



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:55 am GMT

PDB ID : 3PIP
Title : Crystal structure of the synergistic antibiotic pair lankamycin and lankacidin in complex with the large ribosomal subunit
Authors : Belousoff, M.J.; Shapira, T.; Bashan, A.; Zimmerman, E.; Kinashi, H.; Rozenberg, H.; Yonath, A.
Deposited on : 2010-11-07
Resolution : 3.45 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

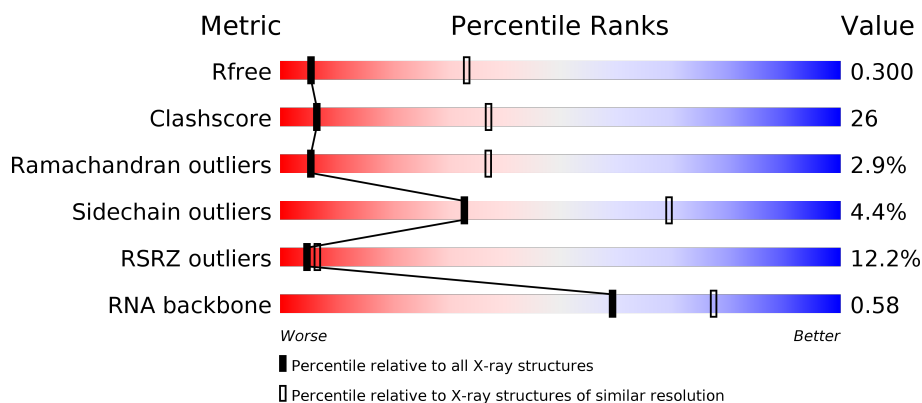
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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}	100719	1135 (3.56-3.36)
Clashscore	112137	1040 (3.52-3.40)
Ramachandran outliers	110173	1009 (3.52-3.40)
Sidechain outliers	110143	1010 (3.52-3.40)
RSRZ outliers	101464	1017 (3.54-3.38)
RNA backbone	2435	1020 (4.02-2.86)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	X	2880	
2	Y	123	
3	A	274	
4	B	211	

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	<div> <div>89%</div> <div>62%35%</div> </div>

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
31	LC2	X	2881	-	-	-	X
32	LMA	X	2882	-	-	X	X
33	MG	X	2884	-	-	-	X
33	MG	X	2886	-	-	-	X
33	MG	X	2887	-	-	-	X
33	MG	X	2890	-	-	-	X
33	MG	X	2891	-	-	-	X
33	MG	X	2892	-	-	-	X
33	MG	X	2899	-	-	-	X
33	MG	X	2900	-	-	-	X
33	MG	X	2901	-	-	-	X
33	MG	X	2905	-	-	-	X
33	MG	X	2908	-	-	-	X
33	MG	X	2918	-	-	-	X
33	MG	X	2919	-	-	-	X
33	MG	X	2922	-	-	-	X
33	MG	X	2926	-	-	-	X
33	MG	X	2932	-	-	-	X
33	MG	X	2934	-	-	-	X
33	MG	X	2937	-	-	-	X
33	MG	X	2940	-	-	-	X
33	MG	X	2948	-	-	-	X
33	MG	X	2950	-	-	-	X
33	MG	X	2951	-	-	-	X
35	NA	X	2958	-	-	-	X
35	NA	X	2961	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 83963 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 RNA chain called RIBOSOMAL 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2644	Total	C	N	O	P	0	0	0
			56750	25314	10473	18320	2643			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	253	Total	C	N	O	S	0	0	0
			1920	1196	382	340	2			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1394	889	244	254	7			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	63	Total	C	N	O	S	0	0	0
			451	280	82	86	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	134	Total	C	N	O	S	0	0	0
			1005	616	203	186				

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	126	Total	C	N	O	S	0	0	0
			1004	633	197	172	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			714	452	130	130	2			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	74	Total	C	N	O	S	0	0	0
			556	351	107	97	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O		0	0	0
			537	334	110	93				

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	57	Total	C	N	O	S	0	0	0
			452	278	93	76	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

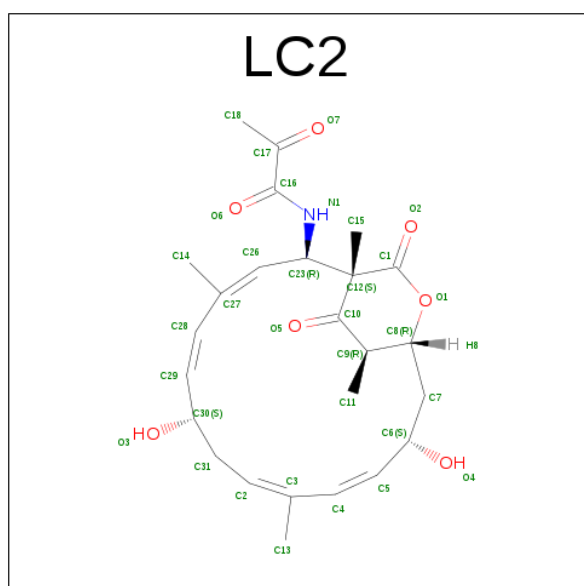
- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- Molecule 30 is a protein called 50S ribosomal protein L36.

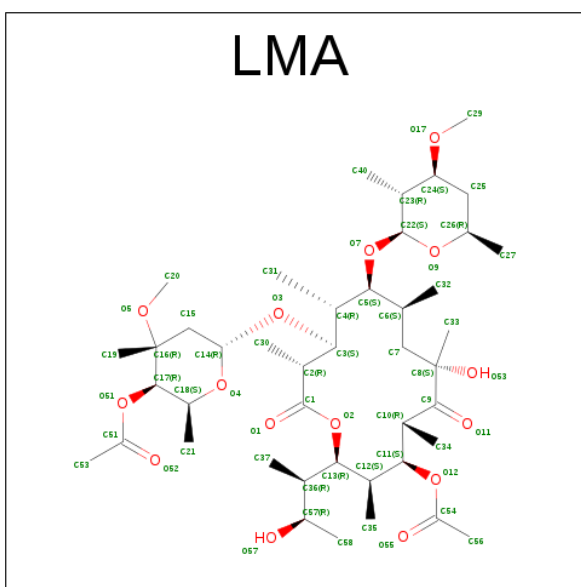
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	37	Total	C	N	O	S	0	0	0
			297	179	66	47	5			

- Molecule 31 is N-[(1S,2R,3E,5E,7S,9E,11E,13S,15R,19R)-7,13-DIHYDROXY-1,4,10,19-TE TRAMETHYL-17,18-DIOXO-16-OXABICYCLO[13.2.2]NONADECA-3,5,9,11-TETRAEN-2-YL]-2-OXOPROPANAMIDE (three-letter code: LC2) (formula: C₂₅H₃₃NO₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	X	1	Total	C	N	O	0	0
			33	25	1	7		

- Molecule 32 is LANKAMYCIN (three-letter code: LMA) (formula: C₄₃H₇₄O₁₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	O	0	0
			58	43	15		

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	X	71	Total Mg 71 71	0	0
33	I	1	Total Mg 1 1	0	0
33	U	1	Total Mg 1 1	0	0

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	X	4	Total K 4 4	0	0

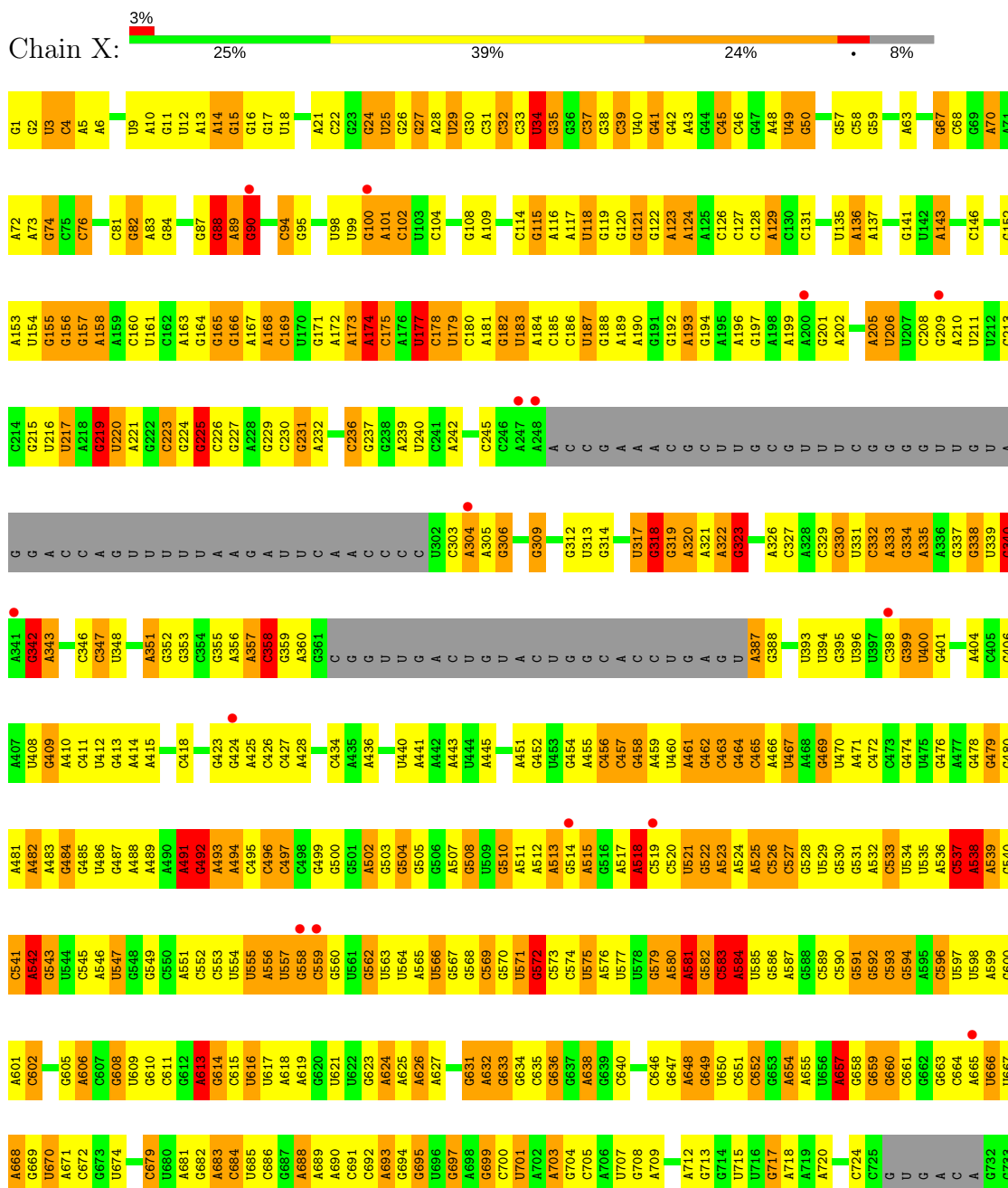
- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	X	5	Total Na 5 5	0	0

3 Residue-property plots

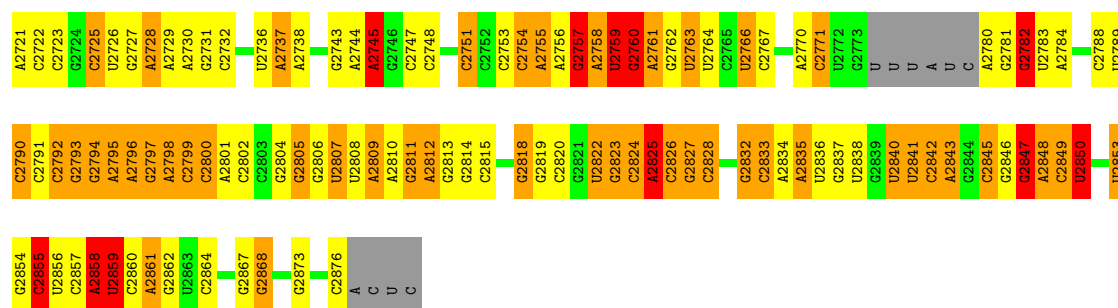
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: RIBOSOMAL 23S RNA

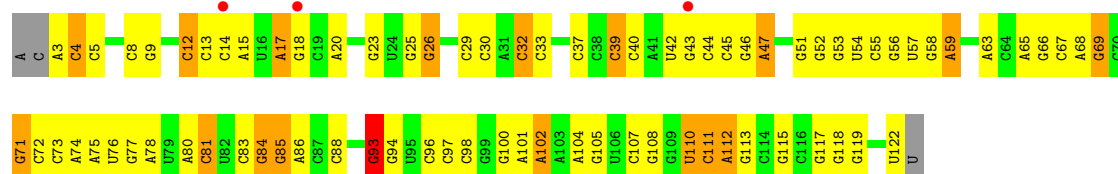




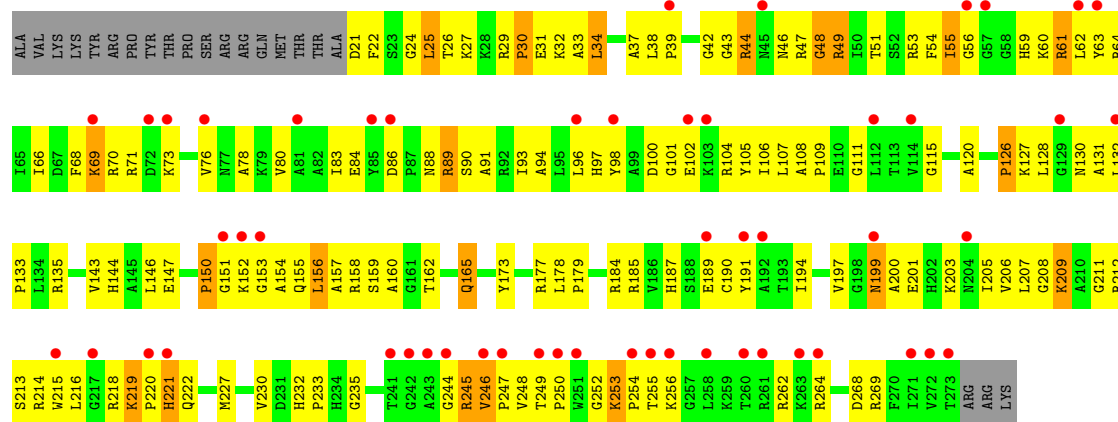




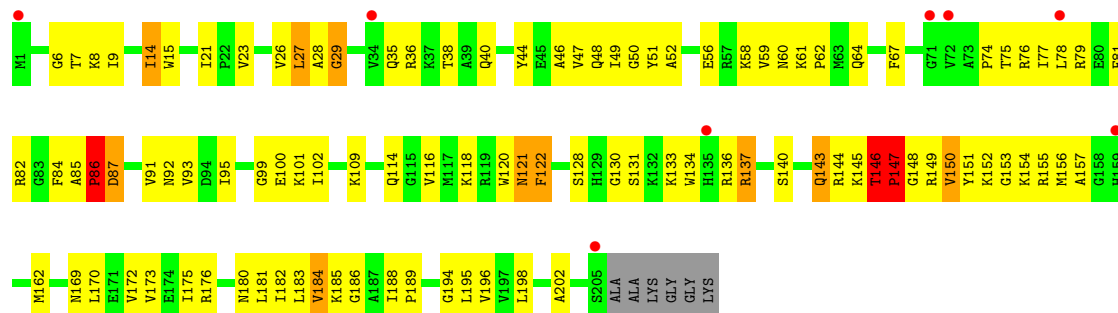
• Molecule 2: 5S ribosomal RNA



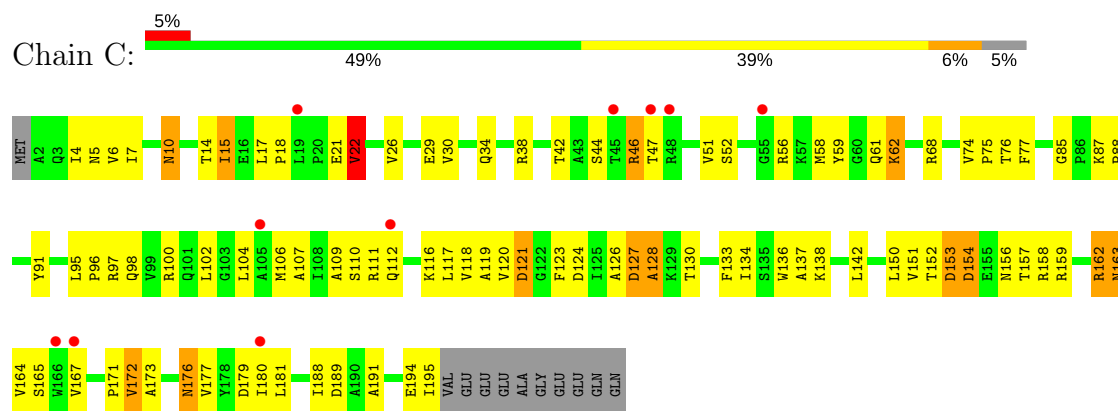
• Molecule 3: 50S ribosomal protein L2



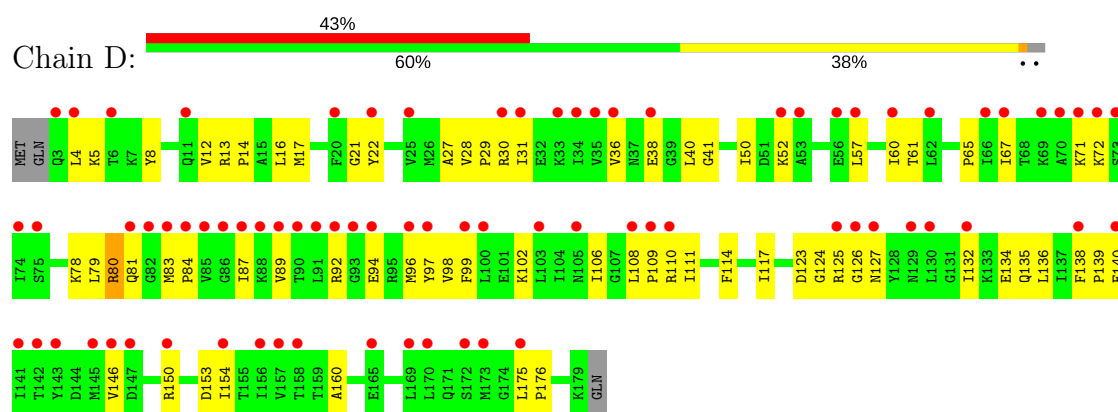
• Molecule 4: 50S ribosomal protein L3



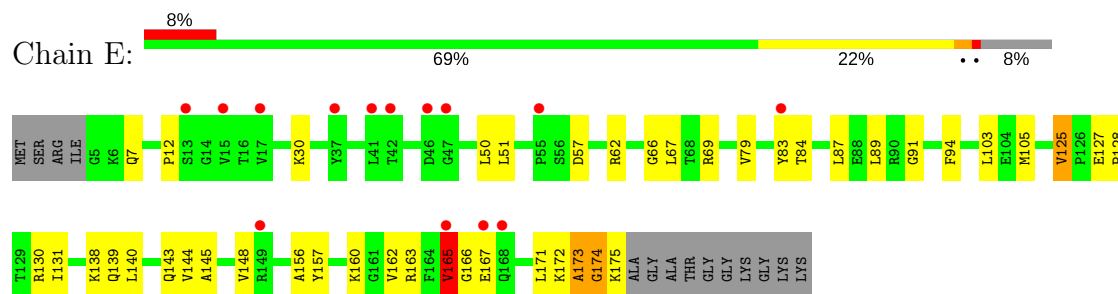
- Molecule 5: 50S ribosomal protein L4



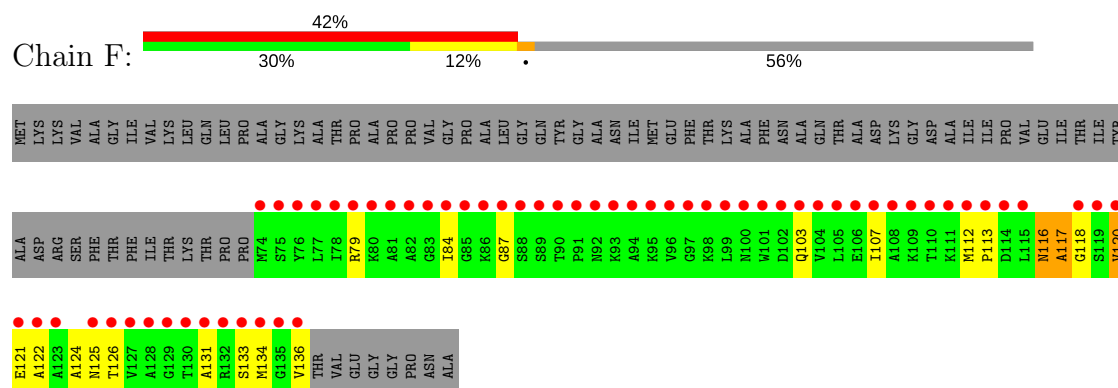
- Molecule 6: 50S ribosomal protein L5



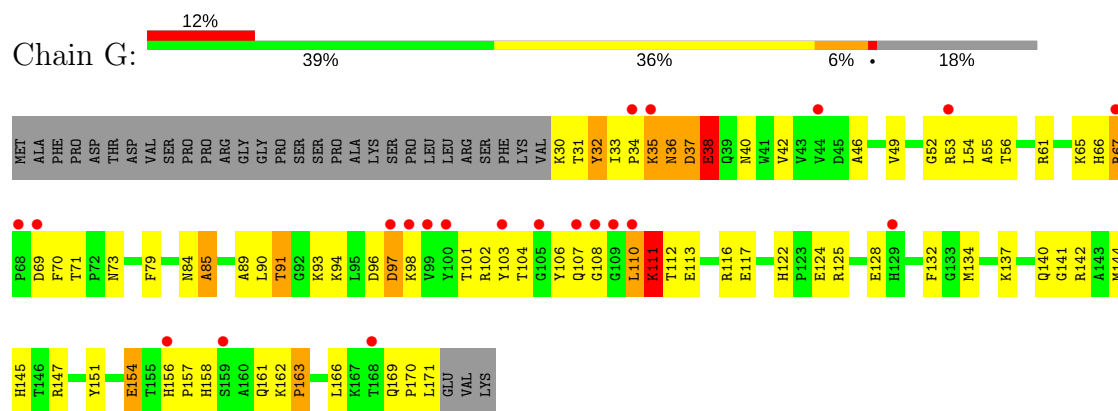
- Molecule 7: 50S ribosomal protein L6



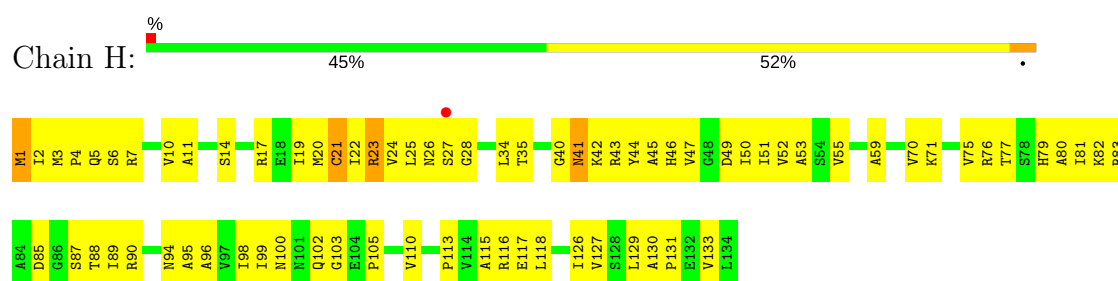
- Molecule 8: 50S ribosomal protein L11



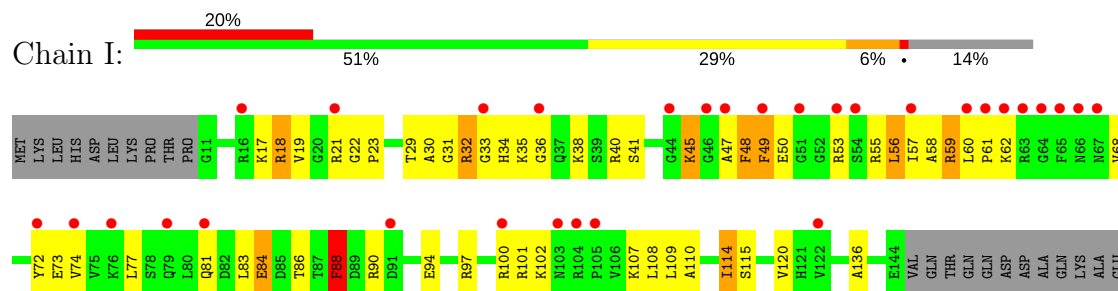
- Molecule 9: 50S ribosomal protein L13



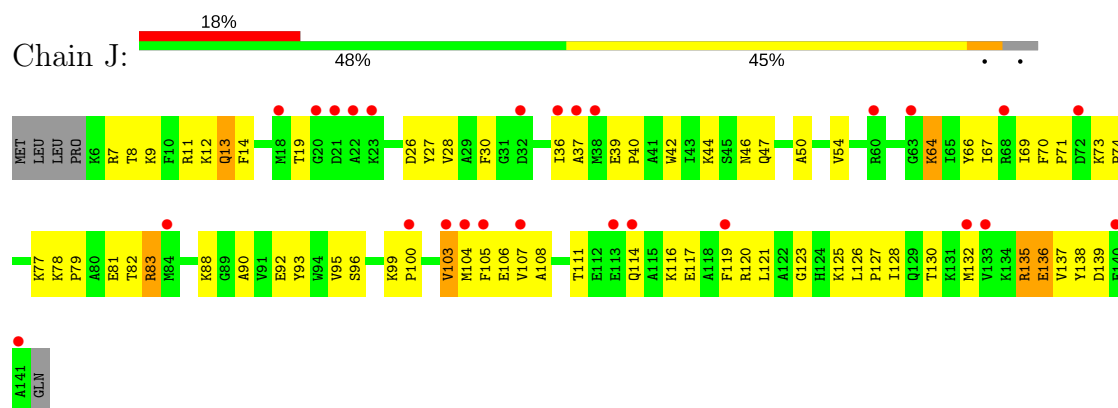
- Molecule 10: 50S ribosomal protein L14



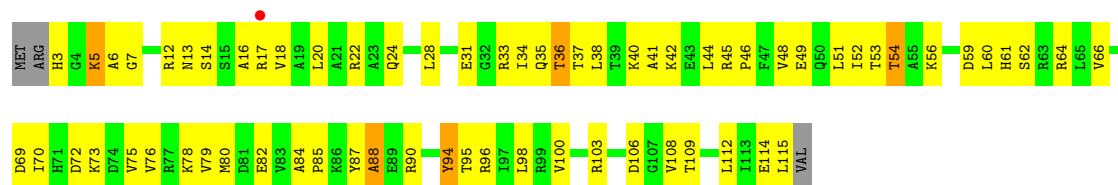
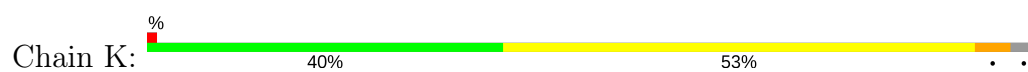
- Molecule 11: 50S ribosomal protein L15



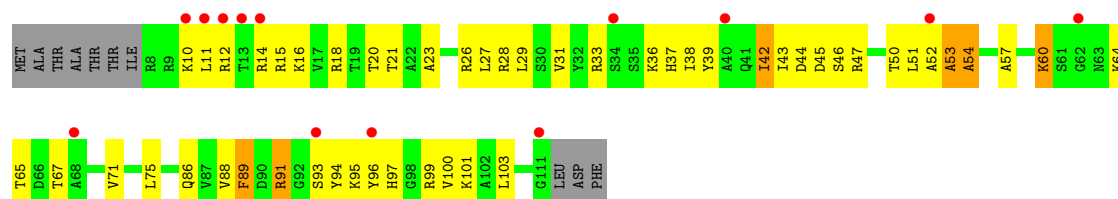
- Molecule 12: 50S ribosomal protein L16



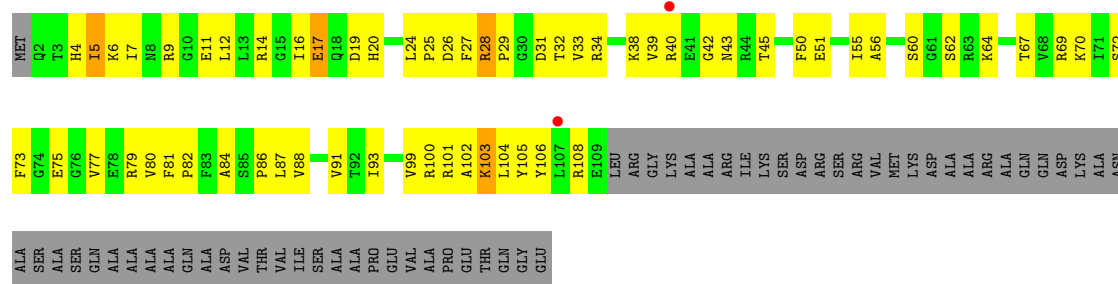
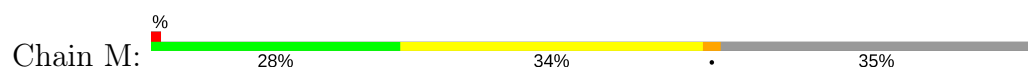
- Molecule 13: 50S ribosomal protein L17



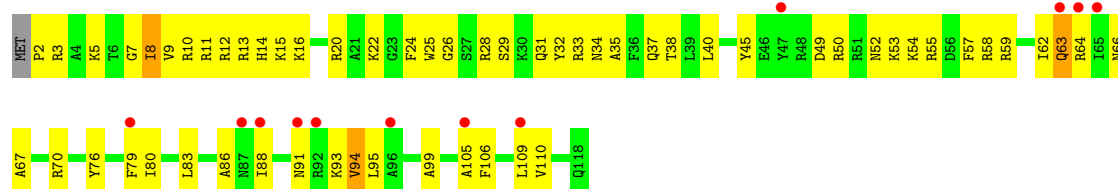
• Molecule 14: 50S ribosomal protein L18



• Molecule 15: 50S ribosomal protein L19



• Molecule 16: 50S ribosomal protein L20

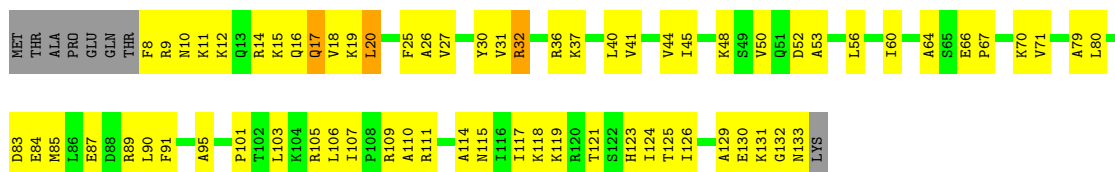


• Molecule 17: 50S ribosomal protein L21



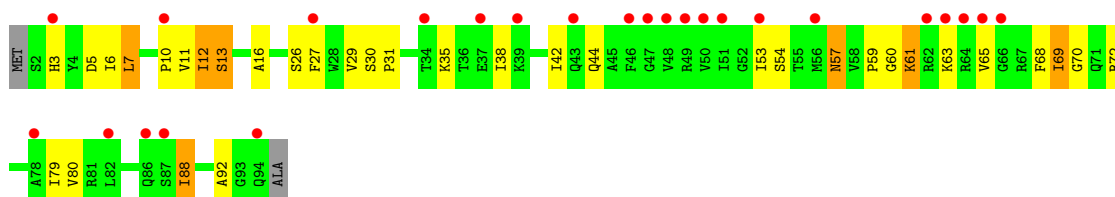
- Molecule 18: 50S ribosomal protein L22

Chain P:  43% 49% 6%



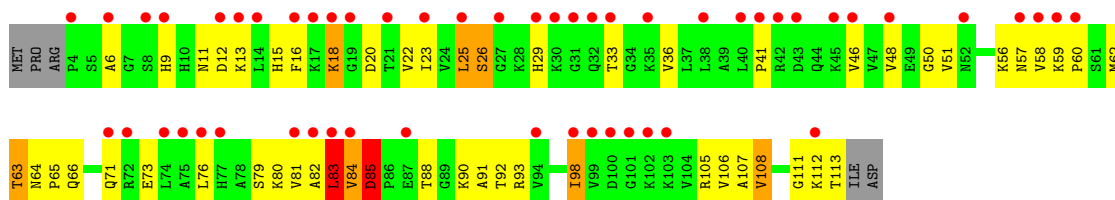
- Molecule 19: 50S ribosomal protein L23

Chain Q: 



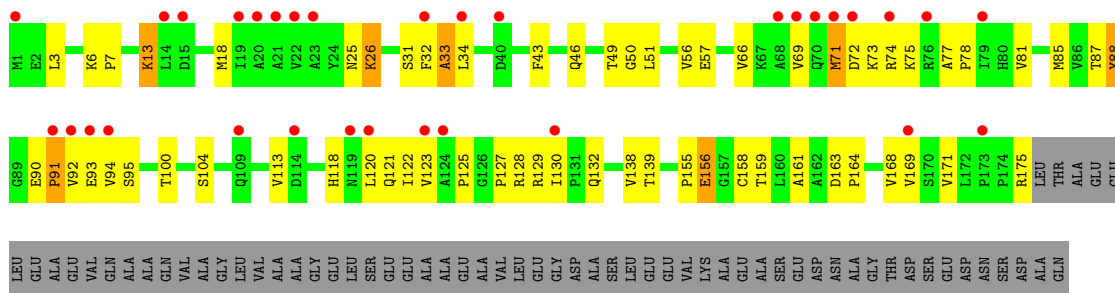
- Molecule 20: 50S ribosomal protein L24

Chain R: 



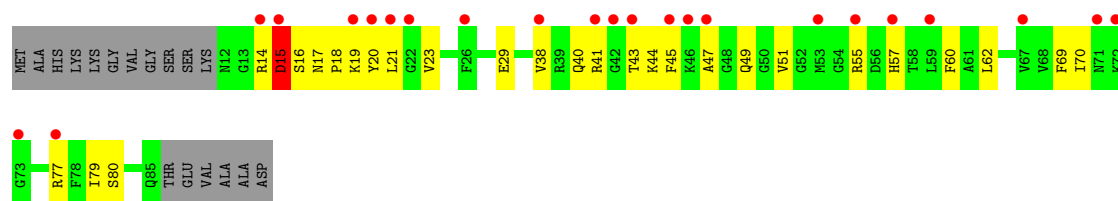
- Molecule 21: 50S ribosomal protein L25

Chain S: 

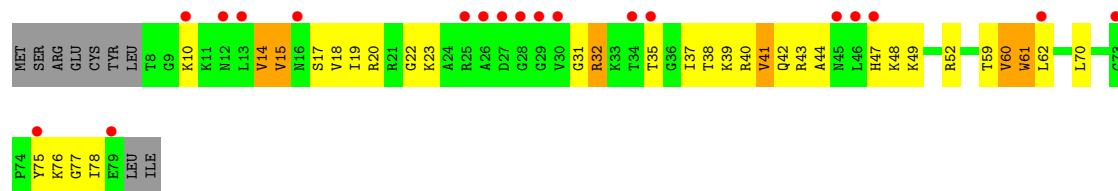


- Molecule 22: 50S ribosomal protein L27

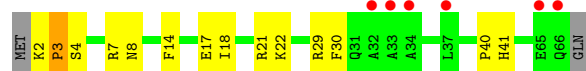
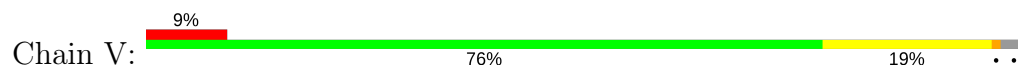
Chain T: 25% 51% 30% 19%



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L32

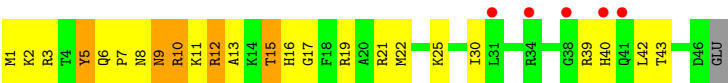


- Molecule 27: 50S ribosomal protein L33

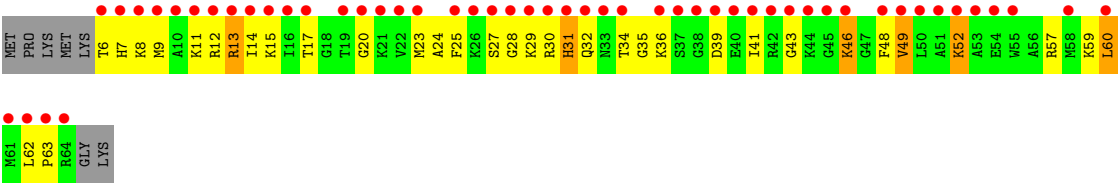
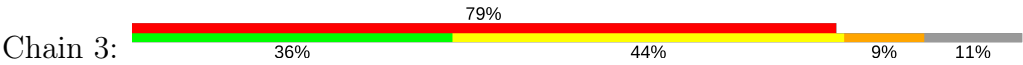


- Molecule 28: 50S ribosomal protein L34

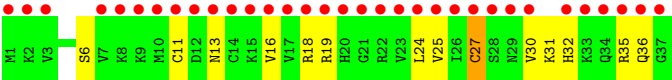
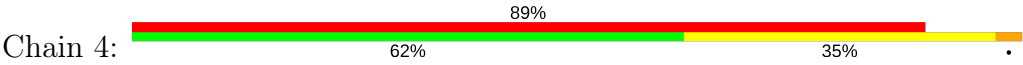




• Molecule 29: 50S ribosomal protein L35



• Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.72Å 408.56Å 693.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.45 93.01 – 3.44	Depositor EDS
% Data completeness (in resolution range)	83.3 (20.00-3.45) 82.4 (93.01-3.44)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.41Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, R_{free}	0.257 , 0.301 0.261 , 0.300	Depositor DCC
R_{free} test set	2643 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	83963	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, K, LC2, MG, LMA

