



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 8, 2019 – 08:24 PM EST

PDB ID : 5A2Q
EMDB ID: : EMD-3019
Title : Structure of the HCV IRES bound to the human ribosome
Authors : Quade, N.; Leiundgut, M.; Boehringer, D.; Heuvel, J.v.d.; Ban, N.
Deposited on : 2015-05-21
Resolution : 3.90 Å(reported)
Based on PDB ID : 4W23

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

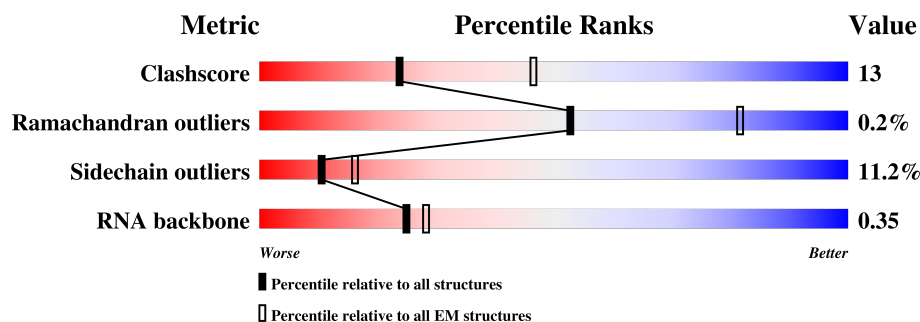
1 Overall quality at a glance

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.







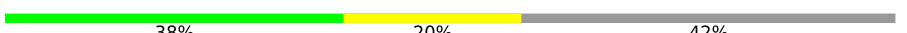
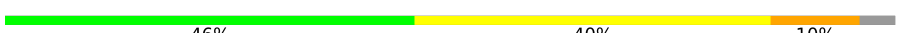





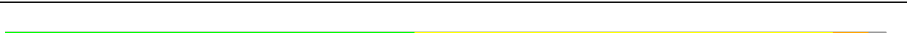











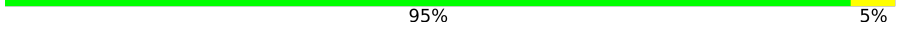
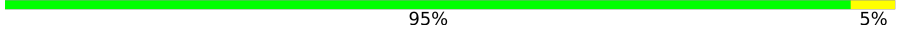
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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	2	1868	<div> <div>32%</div> <div>36%</div> <div>17%</div> <div>•</div> <div>11%</div> </div>
2	3	257	<div> <div>32%</div> <div>39%</div> <div>27%</div> <div>•</div> </div>
3	A	295	<div> <div>46%</div> <div>25%</div> <div>•</div> <div>27%</div> </div>
4	B	264	<div> <div>51%</div> <div>26%</div> <div>•</div> <div>19%</div> </div>
5	C	293	<div> <div>42%</div> <div>25%</div> <div>7%</div> <div>26%</div> </div>
6	D	243	<div> <div>63%</div> <div>27%</div> <div>•</div> <div>7%</div> </div>
7	E	263	<div> <div>54%</div> <div>37%</div> <div>8%</div> </div>
8	F	204	<div> <div>69%</div> <div>23%</div> <div>7%</div> </div>

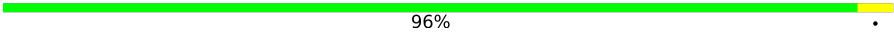
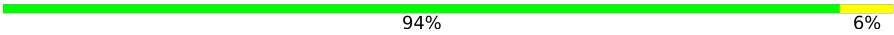


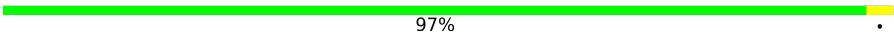
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Mol	Chain	Length	Quality of chain
9	G	249	
10	H	194	
11	I	208	
12	J	194	
13	K	165	
14	L	158	
15	M	132	
16	N	151	
17	O	151	
18	P	145	
19	Q	146	
20	R	135	
21	S	152	
22	T	146	
23	U	119	
24	V	83	
25	W	130	
26	X	143	
27	Y	130	
28	Z	125	
29	a	101	
30	b	82	
31	c	61	
32	d	55	
33	e	56	

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Mol	Chain	Length	Quality of chain
34	f	72	 96% .
35	g	315	 94% 6%
36	h	24	 88% 13%
37	r	13	 92% 8%
38	w	62	 97% .

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 80749 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	2	1665	Total	C	N	O	P	0	0
			35552	15869	6385	11633	1665		

- Molecule 2 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	257	Total	C	N	O	P	0	0
			5485	2444	979	1805	257		

- Molecule 3 is a protein called RIBOSOMAL PROTEIN US2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 4 is a protein called RIBOSOMAL PROTEIN ES1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 5 is a protein called RIBOSOMAL PROTEIN US5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 6 is a protein called RIBOSOMAL PROTEIN US3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 7 is a protein called RIBOSOMAL PROTEIN ES4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 8 is a protein called RIBOSOMAL PROTEIN US7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 9 is a protein called RIBOSOMAL PROTEIN ES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	230	Total	C	N	O	S	0	0
			1864	1164	373	320	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	221	ARG	LYS	conflict	UNP P62753

- Molecule 10 is a protein called RIBOSOMAL PROTEIN ES7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 11 is a protein called RIBOSOMAL PROTEIN ES8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 12 is a protein called RIBOSOMAL PROTEIN US4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 13 is a protein called RIBOSOMAL PROTEIN ES10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	95	Total	C	N	O	S	0	0
			800	522	142	131	5		

- Molecule 14 is a protein called RIBOSOMAL PROTEIN US17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 15 is a protein called RIBOSOMAL PROTEIN ES12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 16 is a protein called RIBOSOMAL PROTEIN US15.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN US11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 18 is a protein called RIBOSOMAL PROTEIN US19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 19 is a protein called RIBOSOMAL PROTEIN US9.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN ES17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	132	Total	C	N	O	S	0	0
			1066	669	199	194	4		

- Molecule 21 is a protein called RIBOSOMAL PROTEIN US13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 22 is a protein called RIBOSOMAL PROTEIN ES19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	145	Total	C	N	O	S	0	0
			1128	706	218	201	3		

- Molecule 23 is a protein called RIBOSOMAL PROTEIN US10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 24 is a protein called RIBOSOMAL PROTEIN ES21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 25 is a protein called RIBOSOMAL PROTEIN US8.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 27 is a protein called RIBOSOMAL PROTEIN ES24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 28 is a protein called RIBOSOMAL PROTEIN ES25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 29 is a protein called RIBOSOMAL PROTEIN ES26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	101	Total	C	N	O	S	0	0
			816	509	170	132	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	78	VAL	ALA	conflict	UNP P62854

- Molecule 30 is a protein called RIBOSOMAL PROTEIN ES27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 31 is a protein called RIBOSOMAL PROTEIN ES28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 32 is a protein called RIBOSOMAL PROTEIN US14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 33 is a protein called RIBOSOMAL PROTEIN ES30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	56	Total	C	N	O	S	0	0
			442	273	96	72	1		

- Molecule 34 is a protein called RIBOSOMAL PROTEIN ES31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	72	Total	C	N	O	S	0	0
			585	366	114	97	8		

- Molecule 35 is a protein called RIBOSOMAL PROTEIN RACK1.

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

- Molecule 36 is a protein called RIBOSOMAL PROTEIN EL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	24	Total	C	N	O	S	0	0
			231	140	63	26	2		

- Molecule 37 is a protein called RIBOSOMAL PROTEIN EL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	r	13	Total	C	N	O	0	0
			118	68	31	19		

- Molecule 38 is a protein called RIBOSOMAL PROTEIN EL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	62	Total	C	N	O	S	0	0
			452	279	92	80	1		

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

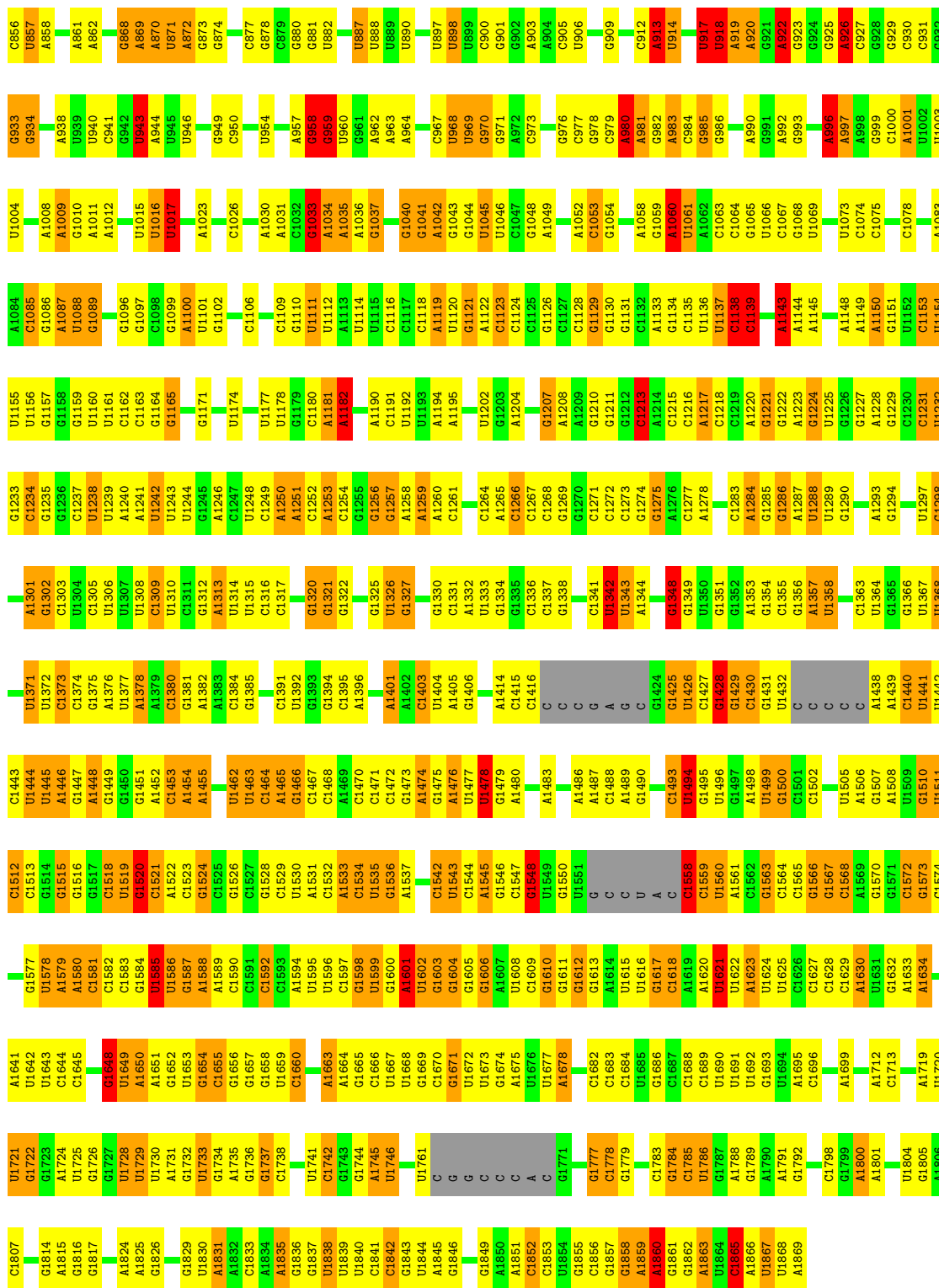
Mol	Chain	Residues	Atoms		AltConf
39	2	98	Total	Mg	0
			98	98	

- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	a	1	Total 1	Zn 1	0
40	d	1	Total 1	Zn 1	0
40	f	1	Total 1	Zn 1	0

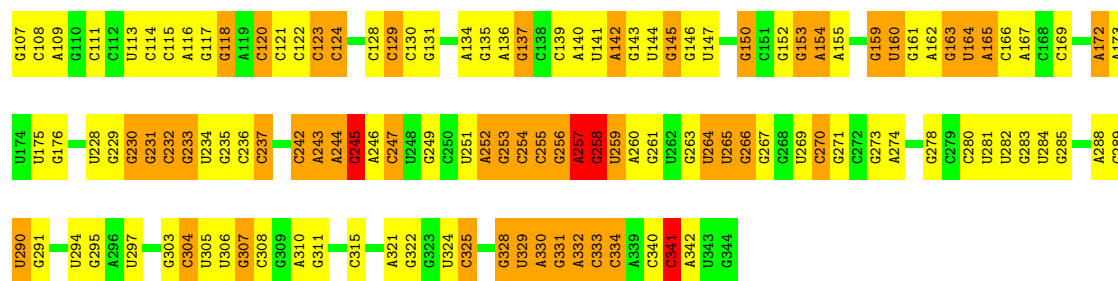
- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	2	141	Total 141	O 141	0
41	C	2	Total 2	O 2	0
41	e	1	Total 1	O 1	0

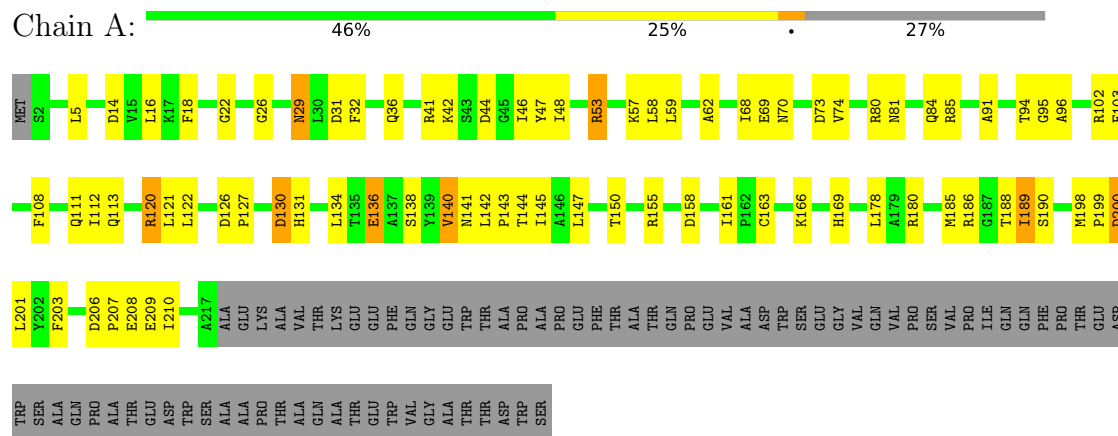


- Molecule 2: HCV IRES

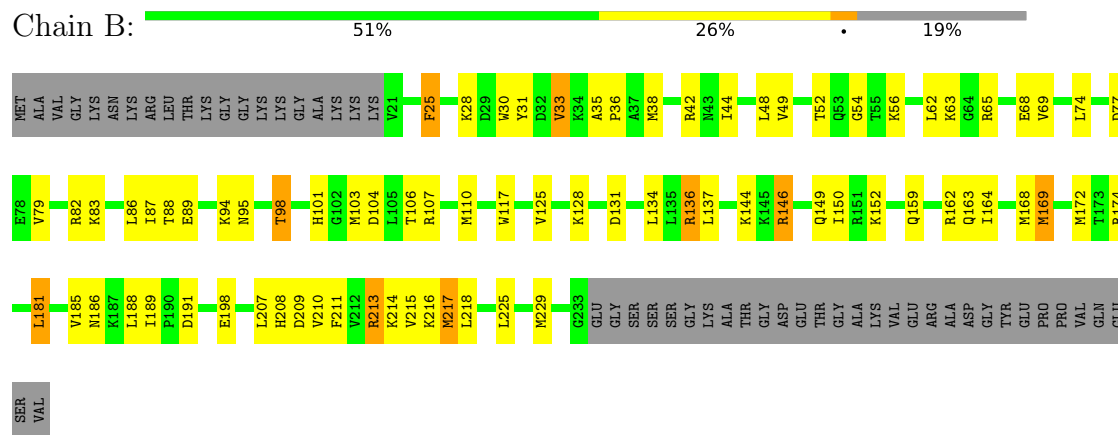




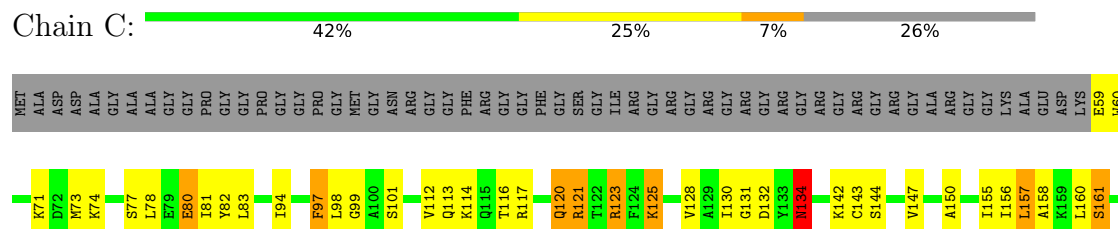
• Molecule 3: RIBOSOMAL PROTEIN US2

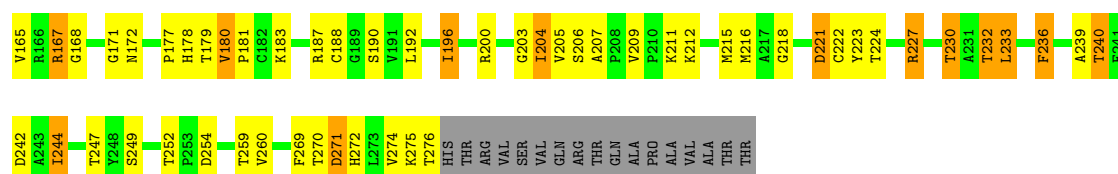


• Molecule 4: RIBOSOMAL PROTEIN ES1



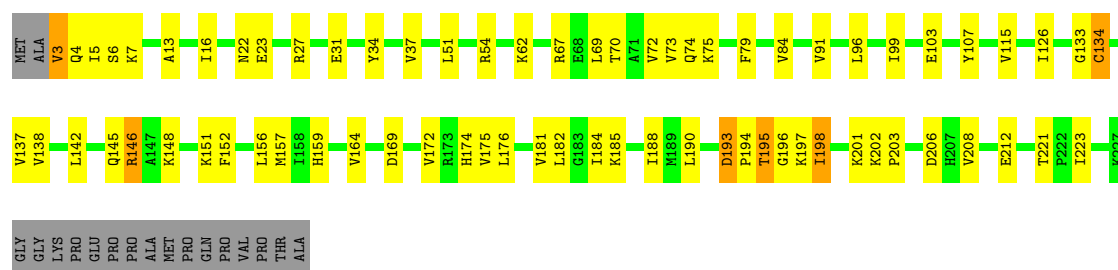
• Molecule 5: RIBOSOMAL PROTEIN US5





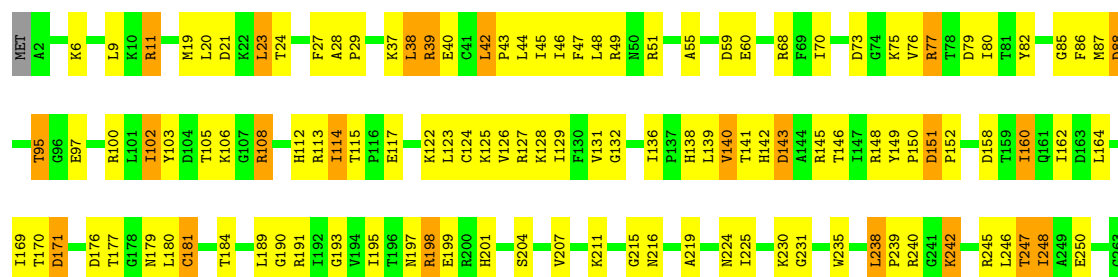
• Molecule 6: RIBOSOMAL PROTEIN US3

Chain D: 63% 27% 7%



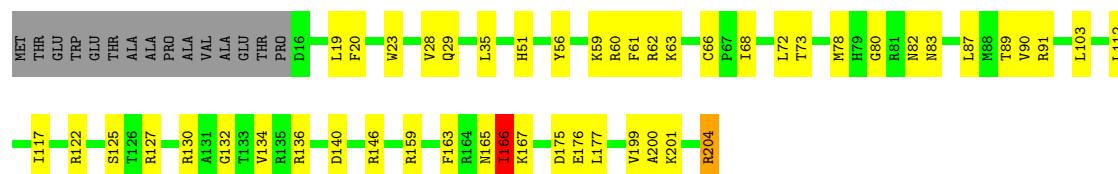
• Molecule 7: RIBOSOMAL PROTEIN ES4

Chain E: 54% 37% 8%



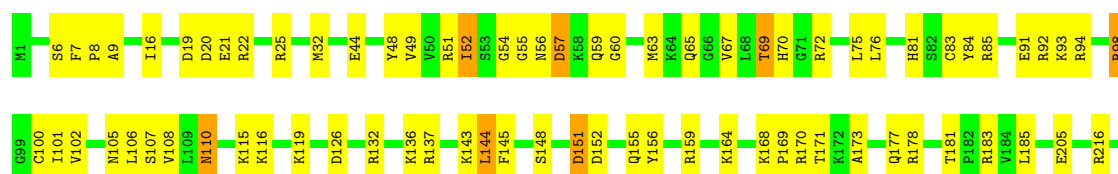
• Molecule 8: RIBOSOMAL PROTEIN US7

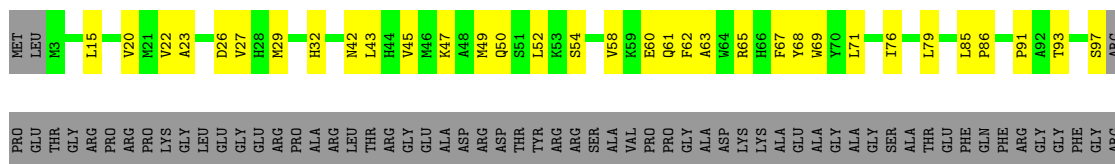
Chain F: 69% 23% 7%



• Molecule 9: RIBOSOMAL PROTEIN ES6

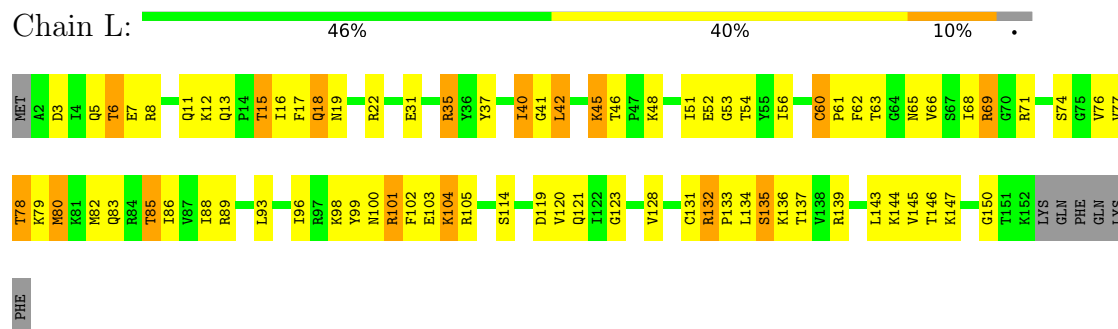
Chain G: 61% 29% 8%



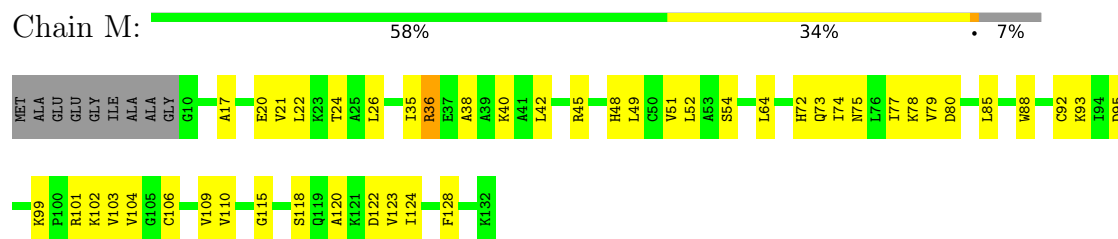


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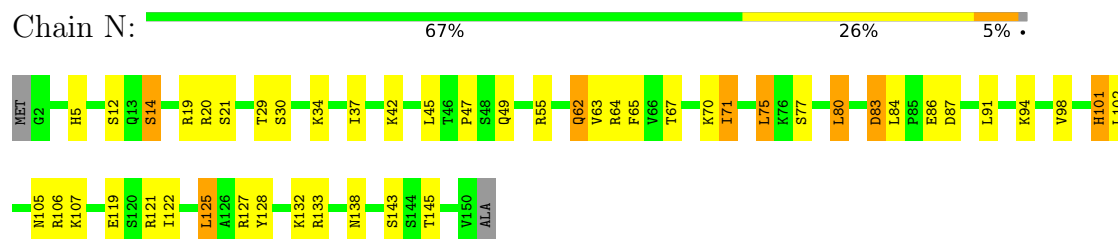
• Molecule 14: RIBOSOMAL PROTEIN US17



