



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:31 PM BST

PDB ID : 5FLX
EMDB ID: : EMD-3221
Title : Mammalian 40S HCV-IRES complex
Authors : Yamamoto, H.; Collier, M.; Loerke, J.; Ismer, J.; Schmidt, A.; Hilal, T.;
Sprink, T.; Yamamoto, K.; Mielke, T.; Burger, J.; Shaikh, T.R.; Dabrowski,
M.; Hildebrand, P.W.; Scheerer, P.; Spahn, C.M.T.
Deposited on : 2015-10-28
Resolution : 3.90 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

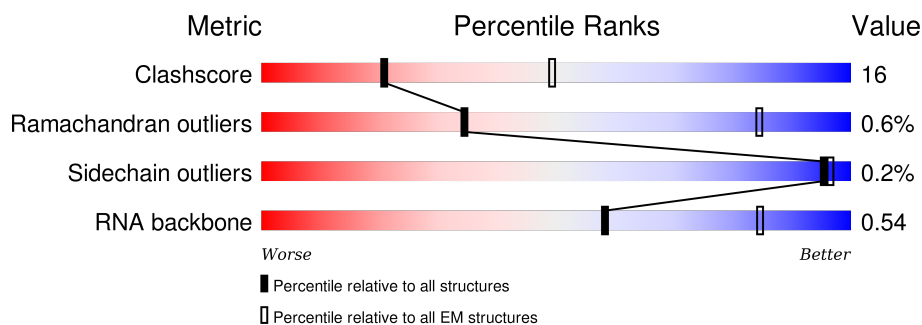
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	1869	
2	A	295	
3	B	264	
4	C	293	
5	D	243	
6	E	263	
7	F	204	
8	G	249	

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Mol	Chain	Length	Quality of chain
9	H	194	
10	I	208	
11	J	194	
12	K	165	
13	L	158	
14	M	132	
15	N	151	
16	O	151	
17	P	145	
18	Q	146	
19	R	135	
20	S	152	
21	T	145	
22	U	119	
23	V	83	
24	W	130	
25	X	143	
26	Y	133	
27	Z	125	
28	a	115	
29	b	84	
30	c	69	
31	d	56	
32	e	59	
33	f	156	

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Mol	Chain	Length	Quality of chain
34	g	317	<div><div></div><div>99%</div><div>.</div></div>
35	z	504	<div><div><div></div><div>42%</div></div><div><div></div><div>10%</div><div>.</div></div><div><div></div><div>48%</div></div></div>

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 80592 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 18S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	1708	Total	C	N	O	P	0	0
			36456	16274	6546	11928	1708		

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	215	Total	C	N	O	S	0	0
			1704	1083	298	315	8		

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	222	Total	C	N	O	S	0	0
			1724	1114	296	304	10		

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	220	Total	C	N	O	S	0	0
			1709	1090	308	304	7		

- Molecule 6 is a protein called 40S RIBOSOMAL PROTEIN S4, Y ISOFORM 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

- Molecule 7 is a protein called 40S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	190	Total	C	N	O	S	0	0
			1502	939	285	271	7		

- Molecule 8 is a protein called 40S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	232	Total	C	N	O	S	0	0
			1884	1176	379	322	7		

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	183	Total	C	N	O	S	0	0
			1479	941	272	265	1		

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	207	Total	C	N	O	S	0	0
			1696	1064	334	293	5		

- Molecule 11 is a protein called 40S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	153	Total	C	N	O	S	0	0
			1258	804	235	213	6		

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	120	Total	C	N	O	S	0	0
			931	584	164	174	9		

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called 40S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	120	Total	C	N	O	S	0	0
			999	636	188	168	7		

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	121	Total	C	N	O	S	0	0
			985	618	183	181	3		

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	139	Total	C	N	O	S	0	0
			1154	725	233	195	1		

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	97	Total	C	N	O	S	0	0
			769	483	144	138	4		

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0
			585	374	108	102	1		

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	97	Total	C	N	O	S	0	0
			774	481	160	128	5		

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	80	Total	C	N	O	S	0	0
			625	391	116	111	7		

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	61	Total	C	N	O	S	0	0
			480	291	96	91	2		

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	51	Total	C	N	O	S	0	0
			427	269	87	66	5		

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	55	Total	C	N	O	S	0	0
			437	272	96	68	1		

- Molecule 33 is a protein called UBIQUITIN-40S RIBOSOMAL PROTEIN S27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	73	Total	C	N	O	S	0	0
			601	379	115	100	7		

- Molecule 34 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 35 is a RNA chain called HCV-IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	264	Total	C	N	O	P	0	0
			5637	2512	1009	1852	264		

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	X	1	Total	Mg	0
			1	1	
36	1	72	Total	Mg	0
			72	72	
36	D	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

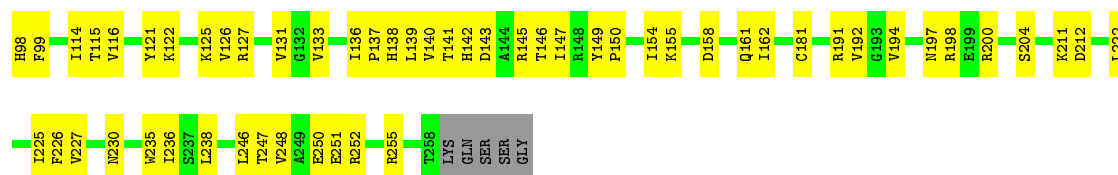
Mol	Chain	Residues	Atoms		AltConf
37	a	1	Total	Zn	0
			1	1	
37	d	1	Total	Zn	0
			1	1	

• Molecule 2: 40S RIBOSOMAL PROTEIN SA

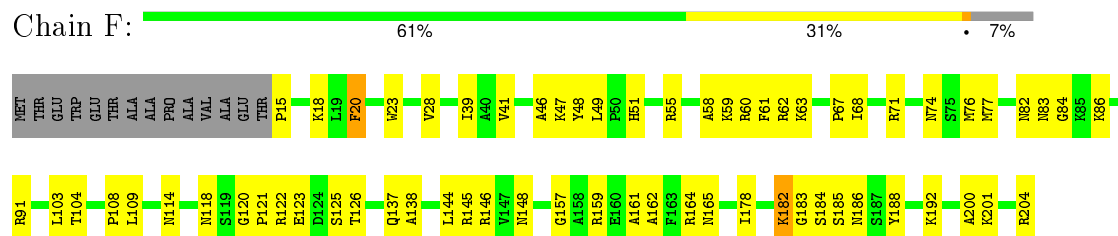
Response	Percentage
Yes	49%
No	23%
Don't know	27%

WORLDWIDE
PDB
PROTEIN DATA BANK

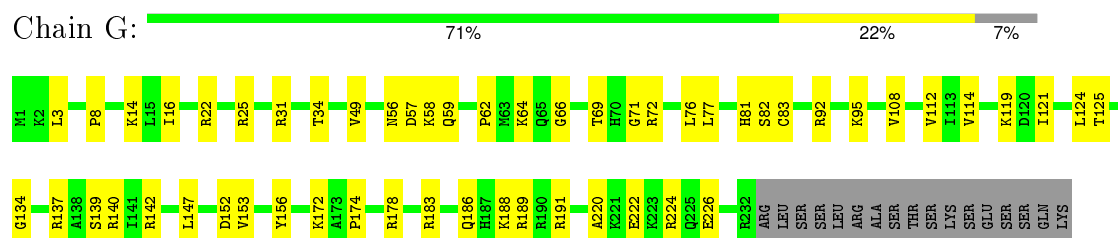
 **EMDataBank**
Unified Data Resource for 3DEM



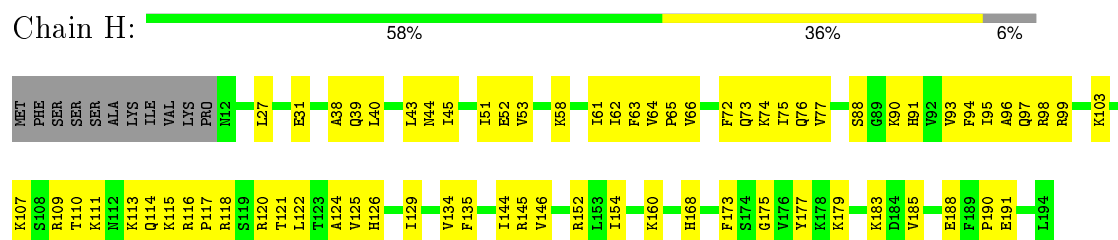
• Molecule 7: 40S RIBOSOMAL PROTEIN S5



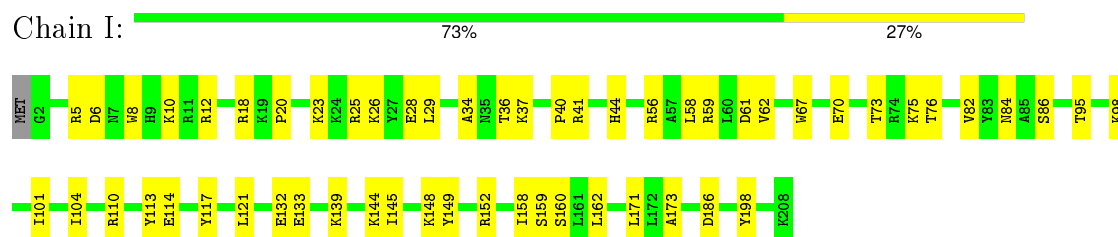
• Molecule 8: 40S RIBOSOMAL PROTEIN S6



• Molecule 9: 40S RIBOSOMAL PROTEIN S7

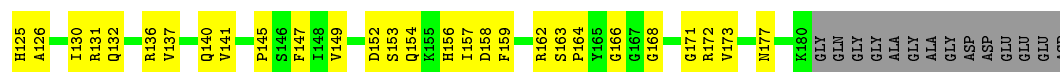


• Molecule 10: 40S RIBOSOMAL PROTEIN S8

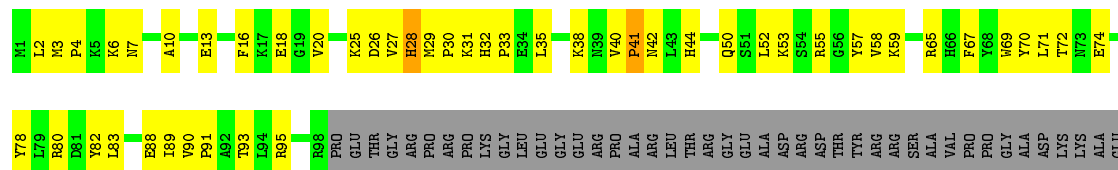
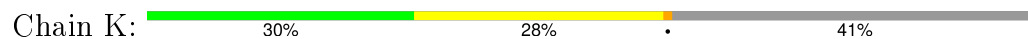


• Molecule 11: 40S RIBOSOMAL PROTEIN S9

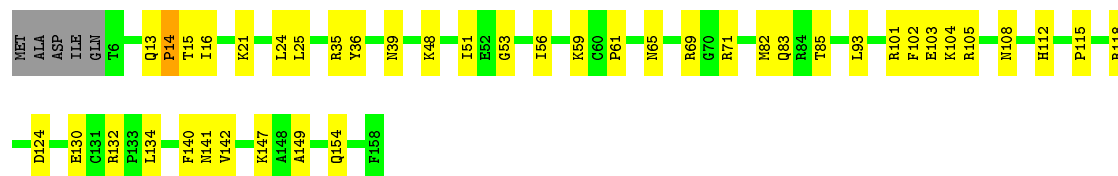




• Molecule 12: 40S RIBOSOMAL PROTEIN S10



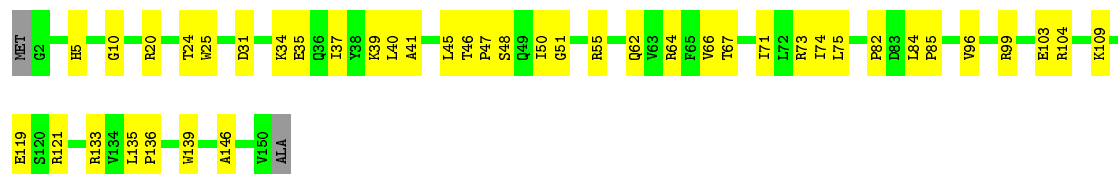
• Molecule 13: 40S RIBOSOMAL PROTEIN S11



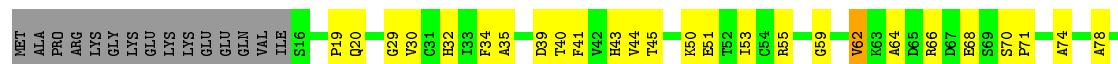
• Molecule 14: 40S RIBOSOMAL PROTEIN S12



• Molecule 15: 40S RIBOSOMAL PROTEIN S13

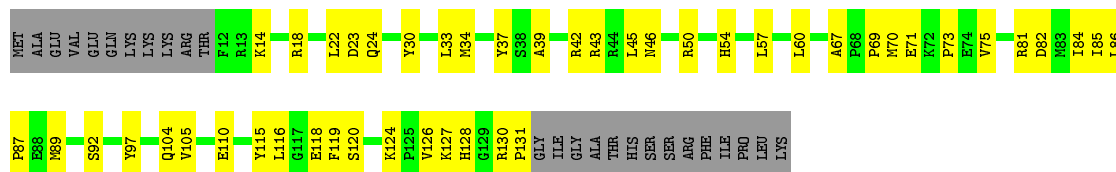


• Molecule 16: 40S RIBOSOMAL PROTEIN S14

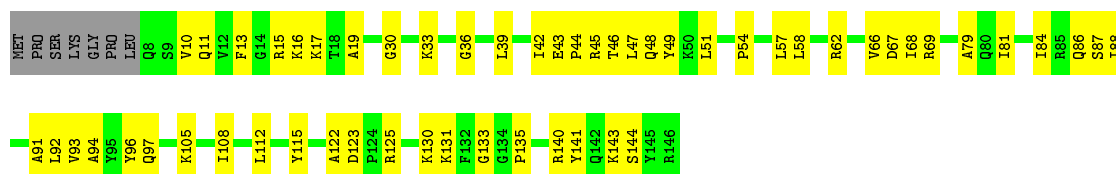




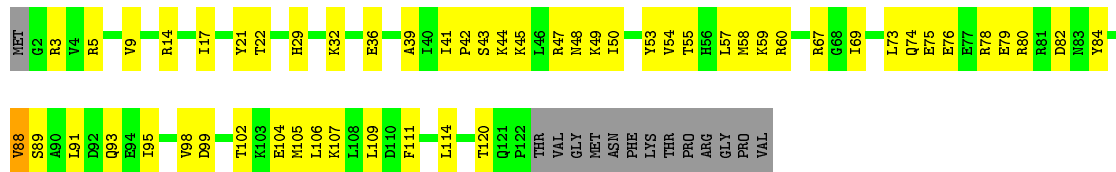
• Molecule 17: 40S RIBOSOMAL PROTEIN S15



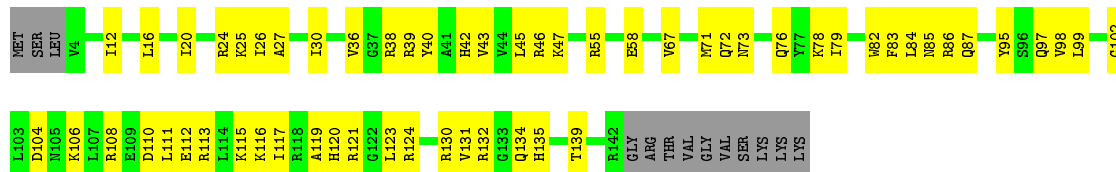
• Molecule 18: 40S RIBOSOMAL PROTEIN S16



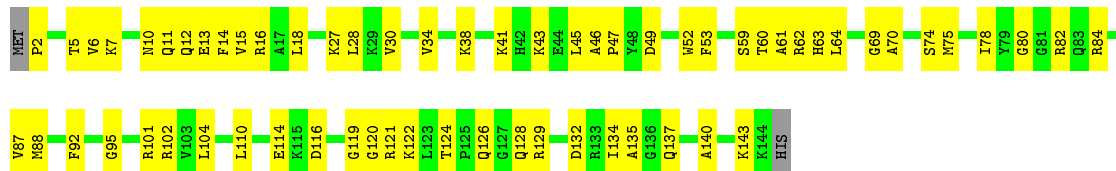
• Molecule 19: 40S RIBOSOMAL PROTEIN S17



• Molecule 20: 40S RIBOSOMAL PROTEIN S18

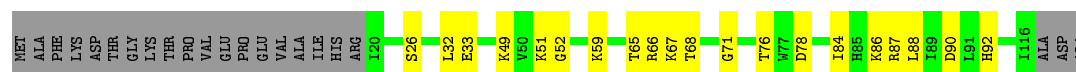


• Molecule 21: 40S RIBOSOMAL PROTEIN S19



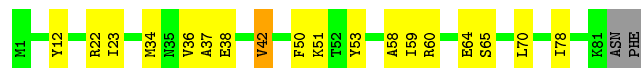
● Molecule 22: 40S RIBOSOMAL PROTEIN S20

Chain U: 65% 17% 18%



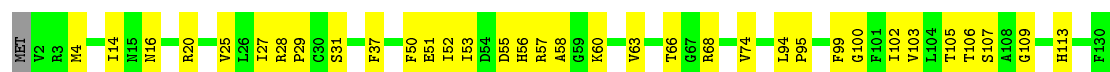
● Molecule 23: 40S RIBOSOMAL PROTEIN S21

Chain V: 76% 20% ..



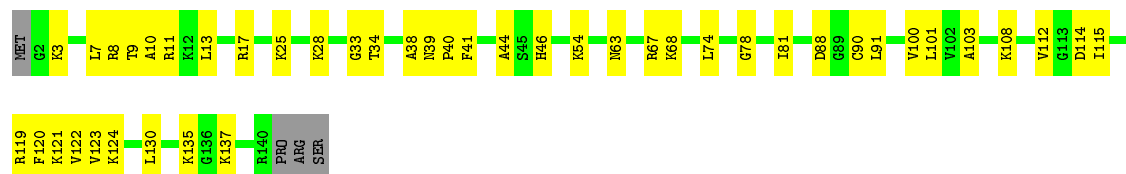
• Molecule 24: 40S RIBOSOMAL PROTEIN S15A

Chain W:  73% 26%



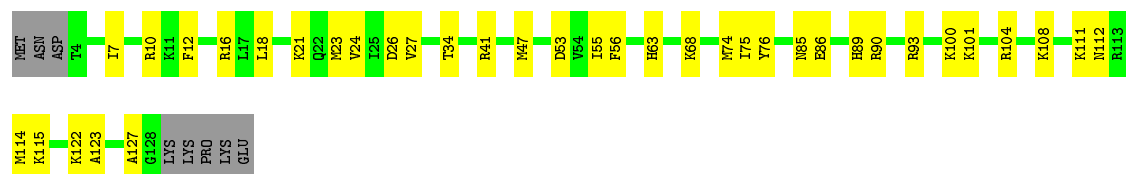
• Molecule 25: 40S RIBOSOMAL PROTEIN S23

Chain X:  66% 31% .

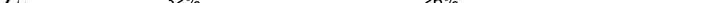


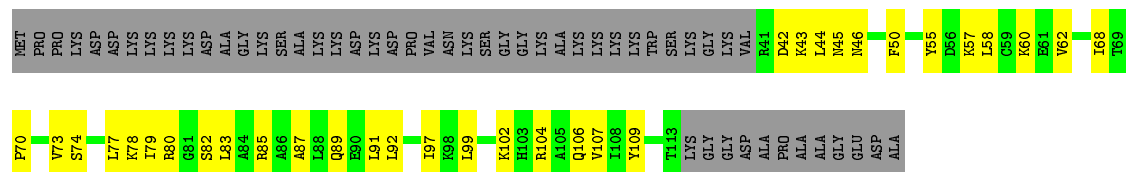
● Molecule 26: 40S RIBOSOMAL PROTEIN S24

Chain Y:  66% 28% 6%




● Molecule 27: 40S RIBOSOMAL PROTEIN S25

Chain Z:  32% 26% 42%




● Molecule 28: 40S RIBOSOMAL PROTEIN S26

Chain a:  75% 8% 16%




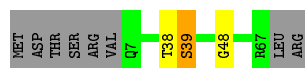
- Molecule 29: 40S RIBOSOMAL PROTEIN S27

Chain b:  90% 5%




- Molecule 30: 40S RIBOSOMAL PROTEIN S28

Chain c:  84% 12%



- Molecule 31: 40S RIBOSOMAL PROTEIN S29

Chain d:  91% 9%



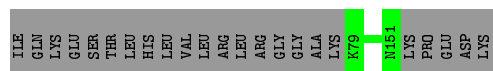
- Molecule 32: 40S RIBOSOMAL PROTEIN S30

Chain e:  92% 7%



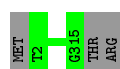
- Molecule 33: UBIQUITIN-40S RIBOSOMAL PROTEIN S27A

Chain f:  47% 53%

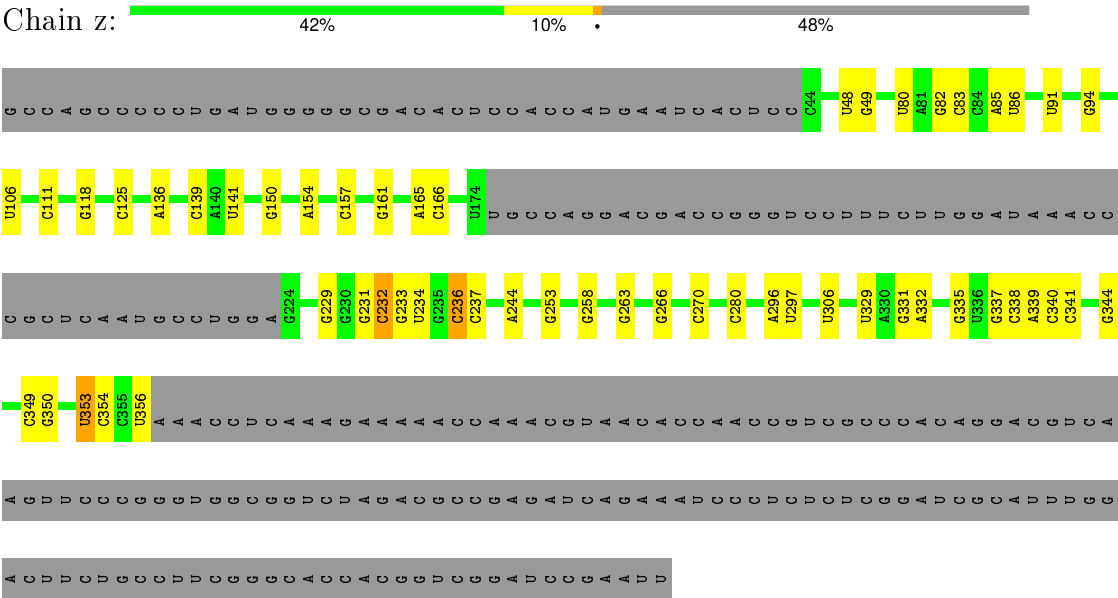


- Molecule 34: GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1

Chain g:  99%



- Molecule 35: HCV-IRES



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTFFIND3, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.19	1/40766 (0.0%)	0.78	23/63532 (0.0%)
10	I	0.24	0/1725	0.44	0/2298
11	J	0.23	0/1520	0.40	0/2030
12	K	0.25	0/851	0.48	0/1147
13	L	0.24	0/1281	0.49	0/1710
14	M	0.24	0/941	0.42	0/1264
15	N	0.23	0/1226	0.44	0/1649
16	O	0.25	0/1029	0.50	0/1380
17	P	0.24	0/1019	0.49	0/1361
18	Q	0.24	0/1126	0.49	0/1506
19	R	0.25	0/997	0.48	0/1338
2	A	0.25	0/1741	0.46	0/2366
20	S	0.24	0/1172	0.44	0/1570
21	T	0.25	0/1131	0.44	0/1515
22	U	0.22	0/778	0.43	0/1045
23	V	0.24	0/623	0.41	0/833
24	W	0.24	0/1051	0.44	0/1406
25	X	0.24	0/1097	0.44	0/1464
26	Y	0.24	0/1032	0.43	0/1371
27	Z	0.24	0/591	0.49	0/794
28	a	0.71	4/786 (0.5%)	1.26	6/1053 (0.6%)
29	b	0.25	0/637	0.54	0/854
3	B	0.23	0/1749	0.48	0/2340
30	c	1.01	1/482 (0.2%)	1.07	5/645 (0.8%)
31	d	0.27	0/437	0.50	0/580
32	e	0.65	3/443 (0.7%)	0.83	2/583 (0.3%)
33	f	0.24	0/613	0.48	0/811
34	g	0.24	0/2497	0.44	0/3399
35	z	0.34	4/6299 (0.1%)	0.92	24/9818 (0.2%)
4	C	0.25	0/1761	0.43	0/2379
5	D	0.25	0/1736	0.44	0/2338
6	E	0.24	0/2072	0.45	0/2793