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	X	1.17	260/63542 (0.4%)	1.58	1813/99100 (1.8%)
2	Y	0.80	1/2863 (0.0%)	1.13	21/4461 (0.5%)
3	A	0.65	0/1958	0.83	2/2638 (0.1%)
4	B	0.85	0/1567	0.93	2/2105 (0.1%)
5	C	0.84	0/1504	0.84	1/2036 (0.0%)
6	D	0.46	0/1413	0.56	0/1896
7	E	0.57	0/1308	0.60	0/1771
8	F	0.37	0/455	0.45	0/611
9	G	0.75	0/1138	0.82	0/1539
10	H	0.94	0/1007	0.99	0/1352
11	I	0.62	0/1016	0.71	0/1359
12	J	0.80	0/1113	0.80	0/1486
13	K	0.93	1/886 (0.1%)	1.01	0/1188
14	L	0.72	0/785	0.93	1/1048 (0.1%)
15	M	0.99	0/884	1.07	1/1186 (0.1%)
16	N	0.93	0/994	0.85	0/1323
17	O	0.77	0/750	0.81	0/1000
18	P	1.01	2/1017 (0.2%)	0.97	1/1362 (0.1%)
19	Q	0.66	0/725	0.69	0/974
20	R	0.66	0/835	0.72	1/1121 (0.1%)
21	S	0.51	0/1370	0.60	1/1862 (0.1%)
22	T	0.74	0/563	0.77	0/747
23	U	0.57	0/541	0.70	1/723 (0.1%)
24	V	0.67	0/529	0.63	0/704
25	W	0.60	0/426	0.71	0/568
26	Z	0.89	0/464	0.94	1/622 (0.2%)
27	1	0.32	0/438	0.60	0/583
28	2	0.57	0/387	0.54	0/509
29	3	0.22	0/468	0.38	0/614
30	4	0.69	1/298 (0.3%)	0.58	0/390
All	All	1.06	265/91244 (0.3%)	1.42	1846/136878 (1.3%)

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
7	E	0	4
8	F	0	3
9	G	0	8
10	H	0	2
11	I	0	1
12	J	0	1
All	All	0	19

All (265) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	616	U	C3'-C2'	-13.53	1.37	1.52
1	X	1775	A	O3'-P	-11.52	1.47	1.61
1	X	1299	A	N9-C4	-11.34	1.31	1.37
1	X	1260	A	N9-C4	-11.21	1.31	1.37
1	X	2669	C	N1-C6	-10.57	1.30	1.37
1	X	2524	G	N7-C5	-10.21	1.33	1.39
1	X	747	A	N9-C8	-9.54	1.30	1.37
1	X	1316	G	N3-C4	-9.29	1.28	1.35
1	X	581	A	N9-C4	-9.27	1.32	1.37
1	X	1635	G	N3-C4	-9.03	1.29	1.35
1	X	1290	A	N9-C8	-8.96	1.30	1.37
1	X	2486	C	C4-C5	-8.89	1.35	1.43
1	X	461	A	N7-C5	-8.61	1.34	1.39
1	X	2745	A	N9-C4	-8.54	1.32	1.37
1	X	542	A	N9-C4	-8.43	1.32	1.37
1	X	2799	C	N3-C4	-8.35	1.28	1.33
1	X	2381	A	C2'-C1'	-8.28	1.44	1.53
1	X	982	C	N1-C6	-8.23	1.32	1.37
1	X	2669	C	C2-O2	8.22	1.31	1.24
1	X	827	C	N1-C6	-7.90	1.32	1.37
1	X	583	C	C4-C5	-7.69	1.36	1.43
1	X	955	G	O3'-P	-7.68	1.51	1.61
1	X	691	C	N3-C4	-7.60	1.28	1.33
1	X	2826	C	N1-C6	-7.53	1.32	1.37
1	X	1284	G	N3-C4	-7.51	1.30	1.35
1	X	2540	A	N9-C4	-7.51	1.33	1.37
1	X	679	C	N1-C6	-7.50	1.32	1.37
1	X	1975	G	N3-C4	-7.41	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2314	A	N9-C8	-7.33	1.31	1.37
1	X	975	C	N1-C6	-7.25	1.32	1.37
1	X	1655	C	N1-C6	-7.24	1.32	1.37
1	X	754	G	C5-C4	-7.16	1.33	1.38
1	X	2531	U	N1-C6	-7.16	1.31	1.38
1	X	586	G	N7-C5	-7.09	1.34	1.39
1	X	2674	C	N1-C2	-7.07	1.33	1.40
1	X	2712	G	N3-C4	-7.06	1.30	1.35
1	X	1288	A	C5-C4	7.02	1.43	1.38
1	X	2790	C	N1-C6	-7.00	1.32	1.37
1	X	522	G	C5-C4	6.99	1.43	1.38
1	X	579	G	C5-C6	6.91	1.49	1.42
1	X	1333	G	N9-C4	-6.86	1.32	1.38
1	X	1333	G	N3-C4	-6.83	1.30	1.35
1	X	1621	C	C3'-C2'	-6.82	1.45	1.52
1	X	2696	A	C5-C4	-6.80	1.33	1.38
1	X	2312	A	N7-C5	-6.80	1.35	1.39
1	X	1246	G	C6-N1	-6.79	1.34	1.39
1	X	1770	U	N3-C4	-6.76	1.32	1.38
1	X	2382	C	O3'-P	6.76	1.69	1.61
1	X	1717	A	N3-C4	-6.71	1.30	1.34
1	X	1674	C	N1-C6	-6.70	1.33	1.37
1	X	1744	G	C6-N1	-6.69	1.34	1.39
1	X	2807	U	N1-C2	6.67	1.44	1.38
1	X	575	U	N1-C2	-6.65	1.32	1.38
1	X	2432	A	N7-C5	-6.65	1.35	1.39
1	X	836	G	N7-C5	-6.64	1.35	1.39
1	X	465	C	N1-C6	-6.61	1.33	1.37
1	X	1675	C	N1-C6	-6.58	1.33	1.37
1	X	1261	G	N7-C5	-6.58	1.35	1.39
1	X	569	C	C4-N4	-6.57	1.28	1.33
1	X	1672	A	N9-C4	-6.56	1.33	1.37
1	X	1986	G	O3'-P	-6.52	1.53	1.61
1	X	2226	A	N9-C4	-6.47	1.33	1.37
1	X	1292	A	N7-C5	6.46	1.43	1.39
1	X	2617	G	N9-C8	-6.44	1.33	1.37
1	X	740	A	N3-C4	-6.43	1.30	1.34
1	X	2486	C	N1-C6	-6.39	1.33	1.37
1	X	2807	U	C4-C5	6.38	1.49	1.43
1	X	1250	A	N9-C4	-6.34	1.34	1.37
1	X	2702	G	N9-C8	6.34	1.42	1.37
1	X	1265	G	N9-C8	-6.34	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	753	U	N1-C2	-6.33	1.32	1.38
1	X	2065	A	N7-C5	-6.30	1.35	1.39
1	X	1334	A	N7-C5	-6.29	1.35	1.39
2	Y	101	A	C6-N1	-6.29	1.31	1.35
1	X	2039	G	C2-N3	-6.27	1.27	1.32
1	X	2691	C	N3-C4	6.26	1.38	1.33
1	X	461	A	N9-C8	-6.25	1.32	1.37
1	X	1281	A	C6-N6	6.20	1.39	1.33
1	X	2694	G	N9-C4	6.19	1.43	1.38
1	X	2815	C	N1-C6	6.19	1.40	1.37
1	X	2352	A	N3-C4	-6.15	1.31	1.34
1	X	1332	G	N9-C8	-6.12	1.33	1.37
1	X	2054	A	C6-N1	-6.10	1.31	1.35
1	X	986	A	N9-C4	-6.09	1.34	1.37
1	X	499	G	N1-C2	-6.09	1.32	1.37
1	X	690	A	N3-C4	-6.09	1.31	1.34
1	X	2602	G	N9-C4	6.07	1.42	1.38
1	X	2515	G	N3-C4	-6.07	1.31	1.35
1	X	2398	U	C4-O4	6.07	1.28	1.23
1	X	571	U	N1-C2	-6.06	1.33	1.38
1	X	1629	G	N7-C5	-6.05	1.35	1.39
1	X	807	A	N9-C4	-6.05	1.34	1.37
1	X	2530	C	N1-C6	-6.04	1.33	1.37
1	X	1288	A	N9-C8	6.03	1.42	1.37
1	X	2759	U	N1-C6	-6.03	1.32	1.38
1	X	1166	A	N9-C4	6.02	1.41	1.37
1	X	157	G	P-O5'	-5.98	1.53	1.59
1	X	2218	G	C5-C6	-5.97	1.36	1.42
1	X	1653	C	N1-C6	-5.96	1.33	1.37
1	X	2555	G	N9-C4	-5.94	1.33	1.38
1	X	815	A	N9-C4	-5.94	1.34	1.37
1	X	1687	C	N1-C6	-5.90	1.33	1.37
1	X	1624	A	N3-C4	-5.90	1.31	1.34
1	X	1290	A	N9-C4	-5.89	1.34	1.37
1	X	2523	G	C6-N1	-5.86	1.35	1.39
1	X	1672	A	N3-C4	-5.84	1.31	1.34
1	X	1290	A	N3-C4	-5.84	1.31	1.34
1	X	841	G	N9-C4	-5.82	1.33	1.38
1	X	2495	G	N1-C2	-5.81	1.33	1.37
1	X	522	G	N1-C2	5.80	1.42	1.37
1	X	1699	A	C5-C6	-5.75	1.35	1.41
1	X	351	A	N3-C4	-5.74	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1671	A	N3-C4	5.73	1.38	1.34
1	X	1223	G	N3-C4	-5.73	1.31	1.35
1	X	1313	U	N3-C4	-5.72	1.33	1.38
1	X	2699	G	P-O5'	-5.72	1.54	1.59
1	X	2854	G	N9-C8	5.72	1.41	1.37
1	X	156	G	N9-C4	-5.71	1.33	1.38
1	X	2015	G	N9-C8	5.71	1.41	1.37
1	X	1700	C	N1-C6	-5.70	1.33	1.37
1	X	2574	G	C5-C4	-5.70	1.34	1.38
1	X	2258	G	N9-C8	-5.70	1.33	1.37
1	X	596	C	N1-C6	-5.70	1.33	1.37
1	X	2696	A	N7-C5	-5.69	1.35	1.39
1	X	174	A	C3'-O3'	-5.69	1.34	1.42
1	X	1268	U	O3'-P	-5.67	1.54	1.61
1	X	1761	G	C2-N2	-5.67	1.28	1.34
1	X	320	A	N9-C4	-5.66	1.34	1.37
1	X	1288	A	C6-N6	-5.66	1.29	1.33
1	X	2355	A	C5-C4	-5.65	1.34	1.38
1	X	2424	G	N9-C8	-5.65	1.33	1.37
1	X	1012	A	N9-C4	-5.63	1.34	1.37
1	X	950	G	N3-C4	-5.63	1.31	1.35
1	X	393	U	C4-O4	5.61	1.28	1.23
18	P	17	GLN	CD-OE1	5.61	1.36	1.24
1	X	1665	C	N1-C6	-5.60	1.33	1.37
1	X	322	A	N7-C5	5.60	1.42	1.39
1	X	2258	G	C6-N1	-5.59	1.35	1.39
1	X	1940	C	N1-C6	-5.59	1.33	1.37
1	X	1267	A	O3'-P	5.58	1.67	1.61
1	X	2688	G	N7-C5	5.58	1.42	1.39
1	X	1474	A	N9-C4	5.57	1.41	1.37
1	X	1334	A	N9-C4	-5.57	1.34	1.37
1	X	2492	G	P-O5'	-5.57	1.54	1.59
1	X	2014	A	N7-C5	-5.57	1.35	1.39
1	X	520	C	N1-C2	-5.56	1.34	1.40
1	X	1678	G	N7-C5	5.56	1.42	1.39
1	X	1985	G	O3'-P	-5.55	1.54	1.61
1	X	538	A	N9-C4	5.54	1.41	1.37
1	X	2527	G	C5-C4	-5.54	1.34	1.38
1	X	2007	G	C6-O6	5.53	1.29	1.24
1	X	513	A	C6-N1	-5.53	1.31	1.35
1	X	72	A	C6-N1	-5.53	1.31	1.35
1	X	1325	U	N1-C6	-5.52	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1282	A	C5-C6	-5.52	1.36	1.41
1	X	2039	G	N7-C5	-5.52	1.35	1.39
1	X	1287	A	C6-N1	-5.51	1.31	1.35
1	X	2498	U	P-O5'	-5.51	1.54	1.59
1	X	1673	C	N1-C6	-5.51	1.33	1.37
1	X	752	G	N3-C4	-5.48	1.31	1.35
1	X	1232	U	N1-C2	-5.48	1.33	1.38
1	X	1625	A	N9-C4	-5.48	1.34	1.37
1	X	718	A	N3-C4	-5.48	1.31	1.34
1	X	1278	A	C5-C6	-5.48	1.36	1.41
1	X	562	G	N9-C8	-5.46	1.34	1.37
1	X	2540	A	C5-C4	-5.46	1.34	1.38
1	X	2698	G	N7-C5	-5.45	1.35	1.39
1	X	1265	G	N7-C5	-5.45	1.35	1.39
1	X	2226	A	N3-C4	-5.45	1.31	1.34
1	X	991	A	C5-C6	-5.44	1.36	1.41
1	X	2680	U	C4-O4	5.44	1.27	1.23
1	X	542	A	N3-C4	-5.43	1.31	1.34
1	X	2802	C	N1-C2	-5.43	1.34	1.40
1	X	2815	C	C4-C5	5.43	1.47	1.43
1	X	1150	C	P-O5'	-5.43	1.54	1.59
1	X	970	A	N7-C5	-5.41	1.36	1.39
1	X	1968	G	N9-C8	-5.40	1.34	1.37
1	X	1172	U	N1-C2	-5.40	1.33	1.38
1	X	1678	G	C6-N1	-5.40	1.35	1.39
1	X	2825	A	C6-N1	-5.40	1.31	1.35
1	X	928	G	N7-C5	-5.40	1.36	1.39
1	X	168	A	N3-C4	-5.39	1.31	1.34
1	X	1778	U	N1-C2	-5.38	1.33	1.38
1	X	1298	G	N9-C8	-5.38	1.34	1.37
1	X	1260	A	N3-C4	-5.38	1.31	1.34
1	X	1670	G	C5-C4	-5.38	1.34	1.38
1	X	462	G	C6-O6	5.36	1.28	1.24
1	X	2042	A	N7-C5	-5.36	1.36	1.39
1	X	1449	C	N1-C6	5.36	1.40	1.37
1	X	1665	C	N3-C4	-5.36	1.30	1.33
1	X	2674	C	N3-C4	-5.34	1.30	1.33
1	X	1041	G	N9-C4	-5.34	1.33	1.38
1	X	2471	U	C4-O4	-5.32	1.19	1.23
1	X	947	C	N1-C6	-5.32	1.33	1.37
1	X	2596	C	C2-O2	5.30	1.29	1.24
1	X	2681	A	N9-C4	-5.30	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2634	G	N9-C8	-5.30	1.34	1.37
1	X	693	A	N9-C4	-5.29	1.34	1.37
1	X	1276	U	P-O5'	-5.29	1.54	1.59
1	X	572	G	N3-C4	-5.29	1.31	1.35
1	X	482	A	P-O5'	-5.27	1.54	1.59
1	X	1151	U	N1-C6	-5.27	1.33	1.38
1	X	2218	G	N7-C5	-5.26	1.36	1.39
1	X	991	A	N7-C5	-5.26	1.36	1.39
1	X	1333	G	N9-C8	5.25	1.41	1.37
1	X	2837	G	C5-C4	-5.25	1.34	1.38
1	X	536	A	N9-C4	5.24	1.41	1.37
1	X	1278	A	N3-C4	-5.24	1.31	1.34
1	X	841	G	N9-C8	5.24	1.41	1.37
1	X	1666	G	C8-N7	5.24	1.34	1.30
1	X	1942	G	N9-C4	-5.24	1.33	1.38
1	X	2520	A	P-O5'	-5.23	1.54	1.59
1	X	2229	G	C5-C6	5.23	1.47	1.42
1	X	1472	C	N3-C4	5.22	1.37	1.33
1	X	2540	A	C6-N6	-5.22	1.29	1.33
1	X	2508	G	C5-C6	-5.22	1.37	1.42
1	X	1282	A	N7-C5	-5.22	1.36	1.39
1	X	1287	A	N3-C4	-5.21	1.31	1.34
1	X	2303	C	N1-C6	-5.21	1.34	1.37
1	X	1938	U	C2'-C1'	-5.20	1.47	1.53
1	X	1270	C	N3-C4	-5.19	1.30	1.33
1	X	2372	A	N7-C5	-5.19	1.36	1.39
1	X	2823	G	N9-C8	-5.19	1.34	1.37
1	X	24	G	N7-C5	-5.18	1.36	1.39
1	X	2673	G	C5-C4	-5.18	1.34	1.38
1	X	2244	C	N1-C6	-5.18	1.34	1.37
1	X	538	A	C2'-C1'	5.18	1.59	1.53
1	X	2039	G	C5-C6	-5.16	1.37	1.42
1	X	2693	U	N3-C4	-5.16	1.33	1.38
1	X	1337	G	O3'-P	-5.16	1.54	1.61
1	X	461	A	C6-N1	5.16	1.39	1.35
1	X	691	C	N1-C6	-5.15	1.34	1.37
1	X	1761	G	C5-C4	-5.14	1.34	1.38
1	X	1952	A	N3-C4	-5.14	1.31	1.34
1	X	523	A	N9-C8	-5.13	1.33	1.37
1	X	920	G	C5-C4	-5.13	1.34	1.38
1	X	1265	G	C6-N1	5.13	1.43	1.39
13	K	88	ALA	CA-CB	-5.12	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	703	A	N3-C4	-5.11	1.31	1.34
1	X	745	C	N1-C6	-5.11	1.34	1.37
1	X	1778	U	C4-O4	-5.11	1.19	1.23
1	X	2348	A	N9-C4	-5.11	1.34	1.37
1	X	2745	A	C5-C6	-5.11	1.36	1.41
1	X	522	G	N9-C8	5.11	1.41	1.37
1	X	1813	A	N7-C5	-5.10	1.36	1.39
1	X	2812	A	N7-C5	-5.10	1.36	1.39
1	X	1054	C	N1-C6	-5.10	1.34	1.37
1	X	2015	G	C8-N7	5.09	1.34	1.30
1	X	584	A	N3-C4	-5.07	1.31	1.34
1	X	522	G	P-O5'	-5.07	1.54	1.59
1	X	718	A	N9-C4	-5.07	1.34	1.37
1	X	1278	A	N7-C5	-5.06	1.36	1.39
30	4	27	CYS	CB-SG	5.06	1.90	1.82
18	P	31	VAL	CB-CG1	-5.06	1.42	1.52
1	X	1650	A	P-O5'	-5.05	1.54	1.59
1	X	1240	G	N9-C8	-5.05	1.34	1.37
1	X	1778	U	C2-O2	-5.04	1.17	1.22
1	X	1246	G	C5-C4	-5.04	1.34	1.38
1	X	2856	U	N1-C2	-5.04	1.34	1.38
1	X	1763	G	N9-C8	-5.02	1.34	1.37
1	X	755	C	N1-C6	-5.02	1.34	1.37
1	X	1671	A	N9-C4	5.02	1.40	1.37
1	X	743	A	N3-C4	-5.02	1.31	1.34
1	X	762	A	C5-C6	-5.01	1.36	1.41
1	X	2331	A	N3-C4	-5.00	1.31	1.34