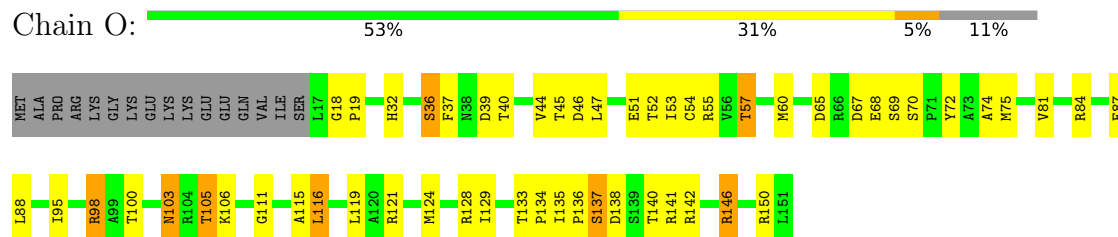
• Molecule 15: RIBOSOMAL PROTEIN ES12



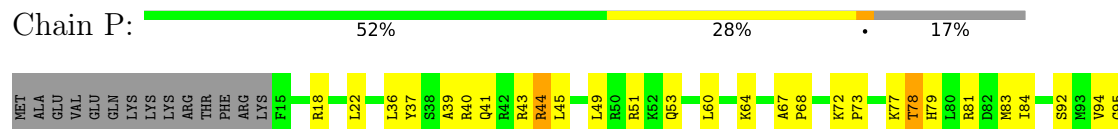
• Molecule 16: RIBOSOMAL PROTEIN US15



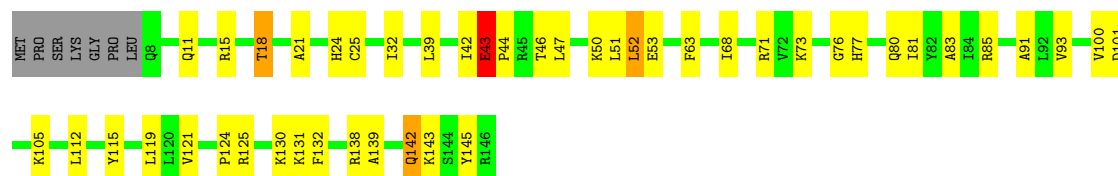
• Molecule 17: RIBOSOMAL PROTEIN US11



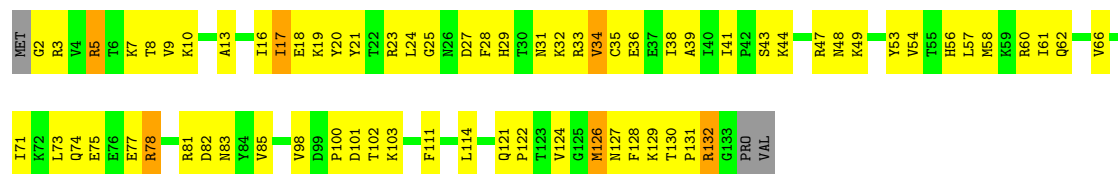
• Molecule 18: RIBOSOMAL PROTEIN US19



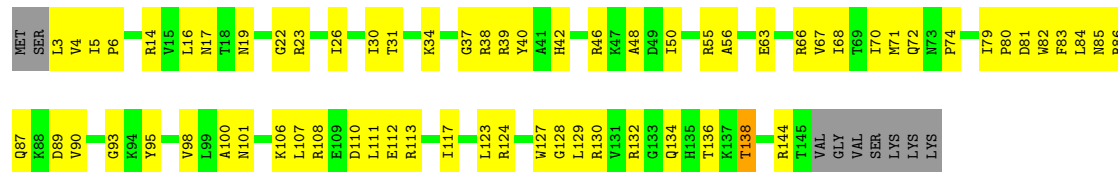
● Molecule 19: RIBOSOMAL PROTEIN US9



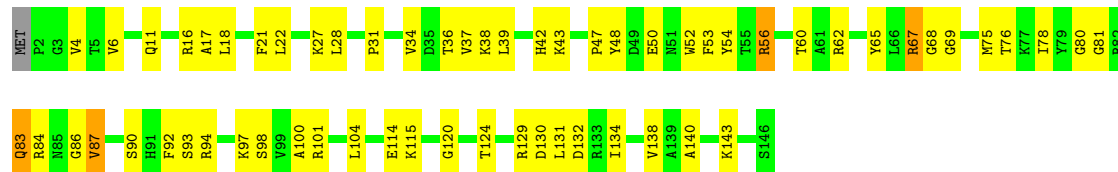
• Molecule 20: RIBOSOMAL PROTEIN ES17



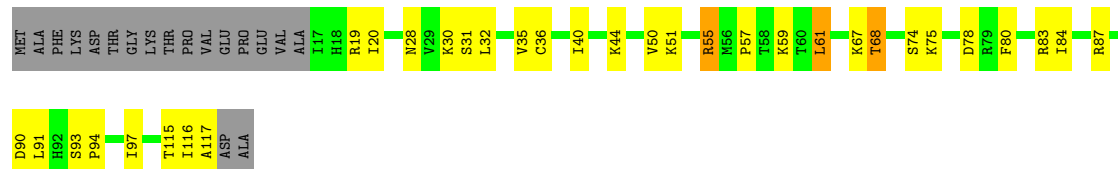
● Molecule 21: RIBOSOMAL PROTEIN US13



• Molecule 22: RIBOSOMAL PROTEIN ES19



• Molecule 23: RIBOSOMAL PROTEIN US10



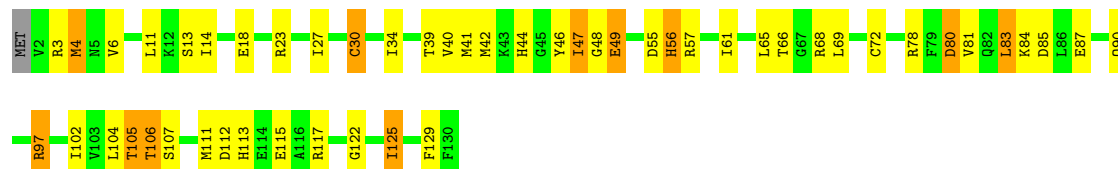
- Molecule 24: RIBOSOMAL PROTEIN ES21

Chain V:  66% 24% 8%



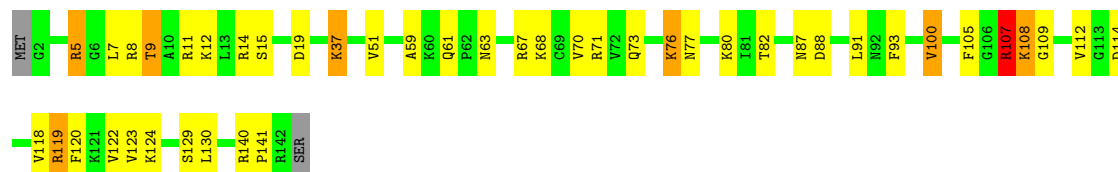
● Molecule 25: RIBOSOMAL PROTEIN US8

Chain W:  60% 31% 8%



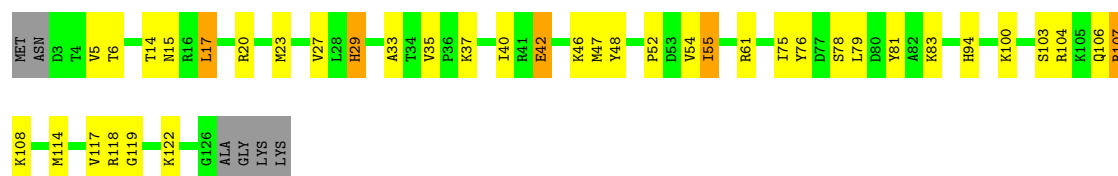
• Molecule 26: RIBOSOMAL PROTEIN US12

Chain X: 68% 25% 5% ..



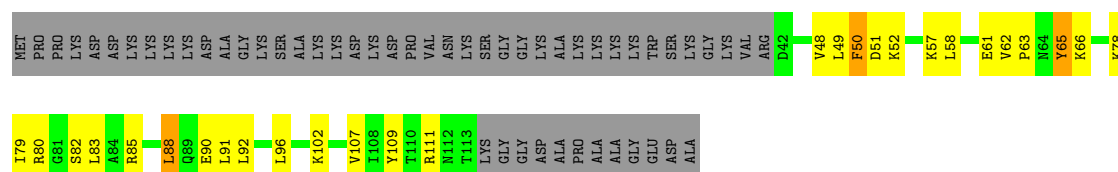
• Molecule 27: RIBOSOMAL PROTEIN ES24

Chain Y: 65% 26% 9%



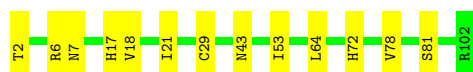
• Molecule 28: RIBOSOMAL PROTEIN ES25

Chain Z: 36% 19% . 42%



• Molecule 29: RIBOSOMAL PROTEIN ES26

Chain a:  87% 13%



- Molecule 30: RIBOSOMAL PROTEIN ES27

Chain b: 87% 13%



- Molecule 31: RIBOSOMAL PROTEIN ES28

Chain c: 95% 5%



- Molecule 32: RIBOSOMAL PROTEIN US14

Chain d: 95% 5%



- Molecule 33: RIBOSOMAL PROTEIN ES30

Chain e: 84% 16%



- Molecule 34: RIBOSOMAL PROTEIN ES31

Chain f: 96% 4%



- Molecule 35: RIBOSOMAL PROTEIN RACK1

Chain g: 94% 6%



- Molecule 36: RIBOSOMAL PROTEIN EL41

Chain h: 88% 13%



- Molecule 37: RIBOSOMAL PROTEIN EL19

Chain r:  92% 8%



- Molecule 38: RIBOSOMAL PROTEIN EL24

Chain w:  97% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	404357	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	INDIVIDUAL FRAMES	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20.00	Depositor
Minimum defocus (nm)	1500.00	Depositor
Maximum defocus (nm)	3400.00	Depositor
Magnification	100719	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	2	0.74	11/39755 (0.0%)	1.24	222/61954 (0.4%)
10	H	0.44	0/1524	0.61	0/2042
11	I	0.51	0/1711	0.66	1/2282 (0.0%)
12	J	0.57	0/1524	0.67	0/2035
13	K	0.32	0/824	0.46	0/1112
14	L	0.62	0/1250	0.72	0/1673
15	M	0.32	0/963	0.50	0/1291
16	N	0.51	0/1226	0.66	0/1649
17	O	0.52	0/1023	0.75	0/1372
18	P	0.34	0/1003	0.52	0/1341
19	Q	0.35	0/1126	0.55	1/1506 (0.1%)
2	3	0.40	0/6127	1.02	8/9547 (0.1%)
20	R	0.39	0/1080	0.58	0/1449
21	S	0.33	0/1202	0.50	0/1610
22	T	0.35	0/1148	0.50	0/1538
23	U	0.34	0/813	0.52	0/1092
24	V	0.51	0/631	0.63	0/844
25	W	0.65	0/1051	0.73	0/1406
26	X	0.62	0/1116	0.71	0/1490
27	Y	0.51	0/1031	0.64	0/1370
28	Z	0.28	0/580	0.48	0/780
29	a	0.56	0/830	0.64	0/1112
3	A	0.48	0/1742	0.63	0/2367
30	b	0.51	0/653	0.69	0/876
31	c	0.38	0/481	0.59	0/643
32	d	0.36	0/469	0.59	0/623
33	e	0.46	0/447	0.59	0/587
34	f	0.30	0/595	0.50	0/785
35	g	0.31	0/2497	0.52	0/3399
36	h	0.57	0/232	0.65	0/295
37	r	0.29	0/117	0.44	0/149
38	w	0.37	0/368	0.43	0/485

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
4	B	0.52	0/1756	0.68	0/2350
5	C	0.61	0/1726	0.77	4/2332 (0.2%)
6	D	0.35	0/1780	0.53	0/2397
7	E	0.57	0/2118	0.69	0/2849
8	F	0.34	0/1516	0.55	0/2037
9	G	0.42	0/1887	0.60	0/2513
All	All	0.60	11/85922 (0.0%)	1.00	236/125182 (0.2%)

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
10	H	0	1
26	X	0	2
27	Y	0	1
35	g	0	1
6	D	0	1
All	All	0	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1353	A	N9-C4	-6.78	1.33	1.37
1	2	1085	C	N1-C6	-6.62	1.33	1.37
1	2	599	A	N9-C4	-6.35	1.34	1.37
1	2	1000	C	N1-C6	-6.09	1.33	1.37
1	2	808	A	N9-C4	-5.94	1.34	1.37
1	2	476	A	N9-C4	-5.59	1.34	1.37
1	2	1825	A	N9-C4	5.32	1.41	1.37
1	2	813	A	N9-C4	-5.28	1.34	1.37
1	2	348	A	N9-C4	-5.27	1.34	1.37
1	2	1396	A	N9-C4	5.25	1.41	1.37
1	2	474	G	C6-N1	-5.08	1.35	1.39

