



wwPDB EM Map/Model Validation Report ⓘ

Oct 3, 2016 – 04:41 PM EDT

PDB ID : 5GAF
EMDB ID: : EMD-8002
Title : RNC in complex with SRP
Authors : Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.
Deposited on : 2015-11-25
Resolution : 4.30 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

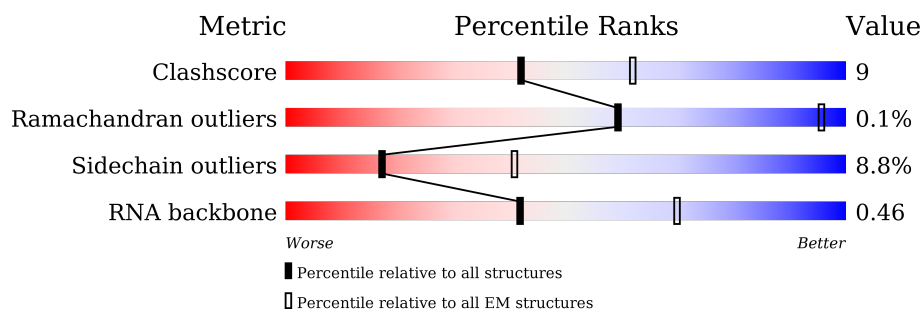
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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























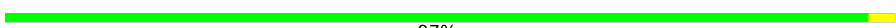




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	113	10% 19% 8% . 62%
2	2	3	33% 33% 33%
3	A	2883	55% 36% 8% .
4	B	120	74% 23% .
5	C	271	71% 26% .
6	D	209	78% 20% .
7	E	201	77% 21% .
8	F	177	60% 35% 5%

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Mol	Chain	Length	Quality of chain
9	G	176	 69% 29% .
10	H	149	 66% 32% .
11	I	125	 66% 33% .
12	J	134	 57% 39% .
13	K	142	 73% 23% .
14	L	123	 67% 31% .
15	M	144	 75% 23% .
16	N	136	 72% 26% .
17	O	125	 71% 26% .
18	P	117	 65% 32% .
19	Q	114	 75% 25% .
20	R	117	 74% 21% .
21	S	103	 70% 28% .
22	T	110	 78% 20% .
23	U	95	 78% 20% .
24	V	102	 70% 29% .
25	W	94	 74% 24% .
26	X	76	 66% 32% .
27	Y	77	 65% 34% .
28	Z	62	 65% 31% 5%
29	a	58	 97% .
30	b	56	 79% 21%
31	c	51	 90% 10%
32	d	46	 87% 13%
33	e	64	 94% 6%

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Mol	Chain	Length	Quality of chain
34	f	38	<div><div></div><div>92%</div><div>8%</div></div>
35	i	398	<div><div></div><div>95%</div><div><div></div><div></div></div></div>
36	k	18	<div><div></div><div>89%</div><div>11%</div></div>

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 96182 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 SRP 4.5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	43	Total	C	N	O	P	0	0
			926	413	174	296	43		

- Molecule 2 is a RNA chain called tRNA CCAend.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 3 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	2883	Total	C	N	O	P	0	0
			61902	27613	11397	20009	2883		

- Molecule 4 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	125	Total	C	N	O	S	0	0
			946	599	169	175	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	85	VAL	SER	conflict	UNP P0A7J3
I	86	THR	MET	conflict	UNP P0A7J3

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	V	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	51	Total	C	N	O	0	0
			414	266	76	72		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a protein called Signal recognition particle protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	398	Total	C	N	O	S	0	0
			3036	1910	548	560	18		

- Molecule 36 is a protein called 1A9L SS.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	18	Total	C	N	O	S	0	0
			137	94	20	22	1		

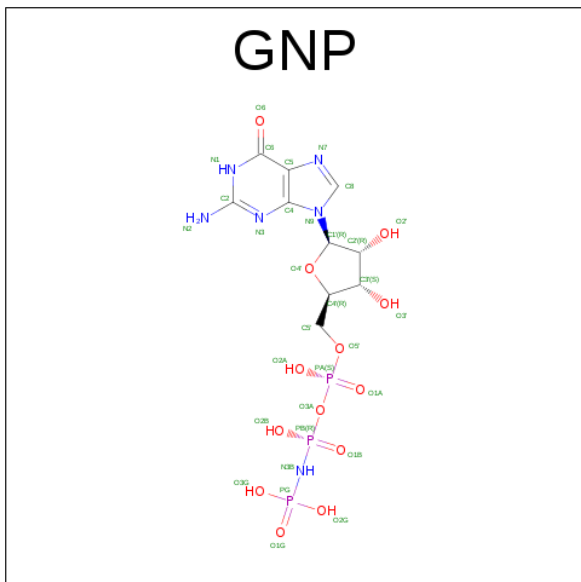
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	P	1	Total	Mg	0
			1	1	
37	D	1	Total	Mg	0
			1	1	
37	E	1	Total	Mg	0
			1	1	
37	B	11	Total	Mg	0
			11	11	
37	b	1	Total	Mg	0
			1	1	
37	C	2	Total	Mg	0
			2	2	
37	A	412	Total	Mg	0
			412	412	
37	2	1	Total	Mg	0
			1	1	
37	R	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	f	1	Total	Zn	0
			1	1	

- Molecule 39 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{13}\text{P}_3$).

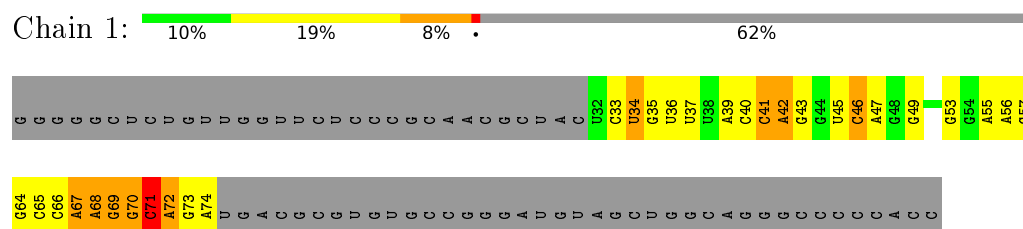


Mol	Chain	Residues	Atoms					AltConf
39	i	1	Total	C	N	O	P	0
			32	10	6	13	3	

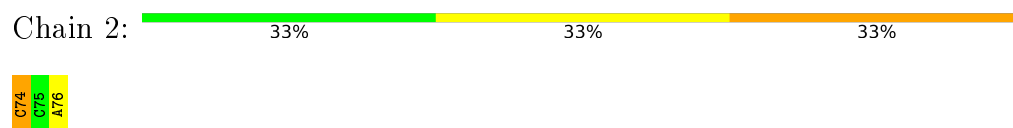
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

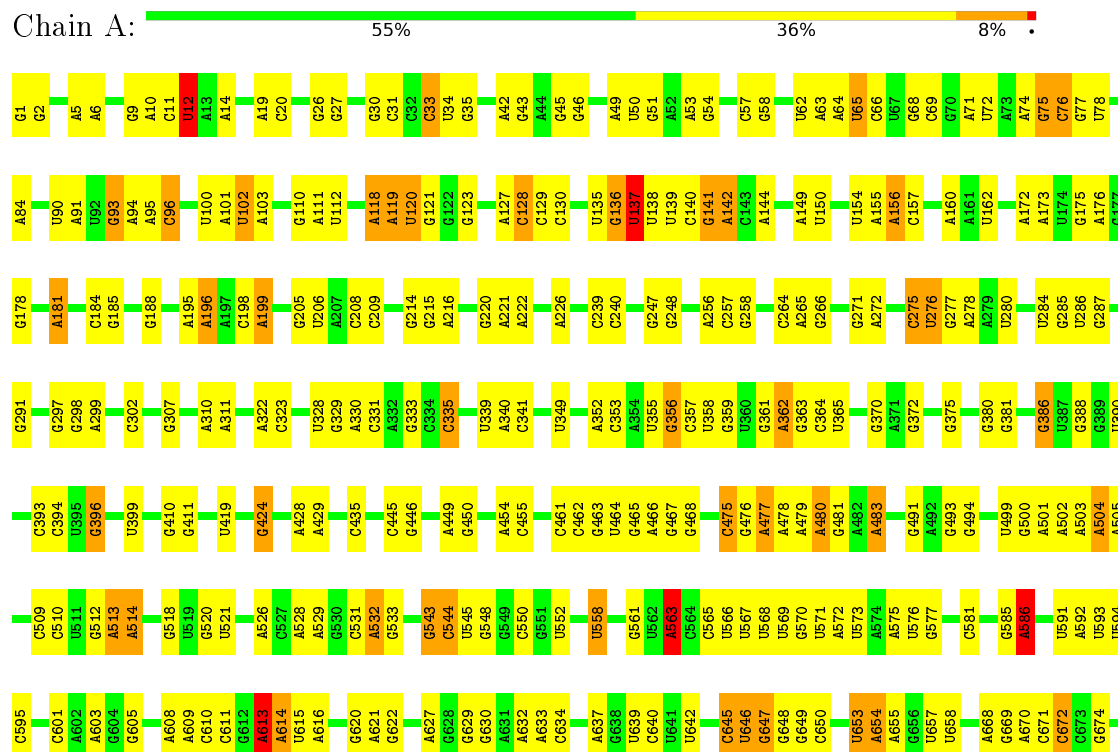
• Molecule 1: SRP 4.5S RNA



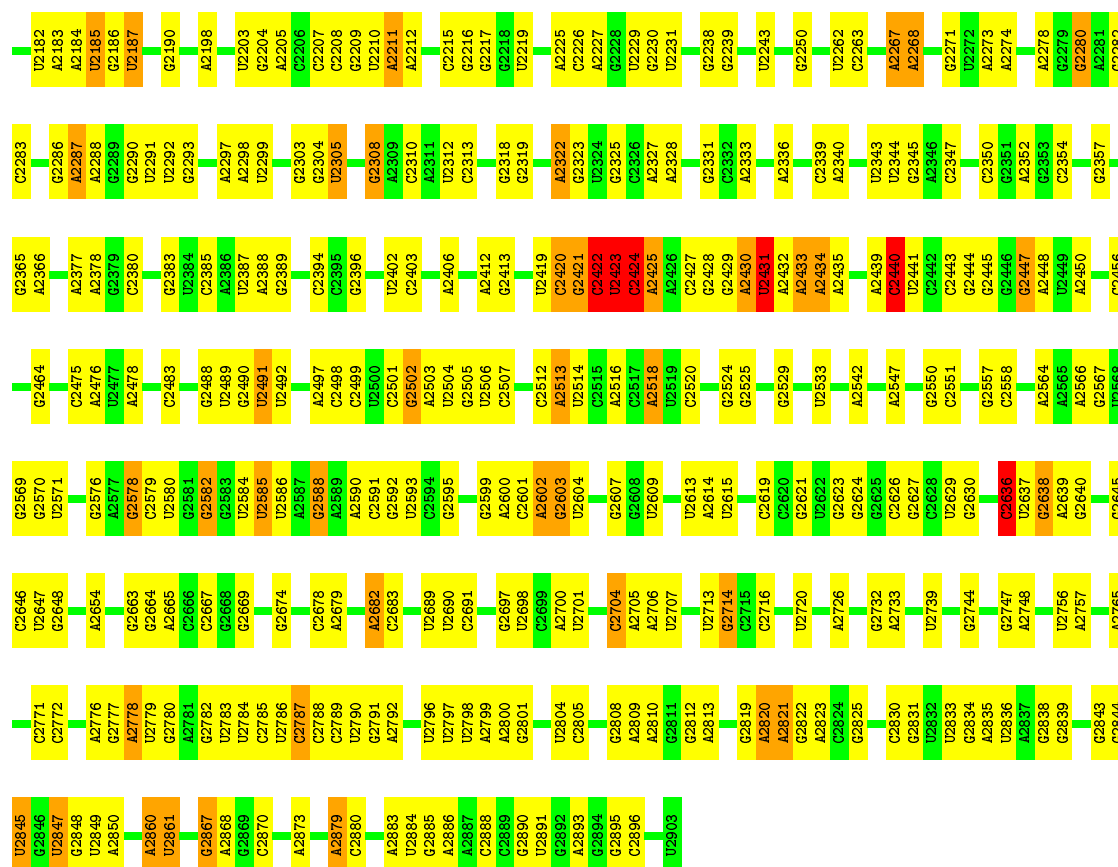
• Molecule 2: tRNA CCAend

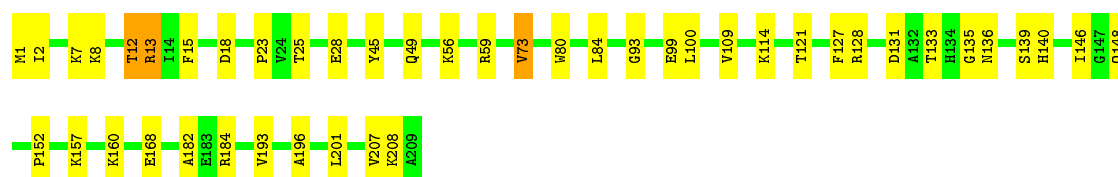


• Molecule 3: 23S ribosomal RNA



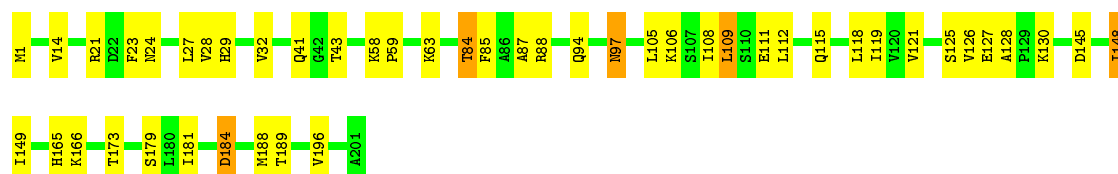




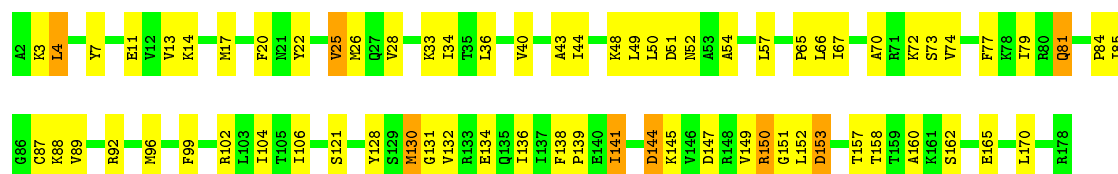
• Molecule 7: 50S ribosomal protein L4

Chain E: 77% 21% .



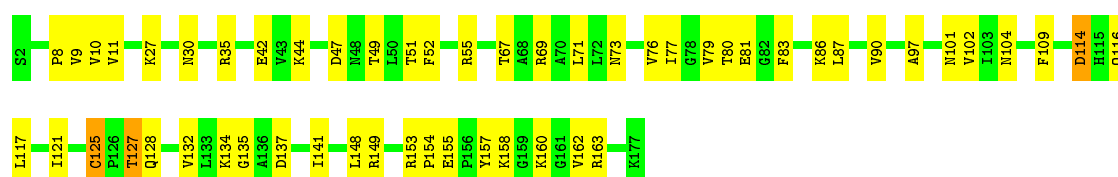
• Molecule 8: 50S ribosomal protein L5

Chain F: 60% 35% 5% .



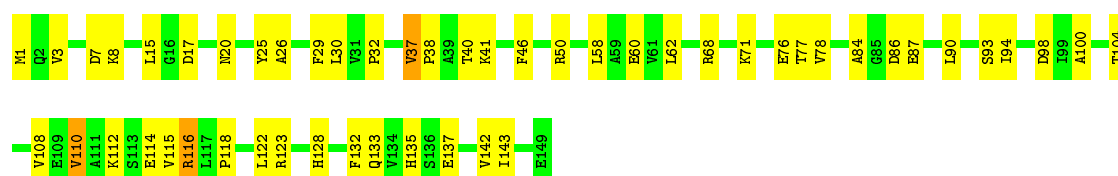
• Molecule 9: 50S ribosomal protein L6

Chain G: 69% 29% .



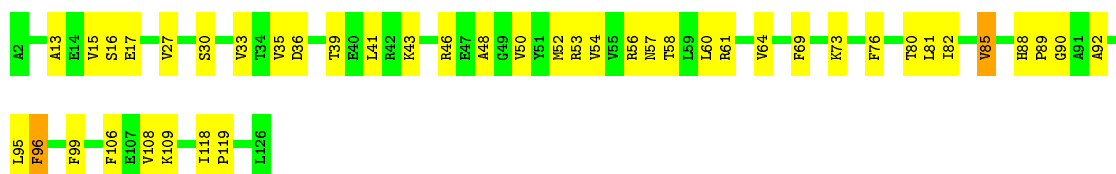
• Molecule 10: 50S ribosomal protein L9

Chain H: 66% 32% .



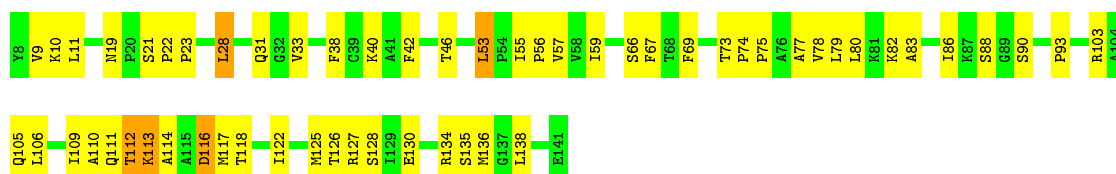
• Molecule 11: 50S ribosomal protein L10

Chain I: 66% 33% .



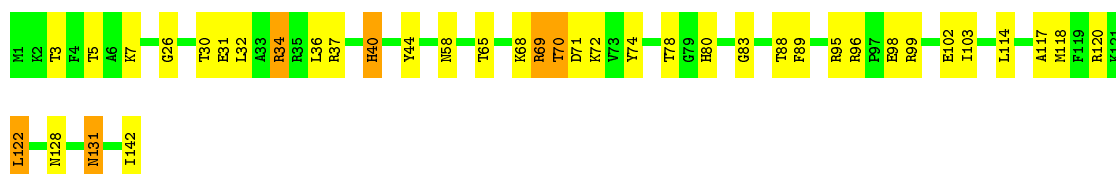
- Molecule 12: 50S ribosomal protein L11

Chain J: 57% 39% .



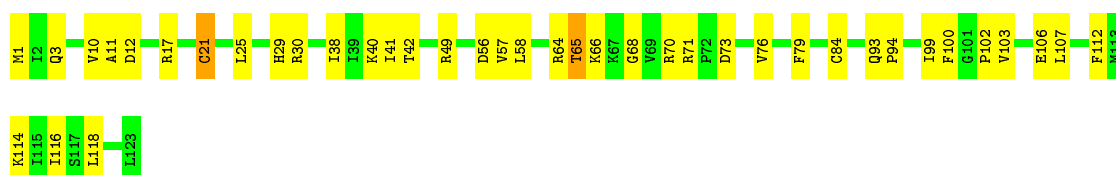
- Molecule 13: 50S ribosomal protein L13

Chain K: 73% 23% .



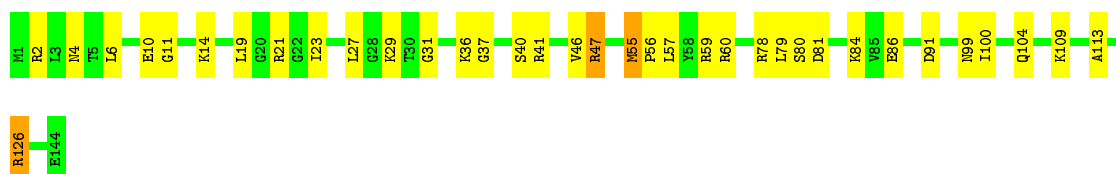
- Molecule 14: 50S ribosomal protein L14

Chain L: 67% 31% .



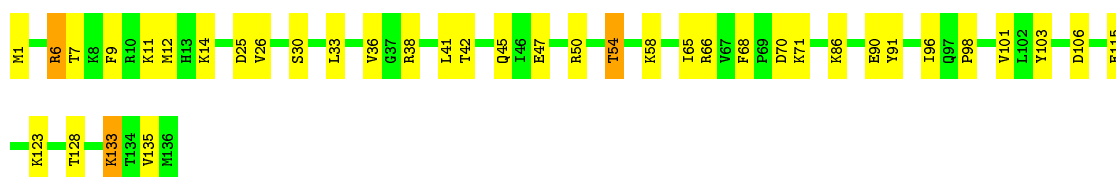
- Molecule 15: 50S ribosomal protein L15

Chain M: 75% 23% .



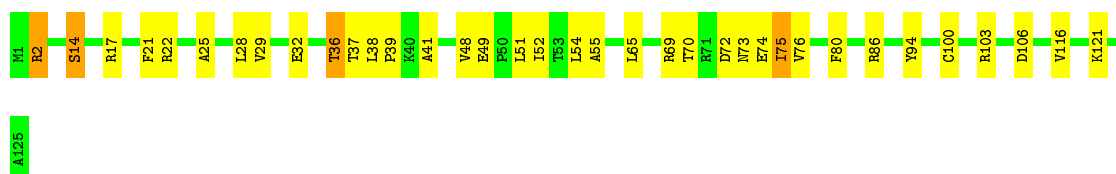
- Molecule 16: 50S ribosomal protein L16

Chain N: 72% 26% .



