Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 10:29 AM EST

PDB ID	:	3CCU
Title	:	Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2482C
Authors	:	Blaha, G.; Gurel, G.
Deposited on	:	2008-02-26
Resolution	:	2.80 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:

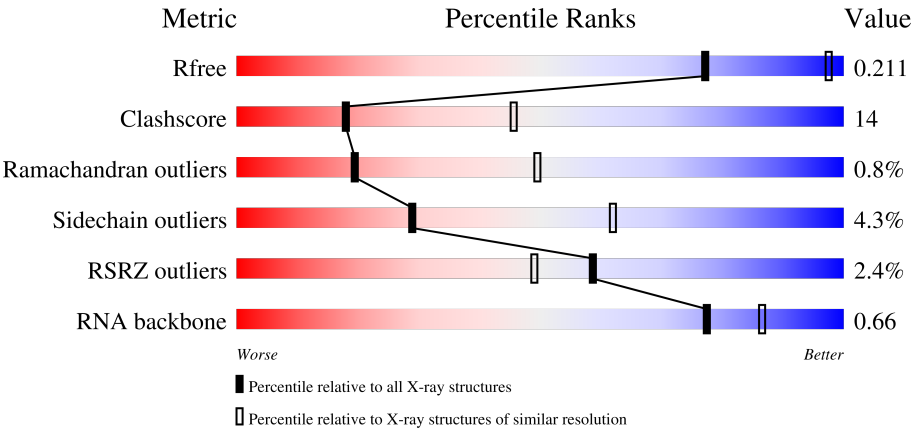
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	2%, 72%, 24%, ••
2	B	338	65%, 31%, •
3	C	246	74%, 23%, •
4	D	177	15%, 44%, 35%, 21%

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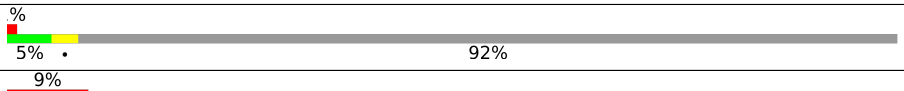
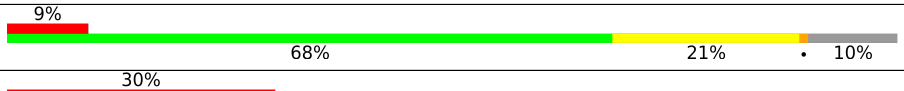
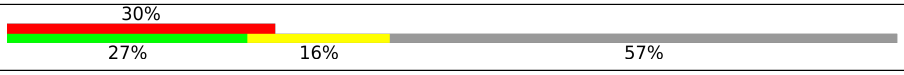
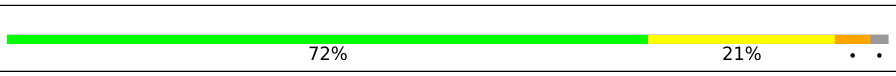
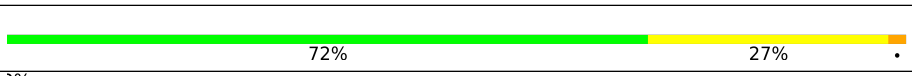
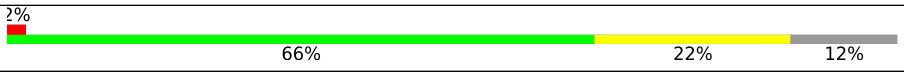
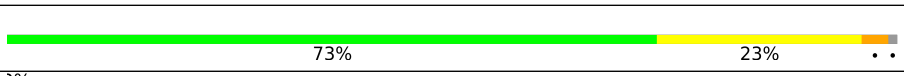
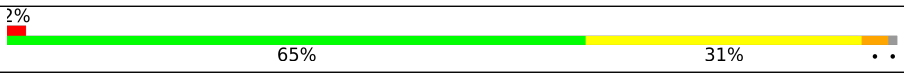
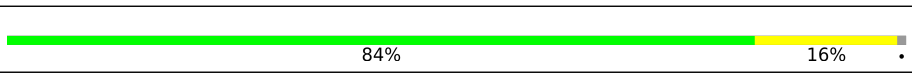
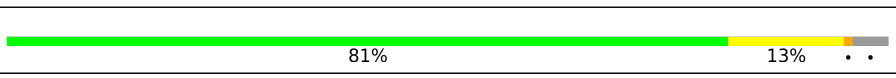
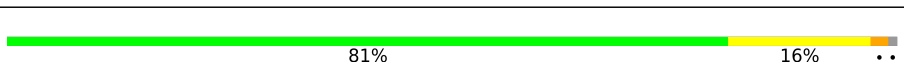
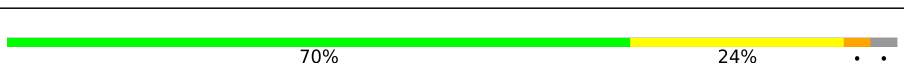
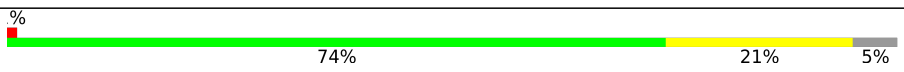
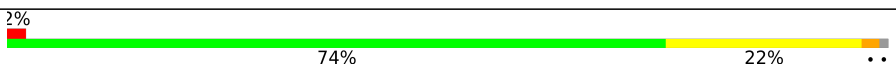
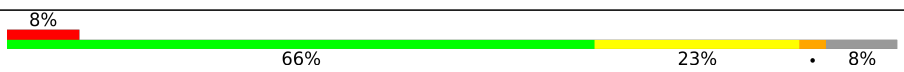
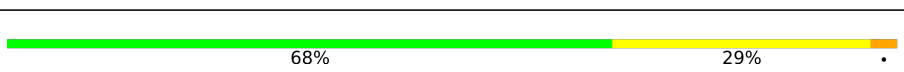
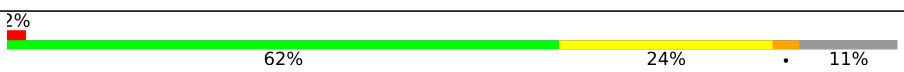
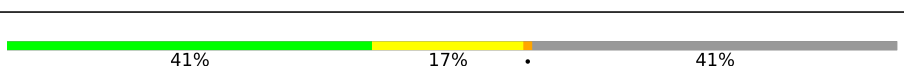
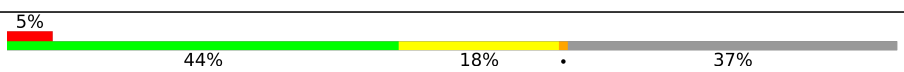
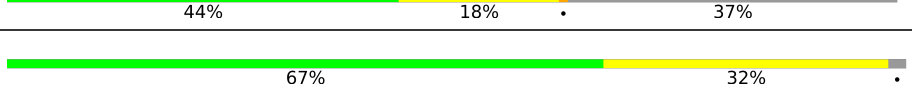
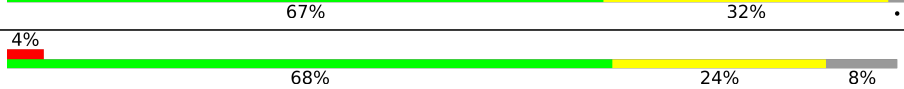
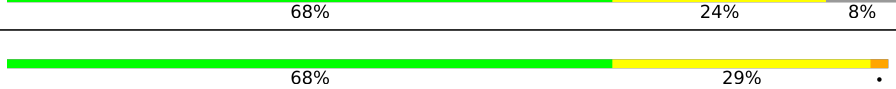
Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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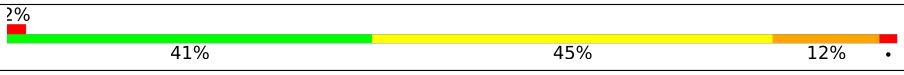
Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CL	J	8801	-	-	X	-
34	SR	0	9006	-	-	-	X
34	SR	J	8986	-	-	-	X
37	K	0	8401	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99119 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
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

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

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

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

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

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

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

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

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

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

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

- 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
			59017	26348	10871	19053	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	84	Total	Mg	0	0
			84	84		
32	9	2	Total	Mg	0	0
			2	2		

- 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	K	1	Total Cl 1 1	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	9	Total Cl 9 9	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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	92	Total Sr 92 92	0	0
34	9	3	Total Sr 3 3	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	H	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	1	Total Na 1 1	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	110	Total O 110 110	0	0
38	B	144	Total O 144 144	0	0
38	C	178	Total O 178 178	0	0
38	D	45	Total O 45 45	0	0
38	E	43	Total O 43 43	0	0
38	F	27	Total O 27 27	0	0
38	G	17	Total O 17 17	0	0
38	H	69	Total O 69 69	0	0
38	I	6	Total O 6 6	0	0
38	J	53	Total O 53 53	0	0
38	K	56	Total O 56 56	0	0
38	L	92	Total O 92 92	0	0
38	M	129	Total O 129 129	0	0
38	N	63	Total O 63 63	0	0
38	O	40	Total O 40 40	0	0
38	P	66	Total O 66 66	0	0
38	Q	46	Total O 46 46	0	0
38	R	76	Total O 76 76	0	0
38	S	39	Total O 39 39	0	0

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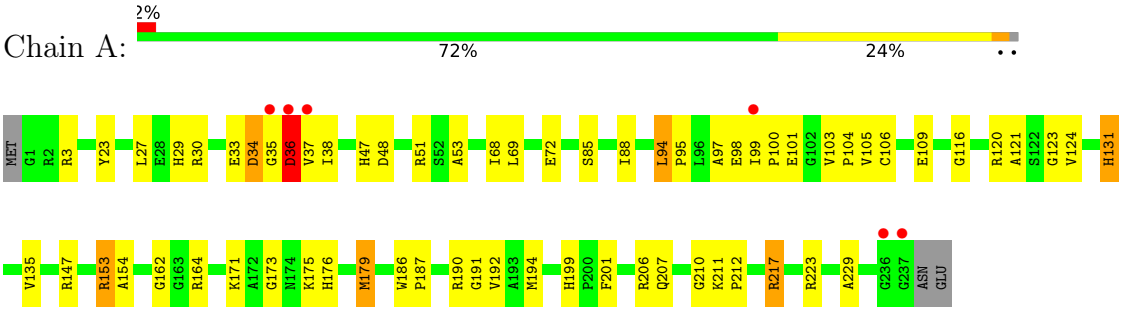
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	T	35	Total O 35 35	0	0
38	U	28	Total O 28 28	0	0
38	V	13	Total O 13 13	0	0
38	W	69	Total O 69 69	0	0
38	X	27	Total O 27 27	0	0
38	Y	91	Total O 91 91	0	0
38	Z	25	Total O 25 25	0	0
38	1	56	Total O 56 56	0	0
38	2	38	Total O 38 38	0	0
38	3	65	Total O 65 65	0	0
38	0	5933	Total O 5933 5933	0	0
38	9	144	Total O 144 144	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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

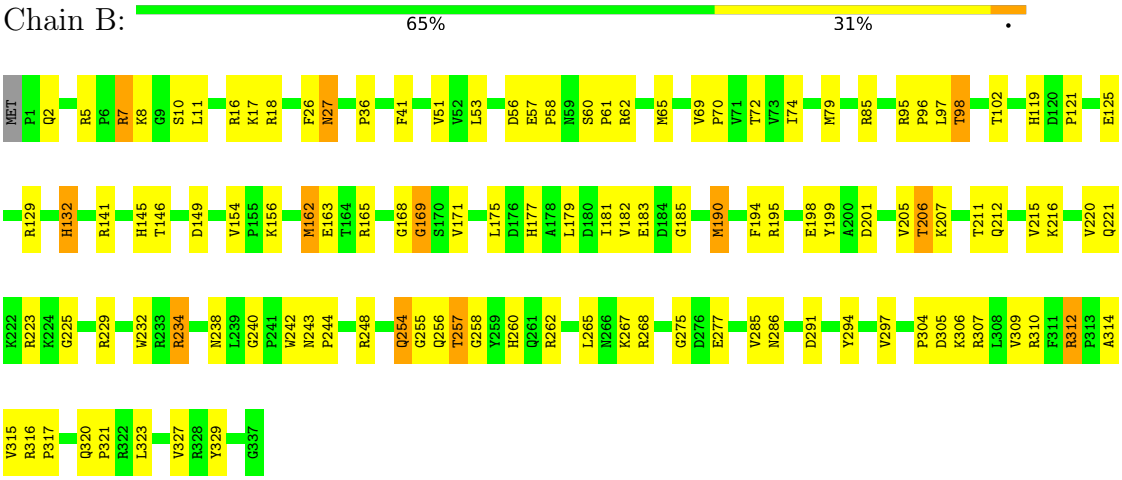
• Molecule 1: 50S ribosomal protein L2P

Chain A:



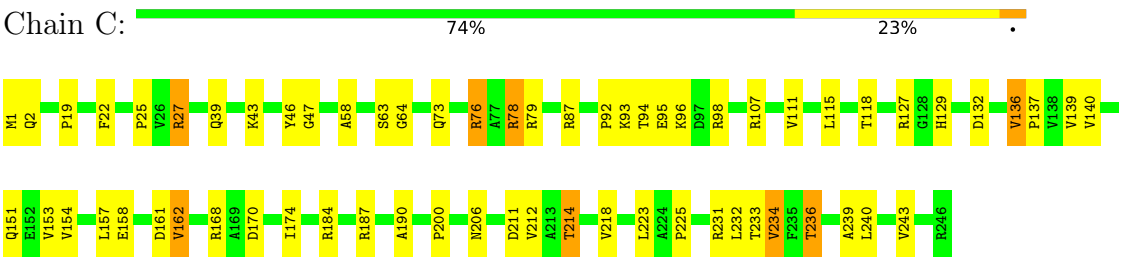
• Molecule 2: 50S ribosomal protein L3P

Chain B:



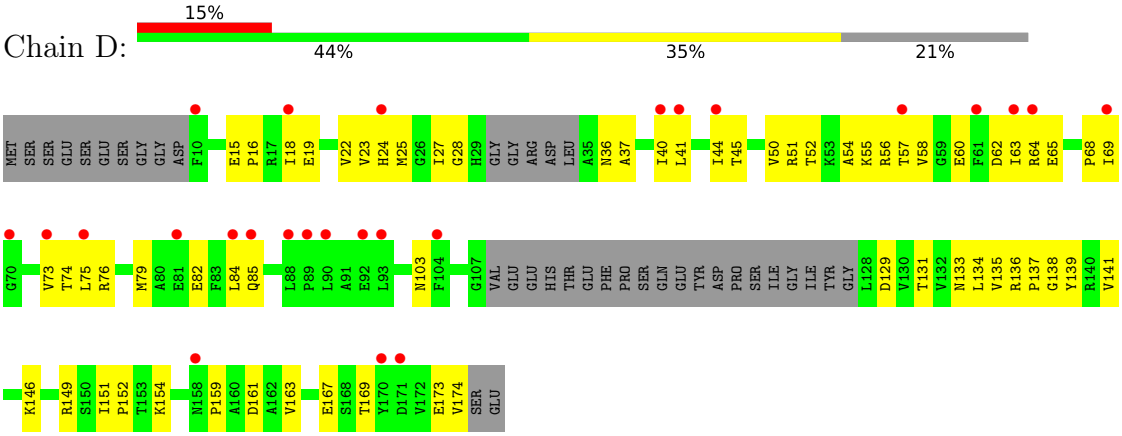
• Molecule 3: 50S ribosomal protein L4P

Chain C:



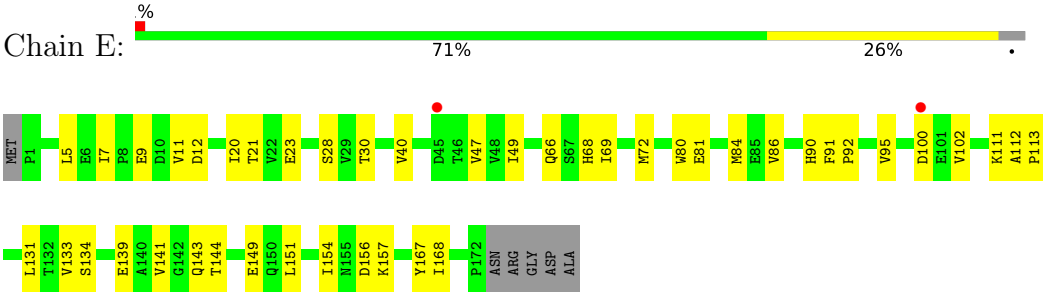
• Molecule 4: 50S ribosomal protein L5P

Chain D:



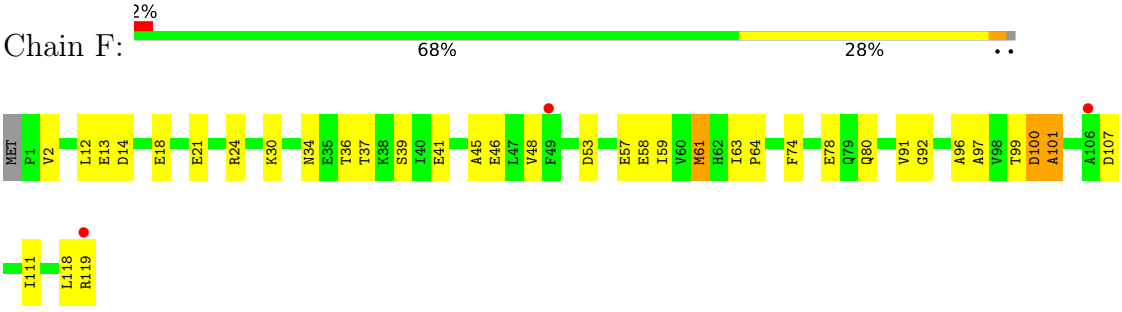
• Molecule 5: 50S ribosomal protein L6P

Chain E:



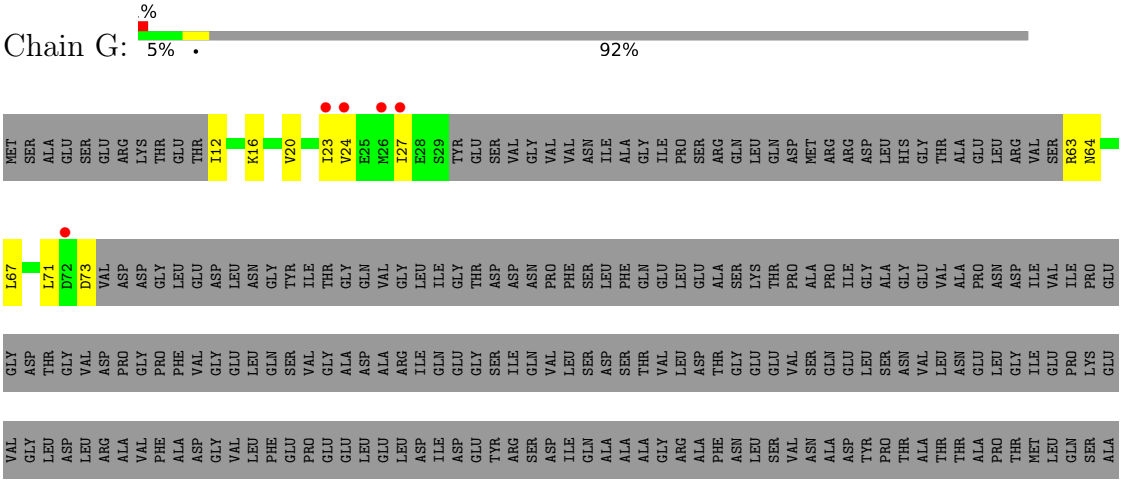
• Molecule 6: 50S ribosomal protein L7Ae

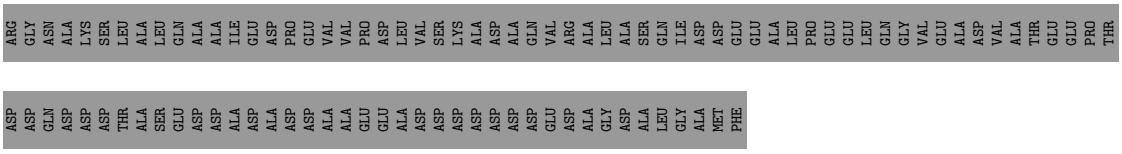
Chain F:



• Molecule 7: 50S ribosomal protein L10E

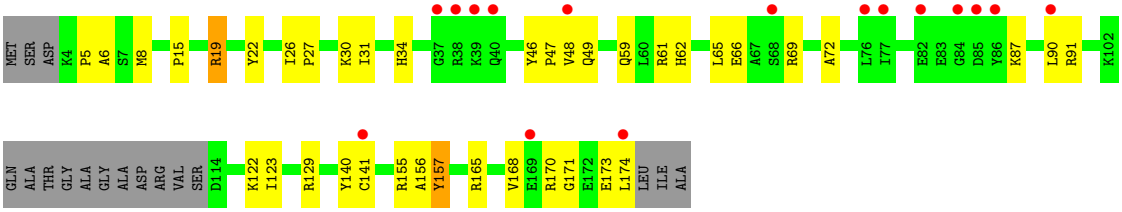
Chain G:





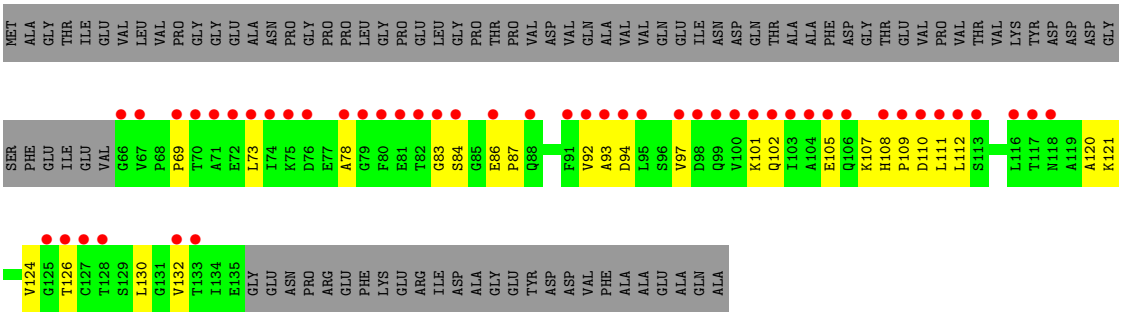
• Molecule 8: 50S ribosomal protein L10e

Chain H:



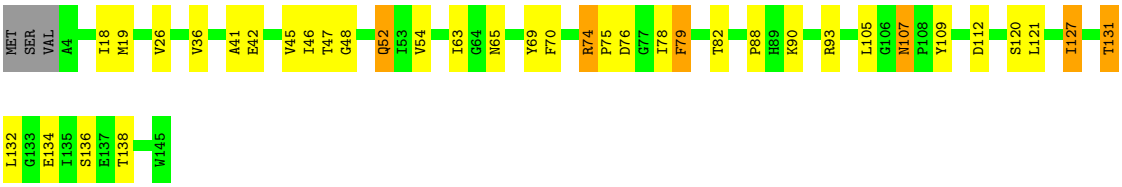
• Molecule 9: 50S ribosomal protein L11P

Chain I:



• Molecule 10: 50S ribosomal protein L13P

Chain J:

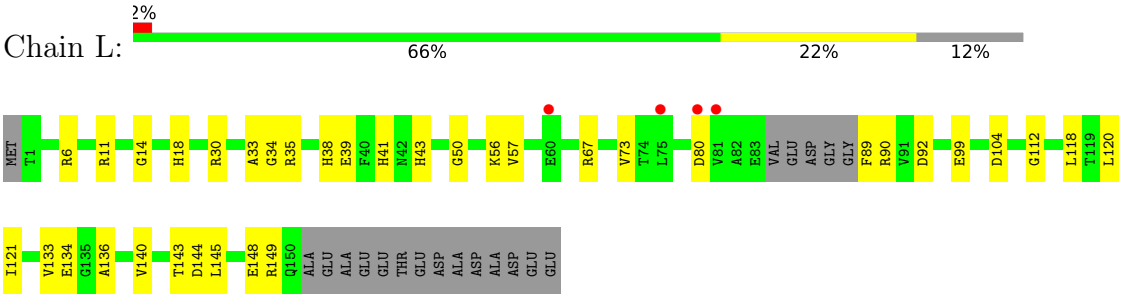


• Molecule 11: 50S ribosomal protein L14P

Chain K:

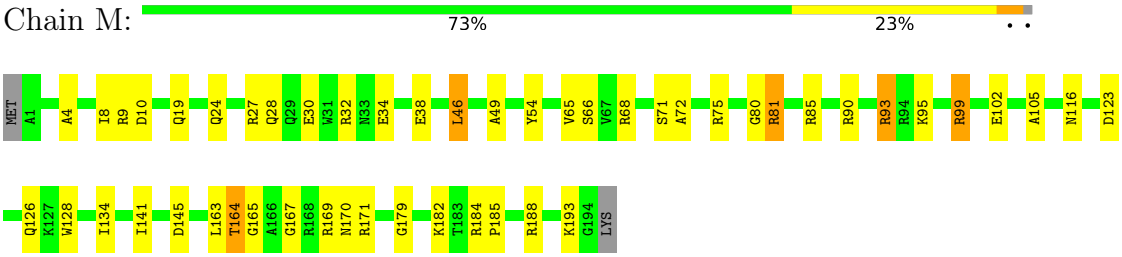
• Molecule 12: 50S ribosomal protein L15P

Chain L:



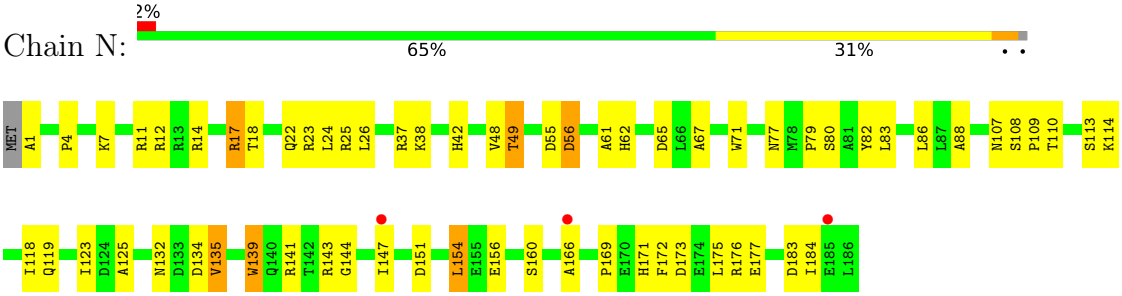
• Molecule 13: 50S ribosomal protein L15e

Chain M:



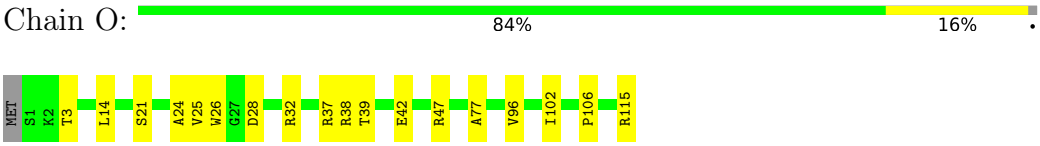
• Molecule 14: 50S ribosomal protein L18P

Chain N:



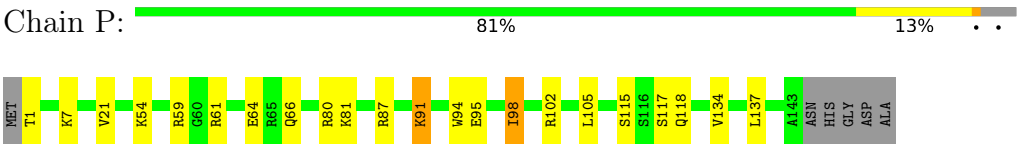
• Molecule 15: 50S ribosomal protein L18e

Chain O:



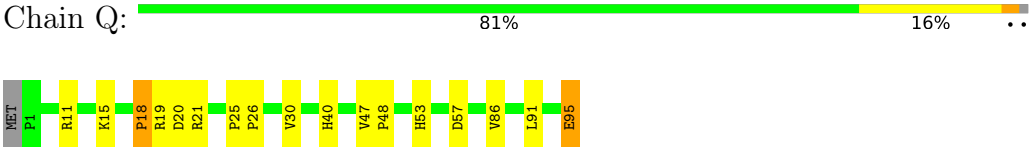
• Molecule 16: 50S ribosomal protein L19e

Chain P:



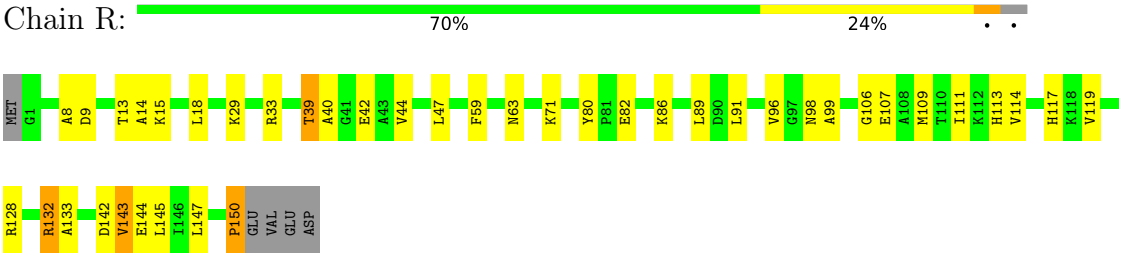
• Molecule 17: 50S ribosomal protein L21e

Chain Q:



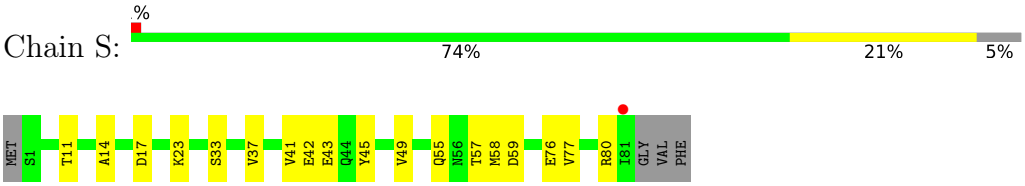
• Molecule 18: 50S ribosomal protein L22P