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	501	C	N1-C2-O2	10.93	125.45	118.90
1	2	501	C	C2-N1-C1'	10.11	129.93	118.80
1	2	1842	C	C6-N1-C2	-9.59	116.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	501	C	C6-N1-C1'	-9.28	109.67	120.80
1	2	1139	C	C6-N1-C2	-9.27	116.59	120.30
1	2	1842	C	N3-C4-C5	-9.24	118.20	121.90
1	2	1520	G	C4-N9-C1'	9.04	138.25	126.50
1	2	1060	A	O4'-C1'-N9	8.61	115.09	108.20
1	2	853	C	N3-C2-O2	-8.50	115.95	121.90
1	2	1213	C	C6-N1-C2	8.42	123.67	120.30
1	2	1655	C	C6-N1-C2	-8.24	117.00	120.30
1	2	60	A	N1-C2-N3	8.15	133.38	129.30
1	2	958	G	C8-N9-C4	-8.04	103.18	106.40
1	2	1085	C	C6-N1-C2	7.95	123.48	120.30
1	2	1085	C	C5-C6-N1	-7.89	117.06	121.00
1	2	508	A	C8-N9-C4	-7.82	102.67	105.80
1	2	1253	A	P-O3'-C3'	7.73	128.98	119.70
1	2	1858	G	C4-C5-N7	7.64	113.86	110.80
1	2	1314	U	C2-N1-C1'	7.61	126.83	117.70
1	2	913	A	O4'-C1'-N9	7.54	114.23	108.20
1	2	1835	A	P-O3'-C3'	7.45	128.64	119.70
1	2	447	A	N1-C6-N6	-7.33	114.20	118.60
1	2	639	C	C6-N1-C2	-7.31	117.38	120.30
1	2	1520	G	C8-N9-C1'	-7.29	117.52	127.00
1	2	1357	A	N1-C2-N3	7.28	132.94	129.30
1	2	1838	U	P-O3'-C3'	7.24	128.38	119.70
1	2	686	U	N1-C2-O2	-7.22	117.74	122.80
1	2	501	C	N3-C2-O2	-7.17	116.88	121.90
1	2	1139	C	N3-C4-C5	-7.16	119.04	121.90
1	2	30	C	C6-N1-C2	-7.08	117.47	120.30
1	2	983	A	C6-N1-C2	-6.96	114.43	118.60
1	2	943	U	C2-N3-C4	-6.92	122.85	127.00
1	2	813	A	C2-N3-C4	-6.81	107.20	110.60
1	2	1139	C	N3-C2-O2	-6.77	117.16	121.90
1	2	823	U	N3-C2-O2	-6.73	117.49	122.20
1	2	408	A	P-O3'-C3'	6.72	127.76	119.70
1	2	868	G	N3-C4-C5	6.71	131.96	128.60
1	2	65	C	C6-N1-C2	-6.67	117.63	120.30
1	2	370	G	C8-N9-C4	6.66	109.06	106.40
1	2	834	C	C6-N1-C2	-6.63	117.65	120.30
1	2	65	C	C5-C6-N1	6.59	124.29	121.00
1	2	830	A	C6-N1-C2	-6.58	114.65	118.60
1	2	958	G	O4'-C1'-N9	6.57	113.46	108.20
1	2	1069	U	C6-N1-C2	6.56	124.94	121.00
1	2	958	G	N7-C8-N9	6.56	116.38	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1182	A	C8-N9-C4	-6.56	103.18	105.80
1	2	958	G	P-O3'-C3'	6.54	127.55	119.70
1	2	659	G	N3-C4-N9	6.53	129.92	126.00
5	C	233	LEU	CA-CB-CG	-6.51	100.32	115.30
1	2	1453	C	C2-N1-C1'	6.51	125.96	118.80
1	2	595	U	N1-C2-N3	6.51	118.81	114.90
1	2	1123	C	C6-N1-C2	-6.49	117.70	120.30
1	2	1865	C	N3-C2-O2	-6.37	117.44	121.90
1	2	1520	G	C6-C5-N7	-6.35	126.59	130.40
1	2	447	A	N9-C4-C5	6.35	108.34	105.80
1	2	604	A	N1-C2-N3	6.33	132.47	129.30
1	2	667	U	C5-C6-N1	-6.33	119.53	122.70
1	2	1520	G	N7-C8-N9	6.30	116.25	113.10
1	2	926	A	C8-N9-C4	-6.27	103.29	105.80
1	2	1182	A	N7-C8-N9	6.25	116.92	113.80
5	C	99	GLY	N-CA-C	-6.24	97.49	113.10
1	2	1804	U	N1-C2-O2	6.24	127.16	122.80
1	2	356	C	N1-C2-O2	6.23	122.64	118.90
1	2	1037	G	C8-N9-C4	-6.18	103.93	106.40
1	2	114	G	P-O3'-C3'	6.17	127.10	119.70
1	2	1860	A	O5'-P-OP2	-6.16	100.15	105.70
1	2	1621	U	C2-N1-C1'	6.15	125.08	117.70
1	2	71	G	C8-N9-C4	-6.14	103.94	106.40
1	2	382	C	P-O3'-C3'	6.07	126.99	119.70
1	2	1348	G	N3-C4-C5	-6.07	125.57	128.60
1	2	1520	G	N3-C4-N9	6.06	129.64	126.00
1	2	1648	G	P-O3'-C3'	6.04	126.95	119.70
2	3	245	G	O5'-P-OP1	-6.01	100.29	105.70
1	2	1520	G	N3-C4-C5	-5.97	125.61	128.60
1	2	1153	C	C2-N1-C1'	5.93	125.32	118.80
1	2	73	C	C6-N1-C2	-5.92	117.93	120.30
1	2	659	G	C6-N1-C2	-5.91	121.55	125.10
1	2	102	A	C8-N9-C4	-5.91	103.44	105.80
1	2	1585	U	P-O3'-C3'	5.86	126.73	119.70
1	2	960	U	N3-C2-O2	-5.85	118.11	122.20
1	2	73	C	C5-C6-N1	5.83	123.91	121.00
1	2	1342	U	P-O3'-C3'	5.79	126.64	119.70
1	2	926	A	N7-C8-N9	5.77	116.69	113.80
1	2	532	C	C6-N1-C2	-5.76	118.00	120.30
1	2	1601	A	P-O3'-C3'	5.76	126.61	119.70
1	2	342	C	C2-N1-C1'	5.76	125.13	118.80
1	2	1471	C	C6-N1-C2	-5.75	118.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1684	C	C6-N1-C2	-5.74	118.00	120.30
1	2	830	A	N1-C2-N3	5.74	132.17	129.30
1	2	660	C	C6-N1-C2	5.72	122.59	120.30
1	2	599	A	C8-N9-C4	5.71	108.08	105.80
1	2	604	A	C8-N9-C4	-5.71	103.52	105.80
1	2	1733	U	N3-C2-O2	-5.68	118.22	122.20
1	2	1842	C	C5-C6-N1	5.68	123.84	121.00
1	2	337	C	C2-N1-C1'	5.67	125.04	118.80
1	2	1085	C	C2-N3-C4	-5.64	117.08	119.90
1	2	1155	U	C5-C6-N1	-5.63	119.89	122.70
1	2	1033	G	N3-C4-N9	5.62	129.37	126.00
1	2	682	U	C5-C6-N1	-5.61	119.89	122.70
1	2	64	A	C2-N3-C4	-5.61	107.79	110.60
1	2	427	U	N3-C2-O2	-5.61	118.27	122.20
1	2	853	C	C2-N1-C1'	5.60	124.96	118.80
1	2	661	U	C5-C6-N1	-5.59	119.90	122.70
1	2	1520	G	C8-N9-C4	-5.59	104.16	106.40
1	2	1034	A	C8-N9-C4	5.59	108.04	105.80
1	2	1314	U	C6-N1-C1'	-5.58	113.39	121.20
1	2	1558	C	C6-N1-C2	-5.57	118.07	120.30
1	2	855	G	C8-N9-C4	5.57	108.63	106.40
1	2	1138	C	C6-N1-C2	5.56	122.53	120.30
2	3	307	G	C4-N9-C1'	5.56	133.73	126.50
1	2	1524	G	N3-C4-N9	5.55	129.33	126.00
1	2	857	U	N1-C2-O2	5.55	126.68	122.80
1	2	959	G	C6-C5-N7	-5.54	127.08	130.40
1	2	1111	U	C2-N1-C1'	5.53	124.34	117.70
1	2	604	A	P-O3'-C3'	5.53	126.33	119.70
1	2	1865	C	N1-C2-O2	5.52	122.21	118.90
1	2	1842	C	C2-N3-C4	5.51	122.66	119.90
1	2	112	U	C5-C6-N1	-5.51	119.94	122.70
1	2	314	U	P-O3'-C3'	5.51	126.31	119.70
1	2	842	C	C2-N1-C1'	5.51	124.86	118.80
1	2	917	U	C2-N3-C4	5.51	130.30	127.00
1	2	1174	U	C6-N1-C2	-5.50	117.70	121.00
1	2	1151	G	C8-N9-C4	5.50	108.60	106.40
1	2	684	G	N3-C4-C5	5.50	131.35	128.60
1	2	1314	U	N1-C2-O2	5.49	126.64	122.80
1	2	474	G	N3-C4-C5	-5.49	125.86	128.60
1	2	1064	C	C6-N1-C2	-5.48	118.11	120.30
1	2	1488	C	C6-N1-C2	-5.47	118.11	120.30
1	2	620	G	P-O3'-C3'	5.46	126.25	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	43	GLU	C-N-CD	5.46	139.86	128.40
1	2	130	G	C4-N9-C1'	5.45	133.59	126.50
1	2	686	U	N3-C2-O2	5.45	126.02	122.20
1	2	508	A	N7-C8-N9	5.45	116.53	113.80
1	2	601	G	C3'-C2'-C1'	5.45	105.86	101.50
1	2	124	U	C2-N1-C1'	5.43	124.22	117.70
1	2	422	U	N1-C2-N3	5.42	118.15	114.90
1	2	71	G	N3-C4-C5	-5.40	125.90	128.60
1	2	1478	U	N1-C2-O2	5.39	126.57	122.80
1	2	90	G	N3-C4-C5	-5.39	125.91	128.60
1	2	102	A	P-O3'-C3'	5.38	126.16	119.70
1	2	853	C	N1-C2-O2	5.38	122.13	118.90
1	2	452	G	P-O3'-C3'	5.38	126.15	119.70
1	2	811	A	P-O3'-C3'	5.38	126.15	119.70
1	2	130	G	N3-C4-C5	-5.37	125.91	128.60
1	2	1234	C	N1-C2-O2	5.37	122.12	118.90
2	3	258	G	O4'-C1'-N9	5.37	112.49	108.20
1	2	465	A	P-O3'-C3'	5.36	126.13	119.70
1	2	918	U	N1-C2-N3	5.36	118.11	114.90
1	2	447	A	C6-N1-C2	-5.35	115.39	118.60
1	2	641	A	N1-C2-N3	5.35	131.97	129.30
2	3	70	A	C4-N9-C1'	5.35	135.93	126.30
2	3	257	A	P-O3'-C3'	5.34	126.11	119.70
2	3	48	U	P-O3'-C3'	5.33	126.09	119.70
1	2	1139	C	C5-C4-N4	5.33	123.93	120.20
1	2	1476	A	P-O3'-C3'	5.33	126.09	119.70
1	2	46	A	N9-C4-C5	5.31	107.92	105.80
1	2	1143	A	N9-C4-C5	5.30	107.92	105.80
1	2	620	G	N9-C4-C5	5.29	107.52	105.40
1	2	996	A	C3'-C2'-C1'	5.29	105.73	101.50
1	2	215	G	C4-N9-C1'	5.28	133.37	126.50
1	2	659	G	C8-N9-C1'	-5.28	120.13	127.00
1	2	1351	G	N3-C4-C5	-5.28	125.96	128.60
1	2	1368	U	N1-C2-N3	5.28	118.07	114.90
1	2	1478	U	C2-N1-C1'	5.28	124.03	117.70
1	2	1129	G	N3-C4-C5	-5.28	125.96	128.60
1	2	1139	C	C4-C5-C6	5.27	120.03	117.40
1	2	1494	U	P-O3'-C3'	5.27	126.02	119.70
1	2	1128	C	C6-N1-C2	5.26	122.40	120.30
1	2	369	C	C2-N1-C1'	5.25	124.58	118.80
1	2	334	C	C6-N1-C2	-5.25	118.20	120.30
1	2	1592	C	C6-N1-C2	-5.25	118.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1378	A	C8-N9-C4	-5.25	103.70	105.80
1	2	1302	G	P-O3'-C3'	5.25	126.00	119.70
1	2	382	C	C5-C6-N1	5.24	123.62	121.00
1	2	24	C	C6-N1-C2	5.24	122.39	120.30
1	2	1035	A	C8-N9-C4	5.23	107.89	105.80
1	2	476	A	C8-N9-C4	5.23	107.89	105.80
1	2	30	C	N3-C2-O2	-5.23	118.24	121.90
1	2	639	C	C2-N1-C1'	5.23	124.55	118.80
1	2	922	A	N1-C2-N3	5.23	131.91	129.30
1	2	1123	C	C5-C6-N1	5.22	123.61	121.00
1	2	1016	U	N3-C2-O2	-5.22	118.54	122.20
11	I	67	TRP	CA-CB-CG	5.22	123.62	113.70
1	2	983	A	C5-C6-N6	-5.22	119.53	123.70
1	2	1478	U	N3-C2-O2	-5.21	118.55	122.20
1	2	92	A	C6-N1-C2	-5.21	115.47	118.60
1	2	1164	G	C6-N1-C2	-5.20	121.98	125.10
1	2	1363	C	C6-N1-C2	5.20	122.38	120.30
1	2	630	U	N1-C2-O2	5.20	126.44	122.80
1	2	595	U	C2-N3-C4	-5.20	123.88	127.00
1	2	370	G	N7-C8-N9	-5.19	110.51	113.10
1	2	382	C	C6-N1-C2	-5.19	118.22	120.30
1	2	1403	C	P-O3'-C3'	5.19	125.92	119.70
1	2	1863	A	N1-C6-N6	-5.19	115.49	118.60
1	2	1428	G	C8-N9-C4	-5.18	104.33	106.40
1	2	1524	G	C8-N9-C1'	-5.16	120.30	127.00
1	2	658	U	C5-C6-N1	-5.14	120.13	122.70
1	2	453	C	C3'-C2'-C1'	5.13	105.60	101.50
1	2	1867	U	C6-N1-C1'	-5.13	114.02	121.20
1	2	681	U	N3-C2-O2	-5.13	118.61	122.20
1	2	659	G	C5-C6-N1	5.12	114.06	111.50
1	2	1696	C	C6-N1-C2	-5.12	118.25	120.30
1	2	1502	C	C6-N1-C2	-5.12	118.25	120.30
1	2	547	G	P-O3'-C3'	5.11	125.84	119.70
1	2	922	A	C6-N1-C2	-5.11	115.53	118.60
5	C	134	ASN	N-CA-C	5.11	124.80	111.00
1	2	472	C	N1-C2-O2	-5.11	115.84	118.90
1	2	662	G	C4-C5-N7	5.10	112.84	110.80
1	2	1165	G	C5-C6-N1	5.10	114.05	111.50
5	C	171	GLY	N-CA-C	-5.10	100.35	113.10
1	2	315	C	C6-N1-C2	-5.09	118.27	120.30
1	2	887	U	C2-N1-C1'	5.08	123.79	117.70
1	2	64	A	O5'-P-OP2	-5.07	101.13	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1624	U	C2-N1-C1'	5.07	123.78	117.70
1	2	1106	C	C6-N1-C2	-5.07	118.27	120.30
1	2	667	U	C2-N3-C4	-5.07	123.96	127.00
1	2	1015	U	C2-N1-C1'	-5.07	111.62	117.70
1	2	1182	A	C6-C5-N7	-5.07	128.75	132.30
1	2	1462	U	C2-N1-C1'	5.07	123.78	117.70
1	2	116	U	C6-N1-C2	-5.06	117.96	121.00
1	2	595	U	C5-C6-N1	-5.06	120.17	122.70
2	3	137	G	C4-N9-C1'	5.06	133.08	126.50
1	2	660	C	N1-C2-N3	-5.06	115.66	119.20
1	2	1472	C	C6-N1-C2	-5.05	118.28	120.30
1	2	293	C	N3-C2-O2	-5.05	118.37	121.90
1	2	1548	G	C8-N9-C4	-5.05	104.38	106.40
1	2	934	G	O5'-P-OP2	-5.04	101.16	105.70
1	2	1371	U	C5-C6-N1	-5.04	120.18	122.70
1	2	980	A	P-O3'-C3'	5.04	125.75	119.70
1	2	1017	U	N3-C2-O2	-5.03	118.68	122.20
2	3	341	C	C6-N1-C2	-5.03	118.29	120.30
1	2	1357	A	C2-N3-C4	-5.03	108.09	110.60
1	2	808	A	C8-N9-C4	5.02	107.81	105.80
1	2	686	U	C2-N1-C1'	-5.02	111.68	117.70
1	2	985	G	C6-N1-C2	-5.02	122.09	125.10
1	2	1858	G	C5-N7-C8	-5.00	101.80	104.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	D	193	ASP	Peptide
10	H	134	VAL	Peptide
26	X	107	ARG	Peptide
26	X	112	VAL	Peptide
27	Y	118	ARG	Peptide
35	g	190	GLY	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	2	35552	0	17948	699	0
2	3	5485	0	2776	79	0
3	A	1705	0	1706	54	0
4	B	1729	0	1803	57	0
5	C	1690	0	1777	55	0
6	D	1752	0	1848	57	0
7	E	2076	0	2177	81	0
8	F	1495	0	1549	32	0
9	G	1864	0	2018	61	0
10	H	1501	0	1593	41	0
11	I	1682	0	1769	58	0
12	J	1499	0	1618	59	0
13	K	800	0	818	23	0
14	L	1229	0	1302	51	0
15	M	953	0	990	27	0
16	N	1202	0	1289	34	0
17	O	1010	0	1034	43	0
18	P	984	0	1028	34	0
19	Q	1109	0	1174	35	0
20	R	1066	0	1116	52	0
21	S	1184	0	1244	64	0
22	T	1128	0	1158	56	0
23	U	803	0	873	26	0
24	V	625	0	628	17	0
25	W	1034	0	1080	29	0
26	X	1098	0	1167	36	0
27	Y	1014	0	1082	23	0
28	Z	574	0	627	24	0
29	a	816	0	867	0	0
30	b	640	0	665	0	0
31	c	479	0	507	0	0
32	d	458	0	448	0	0
33	e	442	0	487	0	0
34	f	585	0	615	0	0
35	g	2440	0	2396	0	0
36	h	231	0	277	0	0
37	r	118	0	132	0	0
38	w	452	0	493	0	0
39	2	98	0	0	0	0
40	a	1	0	0	0	0
40	d	1	0	0	0	0
40	f	1	0	0	0	0
41	2	141	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	C	2	0	0	0	0
41	e	1	0	0	0	0
All	All	80749	0	62079	1639	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1639) 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)
15:M:20:GLU:HB3	15:M:120:ALA:HB2	1.50	0.94
1:2:1622:U:H3	18:P:122:THR:HG1	1.11	0.90
22:T:69:GLY:HA2	22:T:120:GLY:HA3	1.55	0.89
1:2:1256:G:H21	1:2:1659:U:H5'	1.37	0.89
1:2:560:A:H5'	12:J:174:LYS:HG3	1.56	0.88
1:2:958:G:N2	17:O:68:GLU:OE2	2.08	0.86
1:2:1337:C:H2'	1:2:1338:G:H8	1.42	0.85
12:J:136:ARG:HD2	12:J:160:SER:HA	1.57	0.85
21:S:50:ILE:HD12	21:S:67:VAL:CG2	2.06	0.84
1:2:384:U:O4	11:I:5:ARG:NH2	2.11	0.83
4:B:87:ILE:HG12	4:B:101:HIS:HB2	1.60	0.83
1:2:589:G:N2	41:2:2001:HOH:O	2.08	0.83
25:W:80:ASP:OD1	25:W:80:ASP:N	2.11	0.83
22:T:76:THR:HG22	22:T:94:ARG:HB3	1.61	0.82
1:2:76:U:H5'	9:G:159:ARG:HH22	1.41	0.82
11:I:141:ARG:HD3	11:I:146:GLN:HA	1.60	0.82
26:X:67:ARG:NH2	26:X:114:ASP:OD2	2.10	0.81
9:G:59:GLN:HG3	9:G:72:ARG:NH2	1.95	0.81
20:R:34:VAL:HG13	20:R:38:ILE:HD12	1.63	0.81
1:2:297:A:H5'	7:E:132:GLY:HA2	1.63	0.81
1:2:685:A:H62	1:2:918:U:H3	1.26	0.80
1:2:64:A:H2	1:2:83:A:H62	1.23	0.80
1:2:1241:A:HO2'	1:2:1266:C:HO2'	1.26	0.80
26:X:68:LYS:HB3	26:X:91:LEU:HD22	1.63	0.79
26:X:93:PHE:O	26:X:140:ARG:NH1	2.16	0.79
1:2:1601:A:H4'	1:2:1602:U:H5'	1.62	0.79
1:2:587:A:N3	41:2:2005:HOH:O	2.14	0.79
1:2:943:U:OP1	4:B:214:LYS:NZ	2.15	0.79
1:2:1579:A:H4'	1:2:1581:C:H5	1.49	0.79
1:2:115:U:OP1	1:2:382:C:O2'	2.01	0.78
2:3:71:G:O6	2:3:94:G:O2'	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:86:ARG:HD2	21:S:106:LYS:HD3	1.66	0.77
2:3:42:C:H42	2:3:120:C:H42	1.32	0.77
1:2:1649:U:OP2	1:2:1674:G:N1	2.16	0.77
1:2:499:G:H2'	1:2:501:C:H5	1.48	0.77
1:2:1521:C:OP2	21:S:124:ARG:NH1	2.18	0.77
4:B:144:LYS:HB2	4:B:208:HIS:HB2	1.65	0.76
11:I:122:GLY:HA2	11:I:167:GLN:HG2	1.67	0.76
18:P:44:ARG:HD2	18:P:84:ILE:HD11	1.65	0.76
1:2:121:U:H5''	7:E:77:ARG:HH21	1.49	0.76
1:2:1446:A:OP1	23:U:57:PRO:HA	1.86	0.76
21:S:17:ASN:HD22	21:S:101:ASN:HD21	1.34	0.76
1:2:925:G:H2'	1:2:926:A:H5''	1.66	0.75
1:2:1068:G:N7	41:2:2008:HOH:O	2.20	0.74
1:2:1310:U:OP2	15:M:36:ARG:NH2	2.19	0.74
1:2:103:A:OP2	1:2:356:C:N4	2.20	0.74
1:2:1333:U:H2'	1:2:1334:G:H8	1.51	0.74
12:J:47:LYS:HA	12:J:102:ILE:HD11	1.70	0.74
12:J:121:LYS:H	12:J:125:HIS:HD2	1.35	0.74
6:D:96:LEU:HD12	6:D:198:ILE:HG21	1.67	0.74
21:S:34:LYS:HB2	21:S:100:ALA:HA	1.68	0.74
4:B:198:GLU:HB2	4:B:210:VAL:HG11	1.70	0.74
1:2:1738:C:OP1	9:G:92:ARG:NH2	2.21	0.73
2:3:150:G:H1	2:3:242:C:H42	1.36	0.73
13:K:27:VAL:HG13	13:K:43:LEU:HD13	1.71	0.73
15:M:21:VAL:HG21	15:M:124:ILE:HD12	1.69	0.73
1:2:190:G:O2'	1:2:209:A:N6	2.22	0.73
5:C:60:TRP:O	5:C:71:LYS:NZ	2.21	0.73
16:N:101:HIS:CE1	16:N:105:ASN:HD22	2.06	0.73
18:P:41:GLN:NE2	18:P:113:GLY:O	2.22	0.73
1:2:390:C:H4'	14:L:8:ARG:HH22	1.52	0.73
1:2:525:A:N7	41:2:2009:HOH:O	2.21	0.73
1:2:1542:C:H4'	22:T:11:GLN:HB2	1.70	0.73
2:3:92:U:H5'	2:3:93:A:H2'	1.69	0.72
4:B:101:HIS:O	4:B:217:MET:HG3	1.88	0.72
2:3:70:A:H61	2:3:97:U:H3	1.37	0.72
20:R:31:ASN:HA	20:R:34:VAL:HB	1.71	0.72
1:2:1395:C:OP1	19:Q:15:ARG:NH1	2.22	0.72
1:2:925:G:H1	1:2:1017:U:H3	1.37	0.72
6:D:208:VAL:HG12	20:R:41:ILE:HG22	1.71	0.72
1:2:171:A:H5''	9:G:177:GLN:HG2	1.72	0.72
23:U:51:LYS:HB2	23:U:90:ASP:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:48:LEU:HD22	7:E:70:ILE:HD11	1.70	0.72
14:L:131:CYS:SG	14:L:132:ARG:N	2.63	0.72
1:2:1478:U:H2'	1:2:1479:G:C8	2.25	0.71
8:F:127:ARG:HH22	8:F:132:GLY:H	1.38	0.71
19:Q:53:GLU:OE1	19:Q:85:ARG:NH2	2.23	0.71
1:2:387:C:OP2	11:I:10:LYS:NZ	2.24	0.71
2:3:70:A:H3'	2:3:71:G:H5'	1.71	0.71
6:D:27:ARG:HG3	13:K:63:ALA:HB2	1.72	0.71
1:2:1337:C:H2'	1:2:1338:G:C8	2.26	0.71
6:D:67:ARG:NH1	13:K:93:THR:O	2.23	0.71
12:J:88:ASP:N	12:J:88:ASP:OD1	2.23	0.71
6:D:172:VAL:HG22	6:D:185:LYS:HG2	1.71	0.71
1:2:446:G:OP2	11:I:47:ARG:NH2	2.23	0.70
26:X:140:ARG:HD2	26:X:141:PRO:HD2	1.74	0.70
14:L:22:ARG:HH22	14:L:31:GLU:HG3	1.55	0.70
1:2:381:C:H5'	11:I:49:ARG:HB2	1.73	0.70
5:C:134:ASN:HA	5:C:218:GLY:HA3	1.74	0.70
1:2:1534:C:H4'	1:2:1535:U:O5'	1.91	0.69
12:J:109:ARG:NH2	12:J:146:SER:OG	2.24	0.69
15:M:21:VAL:HG23	15:M:120:ALA:HB1	1.74	0.69
1:2:1269:G:H1	1:2:1513:C:H42	1.40	0.69
1:2:475:C:OP2	41:2:2002:HOH:O	2.10	0.69
1:2:619:A:N1	26:X:114:ASP:HB2	2.08	0.69
1:2:9:U:OP2	41:2:2003:HOH:O	2.10	0.69
2:3:92:U:O4	2:3:93:A:N6	2.26	0.69
1:2:996:A:H2'	1:2:997:A:C8	2.28	0.69
20:R:41:ILE:HD13	20:R:47:ARG:HB2	1.74	0.69
1:2:615:C:O2'	1:2:616:A:O4'	2.11	0.69
14:L:80:MET:HB3	14:L:86:ILE:HG22	1.75	0.69
21:S:50:ILE:CD1	21:S:67:VAL:CG2	2.70	0.69
5:C:271:ASP:OD1	5:C:271:ASP:N	2.26	0.68
1:2:65:C:OP1	9:G:136:LYS:NZ	2.26	0.68
1:2:688:U:H5	10:H:103:LYS:H	1.41	0.68
5:C:209:VAL:HG21	5:C:233:LEU:HD11	1.75	0.68
11:I:69:SER:OG	11:I:191:GLU:OE1	2.08	0.68
1:2:1332:A:O2'	6:D:145:GLN:OE1	2.11	0.68
7:E:11:ARG:NH2	7:E:24:THR:OG1	2.27	0.68
9:G:159:ARG:HH11	9:G:171:THR:HG21	1.57	0.68
1:2:1721:U:H4'	1:2:1722:G:H5''	1.76	0.68
1:2:643:A:OP1	12:J:39:ASN:ND2	2.27	0.68
25:W:81:VAL:HG21	25:W:125:ILE:HG13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:18:ARG:HG3	18:P:36:LEU:HB3	1.75	0.68
27:Y:78:SER:HB3	27:Y:81:TYR:HD2	1.59	0.68
1:2:617:G:H4'	26:X:88:ASP:HB3	1.77	0.67
1:2:145:G:H2'	1:2:146:G:C8	2.30	0.67
18:P:98:ASN:ND2	18:P:103:ASN:OD1	2.28	0.67
21:S:50:ILE:CD1	21:S:67:VAL:HG23	2.23	0.67
2:3:146:G:H1	2:3:247:C:H42	1.43	0.67
3:A:85:ARG:HH21	3:A:201:LEU:HD12	1.58	0.67
10:H:9:VAL:HG12	10:H:11:PRO:HD3	1.77	0.67
22:T:22:LEU:HB3	22:T:54:TYR:HD1	1.58	0.67
1:2:499:G:H2'	1:2:501:C:C5	2.30	0.67
22:T:140:ALA:HA	22:T:143:LYS:HE2	1.77	0.67
1:2:1649:U:O2'	1:2:1650:A:OP1	2.13	0.67
3:A:53:ARG:NH2	24:V:82:ASN:O	2.27	0.66
1:2:1048:G:OP2	41:2:2004:HOH:O	2.12	0.66
1:2:1333:U:H2'	1:2:1334:G:C8	2.29	0.66
1:2:1579:A:H4'	1:2:1581:C:C5	2.31	0.66
1:2:76:U:H3'	1:2:77:A:H5'	1.77	0.66
4:B:65:ARG:NH2	17:O:51:GLU:OE2	2.18	0.66
8:F:35:LEU:HD21	8:F:146:ARG:HD2	1.78	0.66
12:J:104:ASP:OD1	12:J:104:ASP:N	2.28	0.66
6:D:157:MET:HG3	6:D:159:HIS:CE1	2.30	0.66
1:2:309:G:OP2	11:I:55:TYR:OH	2.11	0.66
20:R:27:ASP:O	20:R:31:ASN:ND2	2.28	0.66
21:S:16:LEU:HD21	21:S:72:GLN:HE22	1.58	0.66
2:3:329:U:O2'	2:3:330:A:O5'	2.10	0.66
9:G:69:THR:HG22	9:G:70:HIS:H	1.61	0.65
1:2:1857:G:N7	17:O:146:ARG:NH1	2.43	0.65
1:2:996:A:O2'	1:2:997:A:O4'	2.10	0.65
8:F:72:LEU:HD22	8:F:112:LEU:HD11	1.76	0.65
8:F:78:MET:H	8:F:159:ARG:HH22	1.44	0.65
1:2:1342:U:H4'	1:2:1343:U:O5'	1.96	0.65
6:D:195:THR:HG22	6:D:201:LYS:HE2	1.79	0.65
17:O:103:ASN:N	17:O:103:ASN:OD1	2.28	0.65
1:2:1622:U:O4	18:P:81:ARG:NH2	2.30	0.65
2:3:252:A:H4'	2:3:253:G:H5'	1.79	0.65
2:3:330:A:O2'	2:3:331:G:O5'	2.15	0.65
14:L:68:ILE:HG21	14:L:143:LEU:HD11	1.77	0.65
2:3:144:U:H2'	2:3:145:G:H8	1.60	0.65
2:3:333:C:O2'	2:3:334:C:OP1	2.14	0.65
1:2:632:C:OP2	41:2:2006:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:54:GLY:H	9:G:110:ASN:HB2	1.62	0.64
1:2:841:G:H2'	1:2:842:C:H6	1.62	0.64
1:2:1543:U:O2'	19:Q:43:GLU:OE2	2.15	0.64
5:C:179:THR:OG1	5:C:180:VAL:N	2.31	0.64
11:I:123:ARG:NH1	11:I:133:GLU:OE2	2.28	0.64
12:J:169:ARG:HE	12:J:175:ARG:HH21	1.43	0.64
22:T:52:TRP:O	22:T:56:ARG:HB2	1.98	0.64
1:2:1284:A:O4'	1:2:1312:G:N2	2.31	0.64
1:2:1453:C:OP1	20:R:48:ASN:ND2	2.26	0.64
1:2:640:A:H2'	1:2:641:A:C8	2.32	0.64
1:2:1599:U:C4	8:F:166:ILE:HD12	2.33	0.64
12:J:169:ARG:HH21	12:J:175:ARG:HH22	1.46	0.63
13:K:60:GLU:HG2	13:K:69:TRP:CD1	2.34	0.63
1:2:918:U:H3'	16:N:64:ARG:HH22	1.63	0.63
22:T:75:MET:HB3	22:T:100:ALA:HB1	1.80	0.63
2:3:232:C:H2'	2:3:233:G:H5''	1.79	0.63
2:3:243:A:O2'	2:3:244:A:OP1	2.16	0.63
3:A:42:LYS:HE2	3:A:46:ILE:HB	1.79	0.63
14:L:119:ASP:O	14:L:147:LYS:NZ	2.30	0.63
1:2:1428:G:O6	19:Q:71:ARG:NH2	2.30	0.63
1:2:1606:G:H5'	22:T:86:GLY:HA2	1.79	0.63
1:2:1277:C:H2'	1:2:1278:A:H8	1.64	0.63
3:A:198:MET:HG2	3:A:200:ASP:HB2	1.80	0.63
1:2:639:C:HO2'	1:2:640:A:H8	1.46	0.63
1:2:1598:G:H3'	28:Z:80:ARG:HG2	1.81	0.63
1:2:1139:C:H5	1:2:1149:A:H62	1.47	0.63
1:2:816:A:P	12:J:10:ARG:HH22	2.22	0.63
1:2:925:G:C2'	1:2:926:A:H5''	2.28	0.63
5:C:259:THR:HG21	24:V:16:LYS:H	1.62	0.63
28:Z:79:ILE:HG23	28:Z:83:LEU:HD23	1.80	0.63
1:2:808:A:O2'	1:2:809:A:O5'	2.15	0.63
1:2:1650:A:OP1	19:Q:138:ARG:HB2	1.99	0.62
18:P:72:LYS:NZ	18:P:106:GLU:OE2	2.32	0.62
1:2:1590:C:H41	19:Q:77:HIS:CE1	2.16	0.62
1:2:75:G:H22	9:G:155:GLN:HG3	1.63	0.62
13:K:23:ALA:HB3	13:K:67:PHE:HB2	1.81	0.62
1:2:114:G:OP1	14:L:69:ARG:NH1	2.32	0.62
23:U:61:LEU:HD11	23:U:84:ILE:HD11	1.80	0.62
1:2:1857:G:OP2	17:O:141:ARG:NH2	2.32	0.62
1:2:71:G:O2'	1:2:79:A:N6	2.32	0.62
1:2:1567:G:H2'	22:T:37:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1277:C:H2'	1:2:1278:A:C8	2.35	0.62
1:2:1498:A:OP2	6:D:27:ARG:NH1	2.30	0.62
1:2:559:G:HO2'	1:2:560:A:H8	1.46	0.62
1:2:843:C:H2'	1:2:844:U:O4'	1.99	0.62
5:C:178:HIS:H	5:C:178:HIS:CD2	2.17	0.62
1:2:980:A:H2'	1:2:981:A:C8	2.34	0.62
1:2:1237:C:H2'	1:2:1238:U:O4'	1.99	0.62
1:2:1824:A:OP2	26:X:61:GLN:NE2	2.33	0.62
5:C:206:SER:HB3	5:C:224:THR:HB	1.81	0.62
1:2:919:A:OP2	16:N:64:ARG:NH1	2.32	0.62
1:2:943:U:OP2	4:B:216:LYS:NZ	2.28	0.62
1:2:1859:A:H5'	1:2:1860:A:OP2	1.99	0.62
1:2:1616:U:OP2	18:P:43:ARG:NH2	2.33	0.62
11:I:72:CYS:SG	11:I:73:THR:N	2.72	0.61
1:2:1190:A:H2'	1:2:1191:C:O4'	2.00	0.61
1:2:618:C:OP1	26:X:87:ASN:HA	2.01	0.61
1:2:870:A:H4'	1:2:871:U:H5'	1.81	0.61
1:2:816:A:OP2	12:J:10:ARG:NH2	2.33	0.61
1:2:1605:G:OP1	22:T:84:ARG:NH2	2.33	0.61
1:2:1589:A:OP1	22:T:80:GLY:HA3	2.00	0.61
1:2:1605:G:O2'	1:2:1634:A:N6	2.32	0.61
21:S:22:GLY:HA2	21:S:56:ALA:HB3	1.83	0.61
25:W:55:ASP:OD1	25:W:56:HIS:N	2.33	0.61
2:3:165:A:N6	2:3:237:C:O2'	2.33	0.61
1:2:1380:C:O2'	3:A:113:GLN:OE1	2.14	0.61
1:2:1395:C:H1'	1:2:1474:A:C4	2.35	0.61
1:2:1518:C:OP1	1:2:1520:G:H8	1.82	0.61
1:2:1565:C:OP2	22:T:101:ARG:NH1	2.33	0.61
3:A:41:ARG:HB2	3:A:47:TYR:CE1	2.35	0.61
1:2:1036:A:N3	1:2:1844:U:O2'	2.33	0.61
1:2:683:G:H4'	25:W:4:MET:HB3	1.83	0.61
21:S:68:ILE:HG23	21:S:72:GLN:HE21	1.66	0.61
17:O:98:ARG:HG3	17:O:98:ARG:HH11	1.65	0.61
8:F:35:LEU:HD12	8:F:117:ILE:HG12	1.83	0.61
1:2:1016:U:H5''	16:N:14:SER:HB3	1.83	0.60
1:2:634:A:H2'	1:2:635:G:C8	2.37	0.60
8:F:127:ARG:HH22	8:F:132:GLY:N	1.98	0.60
9:G:148:SER:OG	9:G:151:ASP:OD1	2.18	0.60
1:2:940:U:H2'	1:2:941:C:C6	2.36	0.60
1:2:76:U:OP1	9:G:159:ARG:NH1	2.27	0.60
1:2:792:C:H2'	1:2:793:G:C8	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:841:G:H2'	1:2:842:C:C6	2.37	0.60
1:2:963:A:H2'	1:2:964:A:C8	2.36	0.60
2:3:253:G:O2'	2:3:254:C:H5'	2.02	0.60
4:B:136:ARG:HG3	4:B:218:LEU:HD11	1.84	0.60
13:K:58:VAL:HG12	13:K:71:LEU:HD23	1.82	0.60
1:2:1231:C:H2'	1:2:1232:U:O4'	2.02	0.60
10:H:9:VAL:HG23	10:H:24:SER:HB3	1.83	0.60
22:T:42:HIS:CG	22:T:81:GLY:HA3	2.36	0.60
1:2:1207:G:N2	2:3:341:C:OP2	2.33	0.60
1:2:1224:G:H2'	1:2:1225:U:C6	2.37	0.60
1:2:163:U:O3'	9:G:83:CYS:HA	2.02	0.60
1:2:164:A:H3'	1:2:165:G:N2	2.17	0.60
5:C:59:GLU:OE2	5:C:71:LYS:NZ	2.30	0.60
6:D:115:VAL:HG21	6:D:142:LEU:HD22	1.83	0.60
1:2:1566:G:H1'	1:2:1570:G:N2	2.17	0.60
1:2:91:A:H5''	1:2:92:A:H5''	1.84	0.60
5:C:259:THR:HG21	24:V:15:ARG:HA	1.84	0.60
7:E:42:LEU:HD13	7:E:47:PHE:HB2	1.82	0.60
11:I:31:ARG:HB3	11:I:32:PRO:HD2	1.83	0.60
14:L:82:MET:HB3	14:L:85:THR:HG23	1.83	0.60
21:S:23:ARG:HB2	28:Z:48:VAL:HG21	1.82	0.60
6:D:212:GLU:HG2	20:R:19:LYS:HZ3	1.66	0.60
7:E:102:ILE:HD12	7:E:239:PRO:HD3	1.84	0.60
1:2:1857:G:H3'	17:O:146:ARG:NH2	2.17	0.60
1:2:128:U:O2'	1:2:130:G:O6	2.21	0.59
6:D:96:LEU:HD12	6:D:198:ILE:HD13	1.84	0.59
17:O:106:LYS:NZ	17:O:135:ILE:HG13	2.17	0.59
20:R:57:LEU:HD11	20:R:66:VAL:HG11	1.84	0.59
22:T:18:LEU:HD13	22:T:134:ILE:HD13	1.84	0.59
1:2:1001:A:H5''	1:2:1001:A:H8	1.66	0.59
1:2:1480:A:OP1	19:Q:131:LYS:NZ	2.35	0.59
4:B:146:ARG:HA	4:B:146:ARG:HH11	1.67	0.59
15:M:72:HIS:O	15:M:73:GLN:HG2	2.02	0.59
19:Q:44:PRO:HG2	19:Q:47:LEU:HB2	1.83	0.59
7:E:43:PRO:HG2	7:E:46:ILE:HD13	1.84	0.59
12:J:136:ARG:HD3	12:J:158:ASP:HB2	1.84	0.59
1:2:1240:A:C4	18:P:100:LYS:HB2	2.37	0.59
1:2:1629:C:H5'	21:S:39:ARG:HG2	1.83	0.59
23:U:20:ILE:HG23	23:U:116:ILE:HG12	1.84	0.59
7:E:181:CYS:SG	7:E:195:ILE:HG13	2.43	0.59
22:T:42:HIS:CD2	22:T:43:LYS:HG3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:294:U:C4	14:L:65:ASN:HB2	2.37	0.59
1:2:1623:A:C8	21:S:132:ARG:HD2	2.38	0.59
20:R:5:ARG:HG3	20:R:10:LYS:HE2	1.85	0.59
1:2:1470:C:OP2	8:F:59:LYS:NZ	2.35	0.59
26:X:71:ARG:HD2	26:X:82:THR:HG22	1.84	0.59
1:2:525:A:H2'	1:2:526:A:C8	2.37	0.58
2:3:163:G:O2'	2:3:164:U:H4'	2.02	0.58
8:F:59:LYS:HG3	8:F:62:ARG:HB2	1.84	0.58
12:J:169:ARG:HH21	12:J:175:ARG:NH2	2.01	0.58
5:C:131:GLY:HA3	5:C:216:MET:HB3	1.84	0.58
2:3:61:U:O2'	2:3:62:C:OP1	2.19	0.58
21:S:85:ASN:HD22	21:S:98:VAL:HB	1.68	0.58
7:E:179:ASN:HD22	7:E:231:GLY:H	1.51	0.58
12:J:77:LEU:HA	12:J:80:ARG:HH11	1.67	0.58
14:L:22:ARG:NH2	14:L:31:GLU:HG3	2.17	0.58
20:R:33:ARG:NH1	20:R:36:GLU:OE1	2.35	0.58
1:2:1746:U:H4'	9:G:65:GLN:NE2	2.19	0.58
7:E:127:ARG:NH2	7:E:142:HIS:HB2	2.19	0.58
14:L:60:CYS:HB2	14:L:114:SER:HB2	1.84	0.58
15:M:118:SER:O	15:M:122:ASP:HB2	2.04	0.58
9:G:44:GLU:HA	9:G:119:LYS:HD2	1.85	0.58
1:2:1608:U:H4'	21:S:130:ARG:NH1	2.18	0.58
1:2:172:U:OP1	1:2:314:U:O2'	2.22	0.58
1:2:926:A:H2'	1:2:927:C:O4'	2.04	0.58
10:H:76:GLN:HE22	10:H:94:PHE:HB2	1.68	0.58
17:O:95:ILE:HB	17:O:129:ILE:HD13	1.85	0.58
23:U:19:ARG:HG3	23:U:117:ALA:HA	1.86	0.58
4:B:62:LEU:HA	4:B:65:ARG:HE	1.69	0.57
1:2:979:C:H2'	1:2:980:A:C8	2.39	0.57
6:D:13:ALA:HA	6:D:16:ILE:HD12	1.86	0.57
20:R:57:LEU:O	20:R:61:ILE:HG13	2.04	0.57
21:S:80:PRO:HB2	21:S:83:PHE:HD2	1.69	0.57
1:2:525:A:H2'	1:2:526:A:H8	1.69	0.57
1:2:64:A:H2	1:2:83:A:N6	1.99	0.57
19:Q:25:CYS:SG	19:Q:91:ALA:HB1	2.44	0.57
1:2:407:G:N3	1:2:407:G:H2'	2.19	0.57
12:J:169:ARG:HE	12:J:175:ARG:NH2	2.03	0.57
20:R:25:GLY:O	20:R:31:ASN:ND2	2.33	0.57
1:2:1275:G:N2	1:2:1506:A:OP2	2.36	0.57
14:L:135:SER:OG	14:L:136:LYS:N	2.38	0.57
1:2:1392:U:OP1	23:U:83:ARG:NH1	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1217:A:H2'	1:2:1218:C:C6	2.39	0.57
1:2:1537:A:O2'	1:2:1604:G:OP1	2.22	0.57
1:2:1612:G:H1'	21:S:87:GLN:HG3	1.86	0.57
8:F:125:SER:HB3	8:F:136:ARG:HB3	1.86	0.57
17:O:54:CYS:HB3	17:O:81:VAL:HG23	1.86	0.57
25:W:18:GLU:OE1	25:W:65:LEU:HD13	2.04	0.57
1:2:1241:A:H2'	1:2:1242:U:H4'	1.85	0.57
11:I:11:ARG:HB3	11:I:15:GLY:HA2	1.87	0.57
21:S:68:ILE:O	21:S:72:GLN:HG2	2.05	0.57
1:2:1137:U:O2'	1:2:1138:C:OP1	2.21	0.57
2:3:150:G:H1	2:3:242:C:N4	2.01	0.57
12:J:89:GLU:OE1	12:J:89:GLU:N	2.37	0.57
1:2:146:G:OP1	9:G:143:LYS:NZ	2.38	0.57
1:2:376:A:H2'	1:2:377:G:O4'	2.05	0.57
1:2:1374:C:H2'	1:2:1375:G:O4'	2.05	0.56
11:I:13:LYS:HG3	14:L:137:THR:HG21	1.85	0.56
1:2:1785:C:O2'	1:2:1786:U:O5'	2.20	0.56
27:Y:55:ILE:HG22	27:Y:75:ILE:HG23	1.87	0.56
1:2:589:G:N2	41:2:2015:HOH:O	2.37	0.56
1:2:798:G:H3'	1:2:799:U:C5'	2.35	0.56
2:3:256:G:H5'	2:3:257:A:H5''	1.86	0.56
7:E:11:ARG:NH1	7:E:20:LEU:HD22	2.21	0.56
17:O:36:SER:OG	17:O:37:PHE:N	2.35	0.56
26:X:100:VAL:HG13	26:X:122:VAL:HG13	1.86	0.56
7:E:136:ILE:HG12	7:E:149:TYR:HE1	1.70	0.56
11:I:80:ASP:OD1	11:I:81:VAL:N	2.39	0.56
1:2:165:G:H2'	1:2:166:A:H8	1.69	0.56
2:3:144:U:H2'	2:3:145:G:C8	2.39	0.56
1:2:1334:G:O2'	6:D:174:HIS:HD2	1.88	0.56
7:E:97:GLU:OE2	7:E:113:ARG:NH1	2.37	0.56
23:U:40:ILE:O	23:U:44:LYS:HB2	2.05	0.56
26:X:19:ASP:N	26:X:19:ASP:OD1	2.39	0.56
11:I:141:ARG:HD3	11:I:146:GLN:CA	2.34	0.56
15:M:24:THR:HB	15:M:115:GLY:HA3	1.86	0.56
20:R:111:PHE:O	20:R:114:LEU:HG	2.06	0.56
1:2:1001:A:H5''	1:2:1001:A:C8	2.41	0.56
2:3:81:A:N6	2:3:84:C:O2'	2.39	0.56
5:C:187:ARG:HD3	5:C:192:LEU:HD23	1.88	0.56
1:2:1428:G:H4'	1:2:1429:G:C5'	2.36	0.56
1:2:1498:A:P	6:D:27:ARG:HH12	2.29	0.56
4:B:28:LYS:HB3	4:B:48:LEU:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:85:GLY:O	7:E:88:ASP:HB2	2.05	0.56
12:J:132:GLN:HB3	12:J:134:HIS:CD2	2.40	0.56
1:2:958:G:O2'	1:2:959:G:O5'	2.24	0.56
2:3:294:U:H2'	2:3:295:G:H2'	1.87	0.56
3:A:198:MET:HG3	3:A:199:PRO:HD2	1.88	0.56
1:2:122:G:H21	7:E:146:THR:HG21	1.70	0.56
7:E:179:ASN:HD21	7:E:230:LYS:HD2	1.71	0.56
8:F:166:ILE:N	8:F:166:ILE:HD13	2.21	0.56
11:I:9:HIS:O	11:I:9:HIS:CG	2.59	0.56
16:N:87:ASP:N	16:N:87:ASP:OD1	2.37	0.56
7:E:122:LYS:NZ	7:E:143:ASP:OD2	2.29	0.55
15:M:93:LYS:HB2	15:M:102:LYS:HB3	1.88	0.55
17:O:72:TYR:O	17:O:75:MET:HB2	2.05	0.55
1:2:1446:A:HO2'	1:2:1447:G:H8	1.50	0.55
4:B:52:THR:HG22	4:B:54:GLY:H	1.71	0.55
7:E:138:HIS:CD2	7:E:148:ARG:HB3	2.42	0.55
1:2:585:C:OP1	12:J:179:LYS:NZ	2.39	0.55
24:V:21:ASN:ND2	24:V:21:ASN:O	2.37	0.55
12:J:136:ARG:HB3	12:J:160:SER:HB3	1.88	0.55
1:2:1578:U:O2'	6:D:6:SER:HA	2.05	0.55
12:J:77:LEU:HA	12:J:80:ARG:NH1	2.21	0.55
1:2:1284:A:H5''	1:2:1286:G:O4'	2.07	0.55
1:2:84:A:H4'	27:Y:119:GLY:O	2.07	0.55
1:2:1475:G:H5'	19:Q:124:PRO:HG3	1.89	0.55
1:2:1225:U:H1'	19:Q:142:GLN:HE22	1.71	0.55
