	0.56
1:A:945:G:H2'	1:A:945:G:N3	2.20	0.56
1:A:1402:C:H2'	1:A:1403:C:O4'	2.06	0.56
4:D:29:PRO:O	4:D:35:ARG:CD	2.48	0.56
12:L:33:ARG:HB3	12:L:60:LEU:HD12	1.86	0.56
14:N:21:TYR:CD1	14:N:21:TYR:N	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:G:N2	1:A:90:U:H1'	2.21	0.56
1:A:89:C:C4	1:A:90:U:C5	2.94	0.56
1:A:171:A:H2'	1:A:172:A:C8	2.41	0.56
3:C:8:ILE:O	3:C:12:LEU:N	2.38	0.56
1:A:30:U:H3'	1:A:31:G:C5'	2.36	0.56
1:A:76:C:H2'	1:A:77:G:C8	2.41	0.56
1:A:621:A:H2'	1:A:622:A:C8	2.41	0.56
1:A:946:A:H5'	1:A:946:A:C8	2.39	0.56
1:A:1466:C:H2'	1:A:1467:G:O4'	2.06	0.56
3:C:12:LEU:CD2	3:C:18:TRP:CE2	2.87	0.56
20:T:44:ALA:HB1	20:T:91:LEU:CB	2.36	0.56
1:A:82:U:H2'	1:A:83:U:O4'	2.05	0.56
1:A:424:G:H8	1:A:424:G:O5'	1.89	0.56
9:I:8:GLY:HA3	9:I:76:ALA:O	2.05	0.56
1:A:745:C:H2'	1:A:746:A:H8	1.69	0.56
22:W:23:ARG:NE	22:W:33:LEU:HD22	2.11	0.56
5:E:76:ILE:CD1	5:E:118:ILE:HG21	2.36	0.56
15:O:41:GLU:O	15:O:44:LYS:HB2	2.05	0.56
1:A:174:C:H2'	1:A:175:C:C6	2.40	0.55
1:A:1382:C:H2'	1:A:1383:C:H6	1.71	0.55
1:A:1434:A:H2'	1:A:1435:G:O4'	2.06	0.55
1:A:266:G:H5''	1:A:266:G:H8	1.71	0.55
1:A:707:C:H4'	11:K:20:TYR:CD2	2.41	0.55
3:C:8:ILE:HG23	3:C:16:ARG:NE	2.21	0.55
1:A:1239:A:H62	1:A:1299:A:N6	2.05	0.55
4:D:62:GLN:O	4:D:66:ARG:HD2	2.07	0.55
14:N:9:LYS:CD	14:N:21:TYR:O	2.55	0.55
1:A:107:G:C2	1:A:108:G:H1'	2.41	0.55
1:A:269:C:H2'	1:A:270:A:H8	1.70	0.55
1:A:323:U:H5'	20:T:23:ARG:HB2	1.87	0.55
5:E:82:VAL:HG11	5:E:137:GLU:HB3	1.89	0.55
19:S:22:LEU:HD13	19:S:28:LYS:HB3	1.88	0.55
1:A:321:A:H2'	1:A:322:C:H6	1.70	0.55
1:A:657:G:H1	1:A:749:C:N4	2.04	0.55
1:A:1103:C:H5'	2:B:98:LEU:HD22	1.89	0.55
1:A:1459:C:H2'	1:A:1460:A:O4'	2.07	0.55
10:J:21:GLN:HA	10:J:24:VAL:HB	1.88	0.55
1:A:636:U:H2'	1:A:637:G:C8	2.42	0.55
1:A:1292:U:H2'	1:A:1293:G:C8	2.40	0.55
9:I:9:ARG:HG2	9:I:14:VAL:HG12	1.88	0.55
12:L:85:ILE:HA	12:L:99:HIS:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:ILE:HG22	3:C:12:LEU:HD12	1.89	0.55
1:A:589:C:O2	1:A:651:C:O2	2.25	0.55
1:A:790:A:C4	24:Y:36:A:N6	2.75	0.55
1:A:1144:G:N2	1:A:1146:A:H62	2.04	0.55
1:A:1386:G:H2'	1:A:1387:G:H8	1.72	0.55
2:B:24:TRP:CB	2:B:190:THR:OG1	2.53	0.55
6:F:3:ARG:HB3	6:F:93:SER:HB2	1.89	0.55
11:K:84:VAL:HG11	11:K:95:ILE:HD11	1.87	0.55
12:L:60:LEU:HB3	12:L:62:SER:H	1.71	0.55
1:A:734:G:C2	1:A:735:C:C2	2.94	0.54
1:A:1151:A:O2'	1:A:1152:A:C8	2.44	0.54
1:A:1464:G:N2	1:A:1465:C:C2	2.75	0.54
1:A:1513:A:H2'	1:A:1514:C:H6	1.67	0.54
1:A:70:G:C2	1:A:100:C:C2	2.95	0.54
1:A:269:C:H2'	1:A:270:A:C8	2.41	0.54
1:A:568:G:C2	1:A:883:C:C2	2.95	0.54
1:A:1093:A:O2'	1:A:1094:G:H3'	2.06	0.54
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.73	0.54
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.90	0.54
2:B:111:ARG:HD3	2:B:145:LEU:HD21	1.88	0.54
5:E:129:ILE:H	5:E:129:ILE:HD12	1.71	0.54
1:A:111:G:O6	1:A:330:C:N4	2.39	0.54
1:A:148:G:C2	1:A:175:C:C2	2.95	0.54
1:A:1326:C:H2'	1:A:1327:C:C6	2.42	0.54
1:A:19:C:H2'	1:A:20:U:C6	2.38	0.54
1:A:1354:C:H2'	1:A:1355:G:C8	2.43	0.54
1:A:1428:A:H2'	1:A:1429:C:C6	2.42	0.54
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.88	0.54
1:A:419:C:H42	1:A:424:G:H1	1.55	0.54
1:A:777:A:H2'	1:A:778:G:C8	2.42	0.54
1:A:826:C:H2'	1:A:827:U:C6	2.43	0.54
1:A:89:C:C2'	1:A:90:U:C5'	2.54	0.54
1:A:243:A:H4'	1:A:244:U:O5'	2.07	0.54
1:A:1320:C:N3	19:S:36:ARG:HD3	2.22	0.54
1:A:1349:A:P	9:I:118:LYS:CD	2.94	0.54
1:A:1475:G:H2'	1:A:1476:G:H8	1.72	0.54
2:B:129:GLU:O	2:B:130:ARG:HD2	2.08	0.54
11:K:32:ILE:HG21	11:K:72:ALA:HB2	1.90	0.54
1:A:109:A:C6	1:A:326:G:C6	2.96	0.54
1:A:452:A:HO2'	1:A:453:A:H8	1.54	0.54
1:A:624:C:H2'	1:A:625:G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:110:ASP:HB3	18:R:85:LEU:HB3	1.89	0.54
15:O:26:GLU:HA	15:O:81:LEU:HD21	1.89	0.54
23:X:17:ARG:HH22	23:X:25:GLN:HA	1.73	0.54
1:A:437:U:H2'	1:A:438:G:O4'	2.07	0.54
1:A:580:U:H5''	15:O:58:MET:HG3	1.89	0.54
1:A:1367:C:H2'	1:A:1368:G:O4'	2.08	0.54
5:E:15:ARG:NH2	5:E:26:PHE:CG	2.62	0.54
9:I:26:VAL:HG22	9:I:61:ALA:HB3	1.90	0.54
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.90	0.54
20:T:33:ILE:HG13	20:T:62:LEU:HB3	1.89	0.54
1:A:1161:C:H2'	1:A:1162:C:H6	1.72	0.54
1:A:1411:C:H2'	1:A:1412:C:O4'	2.08	0.54
5:E:76:ILE:O	5:E:93:PRO:HB3	2.07	0.54
12:L:27:LEU:HG	12:L:28:LYS:H	1.73	0.54
1:A:193:C:H2'	1:A:194:C:C6	2.43	0.54
1:A:568:G:N1	1:A:883:C:C4	2.76	0.54
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.43	0.54
24:Y:21:G:H2'	24:Y:22:G:H8	1.72	0.54
1:A:312:C:C2'	1:A:313:A:H8	2.20	0.53
1:A:337:C:H2'	1:A:338:A:C8	2.43	0.53
1:A:953:G:H2'	1:A:954:G:O4'	2.08	0.53
1:A:1328:C:H2'	1:A:1329:A:O4'	2.07	0.53
1:A:1438:G:N2	1:A:1439:C:C2	2.76	0.53
2:B:17:PHE:O	2:B:42:ILE:N	2.37	0.53
2:B:102:LEU:HB3	2:B:180:LEU:HD11	1.89	0.53
1:A:236:G:C6	1:A:237:C:N3	2.76	0.53
1:A:514:C:H2'	1:A:515:G:H8	1.73	0.53
1:A:567:G:H5'	1:A:567:G:H8	1.73	0.53
1:A:962:C:H1'	1:A:1201:A:N6	2.24	0.53
1:A:1004:A:H5''	1:A:1025:U:C5	2.43	0.53
1:A:1162:C:C2	1:A:1175:G:N2	2.77	0.53
23:X:85:VAL:HA	23:X:115:LYS:O	2.08	0.53
1:A:92:C:H2'	1:A:93:G:C8	2.43	0.53
1:A:225:C:H2'	1:A:226:G:H8	1.73	0.53
1:A:370:C:N3	1:A:392:G:C2	2.76	0.53
1:A:524:G:C2	1:A:525:C:N3	2.76	0.53
1:A:1352:C:H2'	1:A:1353:G:C8	2.43	0.53
7:G:62:PHE:HD1	7:G:124:LEU:HD21	1.72	0.53
17:Q:41:LYS:HE2	17:Q:88:TYR:HE1	1.74	0.53
1:A:865:A:H2'	1:A:866:C:C6	2.43	0.53
1:A:1239:A:H62	1:A:1299:A:H62	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:G:N2	1:A:1242:C:C2	2.77	0.53
4:D:33:MET:HB2	4:D:34:GLU:OE1	2.09	0.53
2:B:12:GLU:HG3	2:B:16:HIS:HB2	1.90	0.53
6:F:4:TYR:HB2	6:F:65:VAL:HG22	1.89	0.53
1:A:172:A:H2'	1:A:174:C:C5	2.42	0.53
1:A:1038:C:H2'	1:A:1039:C:H6	1.74	0.53
1:A:1172:C:H2'	1:A:1173:G:C8	2.44	0.53
1:A:1404:C:H2'	1:A:1405:G:C8	2.43	0.53
2:B:94:ASN:HD22	2:B:95:GLN:HG2	1.73	0.53
1:A:669:U:H2'	1:A:670:G:H8	1.73	0.53
1:A:1308:U:H2'	1:A:1309:G:H8	1.72	0.53
4:D:65:ARG:HB3	4:D:65:ARG:HH11	1.73	0.53
9:I:42:ARG:O	9:I:42:ARG:HG2	2.08	0.53
9:I:69:GLY:O	9:I:73:GLN:HG3	2.09	0.53
23:X:17:ARG:HH21	23:X:19:VAL:HG22	1.73	0.53
23:X:34:ALA:HB1	23:X:45:LEU:HD13	1.91	0.53
1:A:582:U:H2'	1:A:583:A:C8	2.44	0.53
1:A:1258:G:C6	1:A:1259:C:N4	2.77	0.53
3:C:114:PRO:HA	3:C:185:GLY:HA3	1.89	0.53
13:M:64:TRP:HE3	13:M:66:LEU:HD11	1.74	0.53
1:A:1172:C:H2'	1:A:1173:G:H8	1.74	0.53
1:A:1298:C:C4	7:G:114:ARG:HD2	2.44	0.53
2:B:28:PHE:CD2	2:B:190:THR:HA	2.44	0.53
11:K:15:ALA:HA	11:K:77:MET:HA	1.91	0.53
22:W:22:PHE:CD1	22:W:22:PHE:N	2.73	0.53
1:A:97:G:H2'	1:A:98:G:C8	2.44	0.53
1:A:512:U:H2'	1:A:513:C:C6	2.44	0.53
1:A:575:G:H4'	1:A:576:G:C5'	2.38	0.53
1:A:908:A:H2'	1:A:909:A:C8	2.44	0.53
1:A:998:G:N1	1:A:999:C:C4	2.77	0.53
1:A:617:G:N2	1:A:618:C:C2	2.77	0.52
1:A:774:G:N2	1:A:806:C:C2	2.78	0.52
1:A:1182:G:H4'	1:A:1183:A:C5'	2.39	0.52
23:X:46:VAL:HG21	23:X:62:TYR:HB2	1.90	0.52
1:A:79:G:N1	1:A:91:C:C2	2.74	0.52
1:A:678:U:H2'	1:A:679:C:H6	1.72	0.52
1:A:1292:U:H2'	1:A:1293:G:H8	1.74	0.52
2:B:55:PHE:CZ	2:B:217:ARG:HB3	2.44	0.52
1:A:344:A:H5''	1:A:345:C:H5	1.73	0.52
1:A:975:A:O5'	1:A:976:G:H5'	2.09	0.52
1:A:1396:A:H4'	1:A:1397:C:H5''	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1416:G:H2'	1:A:1417:G:O4'	2.09	0.52
19:S:49:ILE:HG21	19:S:71:LEU:CD1	2.39	0.52
1:A:216:G:C2	1:A:217:C:N3	2.77	0.52
1:A:939:G:C6	1:A:940:C:N4	2.78	0.52
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.08	0.52
1:A:1148:U:H2'	1:A:1149:C:O4'	2.09	0.52
1:A:299:G:H2'	1:A:300:A:C8	2.45	0.52
1:A:1164:G:N2	1:A:1165:C:C2	2.76	0.52
1:A:1435:G:H2'	1:A:1436:U:C6	2.44	0.52
3:C:14:ILE:N	3:C:14:ILE:CD1	2.73	0.52
15:O:33:THR:HA	15:O:63:ARG:HH11	1.73	0.52
23:X:61:ASP:HB3	23:X:64:LYS:HB3	1.92	0.52
1:A:128:G:C2	1:A:234:C:C2	2.97	0.52
1:A:521:G:N2	1:A:522:C:C2	2.78	0.52
1:A:974:A:C8	14:N:31:ARG:HG2	2.44	0.52
9:I:14:VAL:HG23	9:I:66:ARG:HB3	1.91	0.52
19:S:72:GLY:O	19:S:73:GLU:C	2.45	0.52
1:A:542:G:N2	1:A:543:C:C2	2.78	0.52
1:A:673:G:H5''	6:F:87:ARG:CZ	2.40	0.52
1:A:928:G:H1	1:A:1389:C:N4	2.06	0.52
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.43	0.52
1:A:1133:G:H1	1:A:1141:C:H42	1.58	0.52
2:B:184:VAL:HG13	2:B:197:VAL:HA	1.92	0.52
14:N:14:PRO:C	14:N:16:PHE:H	2.13	0.52
1:A:949:A:H2'	1:A:950:U:O4'	2.10	0.52
1:A:1475:G:H2'	1:A:1476:G:C8	2.44	0.52
21:V:3:LYS:H	21:V:10:ARG:HG2	1.74	0.52
23:X:149:VAL:HG13	23:X:168:VAL:HG22	1.91	0.52
1:A:351:G:H8	1:A:351:G:OP2	1.93	0.52
1:A:793:U:C3'	1:A:794:A:H5''	2.20	0.52
1:A:955:U:H2'	1:A:956:U:C6	2.43	0.52
1:A:1129:C:P	1:A:1130:A:H5'	2.50	0.52
2:B:49:GLU:O	2:B:52:GLU:HG2	2.09	0.52
10:J:62:HIS:HB2	14:N:59:ALA:HB3	1.91	0.52
1:A:16:A:O2'	5:E:16:THR:OG1	2.19	0.51
1:A:129(A):G:H4'	1:A:130:A:O5'	2.09	0.51
1:A:352:C:H4'	1:A:354:G:OP1	2.10	0.51
1:A:491:G:H2'	1:A:492:G:O4'	2.10	0.51
1:A:999:C:N3	1:A:1043:C:N3	2.58	0.51
1:A:1064:G:H1'	1:A:1190:G:H21	1.75	0.51
1:A:1365:G:C2	1:A:1366:C:C2	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:G:N2	1:A:726:C:C2	2.78	0.51
4:D:9:CYS:SG	4:D:26:CYS:SG	3.08	0.51
10:J:5:ARG:HG2	10:J:71:LEU:HD21	1.91	0.51
1:A:522:C:OP2	12:L:69:TYR:OH	2.27	0.51
4:D:100:ARG:NH1	4:D:137:SER:HA	2.25	0.51
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.93	0.51
1:A:362:G:H5''	12:L:61:THR:HB	1.92	0.51
1:A:662:G:C2	1:A:744:C:O2	2.64	0.51
1:A:673:G:H2'	1:A:674:G:C8	2.45	0.51
1:A:174:C:H2'	1:A:175:C:H6	1.75	0.51
1:A:1030:C:H42	1:A:1031:G:H1	1.59	0.51
5:E:40:ARG:HH11	5:E:40:ARG:CG	2.21	0.51
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.91	0.51
19:S:49:ILE:HG22	19:S:71:LEU:HD11	1.91	0.51
1:A:320:C:H2'	1:A:321:A:C8	2.46	0.51
1:A:884:U:H4'	1:A:885:G:H5''	1.93	0.51
4:D:110:PHE:HD1	4:D:110:PHE:H	1.57	0.51
11:K:18:ARG:HG3	11:K:81:ASP:HB3	1.92	0.51
1:A:1001(A):G:N1	1:A:1002:G:C6	2.78	0.51
1:A:1364:U:C6	21:V:14:TRP:HH2	2.29	0.51
1:A:1405:G:H2'	1:A:1406:U:H6	1.75	0.51
1:A:1506:U:O2'	1:A:1507:A:O5'	2.27	0.51
2:B:130:ARG:CD	2:B:130:ARG:N	2.73	0.51
12:L:32:PHE:HE1	12:L:86:ARG:HG3	1.76	0.51
1:A:49:U:H3'	1:A:50:A:H5''	1.93	0.51
1:A:77:G:C8	1:A:77:G:H3'	2.46	0.51
1:A:981:U:C4'	14:N:21:TYR:CE2	2.81	0.51
4:D:120:LEU:HD12	4:D:125:HIS:HD2	1.76	0.51
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.91	0.51
19:S:45:VAL:HA	19:S:62:ILE:HG22	1.93	0.51
1:A:374:A:C6	1:A:375:U:C4	2.99	0.51
1:A:441:A:H3'	1:A:442:C:C6	2.46	0.51
1:A:582:U:H2'	1:A:583:A:H8	1.75	0.51
1:A:613:C:H2'	1:A:614:A:H8	1.74	0.51
1:A:1272:G:H2'	1:A:1273:G:C8	2.46	0.51
1:A:1502:A:H2	1:A:1505:G:H1	1.57	0.51
1:A:59:A:H5''	1:A:387:U:H5''	1.93	0.50
1:A:563:A:N6	1:A:884:U:C2	2.72	0.50
10:J:6:ILE:HG13	10:J:72:VAL:O	2.11	0.50
23:X:130:PRO:HD2	23:X:131:GLU:OE2	2.11	0.50
1:A:31:G:OP1	1:A:31:G:H2'	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:G:C6	20:T:15:ARG:HG3	2.46	0.50
1:A:123:C:H2'	1:A:124:G:H8	1.76	0.50
1:A:698:G:C6	1:A:699:C:N4	2.79	0.50
1:A:1495:U:OP1	23:X:93:LYS:HE3	2.10	0.50
1:A:1537:U:H3	24:Y:28:A:H61	1.59	0.50
23:X:91:ARG:H	23:X:94:ILE:HD11	0.49	0.50
1:A:254:G:H21	17:Q:16:GLN:HE22	1.58	0.50
1:A:578:C:H6	1:A:578:C:H5''	1.76	0.50
1:A:884:U:H4'	1:A:885:G:C5'	2.40	0.50
1:A:895:G:H1	1:A:904:C:H42	1.58	0.50
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.92	0.50
1:A:1422:G:N2	1:A:1479:C:C2	2.80	0.50
12:L:84:LEU:HB2	12:L:105:TYR:HE2	1.75	0.50
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.92	0.50
1:A:266:G:O3'	17:Q:67:LYS:HB2	2.10	0.50
1:A:657:G:H4'	15:O:28:GLN:HG3	1.93	0.50
1:A:713:G:H2'	1:A:714:G:C8	2.46	0.50
1:A:975:A:H4'	1:A:976:G:O5'	2.12	0.50
1:A:1368:G:N2	1:A:1369:C:C2	2.80	0.50
3:C:131:ARG:HG2	3:C:131:ARG:NH1	2.26	0.50
4:D:8:VAL:O	4:D:11:LEU:N	2.43	0.50
24:Y:23:C:H2'	24:Y:24:A:O4'	2.12	0.50
1:A:156:G:H1	1:A:165:C:H42	1.60	0.50
1:A:544:G:OP1	4:D:62:GLN:HG3	2.11	0.50
1:A:1129:C:OP1	1:A:1130:A:H5'	2.12	0.50
1:A:1216:G:N2	1:A:1217:C:C2	2.79	0.50
1:A:1258:G:C2	1:A:1259:C:N3	2.79	0.50
1:A:1409:C:H2'	1:A:1410:G:C8	2.47	0.50
3:C:113:ALA:HA	3:C:202:ILE:HD13	1.93	0.50
12:L:84:LEU:HB2	12:L:105:TYR:CE2	2.46	0.50
1:A:70:G:C2	1:A:100:C:O2	2.65	0.50
1:A:794:A:H2'	1:A:795:C:H6	1.77	0.50
1:A:1272:G:H2'	1:A:1273:G:H8	1.75	0.50
2:B:130:ARG:HE	2:B:130:ARG:N	2.10	0.50
5:E:11:ILE:HD12	5:E:31:LEU:CD1	2.42	0.50
12:L:32:PHE:CB	12:L:84:LEU:HD11	2.42	0.50
1:A:671:G:N2	1:A:736:C:C2	2.80	0.50
1:A:945:G:H2'	1:A:946:A:H5''	1.93	0.50
1:A:985:C:C2	1:A:1221:G:C2	3.00	0.50
1:A:1310:G:N2	1:A:1328:C:C2	2.80	0.50
18:R:26:LEU:HD21	18:R:39:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:72:GLY:C	19:S:74:PHE:N	2.58	0.50
1:A:11:G:H2'	1:A:12:U:O4'	2.11	0.50
1:A:34:C:H2'	1:A:35:G:C8	2.47	0.50
1:A:247:G:OP2	17:Q:100:LYS:N	2.45	0.50
2:B:24:TRP:NE1	2:B:40:HIS:HE1	2.06	0.50
3:C:46:GLU:HB2	3:C:47:LEU:HD12	1.93	0.50
14:N:23:ARG:HG3	14:N:30:ALA:CA	2.38	0.50
19:S:15:LEU:HD23	19:S:33:THR:HG21	1.94	0.50
1:A:17:U:H2'	1:A:18:C:C6	2.46	0.50
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.46	0.50
1:A:331:G:OP1	1:A:332:G:H5'	2.11	0.50
1:A:474:G:H2'	1:A:475:G:H8	1.76	0.50
1:A:662:G:C6	1:A:744:C:N3	2.80	0.50
1:A:1000:U:C6	1:A:1000:U:C3'	2.94	0.50
1:A:1190:G:H5'	3:C:176:HIS:CE1	2.47	0.50
1:A:1248:A:H2'	1:A:1249:C:C6	2.47	0.50
1:A:1355:G:H1	1:A:1367:C:H42	1.60	0.50
3:C:29:TYR:CD1	3:C:29:TYR:C	2.85	0.50
4:D:8:VAL:HG21	4:D:115:ARG:HE	1.76	0.50
9:I:79:LEU:O	9:I:83:ARG:HG3	2.12	0.50
2:B:25:ASN:ND2	2:B:27:LYS:H	2.10	0.49
2:B:28:PHE:O	2:B:30:ARG:CA	2.57	0.49
2:B:130:ARG:CA	2:B:130:ARG:NE	2.73	0.49
23:X:131:GLU:O	23:X:135:ARG:HB2	2.11	0.49
1:A:44:G:C2	1:A:45:U:H1'	2.47	0.49
1:A:44:G:H2'	1:A:45:U:O4'	2.12	0.49
1:A:51:A:H4'	1:A:52:G:C5'	2.42	0.49
1:A:132:C:C5'	20:T:75:ASN:HD22	2.24	0.49
1:A:407:G:C2	1:A:436:C:C2	3.00	0.49
1:A:824:C:H2'	1:A:825:G:H8	1.77	0.49
1:A:897:C:O2	1:A:903:G:C2	2.65	0.49
1:A:84:U:H2'	1:A:88:A:O4'	2.12	0.49
1:A:765:G:C6	1:A:812:C:C4	3.00	0.49
1:A:925:G:H1	1:A:1391:U:H3	1.61	0.49
1:A:1095:U:P	1:A:1108:G:H1	2.35	0.49
4:D:56:VAL:HG12	4:D:202:LEU:CD2	2.42	0.49
1:A:403:C:H5''	4:D:136:PRO:HD2	1.94	0.49
1:A:778:G:N1	1:A:779:C:C2	2.81	0.49
1:A:825:G:C6	1:A:826:C:C4	3.00	0.49
1:A:975:A:H5'	1:A:975:A:H8	1.76	0.49
1:A:1348:U:H2'	1:A:1349:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.94	0.49
23:X:94:ILE:CG2	23:X:98:ASP:OD1	2.61	0.49
1:A:201:C:H42	1:A:216:G:H1	1.59	0.49
1:A:354:G:N1	1:A:355:C:C4	2.80	0.49
1:A:438:G:OP1	4:D:125:HIS:HE1	1.95	0.49
1:A:1158:C:H3'	1:A:1158:C:O2	2.12	0.49
2:B:178:ARG:HD3	2:B:196:LEU:HD23	1.94	0.49
12:L:71:PRO:O	12:L:102:ARG:HD2	2.12	0.49
1:A:77:G:H8	1:A:77:G:OP2	1.96	0.49
1:A:1431:C:H2'	1:A:1432:G:O4'	2.13	0.49
5:E:15:ARG:HD3	5:E:28:PHE:CZ	2.47	0.49
6:F:52:ILE:HD11	18:R:77:GLY:HA3	1.95	0.49
1:A:370:C:C2	1:A:392:G:C2	3.01	0.49
1:A:1017:G:C2	1:A:1018:C:C2	3.01	0.49
1:A:1125:U:H5'	1:A:1126:U:O4	2.13	0.49
1:A:1128:C:H2'	1:A:1139:G:N7	2.26	0.49
1:A:1363(A):A:H1'	1:A:1365:G:N7	2.27	0.49
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.93	0.49
10:J:38:ILE:CG2	10:J:71:LEU:HD13	2.43	0.49
1:A:51:A:H4'	1:A:52:G:H5'	1.94	0.49
1:A:264:U:H2'	1:A:265:G:O4'	2.12	0.49
1:A:424:G:H2'	1:A:425:G:C8	2.47	0.49
1:A:911:U:H2'	1:A:912:C:C6	2.47	0.49
1:A:1128:C:H42	1:A:1143:G:H1	1.60	0.49
1:A:1315:U:H2'	1:A:1316:G:C8	2.48	0.49
2:B:19:HIS:CD2	2:B:20:GLU:HG2	2.48	0.49
1:A:93:G:C3'	1:A:96:U:O4'	2.60	0.49
1:A:286:G:H2'	1:A:287:U:O4'	2.13	0.49
1:A:456:C:C2	1:A:476:G:C2	3.01	0.49
1:A:658:G:C6	1:A:749:C:N4	2.81	0.49
1:A:1124:G:H1	1:A:1149:C:H42	1.61	0.49
1:A:1495:U:C5'	23:X:93:LYS:O	2.54	0.49
3:C:113:ALA:N	3:C:114:PRO:CD	2.76	0.49
1:A:837:G:H1	1:A:849:C:H42	1.59	0.49
1:A:945:G:C2	1:A:946:A:C8	3.01	0.49
1:A:1300:G:H1'	1:A:1301:U:H5	1.77	0.49
2:B:33:TYR:HB2	2:B:43:ASP:HA	1.95	0.49
10:J:11:PHE:HB3	14:N:55:GLY:HA3	1.95	0.49
24:Y:22:G:C6	24:Y:23:C:N4	2.80	0.49
1:A:124:G:H2'	1:A:125:U:O4'	2.13	0.48
1:A:411:A:H2'	1:A:412:A:H4'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:C:C2	1:A:476:G:N2	2.81	0.48
1:A:486:U:H2'	1:A:487:A:C8	2.41	0.48
1:A:707:C:H2'	1:A:708:C:C6	2.48	0.48
1:A:1251:A:H5'	9:I:12:GLU:OE1	2.13	0.48
2:B:10:LEU:CA	2:B:48:MET:HE2	2.42	0.48
4:D:10:ARG:HH11	4:D:10:ARG:HG3	1.78	0.48
4:D:174:LEU:HD23	4:D:185:PHE:HA	1.95	0.48
14:N:22:THR:HB	14:N:33:VAL:HG11	1.95	0.48
24:Y:21:G:H2'	24:Y:22:G:C8	2.48	0.48
1:A:73:G:C6	1:A:97:G:C6	3.01	0.48
1:A:187:C:H2'	1:A:188:C:C6	2.49	0.48
1:A:457:C:H2'	1:A:458:C:C6	2.48	0.48
1:A:457:C:H2'	1:A:458:C:H6	1.77	0.48
1:A:1094:G:O2'	1:A:1095:U:P	2.71	0.48
3:C:201:TYR:N	3:C:201:TYR:CD1	2.82	0.48
1:A:441:A:H3'	1:A:442:C:H6	1.78	0.48
2:B:129:GLU:C	2:B:130:ARG:CD	2.75	0.48
5:E:71:LEU:HD11	5:E:115:VAL:HG23	1.94	0.48
23:X:7:THR:HG22	23:X:46:VAL:HG13	1.94	0.48
1:A:382:A:H2'	1:A:383:A:C8	2.48	0.48
1:A:1164:G:N1	1:A:1165:C:C4	2.80	0.48
1:A:1326:C:H5''	21:V:12:LYS:NZ	2.28	0.48
1:A:333:G:N1	1:A:334:C:C4	2.82	0.48
1:A:393:A:C2	1:A:394:G:C8	3.01	0.48
1:A:623:C:H2'	1:A:624:C:O4'	2.13	0.48
1:A:952:U:H2'	1:A:953:G:H8	1.79	0.48
1:A:986:A:H2'	1:A:987:G:O4'	2.13	0.48
1:A:1308:U:OP1	13:M:98:VAL:N	2.45	0.48
1:A:1320:C:C5'	19:S:73:GLU:OE2	2.61	0.48
2:B:103:THR:H	2:B:176:GLU:CD	2.16	0.48
6:F:68:PRO:HG2	6:F:71:ARG:HH21	1.78	0.48
7:G:150:ALA:HB1	11:K:57:THR:HG21	1.96	0.48
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.96	0.48
12:L:75:HIS:C	12:L:77:LEU:H	2.15	0.48
12:L:93:LEU:H	12:L:93:LEU:HD12	1.77	0.48
1:A:90:U:H2'	1:A:91:C:C6	2.49	0.48
1:A:563:A:H2	12:L:15:ARG:CZ	2.26	0.48
1:A:570:G:C5	1:A:873:A:C2	3.01	0.48
1:A:679:C:H2'	1:A:680:C:C6	2.48	0.48
1:A:784:C:C2	1:A:799:G:N2	2.81	0.48
1:A:1299:A:O2'	1:A:1301:U:C6	2.64	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:50:LEU:HD23	9:I:85:LEU:HD11	1.95	0.48
14:N:24:CYS:O	14:N:28:GLY:HA2	2.13	0.48
23:X:94:ILE:CG2	23:X:98:ASP:CG	2.80	0.48
1:A:802:A:H2'	1:A:803:G:O4'	2.14	0.48
1:A:1464:G:N1	1:A:1465:C:C4	2.81	0.48
4:D:39:PRO:O	4:D:44:GLY:HA2	2.14	0.48
4:D:64:LEU:HG	4:D:198:VAL:HG21	1.95	0.48
7:G:62:PHE:HA	7:G:124:LEU:HD22	1.96	0.48