All (1846) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	29	ARG	C-N-CD	-19.10	78.58	120.60
1	X	1678	G	N1-C6-O6	-18.90	108.56	119.90
1	X	2486	C	C5-C6-N1	17.23	129.62	121.00
1	X	2815	C	C6-N1-C2	17.04	127.12	120.30
14	L	54	ALA	CB-CA-C	16.51	134.87	110.10
1	X	2486	C	O5'-P-OP1	-16.31	91.02	105.70
1	X	747	A	C8-N9-C4	15.93	112.17	105.80
1	X	2815	C	C5-C6-N1	-15.67	113.17	121.00
1	X	1282	A	N1-C6-N6	14.72	127.43	118.60
1	X	1674	C	C6-N1-C2	14.58	126.13	120.30
1	X	1290	A	N7-C8-N9	13.97	120.79	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2565	C	C6-N1-C2	-13.92	114.73	120.30
1	X	2550	C	C6-N1-C2	-13.26	115.00	120.30
1	X	491	A	C8-N9-C4	13.16	111.06	105.80
1	X	2034	A	C8-N9-C4	-13.14	100.54	105.80
1	X	545	C	C6-N1-C2	13.09	125.53	120.30
1	X	841	G	C5-N7-C8	-12.85	97.88	104.30
1	X	1292	A	C8-N9-C4	12.70	110.88	105.80
1	X	579	G	C4-C5-N7	-12.46	105.82	110.80
1	X	982	C	C5-C6-N1	12.42	127.21	121.00
1	X	1670	G	N7-C8-N9	-12.17	107.01	113.10
1	X	2008	C	N3-C4-C5	-12.14	117.04	121.90
1	X	527	C	C6-N1-C2	-12.10	115.46	120.30
1	X	1991	C	C5-C4-N4	11.94	128.56	120.20
1	X	1991	C	N3-C4-N4	-11.90	109.67	118.00
1	X	1305	C	C6-N1-C2	11.86	125.04	120.30
1	X	2802	C	N1-C2-O2	-11.85	111.79	118.90
1	X	174	A	P-O3'-C3'	-11.76	105.59	119.70
1	X	1333	G	N3-C4-C5	11.73	134.47	128.60
1	X	1770	U	C5-C6-N1	-11.71	116.84	122.70
1	X	2371	A	C8-N9-C4	-11.71	101.11	105.80
1	X	850	C	N3-C4-C5	-11.63	117.25	121.90
1	X	1678	G	C5-C6-O6	11.57	135.54	128.60
1	X	37	C	C6-N1-C2	-11.52	115.69	120.30
1	X	1676	U	P-O3'-C3'	-11.50	105.90	119.70
1	X	2524	G	C8-N9-C4	-11.47	101.81	106.40
1	X	805	G	N1-C6-O6	-11.37	113.08	119.90
1	X	2039	G	N1-C6-O6	11.35	126.71	119.90
1	X	1771	A	C8-N9-C4	-11.35	101.26	105.80
1	X	2486	C	C6-N1-C2	-11.32	115.77	120.30
1	X	2008	C	C6-N1-C2	-11.31	115.78	120.30
1	X	1993	G	N1-C6-O6	11.30	126.68	119.90
1	X	2034	A	N9-C4-C5	11.30	110.32	105.80
1	X	1235	C	C6-N1-C2	11.21	124.78	120.30
1	X	496	C	C6-N1-C2	11.15	124.76	120.30
1	X	2807	U	C5-C6-N1	-11.14	117.13	122.70
1	X	1290	A	C5-N7-C8	-11.10	98.35	103.90
1	X	57	G	C8-N9-C4	-11.04	101.98	106.40
1	X	1255	A	N1-C6-N6	-11.02	111.99	118.60
1	X	2347	C	C6-N1-C2	11.01	124.70	120.30
1	X	1667	A	N1-C6-N6	11.00	125.20	118.60
1	X	761	G	C8-N9-C4	10.99	110.79	106.40
1	X	1665	C	C5-C6-N1	-10.98	115.51	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2229	G	N1-C6-O6	-10.96	113.32	119.90
1	X	1995	G	N1-C2-N2	-10.92	106.37	116.20
1	X	830	C	C6-N1-C2	10.90	124.66	120.30
1	X	2855	C	N3-C2-O2	10.90	129.53	121.90
1	X	1708	C	C6-N1-C2	10.82	124.63	120.30
1	X	1288	A	C8-N9-C4	-10.79	101.48	105.80
1	X	2825	A	C8-N9-C4	-10.75	101.50	105.80
1	X	579	G	C5-C6-O6	10.74	135.05	128.60
1	X	2655	C	C6-N1-C2	10.70	124.58	120.30
1	X	1702	C	C6-N1-C2	10.62	124.55	120.30
1	X	1773	C	C6-N1-C2	10.60	124.54	120.30
1	X	1991	C	C5-C6-N1	-10.56	115.72	121.00
1	X	2303	C	C6-N1-C2	10.56	124.53	120.30
1	X	1937	G	C8-N9-C4	10.54	110.62	106.40
1	X	2035	G	N1-C6-O6	-10.49	113.60	119.90
1	X	1333	G	N3-C4-N9	-10.47	119.72	126.00
1	X	2672	U	N3-C2-O2	-10.46	114.88	122.20
1	X	1670	G	C8-N9-C4	10.44	110.58	106.40
1	X	504	G	N1-C6-O6	10.43	126.16	119.90
1	X	1993	G	C2-N3-C4	-10.38	106.71	111.90
1	X	2811	G	C8-N9-C4	10.38	110.55	106.40
1	X	841	G	C4-C5-N7	10.31	114.92	110.80
1	X	806	A	N1-C6-N6	-10.31	112.42	118.60
1	X	1670	G	C5-N7-C8	10.24	109.42	104.30
1	X	481	A	N1-C6-N6	10.24	124.74	118.60
1	X	1009	C	C6-N1-C2	10.19	124.38	120.30
1	X	2540	A	C8-N9-C4	10.19	109.88	105.80
1	X	2229	G	C5-C6-O6	10.17	134.70	128.60
1	X	985	G	C8-N9-C4	-10.15	102.34	106.40
1	X	1674	C	C5-C6-N1	-10.13	115.94	121.00
1	X	985	G	C5-N7-C8	-10.12	99.24	104.30
1	X	1298	G	C8-N9-C4	10.12	110.45	106.40
1	X	520	C	N1-C2-O2	-10.11	112.83	118.90
1	X	982	C	O4'-C1'-N1	10.11	116.29	108.20
1	X	2034	A	C2-N3-C4	10.06	115.63	110.60
1	X	2523	G	N1-C6-O6	-10.03	113.88	119.90
1	X	522	G	N1-C6-O6	10.02	125.91	119.90
1	X	1201	G	C8-N9-C4	-10.02	102.39	106.40
1	X	1663	C	N1-C2-O2	9.99	124.89	118.90
1	X	1288	A	N7-C8-N9	9.99	118.79	113.80
1	X	1699	A	N1-C6-N6	9.97	124.58	118.60
1	X	985	G	N7-C8-N9	9.96	118.08	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1680	U	C5-C6-N1	-9.91	117.75	122.70
1	X	1242	A	C8-N9-C4	9.90	109.76	105.80
1	X	2634	G	C8-N9-C4	9.87	110.35	106.40
1	X	2486	C	C5'-C4'-O4'	9.85	120.92	109.10
1	X	1333	G	C2-N3-C4	-9.84	106.98	111.90
1	X	2056	C	C6-N1-C2	9.83	124.23	120.30
1	X	1535	C	C6-N1-C2	9.81	124.22	120.30
1	X	2815	C	C2-N3-C4	-9.78	115.01	119.90
1	X	2035	G	C5-C6-O6	9.77	134.46	128.60
1	X	309	G	C4-C5-N7	9.75	114.70	110.80
1	X	537	C	C5-C4-N4	9.73	127.01	120.20
1	X	1411	C	C6-N1-C2	9.71	124.19	120.30
1	X	2039	G	C6-C5-N7	-9.68	124.59	130.40
1	X	2524	G	C5-C6-O6	-9.67	122.80	128.60
1	X	1770	U	N3-C4-O4	-9.62	112.67	119.40
1	X	358	C	C6-N1-C2	-9.61	116.45	120.30
1	X	1995	G	N3-C2-N2	9.61	126.63	119.90
1	X	1721	G	C8-N9-C4	9.60	110.24	106.40
1	X	2815	C	N3-C4-C5	9.59	125.74	121.90
1	X	1166	A	C8-N9-C4	-9.55	101.98	105.80
1	X	2039	G	C4-C5-N7	9.55	114.62	110.80
1	X	2553	G	C8-N9-C4	-9.54	102.58	106.40
1	X	2014	A	C8-N9-C4	-9.54	101.98	105.80
1	X	2015	G	C5-N7-C8	-9.51	99.54	104.30
1	X	1944	C	C6-N1-C2	9.50	124.10	120.30
2	Y	20	A	C8-N9-C4	9.48	109.59	105.80
1	X	752	G	N9-C4-C5	9.48	109.19	105.40
1	X	581	A	C8-N9-C4	9.47	109.59	105.80
1	X	752	G	C8-N9-C4	-9.47	102.61	106.40
1	X	2782	G	C8-N9-C4	9.44	110.18	106.40
1	X	1666	G	C8-N9-C4	9.44	110.17	106.40
1	X	1631	C	C6-N1-C2	9.43	124.07	120.30
1	X	985	G	C4-C5-N7	9.39	114.56	110.80
1	X	527	C	N3-C4-C5	-9.37	118.15	121.90
1	X	15	G	C4-C5-N7	-9.36	107.06	110.80
1	X	2486	C	C4-C5-C6	-9.33	112.74	117.40
1	X	50	G	C8-N9-C4	9.33	110.13	106.40
1	X	594	G	N1-C6-O6	-9.30	114.32	119.90
1	X	742	G	C8-N9-C4	-9.30	102.68	106.40
1	X	2725	C	C6-N1-C2	9.28	124.01	120.30
1	X	2745	A	C5-N7-C8	-9.27	99.27	103.90
1	X	2371	A	N9-C4-C5	9.23	109.49	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	747	A	N7-C8-N9	-9.23	109.18	113.80
1	X	1773	C	N1-C2-O2	9.23	124.44	118.90
1	X	717	G	C8-N9-C4	9.22	110.09	106.40
1	X	1717	A	N9-C4-C5	9.21	109.49	105.80
1	X	1744	G	N1-C6-O6	-9.21	114.37	119.90
1	X	821	A	C8-N9-C4	9.20	109.48	105.80
1	X	1289	A	C3'-C2'-C1'	9.19	108.85	101.50
1	X	1158	A	C8-N9-C4	9.14	109.46	105.80
1	X	2807	U	N3-C4-O4	-9.14	113.00	119.40
1	X	538	A	C2-N3-C4	9.12	115.16	110.60
1	X	537	C	N3-C4-N4	-9.11	111.62	118.00
1	X	1779	C	N1-C2-O2	-9.08	113.45	118.90
1	X	479	G	N1-C6-O6	9.08	125.35	119.90
1	X	2247	A	N1-C6-N6	9.07	124.05	118.60
1	X	1678	G	C6-N1-C2	-9.05	119.67	125.10
1	X	2440	C	C5-C6-N1	-9.05	116.47	121.00
1	X	833	A	N1-C6-N6	9.00	124.00	118.60
1	X	1469	U	O4'-C1'-N1	8.99	115.39	108.20
1	X	2825	A	N9-C4-C5	8.98	109.39	105.80
1	X	1931	G	N1-C6-O6	8.97	125.28	119.90
1	X	522	G	C2-N3-C4	-8.96	107.42	111.90
1	X	1664	G	N1-C6-O6	8.96	125.28	119.90
1	X	31	C	N1-C2-O2	-8.95	113.53	118.90
1	X	1792	C	C6-N1-C2	8.95	123.88	120.30
1	X	2688	G	C8-N9-C4	8.93	109.97	106.40
1	X	1201	G	N9-C4-C5	8.92	108.97	105.40
1	X	1992	G	N1-C6-O6	-8.91	114.55	119.90
1	X	533	C	C6-N1-C2	8.91	123.86	120.30
1	X	491	A	N7-C8-N9	-8.90	109.35	113.80
1	X	465	C	C6-N1-C2	8.88	123.85	120.30
1	X	1466	C	C3'-C2'-C1'	8.88	108.60	101.50
1	X	479	G	C5-C6-O6	-8.86	123.28	128.60
1	X	2508	G	C5-C6-O6	-8.85	123.29	128.60
2	Y	101	A	N1-C6-N6	-8.85	113.29	118.60
1	X	2024	U	C6-N1-C2	8.84	126.30	121.00
1	X	2540	A	N1-C2-N3	-8.84	124.88	129.30
1	X	236	C	C6-N1-C2	-8.84	116.77	120.30
1	X	841	G	N7-C8-N9	8.83	117.52	113.10
1	X	1282	A	C5-C6-N6	-8.82	116.64	123.70
1	X	492	G	C2-N3-C4	-8.81	107.49	111.90
1	X	806	A	C5-C6-N6	8.79	130.73	123.70
1	X	1678	G	C5-C6-N1	8.79	115.89	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2468	G	N7-C8-N9	-8.78	108.71	113.10
1	X	1471	G	C8-N9-C4	8.76	109.91	106.40
1	X	2459	C	N1-C2-O2	-8.75	113.65	118.90
1	X	1467	U	O4'-C1'-N1	-8.75	101.20	108.20
1	X	2697	G	N3-C2-N2	8.75	126.02	119.90
1	X	357	A	N1-C6-N6	8.73	123.84	118.60
1	X	1332	G	C8-N9-C4	8.72	109.89	106.40
1	X	1998	A	N1-C6-N6	-8.72	113.37	118.60
1	X	1242	A	C5-C6-N1	8.70	122.05	117.70
1	X	1771	A	N9-C4-C5	8.69	109.28	105.80
1	X	2003	A	C8-N9-C4	-8.69	102.32	105.80
1	X	2431	C	N3-C4-C5	8.66	125.37	121.90
1	X	1288	A	C5-N7-C8	-8.66	99.57	103.90
1	X	1135	C	N1-C2-O2	-8.65	113.71	118.90
1	X	2520	A	N1-C6-N6	-8.65	113.41	118.60
1	X	1016	C	C6-N1-C2	-8.64	116.84	120.30
1	X	1149	G	N1-C6-O6	-8.64	114.72	119.90
1	X	1278	A	C4-C5-C6	8.64	121.32	117.00
1	X	829	C	C2-N3-C4	-8.63	115.58	119.90
1	X	1699	A	C2-N3-C4	-8.63	106.28	110.60
1	X	1717	A	N1-C6-N6	-8.61	113.43	118.60
1	X	2042	A	N1-C6-N6	8.61	123.77	118.60
1	X	2488	G	C5-C6-N1	8.60	115.80	111.50
1	X	2674	C	N1-C2-O2	-8.59	113.75	118.90
1	X	2655	C	N3-C4-C5	8.58	125.33	121.90
1	X	1770	U	C6-N1-C2	8.58	126.15	121.00
1	X	1246	G	N1-C6-O6	-8.57	114.75	119.90
1	X	2555	G	C8-N9-C4	8.57	109.83	106.40
1	X	2856	U	N1-C2-N3	8.55	120.03	114.90
1	X	2627	G	N3-C2-N2	-8.55	113.92	119.90
1	X	2347	C	N1-C2-O2	-8.54	113.77	118.90
1	X	2508	G	C4-C5-N7	8.51	114.20	110.80
1	X	2576	G	N1-C6-O6	8.51	125.01	119.90
1	X	1251	G	C8-N9-C4	-8.50	103.00	106.40
1	X	2039	G	C2-N3-C4	-8.50	107.65	111.90
1	X	1467	U	C5'-C4'-O4'	-8.50	98.90	109.10
1	X	937	C	C6-N1-C2	8.47	123.69	120.30
1	X	1333	G	C5-N7-C8	-8.47	100.06	104.30
1	X	347	C	C6-N1-C2	8.46	123.69	120.30
1	X	596	C	C5-C6-N1	-8.46	116.77	121.00
1	X	1665	C	C6-N1-C2	8.45	123.68	120.30
1	X	1664	G	C5-C6-O6	-8.45	123.53	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1994	U	N3-C2-O2	8.45	128.11	122.20
1	X	1617	G	N1-C6-O6	8.44	124.97	119.90
1	X	2496	C	C6-N1-C2	8.43	123.67	120.30
1	X	2515	G	N1-C6-O6	-8.43	114.84	119.90
1	X	31	C	N3-C2-O2	8.42	127.80	121.90
1	X	2393	G	N1-C6-O6	8.41	124.95	119.90
1	X	2565	C	C5-C6-N1	8.40	125.20	121.00
1	X	2751	C	C6-N1-C2	8.39	123.66	120.30
1	X	409	G	C8-N9-C4	-8.36	103.05	106.40
1	X	2023	C	C6-N1-C2	8.36	123.64	120.30
1	X	1246	G	N9-C4-C5	8.35	108.74	105.40
1	X	508	G	N1-C6-O6	8.34	124.91	119.90
1	X	2519	C	C6-N1-C2	-8.34	116.96	120.30
1	X	2434	G	N1-C6-O6	-8.34	114.90	119.90
1	X	1678	G	N1-C2-N2	-8.33	108.70	116.20
1	X	1778	U	N3-C4-O4	-8.33	113.57	119.40
1	X	1721	G	N9-C4-C5	-8.32	102.07	105.40
1	X	597	U	C5-C6-N1	-8.32	118.54	122.70
1	X	1673	C	N3-C2-O2	8.32	127.72	121.90
1	X	870	C	N1-C2-O2	-8.31	113.91	118.90
1	X	2440	C	C6-N1-C2	8.31	123.62	120.30
1	X	761	G	N9-C4-C5	-8.30	102.08	105.40
1	X	2397	A	C8-N9-C4	8.30	109.12	105.80
1	X	1725	C	C6-N1-C2	-8.25	117.00	120.30
1	X	2035	G	C4-C5-N7	-8.25	107.50	110.80
1	X	2218	G	N1-C6-O6	8.24	124.85	119.90
1	X	2408	G	N9-C4-C5	8.24	108.70	105.40
1	X	1722	G	C8-N9-C4	8.23	109.69	106.40
1	X	1991	C	C4-C5-C6	8.23	121.52	117.40
1	X	864	C	C6-N1-C2	-8.22	117.01	120.30
1	X	2569	A	C8-N9-C4	8.20	109.08	105.80
1	X	2616	U	N3-C4-O4	8.20	125.14	119.40
1	X	2431	C	C6-N1-C2	8.20	123.58	120.30
1	X	2754	C	N3-C4-C5	-8.19	118.62	121.90
1	X	323	G	C8-N9-C4	-8.18	103.13	106.40
1	X	837	U	C5-C6-N1	-8.18	118.61	122.70
1	X	2856	U	N1-C2-O2	-8.18	117.07	122.80
1	X	1966	C	C6-N1-C2	8.18	123.57	120.30
2	Y	88	C	N1-C2-O2	-8.18	114.00	118.90
1	X	2799	C	N1-C2-O2	-8.17	114.00	118.90
1	X	2853	U	C6-N1-C2	8.16	125.90	121.00
1	X	545	C	C5-C6-N1	-8.15	116.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1669	A	O4'-C1'-N9	-8.13	101.69	108.20
1	X	2754	C	C6-N1-C2	-8.13	117.05	120.30
1	X	492	G	C8-N9-C4	8.11	109.64	106.40
1	X	2218	G	C6-C5-N7	-8.11	125.53	130.40
1	X	1225	G	C8-N9-C4	8.11	109.64	106.40
1	X	2669	C	N1-C2-O2	8.10	123.76	118.90
1	X	2408	G	C8-N9-C4	-8.10	103.16	106.40
1	X	1646	G	N1-C6-O6	8.09	124.75	119.90
1	X	479	G	N9-C4-C5	-8.08	102.17	105.40
1	X	2356	A	N1-C6-N6	8.08	123.45	118.60
1	X	2015	G	C4-C5-N7	8.08	114.03	110.80
1	X	1927	U	N3-C2-O2	-8.08	116.55	122.20
1	X	521	U	C6-N1-C2	8.06	125.84	121.00
1	X	2495	G	N3-C2-N2	8.05	125.54	119.90
1	X	2694	G	N3-C4-C5	-8.05	124.57	128.60
1	X	2827	G	N3-C2-N2	8.04	125.53	119.90
1	X	37	C	C5-C6-N1	8.04	125.02	121.00
1	X	456	C	C6-N1-C2	-8.04	117.08	120.30
1	X	2009	U	C5-C6-N1	8.03	126.71	122.70
1	X	2347	C	N3-C2-O2	8.02	127.51	121.90
1	X	2836	U	C5-C6-N1	8.02	126.71	122.70
1	X	1235	C	N3-C4-C5	8.01	125.11	121.90
1	X	2807	U	C6-N1-C2	8.01	125.81	121.00
1	X	569	C	N3-C4-C5	8.00	125.10	121.90
1	X	2745	A	C4-C5-N7	8.00	114.70	110.70
1	X	1942	G	C8-N9-C4	8.00	109.60	106.40
1	X	829	C	N3-C4-C5	8.00	125.10	121.90
1	X	1993	G	C5-C6-N1	-7.99	107.51	111.50
1	X	2802	C	N3-C2-O2	7.98	127.49	121.90
1	X	2435	C	C6-N1-C2	7.98	123.49	120.30
1	X	15	G	C5-C6-O6	7.97	133.38	128.60
1	X	1278	A	N1-C6-N6	7.97	123.38	118.60
1	X	2696	A	N7-C8-N9	-7.96	109.82	113.80
1	X	2468	G	C5-N7-C8	7.95	108.28	104.30
1	X	533	C	C5-C6-N1	-7.95	117.03	121.00
1	X	1678	G	N3-C4-C5	-7.94	124.63	128.60
1	X	29	U	C5-C4-O4	-7.94	121.14	125.90
1	X	850	C	C6-N1-C2	-7.94	117.13	120.30
1	X	1255	A	N9-C4-C5	7.93	108.97	105.80
1	X	863	C	C6-N1-C2	-7.92	117.13	120.30
1	X	555	U	C5-C6-N1	-7.92	118.74	122.70
1	X	2619	G	C5-N7-C8	-7.92	100.34	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1699	A	C5-C6-N1	-7.91	113.74	117.70
1	X	1965	U	N3-C2-O2	-7.90	116.67	122.20
1	X	1104	G	C8-N9-C4	-7.89	103.24	106.40
1	X	1656	U	C5-C6-N1	-7.88	118.76	122.70
1	X	1246	G	C4-C5-N7	-7.87	107.65	110.80
1	X	886	A	C8-N9-C4	-7.85	102.66	105.80
1	X	1242	A	C5-C6-N6	-7.83	117.44	123.70
1	X	594	G	N9-C4-C5	7.82	108.53	105.40
1	X	1242	A	N9-C4-C5	-7.82	102.67	105.80
1	X	34	U	C5-C6-N1	-7.81	118.79	122.70
1	X	1927	U	N1-C2-N3	7.81	119.58	114.90
1	X	1136	G	N1-C6-O6	-7.80	115.22	119.90
1	X	2495	G	N3-C4-C5	-7.80	124.70	128.60
1	X	816	U	C6-N1-C2	-7.80	116.32	121.00
1	X	1038	U	N3-C2-O2	-7.80	116.74	122.20
1	X	508	G	N3-C4-C5	7.79	132.50	128.60
1	X	1379	A	C8-N9-C4	7.78	108.91	105.80
1	X	2311	U	N3-C2-O2	-7.77	116.76	122.20
1	X	2827	G	N3-C4-N9	7.77	130.66	126.00
1	X	2687	G	C8-N9-C4	7.77	109.51	106.40
1	X	981	C	C4'-C3'-C2'	-7.76	94.83	102.60
1	X	1467	U	C5'-C4'-C3'	7.76	128.41	116.00
1	X	1665	C	C4-C5-C6	7.76	121.28	117.40
1	X	2002	A	C8-N9-C4	7.75	108.90	105.80
1	X	2797	G	N3-C4-C5	-7.75	124.73	128.60
1	X	1210	C	N1-C2-O2	-7.74	114.25	118.90
1	X	1041	G	N3-C4-N9	-7.73	121.36	126.00
1	X	1678	G	C4-C5-N7	-7.71	107.71	110.80
1	X	2393	G	C5-C6-O6	-7.71	123.97	128.60
1	X	1290	A	C8-N9-C4	-7.70	102.72	105.80
1	X	583	C	C5-C6-N1	7.70	124.85	121.00
1	X	2540	A	N7-C8-N9	-7.69	109.95	113.80
1	X	1292	A	N7-C8-N9	-7.68	109.96	113.80
1	X	555	U	C2-N3-C4	-7.67	122.40	127.00
1	X	1937	G	N7-C8-N9	-7.66	109.27	113.10
1	X	518	A	C8-N9-C4	-7.66	102.74	105.80
1	X	1278	A	C6-C5-N7	-7.66	126.94	132.30
1	X	1472	C	C6-N1-C2	7.65	123.36	120.30
1	X	1744	G	C5-C6-O6	7.65	133.19	128.60
1	X	2434	G	C8-N9-C4	-7.65	103.34	106.40
1	X	2243	C	N3-C4-C5	-7.64	118.85	121.90
1	X	2832	G	N1-C6-O6	7.64	124.48	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1813	A	C8-N9-C4	-7.63	102.75	105.80
1	X	2560	G	C8-N9-C4	-7.63	103.35	106.40
1	X	2466	G	C8-N9-C4	-7.63	103.35	106.40
1	X	2523	G	C5-C6-O6	7.63	133.18	128.60
1	X	746	G	C8-N9-C1'	-7.62	117.10	127.00
1	X	1617	G	C5-C6-O6	-7.62	124.03	128.60
1	X	2382	C	P-O3'-C3'	-7.61	110.57	119.70
1	X	570	G	C8-N9-C4	7.61	109.44	106.40
1	X	2007	G	C4-C5-N7	-7.61	107.76	110.80
1	X	1286	U	C6-N1-C2	-7.59	116.44	121.00
1	X	2431	C	N1-C2-O2	-7.58	114.35	118.90
1	X	2486	C	O4'-C1'-N1	7.57	114.26	108.20
1	X	2748	C	N1-C2-O2	-7.57	114.36	118.90
1	X	1647	U	N1-C2-N3	7.57	119.44	114.90
1	X	31	C	C6-N1-C2	7.54	123.32	120.30
1	X	50	G	N9-C4-C5	-7.54	102.39	105.40
1	X	572	G	C8-N9-C4	-7.54	103.39	106.40
1	X	583	C	N3-C4-N4	7.53	123.27	118.00
1	X	2753	C	C6-N1-C2	-7.53	117.29	120.30
1	X	1308	C	C6-N1-C2	-7.53	117.29	120.30
1	X	1481	U	N1-C2-O2	-7.52	117.53	122.80
1	X	829	C	C6-N1-C2	7.52	123.31	120.30
1	X	1305	C	C5-C6-N1	-7.51	117.24	121.00
1	X	1278	A	C8-N9-C4	-7.51	102.80	105.80
1	X	2446	C	C6-N1-C2	7.51	123.30	120.30
1	X	471	A	C8-N9-C4	7.50	108.80	105.80
1	X	591	G	C8-N9-C4	7.50	109.40	106.40
1	X	2524	G	C6-C5-N7	-7.50	125.90	130.40
1	X	982	C	C4-C5-C6	-7.50	113.65	117.40
1	X	2855	C	N1-C2-O2	-7.50	114.40	118.90
1	X	2848	A	C6-N1-C2	-7.49	114.11	118.60
1	X	2560	G	N7-C8-N9	7.48	116.84	113.10
1	X	156	G	C8-N9-C4	7.47	109.39	106.40
1	X	175	C	C6-N1-C2	7.47	123.29	120.30
1	X	1172	U	N1-C2-O2	-7.46	117.57	122.80
1	X	1779	C	N3-C2-O2	7.46	127.12	121.90
1	X	2619	G	C4-C5-N7	7.45	113.78	110.80
1	X	1404	C	C6-N1-C2	7.45	123.28	120.30
1	X	2007	G	C5-N7-C8	7.44	108.02	104.30
1	X	805	G	C5-C6-O6	7.43	133.06	128.60
1	X	1449	C	C6-N1-C2	-7.43	117.33	120.30
1	X	1154	A	C2-N3-C4	7.42	114.31	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2694	G	C8-N9-C4	-7.42	103.43	106.40
1	X	1631	C	C5-C6-N1	-7.41	117.29	121.00
1	X	597	U	N1-C2-O2	-7.41	117.61	122.80
1	X	715	U	N1-C2-N3	7.41	119.35	114.90
1	X	2708	U	P-O3'-C3'	-7.41	110.81	119.70
1	X	1928	G	N1-C6-O6	-7.41	115.46	119.90
1	X	508	G	C8-N9-C4	7.40	109.36	106.40
1	X	1994	U	N1-C2-O2	-7.40	117.62	122.80
1	X	1289	A	C4'-C3'-C2'	-7.40	95.20	102.60
1	X	481	A	C5-C6-N6	-7.39	117.78	123.70
1	X	2259	G	C2-N3-C4	-7.39	108.20	111.90
1	X	309	G	C5-C6-O6	-7.38	124.17	128.60
1	X	1735	G	C8-N9-C4	-7.38	103.45	106.40
1	X	2798	A	C2-N3-C4	-7.37	106.91	110.60
1	X	1941	C	C6-N1-C2	7.37	123.25	120.30
1	X	2559	U	C6-N1-C2	7.36	125.42	121.00
1	X	2698	G	N1-C6-O6	7.36	124.32	119.90
1	X	1933	G	C8-N9-C4	-7.36	103.46	106.40
1	X	2495	G	N1-C2-N2	-7.35	109.59	116.20
1	X	1470	G	OP1-P-OP2	-7.34	108.59	119.60
1	X	2627	G	C2-N3-C4	-7.34	108.23	111.90
1	X	1718	A	C8-N9-C4	-7.33	102.87	105.80
1	X	755	C	C4-C5-C6	7.33	121.07	117.40
1	X	2617	G	N3-C4-N9	7.33	130.40	126.00
1	X	2587	G	C8-N9-C4	-7.33	103.47	106.40
1	X	2547	C	C6-N1-C2	7.31	123.23	120.30
1	X	2495	G	N3-C4-N9	7.31	130.39	126.00
1	X	2617	G	C8-N9-C4	7.31	109.32	106.40
1	X	2652	G	C8-N9-C4	7.31	109.32	106.40
1	X	2034	A	N1-C6-N6	-7.31	114.22	118.60
1	X	2693	U	N1-C2-N3	7.29	119.28	114.90
1	X	661	C	C6-N1-C2	-7.29	117.38	120.30
1	X	1766	U	C5-C6-N1	-7.28	119.06	122.70
1	X	1778	U	C2-N3-C4	-7.28	122.63	127.00
1	X	1578	U	C6-N1-C2	7.28	125.37	121.00
1	X	2347	C	C2-N1-C1'	-7.28	110.79	118.80
1	X	2703	C	N3-C4-C5	-7.28	118.99	121.90
1	X	538	A	C5-C6-N1	7.28	121.34	117.70
1	X	2663	U	P-O3'-C3'	7.27	128.43	119.70
1	X	812	G	C8-N9-C4	-7.27	103.49	106.40
1	X	187	U	N1-C2-O2	-7.26	117.72	122.80
1	X	2827	G	N3-C4-C5	-7.26	124.97	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2617	G	C5-N7-C8	7.26	107.93	104.30
1	X	830	C	C5-C6-N1	-7.25	117.38	121.00
1	X	2468	G	N1-C6-O6	-7.25	115.55	119.90
1	X	1272	G	N1-C6-O6	-7.23	115.56	119.90
1	X	1773	C	C6-N1-C1'	-7.23	112.13	120.80
1	X	70	A	C8-N9-C4	-7.23	102.91	105.80
1	X	1009	C	C5-C6-N1	-7.22	117.39	121.00
1	X	1285	A	C2-N3-C4	-7.22	106.99	110.60
1	X	1644	G	C8-N9-C4	7.21	109.28	106.40
1	X	2355	A	C8-N9-C4	7.21	108.68	105.80
1	X	1053	G	P-O3'-C3'	7.21	128.35	119.70
1	X	2474	G	N1-C6-O6	-7.21	115.57	119.90
1	X	2488	G	C5-C6-O6	-7.21	124.28	128.60
1	X	2567	G	C8-N9-C4	-7.21	103.52	106.40
1	X	1758	C	C6-N1-C2	-7.20	117.42	120.30
1	X	2856	U	N3-C4-C5	-7.20	110.28	114.60
1	X	1240	G	C8-N9-C4	7.20	109.28	106.40
1	X	1675	C	N1-C2-O2	-7.20	114.58	118.90
1	X	2807	U	N1-C2-O2	7.19	127.83	122.80
1	X	1667	A	C5-C6-N6	-7.19	117.95	123.70
1	X	1773	C	N3-C4-C5	7.18	124.77	121.90
1	X	15	G	N9-C4-C5	7.18	108.27	105.40
1	X	2838	U	C5-C6-N1	-7.17	119.11	122.70
1	X	1778	U	N1-C2-O2	-7.17	117.78	122.80
1	X	2559	U	N3-C2-O2	7.17	127.22	122.20
1	X	955	G	OP2-P-O3'	7.16	120.96	105.20
1	X	2211	U	C6-N1-C2	7.16	125.30	121.00
1	X	2015	G	N7-C8-N9	7.16	116.68	113.10
1	X	508	G	C5-C6-O6	-7.15	124.31	128.60
1	X	2437	G	N9-C4-C5	-7.15	102.54	105.40
1	X	2019	C	N1-C2-O2	-7.15	114.61	118.90
1	X	2508	G	N1-C6-O6	7.15	124.19	119.90
1	X	1333	G	C4-C5-N7	7.15	113.66	110.80
1	X	1469	U	N1-C2-O2	7.14	127.80	122.80
1	X	1722	G	N9-C4-C5	-7.14	102.54	105.40
1	X	768	U	C5-C4-O4	-7.14	121.62	125.90
1	X	175	C	N3-C4-C5	7.14	124.75	121.90
1	X	562	G	C8-N9-C4	7.13	109.25	106.40
1	X	1645	U	N3-C2-O2	7.12	127.19	122.20
1	X	2566	A	N1-C2-N3	7.12	132.86	129.30
1	X	1472	C	C5-C4-N4	-7.12	115.21	120.20
1	X	1466	C	O4'-C1'-N1	7.12	113.89	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	547	U	N1-C2-O2	-7.12	117.82	122.80
1	X	2014	A	N9-C4-C5	7.12	108.65	105.80
1	X	1741	G	C8-N9-C4	7.11	109.25	106.40
1	X	2699	G	N1-C6-O6	7.11	124.17	119.90
1	X	393	U	N3-C4-O4	7.10	124.37	119.40
1	X	598	U	N1-C2-O2	-7.09	117.84	122.80
1	X	2437	G	C4-C5-N7	7.08	113.63	110.80
1	X	2000	U	N1-C2-O2	-7.08	117.84	122.80
1	X	2811	G	N9-C4-C5	-7.08	102.57	105.40
1	X	670	U	C6-N1-C2	-7.08	116.75	121.00
1	X	479	G	C8-N9-C4	7.08	109.23	106.40
1	X	743	A	C2-N3-C4	-7.07	107.06	110.60
1	X	530	G	C8-N9-C4	7.07	109.23	106.40
1	X	693	A	C2-N3-C4	-7.06	107.07	110.60
1	X	1209	G	N3-C2-N2	-7.06	114.96	119.90
1	X	2553	G	N9-C4-C5	7.06	108.22	105.40
1	X	1287	A	C6-N1-C2	-7.06	114.37	118.60
1	X	745	C	N3-C2-O2	-7.05	116.96	121.90
1	X	970	A	N1-C6-N6	7.05	122.83	118.60
1	X	1300	A	C8-N9-C4	7.05	108.62	105.80
1	X	2496	C	C5-C6-N1	-7.05	117.48	121.00
1	X	2559	U	N1-C2-N3	-7.05	110.67	114.90
1	X	755	C	N3-C4-C5	-7.04	119.08	121.90
1	X	309	G	C5-N7-C8	-7.04	100.78	104.30
1	X	2657	G	C8-N9-C4	-7.04	103.59	106.40
1	X	1698	C	N1-C2-O2	-7.03	114.68	118.90
1	X	2226	A	C2-N3-C4	-7.03	107.08	110.60
1	X	57	G	N7-C8-N9	7.03	116.61	113.10
1	X	1332	G	C5-C6-O6	-7.03	124.38	128.60
1	X	2547	C	N3-C4-C5	7.03	124.71	121.90
1	X	2677	U	N1-C2-O2	-7.02	117.89	122.80
1	X	2243	C	C6-N1-C2	-7.01	117.49	120.30
1	X	165	G	C8-N9-C4	7.01	109.20	106.40
1	X	1771	A	N1-C6-N6	-7.01	114.39	118.60
1	X	494	A	C8-N9-C4	7.01	108.60	105.80
1	X	761	G	N3-C4-N9	7.01	130.21	126.00
1	X	1287	A	N1-C6-N6	-7.01	114.39	118.60
1	X	1032	A	C8-N9-C4	-7.00	103.00	105.80
1	X	9	U	N3-C2-O2	-7.00	117.30	122.20
1	X	21	A	C2-N3-C4	-7.00	107.10	110.60
1	X	1316	G	N9-C4-C5	7.00	108.20	105.40
1	X	2431	C	N3-C2-O2	7.00	126.80	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2457	A	N1-C6-N6	-6.99	114.41	118.60
1	X	1270	C	N1-C2-O2	-6.99	114.71	118.90
1	X	1917	C	C6-N1-C2	-6.98	117.51	120.30
1	X	773	G	C5-C6-N1	-6.98	108.01	111.50
1	X	1160	C	C6-N1-C2	-6.98	117.51	120.30
1	X	2260	C	N1-C2-O2	-6.98	114.71	118.90
1	X	2697	G	C2-N3-C4	6.97	115.39	111.90
1	X	18	U	C6-N1-C2	-6.97	116.82	121.00
1	X	1404	C	C5-C6-N1	-6.97	117.52	121.00
1	X	1985	G	C3'-C2'-C1'	-6.96	95.93	101.50
1	X	661	C	N3-C2-O2	-6.96	117.03	121.90
1	X	1272	G	C5-C6-O6	6.96	132.77	128.60
1	X	1770	U	C2-N3-C4	-6.96	122.83	127.00
1	X	2274	C	C6-N1-C2	6.95	123.08	120.30
1	X	1298	G	N7-C8-N9	-6.95	109.62	113.10
1	X	2025	A	C5-C6-N6	-6.95	118.14	123.70
1	X	2247	A	C5-C6-N6	-6.95	118.14	123.70
1	X	850	C	C5-C4-N4	6.95	125.06	120.20
1	X	1698	C	C6-N1-C2	6.94	123.08	120.30
1	X	465	C	N1-C2-O2	6.94	123.06	118.90
1	X	972	C	C6-N1-C2	-6.94	117.52	120.30
1	X	2652	G	N3-C4-C5	6.94	132.07	128.60
1	X	1818	G	N9-C4-C5	-6.94	102.62	105.40
1	X	2409	A	P-O3'-C3'	6.94	128.03	119.70
1	X	1053	G	O4'-C1'-N9	6.94	113.75	108.20
1	X	2559	U	C5-C4-O4	-6.93	121.74	125.90
1	X	579	G	N1-C6-O6	-6.93	115.74	119.90
1	X	691	C	C5-C6-N1	-6.93	117.53	121.00
1	X	1028	G	C8-N9-C4	6.93	109.17	106.40
1	X	1149	G	C5-C6-O6	6.93	132.76	128.60
1	X	1235	C	C5-C6-N1	-6.93	117.54	121.00
1	X	2498	U	N1-C2-O2	-6.93	117.95	122.80
1	X	1678	G	N3-C2-N2	6.92	124.75	119.90
1	X	2640	G	C5-C6-O6	-6.92	124.44	128.60
1	X	443	A	C8-N9-C4	6.92	108.57	105.80
1	X	1419	G	C8-N9-C4	6.92	109.17	106.40
1	X	2000	U	N3-C2-O2	6.92	127.05	122.20
1	X	1708	C	N3-C4-C5	6.92	124.67	121.90
1	X	2375	G	C8-N9-C4	6.91	109.17	106.40
1	X	2515	G	N3-C4-C5	-6.91	125.14	128.60
1	X	753	U	N1-C2-O2	-6.91	117.96	122.80
1	X	2660	C	C6-N1-C2	6.91	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1240	G	N9-C4-C5	-6.91	102.64	105.40
1	X	504	G	C4-C5-N7	6.91	113.56	110.80
1	X	1292	A	N1-C6-N6	-6.91	114.46	118.60
1	X	850	C	N1-C2-O2	-6.90	114.76	118.90
1	X	1343	C	N3-C4-C5	6.90	124.66	121.90
1	X	2434	G	N9-C4-C5	6.90	108.16	105.40
1	X	2818	G	N1-C6-O6	6.90	124.04	119.90
1	X	579	G	C5-N7-C8	6.89	107.75	104.30
1	X	50	G	N3-C4-C5	6.88	132.04	128.60
1	X	2034	A	N3-C4-C5	-6.88	121.98	126.80
1	X	1708	C	C5-C6-N1	-6.88	117.56	121.00
1	X	2617	G	N7-C8-N9	-6.88	109.66	113.10
1	X	491	A	N9-C4-C5	-6.88	103.05	105.80
1	X	2222	U	C5-C6-N1	-6.88	119.26	122.70
1	X	520	C	C6-N1-C2	-6.87	117.55	120.30
1	X	736	G	C8-N9-C4	6.87	109.15	106.40
1	X	1778	U	N3-C4-C5	6.87	118.72	114.60
1	X	2230	G	C4-C5-N7	6.87	113.55	110.80
1	X	2024	U	C5-C6-N1	-6.87	119.27	122.70
1	X	2038	C	C6-N1-C2	6.87	123.05	120.30
1	X	2267	A	C2-N3-C4	6.87	114.03	110.60
1	X	2848	A	N1-C2-N3	6.86	132.73	129.30
1	X	2230	G	C5-C6-O6	-6.85	124.49	128.60
1	X	190	A	C8-N9-C4	6.85	108.54	105.80
1	X	752	G	C4-C5-N7	-6.85	108.06	110.80
1	X	2748	C	N3-C2-O2	6.84	126.69	121.90
1	X	11	G	N1-C6-O6	6.83	124.00	119.90
1	X	1228	G	N9-C4-C5	6.83	108.13	105.40
1	X	1540	C	C6-N1-C2	-6.83	117.57	120.30
1	X	2495	G	C5-C6-N1	6.83	114.91	111.50
1	X	2745	A	C5-C6-N6	-6.83	118.24	123.70
1	X	1481	U	N3-C2-O2	6.83	126.98	122.20
1	X	806	A	C4-C5-N7	-6.83	107.29	110.70
1	X	2633	A	C5-C6-N1	6.83	121.11	117.70
1	X	1636	G	C8-N9-C4	6.82	109.13	106.40
1	X	1408	A	C8-N9-C4	-6.82	103.07	105.80
1	X	2704	U	N3-C2-O2	-6.82	117.43	122.20
1	X	423	G	C8-N9-C4	6.82	109.13	106.40
1	X	2425	G	N3-C2-N2	-6.81	115.13	119.90
1	X	2399	C	C6-N1-C2	6.81	123.03	120.30
1	X	322	A	C8-N9-C4	6.81	108.52	105.80
1	X	2619	G	N7-C8-N9	6.81	116.50	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1951	G	C8-N9-C4	-6.80	103.68	106.40
1	X	1982	C	C2-N3-C4	-6.80	116.50	119.90
1	X	1006	C	N1-C2-O2	6.79	122.98	118.90
1	X	1242	A	C4-C5-C6	-6.79	113.60	117.00
1	X	697	G	N3-C2-N2	-6.79	115.15	119.90
1	X	2451	G	C5-C6-N1	6.79	114.89	111.50
1	X	742	G	N7-C8-N9	6.79	116.49	113.10
1	X	2007	G	C5-C6-O6	6.78	132.67	128.60
1	X	541	C	C4-C5-C6	6.78	120.79	117.40
1	X	2522	G	C8-N9-C4	-6.78	103.69	106.40
1	X	1821	A	N1-C6-N6	6.78	122.67	118.60
1	X	797	A	C8-N9-C4	6.76	108.51	105.80
1	X	2634	G	N9-C4-C5	-6.76	102.69	105.40