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
7	F	0.24	0/1524	0.45	0/2048
8	G	0.24	0/1907	0.43	0/2538
9	H	0.28	0/1501	0.49	0/2009
All	All	0.25	13/86141 (0.0%)	0.69	60/125767 (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
13	L	0	1
16	O	0	1
17	P	0	1
18	Q	0	1
28	a	2	1
30	c	1	0
5	D	0	1
6	E	0	1
7	F	0	1
All	All	3	8

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	39	SER	CA-CB	-20.82	1.21	1.52
35	z	353	U	N1-C2	-12.82	1.27	1.38
28	a	48	ALA	CA-CB	-11.41	1.28	1.52
1	1	1	U	OP3-P	-10.53	1.48	1.61
28	a	44	ILE	CA-CB	-9.59	1.32	1.54
28	a	48	ALA	CA-C	-9.09	1.29	1.52
35	z	353	U	N3-C4	-8.01	1.31	1.38
35	z	353	U	C2-N3	-7.34	1.32	1.37
32	e	52	LYS	CD-CE	6.85	1.68	1.51
32	e	52	LYS	CG-CD	6.52	1.74	1.52
28	a	44	ILE	N-CA	-6.41	1.33	1.46
32	e	52	LYS	CE-NZ	6.17	1.64	1.49
35	z	353	U	C4-O4	-5.15	1.19	1.23

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	48	ALA	CB-CA-C	29.24	153.96	110.10
30	c	39	SER	CB-CA-C	18.56	145.36	110.10
35	z	234	U	O5'-P-OP1	-16.34	90.99	105.70
35	z	353	U	N3-C4-O4	-16.19	108.06	119.40
35	z	234	U	P-O5'-C5'	15.32	145.42	120.90
35	z	353	U	C2-N1-C1'	-14.99	99.71	117.70
35	z	353	U	C5-C4-O4	14.06	134.34	125.90
32	e	52	LYS	CD-CE-NZ	13.50	142.75	111.70
35	z	353	U	C4-C5-C6	-12.77	112.04	119.70
1	1	1357	A	OP1-P-O3'	-12.55	77.58	105.20
28	a	44	ILE	N-CA-CB	11.92	138.22	110.80
28	a	48	ALA	N-CA-CB	-10.90	94.84	110.10
1	1	1357	A	OP2-P-O3'	-10.35	82.43	105.20
28	a	48	ALA	CA-C-O	-10.03	99.03	120.10
35	z	233	G	C2'-C3'-O3'	10.02	131.55	109.50
35	z	233	G	P-O3'-C3'	9.83	131.49	119.70
28	a	48	ALA	CA-C-N	9.49	138.08	117.20
35	z	353	U	N1-C2-N3	-9.42	109.25	114.90
1	1	1358	U	OP1-P-OP2	9.19	133.38	119.60
35	z	234	U	O5'-P-OP2	9.19	121.72	110.70
35	z	353	U	C6-N1-C1'	8.98	133.77	121.20
30	c	39	SER	CA-C-O	-8.50	102.25	120.10
35	z	234	U	O4'-C1'-N1	8.13	114.70	108.20
1	1	67	C	N1-C2-O2	7.85	123.61	118.90
1	1	67	C	C2-N1-C1'	7.79	127.37	118.80
35	z	233	G	O5'-P-OP1	-7.77	98.71	105.70
35	z	353	U	C6-N1-C2	7.75	125.65	121.00
32	e	52	LYS	CA-CB-CG	7.71	130.37	113.40
30	c	39	SER	CA-C-N	7.70	134.14	117.20
1	1	1022	U	C2-N1-C1'	6.97	126.07	117.70
35	z	353	U	N3-C2-O2	6.75	126.93	122.20
35	z	233	G	P-O5'-C5'	-6.57	110.39	120.90
28	a	44	ILE	CA-CB-CG1	-6.57	98.53	111.00
1	1	67	C	N3-C2-O2	-6.43	117.40	121.90
35	z	234	U	P-O3'-C3'	-6.39	112.03	119.70
35	z	353	U	C2-N3-C4	6.30	130.78	127.00
35	z	234	U	O5'-C5'-C4'	-6.16	99.99	111.70
30	c	39	SER	CA-CB-OG	6.12	127.72	111.20
35	z	233	G	O4'-C1'-C2'	6.00	113.00	107.60
1	1	1271	C	C2-N1-C1'	5.91	125.30	118.80
1	1	1271	C	N1-C2-O2	5.89	122.43	118.90
35	z	232	C	O3'-P-O5'	-5.88	92.83	104.00
35	z	232	C	C4'-C3'-O3'	5.71	124.41	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	89	C	C2-N1-C1'	5.66	125.02	118.80
35	z	232	C	P-O3'-C3'	5.60	126.42	119.70
1	1	797	C	OP2-P-O3'	5.49	117.29	105.20
1	1	1756	C	P-O3'-C3'	5.42	126.20	119.70
1	1	546	G	OP2-P-O3'	5.39	117.05	105.20
35	z	236	C	O5'-P-OP2	-5.38	100.86	105.70
1	1	96	C	C2-N1-C1'	5.35	124.69	118.80
1	1	67	C	C6-N1-C2	-5.34	118.16	120.30
1	1	1464	C	C2-N1-C1'	5.32	124.65	118.80
1	1	1464	C	N1-C2-O2	5.31	122.08	118.90
1	1	67	C	C6-N1-C1'	-5.30	114.43	120.80
1	1	1398	G	C4-N9-C1'	5.22	133.28	126.50
1	1	797	C	P-O3'-C3'	5.14	125.87	119.70
1	1	1116	C	C2-N1-C1'	5.09	124.40	118.80
30	c	48	GLY	C-N-CD	5.06	139.03	128.40
1	1	174	C	C5-C6-N1	5.03	123.52	121.00
1	1	118	C	C2-N1-C1'	5.01	124.31	118.80

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	a	44	ILE	CA
28	a	48	ALA	CA
30	c	39	SER	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	D	76	ARG	Peptide
6	E	92	ILE	Peptide
7	F	20	PHE	Peptide
13	L	15	THR	Peptide
16	O	141	ARG	Peptide
17	P	67	ALA	Peptide
18	Q	13	PHE	Peptide
28	a	28	ARG	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	1	36456	0	18413	792	0
2	A	1704	0	1704	68	0
3	B	1722	0	1793	60	0
4	C	1724	0	1808	59	0
5	D	1709	0	1803	34	0
6	E	2031	0	2138	74	0
7	F	1502	0	1556	53	0
8	G	1884	0	2044	38	0
9	H	1479	0	1564	98	0
10	I	1696	0	1785	50	0
11	J	1495	0	1615	50	0
12	K	827	0	854	40	0
13	L	1258	0	1334	36	0
14	M	931	0	961	33	0
15	N	1202	0	1289	37	0
16	O	1016	0	1039	60	0
17	P	999	0	1046	35	0
18	Q	1109	0	1174	50	0
19	R	985	0	1035	45	0
20	S	1154	0	1210	49	0
21	T	1112	0	1146	52	0
22	U	769	0	837	13	0
23	V	617	0	622	14	0
24	W	1034	0	1080	31	0
25	X	1080	0	1147	37	0
26	Y	1015	0	1086	28	0
27	Z	585	0	640	45	0
28	a	774	0	819	0	0
29	b	625	0	646	0	0
30	c	480	0	502	0	0
31	d	427	0	428	0	0
32	e	437	0	483	0	0
33	f	601	0	622	0	0
34	g	2440	0	2396	0	0
35	z	5637	0	2849	0	0
36	1	72	0	0	0	0
36	D	1	0	0	0	0
36	X	1	0	0	0	0
37	a	1	0	0	0	0
37	d	1	0	0	0	0
All	All	80592	0	61468	1693	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 16.