9:I:6:GLY:HA3	9:I:80:GLY:O	2.12	0.48
9:I:96:LEU:HG	9:I:101:PHE:HB2	1.95	0.48
13:M:10:PRO:HG2	13:M:45:VAL:HG11	1.96	0.48
1:A:80:G:C2	1:A:90:U:H1'	2.49	0.48
1:A:246:A:N6	1:A:281:G:H1'	2.29	0.48
1:A:545:C:H5'	4:D:72:GLU:HB2	1.95	0.48
1:A:1134:G:N2	1:A:1141:C:C2	2.81	0.48
1:A:1367:C:H5''	9:I:114:TYR:HB3	1.95	0.48
2:B:24:TRP:CZ3	2:B:29:ALA:HB2	2.49	0.48
2:B:103:THR:N	2:B:176:GLU:OE1	2.47	0.48
1:A:580:U:H3	1:A:761:G:H1	1.61	0.48
1:A:590:C:C2	1:A:650:G:C2	3.02	0.48
1:A:734:G:C6	1:A:735:C:C4	3.01	0.48
1:A:834:C:C2	1:A:853:G:C2	3.02	0.48
1:A:918:A:H2'	1:A:919:A:O4'	2.14	0.48
1:A:424:G:H2'	1:A:425:G:H8	1.76	0.48
1:A:722:A:H3'	1:A:722:A:N3	2.28	0.48
1:A:728:A:OP1	1:A:742:G:O2'	2.31	0.48
1:A:825:G:C2	1:A:826:C:C2	3.02	0.48
1:A:1041:A:H2'	1:A:1042:G:C8	2.49	0.48
1:A:1129:C:O5'	1:A:1130:A:H5'	2.13	0.48
1:A:1361:G:C6	1:A:1362:C:N3	2.82	0.48
1:A:1419:G:C6	1:A:1420:C:C4	3.02	0.48
2:B:130:ARG:N	2:B:130:ARG:NE	2.62	0.48
14:N:9:LYS:CG	14:N:21:TYR:O	2.61	0.48
22:W:32:ILE:N	22:W:32:ILE:CD1	2.73	0.48
1:A:434:U:H2'	1:A:435:C:H6	1.78	0.47
1:A:778:G:C6	1:A:779:C:N3	2.82	0.47
1:A:829:G:C1'	2:B:26:PRO:CG	2.89	0.47
1:A:1354:C:H2'	1:A:1355:G:H8	1.79	0.47
1:A:1489:G:C2	1:A:1490:C:C2	3.02	0.47
1:A:1507:A:H2'	1:A:1508:G:C8	2.49	0.47
5:E:102:ALA:O	5:E:107:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:61:ALA:CB	11:K:90:GLY:HA3	2.44	0.47
23:X:137:LEU:HD22	23:X:163:MET:SD	2.53	0.47
1:A:69:G:H1	1:A:100:C:H42	1.62	0.47
1:A:145:G:N2	1:A:178:C:C2	2.82	0.47
1:A:563:A:N1	1:A:884:U:C4	2.82	0.47
1:A:626:U:H5''	16:P:38:TYR:CG	2.48	0.47
1:A:632:A:H2'	1:A:633:G:O4'	2.14	0.47
1:A:778:G:C6	1:A:779:C:C4	3.02	0.47
1:A:932:C:H42	1:A:1385:G:H1	1.62	0.47
1:A:1232:U:OP1	9:I:124:GLN:NE2	2.44	0.47
1:A:1250:A:H2'	1:A:1251:A:C8	2.49	0.47
1:A:1255:G:O2'	1:A:1258:G:H1'	2.14	0.47
1:A:1326:C:H5''	21:V:12:LYS:HZ1	1.79	0.47
2:B:19:HIS:O	2:B:190:THR:HG22	2.14	0.47
1:A:18:C:H2'	1:A:19:C:O4'	2.14	0.47
1:A:778:G:H2'	1:A:779:C:O4'	2.14	0.47
1:A:802:A:H3'	1:A:803:G:H8	1.79	0.47
1:A:1112:C:H1'	3:C:179:ARG:HE	1.79	0.47
1:A:1371:G:P	9:I:12:GLU:CG	3.01	0.47
3:C:12:LEU:HD22	3:C:18:TRP:NE1	2.27	0.47
7:G:106:GLN:O	7:G:110:GLN:HG2	2.14	0.47
8:H:30:ARG:HA	8:H:30:ARG:HD3	1.63	0.47
1:A:585:G:C6	1:A:586:C:C4	3.01	0.47
1:A:1069:C:H2'	1:A:1070:U:O4'	2.14	0.47
1:A:1489:G:C6	1:A:1490:C:C4	3.02	0.47
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.96	0.47
13:M:87:TYR:O	13:M:91:ARG:HG2	2.14	0.47
1:A:652:U:C2	1:A:752:G:N2	2.83	0.47
1:A:769:G:N2	1:A:770:C:C2	2.82	0.47
1:A:225:C:H2'	1:A:226:G:C8	2.50	0.47
1:A:351:G:H4'	1:A:352:C:OP1	2.15	0.47
1:A:512:U:H2'	1:A:513:C:H6	1.79	0.47
1:A:546:G:H4'	1:A:548:G:H4'	1.96	0.47
1:A:834:C:H5''	18:R:60:ALA:CB	2.44	0.47
2:B:55:PHE:HZ	2:B:217:ARG:HB3	1.79	0.47
13:M:54:VAL:O	13:M:58:GLU:HG2	2.14	0.47
1:A:100:C:H2'	1:A:101:A:C8	2.49	0.47
1:A:130:A:H8	1:A:130:A:OP1	1.98	0.47
1:A:189(K):U:H2'	1:A:189(L):G:H8	1.79	0.47
1:A:317:G:C2	1:A:337:C:O2	2.68	0.47
1:A:330:C:C6	1:A:330:C:H5''	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:U:H2'	1:A:341:C:H6	1.79	0.47
1:A:370:C:C4	1:A:392:G:N1	2.83	0.47
1:A:834:C:O2	1:A:853:G:C2	2.68	0.47
1:A:1117:G:C5'	1:A:1117:G:H8	2.28	0.47
1:A:1233:G:C2	1:A:1234:C:C2	3.03	0.47
1:A:1356:G:H2'	1:A:1357:A:C8	2.49	0.47
6:F:30:LEU:HD23	6:F:75:LEU:HD21	1.97	0.47
9:I:92:TYR:O	9:I:96:LEU:HB2	2.13	0.47
13:M:67:GLU:O	13:M:71:ARG:HG3	2.14	0.47
17:Q:41:LYS:HE2	17:Q:88:TYR:CE1	2.49	0.47
19:S:72:GLY:C	19:S:74:PHE:H	2.16	0.47
22:W:17:LEU:HB3	22:W:18:PRO:CD	2.45	0.47
1:A:73:G:H2'	1:A:73:G:N3	2.30	0.47
1:A:372:C:H42	1:A:389:A:H62	1.63	0.47
1:A:502:G:C2	1:A:503:C:C2	3.03	0.47
1:A:1033:G:H2'	1:A:1034:G:C8	2.50	0.47
1:A:1122:U:H2'	1:A:1123:A:O4'	2.14	0.47
1:A:1255:G:H2'	1:A:1279:A:N6	2.29	0.47
1:A:1279:A:H5''	10:J:7:LYS:HE2	1.96	0.47
1:A:1362:C:HO2'	1:A:1363:C:H6	1.60	0.47
1:A:1443:G:N2	1:A:1444:C:C2	2.83	0.47
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.97	0.47
4:D:79:PHE:CZ	4:D:204:ILE:HA	2.50	0.47
20:T:10:LEU:HG	20:T:12:ALA:H	1.79	0.47
1:A:28:G:H2'	1:A:29:G:O4'	2.14	0.47
1:A:492:G:H2'	1:A:492:G:N3	2.29	0.47
9:I:117:HIS:ND1	9:I:117:HIS:N	2.63	0.47
19:S:49:ILE:HG21	19:S:71:LEU:HD11	1.96	0.47
20:T:56:MET:HG2	20:T:84:LEU:HD21	1.96	0.47
22:W:23:ARG:HH11	22:W:23:ARG:HG3	1.77	0.47
1:A:10:A:H2'	1:A:11:G:C8	2.48	0.47
1:A:337:C:H2'	1:A:338:A:H8	1.80	0.47
1:A:536:C:H2'	1:A:537:G:H8	1.79	0.47
1:A:588:G:N1	1:A:589:C:C4	2.83	0.47
1:A:1058:G:H2'	1:A:1059:C:O4'	2.14	0.47
1:A:1507:A:H8	1:A:1507:A:C5'	2.27	0.47
5:E:16:THR:HG22	5:E:27:ARG:O	2.14	0.47
1:A:189:G:C2	1:A:189(A):C:C2	3.03	0.46
1:A:881:G:C2	1:A:882:C:C2	3.04	0.46
2:B:10:LEU:HB2	2:B:48:MET:HE3	1.40	0.46
17:Q:43:LEU:HD13	17:Q:68:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:G:N2	1:A:67:C:C2	2.83	0.46
1:A:153:C:N4	1:A:154:C:N4	2.63	0.46
1:A:199:G:N2	1:A:219:C:C2	2.83	0.46
1:A:247:G:P	17:Q:99:SER:HG	2.38	0.46
1:A:408:A:H2'	1:A:409:G:O4'	2.14	0.46
1:A:426:G:P	4:D:36:ARG:NH2	2.87	0.46
1:A:865:A:H2'	1:A:866:C:H6	1.78	0.46
5:E:115:VAL:CG1	5:E:118:ILE:HG23	2.45	0.46
11:K:33:THR:HA	11:K:40:ILE:H	1.80	0.46
12:L:6:THR:O	12:L:9:GLN:HB2	2.16	0.46
18:R:48:GLY:N	18:R:83:GLU:HB2	2.30	0.46
1:A:44:G:OP2	16:P:12:LYS:HE3	2.15	0.46
1:A:122:G:C2	1:A:123:C:C2	3.03	0.46
1:A:389:A:H3'	1:A:390:C:C6	2.51	0.46
1:A:585:G:C2	1:A:586:C:C2	3.04	0.46
1:A:663:A:H2'	1:A:664:G:O4'	2.15	0.46
1:A:902:G:H2'	1:A:903:G:H8	1.79	0.46
1:A:910:C:H4'	1:A:1413:A:H4'	1.98	0.46
1:A:961:U:C4	1:A:1201:A:N1	2.81	0.46
1:A:1010:G:H2'	1:A:1011:G:C8	2.51	0.46
1:A:1062:U:H2'	1:A:1063:C:C6	2.50	0.46
1:A:1226:C:P	13:M:91:ARG:HH12	2.39	0.46
1:A:89:C:H2'	1:A:90:U:O4'	2.14	0.46
1:A:255:G:H2'	1:A:256:U:C6	2.50	0.46
1:A:688:G:C2	1:A:689:C:C2	3.03	0.46
1:A:743:U:H2'	1:A:744:C:C6	2.51	0.46
1:A:1268:A:H2'	1:A:1269:A:C8	2.50	0.46
1:A:1430:C:C2	1:A:1471:G:N2	2.83	0.46
2:B:187:LEU:HD12	2:B:211:ILE:HG23	1.98	0.46
3:C:33:LEU:HD11	14:N:53:LEU:HD23	1.97	0.46
4:D:10:ARG:HG3	4:D:10:ARG:NH1	2.30	0.46
15:O:25:THR:HG23	15:O:66:LEU:HD23	1.97	0.46
1:A:31:G:C6	1:A:48:C:O4'	2.68	0.46
1:A:538:G:H5''	12:L:114:LYS:HB2	1.97	0.46
1:A:539:A:H2'	1:A:540:G:C8	2.51	0.46
1:A:1042:G:N2	1:A:1043:C:C2	2.84	0.46
1:A:108:G:H5'	1:A:109:A:H5''	1.97	0.46
1:A:193:C:H2'	1:A:194:C:H6	1.81	0.46
1:A:457:C:C2	1:A:475:G:N2	2.83	0.46
1:A:1163:C:C2	1:A:1174:G:N2	2.84	0.46
1:A:1266:G:N2	1:A:1270:C:C2	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1287:A:H2'	1:A:1288:A:H8	1.76	0.46
1:A:1502:A:H2'	1:A:1504:G:N7	2.30	0.46
3:C:146:ALA:C	3:C:148:GLY:H	2.19	0.46
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.51	0.46
17:Q:43:LEU:HD13	17:Q:68:ARG:HH22	1.80	0.46
23:X:48:VAL:HG23	23:X:56:VAL:HG12	1.98	0.46
1:A:15:G:H2'	1:A:16:A:H8	1.80	0.46
1:A:542:G:H5'	4:D:41:GLY:HA3	1.97	0.46
1:A:638:G:H2'	1:A:639:G:O4'	2.15	0.46
2:B:77:ALA:HA	2:B:80:ILE:HD12	1.97	0.46
1:A:256:U:H2'	1:A:257:G:H8	1.81	0.46
1:A:369:C:H2'	1:A:370:C:H6	1.80	0.46
1:A:425:G:H2'	1:A:426:G:O4'	2.16	0.46
1:A:786:G:C2	1:A:797:C:C2	3.04	0.46
1:A:1099:G:C2	1:A:1100:C:O2	2.68	0.46
1:A:1127:G:H21	1:A:1147:C:H41	1.64	0.46
1:A:1362:C:O2'	1:A:1363:C:O4'	2.34	0.46
1:A:1381:U:H2'	1:A:1382:C:H6	1.80	0.46
3:C:96:GLY:O	3:C:97:LYS:HG2	2.15	0.46
1:A:245:C:C2	1:A:284:G:C2	3.03	0.46
1:A:812:C:O2'	1:A:813:U:O4'	2.34	0.46
1:A:1504:G:O2'	1:A:1505:G:OP2	2.25	0.46
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.98	0.46
14:N:27:CYS:SG	14:N:28:GLY:N	2.89	0.46
15:O:67:LEU:HD23	15:O:67:LEU:HA	1.64	0.46
24:Y:33:A:H2'	24:Y:33:A:N3	2.31	0.46
1:A:35:G:H2'	1:A:36:C:C6	2.50	0.46
1:A:342:C:C2	1:A:348:G:N2	2.84	0.46
1:A:419:C:N4	1:A:424:G:H1	2.13	0.46
1:A:661:G:C2	1:A:745:C:N3	2.84	0.46
1:A:982:U:H4'	1:A:983:A:O4'	2.15	0.46
1:A:1048:G:H1	1:A:1209:C:N4	2.14	0.46
1:A:1080:A:O3'	5:E:16:THR:OG1	2.34	0.46
1:A:1144:G:H21	1:A:1146:A:H62	1.62	0.46
1:A:1250:A:H4'	9:I:67:GLY:HA2	1.98	0.46
1:A:1355:G:H1	1:A:1367:C:N4	2.14	0.46
1:A:1423:G:C6	1:A:1424:C:C4	3.04	0.46
2:B:29:ALA:HA	2:B:32:ILE:HD12	1.98	0.46
8:H:100:ILE:HD11	8:H:130:GLY:HA2	1.99	0.46
1:A:1132:C:H2'	1:A:1133:G:H8	1.82	0.45
1:A:1308:U:OP1	13:M:97:PRO:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1310:G:C2	1:A:1328:C:N3	2.84	0.45
2:B:211:ILE:H	2:B:211:ILE:HG13	1.52	0.45
3:C:16:ARG:NH1	3:C:16:ARG:HG2	2.31	0.45
3:C:135:LYS:O	3:C:139:GLN:HG2	2.15	0.45
18:R:19:LYS:HG2	18:R:20:ALA:N	2.31	0.45
1:A:70:G:C6	1:A:100:C:N3	2.85	0.45
1:A:157:G:C6	1:A:165:C:N3	2.84	0.45
1:A:317:G:C2	1:A:337:C:C2	3.04	0.45
1:A:774:G:C2	1:A:806:C:N3	2.84	0.45
1:A:1198:G:H2'	1:A:1199:U:O4'	2.15	0.45
1:A:1221:G:H2'	1:A:1222:G:C8	2.51	0.45
1:A:1462:G:C6	1:A:1463:C:N4	2.84	0.45
1:A:1487:G:H2'	1:A:1488:G:C8	2.51	0.45
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.97	0.45
6:F:33:TYR:HD1	6:F:71:ARG:HD2	1.82	0.45
6:F:35:ALA:HA	6:F:67:MET:HB3	1.98	0.45
1:A:32:A:C2	1:A:33:A:C4	3.05	0.45
1:A:189:G:C6	1:A:189(A):C:C4	3.04	0.45
1:A:324:G:H22	1:A:327:A:P	2.40	0.45
1:A:1401:G:H2'	1:A:1402:C:O4'	2.16	0.45
1:A:1458:G:H2'	1:A:1459:C:C6	2.51	0.45
5:E:107:ARG:NH1	5:E:107:ARG:HB2	2.31	0.45
14:N:12:ARG:HH22	14:N:14:PRO:HG3	1.81	0.45
20:T:36:LEU:HB3	20:T:59:ALA:HB2	1.99	0.45
24:Y:30:G:H2'	24:Y:31:U:C6	2.51	0.45
1:A:32:A:H2'	1:A:33:A:C8	2.51	0.45
1:A:133:U:O2	1:A:230:G:C2	2.70	0.45
1:A:536:C:H2'	1:A:537:G:C8	2.51	0.45
1:A:812:C:H4'	1:A:812:C:OP1	2.15	0.45
1:A:1502:A:H2	1:A:1505:G:N1	2.15	0.45
8:H:17:THR:HG22	8:H:63:LEU:HG	1.98	0.45
8:H:17:THR:OG1	8:H:18:ARG:NH1	2.49	0.45
14:N:23:ARG:HH12	14:N:30:ALA:HB2	1.77	0.45
1:A:166:G:H2'	1:A:167:G:C8	2.51	0.45
1:A:166:G:H2'	1:A:167:G:H8	1.81	0.45
1:A:563:A:N3	1:A:563:A:H2'	2.30	0.45
1:A:1048:G:N2	1:A:1210:C:C2	2.85	0.45
8:H:91:ARG:HB2	12:L:7:ILE:HG13	1.99	0.45
14:N:24:CYS:HB3	14:N:28:GLY:H	1.81	0.45
1:A:33:A:O5'	1:A:33:A:H8	1.99	0.45
1:A:446:G:C2	1:A:489:C:C2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:C:O2	1:A:1043:C:O2	2.33	0.45
1:A:1366:C:H2'	1:A:1367:C:C6	2.51	0.45
21:V:2:GLY:O	21:V:4:GLY:N	2.50	0.45
1:A:15:G:H2'	1:A:16:A:C8	2.52	0.45
1:A:243:A:N6	1:A:281:G:O2'	2.49	0.45
1:A:836:G:H1	1:A:850:U:H3	1.65	0.45
1:A:1000:U:H3'	1:A:1000:U:H6	1.81	0.45
1:A:1103:C:H2'	1:A:1104:G:O4'	2.16	0.45
3:C:12:LEU:CD1	14:N:51:GLY:HA2	2.43	0.45
15:O:26:GLU:HG2	15:O:81:LEU:HD11	1.98	0.45
1:A:79:G:O2'	1:A:80:G:H5'	2.16	0.45
1:A:767:A:H2'	1:A:768:A:C8	2.52	0.45
1:A:864:A:C2	1:A:865:A:C2	3.05	0.45
1:A:945:G:C2'	1:A:946:A:H5''	2.47	0.45
1:A:1277:C:HO2'	1:A:1279:A:H8	1.63	0.45
2:B:30:ARG:HH21	2:B:194:PRO:HB2	1.81	0.45
4:D:127:THR:HG23	4:D:131:ARG:H	1.82	0.45
6:F:14:LEU:HD11	6:F:84:ASN:HB3	1.98	0.45
8:H:39:LEU:HD23	8:H:44:PHE:HB2	1.98	0.45
1:A:77:G:C8	1:A:77:G:OP2	2.70	0.45
1:A:585:G:N1	1:A:586:C:C2	2.85	0.45
1:A:672:U:H5'	6:F:80:ARG:HD3	1.98	0.45
1:A:765:G:N1	1:A:812:C:C2	2.85	0.45
1:A:1326:C:H2'	1:A:1327:C:H6	1.82	0.45
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.52	0.45
7:G:42:ILE:HG23	7:G:117:ALA:HA	1.99	0.45
9:I:48:GLU:N	9:I:49:PRO:HD2	2.32	0.45
10:J:6:ILE:HG22	10:J:98:ILE:HA	1.99	0.45
16:P:58:TYR:O	16:P:62:VAL:HG13	2.16	0.45
17:Q:84:LEU:HD12	17:Q:84:LEU:HA	1.88	0.45
19:S:63:THR:HG22	19:S:64:GLU:H	1.81	0.45
1:A:9:G:H5''	5:E:126:ARG:HD2	1.99	0.45
1:A:256:U:H2'	1:A:257:G:C8	2.52	0.45
1:A:376:G:H2'	1:A:377:G:H8	1.82	0.45
1:A:502:G:C6	1:A:503:C:C4	3.05	0.45
1:A:691:G:H22	1:A:695:A:H5''	1.82	0.45
1:A:790:A:N3	24:Y:36:A:N6	2.64	0.45
1:A:1097:C:H2'	1:A:1098:C:C6	2.52	0.45
1:A:1218:C:H2'	1:A:1219:U:C5	2.50	0.45
1:A:1240:U:O4'	7:G:42:ILE:HD11	2.17	0.45
1:A:1284:C:H2'	1:A:1285:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:82:HIS:CD2	8:H:138:TRP:CE2	3.05	0.45
8:H:86:ILE:HB	8:H:133:LEU:HD22	1.98	0.45
18:R:74:ARG:HB3	18:R:81:PHE:CZ	2.52	0.45
1:A:41:G:H2'	1:A:42:G:H8	1.82	0.44
1:A:67:C:H42	1:A:102:G:H1	1.64	0.44
1:A:91:C:C6	1:A:91:C:OP2	2.70	0.44
1:A:394:G:C2	1:A:395:C:C2	3.06	0.44
1:A:399:G:C2	1:A:400:C:C2	3.05	0.44
1:A:518:C:HO2'	12:L:50:SER:HB3	1.83	0.44
1:A:671:G:C2	1:A:736:C:N3	2.85	0.44
1:A:832:C:C2	1:A:855:G:C2	3.04	0.44
1:A:946:A:H2'	1:A:947:G:H8	1.75	0.44
1:A:1004:A:C8	1:A:1038:C:N3	2.85	0.44
18:R:53:ARG:HE	18:R:60:ALA:HA	1.81	0.44
20:T:14:LYS:HA	20:T:17:ARG:CZ	2.47	0.44
1:A:91:C:OP2	1:A:91:C:C5	2.70	0.44
1:A:416:G:C6	1:A:417:C:C4	3.05	0.44
1:A:509:A:H4'	1:A:510:A:OP1	2.16	0.44
1:A:904:C:H2'	1:A:905:U:O4'	2.16	0.44
1:A:1017:G:C6	1:A:1018:C:C4	3.05	0.44
1:A:1240:U:OP1	7:G:116:ALA:HB2	2.17	0.44
1:A:1316:G:N2	1:A:1318:A:H3'	2.33	0.44
14:N:9:LYS:CG	14:N:21:TYR:CD1	3.00	0.44
1:A:428:G:O3'	4:D:13:ARG:NH2	2.50	0.44
1:A:763:G:C6	1:A:764:C:C4	3.06	0.44
1:A:793:U:C3'	1:A:794:A:C5'	2.87	0.44
1:A:861:G:C6	1:A:862:C:C4	3.05	0.44
1:A:1086:U:H2'	1:A:1087:G:H8	1.82	0.44
1:A:1126:U:O2	1:A:1126:U:C2'	2.65	0.44
1:A:1237:C:H5''	1:A:1238:A:O4'	2.18	0.44
1:A:1381:U:H2'	1:A:1382:C:C6	2.53	0.44
1:A:1436:U:H2'	1:A:1437:C:O4'	2.17	0.44
3:C:7:PRO:CB	3:C:11:ARG:HH21	2.30	0.44
5:E:148:VAL:HG21	8:H:107:LEU:HD23	1.99	0.44
11:K:91:ARG:NH1	18:R:88:LYS:HE3	2.20	0.44
15:O:33:THR:HA	15:O:63:ARG:NH1	2.32	0.44
1:A:35:G:C6	1:A:36:C:N4	2.86	0.44
1:A:375:U:C4	1:A:376:G:N7	2.86	0.44
1:A:414:A:H2'	1:A:415:A:O4'	2.18	0.44
1:A:443:C:C2	1:A:492:G:N2	2.86	0.44
1:A:444:C:N3	1:A:491:G:C2	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:U:H2'	1:A:627:G:C8	2.53	0.44
1:A:800:G:H2'	1:A:801:U:C6	2.53	0.44
1:A:1034:G:H2'	1:A:1035:A:H8	1.82	0.44
1:A:1040:U:H2'	1:A:1041:A:C8	2.52	0.44
1:A:1360:A:H2'	1:A:1361:G:C8	2.52	0.44
6:F:46:ARG:HB3	6:F:46:ARG:HH11	1.83	0.44
9:I:97:LYS:N	9:I:98:PRO:HD2	2.31	0.44
16:P:18:ARG:HA	16:P:38:TYR:HA	1.99	0.44
1:A:293:G:C5	1:A:305:G:N2	2.86	0.44
1:A:681:C:C2	1:A:710:G:N2	2.85	0.44
1:A:866:C:H4'	1:A:919:A:H5'	1.99	0.44
1:A:1480:G:H2'	1:A:1481:U:O4'	2.17	0.44
1:A:1495:U:H2'	1:A:1496:C:C6	2.53	0.44
1:A:1504:G:H4'	1:A:1505:G:O5'	2.16	0.44
8:H:64:LYS:HB3	8:H:79:VAL:HG11	1.99	0.44
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.99	0.44
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.99	0.44
1:A:667:G:C2	1:A:740:U:O2	2.71	0.44
1:A:725:G:C6	1:A:726:C:N4	2.85	0.44
1:A:983:A:H5'	1:A:984:C:OP2	2.17	0.44
1:A:1061:G:H5''	10:J:59:SER:OG	2.17	0.44
7:G:150:ALA:HA	11:K:59:TYR:HB3	2.00	0.44
1:A:41:G:H2'	1:A:42:G:C8	2.52	0.44
1:A:563:A:N3	1:A:563:A:C2'	2.81	0.44
1:A:577:G:C2	1:A:578:C:C2	3.05	0.44
1:A:916:G:H2'	1:A:917:G:C8	2.49	0.44
1:A:973:G:C3'	1:A:974:A:H5''	2.34	0.44
1:A:1253:G:C6	1:A:1254:C:C4	3.06	0.44
4:D:10:ARG:NH1	4:D:40:PRO:HG3	2.32	0.44
8:H:82:HIS:CD2	8:H:82:HIS:C	2.91	0.44
11:K:58:PRO:HD3	11:K:89:ALA:HB1	1.99	0.44
1:A:132:C:C2	1:A:231:G:N2	2.86	0.44
1:A:416:G:C2	1:A:417:C:C2	3.05	0.44
1:A:748:C:H4'	1:A:749:C:O5'	2.18	0.44
1:A:988:G:C6	1:A:989:C:N3	2.86	0.44
1:A:1030:C:N4	1:A:1031:G:H1	2.16	0.44
1:A:1419:G:C2	1:A:1420:C:C2	3.06	0.44
17:Q:29:HIS:HB2	17:Q:36:ILE:HG13	2.00	0.44
1:A:109:A:C6	1:A:327:A:C6	3.06	0.44
1:A:860:A:H2'	1:A:861:G:O4'	2.18	0.44
1:A:866:C:N3	1:A:867:G:H1'	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1061:G:C5'	10:J:59:SER:OG	2.66	0.44
1:A:1182:G:H4'	1:A:1183:A:O5'	2.18	0.44
2:B:24:TRP:CG	2:B:24:TRP:O	2.71	0.44
6:F:53:ALA:HB3	6:F:86:ARG:HD3	1.99	0.44
14:N:24:CYS:CB	14:N:29:ARG:H	2.28	0.44
16:P:13:HIS:C	16:P:15:PRO:HD3	2.38	0.44
1:A:42:G:C6	1:A:43:C:C4	3.06	0.43
1:A:112:G:OP2	16:P:27:LYS:HE2	2.18	0.43
1:A:164:U:H2'	1:A:165:C:C6	2.53	0.43
1:A:310:G:C6	1:A:311:C:C4	3.05	0.43
1:A:481:G:O2'	1:A:483:C:N4	2.49	0.43
1:A:830:G:N2	1:A:857:C:C2	2.86	0.43
1:A:947:G:C2	1:A:948:C:C2	3.06	0.43
1:A:981:U:H5'	14:N:21:TYR:HE2	1.82	0.43
1:A:1018:C:H2'	1:A:1019:C:C6	2.53	0.43
1:A:1164:G:H1	1:A:1172:C:N4	2.16	0.43
2:B:47:THR:HG23	2:B:202:PRO:HD2	2.00	0.43
8:H:86:ILE:HG22	8:H:93:VAL:HG21	2.00	0.43
1:A:64:G:H4'	1:A:65:U:H5''	1.99	0.43
1:A:413:G:N2	1:A:429:U:OP2	2.47	0.43
1:A:521:G:N1	1:A:522:C:C4	2.86	0.43
1:A:690:G:OP2	11:K:27:ASN:HB3	2.18	0.43
1:A:717:C:H4'	11:K:117:ASN:HB3	1.99	0.43
1:A:927:G:H1	1:A:1390:U:H3	1.65	0.43
1:A:1064:G:N2	1:A:1190:G:O2'	2.51	0.43
1:A:1133:G:H1	1:A:1141:C:N4	2.16	0.43
1:A:1196:U:H5'	1:A:1197:G:C5'	2.48	0.43
1:A:1276:G:H2'	1:A:1277:C:O4'	2.18	0.43
2:B:23:ARG:HG3	2:B:23:ARG:O	2.17	0.43
2:B:24:TRP:CD1	2:B:24:TRP:N	2.86	0.43
4:D:35:ARG:CB	4:D:35:ARG:NH1	2.73	0.43
15:O:65:ARG:HG2	15:O:65:ARG:NH1	2.21	0.43
22:W:45:ILE:HG21	22:W:70:ARG:CB	2.48	0.43
23:X:91:ARG:NH1	24:Y:36:A:H2	2.16	0.43
1:A:598:U:H2'	1:A:599:C:C6	2.53	0.43
1:A:829:G:H4'	2:B:26:PRO:CG	2.38	0.43
1:A:855:G:C6	1:A:856:C:C4	3.06	0.43
1:A:933:G:OP2	7:G:3:ARG:HB2	2.18	0.43
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.52	0.43
1:A:1060:C:O2	1:A:1198:G:C2	2.71	0.43
1:A:1423:G:C2	1:A:1424:C:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:LEU:HD23	4:D:156:GLU:H	1.83	0.43
7:G:57:GLU:HA	7:G:58:PRO:HD3	1.88	0.43
11:K:22:HIS:HB3	11:K:29:ILE:HG23	1.98	0.43
12:L:54:LYS:HG2	12:L:75:HIS:CE1	2.51	0.43
13:M:48:LEU:HD13	13:M:53:VAL:HG22	2.00	0.43
17:Q:58:GLU:HB2	17:Q:75:ARG:HG3	2.00	0.43
1:A:123:C:OP1	1:A:311:C:O2'	2.36	0.43
1:A:198:G:H2'	1:A:199:G:C8	2.53	0.43
1:A:217:C:H2'	1:A:218:C:C6	2.53	0.43
1:A:378:G:H2'	1:A:379:C:O4'	2.19	0.43
1:A:616:G:H1	1:A:624:C:H42	1.66	0.43
1:A:728:A:N7	15:O:54:ARG:HD3	2.34	0.43
1:A:731:G:OP1	1:A:766:A:H1'	2.19	0.43
1:A:1163:C:H2'	1:A:1164:G:H8	1.82	0.43
1:A:1253:G:C2	1:A:1254:C:C2	3.07	0.43
1:A:1384:C:H2'	1:A:1385:G:H8	1.81	0.43
1:A:1421:G:H1	1:A:1479:C:H42	1.67	0.43
2:B:15:VAL:HB	2:B:204:ASN:OD1	2.18	0.43
2:B:130:ARG:HD2	2:B:130:ARG:N	2.33	0.43
10:J:54:PHE:H	14:N:41:ARG:NH2	2.16	0.43
20:T:29:LYS:NZ	20:T:65:LYS:HB3	2.32	0.43
1:A:262:A:C6	1:A:263:A:C6	3.06	0.43
1:A:504:C:C2	1:A:542:G:C2	3.06	0.43
1:A:748:C:H1'	1:A:749:C:H5	1.82	0.43
1:A:973:G:OP1	10:J:57:LYS:HD2	2.18	0.43
1:A:1225:A:H4'	19:S:78:ARG:CD	2.48	0.43
1:A:1266:G:C2	1:A:1270:C:N3	2.87	0.43