1	X	549	G	C4-C5-N7	-6.76	108.09	110.80
1	X	1236	G	C4-C5-N7	6.76	113.50	110.80
1	X	1985	G	P-O3'-C3'	6.76	127.81	119.70
1	X	2009	U	C6-N1-C2	-6.76	116.94	121.00
1	X	2515	G	C5-C6-O6	6.76	132.66	128.60
1	X	2565	C	N3-C4-C5	-6.76	119.19	121.90
1	X	2687	G	N7-C8-N9	-6.76	109.72	113.10
1	X	2547	C	C2-N3-C4	-6.76	116.52	119.90
1	X	1166	A	C2-N3-C4	6.76	113.98	110.60
1	X	1253	C	C6-N1-C2	-6.75	117.60	120.30
1	X	2751	C	N3-C4-C5	6.75	124.60	121.90
1	X	1718	A	N9-C4-C5	6.75	108.50	105.80
1	X	2818	G	C5-C6-O6	-6.75	124.55	128.60
1	X	522	G	N3-C4-C5	6.74	131.97	128.60
1	X	1965	U	N1-C2-N3	6.74	118.95	114.90
1	X	2063	A	C8-N9-C4	-6.74	103.10	105.80
2	Y	101	A	N9-C4-C5	6.74	108.50	105.80
1	X	492	G	N3-C4-C5	6.74	131.97	128.60
1	X	1748	U	C5-C4-O4	-6.74	121.86	125.90
1	X	834	A	C4'-C3'-C2'	-6.73	95.87	102.60
1	X	524	A	C6-N1-C2	-6.73	114.56	118.60
1	X	2398	U	N3-C4-C5	-6.73	110.56	114.60
1	X	2266	A	C8-N9-C4	6.72	108.49	105.80
1	X	1993	G	N3-C2-N2	-6.72	115.19	119.90
1	X	2522	G	N9-C4-C5	6.72	108.09	105.40
1	X	2540	A	C4-C5-C6	-6.72	113.64	117.00
1	X	1359	G	N1-C6-O6	-6.72	115.87	119.90
1	X	2764	U	N3-C4-O4	-6.72	114.70	119.40
1	X	2003	A	N7-C8-N9	6.72	117.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	236	C	N3-C2-O2	-6.71	117.20	121.90
1	X	1703	C	C6-N1-C2	6.71	122.98	120.30
1	X	1931	G	C5-C6-O6	-6.71	124.58	128.60
1	X	661	C	N1-C2-O2	6.71	122.92	118.90
1	X	816	U	N3-C2-O2	-6.71	117.50	122.20
1	X	319	G	N3-C4-C5	6.71	131.95	128.60
1	X	82	G	N1-C6-O6	-6.70	115.88	119.90
1	X	137	A	C8-N9-C4	-6.70	103.12	105.80
1	X	752	G	C5-C6-N1	-6.70	108.15	111.50
1	X	2691	C	N3-C2-O2	6.69	126.58	121.90
1	X	323	G	N3-C4-C5	-6.69	125.25	128.60
1	X	480	G	C8-N9-C4	-6.69	103.72	106.40
1	X	1818	G	C8-N9-C4	6.69	109.08	106.40
1	X	2205	C	C6-N1-C2	6.69	122.97	120.30
1	X	991	A	N1-C6-N6	6.68	122.61	118.60
1	X	2008	C	C5-C6-N1	6.68	124.34	121.00
1	X	2815	C	C2-N1-C1'	-6.68	111.45	118.80
1	X	67	G	C4-C5-N7	6.68	113.47	110.80
1	X	1221	C	C6-N1-C2	-6.68	117.63	120.30
1	X	2832	G	C4-C5-N7	6.68	113.47	110.80
1	X	2065	A	C8-N9-C4	-6.67	103.13	105.80
1	X	1635	G	N1-C6-O6	6.67	123.90	119.90
1	X	2548	G	C5-N7-C8	6.67	107.63	104.30
1	X	1912	G	C8-N9-C4	-6.66	103.73	106.40
1	X	2555	G	N3-C4-C5	6.66	131.93	128.60
1	X	474	G	C8-N9-C4	6.66	109.06	106.40
1	X	541	C	C5-C6-N1	-6.66	117.67	121.00
1	X	591	G	N7-C8-N9	-6.65	109.77	113.10
1	X	1328	C	C6-N1-C2	-6.65	117.64	120.30
1	X	2608	A	C8-N9-C4	-6.65	103.14	105.80
1	X	2855	C	C5-C4-N4	-6.65	115.55	120.20
1	X	2490	U	C5-C6-N1	-6.64	119.38	122.70
1	X	692	C	C2-N3-C4	-6.63	116.58	119.90
1	X	771	C	C6-N1-C2	-6.63	117.65	120.30
1	X	2515	G	N9-C4-C5	6.63	108.05	105.40
1	X	2848	A	N9-C4-C5	6.62	108.45	105.80
1	X	2011	U	C5-C6-N1	-6.62	119.39	122.70
1	X	1469	U	C4-C5-C6	-6.62	115.73	119.70
1	X	689	A	N1-C6-N6	6.62	122.57	118.60
1	X	1680	U	C2-N3-C4	-6.61	123.03	127.00
1	X	2696	A	C8-N9-C4	6.61	108.44	105.80
1	X	883	A	N1-C2-N3	-6.60	126.00	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2253	A	N9-C4-C5	-6.60	103.16	105.80
1	X	829	C	C5-C6-N1	-6.59	117.70	121.00
1	X	2655	C	C5-C6-N1	-6.59	117.70	121.00
1	X	25	U	N3-C4-O4	6.59	124.01	119.40
1	X	2790	C	C5-C6-N1	-6.59	117.71	121.00
1	X	2859	U	C4'-C3'-C2'	-6.59	96.01	102.60
2	Y	101	A	C5-C6-N6	6.59	128.97	123.70
1	X	1615	C	C6-N1-C2	6.58	122.93	120.30
1	X	2520	A	C2-N3-C4	6.58	113.89	110.60
1	X	2485	U	C3'-C2'-C1'	6.58	106.76	101.50
1	X	2586	G	N1-C6-O6	-6.58	115.95	119.90
1	X	1747	G	C8-N9-C4	6.57	109.03	106.40
1	X	2757	G	C2-N3-C4	-6.57	108.61	111.90
1	X	166	G	C8-N9-C4	6.57	109.03	106.40
1	X	465	C	C6-N1-C1'	-6.57	112.92	120.80
1	X	2451	G	N1-C6-O6	-6.57	115.96	119.90
1	X	1944	C	N3-C4-C5	6.57	124.53	121.90
1	X	885	A	C8-N9-C4	-6.57	103.17	105.80
1	X	720	A	C2-N3-C4	-6.57	107.32	110.60
1	X	1830	C	C6-N1-C2	6.56	122.93	120.30
1	X	1968	G	C8-N9-C4	6.56	109.03	106.40
1	X	841	G	C8-N9-C4	-6.56	103.78	106.40
1	X	2008	C	N3-C4-N4	6.56	122.59	118.00
1	X	2466	G	N7-C8-N9	6.56	116.38	113.10
1	X	2712	G	N1-C6-O6	-6.56	115.97	119.90
1	X	1009	C	C2-N3-C4	-6.55	116.62	119.90
1	X	596	C	C4-C5-C6	6.55	120.67	117.40
1	X	1656	U	C6-N1-C2	6.55	124.93	121.00
1	X	2853	U	C5-C6-N1	-6.55	119.42	122.70
1	X	1017	C	C6-N1-C2	-6.55	117.68	120.30
1	X	2711	G	N1-C6-O6	-6.54	115.97	119.90
1	X	2485	U	C4-C5-C6	-6.54	115.78	119.70
1	X	2049	C	C6-N1-C2	-6.54	117.69	120.30
1	X	1009	C	N3-C4-C5	6.53	124.51	121.90
1	X	25	U	C5-C4-O4	-6.53	121.98	125.90
1	X	1260	A	C2-N3-C4	-6.53	107.34	110.60
1	X	2704	U	N1-C2-N3	6.53	118.82	114.90
1	X	579	G	N9-C4-C5	6.52	108.01	105.40
1	X	479	G	C4-C5-N7	6.52	113.41	110.80
1	X	858	G	C8-N9-C4	6.52	109.01	106.40
1	X	2792	C	C6-N1-C2	6.52	122.91	120.30
1	X	2347	C	C5-C6-N1	-6.51	117.74	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2623	A	N7-C8-N9	-6.51	110.54	113.80
1	X	1986	G	P-O3'-C3'	-6.51	111.89	119.70
1	X	833	A	N1-C2-N3	-6.50	126.05	129.30
1	X	1270	C	C2-N1-C1'	-6.50	111.65	118.80
1	X	1959	U	N3-C2-O2	-6.50	117.65	122.20
1	X	1256	C	N3-C2-O2	-6.50	117.35	121.90
1	X	1332	G	N9-C4-C5	-6.49	102.80	105.40
1	X	1467	U	N1-C1'-C2'	6.49	122.44	114.00
1	X	2237	C	C6-N1-C2	6.49	122.90	120.30
1	X	918	A	C8-N9-C4	6.49	108.40	105.80
1	X	1762	C	C6-N1-C2	-6.49	117.70	120.30
1	X	401	G	N9-C4-C5	6.49	108.00	105.40
1	X	787	A	C8-N9-C4	6.49	108.39	105.80
1	X	1246	G	C5-C6-O6	6.49	132.49	128.60
1	X	1717	A	C5-C6-N6	6.48	128.88	123.70
1	X	1480	G	N1-C6-O6	6.48	123.79	119.90
1	X	752	G	C5-C6-O6	6.48	132.49	128.60
1	X	1828	C	N3-C4-C5	6.48	124.49	121.90
1	X	34	U	C6-N1-C2	6.48	124.89	121.00
1	X	1304	U	C2-N3-C4	-6.47	123.11	127.00
1	X	1135	C	N3-C2-O2	6.47	126.43	121.90
1	X	323	G	N9-C4-C5	6.47	107.99	105.40
1	X	1916	G	C8-N9-C4	-6.47	103.81	106.40
1	X	1771	A	N7-C8-N9	6.47	117.03	113.80
1	X	1449	C	C5-C6-N1	6.46	124.23	121.00
1	X	1991	C	C2-N1-C1'	-6.46	111.70	118.80
1	X	338	G	C8-N9-C4	-6.45	103.82	106.40
1	X	1770	U	N3-C4-C5	6.45	118.47	114.60
1	X	2847	G	C5-C6-O6	-6.45	124.73	128.60
1	X	1664	G	N3-C4-C5	6.44	131.82	128.60
1	X	32	C	C6-N1-C2	6.44	122.88	120.30
1	X	2822	U	N3-C2-O2	6.44	126.71	122.20
1	X	1673	C	N1-C2-O2	-6.43	115.04	118.90
1	X	2543	A	N9-C4-C5	6.43	108.37	105.80
1	X	2419	C	C5-C6-N1	-6.43	117.78	121.00
1	X	2258	G	N3-C4-N9	6.42	129.85	126.00
1	X	357	A	C2-N3-C4	-6.41	107.39	110.60
1	X	18	U	C5-C6-N1	6.41	125.90	122.70
1	X	751	G	N1-C6-O6	6.40	123.74	119.90
1	X	1240	G	N3-C4-N9	6.40	129.84	126.00
1	X	762	A	N1-C6-N6	6.40	122.44	118.60
1	X	2627	G	C5-C6-N1	-6.40	108.30	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1471	G	N7-C8-N9	-6.40	109.90	113.10
1	X	2540	A	N9-C4-C5	-6.40	103.24	105.80
1	X	528	G	N9-C4-C5	-6.39	102.84	105.40
1	X	2759	U	N3-C4-O4	6.39	123.88	119.40
1	X	693	A	C8-N9-C4	6.39	108.36	105.80
1	X	2588	U	C6-N1-C2	6.39	124.83	121.00
1	X	1673	C	C6-N1-C2	6.38	122.85	120.30
1	X	2195	C	C6-N1-C2	6.38	122.85	120.30
1	X	2468	G	C4-C5-N7	-6.38	108.25	110.80
1	X	340	G	C8-N9-C4	6.38	108.95	106.40
1	X	504	G	C6-C5-N7	-6.38	126.57	130.40
1	X	522	G	C5-C6-N1	-6.38	108.31	111.50
1	X	596	C	C6-N1-C2	6.38	122.85	120.30
1	X	773	G	C2-N3-C4	-6.38	108.71	111.90
1	X	1653	C	N1-C2-O2	-6.38	115.07	118.90
1	X	2835	A	C5-C6-N1	-6.38	114.51	117.70
1	X	1304	U	N3-C4-C5	6.37	118.42	114.60
1	X	1163	C	C6-N1-C2	-6.37	117.75	120.30
1	X	762	A	C4-C5-N7	6.36	113.88	110.70
1	X	1647	U	N3-C4-C5	-6.36	110.78	114.60
1	X	2468	G	C8-N9-C4	6.36	108.94	106.40
1	X	2651	U	N3-C2-O2	6.36	126.66	122.20
1	X	2672	U	N1-C2-O2	6.36	127.25	122.80
1	X	1309	G	N3-C2-N2	6.36	124.35	119.90
1	X	2035	G	N3-C4-C5	-6.36	125.42	128.60
1	X	2008	C	N1-C2-O2	-6.36	115.09	118.90
1	X	1715	A	C5-C6-N6	-6.35	118.62	123.70
1	X	1773	C	C5-C6-N1	-6.35	117.82	121.00
1	X	2524	G	N1-C6-O6	6.34	123.71	119.90
1	X	1470	G	O5'-P-OP2	6.34	118.31	110.70
1	X	1702	C	N3-C4-C5	6.34	124.44	121.90
1	X	2760	G	C8-N9-C4	6.34	108.94	106.40
1	X	1409	U	C6-N1-C2	6.34	124.80	121.00
1	X	1777	A	N7-C8-N9	6.34	116.97	113.80
1	X	950	G	N9-C4-C5	6.34	107.94	105.40
1	X	2655	C	C2-N3-C4	-6.34	116.73	119.90
1	X	2039	G	C5-C6-O6	-6.34	124.80	128.60
1	X	1806	G	C8-N9-C4	-6.33	103.87	106.40
1	X	2437	G	C5-C6-O6	-6.33	124.80	128.60
26	Z	4	HIS	C-N-CD	-6.33	106.67	120.60
1	X	1270	C	C6-N1-C1'	6.33	128.39	120.80
1	X	572	G	N9-C4-C5	6.32	107.93	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	575	U	N1-C2-O2	-6.32	118.37	122.80
1	X	434	C	C6-N1-C2	-6.32	117.77	120.30
1	X	2422	C	C6-N1-C2	-6.32	117.77	120.30
1	X	1766	U	C6-N1-C2	6.32	124.79	121.00
1	X	2422	C	N1-C2-O2	-6.32	115.11	118.90
1	X	2858	A	C4'-C3'-C2'	-6.32	96.28	102.60
1	X	2603	G	C8-N9-C4	-6.31	103.88	106.40
1	X	46	C	C6-N1-C2	-6.31	117.78	120.30
1	X	1679	U	C5-C6-N1	-6.31	119.55	122.70
1	X	1761	G	N1-C2-N3	6.31	127.68	123.90
1	X	1824	C	C6-N1-C2	6.30	122.82	120.30
1	X	2836	U	C6-N1-C2	-6.30	117.22	121.00
1	X	536	A	C2-N3-C4	6.30	113.75	110.60
1	X	827	C	N1-C2-O2	6.30	122.68	118.90
1	X	1018	C	C5-C6-N1	-6.30	117.85	121.00
1	X	985	G	C6-C5-N7	-6.30	126.62	130.40
1	X	2812	A	C2-N3-C4	-6.30	107.45	110.60
1	X	1992	G	C5-C6-O6	6.29	132.38	128.60
1	X	2350	G	N9-C4-C5	6.29	107.92	105.40
1	X	972	C	N3-C4-C5	-6.29	119.38	121.90
1	X	2654	A	C8-N9-C4	6.29	108.32	105.80
1	X	1255	A	C5-C6-N6	6.29	128.73	123.70
1	X	2638	G	C8-N9-C4	-6.29	103.89	106.40
1	X	1299	A	N3-C4-N9	-6.29	122.37	127.40
1	X	1963	G	N9-C4-C5	6.29	107.91	105.40
1	X	2374	C	C5-C4-N4	6.29	124.60	120.20
1	X	2033	C	N1-C2-O2	-6.28	115.13	118.90
1	X	2522	G	C5-C6-O6	6.28	132.37	128.60
1	X	570	G	N3-C2-N2	-6.28	115.51	119.90
1	X	1622	G	N1-C6-O6	-6.28	116.13	119.90
1	X	1054	C	C5-C6-N1	6.27	124.14	121.00
1	X	1236	G	N9-C4-C5	-6.27	102.89	105.40
1	X	1469	U	C5-C6-N1	6.27	125.84	122.70
1	X	527	C	N3-C4-N4	6.27	122.39	118.00
1	X	1675	C	N3-C4-C5	-6.27	119.39	121.90
1	X	804	C	C2-N3-C4	-6.26	116.77	119.90
1	X	1285	A	N1-C2-N3	6.26	132.43	129.30
1	X	1169	C	N1-C2-O2	6.26	122.65	118.90
1	X	2397	A	N9-C4-C5	-6.26	103.30	105.80
1	X	531	G	C8-N9-C4	6.25	108.90	106.40
1	X	536	A	C8-N9-C4	-6.25	103.30	105.80
1	X	2637	C	N3-C2-O2	6.25	126.28	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	549	G	N1-C6-O6	-6.25	116.15	119.90
1	X	393	U	N3-C4-C5	-6.25	110.85	114.60
1	X	594	G	C5-C6-O6	6.25	132.35	128.60
1	X	2698	G	C5-C6-O6	-6.24	124.86	128.60
1	X	1251	G	N7-C8-N9	6.24	116.22	113.10
1	X	2794	G	C5-C6-O6	-6.23	124.86	128.60
1	X	951	G	C8-N9-C4	6.23	108.89	106.40
1	X	2515	G	N1-C2-N2	-6.23	110.59	116.20
1	X	2566	A	C2-N3-C4	-6.22	107.49	110.60
1	X	1314	A	N1-C6-N6	-6.22	114.87	118.60
1	X	1229	C	C5-C4-N4	6.22	124.55	120.20
1	X	1451	C	C6-N1-C2	-6.22	117.81	120.30
1	X	166	G	N3-C4-C5	6.21	131.71	128.60
1	X	1628	C	N1-C2-O2	-6.21	115.17	118.90
1	X	489	A	N1-C6-N6	-6.21	114.88	118.60
1	X	1228	G	C5-C6-O6	6.21	132.32	128.60
1	X	2474	G	N3-C2-N2	6.21	124.25	119.90
1	X	1789	U	N3-C2-O2	-6.20	117.86	122.20
1	X	2693	U	C5-C4-O4	6.20	129.62	125.90
1	X	861	G	C8-N9-C4	-6.20	103.92	106.40
1	X	1256	C	C2-N3-C4	-6.20	116.80	119.90
1	X	686	C	N3-C4-C5	6.20	124.38	121.90
1	X	1333	G	N1-C6-O6	6.20	123.62	119.90
1	X	777	A	C1'-O4'-C4'	-6.19	104.94	109.90
1	X	761	G	N1-C2-N2	-6.19	110.63	116.20
1	X	1658	A	N1-C6-N6	6.19	122.31	118.60
1	X	1719	G	N1-C6-O6	-6.19	116.19	119.90
1	X	2862	G	C8-N9-C4	-6.19	103.92	106.40
1	X	1642	G	C2-N3-C4	-6.19	108.81	111.90
1	X	1721	G	N7-C8-N9	-6.19	110.00	113.10
1	X	2056	C	C5-C6-N1	-6.19	117.91	121.00
1	X	1998	A	C4-C5-N7	-6.19	107.61	110.70
1	X	2782	G	N9-C4-C5	-6.18	102.93	105.40
1	X	2712	G	C5-C6-O6	6.18	132.31	128.60
1	X	1982	C	N1-C2-N3	6.18	123.53	119.20
1	X	219	G	N3-C2-N2	6.17	124.22	119.90
1	X	743	A	N1-C2-N3	6.17	132.39	129.30
1	X	2690	A	N1-C6-N6	6.17	122.30	118.60
1	X	1442	C	N3-C4-C5	6.17	124.37	121.90
1	X	1297	A	C2-N3-C4	-6.16	107.52	110.60
1	X	2524	G	N3-C4-C5	-6.16	125.52	128.60
1	X	507	A	C8-N9-C4	6.16	108.26	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	U	40	ARG	N-CA-CB	6.16	121.68	110.60
1	X	1661	C	C6-N1-C2	6.15	122.76	120.30
1	X	2792	C	C2-N3-C4	-6.15	116.82	119.90
1	X	1282	A	N9-C4-C5	-6.15	103.34	105.80
1	X	2047	C	N1-C2-O2	-6.15	115.21	118.90
1	X	2674	C	N3-C2-O2	6.14	126.20	121.90
1	X	1019	U	C6-N1-C2	6.14	124.69	121.00
1	X	1835	C	N1-C2-O2	-6.14	115.22	118.90
1	X	1255	A	C8-N9-C4	-6.13	103.35	105.80
1	X	27	G	C2-N3-C4	6.13	114.97	111.90
1	X	394	U	C6-N1-C2	6.13	124.68	121.00
1	X	1304	U	N3-C4-O4	-6.13	115.11	119.40
1	X	480	G	N9-C4-C5	6.12	107.85	105.40
1	X	1317	G	C2-N3-C4	-6.12	108.84	111.90
1	X	1648	C	C6-N1-C2	6.12	122.75	120.30
1	X	2619	G	C8-N9-C4	-6.12	103.95	106.40
1	X	126	C	C6-N1-C2	6.12	122.75	120.30
1	X	2343	C	C6-N1-C2	6.12	122.75	120.30
1	X	889	C	N1-C2-O2	6.12	122.57	118.90
1	X	597	U	C2-N1-C1'	-6.11	110.36	117.70
1	X	1292	A	C5-C6-N1	6.11	120.75	117.70
1	X	2697	G	N1-C2-N3	-6.11	120.23	123.90
1	X	1357	U	N3-C2-O2	-6.11	117.92	122.20
1	X	747	A	N9-C4-C5	-6.11	103.36	105.80
1	X	1993	G	C6-C5-N7	-6.10	126.74	130.40
1	X	2068	C	C6-N1-C2	-6.10	117.86	120.30
1	X	1202	U	N1-C2-O2	-6.09	118.53	122.80
1	X	1398	G	C8-N9-C4	6.09	108.84	106.40
1	X	1664	G	C4-C5-N7	6.09	113.24	110.80
1	X	878	C	N3-C4-C5	6.09	124.34	121.90
1	X	1699	A	C8-N9-C4	6.09	108.24	105.80
1	X	735	G	C8-N9-C4	6.09	108.83	106.40
1	X	2617	G	N1-C6-O6	-6.09	116.25	119.90
1	X	2651	U	C6-N1-C2	6.09	124.65	121.00
1	X	29	U	N3-C4-O4	6.08	123.66	119.40
1	X	2603	G	N7-C8-N9	6.08	116.14	113.10
1	X	2855	C	N3-C4-N4	6.08	122.26	118.00
1	X	1993	G	N3-C4-C5	6.08	131.64	128.60
1	X	2688	G	C2-N3-C4	-6.08	108.86	111.90
1	X	2496	C	C2-N3-C4	-6.08	116.86	119.90
1	X	1644	G	N7-C8-N9	-6.07	110.06	113.10
1	X	2711	G	C5-C6-N1	6.07	114.54	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1294	G	C8-N9-C4	-6.07	103.97	106.40
1	X	1711	C	N3-C4-C5	6.07	124.33	121.90
1	X	1710	U	C5-C4-O4	-6.06	122.26	125.90
1	X	2015	G	C8-N9-C4	-6.06	103.97	106.40
1	X	2035	G	C2-N3-C4	6.06	114.93	111.90
1	X	2764	U	C5-C6-N1	-6.06	119.67	122.70
1	X	70	A	N7-C8-N9	6.05	116.83	113.80
1	X	2490	U	N1-C2-N3	6.05	118.53	114.90
1	X	504	G	C2-N3-C4	-6.05	108.87	111.90
1	X	583	C	C6-N1-C2	-6.05	117.88	120.30
1	X	1285	A	C5-C6-N1	-6.05	114.67	117.70
1	X	2550	C	C5-C4-N4	6.05	124.43	120.20
1	X	1318	A	C8-N9-C4	6.04	108.22	105.80
1	X	1629	G	N3-C2-N2	6.04	124.13	119.90
1	X	2371	A	N7-C8-N9	6.04	116.82	113.80
1	X	231	G	C8-N9-C4	-6.04	103.98	106.40
1	X	579	G	C6-C5-N7	6.04	134.02	130.40
1	X	2751	C	C5-C6-N1	-6.04	117.98	121.00
1	X	1721	G	N3-C2-N2	6.03	124.12	119.90
1	X	1939	U	C5-C6-N1	6.03	125.72	122.70
1	X	2034	A	N7-C8-N9	6.03	116.81	113.80
1	X	2437	G	C8-N9-C4	6.03	108.81	106.40
1	X	2605	C	C5-C6-N1	-6.03	117.99	121.00
1	X	2026	C	N1-C2-O2	-6.02	115.29	118.90
1	X	1235	C	C2-N3-C4	-6.02	116.89	119.90
1	X	2039	G	C5-C6-N1	-6.02	108.49	111.50
1	X	2637	C	C6-N1-C2	6.02	122.71	120.30
1	X	581	A	N7-C8-N9	-6.02	110.79	113.80
1	X	761	G	N3-C2-N2	6.01	124.11	119.90
1	X	1963	G	C8-N9-C4	-6.00	104.00	106.40
1	X	1998	A	C6-N1-C2	-6.00	115.00	118.60
1	X	1035	G	N3-C4-C5	-6.00	125.60	128.60
1	X	769	C	C5-C4-N4	-6.00	116.00	120.20
1	X	1472	C	N3-C4-C5	6.00	124.30	121.90
1	X	1636	G	N9-C4-C5	-6.00	103.00	105.40
1	X	581	A	C2-N3-C4	-6.00	107.60	110.60
1	X	1357	U	C6-N1-C2	-6.00	117.40	121.00
1	X	1173	G	N1-C6-O6	-6.00	116.30	119.90
1	X	2230	G	N1-C6-O6	6.00	123.50	119.90
1	X	1255	A	C4-C5-N7	-5.99	107.70	110.70
1	X	1210	C	N3-C2-O2	5.99	126.09	121.90
1	X	527	C	C5-C6-N1	5.99	123.99	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	937	C	N3-C2-O2	5.99	126.09	121.90
1	X	2433	G	C8-N9-C4	5.99	108.80	106.40
1	X	2229	G	C4-C5-N7	-5.99	108.41	110.80
1	X	2682	C	C6-N1-C2	-5.98	117.91	120.30
1	X	841	G	N3-C4-C5	5.98	131.59	128.60
1	X	1699	A	C6-C5-N7	-5.98	128.11	132.30
1	X	15	G	N3-C2-N2	-5.98	115.72	119.90
1	X	2008	C	C2-N3-C4	5.98	122.89	119.90
1	X	1239	A	N9-C4-C5	-5.98	103.41	105.80
1	X	2039	G	C5-N7-C8	-5.98	101.31	104.30
1	X	808	C	C6-N1-C2	5.98	122.69	120.30
1	X	2701	A	N1-C2-N3	5.97	132.29	129.30
1	X	2745	A	C5-C6-N1	5.97	120.69	117.70
1	X	2049	C	N3-C2-O2	-5.97	117.72	121.90
1	X	2811	G	N7-C8-N9	-5.97	110.11	113.10
1	X	2828	C	C4-C5-C6	-5.97	114.42	117.40
1	X	2383	C	C6-N1-C2	-5.97	117.91	120.30
1	X	2331	A	N9-C4-C5	5.96	108.19	105.80
1	X	582	G	N1-C6-O6	5.96	123.48	119.90
1	X	771	C	N3-C2-O2	-5.96	117.73	121.90
1	X	1166	A	N3-C4-C5	-5.96	122.63	126.80
1	X	2862	G	N7-C8-N9	5.96	116.08	113.10
1	X	1477	C	C6-N1-C2	-5.95	117.92	120.30
1	X	1617	G	C8-N9-C4	5.95	108.78	106.40
1	X	571	U	N1-C2-O2	-5.95	118.64	122.80
1	X	753	U	N3-C4-C5	-5.95	111.03	114.60
1	X	1222	G	C8-N9-C4	5.95	108.78	106.40
1	X	2000	U	N3-C4-O4	5.95	123.56	119.40
1	X	1955	G	C8-N9-C4	5.95	108.78	106.40
1	X	2055	G	N3-C4-C5	-5.95	125.63	128.60
1	X	2258	G	C8-N9-C4	5.95	108.78	106.40
1	X	549	G	N9-C4-C5	5.94	107.78	105.40
1	X	2211	U	C5-C6-N1	-5.94	119.73	122.70
1	X	2335	U	N3-C2-O2	-5.94	118.04	122.20
1	X	963	G	C8-N9-C4	5.93	108.77	106.40
1	X	2037	A	N1-C6-N6	-5.93	115.04	118.60
1	X	717	G	N7-C8-N9	-5.93	110.13	113.10
1	X	1262	U	C5-C4-O4	-5.93	122.34	125.90
1	X	2024	U	C2-N3-C4	-5.93	123.44	127.00
1	X	1260	A	N3-C4-N9	-5.93	122.66	127.40
1	X	1404	C	C2-N3-C4	-5.93	116.94	119.90
1	X	1698	C	C5-C6-N1	-5.93	118.04	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1939	U	N1-C2-O2	-5.93	118.65	122.80
1	X	816	U	N1-C2-N3	5.92	118.45	114.90
1	X	67	G	N3-C2-N2	5.92	124.04	119.90
1	X	474	G	N7-C8-N9	-5.92	110.14	113.10
1	X	1570	C	C6-N1-C2	5.91	122.67	120.30
1	X	972	C	N3-C2-O2	-5.91	117.76	121.90
1	X	1678	G	C2-N3-C4	5.91	114.86	111.90
1	X	2035	G	C5-N7-C8	5.91	107.25	104.30
1	X	697	G	N3-C4-N9	-5.91	122.46	126.00
1	X	1763	G	C8-N9-C4	5.91	108.76	106.40
1	X	2824	C	C2-N3-C4	-5.91	116.95	119.90
1	X	2459	C	N3-C2-O2	5.91	126.03	121.90
1	X	1241	G	C8-N9-C4	5.90	108.76	106.40
1	X	387	A	N1-C6-N6	5.90	122.14	118.60
1	X	2703	C	C6-N1-C1'	5.90	127.88	120.80
1	X	327	C	C6-N1-C2	-5.90	117.94	120.30
1	X	1647	U	C4-C5-C6	5.90	123.24	119.70
1	X	521	U	C5-C6-N1	-5.89	119.75	122.70
1	X	985	G	C5-C6-O6	-5.89	125.06	128.60
1	X	1614	C	N1-C2-O2	-5.89	115.36	118.90
1	X	1635	G	N3-C4-N9	-5.89	122.46	126.00
1	X	2597	G	N3-C4-C5	-5.89	125.65	128.60
1	X	1983	G	N7-C8-N9	-5.89	110.16	113.10
1	X	2253	A	C8-N9-C4	5.89	108.16	105.80
1	X	1317	G	N3-C4-C5	5.88	131.54	128.60
1	X	2576	G	C5-C6-O6	-5.88	125.07	128.60
1	X	608	G	N1-C6-O6	-5.88	116.37	119.90
1	X	1041	G	C5-C6-O6	5.88	132.13	128.60
1	X	1717	A	C4-C5-N7	-5.88	107.76	110.70
1	X	2531	U	C2-N3-C4	-5.88	123.47	127.00
1	X	2054	A	N1-C6-N6	-5.88	115.07	118.60
1	X	859	U	N1-C2-O2	-5.88	118.69	122.80
1	X	2848	A	N1-C6-N6	-5.88	115.07	118.60
1	X	2751	C	N3-C4-N4	-5.88	113.89	118.00
1	X	10	A	C8-N9-C4	5.87	108.15	105.80
1	X	1260	A	N1-C6-N6	-5.87	115.08	118.60
1	X	1343	C	N1-C2-O2	-5.87	115.38	118.90
2	Y	42	U	C6-N1-C2	5.87	124.53	121.00
1	X	1939	U	N3-C4-O4	5.87	123.51	119.40
1	X	2524	G	N7-C8-N9	5.87	116.03	113.10
1	X	12	U	N3-C4-C5	-5.86	111.08	114.60
1	X	807	A	C8-N9-C4	5.86	108.14	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2825	A	N7-C8-N9	5.86	116.73	113.80
1	X	1229	C	N1-C2-N3	5.86	123.30	119.20
1	X	2022	C	N3-C4-C5	-5.86	119.56	121.90
1	X	14	A	C2-N3-C4	-5.86	107.67	110.60
1	X	1304	U	C5-C6-N1	-5.86	119.77	122.70
1	X	2753	C	C5-C6-N1	5.86	123.93	121.00
1	X	833	A	C5-C6-N6	-5.85	119.02	123.70
1	X	2218	G	C8-N9-C4	-5.85	104.06	106.40
1	X	2540	A	C5-C6-N1	5.85	120.63	117.70
1	X	806	A	C5-N7-C8	5.85	106.83	103.90
1	X	57	G	N9-C4-C5	5.85	107.74	105.40
1	X	1699	A	N9-C4-C5	-5.84	103.46	105.80
1	X	1616	C	C5-C6-N1	-5.84	118.08	121.00
1	X	2540	A	C2-N3-C4	5.84	113.52	110.60
1	X	2812	A	N1-C2-N3	5.84	132.22	129.30
1	X	2847	G	N1-C6-O6	5.84	123.41	119.90
1	X	1777	A	C5-N7-C8	-5.84	100.98	103.90
1	X	2268	G	C4-C5-N7	-5.84	108.46	110.80
1	X	2559	U	N3-C4-C5	5.84	118.10	114.60
1	X	1313	U	C5-C6-N1	-5.84	119.78	122.70
1	X	1398	G	N9-C4-C5	-5.83	103.07	105.40
1	X	1960	A	C8-N9-C4	5.83	108.13	105.80
1	X	2794	G	N1-C6-O6	5.83	123.40	119.90
1	X	746	G	C4-N9-C1'	5.83	134.09	126.50
1	X	1010	U	C5-C6-N1	-5.83	119.78	122.70
1	X	786	U	C5-C6-N1	-5.83	119.78	122.70
1	X	1006	C	N3-C2-O2	-5.83	117.82	121.90
1	X	2704	U	C5-C4-O4	5.83	129.40	125.90
1	X	157	G	N3-C4-N9	-5.83	122.50	126.00
1	X	2807	U	N3-C4-C5	5.83	118.10	114.60
1	X	2331	A	N1-C6-N6	-5.82	115.11	118.60
1	X	2440	C	C2-N1-C1'	-5.82	112.39	118.80
1	X	619	A	C8-N9-C4	-5.82	103.47	105.80
1	X	1781	C	N3-C4-C5	5.82	124.23	121.90
1	X	2453	C	C6-N1-C2	-5.82	117.97	120.30
2	Y	93	G	N1-C6-O6	5.82	123.39	119.90
1	X	2640	G	C4-C5-N7	5.82	113.13	110.80
1	X	496	C	C5-C6-N1	-5.82	118.09	121.00
1	X	1874	G	C8-N9-C4	-5.82	104.07	106.40
1	X	2745	A	C4-C5-C6	-5.82	114.09	117.00
1	X	1654	A	N1-C6-N6	-5.82	115.11	118.60
1	X	2800	C	N1-C2-O2	5.82	122.39	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	525	A	C2-N3-C4	5.81	113.51	110.60
1	X	1706	A	C6-N1-C2	5.81	122.09	118.60
1	X	2543	A	C8-N9-C4	-5.81	103.47	105.80
1	X	1777	A	C8-N9-C4	-5.81	103.48	105.80
1	X	2486	C	O4'-C1'-C2'	-5.81	99.99	105.80
1	X	981	C	N1-C1'-C2'	5.80	121.55	114.00
1	X	2524	G	C4-C5-N7	5.80	113.12	110.80
1	X	2627	G	N3-C4-N9	-5.80	122.52	126.00
1	X	2210	C	N1-C2-O2	-5.80	115.42	118.90
1	X	330	C	C6-N1-C2	-5.80	117.98	120.30
1	X	569	C	C6-N1-C2	5.80	122.62	120.30
1	X	2853	U	N3-C4-C5	5.80	118.08	114.60
1	X	1272	G	N7-C8-N9	-5.80	110.20	113.10
1	X	1290	A	C2-N3-C4	-5.79	107.70	110.60
1	X	2782	G	N7-C8-N9	-5.79	110.20	113.10
1	X	755	C	N1-C2-N3	5.79	123.25	119.20
1	X	1711	C	C6-N1-C2	5.79	122.62	120.30
1	X	2798	A	N1-C6-N6	5.79	122.07	118.60
1	X	837	U	C2-N3-C4	-5.79	123.53	127.00
1	X	841	G	N3-C4-N9	-5.79	122.53	126.00
1	X	1678	G	C6-C5-N7	5.79	133.87	130.40
1	X	219	G	C5-C6-N1	5.79	114.39	111.50
1	X	744	C	C4-C5-C6	5.78	120.29	117.40
1	X	2861	A	N1-C6-N6	5.78	122.07	118.60
1	X	30	G	C8-N9-C4	-5.78	104.09	106.40
1	X	461	A	N1-C6-N6	5.78	122.07	118.60
1	X	1647	U	C5-C4-O4	5.78	129.37	125.90
1	X	1636	G	C4-C5-N7	5.77	113.11	110.80
1	X	1670	G	C4-C5-N7	-5.77	108.49	110.80
1	X	2471	U	C5-C6-N1	-5.77	119.81	122.70
1	X	875	G	N1-C6-O6	5.77	123.36	119.90
1	X	744	C	N1-C2-N3	5.77	123.24	119.20
1	X	2007	G	N1-C6-O6	-5.77	116.44	119.90
1	X	1459	U	N1-C2-O2	-5.77	118.76	122.80
1	X	323	G	C4-C5-N7	-5.76	108.49	110.80
1	X	1262	U	N3-C4-O4	5.76	123.43	119.40
1	X	2555	G	N9-C4-C5	-5.76	103.10	105.40
1	X	2828	C	C5-C6-N1	5.76	123.88	121.00
1	X	2510	A	N1-C6-N6	5.76	122.06	118.60
1	X	2701	A	C2-N3-C4	-5.76	107.72	110.60
1	X	504	G	C5-C6-O6	-5.76	125.15	128.60
1	X	484	G	N1-C6-O6	5.75	123.35	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	12	U	N3-C4-O4	5.75	123.42	119.40
1	X	864	C	C5-C6-N1	5.75	123.88	121.00
1	X	2003	A	N1-C2-N3	5.75	132.18	129.30
1	X	777	A	O4'-C1'-N9	5.75	112.80	108.20
1	X	1283	C	C5-C6-N1	-5.75	118.13	121.00
1	X	2352	A	N1-C6-N6	-5.75	115.15	118.60
1	X	2687	G	C5-C6-O6	5.75	132.05	128.60
1	X	464	G	C5-C6-O6	5.75	132.05	128.60
1	X	761	G	N7-C8-N9	-5.74	110.23	113.10
1	X	2055	G	N1-C6-O6	-5.74	116.45	119.90
1	X	967	G	C2-N3-C4	5.74	114.77	111.90
1	X	35	G	C5-C6-O6	5.74	132.04	128.60
1	X	1747	G	N7-C8-N9	-5.74	110.23	113.10
1	X	109	A	C8-N9-C4	5.73	108.09	105.80
1	X	818	G	N1-C6-O6	5.73	123.34	119.90
1	X	886	A	N7-C8-N9	5.73	116.67	113.80
1	X	1985	G	C4'-C3'-C2'	-5.73	96.87	102.60
1	X	2228	U	N3-C4-O4	5.73	123.41	119.40
1	X	2267	A	C5-C6-N1	5.73	120.56	117.70
1	X	2701	A	C5-C6-N6	5.73	128.28	123.70
1	X	530	G	N3-C4-C5	5.73	131.46	128.60
1	X	1173	G	N9-C4-C5	5.73	107.69	105.40
1	X	1756	C	N1-C2-O2	-5.72	115.47	118.90
1	X	1479	G	N1-C6-O6	5.72	123.33	119.90
1	X	187	U	N3-C2-O2	5.72	126.20	122.20
1	X	1345	G	N1-C6-O6	-5.72	116.47	119.90
1	X	1751	A	N7-C8-N9	-5.72	110.94	113.80
1	X	2226	A	N1-C2-N3	5.71	132.16	129.30
1	X	2363	G	C5-C6-N1	-5.71	108.64	111.50
1	X	332	C	C6-N1-C2	5.71	122.58	120.30
1	X	2827	G	N1-C2-N2	-5.71	111.06	116.20
1	X	2363	G	N1-C6-O6	5.71	123.33	119.90
1	X	2495	G	C6-N1-C2	-5.71	121.67	125.10
1	X	2818	G	C6-C5-N7	-5.71	126.98	130.40
1	X	322	A	N7-C8-N9	-5.70	110.95	113.80
1	X	1294	G	N7-C8-N9	5.70	115.95	113.10
1	X	1616	C	C6-N1-C2	5.70	122.58	120.30
1	X	2484	G	C8-N9-C4	-5.70	104.12	106.40
1	X	58	C	N1-C2-O2	-5.70	115.48	118.90
1	X	1687	C	C2-N3-C4	-5.70	117.05	119.90
1	X	2515	G	C8-N9-C4	-5.70	104.12	106.40
1	X	2673	G	C4-C5-N7	5.70	113.08	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	507	A	N1-C6-N6	-5.70	115.18	118.60
1	X	545	C	N3-C4-C5	5.70	124.18	121.90
1	X	549	G	C5-C6-O6	5.70	132.02	128.60
1	X	570	G	N1-C2-N2	5.70	121.33	116.20
1	X	780	U	P-O3'-C3'	5.70	126.54	119.70
1	X	1256	C	C5-C6-N1	-5.70	118.15	121.00
1	X	1636	G	N3-C4-C5	5.70	131.45	128.60
1	X	2039	G	N1-C2-N3	5.69	127.32	123.90
1	X	537	C	N3-C2-O2	-5.69	117.92	121.90
1	X	179	U	C5-C6-N1	-5.69	119.86	122.70
1	X	1853	C	N1-C2-O2	-5.69	115.49	118.90
1	X	1675	C	N3-C2-O2	5.69	125.88	121.90
1	X	2055	G	C4-C5-N7	-5.69	108.53	110.80
1	X	2381	A	C3'-C2'-C1'	5.68	106.04	101.50
1	X	2448	A	C8-N9-C4	-5.68	103.53	105.80
1	X	27	G	N3-C2-N2	5.68	123.87	119.90
1	X	715	U	N1-C2-O2	-5.68	118.83	122.80
1	X	1666	G	N7-C8-N9	-5.67	110.26	113.10
1	X	2315	A	C8-N9-C4	5.67	108.07	105.80
1	X	1641	C	C6-N1-C2	5.67	122.57	120.30
1	X	1932	G	N1-C6-O6	-5.67	116.50	119.90
1	X	499	G	N3-C2-N2	5.67	123.87	119.90
1	X	686	C	C6-N1-C2	5.67	122.57	120.30
1	X	1968	G	N7-C8-N9	-5.67	110.27	113.10
1	X	1572	C	N3-C4-C5	-5.67	119.63	121.90
1	X	2753	C	N3-C4-N4	5.67	121.97	118.00
1	X	1316	G	N1-C2-N3	5.67	127.30	123.90
1	X	1773	C	N3-C2-O2	-5.66	117.94	121.90
1	X	1514	C	C6-N1-C2	-5.66	118.03	120.30
1	X	2856	U	C6-N1-C2	-5.66	117.60	121.00
1	X	1018	C	C2-N3-C4	-5.66	117.07	119.90
1	X	1678	G	C5-N7-C8	5.66	107.13	104.30
1	X	1707	A	C8-N9-C4	5.66	108.06	105.80
1	X	2072	C	N1-C2-O2	-5.66	115.50	118.90
1	X	536	A	N3-C4-C5	-5.65	122.84	126.80
1	X	2550	C	N3-C4-C5	-5.65	119.64	121.90
1	X	1166	A	N7-C8-N9	5.65	116.63	113.80
1	X	2440	C	N3-C4-N4	-5.65	114.04	118.00
1	X	566	U	N3-C4-O4	5.65	123.35	119.40
1	X	1616	C	C2-N3-C4	-5.65	117.08	119.90
1	X	211	U	N3-C2-O2	-5.65	118.25	122.20
1	X	634	G	N3-C2-N2	-5.65	115.95	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2515	G	N3-C2-N2	5.65	123.85	119.90