21:S:74:PRO:HA	21:S:79:ILE:HD12	1.88	0.55
21:S:6:PRO:HG2	28:Z:49:LEU:HD13	1.89	0.55
1:2:85:A:H2'	1:2:86:C:H6	1.71	0.55
4:B:104:ASP:N	4:B:104:ASP:OD1	2.40	0.55
1:2:1546:G:H5'	19:Q:18:THR:HG21	1.89	0.55
1:2:1392:U:H3	1:2:1478:U:H3	1.55	0.55
1:2:639:C:O2'	1:2:640:A:H8	1.90	0.55
14:L:133:PRO:HB3	14:L:139:ARG:NH1	2.20	0.55
20:R:20:TYR:HD2	20:R:23:ARG:HD2	1.72	0.55
22:T:22:LEU:HD22	22:T:28:LEU:HD12	1.89	0.55
22:T:75:MET:HG3	22:T:104:LEU:HD11	1.89	0.55
1:2:1511:U:H2'	1:2:1512:C:C6	2.42	0.55
1:2:533:A:H2'	1:2:534:G:O4'	2.06	0.55
1:2:634:A:H2'	1:2:635:G:H8	1.72	0.55
1:2:917:U:O2'	1:2:918:U:O5'	2.25	0.55
16:N:62:GLN:HB2	16:N:65:PHE:CD2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:15:ASN:HB3	27:Y:17:LEU:HD12	1.89	0.55
1:2:1736:G:H2'	1:2:1737:G:C8	2.41	0.54
1:2:217:A:H5'	1:2:218:U:OP2	2.08	0.54
1:2:551:U:H2'	1:2:552:G:C8	2.42	0.54
9:G:159:ARG:HB3	9:G:171:THR:HG23	1.89	0.54
14:L:104:LYS:HZ1	26:X:8:ARG:HD3	1.70	0.54
1:2:1428:G:H4'	1:2:1429:G:H5'	1.87	0.54
1:2:145:G:H2'	1:2:146:G:H8	1.71	0.54
1:2:1590:C:H41	19:Q:77:HIS:HE1	1.55	0.54
21:S:98:VAL:HG11	21:S:106:LYS:HD2	1.89	0.54
27:Y:103:SER:HB3	27:Y:106:GLN:HG2	1.90	0.54
1:2:1546:G:H1	1:2:1655:C:HO2'	1.55	0.54
1:2:73:C:O2'	1:2:74:G:O4'	2.19	0.54
1:2:92:A:H4'	1:2:93:U:OP2	2.06	0.54
27:Y:78:SER:HB3	27:Y:81:TYR:CD2	2.42	0.54
1:2:1719:A:N6	1:2:1814:G:O2'	2.41	0.54
1:2:797:C:O2'	1:2:798:G:OP1	2.21	0.54
1:2:1272:C:H42	1:2:1510:G:H1	1.55	0.54
1:2:1731:A:H2'	1:2:1732:G:C8	2.43	0.54
1:2:65:C:O2'	1:2:67:C:OP2	2.25	0.54
6:D:74:GLN:HE21	6:D:84:VAL:HG12	1.72	0.54
7:E:124:CYS:HB3	7:E:141:THR:HB	1.89	0.54
10:H:184:ASP:N	10:H:184:ASP:OD1	2.40	0.54
12:J:119:LEU:HB3	12:J:159:PHE:CE1	2.42	0.54
19:Q:112:LEU:HD22	19:Q:119:LEU:HD13	1.89	0.54
3:A:143:PRO:HG3	24:V:32:ILE:HG23	1.87	0.54
1:2:1415:C:H5''	22:T:129:ARG:HG3	1.90	0.54
1:2:1493:C:OP1	1:2:1494:U:O2'	2.22	0.54
1:2:1259:A:H61	1:2:1519:U:C5'	2.20	0.54
1:2:1565:C:H3'	1:2:1566:G:H5''	1.89	0.54
1:2:1615:U:O4	18:P:40:ARG:NH1	2.41	0.54
1:2:591:U:O2'	1:2:592:C:H3'	2.08	0.54
3:A:155:ARG:HD2	24:V:61:ARG:O	2.08	0.54
1:2:1613:G:H5''	18:P:39:ALA:HB2	1.88	0.54
1:2:1384:C:H4'	6:D:157:MET:O	2.08	0.54
1:2:1597:C:H3'	1:2:1598:G:C8	2.43	0.54
2:3:150:G:N2	2:3:242:C:N3	2.53	0.54
7:E:151:ASP:OD2	9:G:216:ARG:NH2	2.40	0.54
21:S:84:LEU:HD12	21:S:95:TYR:HB3	1.88	0.54
1:2:830:A:C2	1:2:831:G:C8	2.96	0.54
8:F:87:LEU:HA	8:F:90:VAL:HG22	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:78:LEU:HD13	12:J:92:MET:O	2.07	0.54
16:N:63:VAL:HG21	16:N:71:ILE:HD11	1.90	0.54
25:W:3:ARG:HD3	25:W:6:VAL:HG22	1.89	0.54
23:U:31:SER:O	23:U:35:VAL:HG23	2.08	0.54
1:2:1271:C:H5'	1:2:1301:A:H2	1.72	0.54
1:2:1528:G:O2'	1:2:1666:C:OP1	2.25	0.54
1:2:51:U:H2'	1:2:52:G:C8	2.42	0.54
1:2:70:G:N2	1:2:80:G:N3	2.55	0.54
3:A:134:LEU:HD21	3:A:144:THR:HG21	1.89	0.54
11:I:66:SER:O	11:I:189:VAL:HG23	2.08	0.54
12:J:21:GLU:CD	12:J:24:ARG:HB2	2.29	0.54
1:2:1041:G:H5'	1:2:1042:A:OP2	2.08	0.53
1:2:589:G:O2'	1:2:590:A:OP2	2.19	0.53
4:B:209:ASP:HB3	4:B:211:PHE:HE1	1.73	0.53
3:A:141:ASN:ND2	24:V:29:HIS:O	2.41	0.53
1:2:388:U:H2'	1:2:389:A:H8	1.73	0.53
1:2:554:A:H4'	1:2:555:A:OP1	2.07	0.53
5:C:204:ILE:HG23	5:C:222:CYS:HB3	1.91	0.53
1:2:1217:A:H2'	1:2:1218:C:H6	1.74	0.53
1:2:1643:U:H2'	1:2:1644:C:C6	2.43	0.53
1:2:559:G:H3'	12:J:177:ASN:ND2	2.23	0.53
14:L:99:TYR:O	14:L:101:ARG:HG2	2.09	0.53
1:2:944:A:H5''	17:O:134:PRO:HB3	1.90	0.53
17:O:98:ARG:HH11	17:O:98:ARG:CG	2.21	0.53
26:X:119:ARG:HB2	26:X:120:PHE:CE1	2.44	0.53
26:X:82:THR:O	26:X:118:VAL:HG13	2.08	0.53
1:2:1455:A:OP2	20:R:56:HIS:ND1	2.41	0.53
1:2:1223:A:H4'	1:2:1651:A:H4'	1.91	0.53
1:2:594:A:H61	1:2:643:A:H5''	1.73	0.53
5:C:221:ASP:N	5:C:221:ASP:OD1	2.42	0.53
9:G:55:GLY:HA3	9:G:63:MET:SD	2.48	0.53
10:H:101:LEU:O	10:H:116:ARG:NH1	2.41	0.53
1:2:520:A:H5''	12:J:12:THR:OG1	2.09	0.53
1:2:941:C:H5''	4:B:136:ARG:NH2	2.24	0.53
4:B:87:ILE:HG22	4:B:88:THR:O	2.08	0.53
6:D:79:PHE:CE1	6:D:84:VAL:HB	2.44	0.53
13:K:32:HIS:NE2	13:K:45:VAL:HG11	2.23	0.53
1:2:77:A:H8	1:2:77:A:H5''	1.73	0.53
10:H:80:VAL:O	10:H:84:GLU:HB2	2.08	0.53
1:2:1858:G:OP2	17:O:146:ARG:NH2	2.41	0.53
1:2:1239:U:H4'	18:P:124:LYS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:73:GLN:HG3	26:X:80:LYS:HG3	1.91	0.53
1:2:70:G:C2	1:2:80:G:C2	2.96	0.53
2:3:260:A:C2	2:3:261:G:H1'	2.44	0.53
12:J:95:ASP:OD1	12:J:95:ASP:N	2.41	0.53
2:3:254:C:H4'	2:3:255:C:OP1	2.08	0.53
2:3:86:U:H5''	17:O:72:TYR:CZ	2.44	0.53
6:D:31:GLU:HG2	6:D:107:TYR:HE2	1.74	0.53
14:L:37:TYR:CG	14:L:51:ILE:HG22	2.44	0.53
14:L:7:GLU:HB2	14:L:11:GLN:HE21	1.74	0.53
1:2:1651:A:H2'	1:2:1652:G:H8	1.74	0.53
7:E:87:MET:HE2	7:E:123:LEU:H	1.73	0.53
13:K:62:PHE:CZ	13:K:65:ARG:HA	2.44	0.53
23:U:78:ASP:HB3	23:U:80:PHE:HE1	1.74	0.53
1:2:1259:A:H61	1:2:1519:U:H5'	1.73	0.52
1:2:82:G:HO2'	1:2:83:A:H8	1.57	0.52
1:2:1224:G:H2'	1:2:1225:U:H6	1.73	0.52
1:2:1584:G:C4	1:2:1586:U:H1'	2.44	0.52
1:2:75:G:N2	9:G:155:GLN:HG3	2.24	0.52
1:2:1830:U:OP2	2:3:342:A:O2'	2.27	0.52
8:F:112:LEU:HD13	8:F:177:LEU:HD21	1.91	0.52
8:F:56:TYR:HB3	8:F:63:LYS:HA	1.91	0.52
9:G:110:ASN:N	9:G:110:ASN:OD1	2.42	0.52
9:G:7:PHE:HE1	9:G:9:ALA:HB3	1.74	0.52
18:P:44:ARG:HH21	18:P:53:GLN:HE22	1.58	0.52
21:S:83:PHE:HE2	22:T:36:THR:HG23	1.74	0.52
1:2:1596:U:OP2	28:Z:85:ARG:NH2	2.42	0.52
1:2:601:G:O2'	1:2:602:G:O4'	2.26	0.52
8:F:28:VAL:HG12	8:F:29:GLN:H	1.75	0.52
1:2:317:C:OP2	9:G:183:ARG:NH2	2.42	0.52
11:I:132:GLU:CD	11:I:132:GLU:H	2.13	0.52
24:V:64:GLU:O	24:V:68:SER:OG	2.27	0.52
1:2:1229:G:H21	22:T:87:VAL:HG12	1.74	0.52
3:A:207:PRO:HA	3:A:210:ILE:HD12	1.91	0.52
5:C:200:ARG:O	12:J:54:ARG:NH2	2.40	0.52
16:N:83:ASP:N	16:N:83:ASP:OD1	2.41	0.52
1:2:1643:U:O2'	19:Q:142:GLN:HG2	2.10	0.52
1:2:205:G:H2'	1:2:206:G:O4'	2.08	0.52
4:B:128:LYS:HG3	4:B:134:LEU:HD13	1.92	0.52
6:D:23:GLU:O	6:D:27:ARG:HG2	2.10	0.52
22:T:28:LEU:HD21	22:T:53:PHE:CE1	2.45	0.52
1:2:60:A:H2	1:2:61:A:C2	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:621:C:OP1	26:X:107:ARG:HD2	2.08	0.52
1:2:808:A:H5''	7:E:219:ALA:O	2.09	0.52
1:2:969:U:P	1:2:970:G:H5'	2.49	0.52
10:H:163:GLN:O	10:H:167:GLU:HB2	2.10	0.52
1:2:112:U:H5''	1:2:113:G:H2'	1.92	0.52
1:2:1293:A:H2'	1:2:1294:G:C8	2.44	0.52
1:2:380:G:C6	1:2:382:C:H5''	2.45	0.52
1:2:69:C:N4	1:2:70:G:O6	2.42	0.52
23:U:50:VAL:HG12	23:U:91:LEU:HD22	1.91	0.52
28:Z:91:LEU:HD22	28:Z:96:LEU:HD12	1.91	0.52
1:2:912:C:C2	1:2:914:U:H1'	2.44	0.52
17:O:106:LYS:HZ3	17:O:135:ILE:HA	1.74	0.52
1:2:579:C:O2	27:Y:61:ARG:NH2	2.42	0.52
3:A:29:ASN:OD1	3:A:29:ASN:N	2.42	0.52
9:G:98:ARG:NH2	9:G:101:ILE:O	2.41	0.52
26:X:77:ASN:OD1	26:X:77:ASN:N	2.29	0.52
1:2:1101:U:H2'	1:2:1102:G:C8	2.45	0.52
27:Y:37:LYS:HA	27:Y:40:ILE:HG22	1.90	0.52
1:2:1269:G:H1	1:2:1513:C:N4	2.07	0.51
1:2:1284:A:O2'	15:M:106:CYS:SG	2.65	0.51
1:2:89:C:N4	41:2:2019:HOH:O	2.42	0.51
9:G:151:ASP:OD1	9:G:151:ASP:N	2.43	0.51
24:V:55:ILE:HD11	24:V:69:ILE:HG12	1.92	0.51
1:2:1429:G:HO2'	1:2:1430:C:H6	1.57	0.51
1:2:319:C:O2'	1:2:320:G:OP1	2.25	0.51
2:3:305:U:O2'	2:3:325:C:N4	2.41	0.51
3:A:26:GLY:HA3	3:A:150:THR:HG23	1.93	0.51
7:E:106:LYS:HD2	7:E:108:ARG:NH2	2.25	0.51
15:M:52:LEU:O	15:M:78:LYS:HA	2.10	0.51
22:T:37:VAL:HG22	22:T:38:LYS:N	2.25	0.51
28:Z:58:LEU:HD12	28:Z:62:VAL:HG21	1.92	0.51
1:2:1414:A:N6	1:2:1425:G:O6	2.42	0.51
1:2:957:A:H2'	1:2:958:G:H5'	1.93	0.51
4:B:68:GLU:HG3	4:B:83:LYS:HE2	1.93	0.51
5:C:236:PHE:O	5:C:240:THR:HG22	2.10	0.51
1:2:1298:G:H4'	18:P:77:LYS:O	2.11	0.51
1:2:625:G:O6	26:X:63:ASN:HB2	2.10	0.51
1:2:1542:C:OP1	22:T:62:ARG:NH1	2.41	0.51
2:3:172:A:H2'	2:3:173:A:C8	2.44	0.51
3:A:108:PHE:HB3	3:A:140:VAL:HG21	1.93	0.51
21:S:50:ILE:HD12	21:S:67:VAL:HG21	1.87	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1217:A:C2	1:2:1218:C:C2	2.99	0.51
1:2:1800:A:H5''	1:2:1801:A:OP2	2.11	0.51
1:2:4:C:H5'	5:C:230:THR:HG21	1.91	0.51
1:2:684:G:H1'	1:2:920:A:C2	2.44	0.51
6:D:195:THR:H	6:D:201:LYS:HE2	1.75	0.51
14:L:35:ARG:NH1	14:L:53:GLY:O	2.44	0.51
17:O:37:PHE:HE2	17:O:105:THR:HG21	1.75	0.51
25:W:44:HIS:NE2	25:W:112:ASP:OD2	2.40	0.51
1:2:434:G:H2'	1:2:435:A:C8	2.45	0.51
1:2:559:G:O2'	1:2:560:A:H8	1.94	0.51
3:A:134:LEU:CD2	3:A:144:THR:HG21	2.41	0.51
1:2:345:U:H5''	7:E:37:LYS:HG2	1.92	0.51
9:G:44:GLU:CD	9:G:44:GLU:H	2.14	0.51
1:2:1528:G:H2'	1:2:1529:C:H6	1.75	0.51
12:J:15:THR:HG22	12:J:44:TRP:CZ3	2.46	0.51
12:J:160:SER:O	12:J:162:ARG:N	2.44	0.51
15:M:79:VAL:HG12	15:M:80:ASP:H	1.75	0.51
27:Y:104:ARG:O	27:Y:108:LYS:HB2	2.10	0.51
1:2:70:G:C6	1:2:71:G:C4	2.99	0.51
3:A:189:ILE:HG22	3:A:190:SER:H	1.76	0.51
10:H:100:ILE:HD11	10:H:125:VAL:HG11	1.93	0.51
10:H:138:GLU:OE1	16:N:19:ARG:NH1	2.44	0.51
23:U:32:LEU:HD21	23:U:87:ARG:HE	1.75	0.51
1:2:1037:G:H4'	1:2:1845:A:H4'	1.91	0.51
1:2:1228:A:H2'	1:2:1229:G:C8	2.46	0.51
1:2:180:G:O2'	1:2:181:A:H5'	2.10	0.51
10:H:158:LEU:HD11	10:H:187:PHE:HD2	1.75	0.51
1:2:1650:A:H5'	19:Q:139:ALA:HB2	1.93	0.51
1:2:1692:U:H2'	1:2:1693:G:C8	2.46	0.51
1:2:806:U:C2	1:2:858:A:C2	2.99	0.51
14:L:120:VAL:HG22	14:L:145:VAL:HG11	1.91	0.51
25:W:78:ARG:HH11	25:W:78:ARG:HG2	1.76	0.51
1:2:1391:C:O3'	23:U:83:ARG:NH2	2.43	0.50
1:2:167:G:N7	41:2:2014:HOH:O	2.35	0.50
1:2:29:G:H4'	26:X:129:SER:HB3	1.93	0.50
1:2:478:G:H2'	1:2:479:C:H6	1.77	0.50
1:2:511:U:H2'	1:2:512:A:H8	1.76	0.50
9:G:57:ASP:HA	9:G:107:SER:H	1.75	0.50
1:2:869:A:N1	10:H:114:GLN:NE2	2.59	0.50
10:H:39:GLN:O	10:H:43:LEU:HG	2.11	0.50
20:R:13:ALA:HB3	20:R:53:TYR:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:17:ILE:HG12	20:R:54:VAL:HG13	1.93	0.50
21:S:26:ILE:O	21:S:30:ILE:HG12	2.11	0.50
27:Y:79:LEU:HD21	27:Y:83:LYS:HE3	1.93	0.50
1:2:1550:G:H21	1:2:1577:G:H21	1.59	0.50
1:2:1741:U:H2'	1:2:1742:C:O4'	2.11	0.50
6:D:194:PRO:HA	6:D:201:LYS:HD3	1.91	0.50
7:E:73:ASP:HB3	7:E:164:LEU:HD22	1.93	0.50
1:2:1599:U:C5	8:F:166:ILE:HD12	2.46	0.50
15:M:36:ARG:HE	15:M:40:LYS:NZ	2.08	0.50
1:2:638:C:O2'	1:2:639:C:O5'	2.28	0.50
2:3:153:G:H3'	2:3:154:A:H5'	1.92	0.50
6:D:62:LYS:O	6:D:67:ARG:NH2	2.44	0.50
9:G:126:ASP:N	9:G:126:ASP:OD1	2.45	0.50
15:M:77:ILE:HG12	15:M:128:PHE:HZ	1.76	0.50
19:Q:39:LEU:HD13	19:Q:52:LEU:HD23	1.92	0.50
1:2:1234:C:H5'	1:2:1246:A:H61	1.76	0.50
1:2:189:U:H5'	1:2:190:G:OP2	2.12	0.50
1:2:520:A:H2'	1:2:521:A:H8	1.76	0.50
9:G:216:ARG:O	9:G:219:GLU:HG2	2.11	0.50
1:2:334:C:H5'	1:2:335:G:OP2	2.12	0.50
1:2:85:A:H2'	1:2:86:C:C6	2.46	0.50
2:3:263:G:C2	2:3:264:U:H5	2.29	0.50
2:3:64:U:H3	2:3:103:U:H3	1.59	0.50
5:C:272:HIS:HA	5:C:275:LYS:HD2	1.93	0.50
7:E:103:TYR:CG	7:E:189:LEU:HD11	2.46	0.50
21:S:46:ARG:NE	22:T:50:GLU:OE1	2.45	0.50
21:S:50:ILE:HD11	21:S:67:VAL:HG23	1.91	0.50
1:2:1033:G:H5''	1:2:1034:A:OP1	2.11	0.50
1:2:1136:U:H2'	1:2:1137:U:C6	2.46	0.50
1:2:1597:C:H4'	1:2:1603:G:O6	2.12	0.50
1:2:164:A:H3'	1:2:165:G:H21	1.75	0.50
1:2:871:U:OP2	1:2:871:U:H4'	2.12	0.50
1:2:979:C:H2'	1:2:980:A:H8	1.77	0.50
4:B:144:LYS:HB2	4:B:208:HIS:CB	2.38	0.50
6:D:75:LYS:HB3	13:K:22:VAL:HG21	1.93	0.50
15:M:49:LEU:HD22	15:M:75:ASN:HB2	1.92	0.50
21:S:55:ARG:NH2	28:Z:82:SER:OG	2.45	0.50
1:2:1719:A:H2'	1:2:1720:U:O4'	2.12	0.50
3:A:144:THR:H	3:A:158:ASP:HB2	1.76	0.50
4:B:35:ALA:HB1	4:B:36:PRO:HD2	1.93	0.50
10:H:191:GLU:O	10:H:192:PHE:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:581:U:OP1	12:J:133:ARG:NH2	2.43	0.50
14:L:77:VAL:HA	14:L:88:ILE:HG22	1.94	0.50
15:M:92:CYS:SG	15:M:103:VAL:HG22	2.51	0.50
1:2:389:A:H2'	1:2:390:C:H6	1.77	0.50
1:2:435:A:OP2	1:2:435:A:H8	1.94	0.50
2:3:146:G:H1	2:3:247:C:N4	2.08	0.50
1:2:1578:U:O2	6:D:6:SER:HB2	2.11	0.50
23:U:78:ASP:HB3	23:U:80:PHE:CE1	2.47	0.50
1:2:44:U:O2'	1:2:45:A:H2'	2.12	0.50
4:B:125:VAL:HG22	4:B:169:MET:HG3	1.94	0.50
21:S:86:ARG:NH2	21:S:110:ASP:OD2	2.44	0.50
2:3:98:G:O2'	2:3:99:A:C8	2.62	0.49
4:B:86:LEU:HB3	4:B:98:THR:CG2	2.42	0.49
1:2:296:U:O2'	7:E:131:VAL:O	2.23	0.49
18:P:18:ARG:HA	21:S:93:GLY:HA3	1.94	0.49
1:2:1643:U:H2'	1:2:1644:C:H6	1.77	0.49
1:2:795:A:C2	1:2:796:G:H1'	2.46	0.49
1:2:828:G:H4'	7:E:23:LEU:HD22	1.94	0.49
3:A:122:LEU:HD22	3:A:142:LEU:HD12	1.94	0.49
4:B:146:ARG:N	4:B:149:GLN:OE1	2.44	0.49
7:E:44:LEU:HB3	7:E:80:ILE:O	2.13	0.49
7:E:86:PHE:CE2	7:E:87:MET:HG2	2.47	0.49
9:G:49:VAL:HB	9:G:115:LYS:HB2	1.94	0.49
21:S:128:GLY:O	21:S:144:ARG:NH2	2.45	0.49
5:C:254:ASP:HB3	24:V:1:MET:HG3	1.94	0.49
28:Z:92:LEU:HD21	28:Z:109:TYR:HE1	1.76	0.49
1:2:70:G:N2	1:2:80:G:C2	2.80	0.49
1:2:870:A:H4'	1:2:871:U:C5'	2.42	0.49
5:C:130:ILE:HG22	5:C:158:ALA:HB1	1.94	0.49
7:E:127:ARG:HH21	7:E:142:HIS:HB2	1.78	0.49
11:I:142:SER:H	11:I:145:ILE:HD12	1.77	0.49
14:L:77:VAL:O	14:L:123:GLY:N	2.38	0.49
17:O:39:ASP:HA	17:O:69:SER:HA	1.95	0.49
21:S:86:ARG:HB3	21:S:89:ASP:OD1	2.12	0.49
26:X:59:ALA:HB1	26:X:114:ASP:OD1	2.12	0.49
1:2:1161:U:H2'	1:2:1162:C:C6	2.48	0.49
1:2:1284:A:H61	1:2:1313:A:H2'	1.77	0.49
1:2:1284:A:N6	1:2:1313:A:H2'	2.27	0.49
1:2:1515:G:N2	18:P:99:GLY:O	2.44	0.49
5:C:77:SER:O	5:C:80:GLU:HG2	2.12	0.49
6:D:137:VAL:HG22	6:D:151:LYS:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:137:VAL:HG12	12:J:138:ARG:HG3	1.94	0.49
15:M:42:LEU:HG	15:M:74:ILE:HD13	1.95	0.49
18:P:22:LEU:HD11	18:P:109:PRO:HB3	1.94	0.49
20:R:16:ILE:HD11	20:R:39:ALA:HB2	1.95	0.49
28:Z:50:PHE:CZ	28:Z:58:LEU:HD22	2.46	0.49
1:2:107:A:C2	1:2:355:G:C2	2.99	0.49
9:G:22:ARG:HA	9:G:25:ARG:HG2	1.94	0.49
1:2:433:A:H5''	11:I:25:ARG:HH22	1.77	0.49
16:N:37:ILE:HD11	16:N:63:VAL:HG11	1.95	0.49
16:N:47:PRO:HG2	16:N:86:GLU:HG2	1.94	0.49
19:Q:51:LEU:HD13	19:Q:81:ILE:HG23	1.94	0.49
20:R:20:TYR:CE2	20:R:38:ILE:HG12	2.47	0.49
22:T:17:ALA:CB	22:T:138:VAL:HG21	2.42	0.49
28:Z:57:LYS:O	28:Z:61:GLU:HB3	2.13	0.49
1:2:1232:U:C5	21:S:138:THR:HG21	2.48	0.49
1:2:1354:G:N7	41:2:2013:HOH:O	2.34	0.49
1:2:1733:U:H2'	1:2:1734:G:H5'	1.95	0.49
3:A:18:PHE:O	3:A:22:GLY:N	2.42	0.49
6:D:142:LEU:HB2	6:D:148:LYS:HD2	1.95	0.49
1:2:168:C:O2'	9:G:132:ARG:O	2.31	0.49
20:R:33:ARG:O	20:R:36:GLU:HG2	2.13	0.49
1:2:587:A:H5'	1:2:592:C:N4	2.27	0.49
1:2:857:U:H5''	7:E:201:HIS:CD2	2.48	0.49
2:3:255:C:H3'	2:3:256:G:H5''	1.94	0.49
2:3:332:A:H3'	2:3:333:C:H5'	1.93	0.49
3:A:42:LYS:HD3	3:A:48:ILE:HD11	1.95	0.49
8:F:60:ARG:HG2	8:F:61:PHE:CD2	2.47	0.49
17:O:65:ASP:O	17:O:68:GLU:HB2	2.13	0.49
1:2:1392:U:P	23:U:83:ARG:HH12	2.34	0.49
1:2:1149:A:O2'	1:2:1150:A:H5''	2.12	0.49
1:2:1510:G:H2'	1:2:1511:U:C6	2.48	0.49
1:2:63:U:H5''	1:2:64:A:OP2	2.13	0.49
5:C:168:GLY:HA3	5:C:181:PRO:HA	1.93	0.49
9:G:145:PHE:HD2	9:G:156:TYR:HB3	1.78	0.49
1:2:1293:A:H2'	1:2:1294:G:H8	1.77	0.49
1:2:1592:C:O2'	19:Q:43:GLU:O	2.31	0.49
1:2:1597:C:H4'	1:2:1603:G:C6	2.47	0.49
1:2:309:G:O2'	1:2:310:C:OP2	2.28	0.49
1:2:792:C:H2'	1:2:793:G:H8	1.76	0.49
5:C:77:SER:HA	5:C:97:PHE:HE1	1.78	0.49
6:D:134:CYS:HB2	6:D:188:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:138:VAL:HG12	6:D:182:LEU:HD22	1.95	0.49
10:H:60:ILE:HB	10:H:92:VAL:HG22	1.94	0.49
1:2:1003:U:H2'	1:2:1004:U:H6	1.78	0.49
1:2:1143:A:H5''	1:2:1144:A:OP2	2.13	0.49
1:2:1547:C:H2'	1:2:1548:G:O4'	2.12	0.49
1:2:1816:G:H2'	1:2:1817:G:H8	1.78	0.49
2:3:328:G:C6	2:3:329:U:C4	3.00	0.49
4:B:30:TRP:CE2	4:B:48:LEU:HD13	2.46	0.49
10:H:134:VAL:HG11	10:H:158:LEU:HD22	1.94	0.49
11:I:22:HIS:HB2	11:I:25:ARG:NH2	2.27	0.49
1:2:1063:C:OP1	41:2:2007:HOH:O	2.20	0.48
1:2:60:A:O2'	1:2:61:A:O5'	2.26	0.48
5:C:188:CYS:HB3	5:C:239:ALA:HB2	1.94	0.48
6:D:34:TYR:OH	6:D:37:VAL:HG23	2.13	0.48
1:2:586:G:N7	12:J:172:ARG:HD3	2.28	0.48
12:J:81:LEU:HD23	12:J:84:ILE:HD11	1.93	0.48
14:L:15:THR:O	14:L:16:ILE:HD13	2.12	0.48
18:P:44:ARG:HH21	18:P:53:GLN:NE2	2.11	0.48
22:T:67:ARG:HG3	22:T:68:GLY:O	2.13	0.48
1:2:1045:U:H2'	1:2:1046:U:O4'	2.12	0.48
1:2:1204:A:OP1	5:C:117:ARG:HB3	2.13	0.48
1:2:1244:U:H3	1:2:1257:G:H22	1.59	0.48
1:2:190:G:C6	1:2:208:G:C6	3.01	0.48
1:2:220:U:H2'	1:2:221:A:C8	2.48	0.48
1:2:596:U:H2'	1:2:597:G:O4'	2.13	0.48
1:2:818:A:H5''	1:2:819:G:OP2	2.13	0.48
2:3:164:U:H2'	2:3:165:A:H1'	1.95	0.48
2:3:263:G:N3	2:3:264:U:H5	2.11	0.48
5:C:78:LEU:HD12	5:C:81:ILE:HD12	1.95	0.48
7:E:100:ARG:HB2	7:E:114:ILE:HD12	1.95	0.48
1:2:1267:C:H2'	1:2:1268:C:C6	2.48	0.48
1:2:1735:A:C4	1:2:1800:A:C2	3.00	0.48
1:2:209:A:H2'	1:2:210:U:H5'	1.94	0.48
1:2:553:U:C4	1:2:554:A:N7	2.82	0.48
2:3:134:A:H61	2:3:290:U:H3	1.61	0.48
18:P:45:LEU:HD23	18:P:49:LEU:HD21	1.95	0.48
22:T:42:HIS:HD2	22:T:43:LYS:HG3	1.78	0.48
24:V:76:ASP:HB3	24:V:78:ILE:HG13	1.94	0.48
1:2:1210:G:N2	1:2:1690:U:C2	2.82	0.48
1:2:1440:C:O2'	1:2:1441:U:O5'	2.27	0.48
5:C:196:ILE:HG13	5:C:223:TYR:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:72:C:H5	9:G:170:ARG:HH22	1.60	0.48
11:I:48:VAL:HG22	11:I:52:ASN:O	2.13	0.48
11:I:79:ILE:HG22	11:I:80:ASP:HB2	1.96	0.48
20:R:28:PHE:HD2	20:R:29:HIS:CE1	2.30	0.48
22:T:42:HIS:ND1	22:T:81:GLY:HA3	2.29	0.48
1:2:1181:A:O2'	1:2:1182:A:O4'	2.31	0.48
1:2:1463:U:H4'	1:2:1464:C:H5'	1.95	0.48
1:2:70:G:N2	1:2:79:A:N6	2.61	0.48
2:3:83:C:H5	2:3:84:C:C4	2.32	0.48
7:E:95:THR:HB	7:E:97:GLU:HG3	1.94	0.48
15:M:54:SER:OG	15:M:78:LYS:HB3	2.14	0.48
16:N:98:VAL:O	16:N:102:LEU:HB2	2.13	0.48
20:R:132:ARG:HG3	20:R:132:ARG:H	1.38	0.48
1:2:665:G:N2	1:2:1163:C:H1'	2.28	0.48
1:2:171:A:N7	1:2:173:A:C5	2.82	0.48
5:C:203:GLY:O	5:C:221:ASP:HA	2.14	0.48
7:E:211:LYS:HE2	7:E:215:GLY:HA2	1.94	0.48
11:I:141:ARG:HH22	11:I:153:LYS:NZ	2.12	0.48
1:2:918:U:H5''	16:N:64:ARG:NH2	2.28	0.48
17:O:44:VAL:HG12	17:O:53:ILE:HD12	1.94	0.48
1:2:1558:C:H4'	1:2:1559:C:OP1	2.14	0.48
1:2:1258:A:C2	1:2:1663:A:H2'	2.48	0.48
1:2:946:U:H4'	1:2:1046:U:OP1	2.14	0.48
3:A:102:ARG:HG3	3:A:103:PHE:O	2.13	0.48
4:B:159:GLN:HE22	4:B:162:ARG:NH1	2.12	0.48
4:B:25:PHE:CE2	17:O:88:LEU:HD13	2.49	0.48
5:C:183:LYS:HB3	5:C:196:ILE:HG23	1.96	0.48
11:I:89:GLU:HG2	11:I:92:ARG:NH2	2.28	0.48
1:2:1856:C:OP2	17:O:146:ARG:HB2	2.14	0.48
25:W:112:ASP:OD1	25:W:112:ASP:N	2.46	0.48
1:2:1207:G:O2'	1:2:1837:G:N2	2.46	0.48
1:2:1745:A:O2'	1:2:1746:U:O4'	2.21	0.48
2:3:252:A:H4'	2:3:253:G:C5'	2.44	0.48
2:3:258:G:H1'	2:3:273:G:C6	2.49	0.48
3:A:121:LEU:HD12	3:A:143:PRO:HB2	1.95	0.48
4:B:30:TRP:HE1	17:O:18:GLY:HA2	1.79	0.48
7:E:136:ILE:HG12	7:E:149:TYR:CE1	2.48	0.48
16:N:45:LEU:HB3	16:N:49:GLN:HB2	1.95	0.48
27:Y:20:ARG:HB3	27:Y:76:TYR:CD1	2.49	0.48
1:2:1546:G:H2'	1:2:1547:C:C6	2.49	0.48
1:2:1658:G:OP2	1:2:1660:C:N4	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:563:G:N7	1:2:586:G:N2	2.62	0.48
1:2:587:A:H5'	1:2:592:C:H41	1.79	0.48
1:2:872:A:C8	1:2:874:G:C8	3.02	0.48
1:2:913:A:H2	10:H:99:ARG:H	1.60	0.48
2:3:72:A:H2'	2:3:73:A:O4'	2.13	0.48
7:E:245:ARG:HG2	7:E:246:LEU:H	1.78	0.48
10:H:9:VAL:HG22	10:H:45:ILE:HG12	1.95	0.48
16:N:101:HIS:HE1	16:N:105:ASN:HD22	1.56	0.48
1:2:1320:G:H2'	1:2:1321:G:H5'	1.95	0.48
1:2:130:G:H1	1:2:182:C:H42	1.61	0.48
1:2:380:G:P	11:I:56:ARG:HH22	2.37	0.48
4:B:150:ILE:HG22	20:R:132:ARG:HE	1.79	0.48
22:T:37:VAL:HG22	22:T:38:LYS:H	1.79	0.48
1:2:1154:U:H5''	1:2:1156:U:O4'	2.14	0.47
1:2:1256:G:N2	1:2:1659:U:H5'	2.16	0.47
1:2:316:G:H2'	1:2:317:C:H6	1.78	0.47
1:2:465:A:H5'	1:2:466:G:C5	2.49	0.47
1:2:582:U:H1'	27:Y:33:ALA:HB2	1.95	0.47
2:3:244:A:H1'	2:3:245:G:P	2.54	0.47
4:B:164:ILE:HD13	4:B:207:LEU:HD11	1.96	0.47
4:B:217:MET:HE2	4:B:217:MET:HB3	1.83	0.47
5:C:207:ALA:O	5:C:211:LYS:HB2	2.13	0.47
11:I:79:ILE:HG13	11:I:170:LYS:NZ	2.29	0.47
12:J:64:ASP:OD1	12:J:65:GLU:N	2.47	0.47
5:C:128:VAL:HG11	5:C:155:ILE:HG12	1.96	0.47
11:I:60:LEU:HA	11:I:60:LEU:HD23	1.63	0.47
14:L:40:ILE:HA	14:L:40:ILE:HD13	1.59	0.47
14:L:60:CYS:SG	14:L:62:PHE:N	2.85	0.47
22:T:42:HIS:HA	22:T:83:GLN:OE1	2.14	0.47
1:2:1338:G:OP1	23:U:67:LYS:HD2	2.14	0.47
25:W:111:MET:HB2	25:W:115:GLU:OE1	2.13	0.47
27:Y:37:LYS:O	27:Y:40:ILE:HG22	2.14	0.47
1:2:1610:G:N2	21:S:85:ASN:O	2.47	0.47
1:2:1611:G:O2'	21:S:86:ARG:HG2	2.15	0.47
1:2:608:C:H42	1:2:635:G:H1	1.61	0.47
7:E:38:LEU:HG	7:E:39:ARG:N	2.28	0.47
16:N:5:HIS:CE1	16:N:121:ARG:HG3	2.50	0.47
1:2:1608:U:H5''	21:S:130:ARG:HD3	1.95	0.47
22:T:22:LEU:HB3	22:T:54:TYR:CD1	2.45	0.47
1:2:1603:G:N2	22:T:48:TYR:OH	2.47	0.47
23:U:32:LEU:HD21	23:U:87:ARG:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1011:A:H2'	1:2:1012:A:O4'	2.14	0.47
1:2:389:A:H2'	1:2:390:C:C6	2.48	0.47
5:C:244:ILE:H	5:C:244:ILE:HG12	1.55	0.47
7:E:112:HIS:CE1	7:E:239:PRO:HA	2.48	0.47
10:H:63:PHE:HA	10:H:95:ILE:O	2.14	0.47
1:2:943:U:O2	17:O:137:SER:HB3	2.14	0.47
17:O:142:ARG:HG2	17:O:142:ARG:HH11	1.79	0.47
18:P:78:THR:HG22	18:P:95:GLY:O	2.14	0.47
19:Q:93:VAL:HG12	19:Q:105:LYS:HE3	1.97	0.47
1:2:1224:G:H21	19:Q:142:GLN:NE2	2.11	0.47
1:2:1250:A:H4'	1:2:1251:A:OP2	2.13	0.47
1:2:1649:U:HO2'	1:2:1650:A:P	2.36	0.47
1:2:1777:G:H2'	1:2:1778:C:O4'	2.14	0.47
2:3:153:G:H4'	2:3:154:A:OP2	2.13	0.47
4:B:33:VAL:HB	4:B:44:ILE:HD11	1.96	0.47
9:G:102:VAL:HG13	9:G:106:LEU:HD12	1.96	0.47
10:H:130:LEU:HB2	10:H:177:TYR:HE1	1.79	0.47
10:H:69:LEU:O	10:H:73:GLN:HG2	2.14	0.47
1:2:1415:C:O2'	22:T:132:ASP:OD2	2.28	0.47
26:X:11:ARG:HG3	26:X:12:LYS:N	2.30	0.47
1:2:1210:G:C5'	3:A:85:ARG:HH12	49.13	0.47
1:2:340:C:H2'	1:2:341:C:O4'	2.15	0.47
1:2:656:G:H5'	1:2:662:G:N2	2.30	0.47
4:B:49:VAL:HG21	4:B:62:LEU:HB2	1.97	0.47
6:D:157:MET:HG3	6:D:159:HIS:NE2	2.29	0.47
12:J:123:ILE:O	12:J:126:ALA:HB3	2.15	0.47
12:J:132:GLN:HB3	12:J:134:HIS:HD2	1.79	0.47
14:L:98:LYS:HB3	14:L:99:TYR:CD1	2.50	0.47
14:L:150:GLY:HA3	16:N:133:ARG:NH2	2.28	0.47
25:W:90:GLN:HA	25:W:102:ILE:HD11	1.96	0.47
1:2:1354:G:H5'	1:2:1355:C:OP2	2.15	0.47
1:2:1585:U:H3	19:Q:73:LYS:HE2	1.80	0.47
1:2:1589:A:N3	1:2:1653:U:O2'	2.34	0.47
3:A:141:ASN:HD21	24:V:29:HIS:HA	1.80	0.47
6:D:212:GLU:HG2	20:R:19:LYS:NZ	2.29	0.47
6:D:22:ASN:OD1	6:D:34:TYR:OH	2.25	0.47
11:I:198:TYR:O	11:I:202:ILE:HG13	2.14	0.47
6:D:27:ARG:HB3	13:K:61:GLN:HE21	1.80	0.47
16:N:55:ARG:HH11	16:N:55:ARG:HG2	1.79	0.47
17:O:84:ARG:O	17:O:87:GLU:HB3	2.14	0.47
1:2:448:A:H4'	1:2:449:A:H5'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:488:U:H2'	1:2:488:U:H6	1.51	0.47
1:2:897:U:H2'	1:2:898:U:O4'	2.14	0.47
1:2:925:G:C2	1:2:926:A:C8	3.03	0.47
2:3:304:C:N4	2:3:305:U:O4	2.48	0.47
2:3:65:C:O2'	2:3:66:A:OP1	2.29	0.47
7:E:184:THR:OG1	7:E:224:ASN:O	2.30	0.47
18:P:110:GLU:HB3	21:S:117:ILE:HD11	1.97	0.47
1:2:862:A:N3	25:W:105:THR:OG1	2.48	0.47
1:2:1252:C:OP1	23:U:75:LYS:NZ	2.34	0.47
1:2:1287:A:C6	1:2:1313:A:C8	3.02	0.47
1:2:14:C:OP2	5:C:232:THR:HG21	2.15	0.47
1:2:403:G:H2'	1:2:404:G:H8	1.79	0.47
1:2:900:C:H2'	1:2:901:G:H8	1.79	0.47
7:E:6:LYS:HB2	7:E:6:LYS:HE3	1.65	0.47
11:I:114:GLU:OE1	11:I:123:ARG:NH2	2.46	0.47
12:J:136:ARG:HD2	12:J:160:SER:CA	2.38	0.47
14:L:78:THR:OG1	14:L:79:LYS:N	2.48	0.47
26:X:123:VAL:HG12	26:X:124:LYS:N	2.28	0.47
1:2:1234:C:H4'	1:2:1246:A:N1	2.29	0.47
1:2:1656:G:H1	1:2:1668:U:H3	1.62	0.47
2:3:265:U:O2'	2:3:266:G:OP2	2.31	0.47
2:3:59:U:H2'	2:3:60:G:C8	2.50	0.47
10:H:47:ALA:HB3	10:H:63:PHE:HB2	1.97	0.47
11:I:113:TYR:OH	11:I:156:ALA:HB1	2.15	0.47
21:S:90:VAL:HG21	21:S:113:ARG:NH1	2.30	0.47
1:2:1560:U:H4'	1:2:1583:C:O2'	2.15	0.47
1:2:1651:A:H2'	1:2:1652:G:C8	2.50	0.47
1:2:465:A:H5'	1:2:466:G:C4	2.50	0.47
1:2:594:A:H4'	1:2:595:U:OP1	2.13	0.47
3:A:169:HIS:HA	3:A:203:PHE:CE1	2.50	0.47
11:I:117:TYR:CE1	11:I:156:ALA:HB2	2.49	0.47
11:I:48:VAL:HG11	11:I:54:LYS:HD2	1.96	0.47
25:W:102:ILE:HB	25:W:113:HIS:HB3	1.97	0.47
26:X:7:LEU:O	26:X:9:THR:N	2.48	0.47
1:2:1144:A:H2'	1:2:1145:A:C8	2.50	0.46
1:2:1671:G:H2'	1:2:1672:U:C6	2.50	0.46
1:2:561:A:OP2	12:J:173:VAL:HB	2.15	0.46
2:3:123:C:O2'	2:3:124:C:OP1	2.32	0.46
3:A:206:ASP:OD1	3:A:208:GLU:HG2	2.15	0.46
5:C:116:THR:HG22	5:C:117:ARG:HG2	1.97	0.46
1:2:67:C:C5	9:G:164:LYS:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:18:GLU:HA	20:R:71:ILE:CD1	2.45	0.46
1:2:1577:G:H1'	1:2:1582:C:O2	2.16	0.46
1:2:1609:C:H42	1:2:1630:A:H61	1.62	0.46
1:2:1630:A:OP1	21:S:37:GLY:N	2.38	0.46
1:2:1788:A:H2'	1:2:1789:G:O4'	2.16	0.46
1:2:332:G:H4'	1:2:333:G:OP1	2.15	0.46
1:2:80:G:N2	1:2:81:U:C2	2.83	0.46
5:C:161:SER:HA	24:V:27:LYS:NZ	2.31	0.46
6:D:146:ARG:HD2	6:D:146:ARG:HA	1.63	0.46
6:D:202:LYS:HA	6:D:203:PRO:HD3	1.75	0.46
12:J:128:VAL:O	12:J:132:GLN:HB2	2.16	0.46
15:M:17:ALA:HB3	15:M:123:VAL:HG11	1.97	0.46
1:2:409:C:C2	1:2:432:G:C2	3.04	0.46
1:2:548:C:H2'	1:2:549:C:C6	2.50	0.46
1:2:920:A:C8	1:2:922:A:C8	3.02	0.46
2:3:263:G:C2	2:3:264:U:C5	3.03	0.46
2:3:270:C:HO2'	2:3:271:G:H8	1.54	0.46
1:2:1798:C:H4'	11:I:2:GLY:O	2.15	0.46
16:N:5:HIS:ND1	16:N:121:ARG:HG3	2.29	0.46
16:N:80:LEU:H	16:N:80:LEU:HD22	1.80	0.46
1:2:1373:C:OP1	20:R:7:LYS:N	2.48	0.46
26:X:51:VAL:HG13	26:X:70:VAL:HG13	1.97	0.46
1:2:1177:U:H2'	1:2:1178:U:H6	1.80	0.46
1:2:590:A:H3'	1:2:590:A:OP1	2.15	0.46
7:E:197:ASN:OD1	7:E:198:ARG:N	2.48	0.46
11:I:34:ALA:HB2	11:I:56:ARG:HD3	1.97	0.46
16:N:125:LEU:O	16:N:128:TYR:HB3	2.15	0.46
25:W:6:VAL:HG12	25:W:34:ILE:HD11	1.97	0.46
1:2:1375:G:H2'	1:2:1376:A:H8	1.80	0.46
1:2:1425:G:H2'	1:2:1426:U:C6	2.51	0.46
1:2:439:A:O2'	1:2:440:G:H5'	2.15	0.46
1:2:976:G:H2'	1:2:977:C:C6	2.51	0.46
4:B:69:VAL:HG11	4:B:74:LEU:HD21	1.97	0.46
5:C:77:SER:HA	5:C:97:PHE:CE1	2.50	0.46
7:E:103:TYR:CD1	7:E:189:LEU:HD11	2.51	0.46
10:H:95:ILE:HA	10:H:132:ASP:OD2	2.16	0.46
10:H:30:LEU:O	10:H:34:SER:HB2	2.15	0.46
11:I:76:THR:HG22	11:I:77:ARG:N	2.30	0.46
17:O:57:THR:HG23	17:O:60:MET:HE2	1.98	0.46
1:2:1356:G:H2'	1:2:1357:A:C8	2.51	0.46
1:2:520:A:H2'	1:2:521:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:675:U:H2'	1:2:676:C:H6	1.79	0.46
2:3:230:G:O2'	2:3:231:G:OP1	2.27	0.46
2:3:84:C:O2'	2:3:85:A:O5'	2.26	0.46
9:G:144:LEU:HA	9:G:144:LEU:HD23	1.77	0.46
1:2:1075:C:H5''	16:N:107:LYS:HZ2	1.80	0.46
1:2:19:A:H2'	1:2:20:G:O4'	2.14	0.46
1:2:316:G:H2'	1:2:317:C:C6	2.50	0.46
2:3:102:G:OP1	28:Z:65:TYR:HA	2.16	0.46
10:H:27:LEU:O	10:H:31:GLU:HG3	2.15	0.46
4:B:30:TRP:CE2	17:O:19:PRO:HG3	2.51	0.46
19:Q:131:LYS:HE3	19:Q:131:LYS:HB2	1.73	0.46
3:A:85:ARG:HD2	20:R:82:ASP:OD1	2.15	0.46
1:2:1086:G:O2'	1:2:1087:A:H5'	2.16	0.46
1:2:1628:C:H2'	1:2:1629:C:C6	2.51	0.46
1:2:1833:C:OP1	1:2:1840:U:H4'	2.15	0.46
1:2:68:A:H2'	1:2:69:C:O4'	2.16	0.46
2:3:231:G:N2	2:3:237:C:C2	2.83	0.46
15:M:101:ARG:HG3	15:M:102:LYS:N	2.30	0.46
21:S:50:ILE:CD1	21:S:67:VAL:HG21	2.44	0.46
1:2:1580:A:H5''	23:U:59:LYS:NZ	2.30	0.46
1:2:1040:G:H5'	1:2:1041:G:OP2	2.16	0.46
1:2:1060:A:H4'	1:2:1061:U:O5'	2.16	0.46
1:2:481:C:H5''	1:2:482:G:OP2	2.16	0.46
2:3:231:G:N2	2:3:237:C:O2	2.49	0.46
7:E:23:LEU:HD12	7:E:23:LEU:HA	1.57	0.46
7:E:247:THR:HG23	7:E:250:GLU:OE2	2.16	0.46
8:F:167:LYS:NZ	8:F:175:ASP:OD2	2.49	0.46
22:T:21:PHE:CD2	22:T:134:ILE:HD11	2.51	0.46
1:2:1336:C:H2'	1:2:1337:C:O4'	2.16	0.46
4:B:186:ASN:HA	4:B:189:ILE:HD12	1.98	0.46
4:B:31:TYR:CD2	4:B:94:LYS:HA	2.51	0.46
7:E:199:GLU:HG3	7:E:207:VAL:HB	1.98	0.46
7:E:77:ARG:HG2	7:E:82:TYR:CD2	2.50	0.46
9:G:137:ARG:HD3	9:G:178:ARG:HH11	1.80	0.46
1:2:171:A:C5'	9:G:177:GLN:HG2	2.42	0.46
16:N:42:LYS:HE3	16:N:42:LYS:HB2	1.69	0.46
17:O:46:ASP:OD1	17:O:47:LEU:N	2.46	0.46
21:S:17:ASN:HD22	21:S:101:ASN:ND2	2.09	0.46
1:2:1587:G:H1	22:T:67:ARG:CG	2.29	0.45
1:2:1213:C:H42	1:2:1686:G:H1	1.63	0.45
1:2:525:A:N7	1:2:587:A:C2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:624:C:H41	26:X:63:ASN:HD22	1.64	0.45
2:3:231:G:H5'	2:3:232:C:OP2	2.16	0.45
2:3:290:U:O2'	2:3:315:C:OP2	2.33	0.45
7:E:21:ASP:OD2	7:E:24:THR:OG1	2.24	0.45
7:E:44:LEU:HD21	7:E:70:ILE:HG21	1.98	0.45
9:G:59:GLN:HG3	9:G:72:ARG:HH22	1.78	0.45
10:H:116:ARG:HA	10:H:117:PRO:HD3	1.75	0.45
12:J:174:LYS:HE2	12:J:174:LYS:HB3	1.79	0.45
13:K:20:VAL:HA	13:K:69:TRP:O	2.16	0.45
13:K:26:ASP:HB3	13:K:29:MET:HB2	1.98	0.45
20:R:98:VAL:HG13	20:R:102:THR:HB	1.98	0.45
1:2:1109:C:C4	20:R:126:MET:SD	3.09	0.45
1:2:1454:A:N7	20:R:3:ARG:HD2	2.31	0.45
22:T:31:PRO:HB2	22:T:34:VAL:HG23	1.97	0.45
3:A:36:GLN:HE22	24:V:70:LEU:HD12	1.82	0.45
21:S:5:ILE:HG23	28:Z:50:PHE:O	2.16	0.45
1:2:658:U:H4'	1:2:659:G:O5'	2.16	0.45
1:2:72:C:O2'	1:2:73:C:H2'	2.16	0.45
1:2:917:U:O2'	1:2:918:U:O4'	2.35	0.45
3:A:44:ASP:O	3:A:46:ILE:HG13	2.15	0.45
