Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 07:13 AM EST

PDB ID	:	3CC7
Title	:	Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation C2487U
Authors	:	Blaha, G.; Gurel, G.
Deposited on	:	2008-02-25
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

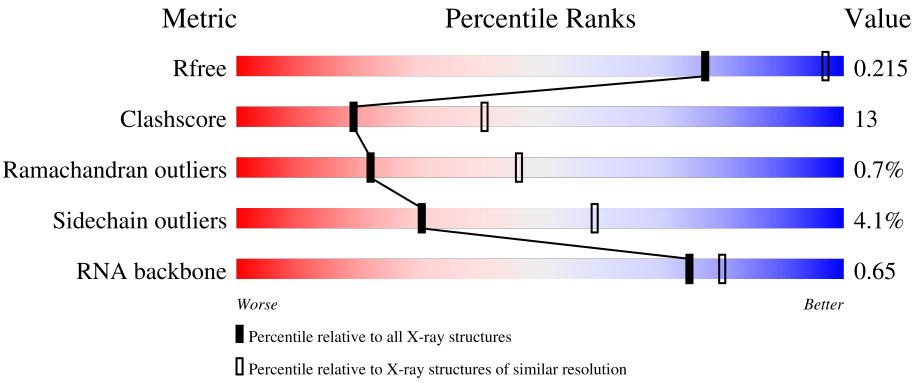
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	240	70% 26% • ••
2	B	338	65% 32% •
3	C	246	74% 22% •
4	D	177	49% 28% • 21%
5	E	178	79% 17% • •
6	F	120	75% 23% ••

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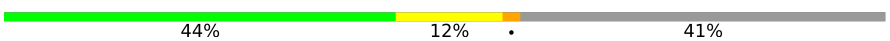
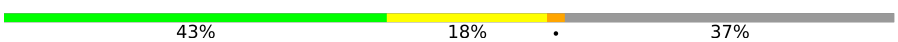
Mol	Chain	Length	Quality of chain
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 99122 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	237	1753	1072	352	324	5	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	337	2625	1616	493	511	5	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	246	1860	1130	345	384	1	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	140	1094	685	195	210	4	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	172	1357	840	224	289	4	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	119	890	551	141	197	1	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O	0	0	0
			1130	686	228	216			

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10872	19054	2745			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	2	Total	Mg	0	0
			2	2		
32	B	2	Total	Mg	0	0
			2	2		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	0	85	Total	Mg	0	0
			85	85		
32	9	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	J	3	Total Cl 3 3	0	0
33	L	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	0	10	Total Cl 10 10	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	3	Total Sr 3 3	0	0
34	B	2	Total Sr 2 2	0	0
34	F	1	Total Sr 1 1	0	0
34	J	1	Total Sr 1 1	0	0
34	R	1	Total Sr 1 1	0	0
34	S	1	Total Sr 1 1	0	0
34	1	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	0	93	Total Sr 93 93	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	9	2	Total Sr 2 2	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0
35	0	66	Total Na 66 66	0	0
35	9	2	Total Na 2 2	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Cd 1 1	0	0
36	U	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	3	1	Total Cd 1 1	0	0

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	111	Total O 111 111	0	0
38	B	153	Total O 153 153	0	0
38	C	165	Total O 165 165	0	0
38	D	46	Total O 46 46	0	0
38	E	44	Total O 44 44	0	0
38	F	23	Total O 23 23	0	0
38	G	19	Total O 19 19	0	0
38	H	71	Total O 71 71	0	0
38	I	10	Total O 10 10	0	0
38	J	54	Total O 54 54	0	0
38	K	56	Total O 56 56	0	0
38	L	80	Total O 80 80	0	0
38	M	130	Total O 130 130	0	0
38	N	59	Total O 59 59	0	0
38	O	41	Total O 41 41	0	0
38	P	61	Total O 61 61	0	0
38	Q	51	Total O 51 51	0	0
38	R	78	Total O 78 78	0	0
38	S	33	Total O 33 33	0	0
38	T	37	Total O 37 37	0	0
38	U	25	Total O 25 25	0	0

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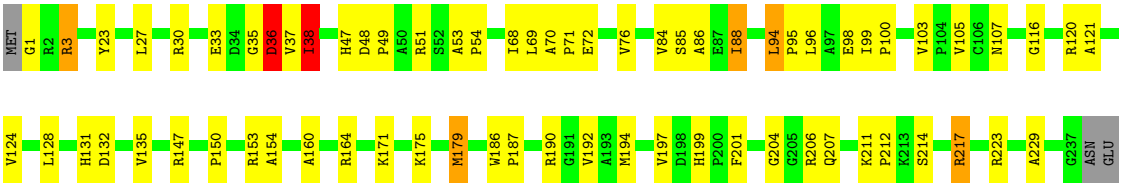
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	V	11	Total O 11 11	0	0
38	W	63	Total O 63 63	0	0
38	X	28	Total O 28 28	0	0
38	Y	91	Total O 91 91	0	0
38	Z	28	Total O 28 28	0	0
38	1	52	Total O 52 52	0	0
38	2	37	Total O 37 37	0	0
38	3	68	Total O 68 68	0	0
38	0	5951	Total O 5951 5951	0	0
38	9	147	Total O 147 147	0	0

3 Residue-property plots (i)

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

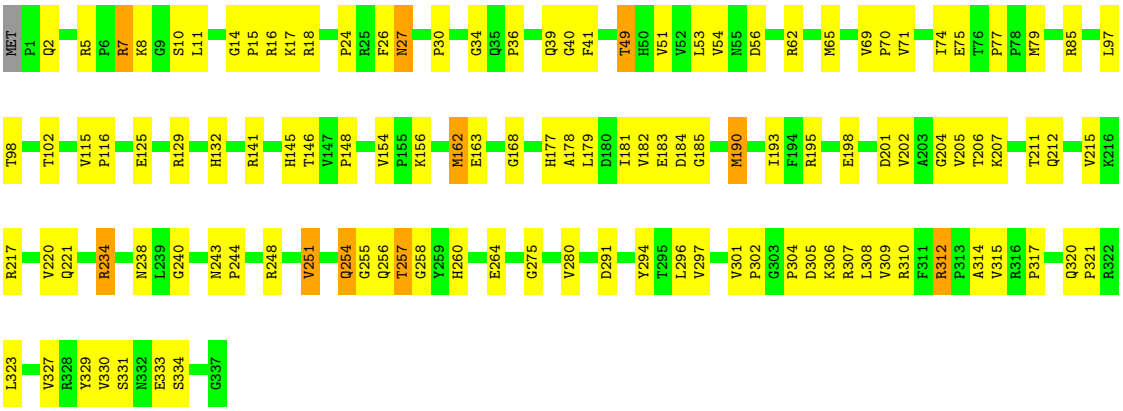
• Molecule 1: 50S ribosomal protein L2P

Chain A:



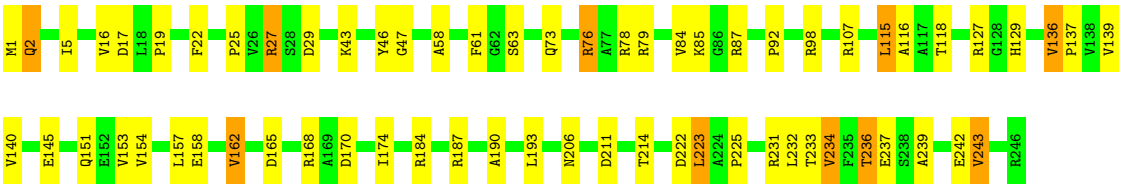
• Molecule 2: 50S ribosomal protein L3P

Chain B:



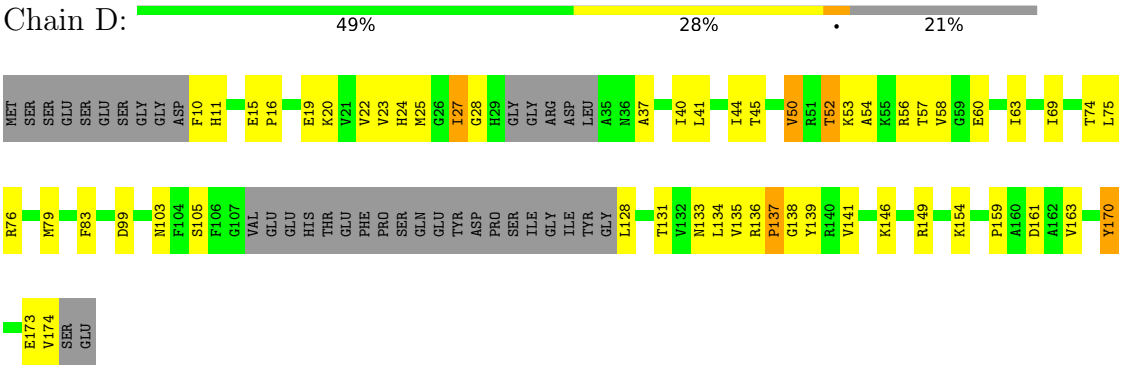
• Molecule 3: 50S ribosomal protein L4P

Chain C:



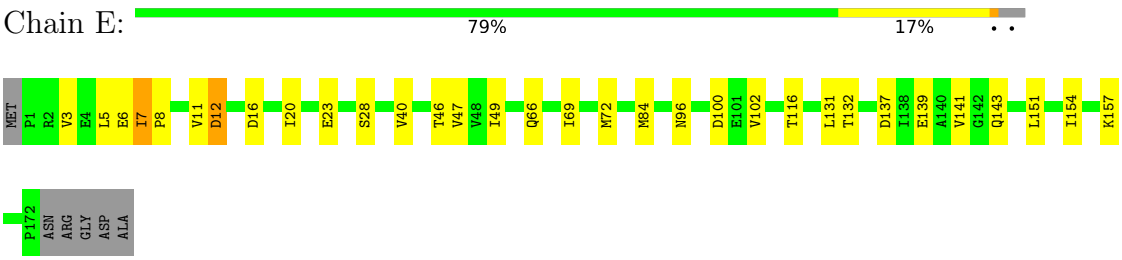
• Molecule 4: 50S ribosomal protein L5P

Chain D:



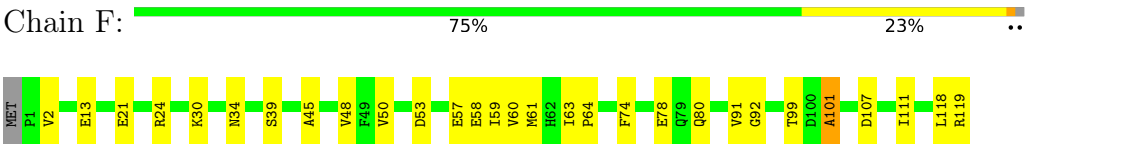
• Molecule 5: 50S ribosomal protein L6P

Chain E:



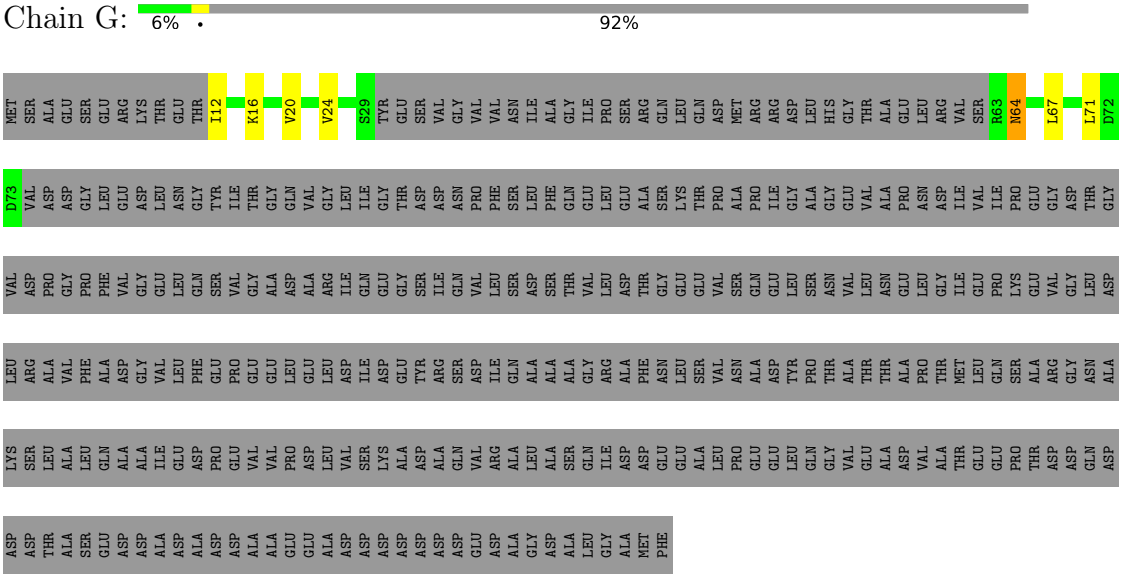
• Molecule 6: 50S ribosomal protein L7Ae

Chain F:



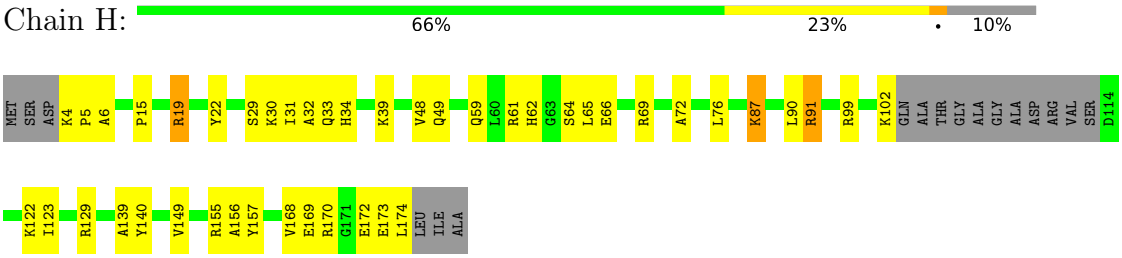
• Molecule 7: 50S ribosomal protein L10E

Chain G:



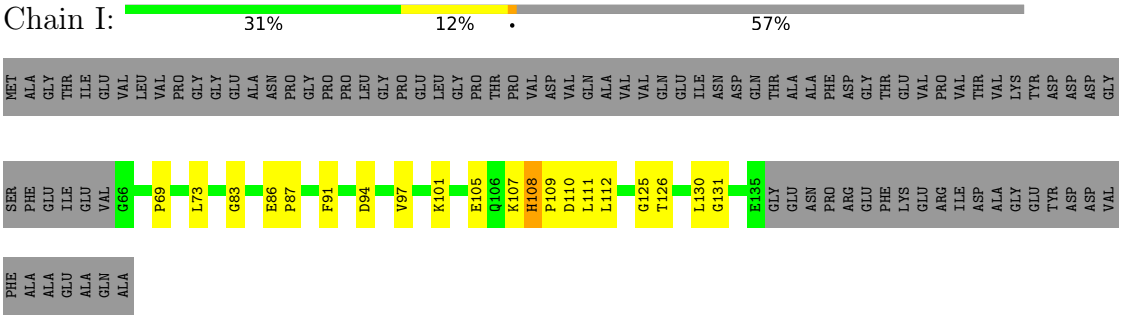
• Molecule 8: 50S ribosomal protein L10e

Chain H:



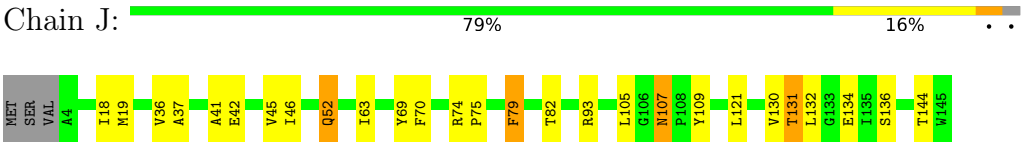
• Molecule 9: 50S ribosomal protein L11P

Chain I:



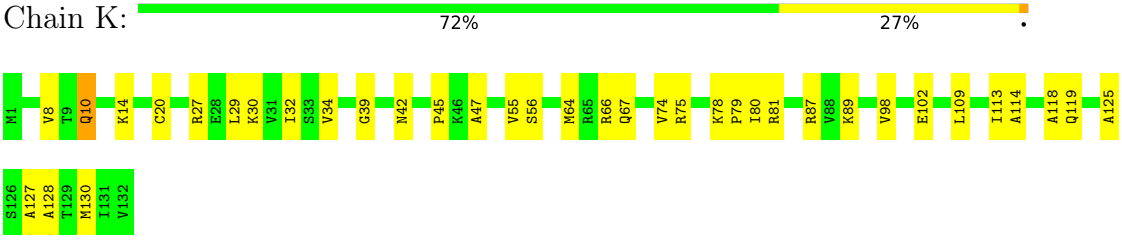
• Molecule 10: 50S ribosomal protein L13P

Chain J:



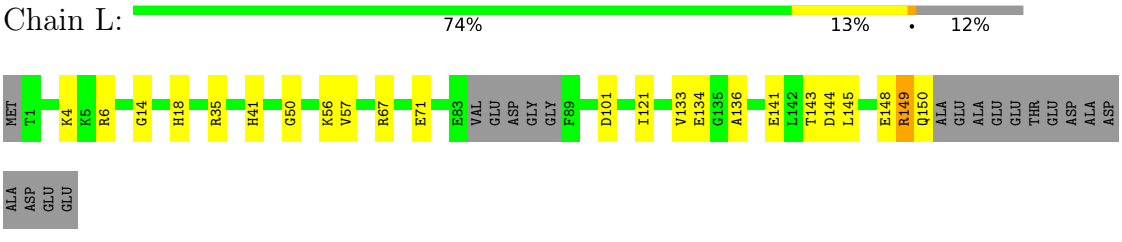
• Molecule 11: 50S ribosomal protein L14P

Chain K:



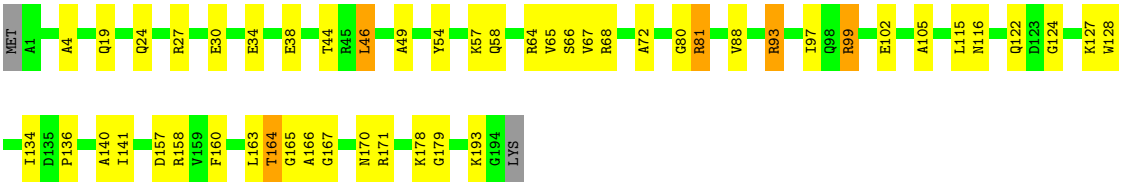
• Molecule 12: 50S ribosomal protein L15P

Chain L:



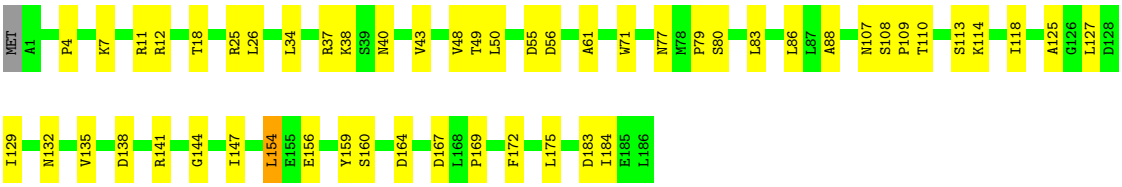
• Molecule 13: 50S ribosomal protein L15e

Chain M:



• Molecule 14: 50S ribosomal protein L18P

Chain N:

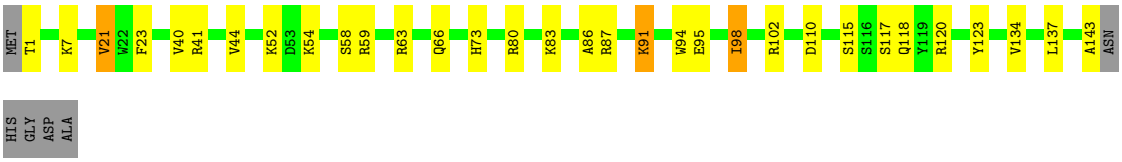


• Molecule 15: 50S ribosomal protein L18e

Chain O:

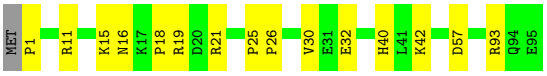
• Molecule 16: 50S ribosomal protein L19e

Chain P:



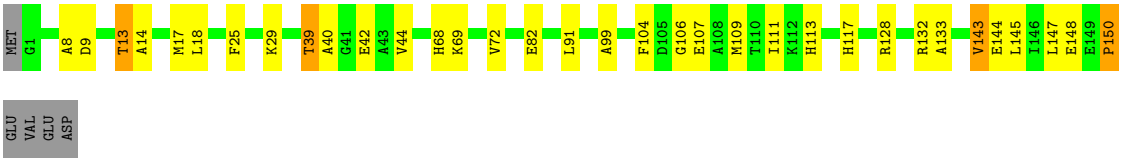
• Molecule 17: 50S ribosomal protein L21e

Chain Q:



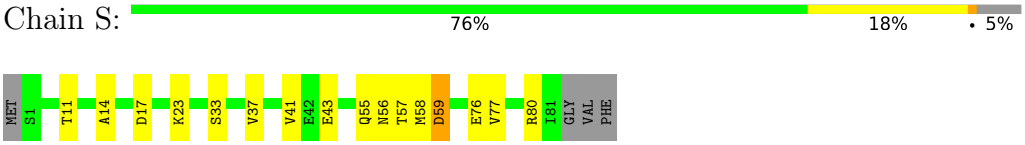
• Molecule 18: 50S ribosomal protein L22P

Chain R:



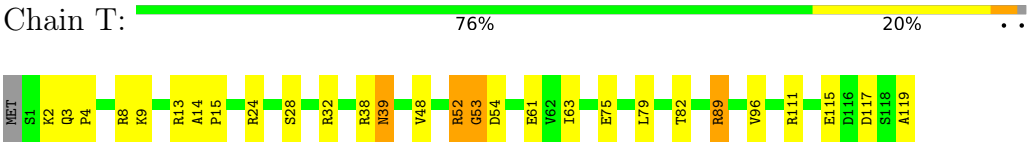
• Molecule 19: 50S ribosomal protein L23P

Chain S:



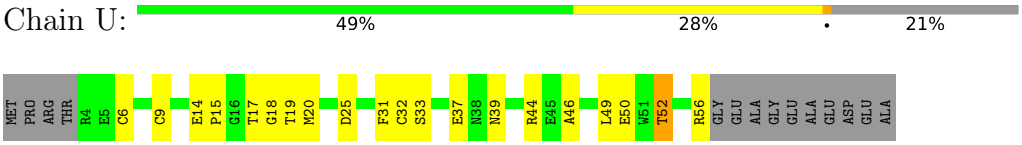
• Molecule 20: 50S ribosomal protein L24P

Chain T:



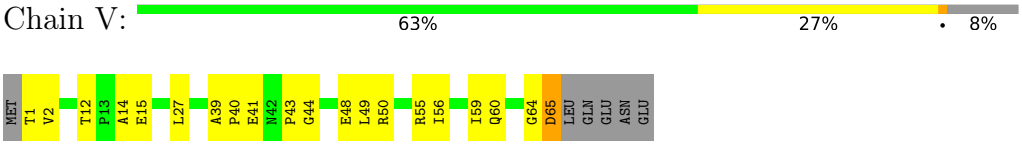
• Molecule 21: 50S ribosomal protein L24e

Chain U:



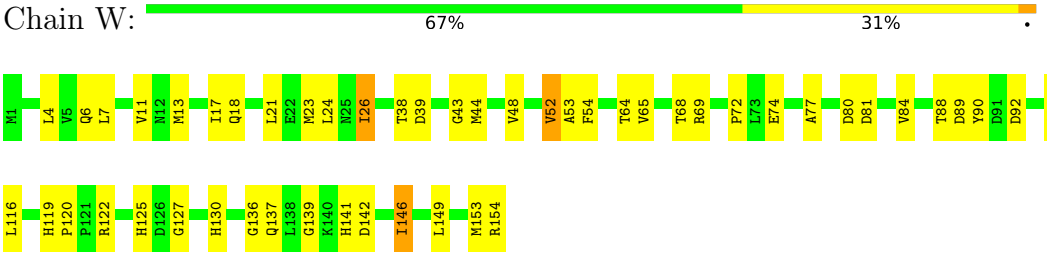
• Molecule 22: 50S ribosomal protein L29P

Chain V:



• Molecule 23: 50S ribosomal protein L30P

Chain W:

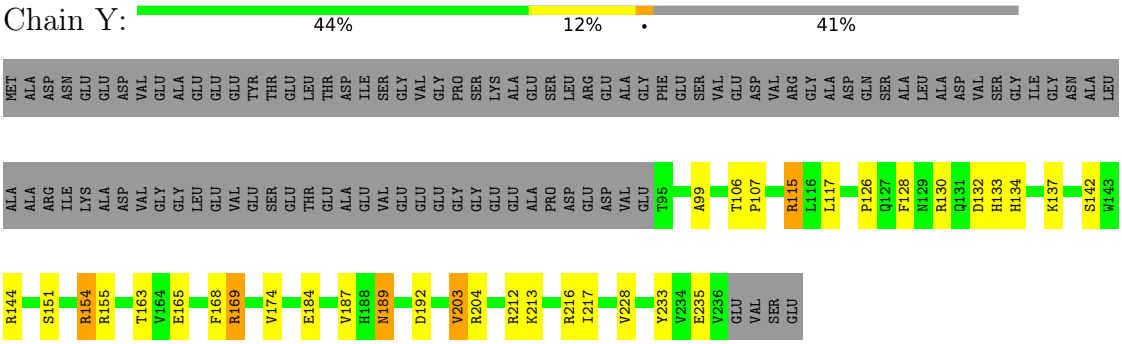


• Molecule 24: 50S ribosomal protein L31e

Chain X:

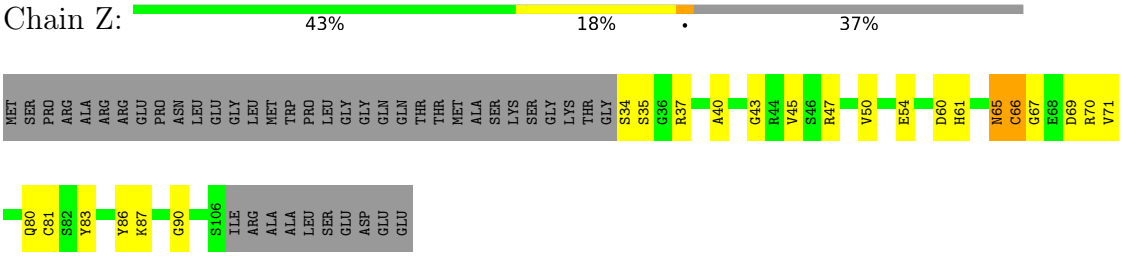
• Molecule 25: 50S ribosomal protein L32e

Chain Y:



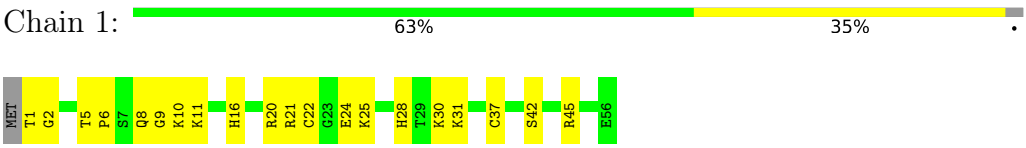
• Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



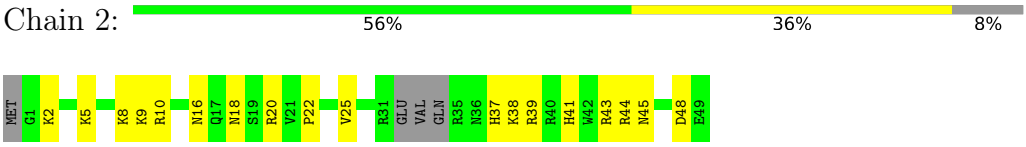
• Molecule 27: 50S ribosomal protein L37e

Chain 1:



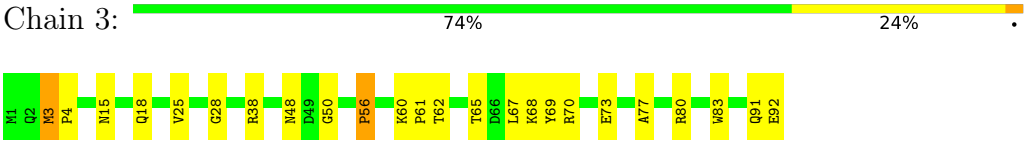
• Molecule 28: 50S ribosomal protein L39e

Chain 2:



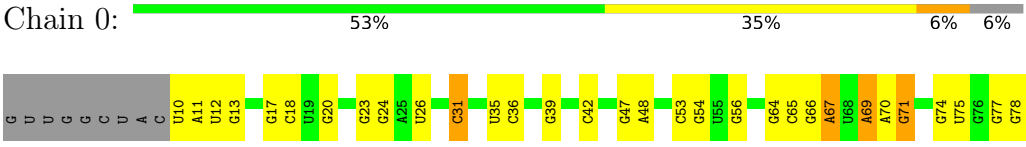
• Molecule 29: 50S ribosomal protein L44E

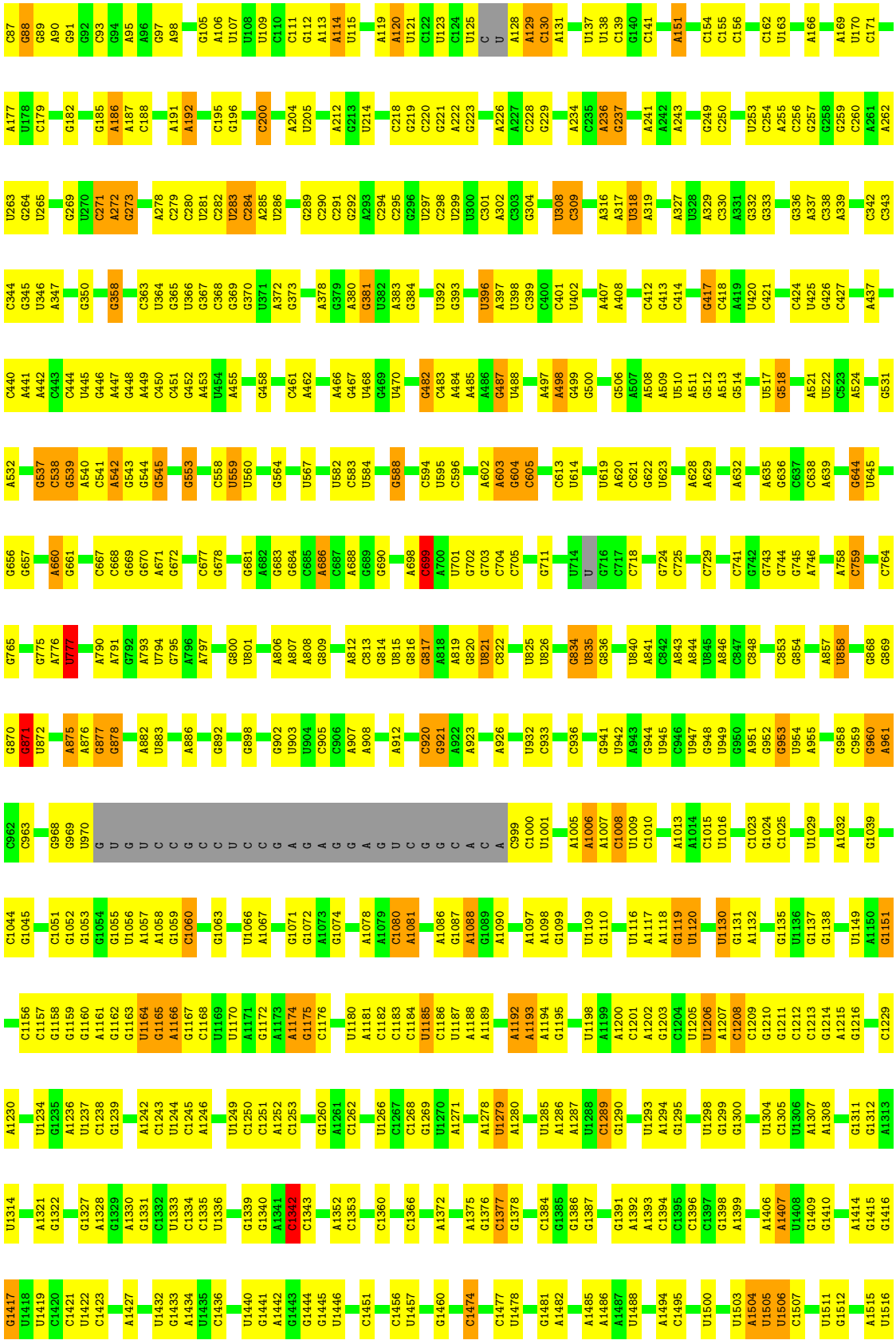
Chain 3:

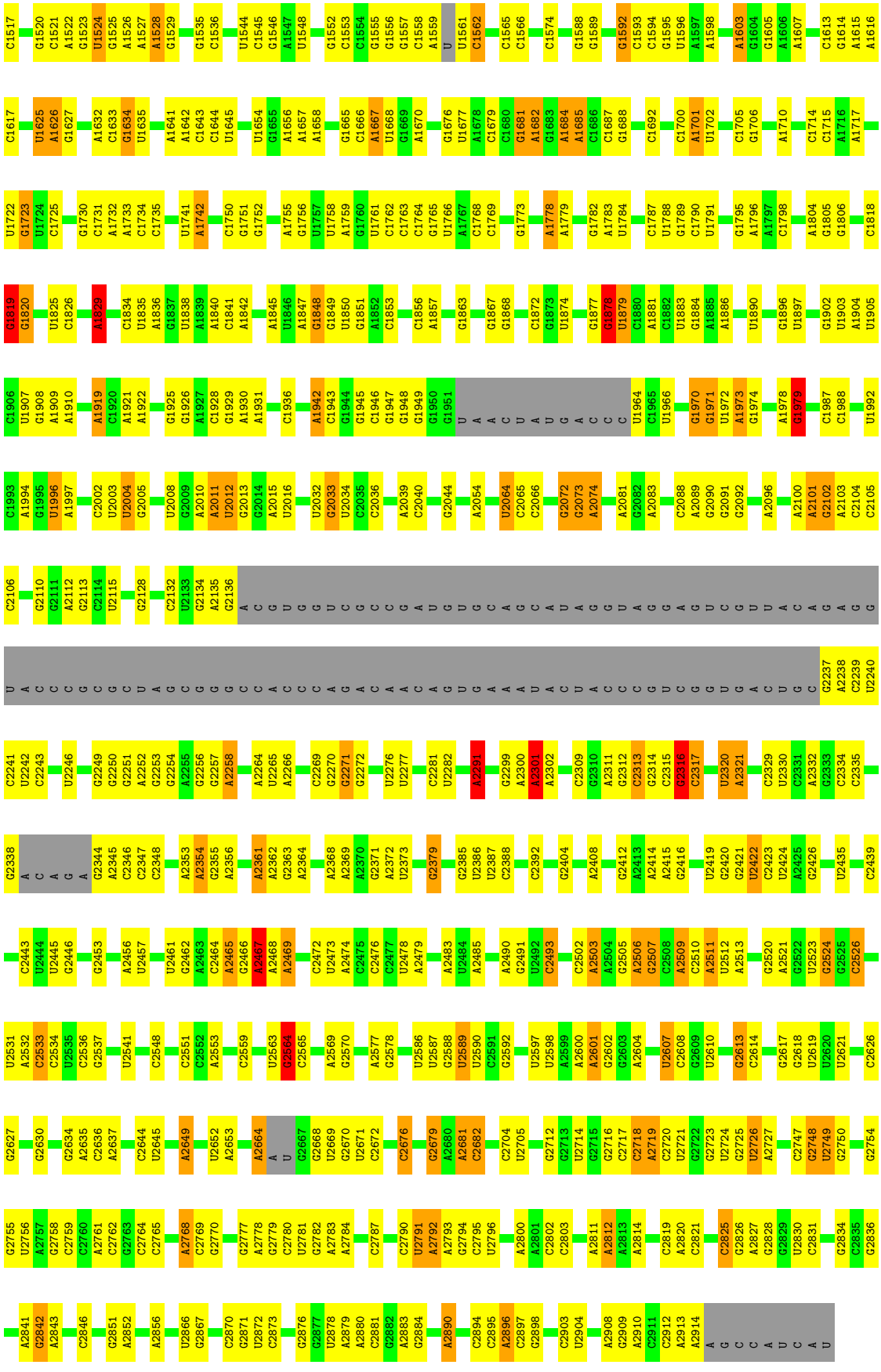


• Molecule 30: 23S ribosomal RNA

Chain 0:

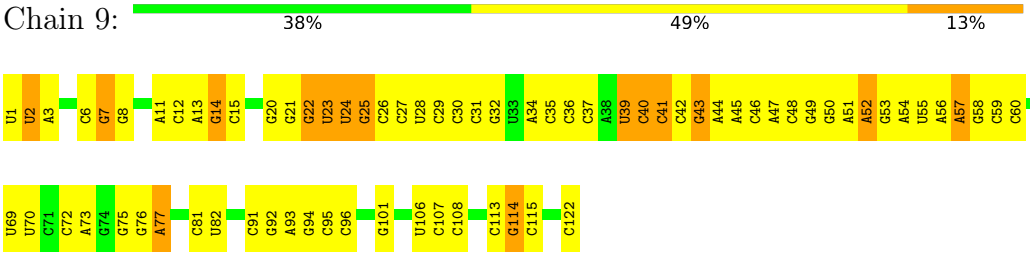






• Molecule 31: 5S ribosomal RNA

Chain 9:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	212.83Å 299.90Å 576.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 2.70 85.81 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.83-2.70) 90.8 (85.81-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.184 , 0.226 0.174 , 0.215	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	47.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 67.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, MG, OMG, K, CD, SR, NA, CL, OMU, PSU, 1MA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.32	0/1786	0.64	0/2408
2	B	0.32	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.31	0/1111	0.55	0/1498
5	E	0.32	0/1382	0.56	0/1880
6	F	0.32	0/901	0.57	0/1224
7	G	0.31	0/241	0.48	0/324
8	H	0.32	0/1302	0.63	0/1743
9	I	0.29	0/526	0.51	0/716
10	J	0.35	0/1136	0.59	0/1530
11	K	0.33	0/1004	0.65	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.34	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.61	0/1999
15	O	0.34	0/874	0.59	1/1181 (0.1%)
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.35	0/749	0.68	0/1005
18	R	1.26	7/1172 (0.6%)	1.11	6/1578 (0.4%)
19	S	0.31	0/648	0.57	0/875
20	T	0.33	0/958	0.62	1/1289 (0.1%)
21	U	0.34	0/417	0.55	0/562
22	V	0.31	0/502	0.52	0/675
23	W	0.34	0/1219	0.64	0/1655
24	X	0.34	0/664	0.58	0/895
25	Y	0.36	0/1146	0.60	0/1536
26	Z	0.35	0/584	0.60	0/781
27	1	0.37	0/438	0.61	0/578
28	2	0.34	0/401	0.55	0/529
29	3	0.36	0/771	0.57	0/1024
30	0	0.36	0/65957	0.68	17/102867 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98701 (0.0%)	0.67	26/147586 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
30	0	0	42
31	9	0	1
All	All	1	43

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.34	2.86	1.50
18	R	150	PRO	CA-C	-18.21	1.16	1.52
18	R	150	PRO	CG-CD	13.97	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.28	1.66	1.47
18	R	150	PRO	N-CD	10.80	1.62	1.47
18	R	150	PRO	CA-CB	7.58	1.68	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	150	PRO	CB-CA-C	-22.47	55.83	112.00
18	R	150	PRO	N-CA-C	-19.39	61.69	112.10
18	R	150	PRO	CA-N-CD	12.31	128.94	111.70
18	R	150	PRO	N-CA-CB	10.98	116.48	103.30
18	R	150	PRO	CA-C-O	-8.51	99.77	120.20
30	0	1878	G	N9-C1'-C2'	-6.59	104.75	112.00
18	R	150	PRO	CA-CB-CG	-6.10	92.41	104.00
30	0	1504	A	C1'-O4'-C4'	-6.07	105.04	109.90
30	0	871	G	C5'-C4'-O4'	-5.99	101.91	109.10
30	0	2291	A	N9-C1'-C2'	5.57	121.24	114.00
31	9	39	U	N1-C1'-C2'	5.48	121.12	114.00
30	0	2467	A	C1'-O4'-C4'	-5.41	105.57	109.90
30	0	1829	A	N9-C1'-C2'	-5.40	106.06	112.00
30	0	1819	G	C5'-C4'-C3'	5.26	124.42	116.00
30	0	2313	C	C5'-C4'-O4'	5.24	115.39	109.10
30	0	1504	A	N9-C1'-C2'	5.23	120.80	114.00
20	T	52	ARG	N-CA-C	5.18	124.97	111.00
30	0	2607	U	N1-C1'-C2'	5.17	120.72	114.00
30	0	2301	A	N9-C1'-C2'	5.15	120.69	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	2313	C	C1'-O4'-C4'	-5.12	105.80	109.90
15	O	66	GLY	N-CA-C	5.08	125.81	113.10
30	0	699	C	C1'-O4'-C4'	-5.07	105.85	109.90
30	0	2316	G	C5'-C4'-C3'	-5.02	107.96	116.00
30	0	841	A	C1'-O4'-C4'	-5.02	105.88	109.90
30	0	777	U	O4'-C1'-N1	5.02	112.21	108.20
30	0	1120	U	C5'-C4'-C3'	-5.00	107.99	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1262	C	Sidechain
30	0	1342	C	Sidechain
30	0	1417	G	Sidechain
30	0	1432	U	Sidechain
30	0	1681	G	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1970	G	Sidechain
30	0	1979	G	Sidechain
30	0	2036	C	Sidechain
30	0	2115	U	Sidechain
30	0	221	G	Sidechain
30	0	2301	A	Sidechain
30	0	2312	G	Sidechain
30	0	2316	G	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2524	G	Sidechain
30	0	2551	C	Sidechain
30	0	2564	G	Sidechain
30	0	26	U	Sidechain
30	0	2607	U	Sidechain
30	0	2679	G	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	686	A	Sidechain
30	0	817	G	Sidechain
30	0	903	U	Sidechain
31	9	94	G	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	75	0
2	B	2625	0	2533	92	0
3	C	1860	0	1813	57	0
4	D	1094	0	1085	40	0
5	E	1357	0	1266	23	0
6	F	890	0	843	26	0
7	G	240	0	231	7	0
8	H	1282	0	1292	37	0
9	I	519	0	500	15	0
10	J	1120	0	1098	30	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	22	0
13	M	1558	0	1573	42	0
14	N	1445	0	1401	45	0
15	O	865	0	873	15	0
16	P	1136	0	1123	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	735	0	729	14	0
18	R	1149	0	1122	34	0
19	S	641	0	605	11	0
20	T	950	0	924	19	0
21	U	410	0	364	19	0
22	V	499	0	511	17	0
23	W	1196	0	1137	55	0
24	X	654	0	653	24	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	16	0
27	1	431	0	426	22	0
28	2	396	0	413	19	0
29	3	755	0	728	20	0
30	0	59020	0	29806	1142	0
31	9	2599	0	1325	101	0
32	0	85	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	10	0	0	2	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	0	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	93	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	2	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	J	1	0	0	0	0
34	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5951	0	0	153	0
38	1	52	0	0	3	0
38	2	37	0	0	2	0
38	3	68	0	0	5	0
38	9	147	0	0	8	0
38	A	111	0	0	5	0
38	B	153	0	0	14	0
38	C	165	0	0	11	0
38	D	46	0	0	2	0
38	E	44	0	0	2	0
38	F	23	0	0	1	0
38	G	19	0	0	0	0
38	H	71	0	0	6	0
38	I	10	0	0	2	0
38	J	54	0	0	1	0
38	K	56	0	0	3	0
38	L	80	0	0	6	0
38	M	130	0	0	5	0
38	N	59	0	0	5	0
38	O	41	0	0	3	0
38	P	61	0	0	1	0
38	Q	51	0	0	2	0
38	R	78	0	0	3	0
38	S	33	0	0	2	0
38	T	37	0	0	2	0
38	U	25	0	0	3	0
38	V	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	W	63	0	0	4	0
38	X	28	0	0	1	0
38	Y	91	0	0	6	0
38	Z	28	0	0	3	0
All	All	99122	0	59907	1937	0