1:A:1320:C:H4'	19:S:73:GLU:OE2	2.18	0.43
1:A:1508:G:C2	1:A:1509:C:C2	3.07	0.43
1:A:1524:C:H2'	1:A:1525:G:C8	2.53	0.43
3:C:191:THR:O	3:C:193:TYR:N	2.52	0.43
4:D:29:PRO:C	4:D:35:ARG:HD3	2.32	0.43
1:A:145:G:C2	1:A:178:C:C2	3.06	0.43
1:A:401:C:H2'	1:A:402:G:H8	1.83	0.43
1:A:613:C:H42	1:A:627:G:H1	1.65	0.43
1:A:690:G:H2'	1:A:691:G:O4'	2.18	0.43
1:A:1050:G:C2	1:A:1209:C:O2	2.71	0.43
1:A:1074:G:C2	1:A:1075:C:C2	3.07	0.43
1:A:1119:C:N4	1:A:1154:G:H1	2.15	0.43
1:A:1162:C:C2	1:A:1175:G:C2	3.06	0.43
1:A:1203:C:H4'	14:N:27:CYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1438:G:N1	1:A:1439:C:C4	2.86	0.43
8:H:80:ILE:H	8:H:80:ILE:HD12	1.83	0.43
9:I:28:VAL:HA	9:I:63:ILE:O	2.19	0.43
11:K:21:ILE:HG12	11:K:30:VAL:HG22	1.99	0.43
23:X:47:LEU:HD11	23:X:55:PRO:HB2	2.01	0.43
1:A:558:G:H3'	1:A:559:A:H3'	2.01	0.43
1:A:858:G:H5''	1:A:869:G:O6	2.19	0.43
1:A:861:G:H2'	1:A:862:C:O4'	2.18	0.43
1:A:961:U:C4	1:A:1201:A:N6	2.69	0.43
1:A:1353:G:N2	1:A:1354:C:C2	2.87	0.43
1:A:1358:U:OP2	1:A:1359:C:H5	2.01	0.43
1:A:1422:G:C2	1:A:1479:C:C2	3.07	0.43
1:A:1444:C:H2'	1:A:1445:C:C6	2.54	0.43
2:B:186:ALA:HB3	2:B:197:VAL:HG11	2.01	0.43
4:D:128:VAL:HB	4:D:133:VAL:HG21	2.01	0.43
7:G:108:ALA:HB1	7:G:120:ILE:HG13	2.00	0.43
23:X:103:LEU:HA	23:X:106:ILE:HD12	2.00	0.43
1:A:44:G:N2	1:A:399:G:C4	2.87	0.43
1:A:115:G:O2'	1:A:289:G:H5''	2.19	0.43
1:A:197:A:H4'	1:A:198:G:OP1	2.17	0.43
1:A:349:A:H2'	1:A:350:G:O4'	2.19	0.43
1:A:407:G:C2	1:A:436:C:O2	2.71	0.43
1:A:542:G:C2	1:A:543:C:C2	3.07	0.43
1:A:763:G:C2	1:A:764:C:C2	3.06	0.43
1:A:1071:C:H2'	1:A:1072:G:C8	2.54	0.43
1:A:1508:G:H2'	1:A:1509:C:C6	2.54	0.43
1:A:1524:C:H2'	1:A:1525:G:O4'	2.18	0.43
6:F:7:ASN:ND2	18:R:34:TYR:OH	2.52	0.43
8:H:111:ILE:HG22	8:H:134:ILE:CD1	2.48	0.43
11:K:91:ARG:O	11:K:95:ILE:HG13	2.18	0.43
15:O:41:GLU:HA	15:O:44:LYS:HD2	1.99	0.43
17:Q:9:VAL:HG11	17:Q:84:LEU:HD23	2.01	0.43
20:T:15:ARG:NH1	20:T:15:ARG:CG	2.81	0.43
1:A:18:C:H4'	1:A:1078:U:O2	2.18	0.43
1:A:270:A:H2'	1:A:271:C:C6	2.54	0.43
1:A:636:U:H2'	1:A:637:G:H8	1.84	0.43
1:A:1001(A):G:C2	1:A:1002:G:C6	3.07	0.43
1:A:1481:U:H2'	1:A:1482:G:O4'	2.18	0.43
3:C:24:ALA:HB2	3:C:32:LEU:HD12	2.00	0.43
4:D:112:VAL:N	4:D:116:GLN:OE1	2.49	0.43
6:F:97:PHE:HB2	18:R:32:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:26:VAL:HA	9:I:61:ALA:O	2.19	0.43
10:J:61:GLU:OE1	10:J:63:PHE:CZ	2.72	0.43
13:M:4:ILE:HA	13:M:57:ARG:HG3	2.00	0.43
20:T:22:ARG:O	20:T:25:ARG:HG2	2.19	0.43
22:W:17:LEU:HB2	22:W:21:THR:HB	2.01	0.43
1:A:48:C:H4'	1:A:49:U:OP1	2.17	0.43
1:A:79:G:C4	1:A:80:G:C8	3.07	0.43
1:A:126:G:H2'	1:A:127:G:O4'	2.19	0.43
1:A:306:G:C6	1:A:307:C:C4	3.07	0.43
1:A:319:G:C6	1:A:320:C:C4	3.07	0.43
1:A:369:C:H2'	1:A:370:C:C6	2.54	0.43
1:A:628:G:H2'	1:A:629:G:O4'	2.19	0.43
1:A:988:G:C6	1:A:989:C:C4	3.07	0.43
1:A:1057:G:H2'	1:A:1058:G:O4'	2.19	0.43
1:A:1095:U:H2'	1:A:1096:C:O4'	2.18	0.43
7:G:46:ALA:HA	7:G:121:ALA:HB2	2.01	0.43
8:H:28:ALA:HB3	8:H:57:PRO:HB2	2.01	0.43
10:J:4:ILE:HD11	10:J:77:PRO:HA	2.00	0.43
12:L:32:PHE:CE1	12:L:86:ARG:HG3	2.54	0.43
1:A:39:G:N2	1:A:40:C:C2	2.87	0.42
1:A:48:C:H5'	1:A:365:U:O4	2.19	0.42
1:A:102:G:C2	1:A:103:C:C2	3.06	0.42
1:A:308:C:H2'	1:A:309:G:H8	1.84	0.42
1:A:768:A:C5	1:A:769:G:C8	3.07	0.42
1:A:920:U:H2'	1:A:921:U:C6	2.54	0.42
1:A:1074:G:C6	1:A:1075:C:N3	2.87	0.42
1:A:1462:G:N2	1:A:1463:C:C2	2.87	0.42
5:E:41:VAL:HG23	5:E:67:VAL:HB	2.01	0.42
5:E:107:ARG:HB2	5:E:107:ARG:HH11	1.83	0.42
9:I:125:TYR:CD2	9:I:125:TYR:O	2.70	0.42
1:A:124:G:C2	1:A:125:U:C2	3.07	0.42
1:A:294:U:O5'	1:A:294:U:H6	2.03	0.42
1:A:518:C:O2'	12:L:50:SER:HB3	2.18	0.42
1:A:545:C:O2'	1:A:549:C:H5''	2.19	0.42
1:A:708:C:H2'	1:A:709:G:H8	1.83	0.42
1:A:953:G:N7	13:M:104:ARG:NH2	2.67	0.42
1:A:986:A:H1'	19:S:54:GLY:O	2.19	0.42
1:A:1463:C:H2'	1:A:1464:G:H8	1.84	0.42
2:B:67:THR:H	2:B:160:ASP:HB2	1.84	0.42
2:B:103:THR:HA	2:B:180:LEU:HD21	2.01	0.42
8:H:87:SER:HA	8:H:93:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:17:LEU:HB3	22:W:18:PRO:HD2	2.01	0.42
1:A:173:U:H5'	1:A:197:A:O4'	2.19	0.42
1:A:279:A:O2'	1:A:280:C:OP2	2.27	0.42
1:A:784:C:N3	1:A:799:G:C2	2.87	0.42
1:A:1347:G:HO2'	1:A:1373:G:H1	1.66	0.42
8:H:104:ARG:O	8:H:105:ARG:C	2.57	0.42
14:N:7:ILE:O	14:N:7:ILE:HG22	2.18	0.42
1:A:34:C:H2'	1:A:35:G:H8	1.84	0.42
1:A:598:U:H4'	8:H:94:TYR:CG	2.54	0.42
1:A:620:C:H2'	1:A:621:A:O4'	2.19	0.42
1:A:736:C:H2'	1:A:737:A:H8	1.83	0.42
1:A:922:G:C2	1:A:923:A:C4	3.07	0.42
1:A:1095:U:H2'	1:A:1096:C:C6	2.54	0.42
1:A:1235:U:H2'	1:A:1236:A:O4'	2.20	0.42
1:A:1357:A:H2'	1:A:1358:U:C6	2.54	0.42
8:H:45:ILE:HG21	8:H:61:VAL:HG12	2.01	0.42
9:I:37:PHE:CE1	9:I:74:ILE:HG13	2.54	0.42
9:I:108:VAL:HG12	9:I:109:VAL:N	2.34	0.42
14:N:14:PRO:C	14:N:16:PHE:N	2.73	0.42
15:O:39:LEU:HD13	15:O:56:LEU:HB2	2.01	0.42
23:X:64:LYS:O	23:X:68:GLU:HG2	2.19	0.42
1:A:394:G:C6	1:A:395:C:C4	3.07	0.42
1:A:570:G:O6	1:A:873:A:C2	2.73	0.42
1:A:688:G:C6	1:A:689:C:C4	3.08	0.42
1:A:744:C:H2'	1:A:745:C:C6	2.55	0.42
1:A:961:U:N3	1:A:1201:A:C6	2.72	0.42
1:A:1345:U:C2	1:A:1377:A:C2	3.08	0.42
1:A:1495:U:H2'	1:A:1496:C:H6	1.84	0.42
7:G:111:ARG:CZ	7:G:122:HIS:HB3	2.49	0.42
8:H:91:ARG:HD3	12:L:7:ILE:HG21	2.01	0.42
8:H:108:GLY:HA3	8:H:138:TRP:HB3	2.01	0.42
15:O:23:GLY:O	15:O:28:GLN:NE2	2.52	0.42
24:Y:22:G:C2	24:Y:23:C:N3	2.88	0.42
1:A:192:U:H5''	20:T:57:ARG:HH21	1.84	0.42
1:A:419:C:C2	1:A:425:G:C2	3.08	0.42
1:A:1001(A):G:C6	1:A:1002:G:O6	2.73	0.42
1:A:1104:G:H5''	1:A:1104:G:H8	1.84	0.42
1:A:1125:U:O2'	1:A:1281:U:O2	2.36	0.42
1:A:1132:C:H2'	1:A:1133:G:C8	2.55	0.42
1:A:1233:G:C6	1:A:1234:C:C4	3.07	0.42
1:A:1283:G:N3	1:A:1283:G:H2'	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:C4	1:A:1373:G:C6	3.08	0.42
1:A:1349:A:H2'	1:A:1350:A:O4'	2.19	0.42
1:A:1500:A:O2'	1:A:1501:C:H5'	2.20	0.42
2:B:21:ARG:HG2	2:B:22:LYS:H	1.84	0.42
4:D:119:GLN:O	4:D:123:HIS:HD2	2.02	0.42
1:A:200:G:N2	1:A:218:C:C2	2.87	0.42
1:A:778:G:C2	1:A:779:C:C2	3.07	0.42
1:A:1054:C:H6	1:A:1054:C:H2'	1.65	0.42
1:A:1118:C:H1'	1:A:1179:A:C5	2.55	0.42
1:A:1168:A:H2'	1:A:1169:A:C8	2.55	0.42
1:A:1233:G:C6	1:A:1234:C:N4	2.87	0.42
1:A:1300:G:H1'	1:A:1301:U:C5	2.53	0.42
1:A:1311:G:N2	1:A:1327:C:C2	2.88	0.42
1:A:1370:G:O3'	9:I:12:GLU:HG3	2.12	0.42
1:A:1510:U:H2'	1:A:1511:G:C8	2.54	0.42
2:B:73:THR:HG23	2:B:95:GLN:O	2.20	0.42
3:C:202:ILE:HG22	3:C:204:LEU:HD23	2.01	0.42
19:S:51:VAL:HG11	19:S:71:LEU:HD23	1.71	0.42
1:A:42:G:C2	1:A:43:C:C2	3.08	0.42
1:A:62:U:H5''	1:A:385:C:O2'	2.20	0.42
1:A:789:U:O4	23:X:86:LYS:NZ	2.53	0.42
1:A:908:A:H2'	1:A:909:A:H8	1.84	0.42
1:A:1022:G:H2'	1:A:1023:G:C8	2.54	0.42
1:A:1113:C:H2'	1:A:1114:C:C6	2.55	0.42
1:A:1262:C:H42	1:A:1273:G:H1	1.67	0.42
1:A:1445:C:C2	1:A:1458:G:C2	3.08	0.42
2:B:132:LYS:HA	2:B:135:GLN:HG2	2.01	0.42
2:B:217:ARG:HD3	2:B:217:ARG:HA	1.71	0.42
5:E:80:ILE:HG23	8:H:104:ARG:HH12	1.85	0.42
10:J:62:HIS:CD2	14:N:61:TRP:HH2	2.37	0.42
12:L:85:ILE:CG2	12:L:86:ARG:N	2.81	0.42
16:P:39:TYR:OH	16:P:41:PRO:HB3	2.19	0.42
17:Q:15:MET:HB2	17:Q:18:THR:HB	2.02	0.42
18:R:19:LYS:HG2	18:R:20:ALA:H	1.85	0.42
22:W:12:VAL:HA	22:W:51:ASP:O	2.20	0.42
23:X:152:MET:HB2	23:X:164:LEU:H	1.84	0.42
1:A:110:C:H2'	1:A:111:G:O4'	2.19	0.42
1:A:244:U:H4'	1:A:245:C:H5''	2.02	0.42
1:A:409:G:H5'	4:D:24:GLU:HB3	2.02	0.42
1:A:696:A:N3	1:A:786:G:O2'	2.52	0.42
1:A:926:G:H2'	1:A:1505:G:N3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:A:H2'	1:A:1015:A:C8	2.55	0.42
1:A:1240:U:H4'	7:G:38:LEU:HD11	2.02	0.42
1:A:1312:G:N2	1:A:1326:C:C2	2.88	0.42
1:A:1464:G:C2	1:A:1465:C:C4	3.08	0.42
2:B:25:ASN:HD21	2:B:27:LYS:N	2.17	0.42
9:I:20:ARG:HH21	9:I:62:TYR:HB3	1.85	0.42
11:K:91:ARG:O	11:K:95:ILE:HD12	2.20	0.42
12:L:24:VAL:HG13	12:L:98:TYR:HE1	1.85	0.42
16:P:1:MET:O	16:P:2:VAL:C	2.57	0.42
17:Q:9:VAL:HG12	17:Q:56:VAL:HB	2.00	0.42
17:Q:66:SER:HB3	17:Q:69:LYS:HB3	2.01	0.42
1:A:6:G:O6	5:E:95:ALA:N	2.43	0.42
1:A:79:G:O6	1:A:91:C:N3	2.52	0.42
1:A:122:G:C6	1:A:123:C:C4	3.07	0.42
1:A:199:G:C2	1:A:219:C:N3	2.88	0.42
1:A:224:C:H2'	1:A:225:C:C6	2.55	0.42
1:A:241:C:C2	1:A:286:G:C2	3.08	0.42
1:A:1001:A:OP2	1:A:1001:A:C8	2.68	0.42
1:A:1074:G:C6	1:A:1075:C:C4	3.07	0.42
7:G:22:LEU:HG	7:G:62:PHE:HE2	1.85	0.42
13:M:22:ILE:HG23	13:M:67:GLU:HG2	2.02	0.42
23:X:91:ARG:HH21	23:X:123:ARG:HH12	1.68	0.42
1:A:83:U:H2'	1:A:84:U:O4'	2.20	0.41
1:A:137:C:C2	1:A:227:G:C2	3.07	0.41
1:A:384:G:C2	1:A:385:C:C2	3.08	0.41
1:A:500:G:H2'	1:A:501:C:C6	2.55	0.41
1:A:568:G:C6	1:A:883:C:N4	2.88	0.41
1:A:641:U:H1'	1:A:642:A:N7	2.35	0.41
1:A:698:G:C2	1:A:699:C:N3	2.88	0.41
1:A:741:G:C5'	15:O:39:LEU:HD11	2.49	0.41
1:A:829:G:O2'	2:B:26:PRO:HD3	2.20	0.41
1:A:881:G:C6	1:A:882:C:C4	3.08	0.41
1:A:1101:A:N6	2:B:176:GLU:HG2	2.35	0.41
1:A:1243:C:H5''	21:V:8:THR:HG21	2.02	0.41
1:A:1350:A:C6	1:A:1351:U:N3	2.88	0.41
1:A:1410:G:H2'	1:A:1411:C:C6	2.55	0.41
2:B:25:ASN:ND2	2:B:25:ASN:C	2.73	0.41
3:C:180:ALA:HB1	3:C:182:ILE:HG13	2.02	0.41
5:E:90:VAL:O	5:E:120:THR:HA	2.21	0.41
1:A:16:A:C2	1:A:920:U:O2	2.73	0.41
1:A:70:G:N1	1:A:100:C:N3	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:C:N4	1:A:216:G:H1	2.18	0.41
1:A:473:G:H2'	1:A:474:G:H8	1.85	0.41
1:A:687:A:N1	1:A:700:G:O2'	2.47	0.41
1:A:765:G:C2	1:A:812:C:C2	3.08	0.41
1:A:955:U:H1'	1:A:1227:A:H61	1.83	0.41
1:A:1095:U:OP1	1:A:1108:G:N1	2.52	0.41
1:A:1134:G:C2	1:A:1141:C:N3	2.88	0.41
1:A:1288:A:H2'	1:A:1289:A:C8	2.55	0.41
1:A:1464:G:C6	1:A:1465:C:N4	2.88	0.41
6:F:4:TYR:O	6:F:64:GLN:HA	2.20	0.41
9:I:89:ASN:O	9:I:92:TYR:HB2	2.20	0.41
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.91	0.41
1:A:254:G:OP1	17:Q:67:LYS:O	2.37	0.41
1:A:262:A:H2'	1:A:263:A:C8	2.55	0.41
1:A:333:G:C6	1:A:334:C:N4	2.87	0.41
1:A:444:C:C2	1:A:491:G:C2	3.08	0.41
1:A:790:A:C6	1:A:791:G:C6	3.08	0.41
1:A:861:G:C2	1:A:862:C:C2	3.07	0.41
1:A:1144:G:C2	1:A:1145:C:N3	2.88	0.41
1:A:1311:G:C2	1:A:1327:C:C2	3.08	0.41
1:A:1513:A:C2	1:A:1523:G:C6	3.09	0.41
2:B:130:ARG:HA	2:B:130:ARG:NE	2.31	0.41
7:G:69:VAL:HG12	7:G:69:VAL:O	2.21	0.41
11:K:91:ARG:O	11:K:95:ILE:CD1	2.68	0.41
18:R:50:ILE:H	18:R:50:ILE:HG13	1.74	0.41
1:A:60:A:N7	1:A:110:C:N4	2.64	0.41
1:A:61:G:H5''	1:A:61:G:H8	1.84	0.41
1:A:236:G:C6	1:A:237:C:C4	3.08	0.41
1:A:389:A:C2	1:A:390:C:H1'	2.55	0.41
1:A:701:C:H1'	1:A:703:G:C6	2.54	0.41
1:A:1117:G:H21	1:A:1180:A:H1'	1.85	0.41
1:A:1216:G:H5''	14:N:5:ALA:CB	2.50	0.41
1:A:1392:G:N2	1:A:1502:A:C8	2.80	0.41
4:D:30:LYS:C	4:D:32:ALA:H	2.24	0.41
10:J:37:PRO:HA	10:J:72:VAL:HG22	2.00	0.41
14:N:26:ARG:HD3	14:N:47:LEU:HD11	2.02	0.41
1:A:188:C:H5'	20:T:89:ARG:HD3	2.02	0.41
1:A:610:G:C4	1:A:611:A:C8	3.08	0.41
1:A:725:G:N1	1:A:726:C:C4	2.87	0.41
1:A:1257:U:H4'	1:A:1258:G:O5'	2.21	0.41
1:A:1324:A:H2'	1:A:1325:C:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1389:C:H2'	1:A:1390:U:O4'	2.20	0.41
2:B:80:ILE:HG21	2:B:212:GLN:HA	2.01	0.41
10:J:38:ILE:HG23	10:J:71:LEU:CB	2.47	0.41
10:J:64:GLU:N	14:N:59:ALA:HB2	2.36	0.41
1:A:376:G:O2'	1:A:377:G:H5'	2.20	0.41
1:A:738:C:H2'	1:A:739:C:C6	2.56	0.41
1:A:952:U:H2'	1:A:953:G:C8	2.56	0.41
4:D:120:LEU:HD12	4:D:125:HIS:CD2	2.55	0.41
9:I:42:ARG:NH2	9:I:71:SER:OG	2.52	0.41
17:Q:57:VAL:HG12	17:Q:76:LEU:HA	2.03	0.41
23:X:92:VAL:CG1	23:X:132:LEU:HD13	2.50	0.41
1:A:435:C:H2'	1:A:436:C:C6	2.55	0.41
1:A:545:C:H5'	4:D:72:GLU:CB	2.51	0.41
1:A:582:U:C2	1:A:760:G:C6	3.09	0.41
1:A:860:A:H3'	1:A:861:G:H8	1.86	0.41
1:A:874:G:C6	1:A:875:C:C4	3.08	0.41
1:A:981:U:H5'	14:N:21:TYR:CE2	2.55	0.41
1:A:1231:G:C6	1:A:1232:U:C4	3.09	0.41
1:A:1507:A:C5'	1:A:1507:A:C8	3.04	0.41
11:K:91:ARG:HG2	11:K:92:GLU:N	2.35	0.41
19:S:10:PHE:HE2	19:S:37:ARG:HB3	1.85	0.41
1:A:19:C:O2	1:A:917:G:C2	2.73	0.41
1:A:22:G:C6	1:A:23:C:C4	3.08	0.41
1:A:66:G:C6	1:A:67:C:C4	3.09	0.41
1:A:411:A:OP2	4:D:25:ARG:NH2	2.52	0.41
1:A:568:G:C6	1:A:569:C:N4	2.89	0.41
1:A:570:G:C4	1:A:571:U:C5	3.09	0.41
1:A:643:C:H4'	8:H:31:PHE:CE2	2.55	0.41
1:A:810:C:H2'	1:A:811:C:O4'	2.20	0.41
1:A:895:G:C2	1:A:896:C:C2	3.08	0.41
1:A:903:G:C2	1:A:904:C:C2	3.08	0.41
1:A:1114:C:C2	1:A:1187:G:C2	3.09	0.41
3:C:28:GLN:H	3:C:28:GLN:CD	2.17	0.41
4:D:207:TYR:HD1	4:D:207:TYR:HA	1.70	0.41
8:H:84:ARG:HH11	8:H:84:ARG:HG3	1.85	0.41
12:L:53:ARG:HG3	12:L:69:TYR:HE1	1.85	0.41
13:M:10:PRO:CB	13:M:18:ALA:HB1	2.51	0.41
18:R:26:LEU:HD13	18:R:42:ARG:HG3	2.03	0.41
19:S:37:ARG:O	19:S:70:LYS:HG3	2.21	0.41
20:T:68:LYS:HE3	20:T:68:LYS:HA	2.03	0.41
1:A:21:G:N2	1:A:22:G:C2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189(L):G:C6	1:A:190:U:O4	2.74	0.41
1:A:264:U:O2	17:Q:64:PRO:HG2	2.21	0.41
1:A:279:A:C4	17:Q:98:LEU:HD12	2.56	0.41
1:A:319:G:N1	1:A:320:C:C2	2.89	0.41
1:A:376:G:H5''	16:P:5:ARG:HB2	2.02	0.41
1:A:542:G:N1	1:A:543:C:C4	2.88	0.41
1:A:734:G:C5	1:A:735:C:C4	3.09	0.41
1:A:826:C:H2'	1:A:827:U:H6	1.83	0.41
1:A:855:G:C2	1:A:856:C:C2	3.08	0.41
1:A:883:C:O2'	1:A:884:U:H5'	2.21	0.41
1:A:1255:G:H2'	1:A:1279:A:H62	1.86	0.41
1:A:1431:C:N3	1:A:1470:G:C2	2.89	0.41
1:A:1437:C:H2'	1:A:1438:G:C8	2.52	0.41
4:D:148:VAL:HG11	4:D:158:ILE:HG21	2.03	0.41
10:J:12:ASP:HB3	10:J:15:THR:HG22	2.03	0.41
12:L:10:LEU:HD12	12:L:10:LEU:HA	1.84	0.41
12:L:32:PHE:HB3	12:L:84:LEU:CD1	2.51	0.41
13:M:107:ALA:HB3	13:M:111:LYS:HE3	2.03	0.41
20:T:89:ARG:HD2	20:T:104:LEU:HD22	2.03	0.41
1:A:155:C:H42	1:A:166:G:H1	1.68	0.41
1:A:259:G:C2	1:A:268:C:C2	3.09	0.41
1:A:502:G:H2'	1:A:503:C:O4'	2.21	0.41
1:A:671:G:C2	1:A:736:C:C2	3.08	0.41
1:A:803:G:H2'	1:A:804:U:O4'	2.20	0.41
1:A:874:G:C2	1:A:875:C:C2	3.09	0.41
1:A:925:G:O2'	1:A:927:G:OP1	2.39	0.41
1:A:931:C:O2	1:A:1387:G:C2	2.74	0.41
1:A:1422:G:C2	1:A:1479:C:N3	2.88	0.41
1:A:1526:G:C2	1:A:1527:C:C2	3.09	0.41
11:K:87:THR:HG21	24:Y:28:A:O2'	2.20	0.41
12:L:41:ARG:HD2	12:L:43:VAL:HG23	2.03	0.41
1:A:113:G:N3	1:A:113:G:H2'	2.35	0.40
1:A:148:G:N2	1:A:175:C:C2	2.90	0.40
1:A:266:G:H8	1:A:266:G:C5'	2.34	0.40
1:A:399:G:C6	1:A:400:C:N4	2.89	0.40
1:A:768:A:H2'	1:A:769:G:O4'	2.21	0.40
1:A:881:G:H2'	1:A:882:C:O4'	2.22	0.40
1:A:929:G:C6	1:A:930:C:C4	3.09	0.40
1:A:977:A:O2'	1:A:979:C:OP2	2.28	0.40
1:A:1011:G:C6	1:A:1012:U:C4	3.09	0.40
1:A:1048:G:C2	1:A:1210:C:C2	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1500:A:H5''	1:A:1508:G:H5''	2.03	0.40
4:D:4:TYR:CE2	4:D:11:LEU:HD21	2.56	0.40
6:F:10:LEU:HA	6:F:85:VAL:HA	2.03	0.40
22:W:18:PRO:C	22:W:20:ALA:H	2.25	0.40
1:A:46:G:H2'	1:A:366:C:H5	1.82	0.40
1:A:725:G:H1	1:A:732:C:H42	1.69	0.40
1:A:798:G:H2'	1:A:799:G:O4'	2.21	0.40
1:A:977:A:C3'	1:A:978:A:H5''	2.51	0.40
1:A:1106:G:C2	1:A:1107:C:C2	3.09	0.40
1:A:1295:G:C6	1:A:1296:C:C4	3.09	0.40
1:A:1320:C:H4'	19:S:73:GLU:HG2	2.02	0.40
1:A:1541:U:H3	24:Y:24:A:H61	1.69	0.40
2:B:95:GLN:HG3	2:B:147:LYS:HG2	2.03	0.40
2:B:126:GLU:HG2	2:B:129:GLU:HB3	2.03	0.40
3:C:177:THR:OG1	3:C:180:ALA:HB2	2.22	0.40
7:G:62:PHE:HD1	7:G:124:LEU:CD2	2.33	0.40
8:H:84:ARG:O	8:H:135:CYS:HB2	2.20	0.40
12:L:10:LEU:O	12:L:14:GLY:N	2.53	0.40
12:L:85:ILE:HG22	12:L:86:ARG:N	2.35	0.40
16:P:20:VAL:HG21	16:P:32:TYR:CD2	2.56	0.40
1:A:506:G:C2	1:A:507:C:C2	3.09	0.40
1:A:663:A:H5''	18:R:61:LYS:HE3	2.03	0.40
1:A:769:G:H2'	1:A:769:G:N3	2.37	0.40
1:A:1320:C:C4'	19:S:73:GLU:OE2	2.69	0.40
4:D:201:GLN:HA	4:D:204:ILE:HD12	2.02	0.40
21:V:14:TRP:HE3	21:V:15:ARG:HG2	1.87	0.40
1:A:142:G:H2'	1:A:143:A:C8	2.57	0.40
1:A:333:G:C2	1:A:334:C:C4	3.09	0.40
1:A:518:C:C5	1:A:529:G:H3'	2.57	0.40
1:A:635:G:C6	1:A:636:U:C4	3.09	0.40
1:A:1216:G:C6	1:A:1217:C:N4	2.90	0.40
1:A:1371:G:P	9:I:12:GLU:HG2	2.57	0.40
1:A:1405:G:H2'	1:A:1406:U:C6	2.56	0.40
1:A:1457:G:H5''	20:T:35:THR:HG21	2.03	0.40
1:A:1476:G:C2	1:A:1477:C:C2	3.09	0.40
3:C:25:GLY:O	3:C:29:TYR:HB2	2.22	0.40
5:E:107:ARG:O	5:E:111:GLU:HB2	2.22	0.40
13:M:34:LEU:HD23	13:M:56:LEU:HD21	2.02	0.40
17:Q:53:LEU:HD23	17:Q:85:VAL:HG11	2.02	0.40
18:R:55:ARG:HA	18:R:55:ARG:HD2	1.88	0.40
1:A:72:C:OP1	1:A:72:C:C4'	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:G:O6	1:A:289:G:H1'	2.22	0.40
1:A:128:G:C2	1:A:234:C:O2	2.74	0.40
1:A:189(C):C:H2'	1:A:189(D):C:O4'	2.22	0.40
1:A:244:U:C6	1:A:894:G:N2	2.90	0.40
1:A:246:A:C4	1:A:282:A:N6	2.90	0.40
1:A:303:A:C4	1:A:304:U:C6	3.10	0.40
1:A:309:G:O2'	1:A:607:A:N1	2.48	0.40
1:A:572:A:N1	1:A:864:A:C5	2.90	0.40
1:A:657:G:N2	1:A:749:C:N3	2.60	0.40
1:A:730:G:C5	1:A:731:G:H1'	2.56	0.40
1:A:917:G:C6	1:A:918:A:C6	3.09	0.40
1:A:1010:G:H2'	1:A:1011:G:H8	1.84	0.40
1:A:1343:G:C5	1:A:1344:C:C4	3.09	0.40
4:D:33:MET:CA	4:D:36:ARG:O	2.69	0.40
4:D:63:LYS:HE3	4:D:63:LYS:HB2	1.83	0.40
11:K:62:GLN:CG	11:K:97:ALA:HB2	2.46	0.40
21:V:9:ARG:HD2	21:V:22:ARG:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	194 (84%)	28 (12%)	10 (4%)	2	19
3	C	204/239 (85%)	176 (86%)	23 (11%)	5 (2%)	4	29
4	D	206/209 (99%)	180 (87%)	23 (11%)	3 (2%)	8	39
5	E	148/162 (91%)	135 (91%)	10 (7%)	3 (2%)	6	34
6	F	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
7	G	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	6	34
8	H	136/138 (99%)	127 (93%)	7 (5%)	2 (2%)	8	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	125/128 (98%)	108 (86%)	13 (10%)	4 (3%)	3	25
10	J	96/105 (91%)	76 (79%)	16 (17%)	4 (4%)	2	19
11	K	118/129 (92%)	98 (83%)	16 (14%)	4 (3%)	3	25
12	L	122/132 (92%)	103 (84%)	15 (12%)	4 (3%)	3	25
13	M	115/126 (91%)	97 (84%)	15 (13%)	3 (3%)	4	28
14	N	58/61 (95%)	44 (76%)	10 (17%)	4 (7%)	1	11
15	O	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	11	43
16	P	81/88 (92%)	73 (90%)	6 (7%)	2 (2%)	4	29
17	Q	97/105 (92%)	82 (84%)	10 (10%)	5 (5%)	1	15
18	R	71/88 (81%)	61 (86%)	9 (13%)	1 (1%)	9	40
19	S	78/93 (84%)	66 (85%)	9 (12%)	3 (4%)	2	22
20	T	97/106 (92%)	84 (87%)	10 (10%)	3 (3%)	3	26
21	V	22/27 (82%)	20 (91%)	1 (4%)	1 (4%)	2	18
22	W	69/72 (96%)	55 (80%)	11 (16%)	3 (4%)	2	19
23	X	166/171 (97%)	145 (87%)	16 (10%)	5 (3%)	3	26
All	All	2579/2781 (93%)	2237 (87%)	269 (10%)	73 (3%)	6	27