1	X	2656	G	C8-N9-C4	5.65	108.66	106.40
1	X	2729	A	N1-C6-N6	-5.65	115.21	118.60
1	X	1958	G	C8-N9-C4	5.64	108.66	106.40
1	X	1494	G	N3-C4-N9	-5.64	122.62	126.00
1	X	1943	A	C8-N9-C4	5.64	108.06	105.80
1	X	746	G	C4-C5-C6	5.64	122.18	118.80
1	X	2352	A	C6-N1-C2	-5.64	115.22	118.60
1	X	1927	U	C2-N3-C4	-5.63	123.62	127.00
1	X	1938	U	C6-N1-C2	5.63	124.38	121.00
1	X	2771	C	C6-N1-C2	-5.63	118.05	120.30
1	X	689	A	C5-C6-N6	-5.63	119.20	123.70
1	X	2328	G	C8-N9-C4	-5.63	104.15	106.40
1	X	1306	U	C2-N3-C4	-5.63	123.62	127.00
1	X	1330	G	C8-N9-C4	5.63	108.65	106.40
1	X	456	C	N3-C4-C5	-5.62	119.65	121.90
1	X	746	G	C5-C6-N1	-5.62	108.69	111.50
1	X	1966	C	N3-C2-O2	5.62	125.83	121.90
1	X	981	C	C6-N1-C2	-5.62	118.05	120.30
1	X	1287	A	N3-C4-C5	-5.62	122.87	126.80
1	X	496	C	N3-C4-C5	5.62	124.15	121.90
1	X	688	A	C5-C6-N6	-5.62	119.20	123.70
1	X	572	G	N7-C8-N9	5.62	115.91	113.10
1	X	1789	U	C6-N1-C2	-5.62	117.63	121.00
1	X	1411	C	C5-C6-N1	-5.62	118.19	121.00
1	X	1272	G	C4-C5-N7	-5.61	108.56	110.80
1	X	1406	A	N1-C6-N6	-5.61	115.23	118.60
1	X	2464	G	C5-C6-O6	-5.61	125.23	128.60
1	X	504	G	C5-C6-N1	-5.61	108.69	111.50
1	X	701	U	C5-C4-O4	5.61	129.27	125.90
1	X	12	U	N1-C2-O2	-5.61	118.87	122.80
1	X	2441	U	N3-C4-O4	-5.61	115.47	119.40
1	X	2764	U	C2-N3-C4	-5.61	123.63	127.00
1	X	1993	G	N1-C2-N3	5.61	127.26	123.90
1	X	1292	A	N9-C4-C5	-5.61	103.56	105.80
1	X	1300	A	C5-C6-N6	-5.61	119.22	123.70
1	X	2329	C	N3-C4-C5	5.61	124.14	121.90
1	X	2578	G	N1-C6-O6	5.61	123.26	119.90
1	X	1212	U	N1-C2-O2	-5.60	118.88	122.80
1	X	861	G	N9-C4-C5	5.60	107.64	105.40
1	X	21	A	N3-C4-C5	5.60	130.72	126.80
1	X	2845	C	C4'-C3'-C2'	-5.60	97.00	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2617	G	N3-C4-C5	-5.60	125.80	128.60
1	X	1653	C	N3-C4-N4	5.60	121.92	118.00
1	X	1715	A	N1-C6-N6	5.60	121.96	118.60
2	Y	102	A	N1-C6-N6	5.60	121.96	118.60
1	X	2350	G	C8-N9-C4	-5.59	104.17	106.40
1	X	1045	G	C8-N9-C4	5.59	108.64	106.40
1	X	638	A	C2-N3-C4	5.59	113.39	110.60
1	X	724	C	C6-N1-C2	-5.59	118.06	120.30
1	X	883	A	C8-N9-C4	5.58	108.03	105.80
1	X	2233	C	C5-C6-N1	-5.58	118.21	121.00
1	X	2763	U	C5-C4-O4	5.58	129.25	125.90
1	X	2792	C	C5-C6-N1	-5.58	118.21	121.00
1	X	22	C	C4-C5-C6	5.58	120.19	117.40
1	X	1228	G	C8-N9-C4	-5.58	104.17	106.40
1	X	1706	A	N1-C6-N6	5.57	121.94	118.60
1	X	220	U	C5-C4-O4	5.57	129.24	125.90
1	X	32	C	C5-C6-N1	-5.57	118.21	121.00
1	X	186	C	C6-N1-C2	5.57	122.53	120.30
1	X	1702	C	C5-C6-N1	-5.57	118.21	121.00
1	X	1572	C	C6-N1-C2	-5.57	118.07	120.30
1	X	1645	U	N1-C2-O2	-5.57	118.90	122.80
1	X	850	C	C4-C5-C6	5.56	120.18	117.40
1	X	953	G	C8-N9-C4	-5.56	104.17	106.40
1	X	346	C	C4-C5-C6	5.56	120.18	117.40
1	X	821	A	N1-C6-N6	5.56	121.94	118.60
1	X	1273	G	C8-N9-C4	5.56	108.62	106.40
1	X	762	A	C5-C6-N6	-5.56	119.25	123.70
1	X	821	A	N9-C4-C5	-5.56	103.58	105.80
1	X	1771	A	N3-C4-C5	-5.56	122.91	126.80
1	X	1173	G	C5-C6-O6	5.56	131.94	128.60
1	X	1172	U	C5-C4-O4	5.56	129.23	125.90
1	X	2553	G	C4-C5-N7	-5.55	108.58	110.80
1	X	2524	G	C6-N1-C2	-5.55	121.77	125.10
1	X	169	C	C5-C6-N1	-5.55	118.23	121.00
1	X	1577	G	N1-C6-O6	-5.55	116.57	119.90
1	X	1312	G	C5-N7-C8	-5.54	101.53	104.30
1	X	306	G	C8-N9-C4	-5.54	104.18	106.40
1	X	502	A	N1-C2-N3	5.54	132.07	129.30
1	X	1158	A	N9-C4-C5	-5.54	103.58	105.80
1	X	2605	C	C2-N3-C4	-5.54	117.13	119.90
1	X	2745	A	N3-C4-C5	5.54	130.68	126.80
1	X	1458	A	C8-N9-C4	5.54	108.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1286	U	N1-C2-N3	5.54	118.22	114.90
1	X	2431	C	C2-N3-C4	-5.54	117.13	119.90
1	X	2441	U	C5-C6-N1	-5.54	119.93	122.70
1	X	2616	U	N3-C4-C5	-5.54	111.28	114.60
1	X	479	G	C6-C5-N7	-5.53	127.08	130.40
1	X	697	G	C8-N9-C4	-5.53	104.19	106.40
1	X	2640	G	N1-C6-O6	5.53	123.22	119.90
1	X	2694	G	N3-C4-N9	5.53	129.32	126.00
2	Y	81	C	N3-C4-N4	5.53	121.87	118.00
1	X	613	A	C4-C5-C6	-5.53	114.23	117.00
1	X	697	G	N9-C4-C5	5.53	107.61	105.40
1	X	1718	A	N1-C2-N3	5.53	132.07	129.30
1	X	2326	C	C5-C6-N1	5.53	123.77	121.00
1	X	2810	A	C8-N9-C4	5.53	108.01	105.80
1	X	606	A	C5-C6-N1	-5.53	114.94	117.70
1	X	1759	A	N1-C6-N6	5.53	121.92	118.60
1	X	1138	A	C6-N1-C2	-5.53	115.28	118.60
1	X	58	C	C6-N1-C2	-5.53	118.09	120.30
1	X	1624	A	N9-C4-C5	5.53	108.01	105.80
1	X	1653	C	N3-C4-C5	-5.53	119.69	121.90
1	X	174	A	C4'-C3'-C2'	5.52	108.12	102.60
2	Y	81	C	C6-N1-C2	-5.52	118.09	120.30
1	X	1085	G	C8-N9-C4	-5.52	104.19	106.40
1	X	1267	A	N1-C6-N6	-5.52	115.29	118.60
1	X	1578	U	N1-C2-N3	-5.52	111.59	114.90
1	X	339	U	C6-N1-C2	-5.52	117.69	121.00
1	X	835	U	N1-C2-N3	5.52	118.21	114.90
1	X	1617	G	N9-C4-C5	-5.52	103.19	105.40
1	X	2468	G	C6-C5-N7	5.51	133.71	130.40
1	X	1346	C	C5-C4-N4	-5.51	116.34	120.20
1	X	2657	G	N3-C2-N2	-5.51	116.04	119.90
1	X	527	C	C2-N1-C1'	5.51	124.86	118.80
1	X	691	C	N3-C4-N4	-5.51	114.14	118.00
1	X	981	C	C3'-C2'-C1'	5.51	105.91	101.50
4	B	121	ASN	N-CA-C	-5.51	96.12	111.00
1	X	1172	U	C2-N1-C1'	-5.51	111.09	117.70
1	X	583	C	C5-C4-N4	-5.50	116.35	120.20
1	X	508	G	N9-C4-C5	-5.50	103.20	105.40
1	X	1944	C	C5-C6-N1	-5.50	118.25	121.00
1	X	2687	G	N1-C6-O6	-5.50	116.60	119.90
1	X	584	A	N9-C4-C5	5.50	108.00	105.80
1	X	1983	G	N1-C6-O6	-5.49	116.60	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	100	G	N1-C6-O6	5.49	123.19	119.90
1	X	2790	C	N3-C4-N4	-5.49	114.16	118.00
1	X	746	G	N1-C2-N3	5.49	127.19	123.90
1	X	883	A	C2-N3-C4	5.49	113.34	110.60
1	X	1383	C	C6-N1-C2	5.49	122.50	120.30
1	X	2631	C	C6-N1-C2	5.49	122.50	120.30
1	X	2693	U	N3-C4-O4	-5.49	115.56	119.40
1	X	1627	C	C6-N1-C2	-5.49	118.11	120.30
1	X	1666	G	N9-C4-C5	-5.49	103.21	105.40
1	X	755	C	C6-N1-C2	-5.48	118.11	120.30
1	X	2618	A	C8-N9-C4	-5.48	103.61	105.80
1	X	2060	A	C2-N3-C4	5.48	113.34	110.60
1	X	2679	G	N9-C4-C5	-5.48	103.21	105.40
1	X	1663	C	C5-C4-N4	-5.47	116.37	120.20
2	Y	42	U	N3-C2-O2	5.47	126.03	122.20
1	X	177	U	C6-N1-C2	-5.47	117.72	121.00
1	X	692	C	C5-C6-N1	-5.47	118.27	121.00
1	X	2617	G	C5-C6-N1	5.47	114.23	111.50
1	X	806	A	C6-C5-N7	5.46	136.13	132.30
1	X	2024	U	N3-C4-C5	5.46	117.88	114.60
1	X	991	A	C5-C6-N6	-5.46	119.33	123.70
1	X	1256	C	N1-C2-N3	5.46	123.02	119.20
1	X	1962	C	N1-C2-O2	-5.46	115.62	118.90
1	X	2020	G	N3-C2-N2	5.46	123.72	119.90
2	Y	93	G	C8-N9-C4	-5.46	104.22	106.40
1	X	1169	C	C6-N1-C2	5.46	122.48	120.30
1	X	1966	C	C2-N1-C1'	-5.45	112.80	118.80
1	X	2025	A	C4-C5-N7	5.45	113.43	110.70
1	X	2504	G	N1-C6-O6	-5.45	116.63	119.90
1	X	1635	G	C8-N9-C4	-5.45	104.22	106.40
1	X	659	G	C8-N9-C4	5.45	108.58	106.40
1	X	1768	U	N1-C2-N3	5.45	118.17	114.90
1	X	2362	G	N3-C4-C5	5.45	131.32	128.60
1	X	21	A	C4-C5-N7	5.45	113.42	110.70
1	X	1396	C	C2-N1-C1'	-5.45	112.81	118.80
1	X	2559	U	C4-C5-C6	-5.45	116.43	119.70
1	X	2807	U	N3-C2-O2	-5.45	118.39	122.20
1	X	1578	U	N3-C2-O2	5.45	126.01	122.20
1	X	2548	G	C4-C5-N7	-5.44	108.62	110.80
1	X	2751	C	C2-N1-C1'	-5.44	112.81	118.80
1	X	2824	C	N3-C4-N4	-5.44	114.19	118.00
2	Y	47	A	C8-N9-C4	-5.44	103.62	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1334	A	N1-C6-N6	5.44	121.86	118.60
1	X	1563	U	N3-C4-C5	5.44	117.86	114.60
1	X	2495	G	C5-C6-O6	-5.44	125.34	128.60
2	Y	32	C	C6-N1-C2	5.44	122.48	120.30
1	X	1033	G	N3-C4-C5	-5.44	125.88	128.60
1	X	1311	C	N3-C2-O2	-5.44	118.09	121.90
1	X	1940	C	C6-N1-C2	5.44	122.47	120.30
1	X	22	C	N1-C2-N3	5.43	123.00	119.20
1	X	502	A	N1-C6-N6	-5.43	115.34	118.60
1	X	1283	C	C2-N1-C1'	-5.43	112.82	118.80
1	X	1314	A	C8-N9-C4	-5.43	103.63	105.80
1	X	2848	A	C4-C5-C6	5.43	119.72	117.00
1	X	570	G	N3-C4-C5	5.43	131.31	128.60
1	X	2809	A	C5-C6-N1	5.43	120.41	117.70
1	X	999	A	N1-C6-N6	-5.43	115.34	118.60
1	X	2832	G	C5-C6-O6	-5.43	125.34	128.60
1	X	1613	G	C8-N9-C4	5.42	108.57	106.40
1	X	2805	G	C5-N7-C8	5.42	107.01	104.30
1	X	502	A	C4-C5-N7	-5.42	107.99	110.70
1	X	2054	A	N9-C4-C5	5.42	107.97	105.80
1	X	2550	C	N1-C2-N3	5.42	123.00	119.20
1	X	225	G	N3-C4-C5	5.42	131.31	128.60
1	X	2799	C	N1-C2-N3	5.42	122.99	119.20
1	X	342	G	N1-C6-O6	5.42	123.15	119.90
1	X	2498	U	N1-C2-N3	5.42	118.15	114.90
1	X	223	C	N1-C2-O2	-5.42	115.65	118.90
1	X	1242	A	N7-C8-N9	-5.42	111.09	113.80
1	X	1764	A	C4'-C3'-C2'	-5.42	97.19	102.60
1	X	357	A	C5-C6-N1	-5.41	114.99	117.70
1	X	2003	A	N9-C4-C5	5.41	107.97	105.80
1	X	2013	A	C8-N9-C4	5.41	107.97	105.80
1	X	2696	A	C5-N7-C8	5.41	106.61	103.90
1	X	1225	G	N9-C4-C5	-5.41	103.23	105.40
1	X	1299	A	N3-C4-C5	5.41	130.59	126.80
1	X	2363	G	C8-N9-C4	5.41	108.56	106.40
1	X	2651	U	N1-C2-O2	-5.41	119.01	122.80
1	X	2656	G	N7-C8-N9	-5.41	110.39	113.10
1	X	231	G	N9-C4-C5	5.41	107.56	105.40
1	X	1939	U	N3-C2-O2	5.41	125.98	122.20
1	X	1998	A	N9-C4-C5	5.41	107.96	105.80
1	X	528	G	C4-C5-N7	5.40	112.96	110.80
1	X	508	G	C4-C5-N7	5.40	112.96	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	923	A	C2-N3-C4	5.40	113.30	110.60
1	X	1467	U	C4'-C3'-C2'	-5.40	97.20	102.60
1	X	597	U	N3-C2-O2	5.40	125.98	122.20
1	X	872	G	N3-C4-N9	5.40	129.24	126.00
1	X	1656	U	C2-N3-C4	-5.40	123.76	127.00
1	X	2444	C	C6-N1-C2	-5.40	118.14	120.30
1	X	2876	C	C6-N1-C2	5.40	122.46	120.30
1	X	1260	A	C5-C6-N6	5.40	128.02	123.70
1	X	1007	A	N9-C4-C5	5.40	107.96	105.80
1	X	2755	A	C8-N9-C4	5.40	107.96	105.80
1	X	522	G	N3-C4-N9	-5.39	122.76	126.00
1	X	530	G	C5-C6-N1	-5.39	108.80	111.50
1	X	593	C	C6-N1-C2	-5.39	118.14	120.30
1	X	1203	A	C5-C6-N1	-5.39	115.00	117.70
1	X	973	U	N1-C2-N3	5.39	118.14	114.90
1	X	1621	C	C3'-C2'-O2'	-5.39	97.66	113.30
1	X	2230	G	C5-N7-C8	-5.39	101.60	104.30
1	X	2682	C	N3-C4-C5	-5.39	119.74	121.90
1	X	2253	A	C2-N3-C4	-5.39	107.91	110.60
1	X	2464	G	C4-C5-N7	5.39	112.96	110.80
1	X	797	A	N9-C4-C5	-5.38	103.65	105.80
1	X	1325	U	N3-C4-C5	-5.38	111.37	114.60
1	X	1705	U	N1-C2-O2	-5.38	119.03	122.80
1	X	2412	A	N1-C6-N6	-5.38	115.37	118.60
1	X	1992	G	N7-C8-N9	-5.38	110.41	113.10
1	X	592	G	N1-C6-O6	5.38	123.13	119.90
1	X	1966	C	C5-C6-N1	-5.38	118.31	121.00
1	X	2247	A	N9-C4-C5	-5.38	103.65	105.80
1	X	493	A	C8-N9-C4	5.37	107.95	105.80
1	X	1028	G	N9-C4-C5	-5.37	103.25	105.40
1	X	695	G	C8-N9-C4	5.37	108.55	106.40
1	X	1641	C	N3-C4-C5	5.37	124.05	121.90
1	X	2222	U	C2-N3-C4	-5.37	123.78	127.00
1	X	1778	U	C5-C6-N1	-5.36	120.02	122.70
1	X	2705	A	P-O3'-C3'	5.36	126.14	119.70
1	X	818	G	C5-C6-O6	-5.36	125.38	128.60
1	X	806	A	N7-C8-N9	-5.36	111.12	113.80
1	X	2527	G	N1-C6-O6	-5.36	116.69	119.90
1	X	2678	C	C4-C5-C6	5.36	120.08	117.40
1	X	1452	U	N3-C4-O4	5.36	123.15	119.40
1	X	1998	A	N7-C8-N9	-5.36	111.12	113.80
1	X	2038	C	C2-N1-C1'	-5.36	112.91	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1236	G	C8-N9-C4	5.35	108.54	106.40
1	X	580	A	N1-C2-N3	5.35	131.98	129.30
1	X	2042	A	C8-N9-C4	5.35	107.94	105.80
1	X	2425	G	N1-C2-N2	5.35	121.02	116.20
1	X	1664	G	N9-C4-C5	-5.35	103.26	105.40
1	X	1718	A	C2-N3-C4	-5.35	107.92	110.60
1	X	2611	A	C8-N9-C4	5.35	107.94	105.80
1	X	686	C	C4-C5-C6	-5.34	114.73	117.40
1	X	1236	G	C5-C6-N1	5.34	114.17	111.50
2	Y	63	A	N9-C4-C5	5.34	107.94	105.80
1	X	745	C	C4-C5-C6	5.34	120.07	117.40
1	X	850	C	C6-N1-C1'	5.34	127.21	120.80
1	X	1673	C	N3-C4-N4	5.34	121.74	118.00
1	X	2855	C	C6-N1-C2	5.34	122.44	120.30
1	X	401	G	N3-C4-N9	-5.34	122.80	126.00
1	X	2835	A	C2-N3-C4	-5.34	107.93	110.60
1	X	510	G	N1-C6-O6	-5.34	116.70	119.90
1	X	1366	A	C8-N9-C4	5.34	107.94	105.80
1	X	156	G	N3-C4-C5	5.33	131.27	128.60
1	X	1991	C	C2-N3-C4	-5.33	117.23	119.90
1	X	660	G	C8-N9-C4	-5.33	104.27	106.40
1	X	1181	C	C6-N1-C2	5.33	122.43	120.30
1	X	1332	G	N1-C6-O6	5.33	123.10	119.90
1	X	484	G	C8-N9-C4	-5.33	104.27	106.40
1	X	2486	C	P-O5'-C5'	5.33	129.43	120.90
1	X	121	G	C8-N9-C4	5.33	108.53	106.40
1	X	1937	G	N9-C4-C5	-5.33	103.27	105.40
1	X	1958	G	N9-C4-C5	-5.33	103.27	105.40
1	X	2019	C	N3-C2-O2	5.32	125.63	121.90
1	X	2623	A	C5-N7-C8	5.32	106.56	103.90
1	X	2864	C	C5-C6-N1	-5.32	118.34	121.00
1	X	12	U	N3-C2-O2	5.32	125.92	122.20
1	X	566	U	C5-C6-N1	5.32	125.36	122.70
1	X	583	C	N3-C2-O2	5.32	125.62	121.90
1	X	739	G	N3-C4-C5	-5.32	125.94	128.60
1	X	1459	U	N3-C2-O2	5.32	125.92	122.20
1	X	787	A	N9-C4-C5	-5.32	103.67	105.80
1	X	1752	U	N3-C2-O2	-5.32	118.48	122.20
1	X	1445	A	N9-C4-C5	-5.31	103.67	105.80
1	X	2362	G	C4-C5-N7	5.31	112.93	110.80
1	X	158	A	N1-C6-N6	-5.31	115.41	118.60
1	X	1768	U	C6-N1-C2	-5.31	117.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	805	G	C6-C5-N7	5.31	133.59	130.40
1	X	175	C	N3-C2-O2	5.31	125.62	121.90
1	X	2021	G	C5-C6-N1	-5.31	108.84	111.50
1	X	1158	A	N7-C8-N9	-5.31	111.15	113.80
1	X	2856	U	C4-C5-C6	5.31	122.88	119.70
1	X	329	C	C6-N1-C2	-5.30	118.18	120.30
1	X	2258	G	N1-C2-N2	-5.30	111.43	116.20
1	X	2823	G	N1-C2-N3	5.30	127.08	123.90
1	X	318	G	N7-C8-N9	-5.30	110.45	113.10
1	X	2678	C	C5-C6-N1	-5.30	118.35	121.00
1	X	2815	C	N3-C4-N4	-5.30	114.29	118.00
1	X	1041	G	N9-C4-C5	5.30	107.52	105.40
1	X	744	C	N1-C2-O2	-5.30	115.72	118.90
1	X	1543	G	C8-N9-C4	-5.30	104.28	106.40
1	X	549	G	N3-C4-C5	-5.29	125.95	128.60
1	X	1948	C	C6-N1-C2	5.29	122.42	120.30
1	X	2513	A	C2-N3-C4	-5.29	107.95	110.60
1	X	2621	G	N3-C2-N2	-5.29	116.20	119.90
1	X	1672	A	N1-C6-N6	5.29	121.77	118.60
1	X	1396	C	C6-N1-C2	5.29	122.42	120.30
1	X	2244	C	N3-C2-O2	-5.29	118.20	121.90
1	X	2303	C	C5-C6-N1	-5.28	118.36	121.00
1	X	2790	C	C2-N3-C4	-5.28	117.26	119.90
1	X	219	G	N3-C4-N9	5.28	129.17	126.00
1	X	739	G	C2-N3-C4	5.28	114.54	111.90
1	X	1667	A	C6-C5-N7	-5.28	128.60	132.30
1	X	2508	G	N9-C4-C5	-5.28	103.29	105.40
1	X	1038	U	N1-C2-N3	5.28	118.07	114.90
1	X	1752	U	N1-C2-N3	5.28	118.07	114.90
1	X	1766	U	N1-C2-O2	-5.28	119.11	122.80
1	X	2243	C	C4-C5-C6	5.28	120.04	117.40
1	X	1135	C	C2-N1-C1'	-5.27	113.00	118.80
1	X	872	G	N3-C4-C5	-5.27	125.96	128.60
1	X	923	A	N1-C2-N3	-5.27	126.66	129.30
1	X	937	C	N1-C2-O2	-5.27	115.74	118.90
1	X	1203	A	C6-N1-C2	5.27	121.76	118.60
1	X	2025	A	N1-C6-N6	5.27	121.76	118.60
1	X	2241	U	C5-C6-N1	-5.27	120.06	122.70
1	X	915	C	C6-N1-C2	5.27	122.41	120.30
1	X	1571	G	C8-N9-C4	-5.27	104.29	106.40
1	X	1983	G	C5-N7-C8	5.27	106.94	104.30
1	X	569	C	C5-C4-N4	-5.27	116.51	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1306	U	C5-C6-N1	-5.27	120.07	122.70
1	X	2849	C	N1-C2-O2	-5.27	115.74	118.90
1	X	971	A	N1-C6-N6	-5.27	115.44	118.60
1	X	2585	C	N1-C2-O2	-5.27	115.74	118.90
1	X	791	G	N1-C6-O6	-5.26	116.74	119.90
1	X	21	A	C5-N7-C8	-5.26	101.27	103.90
1	X	1256	C	C4-C5-C6	5.26	120.03	117.40
1	X	1749	G	C1'-O4'-C4'	-5.26	105.69	109.90
1	X	317	U	N1-C2-O2	-5.26	119.12	122.80
1	X	828	C	C6-N1-C2	5.26	122.40	120.30
1	X	850	C	N1-C2-N3	5.26	122.88	119.20
1	X	2209	G	N9-C4-C5	5.26	107.50	105.40
1	X	746	G	N1-C2-N2	-5.26	111.47	116.20
1	X	237	G	C8-N9-C4	-5.25	104.30	106.40
1	X	529	U	N1-C2-N3	5.25	118.05	114.90
1	X	1671	A	N9-C4-C5	-5.25	103.70	105.80
1	X	2833	C	N1-C2-O2	5.25	122.05	118.90
1	X	10	A	N9-C4-C5	-5.25	103.70	105.80
1	X	504	G	N3-C4-C5	5.25	131.23	128.60
1	X	691	C	N1-C2-O2	-5.25	115.75	118.90
1	X	1282	A	C8-N9-C4	5.25	107.90	105.80
1	X	787	A	N1-C6-N6	5.25	121.75	118.60
1	X	1678	G	N7-C8-N9	-5.25	110.48	113.10
1	X	2848	A	N3-C4-C5	-5.25	123.13	126.80
1	X	340	G	N3-C2-N2	5.24	123.57	119.90
1	X	458	G	N9-C4-C5	5.24	107.50	105.40
1	X	1282	A	C6-C5-N7	-5.24	128.63	132.30
1	X	2290	A	C8-N9-C4	5.24	107.90	105.80
1	X	818	G	N9-C4-C5	-5.24	103.30	105.40
1	X	2809	A	C6-N1-C2	-5.24	115.46	118.60
1	X	2757	G	N1-C2-N3	5.24	127.04	123.90
1	X	586	G	N1-C6-O6	5.24	123.04	119.90
1	X	1104	G	N3-C4-C5	-5.24	125.98	128.60
1	X	1998	A	C5-N7-C8	5.24	106.52	103.90
1	X	1953	A	C8-N9-C4	-5.23	103.71	105.80
1	X	2259	G	N1-C2-N3	5.23	127.04	123.90
1	X	1351	G	C8-N9-C4	5.23	108.49	106.40
1	X	1470	G	O4'-C1'-N9	5.23	112.38	108.20
1	X	2412	A	C5-C6-N1	5.23	120.31	117.70
1	X	2233	C	C6-N1-C2	5.23	122.39	120.30
1	X	2392	G	N3-C4-C5	5.23	131.22	128.60
1	X	457	C	C6-N1-C2	-5.23	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2634	G	N7-C8-N9	-5.23	110.49	113.10
1	X	1622	G	N1-C2-N2	-5.22	111.50	116.20
1	X	2700	U	C4'-C3'-C2'	-5.22	97.38	102.60
1	X	1033	G	C4-C5-N7	-5.22	108.71	110.80
1	X	1212	U	C5-C6-N1	-5.22	120.09	122.70
1	X	2466	G	N1-C6-O6	5.22	123.03	119.90
1	X	1395	A	C8-N9-C4	-5.22	103.71	105.80
1	X	2398	U	C4-C5-C6	5.22	122.83	119.70
1	X	1480	G	C5-C6-O6	-5.22	125.47	128.60
1	X	2051	U	C2-N3-C4	-5.22	123.87	127.00
1	X	2676	G	N3-C4-C5	-5.22	125.99	128.60
1	X	41	G	C8-N9-C4	5.22	108.49	106.40
1	X	2356	A	C5-C6-N6	-5.22	119.53	123.70
1	X	2247	A	N1-C2-N3	-5.22	126.69	129.30
1	X	2848	A	C4-C5-N7	-5.22	108.09	110.70
1	X	1009	C	C6-N1-C1'	-5.21	114.55	120.80
1	X	174	A	C3'-C2'-C1'	-5.21	97.33	101.50
1	X	917	U	C6-N1-C2	-5.21	117.87	121.00
1	X	2522	G	N1-C2-N3	5.21	127.03	123.90
1	X	471	A	C2-N3-C4	-5.21	108.00	110.60
1	X	1922	U	N3-C2-O2	-5.20	118.56	122.20
1	X	2566	A	C6-C5-N7	-5.20	128.66	132.30
1	X	2690	A	C2-N3-C4	-5.20	108.00	110.60
1	X	2031	A	N7-C8-N9	-5.20	111.20	113.80
1	X	2473	G	N1-C6-O6	-5.20	116.78	119.90
1	X	1129	A	C8-N9-C4	-5.20	103.72	105.80
1	X	2850	U	N1-C2-O2	-5.20	119.16	122.80
1	X	1060	C	C6-N1-C2	-5.19	118.22	120.30
1	X	1951	G	N3-C4-C5	-5.19	126.00	128.60
1	X	462	G	N1-C6-O6	5.19	123.02	119.90
1	X	1654	A	N1-C2-N3	5.19	131.90	129.30
1	X	2669	C	N3-C2-O2	-5.19	118.27	121.90
1	X	1780	A	C4-C5-C6	5.19	119.59	117.00
1	X	2832	G	C6-C5-N7	-5.19	127.29	130.40
1	X	440	U	C5-C4-O4	5.19	129.01	125.90
1	X	1325	U	N3-C4-O4	5.19	123.03	119.40
1	X	2348	A	C2-N3-C4	-5.19	108.01	110.60
1	X	1041	G	C2-N3-C4	-5.19	109.31	111.90
1	X	1284	G	C5-C6-O6	5.18	131.71	128.60
1	X	2039	G	N3-C2-N2	-5.18	116.27	119.90
1	X	2415	G	N3-C2-N2	-5.18	116.27	119.90
5	C	46	ARG	NE-CZ-NH1	-5.18	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2698	G	N3-C2-N2	-5.18	116.27	119.90
3	A	253	LYS	C-N-CD	-5.18	109.20	120.60
1	X	2261	G	N1-C6-O6	-5.18	116.79	119.90
1	X	2441	U	C2-N3-C4	-5.18	123.89	127.00
2	Y	96	C	C6-N1-C2	-5.18	118.23	120.30
1	X	1771	A	C2-N3-C4	5.17	113.19	110.60
1	X	2613	A	C8-N9-C4	5.17	107.87	105.80
4	B	146	THR	C-N-CD	-5.17	109.22	120.60
1	X	2258	G	C5-C6-N1	5.17	114.09	111.50
15	M	42	GLY	N-CA-C	-5.17	100.17	113.10
1	X	1654	A	C5-C6-N6	5.17	127.84	123.70
1	X	2523	G	N9-C4-C5	5.17	107.47	105.40
1	X	1297	A	N1-C6-N6	5.17	121.70	118.60
1	X	1396	C	N3-C2-O2	5.17	125.52	121.90
2	Y	39	C	C6-N1-C2	5.17	122.37	120.30
1	X	470	U	N3-C4-O4	-5.17	115.78	119.40
1	X	597	U	C6-N1-C2	5.17	124.10	121.00
1	X	2329	C	C2-N3-C4	-5.17	117.32	119.90
1	X	15	G	N1-C6-O6	-5.16	116.80	119.90
1	X	1288	A	N1-C2-N3	5.16	131.88	129.30
1	X	1928	G	C5-C6-O6	5.16	131.70	128.60
1	X	1995	G	N1-C2-N3	5.16	127.00	123.90
1	X	2798	A	C4-C5-N7	5.16	113.28	110.70
1	X	528	G	N3-C4-N9	5.16	129.09	126.00
1	X	1334	A	C4-C5-C6	5.16	119.58	117.00
1	X	2812	A	C4-C5-C6	5.16	119.58	117.00
1	X	146	C	C6-N1-C2	5.16	122.36	120.30
1	X	767	G	N3-C2-N2	5.15	123.51	119.90
1	X	1964	A	C4'-C3'-C2'	-5.15	97.45	102.60
1	X	1716	G	C5-N7-C8	5.15	106.88	104.30
1	X	1306	U	N3-C4-O4	-5.15	115.80	119.40
1	X	90	G	N1-C6-O6	-5.15	116.81	119.90
1	X	1625	A	C5-N7-C8	-5.15	101.33	103.90
1	X	939	C	C6-N1-C2	5.14	122.36	120.30
1	X	1355	A	C2-N3-C4	-5.14	108.03	110.60
1	X	1466	C	C5'-C4'-O4'	-5.14	102.93	109.10
1	X	985	G	N1-C6-O6	5.14	122.98	119.90
1	X	2336	G	C5-C6-N1	-5.14	108.93	111.50
1	X	2725	C	C5-C6-N1	-5.14	118.43	121.00
1	X	720	A	C5-C6-N1	-5.14	115.13	117.70
1	X	1818	G	N3-C4-N9	5.14	129.08	126.00
1	X	704	G	C8-N9-C4	5.14	108.45	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	827	C	N3-C4-N4	-5.14	114.40	118.00
1	X	2207	G	C8-N9-C4	5.14	108.45	106.40
1	X	489	A	C5-C6-N6	5.14	127.81	123.70
1	X	536	A	N9-C4-C5	5.14	107.86	105.80
1	X	70	A	C5-N7-C8	-5.13	101.33	103.90
1	X	634	G	C4-C5-N7	-5.13	108.75	110.80
1	X	2640	G	C8-N9-C4	5.13	108.45	106.40
1	X	594	G	C8-N9-C4	-5.13	104.35	106.40
1	X	660	G	N3-C4-N9	-5.13	122.92	126.00
1	X	2827	G	C2-N3-C4	5.12	114.46	111.90
1	X	659	G	N7-C8-N9	-5.12	110.54	113.10
1	X	1726	C	N1-C2-O2	-5.12	115.83	118.90
1	X	1718	A	C4-C5-C6	5.12	119.56	117.00
1	X	2219	U	N3-C4-C5	-5.12	111.53	114.60
1	X	2790	C	C5-C4-N4	5.12	123.78	120.20
1	X	213	C	C6-N1-C2	5.12	122.35	120.30
1	X	2415	G	N1-C2-N2	5.12	120.81	116.20
1	X	995	A	C1'-O4'-C4'	-5.11	105.81	109.90
1	X	1316	G	N3-C4-N9	-5.11	122.93	126.00
1	X	1717	A	C8-N9-C4	-5.11	103.75	105.80
1	X	445	A	C8-N9-C4	-5.11	103.76	105.80
1	X	524	A	C5-C6-N1	5.11	120.25	117.70
1	X	1228	G	C4-C5-N7	-5.11	108.76	110.80
1	X	1579	G	N1-C6-O6	5.11	122.97	119.90
1	X	2209	G	C8-N9-C4	-5.11	104.36	106.40
20	R	85	ASP	C-N-CD	-5.11	109.36	120.60
21	S	90	GLU	C-N-CD	-5.11	109.36	120.60
1	X	1017	C	N1-C2-O2	-5.11	115.83	118.90
1	X	2548	G	N3-C4-C5	-5.11	126.05	128.60
1	X	2551	A	N1-C6-N6	-5.11	115.53	118.60
1	X	812	G	N9-C4-C5	5.11	107.44	105.40
1	X	1205	G	N1-C2-N3	5.11	126.96	123.90
1	X	2703	C	N1-C2-O2	-5.11	115.84	118.90
1	X	168	A	N1-C2-N3	5.10	131.85	129.30
1	X	955	G	O3'-P-O5'	-5.10	94.30	104.00
1	X	1766	U	N3-C2-O2	5.10	125.77	122.20
1	X	2669	C	N3-C4-C5	-5.10	119.86	121.90
1	X	787	A	C2-N3-C4	-5.10	108.05	110.60
1	X	1976	U	C4'-C3'-C2'	-5.10	97.50	102.60
1	X	2703	C	C2-N1-C1'	-5.10	113.19	118.80
1	X	736	G	N7-C8-N9	-5.10	110.55	113.10
1	X	339	U	C5-C4-O4	5.10	128.96	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1665	C	C6-N1-C1'	-5.10	114.68	120.80
1	X	462	G	C5-C6-N1	-5.10	108.95	111.50
1	X	2489	C	N1-C2-N3	5.09	122.77	119.20
1	X	102	C	C6-N1-C2	5.09	122.34	120.30
1	X	2035	G	N9-C4-C5	5.09	107.44	105.40
1	X	1311	C	N1-C2-O2	5.09	121.95	118.90
2	Y	12	C	C6-N1-C2	5.09	122.34	120.30
1	X	27	G	N3-C4-C5	-5.09	126.06	128.60
1	X	751	G	C5-C6-O6	-5.09	125.55	128.60
1	X	982	C	C2-N1-C1'	5.09	124.40	118.80
1	X	1479	G	C5-C6-O6	-5.09	125.55	128.60
1	X	1539	U	N3-C4-O4	5.09	122.96	119.40
1	X	2602	G	C2-N3-C4	5.09	114.44	111.90
1	X	613	A	N9-C4-C5	-5.09	103.77	105.80
1	X	953	G	N3-C4-C5	-5.09	126.06	128.60
1	X	2520	A	C4-C5-N7	-5.09	108.16	110.70
1	X	1241	G	N3-C4-N9	5.08	129.05	126.00
2	Y	101	A	C4-C5-N7	-5.08	108.16	110.70
1	X	948	C	C6-N1-C2	5.08	122.33	120.30
1	X	1232	U	N1-C2-O2	-5.08	119.24	122.80
1	X	2036	G	N1-C6-O6	5.08	122.95	119.90
1	X	973	U	N1-C2-O2	-5.08	119.24	122.80
1	X	94	C	C6-N1-C2	5.08	122.33	120.30
1	X	1563	U	C6-N1-C2	5.08	124.05	121.00
1	X	2055	G	C5-N7-C8	5.08	106.84	104.30
1	X	217	U	C6-N1-C2	5.08	124.05	121.00
1	X	530	G	C2-N3-C4	-5.08	109.36	111.90
1	X	833	A	C5-N7-C8	-5.08	101.36	103.90
1	X	115	G	N9-C4-C5	-5.07	103.37	105.40
1	X	670	U	N3-C2-O2	-5.07	118.65	122.20
1	X	2267	A	C8-N9-C4	-5.07	103.77	105.80
1	X	2757	G	C5-C6-N1	-5.07	108.96	111.50
1	X	581	A	N3-C4-C5	5.07	130.35	126.80
1	X	1965	U	C6-N1-C2	-5.07	117.96	121.00
1	X	2660	C	N3-C4-N4	-5.07	114.45	118.00
1	X	2443	C	N3-C4-C5	-5.07	119.87	121.90
1	X	2793	G	C8-N9-C4	5.07	108.43	106.40
1	X	1705	U	N3-C4-O4	-5.07	115.85	119.40
1	X	2243	C	N1-C2-N3	5.07	122.75	119.20
1	X	2688	G	N7-C8-N9	-5.07	110.57	113.10
1	X	1656	U	N3-C4-C5	5.06	117.64	114.60
2	Y	69	G	C4-C5-N7	-5.06	108.77	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1672	A	N3-C4-N9	-5.06	123.35	127.40
1	X	1911	A	C8-N9-C4	-5.06	103.78	105.80
1	X	2019	C	C6-N1-C2	-5.06	118.28	120.30
1	X	2647	G	C8-N9-C4	-5.06	104.38	106.40
1	X	2039	G	N9-C4-C5	-5.06	103.38	105.40
1	X	1238	A	N1-C6-N6	-5.06	115.56	118.60
1	X	2274	C	N3-C2-O2	5.06	125.44	121.90
1	X	2640	G	N3-C4-C5	5.06	131.13	128.60
1	X	529	U	C6-N1-C2	-5.06	117.97	121.00
1	X	1912	G	N7-C8-N9	5.06	115.63	113.10
1	X	1991	C	C6-N1-C1'	5.06	126.87	120.80
1	X	3	U	N3-C2-O2	5.05	125.74	122.20
1	X	236	C	N1-C2-O2	5.05	121.93	118.90
1	X	602	C	N3-C2-O2	5.05	125.44	121.90
18	P	36	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	X	744	C	N3-C4-C5	-5.05	119.88	121.90
1	X	30	G	N9-C4-C5	5.05	107.42	105.40
1	X	1033	G	C5-C6-O6	5.05	131.63	128.60
1	X	2234	G	C5-C6-N1	5.05	114.03	111.50
1	X	2766	U	N3-C4-C5	5.05	117.63	114.60
1	X	1759	A	C5-C6-N6	-5.05	119.66	123.70
1	X	2303	C	C6-N1-C1'	-5.05	114.75	120.80
1	X	165	G	N9-C4-C5	-5.04	103.38	105.40
1	X	1584	G	C4-C5-N7	5.04	112.82	110.80
1	X	1710	U	C6-N1-C2	5.04	124.03	121.00
1	X	2798	A	C5-C6-N1	-5.04	115.18	117.70
1	X	160	C	C6-N1-C2	-5.04	118.28	120.30
1	X	488	A	C5-C6-N1	-5.04	115.18	117.70
1	X	583	C	N1-C2-O2	-5.04	115.88	118.90
1	X	1296	G	C5-C6-O6	5.04	131.62	128.60
1	X	2553	G	C5-N7-C8	5.04	106.82	104.30
1	X	2508	G	C6-C5-N7	-5.04	127.38	130.40
1	X	1041	G	N3-C4-C5	5.04	131.12	128.60
1	X	1316	G	C5-C6-O6	5.04	131.62	128.60
1	X	1780	A	C8-N9-C4	-5.04	103.78	105.80
1	X	1828	C	N3-C4-N4	-5.04	114.47	118.00
1	X	1844	C	C6-N1-C2	-5.04	118.28	120.30
1	X	2412	A	C4-C5-C6	-5.04	114.48	117.00
1	X	531	G	N7-C8-N9	-5.04	110.58	113.10
1	X	2219	U	C6-N1-C2	-5.03	117.98	121.00
1	X	2244	C	N1-C2-O2	5.03	121.92	118.90
1	X	2434	G	C5-C6-O6	5.03	131.62	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	143	A	C8-N9-C4	5.03	107.81	105.80
1	X	2010	G	N3-C4-N9	5.03	129.02	126.00
1	X	2355	A	N7-C8-N9	-5.03	111.28	113.80
1	X	2679	G	C8-N9-C4	5.03	108.41	106.40
1	X	1242	A	C4-C5-N7	5.03	113.21	110.70
1	X	320	A	C8-N9-C4	5.03	107.81	105.80
1	X	1982	C	C4-C5-C6	5.03	119.91	117.40
1	X	1933	G	N9-C4-C5	5.02	107.41	105.40
1	X	1958	G	N1-C6-O6	5.02	122.91	119.90
1	X	2565	C	N3-C2-O2	-5.02	118.38	121.90
1	X	1584	G	N1-C6-O6	5.02	122.91	119.90
1	X	2587	G	N9-C4-C5	5.02	107.41	105.40
1	X	885	A	N9-C4-C5	5.02	107.81	105.80
1	X	1325	U	C6-N1-C2	-5.02	117.99	121.00
1	X	309	G	N9-C4-C5	-5.02	103.39	105.40
1	X	471	A	N9-C4-C5	-5.02	103.79	105.80
1	X	1240	G	N7-C8-N9	-5.02	110.59	113.10
1	X	1399	C	C6-N1-C2	5.02	122.31	120.30
1	X	1214	C	C6-N1-C2	-5.01	118.29	120.30
1	X	2550	C	C5-C6-N1	5.01	123.51	121.00
1	X	657	A	C8-N9-C4	-5.01	103.80	105.80
1	X	1635	G	C5-N7-C8	-5.01	101.79	104.30
1	X	2603	G	N3-C2-N2	-5.01	116.39	119.90
1	X	88	G	C4-C5-N7	5.01	112.80	110.80
1	X	1287	A	C2-N3-C4	5.01	113.10	110.60
1	X	2567	G	C4-C5-C6	5.00	121.80	118.80
1	X	547	U	N3-C2-O2	5.00	125.70	122.20
1	X	746	G	C2-N3-C4	-5.00	109.40	111.90
1	X	1698	C	N3-C2-O2	5.00	125.40	121.90