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

All (1937) 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.44
30:0:1160:G:C5'	30:0:1161:A:H5'	1.81	1.10
31:9:56:A:H2'	31:9:57:A:H5"	1.33	1.08
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07
30:0:871:G:C8	30:0:871:G:H5'	1.87	1.07
14:N:37:ARG:NH1	31:9:6:C:H5"	1.71	1.05
30:0:1160:G:H5'	30:0:1161:A:C5'	1.88	1.03
30:0:381:G:H5"	38:0:4345:HOH:O	1.58	1.02
30:0:1160:G:H5'	30:0:1161:A:H5'	1.02	1.02
30:0:2812:A:H2	30:0:2814:A:H62	1.03	1.02
13:M:171:ARG:HD3	30:0:156:C:H5"	1.40	1.00
10:J:82:THR:HG23	30:0:1242:A:H5'	1.44	1.00
30:0:2717:C:C2'	30:0:2718:C:H5"	1.92	0.99
11:K:10:GLN:HE21	11:K:10:GLN:H	1.06	0.99
31:9:76:G:H3'	31:9:77:A:H5"	1.42	0.99
30:0:182:G:H5'	38:0:5188:HOH:O	1.63	0.98
30:0:871:G:H5'	30:0:871:G:H8	1.23	0.98
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.44	0.98
30:0:1666:C:O2'	30:0:1667:A:H5"	1.61	0.98
30:0:1118:A:H8	30:0:1118:A:H3'	1.29	0.97
30:0:2717:C:H2'	30:0:2718:C:H5"	1.46	0.97
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.47	0.96
30:0:1474:C:H6	30:0:1474:C:H5'	1.29	0.96
15:O:3:THR:HG22	30:0:656:G:H5'	1.46	0.96
30:0:1243:C:H3'	38:0:4869:HOH:O	1.65	0.95
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.12	0.94
30:0:1187:U:HO2'	30:0:1189:A:H2	1.07	0.94
3:C:236:THR:HG22	3:C:239:ALA:H	1.31	0.94
30:0:282:C:O2'	30:0:283:U:H5'	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:115:SER:H	16:P:118:GLN:HE21	0.95	0.92
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.84	0.92
30:0:69:A:H5'	30:0:69:A:H8	1.33	0.92
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.14	0.92
30:0:871:G:H8	30:0:871:G:C5'	1.83	0.91
30:0:1205:U:H2'	30:0:1206:U:C5'	2.00	0.91
30:0:2491:G:H1'	38:0:6910:HOH:O	1.70	0.91
30:0:69:A:H5'	30:0:69:A:C8	2.06	0.91
30:0:1118:A:H3'	30:0:1118:A:C8	2.04	0.91
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.51	0.91
30:0:2533:C:H5'	30:0:2533:C:H6	1.35	0.90
8:H:49:GLN:HE21	8:H:140:TYR:HE2	1.15	0.90
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.53	0.90
4:D:154:LYS:H	4:D:154:LYS:HD2	1.37	0.89
30:0:870:G:H2'	30:0:871:G:H5"	1.53	0.89
30:0:1603:A:H5'	30:0:1605:G:O4'	1.72	0.89
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.37	0.89
30:0:1474:C:H5'	30:0:1474:C:C6	2.08	0.89
30:0:1701:A:H5'	38:0:6316:HOH:O	1.73	0.89
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.19	0.89
30:0:1183:C:H2'	38:0:6276:HOH:O	1.73	0.89
30:0:1184:C:H1'	38:0:7504:HOH:O	1.71	0.88
30:0:542:A:H5'	30:0:542:A:H8	1.38	0.88
30:0:282:C:H1'	30:0:368:C:N4	1.88	0.88
30:0:1666:C:C2'	30:0:1667:A:H5"	2.03	0.88
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.88
30:0:877:G:H5'	30:0:878:G:OP1	1.74	0.88
30:0:2251:G:H2'	30:0:2252:A:C8	2.09	0.87
2:B:238:ASN:HD22	2:B:240:GLY:H	1.20	0.87
30:0:558:C:C2'	30:0:559:U:H5"	2.04	0.87
30:0:1206:U:H5'	30:0:1206:U:H6	1.40	0.87
31:9:56:A:C2'	31:9:57:A:H5"	2.05	0.86
31:9:14:G:H5'	31:9:14:G:H8	1.39	0.86
30:0:10:U:H3'	30:0:10:U:H6	1.40	0.86
14:N:37:ARG:HH12	31:9:6:C:H5"	1.37	0.86
30:0:1372:A:H3'	38:0:7227:HOH:O	1.76	0.85
30:0:1701:A:H4'	30:0:1702:U:H5"	1.56	0.85
16:P:117:SER:HB3	30:0:1593:C:OP1	1.77	0.85
2:B:162:MET:HE3	2:B:308:LEU:HD21	1.57	0.85
30:0:506:G:H22	30:0:509:A:C5'	1.88	0.85
30:0:871:G:C8	30:0:871:G:C5'	2.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1205:U:H2'	30:0:1206:U:H5'	1.56	0.84
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.59	0.84
30:0:545:G:H5'	30:0:545:G:H8	1.39	0.84
30:0:1118:A:H62	30:0:1244:U:H3	1.25	0.84
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.60	0.84
30:0:1667:A:H8	30:0:1667:A:H5'	1.41	0.84
30:0:1116:U:H3	30:0:1246:A:H62	1.26	0.84
30:0:2502:C:C2'	30:0:2503:A:H5'	2.08	0.83
30:0:2506:A:HO2'	30:0:2507:G:H8	0.88	0.83
30:0:541:C:C2'	30:0:542:A:H5"	2.08	0.83
30:0:2769:C:C2'	30:0:2770:G:H5'	2.07	0.83
30:0:214:U:H5'	38:0:6173:HOH:O	1.77	0.83
30:0:1300:G:H1'	38:0:4714:HOH:O	1.78	0.83
30:0:506:G:H22	30:0:509:A:H5'	1.42	0.82
30:0:541:C:H2'	30:0:542:A:H5"	1.60	0.82
30:0:1189:A:H1'	30:0:1209:C:O4'	1.79	0.82
30:0:396:U:H1'	38:0:7666:HOH:O	1.77	0.82
28:2:41:HIS:H	28:2:45:ASN:HD22	1.25	0.82
30:0:1878:G:H1'	38:0:6153:HOH:O	1.79	0.82
30:0:2502:C:H2'	30:0:2503:A:H5'	1.60	0.82
30:0:2506:A:O2'	30:0:2507:G:H8	1.61	0.82
23:W:88:THR:HB	38:W:6679:HOH:O	1.80	0.82
30:0:1183:C:N4	30:0:1184:C:H41	1.78	0.81
30:0:236:A:H4'	30:0:237:G:H5'	1.62	0.81
30:0:1116:U:HO2'	30:0:1118:A:H2	0.82	0.81
30:0:1116:U:O2'	30:0:1118:A:H2	1.63	0.81
30:0:544:G:H2'	30:0:545:G:H5"	1.63	0.81
11:K:39:GLY:HA2	38:0:5251:HOH:O	1.79	0.81
30:0:2783:A:H3'	38:0:5262:HOH:O	1.80	0.81
30:0:559:U:H6	30:0:559:U:H5'	1.43	0.81
30:0:558:C:O2'	30:0:559:U:H5"	1.79	0.81
30:0:380:A:H2'	38:0:7266:HOH:O	1.81	0.80
30:0:1632:A:H2'	30:0:1633:C:H5'	1.63	0.80
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.28	0.80
30:0:1189:A:H3'	38:0:7718:HOH:O	1.80	0.80
30:0:2291:A:C8	30:0:2309:C:H5'	2.16	0.80
30:0:2586:U:H3	30:0:2592:G:H22	1.26	0.80
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.78	0.80
17:Q:15:LYS:HD3	30:0:2364:A:H5"	1.64	0.80
30:0:2426:G:H1'	38:0:6125:HOH:O	1.82	0.80
30:0:1603:A:H5"	30:0:1605:G:H5'	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:115:SER:H	16:P:118:GLN:NE2	1.77	0.80
30:0:1741:U:H5'	30:0:1742:A:OP1	1.82	0.80
30:0:1119:G:N2	30:0:1246:A:C2	2.49	0.79
30:0:2533:C:H5'	30:0:2533:C:C6	2.15	0.79
3:C:139:VAL:HG13	38:C:8641:HOH:O	1.82	0.79
15:O:3:THR:CG2	30:0:656:G:H5'	2.11	0.79
30:0:541:C:H2'	30:0:542:A:C5'	2.12	0.79
30:0:2851:G:O2'	30:0:2852:A:H5'	1.83	0.79
20:T:9:LYS:HE3	20:T:13:ARG:NH1	1.98	0.79
30:0:2896:A:H5"	38:0:6132:HOH:O	1.81	0.78
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.65	0.78
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.48	0.78
30:0:2827:A:H2'	30:0:2828:G:O4'	1.83	0.78
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.13	0.78
33:0:8813:CL:CL	38:0:4714:HOH:O	2.39	0.78
30:0:1634:G:H3'	38:0:3915:HOH:O	1.84	0.77
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.49	0.77
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.99	0.77
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.67	0.77
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.33	0.77
30:0:2769:C:O2'	30:0:2770:G:H5'	1.85	0.77
30:0:1666:C:H2'	30:0:1667:A:C5'	2.14	0.77
13:M:164:THR:HG22	13:M:167:GLY:H	1.50	0.77
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.76
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.50	0.76
22:V:50:ARG:HH12	30:0:56:G:H5"	1.48	0.76
5:E:143:GLN:NE2	30:0:2779:G:H21	1.82	0.76
30:0:1209:C:H2'	30:0:1210:G:H8	1.50	0.76
30:0:2908:A:H2'	30:0:2909:G:O4'	1.85	0.76
30:0:282:C:H1'	30:0:368:C:H42	1.50	0.76
3:C:174:ILE:HD11	30:0:338:C:H4'	1.66	0.76
30:0:558:C:H2'	30:0:559:U:C5'	2.15	0.76
30:0:1080:C:H4'	30:0:1081:A:OP1	1.85	0.76
31:9:2:U:OP2	31:9:3:A:H5'	1.86	0.76
30:0:2768:A:O2'	30:0:2769:C:H5'	1.86	0.76
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.68	0.76
30:0:2004:U:H4'	38:0:5338:HOH:O	1.86	0.76
30:0:31:C:H4'	38:0:7463:HOH:O	1.87	0.75
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.68	0.75
30:0:2637:A:H5'	38:0:4961:HOH:O	1.85	0.75
30:0:2717:C:O2'	30:0:2718:C:H5"	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:283:U:H5	30:0:284:C:C4	2.05	0.74
30:0:1973:A:H5'	30:0:1973:A:H8	1.52	0.74
30:0:2239:C:H2'	30:0:2240:U:H6	1.52	0.74
30:0:603:A:H5"	30:0:604:G:OP1	1.87	0.74
28:2:41:HIS:HD2	28:2:44:ARG:H	1.35	0.74
30:0:2748:G:H5'	38:0:7579:HOH:O	1.85	0.74
30:0:2851:G:C2'	30:0:2852:A:H5'	2.17	0.74
30:0:179:C:H5"	38:0:9320:HOH:O	1.86	0.74
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.69	0.74
30:0:1118:A:C8	30:0:1118:A:C3'	2.69	0.74
30:0:2559:C:H4'	38:0:7294:HOH:O	1.86	0.74
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.69	0.74
14:N:113:SER:HB2	38:N:8854:HOH:O	1.87	0.74
30:0:272:A:H5'	30:0:273:G:OP2	1.88	0.74
31:9:14:G:H5'	31:9:14:G:C8	2.23	0.74
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.69	0.73
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.69	0.73
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.71	0.73
30:0:1942:A:H3'	38:0:7386:HOH:O	1.88	0.73
30:0:1180:U:H2'	30:0:1181:A:O4'	1.89	0.73
16:P:115:SER:N	16:P:118:GLN:HE21	1.79	0.73
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.88	0.73
30:0:10:U:H3'	30:0:10:U:C6	2.23	0.73
30:0:1183:C:H42	30:0:1184:C:H41	1.35	0.73
30:0:2717:C:H2'	30:0:2718:C:C5'	2.19	0.73
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.71	0.72
11:K:10:GLN:H	11:K:10:GLN:NE2	1.83	0.72
30:0:338:C:H5"	38:0:3821:HOH:O	1.89	0.72
30:0:1205:U:H2'	30:0:1206:U:H5"	1.70	0.72
31:9:49:G:O2'	31:9:50:G:H5'	1.88	0.72
30:0:1279:U:O2	30:0:1279:U:H2'	1.88	0.72
30:0:2256:G:O2'	30:0:2257:G:H5'	1.88	0.72
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.87	0.72
18:R:39:THR:HG22	18:R:42:GLU:H	1.53	0.72
30:0:2420:G:O2'	30:0:2421:G:H5'	1.90	0.72
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.70	0.71
30:0:1666:C:H2'	30:0:1667:A:H5'	1.72	0.71
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.73	0.71
30:0:544:G:C2'	30:0:545:G:H5"	2.20	0.71
30:0:1666:C:C2'	30:0:1667:A:C5'	2.68	0.71
18:R:9:ASP:O	18:R:13:THR:HB	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:558:C:H2'	30:0:559:U:H5"	1.70	0.71
30:0:1632:A:C2'	30:0:1633:C:H5'	2.19	0.71
30:0:2679:G:H2'	30:0:2681:A:OP2	1.91	0.71
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.37	0.71
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.72	0.71
30:0:2010:A:H2'	38:0:5990:HOH:O	1.90	0.71
30:0:2578:G:H5'	30:0:2578:G:H8	1.54	0.71
30:0:1964:U:H2'	30:0:1964:U:O2	1.91	0.71
31:9:92:G:H2'	31:9:93:A:C8	2.26	0.71
30:0:1157:C:H2'	30:0:1158:G:H8	1.56	0.70
30:0:2635:A:O2'	30:0:2636:C:H5'	1.90	0.70
30:0:2769:C:H2'	30:0:2770:G:O4'	1.91	0.70
31:9:39:U:H1'	31:9:44:A:H61	1.55	0.70
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.27	0.70
30:0:1527:A:H1'	30:0:1528:A:C8	2.27	0.70
3:C:174:ILE:CD1	30:0:338:C:H4'	2.21	0.70
30:0:1174:A:C5	30:0:1201:C:H4'	2.26	0.70
30:0:31:C:H2'	38:0:7726:HOH:O	1.89	0.70
30:0:1701:A:H4'	30:0:1702:U:C5'	2.20	0.70
22:V:1:THR:HG23	22:V:2:VAL:H	1.56	0.70
30:0:2852:A:H5"	38:0:5264:HOH:O	1.91	0.70
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.05	0.69
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.07	0.69
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.74	0.69
12:L:148:GLU:HA	38:L:8870:HOH:O	1.92	0.69
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.73	0.69
30:0:308:U:H5'	30:0:309:C:OP1	1.91	0.69
30:0:1165:G:O2'	30:0:1174:A:H1'	1.92	0.69
30:0:2507:G:H2'	30:0:2510:C:H42	1.57	0.69
31:9:29:C:H2'	31:9:30:C:H5'	1.73	0.69
3:C:1:MET:HG2	3:C:2:GLN:H	1.55	0.69
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.92	0.69
30:0:814:G:H4'	38:0:3155:HOH:O	1.91	0.69
30:0:1603:A:C5'	30:0:1605:G:H5'	2.22	0.69
31:9:1:U:H4'	31:9:3:A:OP1	1.92	0.69
12:L:133:VAL:HA	38:L:8871:HOH:O	1.92	0.69
30:0:545:G:H5'	30:0:545:G:C8	2.25	0.69
2:B:217:ARG:HG3	2:B:257:THR:HB	1.75	0.68
30:0:281:U:H2'	30:0:282:C:O4'	1.94	0.68
31:9:7:G:H5'	38:9:9099:HOH:O	1.93	0.68
38:Y:8852:HOH:O	33:0:8817:CL:CL	2.49	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:37:ARG:NH1	31:9:6:C:C5'	2.53	0.68
2:B:258:GLY:H	2:B:260:HIS:CE1	2.12	0.68
30:0:1120:U:H5"	30:0:1120:U:C6	2.29	0.68
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.07	0.68
30:0:1819:G:H2'	30:0:1820:G:H4'	1.74	0.68
30:0:870:G:C2'	30:0:871:G:H5"	2.23	0.68
30:0:2256:G:C2'	30:0:2257:G:H5'	2.23	0.68
2:B:244:PRO:HB3	30:0:1234:U:N3	2.09	0.67
13:M:171:ARG:CD	30:0:156:C:H5"	2.20	0.67
10:J:70:PHE:HD1	30:0:2676:C:HO2'	1.40	0.67
14:N:144:GLY:O	14:N:147:ILE:HG22	1.94	0.67
18:R:150:PRO:CG	18:R:150:PRO:O	2.41	0.67
30:0:292:G:H2'	30:0:358:G:N2	2.08	0.67
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.94	0.67
14:N:11:ARG:HD3	31:9:114:G:O6	1.94	0.67
27:1:42:SER:HB2	38:1:354:HOH:O	1.93	0.67
30:0:297:U:H2'	30:0:298:C:C6	2.28	0.67
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.76	0.67
20:T:24:ARG:HH21	20:T:39:ASN:ND2	1.93	0.67
30:0:2812:A:C2	30:0:2814:A:N6	2.58	0.67
31:9:39:U:H1'	31:9:44:A:N6	2.08	0.67
30:0:564:G:H1'	38:0:6342:HOH:O	1.94	0.67
30:0:1667:A:H5'	30:0:1667:A:C8	2.27	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.28	0.66
30:0:1060:C:H6	30:0:1060:C:H5'	1.60	0.66
30:0:1474:C:H6	30:0:1474:C:C5'	2.07	0.66
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.58	0.66
12:L:6:ARG:HD3	30:0:1299:G:O6	1.95	0.66
30:0:2681:A:H4'	30:0:2682:C:H5'	1.75	0.66
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.26	0.66
30:0:1116:U:O2'	30:0:1118:A:C2	2.44	0.66
30:0:1205:U:C2'	30:0:1206:U:C5'	2.72	0.66
12:L:136:ALA:HB3	38:L:8871:HOH:O	1.96	0.66
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.78	0.66
30:0:1289:C:H3'	38:0:6443:HOH:O	1.95	0.66
22:V:50:ARG:NH1	30:0:56:G:H5"	2.10	0.66
30:0:2239:C:H2'	30:0:2240:U:C6	2.30	0.66
3:C:236:THR:HG22	3:C:239:ALA:N	2.09	0.66
30:0:960:G:N3	30:0:960:G:H2'	2.11	0.66
30:0:1016:U:H1'	38:0:3678:HOH:O	1.96	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:125:U:H2'	38:0:3785:HOH:O	1.96	0.65
30:0:2769:C:H2'	30:0:2770:G:H5'	1.77	0.65
30:0:2836:G:H1'	38:0:6880:HOH:O	1.95	0.65
1:A:199:HIS:HD2	1:A:201:PHE:H	1.44	0.65
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.96	0.65
30:0:2795:C:O2'	30:0:2796:U:H5'	1.95	0.65
30:0:283:U:C5	30:0:284:C:C4	2.85	0.65
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.37	0.65
30:0:960:G:N3	30:0:960:G:C2'	2.59	0.65
2:B:212:GLN:HA	30:0:1733:A:H4'	1.79	0.65
16:P:59:ARG:HH22	16:P:66:GLN:NE2	1.94	0.65
30:0:1183:C:N3	30:0:1184:C:C5	2.65	0.65
30:0:1189:A:O2'	30:0:1208:C:H2'	1.96	0.65
30:0:1451:C:H5'	30:0:1505:U:C5	2.32	0.65
30:0:704:C:O2'	30:0:705:C:H5'	1.97	0.65
4:D:103:ASN:ND2	4:D:134:LEU:H	1.95	0.64
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.32	0.64
30:0:363:C:H1'	38:0:5312:HOH:O	1.97	0.64
30:0:1058:A:H2'	30:0:1060:C:H5"	1.78	0.64
30:0:1925:G:O2'	30:0:1926:G:H5'	1.97	0.64
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.62	0.64
30:0:2414:A:H2'	30:0:2415:A:C8	2.32	0.64
2:B:206:THR:HG21	30:0:2716:G:H5"	1.80	0.64
30:0:256:C:H2'	30:0:257:G:O4'	1.96	0.64
30:0:2505:G:O2'	30:0:2506:A:H5'	1.97	0.64
30:0:280:C:H2'	30:0:281:U:O4'	1.97	0.64
30:0:558:C:C2'	30:0:559:U:C5'	2.74	0.64
30:0:1189:A:H1'	30:0:1209:C:C1'	2.28	0.64
30:0:1441:G:O2'	30:0:1442:A:H5'	1.97	0.64
30:0:1741:U:O2'	30:0:2723:G:H4'	1.97	0.64
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.63	0.64
25:Y:204:ARG:HH22	30:0:553:G:P	2.21	0.64
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.78	0.64
3:C:184:ARG:NH2	30:0:450:C:OP1	2.30	0.64
23:W:125:HIS:HD2	23:W:127:GLY:H	1.46	0.64
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.26	0.64
30:0:297:U:H2'	30:0:298:C:H6	1.63	0.64
30:0:2769:C:H2'	30:0:2770:G:C5'	2.28	0.64
1:A:199:HIS:CD2	1:A:201:PHE:H	2.15	0.63
30:0:10:U:C6	30:0:10:U:C3'	2.80	0.63
30:0:1205:U:C2'	30:0:1206:U:H5"	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2256:G:H2'	30:0:2257:G:C5'	2.27	0.63
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.81	0.63
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.79	0.63
29:3:65:THR:HG23	29:3:67:LEU:HG	1.79	0.63
30:0:1187:U:H2'	38:0:6939:HOH:O	1.98	0.63
18:R:128:ARG:NH2	30:0:2054:A:N3	2.46	0.63
21:U:46:ALA:O	21:U:52:THR:HG21	1.98	0.63
24:X:71:ARG:HD3	38:X:2171:HOH:O	1.98	0.63
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.64	0.63
30:0:2533:C:H6	30:0:2533:C:C5'	2.09	0.63
13:M:27:ARG:NH2	13:M:44:THR:HG23	2.13	0.63
30:0:1120:U:H5"	30:0:1120:U:H6	1.63	0.63
30:0:1278:A:H4'	30:0:1279:U:C4	2.33	0.63
30:0:1878:G:O2'	30:0:1879:U:C6	2.49	0.63
31:9:75:G:H1	31:9:106:U:H3	1.47	0.63
9:I:110:ASP:O	30:0:1163:G:H5'	1.99	0.63
30:0:317:A:H4'	38:0:3791:HOH:O	1.98	0.63
30:0:2524:G:H21	30:0:2526:C:N4	1.96	0.63
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.81	0.63
30:0:1835:U:C5	30:0:1840:A:N7	2.60	0.63
30:0:2509:A:H2'	30:0:2510:C:O4'	1.99	0.63
30:0:2649:A:H5'	30:0:2649:A:H8	1.64	0.63
2:B:162:MET:CE	2:B:308:LEU:HD21	2.27	0.63
2:B:264:GLU:HG3	2:B:302:PRO:HD3	1.79	0.63
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.64	0.63
30:0:2604:A:H5'	38:0:5822:HOH:O	1.99	0.62
31:9:54:A:O2'	31:9:55:U:H5'	1.98	0.62
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.96	0.62
23:W:13:MET:HE1	23:W:18:GLN:HA	1.81	0.62
30:0:853:C:H3'	38:0:4580:HOH:O	2.00	0.62
30:0:2250:G:C2	30:0:2251:G:H1'	2.34	0.62
30:0:2256:G:H2'	30:0:2257:G:H5'	1.81	0.62
15:O:73:ASP:HA	15:O:92:VAL:O	2.00	0.62
13:M:178:LYS:HB2	38:0:6916:HOH:O	1.99	0.62
30:0:2421:G:H1'	38:0:7060:HOH:O	1.98	0.62
8:H:168:VAL:HG13	38:H:211:HOH:O	1.98	0.62
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.81	0.62
30:0:1701:A:H5"	30:0:1702:U:H3'	1.82	0.62
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.81	0.62
30:0:1198:U:H1'	30:0:1201:C:H5	1.63	0.62
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:64:ASN:HD22	7:G:64:ASN:N	1.96	0.62
27:1:16:HIS:HD2	30:0:470:U:O2'	1.83	0.62
27:1:20:ARG:HG2	30:0:111:C:O2'	2.00	0.62
30:0:567:U:H5"	38:0:6435:HOH:O	1.99	0.62
31:9:2:U:P	31:9:3:A:H5'	2.40	0.62
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.80	0.62
11:K:10:GLN:HE21	11:K:10:GLN:N	1.87	0.62
29:3:48:ASN:HD21	30:0:2468:A:H61	1.47	0.62
30:0:960:G:N3	30:0:960:G:H3'	2.14	0.62
30:0:1166:A:H61	30:0:1180:U:H3	1.46	0.62
30:0:2404:G:H5"	38:0:5241:HOH:O	2.00	0.62
30:0:2670:G:O2'	30:0:2671:U:H5'	1.99	0.62
6:F:91:VAL:HG12	6:F:92:GLY:N	2.14	0.61
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.82	0.61
25:Y:216:ARG:HD2	38:Y:8865:HOH:O	2.00	0.61
30:0:1170:U:H2'	30:0:1172:G:OP2	2.00	0.61
30:0:1314:U:H2'	38:0:5904:HOH:O	2.00	0.61
11:K:32:ILE:HD11	11:K:56:SER:HB2	1.82	0.61
30:0:848:C:H5'	38:0:7311:HOH:O	2.00	0.61
30:0:958:G:O2'	30:0:959:C:H5'	2.00	0.61
13:M:157:ASP:HB3	13:M:160:PHE:HD1	1.65	0.61
30:0:506:G:H22	30:0:509:A:H5"	1.63	0.61
30:0:2083:A:H3'	38:0:7616:HOH:O	1.99	0.61
30:0:2613:G:O2'	30:0:2614:C:H5'	2.00	0.61
31:9:20:G:O2'	31:9:21:G:H5'	2.00	0.61
2:B:162:MET:HG3	2:B:310:ARG:HD3	1.83	0.61
14:N:4:PRO:HG3	31:9:69:U:OP1	2.00	0.61
23:W:88:THR:HG22	23:W:89:ASP:H	1.65	0.61
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.82	0.61
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.83	0.61
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.81	0.61
30:0:1679:C:H5'	38:0:9334:HOH:O	2.00	0.61
30:0:1759:A:N3	30:0:1818:C:H2'	2.16	0.61
31:9:64:C:C2'	31:9:65:A:H5'	2.30	0.61
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.83	0.61
22:V:1:THR:HB	30:0:93:C:H5"	1.82	0.61
30:0:1506:U:H6	30:0:1506:U:H5'	1.66	0.61
30:0:1641:A:H2'	30:0:1642:A:H5'	1.83	0.61
30:0:1948:G:H2'	30:0:1949:G:O4'	2.01	0.61
27:1:10:LYS:HG3	38:1:2979:HOH:O	2.00	0.61
30:0:2787:C:H5	38:0:4664:HOH:O	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.16	0.61
30:0:558:C:H2'	30:0:559:U:H5'	1.82	0.61
3:C:16:VAL:HG12	3:C:17:ASP:H	1.66	0.61
3:C:236:THR:HG21	38:C:8569:HOH:O	2.00	0.61
1:A:36:ASP:CB	1:A:85:SER:H	2.14	0.60
14:N:141:ARG:HH21	31:9:48:C:H4'	1.66	0.60
23:W:84:VAL:HG12	38:W:6679:HOH:O	2.01	0.60
30:0:2505:G:C2'	30:0:2506:A:H5'	2.31	0.60
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.82	0.60
14:N:40:ASN:ND2	31:9:28:U:H5"	2.16	0.60
30:0:936:C:H5	38:0:5991:HOH:O	1.82	0.60
30:0:2637:A:H4'	38:0:6094:HOH:O	2.00	0.60
30:0:1515:A:H2'	30:0:1516:U:C6	2.37	0.60
38:B:9109:HOH:O	30:0:2672:C:H1'	2.02	0.60
30:0:236:A:H4'	30:0:237:G:OP1	2.01	0.60
30:0:542:A:H5'	30:0:542:A:C8	2.28	0.60
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.84	0.60
23:W:88:THR:HG22	23:W:89:ASP:N	2.17	0.60
30:0:836:G:H5"	38:0:9288:HOH:O	1.99	0.60
4:D:57:THR:HG23	4:D:63:ILE:HA	1.82	0.60
11:K:27:ARG:HD2	38:K:4747:HOH:O	2.01	0.60
10:J:41:ALA:HB3	38:J:5907:HOH:O	2.00	0.60
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.84	0.60
30:0:702:G:O2'	30:0:703:G:H5'	2.02	0.60
30:0:1080:C:O5'	30:0:1080:C:H6	1.85	0.60
30:0:2563:U:H2'	30:0:2565:C:O5'	2.01	0.60
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.84	0.60
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	1.84	0.60
30:0:2089:A:O2'	30:0:2090:G:H5'	2.02	0.60
31:9:3:A:N6	31:9:22:G:H1'	2.16	0.60
6:F:101:ALA:HA	38:F:5413:HOH:O	2.02	0.59
8:H:102:LYS:HD3	8:H:122:LYS:HD3	1.83	0.59
30:0:2419:U:H5"	30:0:2420:G:H5'	1.83	0.59
9:I:87:PRO:HB3	38:I:6825:HOH:O	2.02	0.59
30:0:368:C:H2'	30:0:369:G:H5'	1.84	0.59
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.83	0.59
13:M:80:GLY:O	13:M:81:ARG:HD3	2.01	0.59
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.32	0.59
30:0:567:U:H5"	38:0:5320:HOH:O	2.02	0.59
30:0:271:C:H41	30:0:378:A:H2	1.47	0.59
30:0:1132:A:N6	30:0:1229:C:H2'	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1790:C:H2'	30:0:1791:U:H6	1.67	0.59
30:0:2329:C:O2'	30:0:2330:U:H5'	2.01	0.59
2:B:254:GLN:HG3	38:0:9714:HOH:O	2.01	0.59
8:H:29:SER:HA	8:H:62:HIS:HD2	1.68	0.59
8:H:49:GLN:NE2	8:H:140:TYR:HE2	1.95	0.59
38:Z:8706:HOH:O	30:0:1886:A:H4'	2.03	0.59
30:0:2237:G:H1'	38:0:4887:HOH:O	2.02	0.59
30:0:2718:C:H6	30:0:2718:C:H5'	1.68	0.59
1:A:33:GLU:H	1:A:33:GLU:CD	2.04	0.59
3:C:236:THR:CG2	3:C:239:ALA:H	2.11	0.59
8:H:174:LEU:HA	38:H:222:HOH:O	2.02	0.59
9:I:108:HIS:H	9:I:109:PRO:HD2	1.66	0.59
18:R:39:THR:HG23	18:R:107:GLU:O	2.02	0.59
30:0:119:A:H2'	30:0:120:A:H5"	1.83	0.59
30:0:1377:C:H5'	30:0:1377:C:H6	1.68	0.59
30:0:1595:G:O2'	30:0:1596:U:H5'	2.03	0.59
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.32	0.59
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.37	0.59
30:0:308:U:C4	30:0:342:C:H1'	2.38	0.59
30:0:2344:G:H2'	30:0:2344:G:N3	2.17	0.59
30:0:2756:U:H3	30:0:2896:A:H2	1.43	0.59
1:A:48:ASP:HB3	38:A:9060:HOH:O	2.03	0.59
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.85	0.59
7:G:16:LYS:O	7:G:20:VAL:HG23	2.03	0.59
23:W:125:HIS:CD2	23:W:127:GLY:H	2.21	0.59
7:G:12:ILE:HG23	38:0:5490:HOH:O	2.03	0.59
31:9:64:C:H2'	31:9:65:A:H5'	1.84	0.59
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.85	0.58
2:B:248:ARG:O	2:B:251:VAL:HG13	2.03	0.58
38:C:8655:HOH:O	30:0:2100:A:H5'	2.03	0.58
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.04	0.58
30:0:468:U:H3'	38:0:7607:HOH:O	2.03	0.58
30:0:2812:A:H2	30:0:2814:A:N6	1.87	0.58
31:9:24:U:H3'	31:9:25:G:C5'	2.32	0.58
1:A:171:LYS:HB2	30:0:820:G:C6	2.37	0.58
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.67	0.58
30:0:2534:C:H1'	38:0:3513:HOH:O	2.01	0.58