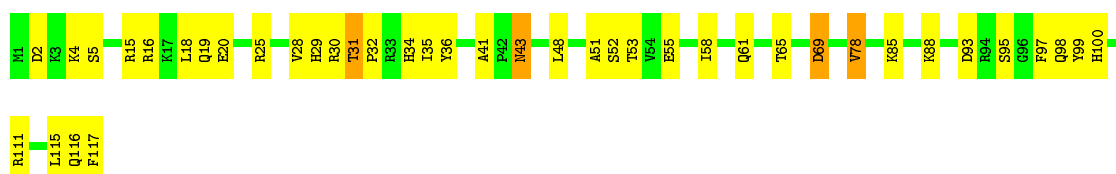
- Molecule 17: 50S ribosomal protein L17

Chain O: 71% 26%



- Molecule 18: 50S ribosomal protein L18

Chain P: 65% 32%



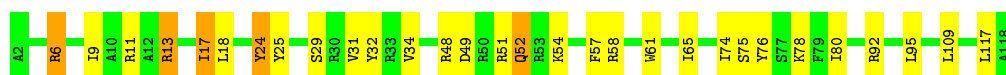
- Molecule 19: 50S ribosomal protein L19

Chain Q: 75% 25%



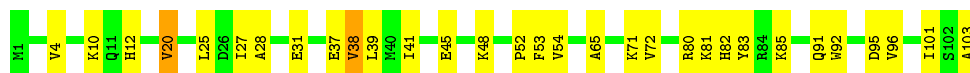
- Molecule 20: 50S ribosomal protein L20

Chain R: 74% 21%



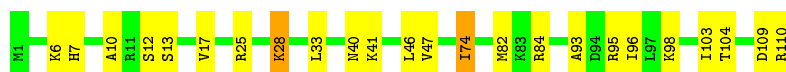
- Molecule 21: 50S ribosomal protein L21

Chain S: 70% 28%



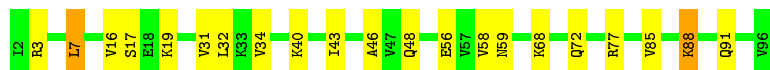
- Molecule 22: 50S ribosomal protein L22

Chain T: 78% 20%



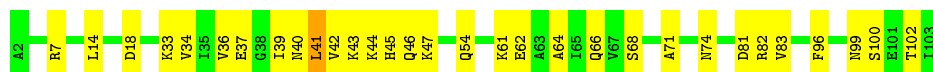
- Molecule 23: 50S ribosomal protein L23

Chain U: 78% 20% .



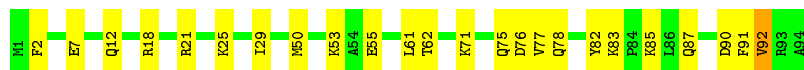
- Molecule 24: 50S ribosomal protein L24

Chain V: 70% 29% .



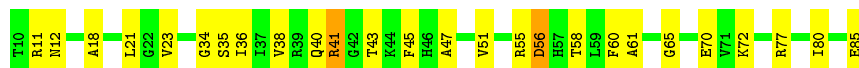
- Molecule 25: 50S ribosomal protein L25

Chain W: 74% 24% .



- Molecule 26: 50S ribosomal protein L27

Chain X: 66% 32% .



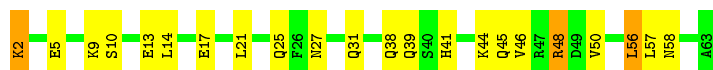
- Molecule 27: 50S ribosomal protein L28

Chain Y: 65% 34% .



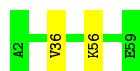
- Molecule 28: 50S ribosomal protein L29

Chain Z: 65% 31% 5% .

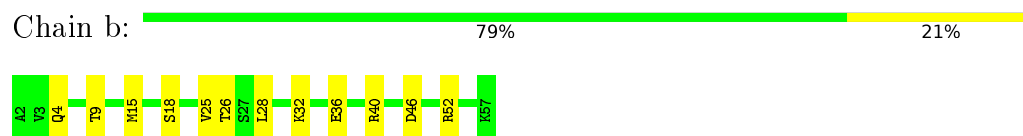


- Molecule 29: 50S ribosomal protein L30

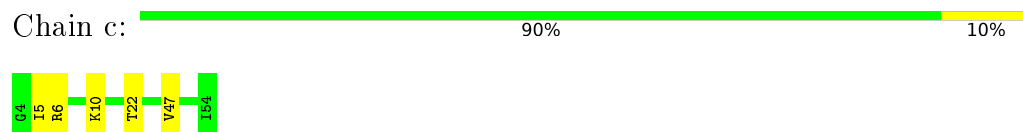
Chain a: 97% .



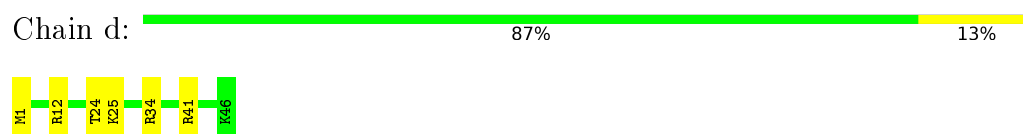
- Molecule 30: 50S ribosomal protein L32



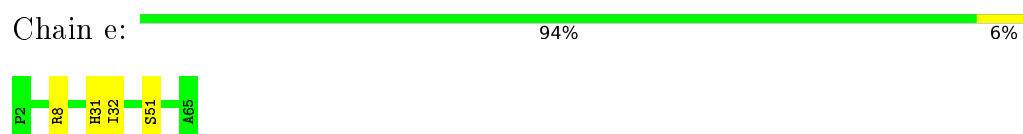
- Molecule 31: 50S ribosomal protein L33



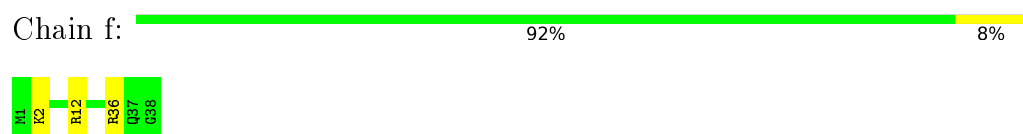
- Molecule 32: 50S ribosomal protein L34



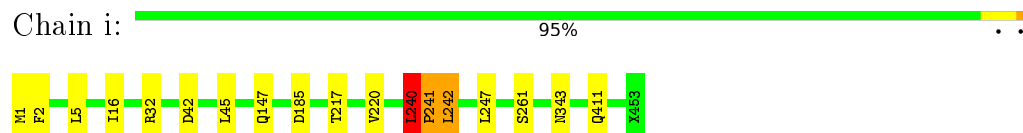
- Molecule 33: 50S ribosomal protein L35



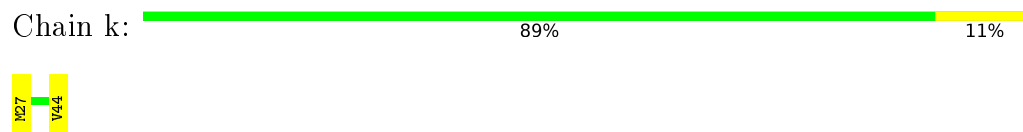
- Molecule 34: 50S ribosomal protein L36



- Molecule 35: Signal recognition particle protein



- Molecule 36: 1A9L SS



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	16407	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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, GNP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	1	0.26	0/1037	0.93	1/1616 (0.1%)
10	H	0.42	0/1121	0.57	0/1515
11	I	0.48	0/958	0.62	1/1292 (0.1%)
12	J	0.58	0/993	0.69	1/1341 (0.1%)
13	K	0.46	0/1152	0.57	0/1551
14	L	0.45	0/955	0.63	0/1279
15	M	0.47	0/1062	0.64	0/1413
16	N	0.48	0/1093	0.60	0/1460
17	O	0.47	0/1006	0.67	0/1345
18	P	0.41	0/910	0.56	0/1219
19	Q	0.48	0/929	0.60	0/1242
2	2	0.58	0/68	1.26	1/103 (1.0%)
20	R	0.56	0/960	0.59	0/1278
21	S	0.46	0/829	0.62	0/1107
22	T	0.52	0/864	0.71	0/1156
23	U	0.63	2/763 (0.3%)	0.76	2/1021 (0.2%)
24	V	0.38	0/788	0.54	0/1051
25	W	0.40	0/766	0.57	0/1025
26	X	0.50	0/587	0.60	0/776
27	Y	0.48	0/635	0.61	0/848
28	Z	0.45	0/502	0.61	0/667
29	a	0.38	0/453	0.56	0/605
3	A	0.68	14/69329 (0.0%)	1.17	181/108152 (0.2%)
30	b	0.43	0/450	0.62	0/599
31	c	0.43	0/421	0.61	0/561
32	d	0.51	0/380	0.66	0/498
33	e	0.47	0/513	0.62	0/676
34	f	0.49	0/303	0.58	0/397
35	i	0.26	0/2954	0.48	1/3967 (0.0%)
36	k	0.30	0/137	0.60	0/186
4	B	0.51	0/2872	1.04	1/4478 (0.0%)
5	C	0.47	0/2122	0.65	0/2852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
6	D	0.47	0/1586	0.63	0/2134
7	E	0.44	0/1571	0.61	1/2113 (0.0%)
8	F	0.39	0/1435	0.56	0/1926
9	G	0.39	0/1343	0.58	0/1816
All	All	0.62	16/103847 (0.0%)	1.04	190/155265 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	J	0	1
35	i	0	2
5	C	0	1
9	G	0	1
All	All	0	5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	U	88	LYS	CA-C	8.36	1.74	1.52
3	A	2542	A	N9-C4	-6.90	1.33	1.37
3	A	1254	A	N9-C4	-6.35	1.34	1.37
3	A	1321	A	N9-C4	6.05	1.41	1.37
3	A	776	G	N9-C4	5.94	1.42	1.38
3	A	2114	A	N9-C4	5.88	1.41	1.37
3	A	1490	A	N9-C4	5.80	1.41	1.37
3	A	563	A	N9-C4	-5.70	1.34	1.37
23	U	88	LYS	C-N	5.61	1.47	1.34
3	A	1254	A	N3-C4	-5.42	1.31	1.34
3	A	586	A	N3-C4	-5.30	1.31	1.34
3	A	1010	A	N9-C4	-5.29	1.34	1.37
3	A	514	A	N9-C4	-5.27	1.34	1.37
3	A	960	A	N9-C4	-5.16	1.34	1.37
3	A	265	A	N9-C4	-5.02	1.34	1.37
3	A	1269	A	N9-C4	-5.01	1.34	1.37

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2423	U	C6-N1-C2	-12.31	113.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1838	C	C6-N1-C2	9.36	124.05	120.30
3	A	2422	C	O4'-C1'-N1	9.24	115.59	108.20
23	U	88	LYS	CB-CA-C	8.84	128.07	110.40
3	A	2423	U	C5-C6-N1	8.78	127.09	122.70
3	A	1584	U	C2-N1-C1'	8.49	127.89	117.70
3	A	776	G	C8-N9-C4	-8.05	103.18	106.40
3	A	2431	U	N3-C2-O2	-7.94	116.64	122.20
3	A	275	C	C6-N1-C2	-7.72	117.21	120.30
3	A	1760	C	C6-N1-C2	7.54	123.31	120.30
3	A	1584	U	N1-C2-O2	7.28	127.90	122.80
3	A	2422	C	N3-C2-O2	-7.27	116.81	121.90
3	A	2207	C	C6-N1-C2	-7.06	117.47	120.30
3	A	2177	C	C6-N1-C2	-7.04	117.48	120.30
3	A	2431	U	C5-C4-O4	6.96	130.07	125.90
3	A	214	G	N3-C4-C5	-6.95	125.13	128.60
3	A	137	U	C5-C4-O4	-6.91	121.75	125.90
3	A	2424	C	O4'-C1'-N1	6.91	113.73	108.20
3	A	2614	A	C6-N1-C2	-6.84	114.49	118.60
3	A	2636	C	C2-N1-C1'	6.84	126.32	118.80
3	A	1992	G	C4-C5-N7	6.83	113.53	110.80
3	A	1064	C	C6-N1-C2	-6.78	117.59	120.30
3	A	2422	C	C6-N1-C2	-6.69	117.62	120.30
3	A	1027	A	C8-N9-C4	6.69	108.47	105.80
3	A	2000	C	C6-N1-C2	6.67	122.97	120.30
3	A	776	G	C4-N9-C1'	6.60	135.07	126.50
3	A	102	U	C2-N1-C1'	6.58	125.60	117.70
3	A	1531	C	C5-C6-N1	6.54	124.27	121.00
3	A	1849	G	C8-N9-C4	-6.50	103.80	106.40
3	A	483	A	C8-N9-C4	6.42	108.37	105.80
3	A	784	G	P-O3'-C3'	6.41	127.40	119.70
3	A	2456	C	C6-N1-C2	-6.41	117.74	120.30
3	A	1607	C	C6-N1-C2	-6.40	117.74	120.30
3	A	2542	A	C2-N3-C4	-6.40	107.40	110.60
3	A	832	U	C5-C6-N1	-6.38	119.51	122.70
3	A	1849	G	N7-C8-N9	6.37	116.29	113.10
3	A	906	U	C5-C4-O4	6.35	129.71	125.90
3	A	1128	G	C8-N9-C4	6.34	108.94	106.40
3	A	1606	C	N3-C2-O2	-6.34	117.46	121.90
3	A	2104	C	C6-N1-C2	-6.33	117.77	120.30
3	A	1313	U	N3-C2-O2	-6.32	117.78	122.20
3	A	1652	A	C8-N9-C4	6.28	108.31	105.80
3	A	758	C	C6-N1-C2	-6.22	117.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	12	U	N3-C2-O2	-6.21	117.85	122.20
3	A	1362	C	C6-N1-C2	-6.20	117.82	120.30
3	A	805	G	C8-N9-C4	6.17	108.87	106.40
3	A	1695	G	N9-C4-C5	-6.15	102.94	105.40
3	A	733	G	C4-C5-N7	6.13	113.25	110.80
3	A	1848	A	C8-N9-C4	-6.12	103.35	105.80
3	A	102	U	N1-C2-O2	6.09	127.06	122.80
3	A	776	G	N3-C4-C5	-6.08	125.56	128.60
3	A	2499	C	N1-C2-O2	6.04	122.52	118.90
3	A	2704	C	C6-N1-C2	-6.03	117.89	120.30
3	A	1584	U	C5-C6-N1	6.01	125.71	122.70
3	A	1470	A	C8-N9-C4	-6.01	103.40	105.80
3	A	1261	C	C6-N1-C2	6.00	122.70	120.30
3	A	2542	A	N3-C4-C5	6.00	131.00	126.80
3	A	1531	C	C6-N1-C2	-6.00	117.90	120.30
3	A	2077	A	C6-N1-C2	-5.99	115.01	118.60
3	A	611	C	C6-N1-C2	-5.96	117.92	120.30
3	A	774	G	C8-N9-C4	5.96	108.78	106.40
3	A	804	A	C8-N9-C4	5.95	108.18	105.80
3	A	130	C	N3-C4-C5	5.94	124.28	121.90
3	A	1272	A	C8-N9-C4	5.93	108.17	105.80
3	A	2171	A	O4'-C1'-N9	5.93	112.94	108.20
3	A	2433	A	N1-C2-N3	5.93	132.26	129.30
3	A	2109	U	C6-N1-C2	-5.93	117.44	121.00
3	A	2440	C	C6-N1-C2	5.92	122.67	120.30
3	A	1992	G	N9-C4-C5	-5.90	103.04	105.40
3	A	1584	U	N3-C2-O2	-5.89	118.08	122.20
3	A	1072	C	C6-N1-C2	-5.88	117.95	120.30
3	A	2153	C	C5-C6-N1	5.88	123.94	121.00
3	A	2582	G	N3-C4-C5	-5.88	125.66	128.60
3	A	2052	A	N1-C6-N6	5.86	122.12	118.60
3	A	790	U	N1-C2-O2	5.86	126.90	122.80
12	J	53	LEU	CA-CB-CG	5.86	128.76	115.30
3	A	2691	C	C6-N1-C2	5.85	122.64	120.30
35	i	242	LEU	CA-CB-CG	5.83	128.70	115.30
3	A	832	U	C2-N3-C4	-5.82	123.51	127.00
3	A	2580	U	C6-N1-C2	-5.76	117.54	121.00
3	A	1643	G	C8-N9-C4	-5.75	104.10	106.40
3	A	2423	U	N3-C4-C5	-5.75	111.15	114.60
3	A	776	G	O4'-C1'-N9	5.75	112.80	108.20
3	A	141	G	N7-C8-N9	5.74	115.97	113.10
1	1	71	C	C6-N1-C2	-5.72	118.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	741	U	C5-C6-N1	-5.71	119.84	122.70
3	A	2588	G	N3-C4-C5	5.71	131.46	128.60
3	A	987	C	N3-C4-C5	5.71	124.19	121.90
7	E	109	LEU	CA-CB-CG	-5.71	102.16	115.30
3	A	1871	A	C8-N9-C4	-5.70	103.52	105.80
3	A	2820	A	C8-N9-C4	5.69	108.07	105.80
3	A	783	A	C8-N9-C4	-5.67	103.53	105.80
3	A	205	G	O4'-C1'-N9	5.67	112.74	108.20
3	A	816	C	C6-N1-C2	-5.67	118.03	120.30
3	A	2845	U	C2-N3-C4	-5.67	123.60	127.00
11	I	95	LEU	CA-CB-CG	5.64	128.26	115.30
3	A	1303	G	C8-N9-C4	5.63	108.65	106.40
3	A	793	A	C5-C6-N6	-5.60	119.22	123.70
3	A	76	C	C5-C6-N1	5.59	123.79	121.00
3	A	1526	C	C6-N1-C2	-5.58	118.07	120.30
3	A	2636	C	C6-N1-C1'	-5.58	114.10	120.80
3	A	1993	U	C5-C6-N1	-5.57	119.91	122.70
3	A	2243	U	C5-C6-N1	-5.57	119.92	122.70
3	A	2498	C	C6-N1-C2	-5.55	118.08	120.30
3	A	1659	G	N3-C4-C5	5.55	131.38	128.60
3	A	1351	C	C6-N1-C2	5.53	122.51	120.30
3	A	776	G	N7-C8-N9	5.52	115.86	113.10
3	A	825	A	C6-N1-C2	-5.52	115.29	118.60
3	A	2145	C	C6-N1-C2	-5.50	118.10	120.30
3	A	1172	C	C6-N1-C2	-5.49	118.10	120.30
3	A	972	A	N1-C6-N6	-5.47	115.32	118.60
23	U	88	LYS	CA-C-N	5.46	129.22	117.20
3	A	2423	U	N1-C2-N3	5.45	118.17	114.90
3	A	128	C	C6-N1-C2	5.45	122.48	120.30
3	A	793	A	C2-N3-C4	5.45	113.32	110.60
3	A	1606	C	N1-C2-O2	5.44	122.17	118.90
3	A	410	G	N3-C4-C5	-5.43	125.89	128.60
3	A	1604	C	C5-C6-N1	-5.42	118.29	121.00
3	A	569	U	C5-C6-N1	-5.42	119.99	122.70
3	A	1078	U	C5-C6-N1	5.41	125.40	122.70
3	A	2380	C	C6-N1-C2	-5.40	118.14	120.30
3	A	1584	U	C6-N1-C1'	-5.40	113.64	121.20
3	A	2614	A	C5-C6-N1	5.40	120.40	117.70
3	A	1314	C	C6-N1-C2	-5.38	118.15	120.30
3	A	613	A	P-O3'-C3'	5.38	126.16	119.70
3	A	206	U	C2-N1-C1'	5.37	124.15	117.70
3	A	755	U	C5-C6-N1	-5.37	120.02	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1125	G	C8-N9-C4	-5.36	104.26	106.40
3	A	2595	G	C4-N9-C1'	-5.35	119.54	126.50
3	A	809	G	N3-C4-C5	-5.35	125.92	128.60
3	A	130	C	C6-N1-C2	5.35	122.44	120.30
3	A	280	U	P-O3'-C3'	5.35	126.12	119.70
3	A	135	U	C5-C6-N1	5.34	125.37	122.70
3	A	2000	C	C5-C6-N1	-5.34	118.33	121.00
3	A	2645	G	N3-C4-C5	-5.33	125.93	128.60
3	A	1045	C	C6-N1-C2	5.32	122.43	120.30
3	A	2542	A	C8-N9-C4	5.32	107.93	105.80
3	A	2022	U	C6-N1-C2	5.32	124.19	121.00
3	A	790	U	C2-N1-C1'	5.31	124.07	117.70
3	A	2153	C	C6-N1-C2	-5.30	118.18	120.30
3	A	642	U	O4'-C1'-N1	5.30	112.44	108.20
3	A	793	A	C5-C6-N1	5.29	120.34	117.70
3	A	1072	C	C5-C6-N1	5.28	123.64	121.00
4	B	42	C	C6-N1-C2	-5.28	118.19	120.30
3	A	1664	A	C8-N9-C4	-5.28	103.69	105.80
3	A	1848	A	N7-C8-N9	5.28	116.44	113.80
3	A	2645	G	C4-N9-C1'	5.27	133.35	126.50
3	A	375	G	N3-C4-N9	5.24	129.15	126.00
3	A	1642	G	N3-C4-C5	5.24	131.22	128.60
3	A	1848	A	O4'-C1'-N9	5.24	112.39	108.20
3	A	1970	A	N1-C2-N3	5.24	131.92	129.30
3	A	906	U	O4'-C1'-N1	5.23	112.39	108.20
3	A	1617	C	C5-C6-N1	-5.23	118.39	121.00
3	A	946	C	N3-C2-O2	-5.23	118.24	121.90
3	A	672	C	N3-C2-O2	-5.22	118.25	121.90
3	A	264	C	N3-C2-O2	-5.20	118.26	121.90
3	A	12	U	N1-C2-O2	5.20	126.44	122.80
3	A	1494	A	P-O3'-C3'	5.19	125.93	119.70
3	A	1769	U	C5-C6-N1	-5.19	120.11	122.70
3	A	906	U	C2-N1-C1'	-5.19	111.48	117.70
3	A	2090	A	C8-N9-C4	5.18	107.87	105.80
3	A	271	G	C8-N9-C4	5.17	108.47	106.40
3	A	375	G	N3-C4-C5	-5.17	126.02	128.60
2	2	74	C	C5-C6-N1	5.16	123.58	121.00
3	A	2074	U	C2-N1-C1'	5.16	123.89	117.70
3	A	2847	U	C5-C6-N1	-5.16	120.12	122.70
3	A	1958	C	C6-N1-C2	-5.15	118.24	120.30
3	A	1617	C	C2-N3-C4	-5.15	117.33	119.90
3	A	972	A	N9-C4-C5	5.14	107.86	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	809	G	C8-N9-C4	-5.13	104.35	106.40
3	A	2516	A	C8-N9-C4	5.12	107.85	105.80
3	A	2114	A	C8-N9-C4	-5.12	103.75	105.80
3	A	66	C	N3-C2-O2	-5.12	118.32	121.90
3	A	828	U	C5-C6-N1	-5.11	120.14	122.70
3	A	878	A	C8-N9-C4	-5.09	103.77	105.80
3	A	2115	G	N3-C4-C5	-5.08	126.06	128.60
3	A	2447	G	O4'-C1'-N9	5.08	112.26	108.20
3	A	2267	A	C8-N9-C4	-5.07	103.77	105.80
3	A	2580	U	N3-C2-O2	-5.06	118.66	122.20
3	A	783	A	N1-C6-N6	-5.05	115.57	118.60
3	A	1570	A	C8-N9-C4	5.05	107.82	105.80
3	A	733	G	C5-N7-C8	-5.04	101.78	104.30
3	A	102	U	C6-N1-C1'	-5.04	114.15	121.20
3	A	30	G	C8-N9-C4	5.03	108.41	106.40
3	A	906	U	C6-N1-C1'	5.03	128.24	121.20
3	A	804	A	C2-N3-C4	-5.02	108.09	110.60
3	A	1652	A	N7-C8-N9	-5.02	111.29	113.80
3	A	981	A	C8-N9-C4	5.02	107.81	105.80
3	A	2074	U	N3-C2-O2	-5.01	118.69	122.20
3	A	2424	C	C5'-C4'-O4'	5.01	115.11	109.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide
12	J	19	ASN	Peptide
35	i	240	LEU	Peptide
35	i	241	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	926	0	467	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	62	0	34	1	0
3	A	61902	0	31132	686	0
4	B	2569	0	1301	19	0
5	C	2083	0	2154	51	0
6	D	1565	0	1616	32	0
7	E	1552	0	1619	27	0
8	F	1411	0	1444	42	0
9	G	1323	0	1371	35	0
10	H	1110	0	1148	23	0
11	I	946	0	978	31	0
12	J	979	0	1028	39	0
13	K	1129	0	1162	24	0
14	L	946	0	1023	22	0
15	M	1053	0	1129	25	0
16	N	1074	0	1157	23	0
17	O	993	0	1034	25	0
18	P	900	0	935	23	0
19	Q	917	0	962	19	0
20	R	947	0	1019	24	0
21	S	816	0	839	20	0
22	T	857	0	922	14	0
23	U	756	0	817	15	0
24	V	780	0	831	18	0
25	W	753	0	780	14	0
26	X	580	0	594	16	0
27	Y	625	0	652	16	0
28	Z	501	0	531	31	0
29	a	449	0	488	0	0
30	b	444	0	458	0	0
31	c	414	0	442	0	0
32	d	377	0	418	0	0
33	e	504	0	572	0	0
34	f	302	0	340	0	0
35	i	3036	0	3154	0	0
36	k	137	0	168	0	0
37	2	1	0	0	0	0
37	A	412	0	0	0	0
37	B	11	0	0	0	0
37	C	2	0	0	0	0
37	D	1	0	0	0	0
37	E	1	0	0	0	0
37	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	R	1	0	0	0	0
37	b	1	0	0	0	0
38	f	1	0	0	0	0
39	i	32	0	13	0	0
All	All	96182	0	64732	1196	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 9.