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	E	125	VAL	Peptide
7	E	130	ARG	Sidechain
7	E	165	VAL	Peptide
7	E	174	GLY	Peptide
8	F	116	ASN	Peptide
8	F	117	ALA	Peptide
8	F	118	GLY	Peptide
9	G	110	LEU	Peptide

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Mol	Chain	Res	Type	Group
9	G	111	LYS	Peptide
9	G	170	PRO	Peptide
9	G	35	LYS	Peptide
9	G	36	ASN	Peptide
9	G	38	GLU	Peptide
9	G	85	ALA	Peptide
9	G	91	THR	Peptide
10	H	40	GLY	Peptide
10	H	41	ASN	Peptide
11	I	18	ARG	Peptide
12	J	83	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	56750	0	28598	2022	3
2	Y	2561	0	1306	67	0
3	A	1920	0	1974	255	0
4	B	1539	0	1600	168	0
5	C	1481	0	1504	122	0
6	D	1394	0	1470	73	0
7	E	1286	0	1336	30	0
8	F	451	0	474	21	0
9	G	1114	0	1144	113	0
10	H	997	0	1046	97	0
11	I	1005	0	1036	117	0
12	J	1090	0	1125	97	0
13	K	878	0	930	93	0
14	L	779	0	820	77	0
15	M	871	0	894	85	3
16	N	978	0	1020	107	0
17	O	741	0	756	66	0
18	P	1004	0	1083	70	0
19	Q	714	0	731	35	0
20	R	825	0	881	78	0
21	S	1345	0	1372	56	0
22	T	556	0	579	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	U	537	0	580	40	0
24	V	525	0	546	20	0
25	W	424	0	470	24	0
26	Z	452	0	457	39	0
27	1	431	0	456	91	0
28	2	383	0	414	51	0
29	3	462	0	506	78	0
30	4	297	0	330	18	0
31	X	33	0	33	18	0
32	X	58	0	69	43	0
33	I	1	0	0	0	0
33	U	1	0	0	0	0
33	X	71	0	0	0	0
34	X	4	0	0	0	0
35	X	5	0	0	0	0
All	All	83963	0	55540	3669	3

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 26.