All (1693) 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)
9:H:52:GLU:HG3	9:H:58:LYS:CG	1.15	1.63
9:H:62:ILE:HD11	9:H:94:PHE:CE1	1.43	1.54
9:H:62:ILE:CD1	9:H:94:PHE:HE1	1.23	1.45
9:H:52:GLU:CG	9:H:58:LYS:CG	2.11	1.26
9:H:52:GLU:HG3	9:H:58:LYS:CD	1.69	1.22
9:H:62:ILE:CD1	9:H:94:PHE:CE1	2.08	1.17
9:H:52:GLU:HG3	9:H:58:LYS:HG3	1.24	1.15
9:H:52:GLU:OE2	9:H:58:LYS:HD2	1.49	1.12
9:H:62:ILE:CG1	9:H:94:PHE:CE1	2.33	1.11
9:H:62:ILE:CG1	9:H:94:PHE:CD1	2.36	1.08
9:H:52:GLU:CG	9:H:58:LYS:HG2	1.77	1.07
9:H:52:GLU:HG3	9:H:58:LYS:HG2	1.09	1.03
9:H:52:GLU:CD	9:H:58:LYS:HD2	1.80	1.01
1:1:442:C:N4	1:1:449:A:H62	1.59	1.01
9:H:52:GLU:CG	9:H:58:LYS:CD	2.38	0.99
9:H:52:GLU:CG	9:H:58:LYS:HD2	1.92	0.99
9:H:93:VAL:HG22	9:H:173:PHE:HE1	1.30	0.97
1:1:442:C:H42	1:1:449:A:N6	1.61	0.96
9:H:62:ILE:HG13	9:H:94:PHE:CD1	2.03	0.93
9:H:52:GLU:CA	9:H:58:LYS:HG2	1.98	0.93
9:H:62:ILE:HG12	9:H:94:PHE:CE1	2.02	0.93
27:Z:44:LEU:HD23	27:Z:45:ASN:N	1.83	0.93
9:H:73:GLN:HA	9:H:135:PHE:HZ	1.34	0.93
1:1:12:U:O2	1:1:1355:C:N3	2.01	0.93
9:H:62:ILE:HG13	9:H:94:PHE:HD1	1.32	0.92
9:H:76:GLN:HG2	9:H:135:PHE:CD1	2.02	0.92
27:Z:77:LEU:O	27:Z:79:ILE:HG12	1.70	0.92
1:1:563:G:C5	1:1:586:G:N2	2.40	0.90
27:Z:73:VAL:O	27:Z:77:LEU:HG	1.71	0.90
1:1:1206:G:H1	1:1:1692:U:H3	0.88	0.86
1:1:1488:C:H3'	1:1:1489:A:H4'	1.55	0.85
15:N:51:GLY:O	15:N:55:ARG:HB2	1.76	0.85
9:H:52:GLU:HA	9:H:58:LYS:HG2	1.57	0.84
1:1:875:A:N6	1:1:912:C:N4	2.25	0.84
1:1:382:C:H41	10:I:5:ARG:HH22	1.25	0.84
16:O:150:ARG:H	16:O:150:ARG:HD3	1.40	0.84
9:H:62:ILE:HG12	9:H:94:PHE:CD1	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:247:THR:O	6:E:251:GLU:HB2	1.78	0.84
1:1:10:G:H1	1:1:1201:U:H3	1.25	0.83
2:A:94:THR:HG23	2:A:96:ALA:H	1.44	0.82
1:1:1752:C:O2	1:1:1780:G:N2	2.12	0.82
1:1:1173:A:H62	1:1:1187:G:H21	1.28	0.82
9:H:52:GLU:CD	9:H:58:LYS:CD	2.49	0.81
1:1:879:C:H3'	1:1:880:G:H21	1.45	0.81
9:H:62:ILE:HD11	9:H:94:PHE:HE1	0.75	0.80
27:Z:74:SER:HA	27:Z:77:LEU:HD12	1.62	0.80
17:P:42:ARG:O	17:P:46:ASN:HB2	1.82	0.80
4:C:114:LYS:HB3	4:C:121:ARG:HB3	1.63	0.80
9:H:93:VAL:HG22	9:H:173:PHE:CE1	2.17	0.80
9:H:52:GLU:CB	9:H:58:LYS:HG2	2.13	0.79
14:M:33:ARG:HD2	14:M:91:LEU:HD21	1.65	0.79
1:1:377:G:H5''	10:I:98:LYS:HB3	1.65	0.78
13:L:101:ARG:HH21	25:X:13:LEU:HD11	1.45	0.78
1:1:442:C:H42	1:1:449:A:H62	0.80	0.77
1:1:10:G:H21	1:1:1357:A:H2'	1.49	0.77
14:M:51:VAL:HB	14:M:109:VAL:HB	1.66	0.77
9:H:76:GLN:HG2	9:H:135:PHE:CE1	2.20	0.76
1:1:976:G:H1'	16:O:50:LYS:HG2	1.67	0.76
1:1:1593:C:H3'	27:Z:104:ARG:HE	1.50	0.76
1:1:509:G:H5''	11:J:3:VAL:HG12	1.69	0.75
1:1:15:U:O2'	1:1:669:A:N6	2.18	0.75
5:D:216:GLU:HG2	5:D:217:ILE:HG12	1.68	0.75
20:S:30:ILE:HG22	20:S:36:VAL:HG11	1.68	0.75
1:1:875:A:C6	1:1:912:C:C4	2.75	0.75
9:H:64:VAL:HB	9:H:96:ALA:HA	1.67	0.75
9:H:44:ASN:OD1	9:H:44:ASN:O	2.06	0.74
9:H:52:GLU:OE2	9:H:58:LYS:CD	2.33	0.74
16:O:150:ARG:HD3	16:O:150:ARG:N	2.02	0.73
1:1:334:C:H2'	1:1:335:G:H8	1.53	0.73
4:C:68:ARG:NH1	4:C:276:THR:OG1	2.21	0.73
1:1:1139:C:O2'	1:1:1140:G:O5'	2.05	0.73
8:G:69:THR:HG22	8:G:71:GLY:H	1.52	0.73
1:1:1546:G:N2	1:1:1670:C:O2	2.20	0.73
1:1:1144:A:N3	1:1:1199:A:O2'	2.21	0.73
18:Q:44:PRO:HG2	18:Q:47:LEU:HB2	1.71	0.72
6:E:45:ILE:O	6:E:49:ARG:HB3	1.88	0.72
3:B:218:LEU:HD12	3:B:219:LYS:HG3	1.70	0.72
1:1:1648:G:N2	1:1:1675:A:OP2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:62:ILE:CD1	9:H:94:PHE:CD1	2.72	0.72
17:P:126:VAL:HG13	17:P:127:LYS:H	1.55	0.72
22:U:65:THR:HB	22:U:78:ASP:HB2	1.71	0.72
6:E:141:THR:HG22	6:E:143:ASP:H	1.54	0.72
16:O:102:GLY:HA2	16:O:136:PRO:HG3	1.70	0.72
1:1:533:A:O2'	1:1:534:G:N7	2.23	0.71
8:G:14:LYS:HB2	8:G:124:LEU:HD21	1.73	0.71
1:1:1614:A:H3'	17:P:43:ARG:HH22	1.55	0.71
1:1:563:G:N7	1:1:586:G:N2	2.39	0.71
1:1:379:C:OP1	10:I:56:ARG:NH1	2.24	0.71
7:F:55:ARG:HE	18:Q:125:ARG:HG3	1.54	0.71
9:H:62:ILE:HD11	9:H:94:PHE:CD1	2.22	0.70
1:1:1004:U:OP1	3:B:165:ARG:NH2	2.22	0.70
11:J:119:LEU:HD21	11:J:159:PHE:HE2	1.55	0.70
1:1:1594:A:N7	27:Z:104:ARG:NH1	2.39	0.70
1:1:1567:G:O2'	21:T:38:LYS:NZ	2.24	0.70
1:1:1101:U:H2'	1:1:1102:G:H8	1.55	0.70
13:L:154:GLN:HE22	15:N:133:ARG:HB3	1.56	0.70
20:S:55:ARG:NH2	27:Z:82:SER:OG	2.24	0.70
1:1:1792:G:H2'	1:1:1793:A:H8	1.56	0.70
2:A:102:ARG:HG2	2:A:104:THR:H	1.54	0.70
25:X:46:HIS:HB3	25:X:101:LEU:HD11	1.73	0.70
1:1:1456:G:OP1	19:R:59:LYS:NZ	2.24	0.70
1:1:1192:U:OP2	25:X:119:ARG:NH2	2.23	0.69
10:I:139:LYS:HB3	10:I:144:LYS:HB2	1.74	0.69
1:1:527:C:H2'	1:1:528:A:C4	2.27	0.69
18:Q:58:LEU:O	18:Q:62:ARG:NH1	2.25	0.69
1:1:1597:C:OP2	27:Z:85:ARG:NH2	2.25	0.69
1:1:665:G:H21	1:1:671:A:H5'	1.57	0.69
1:1:658:U:O3'	25:X:17:ARG:NH2	2.25	0.69
1:1:801:U:H2'	1:1:802:A:H8	1.57	0.69
12:K:26:ASP:O	12:K:42:ASN:ND2	2.26	0.69
8:G:137:ARG:HG3	8:G:178:ARG:HG3	1.74	0.69
18:Q:19:ALA:HB2	18:Q:79:ALA:HB1	1.75	0.69
7:F:126:THR:HG21	7:F:137:GLN:H	1.57	0.69
1:1:957:A:H3'	1:1:958:G:H21	1.57	0.69
18:Q:39:LEU:HD11	18:Q:51:LEU:HD22	1.75	0.69
27:Z:70:PRO:O	27:Z:74:SER:CB	2.41	0.69
1:1:65:C:H42	8:G:134:GLY:H	1.38	0.69
6:E:247:THR:O	6:E:251:GLU:CB	2.41	0.68
10:I:76:THR:HG21	10:I:104:ILE:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:43:LYS:HG3	27:Z:44:LEU:N	2.09	0.68
16:O:95:ILE:HD12	16:O:129:ILE:HG12	1.75	0.68
1:1:1065:G:P	16:O:149:ARG:HH21	2.17	0.68
1:1:331:C:H3'	1:1:332:G:H5''	1.76	0.68
11:J:37:LEU:HD23	11:J:42:GLU:HG3	1.76	0.68
26:Y:12:PHE:HZ	26:Y:21:LYS:HD2	1.60	0.68
1:1:454:U:H2'	1:1:455:A:H8	1.58	0.67
7:F:188:TYR:OH	7:F:192:LYS:NZ	2.23	0.67
1:1:337:C:H2'	1:1:338:G:C8	2.28	0.67
15:N:84:LEU:HD12	15:N:85:PRO:HD2	1.75	0.67
1:1:1271:C:OP1	1:1:1303:C:O2'	2.12	0.67
1:1:397:G:OP2	13:L:108:ASN:ND2	2.28	0.67
11:J:110:LEU:HB2	11:J:147:PHE:HB3	1.77	0.67
1:1:1419:C:O2	1:1:1420:G:N2	2.25	0.67
1:1:1231:C:OP2	20:S:139:THR:OG1	2.12	0.67
5:D:64:ARG:HH21	12:K:72:THR:HA	1.59	0.67
10:I:148:LYS:HG3	10:I:152:ARG:HD2	1.77	0.67
1:1:96:C:H5	1:1:434:G:H1	1.43	0.67
1:1:1395:C:H2'	1:1:1396:A:C8	2.30	0.66
1:1:600:G:H2'	1:1:601:G:H8	1.58	0.66
16:O:146:ARG:O	16:O:147:ARG:HB3	1.95	0.66
22:U:66:ARG:HG3	22:U:68:THR:HG22	1.77	0.66
1:1:190:G:O2'	1:1:209:A:N6	2.28	0.66
13:L:104:LYS:HZ1	25:X:8:ARG:HH11	1.43	0.66
1:1:228:C:H42	1:1:901:G:H1'	1.58	0.66
1:1:1063:C:O3'	16:O:150:ARG:HG2	1.95	0.66
27:Z:42:ASP:O	27:Z:43:LYS:HG2	1.95	0.66
1:1:154:U:O2	1:1:165:G:N2	2.29	0.66
1:1:681:U:H4'	25:X:9:THR:HG22	1.77	0.66
9:H:76:GLN:CB	9:H:135:PHE:CE1	2.79	0.66
1:1:1786:U:H2'	1:1:1787:G:H8	1.60	0.66
17:P:69:PRO:O	17:P:71:GLU:N	2.28	0.66
27:Z:44:LEU:C	27:Z:44:LEU:HD23	2.16	0.66
12:K:4:PRO:HG2	12:K:7:ASN:HB2	1.75	0.66
1:1:562:U:H2'	1:1:563:G:H8	1.61	0.66
1:1:104:A:H4'	10:I:18:ARG:HH21	1.60	0.66
18:Q:130:LYS:NZ	18:Q:135:PRO:O	2.29	0.66
1:1:385:G:N2	1:1:388:U:OP2	2.28	0.66
5:D:106:ARG:HH21	5:D:173:ARG:HB3	1.61	0.66
21:T:75:MET:SD	21:T:121:ARG:NH1	2.70	0.65
1:1:1013:U:OP1	1:1:1129:G:O2'	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:34:THR:O	25:X:38:ALA:CB	2.45	0.65
1:1:1032:C:H5'	15:N:109:LYS:HD3	1.77	0.65
1:1:1454:A:N7	19:R:3:ARG:HD2	2.12	0.65
10:I:40:PRO:HA	10:I:61:ASP:HB2	1.78	0.65
1:1:875:A:N1	1:1:912:C:C4	2.64	0.65
21:T:11:GLN:HE21	21:T:15:VAL:HB	1.62	0.65
1:1:1128:C:H2'	1:1:1129:G:H8	1.62	0.65
1:1:1210:G:H5'	2:A:85:ARG:NH1	47.17	0.65
1:1:493:A:H61	1:1:510:G:H1'	1.63	0.64
9:H:27:LEU:HD13	9:H:43:LEU:HD23	1.79	0.64
3:B:148:ASN:HD22	3:B:148:ASN:N	1.94	0.64
1:1:1171:G:N2	1:1:1188:A:OP2	2.26	0.64
9:H:76:GLN:HB2	9:H:135:PHE:CE1	2.33	0.64
20:S:38:ARG:HH21	21:T:45:LEU:HD11	1.61	0.64
22:U:51:LYS:HD3	22:U:90:ASP:HB2	1.79	0.64
1:1:1606:G:H5''	21:T:87:VAL:HG23	1.80	0.64
12:K:27:VAL:HA	12:K:42:ASN:HD22	1.62	0.64
8:G:153:VAL:HG23	8:G:156:TYR:HB2	1.77	0.64
14:M:124:ILE:O	14:M:128:PHE:HB2	1.98	0.64
6:E:79:ASP:HB3	6:E:82:TYR:HB2	1.80	0.64
18:Q:62:ARG:HD3	18:Q:92:LEU:HD23	1.79	0.64
16:O:70:SER:HB2	16:O:71:PRO:HD2	1.79	0.64
1:1:1674:G:OP1	7:F:51:HIS:NE2	2.30	0.64
1:1:641:A:O2'	1:1:645:C:OP1	2.15	0.64
6:E:115:THR:HG22	6:E:116:VAL:H	1.62	0.64
19:R:14:ARG:HG3	19:R:69:ILE:HG12	1.80	0.64
2:A:189:ILE:HG13	2:A:195:TRP:HZ3	1.62	0.64
12:K:27:VAL:O	12:K:29:MET:N	2.26	0.63
16:O:34:PHE:HB3	16:O:41:PHE:HB2	1.79	0.63
1:1:819:G:O2'	6:E:255:ARG:NH2	2.31	0.63
1:1:524:U:OP1	1:1:525:A:O2'	2.15	0.63
5:D:23:GLU:HA	5:D:26:THR:HG22	1.80	0.63
1:1:925:G:OP1	15:N:121:ARG:NH1	2.30	0.63
17:P:81:ARG:HH12	17:P:120:SER:HB3	1.63	0.63
1:1:1244:U:H2'	1:1:1245:G:H8	1.64	0.63
16:O:62:VAL:HB	16:O:68:GLU:HG2	1.80	0.63
6:E:64:ILE:HG22	26:Y:18:LEU:HD21	1.81	0.63
9:H:115:LYS:HG2	9:H:116:ARG:H	1.62	0.63
1:1:1228:A:H2'	1:1:1229:G:H8	1.63	0.63
1:1:963:A:H8	16:O:66:ARG:HH22	1.46	0.63
1:1:931:C:H2'	1:1:932:G:C8	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:58:LEU:HD13	18:Q:92:LEU:HD22	1.81	0.63
1:1:1270:G:O2'	1:1:1301:A:N6	2.29	0.63
1:1:913:A:H5''	9:H:99:ARG:HD2	1.80	0.63
9:H:73:GLN:HA	9:H:135:PHE:CZ	2.25	0.63
1:1:454:U:H2'	1:1:455:A:C8	2.33	0.63
9:H:52:GLU:CG	9:H:58:LYS:HG3	2.06	0.62
1:1:570:C:O2'	26:Y:34:THR:O	2.17	0.62
15:N:51:GLY:O	15:N:55:ARG:CB	2.46	0.62
1:1:1550:G:O2'	1:1:1558:C:O2	2.16	0.62
7:F:18:LYS:HD3	7:F:46:ALA:HB3	1.80	0.62
2:A:176:TRP:HB2	2:A:202:TYR:HD2	1.64	0.62
1:1:35:C:H5''	1:1:579:C:H5''	1.81	0.62
3:B:82:ARG:NH2	3:B:188:LEU:O	2.31	0.62
16:O:74:ALA:O	16:O:78:ALA:CB	2.47	0.62
5:D:75:LYS:HG3	12:K:20:VAL:HB	1.81	0.62
1:1:1592:C:H2'	1:1:1593:C:C6	2.35	0.62
16:O:64:ALA:O	16:O:68:GLU:HB2	1.99	0.62
1:1:508:A:H3'	1:1:509:G:H8	1.64	0.62
1:1:1538:C:H4'	21:T:45:LEU:HD12	1.81	0.62
1:1:284:C:OP1	1:1:891:G:O2'	2.17	0.62
25:X:103:ALA:O	25:X:121:LYS:N	2.31	0.62
4:C:130:ILE:HG12	4:C:158:ALA:HB1	1.80	0.62
11:J:27:GLN:HA	11:J:30:LYS:HE3	1.80	0.62
2:A:123:VAL:HG22	2:A:145:ILE:HB	1.81	0.62
7:F:71:ARG:NH2	7:F:148:ASN:OD1	2.33	0.62
9:H:74:LYS:HG2	9:H:75:ILE:HG13	1.82	0.62
1:1:392:A:O2'	13:L:83:GLN:NE2	2.33	0.62
12:K:83:LEU:HD22	12:K:88:GLU:HA	1.81	0.62
1:1:1692:U:H2'	1:1:1693:G:C8	2.35	0.61
1:1:1348:G:OP2	4:C:114:LYS:NZ	2.31	0.61
19:R:5:ARG:NH1	19:R:49:LYS:O	2.31	0.61
1:1:226:A:N6	1:1:288:G:OP2	2.33	0.61
19:R:105:MET:O	19:R:109:LEU:HB2	1.99	0.61
9:H:76:GLN:CB	9:H:135:PHE:HE1	2.12	0.61
1:1:1468:C:OP2	19:R:3:ARG:NH2	2.32	0.61
24:W:57:ARG:HG3	24:W:58:ALA:H	1.64	0.61
6:E:68:ARG:HD3	6:E:76:VAL:HG11	1.82	0.61
7:F:103:LEU:HD23	7:F:104:THR:HG23	1.83	0.61
4:C:266:TYR:O	4:C:270:THR:OG1	2.17	0.61
1:1:1610:G:N2	20:S:85:ASN:OD1	2.34	0.61
1:1:170:A:OP1	8:G:140:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1156:U:O4	4:C:194:ARG:NH1	2.31	0.61
1:1:1756:C:O2'	1:1:1757:G:O5'	2.18	0.61
1:1:1528:G:O2'	1:1:1666:C:OP1	2.19	0.61
2:A:204:TYR:O	2:A:205:ARG:HG3	2.00	0.61
1:1:677:G:H21	1:1:1028:A:H62	1.49	0.61
1:1:1287:A:O2'	1:1:1311:C:N4	2.33	0.61
26:Y:10:ARG:NH1	26:Y:26:ASP:OD2	2.32	0.61
27:Z:70:PRO:O	27:Z:74:SER:HB3	2.00	0.61
1:1:1397:U:H4'	1:1:1398:G:N2	2.16	0.61
1:1:869:A:H5'	1:1:874:G:H1'	1.82	0.61
1:1:1033:G:H1	1:1:1080:A:HO2'	0.69	0.61
1:1:563:G:C6	1:1:586:G:N2	2.68	0.61
12:K:7:ASN:HD21	12:K:44:HIS:HB3	1.65	0.61
6:E:90:ILE:HB	6:E:99:PHE:HB2	1.83	0.61
3:B:82:ARG:HH12	3:B:191:ASP:HB2	1.66	0.60
27:Z:58:LEU:HD13	27:Z:77:LEU:HD22	1.81	0.60
1:1:300:U:H2'	1:1:301:A:H8	1.66	0.60
1:1:1259:A:H61	1:1:1518:C:H3'	1.65	0.60
16:O:96:LYS:NZ	16:O:130:GLU:OE1	2.34	0.60
6:E:31:PRO:HG3	6:E:43:PRO:HG3	1.83	0.60
1:1:692:G:H2'	1:1:693:A:H8	1.66	0.60
3:B:52:THR:OG1	3:B:56:LYS:O	2.17	0.60
9:H:63:PHE:HB3	9:H:97:GLN:HB2	1.82	0.60
15:N:99:ARG:NH2	15:N:119:GLU:OE2	2.33	0.60
10:I:104:ILE:HD11	10:I:173:ALA:HB2	1.83	0.60
1:1:639:C:H2'	1:1:640:A:H8	1.64	0.60
1:1:10:G:N2	1:1:1357:A:H2'	2.14	0.60
9:H:111:LYS:HB3	9:H:113:LYS:HD3	1.81	0.60
1:1:982:G:H2'	1:1:983:A:H8	1.66	0.60
6:E:61:VAL:HA	6:E:64:ILE:HG12	1.83	0.60
11:J:35:TYR:O	11:J:111:GLN:NE2	2.35	0.60
1:1:1272:C:H2'	1:1:1273:C:C6	2.36	0.60
15:N:31:ASP:O	15:N:34:LYS:N	2.34	0.60
1:1:1221:G:O2'	1:1:1676:U:O2	2.17	0.60
12:K:6:LYS:O	12:K:10:ALA:HB2	2.02	0.60
1:1:1535:U:O2'	7:F:82:ASN:ND2	2.34	0.60
1:1:1179:G:N2	1:1:1182:A:OP2	2.32	0.60
27:Z:57:LYS:HA	27:Z:60:LYS:HE3	1.81	0.60
20:S:108:ARG:O	20:S:112:GLU:HB2	2.01	0.60
1:1:547:G:H3'	1:1:548:C:H5''	1.83	0.59
1:1:1228:A:H2'	1:1:1229:G:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:104:GLU:HA	19:R:107:LYS:HE2	1.83	0.59
19:R:75:GLU:O	19:R:79:GLU:N	2.28	0.59
22:U:59:LYS:HB2	22:U:84:ILE:HB	1.84	0.59
1:1:1201:U:HO2'	1:1:1358:U:HO2'	1.41	0.59
1:1:1221:G:H2'	1:1:1222:G:H8	1.66	0.59
10:I:104:ILE:HB	10:I:171:LEU:HB3	1.83	0.59
21:T:59:SER:O	21:T:63:HIS:ND1	2.25	0.59
10:I:37:LYS:HB2	10:I:59:ARG:HB3	1.84	0.59
1:1:1447:G:H2'	1:1:1448:A:H8	1.67	0.59
1:1:560:A:H3'	11:J:171:GLY:HA3	1.85	0.59
2:A:176:TRP:CG	2:A:199:PRO:HB3	2.37	0.59
18:Q:16:LYS:HG3	18:Q:17:LYS:H	1.66	0.59
1:1:496:C:H2'	1:1:497:C:H6	1.66	0.59
9:H:75:ILE:HG22	9:H:77:VAL:O	2.02	0.59
1:1:87:U:H4'	1:1:173:A:H4'	1.84	0.59
15:N:135:LEU:HD12	15:N:136:PRO:HD2	1.85	0.59
1:1:1808:U:H2'	1:1:1809:A:H8	1.67	0.59
5:D:18:LYS:O	5:D:22:ASN:HB2	2.02	0.59
1:1:1139:C:O2'	1:1:1140:G:O4'	2.20	0.59
1:1:1137:U:H4'	2:A:155:ARG:HH22	1.67	0.59
19:R:57:LEU:HD23	19:R:60:ARG:HD3	1.85	0.59
1:1:1353:A:H2'	1:1:1354:G:C8	2.38	0.59
6:E:121:TYR:HB3	6:E:161:GLN:HE21	1.67	0.59
19:R:9:VAL:HG13	19:R:50:ILE:HA	1.85	0.59
21:T:126:GLN:OE1	21:T:129:ARG:NH2	2.36	0.59
1:1:1679:A:N6	7:F:58:ALA:O	2.36	0.59
18:Q:42:ILE:HG22	18:Q:44:PRO:HD2	1.85	0.59
16:O:74:ALA:O	16:O:78:ALA:HB2	2.03	0.59
4:C:107:LEU:HD22	4:C:209:VAL:HG13	1.85	0.59
8:G:142:ARG:HG2	8:G:147:LEU:HD11	1.85	0.59
1:1:1049:A:OP2	1:1:1068:G:N2	2.36	0.59
14:M:77:ILE:HD12	14:M:128:PHE:HA	1.83	0.59
1:1:814:U:OP1	6:E:22:LYS:NZ	2.36	0.59
2:A:68:ILE:HG12	2:A:73:ASP:HB2	1.85	0.58
1:1:96:C:H1'	1:1:474:G:H5'	1.85	0.58
1:1:655:A:H4'	1:1:656:G:H3'	1.85	0.58
1:1:177:G:N1	1:1:313:A:OP1	2.31	0.58
2:A:145:ILE:HG12	2:A:159:ILE:HB	1.85	0.58
1:1:692:G:H2'	1:1:693:A:C8	2.38	0.58
1:1:1751:C:O2	1:1:1782:G:N2	2.34	0.58
6:E:114:ILE:HG13	6:E:115:THR:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1286:G:H3'	1:1:1287:A:H5''	1.86	0.58
1:1:1094:C:OP1	24:W:28:ARG:NH2	2.36	0.58
1:1:522:A:O3'	11:J:131:ARG:NH2	2.34	0.58
2:A:7:VAL:HG21	23:V:42:VAL:HA	1.85	0.58
2:A:68:ILE:HD13	2:A:120:ARG:HH11	1.68	0.58
7:F:20:PHE:HB3	7:F:23:TRP:HD1	1.67	0.58
3:B:48:LEU:HD22	16:O:51:GLU:HB3	1.84	0.58
1:1:1204:A:O2'	1:1:1700:C:OP2	2.21	0.58
1:1:1260:A:H61	1:1:1617:G:H1'	1.67	0.58
17:P:105:VAL:HG21	17:P:119:PHE:HB3	1.84	0.58
1:1:1395:C:OP1	18:Q:15:ARG:NH1	2.37	0.58
14:M:125:GLU:HA	14:M:128:PHE:HB3	1.84	0.58
2:A:66:VAL:HG22	2:A:182:VAL:HG13	1.85	0.58
1:1:913:A:OP1	9:H:120:ARG:NH2	2.37	0.58
9:H:76:GLN:CG	9:H:135:PHE:CE1	2.86	0.58
1:1:1561:A:N6	1:1:1574:C:N3	2.46	0.58
7:F:28:VAL:HG11	7:F:109:LEU:HG	1.85	0.58
1:1:1098:C:H2'	1:1:1099:G:C8	2.39	0.58
7:F:120:GLY:HA2	7:F:146:ARG:HD2	1.86	0.58
1:1:173:A:O2'	1:1:174:C:H6	1.86	0.58