10:H:29:GLU:O	10:H:33:ASN:ND2	2.46	0.45
14:L:93:LEU:HB3	14:L:102:PHE:HB3	1.98	0.45
17:O:54:CYS:SG	17:O:84:ARG:HG2	2.57	0.45
22:T:60:THR:HG23	22:T:75:MET:SD	2.57	0.45
25:W:97:ARG:HB3	25:W:97:ARG:HH11	1.80	0.45
26:X:107:ARG:O	26:X:109:GLY:N	2.50	0.45
26:X:76:LYS:HG3	26:X:77:ASN:OD1	2.16	0.45
1:2:1443:C:H2'	1:2:1444:U:H5'	1.98	0.45
1:2:981:A:H2'	1:2:982:G:C8	2.51	0.45
3:A:208:GLU:HG3	3:A:209:GLU:HG3	1.99	0.45
7:E:115:THR:HG22	7:E:117:GLU:HG2	1.98	0.45
7:E:126:VAL:HG22	7:E:158:ASP:O	2.15	0.45
7:E:184:THR:O	7:E:189:LEU:HD13	2.16	0.45
8:F:19:LEU:HG	8:F:20:PHE:HD1	1.81	0.45
10:H:133:LEU:O	10:H:173:PHE:HE1	2.00	0.45
12:J:50:LEU:HD23	12:J:51:ALA:N	2.30	0.45
1:2:1225:U:H1'	19:Q:142:GLN:NE2	2.31	0.45
26:X:37:LYS:HE2	26:X:37:LYS:HB3	1.86	0.45
1:2:963:A:H2'	1:2:964:A:H8	1.77	0.45
7:E:179:ASN:ND2	7:E:231:GLY:H	2.15	0.45
9:G:6:SER:O	9:G:8:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:158:LEU:HD11	10:H:187:PHE:CD2	2.51	0.45
18:P:111:MET:HA	18:P:114:HIS:ND1	2.32	0.45
20:R:58:MET:O	20:R:62:GLN:HG2	2.16	0.45
28:Z:78:LYS:HD3	28:Z:78:LYS:HA	1.69	0.45
1:2:123:G:H5''	1:2:124:U:OP2	2.16	0.45
1:2:466:G:H1'	9:G:59:GLN:NE2	2.32	0.45
1:2:949:G:C6	1:2:950:C:C4	3.05	0.45
18:P:108:LYS:HB3	18:P:109:PRO:HD2	1.98	0.45
1:2:1289:U:H2'	1:2:1290:G:C8	2.52	0.45
1:2:1337:C:O2'	23:U:68:THR:HB	2.17	0.45
1:2:1394:G:H21	1:2:1475:G:H1'	1.81	0.45
7:E:235:TRP:CD1	7:E:235:TRP:N	2.85	0.45
7:E:248:ILE:HG13	7:E:248:ILE:H	1.48	0.45
7:E:55:ALA:HB1	7:E:60:GLU:HB2	1.98	0.45
8:F:73:THR:O	8:F:89:THR:HG21	2.16	0.45
13:K:76:ILE:HD13	13:K:91:PRO:HG3	1.99	0.45
14:L:35:ARG:HH22	14:L:54:THR:C	2.19	0.45
18:P:37:TYR:HB3	18:P:41:GLN:HB2	1.99	0.45
1:2:1358:U:OP1	5:C:114:LYS:HB2	2.16	0.45
1:2:1440:C:HO2'	1:2:1441:U:C5'	2.30	0.45
1:2:1451:G:OP1	20:R:32:LYS:HE2	2.16	0.45
1:2:1583:C:H2'	1:2:1584:G:N7	2.31	0.45
1:2:1657:G:H1	1:2:1667:U:H3	1.64	0.45
1:2:913:A:H2	10:H:98:ARG:HA	1.82	0.45
1:2:933:G:H2'	1:2:993:G:N2	2.31	0.45
4:B:181:LEU:O	4:B:185:VAL:HG23	2.17	0.45
7:E:151:ASP:HA	7:E:152:PRO:HD3	1.81	0.45
11:I:87:ASN:HD22	11:I:88:ASN:N	2.14	0.45
14:L:12:LYS:O	14:L:56:ILE:HD13	2.17	0.45
18:P:122:THR:HG22	18:P:123:TYR:HD2	1.82	0.45
20:R:32:LYS:HG2	20:R:47:ARG:HH21	1.82	0.45
21:S:39:ARG:NH2	22:T:38:LYS:HG3	2.32	0.45
22:T:80:GLY:HA2	22:T:92:PHE:HE1	1.80	0.45
1:2:1043:G:H2'	1:2:1044:G:O4'	2.16	0.45
1:2:1334:G:H22	1:2:1496:U:H3	1.65	0.45
1:2:1642:U:H2'	1:2:1643:U:C6	2.52	0.45
1:2:1656:G:H2'	1:2:1657:G:H8	1.82	0.45
1:2:373:G:OP1	14:L:135:SER:OG	2.35	0.45
1:2:615:C:H2'	1:2:616:A:C8	2.52	0.45
1:2:66:G:OP2	1:2:82:G:N2	2.44	0.45
1:2:78:C:OP1	9:G:173:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:256:G:H5'	2:3:257:A:H2'	1.97	0.45
9:G:32:MET:HA	9:G:52:ILE:HG22	1.98	0.45
12:J:142:VAL:HG12	12:J:144:ILE:H	1.82	0.45
25:W:46:TYR:HB3	25:W:69:LEU:HD13	1.99	0.45
25:W:11:LEU:HD13	25:W:72:CYS:SG	2.57	0.45
1:2:1448:A:H2'	1:2:1449:G:O4'	2.17	0.45
1:2:1671:G:H2'	1:2:1672:U:H6	1.82	0.45
1:2:1674:G:OP1	8:F:51:HIS:NE2	2.50	0.45
1:2:590:A:P	1:2:590:A:H3'	2.57	0.45
1:2:922:A:C2'	1:2:923:G:H5'	2.47	0.45
10:H:53:VAL:HG21	10:H:172:THR:HA	1.99	0.45
20:R:130:THR:HA	20:R:131:PRO:HD3	1.79	0.45
21:S:3:LEU:HD23	21:S:3:LEU:HA	1.81	0.45
23:U:94:PRO:HG2	23:U:97:ILE:HG13	1.99	0.45
2:3:142:A:H2'	2:3:143:G:C8	2.52	0.45
10:H:18:GLU:O	10:H:21:SER:OG	2.33	0.45
1:2:104:A:OP1	11:I:12:ARG:NE	2.50	0.44
1:2:1239:U:H5''	18:P:124:LYS:HD3	1.99	0.44
1:2:528:A:C2	1:2:558:G:C2	3.06	0.44
1:2:604:A:O2'	1:2:605:A:H5'	2.17	0.44
1:2:655:A:H4'	1:2:656:G:H3'	1.99	0.44
5:C:157:LEU:HD12	5:C:157:LEU:HA	1.70	0.44
7:E:170:THR:OG1	7:E:171:ASP:N	2.50	0.44
11:I:141:ARG:HH22	11:I:153:LYS:HZ1	1.63	0.44
11:I:146:GLN:O	11:I:150:ASP:HB2	2.17	0.44
16:N:34:LYS:HE3	16:N:67:THR:HB	1.98	0.44
28:Z:66:LYS:H	28:Z:111:ARG:HD3	1.82	0.44
1:2:674:C:O2	1:2:1031:A:N1	2.50	0.44
1:2:181:A:H2'	1:2:182:C:H2'	1.98	0.44
1:2:536:A:N3	1:2:536:A:H2'	2.33	0.44
3:A:81:ASN:HA	3:A:84:GLN:CG	2.47	0.44
4:B:83:LYS:HB3	4:B:83:LYS:HE2	1.82	0.44
6:D:175:VAL:CG1	6:D:182:LEU:HB2	2.46	0.44
10:H:130:LEU:HB2	10:H:177:TYR:CE1	2.51	0.44
11:I:79:ILE:HG13	11:I:170:LYS:HZ1	1.82	0.44
12:J:119:LEU:HB3	12:J:159:PHE:HE1	1.82	0.44
8:F:103:LEU:HA	15:M:64:LEU:HD11	128.57	0.44
18:P:44:ARG:NH2	18:P:83:MET:HA	2.32	0.44
25:W:69:LEU:HD21	25:W:72:CYS:HB2	1.99	0.44
1:2:1499:U:H2'	1:2:1500:G:H8	1.82	0.44
1:2:1791:A:H2'	1:2:1792:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1852:C:H2'	1:2:1853:C:H6	1.83	0.44
1:2:28:U:H2'	1:2:29:G:C8	2.52	0.44
1:2:488:U:H3'	1:2:489:A:H5'	2.00	0.44
1:2:926:A:H5'	1:2:926:A:H8	1.82	0.44
6:D:72:VAL:HG13	13:K:68:TYR:CE2	2.53	0.44
10:H:133:LEU:HA	10:H:133:LEU:HD12	1.66	0.44
11:I:11:ARG:NH1	11:I:15:GLY:O	2.37	0.44
14:L:104:LYS:HZ1	26:X:8:ARG:CD	2.30	0.44
19:Q:100:VAL:HG12	19:Q:101:ASP:H	1.83	0.44
1:2:1630:A:OP2	21:S:39:ARG:HB3	2.17	0.44
1:2:221:A:H2'	1:2:222:U:H6	1.82	0.44
12:J:28:GLU:HB2	12:J:40:LYS:HZ3	1.83	0.44
25:W:83:LEU:HA	25:W:83:LEU:HD12	1.62	0.44
1:2:1073:U:H2'	1:2:1074:C:H6	1.82	0.44
1:2:1100:A:C2	1:2:1101:U:C2	3.05	0.44
11:I:27:TYR:HB3	11:I:49:ARG:NH2	2.32	0.44
20:R:29:HIS:HA	20:R:32:LYS:HB3	1.99	0.44
1:2:1453:C:O3'	20:R:49:LYS:HG2	2.17	0.44
1:2:1856:C:H2'	1:2:1857:G:C8	2.53	0.44
1:2:60:A:H2	1:2:61:A:N3	2.15	0.44
2:3:330:A:O2'	2:3:331:G:H2'	2.17	0.44
3:A:68:ILE:HD13	3:A:120:ARG:HB3	1.99	0.44
3:A:200:ASP:HA	3:A:203:PHE:CE2	2.53	0.44
5:C:125:LYS:HA	5:C:142:LYS:O	2.18	0.44
6:D:96:LEU:CD1	6:D:198:ILE:HG21	2.43	0.44
9:G:145:PHE:CD2	9:G:156:TYR:HB3	2.52	0.44
9:G:21:GLU:O	9:G:25:ARG:HG2	2.18	0.44
13:K:47:LYS:HE3	13:K:50:GLN:OE1	2.18	0.44
19:Q:85:ARG:HE	19:Q:119:LEU:HD21	1.83	0.44
21:S:82:TRP:CZ2	22:T:36:THR:HG21	2.52	0.44
1:2:1192:U:OP2	26:X:119:ARG:NH2	2.47	0.44
1:2:1670:C:H2'	1:2:1671:G:C8	2.52	0.44
1:2:1672:U:H2'	1:2:1673:U:C6	2.52	0.44
1:2:963:A:P	17:O:65:ASP:HB2	2.57	0.44
2:3:95:U:C2'	2:3:96:A:H5'	2.48	0.44
3:A:70:ASN:HB3	3:A:73:ASP:OD2	2.18	0.44
4:B:225:LEU:O	4:B:229:MET:HG2	2.17	0.44
5:C:167:ARG:HB2	5:C:177:PRO:HB2	2.00	0.44
1:2:1599:U:N3	8:F:166:ILE:HD12	2.33	0.44
11:I:8:TRP:NE1	11:I:22:HIS:HE1	2.16	0.44
12:J:48:PHE:CZ	12:J:52:LYS:HE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:72:VAL:HG22	13:K:20:VAL:HG11	1.99	0.44
1:2:1563:G:OP1	22:T:115:LYS:HE3	2.17	0.44
1:2:72:C:N4	1:2:79:A:N7	2.60	0.44
3:A:5:LEU:HD21	24:V:41:LYS:HA	2.00	0.44
4:B:198:GLU:HB2	4:B:210:VAL:CG1	2.42	0.44
14:L:61:PRO:HA	14:L:66:VAL:CG2	2.47	0.44
14:L:6:THR:HG23	14:L:7:GLU:HG2	2.00	0.44
17:O:74:ALA:HB1	17:O:115:ALA:HB2	1.99	0.44
1:2:1630:A:H5'	21:S:37:GLY:N	2.33	0.44
21:S:63:GLU:HA	21:S:66:ARG:HG2	2.00	0.44
25:W:47:ILE:HG12	25:W:48:GLY:N	2.33	0.44
1:2:1611:G:N2	1:2:1629:C:O2	2.51	0.44
2:3:245:G:OP1	2:3:245:G:C8	2.70	0.44
2:3:61:U:HO2'	2:3:62:C:P	2.39	0.44
3:A:208:GLU:HG3	3:A:209:GLU:N	2.32	0.44
5:C:233:LEU:HA	5:C:233:LEU:HD12	1.52	0.44
8:F:136:ARG:HH11	8:F:199:VAL:HG11	1.82	0.44
11:I:193:LYS:HA	11:I:196:GLU:OE1	2.18	0.44
11:I:97:VAL:HG23	11:I:98:LYS:O	2.18	0.44
12:J:81:LEU:HD23	12:J:81:LEU:HA	1.77	0.44
1:2:1464:C:H2'	1:2:1465:A:C8	2.53	0.43
1:2:494:C:N4	1:2:509:G:H21	2.16	0.43
1:2:533:A:C6	1:2:534:G:C5	3.06	0.43
1:2:70:G:H2'	1:2:71:G:O4'	2.16	0.43
1:2:958:G:C6	1:2:959:G:C2	3.06	0.43
3:A:91:ALA:O	3:A:95:GLY:N	2.50	0.43
4:B:188:LEU:HA	4:B:188:LEU:HD23	1.76	0.43
4:B:63:LYS:HE3	4:B:89:GLU:O	2.18	0.43
6:D:79:PHE:HE1	6:D:84:VAL:HB	1.80	0.43
12:J:161:LEU:O	12:J:167:GLY:HA3	2.17	0.43
20:R:121:GLN:HA	20:R:122:PRO:HD2	1.85	0.43
20:R:77:GLU:HG3	20:R:81:ARG:HE	1.83	0.43
27:Y:20:ARG:HD3	27:Y:76:TYR:HE1	1.83	0.43
1:2:1530:U:H2'	1:2:1531:A:O4'	2.18	0.43
1:2:1677:U:H2'	1:2:1678:A:H8	1.84	0.43
1:2:360:A:C2	1:2:362:C:C2	3.05	0.43
1:2:60:A:HO2'	1:2:61:A:P	2.41	0.43
1:2:749:U:O4	1:2:750:C:N4	2.51	0.43
3:A:69:GLU:HB2	5:C:270:THR:HG21	1.99	0.43
4:B:168:MET:O	4:B:172:MET:HG2	2.17	0.43
18:P:60:LEU:HD22	18:P:92:SER:OG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:108:ARG:O	21:S:112:GLU:HG2	2.18	0.43
21:S:81:ASP:O	21:S:87:GLN:NE2	2.49	0.43
22:T:62:ARG:HA	22:T:65:TYR:HB3	2.01	0.43
1:2:1272:C:N4	1:2:1510:G:H1	2.16	0.43
2:3:45:C:O2	2:3:118:G:N2	2.50	0.43
3:A:41:ARG:HB2	3:A:47:TYR:CD1	2.53	0.43
4:B:42:ARG:HD3	4:B:42:ARG:HA	1.71	0.43
5:C:270:THR:O	5:C:274:VAL:HG23	2.18	0.43
6:D:69:LEU:O	6:D:73:VAL:HG23	2.18	0.43
8:F:56:TYR:CD1	8:F:66:CYS:HB3	2.53	0.43
11:I:196:GLU:HG2	11:I:197:PHE:N	2.33	0.43
14:L:17:PHE:CE1	14:L:19:ASN:HB2	2.52	0.43
21:S:123:LEU:HD22	21:S:127:TRP:CZ2	2.53	0.43
28:Z:48:VAL:HG22	28:Z:80:ARG:HH11	1.83	0.43
1:2:1065:G:H2'	1:2:1066:U:C6	2.53	0.43
1:2:126:G:H1'	1:2:180:G:N2	2.32	0.43
1:2:395:G:H5'	14:L:82:MET:SD	2.59	0.43
6:D:3:VAL:HG12	6:D:4:GLN:H	1.83	0.43
9:G:185:LEU:HD12	9:G:185:LEU:HA	1.76	0.43
14:L:80:MET:H	14:L:80:MET:HG3	1.66	0.43
20:R:71:ILE:O	20:R:75:GLU:HG2	2.19	0.43
26:X:7:LEU:C	26:X:9:THR:H	2.22	0.43
28:Z:62:VAL:HA	28:Z:65:TYR:HD2	1.84	0.43
1:2:1374:C:O2'	1:2:1464:C:O2	2.29	0.43
1:2:1598:G:OP2	1:2:1598:G:H8	2.00	0.43
1:2:72:C:C4	1:2:73:C:N4	2.87	0.43
7:E:189:LEU:HD12	7:E:190:GLY:N	2.34	0.43
8:F:19:LEU:HB3	8:F:23:TRP:HB2	2.00	0.43
9:G:93:LYS:HE2	9:G:93:LYS:HB2	1.72	0.43
13:K:85:LEU:HA	13:K:86:PRO:HD3	1.87	0.43
1:2:919:A:OP1	16:N:20:ARG:NE	2.52	0.43
19:Q:32:ILE:HD11	19:Q:63:PHE:HD1	1.82	0.43
21:S:130:ARG:HD2	21:S:134:GLN:OE1	2.18	0.43
21:S:48:ALA:HB2	21:S:70:ILE:HD12	2.00	0.43
22:T:80:GLY:HA2	22:T:92:PHE:CE1	2.53	0.43
23:U:55:ARG:HB3	23:U:87:ARG:HH11	1.83	0.43
27:Y:104:ARG:NH2	27:Y:108:LYS:HE2	2.33	0.43
1:2:1831:A:O2'	1:2:1852:C:H5'	2.19	0.43
1:2:294:U:O4	14:L:65:ASN:HB2	2.19	0.43
1:2:339:A:H2'	1:2:340:C:C5	2.54	0.43
1:2:842:C:C2'	1:2:843:C:H5'	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:84:A:O3'	27:Y:119:GLY:HA2	2.18	0.43
7:E:176:ASP:OD1	7:E:177:THR:N	2.52	0.43
11:I:121:LEU:HA	11:I:121:LEU:HD23	1.84	0.43
16:N:119:GLU:O	16:N:122:ILE:HB	2.18	0.43
16:N:91:LEU:HD23	16:N:91:LEU:HA	1.72	0.43
20:R:5:ARG:HB3	20:R:9:VAL:HG11	1.99	0.43
21:S:107:LEU:O	21:S:111:LEU:HG	2.18	0.43
25:W:42:MET:HE2	25:W:49:GLU:HA	2.00	0.43
1:2:1073:U:H2'	1:2:1074:C:C6	2.54	0.43
1:2:1271:C:H5'	1:2:1301:A:C2	2.52	0.43
1:2:1287:A:C6	1:2:1288:U:C2	3.06	0.43
1:2:1341:C:H4'	1:2:1342:U:H5'	2.00	0.43
1:2:1542:C:O2'	1:2:1543:U:OP1	2.30	0.43
1:2:60:A:C2	1:2:61:A:C2	3.07	0.43
1:2:796:G:C6	1:2:797:C:C2	3.07	0.43
1:2:926:A:H5'	1:2:926:A:C8	2.54	0.43
1:2:984:C:O2'	17:O:138:ASP:HB3	2.19	0.43
3:A:102:ARG:HG2	3:A:102:ARG:HH11	1.84	0.43
1:2:1277:C:H5'	13:K:54:SER:HB2	2.01	0.43
16:N:70:LYS:HB3	16:N:70:LYS:HE2	1.58	0.43
20:R:41:ILE:O	20:R:41:ILE:HD12	2.17	0.43
28:Z:62:VAL:HA	28:Z:65:TYR:CD2	2.54	0.43
1:2:1009:A:H5'	16:N:94:LYS:HE2	2.00	0.43
1:2:1522:A:N1	18:P:131:PRO:HD3	2.34	0.43
1:2:1692:U:H2'	1:2:1693:G:H8	1.82	0.43
3:A:31:ASP:OD1	3:A:32:PHE:N	2.52	0.43
7:E:9:LEU:HA	7:E:9:LEU:HD12	1.63	0.43
15:M:51:VAL:HB	15:M:109:VAL:HB	2.00	0.43
1:2:986:G:N2	17:O:135:ILE:HD11	2.34	0.43
25:W:106:THR:HB	25:W:122:GLY:O	2.19	0.43
1:2:1118:C:H3'	1:2:1119:A:H5''	2.01	0.43
1:2:1859:A:N6	1:2:1860:A:N6	2.67	0.43
1:2:958:G:O2'	1:2:959:G:O4'	2.28	0.43
2:3:258:G:N2	2:3:273:G:H2'	2.34	0.43
13:K:32:HIS:ND1	13:K:42:ASN:OD1	2.51	0.43
14:L:40:ILE:HD12	14:L:41:GLY:H	1.83	0.43
14:L:96:ILE:HD11	14:L:103:GLU:OE2	2.19	0.43
20:R:21:TYR:CE2	20:R:73:LEU:HD23	2.54	0.43
1:2:1608:U:H5''	21:S:130:ARG:CD	2.49	0.43
22:T:114:GLU:HB2	22:T:124:THR:CG2	2.49	0.43
1:2:1425:G:O2'	1:2:1426:U:OP1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1566:G:OP1	1:2:1566:G:H4'	2.19	0.43
1:2:1731:A:H2'	1:2:1732:G:H8	1.82	0.43
1:2:221:A:H2'	1:2:222:U:C6	2.54	0.43
1:2:958:G:N1	1:2:959:G:C6	2.87	0.43
1:2:99:A:H8	1:2:99:A:O5'	2.01	0.43
4:B:87:ILE:O	4:B:98:THR:HA	2.19	0.43
5:C:144:SER:HB3	5:C:150:ALA:HB2	2.00	0.43
10:H:12:ASN:OD1	10:H:12:ASN:N	2.52	0.43
12:J:13:TYR:CE2	12:J:41:ARG:HD2	2.54	0.43
20:R:43:SER:HB3	20:R:44:LYS:H	1.49	0.43
21:S:3:LEU:N	28:Z:90:GLU:OE2	2.52	0.43
1:2:342:C:H5'	1:2:343:A:OP2	2.19	0.42
3:A:57:LYS:HA	3:A:57:LYS:HD2	1.80	0.42
4:B:137:LEU:HD22	4:B:215:VAL:HG22	2.01	0.42
10:H:138:GLU:OE2	16:N:21:SER:OG	2.35	0.42
11:I:25:ARG:HD3	11:I:25:ARG:HA	1.62	0.42
12:J:134:HIS:ND1	12:J:163:SER:HB2	2.33	0.42
12:J:28:GLU:HB2	12:J:40:LYS:NZ	2.34	0.42
14:L:18:GLN:HG2	14:L:18:GLN:H	1.50	0.42
20:R:17:ILE:HA	20:R:24:LEU:HD11	2.00	0.42
21:S:83:PHE:CE2	22:T:36:THR:HG23	2.54	0.42
23:U:28:ASN:ND2	23:U:30:LYS:HB2	2.34	0.42
1:2:1478:U:H2'	1:2:1479:G:H8	1.79	0.42
1:2:1720:U:H5''	1:2:1721:U:OP2	2.19	0.42
1:2:1730:U:H2'	1:2:1731:A:O4'	2.20	0.42
1:2:441:C:H2'	1:2:442:C:C6	2.55	0.42
1:2:657:U:O2'	1:2:658:U:OP2	2.27	0.42
3:A:147:LEU:HD13	3:A:161:ILE:HB	2.00	0.42
3:A:16:LEU:HA	3:A:16:LEU:HD23	1.67	0.42
4:B:110:MET:HE1	4:B:213:ARG:HB2	2.00	0.42
10:H:101:LEU:HD23	10:H:101:LEU:HA	1.89	0.42
11:I:4:SER:HB3	11:I:24:LYS:HD3	2.00	0.42
1:2:1016:U:OP2	16:N:14:SER:HA	2.18	0.42
17:O:119:LEU:O	17:O:124:MET:HB2	2.18	0.42
18:P:94:VAL:O	18:P:105:VAL:HB	2.19	0.42
20:R:77:GLU:HG3	20:R:81:ARG:NE	2.34	0.42
22:T:6:VAL:HB	22:T:65:TYR:CE1	2.54	0.42
27:Y:47:MET:HB2	27:Y:48:TYR:CD1	2.54	0.42
28:Z:88:LEU:HD12	28:Z:88:LEU:HA	1.87	0.42
1:2:1348:G:C8	1:2:1349:G:C8	3.07	0.42
1:2:1453:C:N4	1:2:1455:A:H1'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1464:C:H2'	1:2:1465:A:H8	1.84	0.42
1:2:1623:A:H5''	21:S:132:ARG:O	2.19	0.42
1:2:71:G:H1'	1:2:79:A:H62	1.84	0.42
2:3:129:C:H2'	2:3:130:C:C6	2.54	0.42
3:A:58:LEU:HD23	3:A:58:LEU:HA	1.81	0.42
7:E:68:ARG:HB3	7:E:76:VAL:HG11	2.02	0.42
1:2:1515:G:H21	18:P:99:GLY:CA	2.32	0.42
25:W:30:CYS:HB2	25:W:61:ILE:HD11	2.01	0.42
1:2:1271:C:H2'	1:2:1272:C:C6	2.54	0.42
1:2:1326:U:H4'	1:2:1327:G:O5'	2.20	0.42
1:2:1445:U:O4	1:2:1446:A:N6	2.52	0.42
1:2:1534:C:H5'	1:2:1536:G:O4'	2.19	0.42
1:2:1566:G:O6	22:T:97:LYS:HB2	2.19	0.42
4:B:86:LEU:HB3	4:B:98:THR:HG22	2.00	0.42
5:C:120:GLN:HG2	5:C:120:GLN:H	1.66	0.42
7:E:75:LYS:HB2	7:E:77:ARG:NH1	2.35	0.42
1:2:1599:U:C4	8:F:166:ILE:HG23	2.54	0.42
12:J:25:LEU:HA	12:J:40:LYS:HZ1	1.84	0.42
15:M:95:ASP:HB2	15:M:99:LYS:HB2	2.00	0.42
25:W:87:GLU:HG2	25:W:117:ARG:NH2	2.34	0.42
27:Y:100:LYS:NZ	27:Y:107:ARG:HD3	2.35	0.42
1:2:1120:U:H3'	1:2:1121:G:H5''	2.00	0.42
1:2:1466:G:H2'	1:2:1467:C:C6	2.54	0.42
1:2:1728:U:H5'	1:2:1729:U:OP2	2.19	0.42
1:2:220:U:H2'	1:2:221:A:H8	1.83	0.42
1:2:123:G:N2	1:2:342:C:C2	2.87	0.42
1:2:638:C:O2'	1:2:639:C:P	2.77	0.42
6:D:169:ASP:OD2	6:D:190:LEU:HD21	2.19	0.42
6:D:138:VAL:HG22	6:D:184:ILE:HG22	2.00	0.42
6:D:221:THR:O	6:D:223:ILE:HG13	2.19	0.42
1:2:152:U:H4'	9:G:132:ARG:NH1	2.35	0.42
17:O:106:LYS:NZ	17:O:136:PRO:HD2	2.33	0.42
19:Q:24:HIS:O	19:Q:68:ILE:HA	2.20	0.42
23:U:30:LYS:HD3	23:U:30:LYS:HA	1.89	0.42
1:2:1052:A:H2'	1:2:1053:C:O4'	2.18	0.42
1:2:1159:G:H2'	1:2:1160:U:O4'	2.20	0.42
1:2:1443:C:C2'	1:2:1444:U:H5'	2.50	0.42
1:2:1273:C:C2	1:2:1506:A:C6	3.07	0.42
1:2:808:A:O2'	1:2:809:A:C8	2.72	0.42
9:G:56:ASN:HB2	9:G:108:VAL:HB	2.01	0.42
12:J:102:ILE:HD13	12:J:102:ILE:HA	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:106:LYS:HZ3	17:O:135:ILE:HG13	1.85	0.42
17:O:142:ARG:HG2	17:O:142:ARG:NH1	2.33	0.42
17:O:95:ILE:HD12	17:O:116:LEU:HD21	2.01	0.42
20:R:74:GLN:O	20:R:78:ARG:HB2	2.19	0.42
1:2:1712:A:H2'	1:2:1713:C:H6	1.85	0.42
1:2:1725:U:C2	1:2:1726:G:C8	3.07	0.42
1:2:446:G:OP1	11:I:50:GLY:N	2.48	0.42
6:D:51:LEU:HB3	6:D:91:VAL:HG22	2.02	0.42
1:2:1568:C:OP2	22:T:98:SER:HB3	2.20	0.42
1:2:1126:G:OP2	20:R:129:LYS:NZ	2.26	0.42
1:2:336:A:H2'	1:2:337:C:O4'	2.20	0.42
1:2:408:A:C2'	1:2:409:C:O5'	2.67	0.42
1:2:465:A:H4'	1:2:466:G:O5'	2.20	0.42
2:3:70:A:C3'	2:3:71:G:H5'	2.44	0.42
16:N:75:LEU:HA	16:N:75:LEU:HD12	1.71	0.42
1:2:1622:U:N3	18:P:122:THR:OG1	2.27	0.42
25:W:66:THR:HG22	25:W:68:ARG:HG3	2.02	0.42
1:2:1134:G:H2'	1:2:1135:C:H6	1.84	0.42
1:2:1528:G:H2'	1:2:1529:C:C6	2.54	0.42
1:2:1568:C:O2	1:2:1627:C:O2'	2.38	0.42
3:A:126:ASP:HA	3:A:127:PRO:HD2	1.85	0.42
14:L:104:LYS:O	14:L:105:ARG:HG3	2.19	0.42
18:P:64:LYS:HA	18:P:73:PRO:HB3	2.01	0.42
22:T:42:HIS:HB3	22:T:93:SER:HB2	2.01	0.42
1:2:1097:G:H4'	3:A:32:PHE:CD1	2.55	0.42
1:2:1159:G:OP2	26:X:5:ARG:NH1	2.53	0.42
1:2:1606:G:O2'	1:2:1633:A:N6	2.53	0.42
1:2:60:A:C2	1:2:61:A:C4	3.07	0.42
8:F:201:LYS:O	8:F:204:ARG:HG3	2.20	0.42
9:G:48:TYR:CZ	9:G:116:LYS:HG3	2.55	0.42
11:I:172:LEU:HD23	11:I:172:LEU:HA	1.78	0.42
13:K:15:LEU:HD23	13:K:79:LEU:HD11	2.01	0.42
1:2:1669:G:OP1	19:Q:132:PHE:N	2.53	0.42
1:2:1520:G:H5''	21:S:136:THR:H	1.84	0.42
1:2:1594:A:O2'	22:T:16:ARG:NH2	2.53	0.42
28:Z:51:ASP:OD1	28:Z:52:LYS:N	2.53	0.42
1:2:1220:A:N6	1:2:1221:G:C6	2.88	0.41
1:2:1264:C:N3	1:2:1265:A:N6	2.67	0.41
1:2:1865:C:H4'	1:2:1866:A:OP2	2.20	0.41
1:2:76:U:H5'	9:G:159:ARG:NH2	2.23	0.41
2:3:159:G:C2	2:3:160:U:C4	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:161:LEU:H	12:J:161:LEU:HG	1.36	0.41
14:L:45:LYS:H	14:L:45:LYS:HD3	1.84	0.41
21:S:16:LEU:HD21	21:S:72:GLN:NE2	2.29	0.41
27:Y:6:THR:O	27:Y:27:VAL:HA	2.20	0.41
1:2:1401:A:N6	1:2:1441:U:O2'	2.53	0.41
1:2:1648:G:H1'	1:2:1649:U:OP2	2.19	0.41
1:2:1691:U:H2'	1:2:1692:U:O4'	2.21	0.41
1:2:403:G:C4	1:2:404:G:C8	3.08	0.41
3:A:74:VAL:O	3:A:96:ALA:HB1	2.20	0.41
4:B:207:LEU:HD23	4:B:207:LEU:HA	1.73	0.41
4:B:213:ARG:HD2	4:B:214:LYS:HB2	2.02	0.41
6:D:133:GLY:HA3	6:D:156:LEU:O	2.21	0.41
17:O:40:THR:HG21	17:O:111:GLY:HA3	2.01	0.41
27:Y:29:HIS:CD2	27:Y:29:HIS:N	2.88	0.41
1:2:1222:G:C6	1:2:1223:A:C6	3.07	0.41
1:2:1563:G:C6	1:2:1564:C:C4	3.09	0.41
1:2:3:C:H5''	5:C:224:THR:O	2.20	0.41
1:2:748:C:O2'	1:2:749:U:OP1	2.33	0.41
4:B:117:TRP:CE2	4:B:152:LYS:HE2	2.55	0.41
4:B:62:LEU:O	4:B:65:ARG:HD2	2.20	0.41
5:C:121:ARG:HH22	5:C:123:ARG:CZ	2.32	0.41
7:E:238:LEU:HA	7:E:238:LEU:HD12	1.76	0.41
12:J:103:GLU:O	12:J:107:GLU:HG2	2.20	0.41
20:R:60:ARG:NH1	20:R:66:VAL:HG13	2.35	0.41
22:T:130:ASP:O	22:T:134:ILE:HD12	2.20	0.41
22:T:39:LEU:HD21	22:T:47:PRO:HG3	2.02	0.41
1:2:1058:A:H2'	1:2:1059:G:C8	2.56	0.41
1:2:1181:A:O2'	1:2:1182:A:C8	2.69	0.41
1:2:1544:C:H5	1:2:1588:A:OP2	2.03	0.41
1:2:1668:U:C4	1:2:1669:G:N7	2.89	0.41
1:2:148:U:C4	1:2:169:U:C4	3.08	0.41
1:2:1845:A:H2'	1:2:1846:G:C8	2.55	0.41
1:2:452:G:O2'	1:2:453:C:H5'	2.20	0.41
1:2:868:G:H5''	1:2:869:A:OP2	2.19	0.41
1:2:929:G:H2'	1:2:930:C:O4'	2.19	0.41
4:B:52:THR:HG23	4:B:56:LYS:O	2.20	0.41
6:D:5:ILE:H	6:D:5:ILE:HG13	1.68	0.41
8:F:200:ALA:O	8:F:204:ARG:HG2	2.20	0.41
8:F:80:GLY:O	8:F:83:ASN:HB2	2.21	0.41
9:G:59:GLN:HG3	9:G:72:ARG:HH21	1.81	0.41
11:I:12:ARG:HG3	11:I:16:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:15:LEU:HD22	13:K:49:MET:SD	2.60	0.41
14:L:134:LEU:HA	14:L:134:LEU:HD23	1.71	0.41
14:L:42:LEU:HD13	14:L:42:LEU:HA	1.53	0.41
1:2:1136:U:H2'	1:2:1137:U:H6	1.84	0.41
1:2:1305:C:H2'	1:2:1306:U:C6	2.55	0.41
1:2:1493:C:H4'	1:2:1494:U:H3'	2.03	0.41
1:2:527:C:O3'	12:J:121:LYS:HD3	2.20	0.41
1:2:973:C:N3	17:O:55:ARG:NH2	2.67	0.41
7:E:179:ASN:HD22	7:E:179:ASN:HA	1.68	0.41
10:H:129:ILE:HD13	10:H:180:LEU:HD13	2.03	0.41
11:I:178:ARG:O	11:I:182:CYS:HB3	2.21	0.41
14:L:63:THR:H	14:L:63:THR:HG1	1.63	0.41
14:L:99:TYR:O	14:L:100:ASN:HB2	2.20	0.41
21:S:40:TYR:HE1	21:S:79:ILE:HG21	1.85	0.41
26:X:51:VAL:HG13	26:X:70:VAL:CG1	2.50	0.41
1:2:1134:G:H2'	1:2:1135:C:C6	2.56	0.41
1:2:1724:A:H2'	1:2:1725:U:H6	1.86	0.41
1:2:71:G:H5''	1:2:72:C:OP2	2.20	0.41
5:C:192:LEU:HD22	5:C:192:LEU:HA	1.90	0.41
5:C:205:VAL:O	5:C:224:THR:HB	2.20	0.41
8:F:51:HIS:O	19:Q:50:LYS:HE3	2.21	0.41
9:G:75:LEU:HA	9:G:75:LEU:HD23	1.90	0.41
10:H:113:LYS:HA	10:H:113:LYS:HD3	1.78	0.41
21:S:31:THR:HG23	21:S:37:GLY:HA2	2.01	0.41
24:V:7:GLU:N	24:V:7:GLU:OE1	2.54	0.41
1:2:1221:G:H2'	1:2:1222:G:C8	2.56	0.41
1:2:12:U:H2'	1:2:13:C:C6	2.56	0.41
1:2:553:U:H2'	1:2:554:A:O4'	2.20	0.41
3:A:130:ASP:OD1	3:A:130:ASP:N	2.54	0.41
4:B:82:ARG:NH1	4:B:191:ASP:HB2	2.36	0.41
5:C:178:HIS:CE1	5:C:179:THR:HG22	2.56	0.41
6:D:138:VAL:HA	6:D:184:ILE:HG22	2.03	0.41
6:D:7:LYS:HD3	6:D:7:LYS:HA	1.84	0.41
7:E:125:LYS:O	7:E:141:THR:HA	2.21	0.41
10:H:100:ILE:HG21	10:H:122:LEU:HD23	2.02	0.41
13:K:60:GLU:HG2	13:K:69:TRP:NE1	2.36	0.41
6:D:67:ARG:HH21	13:K:97:SER:HB3	1.86	0.41
15:M:48:HIS:O	15:M:74:ILE:HG23	2.20	0.41
19:Q:76:GLY:O	19:Q:80:GLN:HG3	2.21	0.41
20:R:78:ARG:O	20:R:82:ASP:HB2	2.21	0.41
25:W:49:GLU:HG3	25:W:49:GLU:H	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1610:G:H2'	1:2:1611:G:O4'	2.20	0.41
4:B:62:LEU:HA	4:B:65:ARG:NE	2.34	0.41
5:C:74:LYS:HB3	5:C:269:PHE:CE1	2.55	0.41
19:Q:53:GLU:OE2	19:Q:115:TYR:OH	2.39	0.41
19:Q:21:ALA:HB2	19:Q:83:ALA:HB1	2.03	0.41
1:2:1010:G:H2'	1:2:1011:A:C8	2.56	0.41
1:2:1445:U:O2'	1:2:1446:A:OP1	2.36	0.41
1:2:1532:C:H5''	1:2:1533:A:O4'	2.21	0.41
1:2:1545:A:N6	1:2:1546:G:O6	2.54	0.41
1:2:48:C:H2'	1:2:49:C:O4'	2.21	0.41
1:2:607:U:H2'	1:2:607:U:H6	1.65	0.41
3:A:59:LEU:O	3:A:62:ALA:HB3	2.21	0.41
6:D:99:ILE:O	6:D:103:GLU:HB2	2.21	0.41
7:E:139:LEU:HG	7:E:150:PRO:HG3	2.03	0.41
7:E:180:LEU:HD12	7:E:193:GLY:O	2.21	0.41
9:G:224:ARG:HD3	9:G:224:ARG:HA	1.83	0.41
9:G:55:GLY:O	9:G:56:ASN:ND2	2.54	0.41
14:L:68:ILE:HG13	14:L:143:LEU:HD21	2.03	0.41
22:T:114:GLU:HB2	22:T:124:THR:HG22	2.03	0.41
1:2:1447:G:OP1	23:U:87:ARG:NH2	2.54	0.41
28:Z:92:LEU:HD23	28:Z:92:LEU:HA	1.96	0.41
1:2:1035:A:H2'	1:2:1036:A:O4'	2.21	0.41
1:2:1368:U:O3'	20:R:2:GLY:HA3	2.21	0.41
1:2:1518:C:H3'	1:2:1519:U:H5'	2.03	0.41
1:2:1620:A:O2'	1:2:1621:U:OP2	2.32	0.41
1:2:1724:A:H2'	1:2:1725:U:C6	2.56	0.41
1:2:1736:G:H2'	1:2:1737:G:H8	1.83	0.41
1:2:1784:G:C2'	1:2:1785:C:H5'	2.51	0.41
1:2:293:C:H2'	1:2:293:C:O2	2.19	0.41
1:2:383:G:C6	1:2:384:U:N3	2.89	0.41
1:2:415:A:H2'	1:2:416:U:O4'	2.21	0.41
1:2:679:A:H2'	1:2:680:G:H5'	2.03	0.41
1:2:941:C:H5''	4:B:136:ARG:HH21	1.84	0.41
1:2:967:C:H3'	1:2:968:U:H5''	2.03	0.41
5:C:206:SER:HB3	5:C:224:THR:CB	2.50	0.41
7:E:11:ARG:HD3	7:E:27:PHE:O	2.21	0.41
9:G:57:ASP:O	9:G:60:GLY:N	2.51	0.41
11:I:65:PHE:HB2	11:I:109:TYR:OH	2.20	0.41
11:I:3:ILE:O	11:I:30:GLY:N	2.27	0.41
14:L:61:PRO:HA	14:L:66:VAL:HG22	2.01	0.41
20:R:100:PRO:O	20:R:103:LYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:93:SER:HB2	23:U:94:PRO:HD2	2.03	0.41
1:2:1026:C:H4'	1:2:1161:U:H4'	2.03	0.41
1:2:219:U:H4'	11:I:182:CYS:SG	2.60	0.41
1:2:528:A:H2'	1:2:529:A:O4'	2.20	0.41
1:2:639:C:O2'	1:2:640:A:C8	2.64	0.41
1:2:969:U:OP2	1:2:970:G:H5'	2.21	0.41
2:3:259:U:H2'	2:3:260:A:H5'	2.02	0.41
5:C:116:THR:HG22	5:C:117:ARG:N	2.35	0.41
6:D:174:HIS:HB3	6:D:181:VAL:HG11	2.03	0.41
9:G:168:LYS:HA	9:G:169:PRO:HD3	1.92	0.41
12:J:25:LEU:HA	12:J:40:LYS:NZ	2.36	0.41
15:M:85:LEU:HB3	15:M:106:CYS:O	2.21	0.41
17:O:32:HIS:N	17:O:32:HIS:CD2	2.89	0.41
25:W:84:LYS:H	25:W:84:LYS:HG3	1.67	0.41
1:2:1088:U:H4'	1:2:1089:G:OP2	2.22	0.40
1:2:1325:G:H5'	1:2:1326:U:P	2.61	0.40
1:2:1428:G:N2	1:2:1585:U:H5''	2.35	0.40
1:2:1572:C:C4	1:2:1573:G:C8	3.09	0.40
1:2:1654:G:OP1	22:T:90:SER:HB2	2.21	0.40
1:2:1842:C:H2'	1:2:1843:G:C8	2.56	0.40
2:3:230:G:HO2'	2:3:231:G:P	2.42	0.40
2:3:245:G:H8	2:3:245:G:OP1	2.03	0.40
2:3:42:C:H42	2:3:120:C:N4	2.09	0.40
4:B:146:ARG:HA	4:B:146:ARG:NH1	2.35	0.40
7:E:216:ASN:H	7:E:216:ASN:ND2	2.19	0.40
7:E:11:ARG:HA	7:E:28:ALA:HB2	2.03	0.40
7:E:79:ASP:OD1	7:E:82:TYR:N	2.54	0.40
9:G:22:ARG:O	9:G:25:ARG:HB2	2.20	0.40
9:G:76:LEU:HB2	9:G:94:ARG:NH1	2.36	0.40
10:H:162:GLN:O	10:H:165:ASN:HB3	2.21	0.40
14:L:69:ARG:HH22	14:L:132:ARG:HA	1.86	0.40
18:P:67:ALA:HA	18:P:68:PRO:HD3	1.97	0.40
1:2:1643:U:H1'	19:Q:142:GLN:HG2	2.03	0.40
22:T:37:VAL:HG13	22:T:38:LYS:O	2.21	0.40
22:T:6:VAL:HB	22:T:65:TYR:CZ	2.56	0.40
24:V:70:LEU:HA	24:V:70:LEU:HD23	1.87	0.40
26:X:130:LEU:HD23	26:X:130:LEU:HA	1.70	0.40
1:2:102:A:HO2'	1:2:103:A:P	2.44	0.40
1:2:1595:U:OP1	28:Z:102:LYS:NZ	2.40	0.40
1:2:1617:G:H3'	1:2:1618:C:C5'	2.51	0.40
1:2:440:G:O2'	1:2:441:C:OP1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:166:LYS:HD2	3:A:166:LYS:HA	1.63	0.40
6:D:175:VAL:HG12	6:D:182:LEU:O	2.21	0.40
6:D:196:GLY:O	6:D:197:LYS:HB2	2.21	0.40
7:E:164:LEU:HD23	7:E:164:LEU:HA	1.79	0.40
7:E:242:LYS:HD3	7:E:242:LYS:HA	1.60	0.40
7:E:105:THR:HG21	7:E:245:ARG:HA	2.03	0.40
1:2:441:C:OP2	11:I:2:GLY:HA3	2.21	0.40
16:N:30:SER:HA	16:N:67:THR:HG22	2.03	0.40
27:Y:114:MET:O	27:Y:122:LYS:HE2	2.21	0.40
27:Y:42:GLU:OE2	27:Y:52:PRO:HB3	2.21	0.40
28:Z:63:PRO:O	28:Z:111:ARG:HB2	2.20	0.40
1:2:1580:A:H5'	23:U:57:PRO:HD2	2.03	0.40
1:2:1667:U:C4	1:2:1668:U:C4	3.09	0.40
1:2:1745:A:H2'	1:2:1746:U:C6	2.56	0.40
1:2:27:A:H2'	1:2:28:U:O4'	2.21	0.40
1:2:819:G:C6	1:2:820:U:C4	3.09	0.40
7:E:129:ILE:HA	7:E:138:HIS:O	2.21	0.40
8:F:165:ASN:OD1	8:F:167:LYS:HB2	2.21	0.40
9:G:54:GLY:HA3	9:G:110:ASN:ND2	2.36	0.40
12:J:121:LYS:HE3	12:J:121:LYS:HB2	1.65	0.40
12:J:111:GLN:CD	12:J:127:ARG:HB2	2.42	0.40
15:M:38:ALA:HB1	15:M:110:VAL:HG23	2.03	0.40
15:M:64:LEU:HA	15:M:64:LEU:HD23	1.93	0.40
15:M:22:LEU:HD12	15:M:88:TRP:HB3	2.03	0.40
21:S:38:ARG:O	21:S:42:HIS:ND1	2.51	0.40
1:2:1297:U:O2'	1:2:1301:A:N6	2.55	0.40
1:2:141:A:N7	1:2:178:C:H1'	2.36	0.40
1:2:846:G:OP2	7:E:108:ARG:NH2	2.53	0.40
1:2:905:C:H2'	1:2:906:U:O4'	2.22	0.40
2:3:70:A:H5'	2:3:71:G:OP2	2.22	0.40
3:A:108:PHE:HD2	3:A:136:GLU:HB3	1.86	0.40
3:A:136:GLU:O	3:A:140:VAL:HG23	2.22	0.40
7:E:128:LYS:O	7:E:140:VAL:HG23	2.21	0.40
7:E:160:ILE:HD12	7:E:162:ILE:HD11	2.03	0.40
7:E:43:PRO:CG	7:E:46:ILE:HD13	2.50	0.40
16:N:101:HIS:ND1	16:N:101:HIS:O	2.55	0.40
19:Q:11:GLN:OE1	19:Q:24:HIS:HD2	2.05	0.40
1:2:1623:A:N9	21:S:132:ARG:HD2	2.36	0.40
1:2:619:A:C6	26:X:114:ASP:HB2	2.56	0.40
1:2:1309:C:H2'	1:2:1310:U:O4'	2.21	0.40
1:2:149:A:OP2	41:2:2010:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:604:A:C8	1:2:604:A:H3'	2.55	0.40
1:2:650:A:OP2	26:X:108:LYS:HE2	2.21	0.40
5:C:192:LEU:HB3	5:C:227:ARG:HG3	2.04	0.40
5:C:82:TYR:HD1	5:C:82:TYR:HA	1.74	0.40
7:E:149:TYR:CD2	9:G:205:GLU:HB3	2.56	0.40
20:R:20:TYR:CE1	20:R:38:ILE:HG23	2.55	0.40
25:W:30:CYS:HB2	25:W:61:ILE:CD1	2.52	0.40
25:W:41:MET:HG2	25:W:129:PHE:CE1	2.56	0.40
27:Y:20:ARG:HD3	27:Y:76:TYR:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	214/295 (72%)	202 (94%)	11 (5%)	1 (0%)	31	71
4	B	211/264 (80%)	200 (95%)	11 (5%)	0	100	100
5	C	216/293 (74%)	213 (99%)	3 (1%)	0	100	100
6	D	223/243 (92%)	214 (96%)	8 (4%)	1 (0%)	36	74
7	E	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
8	F	187/204 (92%)	169 (90%)	16 (9%)	2 (1%)	16	56
9	G	228/249 (92%)	217 (95%)	11 (5%)	0	100	100
10	H	184/194 (95%)	172 (94%)	11 (6%)	1 (0%)	31	71
11	I	203/208 (98%)	196 (97%)	7 (3%)	0	100	100
12	J	178/194 (92%)	172 (97%)	5 (3%)	1 (1%)	27	67
13	K	93/165 (56%)	89 (96%)	4 (4%)	0	100	100
14	L	149/158 (94%)	145 (97%)	4 (3%)	0	100	100
15	M	121/132 (92%)	112 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	N	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
17	O	133/151 (88%)	127 (96%)	6 (4%)	0	100	100
18	P	118/145 (81%)	116 (98%)	2 (2%)	0	100	100
19	Q	137/146 (94%)	131 (96%)	6 (4%)	0	100	100
20	R	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
21	S	141/152 (93%)	136 (96%)	5 (4%)	0	100	100
22	T	143/146 (98%)	138 (96%)	4 (3%)	1 (1%)	24	64
23	U	99/119 (83%)	94 (95%)	5 (5%)	0	100	100
24	V	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
25	W	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
26	X	139/143 (97%)	130 (94%)	8 (6%)	1 (1%)	24	64
27	Y	122/130 (94%)	118 (97%)	4 (3%)	0	100	100
28	Z	70/125 (56%)	66 (94%)	4 (6%)	0	100	100
29	a	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
30	b	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
31	c	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
32	d	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
33	e	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
34	f	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
35	g	312/315 (99%)	295 (95%)	15 (5%)	2 (1%)	27	67
36	h	22/24 (92%)	22 (100%)	0	0	100	100
37	r	11/13 (85%)	11 (100%)	0	0	100	100
38	w	47/62 (76%)	47 (100%)	0	0	100	100
All	All	4860/5459 (89%)	4641 (96%)	209 (4%)	10 (0%)	53	83