All (1196) 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)
23:U:88:LYS:CA	23:U:88:LYS:C	1.74	1.53
28:Z:9:LYS:NZ	28:Z:17:GLU:HG3	1.61	1.15
3:A:96:C:OP1	28:Z:39:GLN:NE2	1.92	1.02
3:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90
28:Z:9:LYS:HZ1	28:Z:17:GLU:HG3	1.34	0.89
3:A:276:U:O2	3:A:278:A:N6	2.08	0.87
3:A:1827:U:OP2	5:C:221:ARG:NH1	2.08	0.85
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.57	0.85
3:A:2135:A:N6	3:A:2156:G:O2'	2.10	0.84
3:A:287:G:O6	3:A:352:A:N6	2.10	0.84
3:A:2135:A:HO2'	3:A:2159:G:HO2'	1.26	0.83
3:A:2107:G:H1	3:A:2182:U:H3	1.22	0.83
5:C:107:PRO:HD2	5:C:110:LEU:HD22	1.59	0.82
3:A:807:U:OP2	15:M:41:ARG:NH1	2.13	0.81
15:M:109:LYS:HG2	15:M:126:ARG:HB2	1.64	0.80
3:A:2128:G:N3	3:A:2173:A:O2'	2.14	0.79
3:A:994:C:O2	21:S:10:LYS:NZ	2.16	0.79
28:Z:9:LYS:NZ	28:Z:17:GLU:CG	2.45	0.78
18:P:15:ARG:NH2	18:P:95:SER:OG	2.18	0.77
11:I:41:LEU:HD21	11:I:96:PHE:HE1	1.50	0.77
5:C:245:VAL:HG12	5:C:251:GLN:HA	1.67	0.76
3:A:95:A:O3'	28:Z:39:GLN:HG2	1.86	0.76
3:A:614:A:O2'	3:A:616:A:N7	2.18	0.76
3:A:2599:G:N7	5:C:236:GLU:HB2	2.02	0.74
3:A:545:U:O2	3:A:548:G:N1	2.18	0.74
1:1:49:G:H1	1:1:60:A:H61	1.36	0.74
3:A:2848:G:O2'	3:A:2867:G:N2	2.19	0.73
5:C:181:MET:HB2	5:C:268:VAL:HB	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:720:U:H2'	3:A:721:A:C8	2.25	0.72
13:K:131:ASN:N	13:K:131:ASN:OD1	2.22	0.72
3:A:2119:A:N6	3:A:2167:U:O2	2.22	0.72
3:A:331:C:H41	3:A:1210:G:H22	1.37	0.72
13:K:70:THR:OG1	13:K:71:ASP:OD1	2.08	0.72
7:E:1:MET:HG3	7:E:14:VAL:HG23	1.71	0.71
23:U:88:LYS:HA	23:U:88:LYS:C	2.05	0.71
3:A:2423:U:H2'	3:A:2424:C:O4'	1.89	0.71
1:1:71:C:H2'	1:1:72:A:C8	2.25	0.71
3:A:331:C:H41	3:A:1210:G:N2	1.89	0.71
14:L:70:ARG:HD3	14:L:76:VAL:HG22	1.72	0.70
3:A:2163:A:OP1	3:A:2170:A:O2'	2.08	0.70
3:A:2310:C:H2'	8:F:77:PHE:HE2	1.54	0.70
3:A:1801:A:OP2	5:C:150:LYS:NZ	2.18	0.70
11:I:50:VAL:HG22	11:I:85:VAL:HG13	1.73	0.70
1:1:42:A:H61	1:1:67:A:H62	1.37	0.70
28:Z:9:LYS:HZ1	28:Z:17:GLU:CG	2.03	0.70
3:A:1069:A:H4'	3:A:1070:A:H5''	1.71	0.70
3:A:971:G:H2'	3:A:972:A:O4'	1.92	0.70
3:A:258:G:H1'	15:M:104:GLN:HE22	1.56	0.69
28:Z:9:LYS:HZ3	28:Z:17:GLU:HG3	1.56	0.69
3:A:513:A:O2'	20:R:11:ARG:NH1	2.26	0.69
9:G:35:ARG:HD3	9:G:71:LEU:HD13	1.74	0.69
14:L:79:PHE:HD1	19:Q:70:VAL:HG22	1.58	0.68
11:I:43:LYS:HG2	11:I:46:ARG:HH22	1.56	0.68
3:A:1536:C:H4'	3:A:1537:G:H5''	1.75	0.68
3:A:2830:C:H5''	6:D:56:LYS:HE3	1.75	0.68
3:A:2135:A:O2'	3:A:2159:G:O2'	2.06	0.68
12:J:79:LEU:HB3	12:J:109:ILE:HG12	1.76	0.68
14:L:21:CYS:HA	14:L:41:ILE:HG22	1.76	0.68
3:A:95:A:O2'	28:Z:41:HIS:HB2	1.94	0.68
3:A:362:A:H3'	3:A:363:G:H8	1.59	0.67
3:A:878:A:H3'	3:A:879:G:H8	1.60	0.67
3:A:358:U:H2'	3:A:359:G:H8	1.60	0.67
18:P:31:THR:HG22	18:P:34:HIS:H	1.59	0.67
3:A:1340:U:OP1	23:U:19:LYS:NZ	2.25	0.67
3:A:2122:U:OP1	3:A:2168:G:N2	2.26	0.67
3:A:286:U:H2'	3:A:287:G:H8	1.60	0.67
28:Z:25:GLN:HB2	28:Z:46:VAL:HG11	1.77	0.67
3:A:2103:C:O2	3:A:2186:G:N1	2.27	0.67
3:A:196:A:OP2	15:M:47:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1105:U:H2'	3:A:1106:G:C8	2.30	0.66
3:A:286:U:H2'	3:A:287:G:C8	2.31	0.66
27:Y:32:ASN:O	27:Y:52:SER:HA	1.95	0.66
3:A:2590:A:H2'	3:A:2591:C:H6	1.61	0.66
3:A:2209:G:H1	3:A:2215:C:H42	1.44	0.66
28:Z:10:SER:N	28:Z:13:GLU:OE1	2.26	0.66
3:A:2216:G:H2'	3:A:2217:G:H8	1.60	0.66
3:A:2713:U:H3'	3:A:2714:G:H5''	1.77	0.66
3:A:2305:U:C2	8:F:151:GLY:HA3	2.31	0.66
10:H:84:ALA:HA	10:H:90:LEU:HA	1.78	0.66
13:K:31:GLU:HG3	13:K:142:ILE:HG13	1.77	0.66
4:B:43:C:O2	8:F:92:ARG:NH2	2.28	0.66
1:1:68:A:H2'	1:1:69:G:C8	2.30	0.66
3:A:572:A:OP2	21:S:80:ARG:NH2	2.27	0.66
3:A:2303:G:O2'	8:F:121:SER:O	2.13	0.65
3:A:1344:U:O2'	3:A:1345:C:OP1	2.14	0.65
3:A:1597:A:H5''	3:A:1598:A:H5'	1.78	0.65
7:E:87:ALA:O	7:E:88:ARG:NH2	2.30	0.65
9:G:9:VAL:HG22	9:G:69:ARG:HE	1.61	0.65
3:A:860:U:H1'	3:A:2268:A:H5'	1.78	0.65
8:F:158:THR:HG22	8:F:160:ALA:H	1.62	0.65
3:A:1794:A:H2'	3:A:1795:C:H6	1.61	0.65
3:A:370:G:O2'	3:A:424:G:OP1	2.11	0.65
16:N:50:ARG:O	16:N:54:THR:OG1	2.13	0.65
3:A:1869:G:N2	3:A:1871:A:O2'	2.30	0.64
3:A:1342:A:O2'	3:A:1344:U:OP2	2.16	0.64
3:A:1007:C:OP1	13:K:37:ARG:NH2	2.29	0.64
3:A:2424:C:H5''	3:A:2425:A:H5'	1.79	0.64
3:A:2674:G:H4'	14:L:30:ARG:HG3	1.78	0.64
26:X:65:GLY:HA2	26:X:85:GLU:HG2	1.78	0.64
3:A:2788:C:O2'	3:A:2809:A:N3	2.28	0.64
3:A:1510:G:H2'	3:A:1511:G:C8	2.32	0.64
3:A:968:C:H2'	3:A:969:G:H8	1.62	0.64
3:A:1105:U:H2'	3:A:1106:G:H8	1.63	0.64
3:A:1094:U:N3	3:A:1097:U:OP2	2.30	0.63
3:A:2102:G:N2	3:A:2187:U:O2	2.31	0.63
3:A:322:A:H5'	3:A:340:A:H1'	1.78	0.63
8:F:74:VAL:HG22	8:F:79:ILE:HD11	1.79	0.63
16:N:14:LYS:O	16:N:71:LYS:NZ	2.32	0.63
3:A:1614:A:N1	22:T:93:ALA:HB2	2.13	0.63
8:F:144:ASP:OD1	8:F:144:ASP:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:74:ILE:HD11	20:R:78:LYS:HB3	1.80	0.63
22:T:82:MET:HB3	22:T:84:ARG:HH22	1.62	0.63
28:Z:21:LEU:HD23	28:Z:50:VAL:HG22	1.79	0.63
3:A:1980:G:O2'	3:A:1982:U:OP2	2.16	0.63
21:S:41:ILE:HB	21:S:48:LYS:HD2	1.79	0.63
3:A:2151:U:H2'	3:A:2152:G:C8	2.34	0.63
3:A:284:U:H3	3:A:356:G:H1	1.44	0.63
19:Q:91:ALA:HB2	19:Q:113:ARG:HA	1.80	0.63
25:W:21:ARG:NH2	25:W:87:GLN:O	2.28	0.63
13:K:117:ALA:HA	13:K:120:ARG:HH21	1.63	0.63
3:A:1187:G:OP1	21:S:85:LYS:NZ	2.31	0.62
28:Z:25:GLN:HB2	28:Z:46:VAL:CG1	2.29	0.62
3:A:2116:G:N7	3:A:2165:C:N4	2.44	0.62
19:Q:4:ILE:H	19:Q:4:ILE:HD12	1.64	0.62
3:A:1433:A:N1	3:A:1434:A:N6	2.47	0.62
17:O:49:GLU:HA	17:O:52:ILE:HD12	1.79	0.62
20:R:58:ARG:HA	20:R:61:TRP:CE3	2.34	0.62
3:A:514:A:N3	3:A:581:C:O2'	2.33	0.62
3:A:784:G:C6	5:C:228:VAL:HG11	2.35	0.62
3:A:825:A:H2'	3:A:826:U:O4'	1.98	0.62
3:A:2809:A:H2'	3:A:2810:A:C8	2.34	0.62
3:A:2590:A:H2'	3:A:2591:C:C6	2.35	0.62
10:H:68:ARG:HA	10:H:71:LYS:HD2	1.81	0.62
3:A:2822:G:O6	17:O:2:ARG:NH1	2.32	0.61
11:I:57:ASN:ND2	11:I:76:PHE:O	2.33	0.61
12:J:53:LEU:HD11	12:J:82:LYS:HD2	1.83	0.61
15:M:57:LEU:HD13	15:M:60:ARG:HH11	1.65	0.61
3:A:1079:C:O2'	12:J:134:ARG:NH1	2.33	0.61
3:A:2636:C:HO2'	6:D:45:TYR:HH	1.47	0.61
3:A:2639:A:H2'	3:A:2640:G:O4'	2.01	0.61
17:O:54:LEU:HD21	17:O:65:LEU:HD23	1.82	0.61
3:A:2310:C:H2'	8:F:77:PHE:CE2	2.35	0.61
11:I:41:LEU:HD21	11:I:96:PHE:CE1	2.34	0.61
3:A:1001:A:H2'	3:A:1002:G:O4'	2.01	0.61
3:A:503:A:H4'	3:A:504:A:H5'	1.82	0.61
5:C:235:GLY:HA3	5:C:239:ASN:HB2	1.83	0.61
3:A:585:G:N7	20:R:6:ARG:NH1	2.48	0.60
6:D:12:THR:OG1	6:D:13:ARG:N	2.34	0.60
3:A:2060:A:H3'	7:E:63:LYS:HZ1	1.65	0.60
1:1:68:A:H2'	1:1:69:G:H8	1.66	0.60
3:A:570:G:H2'	3:A:2030:A:N7	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:6:LYS:HG2	22:T:104:THR:HG23	1.82	0.60
26:X:56:ASP:N	26:X:56:ASP:OD1	2.28	0.60
3:A:1076:C:H2'	3:A:1077:A:C8	2.37	0.60
3:A:1363:C:O2'	3:A:1809:A:N3	2.33	0.60
9:G:137:ASP:O	9:G:141:ILE:HG22	2.01	0.60
3:A:96:C:H1'	28:Z:41:HIS:ND1	2.16	0.60
3:A:1794:A:H2'	3:A:1795:C:C6	2.37	0.60
6:D:2:ILE:HG13	6:D:100:LEU:HD21	1.83	0.60
11:I:27:VAL:HG22	11:I:82:ILE:HG22	1.83	0.60
7:E:97:ASN:OD1	7:E:97:ASN:N	2.34	0.60
15:M:81:ASP:HA	15:M:84:LYS:HD2	1.82	0.60
3:A:776:G:O2'	3:A:777:G:OP1	2.19	0.60
3:A:2831:G:OP1	6:D:56:LYS:NZ	2.35	0.59
8:F:44:ILE:HG21	8:F:79:ILE:HG22	1.83	0.59
28:Z:14:LEU:HB3	28:Z:57:LEU:HD21	1.84	0.59
3:A:355:U:H2'	3:A:356:G:C8	2.38	0.59
3:A:1796:U:H2'	3:A:1797:G:H8	1.67	0.59
3:A:2819:G:H2'	3:A:2821:A:N7	2.17	0.59
3:A:2584:U:H3'	3:A:2585:U:H5''	1.84	0.59
9:G:27:LYS:NZ	9:G:27:LYS:HB3	2.17	0.59
13:K:36:LEU:HD11	13:K:122:LEU:HB2	1.83	0.59
18:P:99:TYR:OH	18:P:111:ARG:NH1	2.36	0.59
3:A:2205:A:H61	3:A:2219:U:H3	1.50	0.59
11:I:64:VAL:HG22	11:I:69:PHE:HB2	1.84	0.59
3:A:878:A:H3'	3:A:879:G:C8	2.38	0.59
24:V:81:ASP:OD1	24:V:82:ARG:N	2.35	0.59
3:A:2127:G:O2'	3:A:2128:G:O5'	2.19	0.59
4:B:7:G:OP1	18:P:4:LYS:NZ	2.27	0.59
3:A:1170:C:O2	3:A:1179:G:N2	2.33	0.58
3:A:2021:C:OP1	20:R:25:TYR:OH	2.21	0.58
3:A:833:A:H2'	3:A:834:G:C8	2.38	0.58
3:A:1130:U:O2'	3:A:1131:G:H8	1.87	0.58
3:A:1808:A:H3'	3:A:1809:A:C8	2.38	0.58
17:O:73:ASN:HA	17:O:76:VAL:HG22	1.86	0.58
21:S:37:GLU:HB3	21:S:53:PHE:CE1	2.39	0.58
3:A:396:G:OP2	27:Y:10:LYS:NZ	2.36	0.58
3:A:2127:G:O2'	3:A:2128:G:O4'	2.20	0.58
25:W:76:ASP:OD1	25:W:77:VAL:N	2.37	0.58
12:J:106:LEU:HB3	12:J:126:THR:HG23	1.85	0.58
3:A:2412:A:H2'	3:A:2413:G:O4'	2.04	0.58
6:D:148:GLN:HB2	6:D:152:PRO:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:41:ALA:HB2	18:P:48:LEU:HD21	1.86	0.57
3:A:1715:G:O2'	3:A:1743:G:O6	2.17	0.57
7:E:21:ARG:HD3	7:E:106:LYS:HB3	1.85	0.57
3:A:2291:U:H2'	3:A:2292:U:C6	2.38	0.57
3:A:2602:A:H4'	3:A:2603:G:O5'	2.04	0.57
3:A:849:A:H2'	3:A:850:U:C6	2.39	0.57
5:C:227:PRO:HG3	5:C:234:GLY:H	1.69	0.57
12:J:59:ILE:HD13	12:J:69:PHE:HB3	1.86	0.57
6:D:157:LYS:HD2	13:K:80:HIS:CE1	2.40	0.57
3:A:1645:G:H5''	3:A:1646:C:H5'	1.86	0.57
3:A:2447:G:N2	3:A:2450:A:OP2	2.37	0.57
3:A:839:U:H2'	3:A:840:C:C6	2.40	0.57
6:D:13:ARG:HD2	6:D:15:PHE:CZ	2.38	0.57
17:O:94:TYR:O	17:O:116:VAL:HG23	2.05	0.57
3:A:340:A:H2'	3:A:341:C:O4'	2.05	0.57
7:E:112:LEU:HB3	7:E:118:LEU:HB2	1.87	0.57
6:D:1:MET:HG2	6:D:2:ILE:H	1.70	0.57
10:H:37:VAL:HG22	10:H:38:PRO:HD2	1.86	0.57
3:A:2216:G:H2'	3:A:2217:G:C8	2.40	0.57
3:A:876:C:H2'	3:A:877:A:O4'	2.05	0.57
8:F:33:LYS:HG2	8:F:157:THR:HB	1.87	0.57
3:A:1796:U:H2'	3:A:1797:G:C8	2.40	0.56
24:V:18:ASP:OD2	24:V:40:ASN:N	2.38	0.56
3:A:1063:G:H5'	12:J:77:ALA:HB1	1.87	0.56
3:A:1800:C:H5'	5:C:146:MET:HE1	1.87	0.56
3:A:1905:C:H2'	3:A:1930:G:C8	2.40	0.56
3:A:299:A:N1	3:A:322:A:O2'	2.27	0.56
3:A:721:A:H2'	3:A:722:A:C8	2.41	0.56
11:I:60:LEU:O	11:I:64:VAL:HB	2.06	0.56
3:A:26:G:C6	3:A:27:G:N1	2.73	0.56
5:C:166:ALA:HB3	5:C:173:THR:HB	1.86	0.56
3:A:2162:G:H5''	3:A:2171:A:H2'	1.86	0.56
3:A:480:A:OP2	24:V:44:LYS:NZ	2.23	0.56
3:A:1790:C:H3'	3:A:1828:G:N2	2.21	0.56
3:A:388:G:N7	3:A:390:U:H2'	2.21	0.56
3:A:1076:C:H2'	3:A:1077:A:H8	1.69	0.56
9:G:30:ASN:HB3	9:G:79:VAL:HA	1.88	0.56
3:A:2133:G:H2'	3:A:2157:G:H1	1.70	0.56
3:A:2491:U:H5''	3:A:2570:G:H5''	1.88	0.56
3:A:2584:U:H3'	3:A:2585:U:C5'	2.36	0.56
4:B:42:C:C5	8:F:66:LEU:HD22	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:73:THR:HB	12:J:112:THR:HG22	1.87	0.56
23:U:56:GLU:HG3	23:U:88:LYS:HG2	1.88	0.56
3:A:1251:C:OP2	20:R:6:ARG:NH2	2.35	0.56
3:A:2430:A:N3	3:A:2430:A:H2'	2.21	0.56
12:J:53:LEU:HD22	12:J:78:VAL:HG13	1.87	0.56
13:K:72:LYS:HE3	13:K:74:TYR:CE1	2.39	0.56
25:W:62:THR:HG22	25:W:71:LYS:HG2	1.88	0.56
3:A:2298:A:H2'	3:A:2299:U:O4'	2.05	0.55
3:A:849:A:H2'	3:A:850:U:H6	1.69	0.55
12:J:127:ARG:HA	12:J:130:GLU:HB2	1.88	0.55
17:O:2:ARG:HB3	17:O:2:ARG:NH1	2.21	0.55
3:A:812:C:H4'	20:R:13:ARG:NH1	2.21	0.55
3:A:1442:U:H2'	3:A:1443:U:C6	2.41	0.55
1:1:70:G:H3'	1:1:71:C:H6	1.71	0.55
3:A:19:A:H2'	3:A:20:C:C6	2.41	0.55
3:A:2171:A:H3'	3:A:2173:A:C8	2.41	0.55
18:P:16:ARG:HA	18:P:16:ARG:HH21	1.71	0.55
3:A:591:U:H2'	3:A:592:A:H8	1.71	0.55
3:A:882:G:H1	3:A:894:U:H3	1.54	0.55
24:V:33:LYS:HB3	24:V:64:ALA:HB1	1.87	0.55
3:A:184:C:H2'	3:A:185:G:C8	2.41	0.55
3:A:2591:C:H2'	3:A:2592:G:C8	2.41	0.55
3:A:2783:U:H2'	3:A:2784:U:C6	2.42	0.55
5:C:160:THR:HG22	5:C:177:ARG:HG2	1.89	0.55
10:H:7:ASP:OD1	10:H:8:LYS:N	2.40	0.55
17:O:48:VAL:O	17:O:51:LEU:HB2	2.05	0.55
18:P:69:ASP:N	18:P:69:ASP:OD1	2.40	0.55
3:A:2070:A:H2'	3:A:2071:A:C8	2.42	0.55
3:A:639:U:H2'	3:A:640:C:C6	2.42	0.55
3:A:2262:U:H2'	3:A:2263:C:H6	1.72	0.55
6:D:8:LYS:HB2	6:D:201:LEU:HD11	1.88	0.55
8:F:132:VAL:HG22	8:F:152:LEU:HB3	1.88	0.55
8:F:134:GLU:HB3	8:F:136:ILE:HG12	1.89	0.54
7:E:88:ARG:HH21	7:E:88:ARG:HA	1.72	0.54
3:A:1837:C:H2'	3:A:1899:A:H61	1.73	0.54
3:A:833:A:H2'	3:A:834:G:H8	1.72	0.54
6:D:184:ARG:NH1	19:Q:7:GLN:OE1	2.40	0.54
12:J:79:LEU:HA	12:J:82:LYS:HG2	1.88	0.54
3:A:2619:C:H5''	6:D:157:LYS:HG3	1.89	0.54
3:A:2424:C:H5''	3:A:2425:A:C5'	2.37	0.54
3:A:586:A:H5'	7:E:84:THR:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:609:A:H2'	3:A:610:C:O4'	2.08	0.54
12:J:56:PRO:HD3	12:J:75:PRO:HD3	1.90	0.54
13:K:34:ARG:HH22	13:K:40:HIS:HB3	1.72	0.54
3:A:172:A:H2'	3:A:173:A:C8	2.43	0.54
3:A:1923:U:H2'	3:A:1924:C:C6	2.43	0.54
3:A:2267:A:H5''	3:A:2268:A:H5''	1.89	0.54
3:A:996:A:OP2	21:S:10:LYS:HD3	2.07	0.54
21:S:48:LYS:HE3	21:S:103:ALA:HB1	1.90	0.54
23:U:68:LYS:HG3	23:U:77:ARG:NH2	2.23	0.54
3:A:2845:U:H5''	19:Q:52:ASN:O	2.08	0.54
3:A:2579:C:O2'	6:D:136:ASN:ND2	2.41	0.54
9:G:104:ASN:ND2	9:G:114:ASP:OD1	2.41	0.54
1:1:69:G:H2'	1:1:70:G:H1'	1.90	0.53
3:A:2834:G:O6	3:A:2879:A:H2'	2.08	0.53
21:S:20:VAL:HG13	21:S:96:VAL:HG23	1.89	0.53
1:1:53:G:HO2'	1:1:55:A:H62	1.56	0.53
3:A:2443:C:H2'	3:A:2444:G:C8	2.43	0.53
5:C:145:GLU:HB2	5:C:188:CYS:HB3	1.89	0.53
3:A:284:U:O2	3:A:356:G:N2	2.37	0.53
3:A:2808:G:O2'	3:A:2890:G:O6	2.21	0.53
3:A:608:A:H2'	3:A:609:A:C8	2.44	0.53
3:A:9:G:O2'	3:A:2800:A:N6	2.42	0.53
14:L:40:LYS:HE3	14:L:57:VAL:HG12	1.91	0.53
1:1:45:U:H3	1:1:64:G:H1	1.55	0.53
3:A:1069:A:C2	3:A:1096:A:H5''	2.44	0.53
3:A:788:A:OP1	3:A:791:C:N4	2.41	0.53
11:I:88:HIS:ND1	11:I:89:PRO:O	2.42	0.53
3:A:2547:A:H4'	14:L:29:HIS:CD2	2.44	0.53
14:L:38:ILE:HD11	14:L:112:PHE:HZ	1.73	0.53