Chain R:



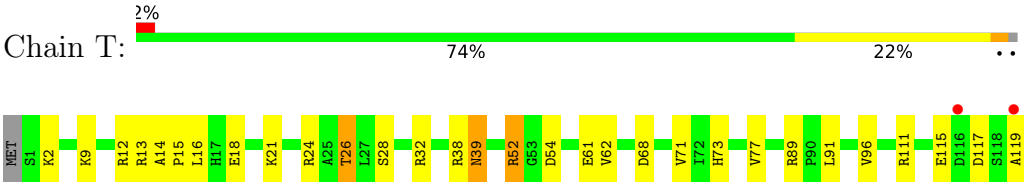
• Molecule 19: 50S ribosomal protein L23P

Chain S:



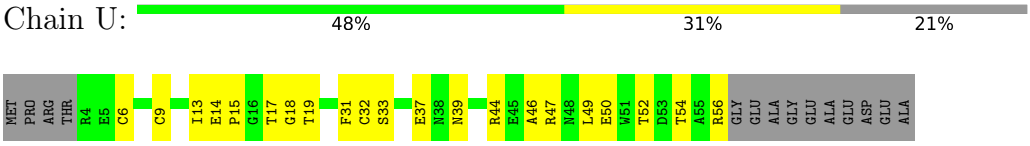
• Molecule 20: 50S ribosomal protein L24P

Chain T:



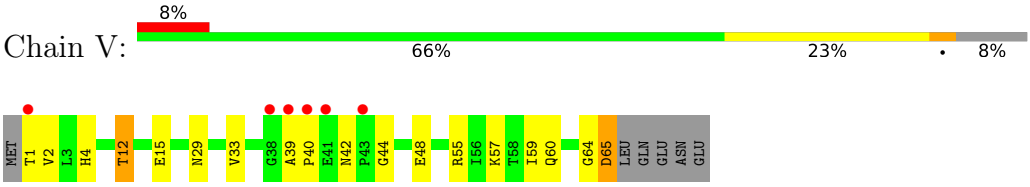
• Molecule 21: 50S ribosomal protein L24e

Chain U:



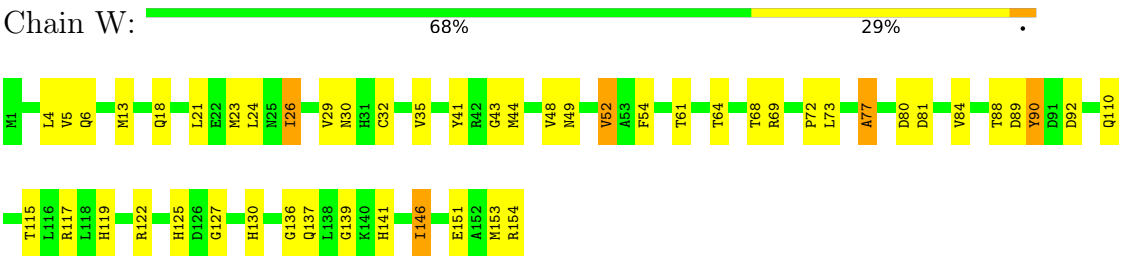
• Molecule 22: 50S ribosomal protein L29P

Chain V:



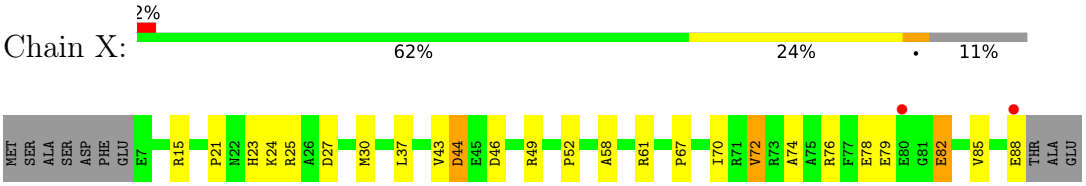
• Molecule 23: 50S ribosomal protein L30P

Chain W:



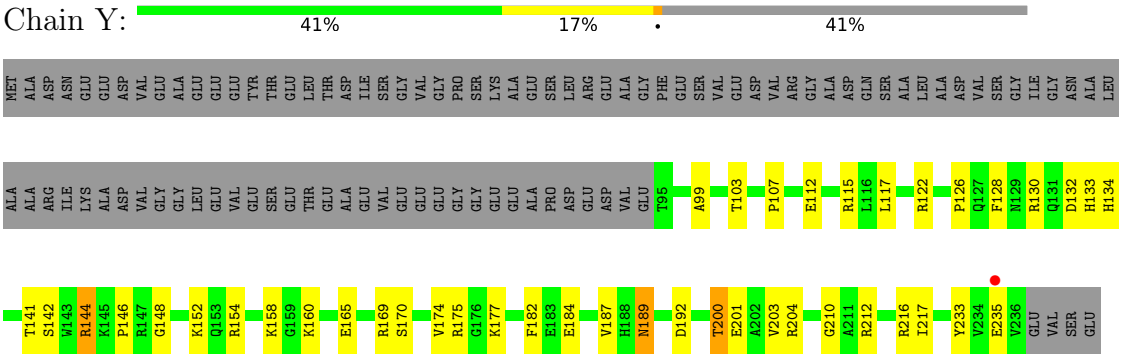
• Molecule 24: 50S ribosomal protein L31e

Chain X:



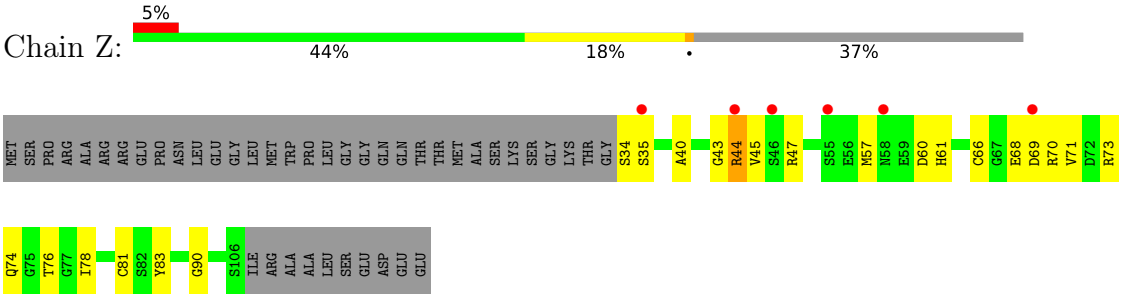
• Molecule 25: 50S ribosomal protein L32e

Chain Y:



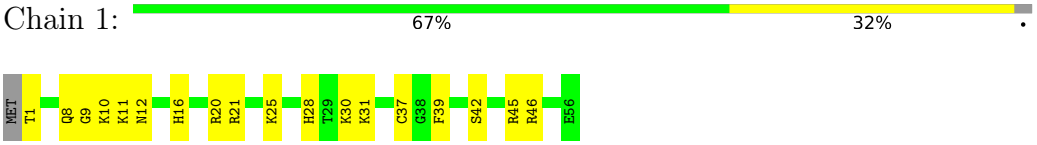
• Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



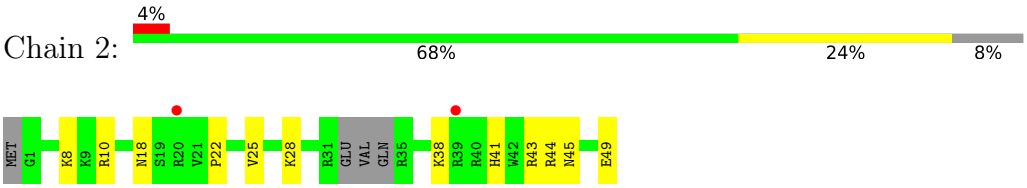
• Molecule 27: 50S ribosomal protein L37e

Chain 1:



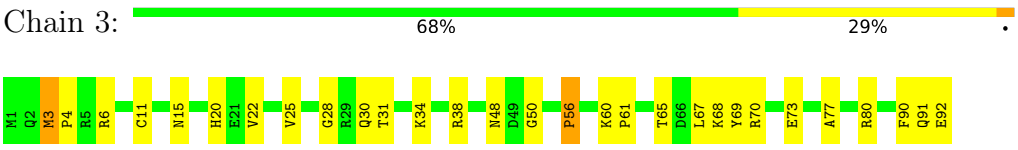
• Molecule 28: 50S ribosomal protein L39e

Chain 2:



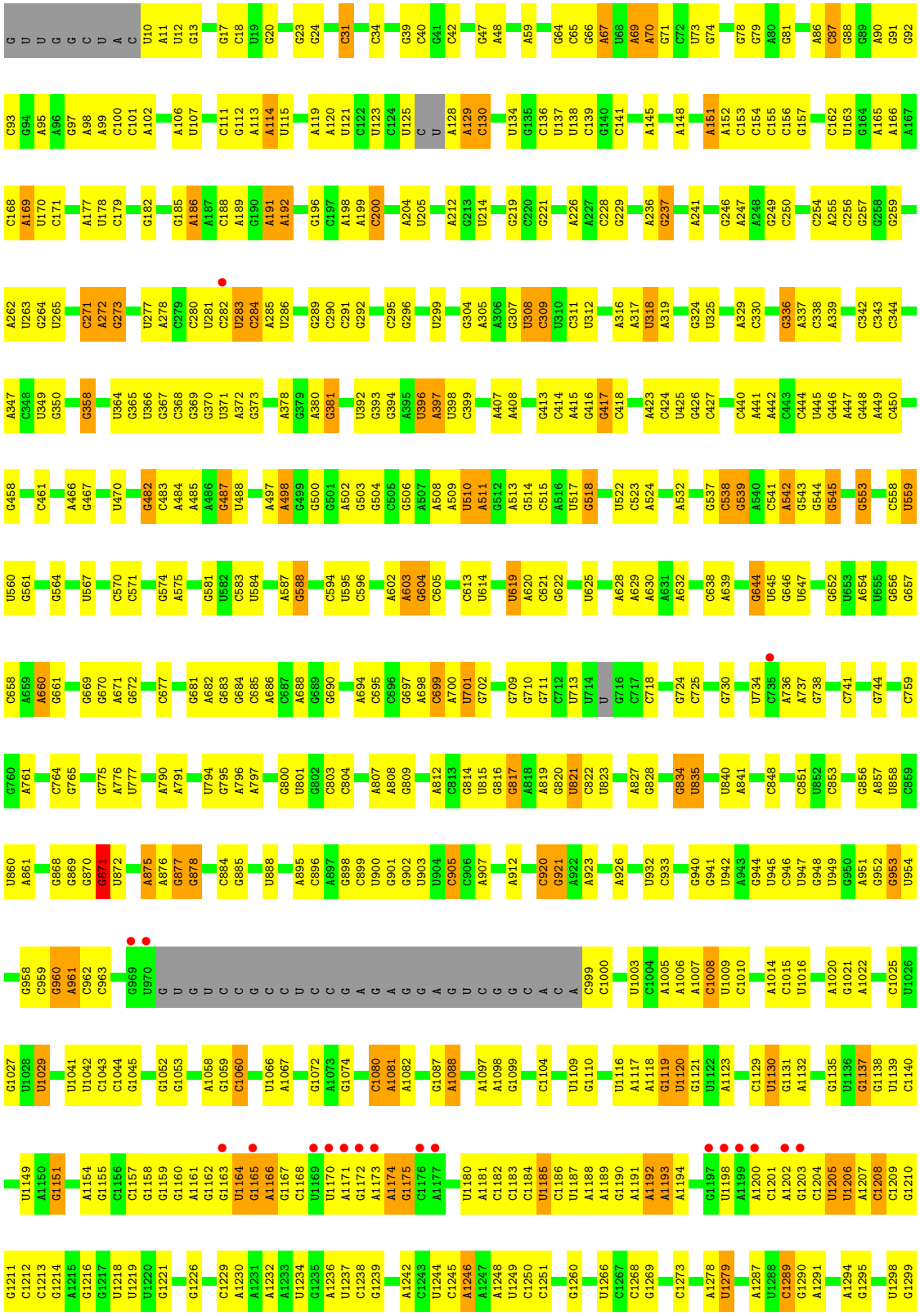
• Molecule 29: 50S ribosomal protein L44E

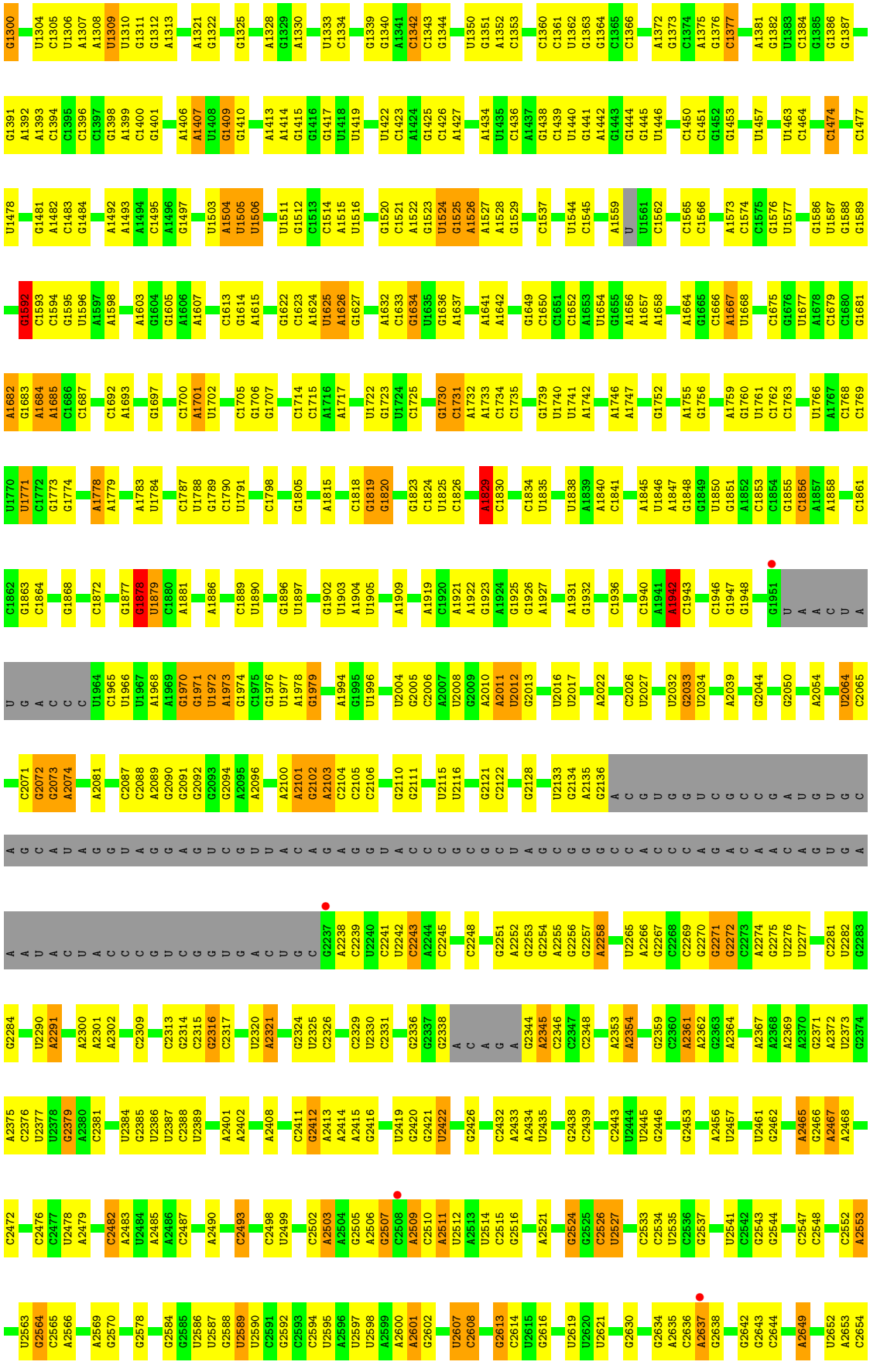
Chain 3:

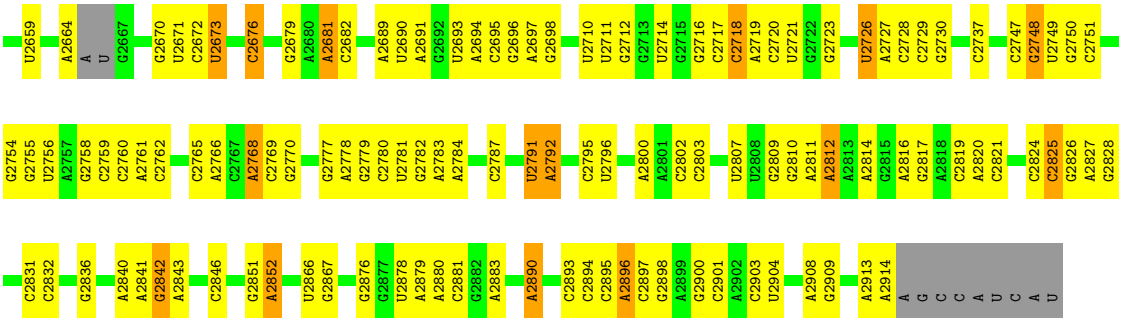


• Molecule 30: 23S RIBOSOMAL RNA

Chain 0:

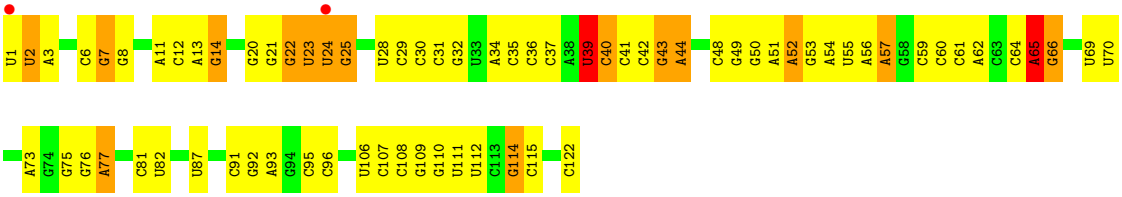






• Molecule 31: 5S RIBOSOMAL RNA

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	211.76Å 299.27Å 574.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 2.80 85.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.99-2.80) 93.0 (85.47-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.179 , 0.223 0.170 , 0.211	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 69.3	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	0.94	EDS
Total number of atoms	99119	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: 1MA, UR3, OMG, CL, NA, OMU, CD, PSU, K, MG, SR

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	0.33	0/1786	0.65	0/2408
2	B	0.33	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.63	0/2552
4	D	0.32	0/1111	0.55	0/1498
5	E	0.32	0/1382	0.58	0/1880
6	F	0.33	0/901	0.57	0/1224
7	G	0.30	0/241	0.48	0/324
8	H	0.33	0/1302	0.61	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.36	0/1136	0.59	0/1530
11	K	0.35	0/1004	0.67	0/1351
12	L	0.32	0/1130	0.63	0/1509
13	M	0.34	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.62	0/1999
15	O	0.33	0/874	0.58	0/1181
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.34	0/749	0.66	0/1005
18	R	1.26	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.33	0/648	0.57	0/875
20	T	0.33	0/958	0.64	1/1289 (0.1%)
21	U	0.34	0/417	0.57	0/562
22	V	0.31	0/502	0.51	0/675
23	W	0.34	0/1219	0.62	0/1655
24	X	0.34	0/664	0.60	0/895
25	Y	0.36	0/1146	0.63	0/1536
26	Z	0.35	0/584	0.59	0/781
27	1	0.39	0/438	0.61	0/578
28	2	0.34	0/401	0.59	0/529
29	3	0.37	0/771	0.57	0/1024
30	0	0.37	0/65953	0.69	16/102860 (0.0%)
31	9	0.31	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98697 (0.0%)	0.67	24/147579 (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
23	W	0	1
30	0	1	34
31	9	0	3
All	All	2	38

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.61	2.88	1.50
18	R	150	PRO	CA-C	-17.92	1.17	1.52
18	R	150	PRO	CG-CD	13.88	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.29	1.66	1.47
18	R	150	PRO	N-CD	10.71	1.62	1.47
18	R	150	PRO	CA-CB	7.49	1.68	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	150	PRO	CB-CA-C	-22.50	55.74	112.00
18	R	150	PRO	N-CA-C	-19.33	61.84	112.10
18	R	150	PRO	CA-N-CD	12.33	128.96	111.70
18	R	150	PRO	N-CA-CB	10.99	116.49	103.30
30	0	2482	C	C2'-C3'-O3'	9.28	129.92	109.50
18	R	150	PRO	CA-C-O	-8.60	99.56	120.20
30	0	1942	A	C5'-C4'-C3'	6.99	127.19	116.00
30	0	1120	U	C5'-C4'-C3'	-6.55	105.51	116.00
30	0	871	G	C5'-C4'-O4'	-6.46	101.35	109.10
18	R	150	PRO	CA-CB-CG	-6.22	92.19	104.00
30	0	1504	A	C1'-O4'-C4'	-6.12	105.00	109.90
31	9	39	U	N1-C1'-C2'	5.91	121.68	114.00
30	0	1592	G	N9-C1'-C2'	5.58	121.26	114.00
30	0	1504	A	N9-C1'-C2'	5.43	121.06	114.00
30	0	2316	G	C5'-C4'-C3'	-5.42	107.33	116.00
30	0	2467	A	C1'-O4'-C4'	-5.41	105.58	109.90
20	T	52	ARG	N-CA-C	5.27	125.23	111.00
30	0	2726	U	N1-C1'-C2'	5.25	120.82	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	1878	G	N9-C1'-C2'	-5.20	106.29	112.00
30	0	2482	C	C4'-C3'-O3'	5.19	123.38	113.00
30	0	841	A	C1'-O4'-C4'	-5.16	105.77	109.90
30	0	1942	A	C1'-O4'-C4'	-5.06	105.85	109.90
30	0	1829	A	N9-C1'-C2'	-5.05	106.44	112.00
30	0	2313	C	O4'-C4'-C3'	-5.01	98.99	104.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA
30	0	2482	C	C3'

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1300	G	Sidechain
30	0	1309	U	Sidechain
30	0	1417	G	Sidechain
30	0	1592	G	Sidechain
30	0	1771	U	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1861	C	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1970	G	Sidechain
30	0	1972	U	Sidechain
30	0	1979	G	Sidechain
30	0	221	G	Sidechain
30	0	2412	G	Sidechain
30	0	246	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2524	G	Sidechain
30	0	2552	C	Sidechain
30	0	2607	U	Sidechain
30	0	2673	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain

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Mol	Chain	Res	Type	Group
30	0	458	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	795	G	Sidechain
30	0	817	G	Sidechain
30	0	888	U	Sidechain
30	0	900	U	Sidechain
31	9	39	U	Sidechain
31	9	65	A	Sidechain
31	9	87	U	Sidechain
23	W	90	TYR	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	71	0
2	B	2625	0	2533	100	0
3	C	1860	0	1813	58	0
4	D	1094	0	1085	44	0
5	E	1357	0	1266	32	0
6	F	890	0	843	30	0
7	G	240	0	231	9	0
8	H	1282	0	1292	33	0
9	I	519	0	500	23	0
10	J	1120	0	1098	38	0
11	K	994	0	1027	35	0
12	L	1118	0	1076	28	0
13	M	1558	0	1573	45	0
14	N	1445	0	1401	57	0
15	O	865	0	873	19	0
16	P	1136	0	1123	18	0
17	Q	735	0	729	16	0
18	R	1149	0	1122	38	0
19	S	641	0	605	16	0
20	T	950	0	924	22	0
21	U	410	0	364	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	V	499	0	511	14	0
23	W	1196	0	1137	48	0
24	X	654	0	653	16	0
25	Y	1130	0	1133	38	0
26	Z	573	0	531	21	0
27	1	431	0	426	23	0
28	2	396	0	413	14	0
29	3	755	0	728	25	0
30	0	59017	0	29810	1217	0
31	9	2599	0	1325	89	0
32	0	84	0	0	0	0
32	9	2	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	9	0	0	1	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	3	0
33	K	1	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	92	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	H	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	1	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	5933	0	0	188	0
38	1	56	0	0	4	0
38	2	38	0	0	0	0
38	3	65	0	0	4	0
38	9	144	0	0	9	0
38	A	110	0	0	6	0
38	B	144	0	0	18	0
38	C	178	0	0	14	0
38	D	45	0	0	3	0
38	E	43	0	0	2	0
38	F	27	0	0	2	0
38	G	17	0	0	0	0
38	H	69	0	0	8	0
38	I	6	0	0	0	0
38	J	53	0	0	2	0
38	K	56	0	0	3	0
38	L	92	0	0	6	0
38	M	129	0	0	4	0
38	N	63	0	0	6	0
38	O	40	0	0	2	0
38	P	66	0	0	1	0
38	Q	46	0	0	1	0
38	R	76	0	0	2	0
38	S	39	0	0	4	0
38	T	35	0	0	3	0
38	U	28	0	0	3	0
38	V	13	0	0	0	0
38	W	69	0	0	5	0
38	X	27	0	0	2	0
38	Y	91	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Z	25	0	0	3	0
All	All	99119	0	59911	2035	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 14.