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.85	0.58
28:2:38:LYS:HE3	38:0:4254:HOH:O	2.01	0.58
30:0:1603:A:H5'	30:0:1605:G:C4'	2.33	0.58
30:0:1972:U:H2'	30:0:1973:A:C5'	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.03	0.58
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.19	0.58
1:A:36:ASP:HB2	1:A:85:SER:H	1.68	0.58
16:P:115:SER:OG	16:P:118:GLN:HG3	2.03	0.58
30:0:1304:U:H2'	30:0:1305:C:C6	2.39	0.58
30:0:2252:A:C5	30:0:2253:G:H1'	2.38	0.58
30:0:2649:A:H5'	30:0:2649:A:C8	2.39	0.58
4:D:103:ASN:HD22	4:D:134:LEU:H	1.49	0.58
28:2:10:ARG:NH2	30:0:121:U:OP2	2.32	0.58
30:0:407:A:H5'	38:0:6057:HOH:O	2.04	0.58
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.34	0.58
30:0:660:A:H4'	30:0:661:G:O5'	2.04	0.58
2:B:238:ASN:HD22	2:B:240:GLY:N	1.96	0.58
23:W:139:GLY:O	23:W:141:HIS:HD2	1.87	0.58
30:0:441:A:H1'	30:0:442:A:N7	2.19	0.58
30:0:2346:C:H6	30:0:2346:C:O5'	1.86	0.58
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.85	0.58
12:L:145:LEU:O	12:L:148:GLU:HG3	2.03	0.57
17:Q:11:ARG:HG3	30:0:2363:G:O2'	2.04	0.57
30:0:1819:G:H5'	38:0:5847:HOH:O	2.04	0.57
30:0:192:A:H5'	38:0:7682:HOH:O	2.03	0.57
30:0:567:U:C5'	38:0:6435:HOH:O	2.52	0.57
30:0:947:U:H2'	30:0:948:G:C8	2.39	0.57
30:0:1477:C:H5'	30:0:1868:G:C5'	2.34	0.57
3:C:79:ARG:O	3:C:87:ARG:HG2	2.04	0.57
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.86	0.57
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.03	0.57
22:V:39:ALA:N	22:V:40:PRO:HD2	2.19	0.57
30:0:88:G:H2'	30:0:89:G:C8	2.39	0.57
30:0:228:C:H2'	30:0:229:G:H5'	1.86	0.57
30:0:644:G:H5'	30:0:644:G:N3	2.19	0.57
30:0:711:G:C2	30:0:718:C:C2	2.92	0.57
31:9:1:U:O3'	31:9:3:A:H5'	2.03	0.57
30:0:2894:C:O2'	30:0:2895:C:H5'	2.05	0.57
30:0:1183:C:C2	30:0:1184:C:C5	2.93	0.57
1:A:51:ARG:HB2	38:A:9060:HOH:O	2.04	0.57
24:X:25:ARG:HD3	24:X:64:ALA:O	2.05	0.57
30:0:512:G:O3'	30:0:513:A:H8	1.87	0.57
30:0:1592:G:H2'	30:0:1593:C:H6	1.69	0.57
30:0:1714:C:O2'	30:0:1715:C:H5'	2.05	0.57
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:68:HIS:O	30:0:2842:G:H5'	2.05	0.57
30:0:2372:A:H2'	30:0:2373:U:C6	2.39	0.57
12:L:41:HIS:HD2	30:0:926:A:O2'	1.88	0.57
30:0:396:U:O2'	30:0:418:C:H4'	2.04	0.57
30:0:541:C:H2'	30:0:542:A:H5'	1.87	0.57
30:0:1768:C:H2'	30:0:1769:C:O4'	2.05	0.57
30:0:1942:A:H5'	38:0:7386:HOH:O	2.05	0.57
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.87	0.56
10:J:74:ARG:NH1	10:J:144:THR:HG21	2.20	0.56
18:R:117:HIS:HD2	30:0:20:G:H21	1.53	0.56
30:0:1477:C:O2'	30:0:1478:U:H5'	2.05	0.56
31:9:49:G:H5"	38:9:9090:HOH:O	2.05	0.56
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.87	0.56
30:0:283:U:C5	30:0:284:C:N3	2.73	0.56
30:0:366:U:H2'	30:0:367:G:O4'	2.05	0.56
30:0:2269:C:H2'	30:0:2270:G:H5'	1.86	0.56
30:0:2320:U:H4'	30:0:2321:A:O4'	2.04	0.56
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.87	0.56
30:0:485:A:N3	30:0:487:G:H5"	2.20	0.56
30:0:2005:G:H3'	30:0:2005:G:OP2	2.06	0.56
30:0:2668:G:H2'	30:0:2669:U:C6	2.40	0.56
31:9:1:U:O3'	31:9:3:A:C5'	2.53	0.56
2:B:71:VAL:HG21	2:B:296:LEU:HB3	1.87	0.56
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.86	0.56
30:0:255:A:H2'	30:0:256:C:H6	1.71	0.56
30:0:542:A:H2'	30:0:543:G:O4'	2.05	0.56
31:9:12:C:H5'	31:9:70:U:O4'	2.04	0.56
8:H:19:ARG:HH12	30:0:1008:C:H5"	1.70	0.56
12:L:134:GLU:HG3	38:L:8854:HOH:O	2.06	0.56
23:W:44:MET:CE	30:0:944:G:H21	2.19	0.56
30:0:319:A:H4'	30:0:338:C:C4	2.40	0.56
3:C:63:SER:OG	30:0:2101:A:H2'	2.05	0.56
10:J:74:ARG:HH12	10:J:144:THR:HG21	1.71	0.56
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.71	0.56
30:0:1206:U:C5'	30:0:1206:U:H6	2.15	0.56
2:B:145:HIS:HD2	2:B:146:THR:O	1.89	0.56
12:L:143:THR:HG22	12:L:144:ASP:H	1.71	0.56
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.79	0.56
30:0:363:C:H2'	30:0:364:U:H6	1.69	0.56
30:0:2472:C:O2'	30:0:2634:G:H4'	2.05	0.56
30:0:2880:A:H2'	30:0:2881:C:H5'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:76:G:C3'	31:9:77:A:H5"	2.28	0.56
31:9:114:G:H2'	31:9:115:C:C6	2.41	0.56
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.41	0.56
29:3:70:ARG:HB3	38:3:9064:HOH:O	2.06	0.56
30:0:2002:C:H2'	30:0:2003:U:H5'	1.87	0.56
2:B:17:LYS:O	2:B:260:HIS:HD2	1.88	0.56
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.41	0.56
27:1:9:GLY:HA2	30:0:1687:C:O2	2.05	0.56
27:1:28:HIS:HE1	30:0:776:A:OP1	1.89	0.56
30:0:1213:C:O2'	30:0:1214:G:H5'	2.06	0.56
30:0:2064:U:H5'	30:0:2652:U:H4'	1.87	0.56
7:G:20:VAL:O	7:G:24:VAL:HG23	2.06	0.56
30:0:583:C:H2'	30:0:584:U:H6	1.70	0.56
14:N:164:ASP:CG	14:N:167:ASP:HA	2.26	0.55
30:0:681:G:N3	30:0:681:G:H5'	2.21	0.55
30:0:834:G:H4'	30:0:835:U:OP2	2.05	0.55
30:0:1209:C:H2'	30:0:1210:G:C8	2.36	0.55
30:0:1766:U:O2	30:0:1778:A:H5'	2.06	0.55
30:0:2316:G:H4'	38:0:6125:HOH:O	2.05	0.55
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.89	0.55
30:0:281:U:O2'	30:0:282:C:H5'	2.06	0.55
30:0:283:U:H5	30:0:284:C:N3	2.04	0.55
30:0:1904:A:H2'	30:0:1905:U:O4'	2.05	0.55
30:0:2269:C:C2'	30:0:2270:G:H5'	2.36	0.55
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.07	0.55
30:0:65:C:O2'	30:0:66:G:H5'	2.06	0.55
30:0:236:A:C4'	30:0:237:G:H5'	2.36	0.55
30:0:1676:G:O2'	30:0:1677:U:H5'	2.06	0.55
30:0:1834:C:H2'	30:0:1840:A:N6	2.20	0.55
2:B:125:GLU:O	2:B:129:ARG:HG3	2.06	0.55
30:0:1973:A:H5'	30:0:1973:A:C8	2.39	0.55
12:L:18:HIS:HD2	30:0:902:G:N7	2.05	0.55
14:N:80:SER:HB2	38:N:8833:HOH:O	2.07	0.55
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	1.89	0.55
30:0:249:G:H2'	30:0:250:C:H6	1.71	0.55
30:0:2748:G:H1'	38:0:7936:HOH:O	2.05	0.55
30:0:2756:U:N3	30:0:2896:A:C2	2.71	0.55
31:9:22:G:H5'	31:9:23:U:OP1	2.06	0.55
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.89	0.55
5:E:11:VAL:HG12	5:E:12:ASP:N	2.22	0.55
30:0:1592:G:H2'	30:0:1593:C:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:37:ARG:HD2	30:0:656:G:OP2	2.07	0.55
26:Z:40:ALA:HA	30:0:1773:G:C8	2.41	0.55
30:0:282:C:C2'	30:0:283:U:H5'	2.35	0.55
30:0:2748:G:H2'	38:0:7579:HOH:O	2.06	0.55
31:9:49:G:C2'	31:9:50:G:H5'	2.37	0.55
12:L:41:HIS:CD2	30:0:926:A:O2'	2.60	0.55
14:N:37:ARG:NH1	31:9:6:C:OP1	2.39	0.55
30:0:1200:A:H3'	38:0:5786:HOH:O	2.06	0.55
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.89	0.55
15:O:35:LYS:HD3	38:0:4645:HOH:O	2.06	0.55
30:0:2768:A:H5"	38:0:4453:HOH:O	2.07	0.55
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.37	0.54
13:M:163:LEU:HD21	30:0:188:C:H5"	1.89	0.54
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.07	0.54
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.42	0.54
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.89	0.54
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.05	0.54
30:0:1157:C:H2'	30:0:1158:G:C8	2.40	0.54
30:0:2064:U:H5'	30:0:2652:U:O3'	2.08	0.54
14:N:110:THR:HB	14:N:113:SER:OG	2.08	0.54
30:0:1165:G:O2'	30:0:1174:A:C1'	2.54	0.54
30:0:1681:G:H5"	30:0:1682:A:H5'	1.88	0.54
30:0:1819:G:H2'	30:0:1820:G:C4'	2.38	0.54
30:0:1878:G:O2'	30:0:1879:U:P	2.66	0.54
2:B:177:HIS:O	2:B:181:ILE:HG13	2.07	0.54
5:E:132:THR:HB	38:E:2227:HOH:O	2.07	0.54
38:I:1549:HOH:O	30:0:1180:U:H1'	2.07	0.54
30:0:350:G:H1'	38:0:5705:HOH:O	2.06	0.54
31:9:47:A:C2	31:9:48:C:C2	2.94	0.54
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.89	0.54
18:R:99:ALA:HB1	18:R:109:MET:CE	2.37	0.54
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.90	0.54
29:3:73:GLU:HB3	38:3:9053:HOH:O	2.08	0.54
30:0:363:C:O2'	30:0:364:U:H5'	2.07	0.54
31:9:23:U:O2'	31:9:24:U:H4'	2.07	0.54
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.08	0.54
8:H:69:ARG:HD3	38:H:231:HOH:O	2.07	0.54
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.73	0.54
30:0:661:G:C5	30:0:686:A:C2	2.96	0.54
30:0:1947:G:H2'	30:0:1948:G:H8	1.73	0.54
9:I:126:THR:O	9:I:130:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:130:HIS:O	23:W:136:GLY:HA3	2.08	0.54
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.89	0.54
30:0:1193:A:H2	30:0:1194:A:N6	2.06	0.54
30:0:1559:A:H4'	38:0:5895:HOH:O	2.07	0.54
30:0:1594:C:O2'	30:0:1607:A:H4'	2.08	0.54
30:0:1755:A:H2'	30:0:1756:G:O4'	2.07	0.54
30:0:1842:A:C4	30:0:1979:G:C6	2.95	0.54
30:0:2135:A:O2'	30:0:2136:G:H5'	2.06	0.54
31:9:3:A:H2	31:9:21:G:N3	2.06	0.54
4:D:138:GLY:HA2	31:9:29:C:O3'	2.08	0.54
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.54
30:0:2415:A:H2'	30:0:2416:G:H5'	1.88	0.54
30:0:2505:G:H2'	30:0:2506:A:H5'	1.89	0.54
30:0:2507:G:H2'	30:0:2510:C:N4	2.23	0.54
30:0:2781:U:C2'	30:0:2782:G:H5'	2.37	0.54
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.90	0.54
16:P:58:SER:HB3	38:0:5659:HOH:O	2.08	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.08	0.54
30:0:877:G:C5'	30:0:878:G:OP1	2.53	0.54
30:0:1878:G:O2'	30:0:1879:U:H6	1.89	0.54
30:0:10:U:O4	30:0:531:G:H2'	2.08	0.54
30:0:1535:G:H2'	30:0:1536:C:C6	2.43	0.54
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.73	0.53
14:N:160:SER:HB2	31:9:51:A:H5'	1.90	0.53
30:0:2073:G:OP2	30:0:2490:A:H5'	2.08	0.53
2:B:198:GLU:HA	38:B:9133:HOH:O	2.07	0.53
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.90	0.53
30:0:407:A:H3'	38:0:4486:HOH:O	2.08	0.53
31:9:49:G:H2'	31:9:50:G:O4'	2.09	0.53
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.38	0.53
10:J:19:MET:CE	10:J:132:LEU:HD11	2.39	0.53
20:T:2:LYS:HG2	30:0:447:A:OP1	2.08	0.53
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.09	0.53
30:0:24:G:N2	30:0:518:G:H1'	2.23	0.53
30:0:1130:U:H2'	30:0:1131:G:O4'	2.08	0.53
30:0:2371:G:H5'	38:0:5041:HOH:O	2.08	0.53
30:0:2502:C:H2'	30:0:2503:A:C5'	2.37	0.53
5:E:137:ASP:O	5:E:141:VAL:HG23	2.08	0.53
17:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.08	0.53
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.39	0.53
30:0:953:G:H4'	30:0:954:U:OP1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1819:G:H2'	30:0:1820:G:C5'	2.38	0.53
30:0:1850:U:H2'	30:0:1851:G:H8	1.73	0.53
30:0:2756:U:N3	30:0:2896:A:H2	2.06	0.53
2:B:294:TYR:HE2	38:B:9124:HOH:O	1.89	0.53
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.09	0.53
30:0:2783:A:H2'	30:0:2784:A:C8	2.44	0.53
21:U:17:THR:HG22	21:U:18:GLY:N	2.24	0.53
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.91	0.53
30:0:138:U:OP2	30:0:139:C:H5	1.91	0.53
30:0:368:C:C2'	30:0:369:G:H5'	2.39	0.53
30:0:1333:U:H2'	30:0:1334:C:C6	2.44	0.53
30:0:1523:G:C6	30:0:1524:U:C4	2.96	0.53
30:0:1787:C:H4'	30:0:2883:A:O4'	2.08	0.53
31:9:2:U:H4'	38:9:9103:HOH:O	2.08	0.53
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.90	0.53
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.90	0.53
21:U:14:GLU:O	21:U:17:THR:HB	2.08	0.53
30:0:67:A:H5"	30:0:69:A:C8	2.44	0.53
30:0:947:U:H2'	30:0:948:G:H8	1.72	0.53
30:0:2249:G:C2	30:0:2253:G:C6	2.96	0.53
31:9:39:U:O2'	31:9:42:C:C5	2.61	0.53
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.90	0.53
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.39	0.53
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.88	0.53
30:0:123:U:H5'	38:0:6694:HOH:O	2.09	0.53
30:0:1206:U:H2'	30:0:1207:A:O4'	2.09	0.53
30:0:1556:G:O2'	30:0:1557:G:H5'	2.09	0.53
30:0:2597:U:H2'	30:0:2598:U:H5'	1.90	0.53
3:C:5:ILE:HD11	3:C:16:VAL:CG2	2.39	0.53
13:M:57:LYS:HE2	13:M:140:ALA:O	2.09	0.53
30:0:960:G:N3	30:0:960:G:C3'	2.72	0.53
30:0:2897:C:O2'	30:0:2898:G:H5'	2.09	0.53
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.23	0.53
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.39	0.53
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.23	0.53
30:0:876:A:H2'	30:0:876:A:N3	2.23	0.53
30:0:1206:U:H5'	30:0:1206:U:C6	2.32	0.53
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.91	0.52
23:W:80:ASP:O	23:W:84:VAL:HG23	2.09	0.52
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.91	0.52
30:0:1524:U:OP1	30:0:1524:U:H4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2781:U:O2'	30:0:2782:G:H5'	2.07	0.52
12:L:4:LYS:HE2	30:0:645:U:OP2	2.09	0.52
25:Y:235:GLU:CD	25:Y:235:GLU:H	2.12	0.52
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.90	0.52
30:0:241:A:C2	30:0:378:A:H4'	2.44	0.52
30:0:1702:U:H1'	38:0:5805:HOH:O	2.08	0.52
30:0:2314:G:C2'	30:0:2315:C:H5'	2.39	0.52
18:R:150:PRO:CG	18:R:150:PRO:CB	2.86	0.52
4:D:159:PRO:O	4:D:163:VAL:HG23	2.09	0.52
13:M:30:GLU:O	13:M:34:GLU:HG3	2.10	0.52
30:0:1174:A:C6	30:0:1201:C:H4'	2.45	0.52
30:0:1377:C:H5'	30:0:1377:C:C6	2.45	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.90	0.52
30:0:2587:OMU:H2'	30:0:2589:U:H5"	1.92	0.52
3:C:153:VAL:O	3:C:157:LEU:HG	2.09	0.52
4:D:50:VAL:HG13	31:9:41:C:O4'	2.10	0.52
17:Q:25:PRO:HB2	38:9:9082:HOH:O	2.10	0.52
19:S:43:GLU:HB3	38:S:8991:HOH:O	2.10	0.52
30:0:113:A:OP2	30:0:114:A:H2'	2.09	0.52
30:0:2478:U:O2'	30:0:2479:A:H5'	2.08	0.52
12:L:143:THR:HG22	12:L:144:ASP:N	2.25	0.52
20:T:38:ARG:NH1	38:0:6725:HOH:O	2.42	0.52
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.45	0.52
28:2:39:ARG:HG2	38:2:3143:HOH:O	2.08	0.52
30:0:1135:G:H5'	38:0:5960:HOH:O	2.09	0.52
1:A:36:ASP:HB2	1:A:84:VAL:N	2.25	0.52
4:D:138:GLY:N	38:D:7597:HOH:O	2.42	0.52
8:H:48:VAL:HA	8:H:170:ARG:O	2.10	0.52
30:0:602:A:O2'	30:0:605:C:H4'	2.09	0.52
30:0:2105:C:H2'	30:0:2106:C:C6	2.44	0.52
30:0:2250:G:H2'	30:0:2251:G:O4'	2.09	0.52
30:0:2664:A:H8	30:0:2664:A:OP1	1.93	0.52
30:0:2681:A:H4'	30:0:2682:C:C5'	2.39	0.52
30:0:2509:A:OP2	30:0:2510:C:H5	1.93	0.52
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.91	0.52
30:0:968:G:O2'	30:0:969:G:H5'	2.10	0.52
30:0:1444:G:O2'	30:0:1445:G:H5'	2.09	0.52
30:0:1921:A:C6	30:0:1922:A:C2	2.98	0.52
30:0:1930:A:H2'	30:0:1931:A:C8	2.45	0.52
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.10	0.52
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:12:U:H2'	30:0:13:G:H5'	1.91	0.52
30:0:704:C:H2'	30:0:705:C:H6	1.75	0.52
30:0:1279:U:O2	30:0:1279:U:C2'	2.58	0.52
30:0:1289:C:O2'	30:0:1290:G:H5'	2.10	0.52
30:0:1805:G:O2'	30:0:1806:G:H5'	2.10	0.52
30:0:2237:G:O2'	30:0:2238:A:C8	2.62	0.52
30:0:2878:U:H2'	30:0:2879:A:O4'	2.10	0.52
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.91	0.51
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.92	0.51
13:M:179:GLY:O	30:0:399:C:H5'	2.10	0.51
23:W:64:THR:O	23:W:68:THR:HG22	2.10	0.51
30:0:185:G:H4'	30:0:186:A:OP1	2.10	0.51
30:0:200:C:H2'	38:0:3463:HOH:O	2.09	0.51
30:0:1130:U:H5'	38:0:7710:HOH:O	2.10	0.51
30:0:1188:A:C6	30:0:1189:A:C6	2.99	0.51
30:0:2531:U:O2'	30:0:2532:A:H5'	2.10	0.51
31:9:24:U:H3'	31:9:25:G:H5'	1.91	0.51
2:B:148:PRO:HD2	38:B:9049:HOH:O	2.10	0.51
6:F:57:GLU:O	6:F:61:MET:HG3	2.10	0.51
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.26	0.51
22:V:12:THR:HG23	22:V:14:ALA:H	1.75	0.51
23:W:119:HIS:HD2	23:W:120:PRO:O	1.92	0.51
30:0:299:U:H5'	38:0:7375:HOH:O	2.09	0.51
30:0:2250:G:N2	30:0:2251:G:H1'	2.25	0.51
30:0:2830:U:O2'	30:0:2831:C:H5'	2.09	0.51
3:C:145:GLU:HG3	38:C:8569:HOH:O	2.09	0.51
23:W:24:LEU:O	23:W:26:ILE:HG22	2.10	0.51
30:0:10:U:O4	30:0:532:A:OP2	2.28	0.51
30:0:363:C:H2'	30:0:364:U:C6	2.46	0.51
30:0:541:C:O2'	30:0:542:A:H5"	2.11	0.51
30:0:1762:C:O2'	30:0:1763:C:H5'	2.10	0.51
31:9:39:U:O2'	31:9:42:C:H5	1.92	0.51
2:B:211:THR:HG21	38:0:7492:HOH:O	2.11	0.51
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.92	0.51
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.92	0.51
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.41	0.51
30:0:228:C:C2'	30:0:229:G:H5'	2.41	0.51
30:0:285:A:H2'	30:0:286:U:O4'	2.10	0.51
30:0:2252:A:H2'	30:0:2253:G:H5'	1.92	0.51
30:0:2825:C:H4'	30:0:2826:G:O5'	2.10	0.51
31:9:1:U:C4'	31:9:3:A:OP1	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.44	0.51
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.93	0.51
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.93	0.51
30:0:414:C:H5'	38:0:9667:HOH:O	2.11	0.51
30:0:958:G:H2'	30:0:959:C:C6	2.45	0.51
30:0:1386:G:O2'	30:0:1387:G:H5'	2.11	0.51
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.11	0.51
25:Y:189:ASN:C	25:Y:189:ASN:HD22	2.14	0.51
30:0:69:A:H8	30:0:69:A:C5'	2.15	0.51
30:0:1205:U:O2'	30:0:1206:U:H5"	2.11	0.51
30:0:2421:G:H3'	30:0:2422:U:H5"	1.92	0.51
30:0:2781:U:H2'	30:0:2782:G:C5'	2.40	0.51
30:0:2826:G:C6	30:0:2913:A:N6	2.78	0.51
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.79	0.51
24:X:23:HIS:HD2	38:0:9973:HOH:O	1.93	0.51
30:0:541:C:C2'	30:0:542:A:C5'	2.79	0.51
30:0:790:A:H2'	30:0:791:A:O4'	2.10	0.51
30:0:1398:G:O2'	30:0:1399:A:H5'	2.11	0.51
30:0:2241:C:O2'	30:0:2242:U:H5'	2.11	0.51
31:9:91:C:H2'	31:9:92:G:O4'	2.10	0.51
2:B:256:GLN:HG2	38:B:9132:HOH:O	2.11	0.51
12:L:14:GLY:O	30:0:1295:G:H5"	2.11	0.51
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.59	0.51
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.41	0.51
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.93	0.51
19:S:33:SER:O	19:S:37:VAL:HG23	2.11	0.51
30:0:282:C:O2'	30:0:283:U:C5'	2.50	0.51
30:0:346:U:H4'	38:0:6884:HOH:O	2.11	0.51
30:0:2764:C:O2'	30:0:2765:C:H5'	2.10	0.51
30:0:2781:U:H2'	30:0:2782:G:H5'	1.92	0.51
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.93	0.51
29:3:15:ASN:O	30:0:2408:A:H4'	2.11	0.51
30:0:952:G:N3	30:0:2302:A:H2'	2.26	0.51
30:0:2251:G:H2'	30:0:2252:A:H8	1.72	0.51
2:B:41:PHE:HA	2:B:79:MET:HE2	1.92	0.51
3:C:233:THR:HG22	3:C:234:VAL:N	2.26	0.51
25:Y:184:GLU:OE2	25:Y:204:ARG:HD2	2.11	0.51
30:0:1419:U:H2'	30:0:1685:A:C2	2.46	0.51
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.76	0.50
30:0:120:A:H2'	30:0:120:A:N3	2.27	0.50
2:B:85:ARG:NH1	38:B:9109:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:56:ILE:O	22:V:60:GLN:HG3	2.11	0.50
30:0:249:G:H2'	30:0:250:C:C6	2.46	0.50
30:0:289:G:O2'	30:0:290:C:H5'	2.12	0.50
30:0:383:A:H4'	38:0:5359:HOH:O	2.10	0.50
30:0:683:G:O2'	30:0:684:G:H5'	2.11	0.50
30:0:1167:G:H2'	30:0:1168:C:C6	2.46	0.50
30:0:1186:C:N4	30:0:1187:U:C4	2.79	0.50
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.45	0.50
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.94	0.50
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.94	0.50
30:0:1183:C:H2'	30:0:1183:C:O2	2.10	0.50
30:0:1202:A:C2'	30:0:1203:G:H5'	2.40	0.50
30:0:1494:A:H1'	30:0:1495:C:C6	2.47	0.50
30:0:1557:G:O2'	30:0:1558:C:H5'	2.11	0.50
30:0:1972:U:C2'	30:0:1973:A:H5"	2.41	0.50
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.27	0.50
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.94	0.50
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.12	0.50
15:O:39:THR:O	15:O:115:ARG:NH2	2.44	0.50
22:V:44:GLY:O	22:V:48:GLU:HG2	2.12	0.50
30:0:559:U:H6	30:0:559:U:C5'	2.20	0.50
30:0:1183:C:H42	30:0:1184:C:N4	2.05	0.50
1:A:135:VAL:HA	1:A:150:PRO:HD3	1.93	0.50
5:E:7:ILE:HG13	5:E:11:VAL:HB	1.93	0.50
8:H:66:GLU:HA	38:H:231:HOH:O	2.11	0.50
11:K:66:ARG:HH22	30:0:1994:A:P	2.35	0.50
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.94	0.50
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.95	0.50
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.11	0.50
30:0:69:A:C8	30:0:69:A:C5'	2.89	0.50
30:0:95:A:H5"	30:0:97:G:O4'	2.11	0.50
30:0:858:U:H5	38:0:5459:HOH:O	1.93	0.50
30:0:2610:U:H4'	38:0:9491:HOH:O	2.12	0.50
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.47	0.50
10:J:42:GLU:O	10:J:131:THR:HG23	2.12	0.50
24:X:61:ARG:NH1	24:X:67:PRO:HD3	2.27	0.50
27:1:16:HIS:HE1	30:0:775:G:OP1	1.94	0.50
30:0:1588:G:C6	30:0:1589:G:N1	2.80	0.50
30:0:1795:G:H2'	30:0:1796:A:O4'	2.12	0.50
30:0:1878:G:C1'	38:0:6153:HOH:O	2.47	0.50
31:9:13:A:O2'	31:9:14:G:H5"	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.47	0.50
5:E:143:GLN:HE22	30:0:2779:G:H21	1.55	0.50
18:R:111:ILE:HG23	18:R:145:LEU:CD1	2.41	0.50
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.30	0.50
23:W:65:VAL:HG12	23:W:116:LEU:HD13	1.94	0.50
23:W:149:LEU:HG	23:W:153:MET:CE	2.41	0.50
30:0:1118:A:H8	30:0:1119:G:H5"	1.76	0.50
30:0:2421:G:H3'	30:0:2422:U:C5'	2.42	0.50
30:0:2793:A:N6	38:0:5912:HOH:O	2.44	0.50
30:0:2883:A:H2'	30:0:2884:G:O4'	2.12	0.50
2:B:310:ARG:HD2	38:B:9122:HOH:O	2.12	0.50
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.93	0.50
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.93	0.50
14:N:132:ASN:O	14:N:135:VAL:HG12	2.12	0.50
23:W:139:GLY:O	23:W:141:HIS:CD2	2.64	0.50
30:0:154:C:H2'	30:0:155:C:H6	1.76	0.50
30:0:264:G:H1'	30:0:265:U:H5	1.77	0.50
30:0:912:A:C4	30:0:1294:A:C2	2.99	0.50
30:0:1667:A:H2'	30:0:1668:U:C6	2.47	0.50
31:9:36:C:C5	31:9:37:C:C5	3.00	0.50
1:A:35:GLY:O	1:A:36:ASP:HB3	2.12	0.50
5:E:69:ILE:HA	5:E:72:MET:CE	2.41	0.50
5:E:84:MET:HB2	5:E:131:LEU:HB2	1.94	0.50
8:H:123:ILE:HD12	8:H:123:ILE:N	2.27	0.50
30:0:79:G:H22	30:0:97:G:H1'	1.77	0.50
30:0:79:G:N2	30:0:97:G:H1'	2.27	0.50
30:0:968:G:C2	30:0:1001:U:O2	2.65	0.50
30:0:969:G:H1	30:0:999:C:N4	2.10	0.50
30:0:2820:A:H2'	30:0:2821:C:C6	2.47	0.50
30:0:2896:A:N3	30:0:2896:A:H2'	2.27	0.50
4:D:52:THR:HG21	30:0:2347:C:H5'	1.94	0.49
19:S:76:GLU:HB3	38:S:8992:HOH:O	2.11	0.49
22:V:39:ALA:H	22:V:40:PRO:HD2	1.76	0.49
30:0:886:A:OP2	30:0:2113:G:H5'	2.11	0.49
30:0:941:G:C5	30:0:942:U:C4	3.00	0.49
30:0:1149:U:H5"	30:0:1151:G:O4'	2.12	0.49
30:0:1644:C:H2'	30:0:1645:U:H6	1.77	0.49
30:0:1848:G:O2'	30:0:1849:G:H5'	2.12	0.49
30:0:2010:A:C2'	38:0:5990:HOH:O	2.56	0.49
30:0:2577:A:H8	38:0:9613:HOH:O	1.95	0.49
31:9:95:C:O2'	31:9:96:C:H5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.77	0.49
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.94	0.49
29:3:60:LYS:HG3	38:0:7595:HOH:O	2.12	0.49
30:0:2256:G:C2'	30:0:2257:G:C5'	2.89	0.49
30:0:2793:A:H2'	30:0:2794:G:H5'	1.94	0.49
2:B:254:GLN:HG2	2:B:255:GLY:N	2.27	0.49
3:C:236:THR:HA	38:C:8644:HOH:O	2.12	0.49
4:D:103:ASN:ND2	4:D:133:ASN:HD22	2.10	0.49
14:N:37:ARG:NH2	38:N:8831:HOH:O	2.45	0.49
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.11	0.49
10:J:131:THR:HB	10:J:134:GLU:HG3	1.95	0.49
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.13	0.49
16:P:41:ARG:HH22	30:0:1500:U:P	2.35	0.49
25:Y:154:ARG:NH1	25:Y:155:ARG:HG3	2.28	0.49
30:0:2092:G:H2'	30:0:2613:G:OP1	2.13	0.49
1:A:51:ARG:NH1	1:A:120:ARG:O	2.46	0.49
2:B:54:VAL:HB	38:B:9087:HOH:O	2.11	0.49
3:C:43:LYS:HG2	30:0:449:A:N7	2.28	0.49
30:0:301:C:O2'	30:0:302:A:H5'	2.13	0.49
30:0:1972:U:H2'	30:0:1973:A:H5"	1.92	0.49
30:0:2724:U:H2'	30:0:2725:G:O4'	2.12	0.49
30:0:2851:G:H2'	30:0:2852:A:H5'	1.91	0.49
2:B:26:PHE:HE1	38:B:9122:HOH:O	1.96	0.49
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.93	0.49
5:E:69:ILE:HA	5:E:72:MET:HE3	1.95	0.49