2:A:103:PHE:CG	2:A:133:PRO:HG3	2.39	0.58
1:1:6:G:O2'	1:1:601:G:N2	2.37	0.58
1:1:104:A:OP1	10:I:12:ARG:NH1	2.37	0.57
25:X:34:THR:O	25:X:38:ALA:HB3	2.03	0.57
2:A:85:ARG:NH2	19:R:84:TYR:OH	2.37	0.57
11:J:108:ARG:NH2	11:J:149:VAL:O	2.37	0.57
6:E:6:LYS:O	6:E:30:ARG:NH1	2.36	0.57
1:1:1536:G:H2'	1:1:1537:A:H8	1.69	0.57
7:F:59:LYS:HE3	7:F:61:PHE:HB2	1.86	0.57
1:1:1260:A:H2'	1:1:1261:C:H6	1.69	0.57
1:1:1096:G:H1	1:1:1136:U:H3	1.51	0.57
1:1:292:A:O2'	13:L:39:ASN:O	2.22	0.57
1:1:406:U:O2'	1:1:408:A:OP1	2.19	0.57
6:E:192:VAL:HG21	6:E:238:LEU:HD11	1.86	0.57
4:C:68:ARG:HH12	4:C:273:LEU:HA	1.69	0.57
1:1:677:G:N2	1:1:1027:A:OP2	2.38	0.57
25:X:68:LYS:HD3	25:X:91:LEU:HD22	1.87	0.57
8:G:59:GLN:OE1	8:G:72:ARG:NH1	2.35	0.57
1:1:1603:G:O4'	20:S:38:ARG:NH1	2.37	0.57
12:K:29:MET:CG	12:K:30:PRO:HD3	2.35	0.57
10:I:148:LYS:O	10:I:152:ARG:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:181:A:H1'	1:1:182:C:C4	2.39	0.57
1:1:305:U:O2'	10:I:41:ARG:NH1	2.38	0.57
4:C:183:LYS:HE2	24:W:95:PRO:HA	1.86	0.57
2:A:180:ARG:HG2	2:A:184:ARG:HH12	1.69	0.57
1:1:1203:G:H3'	1:1:1204:A:H8	1.68	0.57
1:1:1545:A:H2'	1:1:1546:G:C8	2.40	0.57
4:C:131:GLY:HA3	4:C:137:VAL:HG12	1.87	0.57
6:E:139:LEU:HB2	6:E:150:PRO:HG2	1.87	0.57
1:1:1198:G:H2'	1:1:1199:A:C8	2.39	0.57
1:1:1010:G:H2'	1:1:1011:A:H8	1.70	0.57
14:M:32:ALA:HB3	14:M:110:VAL:HB	1.87	0.57
1:1:1622:U:H4'	1:1:1623:A:H5'	1.87	0.57
12:K:6:LYS:O	12:K:10:ALA:CB	2.52	0.57
1:1:1619:A:O2'	17:P:82:ASP:OD2	2.21	0.57
1:1:1131:G:H2'	1:1:1132:C:C6	2.40	0.57
1:1:1562:C:H2'	1:1:1563:G:H8	1.69	0.56
1:1:1288:U:C2	1:1:1315:U:H1'	2.40	0.56
6:E:95:THR:HG22	26:Y:16:ARG:HB2	1.87	0.56
4:C:167:ARG:NH1	4:C:177:PRO:O	2.38	0.56
27:Z:70:PRO:O	27:Z:74:SER:HB2	2.05	0.56
1:1:1613:G:OP1	17:P:42:ARG:NH2	2.38	0.56
7:F:62:ARG:HG3	7:F:63:LYS:H	1.69	0.56
14:M:122:ASP:O	14:M:126:GLU:HG2	2.05	0.56
17:P:50:ARG:O	17:P:54:HIS:CB	2.53	0.56
11:J:117:LEU:HD12	11:J:157:ILE:HD11	1.88	0.56
27:Z:70:PRO:HG2	27:Z:107:VAL:HB	1.85	0.56
7:F:63:LYS:HD2	7:F:144:LEU:HD21	1.86	0.56
18:Q:54:PRO:O	18:Q:58:LEU:HB2	2.04	0.56
21:T:60:THR:HG23	21:T:121:ARG:HH11	1.70	0.56
1:1:1677:U:OP1	7:F:71:ARG:NH2	2.38	0.56
1:1:300:U:H2'	1:1:301:A:C8	2.40	0.56
1:1:1781:A:H2'	1:1:1782:G:C8	2.40	0.56
11:J:108:ARG:HA	11:J:113:GLN:HE21	1.70	0.56
19:R:88:VAL:HG13	19:R:89:SER:H	1.69	0.56
11:J:153:SER:HB2	11:J:156:HIS:HD2	1.70	0.56
1:1:976:G:N3	16:O:50:LYS:NZ	2.53	0.56
21:T:126:GLN:HA	21:T:129:ARG:HE	1.70	0.56
1:1:1239:U:H5''	17:P:124:LYS:HD2	1.86	0.56
27:Z:58:LEU:HD13	27:Z:77:LEU:CD2	2.35	0.56
4:C:114:LYS:N	4:C:121:ARG:O	2.25	0.56
1:1:551:U:H2'	1:1:552:G:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:106:ARG:HG3	5:D:175:VAL:HG22	1.86	0.56
1:1:391:C:H2'	1:1:392:A:H8	1.69	0.56
1:1:293:C:HO2'	1:1:295:C:H6	1.54	0.56
21:T:13:GLU:OE2	21:T:16:ARG:NH2	2.39	0.56
13:L:24:LEU:HD12	13:L:25:LEU:H	1.71	0.56
1:1:1857:G:OP2	16:O:141:ARG:NH2	2.38	0.56
27:Z:44:LEU:HD21	27:Z:46:ASN:OD1	2.05	0.56
17:P:50:ARG:O	17:P:54:HIS:HB2	2.06	0.56
1:1:1688:C:H2'	1:1:1689:C:H6	1.71	0.56
19:R:111:PHE:O	19:R:114:LEU:HD13	2.05	0.56
3:B:81:PHE:CD2	3:B:82:ARG:HG3	2.41	0.56
1:1:5:U:H2'	1:1:6:G:H8	1.70	0.56
1:1:107:A:H2'	1:1:108:G:C8	2.41	0.56
1:1:575:A:OP1	26:Y:93:ARG:NH1	2.28	0.56
10:I:70:GLU:OE2	13:L:21:LYS:NZ	2.32	0.56
18:Q:10:VAL:HG11	18:Q:94:ALA:HB1	1.88	0.56
1:1:77:A:O2'	8:G:174:PRO:O	2.23	0.55
2:A:102:ARG:HB3	19:R:67:ARG:HH21	1.71	0.55
9:H:154:ILE:HB	9:H:185:VAL:HG12	1.88	0.55
7:F:162:ALA:HA	7:F:165:ASN:HD21	1.69	0.55
1:1:495:U:OP1	6:E:58:GLY:N	2.37	0.55
26:Y:55:ILE:HG12	26:Y:75:ILE:HG12	1.88	0.55
1:1:1210:G:C5'	2:A:85:ARG:NH1	47.00	0.55
1:1:1554:C:O2'	1:1:1555:U:OP2	2.22	0.55
1:1:797:C:H4'	1:1:798:G:H5'	1.88	0.55
1:1:1394:G:N2	1:1:1475:G:N3	2.54	0.55
4:C:272:HIS:HA	4:C:275:LYS:HG2	1.87	0.55
11:J:64:ASP:OD2	11:J:66:LYS:NZ	2.33	0.55
2:A:86:ALA:O	2:A:90:PHE:CB	2.55	0.55
2:A:38:ILE:HD11	2:A:47:TYR:HB3	1.88	0.55
7:F:15:PRO:HB2	18:Q:57:LEU:HD22	1.89	0.55
1:1:591:U:H5	1:1:592:C:HO2'	1.55	0.55
4:C:65:LYS:NZ	4:C:273:LEU:HD13	2.22	0.55
1:1:982:G:H2'	1:1:983:A:C8	2.41	0.55
1:1:1474:A:H2'	1:1:1475:G:C8	2.41	0.55
1:1:1653:U:H2'	1:1:1654:G:C8	2.41	0.55
1:1:562:U:H2'	1:1:563:G:C8	2.41	0.55
1:1:1206:G:O6	1:1:1692:U:O4	2.24	0.55
1:1:334:C:H2'	1:1:335:G:C8	2.40	0.55
13:L:35:ARG:NH2	13:L:53:GLY:O	2.40	0.55
16:O:126:ILE:HG22	16:O:127:GLY:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:16:G:H21	1:1:1195:A:H62	1.54	0.55
18:Q:86:GLN:HE22	18:Q:122:ALA:HB2	1.72	0.55
1:1:161:U:H3	26:Y:115:LYS:HE2	1.71	0.55
15:N:37:ILE:HG13	15:N:50:ILE:HG21	1.89	0.55
1:1:1447:G:H2'	1:1:1448:A:C8	2.41	0.55
20:S:78:LYS:HG2	20:S:79:ILE:H	1.72	0.55
1:1:1173:A:H62	1:1:1187:G:N2	2.01	0.55
1:1:88:G:N2	1:1:499:G:O3'	2.40	0.55
1:1:1413:G:H21	1:1:1424:G:H1	1.54	0.55
10:I:159:SER:OG	10:I:160:SER:N	2.40	0.55
1:1:28:U:H2'	1:1:29:G:H8	1.72	0.55
1:1:1093:A:H2'	1:1:1094:C:C6	2.42	0.54
1:1:406:U:H2'	1:1:408:A:C8	2.42	0.54
20:S:16:LEU:HD13	20:S:99:LEU:HG	1.89	0.54
1:1:231:A:OP2	1:1:889:U:O2'	2.24	0.54
1:1:21:U:O2'	11:J:17:ARG:O	2.24	0.54
1:1:5:U:H2'	1:1:6:G:C8	2.42	0.54
1:1:164:A:H5'	8:G:83:CYS:H	1.72	0.54
17:P:118:GLU:HB3	20:S:119:ALA:HA	1.88	0.54
1:1:887:U:HO2'	1:1:888:U:H6	1.56	0.54
2:A:91:ALA:O	2:A:95:GLY:N	2.37	0.54
1:1:1232:U:OP2	20:S:135:HIS:ND1	2.41	0.54
1:1:1314:U:C2	12:K:2:LEU:HB2	2.42	0.54
1:1:1050:A:H62	1:1:1068:G:H21	1.54	0.54
9:H:122:LEU:O	9:H:126:HIS:ND1	2.36	0.54
2:A:149:ASN:OD1	2:A:150:THR:N	2.40	0.54
25:X:25:LYS:HA	25:X:28:LYS:HE2	1.89	0.54
6:E:126:VAL:HG21	6:E:154:ILE:HG21	1.89	0.54
3:B:164:ILE:HD11	3:B:207:LEU:HD21	1.88	0.54
20:S:42:HIS:HB3	20:S:46:ARG:HH12	1.73	0.54
1:1:352:U:H2'	1:1:353:C:C6	2.43	0.54
14:M:63:LYS:HA	14:M:66:GLU:HG2	1.89	0.54
1:1:799:U:H2'	1:1:800:U:C6	2.43	0.54
10:I:8:TRP:CZ3	10:I:20:PRO:HB3	2.43	0.54
1:1:1244:U:H2'	1:1:1245:G:C8	2.43	0.54
22:U:86:LYS:HE2	22:U:88:LEU:HD11	1.89	0.54
4:C:211:LYS:O	4:C:215:MET:HB2	2.08	0.54
13:L:93:LEU:HB3	13:L:102:PHE:HB3	1.89	0.54
6:E:69:PHE:O	6:E:92:ILE:HG23	2.08	0.54
1:1:943:U:O2'	16:O:135:ILE:O	2.26	0.54
7:F:55:ARG:NH2	18:Q:123:ASP:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:175:GLU:O	3:B:179:ASN:ND2	2.41	0.54
7:F:76:MET:O	7:F:159:ARG:NH2	2.40	0.54
1:1:1206:G:N2	1:1:1692:U:O2	2.29	0.54
20:S:39:ARG:HD3	20:S:83:PHE:HE1	1.72	0.54
6:E:45:ILE:O	6:E:49:ARG:CB	2.54	0.54
1:1:933:G:H1'	1:1:1001:A:O4'	2.08	0.54
3:B:144:LYS:HB2	3:B:207:LEU:O	2.08	0.54
20:S:67:VAL:O	20:S:71:MET:HG2	2.08	0.54
2:A:176:TRP:CD2	2:A:199:PRO:HB3	2.43	0.54
1:1:676:C:H5''	15:N:5:HIS:CD2	2.43	0.54
1:1:1452:A:H61	1:1:1473:G:H8	1.56	0.54
1:1:1036:A:H4'	1:1:1855:G:H21	1.73	0.54
9:H:144:ILE:HB	24:W:52:ILE:HB	1.89	0.54
1:1:1492:U:O2'	1:1:1495:G:OP1	2.24	0.54
3:B:119:THR:OG1	3:B:154:SER:O	2.18	0.54
7:F:47:LYS:HE3	7:F:67:PRO:HG3	1.90	0.54
1:1:98:C:OP2	1:1:426:A:O2'	2.20	0.54
1:1:1183:A:H2'	1:1:1184:G:H8	1.72	0.54
4:C:196:ILE:HB	4:C:223:TYR:HB2	1.90	0.54
1:1:1348:G:H4'	4:C:145:LYS:HD3	1.90	0.54
1:1:600:G:H2'	1:1:601:G:C8	2.41	0.54
15:N:75:LEU:HD21	15:N:82:PRO:HD3	1.90	0.54
17:P:110:GLU:HG3	20:S:116:LYS:HE3	1.89	0.54
4:C:253:PRO:O	4:C:256:TRP:HD1	1.91	0.54
2:A:39:TYR:HB2	2:A:50:ASN:HB3	1.89	0.54
23:V:38:GLU:HG2	23:V:51:LYS:HE3	1.90	0.54
4:C:172:ASN:OD1	4:C:173:LYS:N	2.39	0.54
5:D:165:ASN:OD1	5:D:166:TYR:N	2.41	0.54
3:B:36:PRO:HD3	3:B:98:THR:HG23	1.91	0.53
9:H:61:ILE:HG22	9:H:93:VAL:HB	1.89	0.53
27:Z:44:LEU:HD21	27:Z:46:ASN:CG	2.28	0.53
4:C:145:LYS:HG3	4:C:146:GLU:HG3	1.90	0.53
1:1:1594:A:C8	27:Z:104:ARG:CZ	2.91	0.53
1:1:1221:G:H2'	1:1:1222:G:C8	2.44	0.53
7:F:157:GLY:O	7:F:161:ALA:HB2	2.07	0.53
1:1:1277:C:H2'	1:1:1278:A:H8	1.73	0.53
4:C:83:LEU:HD21	23:V:12:TYR:HB2	1.89	0.53
6:E:194:VAL:N	6:E:211:LYS:O	2.34	0.53
7:F:114:ASN:O	7:F:118:ASN:ND2	2.30	0.53
1:1:546:G:H4'	1:1:547:G:OP2	2.07	0.53
1:1:1286:G:H22	14:M:36:ARG:HG3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1562:C:H2'	1:1:1563:G:C8	2.43	0.53
13:L:61:PRO:HD3	13:L:141:ASN:ND2	2.23	0.53
1:1:1786:U:H2'	1:1:1787:G:C8	2.42	0.53
1:1:493:A:H4'	26:Y:89:HIS:CD2	2.43	0.53
3:B:48:LEU:HB2	16:O:51:GLU:HG3	1.89	0.53
1:1:1010:G:H2'	1:1:1011:A:C8	2.43	0.53
14:M:21:VAL:O	14:M:25:ALA:HB2	2.09	0.53
1:1:1624:U:OP1	20:S:132:ARG:NH1	2.40	0.53
1:1:1017:U:H5'	15:N:55:ARG:HD3	1.89	0.53
1:1:1664:A:O2'	1:1:1665:G:O5'	2.25	0.53
11:J:130:ILE:HD12	11:J:145:PRO:HA	1.89	0.53
1:1:973:C:O2	16:O:55:ARG:NH2	2.41	0.53
18:Q:33:LYS:HD3	18:Q:69:ARG:HB2	1.90	0.53
1:1:486:A:O2'	1:1:487:U:O2	2.27	0.53
6:E:125:LYS:H	6:E:142:HIS:CE1	2.26	0.53
15:N:40:LEU:HB3	15:N:45:LEU:HD12	1.91	0.53
7:F:125:SER:OG	7:F:145:ARG:NH2	2.41	0.53
1:1:1745:A:H1'	8:G:66:GLY:HA2	1.90	0.53
1:1:690:G:N2	1:1:691:G:N7	2.57	0.53
1:1:15:U:H2'	1:1:16:G:O4'	2.09	0.53
1:1:407:G:H1	25:X:33:GLY:HA2	1.72	0.53
1:1:1358:U:H2'	1:1:1359:U:C6	2.43	0.53
1:1:1102:G:OP1	3:B:151:ARG:NH2	2.42	0.53
1:1:962:A:H3'	16:O:66:ARG:NH1	2.23	0.53
5:D:75:LYS:NZ	12:K:18:GLU:OE1	2.41	0.53
23:V:36:VAL:O	23:V:51:LYS:N	2.31	0.53
12:K:35:LEU:HD23	12:K:38:LYS:HB2	1.90	0.53
7:F:49:LEU:HG	18:Q:49:TYR:HB2	1.90	0.53
1:1:53:C:OP1	26:Y:112:ASN:ND2	2.41	0.53
3:B:70:SER:HA	3:B:83:LYS:HA	1.91	0.53
1:1:875:A:C6	1:1:912:C:N4	2.75	0.53
6:E:247:THR:HG22	6:E:248:VAL:H	1.73	0.53
1:1:596:U:O2'	1:1:645:C:O2	2.23	0.53
1:1:1012:A:H5''	15:N:10:GLY:HA3	1.90	0.53
11:J:63:LEU:O	11:J:70:ARG:NH1	2.42	0.53
12:K:59:LYS:HB2	12:K:70:TYR:HB3	1.89	0.53
1:1:880:G:H2'	1:1:881:G:H8	1.74	0.53
13:L:101:ARG:HD2	25:X:7:LEU:HA	1.90	0.53
1:1:1197:G:H2'	1:1:1198:G:H8	1.73	0.53
1:1:96:C:H2'	1:1:97:U:C6	2.43	0.53
1:1:406:U:H2'	1:1:408:A:H8	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1845:A:H2'	1:1:1846:G:C8	2.44	0.53
1:1:649:U:H2'	1:1:650:A:H8	1.73	0.53
7:F:182:LYS:H	7:F:182:LYS:HD2	1.74	0.53
3:B:70:SER:HB3	3:B:83:LYS:HG2	1.91	0.53
21:T:63:HIS:CD2	21:T:78:ILE:HG21	2.44	0.53
14:M:75:ASN:HB3	14:M:128:PHE:HE2	1.74	0.53
9:H:51:ILE:HD12	9:H:179:LYS:HE3	1.90	0.53
1:1:92:A:H61	1:1:444:G:H1'	1.72	0.53
22:U:67:LYS:HD2	22:U:76:THR:HG22	1.89	0.52
11:J:153:SER:HB2	11:J:156:HIS:CD2	2.44	0.52
4:C:212:LYS:NZ	4:C:216:MET:SD	2.82	0.52
1:1:1644:C:H4'	18:Q:140:ARG:HB2	1.91	0.52
10:I:6:ASP:HB3	10:I:28:GLU:OE1	2.09	0.52
1:1:433:A:H2'	1:1:434:G:C8	2.44	0.52
3:B:144:LYS:HB3	3:B:206:PRO:HG2	1.90	0.52
9:H:76:GLN:OE1	9:H:76:GLN:HA	2.09	0.52
1:1:800:U:H2'	1:1:801:U:O4'	2.10	0.52
1:1:1473:G:OP2	1:1:1473:G:N2	2.41	0.52
1:1:909:G:H2'	1:1:910:G:H8	1.73	0.52
9:H:117:PRO:HB2	9:H:120:ARG:HG2	1.92	0.52
3:B:161:VAL:HA	3:B:164:ILE:HG22	1.91	0.52
1:1:1278:A:OP1	12:K:55:ARG:NH2	2.39	0.52
6:E:222:LEU:HA	6:E:225:ILE:HD12	1.91	0.52
11:J:32:ILE:O	11:J:36:GLY:N	2.38	0.52
1:1:610:G:O6	1:1:634:A:N6	2.42	0.52
18:Q:30:GLY:N	18:Q:67:ASP:OD1	2.40	0.52
22:U:49:LYS:HB2	22:U:92:HIS:HE1	1.73	0.52
1:1:1048:G:N1	1:1:1069:U:OP2	2.37	0.52
27:Z:58:LEU:O	27:Z:62:VAL:N	2.37	0.52
1:1:1144:A:H2'	1:1:1145:A:C8	2.44	0.52
1:1:815:U:C2	1:1:816:A:C8	2.97	0.52
21:T:5:THR:HG22	21:T:7:LYS:H	1.73	0.52
26:Y:86:GLU:OE1	26:Y:90:ARG:NH1	2.43	0.52
1:1:952:G:H2'	1:1:953:C:C6	2.44	0.52
1:1:24:C:OP1	11:J:11:LYS:NZ	2.38	0.52
1:1:1453:C:O2'	19:R:48:ASN:O	2.24	0.52
1:1:1454:A:C5'	19:R:5:ARG:HH21	2.23	0.52
5:D:39:VAL:HG22	5:D:48:ILE:HG12	1.91	0.52
1:1:980:A:H2'	1:1:981:A:C8	2.44	0.52
1:1:1536:G:H2'	1:1:1537:A:C8	2.44	0.52
1:1:1274:G:N2	12:K:28:HIS:HB3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:27:LEU:HD11	9:H:45:ILE:HD11	1.92	0.52
1:1:1605:G:OP1	21:T:84:ARG:NH2	2.43	0.52
4:C:201:GLY:N	4:C:221:ASP:OD2	2.43	0.52
16:O:117:ARG:O	16:O:121:ARG:HG2	2.10	0.52
1:1:1407:U:O2'	18:Q:11:GLN:NE2	2.42	0.52
17:P:126:VAL:HG23	17:P:128:HIS:HD2	1.75	0.52
12:K:40:VAL:HB	12:K:44:HIS:HB2	1.91	0.52
12:K:7:ASN:ND2	12:K:44:HIS:HB3	2.25	0.52
1:1:1622:U:C5	20:S:120:HIS:HB2	2.44	0.52
4:C:169:TYR:CZ	4:C:177:PRO:HG3	2.45	0.52
1:1:666:U:H5'	1:1:1088:U:O4'	2.09	0.52
9:H:91:HIS:NE2	9:H:168:HIS:HB3	2.25	0.52
2:A:57:LYS:HZ3	23:V:70:LEU:HB3	1.75	0.51
1:1:929:G:H2'	1:1:930:C:O4'	2.10	0.51
8:G:76:LEU:HD11	8:G:92:ARG:HB3	1.91	0.51
3:B:116:LYS:HG2	3:B:117:TRP:CD1	2.45	0.51
4:C:113:GLN:HA	4:C:122:THR:HA	1.92	0.51
16:O:83:GLN:NE2	16:O:87:GLU:OE2	2.42	0.51
1:1:917:U:N3	1:1:918:U:O4	2.43	0.51
2:A:68:ILE:HG13	2:A:70:ASN:H	1.76	0.51
24:W:28:ARG:CG	24:W:29:PRO:HD3	2.40	0.51
21:T:69:GLY:HA2	21:T:120:GLY:H	1.74	0.51
21:T:30:VAL:HG23	21:T:34:VAL:HG23	1.91	0.51
1:1:1691:U:H2'	1:1:1692:U:H5'	1.91	0.51
1:1:1453:C:N4	1:1:1455:A:N3	2.58	0.51
19:R:5:ARG:HH11	19:R:9:VAL:HG11	1.75	0.51
10:I:101:ILE:HD11	10:I:198:TYR:CD1	2.45	0.51
25:X:108:LYS:HE2	25:X:120:PHE:HZ	1.74	0.51
3:B:46:LYS:NZ	16:O:20:GLN:O	2.29	0.51
5:D:167:TYR:OH	5:D:202:LYS:O	2.19	0.51
1:1:1736:G:H2'	1:1:1737:G:C8	2.45	0.51
18:Q:42:ILE:HB	18:Q:48:GLN:HB2	1.92	0.51
5:D:7:LYS:HA	5:D:10:LYS:HE2	1.93	0.51
1:1:525:A:H2'	1:1:526:A:H8	1.76	0.51
18:Q:45:ARG:HH22	21:T:10:ASN:HD22	1.56	0.51
1:1:1146:C:H2'	1:1:1147:C:C6	2.45	0.51
2:A:90:PHE:O	2:A:94:THR:HG22	2.10	0.51
19:R:105:MET:O	19:R:109:LEU:CB	2.58	0.51
1:1:1235:G:H5'	1:1:1247:C:H42	1.76	0.51
1:1:1528:G:H2'	1:1:1529:C:C6	2.46	0.51
1:1:1446:A:HO2'	1:1:1447:G:H8	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1096:G:OP1	24:W:20:ARG:NE	2.43	0.51
5:D:33:GLY:HA3	5:D:53:THR:HB	1.91	0.51
1:1:1389:C:O2'	5:D:163:PRO:HD3	2.10	0.51
17:P:85:ILE:HD11	17:P:116:LEU:HD21	1.91	0.51
1:1:1675:A:O2'	7:F:74:ASN:O	2.29	0.51
1:1:1455:A:N6	1:1:1456:G:O6	2.44	0.51
25:X:39:ASN:HB2	25:X:108:LYS:HZ1	1.74	0.51
16:O:29:GLY:O	16:O:94:HIS:N	2.43	0.51
10:I:36:THR:H	10:I:95:THR:HG23	1.76	0.51
10:I:26:LYS:HD2	10:I:29:LEU:HD21	1.93	0.51
1:1:916:A:O2'	15:N:73:ARG:NH1	2.40	0.51
5:D:65:ARG:HG2	12:K:70:TYR:OH	2.11	0.51
6:E:11:ARG:HA	6:E:28:ALA:HB2	1.93	0.51
1:1:491:C:OP2	26:Y:104:ARG:HD3	2.11	0.51
1:1:1513:C:H2'	1:1:1514:G:H8	1.75	0.51
1:1:941:C:H2'	1:1:942:G:H8	1.74	0.51
8:G:222:GLU:O	8:G:226:GLU:HG2	2.11	0.51
9:H:134:VAL:HG22	9:H:173:PHE:HE2	1.76	0.51
18:Q:51:LEU:HD12	18:Q:81:ILE:HG23	1.92	0.51
1:1:432:G:H2'	1:1:433:A:H8	1.75	0.51
1:1:921:G:H2'	24:W:28:ARG:NH1	2.25	0.51
1:1:486:A:H1'	1:1:513:G:H22	1.76	0.51
1:1:1565:C:OP2	21:T:101:ARG:NH1	2.44	0.51
10:I:110:ARG:O	10:I:114:GLU:CB	2.58	0.51
4:C:88:ILE:HG23	4:C:93:ILE:HD12	1.93	0.51
4:C:270:THR:HA	4:C:273:LEU:HD12	1.92	0.50
12:K:3:MET:SD	12:K:7:ASN:ND2	2.84	0.50
21:T:75:MET:HA	21:T:78:ILE:HD12	1.93	0.50
13:L:147:LYS:HG2	13:L:149:ALA:H	1.76	0.50
19:R:29:HIS:HA	19:R:32:LYS:HE2	1.93	0.50
15:N:66:VAL:HG13	15:N:67:THR:H	1.76	0.50
19:R:73:LEU:O	19:R:78:ARG:NH1	2.44	0.50
1:1:22:A:O2'	11:J:15:THR:HG21	2.11	0.50
10:I:70:GLU:OE1	10:I:117:TYR:OH	2.29	0.50
7:F:182:LYS:N	7:F:182:LYS:HD2	2.26	0.50
20:S:86:ARG:HG3	20:S:98:VAL:HG13	1.93	0.50
1:1:294:U:C4	13:L:65:ASN:HB3	2.46	0.50
20:S:24:ARG:HG3	20:S:25:LYS:H	1.75	0.50
14:M:52:LEU:HD23	14:M:76:LEU:HD11	1.94	0.50