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	189	ILE
10	H	170	VAL
12	J	161	LEU
35	g	145	GLU
26	X	108	LYS
8	F	163	PHE

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Mol	Chain	Res	Type
35	g	119	GLN
6	D	193	ASP
22	T	4	VAL
8	F	166	ILE

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	
3	A	180/243 (74%)	159 (88%)	21 (12%)	6	30
4	B	194/231 (84%)	175 (90%)	19 (10%)	9	36
5	C	184/225 (82%)	140 (76%)	44 (24%)	1	6
6	D	189/202 (94%)	177 (94%)	12 (6%)	20	54
7	E	224/225 (100%)	189 (84%)	35 (16%)	3	20
8	F	159/170 (94%)	149 (94%)	10 (6%)	20	54
9	G	200/218 (92%)	180 (90%)	20 (10%)	8	35
10	H	167/174 (96%)	152 (91%)	15 (9%)	10	41
11	I	178/180 (99%)	153 (86%)	25 (14%)	4	25
12	J	160/168 (95%)	135 (84%)	25 (16%)	3	20
13	K	86/136 (63%)	85 (99%)	1 (1%)	74	87
14	L	135/142 (95%)	104 (77%)	31 (23%)	1	7
15	M	104/108 (96%)	99 (95%)	5 (5%)	28	61
16	N	130/131 (99%)	112 (86%)	18 (14%)	4	25
17	O	105/119 (88%)	87 (83%)	18 (17%)	2	16
18	P	107/130 (82%)	102 (95%)	5 (5%)	29	62
19	Q	115/121 (95%)	104 (90%)	11 (10%)	9	37
20	R	118/122 (97%)	104 (88%)	14 (12%)	6	29
21	S	124/132 (94%)	118 (95%)	6 (5%)	28	61
22	T	115/116 (99%)	108 (94%)	7 (6%)	20	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	93/107 (87%)	87 (94%)	6 (6%)	19	53
24	V	66/67 (98%)	50 (76%)	16 (24%)	1	6
25	W	112/113 (99%)	91 (81%)	21 (19%)	1	13
26	X	113/115 (98%)	103 (91%)	10 (9%)	11	42
27	Y	108/112 (96%)	95 (88%)	13 (12%)	5	29
28	Z	64/103 (62%)	60 (94%)	4 (6%)	20	54
29	a	89/89 (100%)	76 (85%)	13 (15%)	3	22
30	b	74/74 (100%)	63 (85%)	11 (15%)	3	22
31	c	54/54 (100%)	51 (94%)	3 (6%)	23	58
32	d	48/48 (100%)	45 (94%)	3 (6%)	20	54
33	e	45/45 (100%)	36 (80%)	9 (20%)	1	11
34	f	65/65 (100%)	62 (95%)	3 (5%)	29	62
35	g	272/273 (100%)	257 (94%)	15 (6%)	24	58
36	h	23/23 (100%)	20 (87%)	3 (13%)	4	26
37	r	12/12 (100%)	11 (92%)	1 (8%)	12	45
38	w	35/35 (100%)	33 (94%)	2 (6%)	23	57
All	All	4247/4628 (92%)	3772 (89%)	475 (11%)	10	32