All (3669) 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)
1:X:699:G:N2	28:2:5:TYR:CE1	1.89	1.36
27:1:28:ARG:HB2	27:1:30:ASN:OD1	1.24	1.34
1:X:699:G:N2	28:2:5:TYR:HE1	1.25	1.28
1:X:775:U:H5'	1:X:776:G:N2	1.49	1.26
1:X:699:G:N7	28:2:11:LYS:HG3	1.51	1.26
1:X:775:U:H5'	1:X:776:G:C2	1.71	1.25
3:A:66:ILE:CG2	3:A:68:PHE:CZ	2.19	1.24
1:X:1142:G:N2	9:G:101:THR:HG21	1.52	1.23
1:X:2662:C:O2	10:H:82:LYS:NZ	1.71	1.22
1:X:699:G:C8	28:2:11:LYS:HG2	1.75	1.22
1:X:2045:A:C6	32:X:2882:LMA:H27A	1.75	1.21
1:X:1391:A:N7	1:X:1393:G:C6	2.10	1.20
1:X:699:G:C8	28:2:11:LYS:CG	2.26	1.18
1:X:2427:A:N6	11:I:40:ARG:NH2	1.90	1.18
1:X:1692:C:O2	4:B:128:SER:O	1.62	1.17
1:X:400:U:OP2	23:U:37:ILE:HD11	1.44	1.16
32:X:2882:LMA:H34	32:X:2882:LMA:H56B	1.28	1.15
32:X:2882:LMA:C34	32:X:2882:LMA:H56B	1.75	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:41:ASP:OD2	27:1:46:LYS:HD2	1.48	1.13
21:S:13:LYS:HE3	21:S:33:ALA:HB1	1.22	1.13
10:H:75:VAL:HG12	10:H:118:LEU:HD21	1.20	1.12
27:1:14:SER:HB2	27:1:22:TYR:HA	1.24	1.12
1:X:1685:A:N6	1:X:1974:U:O2	1.82	1.12
1:X:699:G:O6	28:2:12:ARG:HA	1.51	1.10
15:M:34:ARG:HD3	15:M:88:VAL:HG22	1.29	1.10
31:X:2881:LC2:C2	31:X:2881:LC2:H28	1.76	1.09
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.32	1.09
1:X:2426:G:H3'	1:X:2479:U:OP2	1.50	1.09
1:X:1142:G:H21	9:G:101:THR:CG2	1.65	1.08
11:I:18:ARG:HB2	11:I:21:ARG:HB2	1.28	1.08
3:A:218:ARG:HG3	3:A:219:LYS:H	0.97	1.08
9:G:35:LYS:CB	9:G:37:ASP:OD2	2.00	1.08
1:X:1673:C:C5'	4:B:136:ARG:HD3	1.83	1.07
3:A:44:ARG:HD2	3:A:44:ARG:H	1.15	1.07
9:G:35:LYS:HG3	9:G:37:ASP:OD2	1.55	1.07
6:D:38:GLU:HB3	6:D:87:ILE:HB	1.35	1.07
3:A:22:PHE:O	3:A:209:LYS:HG3	1.52	1.07
9:G:35:LYS:CG	9:G:37:ASP:OD2	2.03	1.06
1:X:1391:A:C5	1:X:1393:G:C5	2.43	1.06
15:M:33:VAL:HG22	15:M:51:GLU:HB2	1.29	1.05
17:O:21:ARG:NH2	17:O:88:GLN:OE1	1.86	1.05
3:A:218:ARG:HG3	3:A:219:LYS:N	1.57	1.05
3:A:27:LYS:HE2	3:A:205:ILE:CD1	1.85	1.05
1:X:1092:U:H4'	8:F:122:ALA:HB1	1.09	1.05
3:A:66:ILE:HG21	3:A:68:PHE:CZ	1.87	1.05
12:J:92:GLU:HG3	12:J:93:TYR:HD2	1.21	1.05
1:X:1673:C:H5'	4:B:136:ARG:HD3	1.37	1.04
32:X:2882:LMA:H40	32:X:2882:LMA:H29B	1.37	1.03
1:X:1142:G:N2	9:G:101:THR:CG2	2.20	1.03
1:X:2170:C:H3'	1:X:2171:U:H5''	1.40	1.03
1:X:2427:A:N6	11:I:40:ARG:HH22	1.48	1.03
1:X:1142:G:H1'	9:G:103:TYR:CE2	1.94	1.03
18:P:41:VAL:O	18:P:44:VAL:HG22	1.59	1.02
21:S:13:LYS:CE	21:S:33:ALA:HB1	1.89	1.02
1:X:2663:U:O2'	10:H:88:THR:HG21	1.58	1.02
31:X:2881:LC2:O6	31:X:2881:LC2:H14B	1.58	1.02
1:X:763:A:H2'	1:X:764:A:H5''	1.39	1.02
11:I:18:ARG:CB	11:I:21:ARG:HB2	1.88	1.02
3:A:160:ALA:HB2	3:A:199:ASN:ND2	1.72	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2427:A:H61	11:I:40:ARG:NH2	1.54	1.02
21:S:129:ARG:NH2	21:S:156:GLU:OE1	1.93	1.02
1:X:1391:A:C8	1:X:1393:G:O6	2.14	1.01
9:G:67:ARG:HB3	9:G:70:PHE:HA	1.40	1.00
4:B:78:LEU:O	4:B:79:ARG:HD3	1.62	0.99
31:X:2881:LC2:H28	31:X:2881:LC2:C3	1.91	0.99
1:X:577:U:H5'	1:X:956:A:N6	1.77	0.99
9:G:35:LYS:HB2	9:G:37:ASP:OD2	1.61	0.99
1:X:2427:A:H62	11:I:40:ARG:HH22	1.08	0.99
32:X:2882:LMA:H56A	32:X:2882:LMA:H12	1.42	0.99
4:B:133:LYS:HG3	4:B:137:ARG:HD3	1.43	0.99
1:X:971:A:H61	12:J:83:ARG:HH22	0.99	0.99
1:X:2494:C:OP1	9:G:108:GLY:O	1.81	0.99
1:X:309:G:OP1	20:R:93:ARG:O	1.81	0.98
1:X:309:G:OP1	20:R:93:ARG:HB3	1.61	0.98
1:X:775:U:C5'	1:X:776:G:C2	2.45	0.98
1:X:1681:A:H61	1:X:1979:C:H42	0.99	0.98
9:G:70:PHE:CG	16:N:64:ARG:HG2	1.99	0.98
1:X:334:G:H2'	5:C:162:ARG:HE	1.25	0.98
1:X:2350:G:O2'	27:1:46:LYS:HG3	1.64	0.97
1:X:348:U:OP2	20:R:93:ARG:NH2	1.98	0.97
1:X:824:U:H2'	11:I:30:ALA:HA	1.46	0.96
1:X:824:U:C2'	11:I:30:ALA:HA	1.96	0.96
1:X:2378:G:H1'	27:1:22:TYR:OH	1.66	0.96
1:X:1142:G:H21	9:G:101:THR:HG21	0.79	0.96
1:X:309:G:P	20:R:93:ARG:HB3	2.04	0.96
1:X:699:G:N7	28:2:11:LYS:CG	2.28	0.96
1:X:2272:A:H5''	14:L:15:ARG:HH21	1.30	0.95
27:1:8:ILE:HG13	27:1:30:ASN:ND2	1.80	0.95
12:J:50:ALA:HB1	12:J:125:LYS:HD3	1.49	0.95
1:X:2257:A:N6	22:T:15:ASP:OD1	1.99	0.95
12:J:92:GLU:HG3	12:J:93:TYR:CD2	2.00	0.95
1:X:2781:G:H2'	1:X:2782:G:H5''	1.49	0.94
1:X:635:C:H2'	1:X:636:G:H5''	1.49	0.94
1:X:824:U:H2'	11:I:30:ALA:CA	1.97	0.94
20:R:18:LYS:HD3	20:R:18:LYS:H	1.32	0.94
1:X:334:G:N2	5:C:162:ARG:NH2	2.15	0.94
19:Q:88:ILE:HD12	19:Q:92:ALA:HB2	1.50	0.94
3:A:61:ARG:HD3	3:A:88:ASN:OD1	1.66	0.94
1:X:2264:C:H5	27:1:28:ARG:CZ	1.81	0.94
11:I:18:ARG:CG	11:I:21:ARG:HB2	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:699:G:H8	28:2:11:LYS:HG2	1.17	0.94
1:X:775:U:C5'	1:X:776:G:N2	2.30	0.94
15:M:34:ARG:NH1	15:M:88:VAL:HG21	1.83	0.93
1:X:762:A:H2	1:X:766:A:HO2'	1.00	0.93
3:A:27:LYS:CE	3:A:205:ILE:HD13	1.97	0.93
3:A:219:LYS:O	3:A:219:LYS:HD2	1.67	0.93
12:J:27:TYR:HB3	12:J:137:VAL:HG21	1.49	0.93
14:L:89:PHE:HZ	14:L:103:LEU:HD22	1.33	0.93
32:X:2882:LMA:H12	32:X:2882:LMA:C56	1.99	0.93
1:X:1816:G:O2'	3:A:253:LYS:HD3	1.68	0.93
3:A:26:THR:HG22	3:A:27:LYS:N	1.81	0.92
1:X:699:G:C8	28:2:11:LYS:HG3	1.97	0.92
1:X:2264:C:H5	27:1:28:ARG:NH1	1.66	0.92
4:B:76:ARG:HH12	15:M:4:HIS:HB2	1.30	0.92
5:C:154:ASP:O	5:C:157:THR:HG22	1.68	0.92
16:N:7:GLY:O	16:N:9:VAL:HG23	1.70	0.92
1:X:1173:G:H4'	17:O:22:VAL:HG22	1.52	0.92
1:X:1092:U:H4'	8:F:122:ALA:CB	1.98	0.92
27:1:12:MET:HG3	27:1:27:ASN:OD1	1.69	0.92
1:X:2478:C:H6	1:X:2478:C:O5'	1.53	0.92
27:1:9:ILE:HA	27:1:28:ARG:HA	1.52	0.91
11:I:62:LYS:HD3	29:3:12:ARG:CA	2.00	0.91
1:X:1141:U:O4	4:B:147:PRO:HD3	1.68	0.91
1:X:1225:G:H2'	1:X:1249:G:H22	1.36	0.91
1:X:123:A:O2'	28:2:13:ALA:O	1.89	0.91
3:A:248:VAL:HG23	3:A:249:THR:HG23	1.51	0.91
1:X:1291:G:OP1	13:K:36:THR:OG1	1.89	0.90
10:H:75:VAL:HG12	10:H:118:LEU:CD2	2.02	0.90
2:Y:83:C:H2'	2:Y:84:G:H5'	1.51	0.90
3:A:66:ILE:HG21	3:A:89:ARG:HH22	1.37	0.90
1:X:2671:C:OP1	1:X:2846:G:H4'	1.71	0.90
3:A:71:ARG:HH12	3:A:150:PRO:CA	1.85	0.90
1:X:2204:A:H4'	1:X:2205:C:O5'	1.70	0.90
1:X:2757:G:H5''	1:X:2758:A:H5'	1.53	0.90
1:X:1810:U:C5	3:A:158:ARG:HD2	2.07	0.90
20:R:48:VAL:HG12	20:R:50:GLY:H	1.37	0.89
1:X:2064:U:H5'	23:U:41:VAL:HG11	1.53	0.89
1:X:2272:A:H5''	14:L:15:ARG:NH2	1.86	0.89
3:A:84:GLU:OE2	3:A:105:TYR:HE2	1.54	0.89
6:D:4:LEU:HG	6:D:5:LYS:H	1.36	0.89
3:A:66:ILE:HG23	3:A:68:PHE:CZ	2.05	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1656:U:C2'	1:X:1657:A:H5''	2.02	0.89
1:X:2430:A:N1	31:X:2881:LC2:H15A	1.85	0.89
6:D:40:LEU:HD23	6:D:41:GLY:N	1.86	0.89
21:S:13:LYS:HG2	21:S:18:MET:HB2	1.53	0.89
3:A:44:ARG:HD2	3:A:44:ARG:N	1.86	0.89
5:C:102:LEU:O	5:C:102:LEU:HD23	1.72	0.89
15:M:34:ARG:HD3	15:M:88:VAL:CG2	2.02	0.89
1:X:546:A:H4'	16:N:57:PHE:HZ	1.37	0.89
3:A:27:LYS:HE2	3:A:205:ILE:HD13	1.55	0.88
1:X:1681:A:N6	1:X:1979:C:H42	1.70	0.88
18:P:32:ARG:HA	18:P:32:ARG:NE	1.89	0.88
1:X:122:G:H2'	28:2:19:ARG:HH21	1.38	0.88
3:A:90:SER:O	3:A:199:ASN:ND2	2.05	0.88
10:H:23:ARG:HH12	10:H:25:LEU:HD23	1.37	0.88
27:1:8:ILE:HG13	27:1:30:ASN:HD21	1.37	0.88
9:G:53:ARG:HD3	9:G:171:LEU:HD12	1.52	0.88
1:X:2349:G:H21	27:1:46:LYS:NZ	1.71	0.88
11:I:62:LYS:HD3	29:3:12:ARG:HA	1.56	0.88
10:H:19:ILE:O	10:H:19:ILE:HG13	1.71	0.88
14:L:44:ASP:HB3	14:L:47:ARG:O	1.74	0.88
22:T:14:ARG:O	22:T:15:ASP:OD2	1.92	0.88
1:X:1391:A:C8	1:X:1393:G:C6	2.61	0.88
32:X:2882:LMA:H57	32:X:2882:LMA:H56A	1.53	0.88
1:X:748:A:H5''	1:X:748:A:H8	1.38	0.88
1:X:971:A:H61	12:J:83:ARG:NH2	1.71	0.87
1:X:919:U:OP1	12:J:26:ASP:OD2	1.91	0.87
1:X:331:U:H1'	5:C:162:ARG:HH12	1.39	0.87
1:X:609:U:H4'	11:I:18:ARG:NH2	1.89	0.87
1:X:2015:G:H4'	1:X:2016:A:OP1	1.75	0.87
10:H:23:ARG:HB3	10:H:23:ARG:NH2	1.90	0.86
1:X:1810:U:H5	3:A:158:ARG:HD2	1.38	0.86
1:X:1391:A:C4	1:X:1393:G:N7	2.43	0.86
1:X:1441:A:H4'	1:X:1442:C:O5'	1.73	0.86
1:X:2063:A:O3'	23:U:39:LYS:HG2	1.76	0.86
1:X:1142:G:H1'	9:G:103:TYR:HE2	1.40	0.86
15:M:33:VAL:HG22	15:M:51:GLU:CB	2.05	0.86
1:X:2500:C:H6	1:X:2500:C:O5'	1.58	0.86
1:X:2664:G:OP1	10:H:90:ARG:NH1	2.08	0.86
3:A:173:TYR:HA	3:A:187:HIS:HA	1.57	0.86
10:H:116:ARG:NH1	15:M:38:LYS:HE2	1.91	0.86
3:A:207:LEU:HA	3:A:212:ARG:NH1	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2045:A:H61	32:X:2882:LMA:H32B	1.41	0.85
3:A:150:PRO:HD3	3:A:190:CYS:SG	2.16	0.85
1:X:1692:C:C2	4:B:128:SER:O	2.28	0.85
14:L:89:PHE:CZ	14:L:103:LEU:HD22	2.12	0.85
27:1:8:ILE:O	27:1:9:ILE:HG23	1.76	0.85
1:X:552:C:H2'	1:X:553:C:H5''	1.57	0.85
1:X:2371:A:O2'	11:I:59:ARG:HG2	1.76	0.85
3:A:146:LEU:O	3:A:156:LEU:HB2	1.76	0.85
23:U:59:THR:O	23:U:60:VAL:HG22	1.76	0.85
3:A:80:VAL:HB	3:A:115:GLY:H	1.42	0.85
17:O:21:ARG:HH22	17:O:88:GLN:HE22	1.23	0.85
32:X:2882:LMA:O53	32:X:2882:LMA:H32	1.76	0.84
1:X:879:A:H2'	1:X:879:A:N3	1.91	0.84
11:I:31:GLY:HA3	11:I:34:HIS:HB2	1.59	0.84
1:X:1238:A:H5'	17:O:85:GLY:H	1.43	0.84
1:X:2350:G:O2'	27:1:46:LYS:CG	2.25	0.84
1:X:525:A:H2'	1:X:526:C:H5'	1.60	0.84
5:C:164:VAL:HG23	5:C:165:SER:H	1.42	0.84
1:X:123:A:H5'	28:2:19:ARG:NH2	1.93	0.84
1:X:2014:A:C6	1:X:2477:C:H1'	2.12	0.84
12:J:71:PRO:HA	12:J:96:SER:HB2	1.60	0.84
13:K:84:ALA:HB3	13:K:85:PRO:HD3	1.60	0.84
19:Q:53:ILE:HD13	19:Q:80:VAL:HG12	1.60	0.84
14:L:39:TYR:O	14:L:54:ALA:O	1.96	0.84
15:M:39:VAL:HG12	15:M:45:THR:OG1	1.78	0.84
1:X:2366:U:H1'	22:T:41:ARG:NH1	1.93	0.84
4:B:9:ILE:HD11	4:B:27:LEU:HB2	1.59	0.83
15:M:56:ALA:HB3	15:M:67:THR:H	1.42	0.83
15:M:99:VAL:HG21	15:M:104:LEU:HD21	1.60	0.83
1:X:2264:C:C5	27:1:28:ARG:NH1	2.46	0.83
4:B:154:LYS:HE3	4:B:156:MET:SD	2.18	0.83
1:X:1623:C:H4'	1:X:1624:A:O5'	1.78	0.83
32:X:2882:LMA:O9	32:X:2882:LMA:H32A	1.77	0.83
4:B:136:ARG:HG2	4:B:137:ARG:N	1.92	0.83
1:X:1296:G:H22	1:X:1299:A:H5''	1.43	0.83
18:P:41:VAL:O	18:P:44:VAL:CG2	2.27	0.83
1:X:1142:G:H1'	9:G:103:TYR:CD2	2.14	0.83
1:X:1683:G:C2'	1:X:1684:G:H5'	2.09	0.83
1:X:2005:U:H6	1:X:2005:U:OP2	1.61	0.83
2:Y:83:C:H2'	2:Y:84:G:C5'	2.08	0.83
12:J:27:TYR:CB	12:J:137:VAL:HG21	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:162:ARG:CG	5:C:162:ARG:HH11	1.92	0.83
1:X:2621:G:OP1	9:G:110:LEU:HD13	1.79	0.83
1:X:590:C:OP1	16:N:31:GLN:HB3	1.77	0.83
1:X:334:G:N2	5:C:162:ARG:HH21	1.75	0.83
16:N:93:LYS:NZ	17:O:10:LYS:HE2	1.94	0.83
18:P:66:GLU:HB3	18:P:67:PRO:HD3	1.60	0.83
1:X:1681:A:H61	1:X:1979:C:N4	1.77	0.83
3:A:49:ARG:H	3:A:49:ARG:HH11	1.26	0.82
4:B:121:ASN:O	4:B:122:PHE:HB2	1.78	0.82
12:J:135:ARG:HH22	21:S:118:HIS:HD2	1.27	0.82
1:X:1288:A:C8	13:K:16:ALA:HB2	2.14	0.82
1:X:1067:G:H21	1:X:1114:A:H62	1.26	0.82
1:X:1277:G:H8	1:X:1277:G:O5'	1.61	0.82
1:X:6:A:H1'	9:G:162:LYS:CG	2.09	0.82
15:M:103:LYS:O	15:M:104:LEU:HB2	1.78	0.82
1:X:822:G:O2'	1:X:823:U:H5'	1.79	0.82
5:C:176:ASN:HB2	5:C:179:ASP:OD2	1.80	0.82
10:H:76:ARG:HD3	10:H:113:PRO:O	1.79	0.82
4:B:38:THR:HG22	4:B:40:GLN:H	1.45	0.82
19:Q:7:LEU:HD22	19:Q:7:LEU:C	2.00	0.82
1:X:27:G:N2	1:X:522:G:H1'	1.94	0.82
27:1:41:ASP:HB2	27:1:46:LYS:HA	1.59	0.82
12:J:42:TRP:HB3	12:J:95:VAL:HG11	1.61	0.82
1:X:317:U:H2'	1:X:318:G:H5'	1.61	0.82
1:X:1656:U:H2'	1:X:1657:A:H5''	1.60	0.82
17:O:10:LYS:NZ	17:O:37:ALA:HB3	1.95	0.81
20:R:22:VAL:HG11	20:R:80:LYS:HE3	1.62	0.81
3:A:218:ARG:CG	3:A:219:LYS:N	2.39	0.81
14:L:26:ARG:HD3	14:L:86:GLN:HB3	1.61	0.81
1:X:2427:A:H61	11:I:40:ARG:HH21	1.28	0.81
1:X:2827:G:H1	1:X:2840:U:H3	1.27	0.81
1:X:2350:G:O2'	27:1:46:LYS:CB	2.28	0.81
1:X:1437:A:H2'	1:X:1438:G:H8	1.46	0.81
9:G:94:LYS:HG2	9:G:117:GLU:HB2	1.60	0.81
1:X:763:A:C2'	1:X:764:A:H5''	2.11	0.81
11:I:60:LEU:CD2	29:3:13:ARG:HG2	2.11	0.81
13:K:87:TYR:HE1	13:K:94:TYR:HD1	1.25	0.81
1:X:38:G:N2	5:C:42:THR:HG22	1.96	0.81
1:X:971:A:N6	12:J:83:ARG:HH22	1.78	0.81
1:X:759:C:H4'	1:X:759:C:OP1	1.80	0.81
3:A:209:LYS:HE3	3:A:209:LYS:HA	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:26:THR:CG2	3:A:27:LYS:N	2.44	0.81
3:A:49:ARG:NH1	3:A:49:ARG:HB3	1.96	0.81
3:A:69:LYS:H	3:A:69:LYS:HD3	1.46	0.81
14:L:37:HIS:NE2	14:L:39:TYR:CZ	2.49	0.80
3:A:66:ILE:HD11	3:A:107:LEU:HG	1.62	0.80
15:M:5:ILE:HD13	15:M:7:ILE:HG22	1.61	0.80
13:K:87:TYR:HE1	13:K:94:TYR:CD1	2.00	0.80
14:L:21:THR:CG2	14:L:45:ASP:O	2.29	0.80
1:X:1685:A:O4'	1:X:1686:A:C2	2.35	0.80
1:X:2756:A:H4'	1:X:2757:G:O5'	1.79	0.80
9:G:132:PHE:HD2	9:G:145:HIS:CG	1.99	0.80
19:Q:10:PRO:HD3	24:V:30:PHE:CD2	2.17	0.80
1:X:2045:A:C6	32:X:2882:LMA:C27	2.61	0.80
1:X:759:C:H2'	32:X:2882:LMA:H58A	1.63	0.80
1:X:123:A:C5'	28:2:19:ARG:HH21	1.93	0.80
29:3:8:LYS:HD2	29:3:11:LYS:HE3	1.61	0.80
1:X:1816:G:OP1	3:A:53:ARG:HD3	1.80	0.80
1:X:1441:A:H1'	1:X:1442:C:OP2	1.81	0.80
1:X:1696:C:O5'	1:X:1696:C:H6	1.65	0.80
31:X:2881:LC2:C14	31:X:2881:LC2:O6	2.30	0.80
9:G:70:PHE:HB2	16:N:64:ARG:HE	1.47	0.80
17:O:80:TYR:O	17:O:80:TYR:CG	2.34	0.80
3:A:84:GLU:OE2	3:A:105:TYR:CE2	2.34	0.80
1:X:1391:A:C4'	1:X:1392:U:OP1	2.30	0.80
3:A:27:LYS:CE	3:A:205:ILE:CD1	2.59	0.79
1:X:834:A:O2'	1:X:957:G:OP2	1.98	0.79
4:B:59:VAL:HG21	4:B:74:PRO:HB3	1.63	0.79
17:O:10:LYS:HZ2	17:O:37:ALA:HB3	1.45	0.79
1:X:1981:A:H4'	1:X:2704:U:O2'	1.82	0.79
1:X:1391:A:H1'	1:X:1392:U:O5'	1.81	0.79
1:X:845:U:OP1	11:I:38:LYS:NZ	2.14	0.79
4:B:102:ILE:HD11	4:B:184:VAL:CG2	2.13	0.79
4:B:120:TRP:CD2	4:B:155:ARG:HD2	2.18	0.79
17:O:21:ARG:HH22	17:O:88:GLN:NE2	1.80	0.79
1:X:1630:A:N1	18:P:114:ALA:HB2	1.98	0.79
18:P:89:ARG:HG2	18:P:131:LYS:H	1.47	0.79
32:X:2882:LMA:C34	32:X:2882:LMA:C56	2.60	0.79
27:1:28:ARG:CB	27:1:30:ASN:OD1	2.20	0.79
1:X:1391:A:N7	1:X:1393:G:C5	2.47	0.79
1:X:1691:G:N1	1:X:1972:G:O6	2.16	0.79
1:X:331:U:C1'	5:C:162:ARG:HH12	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:X:2881:LC2:C16	31:X:2881:LC2:H14B	2.12	0.78
1:X:2045:A:N6	32:X:2882:LMA:H27A	1.97	0.78
1:X:938:G:O2'	1:X:939:C:H5'	1.82	0.78
1:X:309:G:OP1	20:R:93:ARG:CB	2.31	0.78
1:X:1265:G:O4'	16:N:33:ARG:HD2	1.84	0.78
1:X:2074:U:H1'	23:U:48:LYS:HE3	1.65	0.78
5:C:22:VAL:HG11	5:C:110:SER:OG	1.84	0.78
6:D:65:PRO:HB3	6:D:89:VAL:HG22	1.65	0.78
1:X:596:C:OP2	11:I:29:THR:CG2	2.31	0.78
1:X:761:G:OP2	18:P:109:ARG:HG3	1.83	0.78
17:O:65:ARG:HE	17:O:87:ARG:HD2	1.48	0.78
3:A:66:ILE:CG2	3:A:68:PHE:CE2	2.66	0.78
12:J:13:GLN:O	12:J:74:PRO:HG3	1.82	0.78
16:N:25:TRP:CE3	16:N:26:GLY:N	2.52	0.78
1:X:1173:G:H2'	1:X:1174:G:H8	1.48	0.78
1:X:2264:C:C5	27:I:28:ARG:CZ	2.66	0.78
6:D:72:LYS:HA	6:D:81:GLN:O	1.83	0.78
1:X:1264:C:O2'	1:X:1265:G:H5''	1.82	0.78
3:A:71:ARG:HH12	3:A:150:PRO:HA	1.49	0.78
5:C:46:ARG:HD2	5:C:51:VAL:CG2	2.14	0.78
1:X:1673:C:H5''	4:B:136:ARG:HD3	1.65	0.78
1:X:1391:A:H4'	1:X:1392:U:OP1	1.84	0.78
13:K:17:ARG:HG3	13:K:18:VAL:N	1.99	0.78
23:U:49:LYS:HB3	23:U:61:TRP:CD2	2.19	0.78
1:X:27:G:H22	1:X:522:G:H1'	1.49	0.78
3:A:33:ALA:HB3	3:A:84:GLU:CD	2.05	0.77
1:X:587:A:OP1	1:X:1268:U:O2'	2.03	0.77
10:H:83:ARG:HD2	10:H:89:ILE:HD11	1.67	0.77
21:S:13:LYS:HE3	21:S:33:ALA:CB	2.09	0.77
1:X:1142:G:C1'	9:G:103:TYR:CD2	2.67	0.77
1:X:1324:G:H4'	1:X:1325:U:OP1	1.84	0.77
4:B:136:ARG:HG2	4:B:137:ARG:H	1.49	0.77
4:B:14:ILE:HD12	4:B:23:VAL:HG21	1.65	0.77
1:X:1668:G:N2	1:X:1990:U:C2	2.53	0.77
1:X:1964:A:H5''	1:X:1965:U:OP2	1.84	0.77
1:X:2430:A:C2	31:X:2881:LC2:H15A	2.19	0.77
1:X:822:G:C2'	1:X:823:U:H5'	2.15	0.77
4:B:47:VAL:HG21	4:B:84:PHE:O	1.85	0.77
1:X:824:U:C3'	11:I:30:ALA:HA	2.14	0.77
1:X:1365:U:O2	1:X:1393:G:C2	2.38	0.77
1:X:2663:U:O4	1:X:2664:G:O6	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:4:HIS:CB	26:Z:5:PRO:HD3	2.15	0.77
3:A:96:LEU:HD12	3:A:106:ILE:HD12	1.66	0.77
26:Z:4:HIS:HB2	26:Z:5:PRO:HD3	1.65	0.77
1:X:334:G:C2	5:C:162:ARG:NH2	2.48	0.77
1:X:1225:G:H2'	1:X:1249:G:N2	1.99	0.77
29:3:13:ARG:HG3	29:3:24:ALA:HA	1.66	0.77
3:A:102:GLU:OE2	3:A:104:ARG:NE	2.18	0.77
3:A:71:ARG:NH2	3:A:190:CYS:HA	2.00	0.77
3:A:49:ARG:HH11	3:A:49:ARG:N	1.81	0.77
1:X:45:C:OP2	1:X:192:G:H2'	1.85	0.77
1:X:577:U:H5'	1:X:956:A:H61	1.46	0.77
1:X:817:A:OP1	11:I:45:LYS:HG3	1.84	0.77
27:1:26:LYS:HG2	27:1:28:ARG:NH2	2.00	0.76
3:A:232:HIS:CD2	3:A:233:PRO:HD2	2.20	0.76
5:C:162:ARG:HB3	5:C:162:ARG:HH11	1.51	0.76
5:C:118:VAL:HG12	5:C:188:ILE:HB	1.67	0.76
1:X:1073:G:H21	8:F:133:SER:HB3	1.49	0.76
1:X:122:G:H2'	28:2:19:ARG:NH2	2.00	0.76
1:X:457:C:C2'	1:X:458:G:H5'	2.14	0.76
1:X:1712:G:H2'	1:X:1713:G:H5'	1.66	0.76
1:X:1822:C:H42	1:X:1958:G:H1	1.33	0.76
1:X:1365:U:O2	1:X:1393:G:N2	2.18	0.76
1:X:2825:A:O4'	1:X:2843:A:H2	1.69	0.76
1:X:791:G:C2	1:X:800:U:O2	2.38	0.76
5:C:126:ALA:O	5:C:127:ASP:HB2	1.84	0.76
1:X:1336:G:OP1	18:P:119:LYS:NZ	2.15	0.76
1:X:1668:G:H8	1:X:1668:G:H5''	1.50	0.76
3:A:160:ALA:CB	3:A:199:ASN:CG	2.54	0.76
10:H:2:ILE:HB	10:H:45:ALA:HB3	1.67	0.76
1:X:1682:A:O5'	1:X:1682:A:H8	1.69	0.76
1:X:2000:U:H4'	26:Z:8:LYS:O	1.86	0.76
6:D:60:ILE:HG13	6:D:61:THR:HG23	1.67	0.76
1:X:225:G:C2	1:X:2410:U:H4'	2.20	0.76
32:X:2882:LMA:H40	32:X:2882:LMA:C29	2.16	0.76
1:X:1683:G:H2'	1:X:1684:G:H5'	1.67	0.76
1:X:1983:G:O2'	1:X:1984:A:H5'	1.86	0.75
11:I:31:GLY:CA	11:I:34:HIS:HB2	2.17	0.75
1:X:2855:C:O2'	13:K:90:ARG:NH1	2.19	0.75
4:B:154:LYS:HE3	4:B:156:MET:CG	2.16	0.75
1:X:1203:A:OP1	11:I:33:GLY:O	2.05	0.75
1:X:1322:G:H4'	28:2:7:PRO:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:22:VAL:HA	17:O:91:THR:HG22	1.67	0.75
1:X:1326:U:H4'	1:X:1345:G:H4'	1.68	0.75
1:X:1974:U:H3'	1:X:1974:U:H6	1.51	0.75
26:Z:4:HIS:HB2	26:Z:5:PRO:CD	2.17	0.75
3:A:219:LYS:HD2	3:A:219:LYS:C	2.05	0.75
1:X:161:U:H4'	1:X:194:G:H21	1.51	0.75
1:X:666:U:H2'	1:X:667:U:H5''	1.67	0.75
16:N:28:ARG:HD3	16:N:38:THR:OG1	1.87	0.75
3:A:27:LYS:HE2	3:A:205:ILE:HD11	1.65	0.75
5:C:162:ARG:HG3	5:C:162:ARG:HH11	1.51	0.75
1:X:1289:A:C2	1:X:1290:A:C5	2.74	0.75
1:X:1141:U:C4	4:B:147:PRO:HD3	2.22	0.75
32:X:2882:LMA:H34B	32:X:2882:LMA:H56B	1.66	0.75
1:X:596:C:OP2	11:I:29:THR:HG22	1.86	0.75
3:A:30:PRO:C	3:A:31:GLU:OE1	2.26	0.74
1:X:817:A:H2'	1:X:819:C:C4	2.22	0.74
3:A:70:ARG:HH21	3:A:106:ILE:HG21	1.52	0.74
4:B:76:ARG:NH1	15:M:4:HIS:HB2	2.01	0.74
5:C:30:VAL:HG11	5:C:177:VAL:HG21	1.67	0.74
1:X:863:C:HO2'	25:W:19:THR:HG1	1.26	0.74
1:X:797:A:O2'	1:X:798:G:C8	2.40	0.74
10:H:100:ASN:OD1	10:H:102:GLN:N	2.12	0.74
1:X:824:U:H3'	11:I:30:ALA:HA	1.69	0.74
18:P:60:ILE:HG22	18:P:60:ILE:O	1.85	0.74
21:S:155:PRO:HG2	21:S:158:CYS:SG	2.27	0.74
1:X:2426:G:C3'	1:X:2479:U:OP2	2.33	0.74
4:B:56:GLU:HG2	4:B:74:PRO:HG2	1.69	0.74
4:B:78:LEU:O	4:B:79:ARG:CD	2.35	0.74
9:G:108:GLY:H	9:G:110:LEU:HG	1.51	0.74
21:S:13:LYS:HG2	21:S:18:MET:CB	2.16	0.74
3:A:55:ILE:HG22	3:A:55:ILE:O	1.88	0.74
1:X:679:C:H5''	11:I:49:PHE:CD1	2.23	0.74
9:G:70:PHE:CB	16:N:64:ARG:HG2	2.17	0.74
19:Q:88:ILE:CD1	19:Q:92:ALA:HB2	2.17	0.74
11:I:57:ILE:O	29:3:12:ARG:HD3	1.87	0.74
11:I:83:LEU:O	11:I:84:GLU:HB2	1.87	0.74
1:X:2781:G:C2'	1:X:2782:G:H5''	2.18	0.74
1:X:2841:U:O2'	1:X:2842:C:P	2.46	0.74
1:X:748:A:H5''	1:X:748:A:C8	2.23	0.74
3:A:102:GLU:OE2	3:A:104:ARG:CZ	2.36	0.74
1:X:37:C:H1'	5:C:44:SER:OG	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:309:G:OP1	20:R:93:ARG:C	2.26	0.74
9:G:103:TYR:HB3	9:G:107:GLN:HG2	1.70	0.74
1:X:2272:A:P	14:L:18:ARG:HH12	2.10	0.74
23:U:32:ARG:NE	23:U:32:ARG:H	1.86	0.74
1:X:1107:A:H3'	1:X:1108:U:H5''	1.70	0.74
1:X:1050:G:H1	1:X:1127:C:H42	1.33	0.74
5:C:162:ARG:HH11	5:C:162:ARG:CB	2.01	0.74
1:X:337:G:O2'	20:R:9:HIS:ND1	2.20	0.74
7:E:127:GLU:HG2	7:E:128:PRO:HD2	1.70	0.73
1:X:546:A:H4'	16:N:57:PHE:CZ	2.20	0.73
1:X:1643:A:H61	1:X:1656:U:H3	1.35	0.73
10:H:17:ARG:HE	10:H:59:ALA:HB2	1.52	0.73
15:M:34:ARG:HH11	15:M:88:VAL:HG21	1.50	0.73
21:S:13:LYS:CE	21:S:33:ALA:CB	2.66	0.73
1:X:1265:G:H1	16:N:37:GLN:HE21	1.33	0.73
11:I:18:ARG:HG2	11:I:21:ARG:HD3	1.70	0.73
1:X:2063:A:H5'	23:U:38:THR:HB	1.69	0.73
1:X:824:U:H2'	11:I:30:ALA:N	2.03	0.73
3:A:160:ALA:CB	3:A:199:ASN:ND2	2.51	0.73
1:X:1313:U:H4'	1:X:1314:A:O5'	1.89	0.73
1:X:2015:G:C4'	1:X:2016:A:OP1	2.37	0.73
5:C:46:ARG:HD2	5:C:51:VAL:HG21	1.69	0.73
16:N:59:ARG:O	16:N:63:GLN:OE1	2.07	0.73
1:X:321:A:C2	1:X:323:G:H1'	2.23	0.73
13:K:56:LYS:HE3	13:K:88:ALA:HA	1.70	0.73
2:Y:93:G:OP1	12:J:19:THR:HB	1.88	0.73
17:O:73:LYS:HB2	17:O:82:ARG:HB2	1.71	0.72
1:X:1289:A:C2	1:X:1290:A:C4	2.77	0.72
5:C:158:ARG:HE	5:C:171:PRO:HA	1.53	0.72
1:X:2840:U:C4	1:X:2841:U:C5	2.77	0.72
1:X:626:A:HO2'	5:C:176:ASN:CG	1.92	0.72
6:D:150:ARG:HA	6:D:150:ARG:HH11	1.53	0.72
1:X:2064:U:P	23:U:39:LYS:HG2	2.29	0.72
3:A:66:ILE:HG21	3:A:68:PHE:CE2	2.23	0.72
6:D:80:ARG:HD3	6:D:83:MET:HB3	1.70	0.72
12:J:135:ARG:HH22	21:S:118:HIS:CD2	2.07	0.72
18:P:107:ILE:O	18:P:107:ILE:HG23	1.88	0.72
1:X:517:A:H5''	1:X:518:A:H5'	1.70	0.72
1:X:1780:A:H5''	3:A:222:GLN:OE1	1.88	0.72
3:A:247:PRO:HG2	3:A:249:THR:O	1.89	0.72
1:X:1142:G:C1'	9:G:103:TYR:HD2	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1817:U:H4'	3:A:253:LYS:CE	2.20	0.72
1:X:400:U:OP2	23:U:37:ILE:CD1	2.34	0.72
1:X:648:A:H4'	1:X:649:G:H5'	1.72	0.72
3:A:27:LYS:HE3	3:A:205:ILE:HD13	1.69	0.72
10:H:20:MET:O	10:H:53:ALA:HB1	1.90	0.72
27:1:8:ILE:HA	27:1:29:ARG:HH21	1.54	0.72
3:A:184:ARG:NH1	3:A:184:ARG:HB3	2.05	0.72
5:C:106:MET:O	5:C:109:ALA:HB3	1.89	0.72
15:M:102:ALA:O	15:M:103:LYS:HD3	1.88	0.72
17:O:21:ARG:O	17:O:91:THR:CG2	2.38	0.72
1:X:1007:A:O3'	16:N:93:LYS:HB3	1.88	0.72
1:X:654:A:N3	1:X:654:A:H3'	2.05	0.72
8:F:120:VAL:HG12	8:F:121:GLU:N	2.05	0.72
1:X:923:A:C4	12:J:12:LYS:HE2	2.25	0.72
1:X:2736:U:H5''	30:4:19:ARG:HG2	1.71	0.72
1:X:525:A:C2'	1:X:526:C:H5'	2.20	0.72
3:A:26:THR:CG2	3:A:27:LYS:H	2.03	0.72
29:3:59:LYS:O	29:3:60:LEU:HB2	1.90	0.71
4:B:175:ILE:HG12	4:B:182:ILE:HG13	1.72	0.71
10:H:133:VAL:HG12	10:H:133:VAL:O	1.90	0.71
1:X:334:G:H2'	5:C:162:ARG:NE	2.02	0.71
1:X:609:U:H4'	11:I:18:ARG:CZ	2.20	0.71
1:X:1684:G:O2'	1:X:1974:U:O4	2.08	0.71
1:X:542:A:H8	16:N:28:ARG:HH21	1.37	0.71
3:A:22:PHE:O	3:A:209:LYS:CG	2.35	0.71
1:X:29:U:C4'	16:N:11:ARG:HH12	2.03	0.71
1:X:514:G:C5	18:P:20:LEU:HD22	2.25	0.71
12:J:27:TYR:O	12:J:28:VAL:CG2	2.39	0.71
1:X:1469:U:H5	13:K:64:ARG:HH21	1.36	0.71
13:K:54:THR:HG22	13:K:66:VAL:CG2	2.20	0.71
1:X:1437:A:H2'	1:X:1438:G:C8	2.24	0.71
1:X:1949:A:H1'	1:X:2572:U:H5'	1.72	0.71
27:1:14:SER:HB2	27:1:22:TYR:CA	2.14	0.71
1:X:6:A:H1'	9:G:162:LYS:HG3	1.71	0.71
1:X:1391:A:N7	1:X:1393:G:O6	2.17	0.71
1:X:2040:A:O5'	1:X:2040:A:H8	1.73	0.71
1:X:635:C:C2'	1:X:636:G:H5''	2.19	0.71
1:X:958:G:O2'	1:X:995:A:N1	2.24	0.71
5:C:194:GLU:O	5:C:195:ILE:HG12	1.91	0.71
11:I:61:PRO:HG3	29:3:27:SER:HA	1.72	0.71
29:3:9:MET:HE2	29:3:12:ARG:HH12	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:84:PHE:CD2	4:B:84:PHE:O	2.44	0.71
1:X:1045:G:H5'	30:4:18:ARG:HG3	1.73	0.71
1:X:755:C:H2'	1:X:756:C:C6	2.26	0.71
1:X:798:G:O2'	1:X:1770:U:C5'	2.39	0.71
6:D:123:ASP:OD1	6:D:125:ARG:N	2.23	0.71
27:1:8:ILE:C	27:1:9:ILE:HG23	2.11	0.70
11:I:62:LYS:HD2	29:3:13:ARG:N	2.06	0.70
16:N:40:LEU:HD22	17:O:74:TYR:CE1	2.25	0.70
1:X:2642:G:H2'	1:X:2643:G:O4'	1.90	0.70
31:X:2881:LC2:C2	31:X:2881:LC2:C28	2.51	0.70
1:X:703:A:O2'	1:X:793:G:OP1	2.09	0.70
26:Z:52:TYR:O	26:Z:53:ASP:HB2	1.90	0.70
12:J:44:LYS:HB2	12:J:47:GLN:HG3	1.72	0.70
20:R:92:THR:OG1	20:R:106:VAL:HB	1.91	0.70
1:X:1404:C:H5'	1:X:1405:A:OP2	1.90	0.70
3:A:55:ILE:N	3:A:55:ILE:CD1	2.54	0.70
25:W:3:ILE:HG23	25:W:51:LEU:HD13	1.73	0.70
1:X:2349:G:H21	27:1:46:LYS:HZ1	1.36	0.70
4:B:121:ASN:O	4:B:122:PHE:CB	2.39	0.70
10:H:76:ARG:O	10:H:94:ASN:HA	1.92	0.70
12:J:73:LYS:HB3	12:J:95:VAL:O	1.91	0.70
1:X:2265:A:H61	27:1:25:THR:HG21	1.57	0.70
1:X:1290:A:OP1	13:K:40:LYS:NZ	2.24	0.70
14:L:37:HIS:CD2	14:L:39:TYR:CE1	2.79	0.70
1:X:2698:G:H4'	15:M:103:LYS:HG2	1.72	0.70
9:G:70:PHE:CD1	16:N:64:ARG:HG2	2.26	0.70
20:R:91:ALA:O	20:R:108:VAL:HG22	1.91	0.70
1:X:1333:G:H22	1:X:1344:C:N4	1.88	0.70
3:A:160:ALA:HB2	3:A:199:ASN:CG	2.11	0.70
4:B:61:LYS:HB3	4:B:62:PRO:HD3	1.74	0.70
18:P:41:VAL:HG21	18:P:64:ALA:HB3	1.74	0.70
1:X:1781:C:H2'	1:X:1782:A:C5	2.26	0.70
1:X:2825:A:H2	13:K:61:HIS:CD2	2.10	0.70
11:I:18:ARG:HG3	11:I:21:ARG:HG3	1.73	0.70
10:H:113:PRO:HD3	15:M:73:PHE:HB2	1.73	0.70
1:X:6:A:H1'	9:G:162:LYS:HG2	1.71	0.70
4:B:120:TRP:CE3	4:B:155:ARG:HD2	2.27	0.70
8:F:120:VAL:HG12	8:F:121:GLU:HG3	1.73	0.70
1:X:2692:A:H5''	1:X:2693:U:OP2	1.92	0.70
12:J:77:LYS:O	12:J:79:PRO:HD3	1.91	0.69
1:X:123:A:H5'	28:2:19:ARG:CZ	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:33:ARG:HH11	14:L:100:VAL:HA	1.56	0.69
5:C:7:ILE:O	5:C:120:VAL:O	2.09	0.69
1:X:2044:G:OP1	5:C:62:LYS:HG3	1.91	0.69
3:A:154:ALA:O	3:A:158:ARG:NH2	2.25	0.69
3:A:254:PRO:O	3:A:256:LYS:HG3	1.91	0.69
1:X:116:A:OP1	28:2:22:MET:SD	2.50	0.69
1:X:1391:A:C5	1:X:1393:G:N7	2.60	0.69
1:X:755:C:H2'	1:X:756:C:H6	1.57	0.69
14:L:54:ALA:HB3	14:L:75:LEU:HD13	1.73	0.69
20:R:84:VAL:HA	20:R:90:LYS:HE2	1.74	0.69
1:X:1173:G:H2'	1:X:1174:G:C8	2.27	0.69
1:X:2274:C:OP2	14:L:11:LEU:HD21	1.92	0.69
1:X:555:U:H3'	1:X:556:A:H8	1.56	0.69
29:3:9:MET:HG2	29:3:59:LYS:O	1.92	0.69
3:A:69:LYS:H	3:A:69:LYS:CD	2.06	0.69
20:R:59:LYS:O	20:R:65:PRO:HB3	1.93	0.69
1:X:797:A:C5	3:A:230:VAL:HG21	2.27	0.69
1:X:797:A:C2	3:A:230:VAL:HG11	2.28	0.69
6:D:36:VAL:HB	6:D:89:VAL:HB	1.75	0.69
1:X:123:A:H5'	28:2:19:ARG:HH21	1.53	0.69
1:X:1459:U:H4'	1:X:1460:G:OP2	1.89	0.69
32:X:2882:LMA:O9	32:X:2882:LMA:C32	2.41	0.69
16:N:93:LYS:HD2	16:N:93:LYS:O	1.93	0.69
1:X:2012:A:C2	1:X:2016:A:C5	2.80	0.69
1:X:919:U:OP1	12:J:26:ASP:CG	2.31	0.69
3:A:70:ARG:NH2	3:A:106:ILE:HG21	2.07	0.68
1:X:2590:U:H1'	32:X:2882:LMA:H37B	1.74	0.68
1:X:2045:A:N6	32:X:2882:LMA:H32B	2.08	0.68
4:B:116:VAL:H	4:B:136:ARG:HE	1.41	0.68
4:B:60:ASN:O	4:B:64:GLN:HG3	1.94	0.68
6:D:13:ARG:HB3	6:D:14:PRO:HD3	1.74	0.68
11:I:83:LEU:O	11:I:84:GLU:CB	2.41	0.68
13:K:87:TYR:CE1	13:K:94:TYR:HD1	2.08	0.68
1:X:1327:C:H42	1:X:1351:G:H1	1.40	0.68
3:A:37:ALA:HB1	3:A:63:TYR:O	1.93	0.68
11:I:45:LYS:CE	11:I:47:ALA:HB3	2.23	0.68
1:X:1086:C:H3'	1:X:1087:C:H5''	1.73	0.68
1:X:2811:G:H2'	1:X:2812:A:C8	2.29	0.68
5:C:5:ASN:HA	5:C:118:VAL:HG23	1.74	0.68
24:V:2:LYS:N	24:V:3:PRO:CD	2.56	0.68
25:W:3:ILE:HD12	25:W:51:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2485:U:O4	31:X:2881:LC2:H30	1.93	0.68
1:X:2594:U:H2'	1:X:2594:U:O2	1.92	0.68
32:X:2882:LMA:C12	32:X:2882:LMA:C56	2.70	0.68
1:X:457:C:O2'	1:X:458:G:H5'	1.94	0.68
1:X:1628:C:H5'	28:2:7:PRO:HG2	1.76	0.68
17:O:21:ARG:NH2	17:O:88:GLN:CD	2.47	0.68
18:P:27:VAL:HB	18:P:125:THR:HG22	1.76	0.68
1:X:1750:A:O2'	1:X:2694:G:O2'	2.12	0.68
1:X:2400:G:O6	29:3:32:GLN:HG2	1.93	0.68
1:X:1686:A:O2'	1:X:2528:G:OP1	2.11	0.68
27:1:21:TYR:CD2	27:1:21:TYR:C	2.67	0.68
3:A:160:ALA:HA	3:A:199:ASN:CG	2.14	0.68
13:K:87:TYR:HD1	13:K:90:ARG:HD2	1.58	0.68
20:R:90:LYS:HD2	20:R:108:VAL:HG21	1.75	0.68
1:X:2272:A:OP2	14:L:18:ARG:NH1	2.26	0.68
1:X:2485:U:C4	31:X:2881:LC2:H30	2.29	0.68
4:B:26:VAL:CG1	4:B:196:VAL:HG21	2.24	0.68
13:K:38:LEU:HG	13:K:42:LYS:HE3	1.76	0.68
1:X:1444:C:H42	1:X:1579:G:H1	1.42	0.68
12:J:64:LYS:HD3	12:J:108:ALA:O	1.93	0.68
1:X:334:G:H4'	1:X:335:A:O5'	1.94	0.68
3:A:66:ILE:HG23	3:A:68:PHE:CE2	2.28	0.68
15:M:67:THR:OG1	15:M:80:VAL:HG22	1.94	0.68
1:X:2222:U:H2'	1:X:2223:U:C6	2.29	0.68
1:X:663:G:H3'	1:X:664:C:H5''	1.76	0.68
14:L:67:THR:O	14:L:71:VAL:HG12	1.93	0.67
1:X:1811:A:H1'	1:X:1812:U:OP2	1.94	0.67
1:X:1817:U:C4'	3:A:253:LYS:CD	2.71	0.67
1:X:526:C:O2'	1:X:527:C:H5'	1.94	0.67
9:G:158:HIS:HA	9:G:161:GLN:HG3	1.76	0.67
14:L:60:LYS:NZ	14:L:64:LYS:HE2	2.09	0.67
1:X:2571:G:C2	1:X:2582:G:C2	2.82	0.67
1:X:2692:A:C5'	1:X:2693:U:OP2	2.43	0.67
3:A:71:ARG:HG2	3:A:191:TYR:CE1	2.29	0.67
9:G:132:PHE:HD2	9:G:145:HIS:CD2	2.12	0.67
11:I:74:VAL:HG13	11:I:109:LEU:HD12	1.76	0.67
1:X:116:A:OP2	1:X:117:A:H2'	1.93	0.67
1:X:122:G:C2'	1:X:123:A:H5''	2.24	0.67
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.28	0.67
1:X:167:A:OP2	1:X:182:G:N2	2.27	0.67
14:L:37:HIS:CD2	14:L:39:TYR:CZ	2.82	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2238:G:C8	1:X:2406:C:N4	2.63	0.67
1:X:2790:C:H42	1:X:2806:G:H1	1.42	0.67
32:X:2882:LMA:H56A	32:X:2882:LMA:C57	2.24	0.67
26:Z:4:HIS:CB	26:Z:5:PRO:CD	2.73	0.67
3:A:43:GLY:H	3:A:44:ARG:NH1	1.92	0.67
1:X:1686:A:C6	1:X:1977:C:O2	2.47	0.67
1:X:2484:G:O2'	31:X:2881:LC2:H4	1.94	0.67
1:X:2796:A:H5''	4:B:162:MET:HE3	1.76	0.67
27:1:21:TYR:CD2	27:1:50:PHE:HZ	2.13	0.67
9:G:34:PRO:HB3	9:G:71:THR:HG21	1.75	0.67
18:P:79:ALA:HB1	18:P:85:MET:SD	2.35	0.67
1:X:1404:C:C4	1:X:1406:A:C8	2.82	0.67
1:X:679:C:H5''	11:I:49:PHE:CE1	2.29	0.67
1:X:762:A:H61	1:X:766:A:H2	1.43	0.67
1:X:1982:C:O2'	1:X:1983:G:H5'	1.95	0.67
1:X:2038:C:H2'	1:X:2483:U:H4'	1.75	0.67
3:A:66:ILE:CG2	3:A:68:PHE:CE1	2.78	0.67
10:H:116:ARG:HD2	15:M:38:LYS:HE3	1.74	0.67
17:O:22:VAL:HA	17:O:91:THR:CG2	2.25	0.67
1:X:239:A:H5''	1:X:621:U:H5'	1.76	0.67
3:A:30:PRO:O	3:A:31:GLU:OE1	2.13	0.66
4:B:84:PHE:CE1	4:B:86:PRO:HB2	2.29	0.66
21:S:128:ARG:HG3	21:S:129:ARG:HG3	1.77	0.66
21:S:87:THR:HB	21:S:91:PRO:HB3	1.76	0.66
1:X:1224:A:H5'	18:P:10:ASN:ND2	2.10	0.66
1:X:759:C:C2	32:X:2882:LMA:H37	2.29	0.66
4:B:6:GLY:HA3	4:B:27:LEU:O	1.94	0.66
11:I:58:ALA:O	11:I:59:ARG:CB	2.43	0.66
1:X:1265:G:O4'	16:N:33:ARG:CD	2.44	0.66
1:X:589:C:H4'	16:N:31:GLN:NE2	2.10	0.66
2:Y:83:C:C2'	2:Y:84:G:H5'	2.26	0.66
18:P:40:LEU:HB3	26:Z:25:LEU:HD13	1.77	0.66
5:C:163:ASN:HD22	5:C:163:ASN:C	1.99	0.66
1:X:1614:C:H5''	19:Q:35:LYS:HB3	1.78	0.66
21:S:25:ASN:HB3	21:S:85:MET:HB2	1.77	0.66
1:X:114:C:O2'	1:X:124:A:N3	2.27	0.66
1:X:33:C:O2	1:X:466:A:H2	1.78	0.66
1:X:851:C:O2	1:X:952:A:C2	2.48	0.66
1:X:1774:A:C2	1:X:2566:A:C5	2.84	0.66
1:X:1773:C:N3	1:X:2565:C:N4	2.43	0.66
1:X:2664:G:N2	1:X:2706:U:O2	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:44:ARG:HE	3:A:56:GLY:HA2	1.61	0.66
4:B:67:PHE:CZ	4:B:75:THR:HG22	2.31	0.66
7:E:172:LYS:O	7:E:173:ALA:HB3	1.94	0.66
12:J:105:PHE:C	12:J:106:GLU:OE2	2.33	0.66
14:L:26:ARG:O	14:L:45:ASP:HB3	1.94	0.66
20:R:92:THR:HG22	20:R:108:VAL:HG22	1.77	0.66
2:Y:84:G:N1	2:Y:98:C:C2	2.64	0.66
6:D:106:ILE:HG21	6:D:139:PRO:HB3	1.77	0.66
15:M:99:VAL:HG21	15:M:104:LEU:CD2	2.26	0.66
1:X:128:C:H2'	1:X:129:A:H5''	1.77	0.66
1:X:1290:A:H4'	13:K:20:LEU:HD11	1.78	0.66
1:X:48:A:H8	1:X:50:G:H21	1.43	0.66
1:X:2218:G:O4'	3:A:250:PRO:HG3	1.96	0.66
1:X:2462:C:O2	12:J:125:LYS:NZ	2.28	0.66
1:X:991:A:C2	1:X:1146:G:H4'	2.30	0.66
1:X:1391:A:N3	1:X:1392:U:H3'	2.10	0.66
5:C:14:THR:HG21	5:C:195:ILE:HB	1.78	0.66
11:I:18:ARG:CG	11:I:21:ARG:CB	2.74	0.66
13:K:51:LEU:HD21	13:K:70:ILE:HD11	1.77	0.66
16:N:20:ARG:HH12	17:O:83:ARG:HH22	1.44	0.66
3:A:159:SER:OG	3:A:160:ALA:N	2.28	0.65
7:E:139:GLN:O	7:E:143:GLN:HG3	1.96	0.65
9:G:89:ALA:C	9:G:90:LEU:HD12	2.17	0.65
12:J:37:ALA:HA	12:J:130:THR:HG22	1.77	0.65
1:X:1712:G:C2'	1:X:1713:G:H5'	2.25	0.65
1:X:1770:U:OP2	1:X:1775:A:N6	2.29	0.65
1:X:227:G:OP2	29:3:8:LYS:HG2	1.96	0.65
1:X:2464:G:H4'	12:J:125:LYS:O	1.95	0.65
3:A:201:GLU:HG3	3:A:203:LYS:H	1.61	0.65
4:B:133:LYS:HG3	4:B:137:ARG:CD	2.21	0.65
16:N:93:LYS:HZ1	17:O:10:LYS:HE2	1.60	0.65
1:X:1948:C:C5	1:X:1949:A:N7	2.65	0.65
3:A:54:PHE:HB2	3:A:55:ILE:HD13	1.78	0.65
1:X:797:A:O2'	1:X:798:G:N7	2.29	0.65
10:H:116:ARG:HH21	15:M:40:ARG:HB2	1.62	0.65
12:J:66:TYR:O	12:J:106:GLU:OE1	2.14	0.65
1:X:2668:U:O2	1:X:2693:U:O5'	2.14	0.65
1:X:834:A:C2'	1:X:957:G:OP2	2.45	0.65
4:B:146:THR:HB	4:B:147:PRO:HD2	1.79	0.65
18:P:32:ARG:HA	18:P:32:ARG:HE	1.61	0.65
1:X:923:A:C5	12:J:12:LYS:HE2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:116:ASN:OD1	8:F:117:ALA:N	2.30	0.65
10:H:26:ASN:ND2	10:H:26:ASN:O	2.30	0.65
15:M:56:ALA:HB3	15:M:67:THR:N	2.12	0.65