All (2035) 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	1.43
30:0:1160:G:C5'	30:0:1161:A:H5'	1.74	1.16
31:9:56:A:H2'	31:9:57:A:H5"	1.20	1.16
30:0:1160:G:H5'	30:0:1161:A:C5'	1.77	1.14
14:N:37:ARG:NH1	31:9:6:C:H5"	1.62	1.14
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.32	1.10
15:O:3:THR:HG22	30:0:656:G:H5'	1.30	1.10
31:9:76:G:H3'	31:9:77:A:H5"	1.32	1.09
30:0:871:G:C8	30:0:871:G:H5'	1.87	1.08
10:J:82:THR:HG23	30:0:1242:A:H5'	1.37	1.07
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.06
30:0:381:G:H5"	38:0:4318:HOH:O	1.55	1.05
30:0:545:G:H5'	30:0:545:G:H8	1.19	1.04
30:0:871:G:H5'	30:0:871:G:H8	1.18	1.03
13:M:171:ARG:HD3	30:0:156:C:H5"	1.41	1.01
30:0:2717:C:C2'	30:0:2718:C:H5"	1.90	1.01
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.78	0.98
30:0:1118:A:H8	30:0:1118:A:H3'	1.28	0.98
30:0:1187:U:HO2'	30:0:1189:A:H2	1.00	0.97
30:0:2717:C:H2'	30:0:2718:C:H5"	1.44	0.97
4:D:154:LYS:H	4:D:154:LYS:HD2	1.28	0.97
30:0:1666:C:O2'	30:0:1667:A:H5"	1.65	0.96
16:P:115:SER:H	16:P:118:GLN:HE21	1.11	0.95
30:0:1603:A:H5'	30:0:1605:G:O4'	1.67	0.95
2:B:238:ASN:HD22	2:B:240:GLY:H	1.15	0.94
31:9:56:A:C2'	31:9:57:A:H5"	1.96	0.94
30:0:1474:C:H6	30:0:1474:C:H5'	1.32	0.94
30:0:1701:A:H4'	30:0:1702:U:H5"	1.47	0.94
15:O:3:THR:CG2	30:0:656:G:H5'	1.96	0.94
11:K:10:GLN:HE21	11:K:10:GLN:H	1.03	0.94
22:V:1:THR:HB	30:0:93:C:H5"	1.49	0.93
30:0:1372:A:H3'	38:0:7212:HOH:O	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:164:THR:HG22	13:M:167:GLY:H	1.31	0.93
30:0:1118:A:H3'	30:0:1118:A:C8	2.03	0.93
3:C:236:THR:HG22	3:C:239:ALA:H	1.35	0.92
30:0:542:A:H5'	30:0:542:A:H8	1.35	0.91
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.13	0.91
30:0:545:G:H5'	30:0:545:G:C8	2.06	0.90
30:0:1701:A:H5'	38:0:6304:HOH:O	1.70	0.90
30:0:1835:U:H5	30:0:1840:A:N7	1.69	0.90
30:0:1166:A:H61	30:0:1180:U:H3	1.15	0.90
31:9:29:C:H2'	31:9:30:C:H5'	1.55	0.89
30:0:870:G:H2'	30:0:871:G:H5"	1.53	0.89
30:0:182:G:H5'	38:0:5167:HOH:O	1.71	0.89
30:0:1160:G:H5'	30:0:1161:A:H5'	0.90	0.89
30:0:541:C:H2'	30:0:542:A:H5"	1.55	0.89
30:0:541:C:C2'	30:0:542:A:H5"	2.03	0.89
30:0:506:G:H22	30:0:509:A:C5'	1.85	0.88
30:0:871:G:H8	30:0:871:G:C5'	1.87	0.88
30:0:2291:A:C8	30:0:2309:C:H5'	2.09	0.87
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.21	0.87
30:0:2783:A:H3'	38:0:5241:HOH:O	1.75	0.87
30:0:1118:A:H62	30:0:1244:U:H3	1.21	0.86
30:0:2908:A:H2'	30:0:2909:G:O4'	1.74	0.86
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.57	0.86
30:0:282:C:H1'	30:0:368:C:N4	1.90	0.86
30:0:1474:C:H5'	30:0:1474:C:C6	2.11	0.86
30:0:282:C:O2'	30:0:283:U:H5'	1.76	0.86
30:0:1116:U:HO2'	30:0:1118:A:H2	0.86	0.85
14:N:113:SER:HB2	38:N:8855:HOH:O	1.75	0.85
30:0:2586:U:H3	30:0:2592:G:H22	1.22	0.85
30:0:2506:A:HO2'	30:0:2507:G:H8	0.90	0.85
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.58	0.85
30:0:1165:G:H1'	30:0:1174:A:H1'	1.60	0.83
30:0:1666:C:C2'	30:0:1667:A:H5"	2.08	0.83
30:0:558:C:C2'	30:0:559:U:H5"	2.08	0.83
11:K:39:GLY:HA2	38:0:5229:HOH:O	1.79	0.83
30:0:1183:C:H2'	38:0:6261:HOH:O	1.77	0.83
28:2:41:HIS:H	28:2:45:ASN:HD22	1.25	0.83
30:0:541:C:H2'	30:0:542:A:C5'	2.08	0.83
30:0:2896:A:H5"	38:0:6117:HOH:O	1.77	0.83
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.58	0.83
30:0:1878:G:H1'	38:0:6139:HOH:O	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1189:A:H1'	30:0:1209:C:O4'	1.79	0.82
30:0:2812:A:H2	30:0:2814:A:H62	1.22	0.82
31:9:23:U:O2'	31:9:24:U:H4'	1.78	0.82
30:0:1184:C:H1'	38:0:7491:HOH:O	1.80	0.82
30:0:1116:U:O2'	30:0:1118:A:H2	1.63	0.82
30:0:1116:U:H3	30:0:1246:A:H62	1.27	0.81
30:0:1206:U:H5'	30:0:1206:U:H6	1.44	0.81
1:A:199:HIS:HD2	1:A:201:PHE:H	1.28	0.81
8:H:30:LYS:H	8:H:62:HIS:HD2	1.28	0.81
30:0:69:A:H5'	30:0:69:A:C8	2.15	0.81
30:0:1634:G:H3'	38:0:3895:HOH:O	1.79	0.81
30:0:396:U:H1'	38:0:7650:HOH:O	1.80	0.81
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.46	0.81
31:9:49:G:H5"	38:9:9087:HOH:O	1.80	0.81
30:0:2502:C:C2'	30:0:2503:A:H5'	2.11	0.81
30:0:2005:G:H3'	30:0:2005:G:OP2	1.82	0.80
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.64	0.80
30:0:1300:G:H1'	38:0:4687:HOH:O	1.81	0.80
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.63	0.80
23:W:88:THR:HB	38:W:6679:HOH:O	1.81	0.80
30:0:1119:G:N2	30:0:1246:A:C2	2.49	0.80
30:0:1120:U:H5'	30:0:1121:G:OP2	1.82	0.80
30:0:1667:A:H8	30:0:1667:A:H5'	1.47	0.80
30:0:1666:C:H2'	30:0:1667:A:H5'	1.63	0.80
31:9:14:G:H5'	31:9:14:G:H8	1.48	0.79
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.63	0.79
30:0:506:G:H22	30:0:509:A:H5"	1.48	0.79
30:0:1205:U:H2'	30:0:1206:U:C5'	2.12	0.79
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.27	0.79
30:0:380:A:H2'	38:0:7250:HOH:O	1.83	0.79
30:0:877:G:H5'	30:0:878:G:OP1	1.83	0.79
30:0:1666:C:H2'	30:0:1667:A:C5'	2.12	0.79
30:0:2637:A:H5'	38:0:9273:HOH:O	1.83	0.79
8:H:168:VAL:HG13	38:H:8556:HOH:O	1.83	0.78
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.47	0.78
30:0:2506:A:O2'	30:0:2507:G:H8	1.65	0.78
30:0:69:A:H5'	30:0:69:A:H8	1.49	0.78
30:0:2004:U:H4'	38:0:5316:HOH:O	1.84	0.78
30:0:2502:C:H2'	30:0:2503:A:H5'	1.64	0.78
30:0:2769:C:C2'	30:0:2770:G:H5'	2.14	0.78
30:0:31:C:H2'	38:0:7711:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:603:A:H5”	30:0:604:G:OP1	1.84	0.78
30:0:1183:C:N4	30:0:1184:C:H41	1.82	0.78
30:0:1278:A:H4’	30:0:1279:U:C4	2.19	0.78
3:C:1:MET:HG2	3:C:2:GLN:H	1.48	0.78
30:0:2748:G:H1’	38:0:7918:HOH:O	1.84	0.78
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.78
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.66	0.78
30:0:236:A:H4’	30:0:237:G:H5’	1.66	0.78
30:0:2748:G:H5’	38:0:7565:HOH:O	1.82	0.78
30:0:2756:U:H3	30:0:2896:A:H2	1.31	0.78
10:J:70:PHE:CE1	30:0:2676:C:H4’	2.18	0.77
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.65	0.77
5:E:143:GLN:HE21	30:0:2780:C:H1’	1.48	0.77
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.83	0.77
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.67	0.77
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.65	0.77
38:C:8665:HOH:O	30:0:2100:A:H5’	1.85	0.76
4:D:25:MET:HE2	4:D:41:LEU:HG	1.65	0.76
30:0:1180:U:H1’	38:0:3238:HOH:O	1.85	0.76
30:0:283:U:H5	30:0:284:C:N3	1.83	0.76
30:0:558:C:O2’	30:0:559:U:H5”	1.85	0.76
20:T:61:GLU:HG2	38:T:3851:HOH:O	1.84	0.76
30:0:1603:A:H5”	30:0:1605:G:H5’	1.67	0.76
30:0:1641:A:H2’	30:0:1642:A:H5’	1.64	0.76
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.67	0.76
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.66	0.76
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.67	0.76
25:Y:200:THR:HG22	25:Y:201:GLU:HG3	1.66	0.76
30:0:1201:C:H5”	38:0:6251:HOH:O	1.84	0.76
30:0:1189:A:H3’	38:0:7703:HOH:O	1.85	0.76
30:0:130:C:H2’	38:0:3163:HOH:O	1.85	0.75
30:0:1973:A:H5’	30:0:1973:A:H8	1.51	0.75
30:0:2768:A:O2’	30:0:2769:C:H5’	1.86	0.75
30:0:1118:A:C8	30:0:1118:A:C3’	2.68	0.75
22:V:1:THR:HG23	22:V:2:VAL:H	1.50	0.75
30:0:31:C:H4’	38:0:7449:HOH:O	1.86	0.75
2:B:206:THR:HG21	30:0:2716:G:H5”	1.69	0.75
30:0:2638:G:H5’	38:0:4938:HOH:O	1.86	0.75
30:0:2717:C:O2’	30:0:2718:C:H5”	1.86	0.75
30:0:2578:G:H5’	30:0:2578:G:H8	1.52	0.74
30:0:506:G:H22	30:0:509:A:H5’	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:567:U:H5”	38:0:6425:HOH:O	1.86	0.74
30:0:2507:G:H2’	30:0:2510:C:H42	1.52	0.74
2:B:162:MET:HG3	2:B:310:ARG:NH1	2.02	0.74
10:J:52:GLN:HE22	30:0:1119:G:H2’	1.49	0.74
30:0:255:A:H2’	30:0:256:C:H6	1.51	0.74
30:0:1175:G:H1’	30:0:1193:A:H2’	1.68	0.74
14:N:37:ARG:HH12	31:9:6:C:H5”	1.49	0.74
30:0:2768:A:H5”	38:0:4425:HOH:O	1.88	0.74
30:0:871:G:C8	30:0:871:G:C5’	2.64	0.74
30:0:1172:G:H5”	38:0:7282:HOH:O	1.87	0.74
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.28	0.73
31:9:92:G:H2’	31:9:93:A:C8	2.23	0.73
30:0:619:U:H3’	38:0:3286:HOH:O	1.88	0.73
30:0:2748:G:H2’	38:0:7565:HOH:O	1.88	0.73
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.03	0.73
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.68	0.73
30:0:564:G:H1’	38:0:6331:HOH:O	1.88	0.73
10:J:47:THR:HB	38:0:4845:HOH:O	1.89	0.73
30:0:558:C:H2’	30:0:559:U:C5’	2.17	0.73
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.87	0.73
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.69	0.73
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.68	0.73
30:0:2769:C:O2’	30:0:2770:G:H5’	1.89	0.73
30:0:1441:G:O2’	30:0:1442:A:H5’	1.88	0.73
30:0:281:U:H2’	30:0:282:C:O4’	1.89	0.73
31:9:20:G:O2’	31:9:21:G:H5’	1.89	0.73
1:A:199:HIS:CD2	1:A:201:PHE:H	2.05	0.73
14:N:144:GLY:O	14:N:147:ILE:HG22	1.88	0.72
10:J:70:PHE:HE1	30:0:2676:C:H4’	1.55	0.72
21:U:14:GLU:O	21:U:17:THR:HB	1.90	0.72
38:Y:8907:HOH:O	30:0:1330:A:H5”	1.89	0.72
30:0:1183:C:H42	30:0:1184:C:H41	1.37	0.72
18:R:128:ARG:NH2	30:0:2054:A:N3	2.38	0.72
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.72	0.72
30:0:1666:C:C2’	30:0:1667:A:C5’	2.67	0.72
30:0:2498:C:O2’	30:0:2499:U:H5’	1.90	0.71
21:U:56:ARG:NH2	30:0:2890:A:H1’	2.04	0.71
28:2:43:ARG:HH22	30:0:1684:A:H1’	1.56	0.71
16:P:117:SER:HB3	30:0:1593:C:OP1	1.90	0.71
31:9:2:U:OP2	31:9:3:A:H5’	1.91	0.71
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:34:SER:N	30:0:797:A:H5'	2.04	0.71
30:0:1632:A:H2'	30:0:1633:C:H5'	1.72	0.71
30:0:544:G:H2'	30:0:545:G:H5"	1.73	0.71
30:0:1182:C:H1'	30:0:1192:A:H8	1.54	0.71
30:0:1947:G:H2'	30:0:1948:G:H8	1.55	0.71
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.73	0.71
3:C:139:VAL:HG13	38:C:8650:HOH:O	1.90	0.70
11:K:10:GLN:HE21	11:K:10:GLN:N	1.85	0.70
30:0:960:G:H3'	30:0:960:G:N3	2.05	0.70
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.72	0.70
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.73	0.70
30:0:1172:G:H1'	38:0:4982:HOH:O	1.91	0.70
13:M:171:ARG:CD	30:0:156:C:H5"	2.19	0.70
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.56	0.70
29:3:73:GLU:HB3	38:3:9049:HOH:O	1.91	0.70
30:0:1701:A:H4'	30:0:1702:U:C5'	2.20	0.70
30:0:2768:A:H2'	30:0:2769:C:O4'	1.91	0.70
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.73	0.69
30:0:827:A:H1'	38:0:6233:HOH:O	1.92	0.69
30:0:1525:G:H5'	30:0:1526:A:OP2	1.92	0.69
15:O:3:THR:HG22	30:0:656:G:C5'	2.15	0.69
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.22	0.69
30:0:558:C:H2'	30:0:559:U:H5"	1.72	0.69
30:0:1701:A:H5"	30:0:1702:U:H3'	1.73	0.69
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.75	0.69
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.39	0.69
30:0:870:G:C2'	30:0:871:G:H5"	2.21	0.69
30:0:1058:A:H2'	30:0:1060:C:H5"	1.73	0.69
30:0:2717:C:H2'	30:0:2718:C:C5'	2.19	0.69
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.57	0.69
30:0:1819:G:H2'	30:0:1820:G:H4'	1.73	0.68
12:L:133:VAL:HA	38:L:8878:HOH:O	1.93	0.68
13:M:164:THR:HG22	13:M:167:GLY:N	2.08	0.68
30:0:271:C:H41	30:0:378:A:H2	1.41	0.68
23:W:26:ILE:HB	38:W:5420:HOH:O	1.92	0.68
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.18	0.68
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.75	0.68
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.76	0.68
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.76	0.68
30:0:1679:C:H5'	38:0:9321:HOH:O	1.92	0.68
30:0:1741:U:H5'	30:0:1742:A:OP1	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1730:G:H5'	30:0:1731:C:C5	2.29	0.68
18:R:150:PRO:CG	18:R:150:PRO:O	2.41	0.68
30:0:255:A:H2'	30:0:256:C:C6	2.29	0.68
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.05	0.67
30:0:2256:G:O2'	30:0:2257:G:H5'	1.94	0.67
2:B:162:MET:HG3	2:B:310:ARG:HH11	1.60	0.67
23:W:61:THR:HG23	23:W:151:GLU:HG3	1.76	0.67
30:0:1377:C:H5'	30:0:1377:C:H6	1.59	0.67
30:0:2635:A:O2'	30:0:2636:C:H5'	1.94	0.67
30:0:2769:C:H2'	30:0:2770:G:H5'	1.75	0.67
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.93	0.67
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.77	0.67
30:0:2135:A:O2'	30:0:2136:G:H5'	1.95	0.67
30:0:2827:A:H2'	30:0:2828:G:O4'	1.94	0.67
33:0:8813:CL:CL	38:0:4687:HOH:O	2.50	0.67
31:9:39:U:H1'	31:9:44:A:H61	1.60	0.67
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.59	0.67
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.31	0.67
12:L:6:ARG:HD3	30:0:1299:G:O6	1.95	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.28	0.66
3:C:174:ILE:CD1	30:0:338:C:H4'	2.25	0.66
30:0:185:G:H4'	30:0:186:A:OP1	1.94	0.66
30:0:1189:A:H1'	30:0:1209:C:C1'	2.25	0.66
31:9:14:G:H5'	31:9:14:G:C8	2.29	0.66
9:I:110:ASP:O	30:0:1163:G:H5'	1.96	0.66
30:0:544:G:C2'	30:0:545:G:H5"	2.25	0.66
30:0:1562:C:O2	30:0:1562:C:H2'	1.94	0.66
30:0:2102:G:C2	30:0:2103:A:C6	2.82	0.66
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.78	0.66
5:E:143:GLN:NE2	30:0:2779:G:H21	1.93	0.66
30:0:1205:U:H2'	30:0:1206:U:H5'	1.76	0.66
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.78	0.66
10:J:82:THR:CG2	30:0:1242:A:H5'	2.22	0.66
10:J:107:ASN:HD22	10:J:109:TYR:H	1.43	0.66
30:0:1205:U:H2'	30:0:1206:U:H5"	1.76	0.66
38:B:9099:HOH:O	30:0:2672:C:H1'	1.96	0.66
30:0:2756:U:N3	30:0:2896:A:C2	2.63	0.66
30:0:2787:C:H5	38:0:4636:HOH:O	1.79	0.66
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.78	0.66
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.79	0.65
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1171:A:H2'	30:0:1172:G:H5'	1.78	0.65
30:0:2426:G:H1'	38:0:6110:HOH:O	1.95	0.65
31:9:76:G:H3'	31:9:77:A:C5'	2.20	0.65
30:0:1159:G:H21	30:0:1189:A:H8	1.43	0.65
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.77	0.65
12:L:136:ALA:HB3	38:L:8878:HOH:O	1.96	0.65
3:C:174:ILE:HD11	30:0:338:C:H4'	1.78	0.65
16:P:115:SER:H	16:P:118:GLN:NE2	1.89	0.65
30:0:1835:U:C5	30:0:1840:A:N7	2.58	0.65
30:0:2420:G:O2'	30:0:2421:G:H5'	1.97	0.65
31:9:54:A:O2'	31:9:55:U:H5'	1.97	0.65
30:0:138:U:H5"	30:0:139:C:OP2	1.96	0.65
30:0:2795:C:O2'	30:0:2796:U:H5'	1.97	0.65
14:N:11:ARG:HD3	31:9:114:G:O6	1.97	0.65
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.12	0.65
30:0:308:U:H5'	30:0:309:C:OP1	1.96	0.65
30:0:1947:G:H2'	30:0:1948:G:C8	2.31	0.65
30:0:2769:C:H2'	30:0:2770:G:C5'	2.26	0.65
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.78	0.64
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.12	0.64
2:B:211:THR:HG23	30:0:2840:A:OP1	1.96	0.64
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.80	0.64
25:Y:204:ARG:HH22	30:0:553:G:P	2.21	0.64
30:0:1165:G:N2	30:0:1173:A:H5"	2.13	0.64
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.97	0.64
30:0:1632:A:C2'	30:0:1633:C:H5'	2.27	0.64
27:1:1:THR:HA	38:0:9354:HOH:O	1.98	0.64
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.28	0.64
30:0:542:A:H5'	30:0:542:A:C8	2.25	0.64
30:0:559:U:H6	30:0:559:U:H5'	1.61	0.64
30:0:671:A:O2'	30:0:672:G:H2'	1.98	0.64
30:0:2505:G:O2'	30:0:2506:A:H5'	1.97	0.64
1:A:191:GLY:HA2	1:A:194:MET:CE	2.28	0.64
30:0:1206:U:H2'	30:0:1207:A:O4'	1.96	0.64
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.32	0.63
14:N:37:ARG:NH1	31:9:6:C:C5'	2.50	0.63
24:X:25:ARG:HD2	38:X:5356:HOH:O	1.98	0.63
30:0:1537:C:H1'	38:0:6614:HOH:O	1.97	0.63
1:A:35:GLY:O	1:A:36:ASP:HB3	1.99	0.63
4:D:25:MET:CE	4:D:37:ALA:HB1	2.28	0.63
30:0:272:A:H3'	38:0:7553:HOH:O	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2241:C:O2'	30:0:2242:U:H5'	1.98	0.63
30:0:2526:C:O2'	30:0:2527:U:H5'	1.98	0.63
30:0:2659:U:H5"	38:0:4129:HOH:O	1.98	0.63
31:9:39:U:HO2'	31:9:42:C:H5	1.46	0.63
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.81	0.63
10:J:107:ASN:ND2	10:J:109:TYR:H	1.96	0.63
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.13	0.63
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.80	0.63
8:H:165:ARG:HD2	38:H:8578:HOH:O	1.98	0.63
12:L:41:HIS:HD2	30:0:926:A:O2'	1.82	0.63
30:0:1174:A:C5	30:0:1201:C:H4'	2.33	0.63
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.34	0.63
21:U:9:CYS:HA	21:U:52:THR:HG23	1.81	0.63
30:0:2010:A:H2'	38:0:5975:HOH:O	1.98	0.63
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.81	0.63
16:P:59:ARG:HH22	16:P:66:GLN:NE2	1.96	0.63
30:0:613:C:H2'	30:0:614:U:H6	1.63	0.63
30:0:1342:C:C2'	30:0:1343:C:H5'	2.28	0.63
30:0:2894:C:O2'	30:0:2895:C:H5'	1.98	0.63
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.80	0.63
30:0:1165:G:H21	30:0:1173:A:H5"	1.63	0.63
30:0:1187:U:O2'	30:0:1189:A:H2	1.75	0.63
30:0:441:A:H1'	30:0:442:A:N7	2.14	0.62
23:W:88:THR:HG22	23:W:89:ASP:H	1.64	0.62
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.80	0.62
30:0:2111:G:H1'	38:0:9050:HOH:O	1.98	0.62
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.80	0.62
30:0:281:U:O2'	30:0:282:C:H5'	1.99	0.62
2:B:258:GLY:H	2:B:260:HIS:CE1	2.17	0.62
30:0:1119:G:H22	30:0:1246:A:H2	1.36	0.62
30:0:2756:U:N3	30:0:2896:A:H2	1.95	0.62
30:0:482:G:H4'	30:0:508:A:N1	2.15	0.62
30:0:2851:G:O2'	30:0:2852:A:H5'	2.00	0.62
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.15	0.62
28:2:41:HIS:HD2	28:2:44:ARG:H	1.47	0.62
4:D:154:LYS:HD2	4:D:154:LYS:N	2.09	0.62
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.00	0.62
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.82	0.62
30:0:280:C:H2'	30:0:281:U:O4'	2.00	0.62
30:0:1603:A:C5'	30:0:1605:G:H5'	2.29	0.62
30:0:2256:G:C2'	30:0:2257:G:H5'	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:76:G:C3'	31:9:77:A:H5"	2.20	0.62
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.15	0.61
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.65	0.61
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.82	0.61
30:0:2524:G:H21	30:0:2526:C:N4	1.98	0.61
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.30	0.61
14:N:80:SER:HB2	38:N:8836:HOH:O	1.99	0.61
30:0:1667:A:H5'	30:0:1667:A:C8	2.33	0.61
31:9:7:G:H5'	38:9:9097:HOH:O	2.00	0.61
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.40	0.61
29:3:48:ASN:HD21	30:0:2468:A:H61	1.48	0.61
30:0:1477:C:H5'	30:0:1868:G:C5'	2.30	0.61
30:0:2507:G:H2'	30:0:2510:C:N4	2.15	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.27	0.61
1:A:51:ARG:HB2	38:A:9061:HOH:O	1.99	0.61
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.01	0.61
30:0:125:U:H2'	38:0:3765:HOH:O	1.99	0.61
30:0:2563:U:H2'	30:0:2565:C:O5'	2.00	0.61
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.30	0.61
30:0:812:A:H1'	38:0:3959:HOH:O	2.00	0.61
30:0:2300:A:H4'	30:0:2301:A:O5'	2.01	0.61
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.65	0.61
30:0:1741:U:O2'	30:0:2723:G:H4'	2.00	0.61
2:B:145:HIS:HD2	2:B:146:THR:O	1.83	0.61
2:B:238:ASN:HD22	2:B:240:GLY:N	1.92	0.61
3:C:184:ARG:NH2	30:0:450:C:OP1	2.30	0.61
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.81	0.61
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.01	0.61
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.82	0.61
30:0:1132:A:N6	30:0:1229:C:H2'	2.16	0.61
30:0:2781:U:H2'	30:0:2782:G:H5'	1.82	0.61
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.14	0.61
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.82	0.61
30:0:285:A:H2'	30:0:286:U:O4'	2.00	0.61
31:9:95:C:O2'	31:9:96:C:H5'	2.01	0.61
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.65	0.60
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.83	0.60
30:0:2320:U:H4'	30:0:2321:A:O4'	2.01	0.60
31:9:75:G:H1	31:9:106:U:H3	1.49	0.60
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.82	0.60
11:K:10:GLN:H	11:K:10:GLN:NE2	1.87	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:299:U:H5'	38:0:7361:HOH:O	2.01	0.60
6:F:91:VAL:HG12	6:F:92:GLY:N	2.17	0.60
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.16	0.60
30:0:2781:U:C2'	30:0:2782:G:H5'	2.31	0.60
30:0:1528:A:H2'	30:0:1529:G:O4'	2.01	0.60
30:0:1641:A:C2'	30:0:1642:A:H5'	2.30	0.60
30:0:1819:G:H5'	38:0:4715:HOH:O	2.01	0.60
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.64	0.60
4:D:103:ASN:ND2	4:D:134:LEU:H	1.99	0.60
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.98	0.60
30:0:1972:U:H2'	30:0:1973:A:C5'	2.31	0.60
3:C:214:THR:HG23	38:C:8639:HOH:O	2.01	0.60
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.83	0.60
10:J:90:LYS:HB2	33:J:8802:CL:CL	2.38	0.60
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.82	0.60
28:2:38:LYS:HE3	38:0:4230:HOH:O	2.02	0.60
30:0:123:U:H5'	38:0:6683:HOH:O	2.01	0.60
31:9:55:U:H4'	31:9:56:A:C8	2.36	0.60
22:V:39:ALA:N	22:V:40:PRO:HD2	2.16	0.60
30:0:1730:G:H5"	30:0:1731:C:H6	1.67	0.60
23:W:80:ASP:O	23:W:84:VAL:HG23	2.02	0.60
30:0:510:U:H6	38:0:7463:HOH:O	1.85	0.60
30:0:2252:A:C5	30:0:2253:G:H1'	2.37	0.60
27:1:28:HIS:HE1	30:0:776:A:OP1	1.85	0.60
30:0:2505:G:C2'	30:0:2506:A:H5'	2.32	0.60
1:A:211:LYS:HB2	38:A:9075:HOH:O	2.02	0.59
3:C:236:THR:HG22	3:C:239:ALA:N	2.13	0.59
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.36	0.59
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.31	0.59
25:Y:212:ARG:HD2	38:Y:8896:HOH:O	2.00	0.59
30:0:960:G:N3	30:0:960:G:C2'	2.64	0.59
30:0:2878:U:H2'	30:0:2879:A:O4'	2.01	0.59
30:0:272:A:H5'	30:0:273:G:OP2	2.02	0.59
30:0:681:G:N3	30:0:681:G:H5'	2.17	0.59
31:9:91:C:H2'	31:9:92:G:O4'	2.02	0.59
30:0:1667:A:H2'	30:0:1668:U:C6	2.37	0.59
30:0:1730:G:C5'	30:0:1731:C:C6	2.85	0.59
18:R:117:HIS:HD2	30:0:20:G:H21	1.51	0.59
30:0:204:A:H2'	30:0:205:U:H5'	1.84	0.59
30:0:249:G:O2'	30:0:250:C:H5'	2.03	0.59
7:G:12:ILE:HG23	38:0:5471:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:39:THR:HG23	18:R:107:GLU:O	2.02	0.59
30:0:515:C:H5"	38:0:5654:HOH:O	2.02	0.59
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.03	0.59
30:0:848:C:H5'	38:0:7295:HOH:O	2.02	0.59
30:0:961:A:H4'	38:0:6802:HOH:O	2.01	0.59
30:0:1878:G:O2'	30:0:1879:U:C6	2.54	0.59
26:Z:34:SER:HB2	38:Z:8715:HOH:O	2.02	0.59
30:0:1165:G:H4'	30:0:1174:A:O2'	2.03	0.59
30:0:2670:G:O2'	30:0:2671:U:H5'	2.02	0.59
3:C:236:THR:HA	38:C:8653:HOH:O	2.01	0.59
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.05	0.59
30:0:853:C:H3'	38:0:4553:HOH:O	2.03	0.59
31:9:52:A:O2'	31:9:53:G:H5'	2.03	0.59
3:C:1:MET:HG2	3:C:2:GLN:N	2.18	0.59
19:S:43:GLU:HB3	38:S:8997:HOH:O	2.02	0.59
30:0:1163:G:H1	30:0:1184:C:N4	2.01	0.59
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.03	0.58
4:D:57:THR:HG23	4:D:63:ILE:HA	1.84	0.58
30:0:316:A:N3	30:0:336:G:O2'	2.34	0.58
30:0:2649:A:H5'	30:0:2649:A:H8	1.68	0.58
31:9:22:G:H5'	31:9:23:U:OP1	2.03	0.58
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.85	0.58
30:0:204:A:C2'	30:0:205:U:H5'	2.32	0.58
30:0:2718:C:H6	30:0:2718:C:H5'	1.68	0.58
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.32	0.58
28:2:10:ARG:NH2	30:0:121:U:OP2	2.34	0.58
30:0:283:U:C5	30:0:284:C:N3	2.70	0.58
30:0:1834:C:H2'	30:0:1840:A:N6	2.17	0.58
5:E:111:LYS:HE3	30:0:2690:U:H4'	1.85	0.58
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.86	0.58
30:0:12:U:H2'	30:0:13:G:H5'	1.84	0.58
30:0:485:A:N3	30:0:487:G:H5"	2.18	0.58
30:0:2251:G:H2'	30:0:2252:A:C8	2.39	0.58
30:0:2643:G:H5"	38:0:3928:HOH:O	2.04	0.58
4:D:25:MET:HE1	4:D:37:ALA:HB1	1.84	0.58
30:0:558:C:H2'	30:0:559:U:H5'	1.84	0.58
30:0:2064:U:H5'	30:0:2652:U:O3'	2.04	0.58
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.30	0.58
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.84	0.58
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.86	0.58
30:0:1189:A:O2'	30:0:1208:C:H2'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:1:U:O3'	31:9:3:A:H5"	2.03	0.58
30:0:541:C:H2'	30:0:542:A:H5'	1.85	0.58
30:0:1942:A:H3'	38:0:7371:HOH:O	2.03	0.58
30:0:214:U:H5'	38:0:6160:HOH:O	2.03	0.58
30:0:318:U:H5'	30:0:339:A:C2	2.39	0.58
2:B:41:PHE:HB3	2:B:190:MET:HE1	1.85	0.58
30:0:119:A:H2'	30:0:120:A:H5"	1.84	0.58
31:9:39:U:H1'	31:9:44:A:N6	2.19	0.58
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.34	0.58
30:0:304:G:H1'	30:0:347:A:N6	2.18	0.58
30:0:559:U:C5	30:0:560:U:C5	2.92	0.58
30:0:1181:A:C2'	30:0:1182:C:H5'	2.34	0.58
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.37	0.57
25:Y:174:VAL:HG23	25:Y:177:LYS:HD2	1.85	0.57
2:B:125:GLU:O	2:B:129:ARG:HG3	2.04	0.57
5:E:100:ASP:HB2	38:E:2789:HOH:O	2.03	0.57
30:0:1524:U:OP1	30:0:1524:U:H4'	2.04	0.57
30:0:1603:A:H5'	30:0:1605:G:C4'	2.34	0.57
14:N:37:ARG:HH11	31:9:6:C:H5"	1.64	0.57
15:O:25:VAL:HG12	30:0:709:G:O2'	2.04	0.57
16:P:64:GLU:HG2	38:P:168:HOH:O	2.03	0.57
1:A:179:MET:HG2	1:A:186:TRP:CB	2.35	0.57
3:C:236:THR:HG21	38:C:8577:HOH:O	2.03	0.57
22:V:55:ARG:O	22:V:59:ILE:HG12	2.05	0.57
30:0:1249:U:H2'	30:0:1250:C:C6	2.39	0.57
30:0:2832:C:H5	38:0:7237:HOH:O	1.87	0.57
31:9:52:A:H2'	31:9:53:G:O4'	2.04	0.57
2:B:41:PHE:HA	2:B:79:MET:HE2	1.86	0.57
27:1:25:LYS:HD2	28:2:49:GLU:H	1.69	0.57
30:0:1377:C:H5'	30:0:1377:C:C6	2.40	0.57
30:0:2361:A:H5'	30:0:2361:A:H8	1.70	0.57
7:G:20:VAL:O	7:G:24:VAL:HG23	2.05	0.57
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.85	0.57
30:0:558:C:C2'	30:0:559:U:C5'	2.77	0.57
30:0:2478:U:O2'	30:0:2479:A:H5'	2.04	0.57
1:A:36:ASP:O	1:A:38:ILE:N	2.38	0.57
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.70	0.57
5:E:149:GLU:HG3	5:E:167:TYR:HA	1.84	0.57
30:0:2102:G:H1'	30:0:2103:A:N7	2.20	0.57
17:Q:25:PRO:HB2	38:9:9078:HOH:O	2.04	0.57
30:0:1116:U:O2'	30:0:1118:A:C2	2.46	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:13:MET:HE3	23:W:18:GLN:HA	1.87	0.56
30:0:960:G:N3	30:0:960:G:C3'	2.68	0.56
30:0:1183:C:N3	30:0:1184:C:C5	2.73	0.56
30:0:1200:A:H3'	38:0:5763:HOH:O	2.05	0.56
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.39	0.56
30:0:567:U:H5"	38:0:5297:HOH:O	2.05	0.56
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.05	0.56
12:L:41:HIS:CD2	30:0:926:A:O2'	2.58	0.56
18:R:9:ASP:O	18:R:13:THR:HB	2.05	0.56
27:1:10:LYS:HG3	38:1:8979:HOH:O	2.04	0.56
30:0:2256:G:H2'	30:0:2257:G:C5'	2.35	0.56
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.88	0.56
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.71	0.56
30:0:1160:G:H2'	38:0:5641:HOH:O	2.04	0.56
30:0:1398:G:O2'	30:0:1399:A:H5'	2.06	0.56
30:0:65:C:O2'	30:0:66:G:H5'	2.05	0.56
30:0:1730:G:H5"	30:0:1731:C:C6	2.41	0.56
30:0:2679:G:H2'	30:0:2681:A:OP2	2.06	0.56
30:0:185:G:H4'	30:0:186:A:H4'	1.86	0.56
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.39	0.56
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.06	0.56
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.87	0.56
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.88	0.56
30:0:559:U:H5'	30:0:559:U:C6	2.40	0.56
30:0:856:G:C8	38:0:5439:HOH:O	2.52	0.56
30:0:952:G:H4'	38:0:4035:HOH:O	2.06	0.56
30:0:1778:A:H2'	30:0:1779:A:H5'	1.87	0.56
30:0:2505:G:H2'	30:0:2506:A:H5'	1.87	0.56
30:0:2509:A:OP2	30:0:2510:C:H5	1.89	0.56
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.86	0.56
30:0:73:U:O2'	30:0:74:G:H5'	2.05	0.56
30:0:1044:C:H5"	38:0:9026:HOH:O	2.05	0.56
30:0:1819:G:H2'	30:0:1820:G:C4'	2.36	0.56
1:A:48:ASP:HB3	38:A:9061:HOH:O	2.06	0.56
8:H:30:LYS:H	8:H:62:HIS:CD2	2.16	0.56
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.89	0.56
25:Y:141:THR:HG23	38:Y:8883:HOH:O	2.05	0.56
30:0:567:U:C5'	38:0:6425:HOH:O	2.49	0.56
30:0:2353:A:H4'	30:0:2354:A:O5'	2.06	0.56
22:V:42:ASN:HB3	38:0:7451:HOH:O	2.06	0.56
23:W:84:VAL:HG12	38:W:6679:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:282:C:O2'	30:0:283:U:C5'	2.52	0.56
30:0:1615:A:H5'	38:0:4186:HOH:O	2.04	0.56
30:0:2089:A:O2'	30:0:2090:G:H5'	2.06	0.55
30:0:2316:G:H4'	38:0:6110:HOH:O	2.06	0.55
30:0:2372:A:H2'	30:0:2373:U:C6	2.41	0.55
30:0:999:C:O2'	30:0:1000:C:H5'	2.07	0.55
30:0:1625:U:H6	30:0:1625:U:H3'	1.70	0.55
1:A:51:ARG:NH1	1:A:120:ARG:O	2.39	0.55
3:C:25:PRO:HG2	38:C:8523:HOH:O	2.06	0.55
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.95	0.55
1:A:223:ARG:HD2	30:0:2272:G:OP1	2.06	0.55
4:D:159:PRO:O	4:D:163:VAL:HG23	2.06	0.55
13:M:188:ARG:HD3	30:0:155:C:OP2	2.05	0.55
30:0:1167:G:H2'	30:0:1168:C:O4'	2.07	0.55
30:0:1205:U:C2'	30:0:1206:U:C5'	2.84	0.55
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.88	0.55
27:1:16:HIS:HD2	30:0:470:U:O2'	1.88	0.55
30:0:10:U:O4	30:0:532:A:OP2	2.23	0.55
30:0:1175:G:H1'	30:0:1193:A:C2'	2.34	0.55
30:0:1181:A:H2'	30:0:1182:C:H5'	1.87	0.55
30:0:2649:A:H5'	30:0:2649:A:C8	2.42	0.55
2:B:244:PRO:HB3	30:0:1234:U:N3	2.21	0.55
7:G:64:ASN:HD22	7:G:64:ASN:N	2.04	0.55
24:X:30:MET:HG2	30:0:1384:C:H5'	1.88	0.55
30:0:821:U:H2'	30:0:822:C:H6	1.71	0.55
30:0:1474:C:H6	30:0:1474:C:C5'	2.12	0.55
30:0:1527:A:H1'	30:0:1528:A:C8	2.42	0.55
30:0:2330:U:H4'	30:0:2331:C:OP1	2.06	0.55
30:0:1406:A:H4'	30:0:1407:A:H5"	1.87	0.55
30:0:2238:A:O2'	30:0:2239:C:H5'	2.07	0.55
30:0:2344:G:H2'	30:0:2344:G:N3	2.21	0.55
31:9:1:U:H5"	31:9:3:A:OP1	2.06	0.55
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.16	0.55
4:D:103:ASN:HD22	4:D:134:LEU:H	1.54	0.55
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.86	0.55
25:Y:235:GLU:CD	25:Y:235:GLU:H	2.09	0.55
30:0:941:G:C5	30:0:942:U:C4	2.95	0.55
30:0:1321:A:H2'	30:0:1322:G:C8	2.41	0.55
2:B:305:ASP:O	2:B:306:LYS:HB2	2.07	0.55
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.07	0.55
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.86	0.55
30:0:2472:C:O2'	30:0:2634:G:H4'	2.07	0.55
30:0:2851:G:C2'	30:0:2852:A:H5'	2.36	0.55
18:R:99:ALA:HB1	18:R:109:MET:CE	2.35	0.55
23:W:154:ARG:NH1	30:0:588:G:O6	2.39	0.55
30:0:1202:A:H2'	30:0:1203:G:O4'	2.07	0.55
30:0:1393:A:H2'	30:0:1394:C:C6	2.42	0.55
30:0:2414:A:H2'	30:0:2415:A:C8	2.41	0.55
18:R:39:THR:HG22	18:R:42:GLU:H	1.72	0.54
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.06	0.54
30:0:90:A:H2'	30:0:91:G:O4'	2.07	0.54
30:0:396:U:O2'	30:0:418:C:H4'	2.07	0.54
30:0:960:G:N3	30:0:960:G:H2'	2.20	0.54
30:0:1193:A:C2	30:0:1194:A:N6	2.75	0.54
30:0:1589:G:N2	30:0:1605:G:H1'	2.21	0.54
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.88	0.54
20:T:2:LYS:HG2	30:0:447:A:OP1	2.07	0.54
30:0:1130:U:H2'	30:0:1131:G:O4'	2.07	0.54
30:0:2432:C:O2'	30:0:2433:A:H5'	2.07	0.54
31:9:49:G:H2'	31:9:50:G:O4'	2.07	0.54
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.47	0.54
30:0:595:U:H2'	30:0:596:C:H6	1.72	0.54
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.40	0.54
2:B:62:ARG:HA	2:B:65:MET:CE	2.38	0.54
12:L:18:HIS:HD2	30:0:902:G:N7	2.05	0.54
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.90	0.54
14:N:141:ARG:HH21	31:9:48:C:H4'	1.72	0.54
30:0:128:A:O2'	30:0:129:A:H5'	2.07	0.54
30:0:1080:C:H4'	30:0:1081:A:OP1	2.07	0.54
30:0:1909:A:N1	30:0:2128:G:H1'	2.23	0.54
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.72	0.54
21:U:50:GLU:HB2	30:0:2866:U:C5	2.42	0.54
30:0:522:U:O2'	30:0:1366:C:H5'	2.07	0.54
30:0:794:U:H3	30:0:819:A:H61	1.55	0.54
31:9:36:C:C5	31:9:37:C:C5	2.95	0.54
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.21	0.54
30:0:1279:U:O2	30:0:1279:U:H2'	2.07	0.54
31:9:49:G:O2'	31:9:50:G:H5'	2.08	0.54
1:A:36:ASP:HB2	1:A:85:SER:H	1.73	0.54
1:A:97:ALA:HA	1:A:131:HIS:HE2	1.73	0.54
23:W:64:THR:O	23:W:68:THR:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1972:U:H2'	30:0:1973:A:H5'	1.89	0.54
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.90	0.54
17:Q:15:LYS:HD3	30:0:2364:A:H5"	1.89	0.54
18:R:98:ASN:HD21	30:0:500:G:H21	1.54	0.54
24:X:43:VAL:HG12	24:X:44:ASP:N	2.23	0.54
27:1:20:ARG:HG2	30:0:111:C:O2'	2.08	0.54
30:0:694:A:H2'	30:0:695:C:H5'	1.90	0.54
2:B:212:GLN:HA	30:0:1733:A:H4'	1.89	0.54
9:I:120:ALA:O	9:I:124:VAL:HG23	2.08	0.54
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.40	0.54
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.41	0.54
27:1:9:GLY:HA2	30:0:1687:C:O2	2.08	0.54
30:0:1730:G:H5'	30:0:1731:C:H5	1.72	0.54
30:0:1819:G:H2'	30:0:1820:G:C5'	2.38	0.54
30:0:2419:U:H5"	30:0:2420:G:H5'	1.89	0.54
3:C:132:ASP:HB3	38:C:8566:HOH:O	2.09	0.54
7:G:16:LYS:O	7:G:20:VAL:HG23	2.07	0.54
21:U:52:THR:HG22	21:U:54:THR:H	1.73	0.54
30:0:952:G:N3	30:0:2302:A:H2'	2.23	0.54
30:0:1484:G:H2'	38:0:9107:HOH:O	2.08	0.54
30:0:1947:G:N2	30:0:1966:U:C2	2.76	0.54
15:O:37:ARG:HD2	30:0:656:G:OP2	2.08	0.53
30:0:807:A:O2'	30:0:808:A:H5'	2.08	0.53