1:1:640:A:H2'	1:1:641:A:C8	2.47	0.50
27:Z:83:LEU:O	27:Z:87:ALA:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:104:ASP:HB3	4:C:130:ILE:HG22	1.93	0.50
1:1:918:U:O2'	1:1:919:A:O4'	2.30	0.50
21:T:80:GLY:HA2	21:T:92:PHE:HE1	1.76	0.50
8:G:186:GLN:HB3	8:G:189:ARG:HH21	1.77	0.50
2:A:102:ARG:CZ	2:A:104:THR:HA	2.40	0.50
5:D:71:ALA:O	5:D:75:LYS:HG2	2.12	0.50
6:E:6:LYS:HB2	6:E:30:ARG:HH12	1.75	0.50
9:H:53:VAL:HG13	9:H:175:GLY:HA3	1.93	0.50
16:O:106:LYS:HE2	16:O:136:PRO:HD2	1.93	0.50
26:Y:12:PHE:HD1	26:Y:23:MET:HB3	1.76	0.50
1:1:524:U:H3	1:1:594:A:H62	1.58	0.50
14:M:13:ASP:O	14:M:17:ALA:HB3	2.12	0.50
9:H:98:ARG:NH2	9:H:125:VAL:O	2.45	0.50
1:1:522:A:N6	1:1:644:G:OP1	2.38	0.50
1:1:28:U:H2'	1:1:29:G:C8	2.47	0.50
1:1:355:G:H5''	13:L:105:ARG:NH1	2.26	0.50
10:I:67:TRP:HH2	10:I:162:LEU:HD13	1.77	0.50
24:W:94:LEU:HD22	24:W:100:GLY:HA3	1.93	0.50
14:M:85:LEU:HA	14:M:88:TRP:HD1	1.75	0.50
2:A:94:THR:O	2:A:186:ARG:NH1	2.39	0.50
13:L:101:ARG:NH2	25:X:13:LEU:HD11	2.23	0.50
3:B:151:ARG:NH2	3:B:153:THR:OG1	2.44	0.50
1:1:99:A:H61	1:1:433:A:H1'	1.77	0.50
1:1:1354:G:H2'	1:1:1356:G:N7	2.27	0.50
21:T:134:ILE:HA	21:T:137:GLN:HG2	1.94	0.50
19:R:41:ILE:H	19:R:47:ARG:NH2	2.09	0.50
1:1:291:G:O6	6:E:204:SER:OG	2.29	0.50
1:1:141:A:H4'	1:1:142:C:H5'	1.94	0.50
1:1:122:G:H21	6:E:146:THR:HG21	1.76	0.50
1:1:1036:A:N3	1:1:1844:U:O2'	2.44	0.50
13:L:13:GLN:NE2	13:L:16:ILE:O	2.31	0.50
18:Q:42:ILE:HD12	18:Q:48:GLN:HG3	1.94	0.50
1:1:957:A:H3'	1:1:958:G:N2	2.26	0.50
1:1:301:A:O2'	10:I:73:THR:O	2.27	0.50
1:1:1093:A:H2'	1:1:1094:C:H6	1.76	0.50
1:1:495:U:P	6:E:58:GLY:H	2.35	0.50
1:1:64:A:H2	1:1:83:A:H62	1.59	0.50
1:1:582:U:H2'	1:1:583:A:H8	1.77	0.50
12:K:52:LEU:HA	12:K:57:TYR:HD2	1.76	0.50
26:Y:123:ALA:O	26:Y:127:ALA:HB2	2.11	0.50
3:B:65:ARG:HD3	16:O:50:LYS:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:129:ILE:HG22	16:O:130:GLU:N	2.26	0.49
1:1:601:G:H1	1:1:621:C:H5	1.60	0.49
1:1:1211:G:H2'	1:1:1212:G:C8	2.47	0.49
1:1:962:A:H5''	16:O:66:ARG:HG2	1.93	0.49
20:S:119:ALA:O	20:S:123:LEU:N	2.44	0.49
3:B:144:LYS:HD3	3:B:208:HIS:HD2	1.77	0.49
1:1:352:U:O2	13:L:71:ARG:NE	2.41	0.49
1:1:1337:C:H2'	1:1:1338:G:H8	1.77	0.49
9:H:93:VAL:CG2	9:H:173:PHE:CE1	2.93	0.49
1:1:1198:G:H2'	1:1:1199:A:H8	1.77	0.49
8:G:121:ILE:HG21	8:G:124:LEU:HD12	1.94	0.49
5:D:68:GLU:OE2	12:K:71:LEU:N	2.39	0.49
1:1:744:G:N3	9:H:107:LYS:HB3	2.26	0.49
25:X:100:VAL:HG13	25:X:122:VAL:HG13	1.94	0.49
1:1:1592:C:H5''	7:F:91:ARG:HH12	1.77	0.49
12:K:29:MET:HG3	12:K:30:PRO:HD3	1.94	0.49
1:1:898:U:H2'	1:1:899:U:C6	2.48	0.49
16:O:59:GLY:HA2	16:O:68:GLU:OE1	2.12	0.49
20:S:47:LYS:HE3	20:S:78:LYS:HD3	1.94	0.49
13:L:103:GLU:OE2	13:L:105:ARG:NH2	2.46	0.49
1:1:851:C:O3'	1:1:852:G:N2	2.42	0.49
14:M:26:LEU:HB2	14:M:31:LEU:HD13	1.93	0.49
1:1:792:C:H2'	1:1:793:G:H8	1.78	0.49
2:A:210:ILE:HA	2:A:213:GLU:HB3	1.95	0.49
21:T:116:ASP:HB3	21:T:119:GLY:HA3	1.95	0.49
1:1:1226:G:N1	1:1:1639:G:OP2	2.45	0.49
6:E:87:MET:HE1	6:E:236:ILE:HG13	1.95	0.49
1:1:335:G:C2	1:1:336:A:N7	2.80	0.49
14:M:84:LYS:HB3	14:M:88:TRP:HE1	1.78	0.49
1:1:1839:U:H2'	1:1:1840:U:C6	2.47	0.49
1:1:89:C:H2'	1:1:90:G:C8	2.48	0.49
6:E:96:GLY:O	6:E:97:GLU:HG3	2.13	0.49
1:1:1063:C:O2'	16:O:150:ARG:CG	2.61	0.49
7:F:59:LYS:O	7:F:62:ARG:HG2	2.13	0.49
1:1:998:A:C5	1:1:999:G:H1'	2.48	0.49
21:T:104:LEU:HD21	21:T:121:ARG:HD3	1.95	0.49
1:1:391:C:H2'	1:1:392:A:C8	2.47	0.49
1:1:226:A:H1'	1:1:227:U:H5	1.78	0.49
1:1:145:G:H2'	1:1:146:G:C8	2.48	0.49
2:A:155:ARG:HG2	2:A:156:TYR:CD2	2.47	0.49
1:1:862:A:C8	24:W:107:SER:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:60:TRP:CH2	4:C:67:GLY:HA3	2.48	0.49
1:1:875:A:C6	1:1:912:C:N3	2.81	0.49
1:1:880:G:H2'	1:1:881:G:C8	2.48	0.49
1:1:14:C:H5''	4:C:190:SER:OG	2.13	0.49
14:M:124:ILE:O	14:M:128:PHE:CB	2.60	0.49
1:1:1856:C:H2'	1:1:1857:G:H8	1.78	0.49
1:1:444:G:N2	1:1:447:A:OP2	2.46	0.49
19:R:73:LEU:HD23	19:R:78:ARG:HH12	1.78	0.49
3:B:122:GLU:OE1	3:B:213:ARG:NH1	2.44	0.49
3:B:138:PHE:HB3	3:B:213:ARG:HH21	1.78	0.49
16:O:85:CYS:HB3	16:O:90:ILE:HD11	1.95	0.49
11:J:136:ARG:N	11:J:158:ASP:O	2.39	0.49
11:J:18:ARG:O	11:J:24:ARG:NH2	2.29	0.49
1:1:1593:C:C2	27:Z:104:ARG:NH2	2.80	0.49
1:1:689:U:H2'	1:1:690:G:C4	2.48	0.49
15:N:34:LYS:O	15:N:37:ILE:HG22	2.13	0.49
1:1:1143:A:OP2	4:C:187:ARG:NH2	2.37	0.49
25:X:101:LEU:HB3	25:X:124:LYS:H	1.78	0.49
18:Q:51:LEU:HD11	18:Q:84:ILE:HB	1.95	0.49
1:1:388:U:H2'	1:1:389:A:C8	2.48	0.49
13:L:24:LEU:HD12	13:L:25:LEU:N	2.27	0.49
1:1:1513:C:H2'	1:1:1514:G:C8	2.48	0.49
1:1:1362:U:H5''	1:1:1363:C:H5	1.77	0.49
25:X:90:CYS:HB3	25:X:130:LEU:HD22	1.94	0.49
21:T:41:LYS:HG3	21:T:43:LYS:HG2	1.95	0.48
12:K:3:MET:HB3	12:K:4:PRO:HD2	1.95	0.48
1:1:604:A:N3	1:1:639:C:O2'	2.40	0.48
1:1:1844:U:N3	1:1:1845:A:N7	2.61	0.48
22:U:49:LYS:HB2	22:U:92:HIS:CE1	2.47	0.48
1:1:659:G:O2'	1:1:662:G:O2'	2.24	0.48
1:1:479:C:C2	1:1:480:G:C8	3.01	0.48
19:R:54:VAL:O	19:R:58:MET:HG2	2.13	0.48
16:O:39:ASP:OD1	16:O:40:THR:N	2.45	0.48
12:K:13:GLU:OE1	12:K:82:TYR:OH	2.31	0.48
11:J:41:ARG:O	11:J:45:ARG:HG3	2.13	0.48
1:1:1602:U:O2'	20:S:24:ARG:NH1	2.46	0.48
6:E:198:ARG:HH12	6:E:200:ARG:HD2	1.77	0.48
3:B:149:GLN:HG2	3:B:150:ILE:N	2.28	0.48
1:1:453:C:O2'	8:G:92:ARG:O	2.24	0.48
1:1:1395:C:H2'	1:1:1396:A:H8	1.74	0.48
23:V:34:MET:N	23:V:53:TYR:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1848:U:H2'	1:1:1850:A:OP2	2.13	0.48
20:S:82:TRP:HA	20:S:87:GLN:HE22	1.79	0.48
1:1:1345:G:N7	1:1:1371:U:O2'	2.38	0.48
1:1:1628:C:H2'	1:1:1629:C:C6	2.49	0.48
2:A:63:ARG:NH1	23:V:78:ILE:HG12	2.28	0.48
2:A:76:VAL:HG12	2:A:87:VAL:HG22	1.96	0.48
27:Z:74:SER:HA	27:Z:77:LEU:CD1	2.38	0.48
1:1:875:A:H61	1:1:911:C:H42	1.60	0.48
9:H:43:LEU:HD12	9:H:44:ASN:H	1.78	0.48
9:H:44:ASN:OD1	9:H:65:PRO:HG2	2.13	0.48
22:U:67:LYS:HE2	22:U:78:ASP:OD1	2.13	0.48
1:1:1101:U:H2'	1:1:1102:G:C8	2.42	0.48
1:1:1541:G:H21	21:T:12:GLN:NE2	2.12	0.48
4:C:167:ARG:HB3	4:C:177:PRO:HB2	1.95	0.48
19:R:17:ILE:HA	19:R:21:TYR:HB2	1.95	0.48
1:1:412:G:OP2	1:1:425:G:N2	2.43	0.48
11:J:64:ASP:OD1	11:J:65:GLU:N	2.45	0.48
1:1:855:G:O2'	13:L:71:ARG:NH1	2.44	0.48
3:B:46:LYS:HD3	16:O:19:PRO:HB2	1.96	0.48
1:1:1656:G:H2'	1:1:1657:G:H8	1.79	0.48
9:H:88:SER:HB3	9:H:90:LYS:H	1.78	0.48
1:1:185:G:H2'	1:1:186:C:C6	2.49	0.48
15:N:20:ARG:HH21	24:W:56:HIS:HE1	1.60	0.48
1:1:1705:C:H2'	1:1:1706:G:C8	2.49	0.48
1:1:1441:U:H6	1:1:1443:C:H41	1.62	0.48
2:A:86:ALA:O	2:A:90:PHE:HB2	2.13	0.48
1:1:1348:G:N2	1:1:1381:G:H22	2.10	0.48
1:1:574:A:H4'	26:Y:89:HIS:HB2	1.96	0.48
1:1:17:C:H2'	1:1:18:C:C6	2.48	0.48
10:I:82:VAL:O	10:I:101:ILE:HB	2.14	0.48
1:1:1231:C:H5''	20:S:134:GLN:HE21	1.79	0.48
1:1:900:C:H2'	1:1:901:G:H8	1.78	0.48
1:1:89:C:H2'	1:1:90:G:H8	1.78	0.48
9:H:109:ARG:HG2	9:H:110:THR:HG23	1.94	0.48
12:K:50:GLN:HA	12:K:53:LYS:HG2	1.95	0.48
1:1:219:U:O2'	10:I:186:ASP:OD2	2.29	0.48
1:1:1595:U:H2'	1:1:1596:U:C6	2.49	0.48
8:G:121:ILE:HD13	8:G:124:LEU:HD12	1.95	0.48
1:1:676:C:H2'	1:1:677:G:O4'	2.14	0.48
1:1:1211:G:O2'	1:1:1212:G:OP1	2.26	0.48
7:F:39:ILE:HG23	7:F:68:ILE:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:91:SER:HB2	4:C:159:LYS:HG3	1.95	0.48
27:Z:44:LEU:HD23	27:Z:45:ASN:CA	2.44	0.48
13:L:104:LYS:O	25:X:11:ARG:NH2	2.40	0.48
26:Y:123:ALA:O	26:Y:127:ALA:CB	2.61	0.48
5:D:107:TYR:HD1	5:D:110:LEU:HD12	1.79	0.48
1:1:319:C:H2'	1:1:320:G:C8	2.48	0.48
6:E:133:VAL:O	6:E:136:ILE:HG12	2.13	0.48
2:A:86:ALA:HA	2:A:202:TYR:HD1	1.79	0.48
2:A:120:ARG:NH1	4:C:267:GLN:HE21	2.12	0.48
3:B:148:ASN:N	3:B:148:ASN:ND2	2.60	0.48
1:1:373:G:H2'	1:1:374:G:H8	1.79	0.48
10:I:110:ARG:NH1	10:I:121:LEU:O	2.46	0.48
1:1:72:C:O2'	1:1:73:C:H5''	2.13	0.48
1:1:624:C:H41	25:X:63:ASN:ND2	2.12	0.48
2:A:38:ILE:HD11	2:A:47:TYR:CB	2.44	0.48
1:1:1004:U:H2'	1:1:1005:G:C8	2.48	0.48
1:1:1136:U:H2'	1:1:1137:U:C6	2.49	0.48
1:1:1845:A:H2'	1:1:1846:G:H8	1.79	0.48
1:1:922:A:H2'	1:1:923:G:O4'	2.14	0.48
1:1:383:G:O3'	13:L:132:ARG:NH1	2.47	0.48
6:E:36:HIS:CD2	6:E:85:GLY:HA3	2.49	0.48
6:E:131:VAL:HA	6:E:137:PRO:HA	1.96	0.48
1:1:84:A:H5''	26:Y:122:LYS:HE3	1.96	0.48
17:P:14:LYS:HE3	17:P:22:LEU:HB3	1.95	0.48
1:1:13:C:H5'	4:C:232:THR:HB	1.96	0.47
25:X:10:ALA:HA	25:X:13:LEU:HD12	1.95	0.47
1:1:93:U:OP2	6:E:3:ARG:NH2	2.46	0.47
14:M:26:LEU:HD13	14:M:89:VAL:O	2.14	0.47
5:D:108:LYS:HB3	5:D:113:LEU:HD23	1.95	0.47
18:Q:87:SER:O	18:Q:91:ALA:HB2	2.14	0.47
2:A:206:ASP:OD1	2:A:207:PRO:HD2	2.14	0.47
1:1:869:A:OP1	1:1:874:G:O2'	2.32	0.47
20:S:43:VAL:O	20:S:47:LYS:HG2	2.14	0.47
3:B:207:LEU:HB3	3:B:208:HIS:H	1.52	0.47
1:1:1130:G:H4'	15:N:10:GLY:HA2	1.96	0.47
26:Y:114:MET:HB3	26:Y:122:LYS:HD2	1.96	0.47
24:W:106:THR:OG1	24:W:109:GLY:O	2.29	0.47
8:G:49:VAL:O	8:G:114:VAL:N	2.46	0.47
1:1:1152:U:H1'	24:W:16:ASN:HD21	1.79	0.47
1:1:1468:C:H2'	1:1:1469:A:H8	1.78	0.47
1:1:929:G:N2	1:1:1104:G:H4'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:34:THR:O	25:X:38:ALA:HB2	2.14	0.47
1:1:1210:G:H5''	2:A:85:ARG:HH12	47.31	0.47
1:1:678:U:H2'	1:1:679:A:H8	1.80	0.47
13:L:35:ARG:HG2	13:L:36:TYR:H	1.80	0.47
27:Z:91:LEU:HD23	27:Z:97:ILE:HD12	1.95	0.47
4:C:178:HIS:CD2	4:C:200:ARG:HG2	2.49	0.47
3:B:123:ALA:HB3	3:B:139:CYS:HB3	1.97	0.47
20:S:110:ASP:OD1	20:S:113:ARG:NH1	2.46	0.47
1:1:439:A:H4'	1:1:1799:G:H4'	1.97	0.47
1:1:1099:G:H1	1:1:1133:A:H2	1.58	0.47
1:1:351:G:N3	1:1:351:G:H2'	2.29	0.47
8:G:8:PRO:HD3	8:G:112:VAL:HG13	1.95	0.47
8:G:77:LEU:HD12	8:G:95:LYS:HD3	1.96	0.47
1:1:1788:A:H2'	1:1:1789:G:O4'	2.15	0.47
24:W:53:ILE:HB	24:W:60:LYS:HB2	1.96	0.47
1:1:61:A:H2	1:1:335:G:HO2'	1.61	0.47
17:P:118:GLU:HA	20:S:120:HIS:ND1	2.29	0.47
1:1:1112:U:H1'	3:B:146:ARG:HH22	1.80	0.47
3:B:30:TRP:CE2	16:O:19:PRO:HD3	2.49	0.47
1:1:573:U:H1'	1:1:576:A:N7	2.29	0.47
1:1:322:C:H2'	1:1:323:C:C6	2.49	0.47
8:G:3:LEU:HD12	8:G:16:ILE:HD11	1.96	0.47
1:1:1401:A:H4'	22:U:52:GLY:HA3	1.95	0.47
1:1:827:A:H4'	11:J:8:VAL:HG11	1.96	0.47
16:O:150:ARG:N	16:O:150:ARG:CD	2.73	0.47
1:1:1787:G:H2'	1:1:1788:A:C8	2.50	0.47
9:H:39:GLN:HE21	9:H:72:PHE:HA	1.79	0.47
1:1:652:U:H2'	1:1:653:A:C8	2.50	0.47
1:1:1736:G:H2'	1:1:1737:G:H8	1.78	0.47
1:1:155:G:H2'	1:1:156:G:C8	2.49	0.47
15:N:35:GLU:O	15:N:39:LYS:HG2	2.14	0.47
9:H:134:VAL:O	9:H:134:VAL:HG12	2.15	0.47
20:S:36:VAL:HG13	20:S:40:TYR:HD2	1.79	0.47
1:1:547:G:H3'	1:1:547:G:OP1	2.15	0.47
1:1:1445:U:O4	1:1:1446:A:N6	2.47	0.47
4:C:253:PRO:HD2	24:W:99:PHE:CE1	2.49	0.47
6:E:197:ASN:OD1	6:E:198:ARG:N	2.48	0.47
1:1:598:G:H2'	1:1:599:A:H8	1.80	0.47
1:1:1403:C:OP2	1:1:1405:A:N6	2.35	0.47
7:F:122:ARG:HG3	7:F:123:GLU:HG2	1.95	0.47
1:1:1113:A:H4'	3:B:202:GLN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:6:VAL:HG12	21:T:135:ALA:HB2	1.95	0.47
1:1:387:C:OP1	10:I:10:LYS:NZ	2.25	0.47
24:W:50:PHE:HB3	24:W:63:VAL:HA	1.95	0.47
1:1:511:U:H2'	1:1:512:A:C8	2.49	0.47
2:A:176:TRP:O	2:A:180:ARG:HB2	2.15	0.47
15:N:24:THR:HB	15:N:25:TRP:CE3	2.50	0.47
2:A:36:GLN:HE22	23:V:70:LEU:HD21	1.79	0.47
1:1:875:A:H61	1:1:911:C:N4	2.13	0.47
1:1:1594:A:C8	27:Z:104:ARG:HG2	2.50	0.47
1:1:1650:A:H1'	1:1:1675:A:H61	1.78	0.47
5:D:40:ARG:HB2	5:D:47:GLU:HB3	1.97	0.47
1:1:981:A:H2'	1:1:982:G:C8	2.50	0.47
1:1:498:C:H2'	1:1:499:G:C8	2.49	0.47
1:1:1554:C:O2	5:D:76:ARG:NH2	2.48	0.47
15:N:20:ARG:HH21	24:W:56:HIS:CE1	2.32	0.47
23:V:59:ILE:HG23	23:V:64:GLU:HB3	1.95	0.47
3:B:89:GLU:HG2	3:B:228:LEU:HD22	1.96	0.47
9:H:188:GLU:HG2	9:H:190:PRO:HD3	1.97	0.47
14:M:94:ILE:HG22	14:M:100:PRO:HA	1.97	0.47
27:Z:89:GLN:NE2	27:Z:109:TYR:OH	2.48	0.47
1:1:976:G:H2'	1:1:977:C:C6	2.50	0.47
18:Q:43:GLU:HB2	18:Q:44:PRO:HD3	1.97	0.47
1:1:104:A:H4'	10:I:18:ARG:NH2	2.30	0.47
1:1:1798:C:H2'	1:1:1799:G:O4'	2.15	0.47
1:1:620:G:H2'	1:1:620:G:N3	2.30	0.47
1:1:498:C:H5'	6:E:7:LYS:HD3	1.96	0.47
11:J:84:ILE:O	11:J:108:ARG:NE	2.48	0.47
1:1:1360:U:O2'	1:1:1379:A:OP2	2.25	0.47
20:S:84:LEU:HD12	20:S:95:TYR:HB3	1.96	0.47
2:A:42:LYS:HD3	2:A:48:ILE:HD11	1.97	0.47
9:H:31:GLU:HG2	9:H:40:LEU:HB3	1.97	0.47
22:U:33:GLU:OE2	22:U:87:ARG:NH2	2.36	0.47
1:1:17:C:H2'	1:1:18:C:H6	1.79	0.47
5:D:217:ILE:HG13	5:D:218:LEU:H	1.80	0.47
1:1:1097:G:H4'	2:A:32:PHE:CD1	2.50	0.47
1:1:1101:U:OP1	3:B:151:ARG:HD2	2.14	0.47
6:E:71:LYS:HA	6:E:76:VAL:HA	1.97	0.47
5:D:18:LYS:O	5:D:22:ASN:CB	2.61	0.47
13:L:24:LEU:HD12	13:L:25:LEU:HG	1.95	0.47
1:1:660:C:H5''	25:X:3:LYS:HD3	1.96	0.47
20:S:26:ILE:HG23	20:S:27:ALA:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:171:VAL:HA	2:A:174:MET:HE2	1.96	0.47
4:C:112:VAL:HG23	4:C:123:ARG:HG3	1.97	0.46
1:1:1539:U:H2'	1:1:1540:G:H8	1.80	0.46
1:1:1412:C:H2'	1:1:1413:G:O4'	2.15	0.46
10:I:158:ILE:HB	10:I:162:LEU:HB2	1.96	0.46
2:A:111:GLN:NE2	4:C:64:THR:OG1	2.48	0.46
17:P:30:TYR:O	17:P:34:MET:HG2	2.15	0.46
1:1:430:C:C2	1:1:431:G:C8	3.03	0.46
1:1:448:A:OP1	10:I:25:ARG:NH1	2.49	0.46
15:N:47:PRO:HA	15:N:50:ILE:HB	1.96	0.46
6:E:147:ILE:HG23	6:E:150:PRO:HG3	1.95	0.46
1:1:909:G:H2'	1:1:910:G:C8	2.51	0.46
1:1:1268:C:N4	1:1:1269:G:O6	2.48	0.46
1:1:875:A:H61	1:1:912:C:N4	2.11	0.46
1:1:65:C:C6	8:G:174:PRO:HB3	2.50	0.46
19:R:88:VAL:HG13	19:R:89:SER:N	2.31	0.46
1:1:1411:G:H2'	1:1:1412:C:H6	1.80	0.46
1:1:1268:C:O2	17:P:97:TYR:OH	2.34	0.46
21:T:128:GLN:O	21:T:132:ASP:HB2	2.16	0.46
26:Y:63:HIS:ND1	26:Y:68:LYS:O	2.46	0.46
7:F:77:MET:HB2	7:F:84:GLY:N	2.31	0.46
2:A:73:ASP:HB3	2:A:120:ARG:H	1.80	0.46
6:E:247:THR:HG22	6:E:248:VAL:N	2.30	0.46
1:1:431:G:C2	1:1:432:G:C8	3.03	0.46
1:1:428:U:H4'	11:J:2:PRO:HD2	1.96	0.46
15:N:135:LEU:HD21	15:N:139:TRP:CE3	2.50	0.46
1:1:1782:G:H3'	1:1:1783:C:H5''	1.98	0.46
7:F:41:VAL:HG23	7:F:109:LEU:HD21	1.96	0.46
1:1:317:C:H2'	1:1:318:A:C8	2.50	0.46
17:P:23:ASP:OD1	17:P:24:GLN:N	2.48	0.46
6:E:45:ILE:HB	6:E:80:VAL:HG22	1.98	0.46
10:I:6:ASP:HB2	10:I:8:TRP:CD1	2.50	0.46
1:1:656:G:H1	1:1:1156:U:H5	1.63	0.46
1:1:346:C:H4'	6:E:30:ARG:HH21	1.80	0.46
17:P:34:MET:HG3	17:P:45:LEU:HD13	1.97	0.46
1:1:849:A:O2'	11:J:69:ARG:NH1	2.49	0.46
1:1:179:C:H2'	1:1:180:G:C8	2.51	0.46
19:R:91:LEU:HD13	19:R:93:GLN:HB3	1.97	0.46
1:1:991:G:C6	1:1:1134:G:H4'	2.51	0.46
1:1:1859:A:H2'	1:1:1860:A:C8	2.50	0.46
1:1:1669:G:C8	18:Q:130:LYS:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:595:U:H2'	1:1:596:U:C6	2.51	0.46
21:T:28:LEU:HD11	21:T:53:PHE:HB3	1.97	0.46
1:1:67:C:OP2	8:G:172:LYS:NZ	2.41	0.46
3:B:108:ASP:OD1	3:B:109:LYS:N	2.48	0.46
1:1:996:A:H2'	1:1:997:A:C8	2.51	0.46
3:B:88:THR:HA	3:B:98:THR:HA	1.97	0.46
1:1:1173:A:N6	1:1:1187:G:H21	2.07	0.46
1:1:14:C:H2'	1:1:15:U:C6	2.50	0.46
1:1:1469:A:H2'	1:1:1470:C:C6	2.51	0.46
7:F:201:LYS:HD2	7:F:204:ARG:HH21	1.81	0.46
1:1:167:G:H2'	1:1:168:C:C6	2.50	0.46
1:1:1806:A:H2'	1:1:1807:C:C6	2.51	0.46
1:1:527:C:H4'	11:J:125:HIS:HA	1.98	0.46
4:C:65:LYS:HE3	4:C:266:TYR:CD1	2.50	0.46
14:M:120:ALA:O	14:M:124:ILE:HG12	2.16	0.46
1:1:1286:G:C6	14:M:35:ILE:HD12	2.51	0.46
9:H:95:ILE:HG13	9:H:95:ILE:O	2.15	0.46