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	29	ALA
3	C	192	THR
4	D	37	PRO
17	Q	66	SER
17	Q	98	LEU
19	S	6	LYS
21	V	3	LYS
22	W	20	ALA
23	X	54	PRO
2	B	21	ARG
2	B	130	ARG
2	B	207	ALA
2	B	229	VAL
4	D	170	VAL
7	G	55	GLY
9	I	56	LEU

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Mol	Chain	Res	Type
10	J	34	VAL
10	J	55	LYS
11	K	50	TYR
22	W	70	ARG
23	X	8	ASN
23	X	55	PRO
2	B	20	GLU
3	C	4	LYS
3	C	61	ALA
3	C	108	ASN
4	D	138	TYR
7	G	7	ALA
7	G	149	ARG
8	H	5	PRO
8	H	70	GLN
9	I	29	ASN
11	K	101	SER
12	L	28	LYS
12	L	76	ASN
14	N	14	PRO
15	O	5	LYS
16	P	2	VAL
16	P	31	LYS
17	Q	77	VAL
17	Q	96	GLU
17	Q	97	SER
19	S	35	SER
2	B	208	ILE
2	B	233	SER
9	I	54	ASP
9	I	58	HIS
14	N	17	LYS
14	N	32	SER
18	R	17	SER
19	S	30	LEU
20	T	49	ALA
20	T	95	ALA
22	W	2	LYS
23	X	23	GLY
23	X	81	LYS
5	E	38	GLN
10	J	54	PHE