All (475) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	14	ASP
3	A	29	ASN
3	A	53	ARG
3	A	80	ARG
3	A	94	THR
3	A	111	GLN
3	A	112	ILE
3	A	120	ARG
3	A	130	ASP
3	A	131	HIS
3	A	136	GLU
3	A	138	SER
3	A	140	VAL
3	A	145	ILE
3	A	163	CYS

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Mol	Chain	Res	Type
3	A	178	LEU
3	A	180	ARG
3	A	185	MET
3	A	186	ARG
3	A	188	THR
3	A	200	ASP
4	B	25	PHE
4	B	33	VAL
4	B	38	MET
4	B	77	ASP
4	B	79	VAL
4	B	95	ASN
4	B	98	THR
4	B	103	MET
4	B	106	THR
4	B	107	ARG
4	B	131	ASP
4	B	136	ARG
4	B	146	ARG
4	B	163	GLN
4	B	169	MET
4	B	174	ARG
4	B	181	LEU
4	B	213	ARG
4	B	217	MET
5	C	73	MET
5	C	80	GLU
5	C	83	LEU
5	C	94	ILE
5	C	97	PHE
5	C	98	LEU
5	C	101	SER
5	C	112	VAL
5	C	113	GLN
5	C	120	GLN
5	C	121	ARG
5	C	123	ARG
5	C	125	LYS
5	C	132	ASP
5	C	134	ASN
5	C	143	CYS
5	C	147	VAL

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Mol	Chain	Res	Type
5	C	156	ILE
5	C	157	LEU
5	C	160	LEU
5	C	161	SER
5	C	165	VAL
5	C	167	ARG
5	C	172	ASN
5	C	180	VAL
5	C	190	SER
5	C	196	ILE
5	C	204	ILE
5	C	212	LYS
5	C	215	MET
5	C	221	ASP
5	C	227	ARG
5	C	230	THR
5	C	232	THR
5	C	236	PHE
5	C	240	THR
5	C	242	ASP
5	C	244	ILE
5	C	247	THR
5	C	249	SER
5	C	252	THR
5	C	260	VAL
5	C	271	ASP
5	C	276	THR
6	D	3	VAL
6	D	54	ARG
6	D	70	THR
6	D	126	ILE
6	D	134	CYS
6	D	146	ARG
6	D	152	PHE
6	D	164	VAL
6	D	176	LEU
6	D	195	THR
6	D	198	ILE
6	D	206	ASP
7	E	11	ARG
7	E	19	MET
7	E	23	LEU