1:1:1067:C:H2'	1:1:1068:G:O4'	2.16	0.46
1:1:887:U:O2'	1:1:888:U:H5''	2.16	0.46
1:1:53:C:H4'	26:Y:108:LYS:HD3	1.98	0.46
14:M:53:ALA:HB2	14:M:85:LEU:HD12	1.98	0.46
1:1:740:C:O2'	1:1:741:C:O2	2.28	0.46
26:Y:76:TYR:HE2	26:Y:85:ASN:HD22	1.62	0.46
2:A:141:ASN:HD22	4:C:86:LEU:HD23	1.81	0.46
1:1:877:C:H2'	1:1:878:G:H8	1.81	0.46
25:X:135:LYS:O	25:X:137:LYS:HG2	2.15	0.46
1:1:1165:G:N2	1:1:1165:G:OP2	2.21	0.46
1:1:1539:U:OP1	21:T:43:LYS:HB3	2.16	0.46
1:1:525:A:H2'	1:1:526:A:C8	2.51	0.46
1:1:522:A:H5'	11:J:145:PRO:HG2	1.97	0.46
1:1:1018:U:H5''	15:N:71:ILE:HD11	1.98	0.46
26:Y:41:ARG:HH22	26:Y:53:ASP:HA	1.80	0.46
20:S:111:LEU:O	20:S:115:LYS:HG3	2.16	0.46
1:1:1205:C:H2'	1:1:1206:G:C8	2.50	0.46
1:1:550:C:H2'	1:1:551:U:O4'	2.16	0.46
1:1:962:A:O5'	16:O:66:ARG:NH1	2.47	0.46
1:1:1849:G:H2'	1:1:1850:A:C8	2.50	0.46
19:R:99:ASP:N	19:R:99:ASP:OD1	2.49	0.46
26:Y:7:ILE:HG12	26:Y:27:VAL:HG22	1.98	0.46
1:1:1804:U:H2'	1:1:1805:G:H8	1.81	0.46
7:F:91:ARG:NH2	18:Q:46:THR:OG1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:21:VAL:O	14:M:25:ALA:CB	2.64	0.45
1:1:649:U:H2'	1:1:650:A:C8	2.51	0.45
1:1:1636:G:H21	7:F:164:ARG:HH22	1.64	0.45
1:1:312:G:O2'	8:G:191:ARG:NH1	2.49	0.45
20:S:40:TYR:HD1	20:S:83:PHE:HE2	1.63	0.45
18:Q:58:LEU:HD21	18:Q:112:LEU:HD21	1.97	0.45
1:1:985:G:H3'	1:1:1001:A:O2'	2.16	0.45
21:T:14:PHE:CE2	21:T:18:LEU:HD22	2.51	0.45
11:J:108:ARG:HD2	11:J:113:GLN:NE2	2.30	0.45
25:X:108:LYS:HE2	25:X:120:PHE:CZ	2.50	0.45
1:1:323:C:H2'	1:1:324:C:O4'	2.16	0.45
1:1:436:G:O6	1:1:458:A:N6	2.48	0.45
24:W:14:ILE:HD13	24:W:25:VAL:HG11	1.98	0.45
9:H:146:VAL:HG13	9:H:152:ARG:HG2	1.98	0.45
1:1:602:G:OP2	1:1:603:C:O2'	2.23	0.45
13:L:130:GLU:HA	13:L:140:PHE:CD1	2.52	0.45
16:O:146:ARG:O	16:O:147:ARG:CB	2.61	0.45
1:1:429:C:H2'	1:1:430:C:H6	1.82	0.45
13:L:141:ASN:OD1	13:L:142:VAL:N	2.49	0.45
2:A:111:GLN:HG2	2:A:116:PHE:CZ	2.50	0.45
17:P:33:LEU:HD22	17:P:87:PRO:HG2	1.97	0.45
8:G:22:ARG:HG2	8:G:25:ARG:HH21	1.81	0.45
16:O:35:ALA:HB1	16:O:109:GLY:H	1.81	0.45
1:1:1552:G:OP2	1:1:1578:U:N3	2.32	0.45
11:J:4:ALA:HA	11:J:7:TRP:HH2	1.81	0.45
21:T:114:GLU:HB3	21:T:122:LYS:HG3	1.99	0.45
6:E:246:LEU:HB3	6:E:250:GLU:HB2	1.99	0.45
1:1:1064:C:O3'	16:O:149:ARG:NH2	2.49	0.45
1:1:1745:A:H2'	1:1:1746:U:O4'	2.17	0.45
21:T:11:GLN:HA	21:T:14:PHE:HB3	1.98	0.45
7:F:15:PRO:HA	7:F:48:TYR:OH	2.16	0.45
18:Q:33:LYS:HE3	18:Q:36:GLY:HA2	1.98	0.45
1:1:1643:U:H2'	1:1:1644:C:C6	2.51	0.45
1:1:1377:U:O2'	1:1:1379:A:OP1	2.35	0.45
1:1:1007:C:O2'	15:N:104:ARG:NH2	2.33	0.45
27:Z:77:LEU:C	27:Z:79:ILE:N	2.69	0.45
9:H:134:VAL:HG22	9:H:173:PHE:CE2	2.52	0.45
1:1:1752:C:N3	1:1:1780:G:N1	2.54	0.45
7:F:121:PRO:HD2	7:F:146:ARG:HG3	1.97	0.45
1:1:1593:C:H2'	27:Z:104:ARG:HH21	1.81	0.45
1:1:944:A:H5"	16:O:134:PRO:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:677:G:N2	1:1:1028:A:H62	2.13	0.45
9:H:117:PRO:HD2	9:H:120:ARG:HG3	1.99	0.45
12:K:80:ARG:HA	12:K:83:LEU:HD12	1.99	0.45
9:H:63:PHE:CE1	9:H:95:ILE:HD11	2.52	0.45
1:1:981:A:O2'	1:1:1044:G:OP1	2.28	0.45
1:1:1688:C:H2'	1:1:1689:C:C6	2.51	0.45
4:C:132:ASP:OD1	4:C:133:TYR:N	2.47	0.45
5:D:210:ILE:HG22	19:R:39:ALA:HB2	1.97	0.45
1:1:668:A:H4'	1:1:1197:G:O2'	2.16	0.45
1:1:1541:G:H2'	1:1:1542:C:C6	2.51	0.45
1:1:844:U:H2'	1:1:845:G:H8	1.81	0.45
1:1:1154:U:O2	4:C:194:ARG:NH1	2.46	0.45
1:1:869:A:O4'	9:H:114:GLN:NE2	2.50	0.45
1:1:917:U:H1'	9:H:118:ARG:HG2	1.99	0.45
1:1:375:U:O4	1:1:376:A:N6	2.50	0.45
17:P:57:LEU:HD11	17:P:86:LEU:HD11	1.98	0.45
1:1:118:C:H1'	1:1:445:A:C5	2.51	0.45
1:1:688:U:O5'	9:H:103:LYS:HD2	2.17	0.45
1:1:1358:U:H2'	1:1:1359:U:H6	1.81	0.45
1:1:14:C:H2'	1:1:15:U:H6	1.82	0.45
1:1:1538:C:H2'	1:1:1539:U:C6	2.51	0.45
1:1:1668:U:OP2	18:Q:141:TYR:OH	2.34	0.45
6:E:115:THR:HG22	6:E:116:VAL:N	2.31	0.45
1:1:1099:G:O6	1:1:1133:A:N1	2.49	0.45
19:R:99:ASP:OD2	19:R:102:THR:HB	2.16	0.45
3:B:135:LEU:HB3	3:B:217:MET:SD	2.56	0.45
3:B:171:ILE:HA	3:B:174:ARG:HG2	1.98	0.45
27:Z:99:LEU:HA	27:Z:109:TYR:HA	1.99	0.45
1:1:1592:C:H5''	7:F:91:ARG:NH1	2.31	0.45
1:1:1139:C:O2'	1:1:1140:G:C8	2.70	0.45
1:1:913:A:C5	9:H:98:ARG:HD2	2.52	0.45
3:B:121:ILE:HD13	3:B:164:ILE:HG21	1.98	0.45
1:1:837:A:H1'	26:Y:47:MET:HB3	1.98	0.45
1:1:302:A:H2'	1:1:303:C:C6	2.52	0.45
5:D:203:PRO:HG2	19:R:42:PRO:HB3	1.98	0.45
1:1:635:G:H2'	1:1:636:C:C6	2.52	0.45
1:1:893:U:C2	1:1:894:G:C8	3.05	0.45
18:Q:84:ILE:O	18:Q:88:ILE:HG12	2.17	0.45
1:1:1622:U:H5'	20:S:120:HIS:HD2	1.81	0.45
17:P:115:TYR:O	17:P:116:LEU:HB2	2.17	0.45
1:1:916:A:C5	15:N:73:ARG:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:32:HIS:NE2	12:K:41:PRO:HG3	2.32	0.45
1:1:1417:C:HO2'	21:T:2:PRO:N	2.14	0.45
1:1:906:U:H2'	1:1:907:G:C8	2.52	0.45
6:E:252:ARG:HH12	11:J:72:PHE:HA	1.81	0.45
3:B:82:ARG:NH1	3:B:191:ASP:HB2	2.32	0.44
17:P:39:ALA:HA	17:P:42:ARG:HE	1.82	0.44
1:1:17:C:H4'	1:1:1166:G:C8	2.52	0.44
1:1:1543:U:H4'	18:Q:43:GLU:OE2	2.17	0.44
5:D:29:LEU:HD21	5:D:69:LEU:HD11	1.99	0.44
4:C:144:SER:HB3	4:C:150:ALA:HB2	1.98	0.44
20:S:102:GLY:O	20:S:106:LYS:HG2	2.18	0.44
9:H:52:GLU:CD	9:H:58:LYS:CE	2.85	0.44
1:1:1189:A:H2'	1:1:1190:A:H8	1.82	0.44
1:1:1192:U:H2'	1:1:1193:U:C6	2.53	0.44
1:1:654:A:OP2	1:1:655:A:O2'	2.22	0.44
26:Y:10:ARG:N	26:Y:24:VAL:O	2.40	0.44
1:1:87:U:C2	1:1:88:G:C8	3.05	0.44
6:E:126:VAL:HG22	6:E:139:LEU:HD21	1.99	0.44
4:C:253:PRO:HD3	24:W:68:ARG:HH21	1.82	0.44
16:O:35:ALA:HB3	16:O:99:ALA:HB2	1.99	0.44
1:1:1258:A:N1	1:1:1663:A:H1'	2.32	0.44
25:X:74:LEU:HD21	25:X:81:ILE:HD12	1.98	0.44
1:1:928:G:H1	1:1:1013:U:H3	1.65	0.44
18:Q:33:LYS:HB3	18:Q:69:ARG:HA	1.99	0.44
4:C:178:HIS:HE1	4:C:198:ALA:O	1.99	0.44
1:1:740:C:H2'	1:1:741:C:H2'	1.99	0.44
13:L:69:ARG:O	13:L:130:GLU:HB3	2.17	0.44
10:I:62:VAL:HB	10:I:75:LYS:HE2	1.98	0.44
24:W:102:ILE:HB	24:W:113:HIS:HB2	1.98	0.44
1:1:1216:C:H5''	1:1:1217:A:H5''	2.00	0.44
11:J:168:GLY:O	11:J:172:ARG:NE	2.50	0.44
1:1:1787:G:H2'	1:1:1788:A:H8	1.81	0.44
14:M:13:ASP:O	14:M:17:ALA:CB	2.65	0.44
13:L:14:PRO:HG3	13:L:56:ILE:HG23	1.98	0.44
1:1:1853:C:H2'	1:1:1854:U:C6	2.52	0.44
1:1:16:G:H2'	1:1:17:C:C6	2.53	0.44
1:1:932:G:H4'	1:1:993:G:O2'	2.17	0.44
1:1:1227:G:C2	1:1:1228:A:C8	3.05	0.44
9:H:75:ILE:O	9:H:75:ILE:HG22	2.17	0.44
11:J:113:GLN:OE1	11:J:154:GLN:NE2	2.50	0.44
1:1:352:U:H2'	1:1:353:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:919:A:O2'	1:1:1020:A:N1	2.37	0.44
1:1:1802:C:H2'	1:1:1803:U:C6	2.52	0.44
1:1:1803:U:H2'	1:1:1804:U:C6	2.53	0.44
1:1:682:U:O2'	24:W:4:MET:SD	2.72	0.44
1:1:1683:C:H2'	1:1:1684:C:C6	2.53	0.44
8:G:31:ARG:HB2	8:G:34:THR:HG21	1.99	0.44
13:L:115:PRO:O	13:L:118:ARG:HG3	2.18	0.44
1:1:347:G:H2'	1:1:348:A:C8	2.52	0.44
1:1:490:C:O2'	1:1:574:A:N1	2.40	0.44
1:1:1792:G:H2'	1:1:1793:A:C8	2.45	0.44
5:D:17:PHE:HE2	5:D:39:VAL:HG21	1.82	0.44
12:K:72:THR:HG22	12:K:74:GLU:H	1.83	0.44
1:1:173:A:O2'	1:1:174:C:O5'	2.30	0.44
1:1:497:C:H2'	1:1:498:C:C6	2.53	0.44
1:1:1423:C:OP1	18:Q:33:LYS:HD2	2.18	0.44
1:1:1279:C:H2'	1:1:1280:G:O4'	2.18	0.44
15:N:96:VAL:HG22	15:N:146:ALA:HB1	1.98	0.44
10:I:132:GLU:O	10:I:133:GLU:HG2	2.17	0.44
12:K:90:VAL:HG12	12:K:91:PRO:O	2.18	0.44
12:K:90:VAL:H	12:K:95:ARG:NH2	2.16	0.44
1:1:1594:A:C6	1:1:1595:U:C4	3.06	0.44
1:1:332:G:H1'	1:1:333:G:N7	2.33	0.44
1:1:432:G:H2'	1:1:433:A:C8	2.52	0.44
1:1:620:G:H3'	1:1:621:C:O2	2.18	0.44
16:O:97:LEU:O	16:O:131:ASP:OD1	2.35	0.44
1:1:691:G:H2'	1:1:692:G:H8	1.82	0.44
1:1:693:A:H2'	1:1:694:G:C8	2.52	0.44
24:W:37:PHE:CE1	24:W:103:VAL:HG21	2.53	0.44
15:N:24:THR:HB	15:N:25:TRP:HE3	1.82	0.44
8:G:62:PRO:HG2	8:G:83:CYS:SG	2.58	0.44
1:1:872:A:C8	1:1:874:G:C2	3.06	0.44
1:1:869:A:N3	1:1:915:G:H1'	2.32	0.44
17:P:119:PHE:HE1	20:S:117:ILE:HG23	1.83	0.44
1:1:1588:A:H2'	1:1:1589:A:C8	2.53	0.44
14:M:85:LEU:HA	14:M:88:TRP:CD1	2.53	0.44
4:C:155:ILE:O	4:C:159:LYS:HG2	2.17	0.44
10:I:84:ASN:ND2	10:I:86:SER:OG	2.50	0.44
1:1:1042:A:C6	1:1:1043:G:C6	3.06	0.44
1:1:1157:G:O2'	24:W:74:VAL:O	2.29	0.44
21:T:46:ALA:HB1	21:T:47:PRO:HD2	1.99	0.44
19:R:98:VAL:HG11	19:R:120:THR:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1373:C:H2'	1:1:1374:C:C6	2.53	0.44
4:C:139:LEU:HD11	4:C:237:ALA:HB1	2.00	0.44
21:T:27:LYS:HB3	21:T:110:LEU:HD21	2.00	0.44
1:1:803:C:H2'	1:1:804:U:H6	1.83	0.44
6:E:122:LYS:HB3	6:E:162:ILE:HG23	2.00	0.44
1:1:312:G:C2	1:1:338:G:N1	2.86	0.43
8:G:188:LYS:O	8:G:191:ARG:HG2	2.18	0.43
20:S:55:ARG:HB2	20:S:58:GLU:HG3	2.00	0.43
20:S:58:GLU:OE2	27:Z:50:PHE:HE2	2.01	0.43
1:1:1665:G:OP1	21:T:88:MET:HG3	2.18	0.43
16:O:129:ILE:O	16:O:130:GLU:HG3	2.18	0.43
1:1:438:G:H2'	1:1:439:A:H8	1.82	0.43
21:T:70:ALA:HB3	21:T:121:ARG:HE	1.82	0.43
21:T:14:PHE:HE2	21:T:18:LEU:HD22	1.83	0.43
1:1:815:U:N3	1:1:816:A:N7	2.66	0.43
6:E:149:TYR:N	6:E:150:PRO:HD3	2.33	0.43
1:1:354:U:H2'	1:1:355:G:C8	2.53	0.43
1:1:49:C:H2'	1:1:472:C:H41	1.83	0.43
1:1:945:U:H2'	1:1:946:U:C6	2.52	0.43
18:Q:93:VAL:O	18:Q:97:GLN:HG3	2.17	0.43
2:A:89:LYS:HD3	19:R:80:ARG:HG2	2.00	0.43
1:1:13:C:H1'	1:1:1355:C:C4	2.53	0.43
1:1:941:C:H2'	1:1:942:G:C8	2.53	0.43
1:1:942:G:H2'	1:1:943:U:C6	2.53	0.43
25:X:101:LEU:O	25:X:123:VAL:N	2.44	0.43
19:R:5:ARG:NH1	19:R:53:TYR:HB2	2.33	0.43
1:1:844:U:H2'	1:1:845:G:C8	2.53	0.43
1:1:1519:U:N3	1:1:1623:A:OP2	2.47	0.43
1:1:980:A:H2'	1:1:981:A:H8	1.82	0.43
9:H:126:HIS:HA	9:H:129:ILE:HD12	1.99	0.43
1:1:633:C:N4	1:1:634:A:H62	2.17	0.43
1:1:1533:A:OP1	7:F:164:ARG:NH1	2.52	0.43
16:O:30:VAL:O	16:O:45:THR:N	2.44	0.43
1:1:1661:A:HO2'	1:1:1662:U:H6	1.62	0.43
1:1:1615:U:H2'	1:1:1616:U:C6	2.53	0.43
18:Q:51:LEU:HD23	18:Q:51:LEU:O	2.18	0.43
10:I:101:ILE:HA	10:I:173:ALA:O	2.19	0.43
1:1:148:U:H2'	1:1:149:A:H8	1.82	0.43
2:A:85:ARG:HD3	2:A:204:TYR:HA	1.99	0.43
9:H:38:ALA:HB1	9:H:74:LYS:HD3	2.00	0.43
7:F:49:LEU:HD21	18:Q:49:TYR:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:11:ARG:HE	6:E:28:ALA:HA	1.83	0.43
1:1:1847:G:H2'	1:1:1848:U:C6	2.54	0.43
1:1:1217:A:H2'	1:1:1218:C:C6	2.54	0.43
16:O:44:VAL:HG12	16:O:53:ILE:HB	1.99	0.43
1:1:194:C:H2'	1:1:195:C:H6	1.82	0.43
1:1:1106:C:H2'	1:1:1107:G:H8	1.83	0.43
3:B:223:PHE:CE2	3:B:225:LEU:HB3	2.53	0.43
3:B:157:GLN:HB2	3:B:160:GLN:OE1	2.19	0.43
4:C:74:LYS:HB3	4:C:269:PHE:CE1	2.53	0.43
21:T:11:GLN:OE1	21:T:62:ARG:HD2	2.18	0.43
1:1:1674:G:H5''	7:F:86:LYS:HG3	2.01	0.43
1:1:1353:A:H2'	1:1:1354:G:H8	1.82	0.43
1:1:1407:U:H2'	1:1:1408:U:C6	2.52	0.43
25:X:40:PRO:HD2	25:X:108:LYS:HZ1	1.83	0.43
20:S:24:ARG:HG3	20:S:25:LYS:N	2.34	0.43
3:B:132:GLY:HA3	3:B:221:PRO:HB3	2.00	0.43
2:A:157:VAL:O	23:V:65:SER:OG	2.36	0.43
15:N:46:THR:HG22	15:N:48:SER:H	1.83	0.43
2:A:177:MET:HA	2:A:180:ARG:HB3	2.00	0.43
16:O:32:HIS:N	16:O:43:HIS:O	2.48	0.43
1:1:386:C:H2'	1:1:387:C:C6	2.53	0.43
1:1:685:A:H5''	24:W:31:SER:OG	2.18	0.43
9:H:177:TYR:HE2	9:H:183:LYS:HB2	1.84	0.43
1:1:1587:G:H21	1:1:1587:G:P	2.42	0.43
27:Z:58:LEU:O	27:Z:62:VAL:HG12	2.18	0.43
1:1:639:C:H2'	1:1:640:A:C8	2.51	0.43
19:R:41:ILE:HG22	19:R:43:SER:H	1.82	0.43
1:1:598:G:H2'	1:1:599:A:C8	2.53	0.43
8:G:220:ALA:O	8:G:224:ARG:HG3	2.19	0.43
16:O:103:ASN:OD1	16:O:140:THR:OG1	2.37	0.43
14:M:92:CYS:HB3	14:M:103:VAL:HA	2.01	0.43
1:1:171:A:O2'	1:1:172:U:O5'	2.34	0.43
1:1:26:U:H2'	1:1:27:A:C8	2.54	0.43
2:A:86:ALA:O	2:A:90:PHE:HB3	2.18	0.43
4:C:60:TRP:CZ3	4:C:67:GLY:HA3	2.54	0.43
27:Z:43:LYS:HG3	27:Z:44:LEU:H	1.82	0.43
1:1:563:G:H1	1:1:592:C:H5	1.66	0.43
6:E:247:THR:HG22	6:E:248:VAL:HG23	2.00	0.43
14:M:63:LYS:O	14:M:67:ALA:HB2	2.18	0.43
1:1:976:G:H2'	1:1:977:C:H6	1.84	0.43
12:K:25:LYS:HA	12:K:67:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1468:C:H2'	1:1:1469:A:C8	2.54	0.43
1:1:1597:C:H4'	1:1:1603:G:O6	2.19	0.43
18:Q:16:LYS:HB3	18:Q:19:ALA:HB3	2.00	0.43
1:1:1606:G:H1'	1:1:1632:G:N2	2.34	0.43
1:1:870:A:H62	1:1:915:G:H3'	1.82	0.43
1:1:1394:G:H22	1:1:1475:G:H21	1.65	0.43
1:1:479:C:H2'	1:1:480:G:H8	1.83	0.43
11:J:4:ALA:HA	11:J:7:TRP:CH2	2.53	0.43
1:1:1106:C:H2'	1:1:1107:G:C8	2.53	0.43
1:1:1386:A:C2	1:1:1387:G:H1'	2.54	0.43
1:1:81:U:H2'	1:1:82:G:O4'	2.19	0.43
15:N:62:GLN:HE21	15:N:64:ARG:HB2	1.84	0.43
1:1:1510:G:H2'	1:1:1511:U:O4'	2.17	0.43
1:1:1240:A:N6	1:1:1241:A:N1	2.67	0.43
9:H:52:GLU:HA	9:H:58:LYS:CG	2.39	0.43
21:T:41:LYS:HB3	21:T:95:GLY:HA2	2.00	0.43
1:1:429:C:H2'	1:1:430:C:C6	2.54	0.43
1:1:1259:A:N6	1:1:1518:C:H3'	2.33	0.43
1:1:1411:G:H2'	1:1:1412:C:C6	2.54	0.43
1:1:386:C:OP2	10:I:10:LYS:HG3	2.19	0.43
1:1:1738:C:H2'	1:1:1739:C:H6	1.84	0.43
11:J:137:VAL:N	11:J:140:GLN:O	2.50	0.43
2:A:89:LYS:HB2	2:A:202:TYR:CE1	2.53	0.43
2:A:77:ILE:HB	2:A:124:VAL:HG12	1.99	0.43
9:H:61:ILE:HA	9:H:93:VAL:O	2.18	0.43
8:G:183:ARG:O	8:G:186:GLN:HG2	2.18	0.43
4:C:123:ARG:HA	4:C:145:LYS:HA	1.99	0.43
1:1:1660:C:O3'	1:1:1661:A:H2'	2.19	0.43
1:1:164:A:H5''	8:G:82:SER:HB2	2.00	0.43
1:1:925:G:C2	1:1:926:A:C8	3.07	0.43
7:F:103:LEU:HD22	7:F:178:ILE:HD13	1.99	0.43
15:N:99:ARG:O	15:N:103:GLU:HG2	2.19	0.43
1:1:353:C:H2'	1:1:354:U:C6	2.53	0.43
18:Q:105:LYS:HA	18:Q:108:ILE:HG22	2.01	0.43
14:M:69:CYS:HB3	14:M:74:ILE:O	2.19	0.43
1:1:1711:U:H2'	1:1:1712:A:H8	1.84	0.43
1:1:1593:C:C3'	27:Z:104:ARG:HE	2.27	0.43
12:K:25:LYS:N	12:K:65:ARG:O	2.47	0.43
1:1:933:G:H21	1:1:1000:C:H3'	1.84	0.43
1:1:1094:C:H2'	1:1:1095:C:C6	2.53	0.43
1:1:744:G:H22	1:1:798:G:H21	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:750:C:O2	1:1:793:G:N2	2.35	0.43
1:1:31:U:O2'	1:1:643:A:N1	2.48	0.43
1:1:1367:U:H2'	1:1:1368:U:C6	2.53	0.43
1:1:394:G:C2	1:1:395:G:C8	3.07	0.43
6:E:127:ARG:N	6:E:140:VAL:O	2.47	0.43
1:1:17:C:O2'	1:1:1194:A:N1	2.47	0.42
16:O:106:LYS:HD3	16:O:135:ILE:HD12	2.01	0.42
1:1:1597:C:H4'	1:1:1603:G:C6	2.54	0.42
1:1:1231:C:H42	1:1:1527:C:H42	1.66	0.42
1:1:653:A:H2'	1:1:654:A:O4'	2.18	0.42
5:D:163:PRO:HB2	5:D:167:TYR:CD2	2.54	0.42
21:T:114:GLU:HB2	21:T:124:THR:HG22	2.01	0.42
1:1:1711:U:H2'	1:1:1712:A:C8	2.54	0.42
1:1:1499:U:H2'	1:1:1500:G:H8	1.84	0.42
16:O:138:ASP:OD1	16:O:138:ASP:N	2.52	0.42
1:1:1615:U:OP2	17:P:43:ARG:NH1	2.50	0.42
1:1:1455:A:H61	1:1:1471:C:N4	2.17	0.42
1:1:1454:A:H4'	1:1:1455:A:O5'	2.18	0.42
1:1:1467:C:OP1	19:R:3:ARG:N	2.37	0.42
6:E:31:PRO:HB3	6:E:83:PRO:HB3	2.01	0.42
20:S:134:GLN:HG3	20:S:135:HIS:H	1.85	0.42
1:1:1337:C:H2'	1:1:1338:G:C8	2.54	0.42
1:1:166:A:H2'	1:1:167:G:H8	1.84	0.42
25:X:74:LEU:HB2	25:X:78:GLY:H	1.84	0.42
14:M:69:CYS:HA	14:M:74:ILE:HB	1.99	0.42
3:B:140:VAL:O	3:B:210:VAL:HA	2.19	0.42
21:T:140:ALA:HA	21:T:143:LYS:HE3	2.01	0.42
1:1:422:U:H2'	1:1:423:U:C6	2.54	0.42
1:1:1523:C:H2'	1:1:1524:G:C8	2.54	0.42
5:D:116:ARG:HD3	5:D:152:PHE:HZ	1.84	0.42
20:S:72:GLN:HG3	20:S:73:ASN:H	1.84	0.42
2:A:120:ARG:HH12	4:C:267:GLN:HE21	1.66	0.42
27:Z:43:LYS:CG	27:Z:44:LEU:N	2.78	0.42
1:1:1204:A:H2'	1:1:1205:C:C6	2.54	0.42
1:1:1692:U:H2'	1:1:1693:G:H8	1.84	0.42
1:1:312:G:N3	1:1:338:G:N2	2.67	0.42
18:Q:62:ARG:NE	18:Q:96:TYR:OH	2.49	0.42
1:1:164:A:H2'	1:1:165:G:O4'	2.19	0.42
1:1:1210:G:H5'	2:A:85:ARG:HH11	46.33	0.42