30:0:1158:G:O2'	30:0:1159:G:H5'	2.09	0.53
30:0:1209:C:H2'	30:0:1210:G:H8	1.71	0.53
30:0:1307:A:H2'	30:0:1308:A:C8	2.43	0.53
31:9:39:U:H3'	31:9:40:C:H5"	1.91	0.53
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.73	0.53
6:F:57:GLU:O	6:F:61:MET:HG3	2.08	0.53
30:0:1514:C:O2'	30:0:1515:A:H5'	2.09	0.53
22:V:64:GLY:O	22:V:65:ASP:HB2	2.08	0.53
2:B:265:LEU:HD21	2:B:316:ARG:HD3	1.90	0.53
6:F:101:ALA:HA	38:F:5413:HOH:O	2.09	0.53
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.09	0.53
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.72	0.53
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.44	0.53
30:0:876:A:H2'	30:0:876:A:N3	2.24	0.53
8:H:155:ARG:NH1	30:0:2503:A:H5"	2.23	0.53
21:U:37:GLU:HB3	38:U:408:HOH:O	2.08	0.53
23:W:115:THR:HG23	38:W:5420:HOH:O	2.08	0.53
30:0:1174:A:C6	30:0:1201:C:H4'	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.39	0.53
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.38	0.53
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.24	0.53
30:0:39:G:N2	30:0:444:C:C2	2.77	0.53
30:0:625:U:H5"	30:0:1044:C:N4	2.24	0.53
30:0:1202:A:C2'	30:0:1203:G:H5'	2.39	0.53
30:0:2121:G:O2'	30:0:2122:C:H5'	2.08	0.53
3:C:43:LYS:HG2	30:0:449:A:N7	2.24	0.53
8:H:170:ARG:HD2	38:H:8536:HOH:O	2.08	0.53
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.44	0.53
10:J:74:ARG:O	10:J:78:ILE:HG12	2.08	0.53
30:0:1342:C:O2'	30:0:1343:C:H5'	2.08	0.53
30:0:2598:U:O2	30:0:2600:A:H8	1.92	0.53
31:9:55:U:H4'	31:9:56:A:H8	1.72	0.53
1:A:121:ALA:O	1:A:124:VAL:HG22	2.08	0.53
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.90	0.53
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.44	0.53
30:0:1060:C:H6	30:0:1060:C:H5'	1.73	0.53
30:0:1878:G:O2'	30:0:1879:U:P	2.67	0.53
18:R:29:LYS:HE2	30:0:524:A:H5'	1.91	0.53
30:0:1925:G:O2'	30:0:1926:G:H5'	2.09	0.53
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.39	0.53
20:T:38:ARG:NH1	38:0:6714:HOH:O	2.41	0.53
23:W:21:LEU:O	23:W:26:ILE:HG23	2.09	0.53
25:Y:133:HIS:HD2	38:Y:8876:HOH:O	1.91	0.53
30:0:364:U:H2'	30:0:365:G:O4'	2.09	0.53
30:0:1181:A:N1	30:0:1192:A:O2'	2.39	0.53
30:0:1183:C:H2'	30:0:1183:C:O2	2.08	0.53
30:0:1185:U:H5'	38:0:7491:HOH:O	2.08	0.53
30:0:2578:G:H5'	30:0:2578:G:C8	2.40	0.53
30:0:2781:U:H2'	30:0:2782:G:C5'	2.38	0.53
30:0:2812:A:C2	30:0:2814:A:N6	2.67	0.53
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.38	0.52
11:K:66:ARG:HH22	30:0:1994:A:P	2.32	0.52
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.06	0.52
30:0:138:U:OP2	30:0:139:C:H5	1.92	0.52
30:0:277:U:O2'	30:0:278:A:H5'	2.09	0.52
30:0:814:G:H4'	38:0:3135:HOH:O	2.09	0.52
3:C:95:GLU:HG3	38:C:8680:HOH:O	2.09	0.52
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.72	0.52
4:D:154:LYS:H	4:D:154:LYS:CD	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:44:MET:CE	30:0:944:G:H21	2.22	0.52
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.90	0.52
30:0:1120:U:C5'	30:0:1121:G:OP2	2.56	0.52
30:0:2256:G:H2'	30:0:2257:G:H5'	1.89	0.52
2:B:85:ARG:NH1	38:B:9099:HOH:O	2.42	0.52
30:0:136:C:H2'	30:0:137:U:O4'	2.08	0.52
30:0:1131:G:C6	30:0:1230:A:C4	2.98	0.52
30:0:1714:C:O2'	30:0:1715:C:H5'	2.08	0.52
30:0:2010:A:C2'	38:0:5975:HOH:O	2.54	0.52
30:0:2252:A:H2'	30:0:2253:G:H5'	1.90	0.52
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.91	0.52
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.91	0.52
5:E:69:ILE:HA	5:E:72:MET:CE	2.39	0.52
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.92	0.52
12:L:134:GLU:HG3	38:L:8861:HOH:O	2.09	0.52
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.09	0.52
30:0:545:G:H8	30:0:545:G:C5'	2.06	0.52
30:0:1171:A:C2'	30:0:1172:G:H5'	2.39	0.52
30:0:1787:C:H4'	30:0:2883:A:O4'	2.10	0.52
31:9:64:C:C2'	31:9:65:A:H5'	2.39	0.52
5:E:9:GLU:HA	38:E:5240:HOH:O	2.08	0.52
8:H:30:LYS:N	8:H:62:HIS:HD2	2.02	0.52
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.92	0.52
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.09	0.52
22:V:44:GLY:HA3	30:0:92:G:H4'	1.92	0.52
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.09	0.52
30:0:256:C:H2'	30:0:257:G:O4'	2.10	0.52
30:0:1205:U:C2'	30:0:1206:U:H5"	2.37	0.52
30:0:1206:U:H6	30:0:1206:U:C5'	2.19	0.52
30:0:1268:C:O2'	30:0:1269:G:H5'	2.09	0.52
30:0:2281:C:C2'	30:0:2282:U:H5'	2.39	0.52
31:9:13:A:O2'	31:9:14:G:H5"	2.09	0.52
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.74	0.52
26:Z:40:ALA:HA	30:0:1773:G:C8	2.45	0.52
30:0:228:C:H2'	30:0:229:G:H5'	1.91	0.52
30:0:1339:G:C6	30:0:1340:G:N1	2.78	0.52
30:0:1342:C:H2'	30:0:1343:C:H5'	1.92	0.52
31:9:12:C:H5'	31:9:70:U:O4'	2.09	0.52
22:V:1:THR:CB	30:0:93:C:H5"	2.32	0.52
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.92	0.52
30:0:319:A:H4'	30:0:338:C:C4	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:603:A:H1'	30:0:605:C:C2	2.45	0.52
30:0:1130:U:H5'	38:0:7694:HOH:O	2.08	0.52
30:0:1187:U:H2'	38:0:6927:HOH:O	2.10	0.52
30:0:1636:G:O2'	30:0:1637:A:H5'	2.09	0.52
30:0:2102:G:N3	30:0:2103:A:C5	2.78	0.52
30:0:2493:C:O2	30:0:2493:C:H2'	2.09	0.52
3:C:140:VAL:HB	38:C:8653:HOH:O	2.09	0.52
5:E:69:ILE:HA	5:E:72:MET:HE3	1.91	0.52
6:F:91:VAL:HG11	30:0:262:A:OP2	2.10	0.52
13:M:179:GLY:O	30:0:399:C:H5'	2.10	0.52
17:Q:95:GLU:HA	30:0:949:U:H4'	1.90	0.52
24:X:78:GLU:HG2	24:X:79:GLU:H	1.75	0.52
30:0:369:G:H2'	30:0:370:G:H8	1.75	0.52
30:0:1087:G:H4'	30:0:1088:A:OP1	2.10	0.52
20:T:9:LYS:HB2	38:0:7449:HOH:O	2.10	0.52
1:A:99:ILE:O	1:A:131:HIS:HE1	1.93	0.51
2:B:294:TYR:HE2	38:B:9114:HOH:O	1.93	0.51
26:Z:57:MET:HE3	38:0:6301:HOH:O	2.10	0.51
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.91	0.51
30:0:541:C:C2'	30:0:542:A:C5'	2.76	0.51
30:0:1081:A:H5"	38:0:3155:HOH:O	2.09	0.51
30:0:1182:C:C1'	30:0:1192:A:H8	2.22	0.51
30:0:1205:U:H5	38:0:4440:HOH:O	1.94	0.51
30:0:1406:A:H5'	30:0:1407:A:C8	2.45	0.51
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.40	0.51
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.93	0.51
3:C:233:THR:HG22	3:C:234:VAL:H	1.75	0.51
5:E:11:VAL:HG12	5:E:12:ASP:N	2.26	0.51
8:H:19:ARG:HH12	30:0:1008:C:H5"	1.75	0.51
10:J:107:ASN:HD22	10:J:107:ASN:C	2.11	0.51
13:M:163:LEU:HD21	30:0:188:C:H5"	1.91	0.51
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.11	0.51
30:0:669:G:O2'	30:0:670:G:H5'	2.10	0.51
30:0:1595:G:O2'	30:0:1596:U:H5'	2.10	0.51
30:0:2064:U:H4'	30:0:2653:A:OP1	2.10	0.51
30:0:2415:A:H2'	30:0:2416:G:H5'	1.92	0.51
30:0:2511:A:H2'	30:0:2512:U:O4'	2.09	0.51
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.11	0.51
6:F:96:ALA:HA	38:F:3111:HOH:O	2.09	0.51
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.91	0.51
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:856:G:H2'	38:0:5439:HOH:O	2.08	0.51
30:0:2102:G:N2	30:0:2103:A:C6	2.78	0.51
30:0:2637:A:H4'	38:0:4938:HOH:O	2.10	0.51
31:9:31:C:H2'	31:9:32:G:O4'	2.11	0.51
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.11	0.51
30:0:264:G:H1'	30:0:265:U:H5	1.76	0.51
30:0:644:G:H5'	30:0:644:G:N3	2.25	0.51
30:0:2372:A:H2'	30:0:2373:U:H6	1.74	0.51
2:B:98:THR:HG22	30:0:2820:A:OP1	2.10	0.51
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.91	0.51
3:C:233:THR:HG22	3:C:234:VAL:N	2.25	0.51
4:D:141:VAL:HG21	31:9:57:A:H8	1.76	0.51
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.46	0.51
8:H:66:GLU:HA	38:H:8576:HOH:O	2.10	0.51
16:P:54:LYS:HB2	30:0:1717:A:H5"	1.93	0.51
30:0:1119:G:N2	30:0:1246:A:H2	2.01	0.51
30:0:1766:U:O2	30:0:1778:A:H5'	2.10	0.51
30:0:1838:U:O2'	30:0:2644:C:H5'	2.10	0.51
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.93	0.51
18:R:150:PRO:CG	18:R:150:PRO:CB	2.88	0.51
30:0:69:A:H8	30:0:69:A:C5'	2.23	0.51
30:0:200:C:H2'	38:0:3443:HOH:O	2.10	0.51
30:0:1506:U:H6	30:0:1506:U:H5'	1.75	0.51
1:A:109:GLU:HG2	1:A:116:GLY:N	2.26	0.51
4:D:76:ARG:NE	31:9:44:A:O4'	2.44	0.51
8:H:5:PRO:HD2	8:H:8:MET:SD	2.50	0.51
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.93	0.51
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.91	0.51
30:0:1972:U:H2'	30:0:1973:A:H5"	1.92	0.51
3:C:168:ARG:NH2	3:C:190:ALA:O	2.44	0.51
5:E:84:MET:HG2	5:E:168:ILE:HA	1.92	0.51
30:0:162:C:H2'	30:0:163:U:H5'	1.93	0.51
30:0:1166:A:P	30:0:1174:A:H4'	2.51	0.51
1:A:33:GLU:H	1:A:33:GLU:CD	2.15	0.51
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.92	0.51
30:0:255:A:C5	30:0:256:C:C5	2.99	0.51
30:0:816:G:C6	30:0:817:G:N1	2.79	0.51
30:0:1163:G:C2	30:0:1184:C:N3	2.79	0.51
30:0:1165:G:N2	30:0:1173:A:C5'	2.74	0.51
30:0:1589:G:H22	30:0:1605:G:H1'	1.76	0.51
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:139:GLY:O	23:W:141:HIS:HD2	1.94	0.51
30:0:506:G:N2	30:0:509:A:H5"	2.22	0.51
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.51
30:0:1477:C:O2'	30:0:1478:U:H5'	2.10	0.51
30:0:1878:G:C1'	38:0:6139:HOH:O	2.45	0.51
30:0:2438:G:H2'	30:0:2439:C:O4'	2.11	0.51
30:0:2900:G:H2'	30:0:2901:C:O4'	2.11	0.51
3:C:206:ASN:HB2	30:0:329:A:OP2	2.11	0.50
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.11	0.50
11:K:8:VAL:HG13	11:K:80:ILE:HG22	1.93	0.50
14:N:110:THR:HB	14:N:113:SER:OG	2.11	0.50
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.41	0.50
21:U:33:SER:O	21:U:37:GLU:HG3	2.10	0.50
27:1:42:SER:HB2	38:1:8956:HOH:O	2.12	0.50
29:3:70:ARG:HB3	38:3:9062:HOH:O	2.10	0.50
30:0:1373:G:H1'	38:0:6157:HOH:O	2.10	0.50
31:9:114:G:H2'	31:9:115:C:C6	2.46	0.50
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.93	0.50
9:I:126:THR:O	9:I:130:LEU:HG	2.12	0.50
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.93	0.50
19:S:37:VAL:O	19:S:41:VAL:HG23	2.12	0.50
19:S:76:GLU:HB3	38:S:8999:HOH:O	2.11	0.50
27:1:21:ARG:HD2	27:1:39:PHE:HB2	1.94	0.50
30:0:1586:G:O2'	30:0:1587:U:H5'	2.10	0.50
30:0:2526:C:C6	30:0:2526:C:H5'	2.46	0.50
30:0:2587:OMU:H2'	30:0:2589:U:H5"	1.93	0.50
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.42	0.50
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.93	0.50
20:T:26:THR:HA	20:T:39:ASN:HB3	1.92	0.50
30:0:291:C:H2'	30:0:292:G:O4'	2.11	0.50
30:0:1730:G:C5'	30:0:1731:C:C5	2.93	0.50
30:0:1903:U:O2'	30:0:1904:A:N7	2.43	0.50
1:A:212:PRO:HB2	38:A:9024:HOH:O	2.11	0.50
3:C:79:ARG:O	3:C:87:ARG:HG2	2.12	0.50
7:G:23:ILE:O	7:G:27:ILE:HG13	2.11	0.50
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.93	0.50
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.92	0.50
30:0:369:G:O2'	30:0:370:G:H5'	2.12	0.50
30:0:1202:A:O2'	30:0:1203:G:H5'	2.12	0.50
30:0:2445:U:H2'	30:0:2446:G:C8	2.46	0.50
30:0:2510:C:H5'	30:0:2511:A:OP2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:GLY:HA3	38:B:9031:HOH:O	2.12	0.50
14:N:114:LYS:O	14:N:118:ILE:HG13	2.11	0.50
30:0:407:A:H3'	38:0:4459:HOH:O	2.11	0.50
30:0:1137:G:H1'	38:0:3879:HOH:O	2.11	0.50
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.92	0.50
2:B:51:VAL:CG2	2:B:327:VAL:HG13	2.41	0.50
8:H:48:VAL:HA	8:H:170:ARG:O	2.12	0.50
14:N:37:ARG:NH1	31:9:6:C:OP1	2.43	0.50
30:0:407:A:H2'	30:0:408:A:C8	2.47	0.50
30:0:1020:A:H1'	38:0:7252:HOH:O	2.10	0.50
30:0:1066:U:H2'	30:0:1067:A:C8	2.47	0.50
30:0:1206:U:H5'	30:0:1206:U:C6	2.35	0.50
30:0:1921:A:O2'	30:0:1922:A:H5'	2.12	0.50
30:0:1972:U:C2'	30:0:1973:A:H5"	2.41	0.50
30:0:2502:C:H2'	30:0:2503:A:C5'	2.39	0.50
2:B:17:LYS:O	2:B:260:HIS:HD2	1.94	0.50
4:D:52:THR:HG21	30:0:2346:C:O2'	2.12	0.50
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.93	0.50
29:3:3:MET:O	29:3:90:PHE:HA	2.11	0.50
30:0:292:G:H2'	30:0:358:G:N2	2.26	0.50
30:0:815:U:O2'	30:0:1598:A:H4'	2.12	0.50
30:0:1588:G:C6	30:0:1589:G:C6	3.00	0.50
30:0:2026:C:O2'	30:0:2027:U:H5'	2.11	0.50
1:A:109:GLU:HG2	1:A:116:GLY:H	1.77	0.50
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.50
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.93	0.50
30:0:1183:C:H42	30:0:1184:C:N4	2.07	0.50
30:0:1207:A:C8	30:0:1208:C:C5	3.00	0.50
30:0:2768:A:H3'	38:0:4425:HOH:O	2.10	0.50
30:0:2825:C:H4'	30:0:2826:G:O5'	2.12	0.50
4:D:141:VAL:HG21	31:9:57:A:C8	2.46	0.49
8:H:59:GLN:HG2	8:H:129:ARG:HG2	1.92	0.49
10:J:131:THR:HB	10:J:134:GLU:HG3	1.94	0.49
12:L:143:THR:HG22	12:L:144:ASP:N	2.26	0.49
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.47	0.49
13:M:80:GLY:O	13:M:81:ARG:HD3	2.12	0.49
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.39	0.49
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.11	0.49
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.47	0.49
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.94	0.49
30:0:541:C:O2'	30:0:542:A:H5"	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1343:C:H2'	30:0:1344:G:O5'	2.12	0.49
30:0:2064:U:H5'	30:0:2652:U:H4'	1.93	0.49
30:0:2384:U:H5"	38:0:3492:HOH:O	2.12	0.49
31:9:64:C:H2'	31:9:65:A:H5'	1.94	0.49
29:3:38:ARG:HD2	30:0:396:U:OP2	2.13	0.49
30:0:24:G:N2	30:0:518:G:H1'	2.27	0.49
30:0:1926:G:H2'	30:0:1927:A:C8	2.47	0.49
30:0:2269:C:C2'	30:0:2270:G:H5'	2.42	0.49
30:0:2608:C:H3'	38:0:7829:HOH:O	2.11	0.49
30:0:2697:A:H2'	30:0:2698:G:O4'	2.12	0.49
5:E:80:TRP:O	5:E:134:SER:HA	2.13	0.49
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.22	0.49
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.12	0.49
30:0:1289:C:O2'	30:0:1290:G:H5'	2.12	0.49
30:0:1505:U:H1'	38:0:7609:HOH:O	2.13	0.49
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.94	0.49
20:T:52:ARG:O	30:0:317:A:OP1	2.29	0.49
23:W:24:LEU:O	23:W:26:ILE:HG22	2.13	0.49
30:0:440:C:H2'	30:0:441:A:C8	2.48	0.49
30:0:711:G:C2	30:0:718:C:C2	3.00	0.49
30:0:827:A:H2'	30:0:828:G:O4'	2.12	0.49
30:0:1768:C:H2'	30:0:1769:C:O4'	2.13	0.49
30:0:2607:U:H4'	38:0:9440:HOH:O	2.12	0.49
30:0:2846:C:H4'	38:0:5089:HOH:O	2.12	0.49
31:9:23:U:C2'	31:9:24:U:H4'	2.42	0.49
2:B:267:LYS:HD3	38:0:9562:HOH:O	2.11	0.49
2:B:297:VAL:HB	38:B:9071:HOH:O	2.12	0.49
4:D:23:VAL:HG22	4:D:73:VAL:HB	1.94	0.49
17:Q:19:ARG:HH21	31:9:11:A:P	2.36	0.49
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.60	0.49
30:0:513:A:N3	38:0:3658:HOH:O	2.34	0.49
30:0:1592:G:H2'	30:0:1593:C:C6	2.48	0.49
31:9:60:C:O2'	31:9:61:C:H5'	2.12	0.49
6:F:39:SER:OG	6:F:45:ALA:HB2	2.12	0.49
12:L:14:GLY:O	30:0:1295:G:H5"	2.13	0.49
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.10	0.49
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.13	0.49
30:0:523:C:H2'	30:0:524:A:C8	2.48	0.49
30:0:1157:C:O2'	30:0:1158:G:H5'	2.13	0.49
30:0:2506:A:N6	30:0:2511:A:O2'	2.42	0.49
8:H:69:ARG:HD3	38:H:8576:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:68:ASP:HB2	38:0:5666:HOH:O	2.12	0.49
30:0:1185:U:H2'	30:0:1186:C:C6	2.47	0.49
30:0:2712:G:H5'	38:0:5229:HOH:O	2.12	0.49
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.95	0.49
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.77	0.49
2:B:254:GLN:HG2	2:B:255:GLY:N	2.27	0.49
31:9:29:C:H2'	31:9:30:C:C5'	2.37	0.49
2:B:215:VAL:HA	2:B:220:VAL:HG22	1.95	0.49
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.99	0.49
30:0:447:A:O2'	30:0:448:G:H5'	2.13	0.49
30:0:483:C:C4	30:0:484:A:C6	3.01	0.49
31:9:35:C:H5"	38:9:9074:HOH:O	2.12	0.49
11:K:87:ARG:NH2	30:0:2720:C:O2	2.45	0.49
21:U:52:THR:O	21:U:56:ARG:HG2	2.12	0.49
30:0:78:G:C6	30:0:79:G:C6	3.01	0.49
30:0:255:A:C5	30:0:256:C:C4	3.01	0.49
30:0:343:C:O2'	30:0:344:C:H5'	2.12	0.49
30:0:951:A:O2'	30:0:952:G:H5'	2.13	0.49
30:0:1160:G:H5'	30:0:1161:A:C4'	2.42	0.49
30:0:1173:A:H2	38:0:6300:HOH:O	1.95	0.49
30:0:1762:C:H2'	30:0:1763:C:H6	1.78	0.49
30:0:2281:C:H2'	30:0:2282:U:H5'	1.95	0.49
30:0:2401:A:H2'	30:0:2402:A:C8	2.48	0.49
2:B:36:PRO:HG3	2:B:169:GLY:H	1.78	0.48
2:B:256:GLN:HG2	38:B:9120:HOH:O	2.12	0.48
3:C:63:SER:OG	30:0:2101:A:H2'	2.13	0.48
23:W:4:LEU:O	23:W:32:CYS:HA	2.13	0.48
30:0:120:A:H2'	30:0:120:A:N3	2.28	0.48
30:0:583:C:H2'	30:0:584:U:H6	1.78	0.48
30:0:2324:G:N2	30:0:2377:U:H1'	2.28	0.48
13:M:81:ARG:HG3	13:M:85:ARG:HB2	1.95	0.48
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.33	0.48
19:S:57:THR:HG22	19:S:59:ASP:H	1.78	0.48
27:1:16:HIS:CD2	30:0:470:U:O2'	2.65	0.48
30:0:308:U:C4	30:0:342:C:H1'	2.48	0.48
30:0:629:A:C2	30:0:2074:A:C2	3.01	0.48
30:0:660:A:H4'	30:0:661:G:O5'	2.14	0.48
30:0:807:A:C6	30:0:808:A:C6	3.01	0.48
30:0:1016:U:H1'	38:0:3657:HOH:O	2.13	0.48
30:0:1657:A:H2'	30:0:1658:A:C8	2.48	0.48
30:0:2598:U:O2	30:0:2600:A:C8	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2897:C:O2'	30:0:2898:G:H5'	2.13	0.48
1:A:186:TRP:CG	1:A:187:PRO:HA	2.48	0.48
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.95	0.48
10:J:41:ALA:HB3	38:J:5907:HOH:O	2.12	0.48
30:0:304:G:H1'	30:0:347:A:H61	1.78	0.48
30:0:1067:A:H5'	38:0:4348:HOH:O	2.11	0.48
30:0:1226:G:H5'	38:0:4532:HOH:O	2.13	0.48
30:0:1973:A:H5'	30:0:1973:A:C8	2.39	0.48
30:0:2269:C:H2'	30:0:2270:G:H5'	1.95	0.48
30:0:2435:U:H1'	38:0:5442:HOH:O	2.13	0.48
2:B:51:VAL:HG23	2:B:329:TYR:O	2.13	0.48
14:N:147:ILE:HD12	38:9:9087:HOH:O	2.12	0.48
30:0:2783:A:H2'	30:0:2784:A:C8	2.49	0.48
31:9:1:U:O3'	31:9:3:A:C5'	2.61	0.48
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.29	0.48
3:C:218:VAL:HG12	38:C:8627:HOH:O	2.13	0.48
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.96	0.48
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.44	0.48
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.95	0.48
19:S:33:SER:O	19:S:37:VAL:HG23	2.12	0.48
30:0:366:U:H2'	30:0:367:G:O4'	2.14	0.48
30:0:734:U:O2'	30:0:736:A:N7	2.41	0.48
30:0:1515:A:H2'	30:0:1516:U:C6	2.48	0.48
30:0:1615:A:C5'	38:0:4186:HOH:O	2.62	0.48
30:0:2756:U:C2	30:0:2896:A:H2	2.31	0.48
30:0:2826:G:C6	30:0:2913:A:N6	2.82	0.48
31:9:107:C:O2'	31:9:108:C:H5'	2.13	0.48
3:C:132:ASP:HB2	3:C:161:ASP:HB3	1.94	0.48
10:J:47:THR:HG21	30:0:1244:U:H2'	1.96	0.48
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.39	0.48
15:O:39:THR:O	15:O:115:ARG:NH2	2.46	0.48
18:R:33:ARG:NH1	38:R:8945:HOH:O	2.46	0.48
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.49	0.48
30:0:1451:C:H5'	30:0:1505:U:C5	2.48	0.48
30:0:1666:C:HO2'	30:0:1667:A:H5"	1.73	0.48
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.96	0.48
27:1:45:ARG:HB3	38:1:8965:HOH:O	2.13	0.48
30:0:101:C:H2'	30:0:102:A:H8	1.79	0.48
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.46	0.48
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.60	0.48
15:O:47:ARG:HH11	15:O:47:ARG:HG3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:482:G:O4'	30:0:511:A:C2	2.66	0.48
30:0:652:G:H8	38:0:3013:HOH:O	1.97	0.48
30:0:1298:U:H2'	30:0:1299:G:C8	2.49	0.48
30:0:2104:C:O2	30:0:2485:A:N1	2.47	0.48
30:0:2613:G:O2'	30:0:2614:C:H5'	2.13	0.48
30:0:2689:A:H2'	30:0:2690:U:H5'	1.95	0.48
9:I:78:ALA:HB1	9:I:93:ALA:HB1	1.95	0.48
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.96	0.48
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.62	0.48
19:S:57:THR:HG22	19:S:59:ASP:N	2.29	0.48
30:0:466:A:H2'	30:0:467:G:O4'	2.14	0.48
30:0:545:G:C8	30:0:545:G:C5'	2.89	0.48
30:0:559:U:C6	30:0:559:U:C3'	2.97	0.48
30:0:877:G:C5'	30:0:878:G:OP1	2.58	0.48
30:0:1188:A:C6	30:0:1189:A:C6	3.02	0.48
30:0:1381:A:N3	30:0:1382:G:H1'	2.29	0.48
30:0:1603:A:C5'	30:0:1605:G:O4'	2.51	0.48
30:0:2456:A:H2'	30:0:2457:U:C6	2.49	0.48
31:9:108:C:H2'	31:9:109:G:C8	2.49	0.48
2:B:72:THR:HB	38:B:9071:HOH:O	2.12	0.48
10:J:42:GLU:O	10:J:131:THR:HG23	2.14	0.48
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.96	0.48
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.79	0.48
27:1:45:ARG:NH2	38:1:8973:HOH:O	2.42	0.48
30:0:64:G:H2'	30:0:65:C:O4'	2.14	0.48
30:0:912:A:C4	30:0:1294:A:C2	3.01	0.48
30:0:2336:G:H1'	38:0:6316:HOH:O	2.14	0.48
30:0:2385:G:H2'	30:0:2386:U:C6	2.49	0.48
31:9:3:A:OP2	31:9:25:G:N2	2.47	0.48
1:A:95:PRO:HA	1:A:153:ARG:HA	1.96	0.47
2:B:79:MET:HE1	38:B:9091:HOH:O	2.13	0.47
4:D:62:ASP:HA	38:D:4233:HOH:O	2.14	0.47
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.28	0.47
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.95	0.47
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.95	0.47
30:0:228:C:C2'	30:0:229:G:H5'	2.44	0.47
30:0:724:G:O2'	30:0:725:C:H5'	2.14	0.47
30:0:1135:G:H5'	38:0:5943:HOH:O	2.12	0.47
30:0:1163:G:N1	30:0:1184:C:N4	2.62	0.47
1:A:206:ARG:NH2	30:0:2630:G:O6	2.47	0.47
3:C:78:ARG:HH11	3:C:78:ARG:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:18:ILE:HG22	11:K:93:ASN:HB2	1.95	0.47
30:0:179:C:H5"	38:0:9308:HOH:O	2.13	0.47
30:0:1138:G:H4'	38:0:5714:HOH:O	2.12	0.47
30:0:2072:G:C6	30:0:2533:C:H1'	2.49	0.47
30:0:2781:U:O2'	30:0:2782:G:H5'	2.14	0.47
30:0:602:A:O2'	30:0:605:C:H4'	2.13	0.47
30:0:876:A:N3	30:0:876:A:C2'	2.77	0.47
30:0:1189:A:H1'	30:0:1209:C:H1'	1.96	0.47
30:0:1592:G:H2'	30:0:1593:C:H6	1.78	0.47
30:0:1755:A:H2'	30:0:1756:G:O4'	2.14	0.47
30:0:1790:C:H2'	30:0:1791:U:H6	1.79	0.47
30:0:2534:C:H2'	30:0:2535:U:C6	2.50	0.47
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.95	0.47
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.96	0.47
17:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.14	0.47
20:T:54:ASP:OD2	30:0:316:A:H5'	2.14	0.47
27:1:37:CYS:SG	27:1:39:PHE:HB2	2.54	0.47
30:0:42:C:H1'	38:0:4679:HOH:O	2.14	0.47
30:0:111:C:O2'	30:0:112:G:H5'	2.14	0.47
30:0:247:A:H2'	38:0:3924:HOH:O	2.14	0.47
30:0:497:A:H2'	30:0:498:A:C5'	2.45	0.47
30:0:790:A:H2'	30:0:791:A:O4'	2.14	0.47
30:0:951:A:C2'	30:0:952:G:H5'	2.44	0.47
30:0:2589:U:H2'	30:0:2590:U:C6	2.49	0.47
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.40	0.47
7:G:12:ILE:HG12	38:0:5471:HOH:O	2.14	0.47
13:M:95:LYS:HE2	30:0:157:G:H4'	1.96	0.47
18:R:29:LYS:HE2	30:0:524:A:C5'	2.44	0.47
18:R:132:ARG:HG2	18:R:133:ALA:N	2.28	0.47
19:S:77:VAL:O	19:S:80:ARG:HG2	2.14	0.47
30:0:283:U:H5	30:0:284:C:C4	2.32	0.47
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.47
30:0:1163:G:N2	38:0:4729:HOH:O	2.47	0.47
30:0:1183:C:C2	30:0:1184:C:C5	3.02	0.47
31:9:61:C:H2'	31:9:62:A:H8	1.79	0.47
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.95	0.47
2:B:62:ARG:HA	2:B:65:MET:HE3	1.96	0.47
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.12	0.47
13:M:30:GLU:O	13:M:34:GLU:HG3	2.15	0.47
16:P:91:LYS:O	16:P:95:GLU:HG3	2.15	0.47
30:0:517:U:H1'	38:0:7599:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:821:U:H2'	30:0:822:C:C6	2.50	0.47
30:0:1166:A:C6	30:0:1181:A:C2	3.03	0.47
30:0:1386:G:O2'	30:0:1387:G:H5'	2.14	0.47
30:0:1664:A:H8	30:0:1664:A:OP1	1.96	0.47
30:0:2387:U:H2'	30:0:2388:C:C6	2.49	0.47
30:0:2802:C:H2'	30:0:2803:C:C6	2.49	0.47
31:9:39:U:C2'	31:9:40:C:OP1	2.63	0.47
3:C:118:THR:O	3:C:136:VAL:HG13	2.13	0.47
4:D:36:ASN:HA	38:D:7500:HOH:O	2.15	0.47
13:M:9:ARG:HD2	30:0:380:A:OP2	2.15	0.47
13:M:164:THR:HB	38:M:8819:HOH:O	2.15	0.47
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.15	0.47
22:V:44:GLY:O	22:V:48:GLU:HG2	2.14	0.47
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.14	0.47
26:Z:34:SER:N	30:0:796:A:HO2'	2.13	0.47
30:0:711:G:H1'	38:0:7120:HOH:O	2.13	0.47
30:0:737:A:H2'	30:0:738:G:O4'	2.15	0.47
30:0:932:U:H2'	30:0:933:C:C6	2.49	0.47
30:0:1058:A:H2'	30:0:1060:C:C5'	2.42	0.47
30:0:1214:G:H4'	38:0:4752:HOH:O	2.14	0.47
30:0:1495:C:H1'	30:0:1573:A:H1'	1.97	0.47
30:0:1592:G:O2'	30:0:1593:C:O4'	2.32	0.47
30:0:1741:U:C4	30:0:2033:G:C8	3.02	0.47
30:0:1823:G:O2'	30:0:1824:C:H5'	2.15	0.47
30:0:2032:U:H2'	30:0:2033:G:C5'	2.45	0.47
30:0:2133:U:H4'	30:0:2134:G:H5'	1.95	0.47
30:0:2842:G:H2'	30:0:2843:A:H5'	1.96	0.47
1:A:33:GLU:O	1:A:34:ASP:HB2	2.15	0.47
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.15	0.47
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.42	0.47
26:Z:57:MET:SD	26:Z:73:ARG:HD2	2.55	0.47
30:0:940:G:C5	30:0:1027:G:C2	3.03	0.47
30:0:1029:U:O2'	30:0:1273:C:OP1	2.30	0.47
30:0:1165:G:O3'	30:0:1174:A:H4'	2.14	0.47
30:0:1291:A:H2	38:0:5300:HOH:O	1.97	0.47
30:0:1592:G:O2'	30:0:1593:C:O5'	2.32	0.47
30:0:1878:G:O2'	30:0:1879:U:H6	1.98	0.47
30:0:2361:A:H2'	30:0:2362:A:O4'	2.14	0.47
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.79	0.47
30:0:101:C:H2'	30:0:102:A:C8	2.50	0.47
30:0:396:U:HO2'	30:0:397:A:P	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:734:U:H1'	30:0:737:A:N6	2.30	0.47
30:0:2326:C:H4'	30:0:2412:G:C4'	2.45	0.47
10:J:76:ASP:HA	38:J:5907:HOH:O	2.14	0.47
30:0:445:U:H2'	30:0:446:G:H8	1.80	0.47
30:0:1221:G:H8	38:0:6005:HOH:O	1.97	0.47
30:0:1422:U:H2'	30:0:1423:C:C6	2.49	0.47
31:9:1:U:H4'	31:9:3:A:OP1	2.15	0.47
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.48	0.46
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.97	0.46
8:H:31:ILE:HG23	38:H:8576:HOH:O	2.15	0.46
9:I:101:LYS:O	9:I:105:GLU:HG3	2.15	0.46
10:J:63:ILE:HD11	30:0:1236:A:C8	2.50	0.46
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.96	0.46
21:U:6:CYS:HA	21:U:13:ILE:HD11	1.97	0.46
24:X:43:VAL:HG12	24:X:44:ASP:H	1.79	0.46
30:0:2866:U:H4'	30:0:2867:G:H5'	1.97	0.46
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.98	0.46
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.50	0.46
14:N:4:PRO:HG3	31:9:69:U:OP1	2.15	0.46
21:U:9:CYS:HA	21:U:52:THR:CG2	2.44	0.46
23:W:5:VAL:HG11	23:W:153:MET:CE	2.45	0.46
27:1:25:LYS:HD2	28:2:49:GLU:N	2.30	0.46
30:0:151:A:C2	30:0:152:A:C2	3.04	0.46
30:0:690:G:H4'	30:0:741:C:O2	2.15	0.46
30:0:953:G:H4'	30:0:954:U:OP1	2.15	0.46
30:0:2314:G:C2'	30:0:2315:C:H5'	2.45	0.46
13:M:28:GLN:O	13:M:32:ARG:HG3	2.15	0.46
14:N:169:PRO:O	14:N:172:PHE:HB3	2.16	0.46
15:O:39:THR:HB	38:0:4618:HOH:O	2.14	0.46
20:T:12:ARG:NH1	38:T:3035:HOH:O	2.49	0.46
30:0:255:A:C4	30:0:256:C:C6	3.02	0.46
30:0:1477:C:H5'	30:0:1868:G:H5"	1.97	0.46
30:0:2004:U:H2'	30:0:2005:G:OP1	2.14	0.46
3:C:64:GLY:O	30:0:2100:A:H4'	2.15	0.46
4:D:82:GLU:HA	4:D:85:GLN:HE21	1.81	0.46
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.48	0.46
14:N:154:LEU:C	14:N:156:GLU:H	2.17	0.46
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.98	0.46
23:W:88:THR:HG22	23:W:89:ASP:N	2.29	0.46
30:0:307:G:H3'	38:0:6714:HOH:O	2.15	0.46
30:0:426:G:H2'	30:0:427:C:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1198:U:C6	30:0:1200:A:OP2	2.69	0.46
30:0:1856:C:H5'	30:0:1858:A:O4'	2.16	0.46
30:0:2329:C:O2'	30:0:2330:U:H5'	2.15	0.46
30:0:2515:C:H2'	30:0:2516:G:O4'	2.15	0.46
5:E:133:VAL:HG12	5:E:141:VAL:HG13	1.98	0.46
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.50	0.46
25:Y:148:GLY:HA3	30:0:622:G:P	2.56	0.46
26:Z:45:VAL:HG12	38:Z:8713:HOH:O	2.15	0.46
30:0:17:G:H2'	30:0:18:C:C6	2.51	0.46
30:0:137:U:OP1	30:0:259:G:O2'	2.30	0.46
30:0:177:A:H2'	30:0:178:U:O4'	2.15	0.46
30:0:645:U:O2	30:0:761:A:H2	1.97	0.46
30:0:834:G:H4'	30:0:835:U:OP2	2.15	0.46
30:0:861:A:H4'	30:0:1697:G:H4'	1.98	0.46
30:0:1503:U:H2'	30:0:1504:A:O4'	2.15	0.46
30:0:1634:G:C3'	38:0:3895:HOH:O	2.51	0.46
30:0:2600:A:H2'	30:0:2601:A:O4'	2.15	0.46
1:A:199:HIS:HE1	30:0:1881:A:OP1	1.98	0.46
2:B:27:ASN:HD21	30:0:2807:U:P	2.38	0.46
10:J:19:MET:HE1	10:J:79:PHE:HA	1.98	0.46
14:N:11:ARG:NH1	31:9:8:G:O6	2.49	0.46
14:N:171:HIS:CE1	38:N:8862:HOH:O	2.68	0.46
30:0:1166:A:N6	30:0:1180:U:H3	1.97	0.46
30:0:1181:A:H2'	30:0:1182:C:C5'	2.45	0.46
30:0:1204:C:H2'	30:0:1205:U:O4'	2.15	0.46
30:0:1419:U:H2'	30:0:1685:A:C2	2.51	0.46
30:0:1562:C:O2	30:0:1562:C:C2'	2.61	0.46
30:0:1973:A:H2'	30:0:1974:G:O4'	2.16	0.46
30:0:2071:C:H5'	38:0:9527:HOH:O	2.16	0.46
30:0:2291:A:N9	30:0:2309:C:H5'	2.30	0.46
30:0:2754:G:H2'	30:0:2755:G:O4'	2.16	0.46
30:0:2765:C:H2'	30:0:2766:A:C8	2.50	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.98	0.46
30:0:905:C:H3'	38:0:5195:HOH:O	2.15	0.46
30:0:1202:A:H2'	30:0:1203:G:C5'	2.45	0.46
30:0:1926:G:H2'	30:0:1927:A:H8	1.80	0.46
30:0:1942:A:O2'	30:0:1943:C:H5'	2.16	0.46
30:0:2569:A:H2'	30:0:2570:G:O5'	2.16	0.46
1:A:29:HIS:HB2	1:A:153:ARG:HH12	1.80	0.46
2:B:205:VAL:O	2:B:307:ARG:NE	2.48	0.46
4:D:131:THR:HG21	30:0:2348:C:H1'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.97	0.46
30:0:365:G:C6	30:0:366:U:C4	3.04	0.46
30:0:834:G:H3'	30:0:835:U:H4'	1.97	0.46
30:0:2245:C:H6	30:0:2245:C:O5'	1.99	0.46
30:0:2269:C:H2'	30:0:2270:G:C5'	2.46	0.46
30:0:2371:G:H5'	38:0:5018:HOH:O	2.15	0.46
30:0:2840:A:H3'	38:0:7669:HOH:O	2.15	0.46
1:A:211:LYS:HG2	38:0:7054:HOH:O	2.16	0.46
2:B:234:ARG:HD3	30:0:1734:C:OP1	2.15	0.46
2:B:275:GLY:O	2:B:291:ASP:HA	2.16	0.46
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.98	0.46
27:1:46:ARG:HA	38:0:3021:HOH:O	2.15	0.46
30:0:807:A:H2'	30:0:808:A:C8	2.50	0.46
30:0:1244:U:H4'	30:0:1246:A:O4'	2.16	0.46
30:0:1321:A:H2'	30:0:1322:G:H8	1.80	0.46
30:0:2710:U:O2'	30:0:2711:U:H5'	2.16	0.46
30:0:2895:C:H2'	38:0:9570:HOH:O	2.15	0.46
2:B:254:GLN:HG3	38:0:9698:HOH:O	2.14	0.46
5:E:68:HIS:O	5:E:72:MET:HG3	2.15	0.46
8:H:91:ARG:O	30:0:1003:U:H4'	2.16	0.46
12:L:39:GLU:HG2	30:0:926:A:C4'	2.46	0.46
25:Y:107:PRO:HB3	25:Y:182:PHE:CD2	2.51	0.46
30:0:106:A:H2'	30:0:107:U:O4'	2.16	0.46
30:0:324:G:O2'	30:0:325:U:H5'	2.16	0.46
30:0:1902:G:H2'	30:0:1903:U:O4'	2.16	0.46
30:0:1904:A:H2'	30:0:1905:U:O4'	2.16	0.46
30:0:2433:A:H2'	30:0:2434:A:C8	2.50	0.46
31:9:23:U:HO2'	31:9:24:U:H4'	1.77	0.46
6:F:21:GLU:O	6:F:24:ARG:HG2	2.16	0.45
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.98	0.45
8:H:141:CYS:HB2	38:H:8540:HOH:O	2.17	0.45
12:L:57:VAL:O	12:L:57:VAL:HG12	2.16	0.45
24:X:76:ARG:HG3	24:X:76:ARG:NH1	2.27	0.45
29:3:34:LYS:HE2	38:0:4426:HOH:O	2.16	0.45
30:0:192:A:H5'	38:0:7665:HOH:O	2.15	0.45
30:0:1213:C:O2'	30:0:1214:G:H5'	2.16	0.45
30:0:2301:A:H5"	30:0:2302:A:H5'	1.98	0.45
30:0:2345:A:H3'	30:0:2346:C:C6	2.50	0.45
30:0:2512:U:H4'	30:0:2514:U:O4	2.16	0.45
31:9:108:C:H2'	31:9:109:G:H8	1.81	0.45
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.03	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.46	0.45
7:G:16:LYS:HE2	7:G:63:ARG:NH1	2.31	0.45
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.80	0.45
30:0:271:C:C2	30:0:273:G:O4'	2.69	0.45
30:0:2408:A:H2	38:0:3102:HOH:O	1.98	0.45
30:0:2505:G:H2'	30:0:2506:A:C5'	2.47	0.45
2:B:10:SER:HB2	30:0:2714:U:H4'	1.96	0.45
19:S:45:TYR:O	19:S:80:ARG:NH2	2.49	0.45
29:3:22:VAL:HG11	29:3:67:LEU:HD13	1.98	0.45
30:0:1398:G:H2'	30:0:1399:A:C8	2.51	0.45
30:0:2880:A:H2'	30:0:2881:C:H5'	1.99	0.45
2:B:198:GLU:HA	38:B:9121:HOH:O	2.16	0.45
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.45
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.15	0.45
14:N:1:ALA:HB2	31:9:14:G:O2'	2.17	0.45
14:N:160:SER:HB3	31:9:51:A:H5'	1.97	0.45
18:R:71:LYS:HE2	30:0:2831:C:O3'	2.17	0.45
30:0:484:A:N1	30:0:506:G:H4'	2.31	0.45
30:0:661:G:C5	30:0:686:A:C2	3.05	0.45
30:0:803:C:O2'	30:0:804:C:H5'	2.17	0.45
30:0:1183:C:H1'	30:0:1192:A:N6	2.31	0.45
30:0:1544:U:H2'	30:0:1545:C:C6	2.52	0.45
30:0:2765:C:H2'	30:0:2766:A:H8	1.82	0.45
30:0:2896:A:N3	30:0:2896:A:H2'	2.31	0.45
31:9:59:C:O5'	31:9:59:C:H6	1.99	0.45
12:L:148:GLU:HA	38:L:8877:HOH:O	2.16	0.45
19:S:11:THR:H	19:S:14:ALA:HB3	1.81	0.45
23:W:130:HIS:O	23:W:136:GLY:HA3	2.16	0.45
26:Z:76:THR:HG21	30:0:1652:C:H4'	1.98	0.45
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.51	0.45
30:0:587:A:H5"	38:0:7309:HOH:O	2.17	0.45
30:0:958:G:O2'	30:0:959:C:H5'	2.16	0.45
30:0:1622:G:H2'	30:0:1623:C:H5'	1.99	0.45
30:0:1730:G:C5'	30:0:1731:C:H6	2.27	0.45
30:0:1790:C:H2'	30:0:1791:U:C6	2.51	0.45
31:9:34:A:H2'	31:9:35:C:O4'	2.17	0.45
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.52	0.45
30:0:368:C:H2'	30:0:369:G:H5'	1.98	0.45
30:0:958:G:H2'	30:0:959:C:C6	2.52	0.45
30:0:1521:C:H2'	30:0:1522:A:H8	1.82	0.45
30:0:1596:U:H2'	30:0:1598:A:OP2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1626:A:H2'	30:0:1627:G:C5'	2.46	0.45
30:0:1771:U:O2'	30:0:1773:G:N7	2.48	0.45
30:0:2326:C:H4'	30:0:2412:G:H4'	1.99	0.45
30:0:2748:G:C2'	38:0:7565:HOH:O	2.57	0.45
4:D:18:ILE:HD13	4:D:84:LEU:HD12	1.97	0.45
6:F:107:ASP:O	6:F:111:ILE:HG13	2.16	0.45
10:J:19:MET:CE	10:J:132:LEU:HD11	2.46	0.45
11:K:41:LYS:O	11:K:42:ASN:HB2	2.17	0.45
13:M:24:GLN:NE2	13:M:24:GLN:HA	2.32	0.45
18:R:39:THR:HB	18:R:42:GLU:HG3	1.99	0.45