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Mol	Chain	Res	Type
10	J	83	GLU
12	L	25	PRO
12	L	48	PRO
13	M	104	ARG
13	M	113	PRO
5	E	128	PRO
11	K	14	VAL
13	M	67	GLU
2	B	194	PRO
5	E	115	VAL
11	K	48	ILE
14	N	54	PRO
20	T	103	GLY
3	C	51	GLY

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	202/220 (92%)	142 (70%)	60 (30%)	0	2
3	C	160/188 (85%)	131 (82%)	29 (18%)	1	8
4	D	180/181 (99%)	146 (81%)	34 (19%)	1	7
5	E	115/123 (94%)	90 (78%)	25 (22%)	1	5
6	F	90/90 (100%)	72 (80%)	18 (20%)	1	6
7	G	126/127 (99%)	106 (84%)	20 (16%)	2	12
8	H	119/119 (100%)	90 (76%)	29 (24%)	0	4
9	I	96/99 (97%)	76 (79%)	20 (21%)	1	6
10	J	87/92 (95%)	75 (86%)	12 (14%)	3	17
11	K	91/99 (92%)	72 (79%)	19 (21%)	1	6
12	L	104/109 (95%)	79 (76%)	25 (24%)	0	4
13	M	94/101 (93%)	79 (84%)	15 (16%)	2	12
14	N	49/50 (98%)	41 (84%)	8 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	79/80 (99%)	64 (81%)	15 (19%)	1	7
16	P	72/74 (97%)	59 (82%)	13 (18%)	1	8
17	Q	94/97 (97%)	76 (81%)	18 (19%)	1	7
18	R	64/77 (83%)	52 (81%)	12 (19%)	1	7
19	S	71/80 (89%)	59 (83%)	12 (17%)	1	10
20	T	76/82 (93%)	55 (72%)	21 (28%)	0	3
21	V	19/22 (86%)	15 (79%)	4 (21%)	1	5
22	W	62/63 (98%)	51 (82%)	11 (18%)	1	9
23	X	145/150 (97%)	123 (85%)	22 (15%)	2	14
All	All	2195/2323 (94%)	1753 (80%)	442 (20%)	3	6