1:1:174:C:H2'	1:1:175:A:O4'	2.18	0.42
20:S:26:ILE:HG23	20:S:45:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:564:A:C2	1:1:565:G:H1'	2.54	0.42
1:1:115:U:H2'	1:1:116:U:C6	2.54	0.42
1:1:853:C:C2	1:1:854:A:C8	3.07	0.42
1:1:94:G:C4	1:1:95:G:C8	3.07	0.42
16:O:150:ARG:H	16:O:150:ARG:CD	2.12	0.42
10:I:8:TRP:HB2	10:I:18:ARG:NH1	2.35	0.42
1:1:434:G:OP1	10:I:23:LYS:HG3	2.19	0.42
1:1:1397:U:O2'	1:1:1399:C:OP2	2.30	0.42
1:1:676:C:H5''	15:N:5:HIS:NE2	2.34	0.42
1:1:803:C:H2'	1:1:804:U:C6	2.54	0.42
2:A:91:ALA:HB2	2:A:98:PRO:HB3	2.02	0.42
9:H:43:LEU:HD12	9:H:44:ASN:N	2.34	0.42
1:1:941:C:OP1	3:B:136:ARG:NH2	2.52	0.42
16:O:32:HIS:HA	16:O:96:LYS:HB2	2.01	0.42
1:1:898:U:H2'	1:1:899:U:H6	1.83	0.42
9:H:38:ALA:HB2	9:H:75:ILE:HD12	2.00	0.42
1:1:1782:G:H2'	1:1:1784:G:C8	2.54	0.42
11:J:152:ASP:OD1	11:J:153:SER:N	2.52	0.42
10:I:110:ARG:O	10:I:114:GLU:HB3	2.19	0.42
14:M:84:LYS:HB3	14:M:88:TRP:NE1	2.34	0.42
24:W:14:ILE:HD11	24:W:27:ILE:HD11	2.01	0.42
3:B:204:ILE:HG22	3:B:205:TYR:HD2	1.85	0.42
4:C:84:PHE:CE2	4:C:264:SER:HA	2.55	0.42
1:1:1305:C:C2	1:1:1306:U:C5	3.08	0.42
1:1:1611:G:H2'	1:1:1612:G:O4'	2.20	0.42
16:O:129:ILE:CG2	16:O:130:GLU:N	2.81	0.42
1:1:1634:A:H2'	1:1:1635:C:O4'	2.19	0.42
1:1:1135:C:H2'	1:1:1136:U:C6	2.55	0.42
7:F:15:PRO:HG3	18:Q:115:TYR:CE1	2.55	0.42
13:L:112:HIS:O	13:L:142:VAL:HG23	2.19	0.42
1:1:1047:C:H2'	1:1:1048:G:O4'	2.19	0.42
10:I:110:ARG:O	10:I:114:GLU:HB2	2.18	0.42
19:R:36:GLU:HB2	19:R:47:ARG:HD3	2.01	0.42
1:1:1706:G:H2'	1:1:1707:U:H6	1.83	0.42
1:1:893:U:H2'	1:1:894:G:H8	1.85	0.42
9:H:145:ARG:HA	24:W:51:GLU:HG3	2.01	0.42
13:L:59:LYS:HD3	13:L:134:LEU:HD23	2.00	0.42
1:1:902:G:H2'	1:1:903:A:N3	2.35	0.42
1:1:959:G:O2'	1:1:1065:G:H4'	2.20	0.42
27:Z:44:LEU:C	27:Z:44:LEU:CD2	2.86	0.42
1:1:1594:A:OP2	27:Z:104:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:64:VAL:HA	9:H:72:PHE:HE2	1.85	0.42
10:I:8:TRP:HZ3	10:I:20:PRO:HB3	1.85	0.42
1:1:899:U:H2'	1:1:900:C:O4'	2.18	0.42
1:1:389:A:H2'	1:1:390:C:C6	2.54	0.42
9:H:121:THR:HG23	9:H:124:ALA:H	1.84	0.42
2:A:174:MET:O	2:A:178:LEU:HB2	2.19	0.42
7:F:77:MET:HB2	7:F:84:GLY:H	1.85	0.42
23:V:37:ALA:HA	23:V:50:PHE:HA	2.01	0.42
1:1:539:C:H2'	1:1:540:U:C6	2.55	0.42
1:1:1685:U:H2'	1:1:1686:G:C8	2.55	0.42
1:1:1626:C:H2'	1:1:1627:C:H6	1.84	0.42
19:R:76:GLU:O	19:R:80:ARG:NH1	2.52	0.42
27:Z:55:TYR:HA	27:Z:58:LEU:HD12	2.02	0.42
1:1:1199:A:H3'	1:1:1200:A:H8	1.85	0.42
3:B:147:ASN:C	3:B:148:ASN:ND2	2.73	0.42
1:1:979:C:H2'	1:1:980:A:C8	2.55	0.42
20:S:104:ASP:HB3	20:S:108:ARG:HH12	1.84	0.42
1:1:497:C:H2'	1:1:498:C:H6	1.84	0.42
2:A:156:TYR:HD1	23:V:60:ARG:HE	1.67	0.42
1:1:1679:A:N3	7:F:60:ARG:NH2	2.59	0.42
24:W:28:ARG:HG3	24:W:29:PRO:HD3	2.02	0.42
11:J:126:ALA:O	11:J:130:ILE:HG12	2.18	0.42
1:1:860:G:N2	24:W:107:SER:HG	2.18	0.42
17:P:30:TYR:HA	17:P:33:LEU:HG	2.02	0.42
1:1:839:C:C2	1:1:841:G:H1'	2.55	0.42
17:P:75:VAL:HG21	17:P:104:GLN:HG2	2.02	0.42
9:H:160:LYS:HD2	9:H:191:GLU:HA	2.02	0.42
18:Q:131:LYS:HG3	18:Q:133:GLY:H	1.85	0.42
1:1:617:G:H4'	25:X:88:ASP:OD1	2.19	0.42
27:Z:68:ILE:HG23	27:Z:73:VAL:HG21	2.00	0.42
1:1:1612:G:H2'	1:1:1613:G:C8	2.55	0.42
6:E:141:THR:HB	6:E:145:ARG:H	1.84	0.42
1:1:1756:C:H1'	1:1:1757:G:OP1	2.20	0.42
25:X:54:LYS:HD2	25:X:91:LEU:HD11	2.00	0.42
26:Y:111:LYS:O	26:Y:115:LYS:HB2	2.20	0.42
1:1:1262:C:H3'	1:1:1263:U:C6	2.55	0.42
19:R:55:THR:O	19:R:58:MET:HB2	2.20	0.42
20:S:84:LEU:HD22	20:S:97:GLN:HB2	2.01	0.42
20:S:73:ASN:ND2	20:S:76:GLN:HG3	2.35	0.42
1:1:216:C:HO2'	1:1:217:A:H8	1.66	0.42
4:C:191:VAL:HG11	4:C:236:PHE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:34:ALA:HB1	10:I:58:LEU:HD23	2.02	0.42
1:1:875:A:N6	1:1:912:C:H42	2.14	0.42
1:1:1102:G:N2	1:1:1103:C:C2	2.88	0.42
1:1:1453:C:P	19:R:45:LYS:HG3	2.60	0.42
1:1:433:A:OP1	10:I:25:ARG:NH2	2.52	0.42
1:1:868:G:C2	9:H:115:LYS:HA	2.55	0.42
27:Z:83:LEU:O	27:Z:87:ALA:CB	2.68	0.42
9:H:121:THR:O	9:H:125:VAL:HG23	2.20	0.42
1:1:87:U:N3	1:1:88:G:N7	2.68	0.42
1:1:498:C:C5'	6:E:7:LYS:HD3	2.49	0.42
6:E:11:ARG:HG3	6:E:25:GLY:O	2.20	0.42
6:E:11:ARG:HH12	6:E:24:THR:HB	1.84	0.42
21:T:34:VAL:HB	21:T:53:PHE:HE1	1.84	0.42
1:1:112:U:H2'	1:1:115:U:C5	2.54	0.42
7:F:184:SER:O	7:F:185:SER:HB2	2.19	0.42
6:E:155:LYS:N	6:E:158:ASP:OD2	2.49	0.42
17:P:73:PRO:HG3	17:P:92:SER:HA	2.02	0.42
27:Z:92:LEU:HD22	27:Z:99:LEU:HD21	2.01	0.41
1:1:19:A:O3'	1:1:620:G:O2'	2.31	0.41
1:1:913:A:H1'	9:H:66:VAL:HG21	2.02	0.41
1:1:1856:C:H2'	1:1:1857:G:C8	2.55	0.41
16:O:83:GLN:O	16:O:87:GLU:HG2	2.20	0.41
15:N:66:VAL:HG13	15:N:67:THR:N	2.35	0.41
3:B:198:GLU:O	3:B:202:GLN:NE2	2.44	0.41
3:B:97:LEU:HD21	3:B:228:LEU:HD11	2.02	0.41
1:1:347:G:H2'	1:1:348:A:H8	1.83	0.41
1:1:289:G:H2'	1:1:290:U:C6	2.54	0.41
1:1:1125:C:H2'	1:1:1126:G:H8	1.85	0.41
20:S:12:ILE:HG23	20:S:20:ILE:HG23	2.01	0.41
18:Q:66:VAL:HG12	18:Q:68:ILE:HG13	2.02	0.41
10:I:145:ILE:HG22	10:I:149:TYR:CE2	2.55	0.41
1:1:964:A:H2'	1:1:965:U:C6	2.55	0.41
5:D:70:THR:HA	5:D:86:LEU:HD13	2.01	0.41
1:1:618:C:H41	25:X:67:ARG:NH2	2.18	0.41
6:E:230:ASN:HB2	6:E:235:TRP:HE1	1.85	0.41
13:L:82:MET:HG2	13:L:85:THR:HG23	2.01	0.41
16:O:74:ALA:O	16:O:78:ALA:HB3	2.18	0.41
6:E:125:LYS:NZ	6:E:225:ILE:O	2.29	0.41
14:M:52:LEU:HD22	14:M:62:VAL:HB	2.03	0.41
24:W:55:ASP:OD1	24:W:56:HIS:N	2.53	0.41
3:B:97:LEU:HD22	3:B:228:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:26:SER:HB2	22:U:32:LEU:HB2	2.00	0.41
20:S:124:ARG:NH2	20:S:130:ARG:O	2.42	0.41
17:P:18:ARG:NH1	17:P:37:TYR:HA	2.34	0.41
1:1:1292:C:C2	1:1:1293:A:C8	3.09	0.41
7:F:138:ALA:HB2	7:F:200:ALA:HA	2.03	0.41
16:O:147:ARG:HG2	16:O:147:ARG:O	2.20	0.41
9:H:39:GLN:NE2	9:H:72:PHE:HA	2.35	0.41
1:1:96:C:OP2	11:J:2:PRO:HD3	2.20	0.41
20:S:120:HIS:HA	20:S:123:LEU:HD12	2.03	0.41
15:N:37:ILE:O	15:N:41:ALA:HB2	2.20	0.41
1:1:744:G:C2	9:H:107:LYS:HE3	2.55	0.41
11:J:32:ILE:HD11	11:J:40:LYS:HG2	2.01	0.41
10:I:36:THR:O	10:I:95:THR:HA	2.20	0.41
1:1:178:C:H2'	1:1:179:C:H6	1.85	0.41
6:E:252:ARG:NH1	11:J:72:PHE:HA	2.34	0.41
1:1:172:U:OP1	1:1:314:U:O2'	2.35	0.41
1:1:840:C:H5''	1:1:841:G:H5''	2.02	0.41
1:1:864:A:N1	1:1:865:A:N6	2.68	0.41
6:E:191:ARG:NH2	6:E:212:ASP:OD2	2.50	0.41
1:1:1650:A:H2	7:F:83:ASN:HD21	1.67	0.41
20:S:38:ARG:NH2	21:T:45:LEU:HD11	2.31	0.41
1:1:1127:C:H2'	1:1:1128:C:C6	2.55	0.41
1:1:957:A:C6	1:1:958:G:C6	3.08	0.41
1:1:979:C:H2'	1:1:980:A:H8	1.85	0.41
27:Z:102:LYS:HB2	27:Z:106:GLN:O	2.20	0.41
1:1:561:A:H2'	11:J:132:GLN:NE2	2.36	0.41
13:L:48:LYS:O	13:L:51:ILE:N	2.51	0.41
18:Q:143:LYS:HG3	18:Q:144:SER:H	1.86	0.41
21:T:49:ASP:O	21:T:52:TRP:HE3	2.03	0.41
1:1:1598:G:OP1	27:Z:80:ARG:NH1	2.54	0.41
18:Q:44:PRO:HG3	18:Q:47:LEU:HD12	2.02	0.41
18:Q:135:PRO:HD3	18:Q:141:TYR:CG	2.56	0.41
14:M:17:ALA:HB1	14:M:124:ILE:HD13	2.02	0.41
1:1:651:U:H2'	1:1:652:U:C6	2.55	0.41
1:1:814:U:N3	1:1:815:U:C5	2.88	0.41
1:1:1574:C:H2'	1:1:1575:G:H8	1.85	0.41
6:E:125:LYS:HB2	6:E:226:PHE:CD1	2.55	0.41
1:1:1088:U:H4'	1:1:1089:G:OP2	2.20	0.41
11:J:50:LEU:HD11	11:J:105:PHE:CD2	2.55	0.41
23:V:22:ARG:HH21	23:V:58:ALA:H	1.68	0.41
2:A:89:LYS:HB2	2:A:202:TYR:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1306:U:H2'	1:1:1307:U:O4'	2.21	0.41
1:1:9:U:N3	1:1:12:U:OP2	2.40	0.41
2:A:32:PHE:CE2	2:A:33:GLN:HG3	2.56	0.41
1:1:1256:G:H21	5:D:40:ARG:HD2	36.79	0.41
1:1:428:U:H5'	11:J:2:PRO:HG2	2.01	0.41
8:G:64:LYS:HZ3	8:G:82:SER:H	1.67	0.41
21:T:74:SER:O	21:T:78:ILE:HG13	2.20	0.41
19:R:106:LEU:HD23	19:R:109:LEU:HD22	2.02	0.41
1:1:1518:C:OP1	1:1:1519:U:O2'	2.31	0.41
17:P:50:ARG:O	17:P:54:HIS:HB3	2.21	0.41
1:1:92:A:H4'	1:1:93:U:OP2	2.20	0.41
17:P:84:ILE:HG22	17:P:115:TYR:HD1	1.84	0.41
19:R:78:ARG:O	19:R:82:ASP:N	2.52	0.41
19:R:44:LYS:HG2	19:R:47:ARG:NH1	2.36	0.41
3:B:138:PHE:CD2	3:B:214:LYS:HB3	2.56	0.41
9:H:109:ARG:HG2	9:H:110:THR:N	2.36	0.41
1:1:1712:A:H2'	1:1:1713:C:C6	2.56	0.41
6:E:127:ARG:HB3	6:E:140:VAL:HG12	2.03	0.41
1:1:1414:A:H2'	1:1:1415:C:C6	2.55	0.41
1:1:1819:A:H2'	1:1:1820:G:C8	2.56	0.41
3:B:26:SER:O	3:B:51:ARG:NH1	2.54	0.41
19:R:5:ARG:NH1	19:R:9:VAL:HG11	2.35	0.41
1:1:453:C:C2	1:1:454:U:C5	3.08	0.41
1:1:1541:G:H5''	21:T:59:SER:HB3	2.02	0.41
1:1:1286:G:C5	14:M:35:ILE:HD12	2.56	0.41
1:1:160:U:H3'	1:1:161:U:H5''	2.03	0.41
1:1:1740:C:H2'	1:1:1741:U:C6	2.55	0.41
11:J:173:VAL:HG22	11:J:177:ASN:ND2	2.36	0.41
2:A:89:LYS:HE3	19:R:80:ARG:HA	2.03	0.41
4:C:60:TRP:CD1	4:C:92:GLU:HB2	2.56	0.41
1:1:496:C:H2'	1:1:497:C:C6	2.51	0.41
2:A:126:ASP:O	2:A:130:ASP:HB2	2.20	0.41
1:1:1742:C:H2'	1:1:1743:G:O4'	2.21	0.41
1:1:307:G:N7	10:I:44:HIS:ND1	2.53	0.41
1:1:1501:C:H2'	1:1:1502:C:H6	1.86	0.41
11:J:162:ARG:O	11:J:166:GLY:N	2.53	0.41
26:Y:100:LYS:HG3	26:Y:101:LYS:N	2.36	0.41
8:G:57:ASP:OD1	8:G:58:LYS:N	2.46	0.41
1:1:344:U:H2'	1:1:345:U:C6	2.55	0.41
2:A:176:TRP:HB2	2:A:202:TYR:CD2	2.50	0.41
4:C:66:LEU:O	4:C:70:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1854:U:P	16:O:147:ARG:HH22	2.44	0.41
1:1:1594:A:C5	1:1:1595:U:C5	3.09	0.41
1:1:1650:A:H1'	1:1:1675:A:N6	2.36	0.41
1:1:943:U:C2	1:1:944:A:C8	3.09	0.41
1:1:994:C:N4	1:1:995:G:O6	2.54	0.41
8:G:119:LYS:HG2	8:G:125:THR:HG21	2.02	0.41
1:1:523:A:H2'	1:1:524:U:O4'	2.21	0.41
1:1:430:C:H2'	1:1:431:G:H8	1.86	0.41
12:K:2:LEU:HG	12:K:3:MET:O	2.21	0.41
2:A:81:ASN:ND2	2:A:204:TYR:OH	2.53	0.41
1:1:1228:A:O2'	1:1:1634:A:N3	2.46	0.41
15:N:34:LYS:NZ	15:N:74:ILE:HG23	2.36	0.41
1:1:1050:A:H62	1:1:1068:G:N2	2.19	0.41
1:1:644:G:H5'	11:J:41:ARG:HH22	1.86	0.41
1:1:1410:C:H2'	1:1:1411:G:C8	2.55	0.41
5:D:42:THR:HB	5:D:45:ARG:O	2.20	0.41
21:T:34:VAL:HG11	21:T:102:ARG:NE	2.35	0.41
13:L:124:ASP:HA	13:L:149:ALA:HB2	2.02	0.41
6:E:97:GLU:O	6:E:98:HIS:CG	2.74	0.41
7:F:184:SER:C	7:F:186:ASN:H	2.24	0.41
1:1:1254:C:O2'	22:U:71:GLY:HA3	2.21	0.41
26:Y:56:PHE:HB2	26:Y:74:MET:HB2	2.02	0.41
4:C:251:LEU:HD23	23:V:23:ILE:HG13	2.02	0.41
21:T:61:ALA:O	21:T:64:LEU:HG	2.21	0.41
1:1:11:A:H8	1:1:11:A:O5'	2.03	0.41
1:1:1827:U:H2'	1:1:1828:C:C6	2.56	0.41
1:1:509:G:H2'	1:1:510:G:C8	2.56	0.41
1:1:1615:U:H2'	1:1:1616:U:H6	1.86	0.41
1:1:691:G:H2'	1:1:692:G:C8	2.56	0.41
1:1:559:G:P	1:1:560:A:H5''	2.61	0.41
1:1:1036:A:H4'	1:1:1855:G:N2	2.35	0.41
4:C:256:TRP:HZ3	24:W:66:THR:HG21	1.86	0.41
7:F:49:LEU:HD21	18:Q:49:TYR:CD2	2.56	0.41
12:K:57:TYR:HD1	12:K:78:TYR:CD2	2.38	0.41
25:X:67:ARG:HG3	25:X:115:ILE:HG13	2.03	0.41
11:J:141:VAL:HG21	11:J:162:ARG:HH21	1.86	0.41
1:1:1284:A:H5'	1:1:1285:G:H4'	2.02	0.41
1:1:74:G:H2'	1:1:75:G:O4'	2.21	0.41
1:1:183:G:H2'	1:1:184:G:C8	2.55	0.41
17:P:130:ARG:HB3	17:P:131:PRO:HD3	2.03	0.41
12:K:16:PHE:HZ	12:K:89:ILE:HB	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1059:G:N2	1:1:1829:G:H4'	2.36	0.41
1:1:434:G:OP1	10:I:23:LYS:NZ	2.47	0.40
7:F:23:TRP:CH2	7:F:108:PRO:HD3	2.56	0.40
1:1:1407:U:H2'	1:1:1408:U:H6	1.84	0.40
5:D:68:GLU:HB2	12:K:93:THR:HG21	2.02	0.40
1:1:862:A:N3	24:W:105:THR:HG22	2.36	0.40
6:E:136:ILE:HG13	6:E:138:HIS:CE1	2.55	0.40
1:1:286:U:O2'	1:1:287:U:OP1	2.29	0.40
1:1:834:C:H2'	1:1:835:C:O4'	2.21	0.40
1:1:1590:C:H5'	21:T:82:ARG:HH11	1.86	0.40
1:1:1790:A:H4'	8:G:81:HIS:HE1	1.87	0.40
11:J:163:SER:N	11:J:164:PRO:HD2	2.36	0.40
8:G:56:ASN:HB2	8:G:108:VAL:HB	2.03	0.40
8:G:137:ARG:HG2	8:G:139:SER:H	1.85	0.40
3:B:147:ASN:O	3:B:148:ASN:CB	2.70	0.40
6:E:60:GLU:O	6:E:64:ILE:HG23	2.22	0.40
8:G:142:ARG:NH1	8:G:152:ASP:OD1	2.54	0.40
1:1:1588:A:H2'	1:1:1589:A:H8	1.86	0.40
1:1:291:G:OP2	6:E:200:ARG:NH2	2.54	0.40
1:1:1738:C:H2'	1:1:1739:C:C6	2.57	0.40
1:1:647:U:H2'	1:1:648:A:C8	2.56	0.40
1:1:846:G:H2'	6:E:19:MET:SD	2.61	0.40
12:K:31:LYS:C	12:K:33:PRO:HD3	2.41	0.40
25:X:41:PHE:HB3	25:X:44:ALA:HB3	2.02	0.40
25:X:112:VAL:HG12	25:X:114:ASP:H	1.85	0.40
6:E:181:CYS:HA	6:E:227:VAL:HA	2.02	0.40
1:1:1717:C:H2'	1:1:1718:G:O4'	2.22	0.40
1:1:1351:G:C2	1:1:1352:G:C8	3.10	0.40
1:1:924:G:H2'	1:1:925:G:O4'	2.20	0.40
3:B:52:THR:OG1	3:B:57:ILE:HA	2.21	0.40
1:1:1491:G:H2'	1:1:1492:U:C6	2.57	0.40
10:I:113:TYR:CZ	10:I:121:LEU:HD23	2.57	0.40
6:E:87:MET:CE	6:E:236:ILE:HG13	2.52	0.40
3:B:135:LEU:HD11	3:B:137:LEU:HD23	2.03	0.40
1:1:46:A:H4'	1:1:47:G:H5''	2.03	0.40
3:B:227:LYS:O	3:B:231:LEU:HB2	2.21	0.40
1:1:402:C:C2	1:1:403:G:C8	3.10	0.40
20:S:121:ARG:HG3	20:S:131:VAL:HG11	2.03	0.40
1:1:312:G:C2	1:1:338:G:C2	3.09	0.40
5:D:71:ALA:HB1	5:D:75:LYS:HE2	2.02	0.40
1:1:1287:A:O3'	1:1:1312:G:N2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:35:ARG:HG2	13:L:36:TYR:N	2.36	0.40
3:B:144:LYS:HG3	3:B:146:ARG:H	1.85	0.40
1:1:114:G:O6	1:1:351:G:H1'	2.21	0.40
3:B:106:THR:OG1	3:B:108:ASP:OD1	2.29	0.40
24:W:37:PHE:CD1	24:W:103:VAL:HG21	2.55	0.40
1:1:619:A:H61	25:X:114:ASP:HB3	1.85	0.40
17:P:60:LEU:HD23	17:P:89:MET:HG2	2.03	0.40
2:A:106:GLY:HA2	2:A:109:THR:OG1	2.22	0.40
1:1:1800:A:C2	1:1:1801:A:H1'	2.55	0.40
1:1:1358:U:OP1	4:C:115:GLN:N	2.55	0.40
1:1:1539:U:OP1	21:T:43:LYS:HE3	2.22	0.40
1:1:443:U:H2'	1:1:444:G:O4'	2.22	0.40
1:1:1588:A:H4'	21:T:92:PHE:CE1	2.55	0.40
1:1:745:C:H2'	1:1:746:C:C6	2.56	0.40
12:K:58:VAL:HG11	12:K:69:TRP:HB3	2.02	0.40
19:R:22:THR:HB	19:R:74:GLN:HE22	1.86	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	A	213/295 (72%)	202 (95%)	11 (5%)	0	100	100
3	B	210/264 (80%)	182 (87%)	26 (12%)	2 (1%)	19	64
4	C	220/293 (75%)	209 (95%)	9 (4%)	2 (1%)	21	65
5	D	218/243 (90%)	206 (94%)	11 (5%)	1 (0%)	34	76
6	E	255/263 (97%)	244 (96%)	11 (4%)	0	100	100
7	F	188/204 (92%)	165 (88%)	22 (12%)	1 (0%)	34	76
8	G	230/249 (92%)	221 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	H	181/194 (93%)	165 (91%)	16 (9%)	0	100	100
10	I	205/208 (99%)	186 (91%)	19 (9%)	0	100	100
11	J	177/194 (91%)	163 (92%)	13 (7%)	1 (1%)	30	73
12	K	96/165 (58%)	90 (94%)	4 (4%)	2 (2%)	9	51
13	L	151/158 (96%)	142 (94%)	8 (5%)	1 (1%)	26	70
14	M	118/132 (89%)	111 (94%)	7 (6%)	0	100	100
15	N	147/151 (97%)	131 (89%)	16 (11%)	0	100	100
16	O	134/151 (89%)	119 (89%)	13 (10%)	2 (2%)	13	57
17	P	118/145 (81%)	107 (91%)	10 (8%)	1 (1%)	24	68
18	Q	137/146 (94%)	132 (96%)	5 (4%)	0	100	100
19	R	119/135 (88%)	108 (91%)	9 (8%)	2 (2%)	11	55
20	S	137/152 (90%)	125 (91%)	12 (9%)	0	100	100
21	T	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
22	U	95/119 (80%)	94 (99%)	1 (1%)	0	100	100
23	V	79/83 (95%)	77 (98%)	1 (1%)	1 (1%)	15	59
24	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
25	X	137/143 (96%)	128 (93%)	9 (7%)	0	100	100
26	Y	123/133 (92%)	118 (96%)	5 (4%)	0	100	100
27	Z	71/125 (57%)	64 (90%)	7 (10%)	0	100	100
28	a	95/115 (83%)	78 (82%)	10 (10%)	7 (7%)	1	21
29	b	78/84 (93%)	67 (86%)	7 (9%)	4 (5%)	2	31
30	c	59/69 (86%)	48 (81%)	10 (17%)	1 (2%)	11	55
31	d	49/56 (88%)	43 (88%)	6 (12%)	0	100	100
32	e	53/59 (90%)	49 (92%)	4 (8%)	0	100	100
33	f	71/156 (46%)	66 (93%)	5 (7%)	0	100	100
34	g	312/317 (98%)	298 (96%)	14 (4%)	0	100	100
All	All	4744/5476 (87%)	4395 (93%)	321 (7%)	28 (1%)	34	73