17:O:36:THR:OG1	17:O:37:THR:N	2.42	0.53
11:I:54:VAL:HG22	11:I:81:LEU:HD13	1.90	0.53
3:A:1056:G:H5''	3:A:1057:A:H5'	1.90	0.53
3:A:720:U:H2'	3:A:721:A:H8	1.72	0.53
3:A:1873:G:H2'	3:A:1874:C:H6	1.74	0.53
10:H:116:ARG:HH21	10:H:133:GLN:HB3	1.74	0.53
3:A:1056:G:O2'	3:A:1103:A:N6	2.40	0.52
3:A:2086:U:H2'	3:A:2087:G:C8	2.44	0.52
3:A:2171:A:H3'	3:A:2173:A:H8	1.74	0.52
17:O:36:THR:HG23	17:O:41:ALA:HB2	1.90	0.52
1:1:60:A:H2'	1:1:61:G:O4'	2.10	0.52
3:A:2210:U:H4'	3:A:2211:A:H5'	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:679:C:H2'	3:A:680:C:C6	2.44	0.52
5:C:62:TYR:HA	5:C:86:ASN:HD21	1.73	0.52
3:A:1425:G:H2'	3:A:1426:G:O4'	2.09	0.52
3:A:1428:C:C5	3:A:1569:A:H5''	2.45	0.52
3:A:2280:G:O2'	3:A:2388:A:N1	2.37	0.52
3:A:653:U:H1'	3:A:654:A:H5''	1.91	0.52
13:K:3:THR:HB	20:R:57:PHE:HE1	1.75	0.52
25:W:55:GLU:CD	25:W:55:GLU:H	2.13	0.52
3:A:1791:A:N6	3:A:1828:G:O2'	2.42	0.52
3:A:1993:U:H4'	6:D:133:THR:OG1	2.10	0.52
3:A:671:C:H2'	3:A:672:C:H6	1.74	0.52
3:A:68:G:H2'	3:A:69:C:O4'	2.10	0.52
8:F:99:PHE:HD1	8:F:102:ARG:HH22	1.57	0.52
3:A:1410:G:H1	3:A:1592:C:H42	1.57	0.52
3:A:1421:G:C2	3:A:1422:G:C8	2.98	0.52
3:A:2127:G:H2'	3:A:2128:G:C8	2.45	0.52
21:S:52:PRO:HG2	21:S:53:PHE:CD2	2.45	0.52
3:A:1681:G:H21	3:A:1762:A:H3'	1.75	0.52
3:A:1798:U:H5''	5:C:258:ARG:HB2	1.92	0.52
3:A:2637:U:C2'	3:A:2638:G:H5'	2.39	0.52
3:A:845:A:H61	3:A:932:U:H3	1.58	0.52
3:A:898:C:H2'	3:A:899:A:O4'	2.10	0.52
3:A:90:U:H3'	3:A:91:A:H8	1.74	0.52
4:B:93:C:OP2	25:W:18:ARG:NH1	2.41	0.52
6:D:114:LYS:HD3	6:D:196:ALA:HB2	1.92	0.52
7:E:28:VAL:O	7:E:32:VAL:HG13	2.09	0.52
24:V:74:ASN:HD21	24:V:99:ASN:HD21	1.58	0.52
3:A:1289:C:H2'	3:A:1290:C:C6	2.45	0.52
3:A:1451:C:H1'	3:A:1452:G:C2	2.45	0.52
3:A:2133:G:H21	3:A:2158:A:H62	1.58	0.52
12:J:73:THR:OG1	12:J:113:LYS:NZ	2.40	0.51
1:1:49:G:H1	1:1:60:A:N6	2.04	0.51
3:A:1000:A:OP2	3:A:1154:G:N1	2.32	0.51
3:A:120:U:H4'	3:A:121:G:H5''	1.90	0.51
3:A:1437:C:H2'	3:A:1438:U:C6	2.46	0.51
3:A:2439:A:H4'	3:A:2440:C:H5''	1.91	0.51
3:A:2850:A:N7	3:A:2868:A:O2'	2.39	0.51
28:Z:2:LYS:HG3	28:Z:5:GLU:OE1	2.10	0.51
3:A:1790:C:H2'	3:A:1791:A:C5	2.45	0.51
8:F:128:TYR:HE2	8:F:130:MET:HG2	1.76	0.51
3:A:256:A:H2'	3:A:257:C:H6	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:968:C:H2'	3:A:969:G:C8	2.42	0.51
3:A:141:G:H2'	3:A:142:A:O4'	2.11	0.51
3:A:499:U:H2'	3:A:500:G:O4'	2.10	0.51
7:E:24:ASN:ND2	7:E:27:LEU:HB2	2.25	0.51
7:E:41:GLN:HG2	7:E:43:THR:HG23	1.92	0.51
17:O:55:ALA:HA	17:O:80:PHE:CE2	2.45	0.51
3:A:2720:U:OP1	19:Q:53:ARG:NH2	2.41	0.51
3:A:1115:G:O2'	3:A:1116:G:H5''	2.10	0.51
3:A:1414:C:H2'	3:A:1415:U:O4'	2.11	0.51
3:A:2647:U:H2'	3:A:2648:G:H8	1.76	0.51
3:A:948:C:H2'	3:A:949:G:C8	2.45	0.51
7:E:145:ASP:HA	7:E:166:LYS:HB3	1.92	0.51
20:R:24:TYR:N	20:R:24:TYR:CD1	2.78	0.51
21:S:28:ALA:HB3	21:S:31:GLU:HG3	1.93	0.51
1:I:46:C:H42	1:I:61:G:H3'	1.75	0.51
19:Q:16:ASP:N	19:Q:16:ASP:OD1	2.32	0.51
3:A:364:C:H2'	3:A:365:U:C6	2.45	0.51
3:A:576:U:H2'	3:A:577:G:C8	2.46	0.51
15:M:36:LYS:O	15:M:40:SER:HB3	2.11	0.51
3:A:2502:G:H5''	3:A:2503:A:H5''	1.93	0.51
3:A:621:A:OP2	15:M:99:ASN:ND2	2.40	0.51
3:A:2271:G:H5''	26:X:18:ALA:HB1	1.93	0.51
3:A:1394:U:H4'	3:A:1603:A:H4'	1.92	0.51
3:A:645:C:O2'	3:A:646:U:OP1	2.24	0.51
3:A:2333:A:P	26:X:77:ARG:HH22	2.34	0.50
12:J:113:LYS:HE3	12:J:116:ASP:HB3	1.92	0.50
16:N:30:SER:H	16:N:106:ASP:HB3	1.75	0.50
16:N:1:MET:HA	16:N:47:GLU:HG3	1.94	0.50
3:A:1405:U:H2'	3:A:1406:U:C6	2.46	0.50
3:A:1927:A:H2'	3:A:1928:A:C8	2.46	0.50
13:K:32:LEU:O	13:K:36:LEU:HB2	2.12	0.50
3:A:1132:U:H2'	3:A:1133:A:C8	2.46	0.50
3:A:357:C:H2'	3:A:358:U:C6	2.47	0.50
22:T:40:ASN:O	22:T:41:LYS:HG2	2.10	0.50
8:F:40:VAL:HG11	8:F:43:ALA:HB2	1.92	0.50
14:L:64:ARG:NH1	14:L:102:PRO:O	2.44	0.50
15:M:23:ILE:HG12	21:S:82:HIS:CD2	2.47	0.50
3:A:1342:A:OP1	23:U:40:LYS:NZ	2.33	0.50
3:A:2282:G:C6	3:A:2425:A:C2	3.00	0.50
20:R:65:ILE:HD11	20:R:95:LEU:HB2	1.93	0.50
3:A:128:C:H2'	3:A:129:C:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2024:G:H2'	3:A:2025:C:H6	1.77	0.50
3:A:256:A:H2'	3:A:257:C:C6	2.47	0.50
3:A:2183:A:H2'	3:A:2184:A:C8	2.46	0.50
23:U:7:LEU:HD13	23:U:46:ALA:HA	1.92	0.50
23:U:88:LYS:CA	23:U:88:LYS:O	2.51	0.50
24:V:46:GLN:OE1	24:V:54:GLN:NE2	2.44	0.50
3:A:2308:G:H3'	3:A:2310:C:OP2	2.11	0.50
3:A:90:U:C2	3:A:91:A:N7	2.80	0.50
9:G:127:THR:HG22	9:G:128:GLN:H	1.77	0.50
20:R:76:TYR:CZ	20:R:80:ILE:HG13	2.46	0.50
3:A:738:G:H1'	3:A:759:G:N2	2.27	0.50
4:B:2:G:H2'	4:B:3:C:C6	2.47	0.50
5:C:132:MET:HG2	5:C:135:ILE:HD12	1.94	0.50
8:F:17:MET:SD	8:F:22:TYR:HB2	2.52	0.50
10:H:94:ILE:HB	10:H:122:LEU:HB2	1.94	0.50
12:J:83:ALA:O	12:J:105:GLN:NE2	2.45	0.50
3:A:1638:C:H1'	3:A:2698:U:O2'	2.12	0.49
3:A:613:A:O2'	3:A:614:A:O5'	2.30	0.49
3:A:878:A:N6	3:A:899:A:O2'	2.45	0.49
9:G:83:PHE:O	9:G:134:LYS:HA	2.12	0.49
18:P:30:ARG:HG3	18:P:35:ILE:HD12	1.93	0.49
28:Z:38:GLN:HG3	28:Z:39:GLN:H	1.77	0.49
28:Z:21:LEU:HD23	28:Z:50:VAL:CG2	2.41	0.49
3:A:1021:A:N3	3:A:1021:A:H3'	2.27	0.49
3:A:1187:G:HO2'	3:A:1188:U:H6	1.60	0.49
3:A:1327:A:N6	3:A:1647:U:O2	2.45	0.49
8:F:50:LEU:O	8:F:54:ALA:N	2.38	0.49
9:G:8:PRO:HB3	9:G:51:THR:HG22	1.94	0.49
17:O:14:SER:HA	17:O:17:ARG:NH1	2.27	0.49
19:Q:23:GLY:O	19:Q:90:GLY:HA3	2.11	0.49
25:W:75:GLN:HB2	25:W:92:VAL:HG12	1.94	0.49
3:A:2171:A:H5'	3:A:2173:A:N7	2.26	0.49
3:A:2747:G:O2'	9:G:67:THR:HG23	2.12	0.49
26:X:34:GLY:N	26:X:61:ALA:O	2.37	0.49
3:A:1506:U:H2'	3:A:1507:C:C6	2.48	0.49
3:A:2073:C:H2'	3:A:2074:U:H6	1.77	0.49
3:A:2809:A:H2'	3:A:2810:A:H8	1.75	0.49
3:A:1088:A:N6	12:J:135:SER:HB3	2.26	0.49
9:G:101:ASN:ND2	9:G:116:GLN:OE1	2.46	0.49
3:A:1939:U:OP1	3:A:2604:U:O2'	2.28	0.49
3:A:2576:G:O2'	3:A:2579:C:OP2	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2626:C:H2'	3:A:2627:G:O4'	2.12	0.49
3:A:27:G:N2	3:A:512:G:H1'	2.27	0.49
3:A:671:C:H2'	3:A:672:C:C6	2.47	0.49
7:E:184:ASP:N	7:E:184:ASP:OD1	2.43	0.49
15:M:4:ASN:OD1	15:M:4:ASN:N	2.39	0.49
3:A:1243:C:H1'	15:M:4:ASN:O	2.13	0.49
11:I:33:VAL:HG21	11:I:106:PHE:CE2	2.47	0.49
14:L:10:VAL:HG12	14:L:12:ASP:H	1.77	0.49
3:A:1606:C:H5'	3:A:1607:C:OP1	2.13	0.49
3:A:563:A:C4	3:A:2018:G:C2	3.01	0.49
3:A:1819:A:H5''	5:C:160:THR:HG21	1.94	0.49
7:E:23:PHE:CD1	7:E:111:GLU:HG3	2.48	0.49
10:H:110:VAL:HG12	10:H:114:GLU:HB2	1.94	0.49
15:M:19:LEU:HD23	15:M:27:LEU:HD13	1.95	0.49
21:S:65:ALA:HB3	21:S:95:ASP:HB2	1.94	0.49
3:A:1005:C:H2'	3:A:1006:C:C6	2.47	0.49
3:A:184:C:H2'	3:A:185:G:H8	1.76	0.49
3:A:2151:U:H2'	3:A:2152:G:H8	1.77	0.49
3:A:2564:A:OP1	3:A:2648:G:O2'	2.20	0.49
3:A:1093:G:C2'	3:A:1098:A:H61	2.26	0.48
3:A:1903:G:C2	3:A:1904:G:C8	3.00	0.48
3:A:2483:C:N3	16:N:123:LYS:NZ	2.60	0.48
4:B:116:G:H2'	4:B:117:G:C8	2.48	0.48
3:A:1790:C:H3'	3:A:1828:G:H22	1.77	0.48
3:A:2290:G:H2'	3:A:2291:U:O4'	2.13	0.48
3:A:719:C:H2'	3:A:720:U:H6	1.78	0.48
3:A:784:G:H5'	3:A:785:G:OP1	2.13	0.48
12:J:113:LYS:O	12:J:117:MET:N	2.46	0.48
3:A:140:C:H4'	3:A:141:G:OP1	2.13	0.48
3:A:1654:A:H2'	3:A:1655:A:H8	1.79	0.48
3:A:2116:G:C5	3:A:2165:C:N4	2.82	0.48
27:Y:6:GLN:NE2	27:Y:76:GLU:OE2	2.39	0.48
3:A:813:U:H2'	3:A:814:C:C6	2.49	0.48
5:C:175:ARG:HG3	5:C:181:MET:HE1	1.95	0.48
9:G:80:THR:OG1	9:G:81:GLU:N	2.46	0.48
18:P:51:ALA:HB3	18:P:78:VAL:HG13	1.95	0.48
26:X:40:GLN:NE2	26:X:43:THR:HA	2.29	0.48
27:Y:17:ASN:HB2	27:Y:25:THR:OG1	2.13	0.48
27:Y:17:ASN:OD1	27:Y:27:ARG:HD2	2.13	0.48
3:A:136:G:H2'	3:A:137:U:O4'	2.13	0.48
3:A:1773:A:N7	3:A:1829:A:H1'	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:467:G:H2'	3:A:468:G:O4'	2.13	0.48
13:K:72:LYS:HE3	13:K:74:TYR:CZ	2.48	0.48
17:O:38:LEU:HB3	17:O:39:PRO:HD3	1.95	0.48
3:A:1179:G:H2'	3:A:1180:U:C6	2.48	0.48
3:A:175:G:N2	3:A:176:A:N3	2.62	0.48
3:A:2158:A:H4'	3:A:2159:G:O5'	2.14	0.48
3:A:2428:G:H21	15:M:60:ARG:NH2	2.12	0.48
5:C:145:GLU:HG2	5:C:151:GLY:C	2.34	0.48
9:G:86:LYS:HG2	9:G:132:VAL:HG22	1.96	0.48
28:Z:27:ASN:O	28:Z:31:GLN:HG3	2.14	0.48
3:A:428:A:H2'	3:A:429:A:C8	2.49	0.48
3:A:1386:C:H2'	3:A:1387:A:C8	2.49	0.48
3:A:160:A:N3	3:A:2208:C:O2'	2.43	0.48
3:A:2209:G:H1	3:A:2215:C:N4	2.12	0.48
3:A:2834:G:H2'	3:A:2879:A:N6	2.29	0.48
3:A:782:A:N7	5:C:220:VAL:HG21	2.29	0.48
5:C:260:ASN:OD1	5:C:262:ARG:N	2.37	0.48
3:A:2305:U:H5''	8:F:131:GLY:HA3	1.96	0.48
8:F:7:TYR:CD1	8:F:11:GLU:HG3	2.48	0.48
10:H:115:VAL:HG22	10:H:132:PHE:CE2	2.48	0.48
23:U:58:VAL:HG22	23:U:85:VAL:HG22	1.96	0.48
23:U:68:LYS:HG3	23:U:77:ARG:HH21	1.79	0.48
3:A:2433:A:H2	27:Y:21:ALA:HB1	1.79	0.48
3:A:1527:G:N1	3:A:1544:A:OP2	2.32	0.48
3:A:156:A:H2'	3:A:157:C:O4'	2.13	0.48
3:A:1846:G:H5''	3:A:1847:A:OP2	2.14	0.48
3:A:2570:G:H2'	3:A:2571:U:O4'	2.14	0.48
3:A:914:G:H5'	3:A:915:C:OP2	2.14	0.48
6:D:25:THR:HG21	6:D:193:VAL:HG22	1.95	0.48
10:H:142:VAL:HG12	10:H:143:ILE:H	1.79	0.48
16:N:11:LYS:HD3	16:N:86:LYS:HD3	1.96	0.48
16:N:41:LEU:HG	16:N:96:ILE:HG13	1.95	0.48
3:A:1132:U:H3'	3:A:1133:A:H5''	1.95	0.47
3:A:2226:C:H2'	3:A:2227:A:O4'	2.13	0.47
9:G:155:GLU:OE1	9:G:157:TYR:N	2.45	0.47
13:K:58:ASN:ND2	13:K:128:ASN:OD1	2.42	0.47
3:A:483:A:O4'	24:V:45:HIS:HB3	2.14	0.47
28:Z:21:LEU:HD11	28:Z:46:VAL:HG22	1.96	0.47
3:A:2060:A:H3'	7:E:63:LYS:NZ	2.29	0.47
3:A:477:A:H2'	3:A:478:A:C8	2.49	0.47
3:A:910:A:H2'	3:A:911:A:C8	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:78:THR:HG23	13:K:83:GLY:O	2.13	0.47
22:T:96:ILE:HA	22:T:96:ILE:HD13	1.73	0.47
1:1:42:A:N6	1:1:67:A:H62	2.09	0.47
3:A:1027:A:C6	3:A:1126:A:C4	3.02	0.47
3:A:112:U:H5'	28:Z:58:ASN:HD21	1.80	0.47
3:A:1268:A:H2'	3:A:1269:A:O4'	2.13	0.47
3:A:208:C:H2'	3:A:209:C:H6	1.78	0.47
3:A:2444:G:OP2	7:E:63:LYS:HD2	2.14	0.47
3:A:795:C:H2'	3:A:796:C:C6	2.49	0.47
6:D:56:LYS:HB2	6:D:59:ARG:HB2	1.95	0.47
9:G:35:ARG:CD	9:G:71:LEU:HD13	2.44	0.47
12:J:10:LYS:O	12:J:11:LEU:HD12	2.15	0.47
3:A:1873:G:H2'	3:A:1874:C:C6	2.49	0.47
3:A:957:C:C5	3:A:959:A:C5	3.01	0.47
10:H:93:SER:HB3	10:H:123:ARG:HG2	1.95	0.47
12:J:42:PHE:O	12:J:46:THR:OG1	2.32	0.47
13:K:114:LEU:O	13:K:118:MET:HG3	2.14	0.47
24:V:14:LEU:HD11	24:V:71:ALA:HB2	1.95	0.47
3:A:1438:U:H2'	3:A:1439:A:H8	1.79	0.47
3:A:1446:C:H2'	3:A:1447:C:C6	2.49	0.47
3:A:995:C:OP2	20:R:54:LYS:NZ	2.44	0.47
11:I:85:VAL:HG22	11:I:92:ALA:HB2	1.96	0.47
12:J:40:LYS:N	12:J:40:LYS:HD2	2.30	0.47
15:M:55:MET:SD	15:M:56:PRO:HD2	2.55	0.47
6:D:121:THR:HB	6:D:127:PHE:CD2	2.49	0.47
18:P:43:ASN:ND2	18:P:43:ASN:H	2.13	0.47
25:W:2:PHE:HB3	25:W:50:MET:CE	2.45	0.47
27:Y:62:LYS:HE3	27:Y:66:THR:HG21	1.96	0.47
3:A:1007:C:H5''	13:K:37:ARG:NH2	2.29	0.47
3:A:127:A:H5''	3:A:128:C:O4'	2.14	0.47
3:A:911:A:H2'	16:N:9:PHE:HZ	1.78	0.47
7:E:125:SER:OG	7:E:126:VAL:N	2.46	0.47
3:A:911:A:H2'	16:N:9:PHE:CZ	2.50	0.47
18:P:31:THR:HG23	18:P:32:PRO:HD2	1.96	0.47
3:A:1672:A:C6	3:A:1673:G:C6	3.03	0.47
3:A:2431:U:H5	3:A:2433:A:H5''	1.79	0.47
3:A:2557:G:H2'	3:A:2558:C:C6	2.49	0.47
3:A:2592:G:C6	3:A:2593:U:N3	2.83	0.47
9:G:102:VAL:HG22	9:G:116:GLN:HE22	1.78	0.47
18:P:30:ARG:HB3	18:P:97:PHE:CE1	2.50	0.47
3:A:323:C:C4	3:A:333:G:C8	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:149:ILE:HB	7:E:188:MET:HG2	1.96	0.47
8:F:25:VAL:O	8:F:28:VAL:HG12	2.14	0.47
10:H:29:PHE:O	10:H:32:PRO:HD2	2.15	0.47
3:A:1085:A:H61	11:I:35:VAL:HG22	1.78	0.47
22:T:7:HIS:CE1	22:T:10:ALA:HB2	2.49	0.47
3:A:1799:G:C5	5:C:176:LEU:HD13	2.50	0.47
3:A:861:A:C6	3:A:917:A:C8	3.03	0.47
3:A:998:C:H2'	3:A:999:U:O4'	2.14	0.47
12:J:75:PRO:HD2	12:J:78:VAL:HB	1.96	0.47
17:O:25:ALA:O	17:O:29:VAL:HG23	2.15	0.47
3:A:2039:U:H2'	3:A:2040:G:C8	2.50	0.47
3:A:2419:U:O2'	3:A:2420:C:H5'	2.15	0.47
3:A:713:G:H2'	3:A:714:U:C6	2.50	0.47
3:A:975:A:H1'	3:A:990:A:C2	2.50	0.47
8:F:73:SER:OG	8:F:81:GLN:N	2.33	0.47
9:G:42:GLU:CG	9:G:55:ARG:HH21	2.29	0.47
11:I:39:THR:HG22	11:I:43:LYS:HE3	1.98	0.47
12:J:28:LEU:HD11	12:J:33:VAL:HG11	1.97	0.47
24:V:41:LEU:HD22	24:V:62:GLU:HG2	1.96	0.47
27:Y:40:VAL:HG12	27:Y:43:GLU:H	1.80	0.47
3:A:1060:U:C2	3:A:1062:G:H5'	2.50	0.46
3:A:1097:U:H2'	3:A:1098:A:O4'	2.15	0.46
3:A:1689:A:C6	3:A:1700:A:C2	3.03	0.46
3:A:1946:U:H2'	3:A:1947:C:C6	2.50	0.46
3:A:2339:C:H2'	3:A:2340:A:H8	1.80	0.46
3:A:825:A:C2	3:A:833:A:C2	3.03	0.46
3:A:857:G:H2'	3:A:858:G:O4'	2.16	0.46
5:C:252:THR:OG1	5:C:253:LYS:N	2.48	0.46
3:A:1038:G:H2'	3:A:1039:A:C8	2.50	0.46
3:A:1028:A:N6	3:A:1125:G:H2'	2.30	0.46
3:A:144:A:H1'	23:U:3:ARG:HH22	1.80	0.46
3:A:247:G:H4'	3:A:386:G:C5	2.50	0.46
3:A:871:U:H2'	3:A:872:U:C6	2.50	0.46
4:B:116:G:H2'	4:B:117:G:H8	1.80	0.46
10:H:40:THR:HG22	10:H:41:LYS:H	1.79	0.46
15:M:21:ARG:HD3	15:M:21:ARG:HA	1.66	0.46
19:Q:88:ARG:NH2	19:Q:112:GLU:HB2	2.31	0.46
21:S:38:VAL:O	21:S:54:VAL:HG23	2.15	0.46
3:A:2047:C:O2'	3:A:2823:A:N1	2.42	0.46
3:A:796:C:H2'	3:A:797:G:C8	2.51	0.46
13:K:98:GLU:N	13:K:98:GLU:OE1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:49:ASP:HA	20:R:52:GLN:HB2	1.96	0.46
3:A:96:C:P	28:Z:39:GLN:HG2	2.55	0.46
3:A:75:G:H4'	28:Z:48:ARG:CZ	2.45	0.46
3:A:1420:A:N7	3:A:2211:A:N6	2.62	0.46
3:A:1808:A:H3'	3:A:1809:A:H8	1.79	0.46