All (442) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	10	LEU
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	22	LYS
2	B	23	ARG
2	B	25	ASN
2	B	28	PHE
2	B	30	ARG
2	B	39	ILE
2	B	44	LEU
2	B	48	MET
2	B	51	LEU
2	B	53	ARG
2	B	55	PHE
2	B	59	GLU
2	B	60	ASP
2	B	61	LEU
2	B	75	LYS
2	B	79	ASP
2	B	83	MET
2	B	95	GLN
2	B	96	ARG

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Mol	Chain	Res	Type
2	B	97	TRP
2	B	101	MET
2	B	107	THR
2	B	110	GLN
2	B	111	ARG
2	B	112	VAL
2	B	113	HIS
2	B	114	ARG
2	B	115	LEU
2	B	116	GLU
2	B	118	LEU
2	B	121	LEU
2	B	126	GLU
2	B	130	ARG
2	B	135	GLN
2	B	140	HIS
2	B	144	ARG
2	B	145	LEU
2	B	155	LEU
2	B	157	ARG
2	B	165	VAL
2	B	168	THR
2	B	172	ILE
2	B	176	GLU
2	B	178	ARG
2	B	180	LEU
2	B	187	LEU
2	B	189	ASP
2	B	196	LEU
2	B	198	ASP
2	B	205	ASP
2	B	211	ILE
2	B	217	ARG
2	B	229	VAL
2	B	231	GLU
3	C	3	ASN
3	C	12	LEU
3	C	14	ILE
3	C	16	ARG
3	C	28	GLN
3	C	30	ARG
3	C	33	LEU

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Mol	Chain	Res	Type
3	C	34	LEU
3	C	36	ASP
3	C	44	GLU
3	C	45	LYS
3	C	56	ASP
3	C	70	VAL
3	C	82	GLU
3	C	89	GLU
3	C	94	LEU
3	C	127	ARG
3	C	131	ARG
3	C	132	ARG
3	C	135	LYS
3	C	138	VAL
3	C	162	GLN
3	C	166	GLU
3	C	172	ARG
3	C	188	LEU
3	C	190	ARG
3	C	191	THR
3	C	201	TYR
3	C	204	LEU
4	D	3	ARG
4	D	10	ARG
4	D	26	CYS
4	D	34	GLU
4	D	35	ARG
4	D	36	ARG
4	D	42	GLN
4	D	49	ARG
4	D	50	ARG
4	D	58	LEU
4	D	59	ARG
4	D	61	LYS
4	D	64	LEU
4	D	65	ARG
4	D	66	ARG
4	D	70	ILE
4	D	83	SER
4	D	92	VAL
4	D	104	VAL
4	D	110	PHE

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Mol	Chain	Res	Type
4	D	114	ARG
4	D	122	ARG
4	D	127	THR
4	D	131	ARG
4	D	132	ARG
4	D	139	ARG
4	D	140	VAL
4	D	141	ARG
4	D	155	LEU
4	D	157	LEU
4	D	165	MET
4	D	176	LEU
4	D	181	MET
4	D	207	TYR
5	E	10	MET
5	E	13	ILE
5	E	14	ARG
5	E	15	ARG
5	E	19	MET
5	E	20	GLN
5	E	24	ARG
5	E	34	VAL
5	E	38	GLN
5	E	40	ARG
5	E	41	VAL
5	E	47	LYS
5	E	64	ARG
5	E	71	LEU
5	E	80	ILE
5	E	89	ILE
5	E	91	LEU
5	E	107	ARG
5	E	116	THR
5	E	117	ASP
5	E	118	ILE
5	E	136	MET
5	E	137	GLU
5	E	144	THR
5	E	150	ARG
6	F	3	ARG
6	F	8	ILE
6	F	15	ASP

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Mol	Chain	Res	Type
6	F	24	GLU
6	F	27	GLN
6	F	28	ARG
6	F	31	GLU
6	F	32	ASN
6	F	36	ARG
6	F	39	LYS
6	F	40	VAL
6	F	47	ARG
6	F	61	LEU
6	F	75	LEU
6	F	77	ARG
6	F	87	ARG
6	F	89	MET
6	F	94	GLN
7	G	6	ARG
7	G	16	LEU
7	G	37	ASN
7	G	59	LEU
7	G	72	ARG
7	G	74	GLU
7	G	75	VAL
7	G	94	ARG
7	G	95	ARG
7	G	96	GLN
7	G	104	LEU
7	G	106	GLN
7	G	115	ARG
7	G	126	ASP
7	G	137	LYS
7	G	139	GLU
7	G	141	VAL
7	G	142	GLU
7	G	149	ARG
7	G	156	TRP
8	H	1	MET
8	H	8	ASP
8	H	18	ARG
8	H	26	VAL
8	H	29	SER
8	H	30	ARG
8	H	31	PHE

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Mol	Chain	Res	Type
8	H	34	GLU
8	H	39	LEU
8	H	41	ARG
8	H	45	ILE
8	H	50	ARG
8	H	56	LYS
8	H	59	LEU
8	H	70	GLN
8	H	77	GLU
8	H	78	GLN
8	H	79	VAL
8	H	80	ILE
8	H	82	HIS
8	H	92	ARG
8	H	102	ARG
8	H	105	ARG
8	H	112	LEU
8	H	116	LYS
8	H	119	LEU
8	H	120	THR
8	H	121	ASP
8	H	127	LEU
9	I	12	GLU
9	I	14	VAL
9	I	25	LYS
9	I	38	GLN
9	I	40	LEU
9	I	48	GLU
9	I	54	ASP
9	I	71	SER
9	I	75	ASP
9	I	85	LEU
9	I	95	LYS
9	I	99	LEU
9	I	102	LEU
9	I	104	ARG
9	I	116	LYS
9	I	117	HIS
9	I	118	LYS
9	I	121	ARG
9	I	124	GLN
9	I	125	TYR

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Mol	Chain	Res	Type
10	J	4	ILE
10	J	16	LEU
10	J	57	LYS
10	J	61	GLU
10	J	65	LEU
10	J	67	THR
10	J	71	LEU
10	J	74	ILE
10	J	75	ILE
10	J	82	ILE
10	J	85	LEU
10	J	87	THR
11	K	16	SER
11	K	18	ARG
11	K	32	ILE
11	K	34	ASP
11	K	47	VAL
11	K	54	ARG
11	K	55	LYS
11	K	57	THR
11	K	77	MET
11	K	80	VAL
11	K	84	VAL
11	K	85	ARG
11	K	93	GLN
11	K	98	LEU
11	K	101	SER
11	K	109	VAL
11	K	110	ASP
11	K	116	HIS
11	K	117	ASN
12	L	7	ILE
12	L	10	LEU
12	L	27	LEU
12	L	33	ARG
12	L	34	ARG
12	L	39	VAL
12	L	41	ARG
12	L	42	THR
12	L	46	LYS
12	L	53	ARG
12	L	55	VAL

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Mol	Chain	Res	Type
12	L	59	ARG
12	L	65	GLU
12	L	67	THR
12	L	70	ILE
12	L	79	GLU
12	L	81	SER
12	L	82	VAL
12	L	89	ARG
12	L	91	LYS
12	L	97	ARG
12	L	104	VAL
12	L	106	ASP
12	L	113	ARG
12	L	114	LYS
13	M	3	ARG
13	M	9	ILE
13	M	11	ARG
13	M	27	LYS
13	M	32	GLU
13	M	45	VAL
13	M	46	LYS
13	M	65	LYS
13	M	66	LEU
13	M	71	ARG
13	M	77	ASN
13	M	90	LEU
13	M	101	GLN
13	M	105	THR
13	M	115	LYS
14	N	3	ARG
14	N	4	LYS
14	N	12	ARG
14	N	16	PHE
14	N	17	LYS
14	N	21	TYR
14	N	31	ARG
14	N	41	ARG
15	O	4	THR
15	O	10	LYS
15	O	17	ARG
15	O	22	THR
15	O	28	GLN

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Mol	Chain	Res	Type
15	O	34	LEU
15	O	35	ARG
15	O	56	LEU
15	O	58	MET
15	O	64	ARG
15	O	65	ARG
15	O	66	LEU
15	O	70	LEU
15	O	79	ARG
15	O	88	ARG
16	P	1	MET
16	P	8	ARG
16	P	12	LYS
16	P	20	VAL
16	P	22	THR
16	P	28	ARG
16	P	45	THR
16	P	49	LEU
16	P	50	LYS
16	P	71	ARG
16	P	72	ARG
16	P	73	LEU
16	P	81	ARG
17	Q	15	MET
17	Q	16	GLN
17	Q	22	LEU
17	Q	25	ARG
17	Q	34	LYS
17	Q	38	ARG
17	Q	53	LEU
17	Q	63	ARG
17	Q	65	ILE
17	Q	66	SER
17	Q	75	ARG
17	Q	76	LEU
17	Q	84	LEU
17	Q	90	ILE
17	Q	92	ARG
17	Q	93	GLN
17	Q	98	LEU
17	Q	100	LYS
18	R	19	LYS

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Mol	Chain	Res	Type
18	R	31	LEU
18	R	36	ASN
18	R	37	VAL
18	R	38	GLU
18	R	47	THR
18	R	53	ARG
18	R	54	ARG
18	R	68	LYS
18	R	69	THR
18	R	75	ILE
18	R	78	LEU
19	S	3	ARG
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	15	LEU
19	S	18	LYS
19	S	25	LYS
19	S	39	THR
19	S	41	VAL
19	S	63	THR
19	S	67	VAL
19	S	77	THR
20	T	8	ARG
20	T	11	SER
20	T	13	LEU
20	T	14	LYS
20	T	15	ARG
20	T	19	SER
20	T	22	ARG
20	T	23	ARG
20	T	46	GLU
20	T	51	GLU
20	T	54	LYS
20	T	55	ILE
20	T	57	ARG
20	T	62	LEU
20	T	64	ASP
20	T	68	LYS
20	T	74	LYS
20	T	75	ASN
20	T	83	ARG

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Mol	Chain	Res	Type
20	T	84	LEU
20	T	90	GLN
21	V	6	ARG
21	V	9	ARG
21	V	10	ARG
21	V	12	LYS
22	W	15	GLU
22	W	19	ASN
22	W	22	PHE
22	W	23	ARG
22	W	32	ILE
22	W	33	LEU
22	W	47	ILE
22	W	48	LEU
22	W	51	ASP
22	W	58	THR
22	W	68	VAL
23	X	22	ASP
23	X	35	LEU
23	X	69	GLN
23	X	87	SER
23	X	91	ARG
23	X	93	LYS
23	X	95	ASP
23	X	98	ASP
23	X	100	GLN
23	X	119	THR
23	X	120	ILE
23	X	121	MET
23	X	123	ARG
23	X	132	LEU
23	X	134	GLU
23	X	135	ARG
23	X	147	LEU
23	X	156	MET
23	X	160	ASP
23	X	162	ASN
23	X	163	MET
23	X	164	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
2	B	40	HIS
2	B	95	GLN
2	B	204	ASN
3	C	3	ASN
3	C	108	ASN
3	C	176	HIS
4	D	77	ASN
4	D	123	HIS
4	D	125	HIS
4	D	129	ASN
4	D	201	GLN
5	E	20	GLN
5	E	72	GLN
6	F	7	ASN
6	F	11	ASN
6	F	13	ASN
6	F	100	ASN
8	H	82	HIS
9	I	3	GLN
9	I	117	HIS
9	I	124	GLN
10	J	62	HIS
11	K	117	ASN
12	L	8	ASN
12	L	49	ASN
12	L	75	HIS
13	M	106	ASN
15	O	37	ASN
15	O	62	GLN
17	Q	16	GLN
20	T	26	ASN
20	T	75	ASN
23	X	69	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	447 (29%)	99 (6%)
24	Y	19/42 (45%)	12 (63%)	2 (10%)
All	All	1527/1564 (97%)	459 (30%)	101 (6%)

All (459) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	31	G
1	A	32	A
1	A	35	G
1	A	39	G
1	A	44	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	53	A
1	A	54	C
1	A	58	C
1	A	63	C
1	A	72	C
1	A	77	G
1	A	78	G
1	A	79	G
1	A	81	U
1	A	82	U
1	A	90	U
1	A	91	C
1	A	92	C
1	A	96	U
1	A	98	G
1	A	105	G
1	A	108	G
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	142	G
1	A	144	G
1	A	151	A

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Mol	Chain	Res	Type
1	A	152	A
1	A	163	C
1	A	181	G
1	A	182	U
1	A	187	C
1	A	189(D)	C
1	A	189(E)	U
1	A	189(F)	U
1	A	189(G)	G
1	A	189(H)	G
1	A	195	A
1	A	197	A
1	A	198	G
1	A	201	C
1	A	203	U
1	A	204	U
1	A	219	C
1	A	220	G
1	A	222	U
1	A	223	U
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	272	C
1	A	279	A
1	A	280	C
1	A	281	G
1	A	282	A
1	A	283	C
1	A	289	G
1	A	296	U
1	A	298	A
1	A	301	G
1	A	303	A
1	A	306	G
1	A	315	A
1	A	316	G
1	A	319	G
1	A	321	A

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Mol	Chain	Res	Type
1	A	324	G
1	A	325	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	342	C
1	A	344	A
1	A	345	C
1	A	346	G
1	A	348	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	369	C
1	A	372	C
1	A	373	A
1	A	375	U
1	A	378	G
1	A	379	C
1	A	381	C
1	A	390	C
1	A	392	G
1	A	395	C
1	A	397	A
1	A	398	C
1	A	399	G
1	A	406	G
1	A	412	A
1	A	413	G
1	A	419	C
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	426	G
1	A	428	G
1	A	429	U
1	A	438	G
1	A	439	A

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Mol	Chain	Res	Type
1	A	441	A
1	A	452	A
1	A	453	A
1	A	470	C
1	A	472	A
1	A	477	A
1	A	484	G
1	A	485	G
1	A	486	U
1	A	495	A
1	A	496	A
1	A	498	U
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	521	G
1	A	524	G
1	A	527	G
1	A	528	C
1	A	529	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U
1	A	535	A
1	A	542	G
1	A	545	C
1	A	546	G
1	A	547	A
1	A	550	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	574	A

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Mol	Chain	Res	Type
1	A	576	G
1	A	577	G
1	A	578	C
1	A	579	G
1	A	582	U
1	A	587	G
1	A	595	G
1	A	596	C
1	A	607	A
1	A	617	G
1	A	618	C
1	A	619	U
1	A	641	U
1	A	642	A
1	A	653	A
1	A	654	G
1	A	662	G
1	A	665	A
1	A	666	G
1	A	671	G
1	A	672	U
1	A	673	G
1	A	678	U
1	A	687	A
1	A	688	G
1	A	692	U
1	A	693	G
1	A	695	A
1	A	697	U
1	A	701	C
1	A	702	A
1	A	703	G
1	A	715	A
1	A	717	C
1	A	720	C
1	A	721	G
1	A	723	U
1	A	728	A
1	A	729	A
1	A	731	G
1	A	748	C
1	A	749	C

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Mol	Chain	Res	Type
1	A	753	A
1	A	755	G
1	A	759	A
1	A	762	C
1	A	774	G
1	A	777	A
1	A	782	A
1	A	786	G
1	A	787	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	799	G
1	A	812	C
1	A	815	A
1	A	816	A
1	A	817	C
1	A	819	A
1	A	821	G
1	A	828	A
1	A	835	U
1	A	839	U
1	A	840	C
1	A	841	U
1	A	849	C
1	A	851	G
1	A	867	G
1	A	871	U
1	A	873	A
1	A	876	G
1	A	883	C
1	A	884	U
1	A	885	G
1	A	888	G
1	A	889	A
1	A	891	U
1	A	900	A
1	A	911	U
1	A	914	A
1	A	922	G
1	A	926	G

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Mol	Chain	Res	Type
1	A	927	G
1	A	931	C
1	A	932	C
1	A	933	G
1	A	934	C
1	A	935	A
1	A	938	A
1	A	942	G
1	A	945	G
1	A	946	A
1	A	947	G
1	A	960	U
1	A	961	U
1	A	966	G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	984	C
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1000	U
1	A	1001	A
1	A	1002	G
1	A	1003	G
1	A	1005	A
1	A	1007	C
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1028	C
1	A	1029	C
1	A	1038	C
1	A	1042	G
1	A	1045	C

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Mol	Chain	Res	Type
1	A	1046	A
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1070	U
1	A	1078	U
1	A	1086	U
1	A	1089	G
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1100	C
1	A	1101	A
1	A	1102	A
1	A	1103	C
1	A	1104	G
1	A	1108	G
1	A	1117	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1146	A
1	A	1151	A
1	A	1152	A
1	A	1157	A
1	A	1159	U
1	A	1169	A

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Mol	Chain	Res	Type
1	A	1177	G
1	A	1183	A
1	A	1184	G
1	A	1185	G
1	A	1191	A
1	A	1195	C
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1209	C
1	A	1212	U
1	A	1213	A
1	A	1215	G
1	A	1221	G
1	A	1226	C
1	A	1227	A
1	A	1231	G
1	A	1236	A
1	A	1238	A
1	A	1239	A
1	A	1240	U
1	A	1249	C
1	A	1250	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1266	G
1	A	1267	C
1	A	1270	C
1	A	1277	C
1	A	1278	U
1	A	1279	A
1	A	1281	U
1	A	1283	G
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1288	A

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Mol	Chain	Res	Type
1	A	1296	C
1	A	1297	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1315	U
1	A	1316	G
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1323	G
1	A	1331	G
1	A	1332	A
1	A	1335	C
1	A	1336	C
1	A	1337	G
1	A	1340	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1357	A
1	A	1363	C
1	A	1363(A)	A
1	A	1364	U
1	A	1368	G
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1380	U
1	A	1381	U
1	A	1388	C
1	A	1394	A
1	A	1397	C
1	A	1398	A
1	A	1399	C
1	A	1400	C
1	A	1415	G
1	A	1434	A
1	A	1442	G

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Mol	Chain	Res	Type
1	A	1443	G
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1457	G
1	A	1459	C
1	A	1486	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1519	A
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1532	U
1	A	1536	C
1	A	1538	C
24	Y	23	C
24	Y	24	A
24	Y	28	A
24	Y	30	G
24	Y	32	A
24	Y	33	A
24	Y	34	A
24	Y	35	A
24	Y	36	A
24	Y	37	U
24	Y	38	G
24	Y	39	U

All (101) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	A	7	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	77	G
1	A	108	G
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	197	A
1	A	202	U
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	279	A
1	A	280	C
1	A	281	G
1	A	288	A
1	A	329	A
1	A	344	A
1	A	351	G
1	A	372	C
1	A	389	A
1	A	421	U
1	A	428	G
1	A	484	G
1	A	495	A
1	A	496	A
1	A	509	A
1	A	518	C
1	A	531	U
1	A	535	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	576	G
1	A	595	G
1	A	641	U
1	A	672	U

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Mol	Chain	Res	Type
1	A	687	A
1	A	701	C
1	A	702	A
1	A	717	C
1	A	748	C
1	A	792	A
1	A	820	U
1	A	840	C
1	A	872	A
1	A	873	A
1	A	897	C
1	A	934	C
1	A	946	A
1	A	965	A
1	A	975	A
1	A	992	U
1	A	993	G
1	A	1000	U
1	A	1049	U
1	A	1054	C
1	A	1064	G
1	A	1065	U
1	A	1085	U
1	A	1101	A
1	A	1126	U
1	A	1128	C
1	A	1137	C
1	A	1145	C
1	A	1151	A
1	A	1182	G
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1211	U
1	A	1212	U
1	A	1214	C
1	A	1239	A
1	A	1257	U
1	A	1266	G
1	A	1278	U
1	A	1285	A
1	A	1299	A

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Mol	Chain	Res	Type
1	A	1300	G
1	A	1301	U
1	A	1322	C
1	A	1331	G
1	A	1346	A
1	A	1363(A)	A
1	A	1380	U
1	A	1399	C
1	A	1442(B)	A
1	A	1447	A
1	A	1452	C
1	A	1493	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1507	A
24	Y	32	A
24	Y	33	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 129 ligands modelled in this entry, 129 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	84:U	O3'	88:A	P	5.75
1	A	1442(A):G	O3'	1442(B):A	P	5.10
1	A	841:U	O3'	848:C	P	4.14
1	A	204:U	O3'	216:G	P	3.78

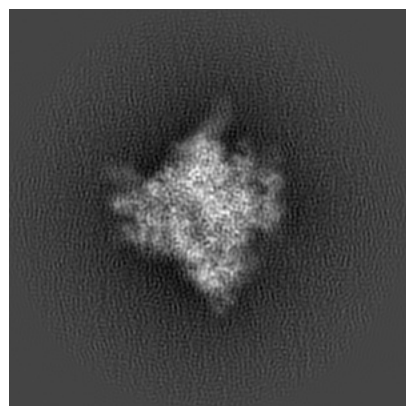
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4073. These allow visual inspection of the internal detail of the map and identification of artifacts.