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.99	0.45
30:0:48:A:N1	30:0:148:A:O2'	2.42	0.45
30:0:371:U:H2'	30:0:372:A:H8	1.82	0.45
30:0:570:C:O5'	30:0:570:C:H6	2.00	0.45
30:0:1008:C:O2'	30:0:1009:U:H5'	2.17	0.45
30:0:1123:A:C2	30:0:1129:C:H4'	2.52	0.45
30:0:1186:C:N4	30:0:1187:U:C4	2.84	0.45
30:0:1190:G:H2'	38:0:4061:HOH:O	2.16	0.45
30:0:1477:C:H5'	30:0:1868:G:H5'	1.96	0.45
30:0:1762:C:O2'	30:0:1763:C:H5'	2.17	0.45
30:0:2102:G:C2	30:0:2104:C:C4	3.05	0.45
31:9:3:A:H2	31:9:21:G:N3	2.15	0.45
2:B:223:ARG:HG3	2:B:232:TRP:O	2.16	0.45
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.84	0.45
30:0:95:A:H5"	30:0:97:G:O4'	2.16	0.45
30:0:960:G:H8	38:0:5988:HOH:O	1.99	0.45
30:0:1149:U:H5"	30:0:1151:G:O4'	2.17	0.45
30:0:1588:G:C6	30:0:1589:G:N1	2.85	0.45
30:0:1931:A:H2'	30:0:1932:G:H5'	1.99	0.45
30:0:2691:A:H5'	30:0:2693:U:H1'	1.99	0.45
30:0:2729:C:O2'	30:0:2730:G:H5'	2.16	0.45
30:0:2769:C:H2'	30:0:2770:G:O4'	2.16	0.45
1:A:210:GLY:HA3	38:0:5306:HOH:O	2.16	0.45
3:C:76:ARG:HH22	30:0:1363:G:P	2.40	0.45
8:H:174:LEU:HA	38:H:8567:HOH:O	2.17	0.45
10:J:75:PRO:HD3	10:J:136:SER:OG	2.17	0.45
12:L:80:ASP:HB2	12:L:90:ARG:O	2.17	0.45
14:N:37:ARG:NH2	38:N:8834:HOH:O	2.48	0.45
15:O:77:ALA:HA	15:O:96:VAL:O	2.16	0.45
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.44	0.45
24:X:72:VAL:HG22	24:X:85:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:254:C:O2	30:0:254:C:H2'	2.15	0.45
30:0:559:U:C6	30:0:559:U:H3'	2.51	0.45
30:0:594:C:C4	30:0:595:U:C4	3.05	0.45
30:0:1154:A:H2'	30:0:1155:G:C8	2.52	0.45
30:0:1434:A:H2'	30:0:1436:C:C5	2.51	0.45
30:0:2265:U:H2'	30:0:2266:A:C8	2.51	0.45
30:0:2553:A:H2'	30:0:2553:A:N3	2.31	0.45
2:B:229:ARG:HD2	38:0:9112:HOH:O	2.17	0.45
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.78	0.45
30:0:407:A:H8	38:0:4459:HOH:O	2.00	0.45
30:0:657:G:H2'	30:0:658:C:C6	2.52	0.45
30:0:1245:C:O5'	30:0:1245:C:H6	1.99	0.45
30:0:1278:A:H4'	30:0:1279:U:N3	2.32	0.45
30:0:1444:G:O2'	30:0:1445:G:H5'	2.17	0.45
30:0:1576:G:H2'	30:0:1577:U:O4'	2.17	0.45
30:0:2092:G:H2'	30:0:2613:G:OP1	2.16	0.45
30:0:2106:C:H5'	30:0:2284:G:H21	1.81	0.45
9:I:84:SER:HB3	9:I:92:VAL:CG2	2.47	0.44
12:L:92:ASP:HA	12:L:121:ILE:HB	1.98	0.44
13:M:182:LYS:HE2	30:0:392:U:O2'	2.17	0.44
15:O:24:ALA:HB3	30:0:710:G:OP1	2.17	0.44
38:Y:8907:HOH:O	30:0:1330:A:C5'	2.54	0.44
30:0:111:C:C2'	30:0:112:G:H5'	2.48	0.44
30:0:1413:A:H2'	30:0:1414:A:O4'	2.17	0.44
30:0:1457:U:H5	38:0:7895:HOH:O	2.00	0.44
30:0:1878:G:H5'	38:0:4371:HOH:O	2.18	0.44
30:0:2072:G:H3'	30:0:2073:G:C5'	2.48	0.44
30:0:2566:A:C2	30:0:2696:G:O4'	2.70	0.44
30:0:2672:C:O2'	30:0:2673:U:H5'	2.17	0.44
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.82	0.44
9:I:93:ALA:HB3	9:I:132:VAL:HG22	1.99	0.44
15:O:25:VAL:CG1	30:0:710:G:H5'	2.48	0.44
29:3:91:GLN:O	29:3:92:GLU:HB2	2.18	0.44
30:0:941:G:C6	30:0:942:U:C4	3.06	0.44
30:0:1165:G:H21	30:0:1173:A:C5'	2.27	0.44
30:0:1453:G:N2	30:0:1675:C:C2	2.86	0.44
30:0:2487:C:H5	38:0:4897:HOH:O	2.01	0.44
30:0:2717:C:C2'	30:0:2718:C:C5'	2.78	0.44
2:B:16:ARG:NH2	38:B:9020:HOH:O	2.42	0.44
2:B:310:ARG:HB3	38:B:9112:HOH:O	2.18	0.44
3:C:2:GLN:HB3	38:C:8588:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:ARG:O	3:C:111:VAL:HG23	2.17	0.44
4:D:135:VAL:HG22	4:D:136:ARG:H	1.82	0.44
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.99	0.44
6:F:58:GLU:HA	6:F:61:MET:HG3	2.00	0.44
30:0:1184:C:O2'	30:0:1185:U:OP2	2.33	0.44
30:0:1739:G:O2'	30:0:1740:U:H5'	2.17	0.44
30:0:1972:U:C2'	30:0:1973:A:C5'	2.95	0.44
30:0:1976:G:O2'	30:0:1977:U:H5'	2.18	0.44
30:0:2134:G:C6	30:0:2258:A:C8	3.06	0.44
31:9:52:A:C2'	31:9:53:G:H5'	2.48	0.44
6:F:46:GLU:OE2	6:F:100:ASP:HA	2.17	0.44
10:J:47:THR:HG22	10:J:48:GLY:N	2.32	0.44
20:T:62:VAL:N	38:T:3851:HOH:O	2.51	0.44
30:0:69:A:C8	30:0:69:A:C5'	2.95	0.44
30:0:488:U:H2'	38:0:4010:HOH:O	2.18	0.44
30:0:962:C:H2'	30:0:963:C:H5'	2.00	0.44
30:0:1406:A:H4'	30:0:1407:A:C5'	2.48	0.44
30:0:1589:G:C2	30:0:1605:G:N3	2.86	0.44
30:0:1850:U:H2'	30:0:1851:G:H8	1.82	0.44
30:0:1940:C:H4'	38:0:7371:HOH:O	2.17	0.44
31:9:3:A:N6	31:9:22:G:H1'	2.32	0.44
2:B:41:PHE:HB3	2:B:190:MET:CE	2.45	0.44
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.99	0.44
6:F:48:VAL:HG23	6:F:74:PHE:CB	2.46	0.44
6:F:59:ILE:CD1	30:0:263:U:C2	3.01	0.44
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.33	0.44
12:L:34:GLY:HA2	38:0:5421:HOH:O	2.17	0.44
13:M:75:ARG:HH11	30:0:1864:C:H5	1.61	0.44
14:N:132:ASN:O	14:N:135:VAL:HG12	2.17	0.44
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.49	0.44
16:P:115:SER:OG	16:P:118:GLN:HG3	2.17	0.44
23:W:23:MET:O	30:0:1025:C:H5'	2.17	0.44
26:Z:44:ARG:HB2	30:0:1886:A:O2'	2.17	0.44
30:0:646:G:H2'	30:0:647:U:C6	2.53	0.44
30:0:1783:A:O2'	30:0:1784:U:H5'	2.17	0.44
30:0:2498:C:C2'	30:0:2499:U:H5'	2.47	0.44
9:I:102:GLN:HA	9:I:105:GLU:OE2	2.18	0.44
15:O:25:VAL:HG23	15:O:26:TRP:N	2.33	0.44
30:0:1497:G:H4'	30:0:1627:G:O2'	2.18	0.44
30:0:1520:G:H2'	30:0:1521:C:C6	2.52	0.44
30:0:1588:G:C5	30:0:1589:G:C6	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1683:G:C2	30:0:1693:A:O4'	2.71	0.44
30:0:2256:G:C2'	30:0:2257:G:C5'	2.96	0.44
3:C:184:ARG:HD2	30:0:1306:U:OP1	2.18	0.44
12:L:89:PHE:N	38:L:8876:HOH:O	2.50	0.44
13:M:164:THR:HG23	13:M:165:GLY:N	2.33	0.44
14:N:109:PRO:HB3	30:0:2413:A:N7	2.33	0.44
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.47	0.44
29:3:11:CYS:HB2	29:3:20:HIS:HE1	1.82	0.44
30:0:629:A:H2'	30:0:630:A:O4'	2.18	0.44
30:0:920:C:H5"	30:0:921:G:O5'	2.17	0.44
30:0:932:U:H2'	30:0:933:C:H6	1.83	0.44
30:0:1021:G:O2'	30:0:1022:A:H5'	2.17	0.44
30:0:1624:A:H5'	30:0:1626:A:O4'	2.17	0.44
30:0:2421:G:H3'	30:0:2422:U:C5'	2.47	0.44
1:A:53:ALA:HB3	38:A:9061:HOH:O	2.18	0.44
2:B:5:ARG:HD2	2:B:8:LYS:NZ	2.33	0.44
2:B:243:ASN:HA	2:B:244:PRO:C	2.37	0.44
9:I:69:PRO:HA	30:0:1164:U:OP1	2.18	0.44
14:N:23:ARG:NH1	38:N:8865:HOH:O	2.51	0.44
15:O:32:ARG:O	15:O:32:ARG:HD3	2.18	0.44
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.48	0.44
23:W:125:HIS:HB2	23:W:137:GLN:HG2	1.99	0.44
28:2:41:HIS:CD2	28:2:44:ARG:H	2.33	0.44
30:0:538:C:H5"	30:0:539:G:C8	2.53	0.44
30:0:823:U:H3'	38:0:4445:HOH:O	2.18	0.44
30:0:1218:U:H2'	30:0:1219:U:C6	2.52	0.44
30:0:1350:U:H4'	38:0:5132:HOH:O	2.17	0.44
30:0:1762:C:H2'	30:0:1763:C:C6	2.53	0.44
30:0:2506:A:C4	38:0:6073:HOH:O	2.70	0.44
3:C:153:VAL:O	3:C:157:LEU:HG	2.17	0.44
6:F:91:VAL:CG1	6:F:92:GLY:N	2.79	0.44
25:Y:165:GLU:HB3	38:Y:8888:HOH:O	2.17	0.44
38:Z:8706:HOH:O	30:0:1886:A:H4'	2.18	0.44
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.53	0.44
29:3:3:MET:HG3	29:3:4:PRO:HD2	1.99	0.44
29:3:70:ARG:HD3	38:3:9062:HOH:O	2.18	0.44
30:0:113:A:OP2	30:0:114:A:H2'	2.18	0.44
30:0:523:C:H2'	30:0:524:A:H8	1.83	0.44
30:0:1015:C:H2'	30:0:1016:U:H6	1.83	0.44
30:0:1477:C:C5'	30:0:1868:G:H5"	2.47	0.44
30:0:1544:U:H2'	30:0:1545:C:H6	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1702:U:H1'	38:0:5781:HOH:O	2.18	0.44
31:9:59:C:H2'	31:9:60:C:C6	2.53	0.44
1:A:105:VAL:HG12	1:A:106:CYS:N	2.31	0.43
2:B:8:LYS:HG3	2:B:220:VAL:HG12	2.00	0.43
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.53	0.43
14:N:42:HIS:HB3	14:N:62:HIS:CE1	2.53	0.43
14:N:132:ASN:HD22	30:0:2413:A:H4'	1.83	0.43
23:W:43:GLY:HA3	30:0:945:U:O2'	2.18	0.43
25:Y:152:LYS:HB3	25:Y:160:LYS:HG3	2.00	0.43
30:0:212:A:O4'	30:0:214:U:C6	2.71	0.43
30:0:861:A:C4'	30:0:1697:G:H4'	2.48	0.43
30:0:1427:A:H61	30:0:1440:U:H1'	1.82	0.43
30:0:1520:G:C6	30:0:1521:C:C4	3.06	0.43
30:0:2252:A:C2'	30:0:2253:G:H5'	2.47	0.43
30:0:2642:G:H2'	30:0:2643:G:O4'	2.18	0.43
30:0:2777:G:O2'	30:0:2778:A:H5'	2.18	0.43
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.99	0.43
12:L:33:ALA:HB2	30:0:165:A:H5"	2.00	0.43
30:0:349:U:O2'	30:0:350:G:H5'	2.18	0.43
30:0:1192:A:H3'	30:0:1193:A:H5'	1.99	0.43
30:0:1878:G:O2'	30:0:1879:U:OP2	2.36	0.43
30:0:2087:C:O2'	30:0:2088:C:H5'	2.18	0.43
30:0:2133:U:H4'	30:0:2134:G:C5'	2.47	0.43
30:0:2375:A:H2'	30:0:2376:C:C6	2.53	0.43
30:0:2816:A:H5"	30:0:2817:G:H5'	2.00	0.43
2:B:177:HIS:O	2:B:181:ILE:HG13	2.19	0.43
3:C:170:ASP:OD2	30:0:330:C:H5	2.02	0.43
4:D:138:GLY:N	38:D:7597:HOH:O	2.51	0.43
12:L:18:HIS:HE1	30:0:901:G:OP2	2.00	0.43
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.18	0.43
30:0:684:G:H2'	30:0:685:C:C6	2.54	0.43
30:0:1014:A:H2'	30:0:1015:C:H5'	2.00	0.43
30:0:1681:G:H5"	30:0:1682:A:H5'	2.00	0.43
30:0:1705:C:H2'	30:0:1706:G:O4'	2.18	0.43
30:0:1815:A:H4'	30:0:2751:C:O4'	2.19	0.43
30:0:1850:U:H2'	30:0:1851:G:C8	2.52	0.43
1:A:173:GLY:O	1:A:176:HIS:HB3	2.18	0.43
2:B:10:SER:O	2:B:16:ARG:NH1	2.48	0.43
4:D:58:VAL:HB	4:D:62:ASP:HB2	1.99	0.43
5:E:90:HIS:CE1	30:0:2694:A:H5"	2.53	0.43
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:423:A:C5	30:0:424:C:C5	3.07	0.43
30:0:700:A:H5"	30:0:701:U:H5'	2.00	0.43
30:0:945:U:H2'	30:0:946:C:C6	2.53	0.43
30:0:1463:U:H2'	30:0:1464:C:C6	2.54	0.43
30:0:1625:U:H3'	30:0:1625:U:C6	2.52	0.43
30:0:2271:G:N3	30:0:2271:G:H2'	2.33	0.43
30:0:2791:U:H1'	30:0:2792:A:H5"	2.00	0.43
2:B:62:ARG:HA	2:B:65:MET:HE2	2.00	0.43
2:B:248:ARG:NH2	38:B:8994:HOH:O	2.51	0.43
3:C:39:GLN:O	3:C:43:LYS:HD3	2.18	0.43
3:C:240:LEU:HB2	38:C:8650:HOH:O	2.18	0.43
4:D:25:MET:SD	4:D:40:ILE:HD11	2.59	0.43
9:I:108:HIS:H	9:I:109:PRO:HD2	1.83	0.43
30:0:398:U:H2'	30:0:399:C:C6	2.54	0.43
30:0:638:C:H2'	30:0:639:A:C8	2.54	0.43
30:0:899:C:H5'	38:0:3205:HOH:O	2.18	0.43
30:0:2421:G:H3'	30:0:2422:U:H5"	2.01	0.43
30:0:2809:G:H2'	30:0:2810:G:O4'	2.19	0.43
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.48	0.43
20:T:28:SER:O	20:T:32:ARG:HG3	2.18	0.43
22:V:29:ASN:O	22:V:33:VAL:HG23	2.19	0.43
29:3:48:ASN:ND2	29:3:50:GLY:H	2.16	0.43
30:0:170:U:H2'	30:0:171:C:H5'	1.99	0.43
30:0:1042:U:O2'	30:0:1043:C:H5'	2.18	0.43
30:0:1333:U:H2'	30:0:1334:C:H6	1.84	0.43
30:0:1400:C:O2'	30:0:1401:G:H5'	2.19	0.43
30:0:1409:G:C2	30:0:1410:G:C8	3.07	0.43
30:0:1706:G:C6	30:0:1707:G:C6	3.06	0.43
30:0:1761:U:H2'	30:0:1762:C:C6	2.54	0.43
3:C:93:LYS:O	3:C:98:ARG:NH2	2.51	0.43
11:K:55:VAL:HG12	11:K:56:SER:N	2.34	0.43
12:L:145:LEU:O	12:L:148:GLU:HG3	2.19	0.43
14:N:65:ASP:HB3	38:N:8824:HOH:O	2.18	0.43
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.49	0.43
19:S:57:THR:C	19:S:59:ASP:H	2.22	0.43
29:3:30:GLN:NE2	38:3:9042:HOH:O	2.51	0.43
30:0:1773:G:N2	30:0:1774:G:C8	2.86	0.43
30:0:1838:U:H3'	38:0:5534:HOH:O	2.19	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.34	0.43
31:9:28:U:H5	38:9:9019:HOH:O	2.02	0.43
31:9:73:A:N1	31:9:108:C:O2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:MET:SD	30:0:875:A:C2	3.12	0.43
9:I:84:SER:HB3	9:I:92:VAL:HG21	1.99	0.43
13:M:49:ALA:C	13:M:54:TYR:HB3	2.39	0.43
15:O:38:ARG:HD3	30:0:654:A:OP2	2.19	0.43
22:V:39:ALA:N	22:V:40:PRO:CD	2.80	0.43
25:Y:158:LYS:HD3	38:0:6305:HOH:O	2.18	0.43
26:Z:61:HIS:O	26:Z:69:ASP:HA	2.19	0.43
28:2:28:LYS:O	30:0:87:C:H2'	2.19	0.43
30:0:106:A:O2'	30:0:107:U:H5'	2.19	0.43
30:0:111:C:H2'	30:0:112:G:C5'	2.48	0.43
30:0:907:A:H4'	30:0:1328:A:C2	2.53	0.43
30:0:1118:A:H8	30:0:1119:G:H5"	1.83	0.43
30:0:1170:U:O2'	30:0:1172:G:N7	2.45	0.43
30:0:1622:G:C2'	30:0:1623:C:H5'	2.48	0.43
30:0:2597:U:H2'	30:0:2598:U:H5'	2.00	0.43
30:0:2616:G:H1'	38:0:9424:HOH:O	2.18	0.43
3:C:78:ARG:NH1	3:C:78:ARG:HG3	2.33	0.43
4:D:23:VAL:HG23	4:D:23:VAL:O	2.19	0.43
8:H:122:LYS:HE3	8:H:122:LYS:HB2	1.89	0.43
13:M:171:ARG:NH2	30:0:189:A:OP1	2.52	0.43
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.34	0.43
18:R:82:GLU:O	18:R:86:LYS:HG3	2.19	0.43
25:Y:107:PRO:HB3	25:Y:182:PHE:CE2	2.54	0.43
30:0:191:A:C4	30:0:237:G:N7	2.87	0.43
30:0:289:G:O2'	30:0:290:C:H5'	2.19	0.43
30:0:613:C:H2'	30:0:614:U:C6	2.50	0.43
30:0:1074:G:H4'	30:0:1260:G:C6	2.54	0.43
30:0:1311:G:C2	30:0:1312:G:C8	3.06	0.43
30:0:2004:U:H2'	30:0:2004:U:O2	2.19	0.43
2:B:16:ARG:NE	38:B:9020:HOH:O	2.38	0.43
2:B:154:VAL:HG12	2:B:156:LYS:HG2	2.01	0.43
6:F:37:THR:O	6:F:41:GLU:HG3	2.19	0.43
18:R:47:LEU:HB2	18:R:89:LEU:HD21	2.01	0.43
22:V:4:HIS:HB3	38:0:7000:HOH:O	2.19	0.43
28:2:41:HIS:HE1	30:0:1439:C:OP1	2.02	0.43
30:0:69:A:H2'	30:0:70:A:OP2	2.18	0.43
30:0:168:C:O5'	30:0:168:C:H6	2.01	0.43
30:0:305:A:C5	30:0:329:A:C2	3.07	0.43
30:0:1170:U:H1'	30:0:1172:G:N7	2.34	0.43
30:0:1343:C:C2'	30:0:1344:G:O5'	2.66	0.43
30:0:1503:U:H6	30:0:1503:U:H3'	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1525:G:H4'	30:0:1525:G:OP1	2.19	0.43
30:0:2102:G:C2	30:0:2103:A:N6	2.87	0.43
30:0:2134:G:N2	30:0:2242:U:C2	2.87	0.43
30:0:2253:G:H2'	30:0:2254:G:H8	1.84	0.43
30:0:2379:G:N7	30:0:2408:A:N1	2.67	0.43
30:0:2506:A:O2'	30:0:2507:G:P	2.77	0.43
1:A:175:LYS:HG3	30:0:1847:A:OP1	2.19	0.42
2:B:162:MET:SD	2:B:310:ARG:HD3	2.59	0.42
2:B:171:VAL:O	2:B:175:LEU:HB2	2.19	0.42
2:B:314:ALA:HB3	2:B:317:PRO:HG3	2.01	0.42
3:C:129:HIS:CE1	3:C:232:LEU:H	2.37	0.42
7:G:67:LEU:O	7:G:71:LEU:HG	2.18	0.42
10:J:88:PRO:HD3	30:0:1104:C:H4'	2.00	0.42
21:U:17:THR:CG2	21:U:18:GLY:N	2.81	0.42
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.54	0.42
25:Y:146:PRO:O	25:Y:154:ARG:HG3	2.19	0.42
29:3:69:TYR:CZ	29:3:80:ARG:HD2	2.54	0.42
30:0:134:U:C2	30:0:145:A:C2	3.07	0.42
30:0:503:G:H2'	30:0:504:G:H8	1.84	0.42
30:0:694:A:C2'	30:0:695:C:H5'	2.49	0.42
30:0:1041:U:H4'	30:0:1295:G:H5'	2.01	0.42
30:0:2274:A:O2'	30:0:2275:G:H5'	2.19	0.42
30:0:2638:G:H1'	38:0:7780:HOH:O	2.19	0.42
30:0:2769:C:C2'	30:0:2770:G:C5'	2.87	0.42
2:B:216:LYS:HA	38:0:5091:HOH:O	2.20	0.42
3:C:218:VAL:N	38:C:8627:HOH:O	2.51	0.42
4:D:63:ILE:HG13	4:D:64:ARG:N	2.34	0.42
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.01	0.42
6:F:46:GLU:CD	6:F:100:ASP:HA	2.39	0.42
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.01	0.42
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.85	0.42
30:0:1206:U:C6	30:0:1206:U:C3'	3.03	0.42
30:0:1211:G:H2'	30:0:1212:C:C6	2.54	0.42
30:0:1438:G:HO2'	30:0:1684:A:H2	1.67	0.42
30:0:1759:A:N3	30:0:1818:C:H2'	2.34	0.42
30:0:2011:A:H4'	30:0:2012:U:O5'	2.19	0.42
30:0:2039:A:H4'	30:0:2760:C:O2'	2.19	0.42
30:0:2252:A:H2'	30:0:2253:G:C5'	2.49	0.42
30:0:2543:G:H2'	30:0:2544:G:O4'	2.18	0.42
31:9:1:U:C4'	31:9:3:A:OP1	2.67	0.42
31:9:3:A:H1'	38:9:9036:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:73:VAL:HG11	12:L:118:LEU:HD21	2.01	0.42
12:L:120:LEU:HD12	12:L:133:VAL:HG21	2.01	0.42
14:N:139:TRP:HA	14:N:139:TRP:HE3	1.83	0.42
23:W:119:HIS:CG	38:0:5297:HOH:O	2.71	0.42
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.49	0.42
30:0:99:A:C8	30:0:100:C:C5	3.07	0.42
30:0:152:A:O2'	30:0:153:C:H5'	2.18	0.42
30:0:284:C:H4'	30:0:285:A:H8	1.84	0.42
30:0:820:G:O2'	30:0:856:G:H4'	2.20	0.42
30:0:1654:U:H5"	38:0:7446:HOH:O	2.18	0.42
30:0:2758:G:H2'	30:0:2759:C:C6	2.54	0.42
2:B:74:ILE:HG13	38:B:9071:HOH:O	2.20	0.42
3:C:46:TYR:CE1	30:0:450:C:H4'	2.54	0.42
20:T:21:LYS:HA	20:T:24:ARG:HG3	2.01	0.42
25:Y:184:GLU:OE2	25:Y:204:ARG:HD2	2.20	0.42
30:0:154:C:H2'	30:0:155:C:H6	1.84	0.42
30:0:413:G:H2'	30:0:414:C:C6	2.54	0.42
30:0:1202:A:H2'	30:0:1203:G:H5'	2.00	0.42
30:0:1574:C:O5'	30:0:1574:C:H6	2.02	0.42
30:0:1632:A:C3'	30:0:1633:C:H5'	2.50	0.42
30:0:2105:C:O2'	30:0:2284:G:N2	2.53	0.42
31:9:39:U:O2'	31:9:42:C:C5	2.72	0.42
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.52	0.42
16:P:94:TRP:CZ2	16:P:98:ILE:HG13	2.55	0.42
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.55	0.42
27:1:16:HIS:HE1	30:0:775:G:OP1	2.02	0.42
29:3:69:TYR:O	29:3:77:ALA:HA	2.19	0.42
30:0:17:G:H2'	30:0:18:C:H6	1.83	0.42
30:0:677:C:P	38:0:7159:HOH:O	2.76	0.42
30:0:947:U:O2'	30:0:948:G:H5'	2.20	0.42
30:0:1119:G:N2	30:0:1246:A:N1	2.67	0.42
30:0:1161:A:O5'	30:0:1161:A:H8	2.02	0.42
30:0:1246:A:C4	30:0:1248:A:C8	3.08	0.42
30:0:1615:A:H4'	38:0:5897:HOH:O	2.17	0.42
30:0:2842:G:C2'	30:0:2843:A:H5'	2.49	0.42
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.52	0.42
2:B:60:SER:HA	2:B:61:PRO:HD3	1.89	0.42
2:B:307:ARG:HB3	38:B:9117:HOH:O	2.20	0.42
3:C:107:ARG:NH2	38:0:7159:HOH:O	2.53	0.42
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.91	0.42
14:N:119:GLN:O	14:N:123:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:151:ASP:OD1	14:N:166:ALA:HA	2.19	0.42
30:0:47:G:N3	30:0:114:A:C2	2.88	0.42
30:0:764:C:H2'	30:0:765:G:O4'	2.19	0.42
30:0:1309:U:O2'	30:0:1310:U:H5'	2.20	0.42
30:0:1746:A:O4'	30:0:1747:A:C2	2.72	0.42
30:0:1760:G:H5'	30:0:1818:C:O2'	2.19	0.42
30:0:2090:G:H2'	30:0:2091:G:C8	2.53	0.42
30:0:2094:G:O6	30:0:2649:A:H2	2.01	0.42
30:0:2820:A:H2'	30:0:2821:C:C6	2.54	0.42
31:9:92:G:C6	31:9:93:A:C6	3.08	0.42
1:A:212:PRO:HA	30:0:1943:C:O4'	2.20	0.42
2:B:26:PHE:HE1	38:B:9112:HOH:O	2.02	0.42
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.87	0.42
5:E:91:PHE:HE1	30:0:2694:A:C4'	2.31	0.42
7:G:64:ASN:N	7:G:64:ASN:ND2	2.67	0.42
19:S:57:THR:HG23	38:S:8982:HOH:O	2.19	0.42
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.20	0.42
29:3:65:THR:CG2	29:3:67:LEU:HG	2.50	0.42
30:0:23:G:C6	30:0:24:G:N1	2.88	0.42
30:0:295:C:H2'	30:0:296:G:O4'	2.19	0.42
30:0:699:C:H6	30:0:744:G:O4'	2.03	0.42
30:0:1183:C:H41	30:0:1192:A:P	2.43	0.42
30:0:1211:G:H2'	30:0:1212:C:H6	1.84	0.42
30:0:1441:G:H1'	38:0:7786:HOH:O	2.19	0.42
30:0:2594:C:O2'	30:0:2595:U:H5'	2.20	0.42
30:0:2653:A:H2'	30:0:2654:C:C6	2.55	0.42
31:9:65:A:N6	31:9:112:U:C6	2.88	0.42
1:A:36:ASP:CB	1:A:85:SER:H	2.33	0.42
2:B:132:HIS:CE1	2:B:171:VAL:HG23	2.55	0.42
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.55	0.42
2:B:211:THR:HG21	38:0:7480:HOH:O	2.19	0.42
11:K:89:LYS:HE2	21:U:19:THR:HG21	2.02	0.42
14:N:22:GLN:HA	14:N:25:ARG:CZ	2.50	0.42
20:T:77:VAL:HG11	20:T:91:LEU:HD11	2.02	0.42
30:0:40:C:H4'	38:0:7030:HOH:O	2.20	0.42
30:0:1139:U:H2'	30:0:1140:C:C6	2.55	0.42
30:0:2064:U:H2'	30:0:2065:C:H6	1.85	0.42
30:0:2105:C:H2'	30:0:2106:C:C6	2.55	0.42
30:0:2819:C:H2'	30:0:2820:A:C8	2.54	0.42
31:9:42:C:H5'	31:9:43:G:OP2	2.19	0.42
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:ARG:NH1	30:0:2547:C:OP2	2.53	0.42
2:B:141:ARG:HG2	2:B:165:ARG:HA	2.02	0.42
14:N:61:ALA:CB	14:N:88:ALA:HB2	2.49	0.42
14:N:108:SER:HA	14:N:109:PRO:HD3	1.74	0.42
27:1:12:ASN:O	30:0:1415:G:H5'	2.20	0.42
30:0:128:A:C8	30:0:128:A:H3'	2.55	0.42
30:0:542:A:H1'	38:0:4680:HOH:O	2.20	0.42
30:0:595:U:H2'	30:0:596:C:C6	2.54	0.42
30:0:860:U:H2'	30:0:861:A:C8	2.54	0.42
30:0:1902:G:N2	30:0:1936:C:C2	2.88	0.42
30:0:2354:A:C2	30:0:2367:A:C8	3.08	0.42
30:0:2415:A:C2'	30:0:2416:G:H5'	2.49	0.42
30:0:2824:C:O3'	30:0:2825:C:H6	2.02	0.42
1:A:88:ILE:O	1:A:88:ILE:HG22	2.19	0.42
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.84	0.42
10:J:26:VAL:HG13	10:J:36:VAL:HG11	2.02	0.42
13:M:46:LEU:HG	38:M:8922:HOH:O	2.18	0.42
13:M:167:GLY:O	13:M:171:ARG:HG3	2.20	0.42
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.50	0.42
17:Q:86:VAL:HG13	17:Q:91:LEU:HD11	2.01	0.42
18:R:40:ALA:O	18:R:44:VAL:HG23	2.19	0.42
30:0:59:A:H5'	38:0:4331:HOH:O	2.20	0.42
30:0:851:C:O2	30:0:2022:A:H2	2.03	0.42
30:0:920:C:H5'	30:0:921:G:C4	2.55	0.42
30:0:1825:U:O2'	30:0:1826:C:H5'	2.20	0.42
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.42
30:0:1946:C:H2'	30:0:1971:G:C8	2.55	0.42
30:0:2379:G:H5'	30:0:2381:C:O4'	2.20	0.42
30:0:2691:A:H8	30:0:2691:A:OP1	2.03	0.42
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.20	0.41
3:C:200:PRO:HB3	3:C:212:VAL:HG23	2.02	0.41
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.84	0.41
6:F:30:LYS:HE2	6:F:99:THR:HG21	2.01	0.41
16:P:81:LYS:HG2	38:0:9537:HOH:O	2.19	0.41
23:W:122:ARG:NH2	38:0:6425:HOH:O	2.53	0.41
30:0:441:A:H8	30:0:441:A:O5'	2.03	0.41
30:0:559:U:H2'	30:0:560:U:O4'	2.20	0.41
30:0:699:C:C6	30:0:744:G:C4	3.08	0.41
30:0:1425:G:O2'	30:0:1426:C:H5'	2.20	0.41
30:0:1788:U:C2	30:0:1805:G:N2	2.88	0.41
1:A:29:HIS:HB2	1:A:153:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.07	0.41
10:J:45:VAL:HG11	10:J:121:LEU:HD22	2.02	0.41
18:R:114:VAL:HA	18:R:144:GLU:O	2.20	0.41
27:1:28:HIS:HD2	27:1:30:LYS:H	1.66	0.41
29:3:22:VAL:CG1	29:3:67:LEU:HD13	2.51	0.41
30:0:1481:G:H2'	30:0:1482:A:O4'	2.20	0.41
30:0:1625:U:C6	30:0:1625:U:C3'	3.03	0.41
30:0:1706:G:C6	30:0:1707:G:N1	2.87	0.41
30:0:1788:U:O2'	30:0:1789:G:H5'	2.20	0.41
30:0:2461:U:O2	30:0:2466:G:H1'	2.19	0.41
30:0:2718:C:H5'	30:0:2718:C:C6	2.53	0.41
30:0:2754:G:C2'	30:0:2755:G:H5'	2.50	0.41
4:D:167:GLU:C	4:D:169:THR:H	2.24	0.41
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.47	0.41
30:0:1163:G:H2'	30:0:1164:U:C5	2.54	0.41
30:0:1250:C:O2'	30:0:1251:C:H5'	2.20	0.41
30:0:1511:U:O2'	30:0:1512:G:H5'	2.20	0.41
30:0:1921:A:C6	30:0:1922:A:C2	3.09	0.41
30:0:2325:U:O2'	30:0:2411:C:H1'	2.20	0.41
30:0:2802:C:H2'	30:0:2803:C:H6	1.85	0.41
30:0:2893:C:O2'	30:0:2894:C:H5'	2.19	0.41
1:A:23:TYR:HB2	30:0:1872:C:C5	2.55	0.41
2:B:57:GLU:HA	2:B:58:PRO:HD2	1.91	0.41
2:B:95:ARG:HA	2:B:96:PRO:HD3	1.93	0.41
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.01	0.41
5:E:118:ILE:HG23	5:E:144:THR:HG21	2.01	0.41
16:P:1:THR:O	30:0:1396:C:H1'	2.19	0.41
20:T:18:GLU:O	20:T:21:LYS:HG2	2.20	0.41
30:0:311:C:H2'	30:0:312:U:C6	2.55	0.41
30:0:567:U:O5'	30:0:567:U:H6	2.03	0.41
30:0:1304:U:H2'	30:0:1305:C:C6	2.56	0.41
30:0:1855:G:H4'	30:0:1856:C:O5'	2.20	0.41
30:0:2359:G:H3'	38:0:5696:HOH:O	2.21	0.41
30:0:2510:C:H42	30:0:2564:G:H22	1.68	0.41
3:C:19:PRO:HG2	3:C:22:PHE:CD1	2.56	0.41
4:D:55:LYS:HB2	38:0:6341:HOH:O	2.20	0.41
5:E:95:VAL:HG11	5:E:131:LEU:HD11	2.02	0.41
14:N:37:ARG:HD3	33:N:8807:CL:CL	2.57	0.41
15:O:21:SER:OG	15:O:106:PRO:HB2	2.20	0.41
23:W:139:GLY:O	23:W:141:HIS:CD2	2.72	0.41
27:1:25:LYS:HE3	38:0:7430:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:241:A:C2	30:0:378:A:H4'	2.56	0.41
30:0:699:C:C2	30:0:744:G:C2	3.08	0.41
30:0:1118:A:C8	30:0:1119:G:H5"	2.55	0.41
30:0:1175:G:H1'	30:0:1193:A:C8	2.55	0.41
30:0:1183:C:N3	30:0:1184:C:N4	2.68	0.41
30:0:1700:C:H5"	30:0:1701:A:OP2	2.19	0.41
30:0:2255:A:N1	30:0:2256:G:C4	2.88	0.41
30:0:2727:A:C6	30:0:2756:U:C2	3.09	0.41
1:A:123:GLY:HA3	1:A:162:GLY:HA2	2.03	0.41
1:A:164:ARG:NE	38:0:5420:HOH:O	2.54	0.41
16:P:134:VAL:O	16:P:137:LEU:HB3	2.21	0.41
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.56	0.41
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.35	0.41
25:Y:216:ARG:HD2	38:Y:8866:HOH:O	2.19	0.41
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	2.03	0.41
30:0:571:C:O5'	30:0:571:C:H6	2.04	0.41
30:0:861:A:H4'	30:0:1697:G:C4'	2.51	0.41
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.41
30:0:1180:U:O2'	30:0:1181:A:H5'	2.20	0.41
30:0:1361:C:H2'	30:0:1362:U:C6	2.55	0.41
30:0:1845:A:O2'	30:0:1846:U:H5'	2.19	0.41
30:0:2564:G:OP2	30:0:2565:C:H5"	2.21	0.41
2:B:119:HIS:O	2:B:121:PRO:HD3	2.20	0.41
3:C:154:VAL:O	3:C:158:GLU:HG3	2.20	0.41
38:C:8571:HOH:O	20:T:2:LYS:HE2	2.19	0.41
13:M:184:ARG:HG3	13:M:185:PRO:HA	2.03	0.41
17:Q:15:LYS:HB3	17:Q:15:LYS:HE2	1.82	0.41
20:T:9:LYS:HD2	38:0:7449:HOH:O	2.20	0.41
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.33	0.41
30:0:553:G:O4'	30:0:1325:G:H5'	2.21	0.41
30:0:1523:G:C6	30:0:1524:U:O4	2.74	0.41
30:0:1565:C:H2'	30:0:1566:C:C6	2.56	0.41
30:0:1594:C:O2'	30:0:1607:A:H4'	2.20	0.41
30:0:2248:C:H3'	38:0:5454:HOH:O	2.20	0.41
30:0:2276:U:H2'	30:0:2277:U:C6	2.56	0.41
30:0:2329:C:H2'	30:0:2330:U:C6	2.56	0.41
30:0:2584:G:H4'	38:0:7141:HOH:O	2.20	0.41
30:0:2587:OMU:O3'	30:0:2587:OMU:HM22	2.21	0.41
31:9:2:U:P	31:9:3:A:H5'	2.61	0.41
2:B:262:ARG:HG3	30:0:2716:G:H5'	2.02	0.41
6:F:14:ASP:O	6:F:18:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.21	0.41
9:I:87:PRO:HG2	30:0:1181:A:H4'	2.03	0.41
13:M:169:ARG:NH2	38:M:8849:HOH:O	2.49	0.41
18:R:114:VAL:HG13	18:R:114:VAL:O	2.20	0.41
19:S:80:ARG:NH1	38:S:8999:HOH:O	2.54	0.41
25:Y:117:LEU:HB2	25:Y:174:VAL:HG21	2.02	0.41
28:2:41:HIS:HB3	28:2:44:ARG:HB2	2.03	0.41
30:0:11:A:N3	30:0:11:A:H2'	2.36	0.41
30:0:407:A:H5'	38:0:6043:HOH:O	2.19	0.41
30:0:1098:A:H2'	30:0:1099:G:O4'	2.20	0.41
30:0:1193:A:H2	30:0:1194:A:N6	2.18	0.41
30:0:1364:G:H1'	38:0:4805:HOH:O	2.21	0.41
30:0:1829:A:H2'	30:0:1830:C:H5'	2.03	0.41
30:0:2089:A:C2'	30:0:2090:G:H5'	2.50	0.41
30:0:2115:U:H2'	30:0:2116:U:C6	2.56	0.41
1:A:105:VAL:HG11	1:A:154:ALA:CB	2.49	0.41
1:A:164:ARG:CZ	38:0:5420:HOH:O	2.68	0.41
2:B:53:LEU:HD11	2:B:327:VAL:HG22	2.02	0.41
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.36	0.41
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.20	0.41
5:E:21:THR:HG23	5:E:30:THR:OG1	2.21	0.41
5:E:23:GLU:HG2	5:E:28:SER:HB3	2.02	0.41
8:H:34:HIS:HD2	8:H:90:LEU:O	2.03	0.41
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.84	0.41
11:K:63:GLU:HG2	38:K:6344:HOH:O	2.20	0.41
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.21	0.41
17:Q:47:VAL:HA	17:Q:48:PRO:HD3	1.81	0.41
18:R:119:VAL:HG12	18:R:119:VAL:O	2.21	0.41
19:S:42:GLU:HG2	19:S:49:VAL:HG23	2.02	0.41
19:S:57:THR:CG2	19:S:58:MET:N	2.83	0.41
20:T:16:LEU:HB2	30:0:100:C:H4'	2.03	0.41
21:U:46:ALA:HB1	21:U:52:THR:HG21	2.03	0.41
24:X:30:MET:HE1	24:X:58:ALA:HB3	2.02	0.41
38:X:2479:HOH:O	30:0:2904:U:H4'	2.20	0.41
25:Y:144:ARG:NH2	38:Y:8907:HOH:O	2.54	0.41
26:Z:74:GLN:HB2	26:Z:78:ILE:HG22	2.03	0.41
29:3:15:ASN:O	30:0:2408:A:H4'	2.20	0.41
29:3:31:THR:O	30:0:1923:G:H4'	2.21	0.41
30:0:196:G:H1'	30:0:198:A:N7	2.36	0.41
30:0:199:A:H8	38:0:6963:HOH:O	2.04	0.41
30:0:226:A:H1'	30:0:393:G:C5	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:393:G:C6	30:0:394:G:C6	3.08	0.41
30:0:424:C:H2'	30:0:425:U:C6	2.56	0.41
30:0:506:G:N2	30:0:509:A:C5'	2.69	0.41
30:0:506:G:N2	30:0:509:A:H5'	2.28	0.41
30:0:697:G:H4'	30:0:730:G:O3'	2.21	0.41
30:0:1185:U:C5'	38:0:7491:HOH:O	2.67	0.41
30:0:1191:A:C2	30:0:1207:A:C2	3.08	0.41
30:0:1207:A:N6	38:0:5641:HOH:O	2.53	0.41
30:0:1209:C:O2'	30:0:1210:G:H5'	2.21	0.41
30:0:1482:A:O2'	30:0:1483:C:H5'	2.21	0.41
30:0:1504:A:H5'	38:0:4416:HOH:O	2.21	0.41
30:0:1626:A:H2'	30:0:1627:G:H5'	2.02	0.41
30:0:1649:G:O2'	30:0:1650:C:H5'	2.21	0.41
30:0:1840:A:H4'	30:0:1841:C:O5'	2.21	0.41
30:0:1889:C:H2'	30:0:1890:U:O4'	2.21	0.41
30:0:1976:G:O2'	30:0:1977:U:C5'	2.69	0.41
30:0:2073:G:OP2	30:0:2490:A:H5'	2.21	0.41
31:9:57:A:N6	38:9:9060:HOH:O	2.53	0.41
3:C:19:PRO:HD2	3:C:240:LEU:HD11	2.02	0.41
3:C:118:THR:CG2	3:C:137:PRO:HB3	2.50	0.41
11:K:4:LEU:HD22	11:K:116:GLU:HB3	2.02	0.41
14:N:42:HIS:CG	14:N:62:HIS:HE1	2.38	0.41
14:N:82:TYR:OH	14:N:176:ARG:NH1	2.54	0.41
18:R:80:TYR:O	30:0:2050:G:H5"	2.20	0.41
25:Y:210:GLY:H	30:0:1313:A:H5"	1.85	0.41
29:3:6:ARG:HA	29:3:20:HIS:O	2.21	0.41
30:0:34:C:H1'	38:0:9175:HOH:O	2.19	0.41
30:0:1495:C:OP2	30:0:1505:U:N3	2.53	0.41
30:0:2252:A:H2'	30:0:2253:G:O4'	2.21	0.41
30:0:2445:U:H2'	30:0:2446:G:H8	1.83	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.39	0.41
30:0:2754:G:O2'	30:0:2755:G:H5'	2.21	0.41
6:F:48:VAL:HG12	6:F:97:ALA:CB	2.51	0.40
6:F:118:LEU:O	6:F:119:ARG:HB3	2.21	0.40
11:K:1:MET:HE1	38:K:6646:HOH:O	2.21	0.40
14:N:141:ARG:NH2	31:9:48:C:H4'	2.35	0.40
30:0:397:A:O2'	30:0:417:G:N3	2.38	0.40
30:0:682:A:H2'	30:0:683:G:O4'	2.20	0.40
30:0:1015:C:H2'	30:0:1016:U:C6	2.56	0.40
30:0:1559:A:C1'	38:0:5876:HOH:O	2.68	0.40
30:0:1603:A:C5'	30:0:1605:G:C5'	2.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2016:U:H2'	30:0:2017:U:O4'	2.20	0.40
30:0:2135:A:O4'	30:0:2243:C:N4	2.54	0.40
31:9:65:A:C2'	31:9:66:G:OP2	2.68	0.40
31:9:81:C:C2'	31:9:82:U:H5'	2.51	0.40
1:A:101:GLU:HG2	38:A:9034:HOH:O	2.20	0.40
1:A:223:ARG:HB2	30:0:2272:G:H5'	2.03	0.40
2:B:321:PRO:HG3	38:B:9065:HOH:O	2.21	0.40
8:H:49:GLN:HG3	8:H:140:TYR:CE2	2.56	0.40
10:J:127:ILE:CG2	33:J:8801:CL:CL	3.02	0.40
12:L:50:GLY:C	30:0:2453:G:H4'	2.41	0.40
16:P:105:LEU:HD21	16:P:137:LEU:HD11	2.04	0.40
18:R:15:LYS:HE3	38:R:8976:HOH:O	2.21	0.40
18:R:59:PHE:O	18:R:63:ASN:HB3	2.21	0.40
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.57	0.40
23:W:29:VAL:O	23:W:30:ASN:HB2	2.21	0.40
25:Y:122:ARG:NH2	38:Y:8833:HOH:O	2.54	0.40
30:0:67:A:H5"	30:0:69:A:C8	2.57	0.40
30:0:81:G:N3	30:0:98:A:C2	2.89	0.40
30:0:542:A:H2'	30:0:543:G:O4'	2.21	0.40
30:0:570:C:H2'	30:0:571:C:H5'	2.02	0.40
30:0:1896:G:C6	30:0:1897:U:C4	3.09	0.40
30:0:2314:G:H2'	30:0:2315:C:H5'	2.03	0.40
1:A:103:VAL:HA	1:A:104:PRO:HD3	1.92	0.40
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.85	0.40
38:M:8835:HOH:O	30:0:169:A:H5"	2.22	0.40
20:T:9:LYS:HD3	38:0:3755:HOH:O	2.20	0.40
21:U:49:LEU:HG	38:U:3805:HOH:O	2.21	0.40
23:W:125:HIS:NE2	30:0:1097:A:H5"	2.36	0.40
25:Y:112:GLU:OE2	25:Y:115:ARG:NH1	2.55	0.40
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.21	0.40
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	2.04	0.40
30:0:282:C:C2'	30:0:283:U:H5'	2.51	0.40
30:0:560:U:H2'	30:0:561:G:H8	1.86	0.40
30:0:574:G:O2'	30:0:575:A:H5'	2.21	0.40
30:0:1081:A:C6	30:0:1082:A:N1	2.89	0.40
30:0:1375:A:C2'	30:0:1376:G:H5'	2.50	0.40
30:0:1613:C:H2'	30:0:1614:G:O4'	2.21	0.40
30:0:2566:A:H2	30:0:2695:C:O2	2.03	0.40
31:9:110:G:C5	31:9:111:U:C5	3.09	0.40
2:B:285:VAL:O	2:B:286:ASN:HB2	2.21	0.40
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:GLN:NE2	30:0:1119:G:H8	2.19	0.40
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.56	0.40
18:R:113:HIS:O	18:R:145:LEU:HD12	2.20	0.40
23:W:125:HIS:CD2	23:W:127:GLY:H	2.39	0.40
25:Y:130:ARG:HD2	38:Y:8850:HOH:O	2.19	0.40
30:0:282:C:H1'	30:0:368:C:H41	1.78	0.40
30:0:372:A:H2'	30:0:373:G:C8	2.57	0.40
30:0:502:A:H2'	30:0:503:G:O4'	2.21	0.40
30:0:1117:A:C2	30:0:1244:U:C2	3.10	0.40
30:0:1160:G:O2'	30:0:1190:G:H1'	2.22	0.40
30:0:1268:C:H2'	30:0:1269:G:H8	1.87	0.40
30:0:1294:A:H2'	30:0:1295:G:O4'	2.21	0.40
30:0:1391:G:H2'	30:0:1392:A:H5'	2.03	0.40
30:0:1450:C:H4'	30:0:1493:A:C5	2.56	0.40
30:0:2266:A:H2'	30:0:2267:G:C8	2.57	0.40
30:0:2346:C:H6	30:0:2346:C:O5'	2.03	0.40
30:0:2727:A:N1	30:0:2756:U:C2	2.90	0.40
31:9:3:A:H2'	38:9:9039:HOH:O	2.21	0.40
2:B:215:VAL:HB	38:B:9085:HOH:O	2.21	0.40
8:H:157:TYR:CD1	8:H:157:TYR:C	2.94	0.40
12:L:11:ARG:NH1	30:0:903:U:OP2	2.54	0.40
12:L:30:ARG:NH2	38:L:8822:HOH:O	2.53	0.40
13:M:193:LYS:HB3	30:0:392:U:C5'	2.52	0.40
14:N:17:ARG:HH11	14:N:17:ARG:HB3	1.86	0.40
30:0:415:A:O2'	30:0:416:G:H5'	2.21	0.40
30:0:713:U:H6	30:0:713:U:O5'	2.04	0.40
30:0:800:G:H2'	30:0:801:U:C6	2.56	0.40
30:0:895:A:H2'	30:0:896:C:C6	2.56	0.40
30:0:1052:G:N3	30:0:1052:G:H2'	2.36	0.40
30:0:1201:C:H2'	30:0:1202:A:H5'	2.04	0.40
30:0:1970:G:N3	30:0:1970:G:H2'	2.36	0.40
30:0:2290:U:H2'	38:0:7160:HOH:O	2.22	0.40
30:0:2712:G:P	38:0:5229:HOH:O	2.80	0.40
30:0:2728:C:O5'	30:0:2728:C:H6	2.04	0.40
31:9:28:U:H2'	31:9:29:C:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	19 (8%)	4 (2%)	9 29
2	B	335/338 (99%)	307 (92%)	24 (7%)	4 (1%)	13 39
3	C	244/246 (99%)	224 (92%)	20 (8%)	0	100 100
4	D	134/177 (76%)	110 (82%)	20 (15%)	4 (3%)	4 15
5	E	170/178 (96%)	162 (95%)	8 (5%)	0	100 100
6	F	117/120 (98%)	106 (91%)	8 (7%)	3 (3%)	5 18
7	G	25/348 (7%)	25 (100%)	0	0	100 100
8	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	12 36
9	I	68/162 (42%)	52 (76%)	15 (22%)	1 (2%)	10 33
10	J	140/145 (97%)	129 (92%)	10 (7%)	1 (1%)	22 53
11	K	130/132 (98%)	122 (94%)	7 (5%)	1 (1%)	19 49
12	L	141/165 (86%)	128 (91%)	12 (8%)	1 (1%)	22 53
13	M	192/196 (98%)	184 (96%)	7 (4%)	1 (0%)	29 61
14	N	184/187 (98%)	168 (91%)	12 (6%)	4 (2%)	6 22
15	O	113/116 (97%)	111 (98%)	2 (2%)	0	100 100
16	P	141/149 (95%)	139 (99%)	2 (1%)	0	100 100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100 100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100 100
20	T	117/120 (98%)	112 (96%)	5 (4%)	0	100 100
21	U	51/67 (76%)	47 (92%)	4 (8%)	0	100 100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100 100
23	W	152/154 (99%)	150 (99%)	0	2 (1%)	12 36
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	12 36
25	Y	140/241 (58%)	140 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	63 (89%)	7 (10%)	1 (1%)	11	34
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	14	41
All	All	3705/4472 (83%)	3453 (93%)	221 (6%)	31 (1%)	19	49