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	O	62	VAL
23	V	42	VAL

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Mol	Chain	Res	Type
28	a	92	ARG
28	a	94	ASP
29	b	74	THR
29	b	78	SER
7	F	183	GLY
11	J	3	VAL
13	L	14	PRO
16	O	141	ARG
17	P	70	MET
28	a	46	GLU
3	B	148	ASN
12	K	28	HIS
12	K	41	PRO
4	C	174	ILE
5	D	217	ILE
19	R	88	VAL
28	a	14	GLY
28	a	45	VAL
28	a	48	ALA
29	b	75	GLU
30	c	38	THR
28	a	82	LYS
4	C	63	VAL
3	B	210	VAL
19	R	95	ILE
29	b	62	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	180/243 (74%)	180 (100%)	0	100	100
3	B	193/231 (84%)	192 (100%)	1 (0%)	92	96
4	C	188/225 (84%)	188 (100%)	0	100	100
5	D	183/202 (91%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	E	220/225 (98%)	220 (100%)	0	100	100
7	F	160/170 (94%)	159 (99%)	1 (1%)	90	95
8	G	202/218 (93%)	202 (100%)	0	100	100
9	H	164/174 (94%)	164 (100%)	0	100	100
10	I	179/180 (99%)	179 (100%)	0	100	100
11	J	160/168 (95%)	160 (100%)	0	100	100
12	K	89/136 (65%)	89 (100%)	0	100	100
13	L	138/142 (97%)	138 (100%)	0	100	100
14	M	102/108 (94%)	102 (100%)	0	100	100
15	N	130/131 (99%)	130 (100%)	0	100	100
16	O	106/119 (89%)	105 (99%)	1 (1%)	84	92
17	P	109/130 (84%)	109 (100%)	0	100	100
18	Q	115/121 (95%)	115 (100%)	0	100	100
19	R	110/122 (90%)	110 (100%)	0	100	100
20	S	121/132 (92%)	121 (100%)	0	100	100
21	T	113/115 (98%)	113 (100%)	0	100	100
22	U	90/107 (84%)	90 (100%)	0	100	100
23	V	65/67 (97%)	65 (100%)	0	100	100
24	W	112/113 (99%)	112 (100%)	0	100	100
25	X	111/115 (96%)	111 (100%)	0	100	100
26	Y	107/115 (93%)	107 (100%)	0	100	100
27	Z	65/103 (63%)	64 (98%)	1 (2%)	72	89
28	a	84/98 (86%)	81 (96%)	3 (4%)	42	76
29	b	72/76 (95%)	71 (99%)	1 (1%)	74	89
30	c	54/62 (87%)	53 (98%)	1 (2%)	65	86
31	d	45/49 (92%)	45 (100%)	0	100	100
32	e	44/48 (92%)	44 (100%)	0	100	100
33	f	66/140 (47%)	66 (100%)	0	100	100
34	g	272/275 (99%)	272 (100%)	0	100	100
All	All	4149/4660 (89%)	4140 (100%)	9 (0%)	95	97

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	148	ASN
7	F	182	LYS
16	O	150	ARG
27	Z	78	LYS
28	a	15	ARG
28	a	46	GLU
28	a	89	ARG
29	b	75	GLU
30	c	39	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	36	GLN
2	A	81	ASN
2	A	111	GLN
2	A	132	GLN
3	B	101	HIS
3	B	148	ASN
4	C	267	GLN
5	D	159	HIS
6	E	8	HIS
6	E	138	HIS
6	E	142	HIS
6	E	161	GLN
7	F	82	ASN
7	F	114	ASN
7	F	203	ASN
8	G	13	GLN
8	G	81	HIS
9	H	39	GLN
9	H	114	GLN
9	H	193	GLN
10	I	84	ASN
10	I	88	ASN
11	J	113	GLN
11	J	134	HIS
11	J	154	GLN
11	J	156	HIS
12	K	7	ASN
12	K	28	HIS
12	K	42	ASN
13	L	83	GLN

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Mol	Chain	Res	Type
13	L	154	GLN
15	N	62	GLN
16	O	32	HIS
16	O	103	ASN
17	P	35	GLN
17	P	41	GLN
17	P	103	ASN
17	P	128	HIS
18	Q	11	GLN
18	Q	86	GLN
20	S	42	HIS
20	S	87	GLN
20	S	134	GLN
21	T	10	ASN
21	T	42	HIS
21	T	85	ASN
22	U	81	GLN
22	U	85	HIS
23	V	29	HIS
23	V	47	ASN
24	W	16	ASN
24	W	24	GLN
25	X	31	HIS
25	X	63	ASN
26	Y	19	GLN
27	Z	89	GLN
30	c	24	GLN
34	g	20	GLN
34	g	56	GLN
34	g	143	GLN
34	g	191	HIS
34	g	226	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1700/1869 (90%)	286 (16%)	9 (0%)
35	z	262/504 (51%)	52 (19%)	0
All	All	1962/2373 (82%)	338 (17%)	9 (0%)

All (338) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	C
1	1	33	G
1	1	41	G
1	1	42	A
1	1	49	C
1	1	67	C
1	1	68	A
1	1	72	C
1	1	73	C
1	1	76	U
1	1	77	A
1	1	103	A
1	1	112	U
1	1	113	G
1	1	114	G
1	1	115	U
1	1	125	C
1	1	142	C
1	1	143	U
1	1	155	G
1	1	158	A
1	1	161	U
1	1	171	A
1	1	172	U
1	1	174	C
1	1	175	A
1	1	187	G
1	1	217	A
1	1	226	A
1	1	228	C
1	1	229	A
1	1	230	A
1	1	238	C
1	1	239	C
1	1	284	C
1	1	286	U
1	1	287	U
1	1	292	A
1	1	306	C
1	1	314	U
1	1	319	C
1	1	320	G
1	1	325	C

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Mol	Chain	Res	Type
1	1	327	G
1	1	328	U
1	1	329	G
1	1	331	C
1	1	332	G
1	1	333	G
1	1	339	A
1	1	351	G
1	1	364	A
1	1	368	U
1	1	370	G
1	1	371	A
1	1	385	G
1	1	386	C
1	1	407	G
1	1	408	A
1	1	409	C
1	1	448	A
1	1	450	C
1	1	452	G
1	1	463	C
1	1	465	A
1	1	466	G
1	1	472	C
1	1	474	G
1	1	476	A
1	1	487	U
1	1	489	A
1	1	492	C
1	1	509	G
1	1	516	A
1	1	523	A
1	1	525	A
1	1	526	A
1	1	533	A
1	1	534	G
1	1	535	G
1	1	536	A
1	1	541	U
1	1	542	U
1	1	544	G
1	1	545	A

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Mol	Chain	Res	Type
1	1	546	G
1	1	547	G
1	1	548	C
1	1	553	U
1	1	554	A
1	1	560	A
1	1	561	A
1	1	562	U
1	1	576	A
1	1	587	A
1	1	590	A
1	1	591	U
1	1	592	C
1	1	607	U
1	1	608	C
1	1	611	G
1	1	614	C
1	1	617	G
1	1	620	G
1	1	629	A
1	1	643	A
1	1	644	G
1	1	645	C
1	1	661	U
1	1	668	A
1	1	669	A
1	1	671	A
1	1	672	A
1	1	673	G
1	1	688	U
1	1	689	U
1	1	690	G
1	1	695	C
1	1	741	C
1	1	742	U
1	1	743	U
1	1	744	G
1	1	746	C
1	1	748	C
1	1	750	C
1	1	751	G
1	1	797	C

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Mol	Chain	Res	Type
1	1	798	G
1	1	799	U
1	1	801	U
1	1	804	U
1	1	805	U
1	1	837	A
1	1	839	C
1	1	841	G
1	1	847	A
1	1	865	A
1	1	868	G
1	1	870	A
1	1	874	G
1	1	913	A
1	1	914	U
1	1	917	U
1	1	919	A
1	1	920	A
1	1	928	G
1	1	929	G
1	1	930	C
1	1	933	G
1	1	943	U
1	1	956	G
1	1	959	G
1	1	960	U
1	1	961	G
1	1	963	A
1	1	969	U
1	1	990	A
1	1	992	A
1	1	994	C
1	1	997	A
1	1	1002	U
1	1	1008	A
1	1	1015	U
1	1	1023	A
1	1	1044	G
1	1	1055	A
1	1	1061	U
1	1	1066	U
1	1	1085	C

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Mol	Chain	Res	Type
1	1	1109	C
1	1	1110	G
1	1	1114	U
1	1	1116	C
1	1	1121	G
1	1	1133	A
1	1	1139	C
1	1	1140	G
1	1	1149	A
1	1	1150	A
1	1	1195	A
1	1	1199	A
1	1	1207	G
1	1	1212	G
1	1	1215	C
1	1	1224	G
1	1	1237	C
1	1	1242	U
1	1	1251	A
1	1	1256	G
1	1	1257	G
1	1	1258	A
1	1	1259	A
1	1	1261	C
1	1	1275	G
1	1	1285	G
1	1	1286	G
1	1	1287	A
1	1	1288	U
1	1	1289	U
1	1	1290	G
1	1	1301	A
1	1	1302	G
1	1	1330	G
1	1	1333	U
1	1	1342	U
1	1	1351	G
1	1	1356	G
1	1	1358	U
1	1	1371	U
1	1	1372	U
1	1	1375	G

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Mol	Chain	Res	Type
1	1	1378	A
1	1	1382	A
1	1	1394	G
1	1	1399	C
1	1	1409	A
1	1	1418	C
1	1	1420	G
1	1	1421	A
1	1	1439	A
1	1	1442	U
1	1	1444	U
1	1	1454	A
1	1	1456	G
1	1	1462	U
1	1	1463	U
1	1	1476	A
1	1	1477	U
1	1	1478	U
1	1	1484	A
1	1	1489	A
1	1	1497	G
1	1	1498	A
1	1	1505	U
1	1	1508	A
1	1	1519	U
1	1	1521	C
1	1	1522	A
1	1	1531	A
1	1	1533	A
1	1	1537	A
1	1	1544	C
1	1	1545	A
1	1	1554	C
1	1	1555	U
1	1	1558	C
1	1	1580	A
1	1	1585	U
1	1	1586	U
1	1	1588	A
1	1	1589	A
1	1	1601	A
1	1	1604	G

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Mol	Chain	Res	Type
1	1	1606	G
1	1	1620	A
1	1	1621	U
1	1	1622	U
1	1	1624	U
1	1	1625	U
1	1	1660	C
1	1	1661	A
1	1	1662	U
1	1	1665	G
1	1	1671	G
1	1	1678	A
1	1	1683	C
1	1	1690	U
1	1	1692	U
1	1	1721	U
1	1	1742	C
1	1	1745	A
1	1	1757	G
1	1	1823	A
1	1	1831	A
1	1	1834	A
1	1	1835	A
1	1	1838	U
1	1	1839	U
1	1	1849	G
1	1	1861	G
1	1	1862	G
1	1	1863	A
1	1	1864	U
1	1	1865	C
1	1	1866	A
1	1	1869	A
35	z	48	U
35	z	49	G
35	z	80	U
35	z	82	G
35	z	83	C
35	z	85	A
35	z	86	U
35	z	91	U
35	z	94	G

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Mol	Chain	Res	Type
35	z	106	U
35	z	111	C
35	z	118	G
35	z	125	C
35	z	136	A
35	z	139	C
35	z	141	U
35	z	150	G
35	z	154	A
35	z	157	C
35	z	161	G
35	z	165	A
35	z	166	C
35	z	229	G
35	z	231	G
35	z	232	C
35	z	236	C
35	z	237	C
35	z	244	A
35	z	253	G
35	z	258	G
35	z	263	G
35	z	266	G
35	z	270	C
35	z	280	C
35	z	296	A
35	z	297	U
35	z	306	U
35	z	329	U
35	z	331	G
35	z	332	A
35	z	335	G
35	z	337	G
35	z	338	C
35	z	339	A
35	z	340	C
35	z	341	C
35	z	344	G
35	z	349	C
35	z	350	G
35	z	353	U
35	z	354	C

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Mol	Chain	Res	Type
35	z	356	U

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	227	U
1	1	286	U
1	1	369	C
1	1	546	G
1	1	797	C
1	1	869	A
1	1	1211	G
1	1	1554	C
1	1	1756	C

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 76 ligands modelled in this entry, 76 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 ⓘ

There are no chain breaks in this entry.