13:M:193:LYS:HB3	30:0:392:U:H4'	1.94	0.49
16:P:54:LYS:HB2	30:0:1717:A:H5"	1.93	0.49
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.95	0.49
20:T:54:ASP:OD2	30:0:316:A:H5'	2.12	0.49
21:U:33:SER:O	21:U:37:GLU:HG3	2.13	0.49
30:0:671:A:O2'	30:0:672:G:H2'	2.13	0.49
30:0:1198:U:C6	30:0:1200:A:OP2	2.65	0.49
31:9:39:U:HO2'	31:9:42:C:H5	1.52	0.49
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.42	0.49
30:0:255:A:C4	30:0:256:C:C6	3.00	0.49
30:0:1666:C:HO2'	30:0:1667:A:H5"	1.70	0.49
30:0:2265:U:H2'	30:0:2266:A:C8	2.48	0.49
30:0:2356:A:H5'	38:0:5666:HOH:O	2.12	0.49
30:0:2467:A:H2'	38:0:5488:HOH:O	2.12	0.49
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.95	0.49
20:T:52:ARG:O	30:0:317:A:OP1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1008:C:O2'	30:0:1009:U:H5'	2.13	0.49
30:0:1552:G:H2'	30:0:1553:C:C6	2.47	0.49
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.94	0.49
8:H:30:LYS:H	8:H:62:HIS:CD2	2.30	0.49
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.93	0.49
25:Y:154:ARG:HH21	30:0:1293:U:H5'	1.78	0.49
30:0:255:A:H2'	30:0:256:C:C6	2.47	0.49
30:0:304:G:H1'	30:0:347:A:N6	2.28	0.49
30:0:790:A:H1'	30:0:1710:A:H2'	1.95	0.49
30:0:2453:G:H5"	38:0:4755:HOH:O	2.13	0.49
30:0:2717:C:C2'	30:0:2718:C:C5'	2.79	0.49
30:0:2769:C:C2'	30:0:2770:G:C5'	2.84	0.49
30:0:154:C:H2'	30:0:155:C:C6	2.48	0.49
30:0:513:A:N3	38:0:3679:HOH:O	2.35	0.49
30:0:1857:A:H5"	38:0:6744:HOH:O	2.12	0.49
30:0:2002:C:C2'	30:0:2003:U:H5'	2.42	0.49
30:0:2316:G:OP1	30:0:2317:C:H1'	2.13	0.49
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.94	0.48
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.95	0.48
7:G:67:LEU:O	7:G:71:LEU:HG	2.12	0.48
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.42	0.48
21:U:37:GLU:HB3	38:U:408:HOH:O	2.11	0.48
22:V:1:THR:HG23	22:V:2:VAL:HG23	1.94	0.48
30:0:282:C:O2	30:0:282:C:H2'	2.13	0.48
30:0:1158:G:O2'	30:0:1159:G:H5'	2.13	0.48
30:0:1391:G:H2'	30:0:1392:A:H5'	1.95	0.48
30:0:1562:C:O2	30:0:1562:C:H2'	2.12	0.48
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.45	0.48
10:J:75:PRO:HB3	10:J:132:LEU:HB3	1.95	0.48
12:L:6:ARG:NH1	30:0:1299:G:N7	2.62	0.48
16:P:83:LYS:HG2	30:0:793:A:H5"	1.94	0.48
24:X:43:VAL:HG12	24:X:44:ASP:N	2.28	0.48
27:1:1:THR:O	30:0:1836:A:H1'	2.13	0.48
30:0:195:C:H2'	30:0:196:G:H5'	1.95	0.48
30:0:1159:G:H1	30:0:1208:C:H42	1.58	0.48
30:0:1825:U:O2'	30:0:1826:C:H5'	2.12	0.48
2:B:205:VAL:O	2:B:307:ARG:NE	2.47	0.48
3:C:136:VAL:HG22	3:C:137:PRO:HA	1.95	0.48
15:O:32:ARG:O	15:O:32:ARG:HD3	2.12	0.48
19:S:37:VAL:O	19:S:41:VAL:HG23	2.13	0.48
23:W:23:MET:O	30:0:1025:C:H5'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:212:ARG:HD2	38:Y:8896:HOH:O	2.12	0.48
26:Z:80:GLN:HA	26:Z:86:TYR:O	2.12	0.48
30:0:137:U:H2'	30:0:139:C:C5	2.47	0.48
30:0:1087:G:H4'	30:0:1088:A:OP1	2.13	0.48
30:0:1528:A:H2'	30:0:1529:G:O4'	2.13	0.48
30:0:1632:A:C3'	30:0:1633:C:H5'	2.43	0.48
1:A:121:ALA:O	1:A:124:VAL:HG22	2.13	0.48
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.95	0.48
20:T:8:ARG:HD2	30:0:31:C:OP2	2.13	0.48
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.48
30:0:1321:A:H2'	30:0:1322:G:C8	2.48	0.48
30:0:2300:A:H4'	30:0:2301:A:O5'	2.13	0.48
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.48
2:B:49:THR:HG21	2:B:331:SER:O	2.14	0.48
2:B:255:GLY:O	2:B:257:THR:HG22	2.14	0.48
3:C:236:THR:H	3:C:239:ALA:HB3	1.78	0.48
6:F:48:VAL:HG23	6:F:74:PHE:CB	2.42	0.48
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.95	0.48
30:0:961:A:H4'	38:0:6814:HOH:O	2.12	0.48
30:0:1883:U:O2'	30:0:1884:G:H5'	2.13	0.48
30:0:2301:A:H5"	30:0:2302:A:H5'	1.95	0.48
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.96	0.48
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.95	0.48
30:0:447:A:O2'	30:0:448:G:H5'	2.14	0.48
30:0:1165:G:H4'	30:0:1174:A:O2'	2.13	0.48
30:0:2269:C:H2'	30:0:2270:G:C5'	2.44	0.48
10:J:107:ASN:C	10:J:107:ASN:HD22	2.17	0.48
30:0:222:A:H2'	30:0:223:G:O4'	2.14	0.48
30:0:2564:G:OP2	30:0:2565:C:H5"	2.14	0.48
6:F:21:GLU:O	6:F:24:ARG:HG2	2.14	0.48
18:R:104:PHE:HB3	18:R:109:MET:HE1	1.96	0.48
30:0:484:A:N1	30:0:506:G:H4'	2.28	0.48
30:0:920:C:H5'	30:0:921:G:C4	2.49	0.48
30:0:1130:U:H4'	38:0:6158:HOH:O	2.13	0.48
31:9:45:A:H2'	31:9:46:C:H6	1.79	0.48
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.94	0.48
3:C:140:VAL:HB	38:C:8644:HOH:O	2.13	0.48
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.46	0.48
15:O:57:THR:HB	15:O:111:VAL:HG23	1.95	0.48
29:3:48:ASN:ND2	29:3:50:GLY:H	2.11	0.48
30:0:960:G:H3'	30:0:960:G:C4	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1051:C:H2'	30:0:1052:G:O4'	2.14	0.48
30:0:1131:G:C6	30:0:1230:A:C4	3.02	0.48
30:0:1545:C:H2'	30:0:1546:G:O4'	2.14	0.48
30:0:2912:C:H2'	30:0:2913:A:O4'	2.14	0.48
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.44	0.48
2:B:275:GLY:O	2:B:291:ASP:HA	2.14	0.48
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.79	0.48
12:L:121:ILE:HG12	12:L:141:GLU:HB2	1.96	0.48
30:0:1477:C:H5'	30:0:1868:G:H5"	1.96	0.48
30:0:1625:U:H5"	38:0:6053:HOH:O	2.13	0.48
30:0:2439:C:H5'	38:0:5518:HOH:O	2.12	0.48
1:A:3:ARG:HD3	30:0:870:G:OP2	2.14	0.47
3:C:22:PHE:HA	3:C:116:ALA:HA	1.94	0.47
13:M:64:ARG:HD2	38:M:8881:HOH:O	2.14	0.47
14:N:43:VAL:HG13	14:N:118:ILE:HD11	1.96	0.47
14:N:114:LYS:O	14:N:118:ILE:HG13	2.14	0.47
14:N:169:PRO:O	14:N:172:PHE:HB3	2.14	0.47
23:W:65:VAL:HA	23:W:68:THR:HG22	1.95	0.47
27:1:28:HIS:HD2	27:1:30:LYS:H	1.60	0.47
30:0:90:A:H2'	30:0:91:G:O4'	2.14	0.47
30:0:2314:G:H2'	30:0:2315:C:H5'	1.96	0.47
4:D:76:ARG:NE	31:9:44:A:O4'	2.47	0.47
21:U:9:CYS:HA	21:U:52:THR:OG1	2.14	0.47
30:0:398:U:H2'	30:0:399:C:C6	2.49	0.47
30:0:1666:C:H2'	30:0:1667:A:H5"	1.78	0.47
30:0:1838:U:O2'	30:0:2644:C:H5'	2.14	0.47
30:0:1850:U:H2'	30:0:1851:G:C8	2.48	0.47
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.27	0.47
8:H:61:ARG:HG3	8:H:61:ARG:NH1	2.29	0.47
27:1:25:LYS:HD2	28:2:48:ASP:HA	1.96	0.47
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.47
30:0:1422:U:H2'	30:0:1423:C:C6	2.50	0.47
30:0:1641:A:C2'	30:0:1642:A:H5'	2.44	0.47
30:0:1788:U:O2'	30:0:1789:G:H5'	2.14	0.47
30:0:2264:A:H2'	30:0:2265:U:C6	2.48	0.47
30:0:2506:A:H1'	38:0:3766:HOH:O	2.13	0.47
1:A:30:ARG:NH2	1:A:38:ILE:HG13	2.28	0.47
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.79	0.47
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.50	0.47
6:F:107:ASP:O	6:F:111:ILE:HG13	2.14	0.47
16:P:143:ALA:HA	38:P:184:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:154:ARG:NH1	30:0:588:G:O6	2.47	0.47
30:0:955:A:C2	30:0:1013:A:C4	3.03	0.47
30:0:1268:C:O2'	30:0:1269:G:H5'	2.14	0.47
30:0:1280:A:OP1	30:0:1280:A:H3'	2.15	0.47
30:0:2064:U:H4'	30:0:2653:A:OP1	2.13	0.47
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.30	0.47
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.47
14:N:40:ASN:HD21	31:9:28:U:H5"	1.80	0.47
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.49	0.47
30:0:137:U:OP1	30:0:259:G:O2'	2.33	0.47
30:0:1193:A:C2	30:0:1194:A:N6	2.78	0.47
30:0:1252:A:H2'	30:0:1253:C:O4'	2.14	0.47
31:9:56:A:C3'	31:9:57:A:H5"	2.44	0.47
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.97	0.47
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.48	0.47
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.15	0.47
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.45	0.47
16:P:120:ARG:NH1	30:0:1594:C:C5	2.82	0.47
24:X:85:VAL:HG12	24:X:86:GLU:N	2.30	0.47
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	1.97	0.47
30:0:407:A:H2'	30:0:408:A:C8	2.50	0.47
30:0:1393:A:H2'	30:0:1394:C:C6	2.49	0.47
30:0:2271:G:H5'	38:0:4783:HOH:O	2.14	0.47
30:0:2469:A:H2'	38:0:7512:HOH:O	2.15	0.47
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.47	0.47
4:D:10:PHE:CG	4:D:11:HIS:N	2.81	0.47
12:L:149:ARG:O	12:L:150:GLN:HB2	2.14	0.47
17:Q:32:GLU:O	17:Q:93:ARG:NH2	2.48	0.47
30:0:283:U:H5	30:0:284:C:N4	2.12	0.47
30:0:440:C:H2'	30:0:441:A:C8	2.50	0.47
30:0:1118:A:C8	30:0:1119:G:H5"	2.49	0.47
30:0:1176:C:N4	38:0:5775:HOH:O	2.48	0.47
30:0:1762:C:H2'	30:0:1763:C:H6	1.80	0.47
30:0:2353:A:H4'	30:0:2354:A:O5'	2.14	0.47
13:M:164:THR:HG22	13:M:166:ALA:N	2.29	0.47
23:W:11:VAL:HG11	30:0:1086:A:C6	2.49	0.47
27:1:22:CYS:SG	27:1:24:GLU:HB2	2.55	0.47
29:3:65:THR:HB	29:3:83:TRP:H	1.79	0.47
30:0:426:G:H2'	30:0:427:C:O4'	2.15	0.47
30:0:483:C:C4	30:0:484:A:C6	3.03	0.47
30:0:2791:U:H1'	30:0:2792:A:H5"	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:52:A:H2'	31:9:53:G:O4'	2.15	0.47
6:F:91:VAL:HG12	6:F:92:GLY:H	1.78	0.47
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.45	0.47
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.44	0.47
30:0:1682:A:H2'	38:0:9820:HOH:O	2.14	0.47
30:0:2533:C:C6	30:0:2533:C:C5'	2.92	0.47
31:9:55:U:H4'	31:9:56:A:C8	2.49	0.47
2:B:297:VAL:HB	38:B:9080:HOH:O	2.15	0.47
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.97	0.47
30:0:816:G:C6	30:0:817:G:N1	2.83	0.47
30:0:1249:U:H2'	30:0:1250:C:C6	2.50	0.47
30:0:1477:C:C5'	30:0:1868:G:H5"	2.44	0.47
30:0:1928:C:H2'	30:0:1929:G:H5'	1.96	0.47
30:0:2281:C:H2'	30:0:2282:U:H5'	1.97	0.47
30:0:2372:A:H2'	30:0:2373:U:H6	1.78	0.47
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.30	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.15	0.46
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.35	0.46
26:Z:34:SER:HB3	30:0:797:A:H4'	1.96	0.46
30:0:170:U:H2'	30:0:171:C:H5'	1.95	0.46
30:0:2011:A:H4'	30:0:2012:U:O5'	2.15	0.46
30:0:2238:A:H3'	38:0:6711:HOH:O	2.15	0.46
30:0:2589:U:H2'	30:0:2590:U:C6	2.50	0.46
1:A:175:LYS:HG3	30:0:1847:A:OP1	2.16	0.46
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.19	0.46
8:H:172:GLU:HB3	38:H:243:HOH:O	2.15	0.46
21:U:50:GLU:HB2	30:0:2866:U:C5	2.50	0.46
24:X:43:VAL:HG12	24:X:47:ALA:HB3	1.97	0.46
25:Y:165:GLU:HB3	38:0:6747:HOH:O	2.15	0.46
27:1:11:LYS:HG2	30:0:777:U:O2'	2.15	0.46
31:9:28:U:H2'	31:9:29:C:C6	2.50	0.46
14:N:141:ARG:NH2	31:9:48:C:H4'	2.30	0.46
16:P:1:THR:O	30:0:1396:C:H1'	2.15	0.46
30:0:304:G:H1'	30:0:347:A:H61	1.80	0.46
30:0:559:U:C5	30:0:560:U:C5	3.03	0.46
30:0:800:G:H2'	30:0:801:U:C6	2.50	0.46
30:0:969:G:H1	30:0:999:C:H42	1.62	0.46
30:0:1907:U:O2'	30:0:1908:G:H5'	2.15	0.46
1:A:88:ILE:O	1:A:88:ILE:HG22	2.14	0.46
1:A:132:ASP:HB3	1:A:135:VAL:H	1.80	0.46
3:C:129:HIS:HD2	3:C:165:ASP:OD2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.15	0.46
23:W:122:ARG:NH2	38:0:5320:HOH:O	2.48	0.46
25:Y:115:ARG:NH2	30:0:1266:U:H4'	2.30	0.46
30:0:105:G:O2'	30:0:106:A:H5'	2.15	0.46
30:0:690:G:H4'	30:0:741:C:O2	2.15	0.46
30:0:699:C:C2	30:0:744:G:C2	3.03	0.46
30:0:2103:A:H2'	30:0:2104:C:H5'	1.96	0.46
2:B:320:GLN:HE21	2:B:321:PRO:CD	2.24	0.46
8:H:139:ALA:HB3	8:H:149:VAL:HG21	1.97	0.46
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.31	0.46
10:J:82:THR:CG2	30:0:1242:A:H5'	2.30	0.46
10:J:107:ASN:HD22	10:J:109:TYR:H	1.64	0.46
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.96	0.46
23:W:125:HIS:CE1	30:0:1097:A:H5"	2.51	0.46
30:0:343:C:O2'	30:0:344:C:H5'	2.15	0.46
30:0:638:C:H2'	30:0:639:A:C8	2.51	0.46
30:0:920:C:H5"	30:0:921:G:O5'	2.15	0.46
30:0:1117:A:C2	30:0:1244:U:C2	3.04	0.46
30:0:1657:A:H2'	30:0:1658:A:C8	2.51	0.46
31:9:101:G:H5"	38:9:9140:HOH:O	2.15	0.46
1:A:51:ARG:HD2	30:0:1874:U:OP1	2.15	0.46
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.95	0.46
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.82	0.46
20:T:28:SER:O	20:T:32:ARG:HG3	2.15	0.46
30:0:11:A:H5'	30:0:12:U:OP2	2.15	0.46
30:0:583:C:C2	30:0:584:U:C5	3.03	0.46
30:0:1503:U:H2'	30:0:1504:A:O4'	2.15	0.46
30:0:1596:U:H2'	30:0:1598:A:OP2	2.15	0.46
30:0:2712:G:H5'	38:0:5251:HOH:O	2.15	0.46
18:R:104:PHE:CB	18:R:109:MET:HE1	2.46	0.46
24:X:30:MET:CE	24:X:58:ALA:HB3	2.45	0.46
27:1:1:THR:HA	38:0:9368:HOH:O	2.16	0.46
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.54	0.46
30:0:613:C:H2'	30:0:614:U:H6	1.80	0.46
30:0:812:A:H2'	30:0:813:C:O4'	2.16	0.46
30:0:1883:U:C2'	30:0:1884:G:H5'	2.46	0.46
31:9:39:U:C2'	31:9:40:C:OP1	2.63	0.46
1:A:214:SER:HB2	38:0:4392:HOH:O	2.15	0.46
3:C:206:ASN:HB2	30:0:329:A:OP2	2.15	0.46
4:D:27:ILE:HB	4:D:69:ILE:O	2.15	0.46
8:H:61:ARG:HG3	38:0:5004:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:132:ARG:NH1	38:R:8984:HOH:O	2.48	0.46
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.98	0.46
30:0:1202:A:O2'	30:0:1203:G:H5'	2.16	0.46
30:0:1928:C:C2'	30:0:1929:G:H5'	2.46	0.46
6:F:91:VAL:HG11	30:0:262:A:OP2	2.16	0.46
10:J:63:ILE:CD1	30:0:1236:A:C8	2.99	0.46
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.97	0.46
18:R:29:LYS:HD3	30:0:524:A:H5"	1.98	0.46
28:2:20:ARG:HD3	38:0:6163:HOH:O	2.16	0.46
30:0:71:G:H5"	38:0:3932:HOH:O	2.16	0.46
30:0:622:G:O2'	30:0:623:U:H5'	2.16	0.46
30:0:711:G:H1'	38:0:7133:HOH:O	2.14	0.46
30:0:2065:C:O2'	30:0:2066:C:H5'	2.16	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.51	0.46
30:0:2758:G:H2'	30:0:2759:C:C6	2.51	0.46
31:9:29:C:C2'	31:9:30:C:H5'	2.42	0.46
1:A:206:ARG:NH2	30:0:2630:G:O6	2.49	0.46
2:B:141:ARG:N	38:B:9048:HOH:O	2.48	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.98	0.46
30:0:1311:G:C2	30:0:1312:G:C8	3.04	0.46
30:0:1790:C:H2'	30:0:1791:U:C6	2.50	0.46
30:0:2241:C:H2'	30:0:2242:U:C6	2.51	0.46
30:0:2379:G:N7	30:0:2408:A:N1	2.63	0.46
1:A:194:MET:HG2	30:0:875:A:C2	2.52	0.45
2:B:62:ARG:HA	2:B:65:MET:CE	2.46	0.45
29:3:62:THR:HB	38:3:9044:HOH:O	2.15	0.45
30:0:78:G:C6	30:0:79:G:C6	3.04	0.45
30:0:162:C:H2'	30:0:163:U:H5'	1.98	0.45
30:0:278:A:H2'	30:0:279:C:O4'	2.16	0.45
30:0:372:A:H2'	30:0:373:G:C8	2.51	0.45
30:0:876:A:N3	30:0:876:A:C2'	2.80	0.45
30:0:1511:U:O2'	30:0:1512:G:H5'	2.16	0.45
30:0:1522:A:C2	30:0:1665:G:C6	3.04	0.45
30:0:2415:A:C2'	30:0:2416:G:H5'	2.46	0.45
30:0:2831:C:H42	30:0:2909:G:H1	1.64	0.45
30:0:2872:U:H2'	30:0:2873:C:H6	1.81	0.45
30:0:2880:A:C2'	30:0:2881:C:H5'	2.46	0.45
10:J:75:PRO:HD3	10:J:136:SER:OG	2.16	0.45
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.31	0.45
20:T:63:ILE:HD11	20:T:75:GLU:HB2	1.99	0.45
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:53:C:H2'	30:0:54:G:O4'	2.16	0.45
30:0:412:C:O2'	30:0:413:G:H5'	2.16	0.45
30:0:669:G:O2'	30:0:670:G:H5'	2.16	0.45
30:0:758:A:H2'	30:0:759:C:O4'	2.17	0.45
30:0:1074:G:H4'	30:0:1260:G:C6	2.51	0.45
30:0:1194:A:O2'	30:0:1195:G:H5'	2.16	0.45
30:0:1339:G:C6	30:0:1340:G:N1	2.85	0.45
30:0:1778:A:H2'	30:0:1779:A:H5'	1.97	0.45
3:C:19:PRO:HG2	3:C:22:PHE:CD1	2.51	0.45
7:G:64:ASN:N	7:G:64:ASN:ND2	2.63	0.45
23:W:38:THR:HG22	23:W:39:ASP:N	2.31	0.45
30:0:407:A:H8	38:0:4486:HOH:O	2.00	0.45
30:0:445:U:H2'	30:0:446:G:H8	1.81	0.45
30:0:2456:A:H2'	30:0:2457:U:C6	2.51	0.45
6:F:91:VAL:CG1	6:F:92:GLY:N	2.80	0.45
10:J:19:MET:HE1	10:J:79:PHE:HA	1.99	0.45
13:M:49:ALA:C	13:M:54:TYR:HB3	2.37	0.45
30:0:253:U:H1'	30:0:256:C:H41	1.82	0.45
30:0:281:U:H2'	30:0:282:C:H6	1.82	0.45
30:0:506:G:N2	30:0:509:A:H5'	2.22	0.45
30:0:522:U:O2'	30:0:1366:C:H5'	2.16	0.45
30:0:1333:U:H2'	30:0:1334:C:H6	1.82	0.45
30:0:2271:G:N3	30:0:2271:G:H2'	2.31	0.45
31:9:3:A:OP2	31:9:25:G:N2	2.49	0.45
31:9:53:G:O2'	31:9:54:A:H5'	2.16	0.45
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.35	0.45
11:K:113:ILE:HG22	11:K:114:ALA:N	2.32	0.45
15:O:10:LEU:HD13	15:O:99:GLU:HG3	1.99	0.45
30:0:1919:A:H4'	38:0:4883:HOH:O	2.15	0.45
30:0:2493:C:O2	30:0:2493:C:H2'	2.15	0.45
31:9:40:C:H2'	31:9:41:C:OP1	2.17	0.45
31:9:57:A:N6	38:9:9066:HOH:O	2.47	0.45
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.51	0.45
4:D:20:LYS:HG2	4:D:133:ASN:HB3	1.97	0.45
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.51	0.45
11:K:125:ALA:C	11:K:127:ALA:H	2.20	0.45
18:R:132:ARG:HG2	18:R:133:ALA:N	2.31	0.45
24:X:78:GLU:HG2	24:X:79:GLU:H	1.81	0.45
30:0:603:A:H1'	30:0:605:C:C2	2.52	0.45
30:0:1202:A:H2'	30:0:1203:G:H5'	1.99	0.45
30:0:1588:G:C6	30:0:1589:G:C6	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1947:G:H2'	30:0:1948:G:C8	2.52	0.45
30:0:2598:U:O2	30:0:2600:A:H8	2.00	0.45
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.99	0.45
1:A:164:ARG:NE	38:A:9043:HOH:O	2.49	0.45
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.99	0.45
13:M:99:ARG:HG3	38:M:8855:HOH:O	2.16	0.45
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.99	0.45
16:P:134:VAL:O	16:P:137:LEU:HB3	2.17	0.45
17:Q:1:PRO:HA	30:0:2299:G:O6	2.16	0.45
30:0:42:C:H1'	38:0:4707:HOH:O	2.15	0.45
30:0:821:U:H3'	38:0:3789:HOH:O	2.15	0.45
30:0:1183:C:N3	30:0:1184:C:H5	2.15	0.45
30:0:2090:G:H2'	30:0:2091:G:C8	2.51	0.45
30:0:2281:C:C2'	30:0:2282:U:H5'	2.47	0.45
30:0:2812:A:N7	38:0:7555:HOH:O	2.36	0.45
1:A:96:LEU:HD22	1:A:128:LEU:HD13	1.99	0.45
1:A:99:ILE:O	1:A:131:HIS:HE1	2.00	0.45
1:A:186:TRP:CG	1:A:187:PRO:HA	2.52	0.45
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.98	0.45
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.99	0.45
8:H:34:HIS:HD2	8:H:90:LEU:O	2.00	0.45
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.97	0.45
23:W:149:LEU:HG	23:W:153:MET:HE2	1.99	0.45
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.32	0.45
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.52	0.45
30:0:1987:C:H2'	30:0:1988:C:C6	2.51	0.45
3:C:84:VAL:O	3:C:85:LYS:HB2	2.17	0.45
12:L:50:GLY:C	30:0:2453:G:H4'	2.37	0.45
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.99	0.45
18:R:113:HIS:O	18:R:145:LEU:HD12	2.17	0.45
19:S:77:VAL:O	19:S:80:ARG:HG2	2.16	0.45
23:W:119:HIS:HE1	38:0:9565:HOH:O	2.00	0.45
30:0:128:A:C8	30:0:128:A:H3'	2.52	0.45
30:0:1902:G:N2	30:0:1936:C:C2	2.85	0.45
30:0:2506:A:O2'	30:0:2507:G:P	2.75	0.45
31:9:81:C:O2'	31:9:82:U:H5'	2.17	0.45
3:C:168:ARG:NH2	3:C:190:ALA:O	2.50	0.45
23:W:74:GLU:OE1	30:0:1285:U:H4'	2.17	0.45
25:Y:137:LYS:HD2	30:0:521:A:H5"	1.99	0.45
27:1:2:GLY:O	27:1:6:PRO:HG2	2.17	0.45
30:0:77:G:C2'	30:0:78:G:H5'	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:951:A:O2'	30:0:952:G:H5'	2.17	0.45
30:0:969:G:N2	30:0:1000:C:C2	2.84	0.45
30:0:1615:A:H5'	38:0:4210:HOH:O	2.16	0.45
30:0:1626:A:H2'	30:0:1627:G:O4'	2.17	0.45
31:9:1:U:O3'	31:9:3:A:OP1	2.35	0.45
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.00	0.44
2:B:62:ARG:HA	2:B:65:MET:HE2	1.99	0.44
13:M:164:THR:HB	38:M:8819:HOH:O	2.15	0.44
30:0:542:A:O2'	30:0:543:G:H5'	2.16	0.44
30:0:1783:A:O2'	30:0:1784:U:H5'	2.16	0.44
30:0:1896:G:C6	30:0:1897:U:C4	3.05	0.44
30:0:1942:A:O2'	30:0:1943:C:H5'	2.17	0.44
30:0:2754:G:H2'	30:0:2755:G:O4'	2.17	0.44
1:A:53:ALA:HB3	38:A:9060:HOH:O	2.16	0.44
4:D:135:VAL:HG22	4:D:136:ARG:N	2.32	0.44
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.98	0.44
26:Z:37:ARG:HD2	38:Z:8719:HOH:O	2.17	0.44
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.64	0.44
29:3:65:THR:CG2	29:3:67:LEU:HG	2.46	0.44
30:0:291:C:H2'	30:0:292:G:O4'	2.17	0.44
30:0:812:A:H2'	30:0:813:C:C6	2.52	0.44
30:0:1406:A:H4'	30:0:1407:A:H5"	1.99	0.44
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.76	0.44
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.38	0.44
11:K:14:LYS:HG3	11:K:32:ILE:O	2.18	0.44
14:N:108:SER:HA	14:N:109:PRO:HD3	1.81	0.44
30:0:187:A:H3'	30:0:188:C:H6	1.82	0.44
30:0:204:A:H2'	30:0:205:U:H5'	1.98	0.44
30:0:582:U:H2'	30:0:583:C:C6	2.53	0.44
30:0:1182:C:HO2'	30:0:1183:C:H5	1.64	0.44
30:0:2032:U:H2'	30:0:2033:G:C5'	2.47	0.44
13:M:58:GLN:HG3	38:M:8906:HOH:O	2.18	0.44
25:Y:144:ARG:NH2	38:Y:8907:HOH:O	2.51	0.44
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.44
30:0:451:C:O2'	30:0:452:G:H5'	2.18	0.44
30:0:453:A:H4'	30:0:455:A:N7	2.32	0.44
30:0:2385:G:H2'	30:0:2386:U:C6	2.52	0.44
30:0:2464:C:H5"	30:0:2465:A:OP1	2.17	0.44
30:0:2473:U:O3'	30:0:2474:A:H3'	2.17	0.44
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.47	0.44
16:P:120:ARG:NH2	16:P:123:TYR:CD2	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:185:G:H4'	30:0:186:A:H4'	1.99	0.44
30:0:558:C:HO2'	30:0:559:U:H5"	1.80	0.44
30:0:815:U:O2'	30:0:1598:A:H4'	2.17	0.44
30:0:825:U:H5"	30:0:826:U:OP1	2.18	0.44
30:0:947:U:O2'	30:0:948:G:H5'	2.16	0.44
30:0:1342:C:C2'	30:0:1343:C:H5'	2.47	0.44
30:0:1973:A:H2'	30:0:1974:G:O4'	2.18	0.44
30:0:2635:A:C2'	30:0:2636:C:H5'	2.46	0.44
2:B:74:ILE:HG13	38:B:9080:HOH:O	2.17	0.44
4:D:53:LYS:HE3	31:9:40:C:H42	1.82	0.44
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.17	0.44
13:M:46:LEU:HG	38:M:8922:HOH:O	2.18	0.44
28:2:2:LYS:HG3	30:0:1486:A:C5	2.52	0.44
30:0:77:G:H2'	30:0:78:G:H5'	1.99	0.44
30:0:218:C:C5	30:0:220:C:C4	3.06	0.44
30:0:816:G:H5'	30:0:1598:A:H4'	1.99	0.44
30:0:1427:A:H61	30:0:1440:U:C1'	2.30	0.44
30:0:1592:G:C4	30:0:1593:C:C5	3.06	0.44
30:0:1592:G:O2'	30:0:1593:C:O5'	2.35	0.44
30:0:2276:U:H2'	30:0:2277:U:C6	2.53	0.44
30:0:2636:C:H4'	38:0:6666:HOH:O	2.18	0.44
31:9:76:G:H3'	31:9:77:A:C5'	2.31	0.44
2:B:79:MET:HE1	38:B:9100:HOH:O	2.17	0.44
14:N:11:ARG:NH1	31:9:8:G:O6	2.50	0.44
16:P:91:LYS:O	16:P:95:GLU:HG3	2.17	0.44
30:0:204:A:C2'	30:0:205:U:H5'	2.47	0.44
30:0:764:C:H2'	30:0:765:G:O4'	2.17	0.44
30:0:794:U:C2'	30:0:795:G:H5'	2.48	0.44
30:0:1603:A:C5'	30:0:1605:G:C5'	2.94	0.44
30:0:1878:G:O2'	30:0:1879:U:OP2	2.36	0.44
1:A:204:GLY:N	30:0:2634:G:OP2	2.48	0.44
2:B:280:VAL:HG13	2:B:333:GLU:O	2.17	0.44
4:D:131:THR:HG21	30:0:2348:C:H1'	1.99	0.44
4:D:135:VAL:HG22	4:D:136:ARG:H	1.82	0.44
5:E:6:GLU:HG2	5:E:46:THR:HG22	1.99	0.44
6:F:60:VAL:HG13	6:F:63:ILE:HG13	1.99	0.44
8:H:30:LYS:H	8:H:62:HIS:HD2	1.65	0.44
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.83	0.44
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.53	0.44
30:0:441:A:H8	30:0:441:A:O5'	1.99	0.44
30:0:497:A:H2'	30:0:498:A:C5'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:807:A:O2'	30:0:808:A:H5'	2.17	0.44
30:0:1006:A:N1	30:0:2311:A:H1'	2.33	0.44
30:0:1044:C:H5"	38:0:9028:HOH:O	2.18	0.44
30:0:2461:U:O2	30:0:2466:G:H1'	2.18	0.44
30:0:2511:A:H2'	30:0:2512:U:O4'	2.17	0.44
30:0:2565:C:H4'	38:0:4868:HOH:O	2.18	0.44
31:9:107:C:O2'	31:9:108:C:H5'	2.18	0.44
1:A:76:VAL:HG23	26:Z:87:LYS:HB3	2.00	0.44
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.66	0.44
11:K:89:LYS:HE2	21:U:19:THR:HG21	2.00	0.44
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.49	0.44
21:U:49:LEU:HG	38:U:3805:HOH:O	2.17	0.44
30:0:66:G:C2	30:0:109:U:C4	3.06	0.44
30:0:88:G:H2'	30:0:89:G:H8	1.83	0.44
30:0:383:A:H2'	30:0:384:G:O4'	2.18	0.44
30:0:629:A:C2	30:0:2074:A:C2	3.06	0.44
30:0:1066:U:H2'	30:0:1067:A:C8	2.52	0.44
30:0:1189:A:H1'	30:0:1209:C:H1'	1.99	0.44