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	VAL
6	F	101	ALA
8	H	19	ARG
12	L	149	ARG
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
23	W	77	ALA
1	A	34	ASP
2	B	185	GLY
4	D	137	PRO
2	B	2	GLN
6	F	100	ASP
11	K	127	ALA
1	A	36	ASP
2	B	169	GLY
2	B	206	THR
4	D	27	ILE
4	D	56	ARG
4	D	65	GLU
6	F	61	MET
13	M	71	SER
14	N	139	TRP
23	W	49	ASN
24	X	70	ILE
26	Z	44	ARG
29	3	56	PRO
10	J	65	ASN
8	H	171	GLY
9	I	83	GLY

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%)	169 (94%)	10 (6%)	21 51
2	B	282/283 (100%)	267 (95%)	15 (5%)	22 54
3	C	193/193 (100%)	178 (92%)	15 (8%)	12 35
4	D	117/148 (79%)	112 (96%)	5 (4%)	29 62
5	E	152/156 (97%)	148 (97%)	4 (3%)	46 79
6	F	93/94 (99%)	92 (99%)	1 (1%)	73 92
7	G	27/282 (10%)	26 (96%)	1 (4%)	34 68
8	H	134/145 (92%)	130 (97%)	4 (3%)	41 75
9	I	58/130 (45%)	57 (98%)	1 (2%)	60 87
10	J	118/121 (98%)	108 (92%)	10 (8%)	10 31
11	K	106/106 (100%)	102 (96%)	4 (4%)	33 67
12	L	113/127 (89%)	108 (96%)	5 (4%)	28 61
13	M	158/160 (99%)	149 (94%)	9 (6%)	20 50
14	N	149/150 (99%)	141 (95%)	8 (5%)	22 53
15	O	93/94 (99%)	92 (99%)	1 (1%)	73 92
16	P	113/117 (97%)	111 (98%)	2 (2%)	59 86
17	Q	79/80 (99%)	75 (95%)	4 (5%)	24 55
18	R	117/122 (96%)	114 (97%)	3 (3%)	46 79
19	S	71/74 (96%)	71 (100%)	0	100 100
20	T	105/106 (99%)	97 (92%)	8 (8%)	13 36
21	U	44/53 (83%)	43 (98%)	1 (2%)	50 82
22	V	51/57 (90%)	49 (96%)	2 (4%)	32 66
23	W	130/130 (100%)	126 (97%)	4 (3%)	40 74
24	X	66/74 (89%)	57 (86%)	9 (14%)	3 11
25	Y	120/196 (61%)	115 (96%)	5 (4%)	30 63
26	Z	60/94 (64%)	60 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	1	46/47 (98%)	46 (100%)	0	100 100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49 81
29	3	79/79 (100%)	77 (98%)	2 (2%)	47 80
All	All	3095/3646 (85%)	2961 (96%)	134 (4%)	29 62