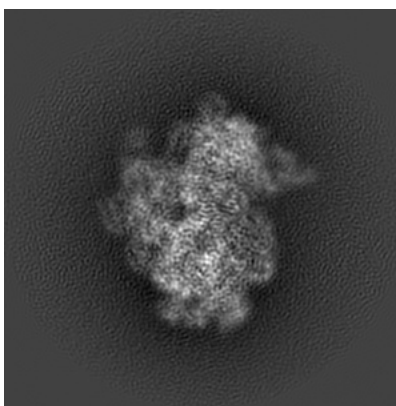
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

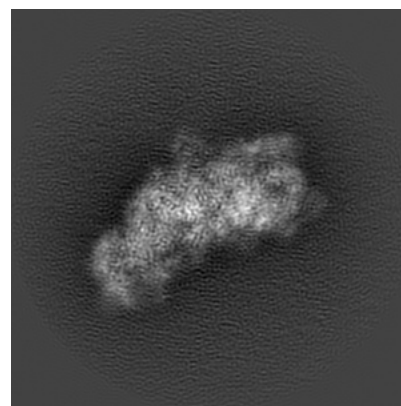
6.1.1 Primary map



X

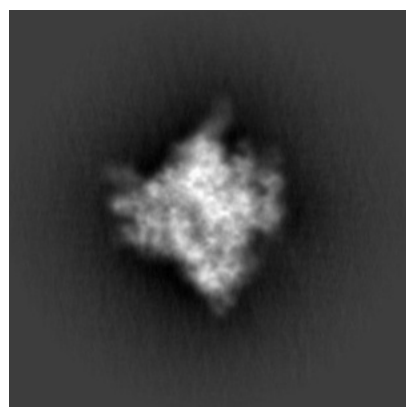


Y

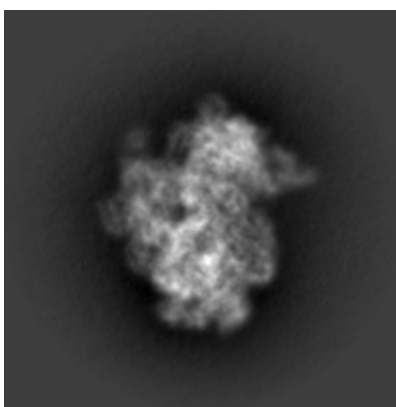


Z

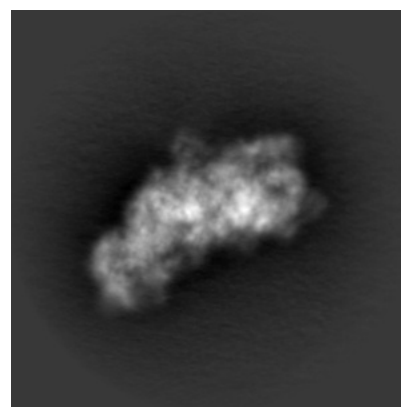
6.1.2 Raw map



X



Y

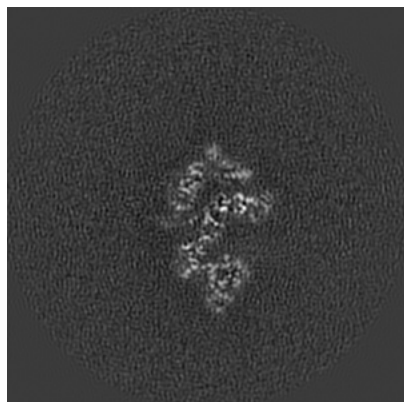


Z

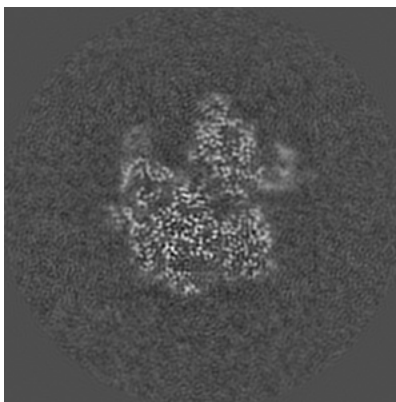
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

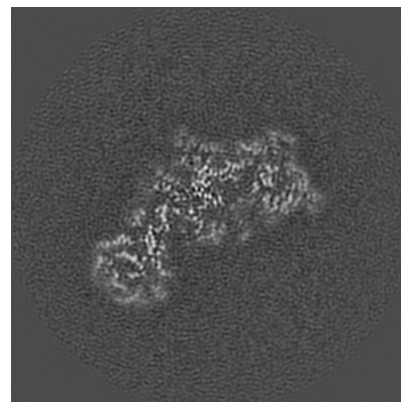
6.2.1 Primary map



X Index: 130

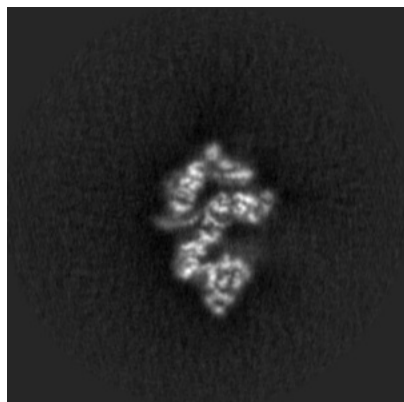


Y Index: 130

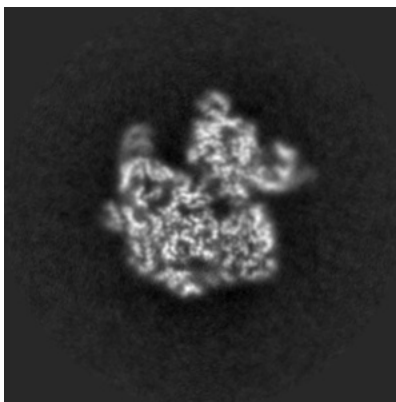


Z Index: 130

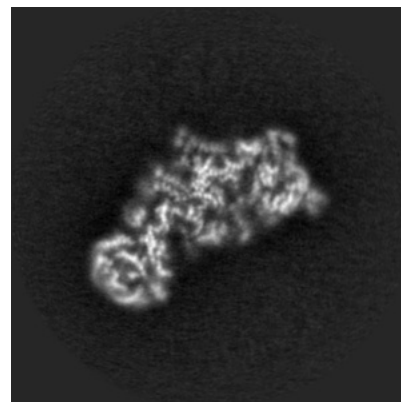
6.2.2 Raw map



X Index: 130



Y Index: 130

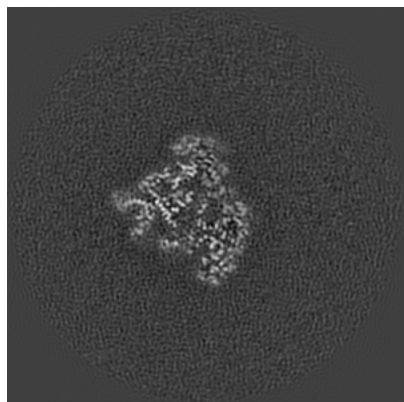


Z Index: 130

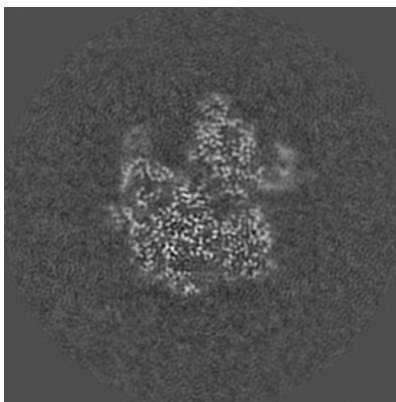
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

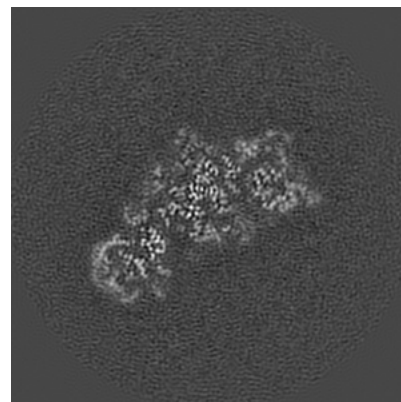
6.3.1 Primary map



X Index: 95

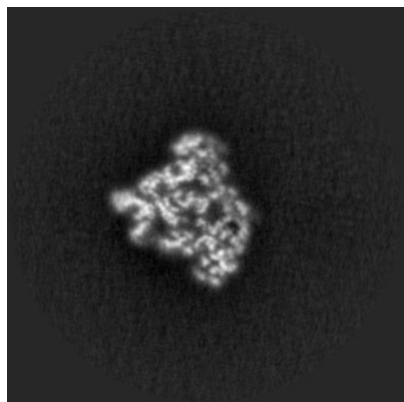


Y Index: 130

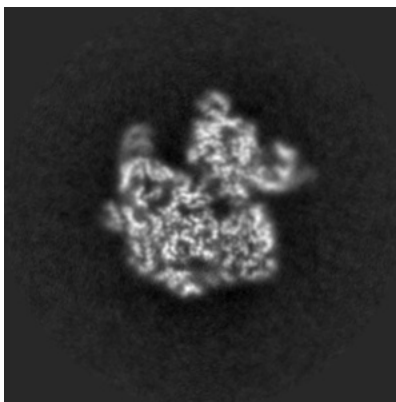


Z Index: 128

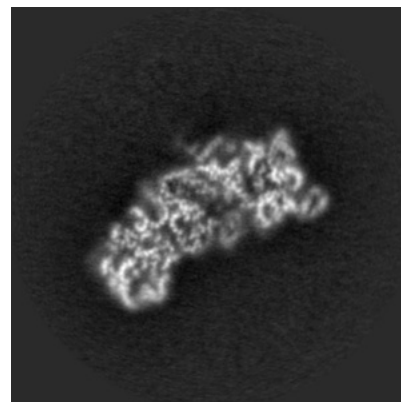
6.3.2 Raw map



X Index: 96



Y Index: 130

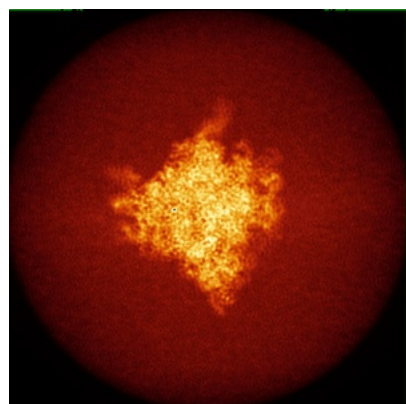


Z Index: 136

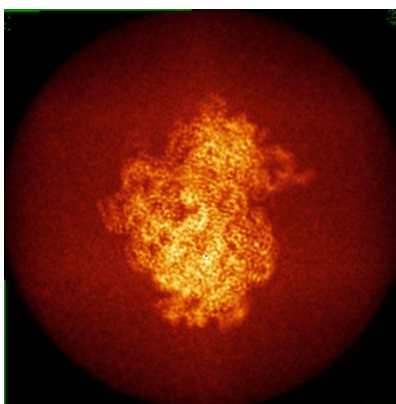
The images above show the largest variance slices of the map in three orthogonal directions.

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

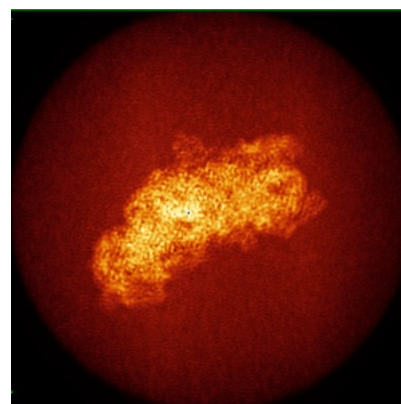
6.4.1 Primary map



X



Y



Z

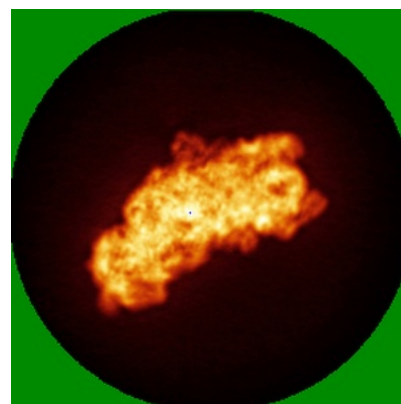
6.4.2 Raw map



X



Y

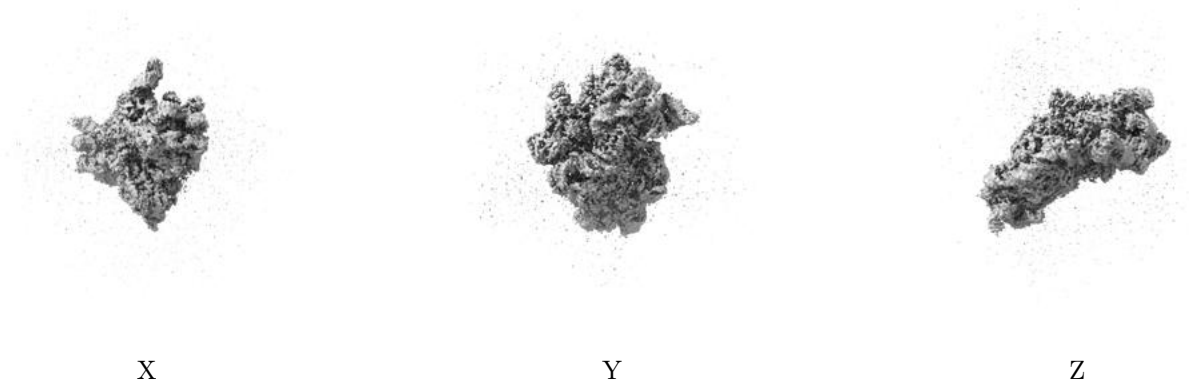


Z

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

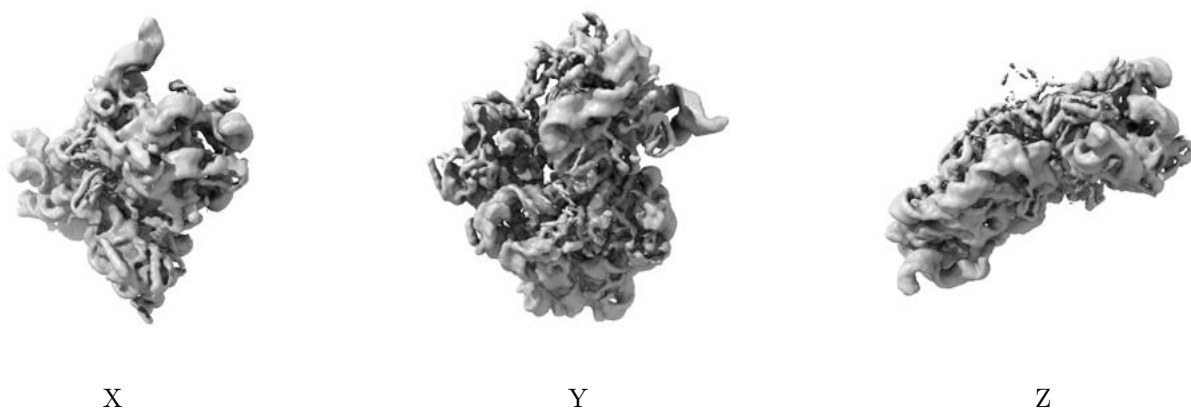
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

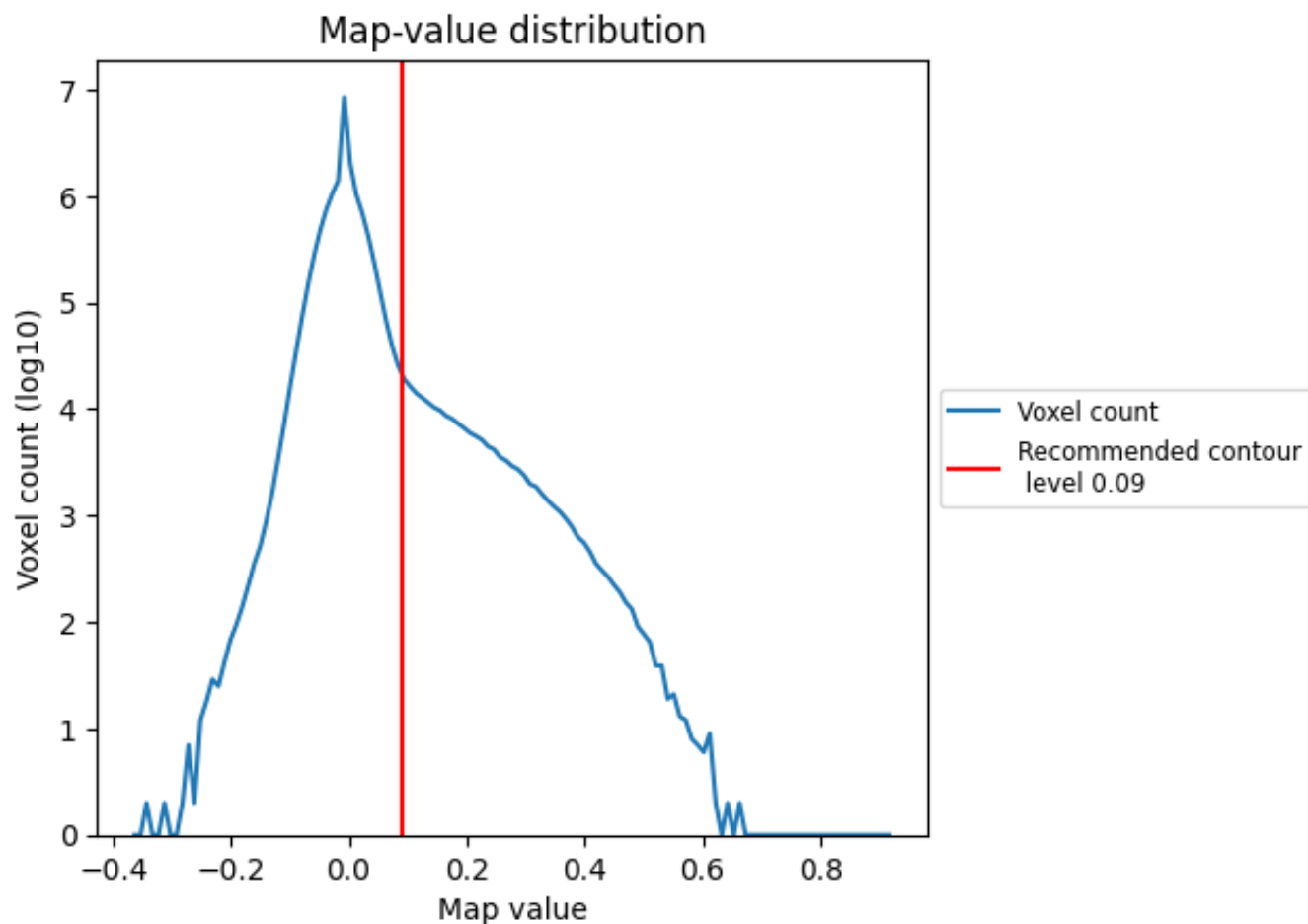
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