30:0:1375:A:C2'	30:0:1376:G:H5'	2.47	0.44
30:0:1588:G:C5	30:0:1589:G:C6	3.06	0.44
30:0:1903:U:O2'	30:0:1904:A:N7	2.50	0.44
30:0:2015:A:H2'	30:0:2016:U:O4'	2.18	0.44
30:0:2238:A:O2'	30:0:2239:C:H5'	2.18	0.44
30:0:2506:A:O2'	30:0:2507:G:O5'	2.36	0.44
30:0:2569:A:H2'	30:0:2570:G:O5'	2.18	0.44
1:A:190:ARG:HH11	30:0:1845:A:P	2.41	0.43
2:B:53:LEU:HD11	2:B:327:VAL:HG22	1.99	0.43
3:C:170:ASP:OD2	30:0:330:C:H5	2.01	0.43
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.99	0.43
10:J:70:PHE:HD1	30:0:2676:C:O2'	2.00	0.43
14:N:37:ARG:HH12	31:9:6:C:C5'	2.21	0.43
14:N:37:ARG:NE	38:N:8831:HOH:O	2.51	0.43
16:P:73:HIS:HE1	30:0:1789:G:O6	2.01	0.43
17:Q:19:ARG:HH21	31:9:11:A:P	2.41	0.43
30:0:177:A:O2'	30:0:892:G:H4'	2.17	0.43
30:0:499:G:O2'	30:0:500:G:H5'	2.16	0.43
30:0:594:C:C4	30:0:595:U:C4	3.06	0.43
30:0:1632:A:H2'	30:0:1633:C:C5'	2.42	0.43
30:0:2842:G:H2'	30:0:2843:A:H5'	2.00	0.43
31:9:55:U:H4'	31:9:56:A:H8	1.83	0.43
2:B:10:SER:HB2	30:0:2714:U:H4'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.51	0.43
13:M:134:ILE:O	13:M:136:PRO:HD3	2.19	0.43
14:N:50:LEU:HD12	14:N:50:LEU:HA	1.86	0.43
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.53	0.43
29:3:91:GLN:O	29:3:92:GLU:HB2	2.18	0.43
30:0:963:C:O2	30:0:1005:A:N1	2.51	0.43
30:0:1119:G:N2	30:0:1246:A:H2	2.13	0.43
31:9:31:C:H2'	31:9:32:G:O4'	2.18	0.43
31:9:114:G:H2'	31:9:115:C:H6	1.81	0.43
1:A:1:GLY:HA2	1:A:197:VAL:HG23	1.99	0.43
1:A:95:PRO:O	1:A:99:ILE:HG12	2.19	0.43
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.84	0.43
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.16	0.43
18:R:40:ALA:O	18:R:44:VAL:HG23	2.18	0.43
28:2:16:ASN:HB2	38:2:5203:HOH:O	2.17	0.43
30:0:271:C:C2	30:0:273:G:O4'	2.70	0.43
30:0:1056:U:H2'	30:0:1057:A:O4'	2.18	0.43
30:0:1156:C:O5'	30:0:1156:C:H6	2.01	0.43
30:0:1517:C:O2	30:0:1670:A:C2	2.71	0.43
30:0:1565:C:H2'	30:0:1566:C:H6	1.83	0.43
30:0:2870:C:O2'	30:0:2871:G:H5'	2.19	0.43
31:9:3:A:C2	31:9:21:G:N3	2.85	0.43
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.43
3:C:61:PHE:HB3	38:C:8639:HOH:O	2.18	0.43
7:G:12:ILE:HG12	38:0:5490:HOH:O	2.19	0.43
30:0:17:G:H2'	30:0:18:C:C6	2.53	0.43
30:0:212:A:O4'	30:0:214:U:C6	2.72	0.43
30:0:294:C:H2'	30:0:295:C:O4'	2.18	0.43
30:0:559:U:H2'	30:0:560:U:O4'	2.18	0.43
30:0:677:C:O2'	30:0:678:G:H5'	2.18	0.43
30:0:960:G:C3'	30:0:960:G:C4	3.01	0.43
30:0:1434:A:H2'	30:0:1436:C:C5	2.53	0.43
30:0:1456:C:H2'	30:0:1457:U:C6	2.54	0.43
30:0:1789:G:H2'	30:0:1790:C:O5'	2.18	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.96	0.43
2:B:305:ASP:O	2:B:306:LYS:HB2	2.19	0.43
3:C:242:GLU:HB2	38:C:8577:HOH:O	2.17	0.43
11:K:8:VAL:HG13	11:K:80:ILE:HG22	2.00	0.43
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.89	0.43
22:V:1:THR:HG23	22:V:2:VAL:N	2.30	0.43
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:41:HIS:CD2	28:2:44:ARG:H	2.26	0.43
30:0:365:G:C6	30:0:366:U:C4	3.06	0.43
30:0:424:C:H2'	30:0:425:U:C6	2.53	0.43
30:0:951:A:C2'	30:0:952:G:H5'	2.48	0.43
30:0:1946:C:H2'	30:0:1971:G:C8	2.53	0.43
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.82	0.43
30:0:35:U:H2'	30:0:36:C:C6	2.53	0.43
30:0:226:A:H1'	30:0:393:G:C5	2.54	0.43
31:9:42:C:H5'	31:9:43:G:OP2	2.19	0.43
31:9:58:G:H3'	31:9:59:C:C6	2.54	0.43
1:A:94:LEU:HG	1:A:99:ILE:HD13	2.01	0.43
6:F:59:ILE:CD1	30:0:263:U:C2	3.01	0.43
8:H:64:SER:OG	30:0:2520:G:H5'	2.17	0.43
30:0:130:C:H5'	38:0:5243:HOH:O	2.19	0.43
30:0:512:G:O3'	30:0:513:A:C8	2.71	0.43
30:0:794:U:H2'	30:0:795:G:H5'	2.01	0.43
30:0:794:U:H3	30:0:819:A:H61	1.65	0.43
30:0:844:A:C6	30:0:882:A:C5	3.06	0.43
30:0:1764:C:H2'	30:0:1765:G:O4'	2.18	0.43
30:0:1970:G:H2'	30:0:1970:G:N3	2.33	0.43
30:0:1992:U:H2'	30:0:1994:A:OP2	2.18	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.34	0.43
30:0:2523:U:O2'	30:0:2524:G:H5'	2.19	0.43
3:C:98:ARG:NH1	38:C:8554:HOH:O	2.51	0.43
6:F:59:ILE:HD13	30:0:263:U:O4'	2.19	0.43
6:F:99:THR:HG23	6:F:99:THR:O	2.19	0.43
11:K:130:MET:SD	21:U:25:ASP:O	2.77	0.43
19:S:57:THR:HG22	19:S:58:MET:N	2.33	0.43
22:V:55:ARG:O	22:V:59:ILE:HG12	2.19	0.43
30:0:1250:C:O2'	30:0:1251:C:H5'	2.19	0.43
30:0:1589:G:N2	30:0:1605:G:H1'	2.34	0.43
30:0:2387:U:H2'	30:0:2388:C:C6	2.54	0.43
3:C:151:GLN:HG3	30:0:327:A:OP2	2.19	0.43
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.19	0.43
10:J:36:VAL:HG12	10:J:37:ALA:N	2.34	0.43
11:K:64:MET:HA	11:K:67:GLN:HE21	1.84	0.43
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.49	0.43
16:P:40:VAL:O	16:P:44:VAL:HG23	2.19	0.43
21:U:49:LEU:O	21:U:52:THR:HG22	2.17	0.43
25:Y:133:HIS:HD2	38:Y:8877:HOH:O	2.02	0.43
25:Y:168:PHE:CE2	30:0:1090:A:H4'	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:537:G:O4'	30:0:538:C:C5	2.71	0.43
30:0:941:G:C6	30:0:942:U:C4	3.07	0.43
30:0:1245:C:O5'	30:0:1245:C:H6	2.02	0.43
30:0:1421:C:O2'	30:0:1422:U:H5'	2.18	0.43
30:0:1616:A:H5"	30:0:1617:C:OP1	2.19	0.43
31:9:59:C:H2'	31:9:60:C:C6	2.54	0.43
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.90	0.43
4:D:99:ASP:HB3	4:D:103:ASN:H	1.84	0.43
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.43
14:N:38:LYS:HB2	14:N:38:LYS:HE3	1.77	0.43
18:R:109:MET:HG2	18:R:148:GLU:C	2.40	0.43
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.19	0.43
27:1:25:LYS:O	27:1:25:LYS:HG2	2.19	0.43
30:0:488:U:H2'	38:0:4031:HOH:O	2.18	0.43
30:0:1032:A:H2'	30:0:1032:A:N3	2.33	0.43
30:0:1160:G:H5'	30:0:1161:A:C4'	2.46	0.43
30:0:1187:U:O2'	30:0:1189:A:H2	1.85	0.43
30:0:1555:G:O2'	30:0:1556:G:H5'	2.19	0.43
30:0:1644:C:C2	30:0:1645:U:C6	3.07	0.43
30:0:1996:U:O2'	30:0:1997:A:H5'	2.18	0.43
30:0:2524:G:N2	30:0:2526:C:H41	2.17	0.43
31:9:52:A:O2'	31:9:53:G:H5'	2.19	0.43
2:B:5:ARG:NH1	2:B:8:LYS:HE2	2.34	0.42
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.34	0.42
9:I:86:GLU:HG2	30:0:1180:U:H4'	2.01	0.42
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.18	0.42
30:0:39:G:N2	30:0:444:C:C2	2.87	0.42
30:0:332:G:O2'	30:0:333:G:H5'	2.19	0.42
30:0:1202:A:H2'	30:0:1203:G:C5'	2.48	0.42
30:0:1788:U:C2	30:0:1805:G:N2	2.87	0.42
30:0:2252:A:C6	30:0:2253:G:H1'	2.53	0.42
30:0:2435:U:H1'	38:0:5462:HOH:O	2.19	0.42
31:9:45:A:H2'	31:9:46:C:C6	2.54	0.42
1:A:99:ILE:O	1:A:131:HIS:CE1	2.72	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.18	0.42
3:C:25:PRO:HG2	38:C:8520:HOH:O	2.18	0.42
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.20	0.42
18:R:113:HIS:HE1	18:R:144:GLU:CD	2.22	0.42
30:0:1015:C:O5'	30:0:1015:C:H6	2.02	0.42
30:0:1761:U:H2'	30:0:1762:C:C6	2.54	0.42
31:9:2:U:OP2	31:9:2:U:H4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:2:U:C4'	38:9:9103:HOH:O	2.67	0.42
31:9:14:G:H2'	31:9:15:C:H5'	2.01	0.42
31:9:72:C:O2'	31:9:73:A:H5'	2.19	0.42
1:A:179:MET:HG2	1:A:186:TRP:CG	2.55	0.42
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.51	0.42
8:H:31:ILE:HG23	38:H:231:HOH:O	2.18	0.42
12:L:67:ARG:O	12:L:71:GLU:HG3	2.20	0.42
38:Q:2875:HOH:O	30:0:2392:C:H4'	2.20	0.42
29:3:3:MET:HG3	29:3:4:PRO:HD2	2.01	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.46	0.42
30:0:1634:G:C6	30:0:1635:U:C4	3.07	0.42
30:0:1762:C:H2'	30:0:1763:C:C6	2.54	0.42
30:0:2004:U:H2'	30:0:2005:G:OP1	2.19	0.42
30:0:2423:C:H2'	30:0:2424:U:C6	2.54	0.42
30:0:2819:C:H2'	30:0:2820:A:C8	2.54	0.42
1:A:179:MET:HG2	1:A:186:TRP:CB	2.49	0.42
2:B:178:ALA:O	2:B:182:VAL:HG23	2.20	0.42
6:F:118:LEU:O	6:F:119:ARG:HB3	2.19	0.42
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.84	0.42
9:I:111:LEU:HD23	30:0:1163:G:H4'	2.01	0.42
16:P:59:ARG:NH2	16:P:66:GLN:HE22	2.10	0.42
23:W:43:GLY:HA3	30:0:945:U:O2'	2.19	0.42
24:X:15:ARG:HH22	30:0:2856:A:P	2.42	0.42
30:0:254:C:O2	30:0:254:C:H2'	2.19	0.42
30:0:1175:G:H1'	30:0:1193:A:H2'	2.02	0.42
30:0:1416:G:C2'	30:0:1417:G:H5'	2.49	0.42
30:0:1561:U:O2	30:0:1561:U:H2'	2.18	0.42
30:0:2104:C:O2	30:0:2485:A:N1	2.53	0.42
10:J:93:ARG:HB3	10:J:93:ARG:HH11	1.83	0.42
20:T:32:ARG:NH1	20:T:38:ARG:HH12	2.17	0.42
23:W:13:MET:CE	23:W:17:ILE:HG22	2.49	0.42
23:W:80:ASP:HB2	38:W:3312:HOH:O	2.18	0.42
30:0:344:C:H2'	30:0:345:G:O4'	2.20	0.42
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.42
30:0:2134:G:N2	30:0:2242:U:C2	2.87	0.42
30:0:2414:A:N1	30:0:2415:A:C6	2.88	0.42
30:0:2719:A:H5"	38:0:3702:HOH:O	2.19	0.42
2:B:14:GLY:HA2	2:B:15:PRO:C	2.39	0.42
4:D:23:VAL:HG11	4:D:83:PHE:CZ	2.55	0.42
14:N:34:LEU:HD22	14:N:129:ILE:HD13	2.01	0.42
21:U:17:THR:CG2	21:U:18:GLY:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:243:A:H61	30:0:269:G:H1'	1.84	0.42
30:0:284:C:H4'	30:0:285:A:H8	1.84	0.42
30:0:544:G:C3'	30:0:545:G:H5"	2.48	0.42
30:0:603:A:H4'	30:0:604:G:O5'	2.20	0.42
30:0:843:A:C2	30:0:846:A:C8	3.08	0.42
30:0:1206:U:C6	30:0:1206:U:C3'	3.02	0.42
30:0:1211:G:O2'	30:0:1212:C:H5'	2.19	0.42
30:0:1451:C:H5'	30:0:1505:U:C4	2.54	0.42
30:0:1987:C:H2'	30:0:1988:C:H6	1.85	0.42
30:0:2134:G:C6	30:0:2258:A:C8	3.08	0.42
30:0:2361:A:H2'	30:0:2362:A:O4'	2.19	0.42
30:0:2578:G:H5'	30:0:2578:G:C8	2.44	0.42
30:0:2754:G:C2'	30:0:2755:G:H5'	2.49	0.42
31:9:14:G:H2'	31:9:15:C:C5'	2.50	0.42
2:B:314:ALA:CB	2:B:317:PRO:HG3	2.50	0.42
14:N:25:ARG:HB3	30:0:2415:A:C2	2.54	0.42
23:W:7:LEU:HD12	23:W:53:ALA:HB2	2.00	0.42
26:Z:45:VAL:HG12	38:Z:8713:HOH:O	2.19	0.42
30:0:369:G:C2	30:0:370:G:C8	3.08	0.42
30:0:466:A:H2'	30:0:467:G:O4'	2.20	0.42
30:0:1307:A:H2'	30:0:1308:A:C8	2.55	0.42
30:0:2505:G:H2'	30:0:2506:A:C5'	2.50	0.42
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.85	0.42
3:C:85:LYS:HA	3:C:85:LYS:HD2	1.90	0.42
4:D:170:TYR:CD1	4:D:170:TYR:N	2.87	0.42
8:H:4:LYS:HA	8:H:5:PRO:HD3	1.86	0.42
8:H:87:LYS:NZ	8:H:87:LYS:HB2	2.35	0.42
13:M:124:GLY:HA3	30:0:2132:C:H1'	2.02	0.42
15:O:96:VAL:HG12	15:O:97:SER:O	2.20	0.42
18:R:69:LYS:HB2	18:R:72:VAL:HG23	2.01	0.42
22:V:12:THR:HG22	22:V:15:GLU:CG	2.47	0.42
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.30	0.42
24:X:37:LEU:O	24:X:41:PHE:HB2	2.19	0.42
30:0:539:G:H2'	30:0:540:A:C8	2.54	0.42
30:0:790:A:H8	38:0:6134:HOH:O	2.01	0.42
30:0:1023:C:H2'	30:0:1024:G:O4'	2.20	0.42
30:0:1244:U:H4'	30:0:1246:A:O4'	2.20	0.42
30:0:1298:U:H2'	30:0:1299:G:C8	2.54	0.42
30:0:1782:G:O2'	30:0:1783:A:H5'	2.19	0.42
30:0:2252:A:C2'	30:0:2253:G:H5'	2.49	0.42
30:0:2756:U:C2	30:0:2896:A:H2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2909:G:H2'	30:0:2910:A:H8	1.84	0.42
1:A:23:TYR:HD1	30:0:1872:C:H2'	1.85	0.42
1:A:94:LEU:HD23	1:A:94:LEU:N	2.34	0.42
2:B:27:ASN:HD22	2:B:27:ASN:H	1.67	0.42
14:N:159:TYR:HE1	31:9:50:G:H5"	1.85	0.42
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.19	0.42
19:S:56:ASN:O	28:2:8:LYS:NZ	2.51	0.42
24:X:8:ARG:NH1	30:0:2904:U:H4'	2.35	0.42
24:X:37:LEU:HD21	24:X:72:VAL:HG11	2.02	0.42
30:0:417:G:P	38:0:7457:HOH:O	2.77	0.42
30:0:1198:U:H1'	30:0:1201:C:C5	2.50	0.42
30:0:1433:G:O2'	30:0:1434:A:H5'	2.20	0.42
30:0:1676:G:C2'	30:0:1677:U:H5'	2.50	0.42
30:0:2783:A:O2'	30:0:2784:A:H5'	2.19	0.42
1:A:54:PRO:HG2	1:A:160:ALA:HB3	2.02	0.42
1:A:107:ASN:OD1	1:A:116:GLY:HA3	2.20	0.42
1:A:211:LYS:HB2	38:A:9075:HOH:O	2.19	0.42
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.85	0.42
2:B:243:ASN:HA	2:B:244:PRO:C	2.40	0.42
3:C:5:ILE:HD11	3:C:16:VAL:HG23	2.01	0.42
10:J:45:VAL:HG11	10:J:121:LEU:HD22	2.02	0.42
18:R:29:LYS:NZ	38:R:8944:HOH:O	2.53	0.42
30:0:128:A:C8	30:0:128:A:C3'	3.03	0.42
30:0:1334:C:H2'	30:0:1335:C:H6	1.85	0.42
30:0:2509:A:OP2	30:0:2510:C:C5	2.72	0.42
30:0:2712:G:P	38:0:5251:HOH:O	2.77	0.42
30:0:2718:C:H5'	30:0:2718:C:C6	2.53	0.42
30:0:2908:A:C2'	30:0:2909:G:H5'	2.49	0.42
4:D:105:SER:OG	30:0:2338:G:H1'	2.20	0.41
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.20	0.41
6:F:39:SER:HB3	6:F:45:ALA:HB2	2.02	0.41
10:J:131:THR:HG22	10:J:134:GLU:H	1.85	0.41
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.17	0.41
14:N:147:ILE:HB	38:9:9090:HOH:O	2.19	0.41
25:Y:154:ARG:HH22	30:0:1071:G:H4'	1.85	0.41
29:3:18:GLN:HG3	38:3:9009:HOH:O	2.20	0.41
30:0:129:A:O2'	30:0:131:A:OP1	2.36	0.41
30:0:259:G:O2'	30:0:260:C:H5'	2.20	0.41
30:0:821:U:H2'	30:0:822:C:H6	1.84	0.41
30:0:883:U:O2	30:0:883:U:C2'	2.67	0.41
30:0:960:G:H2'	30:0:961:A:OP2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1335:C:H2'	30:0:1336:U:C6	2.55	0.41
30:0:1406:A:H4'	30:0:1407:A:C5'	2.50	0.41
30:0:1562:C:N4	38:0:5895:HOH:O	2.53	0.41
30:0:1789:G:C2'	30:0:1790:C:O5'	2.68	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.20	0.41
30:0:2727:A:C6	30:0:2756:U:C2	3.08	0.41
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.51	0.41
2:B:40:GLY:O	2:B:193:ILE:HD13	2.20	0.41
3:C:193:LEU:HD12	3:C:211:ASP:O	2.20	0.41
4:D:22:VAL:HG22	4:D:74:THR:HG22	2.00	0.41
4:D:37:ALA:O	4:D:40:ILE:HG12	2.20	0.41
12:L:150:GLN:HB3	38:L:8868:HOH:O	2.20	0.41
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.44	0.41
19:S:11:THR:H	19:S:14:ALA:HB3	1.84	0.41
25:Y:142:SER:OG	30:0:1331:G:OP2	2.34	0.41
30:0:64:G:H2'	30:0:65:C:O4'	2.20	0.41
30:0:420:U:H2'	30:0:421:C:C6	2.55	0.41
30:0:1052:G:C5	30:0:1063:G:C6	3.09	0.41
31:9:47:A:H2'	31:9:48:C:O4'	2.20	0.41
2:B:75:GLU:C	2:B:77:PRO:HD3	2.40	0.41
2:B:248:ARG:NH1	38:B:9090:HOH:O	2.53	0.41
4:D:141:VAL:HG21	31:9:57:A:H8	1.85	0.41
9:I:69:PRO:HA	30:0:1164:U:OP1	2.21	0.41
14:N:37:ARG:HD3	33:N:8807:CL:CL	2.57	0.41
27:1:45:ARG:HB3	38:1:988:HOH:O	2.20	0.41
28:2:41:HIS:CD2	28:2:43:ARG:H	2.39	0.41
30:0:506:G:N2	30:0:509:A:H5"	2.32	0.41
30:0:1167:G:C2	30:0:1168:C:C2	3.08	0.41
30:0:1185:U:H5'	38:0:7504:HOH:O	2.20	0.41
30:0:1840:A:H4'	30:0:1841:C:O5'	2.20	0.41
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.41
9:I:101:LYS:O	9:I:105:GLU:HG3	2.21	0.41
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.01	0.41
28:2:41:HIS:N	28:2:45:ASN:HD22	2.03	0.41
30:0:151:A:C2	30:0:442:A:C8	3.09	0.41
30:0:635:A:H2'	30:0:636:G:H5"	2.02	0.41
30:0:729:C:C2	30:0:743:G:C2	3.08	0.41
30:0:1422:U:O2'	30:0:1423:C:H5'	2.20	0.41
30:0:1474:C:C6	30:0:1474:C:C5'	2.89	0.41
30:0:1909:A:H2'	30:0:1910:A:C8	2.54	0.41
31:9:45:A:C5	31:9:46:C:C5	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:O	1:A:38:ILE:N	2.53	0.41
3:C:223:LEU:HD12	3:C:223:LEU:HA	1.91	0.41
16:P:7:LYS:HG2	16:P:23:PHE:CE2	2.55	0.41
24:X:39:LYS:HE2	30:0:2834:G:OP1	2.20	0.41
28:2:37:HIS:CE1	30:0:462:A:C8	3.08	0.41
30:0:834:G:H3'	30:0:835:U:H4'	2.01	0.41
30:0:1138:G:H4'	38:0:5739:HOH:O	2.18	0.41
30:0:1342:C:O2'	30:0:1343:C:H5'	2.20	0.41
30:0:1667:A:C2	30:0:1668:U:C2	3.08	0.41
30:0:1903:U:O2'	30:0:1904:A:C8	2.68	0.41
30:0:2421:G:H4'	38:0:4814:HOH:O	2.20	0.41
30:0:2704:C:H2'	30:0:2705:U:O4'	2.20	0.41
2:B:215:VAL:HA	2:B:220:VAL:HG22	2.02	0.41
3:C:154:VAL:O	3:C:158:GLU:HG3	2.21	0.41
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.20	0.41
10:J:52:GLN:HE22	30:0:1119:G:H8	1.69	0.41
16:P:59:ARG:O	16:P:63:ARG:HG3	2.21	0.41
19:S:57:THR:C	19:S:59:ASP:H	2.24	0.41
24:X:43:VAL:HG11	24:X:82:GLU:HA	2.01	0.41
29:3:38:ARG:HD2	30:0:396:U:OP2	2.21	0.41
30:0:243:A:H61	30:0:269:G:C1'	2.34	0.41
30:0:290:C:H1'	38:0:6136:HOH:O	2.21	0.41
30:0:318:U:H5'	30:0:339:A:C2	2.56	0.41
30:0:482:G:H4'	30:0:508:A:N1	2.36	0.41
30:0:2102:G:C2	30:0:2104:C:C4	3.08	0.41
30:0:2361:A:H5'	30:0:2361:A:H8	1.86	0.41
30:0:2419:U:H5"	30:0:2420:G:C5'	2.50	0.41
30:0:2637:A:C5'	38:0:4961:HOH:O	2.59	0.41
30:0:2791:U:H4'	30:0:2792:A:OP1	2.20	0.41
30:0:2802:C:H2'	30:0:2803:C:C6	2.55	0.41
1:A:212:PRO:HB2	38:0:4392:HOH:O	2.20	0.41
1:A:217:ARG:HG2	1:A:229:ALA:HB2	2.03	0.41
2:B:280:VAL:CG1	2:B:334:SER:HA	2.50	0.41
13:M:67:VAL:HB	13:M:97:ILE:HG23	2.03	0.41
16:P:94:TRP:CZ2	16:P:98:ILE:HG13	2.56	0.41
25:Y:213:LYS:HE3	25:Y:213:LYS:HB2	1.90	0.41
27:1:5:THR:HG23	30:0:1688:G:O2'	2.20	0.41
29:3:69:TYR:CZ	29:3:80:ARG:HD2	2.56	0.41
30:0:290:C:O2'	30:0:291:C:H5'	2.20	0.41
30:0:559:U:H5'	30:0:559:U:C6	2.35	0.41
30:0:1377:C:H6	30:0:1377:C:C5'	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1481:G:H2'	30:0:1482:A:O4'	2.20	0.41
30:0:1548:U:H1'	38:0:6897:HOH:O	2.19	0.41
30:0:2089:A:C2'	30:0:2090:G:H5'	2.49	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.20	0.41
1:A:95:PRO:HA	1:A:153:ARG:HA	2.03	0.41
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.48	0.41
11:K:30:LYS:HB3	11:K:56:SER:HB3	2.03	0.41
13:M:167:GLY:O	13:M:171:ARG:HG3	2.21	0.41
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.21	0.41
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.56	0.41
14:N:160:SER:CB	31:9:51:A:H5'	2.50	0.41
15:O:98:LEU:O	15:O:102:ILE:HG13	2.21	0.41
16:P:83:LYS:O	16:P:86:ALA:HB3	2.21	0.41
18:R:17:MET:SD	38:R:8951:HOH:O	2.62	0.41
22:V:27:LEU:HA	22:V:49:LEU:HD13	2.02	0.41
23:W:48:VAL:HG12	23:W:48:VAL:O	2.19	0.41
30:0:81:G:N3	30:0:98:A:C2	2.88	0.41
30:0:667:C:H2'	30:0:668:C:H6	1.85	0.41
30:0:1544:U:O2'	30:0:1545:C:H5'	2.20	0.41
30:0:1714:C:C2'	30:0:1715:C:H5'	2.51	0.41
30:0:1804:A:H2'	30:0:1805:G:C8	2.56	0.41
30:0:2617:G:C2	30:0:2618:G:C8	3.08	0.41
30:0:2802:C:H2'	30:0:2803:C:H6	1.84	0.41
31:9:13:A:OP1	31:9:113:C:H5'	2.21	0.41
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.85	0.41
2:B:154:VAL:CG1	2:B:156:LYS:HG2	2.51	0.41
3:C:76:ARG:HB3	3:C:76:ARG:NH1	2.36	0.41
4:D:25:MET:HE1	4:D:37:ALA:O	2.21	0.41
38:K:7438:HOH:O	21:U:20:MET:HE2	2.21	0.41
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.49	0.41
13:M:164:THR:CG2	13:M:165:GLY:N	2.83	0.41
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.51	0.41
38:N:8830:HOH:O	30:0:2368:A:H8	2.04	0.41
15:O:115:ARG:NH1	38:O:6194:HOH:O	2.54	0.41
20:T:79:LEU:HG	20:T:89:ARG:HB2	2.03	0.41
22:V:39:ALA:C	22:V:41:GLU:H	2.23	0.41
26:Z:50:VAL:O	26:Z:54:GLU:HG3	2.20	0.41
30:0:23:G:C6	30:0:24:G:N1	2.89	0.41
30:0:130:C:H2'	38:0:3183:HOH:O	2.20	0.41
30:0:969:G:H2'	30:0:970:U:C6	2.56	0.41
30:0:1166:A:N3	30:0:1166:A:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1184:C:O2'	30:0:1185:U:OP2	2.36	0.41
30:0:1634:G:C5	30:0:1635:U:C4	3.08	0.41
30:0:1909:A:N1	30:0:2128:G:H1'	2.35	0.41
30:0:1945:G:O2'	30:0:1946:C:H5'	2.20	0.41
30:0:2039:A:H2'	30:0:2040:C:C6	2.56	0.41
30:0:2246:U:N3	30:0:2256:G:C2	2.89	0.41
31:9:34:A:H2'	31:9:35:C:O4'	2.21	0.41
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.02	0.41
29:3:70:ARG:HD3	38:3:9064:HOH:O	2.21	0.41
30:0:595:U:O2'	30:0:596:C:H5'	2.21	0.41
30:0:1119:G:N2	30:0:1246:A:N1	2.69	0.41
30:0:1163:G:N2	38:0:6078:HOH:O	2.54	0.41
30:0:1271:A:C2	30:0:1286:A:C2	3.09	0.41
30:0:1522:A:C2'	30:0:1523:G:H5'	2.51	0.41
30:0:1574:C:O5'	30:0:1574:C:H6	2.04	0.41
30:0:1613:C:H2'	30:0:1614:G:O4'	2.21	0.41
30:0:2072:G:N2	38:0:6910:HOH:O	2.54	0.41
30:0:2251:G:C6	30:0:2252:A:C6	3.09	0.41
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.86	0.40
2:B:154:VAL:HG12	2:B:156:LYS:HG2	2.02	0.40
4:D:25:MET:HE3	4:D:37:ALA:HB1	2.04	0.40
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.03	0.40
25:Y:106:THR:HG23	25:Y:107:PRO:HD2	2.03	0.40
25:Y:189:ASN:ND2	25:Y:192:ASP:H	2.19	0.40
30:0:106:A:H2'	30:0:107:U:O4'	2.21	0.40
30:0:369:G:O2'	30:0:370:G:H5'	2.21	0.40
30:0:401:C:H2'	30:0:402:U:C6	2.56	0.40
30:0:745:G:H5"	30:0:746:A:OP1	2.21	0.40
30:0:1098:A:H2'	30:0:1099:G:O4'	2.21	0.40
30:0:1182:C:O2'	30:0:1183:C:H5	2.04	0.40
30:0:1515:A:H2'	30:0:1516:U:H6	1.82	0.40
30:0:1520:G:C6	30:0:1521:C:C4	3.09	0.40
30:0:1536:C:H6	30:0:1536:C:O5'	2.03	0.40
30:0:1750:C:N4	30:0:1751:G:C6	2.89	0.40
30:0:1758:U:H2'	30:0:1759:A:O4'	2.22	0.40
30:0:2332:A:C2	30:0:2355:G:C5	3.09	0.40
30:0:2334:C:O2'	30:0:2335:C:H5'	2.21	0.40
31:9:64:C:O2'	31:9:65:A:H5'	2.21	0.40
2:B:234:ARG:HD3	30:0:1734:C:OP1	2.21	0.40
12:L:143:THR:HG21	38:L:8837:HOH:O	2.21	0.40
14:N:154:LEU:C	14:N:156:GLU:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:74:G:H2'	30:0:75:U:C6	2.56	0.40
30:0:278:A:C6	30:0:279:C:C4	3.09	0.40
30:0:1192:A:H3'	30:0:1193:A:H5'	2.02	0.40
30:0:1327:G:N1	30:0:1330:A:OP2	2.52	0.40
30:0:1377:C:H2'	30:0:1723:G:O6	2.21	0.40
30:0:1617:C:C4	30:0:1643:C:H4'	2.56	0.40
30:0:1700:C:H5"	30:0:1701:A:OP2	2.22	0.40
30:0:1947:G:C8	30:0:1970:G:C8	3.09	0.40
30:0:2253:G:C2	30:0:2254:G:C8	3.09	0.40
30:0:2524:G:H21	30:0:2526:C:H41	1.67	0.40
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.80	0.40
8:H:76:LEU:HD21	8:H:149:VAL:HA	2.02	0.40
8:H:91:ARG:H	8:H:91:ARG:HG2	1.59	0.40
20:T:24:ARG:NH2	20:T:39:ASN:HD22	2.07	0.40
30:0:111:C:O2'	30:0:112:G:H5'	2.21	0.40
30:0:200:C:H6	38:0:3463:HOH:O	2.03	0.40
30:0:255:A:C5	30:0:256:C:C5	3.09	0.40
30:0:932:U:H2'	30:0:933:C:C6	2.57	0.40
30:0:1163:G:C4	30:0:1164:U:C5	3.09	0.40
30:0:1183:C:O2	30:0:1183:C:C2'	2.69	0.40
30:0:1409:G:C2	30:0:1410:G:C8	3.10	0.40
30:0:1896:G:H1'	38:0:4284:HOH:O	2.21	0.40
30:0:1947:G:N2	30:0:1966:U:C2	2.90	0.40
30:0:2626:C:H2'	30:0:2627:G:C8	2.56	0.40
30:0:2727:A:N1	30:0:2756:U:C2	2.90	0.40
30:0:2782:G:O6	30:0:2790:C:H5"	2.21	0.40
31:9:26:C:H2'	31:9:27:C:C6	2.57	0.40
1:A:86:ALA:HB3	1:A:94:LEU:HD22	2.03	0.40
2:B:202:VAL:HG11	2:B:301:VAL:HG13	2.04	0.40
3:C:107:ARG:HB3	3:C:107:ARG:NH1	2.37	0.40
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.95	0.40
23:W:90:TYR:CE2	23:W:99:ALA:HB2	2.56	0.40
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.37	0.40
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.21	0.40
30:0:445:U:H2'	30:0:446:G:C8	2.56	0.40
30:0:724:G:O2'	30:0:725:C:H5'	2.22	0.40
30:0:806:A:H2'	30:0:807:A:O4'	2.22	0.40
30:0:853:C:H2'	30:0:854:G:O4'	2.21	0.40
30:0:1149:U:C5	30:0:1215:A:C5	3.09	0.40
30:0:1414:A:H2'	30:0:1415:G:O4'	2.21	0.40
30:0:1503:U:H6	30:0:1503:U:H3'	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1741:U:C5'	30:0:1742:A:OP1	2.63	0.40
30:0:2112:A:H2'	30:0:2113:G:C8	2.56	0.40
30:0:2726:U:O2	30:0:2749:U:O5'	2.40	0.40
30:0:2842:G:C2'	30:0:2843:A:H5'	2.51	0.40
31:9:39:U:H3'	31:9:40:C:H5"	2.02	0.40
3:C:2:GLN:HB3	38:C:8530:HOH:O	2.21	0.40
3:C:16:VAL:HG12	3:C:17:ASP:N	2.36	0.40
3:C:118:THR:O	3:C:136:VAL:HG13	2.22	0.40
3:C:236:THR:HG22	3:C:239:ALA:CB	2.51	0.40
8:H:155:ARG:NH1	30:0:2503:A:H5"	2.36	0.40
20:T:82:THR:HG21	30:0:488:U:O2'	2.21	0.40
23:W:149:LEU:HG	23:W:153:MET:HE1	2.03	0.40
25:Y:144:ARG:NH1	38:Y:8871:HOH:O	2.53	0.40
28:2:5:LYS:O	28:2:9:LYS:HG3	2.22	0.40
30:0:47:G:N3	30:0:114:A:C2	2.90	0.40
30:0:138:U:OP2	30:0:139:C:C5	2.73	0.40
30:0:234:A:H4'	30:0:437:A:O4'	2.22	0.40
30:0:517:U:H1'	38:0:7614:HOH:O	2.21	0.40
30:0:907:A:H2'	30:0:908:A:H8	1.85	0.40
30:0:1705:C:H2'	30:0:1706:G:O4'	2.20	0.40
30:0:1878:G:H2'	38:0:3278:HOH:O	2.21	0.40
30:0:2016:U:O5'	30:0:2016:U:H6	2.05	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 X-ray entries followed by that with respect to entries of similar resolution.