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	36	ASP
1	A	68	ILE
1	A	69	LEU
1	A	94	LEU
1	A	131	HIS
1	A	153	ARG
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN
2	B	56	ASP
2	B	97	LEU
2	B	98	THR
2	B	132	HIS
2	B	149	ASP
2	B	162	MET
2	B	190	MET
2	B	234	ARG
2	B	254	GLN
2	B	257	THR
2	B	277	GLU
2	B	312	ARG
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	94	THR
3	C	115	LEU
3	C	136	VAL
3	C	151	GLN
3	C	162	VAL

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Mol	Chain	Res	Type
3	C	187	ARG
3	C	211	ASP
3	C	214	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	243	VAL
4	D	19	GLU
4	D	24	HIS
4	D	50	VAL
4	D	149	ARG
4	D	161	ASP
5	E	7	ILE
5	E	86	VAL
5	E	102	VAL
5	E	156	ASP
6	F	12	LEU
7	G	73	ASP
8	H	65	LEU
8	H	87	LYS
8	H	157	TYR
8	H	173	GLU
9	I	94	ASP
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	93	ARG
10	J	107	ASN
10	J	112	ASP
10	J	120	SER
10	J	127	ILE
10	J	131	THR
11	K	7	ASP
11	K	10	GLN
11	K	98	VAL
11	K	119	GLN
12	L	35	ARG
12	L	43	HIS
12	L	99	GLU
12	L	104	ASP
12	L	140	VAL

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Mol	Chain	Res	Type
13	M	10	ASP
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	145	ASP
13	M	164	THR
14	N	17	ARG
14	N	26	LEU
14	N	49	THR
14	N	56	ASP
14	N	134	ASP
14	N	135	VAL
14	N	173	ASP
14	N	177	GLU
15	O	28	ASP
16	P	91	LYS
16	P	98	ILE
17	Q	18	PRO
17	Q	20	ASP
17	Q	57	ASP
17	Q	95	GLU
18	R	39	THR
18	R	132	ARG
18	R	143	VAL
20	T	26	THR
20	T	39	ASN
20	T	71	VAL
20	T	73	HIS
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	47	ARG
22	V	12	THR
22	V	65	ASP
23	W	26	ILE
23	W	52	VAL
23	W	73	LEU
23	W	146	ILE

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Mol	Chain	Res	Type
24	X	15	ARG
24	X	27	ASP
24	X	44	ASP
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	103	THR
25	Y	144	ARG
25	Y	189	ASN
25	Y	200	THR
25	Y	203	VAL
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 (79) 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	260	HIS
2	B	320	GLN
2	B	332	ASN
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	90	HIS
5	E	119	HIS
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN

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Mol	Chain	Res	Type
8	H	62	HIS
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
11	K	119	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	107	ASN
14	N	132	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
19	S	44	GLN
19	S	53	ASN
19	S	55	GLN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	60	GLN
23	W	12	ASN
23	W	14	HIS
23	W	27	HIS
23	W	28	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS

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Mol	Chain	Res	Type
24	X	23	HIS
24	X	36	HIS
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	15	ASN
29	3	20	HIS
29	3	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	236 (8%)	30 (1%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	254 (8%)	31 (1%)

All (254) 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	130	C
30	0	141	C
30	0	151	A
30	0	166	A

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Mol	Chain	Res	Type
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
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
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	581	G
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	698	A

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Mol	Chain	Res	Type
30	0	701	U
30	0	702	G
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	884	C
30	0	885	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
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

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Mol	Chain	Res	Type
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	1205	U
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	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1492	A
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1592	G
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

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Mol	Chain	Res	Type
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1732	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	1965	C
30	0	1968	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1996	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
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	2103	A
30	0	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G

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Mol	Chain	Res	Type
30	0	2291	A
30	0	2317	C
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	2465	A
30	0	2467	A
30	0	2476	C
30	0	2482	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2527	U
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2637	A
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

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Mol	Chain	Res	Type
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2836	G
30	0	2852	A
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	39	U
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (31) 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	644	G
30	0	699	C
30	0	834	G
30	0	857	A