3:A:2126:A:H61	3:A:2163:A:H5'	1.80	0.46
3:A:2230:G:H2'	3:A:2231:U:C6	2.51	0.46
3:A:861:A:H2'	3:A:862:G:O4'	2.15	0.46
9:G:121:ILE:HD13	9:G:135:GLY:HA3	1.98	0.46
11:I:27:VAL:HG13	11:I:80:THR:HG23	1.97	0.46
3:A:1062:G:N2	12:J:93:PRO:HG2	2.29	0.46
18:P:53:THR:HB	18:P:65:THR:HB	1.98	0.46
20:R:18:LEU:HD11	20:R:32:TYR:HA	1.97	0.46
3:A:2788:C:H2'	3:A:2789:C:C6	2.50	0.46
14:L:73:ASP:OD1	14:L:73:ASP:N	2.39	0.46
3:A:483:A:H5''	24:V:47:LYS:HG2	1.97	0.46
3:A:1709:U:H2'	3:A:1710:G:H8	1.80	0.46
3:A:2821:A:H2'	3:A:2822:G:C8	2.51	0.46
5:C:176:LEU:HA	5:C:176:LEU:HD23	1.80	0.46
13:K:95:ARG:HG2	13:K:96:ARG:N	2.29	0.46
14:L:25:LEU:HD23	14:L:25:LEU:HA	1.67	0.46
3:A:1510:G:H2'	3:A:1511:G:H8	1.79	0.46
3:A:358:U:H2'	3:A:359:G:C8	2.44	0.46
5:C:125:LYS:HB2	5:C:125:LYS:HE2	1.77	0.46
5:C:232:HIS:NE2	5:C:244:PRO:HA	2.31	0.46
22:T:25:ARG:NH2	22:T:74:ILE:O	2.49	0.46
3:A:1342:A:C6	3:A:1397:U:C5	3.04	0.46
3:A:1387:A:H5'	3:A:1469:A:H1'	1.97	0.46
16:N:66:ARG:HB2	16:N:101:VAL:O	2.16	0.46
3:A:2069:G:N2	3:A:2443:C:C2	2.83	0.46
3:A:2786:U:H2'	3:A:2787:C:H6	1.80	0.46
3:A:878:A:H5'	3:A:879:G:OP2	2.16	0.46
5:C:33:LEU:HA	5:C:33:LEU:HD23	1.58	0.46
9:G:155:GLU:OE2	9:G:158:LYS:N	2.48	0.46
11:I:30:SER:HB3	11:I:81:LEU:HB2	1.98	0.46
19:Q:106:LYS:O	19:Q:109:ARG:NH2	2.45	0.46
3:A:1785:A:O2'	3:A:1786:A:H2'	2.16	0.46
3:A:1869:G:N2	3:A:1873:G:C5	2.83	0.46
3:A:2229:U:H2'	3:A:2230:G:C8	2.51	0.46
3:A:880:G:N2	3:A:898:C:C2	2.84	0.46
4:B:95:U:H2'	4:B:96:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:28:LEU:O	17:O:32:GLU:N	2.45	0.46
3:A:1466:U:H5''	3:A:1467:U:H5'	1.98	0.45
3:A:532:A:H2'	3:A:532:A:N3	2.31	0.45
6:D:99:GLU:OE2	6:D:182:ALA:HB2	2.15	0.45
14:L:17:ARG:HD3	14:L:17:ARG:HA	1.77	0.45
3:A:1086:A:H4'	3:A:1103:A:C2	2.52	0.45
3:A:1563:U:H2'	3:A:1564:C:C6	2.51	0.45
3:A:1570:A:H5'	5:C:36:LYS:HB2	1.98	0.45
3:A:772:C:H2'	3:A:773:U:C6	2.52	0.45
15:M:27:LEU:O	15:M:31:GLY:HA2	2.16	0.45
24:V:81:ASP:OD2	24:V:96:PHE:HB3	2.16	0.45
1:1:67:A:C4	1:1:68:A:C8	3.04	0.45
3:A:1848:A:H3'	3:A:1849:G:H8	1.80	0.45
3:A:208:C:H2'	3:A:209:C:C6	2.52	0.45
5:C:160:THR:O	5:C:195:VAL:HG23	2.17	0.45
12:J:80:LEU:HB3	12:J:138:LEU:CD1	2.46	0.45
14:L:79:PHE:CD1	19:Q:70:VAL:HG22	2.46	0.45
6:D:184:ARG:HH11	19:Q:7:GLN:CD	2.20	0.45
22:T:13:SER:O	22:T:17:VAL:HG23	2.17	0.45
24:V:37:GLU:O	24:V:39:ILE:HG12	2.17	0.45
3:A:1706:C:O2'	3:A:1757:A:H5'	2.17	0.45
14:L:114:LYS:HZ2	14:L:118:LEU:HD11	1.82	0.45
18:P:88:LYS:HG2	18:P:116:GLN:HB2	1.98	0.45
3:A:111:A:H2'	3:A:112:U:O4'	2.16	0.45
3:A:1149:G:H2'	3:A:1150:C:C6	2.50	0.45
3:A:172:A:H2'	3:A:173:A:H8	1.81	0.45
3:A:831:G:H5''	15:M:37:GLY:HA2	1.97	0.45
6:D:207:VAL:HG13	6:D:208:LYS:HG3	1.97	0.45
8:F:20:PHE:CZ	8:F:165:GLU:HA	2.51	0.45
3:A:499:U:H5''	24:V:43:LYS:HE3	1.99	0.45
3:A:1545:A:H2'	3:A:1546:G:O4'	2.17	0.45
3:A:2052:A:OP1	6:D:146:ILE:HG12	2.17	0.45
6:D:49:GLN:HA	6:D:80:TRP:O	2.16	0.45
10:H:62:LEU:HD23	10:H:135:HIS:CD2	2.52	0.45
11:I:53:ARG:O	11:I:81:LEU:HD12	2.16	0.45
3:A:908:C:O2'	16:N:70:ASP:OD2	2.30	0.45
3:A:1653:G:H3'	17:O:2:ARG:HG3	1.98	0.45
25:W:25:LYS:HB3	25:W:25:LYS:HE2	1.71	0.45
25:W:83:LYS:HB3	25:W:85:LYS:HG3	1.98	0.45
26:X:23:VAL:HG22	26:X:38:VAL:HB	1.99	0.45
3:A:1416:G:N2	3:A:1582:C:O2	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1313:U:H2'	3:A:1610:A:C2	2.51	0.45
3:A:1631:G:N2	3:A:1634:A:OP2	2.32	0.45
3:A:1972:G:H2'	3:A:1973:G:H8	1.81	0.45
3:A:2134:A:H1'	3:A:2159:G:H21	1.82	0.45
3:A:2327:A:H2'	3:A:2328:A:C8	2.51	0.45
3:A:257:C:H2'	3:A:258:G:O4'	2.16	0.45
3:A:629:G:H5''	3:A:650:C:O2'	2.16	0.45
10:H:100:ALA:O	10:H:104:THR:HG23	2.17	0.45
14:L:99:ILE:HG12	14:L:118:LEU:HB2	1.98	0.45
14:L:66:LYS:HB3	14:L:66:LYS:HE2	1.64	0.45
23:U:34:VAL:HG21	23:U:43:ILE:HD11	1.99	0.45
3:A:1022:G:O2'	3:A:1024:G:O6	2.27	0.45
3:A:1287:A:H3'	3:A:1288:G:N2	2.32	0.45
3:A:1848:A:N3	3:A:1849:G:C8	2.85	0.45
3:A:1918:A:O2'	3:A:1920:C:N4	2.50	0.45
3:A:2396:G:N3	3:A:2421:G:N2	2.64	0.45
3:A:239:C:H2'	3:A:240:C:O4'	2.16	0.45
3:A:2433:A:H5'	3:A:2434:A:P	2.57	0.45
3:A:96:C:C1'	28:Z:41:HIS:ND1	2.78	0.45
3:A:2667:C:H1'	9:G:109:PHE:CD1	2.52	0.45
9:G:148:LEU:HD23	9:G:148:LEU:HA	1.71	0.45
17:O:17:ARG:HG2	17:O:21:PHE:HE2	1.82	0.45
17:O:2:ARG:CZ	17:O:2:ARG:HB3	2.47	0.45
1:1:53:G:N2	1:1:56:A:OP2	2.43	0.45
1:1:70:G:H5'	1:1:71:C:OP2	2.16	0.45
3:A:2165:C:H2'	3:A:2166:U:O4'	2.16	0.45
3:A:593:U:H2'	3:A:594:U:C6	2.52	0.45
3:A:657:U:H2'	3:A:658:U:C6	2.52	0.45
3:A:706:A:C2	3:A:707:G:H1'	2.52	0.45
3:A:718:A:H2'	3:A:719:C:O4'	2.16	0.45
3:A:948:C:H1'	3:A:984:A:C8	2.52	0.45
13:K:69:ARG:O	13:K:89:PHE:HB3	2.17	0.45
3:A:2273:A:H2'	3:A:2274:A:C8	2.52	0.45
3:A:2313:C:H5''	8:F:88:LYS:HD3	1.98	0.45
3:A:2524:G:H2'	3:A:2525:G:O4'	2.16	0.45
3:A:764:A:H5'	5:C:209:GLY:HA2	1.98	0.45
8:F:136:ILE:HG22	8:F:141:ILE:HG21	1.98	0.45
11:I:41:LEU:HB2	11:I:99:PHE:CE1	2.52	0.45
12:J:86:ILE:CD1	12:J:138:LEU:HD21	2.46	0.45
18:P:18:LEU:HD23	18:P:18:LEU:HA	1.71	0.45
19:Q:89:ARG:HB3	19:Q:113:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2230:G:H1'	27:Y:32:ASN:HB2	1.99	0.45
28:Z:14:LEU:HA	28:Z:14:LEU:HD23	1.84	0.45
3:A:1177:G:H2'	3:A:1178:C:C6	2.52	0.44
3:A:154:U:H2'	3:A:155:A:C8	2.53	0.44
3:A:2396:G:C2	3:A:2421:G:C2	3.05	0.44
3:A:594:U:H2'	3:A:595:C:C6	2.51	0.44
5:C:243:HIS:HA	5:C:244:PRO:HD3	1.79	0.44
6:D:7:LYS:HB3	6:D:7:LYS:HE2	1.78	0.44
3:A:2667:C:H1'	9:G:109:PHE:HD1	1.82	0.44
12:J:117:MET:HB2	12:J:125:MET:HG2	1.99	0.44
13:K:65:THR:O	13:K:68:LYS:HB2	2.16	0.44
3:A:1667:G:N2	3:A:1992:G:OP2	2.44	0.44
3:A:2683:C:H4'	6:D:13:ARG:HH12	1.81	0.44
12:J:130:GLU:HB3	12:J:134:ARG:NH2	2.32	0.44
16:N:65:ILE:HG12	16:N:103:TYR:CD2	2.51	0.44
16:N:90:GLU:HB3	16:N:91:TYR:CD1	2.53	0.44
21:S:4:VAL:HA	21:S:12:HIS:O	2.17	0.44
3:A:1450:G:C6	3:A:1451:C:N4	2.86	0.44
3:A:198:C:O2'	3:A:199:A:H5'	2.17	0.44
3:A:2489:U:C4	3:A:2490:G:C6	3.06	0.44
3:A:2569:G:C2	3:A:2570:G:C8	3.05	0.44
3:A:620:G:H4'	3:A:621:A:O5'	2.17	0.44
3:A:77:G:H2'	3:A:78:U:O4'	2.16	0.44
7:E:121:VAL:O	7:E:189:THR:HA	2.18	0.44
11:I:52:MET:HE3	11:I:81:LEU:HD11	1.99	0.44
21:S:27:ILE:HG22	21:S:28:ALA:O	2.18	0.44
3:A:1198:U:H2'	3:A:1199:U:C6	2.52	0.44
3:A:2318:G:C6	3:A:2319:G:N1	2.85	0.44
3:A:2776:A:C8	3:A:2782:G:C5	3.05	0.44
9:G:117:LEU:HD13	9:G:121:ILE:HG22	1.99	0.44
15:M:10:GLU:OE2	15:M:11:GLY:N	2.50	0.44
25:W:21:ARG:HE	25:W:87:GLN:HA	1.83	0.44
26:X:55:ARG:HE	26:X:55:ARG:HB2	1.45	0.44
28:Z:56:LEU:HA	28:Z:56:LEU:HD22	1.82	0.44
3:A:141:G:H3'	3:A:141:G:C8	2.51	0.44
3:A:1508:A:O2'	3:A:1509:A:O4'	2.19	0.44
3:A:1420:A:N7	3:A:2211:A:C6	2.86	0.44
3:A:2704:C:H2'	3:A:2705:A:O4'	2.17	0.44
3:A:356:G:H2'	3:A:357:C:O4'	2.17	0.44
3:A:57:C:H2'	3:A:58:G:O4'	2.18	0.44
8:F:67:ILE:HD12	8:F:84:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:122:ILE:O	12:J:126:THR:OG1	2.22	0.44
19:Q:62:ARG:NH2	19:Q:101:ARG:HG2	2.33	0.44
3:A:2387:U:H1'	26:X:41:ARG:NH1	2.33	0.44
26:X:36:ILE:HG23	26:X:58:THR:HG23	2.00	0.44
3:A:1230:A:H2'	3:A:1231:U:O4'	2.17	0.44
3:A:1591:A:H2'	3:A:1592:C:C6	2.53	0.44
3:A:2377:A:H2'	3:A:2378:A:C8	2.53	0.44
8:F:147:ASP:OD1	8:F:150:ARG:NH2	2.51	0.44
14:L:3:GLN:HB3	14:L:3:GLN:HE21	1.66	0.44
3:A:997:G:H5''	20:R:92:ARG:NH1	2.33	0.44
27:Y:59:ILE:HG12	27:Y:67:VAL:HG21	1.99	0.44
3:A:1082:U:O2'	11:I:39:THR:HG23	2.18	0.44
3:A:149:A:C2	3:A:150:U:C2	3.06	0.44
3:A:870:U:OP1	16:N:6:ARG:NH1	2.51	0.44
3:A:1205:A:H2'	7:E:165:HIS:HE1	1.83	0.44
3:A:1301:A:H2'	3:A:1301:A:N3	2.33	0.44
3:A:1614:A:C2	22:T:93:ALA:HB2	2.52	0.44
3:A:181:A:H1'	3:A:435:C:O4'	2.17	0.44
3:A:2024:G:H2'	3:A:2025:C:C6	2.53	0.44
3:A:2678:C:H2'	3:A:2679:A:O4'	2.18	0.44
3:A:33:C:N4	3:A:446:G:O2'	2.45	0.44
3:A:630:G:N2	3:A:633:A:OP2	2.43	0.44
3:A:2683:C:H4'	6:D:13:ARG:NH1	2.33	0.44
8:F:128:TYR:CE2	8:F:130:MET:HG2	2.53	0.44
10:H:26:ALA:HA	10:H:30:LEU:HB2	1.99	0.44
19:Q:53:ARG:HB2	19:Q:56:HIS:HB2	1.99	0.44
3:A:1056:G:H1'	3:A:1103:A:N6	2.33	0.44
3:A:1082:U:H4'	11:I:46:ARG:NH1	2.33	0.44
3:A:1093:G:H1'	3:A:1099:G:N1	2.32	0.44
3:A:1853:A:N6	3:A:1888:G:O2'	2.51	0.44
3:A:277:G:H4'	3:A:278:A:N7	2.33	0.44
9:G:42:GLU:HG3	9:G:55:ARG:HH21	1.83	0.44
18:P:52:SER:O	18:P:58:ILE:HD12	2.18	0.44
23:U:31:VAL:O	23:U:32:LEU:HD23	2.18	0.44
25:W:2:PHE:HB3	25:W:50:MET:HE3	2.00	0.44
3:A:1287:A:H5'	17:O:103:ARG:HD2	1.98	0.43
3:A:1962:C:H4'	3:A:1963:U:C5	2.52	0.43
3:A:1266:G:N2	3:A:2012:G:H2'	2.33	0.43
3:A:1266:G:O2'	3:A:2012:G:O6	2.34	0.43
3:A:2292:U:H2'	3:A:2293:G:C8	2.52	0.43
3:A:2443:C:H2'	3:A:2444:G:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:475:C:N4	3:A:476:G:C6	2.86	0.43
3:A:96:C:OP1	28:Z:39:GLN:CD	2.52	0.43
4:B:114:C:H2'	4:B:115:A:H8	1.83	0.43
18:P:85:LYS:HB3	18:P:85:LYS:HE2	1.79	0.43
19:Q:100:LEU:HD23	19:Q:100:LEU:HA	1.67	0.43
19:Q:25:THR:HB	19:Q:88:ARG:HG2	1.99	0.43
3:A:1710:G:H2'	3:A:1711:A:C8	2.53	0.43
3:A:2172:U:H4'	3:A:2173:A:H5'	2.00	0.43
3:A:2654:A:OP1	3:A:2654:A:H8	2.01	0.43
5:C:141:VAL:HG12	5:C:192:LEU:HA	1.99	0.43
12:J:90:SER:HB2	12:J:136:MET:O	2.18	0.43
21:S:91:GLN:NE2	21:S:92:TRP:H	2.16	0.43
3:A:1351:C:H4'	3:A:1572:A:O4'	2.19	0.43
3:A:677:A:O2'	3:A:2071:A:H5'	2.18	0.43
3:A:969:G:H2'	3:A:970:U:C6	2.53	0.43
12:J:110:ALA:O	12:J:114:ALA:HB2	2.18	0.43
1:1:68:A:O2'	1:1:69:G:OP1	2.35	0.43
3:A:1048:A:N1	3:A:1112:G:O2'	2.36	0.43
3:A:1044:C:O2'	3:A:1111:A:N1	2.45	0.43
3:A:2647:U:H2'	3:A:2648:G:C8	2.54	0.43
3:A:380:G:H2'	3:A:381:G:O4'	2.19	0.43
3:A:776:G:HO2'	3:A:777:G:P	2.39	0.43
8:F:145:LYS:HA	8:F:145:LYS:HD3	1.89	0.43
10:H:46:PHE:HD1	10:H:50:ARG:NH2	2.16	0.43
15:M:80:SER:O	15:M:84:LYS:HE3	2.19	0.43
20:R:24:TYR:O	20:R:29:SER:HB3	2.19	0.43
22:T:47:VAL:HG22	22:T:103:ILE:HD13	2.00	0.43
3:A:1354:A:H2'	3:A:1355:G:O4'	2.19	0.43
3:A:1627:G:C2	3:A:1628:G:C8	3.07	0.43
3:A:1735:A:H2'	3:A:1736:U:O4'	2.18	0.43
3:A:2292:U:H2'	3:A:2293:G:H8	1.84	0.43
3:A:834:G:C2	3:A:835:C:C2	3.06	0.43
4:B:49:C:H2'	4:B:50:A:C8	2.54	0.43
5:C:153:GLN:O	5:C:156:ARG:HG3	2.18	0.43
7:E:108:ILE:O	7:E:112:LEU:HG	2.18	0.43
3:A:973:A:OP2	21:S:81:LYS:HE3	2.18	0.43
3:A:112:U:H5'	28:Z:58:ASN:ND2	2.34	0.43
3:A:11:C:H2'	3:A:12:U:H5'	2.00	0.43
3:A:1515:A:H3'	3:A:1516:G:H8	1.84	0.43
3:A:2847:U:H2'	3:A:2848:G:O4'	2.18	0.43
6:D:131:ASP:O	6:D:140:HIS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:26:VAL:HB	16:N:133:LYS:HB2	2.00	0.43
17:O:86:ARG:HD3	17:O:121:LYS:HG3	1.99	0.43
20:R:74:ILE:HG12	20:R:75:SER:N	2.34	0.43
21:S:4:VAL:HG12	21:S:39:LEU:HB2	2.00	0.43
3:A:976:G:HO2'	3:A:1155:A:HO2'	1.60	0.43
3:A:1434:A:C2	3:A:1435:G:C5	3.07	0.43
3:A:14:A:C6	3:A:526:A:C2	3.07	0.43
3:A:1858:A:H2'	3:A:1859:U:O4'	2.17	0.43
3:A:239:C:HO2'	3:A:622:G:HO2'	1.62	0.43
3:A:2588:G:O6	3:A:2607:G:C6	2.72	0.43
3:A:2786:U:H2'	3:A:2787:C:C6	2.53	0.43
3:A:591:U:H2'	3:A:592:A:C8	2.53	0.43
5:C:90:ASN:ND2	5:C:197:ASN:HB2	2.34	0.43
7:E:128:ALA:O	7:E:130:LYS:N	2.51	0.43
8:F:138:PHE:HA	8:F:139:PRO:HD3	1.90	0.43
15:M:6:LEU:HA	15:M:6:LEU:HD23	1.82	0.43
3:A:1542:U:H2'	3:A:1543:G:O4'	2.18	0.43
3:A:1597:A:C5'	3:A:1598:A:H5'	2.47	0.43
3:A:2114:A:C2	3:A:2166:U:H2'	2.53	0.43
3:A:2130:U:O2'	3:A:2133:G:O2'	2.32	0.43
3:A:2138:G:C6	3:A:2154:A:C2	3.06	0.43
3:A:2512:C:H5''	3:A:2513:A:OP2	2.17	0.43
3:A:463:G:N1	3:A:467:G:C6	2.86	0.43
5:C:245:VAL:HA	5:C:252:THR:HG22	2.01	0.43
10:H:104:THR:HA	10:H:108:VAL:O	2.18	0.43
10:H:62:LEU:HD22	10:H:137:GLU:OE1	2.19	0.43
3:A:566:U:H5''	15:M:29:LYS:HE3	1.99	0.43
16:N:33:LEU:HD11	16:N:128:THR:HB	2.00	0.43
20:R:9:ILE:HD12	20:R:9:ILE:H	1.84	0.43
22:T:46:LEU:HA	22:T:46:LEU:HD23	1.82	0.43
3:A:1341:G:O2'	23:U:59:ASN:ND2	2.47	0.43
3:A:1501:G:H2'	3:A:1502:A:H8	1.84	0.43
3:A:493:G:H2'	3:A:494:G:O4'	2.19	0.43
3:A:76:C:H6	3:A:76:C:O5'	2.02	0.43
3:A:93:G:H2'	3:A:94:A:H8	1.84	0.43
6:D:148:GLN:N	6:D:148:GLN:OE1	2.51	0.43
6:D:109:VAL:HG12	6:D:201:LEU:HD22	2.01	0.43
11:I:118:ILE:HA	11:I:119:PRO:HD2	1.84	0.43
12:J:33:VAL:HG13	12:J:67:PHE:CD2	2.54	0.43
13:K:26:GLY:O	13:K:30:THR:HG23	2.18	0.43
20:R:17:ILE:HD13	20:R:17:ILE:HA	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:47:ALA:HB1	26:X:51:VAL:O	2.19	0.43
3:A:1141:U:H4'	3:A:1142:A:O4'	2.19	0.43
3:A:1473:G:H2'	3:A:1474:U:O4'	2.19	0.43
3:A:1517:G:C2	3:A:1732:C:N3	2.86	0.43
3:A:2038:G:H2'	3:A:2039:U:O4'	2.17	0.43
3:A:5:A:H2'	3:A:6:A:C8	2.54	0.43
5:C:8:PRO:HB3	5:C:14:ARG:HG3	1.99	0.43
25:W:29:ILE:O	25:W:91:PHE:HB2	2.19	0.43
3:A:1494:A:H2'	3:A:1495:A:H8	1.83	0.42
3:A:1759:A:H2'	3:A:1760:C:C6	2.54	0.42
3:A:2144:G:N2	3:A:2148:G:O6	2.52	0.42
3:A:2700:A:H2'	3:A:2701:U:C6	2.54	0.42
3:A:2646:C:OP2	3:A:2732:G:O2'	2.35	0.42
3:A:2843:G:H2'	3:A:2844:G:C8	2.54	0.42
3:A:461:C:H2'	3:A:462:C:H6	1.84	0.42
3:A:783:A:C5	3:A:785:G:H1'	2.54	0.42
3:A:674:G:H2'	3:A:804:A:H61	1.83	0.42
8:F:170:LEU:HD23	8:F:170:LEU:HA	1.75	0.42
9:G:44:LYS:HB2	9:G:44:LYS:HE3	1.80	0.42
3:A:1088:A:H61	12:J:135:SER:HB3	1.82	0.42
17:O:72:ASP:OD1	17:O:73:ASN:N	2.51	0.42
23:U:34:VAL:HG11	23:U:43:ILE:HD13	2.01	0.42
3:A:141:G:C8	3:A:142:A:O4'	2.72	0.42
3:A:2184:A:H2'	3:A:2185:U:C6	2.53	0.42