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
1	A	235/240 (98%)	212 (90%)	18 (8%)	5 (2%)	7 18
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	17 40
3	C	244/246 (99%)	228 (93%)	16 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	6 17
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100 100
6	F	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	17 40
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100 100
8	H	156/177 (88%)	149 (96%)	6 (4%)	1 (1%)	25 50
9	I	68/162 (42%)	55 (81%)	10 (15%)	3 (4%)	2 5
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100 100
11	K	130/132 (98%)	125 (96%)	5 (4%)	0	100 100
12	L	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	22 46
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	29 54
14	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	9 24
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100 100
16	P	141/149 (95%)	141 (100%)	0	0	100 100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
18	R	148/155 (96%)	140 (95%)	8 (5%)	0	100 100
19	S	79/85 (93%)	78 (99%)	1 (1%)	0	100 100
20	T	117/120 (98%)	110 (94%)	6 (5%)	1 (1%)	17 40
21	U	51/67 (76%)	47 (92%)	4 (8%)	0	100 100
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	9 24
23	W	152/154 (99%)	148 (97%)	4 (3%)	0	100 100
24	X	80/92 (87%)	73 (91%)	6 (8%)	1 (1%)	12 30
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100 100
26	Z	71/116 (61%)	61 (86%)	8 (11%)	2 (3%)	5 11
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100 100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100 100
29	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	14 34
All	All	3705/4472 (83%)	3458 (93%)	220 (6%)	27 (1%)	22 46