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Mol	Chain	Res	Type
7	E	29	PRO
7	E	38	LEU
7	E	39	ARG
7	E	40	GLU
7	E	42	LEU
7	E	45	ILE
7	E	49	ARG
7	E	51	ARG
7	E	59	ASP
7	E	77	ARG
7	E	88	ASP
7	E	95	THR
7	E	102	ILE
7	E	108	ARG
7	E	114	ILE
7	E	140	VAL
7	E	143	ASP
7	E	145	ARG
7	E	151	ASP
7	E	160	ILE
7	E	169	ILE
7	E	171	ASP
7	E	181	CYS
7	E	191	ARG
7	E	198	ARG
7	E	204	SER
7	E	225	ILE
7	E	238	LEU
7	E	240	ARG
7	E	242	LYS
7	E	247	THR
7	E	248	ILE
8	F	68	ILE
8	F	82	ASN
8	F	91	ARG
8	F	122	ARG
8	F	130	ARG
8	F	134	VAL
8	F	140	ASP
8	F	166	ILE
8	F	176	GLU
8	F	204	ARG

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Mol	Chain	Res	Type
9	G	16	ILE
9	G	19	ASP
9	G	20	ASP
9	G	51	ARG
9	G	52	ILE
9	G	57	ASP
9	G	67	VAL
9	G	69	THR
9	G	81	HIS
9	G	84	TYR
9	G	85	ARG
9	G	91	GLU
9	G	98	ARG
9	G	100	CYS
9	G	105	ASN
9	G	110	ASN
9	G	144	LEU
9	G	151	ASP
9	G	152	ASP
9	G	181	THR
10	H	12	ASN
10	H	46	THR
10	H	51	ILE
10	H	70	LYS
10	H	75	ILE
10	H	84	GLU
10	H	87	PHE
10	H	105	THR
10	H	121	THR
10	H	122	LEU
10	H	123	THR
10	H	134	VAL
10	H	153	LEU
10	H	180	LEU
10	H	184	ASP
11	I	5	ARG
11	I	17	LYS
11	I	18	ARG
11	I	22	HIS
11	I	29	LEU
11	I	35	ASN
11	I	47	ARG

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Mol	Chain	Res	Type
11	I	49	ARG
11	I	62	VAL
11	I	72	CYS
11	I	87	ASN
11	I	95	THR
11	I	106	SER
11	I	121	LEU
11	I	128	LYS
11	I	130	THR
11	I	144	LYS
11	I	170	LYS
11	I	175	ILE
11	I	177	SER
11	I	178	ARG
11	I	184	ARG
11	I	191	GLU
11	I	194	GLU
11	I	196	GLU
12	J	3	VAL
12	J	12	THR
12	J	21	GLU
12	J	29	LEU
12	J	42	GLU
12	J	50	LEU
12	J	61	LEU
12	J	70	ARG
12	J	83	ARG
12	J	88	ASP
12	J	94	LEU
12	J	95	ASP
12	J	102	ILE
12	J	104	ASP
12	J	108	ARG
12	J	122	SER
12	J	128	VAL
12	J	131	ARG
12	J	132	GLN
12	J	136	ARG
12	J	144	ILE
12	J	150	ARG
12	J	153	SER
12	J	156	HIS

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Mol	Chain	Res	Type
12	J	161	LEU
13	K	52	LEU
14	L	3	ASP
14	L	5	GLN
14	L	6	THR
14	L	13	GLN
14	L	15	THR
14	L	18	GLN
14	L	35	ARG
14	L	40	ILE
14	L	42	LEU
14	L	45	LYS
14	L	46	THR
14	L	48	LYS
14	L	52	GLU
14	L	60	CYS
14	L	69	ARG
14	L	71	ARG
14	L	74	SER
14	L	76	VAL
14	L	78	THR
14	L	80	MET
14	L	83	GLN
14	L	85	THR
14	L	89	ARG
14	L	101	ARG
14	L	104	LYS
14	L	121	GLN
14	L	128	VAL
14	L	132	ARG
14	L	135	SER
14	L	144	LYS
14	L	146	THR
15	M	26	LEU
15	M	35	ILE
15	M	36	ARG
15	M	45	ARG
15	M	104	VAL
16	N	12	SER
16	N	14	SER
16	N	29	THR
16	N	62	GLN

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Mol	Chain	Res	Type
16	N	71	ILE
16	N	75	LEU
16	N	77	SER
16	N	80	LEU
16	N	83	ASP
16	N	84	LEU
16	N	101	HIS
16	N	106	ARG
16	N	125	LEU
16	N	127	ARG
16	N	132	LYS
16	N	138	ASN
16	N	143	SER
16	N	145	THR
17	O	36	SER
17	O	45	THR
17	O	52	THR
17	O	57	THR
17	O	67	ASP
17	O	70	SER
17	O	98	ARG
17	O	100	THR
17	O	103	ASN
17	O	105	THR
17	O	116	LEU
17	O	121	ARG
17	O	128	ARG
17	O	133	THR
17	O	137	SER
17	O	140	THR
17	O	146	ARG
17	O	150	ARG
18	P	44	ARG
18	P	51	ARG
18	P	78	THR
18	P	79	HIS
18	P	122	THR
19	Q	18	THR
19	Q	42	ILE
19	Q	43	GLU
19	Q	46	THR
19	Q	52	LEU

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Mol	Chain	Res	Type
19	Q	121	VAL
19	Q	125	ARG
19	Q	130	LYS
19	Q	142	GLN
19	Q	143	LYS
19	Q	145	TYR
20	R	5	ARG
20	R	8	THR
20	R	17	ILE
20	R	34	VAL
20	R	35	CYS
20	R	78	ARG
20	R	83	ASN
20	R	85	VAL
20	R	101	ASP
20	R	124	VAL
20	R	126	MET
20	R	127	ASN
20	R	128	PHE
20	R	132	ARG
21	S	4	VAL
21	S	14	ARG
21	S	19	ASN
21	S	71	MET
21	S	129	LEU
21	S	138	THR
22	T	27	LYS
22	T	56	ARG
22	T	67	ARG
22	T	78	ILE
22	T	83	GLN
22	T	87	VAL
22	T	131	LEU
23	U	36	CYS
23	U	55	ARG
23	U	61	LEU
23	U	68	THR
23	U	74	SER
23	U	115	THR
24	V	1	MET
24	V	2	GLN
24	V	4	ASP

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Mol	Chain	Res	Type
24	V	7	GLU
24	V	9	VAL
24	V	15	ARG
24	V	18	SER
24	V	21	ASN
24	V	31	SER
24	V	34	MET
24	V	43	THR
24	V	62	MET
24	V	67	ASP
24	V	68	SER
24	V	70	LEU
24	V	76	ASP
25	W	4	MET
25	W	13	SER
25	W	14	ILE
25	W	23	ARG
25	W	27	ILE
25	W	30	CYS
25	W	39	THR
25	W	40	VAL
25	W	47	ILE
25	W	49	GLU
25	W	56	HIS
25	W	57	ARG
25	W	80	ASP
25	W	83	LEU
25	W	85	ASP
25	W	97	ARG
25	W	104	LEU
25	W	105	THR
25	W	106	THR
25	W	107	SER
25	W	125	ILE
26	X	5	ARG
26	X	9	THR
26	X	14	ARG
26	X	15	SER
26	X	37	LYS
26	X	76	LYS
26	X	100	VAL
26	X	105	PHE

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Mol	Chain	Res	Type
26	X	107	ARG
26	X	119	ARG
27	Y	5	VAL
27	Y	14	THR
27	Y	17	LEU
27	Y	23	MET
27	Y	29	HIS
27	Y	35	VAL
27	Y	42	GLU
27	Y	46	LYS
27	Y	54	VAL
27	Y	55	ILE
27	Y	94	HIS
27	Y	107	ARG
27	Y	117	VAL
28	Z	50	PHE
28	Z	65	TYR
28	Z	88	LEU
28	Z	107	VAL
29	a	2	THR
29	a	6	ARG
29	a	7	ASN
29	a	17	HIS
29	a	18	VAL
29	a	21	ILE
29	a	29	CYS
29	a	43	ASN
29	a	53	ILE
29	a	64	LEU
29	a	72	HIS
29	a	78	VAL
29	a	81	SER
30	b	3	LEU
30	b	17	ARG
30	b	20	LYS
30	b	23	ARG
30	b	37	CYS
30	b	43	ILE
30	b	53	VAL
30	b	54	VAL
30	b	56	CYS
30	b	63	LEU

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Mol	Chain	Res	Type
30	b	83	GLN
31	c	26	GLN
31	c	37	ASP
31	c	55	VAL
32	d	8	TRP
32	d	28	HIS
32	d	40	ARG
33	e	5	SER
33	e	8	ARG
33	e	11	LYS
33	e	12	VAL
33	e	27	LYS
33	e	29	THR
33	e	34	ARG
33	e	45	VAL
33	e	58	ASN
34	f	86	THR
34	f	98	VAL
34	f	116	ARG
35	g	31	ILE
35	g	46	THR
35	g	65	PHE
35	g	74	ASP
35	g	96	THR
35	g	97	THR
35	g	102	VAL
35	g	110	SER
35	g	118	ARG
35	g	155	ARG
35	g	195	LEU
35	g	272	GLN
35	g	297	THR
35	g	306	LEU
35	g	309	VAL
36	h	9	ARG
36	h	14	LYS
36	h	23	ARG
37	r	162	ARG
38	w	91	MET
38	w	94	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	111	GLN
3	A	132	GLN
3	A	141	ASN
4	B	40	ASN
4	B	159	GLN
5	C	178	HIS
6	D	56	GLN
6	D	74	GLN
6	D	174	HIS
6	D	179	GLN
7	E	8	HIS
7	E	112	HIS
7	E	179	ASN
7	E	214	ASN
7	E	216	ASN
8	F	83	ASN
8	F	137	GLN
8	F	203	ASN
9	G	59	GLN
9	G	65	GLN
9	G	105	ASN
9	G	146	ASN
10	H	76	GLN
10	H	157	HIS
11	I	22	HIS
11	I	84	ASN
11	I	87	ASN
11	I	168	GLN
12	J	124	HIS
12	J	125	HIS
13	K	61	GLN
14	L	11	GLN
14	L	65	ASN
16	N	58	HIS
16	N	105	ASN
17	O	32	HIS
17	O	43	HIS
18	P	53	GLN
18	P	79	HIS
19	Q	24	HIS
19	Q	77	HIS
19	Q	142	GLN
21	S	72	GLN

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Mol	Chain	Res	Type
21	S	101	ASN
26	X	31	HIS
26	X	61	GLN
26	X	63	ASN
27	Y	63	HIS
28	Z	46	ASN
28	Z	103	HIS
31	c	29	GLN
32	d	3	HIS
33	e	37	GLN
33	e	56	ASN
34	f	111	ASN
35	g	20	GLN
35	g	147	HIS
35	g	178	ASN
38	w	95	ASN
38	w	96	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1656/1868 (88%)	595 (35%)	83 (5%)
2	3	254/257 (98%)	148 (58%)	25 (9%)
All	All	1910/2125 (89%)	743 (38%)	108 (5%)

All (743) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	4	C
1	2	5	U
1	2	8	U
1	2	9	U
1	2	17	C
1	2	23	G
1	2	25	A
1	2	26	U
1	2	31	U
1	2	33	G
1	2	37	C
1	2	41	G

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Mol	Chain	Res	Type
1	2	46	A
1	2	49	C
1	2	50	A
1	2	56	G
1	2	58	C
1	2	60	A
1	2	61	A
1	2	63	U
1	2	65	C
1	2	66	G
1	2	67	C
1	2	68	A
1	2	69	C
1	2	70	G
1	2	71	G
1	2	72	C
1	2	75	G
1	2	76	U
1	2	77	A
1	2	78	C
1	2	79	A
1	2	81	U
1	2	102	A
1	2	103	A
1	2	104	A
1	2	110	U
1	2	111	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	116	U
1	2	123	G
1	2	124	U
1	2	125	C
1	2	126	G
1	2	127	C
1	2	129	C
1	2	130	G
1	2	141	A
1	2	142	C
1	2	143	U
1	2	144	U

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Mol	Chain	Res	Type
1	2	150	A
1	2	153	G
1	2	154	U
1	2	155	G
1	2	163	U
1	2	167	G
1	2	168	C
1	2	170	A
1	2	173	A
1	2	175	A
1	2	179	C
1	2	181	A
1	2	182	C
1	2	184	G
1	2	188	C
1	2	189	U
1	2	190	G
1	2	191	A
1	2	192	C
1	2	200	G
1	2	206	G
1	2	209	A
1	2	210	U
1	2	213	G
1	2	214	U
1	2	215	G
1	2	216	C
1	2	217	A
1	2	290	U
1	2	291	G
1	2	292	A
1	2	294	U
1	2	295	C
1	2	297	A
1	2	302	A
1	2	307	G
1	2	308	G
1	2	310	C
1	2	311	C
1	2	312	G
1	2	315	C
1	2	317	C

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Mol	Chain	Res	Type
1	2	319	C
1	2	320	G
1	2	321	C
1	2	332	G
1	2	333	G
1	2	334	C
1	2	335	G
1	2	336	A
1	2	338	G
1	2	339	A
1	2	342	C
1	2	347	G
1	2	351	G
1	2	360	A
1	2	362	C
1	2	364	A
1	2	368	U
1	2	369	C
1	2	370	G
1	2	377	G
1	2	381	C
1	2	382	C
1	2	383	G
1	2	384	U
1	2	385	G
1	2	386	C
1	2	398	A
1	2	400	C
1	2	407	G
1	2	408	A
1	2	409	C
1	2	417	C
1	2	418	A
1	2	421	G
1	2	425	G
1	2	426	A
1	2	427	U
1	2	434	G
1	2	438	G
1	2	441	C
1	2	447	A
1	2	448	A

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Mol	Chain	Res	Type
1	2	450	C
1	2	453	C
1	2	454	U
1	2	464	A
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	476	A
1	2	482	G
1	2	485	A
1	2	487	U
1	2	489	A
1	2	492	C
1	2	496	C
1	2	500	A
1	2	502	C
1	2	507	G
1	2	508	A
1	2	509	G
1	2	523	A
1	2	530	U
1	2	531	A
1	2	532	C
1	2	534	G
1	2	535	G
1	2	536	A
1	2	537	C
1	2	542	U
1	2	544	G
1	2	546	G
1	2	548	C
1	2	550	C
1	2	552	G
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	562	U
1	2	563	G

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Mol	Chain	Res	Type
1	2	564	A
1	2	568	C
1	2	570	C
1	2	576	A
1	2	583	A
1	2	585	C
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	593	C
1	2	594	A
1	2	595	U
1	2	596	U
1	2	598	G
1	2	601	G
1	2	602	G
1	2	603	C
1	2	604	A
1	2	605	A
1	2	606	G
1	2	607	U
1	2	608	C
1	2	614	C
1	2	615	C
1	2	616	A
1	2	617	G
1	2	618	C
1	2	621	C
1	2	626	G
1	2	627	U
1	2	628	A
1	2	629	A
1	2	631	U
1	2	632	C
1	2	638	C
1	2	639	C
1	2	640	A
1	2	643	A
1	2	644	G
1	2	647	U

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Mol	Chain	Res	Type
1	2	657	U
1	2	658	U
1	2	659	G
1	2	660	C
1	2	668	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	683	G
1	2	684	G
1	2	685	A
1	2	686	U
1	2	687	C
1	2	688	U
1	2	748	C
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C
1	2	793	G
1	2	794	A
1	2	796	G
1	2	797	C
1	2	798	G
1	2	799	U
1	2	807	G
1	2	808	A
1	2	809	A
1	2	810	A
1	2	811	A
1	2	812	A
1	2	818	A
1	2	821	G
1	2	822	U
1	2	823	U
1	2	824	C
1	2	830	A
1	2	834	C
1	2	842	C
1	2	843	C

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Mol	Chain	Res	Type
1	2	845	G
1	2	847	A
1	2	852	G
1	2	856	C
1	2	861	A
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	877	C
1	2	878	G
1	2	880	G
1	2	881	G
1	2	882	U
1	2	887	U
1	2	888	U
1	2	890	U
1	2	898	U
1	2	903	A
1	2	909	G
1	2	913	A
1	2	914	U
1	2	917	U
1	2	918	U
1	2	919	A
1	2	920	A
1	2	922	A
1	2	926	A
1	2	931	C
1	2	933	G
1	2	934	G
1	2	938	A
1	2	943	U
1	2	954	U
1	2	959	G
1	2	962	A
1	2	968	U
1	2	969	U
1	2	970	G
1	2	971	G
1	2	978	G

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Mol	Chain	Res	Type
1	2	980	A
1	2	981	A
1	2	983	A
1	2	985	G
1	2	990	A
1	2	992	A
1	2	996	A
1	2	997	A
1	2	999	G
1	2	1001	A
1	2	1008	A
1	2	1009	A
1	2	1017	U
1	2	1023	A
1	2	1030	A
1	2	1033	G
1	2	1040	G
1	2	1041	G
1	2	1042	A
1	2	1045	U
1	2	1049	A
1	2	1053	C
1	2	1054	G
1	2	1060	A
1	2	1061	U
1	2	1067	C
1	2	1078	C
1	2	1083	A
1	2	1085	C
1	2	1087	A
1	2	1088	U
1	2	1089	G
1	2	1096	G
1	2	1099	G
1	2	1100	A
1	2	1110	G
1	2	1111	U
1	2	1112	U
1	2	1114	U
1	2	1116	C
1	2	1119	A
1	2	1121	G

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Mol	Chain	Res	Type
1	2	1122	A
1	2	1123	C
1	2	1124	C
1	2	1130	G
1	2	1131	G
1	2	1133	A
1	2	1137	U
1	2	1138	C
1	2	1139	C
1	2	1143	A
1	2	1148	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1157	G
1	2	1171	G
1	2	1181	A
1	2	1182	A
1	2	1194	A
1	2	1195	A
1	2	1202	U
1	2	1207	G
1	2	1208	A
1	2	1211	G
1	2	1213	C
1	2	1215	C
1	2	1216	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1232	U
1	2	1233	G
1	2	1235	G
1	2	1238	U
1	2	1242	U
1	2	1243	U
1	2	1248	U
1	2	1249	C
1	2	1250	A
1	2	1251	A
1	2	1253	A

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Mol	Chain	Res	Type
1	2	1254	C
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1260	A
1	2	1261	C
1	2	1266	C
1	2	1274	G
1	2	1275	G
1	2	1283	C
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1288	U
1	2	1298	G
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1308	U
1	2	1309	C
1	2	1313	A
1	2	1315	U
1	2	1317	C
1	2	1320	G
1	2	1321	G
1	2	1322	G
1	2	1326	U
1	2	1327	G
1	2	1330	G
1	2	1331	C
1	2	1343	U
1	2	1344	A
1	2	1348	G
1	2	1358	U
1	2	1364	U
1	2	1366	G
1	2	1367	U
1	2	1371	U
1	2	1372	U
1	2	1373	C
1	2	1377	U
1	2	1378	A

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Mol	Chain	Res	Type
1	2	1380	C
1	2	1381	G
1	2	1382	A
1	2	1385	G
1	2	1401	A
1	2	1404	U
1	2	1405	A
1	2	1406	G
1	2	1416	C
1	2	1426	U
1	2	1427	C
1	2	1428	G
1	2	1429	G
1	2	1430	C
1	2	1431	G
1	2	1432	U
1	2	1439	A
1	2	1441	U
1	2	1442	U
1	2	1444	U
1	2	1446	A
1	2	1448	A
1	2	1452	A
1	2	1454	A
1	2	1455	A
1	2	1462	U
1	2	1463	U
1	2	1464	C
1	2	1465	A
1	2	1466	G
1	2	1468	C
1	2	1473	G
1	2	1474	A
1	2	1477	U
1	2	1478	U
1	2	1483	A
1	2	1486	A
1	2	1487	A
1	2	1489	A
1	2	1490	G
1	2	1493	C
1	2	1494	U

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Mol	Chain	Res	Type
1	2	1495	G
1	2	1499	U
1	2	1500	G
1	2	1505	U
1	2	1507	G
1	2	1508	A
1	2	1510	G
1	2	1512	C
1	2	1515	G
1	2	1516	G
1	2	1518	C
1	2	1519	U
1	2	1520	G
1	2	1521	C
1	2	1523	C
1	2	1524	G
1	2	1526	G
1	2	1533	A
1	2	1535	U
1	2	1536	G
1	2	1543	U
1	2	1545	A
1	2	1548	G
1	2	1559	C
1	2	1560	U
1	2	1561	A
1	2	1563	G
1	2	1566	G
1	2	1567	G
1	2	1568	C
1	2	1572	C
1	2	1573	G
1	2	1574	C
1	2	1578	U
1	2	1579	A
1	2	1580	A
1	2	1581	C
1	2	1585	U
1	2	1586	U
1	2	1587	G
1	2	1588	A
1	2	1598	G

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Mol	Chain	Res	Type
1	2	1599	U
1	2	1600	G
1	2	1601	A
1	2	1602	U
1	2	1603	G
1	2	1604	G
1	2	1606	G
1	2	1610	G
1	2	1612	G
1	2	1617	G
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1625	U
1	2	1630	A
1	2	1632	G
1	2	1634	A
1	2	1641	A
1	2	1645	C
1	2	1648	G
1	2	1649	U
1	2	1650	A
1	2	1654	G
1	2	1660	C
1	2	1663	A
1	2	1664	A
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1678	A
1	2	1682	C
1	2	1683	C
1	2	1688	C
1	2	1689	C
1	2	1695	A
1	2	1699	A
1	2	1721	U
1	2	1722	G
1	2	1728	U
1	2	1729	U
1	2	1737	G
1	2	1742	C

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Mol	Chain	Res	Type
1	2	1744	G
1	2	1745	A
1	2	1746	U
1	2	1761	U
1	2	1777	G
1	2	1778	C
1	2	1779	G
1	2	1783	C
1	2	1784	G
1	2	1785	C
1	2	1786	U
1	2	1800	A
1	2	1805	G
1	2	1807	C
1	2	1815	A
1	2	1826	G
1	2	1829	G
1	2	1831	A
1	2	1835	A
1	2	1836	G
1	2	1838	U
1	2	1839	U
1	2	1841	C
1	2	1849	G
1	2	1851	A
1	2	1852	C
1	2	1855	G
1	2	1859	A
1	2	1860	A
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1865	C
1	2	1867	U
1	2	1868	U
1	2	1869	A
2	3	41	U
2	3	42	C
2	3	43	C
2	3	44	C
2	3	45	C
2	3	46	U

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Mol	Chain	Res	Type
2	3	47	G
2	3	48	U
2	3	49	G
2	3	52	G
2	3	55	C
2	3	57	A
2	3	58	C
2	3	59	U
2	3	61	U
2	3	62	C
2	3	63	U
2	3	65	C
2	3	66	A
2	3	68	G
2	3	70	A
2	3	71	G
2	3	72	A
2	3	73	A
2	3	74	A
2	3	75	G
2	3	78	U
2	3	83	C
2	3	84	C
2	3	85	A
2	3	86	U
2	3	87	G
2	3	92	U
2	3	93	A
2	3	95	U
2	3	96	A
2	3	97	U
2	3	99	A
2	3	100	G
2	3	101	U
2	3	102	G
2	3	106	U
2	3	107	G
2	3	108	C
2	3	109	A
2	3	111	C
2	3	113	U
2	3	114	C

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Mol	Chain	Res	Type
2	3	115	C
2	3	116	A
2	3	117	G
2	3	118	G
2	3	120	C
2	3	121	C
2	3	122	C
2	3	123	C
2	3	124	C
2	3	128	C
2	3	129	C
2	3	131	G
2	3	135	G
2	3	137	G
2	3	139	C
2	3	140	A
2	3	141	U
2	3	142	A
2	3	145	G
2	3	147	U
2	3	150	G
2	3	152	G
2	3	153	G
2	3	154	A
2	3	155	A
2	3	159	G
2	3	160	U
2	3	161	G
2	3	162	A
2	3	163	G
2	3	164	U
2	3	165	A
2	3	166	C
2	3	167	A
2	3	169	C
2	3	172	A
2	3	175	U
2	3	176	G
2	3	228	U
2	3	229	G
2	3	231	G
2	3	232	C

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Mol	Chain	Res	Type
2	3	233	G
2	3	234	U
2	3	235	G
2	3	236	C
2	3	237	C
2	3	242	C
2	3	243	A
2	3	244	A
2	3	245	G
2	3	246	A
2	3	247	C
2	3	249	G
2	3	251	U
2	3	252	A
2	3	253	G
2	3	254	C
2	3	255	C
2	3	256	G
2	3	257	A
2	3	258	G
2	3	259	U
2	3	264	U
2	3	265	U
2	3	266	G
2	3	267	G
2	3	269	U
2	3	270	C
2	3	274	A
2	3	278	G
2	3	280	C
2	3	281	U
2	3	282	U
2	3	283	G
2	3	284	U
2	3	285	G
2	3	288	A
2	3	290	U
2	3	291	G
2	3	297	U
2	3	303	G
2	3	304	C
2	3	306	U

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Mol	Chain	Res	Type
2	3	307	G
2	3	308	C
2	3	310	A
2	3	311	G
2	3	321	A
2	3	322	G
2	3	324	U
2	3	325	C
2	3	328	G
2	3	330	A
2	3	331	G
2	3	332	A
2	3	333	C
2	3	334	C
2	3	340	C
2	3	341	C

All (108) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	60	A
1	2	65	C
1	2	102	A
1	2	114	G
1	2	126	G
1	2	143	U
1	2	180	G
1	2	291	G
1	2	314	U
1	2	319	C
1	2	332	G
1	2	368	U
1	2	381	C
1	2	382	C
1	2	408	A
1	2	437	G
1	2	440	G
1	2	453	C
1	2	465	A
1	2	547	G
1	2	554	A

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Mol	Chain	Res	Type
1	2	590	A
1	2	594	A
1	2	601	G
1	2	604	A
1	2	615	C
1	2	620	G
1	2	657	U
1	2	670	A
1	2	748	C
1	2	750	C
1	2	793	G
1	2	797	C
1	2	811	A
1	2	870	A
1	2	917	U
1	2	920	A
1	2	926	A
1	2	958	G
1	2	980	A
1	2	996	A
1	2	1001	A
1	2	1060	A
1	2	1129	G
1	2	1137	U
1	2	1165	G
1	2	1180	C
1	2	1181	A
1	2	1231	C
1	2	1250	A
1	2	1253	A
1	2	1302	G
1	2	1308	U
1	2	1316	C
1	2	1321	G
1	2	1330	G
1	2	1342	U
1	2	1403	C
1	2	1404	U
1	2	1425	G
1	2	1428	G
1	2	1430	C
1	2	1438	A

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Mol	Chain	Res	Type
1	2	1440	C
1	2	1445	U
1	2	1464	C
1	2	1476	A
1	2	1493	C
1	2	1494	U
1	2	1511	U
1	2	1534	C
1	2	1542	C
1	2	1558	C
1	2	1585	U
1	2	1587	G
1	2	1601	A
1	2	1648	G
1	2	1649	U
1	2	1745	A
1	2	1783	C
1	2	1835	A
1	2	1838	U
2	3	48	U
2	3	61	U
2	3	62	C
2	3	65	C
2	3	77	G
2	3	98	G
2	3	99	A
2	3	116	A
2	3	123	C
2	3	136	A
2	3	160	U
2	3	163	G
2	3	230	G
2	3	243	A
2	3	244	A
2	3	245	G
2	3	252	A
2	3	254	C
2	3	257	A
2	3	280	C
2	3	281	U
2	3	289	C
2	3	306	U

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Mol	Chain	Res	Type
2	3	329	U
2	3	330	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 101 ligands modelled in this entry, 101 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3	177:C	O3'	222:G	P	17.37

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3	334:C	O3'	339:A	P	15.84