3:A:2533:U:OP1	3:A:2665:A:O2'	2.34	0.42
3:A:2771:C:H2'	3:A:2772:C:C6	2.54	0.42
3:A:464:U:C2	3:A:788:A:C6	3.07	0.42
4:B:66:A:H61	4:B:107:G:H2'	1.84	0.42
5:C:133:ARG:HD2	10:H:123:ARG:NH1	2.35	0.42
5:C:200:HIS:C	5:C:200:HIS:CD2	2.92	0.42
5:C:210:ALA:HA	5:C:213:TRP:CE3	2.53	0.42
8:F:79:ILE:HG21	8:F:85:ILE:HD11	2.01	0.42
14:L:65:THR:HB	14:L:68:GLY:H	1.84	0.42
3:A:195:A:H5''	15:M:47:ARG:HH22	1.84	0.42
20:R:24:TYR:HD1	20:R:24:TYR:N	2.17	0.42
3:A:1064:C:H5''	12:J:88:SER:HB2	2.01	0.42
3:A:1590:A:H2'	3:A:1591:A:C8	2.54	0.42
3:A:1614:A:H8	3:A:1614:A:O5'	2.03	0.42
3:A:1637:A:H2'	3:A:1638:C:C6	2.54	0.42
3:A:1736:U:H2'	3:A:1737:G:O4'	2.18	0.42
3:A:1922:G:H2'	3:A:1923:U:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2790:U:H5'	3:A:2893:A:N7	2.34	0.42
4:B:106:G:H2'	4:B:107:G:O4'	2.19	0.42
7:E:29:HIS:O	7:E:32:VAL:HG22	2.19	0.42
3:A:571:U:H3'	21:S:80:ARG:NH2	2.34	0.42
28:Z:17:GLU:HA	28:Z:17:GLU:OE1	2.19	0.42
1:1:47:A:OP2	1:1:61:G:N1	2.52	0.42
3:A:1524:G:H2'	3:A:1525:A:O4'	2.20	0.42
3:A:1751:U:H2'	3:A:1752:C:C6	2.54	0.42
3:A:729:G:H2'	3:A:1775:U:H1'	2.01	0.42
3:A:543:G:H5'	3:A:544:C:OP2	2.18	0.42
3:A:653:U:C1'	3:A:654:A:H5''	2.48	0.42
8:F:48:LYS:HE2	8:F:48:LYS:HB2	1.85	0.42
9:G:149:ARG:HG3	9:G:162:VAL:O	2.20	0.42
12:J:113:LYS:HA	12:J:116:ASP:HB2	2.02	0.42
24:V:61:LYS:HG2	24:V:62:GLU:H	1.85	0.42
25:W:2:PHE:HE1	25:W:53:LYS:HD2	1.84	0.42
16:N:36:VAL:HG13	25:W:82:TYR:CD2	2.55	0.42
1:1:35:G:H2'	1:1:36:U:O4'	2.19	0.42
1:1:72:A:H2'	1:1:73:G:H8	1.84	0.42
3:A:123:G:N2	3:A:129:C:C2	2.87	0.42
3:A:794:A:H2'	3:A:795:C:C6	2.55	0.42
3:A:1902:C:H4'	5:C:242:LYS:O	2.19	0.42
5:C:24:LEU:HD12	5:C:24:LEU:HA	1.66	0.42
12:J:38:PHE:CD1	12:J:59:ILE:HD11	2.54	0.42
3:A:1039:A:H2'	3:A:1040:A:O4'	2.20	0.42
3:A:1387:A:H2'	3:A:1388:G:O4'	2.19	0.42
3:A:1759:A:C2	3:A:2697:G:H1'	2.54	0.42
3:A:1798:U:OP2	5:C:271:ARG:NH2	2.52	0.42
3:A:2322:A:C4	3:A:2323:G:C8	3.07	0.42
3:A:2518:A:N3	3:A:2518:A:H2'	2.34	0.42
3:A:307:G:N1	3:A:310:A:OP2	2.52	0.42
3:A:729:G:C5	5:C:207:LYS:HB2	2.55	0.42
10:H:94:ILE:HG23	10:H:98:ASP:HB2	2.01	0.42
11:I:15:VAL:HG11	11:I:60:LEU:CD2	2.50	0.42
11:I:85:VAL:HG21	11:I:90:GLY:O	2.20	0.42
12:J:103:ARG:H	12:J:103:ARG:HD2	1.83	0.42
19:Q:106:LYS:O	19:Q:109:ARG:HD3	2.20	0.42
3:A:1327:A:H2'	3:A:1328:A:O4'	2.19	0.42
3:A:2304:G:H22	3:A:2312:U:H3	1.67	0.42
3:A:2796:U:HO2'	3:A:2797:U:H6	1.63	0.42
3:A:647:G:H2'	3:A:648:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:812:C:C2	3:A:1250:G:N1	2.87	0.42
3:A:819:A:N3	3:A:819:A:H2'	2.34	0.42
3:A:877:A:C6	3:A:899:A:C6	3.08	0.42
4:B:57:A:C4	8:F:26:MET:HB3	2.54	0.42
10:H:1:MET:O	10:H:20:ASN:HA	2.20	0.42
12:J:22:PRO:HB2	12:J:23:PRO:HD3	2.02	0.42
12:J:74:PRO:HA	12:J:75:PRO:HD3	1.89	0.42
17:O:75:ILE:HD12	17:O:75:ILE:HA	1.82	0.42
20:R:117:LEU:HD23	20:R:117:LEU:HA	1.77	0.42
1:1:40:C:H3'	1:1:41:C:H5''	2.02	0.42
1:1:65:C:H2'	1:1:66:C:C6	2.55	0.42
3:A:1047:G:OP1	11:I:56:ARG:NH1	2.52	0.42
3:A:1065:U:H2'	3:A:1066:U:O4'	2.19	0.42
3:A:1110:G:HO2'	3:A:1111:A:P	2.43	0.42
3:A:1324:G:C4	3:A:1328:A:N6	2.87	0.42
3:A:2776:A:C2	3:A:2778:A:C4	3.07	0.42
14:L:11:ALA:O	14:L:100:PHE:N	2.46	0.42
3:A:1056:G:H5'	11:I:35:VAL:HG21	2.01	0.42
3:A:1068:G:N2	3:A:1095:A:O3'	2.44	0.42
3:A:1400:U:H2'	3:A:1401:G:O4'	2.19	0.42
3:A:1463:C:H2'	3:A:1464:G:H8	1.85	0.42
3:A:1509:A:O2'	3:A:1510:G:H8	2.03	0.42
3:A:2433:A:H5'	3:A:2434:A:OP2	2.19	0.42
3:A:565:C:H4'	3:A:1253:A:C6	2.55	0.42
16:N:42:THR:N	16:N:45:GLN:OE1	2.47	0.42
17:O:103:ARG:HB3	17:O:106:ASP:OD1	2.20	0.42
3:A:1484:U:H2'	3:A:1485:U:C6	2.55	0.42
3:A:1499:C:H2'	3:A:1500:G:H8	1.85	0.42
3:A:1607:C:O2'	3:A:1608:A:OP1	2.37	0.42
3:A:2119:A:H62	3:A:2167:U:H1'	1.85	0.42
3:A:669:G:N2	3:A:670:A:C2	2.88	0.42
3:A:910:A:C6	3:A:911:A:C6	3.08	0.42
5:C:205:LEU:HD23	5:C:205:LEU:HA	1.68	0.42
8:F:4:LEU:HA	8:F:4:LEU:HD23	1.73	0.42
8:F:34:ILE:HB	8:F:96:MET:HG3	2.02	0.42
11:I:43:LYS:HE2	12:J:118:THR:HA	2.02	0.42
20:R:31:VAL:HG12	20:R:34:VAL:H	1.85	0.42
28:Z:21:LEU:HD23	28:Z:50:VAL:HA	2.02	0.42
3:A:1417:C:H2'	3:A:1418:G:C8	2.55	0.41
3:A:1449:G:N2	3:A:1463:C:C2	2.88	0.41
3:A:1877:A:H2'	3:A:1878:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1880:U:H2'	3:A:1881:C:C6	2.55	0.41
3:A:1946:U:H2'	3:A:1947:C:H6	1.84	0.41
3:A:2706:A:C2	3:A:2707:U:C2	3.08	0.41
3:A:648:G:C2	3:A:649:G:C5	3.08	0.41
3:A:1463:C:H2'	3:A:1464:G:C8	2.55	0.41
3:A:1780:A:H3'	3:A:1781:U:H2'	2.01	0.41
3:A:2209:G:C2	3:A:2216:G:C2	3.08	0.41
3:A:848:C:H42	3:A:930:G:H1	1.68	0.41
3:A:981:A:N1	3:A:2027:G:O2'	2.42	0.41
7:E:109:LEU:HA	7:E:109:LEU:HD23	1.79	0.41
8:F:79:ILE:HD12	8:F:79:ILE:O	2.20	0.41
8:F:57:LEU:HD12	8:F:87:CYS:SG	2.61	0.41
9:G:97:ALA:HB3	9:G:104:ASN:HB2	2.01	0.41
16:N:133:LYS:HE3	16:N:133:LYS:HB3	1.42	0.41
22:T:28:LYS:HE2	22:T:28:LYS:HB2	1.41	0.41
3:A:1432:G:H2'	3:A:1433:A:C8	2.55	0.41
3:A:1825:U:O2	5:C:253:LYS:NZ	2.31	0.41
3:A:1770:G:C6	3:A:1983:G:C6	3.07	0.41
3:A:2339:C:O3'	4:B:41:G:N2	2.52	0.41
3:A:2838:G:H2'	3:A:2839:G:O4'	2.20	0.41
3:A:393:C:H2'	3:A:394:C:H6	1.85	0.41
3:A:449:A:C4	3:A:450:G:C8	3.08	0.41
3:A:53:A:H2'	3:A:54:G:O4'	2.21	0.41
7:E:181:ILE:H	7:E:181:ILE:HG13	1.69	0.41
9:G:76:VAL:O	9:G:80:THR:HG23	2.20	0.41
9:G:73:ASN:O	9:G:77:ILE:HG13	2.20	0.41
9:G:83:PHE:HB2	9:G:135:GLY:O	2.20	0.41
3:A:1005:C:H2'	3:A:1006:C:H6	1.84	0.41
3:A:1078:U:O2	3:A:1088:A:H3'	2.21	0.41
3:A:118:A:N3	3:A:178:G:H1'	2.36	0.41
3:A:1482:G:H2'	3:A:1483:G:H8	1.84	0.41
3:A:2860:A:H5''	3:A:2861:U:OP2	2.21	0.41
3:A:297:G:H2'	3:A:298:G:O4'	2.20	0.41
5:C:176:LEU:HB2	5:C:180:GLU:O	2.20	0.41
8:F:13:VAL:O	8:F:17:MET:HB2	2.20	0.41
8:F:70:ALA:HB3	8:F:81:GLN:HA	2.02	0.41
14:L:93:GLN:HA	14:L:94:PRO:HD3	1.88	0.41
1:1:34:U:H2'	1:1:35:G:C8	2.54	0.41
2:2:74:C:O5'	2:2:74:C:H6	2.03	0.41
3:A:1972:G:H2'	3:A:1973:G:C8	2.55	0.41
3:A:2895:G:H2'	3:A:2896:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:31:C:O3'	3:A:1238:G:H5'	2.21	0.41
4:B:48:U:H4'	18:P:100:HIS:HD2	1.84	0.41
4:B:71:C:C2	4:B:106:G:C2	3.08	0.41
6:D:73:VAL:HG11	6:D:93:GLY:HA2	2.02	0.41
3:A:1073:A:H2'	3:A:1074:G:O4'	2.21	0.41
3:A:1366:A:H2'	3:A:1367:A:O4'	2.20	0.41
3:A:1709:U:H2'	3:A:1710:G:C8	2.55	0.41
3:A:2102:G:C2	3:A:2187:U:O2	2.73	0.41
3:A:2267:A:H5''	3:A:2268:A:C5'	2.50	0.41
3:A:2550:G:C6	3:A:2551:C:C4	3.09	0.41
3:A:2682:A:C2	6:D:23:PRO:HB3	2.56	0.41
3:A:2812:G:H2'	3:A:2813:A:O4'	2.20	0.41
3:A:335:C:H5''	24:V:82:ARG:HD2	2.02	0.41
3:A:528:A:C8	3:A:2042:A:C2	3.09	0.41
3:A:558:U:OP1	13:K:114:LEU:N	2.46	0.41
3:A:75:G:H4'	28:Z:48:ARG:NH2	2.35	0.41
3:A:807:U:H2'	3:A:808:G:H8	1.85	0.41
3:A:1821:A:H2'	3:A:1822:C:C6	2.55	0.41
3:A:1869:G:C2	3:A:1873:G:C6	3.09	0.41
3:A:678:C:H2'	3:A:679:C:H6	1.84	0.41
8:F:36:LEU:HA	8:F:153:ASP:O	2.21	0.41
14:L:71:ARG:HD3	14:L:71:ARG:HA	1.81	0.41
3:A:2365:G:H4'	26:X:60:PHE:CE2	2.55	0.41
27:Y:3:ARG:NE	27:Y:30:LEU:HD13	2.35	0.41
3:A:1057:A:N7	3:A:1086:A:H2'	2.35	0.41
3:A:2286:G:C8	3:A:2287:A:N6	2.88	0.41
3:A:396:G:H1'	27:Y:29:PHE:HB3	2.02	0.41
3:A:465:G:C6	3:A:466:A:N6	2.89	0.41
3:A:520:G:H2'	3:A:521:U:C6	2.56	0.41
3:A:997:G:OP1	20:R:92:ARG:HD2	2.20	0.41
4:B:95:U:H2'	4:B:96:G:C8	2.56	0.41
9:G:154:PRO:HA	9:G:160:LYS:O	2.21	0.41
9:G:71:LEU:HD23	9:G:71:LEU:HA	1.83	0.41
15:M:78:ARG:HG2	15:M:113:ALA:HB3	2.03	0.41
22:T:33:LEU:HD23	22:T:33:LEU:HA	1.66	0.41
3:A:2352:A:N1	26:X:34:GLY:HA3	2.35	0.41
26:X:41:ARG:HD3	26:X:41:ARG:HA	1.53	0.41
1:1:71:C:H2'	1:1:72:A:H8	1.83	0.41
3:A:1275:A:OP2	3:A:1646:C:N4	2.53	0.41
3:A:1341:G:C2	3:A:1398:C:H4'	2.56	0.41
3:A:1789:A:H2'	3:A:1790:C:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2061:G:H2'	3:A:2501:C:O2'	2.21	0.41
3:A:2343:U:H2'	3:A:2344:U:C6	2.55	0.41
3:A:2785:C:H2'	3:A:2786:U:H6	1.85	0.41
3:A:601:C:O2'	3:A:605:G:H5''	2.21	0.41
3:A:779:U:H2'	3:A:780:G:C8	2.56	0.41
3:A:799:G:C6	3:A:800:A:C6	3.08	0.41
4:B:7:G:H5''	18:P:29:HIS:CE1	2.56	0.41
11:I:48:ALA:HB3	11:I:50:VAL:HG23	2.03	0.41
13:K:32:LEU:O	13:K:36:LEU:HG	3.31	0.41
3:A:328:U:H4'	24:V:66:GLN:HE21	1.86	0.41
27:Y:54:LYS:O	27:Y:58:VAL:HG23	2.20	0.41
3:A:1374:G:H8	3:A:1374:G:OP2	2.04	0.41
3:A:1423:G:N2	3:A:1576:U:O2	2.54	0.41
3:A:2578:G:OP2	3:A:2578:G:H4'	2.20	0.41
3:A:2663:G:H2'	3:A:2664:G:O4'	2.21	0.41
3:A:64:A:C6	3:A:65:U:C4	3.09	0.41
3:A:681:G:C2	3:A:797:G:C2	3.09	0.41
3:A:743:A:OP1	6:D:135:GLY:HA2	2.21	0.41
10:H:128:HIS:O	10:H:143:ILE:HA	2.20	0.41
14:L:103:VAL:HB	14:L:107:LEU:HD12	2.02	0.41
16:N:6:ARG:HB2	16:N:6:ARG:CZ	2.50	0.41
27:Y:74:ARG:HB3	27:Y:74:ARG:HE	1.45	0.41
3:A:811:U:C2	3:A:1251:C:C5	3.09	0.41
3:A:2229:U:H2'	3:A:2230:G:H8	1.85	0.41
3:A:561:G:H4'	20:R:48:ARG:HH22	1.86	0.41
3:A:948:C:H2'	3:A:949:G:H8	1.85	0.41
15:M:81:ASP:HB3	15:M:100:ILE:HD13	2.02	0.41
16:N:38:ARG:HB2	16:N:98:PRO:HD3	2.03	0.41
18:P:115:LEU:HD23	18:P:117:PHE:CE2	2.56	0.41
3:A:1045:C:OP1	3:A:1046:A:O2'	2.37	0.40
3:A:141:G:C8	3:A:141:G:C3'	3.04	0.40
3:A:2143:C:H2'	3:A:2144:G:O4'	2.21	0.40
3:A:199:A:N6	3:A:2434:A:C5	2.89	0.40
3:A:2804:U:H2'	3:A:2805:C:C6	2.56	0.40
3:A:778:G:H5''	3:A:779:U:OP2	2.21	0.40
9:G:9:VAL:HG23	9:G:52:PHE:HE1	1.86	0.40
11:I:61:ARG:HG2	11:I:73:LYS:HG2	2.02	0.40
21:S:85:LYS:HE2	21:S:85:LYS:HB3	1.80	0.40
27:Y:3:ARG:O	27:Y:12:PRO:HD3	2.21	0.40
27:Y:72:ARG:HG3	27:Y:78:TYR:HE2	1.86	0.40
3:A:1024:G:C6	3:A:1025:G:C6	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1071:G:O2'	3:A:1089:A:OP2	2.36	0.40
3:A:1818:U:C5	5:C:156:ARG:NH2	2.90	0.40
3:A:2421:G:H4'	3:A:2421:G:OP1	2.21	0.40
3:A:2423:U:H2'	3:A:2424:C:C1'	2.51	0.40
3:A:2431:U:O2	3:A:2431:U:O4'	2.39	0.40
3:A:277:G:H4'	3:A:278:A:C5	2.57	0.40
3:A:42:A:C6	3:A:43:G:C5	3.10	0.40
3:A:501:A:H2'	3:A:502:A:C8	2.56	0.40
3:A:863:A:H2'	3:A:864:G:C8	2.57	0.40
3:A:863:A:H2'	3:A:864:G:H8	1.86	0.40
5:C:34:LEU:HD21	5:C:63:ARG:HG3	2.03	0.40
9:G:125:CYS:HB2	9:G:127:THR:O	2.21	0.40
12:J:42:PHE:CE1	12:J:57:VAL:HB	2.56	0.40
16:N:65:ILE:HG12	16:N:103:TYR:HD2	1.86	0.40
17:O:72:ASP:O	17:O:76:VAL:HG13	2.21	0.40
19:Q:40:LEU:HD23	19:Q:40:LEU:HA	1.75	0.40
22:T:109:ASP:OD1	22:T:110:ARG:N	2.54	0.40
24:V:36:VAL:HB	24:V:39:ILE:HB	2.02	0.40
24:V:96:PHE:O	24:V:100:SER:HA	2.21	0.40
3:A:1127:A:N7	3:A:2488:G:O2'	2.54	0.40
3:A:118:A:C8	3:A:119:A:C8	3.09	0.40
3:A:1838:C:H4'	3:A:1839:G:H8	1.85	0.40
3:A:2388:A:H5'	3:A:2389:G:OP2	2.21	0.40
3:A:2603:G:C6	3:A:2604:U:C4	3.10	0.40
3:A:2627:G:H1'	3:A:2777:G:N2	2.36	0.40
3:A:2847:U:C5	3:A:2848:G:C5	3.09	0.40
3:A:445:C:H2'	3:A:446:G:O4'	2.22	0.40
3:A:719:C:H2'	3:A:720:U:C6	2.57	0.40
3:A:822:G:H2'	3:A:823:C:C6	2.56	0.40
11:I:13:ALA:O	11:I:17:GLU:HB2	2.22	0.40
15:M:79:LEU:HB2	15:M:113:ALA:O	2.21	0.40
18:P:25:ARG:O	18:P:25:ARG:HG3	2.22	0.40
18:P:28:VAL:HG12	18:P:93:ASP:O	2.21	0.40
26:X:70:GLU:HG3	26:X:72:LYS:HE2	2.04	0.40
1:I:65:C:H2'	1:I:66:C:H6	1.86	0.40
3:A:987:C:O2'	3:A:1000:A:N3	2.44	0.40
3:A:1672:A:N6	3:A:1673:G:C6	2.89	0.40
3:A:1707:G:C5	3:A:1756:G:C6	3.10	0.40
3:A:1807:G:N2	3:A:1811:G:C5	2.89	0.40
3:A:1:G:H2'	3:A:2:G:C8	2.57	0.40
3:A:2394:C:H42	3:A:2422:C:N4	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2600:A:H2'	3:A:2601:C:C6	2.56	0.40
3:A:339:U:H6	3:A:339:U:O5'	2.05	0.40
7:E:148:ILE:HG12	7:E:148:ILE:H	1.64	0.40
7:E:58:LYS:HA	7:E:59:PRO:HD3	1.94	0.40
8:F:65:PRO:HA	8:F:89:VAL:HG22	2.01	0.40
11:I:99:PHE:HD2	11:I:106:PHE:HZ	1.69	0.40
13:K:99:ARG:HD2	13:K:102:GLU:OE1	2.22	0.40
18:P:115:LEU:HD23	18:P:117:PHE:HE2	1.86	0.40
26:X:45:PHE:CD1	26:X:80:ILE:HD11	2.56	0.40
28:Z:46:VAL:O	28:Z:50:VAL:HG23	2.21	0.40
3:A:1113:U:H2'	3:A:1114:C:H6	1.86	0.40
3:A:1139:G:OP2	3:A:1139:G:H8	2.05	0.40
3:A:729:G:C6	5:C:207:LYS:HB2	2.56	0.40
3:A:871:U:H4'	16:N:68:PHE:CD2	2.57	0.40
4:B:49:C:H2'	4:B:50:A:H8	1.87	0.40
5:C:157:SER:O	5:C:160:THR:OG1	2.38	0.40
9:G:90:VAL:HG21	9:G:163:ARG:NH1	2.37	0.40
17:O:22:ARG:HG3	17:O:70:THR:HA	2.04	0.40
17:O:65:LEU:HD12	17:O:65:LEU:HA	1.84	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	
5	C	269/271 (99%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
9	G	174/176 (99%)	171 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	H	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	26	71
11	I	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	24	70
12	J	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
13	K	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
20	R	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
23	U	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
24	V	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
28	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
29	a	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	b	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
31	c	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	e	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100
35	i	374/398 (94%)	357 (96%)	15 (4%)	2 (0%)	34	77
36	k	16/18 (89%)	11 (69%)	5 (31%)	0	100	100
All	All	3822/3908 (98%)	3685 (96%)	133 (4%)	4 (0%)	59	90