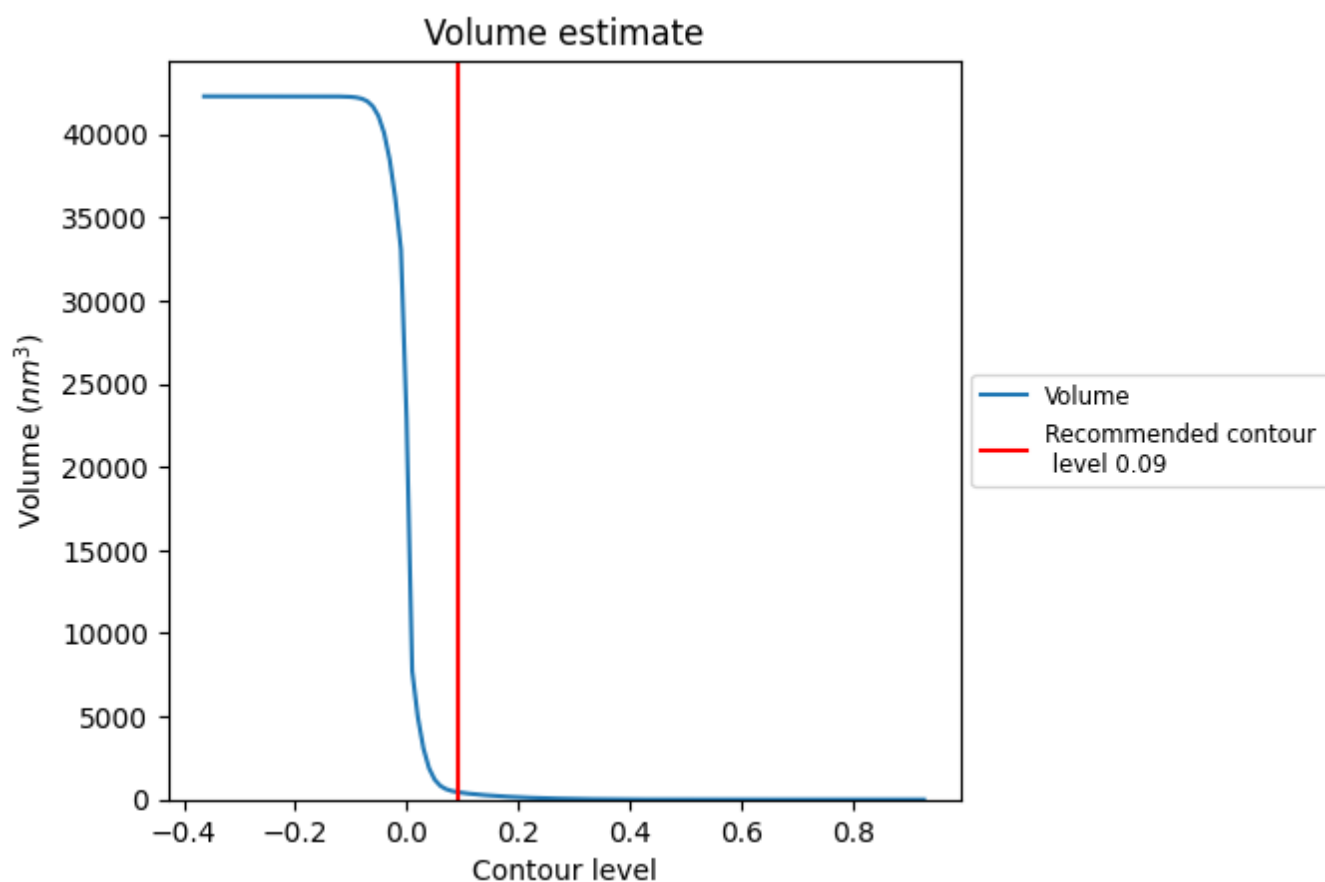
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

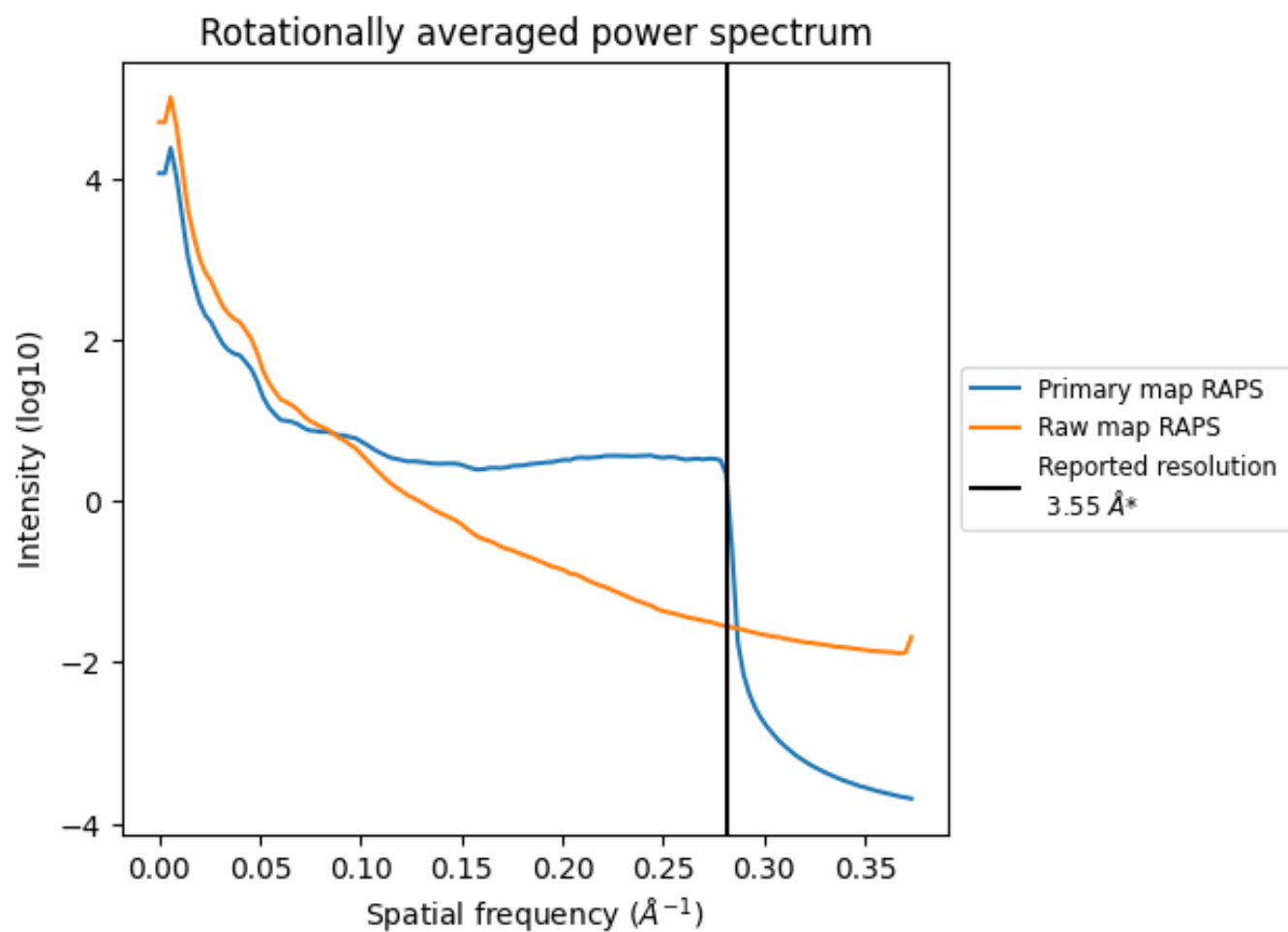
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 454 nm^3 ; this corresponds to an approximate mass of 410 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 ⓘ

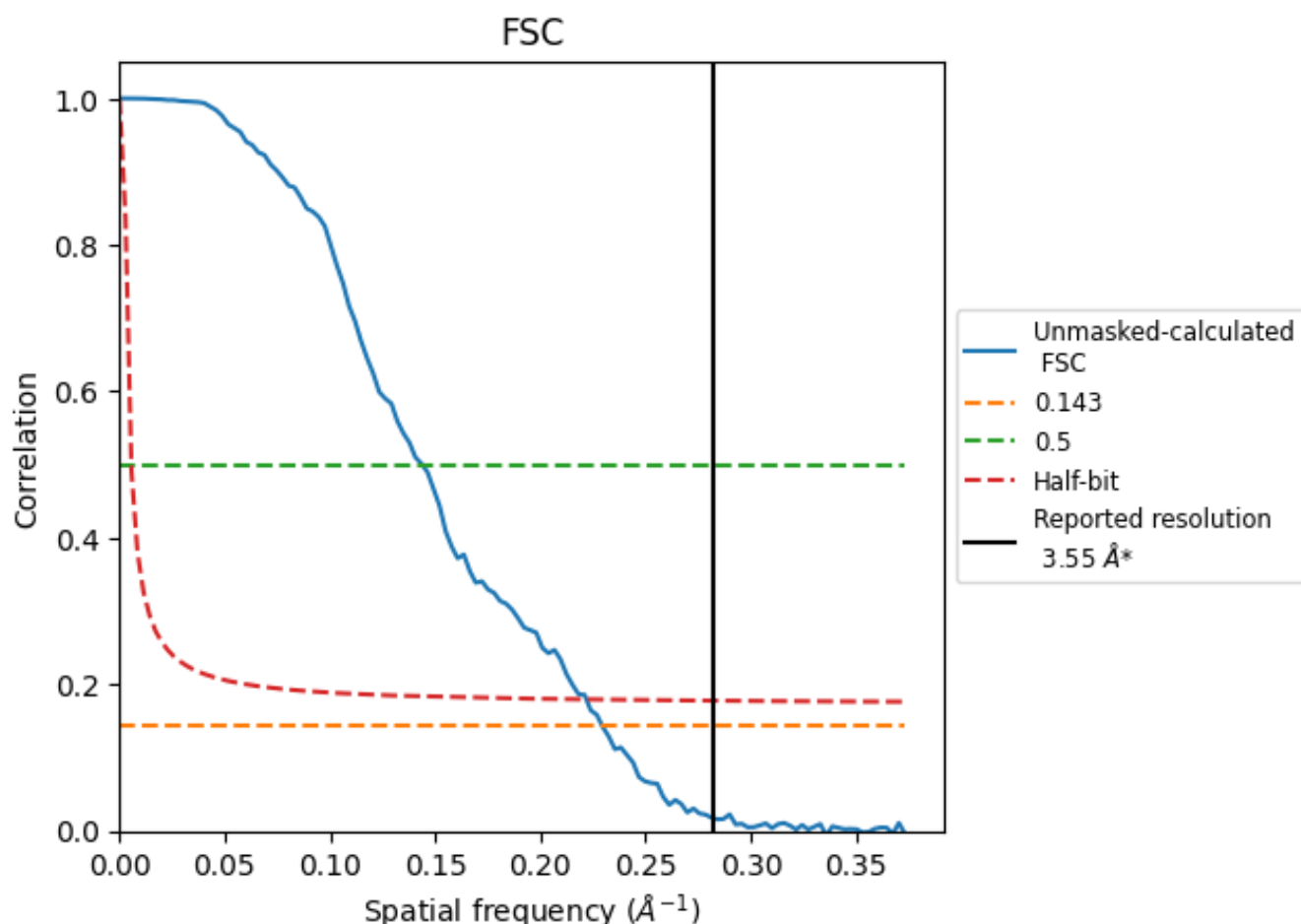


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

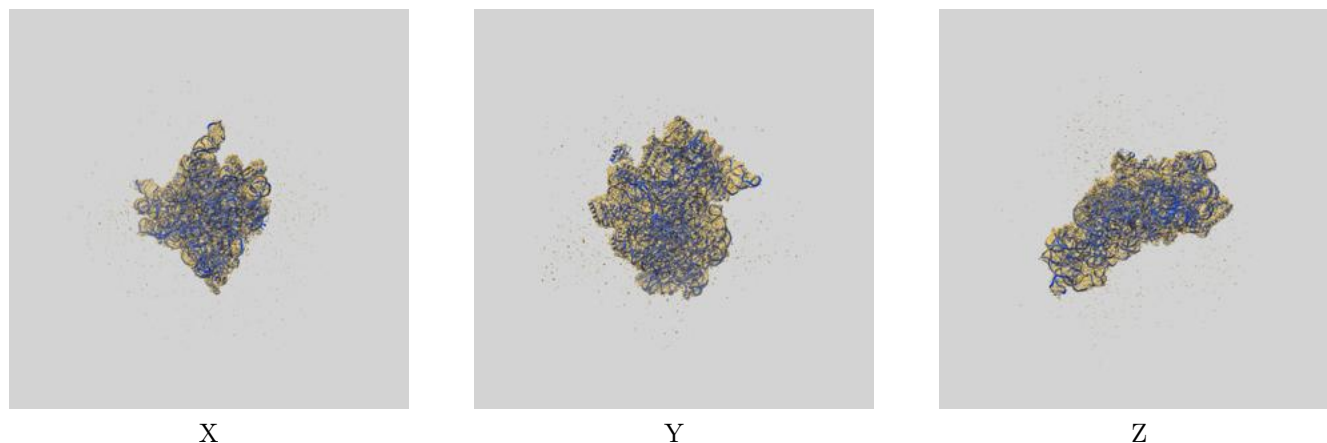
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.55	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.36	6.95	4.51

*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 4.36 differs from the reported value 3.55 by more than 10 %

9 Map-model fit [i](#)

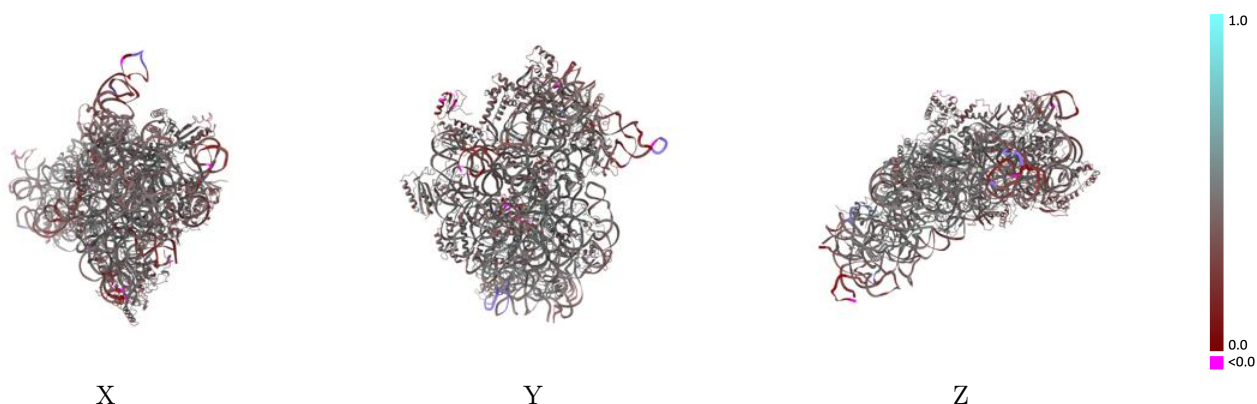
This section contains information regarding the fit between EMDB map EMD-4073 and PDB model 5LMN. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



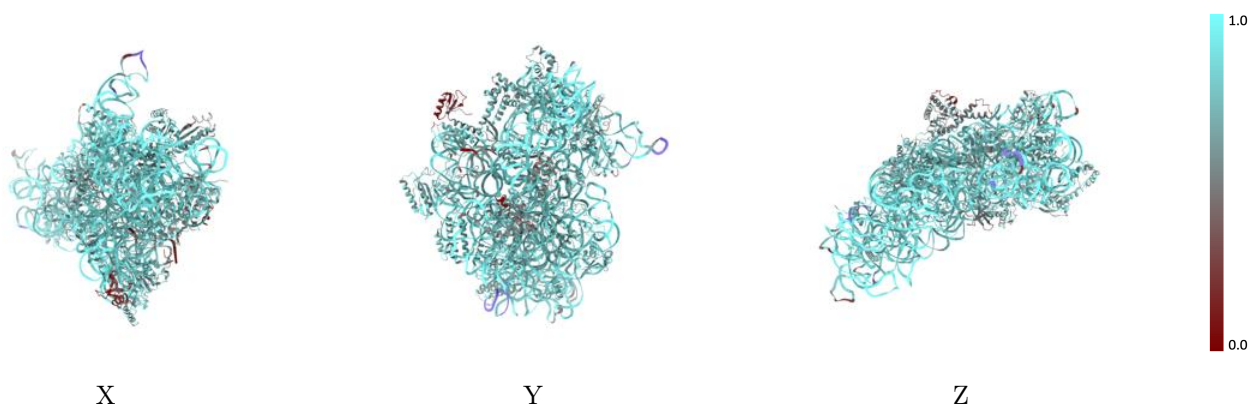
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



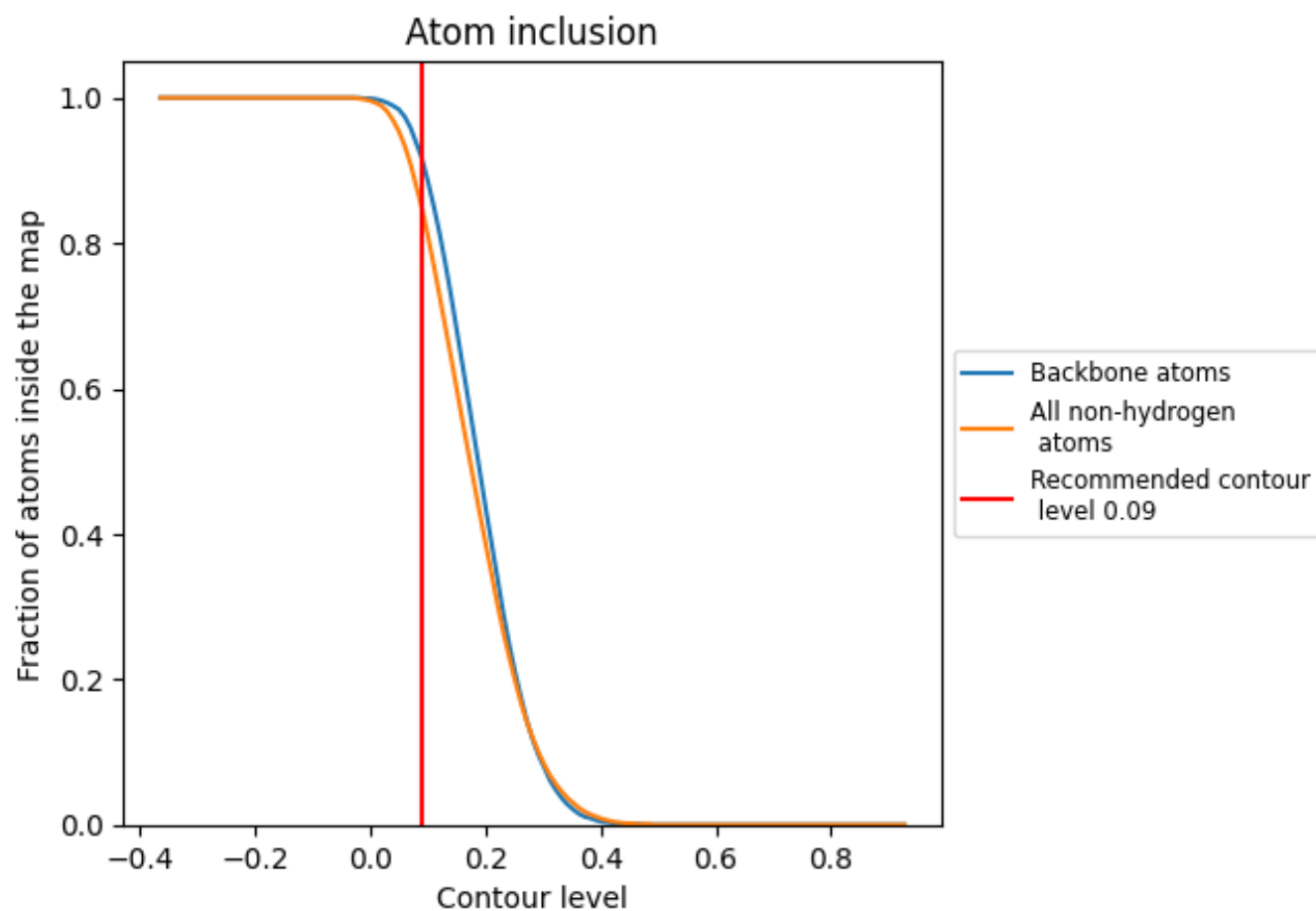
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).



















































9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 85% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8490	 0.4180
A	 0.9280	 0.4200
B	 0.5420	 0.3790
C	 0.7660	 0.4400
D	 0.7930	 0.4340
E	 0.8060	 0.4730
F	 0.7360	 0.4150
G	 0.7400	 0.4120
H	 0.8320	 0.4700
I	 0.7490	 0.4150
J	 0.6730	 0.3930
K	 0.7560	 0.4210
L	 0.8060	 0.4790
M	 0.7440	 0.3800
N	 0.8120	 0.4450
O	 0.8010	 0.4360
P	 0.8460	 0.4810
Q	 0.8370	 0.4740
R	 0.7040	 0.4100
S	 0.7340	 0.3680
T	 0.7550	 0.4170
V	 0.8380	 0.4660
W	 0.5270	 0.3760
X	 0.5130	 0.3180
Y	 0.5220	 0.2420