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	VAL

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Mol	Chain	Res	Type
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
2	B	34	GLY
6	F	101	ALA
12	L	149	ARG
20	T	53	GLY
26	Z	66	CYS
2	B	185	GLY
4	D	27	ILE
4	D	137	PRO
8	H	19	ARG
2	B	2	GLN
22	V	43	PRO
1	A	36	ASP
4	D	56	ARG
9	I	108	HIS
29	3	56	PRO
26	Z	65	ASN
9	I	83	GLY
24	X	70	ILE
1	A	88	ILE
9	I	125	GLY
1	A	38	ILE
13	M	88	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
1	A	179/182 (98%)	171 (96%)	8 (4%)	27	55
2	B	282/283 (100%)	265 (94%)	17 (6%)	19	42
3	C	193/193 (100%)	178 (92%)	15 (8%)	12	29
4	D	117/148 (79%)	109 (93%)	8 (7%)	16	36
5	E	152/156 (97%)	147 (97%)	5 (3%)	38	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	93/94 (99%)	93 (100%)	0	100 100
7	G	27/282 (10%)	26 (96%)	1 (4%)	34 63
8	H	134/145 (92%)	127 (95%)	7 (5%)	23 49
9	I	58/130 (45%)	57 (98%)	1 (2%)	60 84
10	J	118/121 (98%)	112 (95%)	6 (5%)	24 50
11	K	106/106 (100%)	103 (97%)	3 (3%)	43 73
12	L	113/127 (89%)	111 (98%)	2 (2%)	59 83
13	M	158/160 (99%)	150 (95%)	8 (5%)	24 50
14	N	149/150 (99%)	144 (97%)	5 (3%)	37 66
15	O	93/94 (99%)	91 (98%)	2 (2%)	52 79
16	P	113/117 (97%)	108 (96%)	5 (4%)	28 56
17	Q	79/80 (99%)	77 (98%)	2 (2%)	47 76
18	R	117/122 (96%)	113 (97%)	4 (3%)	37 66
19	S	71/74 (96%)	70 (99%)	1 (1%)	67 86
20	T	105/106 (99%)	99 (94%)	6 (6%)	20 44
21	U	44/53 (83%)	43 (98%)	1 (2%)	50 78
22	V	51/57 (90%)	50 (98%)	1 (2%)	55 81
23	W	130/130 (100%)	126 (97%)	4 (3%)	40 69
24	X	66/74 (89%)	60 (91%)	6 (9%)	9 21
25	Y	120/196 (61%)	114 (95%)	6 (5%)	24 51
26	Z	60/94 (64%)	59 (98%)	1 (2%)	60 84
27	1	46/47 (98%)	46 (100%)	0	100 100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49 77
29	3	79/79 (100%)	77 (98%)	2 (2%)	47 76
All	All	3095/3646 (85%)	2967 (96%)	128 (4%)	30 59

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	38	ILE
1	A	68	ILE
1	A	69	LEU

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Mol	Chain	Res	Type
1	A	94	LEU
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	16	ARG
2	B	27	ASN
2	B	49	THR
2	B	56	ASP
2	B	97	LEU
2	B	98	THR
2	B	132	HIS
2	B	162	MET
2	B	184	ASP
2	B	190	MET
2	B	234	ARG
2	B	251	VAL
2	B	254	GLN
2	B	257	THR
2	B	312	ARG
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	115	LEU
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	243	VAL
4	D	19	GLU
4	D	24	HIS
4	D	50	VAL
4	D	52	THR
4	D	137	PRO
4	D	149	ARG
4	D	161	ASP

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Mol	Chain	Res	Type
4	D	170	TYR
5	E	7	ILE
5	E	12	ASP
5	E	16	ASP
5	E	96	ASN
5	E	102	VAL
7	G	64	ASN
8	H	33	GLN
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	169	GLU
8	H	173	GLU
9	I	94	ASP
10	J	46	ILE
10	J	52	GLN
10	J	79	PHE
10	J	107	ASN
10	J	130	VAL
10	J	131	THR
11	K	10	GLN
11	K	55	VAL
11	K	119	GLN
12	L	35	ARG
12	L	101	ASP
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	93	ARG
13	M	99	ARG
13	M	115	LEU
13	M	116	ASN
13	M	164	THR
14	N	26	LEU
14	N	49	THR
14	N	56	ASP
14	N	127	LEU
14	N	138	ASP
15	O	43	VAL
15	O	98	LEU
16	P	21	VAL

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Mol	Chain	Res	Type
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
16	P	110	ASP
17	Q	16	ASN
17	Q	57	ASP
18	R	13	THR
18	R	39	THR
18	R	82	GLU
18	R	143	VAL
19	S	59	ASP
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	52	THR
22	V	65	ASP
23	W	26	ILE
23	W	52	VAL
23	W	142	ASP
23	W	146	ILE
24	X	46	ASP
24	X	49	ARG
24	X	52	PRO
24	X	72	VAL
24	X	82	GLU
24	X	88	GLU
25	Y	115	ARG
25	Y	154	ARG
25	Y	163	THR
25	Y	169	ARG
25	Y	189	ASN
25	Y	203	VAL
26	Z	65	ASN
28	2	18	ASN
29	3	3	MET
29	3	56	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	2	GLN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	85	GLN
4	D	103	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	73	ASN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	40	ASN
14	N	93	GLN
14	N	107	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN

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Mol	Chain	Res	Type
16	P	118	GLN
17	Q	40	HIS
18	R	22	GLN
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
18	R	122	GLN
19	S	44	GLN
20	T	39	ASN
21	U	39	ASN
22	V	60	GLN
23	W	2	HIS
23	W	28	HIS
23	W	87	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	119	GLN
25	Y	133	HIS
25	Y	134	HIS
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	41	HIS
28	2	45	ASN
29	3	20	HIS
29	3	48	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	239 (8%)	32 (1%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	255 (8%)	33 (1%)

All (255) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
30	0	236	A
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G

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Mol	Chain	Res	Type
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	605	C
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	698	A
30	0	701	U
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U

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Mol	Chain	Res	Type
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1151	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1287	A
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1460	G
30	0	1474	C
30	0	1485	A
30	0	1488	U
30	0	1505	U
30	0	1506	U
30	0	1507	C

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Mol	Chain	Res	Type
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1562	C
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1732	A
30	0	1742	A
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1996	U
30	0	2004	U
30	0	2008	U
30	0	2011	A

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Mol	Chain	Res	Type
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2320	U
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2467	A
30	0	2469	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2513	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A

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Mol	Chain	Res	Type
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2645	U
30	0	2649	A
30	0	2664	A
30	0	2676	C
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2867	G
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A

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Mol	Chain	Res	Type
31	9	114	G
31	9	122	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	169	A
30	0	603	A
30	0	604	G
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	869	G
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1237	U
30	0	1352	A
30	0	1377	C
30	0	1474	C
30	0	1506	U
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1856	C
30	0	1878	G
30	0	1979	G
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2761	A
30	0	2791	U
31	9	65	A

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	UR3	0	2619	30	19,22,23	0.43	0	26,32,35	0.64	1 (3%)
30	PSU	0	2621	30	18,21,22	1.46	2 (11%)	22,30,33	1.27	3 (13%)
30	OMG	0	2588	30	18,26,27	1.05	2 (11%)	19,38,41	0.70	1 (5%)
30	1MA	0	628	35,30	16,25,26	1.32	3 (18%)	18,37,40	1.04	2 (11%)
30	OMU	0	2587	30	19,22,23	0.33	0	26,31,34	0.36	0

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
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	1MA	0	628	35,30	-	0/3/25/26	0/3/3/3
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	4.85	1.43	1.36
30	0	628	1MA	C2-N3	3.37	1.33	1.29
30	0	2588	OMG	C5-C6	-2.69	1.42	1.47
30	0	2588	OMG	C8-N7	-2.48	1.30	1.35
30	0	2621	PSU	C6-C5	2.45	1.38	1.35
30	0	628	1MA	C6-N6	2.39	1.33	1.27
30	0	628	1MA	C8-N7	-2.06	1.31	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	2621	PSU	C6-C5-C4	3.46	120.62	118.20
30	0	628	1MA	N1-C2-N3	2.79	129.27	126.02
30	0	2621	PSU	O2-C2-N1	2.73	125.80	122.79
30	0	2621	PSU	C6-N1-C2	-2.57	120.06	122.68
30	0	628	1MA	C5-C6-N1	2.56	117.71	113.90
30	0	2619	UR3	C4-N3-C2	2.42	126.84	124.56
30	0	2588	OMG	O6-C6-C5	2.10	128.48	124.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.