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	i	240	LEU

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Mol	Chain	Res	Type
35	i	241	PRO
10	H	118	PRO
11	I	108	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C	216/216 (100%)	192 (89%)	24 (11%)	8	37
6	D	164/164 (100%)	154 (94%)	10 (6%)	23	63
7	E	165/165 (100%)	152 (92%)	13 (8%)	15	53
8	F	148/148 (100%)	130 (88%)	18 (12%)	6	33
9	G	137/137 (100%)	129 (94%)	8 (6%)	25	64
10	H	114/114 (100%)	100 (88%)	14 (12%)	6	33
11	I	95/95 (100%)	89 (94%)	6 (6%)	22	61
12	J	104/104 (100%)	93 (89%)	11 (11%)	8	39
13	K	116/116 (100%)	105 (90%)	11 (10%)	11	44
14	L	104/104 (100%)	94 (90%)	10 (10%)	10	44
15	M	103/103 (100%)	94 (91%)	9 (9%)	13	48
16	N	109/109 (100%)	100 (92%)	9 (8%)	14	51
17	O	102/102 (100%)	95 (93%)	7 (7%)	19	59
18	P	87/87 (100%)	75 (86%)	12 (14%)	4	29
19	Q	99/99 (100%)	90 (91%)	9 (9%)	12	46
20	R	89/89 (100%)	82 (92%)	7 (8%)	15	53
21	S	84/84 (100%)	76 (90%)	8 (10%)	11	44
22	T	93/93 (100%)	88 (95%)	5 (5%)	27	66
23	U	82/82 (100%)	76 (93%)	6 (7%)	17	57
24	V	83/83 (100%)	76 (92%)	7 (8%)	14	51
25	W	78/78 (100%)	72 (92%)	6 (8%)	16	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	X	57/58 (98%)	51 (90%)	6 (10%)	8	39
27	Y	67/67 (100%)	63 (94%)	4 (6%)	24	63
28	Z	54/54 (100%)	49 (91%)	5 (9%)	11	45
29	a	48/48 (100%)	46 (96%)	2 (4%)	36	72
30	b	47/47 (100%)	35 (74%)	12 (26%)	1	6
31	c	45/46 (98%)	40 (89%)	5 (11%)	8	37
32	d	38/38 (100%)	32 (84%)	6 (16%)	3	23
33	e	51/51 (100%)	47 (92%)	4 (8%)	16	54
34	f	34/34 (100%)	31 (91%)	3 (9%)	12	48
35	i	313/315 (99%)	296 (95%)	17 (5%)	27	66
36	k	17/17 (100%)	15 (88%)	2 (12%)	6	35
All	All	3143/3147 (100%)	2867 (91%)	276 (9%)	17	48

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	3	VAL
5	C	24	LEU
5	C	35	GLU
5	C	51	THR
5	C	72	ASP
5	C	74	ILE
5	C	120	VAL
5	C	130	LEU
5	C	134	ASN
5	C	156	ARG
5	C	180	GLU
5	C	185	GLU
5	C	189	ARG
5	C	195	VAL
5	C	203	ARG
5	C	204	VAL
5	C	228	VAL
5	C	242	LYS
5	C	250	VAL
5	C	251	GLN
5	C	257	THR
5	C	261	LYS

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Mol	Chain	Res	Type
5	C	265	LYS
5	C	271	ARG
6	D	12	THR
6	D	13	ARG
6	D	18	ASP
6	D	28	GLU
6	D	73	VAL
6	D	84	LEU
6	D	128	ARG
6	D	139	SER
6	D	160	LYS
6	D	168	GLU
7	E	84	THR
7	E	85	PHE
7	E	94	GLN
7	E	97	ASN
7	E	105	LEU
7	E	115	GLN
7	E	119	ILE
7	E	127	GLU
7	E	148	ILE
7	E	173	THR
7	E	179	SER
7	E	184	ASP
7	E	196	VAL
8	F	3	LYS
8	F	4	LEU
8	F	14	LYS
8	F	25	VAL
8	F	49	LEU
8	F	51	ASP
8	F	52	ASN
8	F	72	LYS
8	F	81	GLN
8	F	104	ILE
8	F	106	ILE
8	F	130	MET
8	F	141	ILE
8	F	144	ASP
8	F	149	VAL
8	F	150	ARG
8	F	153	ASP