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Mol	Chain	Res	Type
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1165	G
30	0	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1377	C
30	0	1474	C
30	0	1506	U
30	0	1685	A
30	0	1692	C
30	0	1942	A
30	0	2467	A
30	0	2482	C
30	0	2526	C
30	0	2649	A
30	0	2718	C
30	0	2726	U
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	OMG	0	2588	30	18,26,27	1.03	2 (11%)	19,38,41	0.72	1 (5%)
30	1MA	0	628	30	16,25,26	1.35	3 (18%)	18,37,40	1.04	2 (11%)
30	UR3	0	2619	30	19,22,23	0.46	0	26,32,35	0.64	1 (3%)
30	PSU	0	2621	30	18,21,22	1.40	2 (11%)	22,30,33	1.27	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	OMU	0	2587	30	19,22,23	0.31	0	26,31,34	0.37	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	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	1MA	0	628	30	-	0/3/25/26	0/3/3/3
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	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	4.67	1.43	1.36
30	0	628	1MA	C2-N3	3.43	1.33	1.29
30	0	2588	OMG	C5-C6	-2.59	1.42	1.47
30	0	2588	OMG	C8-N7	-2.54	1.30	1.35
30	0	628	1MA	C6-N6	2.46	1.33	1.27
30	0	2621	PSU	C6-C5	2.28	1.38	1.35
30	0	628	1MA	C8-N7	-2.13	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	3.38	120.56	118.20
30	0	628	1MA	N1-C2-N3	2.77	129.25	126.02
30	0	2621	PSU	C6-N1-C2	-2.71	119.91	122.68
30	0	2621	PSU	O2-C2-N1	2.66	125.72	122.79
30	0	628	1MA	C5-C6-N1	2.55	117.71	113.90
30	0	2619	UR3	C4-N3-C2	2.36	126.78	124.56
30	0	2588	OMG	O6-C6-C5	2.16	128.59	124.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	2	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	237/240 (98%)	-0.57	6 (2%) 57 47	22, 48, 85, 107	0
2	B	337/338 (99%)	-0.76	0 100 100	24, 49, 78, 90	0
3	C	246/246 (100%)	-0.72	0 100 100	20, 40, 64, 79	0
4	D	140/177 (79%)	0.92	26 (18%) 1 1	61, 98, 123, 132	0
5	E	172/178 (96%)	-0.46	2 (1%) 79 73	43, 66, 86, 91	0
6	F	119/120 (99%)	-0.01	3 (2%) 57 47	44, 67, 97, 113	0
7	G	29/348 (8%)	0.68	5 (17%) 1 1	77, 94, 103, 104	0
8	H	160/177 (90%)	0.34	16 (10%) 7 4	48, 69, 99, 104	0
9	I	70/162 (43%)	3.42	49 (70%) 0 0	128, 145, 162, 163	0
10	J	142/145 (97%)	-0.73	0 100 100	32, 47, 68, 90	0
11	K	132/132 (100%)	-0.92	0 100 100	30, 44, 67, 73	0
12	L	145/165 (87%)	-0.19	4 (2%) 53 43	25, 62, 112, 124	0
13	M	194/196 (98%)	-0.87	0 100 100	26, 39, 55, 63	0
14	N	186/187 (99%)	-0.31	3 (1%) 72 66	39, 63, 111, 120	0
15	O	115/116 (99%)	-0.74	0 100 100	33, 51, 68, 72	0
16	P	143/149 (95%)	-0.80	0 100 100	33, 49, 65, 73	0
17	Q	95/96 (98%)	-0.75	0 100 100	35, 45, 62, 79	0
18	R	150/155 (96%)	-0.86	0 100 100	27, 42, 62, 77	0
19	S	81/85 (95%)	-0.59	1 (1%) 79 73	38, 54, 74, 87	0
20	T	119/120 (99%)	-0.56	2 (1%) 70 63	37, 52, 80, 109	0
21	U	53/67 (79%)	-0.68	0 100 100	37, 50, 68, 78	0
22	V	65/71 (91%)	0.68	6 (9%) 9 5	47, 68, 117, 122	0
23	W	154/154 (100%)	-0.67	0 100 100	32, 47, 63, 77	0
24	X	82/92 (89%)	-0.46	2 (2%) 59 49	41, 57, 82, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Y	142/241 (58%)	-0.87	1 (0%) 87 84	21, 40, 63, 86	0
26	Z	73/116 (62%)	0.35	6 (8%) 11 6	53, 72, 85, 95	0
27	1	56/57 (98%)	-0.73	0 100 100	22, 28, 36, 44	0
28	2	46/50 (92%)	-0.35	2 (4%) 35 25	30, 56, 84, 98	0
29	3	92/92 (100%)	-0.55	0 100 100	33, 56, 68, 81	0
30	0	2749/2923 (94%)	-0.72	23 (0%) 86 81	19, 42, 86, 163	0
31	9	122/122 (100%)	-0.73	2 (1%) 72 66	34, 64, 87, 144	0
All	All	6646/7517 (88%)	-0.54	159 (2%) 59 49	19, 48, 97, 163	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	12.3
9	I	74	ILE	10.2
22	V	39	ALA	8.6
9	I	104	ALA	8.4
9	I	70	THR	8.0
4	D	63	ILE	7.8
9	I	128	THR	7.2
22	V	40	PRO	6.9
9	I	72	GLU	6.5
9	I	71	ALA	6.5
31	9	1	U	6.4
9	I	102	GLN	6.4
9	I	108	HIS	6.3
9	I	132	VAL	6.1
9	I	66	GLY	6.1
9	I	97	VAL	5.7
9	I	100	VAL	5.6
14	N	166	ALA	5.6
9	I	112	LEU	5.5
9	I	80	PHE	5.4
9	I	99	GLN	5.2
9	I	93	ALA	5.0
22	V	43	PRO	5.0
9	I	106	GLN	4.8
1	A	237	GLY	4.8
9	I	113	SER	4.8
30	0	1198	U	4.6
9	I	109	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
9	I	116	LEU	4.5
9	I	88	GLN	4.5
9	I	98	ASP	4.5
22	V	41	GLU	4.3
9	I	92	VAL	4.2
9	I	91	PHE	4.1
9	I	83	GLY	4.1
9	I	79	GLY	4.0
4	D	57	THR	4.0
4	D	64	ARG	4.0
9	I	103	ILE	3.9
9	I	76	ASP	3.9
9	I	86	GLU	3.8
30	0	1172	G	3.8
4	D	85	GLN	3.7
9	I	110	ASP	3.6
9	I	105	GLU	3.6
30	0	1199	A	3.6
26	Z	46	SER	3.6
12	L	80	ASP	3.6
30	0	970	U	3.6
4	D	90	LEU	3.6
8	H	40	GLN	3.5
22	V	38	GLY	3.5
9	I	78	ALA	3.5
31	9	24	U	3.4
24	X	80	GLU	3.4
9	I	111	LEU	3.4
9	I	82	THR	3.3
9	I	69	PRO	3.2
26	Z	35	SER	3.2
30	0	1202	A	3.2
8	H	77	ILE	3.1
9	I	133	THR	3.1
4	D	18	ILE	3.1
9	I	67	VAL	3.1
8	H	169	GLU	3.1
9	I	95	LEU	3.0
26	Z	69	ASP	3.0
7	G	27	ILE	3.0
26	Z	44	ARG	3.0
9	I	94	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
7	G	23	ILE	2.9
30	0	735	C	2.9
12	L	81	VAL	2.9
8	H	37	GLY	2.9
4	D	40	ILE	2.9
8	H	84	GLY	2.8
4	D	88	LEU	2.8
4	D	89	PRO	2.8
1	A	37	VAL	2.8
9	I	73	LEU	2.8
4	D	44	ILE	2.8
6	F	106	ALA	2.8
25	Y	235	GLU	2.7
4	D	10	PHE	2.7
9	I	81	GLU	2.7
8	H	82	GLU	2.7
4	D	170	TYR	2.7
8	H	86	TYR	2.7
8	H	76	LEU	2.6
24	X	88	GLU	2.6
30	0	282	C	2.6
30	0	1173	A	2.6
9	I	117	THR	2.6
4	D	92	GLU	2.6
8	H	39	LYS	2.6
30	0	1171	A	2.5
4	D	61	PHE	2.5
26	Z	58	ASN	2.5
7	G	26	MET	2.5
30	0	2637	A	2.5
4	D	73	VAL	2.5
30	0	1200	A	2.5
20	T	116	ASP	2.5
30	0	2237	G	2.5
1	A	99	ILE	2.5
28	2	39	ARG	2.4
9	I	84	SER	2.4
8	H	38	ARG	2.4
4	D	69	ILE	2.4
30	0	1177	A	2.4
9	I	118	ASN	2.4
4	D	81	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	93	LEU	2.4
14	N	185	GLU	2.4
6	F	119	ARG	2.3
4	D	75	LEU	2.3
8	H	141	CYS	2.3
30	0	1176	C	2.3
20	T	119	ALA	2.3
19	S	81	ILE	2.3
30	0	1169	U	2.3
9	I	75	LYS	2.3
7	G	24	VAL	2.3
12	L	60	GLU	2.3
30	0	1165	G	2.3
30	0	1203	G	2.3
8	H	48	VAL	2.2
9	I	126	THR	2.2
4	D	41	LEU	2.2
30	0	969	G	2.2
8	H	174	LEU	2.2
12	L	75	LEU	2.2
26	Z	55	SER	2.2
9	I	127	CYS	2.2
4	D	84	LEU	2.2
4	D	171	ASP	2.2
30	0	1951	G	2.2
30	0	2508	C	2.2
5	E	100	ASP	2.2
8	H	90	LEU	2.2
28	2	20	ARG	2.2
4	D	70	GLY	2.2
9	I	101	LYS	2.2
8	H	85	ASP	2.2
4	D	158	ASN	2.1
9	I	125	GLY	2.1
30	0	1163	G	2.1
30	0	1170	U	2.1
4	D	24	HIS	2.1
4	D	104	PHE	2.1
30	0	1197	G	2.1
6	F	49	PHE	2.1
5	E	45	ASP	2.1
8	H	68	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	36	ASP	2.0
7	G	72	ASP	2.0
14	N	147	ILE	2.0
1	A	35	GLY	2.0
1	A	236	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	1MA	0	628	23/24	0.98	0.14	23,27,29,31	0
30	OMG	0	2588	24/25	0.98	0.12	29,31,34,35	0
30	UR3	0	2619	21/22	0.98	0.13	33,36,38,41	0
30	PSU	0	2621	20/21	0.98	0.14	22,26,37,37	0
30	OMU	0	2587	21/22	0.99	0.11	29,31,32,35	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	9	8572	1/1	0.29	0.33	93,93,93,93	0
35	NA	0	8509	1/1	0.53	0.16	56,56,56,56	0
37	K	0	8401	1/1	0.59	0.53	132,132,132,132	0
34	SR	0	8955	1/1	0.60	0.06	187,187,187,187	0
34	SR	0	9006	1/1	0.62	2.89	200,200,200,200	0
32	MG	0	8075	1/1	0.65	0.06	45,45,45,45	0
34	SR	0	8919	1/1	0.67	0.12	159,159,159,159	0
34	SR	0	9001	1/1	0.67	0.17	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8038	1/1	0.68	0.18	65,65,65,65	0
34	SR	0	8982	1/1	0.69	0.31	178,178,178,178	0
34	SR	0	8951	1/1	0.69	0.06	138,138,138,138	0
32	MG	0	8071	1/1	0.70	0.16	49,49,49,49	0
34	SR	0	8944	1/1	0.71	0.10	167,167,167,167	0
32	MG	0	8090	1/1	0.72	0.13	70,70,70,70	0
34	SR	0	8994	1/1	0.73	0.38	200,200,200,200	0
34	SR	S	8961	1/1	0.73	0.09	116,116,116,116	0
32	MG	0	8031	1/1	0.75	0.09	59,59,59,59	0
35	NA	0	8525	1/1	0.76	0.25	71,71,71,71	0
35	NA	0	8506	1/1	0.76	0.10	56,56,56,56	0
34	SR	0	8997	1/1	0.76	0.34	196,196,196,196	0
35	NA	J	8538	1/1	0.77	0.10	51,51,51,51	0
35	NA	0	8544	1/1	0.77	0.14	60,60,60,60	0
34	SR	A	8977	1/1	0.77	0.11	159,159,159,159	0
34	SR	0	8993	1/1	0.77	0.10	170,170,170,170	0
34	SR	0	8947	1/1	0.78	0.23	170,170,170,170	0
35	NA	0	8514	1/1	0.78	0.33	42,42,42,42	0
34	SR	0	8985	1/1	0.79	0.08	115,115,115,115	0
34	SR	J	8986	1/1	0.79	0.81	200,200,200,200	0
32	MG	0	8044	1/1	0.80	0.07	40,40,40,40	0
35	NA	0	8565	1/1	0.80	0.38	66,66,66,66	0
34	SR	0	8922	1/1	0.81	0.13	150,150,150,150	0
34	SR	0	8928	1/1	0.81	0.07	127,127,127,127	0
35	NA	0	8568	1/1	0.81	0.17	36,36,36,36	0
34	SR	0	8957	1/1	0.81	0.11	187,187,187,187	0
34	SR	0	8959	1/1	0.81	0.14	157,157,157,157	0
35	NA	0	8535	1/1	0.82	0.24	47,47,47,47	0
34	SR	0	8927	1/1	0.82	0.10	136,136,136,136	0
34	SR	0	8976	1/1	0.82	0.20	185,185,185,185	0
32	MG	0	8085	1/1	0.83	0.10	76,76,76,76	0
35	NA	0	8562	1/1	0.83	0.66	78,78,78,78	0
34	SR	0	8924	1/1	0.83	0.17	139,139,139,139	0
32	MG	0	8030	1/1	0.84	0.24	60,60,60,60	0
35	NA	0	8542	1/1	0.84	0.39	48,48,48,48	0
35	NA	0	8563	1/1	0.85	0.64	74,74,74,74	0
34	SR	0	8996	1/1	0.85	0.64	200,200,200,200	0
35	NA	0	8533	1/1	0.85	0.15	45,45,45,45	0
35	NA	0	8571	1/1	0.85	0.07	72,72,72,72	0
35	NA	0	8560	1/1	0.85	0.38	74,74,74,74	0
35	NA	0	8520	1/1	0.85	0.09	47,47,47,47	0
34	SR	9	9003	1/1	0.86	0.14	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	8522	1/1	0.86	0.42	73,73,73,73	0
34	SR	0	8995	1/1	0.86	0.15	133,133,133,133	0
35	NA	0	8512	1/1	0.86	0.37	50,50,50,50	0
35	NA	0	8502	1/1	0.86	0.10	62,62,62,62	0
35	NA	0	8530	1/1	0.87	0.22	46,46,46,46	0
34	SR	0	8979	1/1	0.87	0.12	200,200,200,200	0
34	SR	B	8950	1/1	0.87	0.13	121,121,121,121	0
32	MG	0	8078	1/1	0.87	0.35	50,50,50,50	0
34	SR	0	8968	1/1	0.87	0.09	165,165,165,165	0
35	NA	0	8548	1/1	0.87	0.20	56,56,56,56	0
32	MG	T	8057	1/1	0.87	0.09	59,59,59,59	0
34	SR	0	8915	1/1	0.88	0.10	110,110,110,110	0
34	SR	0	9000	1/1	0.89	0.22	160,160,160,160	0
34	SR	0	8963	1/1	0.90	0.05	167,167,167,167	0
35	NA	0	8546	1/1	0.90	0.88	69,69,69,69	0
34	SR	0	8937	1/1	0.90	0.18	100,100,100,100	0
35	NA	0	8555	1/1	0.90	0.58	54,54,54,54	0
35	NA	0	8558	1/1	0.90	0.20	45,45,45,45	0
34	SR	0	8972	1/1	0.90	0.19	163,163,163,163	0
34	SR	0	8974	1/1	0.90	0.21	160,160,160,160	0
32	MG	0	8036	1/1	0.90	0.09	33,33,33,33	0
35	NA	0	8564	1/1	0.90	0.27	61,61,61,61	0
32	MG	0	8037	1/1	0.90	0.20	92,92,92,92	0
32	MG	A	8051	1/1	0.90	0.37	62,62,62,62	0
34	SR	B	8987	1/1	0.90	0.89	200,200,200,200	0
32	MG	0	8010	1/1	0.90	0.13	44,44,44,44	0
32	MG	0	8088	1/1	0.90	0.13	30,30,30,30	0
35	NA	0	8566	1/1	0.91	0.31	43,43,43,43	0
32	MG	0	8053	1/1	0.91	0.06	52,52,52,52	0
35	NA	0	8569	1/1	0.91	0.28	65,65,65,65	0
34	SR	0	8983	1/1	0.91	0.24	169,169,169,169	0
35	NA	0	8505	1/1	0.91	0.28	36,36,36,36	0
34	SR	0	8939	1/1	0.91	0.05	128,128,128,128	0
34	SR	0	8962	1/1	0.92	0.12	168,168,168,168	0
32	MG	0	8066	1/1	0.92	0.18	44,44,44,44	0
35	NA	H	8518	1/1	0.92	0.49	86,86,86,86	0
32	MG	0	8073	1/1	0.92	0.06	65,65,65,65	0
34	SR	0	8971	1/1	0.92	0.04	150,150,150,150	0
32	MG	0	8079	1/1	0.92	0.14	48,48,48,48	0
34	SR	A	8929	1/1	0.92	0.09	123,123,123,123	0
34	SR	0	8914	1/1	0.92	0.24	106,106,106,106	0
32	MG	0	8080	1/1	0.92	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SR	0	8938	1/1	0.92	0.10	158,158,158,158	0
35	NA	0	8574	1/1	0.92	0.52	65,65,65,65	0
35	NA	0	8515	1/1	0.92	0.09	32,32,32,32	0
35	NA	0	8557	1/1	0.92	0.12	56,56,56,56	0
35	NA	0	8559	1/1	0.93	0.18	73,73,73,73	0
35	NA	0	8529	1/1	0.93	0.05	30,30,30,30	0
33	CL	O	8808	1/1	0.93	0.07	58,58,58,58	0
34	SR	0	8981	1/1	0.93	0.14	156,156,156,156	0
32	MG	0	8033	1/1	0.93	0.07	35,35,35,35	0
34	SR	0	8998	1/1	0.93	0.12	148,148,148,148	0
34	SR	0	8956	1/1	0.93	0.07	130,130,130,130	0
34	SR	A	8930	1/1	0.93	0.05	96,96,96,96	0
34	SR	0	8988	1/1	0.93	0.18	159,159,159,159	0
35	NA	0	8549	1/1	0.93	0.47	50,50,50,50	0
34	SR	0	8991	1/1	0.93	0.07	183,183,183,183	0
32	MG	0	8076	1/1	0.93	0.14	38,38,38,38	0
32	MG	9	8040	1/1	0.93	0.09	69,69,69,69	0
32	MG	0	8060	1/1	0.94	0.11	52,52,52,52	0
35	NA	0	8561	1/1	0.94	0.51	76,76,76,76	0
32	MG	0	8077	1/1	0.94	0.07	32,32,32,32	0
35	NA	0	8511	1/1	0.94	0.20	59,59,59,59	0
34	SR	0	8933	1/1	0.94	0.18	136,136,136,136	0
34	SR	0	8970	1/1	0.94	0.04	118,118,118,118	0
34	SR	0	8954	1/1	0.94	0.08	94,94,94,94	0
35	NA	0	8567	1/1	0.94	0.26	77,77,77,77	0
33	CL	0	8815	1/1	0.94	0.06	61,61,61,61	0
35	NA	0	8552	1/1	0.94	0.33	56,56,56,56	0
32	MG	0	8064	1/1	0.94	0.16	36,36,36,36	0
34	SR	0	8975	1/1	0.94	0.07	124,124,124,124	0
32	MG	0	8046	1/1	0.94	0.14	33,33,33,33	0
34	SR	0	8941	1/1	0.94	0.12	99,99,99,99	0
34	SR	0	8921	1/1	0.95	0.10	82,82,82,82	0
33	CL	0	8816	1/1	0.95	0.06	66,66,66,66	0
35	NA	Q	8540	1/1	0.95	0.07	48,48,48,48	0
35	NA	0	8550	1/1	0.95	0.13	51,51,51,51	0
35	NA	S	8510	1/1	0.95	0.10	29,29,29,29	0
35	NA	0	8553	1/1	0.95	0.31	68,68,68,68	0
32	MG	0	8069	1/1	0.95	0.40	99,99,99,99	0
34	SR	0	8926	1/1	0.95	0.13	114,114,114,114	0
34	SR	0	8958	1/1	0.95	0.08	101,101,101,101	0
32	MG	0	8045	1/1	0.95	0.11	28,28,28,28	0
32	MG	0	8072	1/1	0.95	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	Y	8086	1/1	0.95	0.07	34,34,34,34	0
32	MG	0	8011	1/1	0.95	0.18	20,20,20,20	0
32	MG	0	8091	1/1	0.95	0.03	48,48,48,48	0
32	MG	0	8020	1/1	0.95	0.13	37,37,37,37	0
34	SR	0	8911	1/1	0.95	0.09	74,74,74,74	0
35	NA	0	8523	1/1	0.95	0.12	41,41,41,41	0
33	CL	L	8810	1/1	0.95	0.06	53,53,53,53	0
32	MG	0	8041	1/1	0.95	0.20	25,25,25,25	0
34	SR	0	9002	1/1	0.95	0.13	173,173,173,173	0
32	MG	0	8035	1/1	0.95	0.09	49,49,49,49	0
35	NA	0	8573	1/1	0.95	0.22	64,64,64,64	0
34	SR	9	8978	1/1	0.95	0.07	133,133,133,133	0
34	SR	9	8980	1/1	0.95	0.11	168,168,168,168	0
34	SR	0	8953	1/1	0.95	0.15	140,140,140,140	0
33	CL	A	8809	1/1	0.96	0.07	63,63,63,63	0
32	MG	0	8081	1/1	0.96	0.16	64,64,64,64	0
32	MG	0	8039	1/1	0.96	0.16	70,70,70,70	0
34	SR	0	9004	1/1	0.96	0.38	200,200,200,200	0
33	CL	0	8803	1/1	0.96	0.09	46,46,46,46	0
34	SR	0	9007	1/1	0.96	0.43	187,187,187,187	0
34	SR	0	8908	1/1	0.96	0.13	92,92,92,92	0
33	CL	0	8814	1/1	0.96	0.10	48,48,48,48	0
32	MG	0	8063	1/1	0.96	0.26	78,78,78,78	0
35	NA	0	8531	1/1	0.96	0.08	44,44,44,44	0
32	MG	0	8089	1/1	0.96	0.10	43,43,43,43	0
34	SR	0	8989	1/1	0.96	0.18	177,177,177,177	0
35	NA	0	8537	1/1	0.96	0.12	34,34,34,34	0
34	SR	0	8964	1/1	0.96	0.08	118,118,118,118	0
34	SR	0	8966	1/1	0.96	0.06	100,100,100,100	0
35	NA	0	8570	1/1	0.96	0.10	43,43,43,43	0
33	CL	0	8817	1/1	0.96	0.05	50,50,50,50	0
34	SR	0	8945	1/1	0.96	0.08	97,97,97,97	0
32	MG	0	8022	1/1	0.96	0.13	30,30,30,30	0
32	MG	0	8006	1/1	0.96	0.13	25,25,25,25	0
32	MG	0	8068	1/1	0.96	0.09	51,51,51,51	0
37	K	0	8402	1/1	0.96	0.10	69,69,69,69	0
32	MG	0	8021	1/1	0.97	0.07	29,29,29,29	0
35	NA	M	8539	1/1	0.97	0.10	26,26,26,26	0
35	NA	0	8547	1/1	0.97	0.25	43,43,43,43	0
34	SR	0	8984	1/1	0.97	0.09	111,111,111,111	0
32	MG	0	8016	1/1	0.97	0.12	46,46,46,46	0
35	NA	0	8501	1/1	0.97	0.15	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	8551	1/1	0.97	0.11	40,40,40,40	0
32	MG	0	8023	1/1	0.97	0.09	24,24,24,24	0
32	MG	0	8024	1/1	0.97	0.15	55,55,55,55	0
32	MG	0	8092	1/1	0.97	0.02	51,51,51,51	0
35	NA	0	8508	1/1	0.97	0.27	43,43,43,43	0
34	SR	0	8960	1/1	0.97	0.04	135,135,135,135	0
32	MG	0	8026	1/1	0.97	0.10	32,32,32,32	0
32	MG	0	8001	1/1	0.97	0.10	33,33,33,33	0
35	NA	0	8513	1/1	0.97	0.13	42,42,42,42	0
33	CL	J	8801	1/1	0.97	0.06	66,66,66,66	0
33	CL	J	8802	1/1	0.97	0.07	55,55,55,55	0
34	SR	0	8967	1/1	0.97	0.03	127,127,127,127	0
32	MG	0	8070	1/1	0.97	0.18	45,45,45,45	0
33	CL	N	8807	1/1	0.97	0.07	57,57,57,57	0
35	NA	0	8524	1/1	0.97	0.20	39,39,39,39	0
34	SR	0	8942	1/1	0.97	0.08	108,108,108,108	0
34	SR	3	8999	1/1	0.97	0.05	94,94,94,94	0
32	MG	0	8056	1/1	0.97	0.10	48,48,48,48	0
33	CL	Y	8820	1/1	0.97	0.07	35,35,35,35	0
34	SR	0	8949	1/1	0.97	0.05	99,99,99,99	0
32	MG	0	8059	1/1	0.97	0.07	44,44,44,44	0
35	NA	0	8575	1/1	0.97	0.31	86,86,86,86	0
35	NA	9	8543	1/1	0.97	0.15	42,42,42,42	0
33	CL	0	8805	1/1	0.97	0.05	50,50,50,50	0
35	NA	0	8541	1/1	0.97	0.20	53,53,53,53	0
33	CL	0	8813	1/1	0.97	0.06	49,49,49,49	0
34	SR	0	8916	1/1	0.98	0.09	101,101,101,101	0
35	NA	0	8534	1/1	0.98	0.15	37,37,37,37	0
34	SR	0	8917	1/1	0.98	0.12	103,103,103,103	0
35	NA	0	8536	1/1	0.98	0.16	47,47,47,47	0
32	MG	0	8005	1/1	0.98	0.22	31,31,31,31	0
34	SR	0	8920	1/1	0.98	0.03	108,108,108,108	0
33	CL	3	8804	1/1	0.98	0.06	57,57,57,57	0
32	MG	0	8058	1/1	0.98	0.09	18,18,18,18	0
35	NA	0	8545	1/1	0.98	0.13	38,38,38,38	0
34	SR	0	8923	1/1	0.98	0.04	104,104,104,104	0
32	MG	0	8014	1/1	0.98	0.16	21,21,21,21	0
33	CL	0	8811	1/1	0.98	0.11	62,62,62,62	0
34	SR	0	8969	1/1	0.98	0.16	158,158,158,158	0
32	MG	K	8054	1/1	0.98	0.07	34,34,34,34	0
32	MG	0	8082	1/1	0.98	0.17	77,77,77,77	0
34	SR	0	8931	1/1	0.98	0.09	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	R	8532	1/1	0.98	0.07	37,37,37,37	0
35	NA	0	8554	1/1	0.98	0.39	59,59,59,59	0
34	SR	0	8973	1/1	0.98	0.08	124,124,124,124	0
35	NA	0	8556	1/1	0.98	0.56	44,44,44,44	0
32	MG	0	8083	1/1	0.98	0.03	48,48,48,48	0
34	SR	0	8934	1/1	0.98	0.09	104,104,104,104	0
32	MG	0	8061	1/1	0.98	0.21	22,22,22,22	0
32	MG	0	8017	1/1	0.98	0.27	32,32,32,32	0
32	MG	0	8028	1/1	0.98	0.17	22,22,22,22	0
32	MG	0	8029	1/1	0.98	0.15	37,37,37,37	0
32	MG	0	8018	1/1	0.98	0.20	29,29,29,29	0
32	MG	0	8007	1/1	0.98	0.20	29,29,29,29	0
32	MG	0	8093	1/1	0.98	0.09	29,29,29,29	0
32	MG	B	8042	1/1	0.98	0.08	50,50,50,50	0
34	SR	0	8948	1/1	0.98	0.10	94,94,94,94	0
35	NA	0	8519	1/1	0.98	0.12	37,37,37,37	0
34	SR	0	8990	1/1	0.98	0.18	124,124,124,124	0
35	NA	0	8521	1/1	0.98	0.19	52,52,52,52	0
34	SR	R	8912	1/1	0.98	0.17	78,78,78,78	0
32	MG	0	8047	1/1	0.98	0.22	38,38,38,38	0
32	MG	0	8048	1/1	0.98	0.21	19,19,19,19	0
32	MG	0	8049	1/1	0.98	0.27	65,65,65,65	0
35	NA	0	8526	1/1	0.98	0.03	36,36,36,36	0
32	MG	0	8052	1/1	0.98	0.08	39,39,39,39	0
36	CD	O	8705	1/1	0.98	0.08	80,80,80,80	0
32	MG	0	8034	1/1	0.98	0.03	36,36,36,36	0
32	MG	0	8055	1/1	0.98	0.15	35,35,35,35	0
34	SR	0	8904	1/1	0.99	0.18	48,48,48,48	0
34	SR	0	8905	1/1	0.99	0.23	52,52,52,52	0
32	MG	B	8043	1/1	0.99	0.07	38,38,38,38	0
34	SR	0	8910	1/1	0.99	0.05	93,93,93,93	0
33	CL	R	8806	1/1	0.99	0.10	38,38,38,38	0
32	MG	0	8084	1/1	0.99	0.11	31,31,31,31	0
32	MG	0	8025	1/1	0.99	0.07	22,22,22,22	0
32	MG	0	8015	1/1	0.99	0.14	24,24,24,24	0
32	MG	0	8027	1/1	0.99	0.05	29,29,29,29	0
34	SR	0	8918	1/1	0.99	0.11	74,74,74,74	0
34	SR	0	9008	1/1	0.99	0.10	84,84,84,84	0
32	MG	0	8002	1/1	0.99	0.08	25,25,25,25	0
32	MG	0	8008	1/1	0.99	0.12	19,19,19,19	0
32	MG	0	8009	1/1	0.99	0.19	18,18,18,18	0
35	NA	C	8503	1/1	0.99	0.15	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SR	0	8965	1/1	0.99	0.05	117,117,117,117	0
32	MG	0	8004	1/1	0.99	0.18	22,22,22,22	0
32	MG	0	8062	1/1	0.99	0.16	37,37,37,37	0
32	MG	9	8074	1/1	0.99	0.14	62,62,62,62	0
34	SR	0	8925	1/1	0.99	0.10	83,83,83,83	0
33	CL	0	8822	1/1	0.99	0.24	78,78,78,78	0
32	MG	A	8050	1/1	0.99	0.10	34,34,34,34	0
33	CL	B	8819	1/1	0.99	0.04	44,44,44,44	0
35	NA	0	8504	1/1	0.99	0.18	30,30,30,30	0
32	MG	0	8012	1/1	0.99	0.16	15,15,15,15	0
32	MG	0	8065	1/1	0.99	0.08	38,38,38,38	0
35	NA	0	8507	1/1	0.99	0.17	31,31,31,31	0
33	CL	J	8821	1/1	0.99	0.06	60,60,60,60	0
34	SR	0	8935	1/1	0.99	0.10	73,73,73,73	0
34	SR	F	9005	1/1	0.99	0.04	118,118,118,118	0
33	CL	K	8812	1/1	0.99	0.07	39,39,39,39	0
32	MG	0	8013	1/1	0.99	0.04	22,22,22,22	0
34	SR	0	8940	1/1	0.99	0.10	85,85,85,85	0
33	CL	M	8818	1/1	0.99	0.08	34,34,34,34	0
35	NA	0	8516	1/1	0.99	0.07	27,27,27,27	0
35	NA	0	8517	1/1	0.99	0.18	28,28,28,28	0
34	SR	1	8913	1/1	0.99	0.07	76,76,76,76	0
34	SR	0	8943	1/1	0.99	0.05	94,94,94,94	0
34	SR	3	8932	1/1	0.99	0.12	67,67,67,67	0
32	MG	0	8067	1/1	0.99	0.17	31,31,31,31	0
34	SR	0	8946	1/1	0.99	0.17	110,110,110,110	0
34	SR	0	8992	1/1	0.99	0.24	136,136,136,136	0
34	SR	0	8901	1/1	0.99	0.08	74,74,74,74	0
34	SR	0	8902	1/1	0.99	0.13	57,57,57,57	0
36	CD	1	8702	1/1	0.99	0.12	59,59,59,59	0
35	NA	0	8527	1/1	0.99	0.18	53,53,53,53	0
35	NA	0	8528	1/1	0.99	0.13	35,35,35,35	0
34	SR	0	8907	1/1	1.00	0.11	54,54,54,54	0
32	MG	0	8019	1/1	1.00	0.18	24,24,24,24	0
34	SR	0	8909	1/1	1.00	0.14	77,77,77,77	0
32	MG	0	8032	1/1	1.00	0.06	38,38,38,38	0
32	MG	0	8087	1/1	1.00	0.11	29,29,29,29	0
34	SR	0	8903	1/1	1.00	0.15	46,46,46,46	0
34	SR	0	8936	1/1	1.00	0.07	84,84,84,84	0
36	CD	U	8701	1/1	1.00	0.07	48,48,48,48	0
36	CD	Z	8703	1/1	1.00	0.06	79,79,79,79	0
34	SR	1	8952	1/1	1.00	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	CD	3	8704	1/1	1.00	0.06	66,66,66,66	0
32	MG	0	8003	1/1	1.00	0.14	28,28,28,28	0
34	SR	0	8906	1/1	1.00	0.19	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.