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Mol	Chain	Res	Type
8	F	162	SER
9	G	10	VAL
9	G	11	VAL
9	G	49	THR
9	G	87	LEU
9	G	114	ASP
9	G	125	CYS
9	G	127	THR
9	G	153	ARG
10	H	15	LEU
10	H	17	ASP
10	H	25	TYR
10	H	37	VAL
10	H	58	LEU
10	H	60	GLU
10	H	76	GLU
10	H	77	THR
10	H	78	VAL
10	H	86	ASP
10	H	87	GLU
10	H	110	VAL
10	H	112	LYS
10	H	116	ARG
11	I	16	SER
11	I	36	ASP
11	I	58	THR
11	I	85	VAL
11	I	96	PHE
11	I	109	LYS
12	J	9	VAL
12	J	21	SER
12	J	28	LEU
12	J	31	GLN
12	J	55	ILE
12	J	66	SER
12	J	111	GLN
12	J	112	THR
12	J	113	LYS
12	J	116	ASP
12	J	128	SER
13	K	5	THR
13	K	7	LYS

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Mol	Chain	Res	Type
13	K	34	ARG
13	K	40	HIS
13	K	44	TYR
13	K	69	ARG
13	K	70	THR
13	K	88	THR
13	K	103	ILE
13	K	122	LEU
13	K	131	ASN
14	L	1	MET
14	L	21	CYS
14	L	42	THR
14	L	49	ARG
14	L	56	ASP
14	L	58	LEU
14	L	65	THR
14	L	84	CYS
14	L	106	GLU
14	L	116	ILE
15	M	2	ARG
15	M	14	LYS
15	M	46	VAL
15	M	47	ARG
15	M	55	MET
15	M	59	ARG
15	M	86	GLU
15	M	91	ASP
15	M	126	ARG
16	N	6	ARG
16	N	7	THR
16	N	12	MET
16	N	25	ASP
16	N	54	THR
16	N	58	LYS
16	N	115	GLU
16	N	133	LYS
16	N	135	VAL
17	O	2	ARG
17	O	14	SER
17	O	36	THR
17	O	69	ARG
17	O	74	GLU

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Mol	Chain	Res	Type
17	O	75	ILE
17	O	100	CYS
18	P	2	ASP
18	P	5	SER
18	P	19	GLN
18	P	20	GLU
18	P	31	THR
18	P	36	TYR
18	P	43	ASN
18	P	55	GLU
18	P	61	GLN
18	P	69	ASP
18	P	78	VAL
18	P	98	GLN
19	Q	3	ASN
19	Q	7	GLN
19	Q	21	ARG
19	Q	26	VAL
19	Q	51	ARG
19	Q	65	SER
19	Q	68	GLU
19	Q	92	VAL
19	Q	115	ASN
20	R	6	ARG
20	R	13	ARG
20	R	17	ILE
20	R	24	TYR
20	R	51	ARG
20	R	52	GLN
20	R	109	LEU
21	S	20	VAL
21	S	25	LEU
21	S	38	VAL
21	S	45	GLU
21	S	71	LYS
21	S	72	VAL
21	S	83	TYR
21	S	101	ILE
22	T	12	SER
22	T	28	LYS
22	T	74	ILE
22	T	95	ARG

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Mol	Chain	Res	Type
22	T	98	LYS
23	U	7	LEU
23	U	16	VAL
23	U	17	SER
23	U	48	GLN
23	U	72	GLN
23	U	91	GLN
24	V	7	ARG
24	V	34	VAL
24	V	41	LEU
24	V	42	VAL
24	V	68	SER
24	V	83	VAL
24	V	102	THR
25	W	7	GLU
25	W	12	GLN
25	W	61	LEU
25	W	78	GLN
25	W	90	ASP
25	W	92	VAL
26	X	11	ARG
26	X	12	ASN
26	X	21	LEU
26	X	35	SER
26	X	41	ARG
26	X	56	ASP
27	Y	2	SER
27	Y	4	VAL
27	Y	42	SER
27	Y	74	ARG
28	Z	2	LYS
28	Z	44	LYS
28	Z	45	GLN
28	Z	48	ARG
28	Z	56	LEU
29	a	36	VAL
29	a	56	LYS
30	b	4	GLN
30	b	9	THR
30	b	15	MET
30	b	18	SER
30	b	25	VAL

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Mol	Chain	Res	Type
30	b	26	THR
30	b	28	LEU
30	b	32	LYS
30	b	36	GLU
30	b	40	ARG
30	b	46	ASP
30	b	52	ARG
31	c	5	ILE
31	c	6	ARG
31	c	10	LYS
31	c	22	THR
31	c	47	VAL
32	d	1	MET
32	d	12	ARG
32	d	24	THR
32	d	25	LYS
32	d	34	ARG
32	d	41	ARG
33	e	8	ARG
33	e	31	HIS
33	e	32	ILE
33	e	51	SER
34	f	2	LYS
34	f	12	ARG
34	f	36	ARG
35	i	1	MET
35	i	2	PHE
35	i	5	LEU
35	i	16	ILE
35	i	32	ARG
35	i	42	ASP
35	i	45	LEU
35	i	147	GLN
35	i	185	ASP
35	i	217	THR
35	i	220	VAL
35	i	240	LEU
35	i	242	LEU
35	i	247	LEU
35	i	261	SER
35	i	343	ASN
35	i	411	GLN

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Mol	Chain	Res	Type
36	k	27	MET
36	k	44	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
5	C	86	ASN
5	C	90	ASN
5	C	200	HIS
5	C	251	GLN
6	D	136	ASN
6	D	140	HIS
7	E	165	HIS
8	F	81	GLN
8	F	127	ASN
10	H	11	ASN
10	H	33	GLN
10	H	43	ASN
10	H	66	ASN
12	J	31	GLN
13	K	80	HIS
13	K	86	GLN
14	L	3	GLN
14	L	89	ASN
15	M	104	GLN
16	N	3	GLN
17	O	18	GLN
18	P	100	HIS
19	Q	52	ASN
19	Q	66	ASN
20	R	81	ASN
21	S	82	HIS
22	T	7	HIS
23	U	48	GLN
23	U	59	ASN
26	X	46	HIS
28	Z	15	ASN
28	Z	31	GLN
28	Z	36	GLN
28	Z	58	ASN
32	d	26	ASN
32	d	29	GLN

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Mol	Chain	Res	Type
35	i	26	ASN
35	i	62	HIS
35	i	72	GLN
35	i	91	GLN
35	i	147	GLN
35	i	227	GLN
35	i	264	HIS
35	i	411	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	42/113 (37%)	16 (38%)	1 (2%)
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2883 (99%)	518 (17%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3041/3119 (97%)	548 (18%)	20 (0%)

All (548) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	C
1	1	34	U
1	1	37	U
1	1	39	A
1	1	41	C
1	1	42	A
1	1	43	G
1	1	46	C
1	1	57	G
1	1	58	G
1	1	67	A
1	1	69	G
1	1	70	G
1	1	71	C
1	1	72	A
1	1	74	A
2	2	76	A
3	A	10	A
3	A	12	U
3	A	33	C

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Mol	Chain	Res	Type
3	A	34	U
3	A	35	G
3	A	45	G
3	A	46	G
3	A	49	A
3	A	50	U
3	A	51	G
3	A	62	U
3	A	63	A
3	A	65	U
3	A	71	A
3	A	72	U
3	A	74	A
3	A	75	G
3	A	84	A
3	A	93	G
3	A	96	C
3	A	101	A
3	A	102	U
3	A	103	A
3	A	110	G
3	A	118	A
3	A	119	A
3	A	120	U
3	A	136	G
3	A	137	U
3	A	138	U
3	A	139	U
3	A	142	A
3	A	156	A
3	A	162	U
3	A	181	A
3	A	188	G
3	A	196	A
3	A	199	A
3	A	215	G
3	A	216	A
3	A	220	G
3	A	221	A
3	A	222	A
3	A	226	A
3	A	248	G

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Mol	Chain	Res	Type
3	A	266	G
3	A	272	A
3	A	275	C
3	A	276	U
3	A	285	G
3	A	291	G
3	A	302	C
3	A	311	A
3	A	329	G
3	A	330	A
3	A	335	C
3	A	349	U
3	A	353	C
3	A	356	G
3	A	361	G
3	A	362	A
3	A	372	G
3	A	386	G
3	A	396	G
3	A	399	U
3	A	411	G
3	A	419	U
3	A	424	G
3	A	454	A
3	A	455	C
3	A	475	C
3	A	477	A
3	A	479	A
3	A	480	A
3	A	481	G
3	A	491	G
3	A	504	A
3	A	505	A
3	A	509	C
3	A	510	C
3	A	513	A
3	A	518	G
3	A	529	A
3	A	531	C
3	A	532	A
3	A	533	G
3	A	543	G

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Mol	Chain	Res	Type
3	A	544	C
3	A	550	C
3	A	552	U
3	A	558	U
3	A	563	A
3	A	567	U
3	A	568	U
3	A	573	U
3	A	575	A
3	A	586	A
3	A	603	A
3	A	613	A
3	A	614	A
3	A	615	U
3	A	627	A
3	A	632	A
3	A	634	C
3	A	637	A
3	A	645	C
3	A	646	U
3	A	647	G
3	A	653	U
3	A	654	A
3	A	655	A
3	A	668	A
3	A	685	A
3	A	686	U
3	A	711	G
3	A	712	G
3	A	713	G
3	A	718	A
3	A	730	A
3	A	747	U
3	A	753	A
3	A	757	G
3	A	763	G
3	A	764	A
3	A	765	C
3	A	775	G
3	A	777	G
3	A	782	A
3	A	784	G

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Mol	Chain	Res	Type
3	A	785	G
3	A	788	A
3	A	789	A
3	A	790	U
3	A	791	C
3	A	793	A
3	A	794	A
3	A	801	G
3	A	805	G
3	A	812	C
3	A	827	U
3	A	828	U
3	A	831	G
3	A	846	U
3	A	859	G
3	A	865	C
3	A	869	G
3	A	878	A
3	A	896	A
3	A	897	C
3	A	899	A
3	A	907	G
3	A	910	A
3	A	914	G
3	A	915	C
3	A	932	U
3	A	933	A
3	A	946	C
3	A	953	G
3	A	957	C
3	A	961	C
3	A	974	G
3	A	983	A
3	A	990	A
3	A	996	A
3	A	999	U
3	A	1005	C
3	A	1009	A
3	A	1012	U
3	A	1013	C
3	A	1022	G
3	A	1023	U

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Mol	Chain	Res	Type
3	A	1027	A
3	A	1033	U
3	A	1040	A
3	A	1046	A
3	A	1056	G
3	A	1057	A
3	A	1070	A
3	A	1071	G
3	A	1073	A
3	A	1083	U
3	A	1087	G
3	A	1088	A
3	A	1090	A
3	A	1101	U
3	A	1111	A
3	A	1112	G
3	A	1116	G
3	A	1129	A
3	A	1130	U
3	A	1132	U
3	A	1133	A
3	A	1135	C
3	A	1136	G
3	A	1139	G
3	A	1142	A
3	A	1143	A
3	A	1155	A
3	A	1173	U
3	A	1179	G
3	A	1182	G
3	A	1206	G
3	A	1212	G
3	A	1218	G
3	A	1236	G
3	A	1238	G
3	A	1247	A
3	A	1249	U
3	A	1252	G
3	A	1253	A
3	A	1256	G
3	A	1262	A
3	A	1271	G

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Mol	Chain	Res	Type
3	A	1272	A
3	A	1294	U
3	A	1300	G
3	A	1301	A
3	A	1302	A
3	A	1308	A
3	A	1329	U
3	A	1332	G
3	A	1337	G
3	A	1338	G
3	A	1345	C
3	A	1346	G
3	A	1365	A
3	A	1379	U
3	A	1383	A
3	A	1395	A
3	A	1403	A
3	A	1416	G
3	A	1417	C
3	A	1424	G
3	A	1428	C
3	A	1434	A
3	A	1437	C
3	A	1449	G
3	A	1451	C
3	A	1452	G
3	A	1453	A
3	A	1482	G
3	A	1489	C
3	A	1491	G
3	A	1493	C
3	A	1494	A
3	A	1495	A
3	A	1497	U
3	A	1498	C
3	A	1509	A
3	A	1510	G
3	A	1515	A
3	A	1524	G
3	A	1529	G
3	A	1533	C
3	A	1535	A

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Mol	Chain	Res	Type
3	A	1536	C
3	A	1537	G
3	A	1554	U
3	A	1560	G
3	A	1566	A
3	A	1569	A
3	A	1576	U
3	A	1578	U
3	A	1581	G
3	A	1583	A
3	A	1585	C
3	A	1606	C
3	A	1607	C
3	A	1608	A
3	A	1616	A
3	A	1634	A
3	A	1639	C
3	A	1647	U
3	A	1648	U
3	A	1649	G
3	A	1660	G
3	A	1674	G
3	A	1677	A
3	A	1715	G
3	A	1722	A
3	A	1725	U
3	A	1729	U
3	A	1730	C
3	A	1738	G
3	A	1757	A
3	A	1764	C
3	A	1773	A
3	A	1782	U
3	A	1786	A
3	A	1791	A
3	A	1800	C
3	A	1801	A
3	A	1802	A
3	A	1808	A
3	A	1809	A
3	A	1811	G
3	A	1816	C

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Mol	Chain	Res	Type
3	A	1829	A
3	A	1847	A
3	A	1849	G
3	A	1850	G
3	A	1870	C
3	A	1871	A
3	A	1872	A
3	A	1876	A
3	A	1896	G
3	A	1906	G
3	A	1920	C
3	A	1927	A
3	A	1929	G
3	A	1930	G
3	A	1931	U
3	A	1934	C
3	A	1936	A
3	A	1937	A
3	A	1939	U
3	A	1955	U
3	A	1956	U
3	A	1960	A
3	A	1962	C
3	A	1966	A
3	A	1967	C
3	A	1970	A
3	A	1971	U
3	A	1972	G
3	A	1974	C
3	A	1982	U
3	A	1991	U
3	A	1992	G
3	A	1993	U
3	A	1997	C
3	A	2021	C
3	A	2023	C
3	A	2030	A
3	A	2031	A
3	A	2033	A
3	A	2043	C
3	A	2050	C
3	A	2054	A

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Mol	Chain	Res	Type
3	A	2055	C
3	A	2056	G
3	A	2060	A
3	A	2061	G
3	A	2062	A
3	A	2069	G
3	A	2072	C
3	A	2093	G
3	A	2097	A
3	A	2101	A
3	A	2103	C
3	A	2104	C
3	A	2105	U
3	A	2106	U
3	A	2111	U
3	A	2112	G
3	A	2113	U
3	A	2116	G
3	A	2117	A
3	A	2118	U
3	A	2119	A
3	A	2120	G
3	A	2123	G
3	A	2126	A
3	A	2128	G
3	A	2131	U
3	A	2132	U
3	A	2133	G
3	A	2134	A
3	A	2145	C
3	A	2146	C
3	A	2147	A
3	A	2148	G
3	A	2159	G
3	A	2160	C
3	A	2161	C
3	A	2163	A
3	A	2164	C
3	A	2165	C
3	A	2167	U
3	A	2168	G
3	A	2169	A

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Mol	Chain	Res	Type
3	A	2170	A
3	A	2171	A
3	A	2172	U
3	A	2173	A
3	A	2174	C
3	A	2177	C
3	A	2178	C
3	A	2185	U
3	A	2187	U
3	A	2190	G
3	A	2198	A
3	A	2203	U
3	A	2204	G
3	A	2211	A
3	A	2212	A
3	A	2225	A
3	A	2238	G
3	A	2239	G
3	A	2250	G
3	A	2268	A
3	A	2278	A
3	A	2280	G
3	A	2283	C
3	A	2287	A
3	A	2288	A
3	A	2297	A
3	A	2305	U
3	A	2308	G
3	A	2322	A
3	A	2325	G
3	A	2331	G
3	A	2336	A
3	A	2345	G
3	A	2347	C
3	A	2350	C
3	A	2354	C
3	A	2357	G
3	A	2366	A
3	A	2383	G
3	A	2385	C
3	A	2402	U
3	A	2403	C

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Mol	Chain	Res	Type
3	A	2406	A
3	A	2420	C
3	A	2421	G
3	A	2422	C
3	A	2423	U
3	A	2424	C
3	A	2425	A
3	A	2427	C
3	A	2429	G
3	A	2430	A
3	A	2431	U
3	A	2432	A
3	A	2434	A
3	A	2435	A
3	A	2440	C
3	A	2441	U
3	A	2445	G
3	A	2448	A
3	A	2464	G
3	A	2475	C
3	A	2476	A
3	A	2478	A
3	A	2491	U
3	A	2492	U
3	A	2497	A
3	A	2502	G
3	A	2504	U
3	A	2505	G
3	A	2506	U
3	A	2507	C
3	A	2513	A
3	A	2514	U
3	A	2518	A
3	A	2520	C
3	A	2529	G
3	A	2566	A
3	A	2567	G
3	A	2578	G
3	A	2582	G
3	A	2585	U
3	A	2586	U
3	A	2602	A

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Mol	Chain	Res	Type
3	A	2603	G
3	A	2609	U
3	A	2613	U
3	A	2615	U
3	A	2621	G
3	A	2623	G
3	A	2624	G
3	A	2629	U
3	A	2630	G
3	A	2636	C
3	A	2638	G
3	A	2669	G
3	A	2682	A
3	A	2689	U
3	A	2690	U
3	A	2714	G
3	A	2716	C
3	A	2726	A
3	A	2733	A
3	A	2739	U
3	A	2744	G
3	A	2748	A
3	A	2757	A
3	A	2765	A
3	A	2778	A
3	A	2779	U
3	A	2780	G
3	A	2787	C
3	A	2791	G
3	A	2792	A
3	A	2798	U
3	A	2799	A
3	A	2801	G
3	A	2820	A
3	A	2821	A
3	A	2825	G
3	A	2833	U
3	A	2835	A
3	A	2836	U
3	A	2849	U
3	A	2860	A
3	A	2861	U

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Mol	Chain	Res	Type
3	A	2867	G
3	A	2870	C
3	A	2873	A
3	A	2879	A
3	A	2880	C
3	A	2883	A
3	A	2884	U
3	A	2885	G
3	A	2886	A
3	A	2888	C
3	A	2891	U
4	B	24	G
4	B	25	U
4	B	35	C
4	B	41	G
4	B	45	A
4	B	56	G
4	B	66	A
4	B	67	G
4	B	71	C
4	B	88	C
4	B	89	U
4	B	90	C
4	B	109	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	68	A
3	A	100	U
3	A	613	A
3	A	645	C
3	A	653	U
3	A	784	G
3	A	827	U
3	A	830	G
3	A	1110	G
3	A	1344	U
3	A	1494	A
3	A	1721	G
3	A	1939	U
3	A	2127	G

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Mol	Chain	Res	Type
3	A	2158	A
3	A	2422	C
3	A	2424	C
3	A	2430	A
3	A	2602	A
3	A	2756	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 433 ligands modelled in this entry, 432 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	GNP	i	1400	-	29,34,34	2.46	12 (41%)	28,54,54	1.79	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GNP	i	1400	-	-	0/16/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	i	1400	GNP	C4-N9	-6.28	1.39	1.47
39	i	1400	GNP	C5-C6	-3.35	1.46	1.53
39	i	1400	GNP	PB-O2B	-2.50	1.50	1.56
39	i	1400	GNP	PG-O2G	-2.28	1.50	1.56
39	i	1400	GNP	PG-O3G	-2.23	1.50	1.56
39	i	1400	GNP	C8-N9	-2.17	1.40	1.47
39	i	1400	GNP	PG-N3B	3.33	1.72	1.63
39	i	1400	GNP	PB-N3B	3.43	1.72	1.63
39	i	1400	GNP	PB-O1B	3.47	1.49	1.46
39	i	1400	GNP	C1'-N9	3.90	1.49	1.42
39	i	1400	GNP	PG-O1G	4.21	1.50	1.46
39	i	1400	GNP	C6-N1	4.73	1.41	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	i	1400	GNP	O6-C6-N1	-3.19	118.61	122.80
39	i	1400	GNP	O3A-PB-N3B	-2.12	100.23	106.07
39	i	1400	GNP	O2B-PB-O1B	4.33	118.56	110.02
39	i	1400	GNP	C4-C5-N7	4.75	110.09	102.67
39	i	1400	GNP	O6-C6-C5	4.79	128.85	119.69

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
3	A	4
35	i	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	297:MET	C	328:GLY	N	35.34
1	A	882:G	O3'	894:U	P	17.07
1	A	545:U	O3'	548:G	P	16.33
1	A	1912:A	O3'	1917:U	P	16.01
1	i	343:ASN	C	369:ASP	N	12.86
1	A	1173:U	O3'	1177:G	P	12.40