1:X:1445:A:C2	1:X:1579:G:C2	2.84	0.65
3:A:211:GLY:HA2	3:A:214:ARG:HG2	1.78	0.65
3:A:66:ILE:HD12	3:A:89:ARG:CZ	2.27	0.65
5:C:151:VAL:HG12	5:C:173:ALA:HA	1.78	0.65
12:J:136:GLU:O	12:J:136:GLU:HG2	1.95	0.65
16:N:25:TRP:CE3	16:N:26:GLY:CA	2.80	0.65
1:X:1607:A:N3	1:X:1608:U:O4'	2.30	0.65
1:X:764:A:O5'	1:X:764:A:H8	1.80	0.65
10:H:75:VAL:HG22	10:H:96:ALA:HA	1.79	0.65
12:J:13:GLN:O	12:J:74:PRO:CG	2.44	0.65
13:K:79:VAL:O	13:K:84:ALA:HB2	1.97	0.65
21:S:51:LEU:H	21:S:51:LEU:HD23	1.61	0.65
1:X:357:A:H2'	1:X:358:C:H5'	1.78	0.65
1:X:748:A:N6	1:X:749:C:O2	2.30	0.65
1:X:995:A:P	1:X:996:C:H41	2.20	0.65
4:B:122:PHE:HZ	4:B:155:ARG:HB2	1.61	0.65
20:R:58:VAL:HG12	20:R:60:PRO:HD3	1.79	0.65
1:X:2005:U:C6	1:X:2005:U:OP2	2.47	0.65
1:X:2501:U:H6	1:X:2501:U:H5''	1.60	0.65
15:M:67:THR:HA	15:M:79:ARG:O	1.97	0.65
22:T:45:PHE:HA	22:T:77:ARG:HB2	1.77	0.65
5:C:152:THR:CG2	5:C:157:THR:HG21	2.27	0.64
1:X:1991:C:H2'	1:X:1992:G:H8	1.63	0.64
27:1:26:LYS:HG2	27:1:28:ARG:HH21	1.60	0.64
4:B:47:VAL:CG2	4:B:84:PHE:O	2.45	0.64
16:N:28:ARG:O	16:N:35:ALA:HB2	1.97	0.64
17:O:58:ALA:HB2	17:O:95:ILE:HD13	1.79	0.64
1:X:1704:G:N2	1:X:1719:G:C6	2.65	0.64
1:X:1974:U:C6	1:X:1974:U:H3'	2.32	0.64
1:X:2045:A:N6	32:X:2882:LMA:C32	2.60	0.64
1:X:317:U:C2'	1:X:318:G:H5'	2.27	0.64
21:S:127:PRO:O	21:S:128:ARG:HG2	1.97	0.64
23:U:19:ILE:HG22	23:U:42:GLN:HG3	1.79	0.64
1:X:1074:G:H1	1:X:1086:C:N4	1.96	0.64
32:X:2882:LMA:C12	32:X:2882:LMA:H56A	2.22	0.64
1:X:818:G:N2	1:X:842:A:OP1	2.30	0.64
6:D:22:TYR:CD2	6:D:28:VAL:HG22	2.32	0.64
1:X:493:A:H4'	20:R:56:LYS:HE3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1939:U:O2	1:X:2531:U:OP1	2.15	0.64
1:X:1685:A:N6	1:X:1974:U:C2	2.48	0.64
1:X:2398:U:OP2	29:3:41:ILE:HG21	1.98	0.64
4:B:87:ASP:OD2	4:B:87:ASP:N	2.30	0.64
14:L:60:LYS:HZ3	14:L:64:LYS:HE2	1.62	0.64
1:X:1333:G:H22	1:X:1344:C:H41	1.43	0.64
1:X:223:C:N4	29:3:7:HIS:HB3	2.12	0.64
1:X:2571:G:H1	1:X:2580:C:H42	1.45	0.64
1:X:2630:C:O2'	1:X:2631:C:H5'	1.98	0.64
1:X:2676:G:C2	1:X:2690:A:C2	2.86	0.64
1:X:466:A:H4'	1:X:467:U:O5'	1.97	0.64
1:X:992:A:C2	1:X:2011:U:O4'	2.51	0.64
6:D:175:LEU:HD12	6:D:176:PRO:HD2	1.80	0.64
9:G:70:PHE:CB	16:N:64:ARG:HE	2.11	0.64
1:X:1238:A:H5'	17:O:85:GLY:N	2.10	0.64
1:X:333:A:H5'	5:C:162:ARG:HG2	1.80	0.64
1:X:48:A:H4'	1:X:49:U:O5'	1.98	0.64
1:X:623:G:H21	1:X:626:A:H2	1.43	0.64
29:3:29:LYS:HE3	29:3:34:THR:HB	1.80	0.64
7:E:103:LEU:HD21	7:E:131:ILE:HD13	1.80	0.64
11:I:108:LEU:HD22	11:I:120:VAL:HG11	1.80	0.64
1:X:596:C:N4	11:I:36:GLY:HA3	2.12	0.64
16:N:93:LYS:HE3	17:O:5:ILE:HG21	1.79	0.64
20:R:59:LYS:HD2	20:R:62:MET:HG3	1.80	0.64
21:S:155:PRO:CG	21:S:158:CYS:SG	2.86	0.64
23:U:20:ARG:HD3	23:U:43:ARG:NH2	2.12	0.64
1:X:1676:U:H2'	1:X:1677:C:O5'	1.97	0.64
1:X:512:A:H4'	18:P:15:LYS:HB3	1.79	0.64
4:B:6:GLY:HA2	4:B:51:TYR:CE1	2.32	0.64
1:X:2046:C:C5	1:X:2047:C:C4	2.85	0.64
1:X:321:A:N1	1:X:323:G:H1'	2.13	0.64
1:X:605:G:H2'	1:X:606:A:H8	1.63	0.64
1:X:712:A:H2'	1:X:713:G:O4'	1.98	0.64
11:I:57:ILE:HG23	29:3:12:ARG:NH1	2.13	0.64
4:B:120:TRP:HB2	4:B:122:PHE:CE2	2.33	0.64
5:C:47:THR:HG23	5:C:85:GLY:H	1.62	0.64
13:K:73:LYS:O	13:K:76:VAL:HG12	1.97	0.64
1:X:1265:G:O2'	1:X:1266:G:C8	2.51	0.64
1:X:1683:G:N2	1:X:1978:U:N3	2.45	0.64
1:X:1790:G:H4'	1:X:1791:C:O5'	1.94	0.64
1:X:1918:G:H1'	1:X:1947:G:N2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:993:C:H5''	1:X:994:A:OP2	1.98	0.64
1:X:2036:G:OP1	4:B:144:ARG:HG3	1.97	0.63
1:X:2663:U:C5'	15:M:80:VAL:HG11	2.28	0.63
1:X:2663:U:O4	1:X:2664:G:C6	2.51	0.63
4:B:120:TRP:CD1	4:B:155:ARG:HB3	2.33	0.63
1:X:123:A:H5''	28:2:19:ARG:HH21	1.62	0.63
1:X:1333:G:N2	1:X:1344:C:H41	1.96	0.63
1:X:2502:G:H8	1:X:2502:G:O5'	1.79	0.63
4:B:150:VAL:HG21	4:B:154:LYS:HE2	1.79	0.63
1:X:122:G:H2'	1:X:123:A:H5''	1.79	0.63
1:X:1391:A:C6	1:X:1393:G:C4	2.86	0.63
1:X:540:G:C6	1:X:2005:U:O5'	2.51	0.63
1:X:555:U:H3'	1:X:556:A:C8	2.33	0.63
1:X:760:U:C4	26:Z:3:LYS:HG3	2.33	0.63
9:G:132:PHE:HB2	9:G:145:HIS:CD2	2.33	0.63
10:H:22:ILE:HG13	10:H:53:ALA:HA	1.79	0.63
28:2:8:ASN:OD1	28:2:10:ARG:HG2	1.99	0.63
3:A:33:ALA:HB3	3:A:84:GLU:OE1	1.97	0.63
1:X:2796:A:H5''	4:B:162:MET:CE	2.28	0.63
1:X:764:A:O4'	18:P:111:ARG:HA	1.99	0.63
23:U:60:VAL:HG23	23:U:61:TRP:N	2.13	0.63
1:X:590:C:H2'	1:X:591:G:C8	2.33	0.63
1:X:998:C:N4	1:X:999:A:C6	2.66	0.63
15:M:17:GLU:HG3	15:M:62:SER:HB2	1.80	0.63
1:X:1981:A:O2'	1:X:1982:C:H5'	1.98	0.63
1:X:2200:G:H2'	1:X:2201:G:C8	2.34	0.63
1:X:2849:C:H2'	1:X:2850:U:H5'	1.81	0.63
4:B:100:GLU:O	4:B:172:VAL:HG23	1.99	0.63
4:B:44:TYR:HB2	4:B:82:ARG:HH12	1.63	0.63
4:B:85:ALA:N	4:B:86:PRO:CD	2.60	0.63
10:H:23:ARG:HB3	10:H:23:ARG:HH21	1.63	0.63
1:X:2272:A:C5'	14:L:15:ARG:HH21	2.08	0.63
15:M:9:ARG:HA	15:M:12:LEU:HD12	1.80	0.63
1:X:1242:A:O2'	1:X:1243:G:H5'	1.98	0.63
1:X:1584:G:H5''	3:A:62:LEU:HG	1.79	0.63
1:X:2257:A:N6	22:T:15:ASP:CG	2.51	0.63
1:X:2478:C:O5'	1:X:2478:C:C6	2.44	0.63
1:X:1681:A:C2	1:X:2706:U:H1'	2.33	0.63
16:N:66:ASN:CB	16:N:76:TYR:HB2	2.18	0.63
1:X:2660:C:C2	1:X:2704:U:O4	2.52	0.63
1:X:819:C:OP2	11:I:41:SER:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:43:VAL:O	27:1:44:ALA:HB2	1.99	0.63
14:L:33:ARG:HH12	14:L:103:LEU:HB2	1.64	0.63
20:R:20:ASP:O	20:R:22:VAL:HG23	1.99	0.63
1:X:1008:G:C2	1:X:1170:U:O2	2.52	0.63
1:X:2007:G:N2	1:X:2023:C:C2	2.67	0.63
1:X:2266:A:O2'	1:X:2267:A:H2'	1.99	0.63
1:X:2500:C:C6	1:X:2500:C:O5'	2.47	0.63
6:D:60:ILE:HG22	6:D:140:GLU:HB2	1.80	0.62
13:K:33:ARG:HG3	13:K:114:GLU:HB3	1.81	0.62
4:B:182:ILE:C	4:B:183:LEU:HD23	2.19	0.62
1:X:2013:A:H4'	1:X:2014:A:H8	1.63	0.62
1:X:486:U:C2	1:X:492:G:N2	2.67	0.62
1:X:1296:G:N2	1:X:1299:A:H5''	2.14	0.62
1:X:2720:A:N6	1:X:2721:A:C6	2.68	0.62
1:X:966:A:N6	1:X:967:G:C6	2.68	0.62
28:2:1:MET:O	28:2:2:LYS:C	2.36	0.62
3:A:207:LEU:HA	3:A:212:ARG:HH11	1.65	0.62
5:C:21:GLU:C	5:C:22:VAL:HG23	2.19	0.62
9:G:93:LYS:HD3	9:G:93:LYS:N	2.15	0.62
1:X:1142:G:N3	9:G:103:TYR:CD2	2.67	0.62
1:X:1683:G:O5'	1:X:1683:G:H8	1.82	0.62
1:X:166:G:H21	1:X:184:A:H62	1.44	0.62
1:X:1938:U:H4'	1:X:1939:U:OP2	1.96	0.62
1:X:959:C:H1'	1:X:995:A:C2	2.35	0.62
5:C:162:ARG:HD2	5:C:162:ARG:C	2.20	0.62
4:B:152:LYS:HB2	9:G:106:TYR:HB3	1.80	0.62
11:I:18:ARG:HG3	11:I:21:ARG:CG	2.28	0.62
1:X:1164:C:H5'	16:N:76:TYR:HE2	1.63	0.62
1:X:717:G:N3	1:X:739:G:C2	2.67	0.62
29:3:49:VAL:HG11	29:3:52:LYS:HD3	1.82	0.62
3:A:78:ALA:HB2	3:A:98:TYR:HD1	1.64	0.62
21:S:3:LEU:HD23	21:S:56:VAL:HG22	1.82	0.62
1:X:552:C:C2'	1:X:553:C:H5''	2.29	0.62
1:X:571:U:O2'	1:X:581:A:H5'	2.00	0.62
1:X:2264:C:OP2	27:1:28:ARG:NH1	2.33	0.62
3:A:49:ARG:CZ	3:A:49:ARG:HB3	2.30	0.62
9:G:162:LYS:N	9:G:163:PRO:CD	2.63	0.62
20:R:23:ILE:HD12	20:R:23:ILE:C	2.20	0.62
1:X:1380:C:H42	1:X:1799:A:H2	1.48	0.62
1:X:1471:G:O2'	1:X:1472:C:H5'	2.00	0.62
1:X:2045:A:H61	32:X:2882:LMA:C32	2.09	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2201:G:H2'	1:X:2202:G:H8	1.64	0.62
1:X:2710:C:O2'	1:X:2711:G:H5'	1.99	0.62
32:X:2882:LMA:H34B	32:X:2882:LMA:C56	2.27	0.62
1:X:699:G:O6	28:2:12:ARG:CA	2.39	0.62
27:1:41:ASP:CG	27:1:46:LYS:HD2	2.18	0.62
11:I:60:LEU:HD21	29:3:13:ARG:HG2	1.80	0.62
1:X:1291:G:C5'	13:K:34:ILE:HD12	2.29	0.62
1:X:1392:U:H6	1:X:1392:U:O5'	1.82	0.62
3:A:39:PRO:HA	3:A:62:LEU:HD22	1.82	0.62
15:M:33:VAL:CG2	15:M:51:GLU:HB2	2.19	0.62
1:X:67:G:N2	1:X:73:A:N3	2.48	0.62
17:O:75:LYS:O	17:O:78:VAL:HG12	1.99	0.62
22:T:23:VAL:HG13	22:T:38:VAL:HG22	1.81	0.62
1:X:2430:A:OP1	1:X:2476:A:N6	2.30	0.62
1:X:872:G:H22	1:X:928:G:H2'	1.65	0.62
4:B:120:TRP:O	4:B:122:PHE:HD2	1.82	0.61
21:S:113:VAL:HG22	21:S:171:VAL:HG22	1.81	0.61
1:X:1018:C:H3'	1:X:1019:U:C5'	2.28	0.61
1:X:1260:A:O2'	1:X:1261:G:H3'	2.00	0.61
1:X:1677:C:O2	1:X:1984:A:C2	2.52	0.61
1:X:2736:U:H3	1:X:2738:A:H62	1.46	0.61
1:X:567:G:H5'	9:G:140:GLN:OE1	2.00	0.61
1:X:679:C:C5'	11:I:49:PHE:CE1	2.82	0.61
4:B:84:PHE:CZ	4:B:86:PRO:HB2	2.35	0.61
6:D:123:ASP:OD2	6:D:127:ASN:HB2	1.99	0.61
16:N:58:ARG:O	16:N:62:ILE:HG13	2.01	0.61
1:X:537:C:C5	1:X:2759:U:H2'	2.35	0.61
1:X:840:U:H4'	1:X:841:G:C2	2.34	0.61
29:3:60:LEU:HD12	29:3:63:PRO:HG2	1.82	0.61
1:X:1147:G:H2'	1:X:1148:G:C8	2.36	0.61
4:B:154:LYS:CE	4:B:156:MET:SD	2.88	0.61
1:X:1092:U:C4'	8:F:122:ALA:HB1	2.05	0.61
1:X:1182:U:C4'	1:X:1183:C:OP1	2.47	0.61
1:X:1714:A:H5''	1:X:1715:A:H2'	1.80	0.61
1:X:2199:C:H2'	1:X:2200:G:H5'	1.81	0.61
1:X:798:G:O2'	1:X:1770:U:H5'	1.99	0.61
12:J:81:GLU:HG2	12:J:82:THR:HG23	1.82	0.61
1:X:1179:A:C2	1:X:1196:G:C2	2.88	0.61
1:X:1671:A:H5''	1:X:1671:A:H8	1.65	0.61
1:X:192:G:H4'	1:X:193:A:OP1	1.99	0.61
1:X:2349:G:H21	27:1:46:LYS:HZ2	1.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1797:C:H4'	3:A:49:ARG:HD3	1.82	0.61
26:Z:3:LYS:HD3	26:Z:3:LYS:N	2.16	0.61
15:M:32:THR:HG23	15:M:93:ILE:CD1	2.31	0.61
1:X:592:G:OP2	16:N:10:ARG:HD2	2.00	0.61
1:X:94:C:H1'	24:V:40:PRO:HG2	1.83	0.61
1:X:2429:A:C6	1:X:2430:A:N6	2.69	0.61
26:Z:52:TYR:O	26:Z:53:ASP:CB	2.48	0.61
3:A:66:ILE:CD1	3:A:107:LEU:HG	2.30	0.61
3:A:69:LYS:N	3:A:69:LYS:HD3	2.14	0.61
12:J:81:GLU:O	12:J:82:THR:OG1	2.19	0.61
1:X:2257:A:H62	22:T:15:ASP:CG	2.03	0.61
1:X:123:A:H5'	28:2:19:ARG:NE	2.16	0.61
1:X:1774:A:C2	1:X:2566:A:C4	2.89	0.61
1:X:303:C:H2'	1:X:304:A:H5''	1.82	0.61
2:Y:85:G:O6	2:Y:86:A:C6	2.53	0.61
1:X:2399:C:OP2	29:3:34:THR:HG23	2.00	0.61
20:R:18:LYS:H	20:R:18:LYS:CD	2.10	0.61
1:X:1429:A:H1'	1:X:1603:A:C6	2.35	0.61
1:X:1811:A:H4'	1:X:1812:U:O5'	2.01	0.61
1:X:224:G:C2	1:X:229:G:C6	2.88	0.61
4:B:93:VAL:C	4:B:95:ILE:H	2.04	0.61
5:C:152:THR:HG23	5:C:153:ASP:O	2.01	0.61
1:X:1817:U:O4'	3:A:253:LYS:CD	2.49	0.61
3:A:160:ALA:HB1	3:A:199:ASN:HB3	1.82	0.60
20:R:83:LEU:O	20:R:90:LYS:HE2	2.01	0.60
1:X:1508:G:H5'	1:X:1509:A:H5''	1.82	0.60
1:X:1817:U:O4'	3:A:253:LYS:HD2	2.00	0.60
1:X:1755:G:C6	1:X:1972:G:C2	2.89	0.60
1:X:2006:G:N2	1:X:2024:U:C2	2.69	0.60
1:X:459:A:N6	1:X:484:G:C4	2.69	0.60
1:X:746:G:N2	1:X:747:A:N6	2.49	0.60
4:B:136:ARG:CG	4:B:137:ARG:H	2.13	0.60
12:J:44:LYS:HA	12:J:95:VAL:HG22	1.81	0.60
1:X:1683:G:O2'	1:X:1684:G:H5'	2.01	0.60
1:X:762:A:H2	1:X:766:A:O2'	1.77	0.60
16:N:40:LEU:HD22	17:O:74:TYR:CD1	2.35	0.60
1:X:1466:C:O2'	1:X:1467:U:O4'	2.19	0.60
1:X:1764:A:H2'	1:X:1765:C:H5'	1.82	0.60
1:X:2840:U:O4	1:X:2841:U:C4	2.54	0.60
1:X:494:A:C8	1:X:495:C:C5	2.88	0.60
3:A:71:ARG:HH12	3:A:150:PRO:CB	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:248:VAL:CG2	3:A:249:THR:HG23	2.28	0.60
6:D:40:LEU:HD23	6:D:41:GLY:CA	2.31	0.60
10:H:23:ARG:CB	10:H:23:ARG:HH21	2.15	0.60
11:I:18:ARG:HB2	11:I:21:ARG:CB	2.17	0.60
1:X:1701:C:C2	1:X:1722:G:N2	2.70	0.60
1:X:2663:U:H5''	15:M:80:VAL:HG11	1.82	0.60
1:X:749:C:H3'	1:X:749:C:C6	2.36	0.60
4:B:9:ILE:HG23	15:M:9:ARG:HB2	1.83	0.60
10:H:14:SER:OG	10:H:98:ILE:HD12	2.02	0.60
1:X:1223:G:C4'	1:X:1224:A:OP2	2.50	0.60
3:A:147:GLU:HB2	3:A:190:CYS:HB3	1.84	0.60
19:Q:7:LEU:CD2	19:Q:7:LEU:C	2.69	0.60
1:X:615:C:H4'	1:X:669:G:N2	2.16	0.60
1:X:795:A:N1	3:A:227:MET:CE	2.64	0.60
11:I:55:ARG:O	11:I:57:ILE:N	2.29	0.60
14:L:42:ILE:O	14:L:50:THR:HG23	2.01	0.60
14:L:54:ALA:CB	14:L:75:LEU:HD13	2.32	0.60
18:P:37:LYS:HE2	18:P:64:ALA:HB2	1.84	0.60
1:X:1496:G:C4'	1:X:1497:C:OP1	2.50	0.60
1:X:1661:C:O2'	1:X:1662:G:H5'	2.01	0.60
1:X:1681:A:C2	1:X:2706:U:C1'	2.84	0.60
1:X:2840:U:C4	1:X:2841:U:C4	2.89	0.60
1:X:304:A:H62	1:X:356:A:N6	1.98	0.60
1:X:1674:C:OP1	4:B:136:ARG:O	2.20	0.60
6:D:13:ARG:HA	6:D:16:LEU:HD12	1.84	0.60
6:D:38:GLU:HG2	6:D:87:ILE:HD12	1.82	0.60
14:L:37:HIS:HE1	14:L:57:ALA:HB2	1.67	0.60
14:L:96:TYR:CZ	14:L:101:LYS:HG3	2.36	0.60
1:X:1625:A:H1'	1:X:1632:A:H1'	1.84	0.60
1:X:1685:A:O4'	1:X:1686:A:N1	2.34	0.60
1:X:1998:A:C2	26:Z:5:PRO:O	2.53	0.60
1:X:749:C:C3'	1:X:749:C:C6	2.85	0.60
3:A:32:LYS:HE3	3:A:34:LEU:HB2	1.82	0.60
5:C:34:GLN:O	5:C:38:ARG:HG3	2.01	0.60
11:I:72:TYR:HB3	11:I:107:LYS:HB2	1.83	0.60
15:M:34:ARG:CD	15:M:88:VAL:HG22	2.20	0.60
18:P:11:LYS:HA	18:P:14:ARG:HH12	1.65	0.60
1:X:1656:U:H2'	1:X:1657:A:C5'	2.32	0.60
28:2:25:LYS:HE2	28:2:25:LYS:HA	1.83	0.60
3:A:159:SER:O	3:A:197:VAL:HG21	2.02	0.60
10:H:19:ILE:CG1	10:H:19:ILE:O	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:38:PRO:HA	25:W:41:ARG:HD2	1.83	0.60
1:X:1173:G:H4'	17:O:22:VAL:CG2	2.29	0.60
1:X:1182:U:H4'	1:X:1183:C:OP1	2.02	0.60
1:X:1919:A:N7	1:X:1928:G:C6	2.70	0.60
1:X:2720:A:C6	1:X:2721:A:C6	2.89	0.60
29:3:13:ARG:NE	29:3:25:PHE:H	1.99	0.59
3:A:232:HIS:CG	3:A:233:PRO:HD2	2.37	0.59
1:X:583:C:O2	4:B:145:LYS:NZ	2.35	0.59
5:C:177:VAL:O	5:C:180:ILE:HG22	2.01	0.59
1:X:2464:G:C4'	12:J:125:LYS:O	2.50	0.59
14:L:36:LYS:HE3	14:L:64:LYS:O	2.02	0.59
1:X:1407:G:O6	1:X:1408:A:N6	2.34	0.59
1:X:2663:U:O2'	10:H:88:THR:CG2	2.43	0.59
3:A:59:HIS:C	3:A:61:ARG:H	2.05	0.59
1:X:2170:C:H3'	1:X:2171:U:C5'	2.24	0.59
1:X:2564:U:O4	31:X:2881:LC2:H14A	2.03	0.59
1:X:487:G:H4'	1:X:512:A:N1	2.17	0.59
2:Y:83:C:H2'	2:Y:84:G:O5'	2.02	0.59
27:1:14:SER:CB	27:1:23:THR:H	2.13	0.59
29:3:13:ARG:CZ	29:3:25:PHE:H	2.15	0.59
25:W:2:LYS:HE2	25:W:31:SER:HB2	1.84	0.59
1:X:1466:C:H42	1:X:1476:G:H1	1.51	0.59
1:X:1407:G:H4'	1:X:1619:A:H4'	1.83	0.59
1:X:2841:U:H1'	1:X:2843:A:O4'	2.03	0.59
1:X:793:G:C2	1:X:798:G:O6	2.55	0.59
1:X:693:A:C4	1:X:811:G:N2	2.70	0.59
1:X:1277:G:OP1	26:Z:19:ARG:NH2	2.35	0.59
3:A:97:HIS:CE1	3:A:101:GLY:HA2	2.38	0.59
5:C:158:ARG:NE	5:C:171:PRO:HA	2.16	0.59
1:X:2760:G:N1	9:G:128:GLU:OE2	2.35	0.59
10:H:110:VAL:HG23	10:H:129:LEU:CB	2.32	0.59
29:3:46:LYS:HE3	29:3:46:LYS:HA	1.83	0.59
1:X:1817:U:H4'	3:A:253:LYS:CD	2.31	0.59
4:B:6:GLY:CA	4:B:27:LEU:O	2.50	0.59
10:H:51:ILE:HG13	10:H:51:ILE:O	2.03	0.59
1:X:123:A:C5'	28:2:19:ARG:HE	2.16	0.59
1:X:2824:C:O4'	1:X:2843:A:C6	2.55	0.59
1:X:583:C:O2	4:B:145:LYS:CE	2.51	0.59
1:X:2349:G:N2	27:1:46:LYS:NZ	2.48	0.59
1:X:1432:G:O6	1:X:1594:U:H5''	2.03	0.59
1:X:824:U:H2'	11:I:30:ALA:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:57:ILE:O	29:3:12:ARG:CD	2.51	0.59
1:X:583:C:C2	4:B:145:LYS:NZ	2.71	0.59
12:J:42:TRP:HB3	12:J:95:VAL:CG1	2.33	0.59
1:X:2064:U:C5'	23:U:41:VAL:HG11	2.28	0.59
1:X:1764:A:C2'	1:X:1765:C:H5'	2.33	0.59
1:X:709:A:C2	1:X:780:U:C2	2.90	0.59
4:B:170:LEU:HD22	4:B:185:LYS:O	2.01	0.59
17:O:21:ARG:NH2	17:O:88:GLN:NE2	2.51	0.59
1:X:2268:G:H5''	1:X:2363:G:O2'	2.03	0.59
1:X:2616:U:H5''	4:B:82:ARG:NH2	2.17	0.59
2:Y:84:G:C2	2:Y:98:C:O2	2.55	0.59
3:A:109:PRO:HB3	3:A:144:HIS:CE1	2.38	0.59
11:I:18:ARG:HG3	11:I:21:ARG:HB2	1.84	0.59
13:K:51:LEU:HD11	13:K:66:VAL:HG13	1.84	0.59
4:B:181:LEU:HD21	15:M:12:LEU:HD22	1.85	0.59
21:S:71:MET:N	21:S:71:MET:SD	2.74	0.59
1:X:2064:U:OP1	23:U:39:LYS:HG2	2.03	0.59
1:X:2500:C:N3	1:X:2501:U:C4	2.71	0.59
1:X:1042:G:H5'	30:4:6:SER:HG	1.68	0.59
12:J:50:ALA:HB1	12:J:125:LYS:CD	2.29	0.59
13:K:87:TYR:CE1	13:K:94:TYR:CD1	2.88	0.59
32:X:2882:LMA:C54	32:X:2882:LMA:H34B	2.33	0.59
1:X:460:U:C4	1:X:592:G:H1'	2.37	0.59
5:C:194:GLU:HG2	5:C:195:ILE:HG23	1.83	0.58
5:C:7:ILE:HG12	5:C:119:ALA:HB1	1.85	0.58
16:N:20:ARG:NH1	17:O:83:ARG:HH22	2.00	0.58
1:X:2261:G:C4	1:X:2404:A:N6	2.71	0.58
2:Y:85:G:H5'	25:W:49:HIS:CD2	2.37	0.58
1:X:2399:C:H41	29:3:31:HIS:C	2.07	0.58
3:A:59:HIS:O	3:A:61:ARG:N	2.36	0.58
5:C:6:VAL:HG12	5:C:7:ILE:HD13	1.85	0.58
10:H:23:ARG:NH1	10:H:25:LEU:HD23	2.14	0.58
1:X:1265:G:N1	16:N:37:GLN:HB2	2.18	0.58
1:X:2033:C:N4	1:X:2034:A:C6	2.71	0.58
1:X:681:A:H8	1:X:681:A:H5''	1.68	0.58
3:A:70:ARG:HG2	3:A:70:ARG:O	2.03	0.58
8:F:112:MET:HB2	8:F:113:PRO:HD3	1.85	0.58
11:I:62:LYS:HD3	29:3:12:ARG:C	2.23	0.58
20:R:84:VAL:O	20:R:84:VAL:CG2	2.51	0.58
1:X:1234:C:O2	1:X:1242:A:C2	2.56	0.58
32:X:2882:LMA:C40	32:X:2882:LMA:H29B	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:146:LEU:HD23	3:A:156:LEU:HD12	1.85	0.58
1:X:795:A:C6	3:A:227:MET:HE3	2.38	0.58
9:G:84:ASN:O	9:G:85:ALA:HB3	2.02	0.58
22:T:17:ASN:O	22:T:19:LYS:HG2	2.03	0.58
1:X:1724:C:C2	1:X:1747:G:N1	2.72	0.58
1:X:1724:C:C2	1:X:1747:G:C6	2.91	0.58
1:X:2034:A:C2	1:X:2593:A:C2	2.91	0.58
1:X:2691:C:O2'	1:X:2693:U:H5'	2.03	0.58
1:X:2841:U:C1'	1:X:2843:A:O4'	2.51	0.58
1:X:2825:A:OP2	1:X:2843:A:N3	2.36	0.58
1:X:458:G:H4'	1:X:459:A:H5'	1.84	0.58
2:Y:84:G:O2'	2:Y:85:G:C5'	2.51	0.58
27:1:39:LYS:HD3	27:1:39:LYS:O	2.03	0.58
4:B:143:GLN:NE2	4:B:143:GLN:N	2.51	0.58
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.84	0.58
19:Q:68:PHE:O	19:Q:69:ILE:HD12	2.04	0.58
1:X:1202:U:H2'	1:X:1202:U:O2	2.04	0.58
1:X:165:G:H1	1:X:185:C:H42	1.51	0.58
1:X:1717:A:H2'	1:X:1718:A:H5'	1.86	0.58
1:X:219:G:N2	1:X:232:A:OP2	2.35	0.58
1:X:860:U:H3'	1:X:860:U:O2	2.04	0.58
26:Z:16:ARG:HD3	26:Z:20:ARG:CZ	2.34	0.58
27:1:21:TYR:CD2	27:1:50:PHE:CZ	2.91	0.58
4:B:136:ARG:O	4:B:137:ARG:CB	2.51	0.58
10:H:105:PRO:HG3	10:H:126:ILE:HD13	1.85	0.58
14:L:28:ARG:HH21	14:L:43:ILE:HG21	1.69	0.58
1:X:1791:C:OP2	3:A:264:ARG:HG3	2.03	0.58
1:X:2501:U:O2'	1:X:2626:U:H5''	2.03	0.58
1:X:2532:G:H1'	1:X:2561:G:H21	1.69	0.58
1:X:323:G:OP1	1:X:343:A:H5'	2.03	0.58
1:X:788:G:O2'	1:X:789:G:OP2	2.20	0.58
27:1:21:TYR:HD2	27:1:21:TYR:C	2.07	0.58
3:A:71:ARG:HH22	3:A:190:CYS:HA	1.65	0.58
1:X:2805:G:H5''	4:B:58:LYS:NZ	2.18	0.58
12:J:27:TYR:O	12:J:28:VAL:HG23	2.03	0.58
13:K:36:THR:HG22	13:K:41:ALA:HB2	1.86	0.58
15:M:32:THR:HG23	15:M:93:ILE:HD13	1.86	0.58
15:M:55:ILE:HB	15:M:103:LYS:O	2.04	0.58
9:G:70:PHE:HB3	16:N:64:ARG:HG2	1.83	0.58
19:Q:7:LEU:HD22	19:Q:7:LEU:O	2.04	0.58
1:X:839:U:H5''	1:X:2408:G:OP2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2447:G:HO2'	1:X:2448:A:H8	1.50	0.58
1:X:76:C:C2	1:X:108:G:N2	2.72	0.58
1:X:796:A:C2	1:X:1769:U:O2'	2.57	0.58
1:X:817:A:P	11:I:45:LYS:HG3	2.42	0.58
3:A:160:ALA:CA	3:A:199:ASN:CG	2.71	0.58
3:A:209:LYS:CE	3:A:209:LYS:HA	2.32	0.58
12:J:71:PRO:CA	12:J:96:SER:HB2	2.32	0.58
10:H:116:ARG:CZ	15:M:38:LYS:HE2	2.33	0.58
1:X:99:U:H3'	1:X:100:G:H5''	1.86	0.58
1:X:1031:C:H1'	1:X:1032:A:OP2	2.04	0.58
1:X:2793:G:N2	1:X:2804:G:C4	2.72	0.58
1:X:775:U:C4'	1:X:776:G:C2	2.87	0.58
1:X:997:C:O5'	1:X:997:C:H6	1.87	0.58
3:A:66:ILE:CG2	3:A:89:ARG:HH22	2.15	0.58
4:B:120:TRP:CG	4:B:155:ARG:HB3	2.38	0.58
10:H:100:ASN:OD1	10:H:100:ASN:C	2.41	0.58
10:H:77:THR:HA	10:H:94:ASN:OD1	2.03	0.58
11:I:62:LYS:CD	29:3:12:ARG:C	2.72	0.58
12:J:27:TYR:C	12:J:28:VAL:HG23	2.24	0.58
1:X:658:G:H2'	1:X:659:G:H8	1.69	0.58
1:X:67:G:N2	1:X:73:A:C4	2.72	0.58
27:1:9:ILE:HB	27:1:27:ASN:O	2.04	0.58
27:1:9:ILE:HD12	27:1:26:LYS:HG3	1.85	0.58
1:X:1923:U:H1'	1:X:1924:C:OP2	2.03	0.58
1:X:1975:G:H1'	1:X:1976:U:OP2	2.04	0.58
1:X:2659:C:H2'	1:X:2660:C:C6	2.38	0.58
1:X:521:U:O4	1:X:522:G:N2	2.37	0.58
3:A:89:ARG:HG2	3:A:91:ALA:HB3	1.85	0.57
4:B:183:LEU:N	4:B:183:LEU:HD23	2.18	0.57
1:X:1270:C:H4'	5:C:77:PHE:CE2	2.39	0.57
10:H:80:ALA:HB2	10:H:90:ARG:HD3	1.86	0.57
19:Q:29:VAL:HG21	19:Q:38:ILE:HD12	1.85	0.57
20:R:18:LYS:HD3	20:R:18:LYS:N	2.12	0.57
1:X:2533:U:C4	1:X:2534:U:O4	2.56	0.57
1:X:342:G:H4'	1:X:343:A:OP2	2.03	0.57
26:Z:14:SER:O	26:Z:18:MET:HG3	2.04	0.57
14:L:33:ARG:NH1	14:L:100:VAL:HA	2.19	0.57
20:R:84:VAL:HB	20:R:88:THR:O	2.04	0.57
1:X:1429:A:H1'	1:X:1603:A:N1	2.19	0.57
2:Y:85:G:C6	2:Y:86:A:C5	2.92	0.57
1:X:1817:U:H4'	3:A:253:LYS:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:49:PHE:CD1	11:I:50:GLU:N	2.72	0.57
20:R:15:HIS:ND1	20:R:16:PHE:HD2	2.02	0.57
1:X:2312:A:H4'	1:X:2313:G:O5'	2.04	0.57
1:X:2671:C:OP1	1:X:2846:G:C4'	2.49	0.57
1:X:500:G:N7	18:P:70:LYS:NZ	2.51	0.57
1:X:860:U:C2'	1:X:860:U:O2	2.50	0.57
1:X:1673:C:H5''	4:B:136:ARG:HB3	1.85	0.57
5:C:162:ARG:HG3	5:C:162:ARG:NH1	2.14	0.57
1:X:923:A:C6	12:J:12:LYS:HD3	2.40	0.57
1:X:2848:A:H2	13:K:7:GLY:H	1.53	0.57
1:X:1393:G:H1'	1:X:1585:A:H61	1.68	0.57
1:X:2543:A:O2'	1:X:2544:A:H5'	2.04	0.57
1:X:2824:C:H4'	1:X:2825:A:O5'	1.99	0.57
1:X:872:G:N2	1:X:928:G:H2'	2.18	0.57
3:A:38:LEU:HB3	3:A:39:PRO:HD2	1.87	0.57
3:A:66:ILE:HG21	3:A:89:ARG:NH2	2.14	0.57
1:X:334:G:H21	5:C:162:ARG:NH2	2.01	0.57
10:H:1:MET:N	10:H:79:HIS:HB2	2.19	0.57
14:L:10:LYS:O	14:L:14:ARG:HG3	2.04	0.57
15:M:104:LEU:HA	15:M:106:TYR:CE2	2.39	0.57
22:T:18:PRO:C	22:T:19:LYS:HG2	2.25	0.57
1:X:1681:A:C6	1:X:2706:U:C6	2.93	0.57
1:X:1817:U:C4'	3:A:253:LYS:HD3	2.33	0.57
1:X:1970:G:O2'	1:X:1971:C:H5'	2.04	0.57
1:X:2040:A:N6	1:X:2041:A:N6	2.52	0.57
1:X:2355:A:H2'	1:X:2356:A:O4'	2.03	0.57
1:X:2754:C:N4	1:X:2755:A:N6	2.52	0.57
1:X:29:U:H4'	16:N:11:ARG:HH12	1.68	0.57
20:R:62:MET:O	20:R:63:THR:CB	2.53	0.57
1:X:168:A:H2'	1:X:169:C:C6	2.40	0.57
1:X:2639:A:H2'	1:X:2640:G:O4'	2.05	0.57
1:X:496:C:O5'	1:X:496:C:H6	1.88	0.57
1:X:540:G:C5	1:X:2005:U:H5''	2.39	0.57
1:X:851:C:C2	1:X:952:A:N1	2.73	0.57
1:X:88:G:H3'	1:X:89:A:H5''	1.87	0.57
27:I:40:TYR:HB2	27:I:50:PHE:CD2	2.39	0.57
4:B:14:ILE:HD12	4:B:23:VAL:CG2	2.33	0.57
9:G:42:VAL:HG13	9:G:166:LEU:O	2.04	0.57
16:N:93:LYS:HD3	16:N:94:VAL:HG23	1.85	0.57
1:X:1972:G:C5	1:X:1973:C:C4	2.91	0.57
1:X:2711:G:OP1	4:B:169:ASN:CG	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2717:G:H1	1:X:2747:C:H42	1.53	0.57
26:Z:33:CYS:HB2	26:Z:38:GLY:O	2.05	0.57
7:E:94:PHE:HE2	7:E:160:LYS:HB3	1.68	0.57
10:H:85:ASP:OD2	10:H:87:SER:N	2.33	0.57
12:J:103:VAL:O	12:J:103:VAL:HG12	2.02	0.57
18:P:106:LEU:HD23	18:P:106:LEU:C	2.24	0.57
20:R:18:LYS:O	20:R:36:VAL:O	2.21	0.57
25:W:4:LYS:HG3	25:W:52:GLU:HB3	1.86	0.57
1:X:2055:G:O2'	1:X:2056:C:H5'	2.04	0.57
1:X:631:G:N3	1:X:631:G:H2'	2.19	0.57
1:X:94:C:O2'	24:V:40:PRO:HD2	2.05	0.57
30:4:31:LYS:H	30:4:31:LYS:HD2	1.70	0.57
1:X:331:U:O2	5:C:162:ARG:NH2	2.38	0.57
10:H:116:ARG:HD2	15:M:38:LYS:CE	2.34	0.57
1:X:1151:U:C6	9:G:91:THR:HG21	2.39	0.57
1:X:1215:A:C2	1:X:1258:G:C2	2.93	0.57
1:X:2430:A:C6	31:X:2881:LC2:H15A	2.39	0.57
1:X:521:U:C2'	1:X:522:G:H5'	2.35	0.57
3:A:147:GLU:HG2	3:A:154:ALA:HA	1.86	0.56
5:C:126:ALA:O	5:C:127:ASP:CB	2.52	0.56
15:M:24:LEU:HB3	15:M:25:PRO:CD	2.35	0.56
20:R:51:VAL:HG21	20:R:76:LEU:HD11	1.86	0.56
1:X:1442:C:H4'	1:X:1443:G:OP2	2.04	0.56
1:X:1666:G:H1	1:X:1991:C:H42	1.52	0.56
1:X:1681:A:H2'	1:X:1682:A:C8	2.40	0.56
1:X:1823:G:C2	1:X:1958:G:C2	2.93	0.56
1:X:478:G:H2'	1:X:479:G:H8	1.70	0.56
1:X:749:C:O5'	1:X:749:C:H6	1.88	0.56
1:X:832:A:N3	1:X:1203:A:C2	2.73	0.56
2:Y:66:G:C6	2:Y:67:C:N3	2.73	0.56
27:1:40:TYR:H	27:1:50:PHE:CB	2.19	0.56
11:I:62:LYS:NZ	29:3:15:LYS:HE2	2.20	0.56
3:A:151:GLY:C	3:A:153:GLY:H	2.06	0.56
13:K:80:MET:CA	13:K:80:MET:HE2	2.34	0.56
9:G:31:THR:HB	16:N:64:ARG:HH22	1.68	0.56
20:R:29:HIS:CD2	20:R:51:VAL:HG22	2.40	0.56
23:U:32:ARG:NE	23:U:32:ARG:N	2.52	0.56
23:U:49:LYS:HD3	23:U:61:TRP:NE1	2.20	0.56
1:X:1142:G:N2	9:G:101:THR:HG22	2.15	0.56
1:X:2659:C:O2'	1:X:2660:C:H5'	2.04	0.56
1:X:605:G:H2'	1:X:606:A:C8	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:760:U:C4	1:X:2592:U:C5	2.92	0.56
5:C:120:VAL:O	5:C:121:ASP:CB	2.52	0.56
6:D:126:GLY:O	6:D:160:ALA:HB3	2.05	0.56
6:D:22:TYR:OH	6:D:29:PRO:CD	2.52	0.56
25:W:3:ILE:HD11	25:W:44:VAL:HG22	1.86	0.56
1:X:1650:A:N6	1:X:1652:G:C2	2.73	0.56
1:X:579:G:H4'	1:X:994:A:C2	2.40	0.56
1:X:883:A:H1'	12:J:11:ARG:HH21	1.70	0.56
30:4:19:ARG:NH1	30:4:24:LEU:HD22	2.20	0.56
3:A:97:HIS:HE1	3:A:101:GLY:C	2.08	0.56
4:B:121:ASN:O	4:B:122:PHE:CD2	2.58	0.56
1:X:1573:G:H3'	1:X:1574:A:H5''	1.87	0.56
1:X:408:U:H2'	1:X:409:G:C8	2.41	0.56
1:X:2848:A:H2	13:K:6:ALA:HB1	1.70	0.56
19:Q:27:PHE:CZ	19:Q:42:ILE:HD13	2.41	0.56
24:V:14:PHE:O	24:V:18:ILE:HG13	2.04	0.56
1:X:1033:G:C6	1:X:1151:U:C5	2.94	0.56
1:X:1332:G:C6	1:X:1333:G:C6	2.93	0.56
1:X:1683:G:N2	1:X:1978:U:C4	2.70	0.56
1:X:2857:C:H5'	13:K:96:ARG:HB2	1.87	0.56
27:1:13:GLU:O	27:1:52:GLU:O	2.23	0.56
27:1:41:ASP:CB	27:1:46:LYS:HA	2.31	0.56
4:B:116:VAL:O	4:B:121:ASN:O	2.23	0.56
10:H:85:ASP:HB3	15:M:87:LEU:HD12	1.88	0.56
16:N:32:TYR:O	16:N:33:ARG:C	2.43	0.56
20:R:92:THR:HB	20:R:107:ALA:O	2.05	0.56
1:X:1333:G:N2	1:X:1344:C:N4	2.52	0.56
1:X:2422:C:H2'	1:X:2423:G:H8	1.70	0.56
29:3:13:ARG:O	29:3:13:ARG:HG3	2.05	0.56
11:I:45:LYS:HD3	11:I:48:PHE:CZ	2.40	0.56
1:X:1164:C:H5'	16:N:76:TYR:CE2	2.39	0.56
1:X:208:C:N4	1:X:209:G:N2	2.53	0.56
1:X:2595:C:H6	1:X:2595:C:O5'	1.88	0.56
1:X:2825:A:O4'	1:X:2843:A:C2	2.55	0.56
1:X:693:A:H2'	1:X:694:G:C8	2.41	0.56
1:X:2002:A:H62	26:Z:9:LYS:HZ2	1.53	0.56
30:4:19:ARG:HH11	30:4:24:LEU:HD22	1.70	0.56
3:A:66:ILE:HG23	3:A:68:PHE:CE1	2.40	0.56
3:A:66:ILE:HG22	3:A:68:PHE:CZ	2.34	0.56
9:G:101:THR:HG23	9:G:103:TYR:CE1	2.40	0.56
1:X:2669:C:OP2	13:K:14:SER:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2657:G:H1	1:X:2709:C:H42	1.54	0.56
32:X:2882:LMA:O53	32:X:2882:LMA:C32	2.50	0.56
1:X:955:G:N3	1:X:955:G:C5'	2.69	0.56
1:X:1790:G:H5''	3:A:262:ARG:NH2	2.21	0.56
5:C:162:ARG:NH1	5:C:162:ARG:HB3	2.17	0.56
1:X:1166:A:H5''	16:N:55:ARG:HD3	1.88	0.56
22:T:14:ARG:O	22:T:15:ASP:CB	2.54	0.56
23:U:14:VAL:O	23:U:15:VAL:HG22	2.05	0.56
1:X:1804:U:O2'	1:X:1805:G:H5'	2.06	0.56
1:X:1989:C:O2'	1:X:2798:A:O2'	2.22	0.56
1:X:502:A:H2'	1:X:503:G:O4'	2.06	0.56
1:X:834:A:H2'	1:X:957:G:OP2	2.06	0.56
13:K:94:TYR:O	13:K:95:THR:HB	2.06	0.56
15:M:34:ARG:HH21	15:M:91:VAL:HG21	1.69	0.56
1:X:1296:G:N2	1:X:1299:A:C8	2.73	0.56
1:X:2426:G:C8	1:X:2479:U:H3'	2.41	0.56
1:X:2819:G:H2'	1:X:2820:C:C6	2.40	0.56
1:X:521:U:H2'	1:X:522:G:H5'	1.87	0.56
1:X:666:U:C2'	1:X:667:U:H5''	2.36	0.56
1:X:699:G:H2'	1:X:801:A:N1	2.20	0.56
3:A:211:GLY:C	3:A:213:SER:N	2.59	0.56
5:C:112:GLN:HA	5:C:116:LYS:HD3	1.88	0.56
9:G:104:THR:OG1	9:G:106:TYR:O	2.24	0.56
16:N:32:TYR:O	16:N:34:ASN:N	2.39	0.56
1:X:1261:G:O2'	16:N:3:ARG:HA	2.05	0.56
20:R:23:ILE:HG22	20:R:33:THR:HB	1.87	0.56
20:R:16:PHE:HB3	20:R:82:ALA:HB1	1.88	0.56
1:X:1866:G:O2'	1:X:1867:A:H5''	2.06	0.56
1:X:1974:U:C6	1:X:1974:U:C3'	2.87	0.56
1:X:2044:G:N7	1:X:2480:C:H4'	2.21	0.56
1:X:2171:U:H4'	1:X:2171:U:OP1	2.05	0.56
1:X:2756:A:H1'	1:X:2757:G:OP2	2.06	0.56
1:X:538:A:N3	1:X:538:A:H2'	2.20	0.56
9:G:103:TYR:CD2	9:G:111:LYS:HB2	2.41	0.55
1:X:1142:G:C4	9:G:103:TYR:CD2	2.94	0.55
9:G:79:PHE:CE2	9:G:147:ARG:HG2	2.40	0.55
1:X:1288:A:H8	13:K:16:ALA:HB2	1.68	0.55
1:X:1290:A:C4'	13:K:20:LEU:HD11	2.36	0.55
13:K:87:TYR:CD1	13:K:90:ARG:HD2	2.41	0.55
18:P:101:PRO:O	18:P:121:THR:HG23	2.06	0.55
18:P:85:MET:HE1	18:P:129:ALA:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1787:U:H4'	3:A:255:THR:H	1.70	0.55
1:X:2301:A:H2'	1:X:2302:G:O4'	2.06	0.55
1:X:338:G:H5'	20:R:9:HIS:CE1	2.40	0.55
1:X:494:A:N7	1:X:495:C:C4	2.74	0.55
1:X:918:A:H2'	1:X:919:U:H5''	1.87	0.55
29:3:9:MET:HE2	29:3:12:ARG:NH1	2.21	0.55
3:A:150:PRO:CD	3:A:190:CYS:SG	2.92	0.55
16:N:106:PHE:O	16:N:110:VAL:HG23	2.05	0.55
20:R:25:LEU:O	20:R:26:SER:CB	2.53	0.55
1:X:1147:G:H2'	1:X:1148:G:H8	1.71	0.55
1:X:1505:U:H2'	1:X:1506:C:H5''	1.88	0.55
1:X:1816:G:O2'	3:A:253:LYS:CD	2.47	0.55
1:X:2265:A:N6	27:1:25:THR:HG21	2.21	0.55
1:X:2282:G:C2	1:X:2293:G:C2	2.94	0.55
1:X:2670:C:O2	1:X:2698:G:N2	2.34	0.55
1:X:2675:U:H2'	1:X:2676:G:C8	2.41	0.55
1:X:396:U:C4	1:X:398:C:C5	2.94	0.55
27:1:9:ILE:HD12	27:1:26:LYS:CG	2.36	0.55
3:A:160:ALA:HA	3:A:199:ASN:OD1	2.06	0.55
2:Y:45:C:H2'	6:D:92:ARG:NE	2.21	0.55
13:K:98:LEU:HD23	26:Z:45:ILE:HD11	1.86	0.55
14:L:38:ILE:HD12	14:L:39:TYR:N	2.21	0.55
1:X:1074:G:H1	1:X:1086:C:H42	1.51	0.55
1:X:1237:G:H4'	17:O:85:GLY:O	2.06	0.55
1:X:487:G:H21	1:X:491:A:H62	1.52	0.55
1:X:48:A:H4'	1:X:49:U:C5'	2.35	0.55
1:X:599:A:C2	1:X:681:A:C2	2.93	0.55
29:3:13:ARG:HB2	29:3:25:PHE:CD1	2.42	0.55
3:A:165:GLN:OE1	3:A:177:ARG:HB3	2.07	0.55
5:C:107:ALA:HB1	5:C:180:ILE:HG21	1.88	0.55
1:X:2371:A:HO2'	11:I:59:ARG:HG2	1.72	0.55
18:P:30:TYR:H	18:P:123:HIS:CE1	2.24	0.55
1:X:1605:A:C6	1:X:1606:C:N4	2.73	0.55
3:A:59:HIS:C	3:A:61:ARG:N	2.59	0.55
5:C:150:LEU:HD13	5:C:167:VAL:HB	1.88	0.55
10:H:4:PRO:HA	10:H:21:CYS:SG	2.46	0.55
22:T:14:ARG:O	22:T:15:ASP:CG	2.45	0.55
22:T:40:GLN:OE1	22:T:44:LYS:HB3	2.07	0.55
1:X:1681:A:N7	1:X:1682:A:C6	2.75	0.55
1:X:1805:G:N3	3:A:51:THR:HG21	2.22	0.55
1:X:2299:A:H4'	1:X:2300:G:C2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2707:G:N7	1:X:2708:U:C4	2.75	0.55
1:X:332:C:H5''	1:X:333:A:OP2	2.06	0.55
7:E:156:ALA:O	7:E:157:TYR:CG	2.59	0.55
23:U:48:LYS:HG2	23:U:49:LYS:N	2.22	0.55
1:X:1656:U:H4'	1:X:2678:C:H4'	1.88	0.55
1:X:2793:G:O2'	1:X:2794:G:H5'	2.07	0.55
1:X:760:U:C4	1:X:2592:U:C4	2.94	0.55
28:2:12:ARG:HE	28:2:43:THR:CG2	2.20	0.55
29:3:17:THR:HG23	29:3:20:GLY:H	1.72	0.55
29:3:30:ARG:HH21	29:3:31:HIS:CE1	2.24	0.55
5:C:153:ASP:O	5:C:154:ASP:CB	2.55	0.55
7:E:172:LYS:O	7:E:173:ALA:CB	2.55	0.55
12:J:12:LYS:O	12:J:13:GLN:CB	2.54	0.55
20:R:83:LEU:CD2	20:R:113:THR:HB	2.37	0.55
1:X:1223:G:H4'	1:X:1224:A:OP2	2.00	0.55
1:X:1441:A:C4'	1:X:1442:C:O5'	2.53	0.55
1:X:1474:A:H2'	1:X:1474:A:N3	2.20	0.55
1:X:1836:C:H42	1:X:1879:G:H1	1.54	0.55
1:X:1947:G:C6	1:X:1950:C:C4	2.94	0.55
1:X:2707:G:C2'	1:X:2708:U:O5'	2.55	0.55
1:X:2849:C:C2'	1:X:2850:U:H5'	2.37	0.55
1:X:303:C:H42	1:X:359:G:H1	1.54	0.55
18:P:67:PRO:O	18:P:71:VAL:HG23	2.07	0.55
21:S:123:VAL:HG23	21:S:161:ALA:HB2	1.89	0.55
1:X:1989:C:O2'	1:X:2798:A:C2'	2.55	0.55
1:X:201:G:H2'	1:X:202:A:C8	2.42	0.55
1:X:2045:A:C5	32:X:2882:LMA:C27	2.90	0.55
1:X:525:A:N7	1:X:526:C:C4	2.75	0.55
4:B:84:PHE:C	4:B:86:PRO:HD2	2.27	0.55
5:C:172:VAL:O	5:C:173:ALA:C	2.45	0.55
1:X:1128:G:H3'	1:X:1129:A:H5''	1.89	0.55
1:X:1280:U:C5	1:X:1995:G:N2	2.75	0.55
1:X:1888:C:H2'	1:X:1913:G:N7	2.21	0.55
1:X:236:C:H1'	1:X:632:A:O2'	2.07	0.55
1:X:2612:G:C2	1:X:2766:U:O2	2.59	0.55
1:X:869:C:O5'	1:X:869:C:H6	1.90	0.55
2:Y:17:A:H1'	2:Y:112:A:C8	2.42	0.55
11:I:60:LEU:HD23	29:3:13:ARG:HG2	1.89	0.55
13:K:12:ARG:NH2	13:K:20:LEU:HD22	2.22	0.55
1:X:1265:G:H1	16:N:37:GLN:HB2	1.72	0.55
19:Q:7:LEU:H	19:Q:7:LEU:HD13	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1145:C:C6	1:X:1147:G:OP2	2.59	0.55
1:X:1645:U:O2	1:X:2677:U:H4'	2.07	0.55
1:X:457:C:H2'	1:X:458:G:H5'	1.89	0.55
1:X:591:G:H2'	1:X:592:G:C8	2.42	0.55
1:X:608:G:O2'	11:I:18:ARG:HB3	2.07	0.55
27:1:12:MET:CG	27:1:27:ASN:OD1	2.50	0.54
3:A:24:GLY:O	3:A:25:LEU:CB	2.55	0.54
3:A:83:ILE:HA	3:A:94:ALA:HA	1.88	0.54
4:B:21:ILE:O	4:B:21:ILE:HG22	2.07	0.54
6:D:4:LEU:HG	6:D:5:LYS:N	2.16	0.54
10:H:25:LEU:O	10:H:42:LYS:HG2	2.08	0.54
14:L:27:LEU:HD13	14:L:42:ILE:HD11	1.88	0.54
1:X:121:G:H2'	1:X:122:G:O4'	2.07	0.54
1:X:1560:A:O2'	1:X:1561:A:H5'	2.07	0.54
1:X:1563:U:H2'	1:X:1564:U:C6	2.42	0.54
1:X:177:U:O4	1:X:225:G:C2	2.60	0.54
1:X:17:G:C2	1:X:534:U:O2	2.60	0.54
1:X:2020:G:H2'	1:X:2021:G:C8	2.42	0.54
1:X:748:A:N7	1:X:749:C:N3	2.56	0.54
1:X:826:U:OP2	11:I:32:ARG:HG2	2.06	0.54
9:G:30:LYS:O	9:G:30:LYS:HG2	2.06	0.54
10:H:76:ARG:O	10:H:95:ALA:N	2.38	0.54
12:J:135:ARG:O	12:J:136:GLU:CB	2.54	0.54
12:J:27:TYR:O	12:J:28:VAL:HG22	2.07	0.54
20:R:90:LYS:HZ1	20:R:113:THR:HG22	1.71	0.54
1:X:1580:C:O2'	1:X:1581:C:H5'	2.07	0.54
1:X:1838:G:H2'	1:X:1839:A:O4'	2.08	0.54
1:X:1968:G:H2'	1:X:1969:G:H8	1.72	0.54
1:X:832:A:C4	1:X:1203:A:C2	2.95	0.54
4:B:184:VAL:HG13	4:B:185:LYS:N	2.22	0.54
1:X:2659:C:H5'	4:B:189:PRO:HA	1.89	0.54
5:C:111:ARG:HH12	5:C:181:LEU:HD12	1.71	0.54
5:C:152:THR:HG23	5:C:157:THR:HG21	1.89	0.54
7:E:57:ASP:HB3	7:E:62:ARG:HH11	1.72	0.54
9:G:67:ARG:CB	9:G:70:PHE:HA	2.26	0.54
10:H:23:ARG:CB	10:H:23:ARG:NH2	2.66	0.54
1:X:825:C:H6	11:I:30:ALA:HB1	1.73	0.54
21:S:13:LYS:HE2	21:S:33:ALA:CB	2.38	0.54
1:X:1153:A:OP1	1:X:1153:A:H4'	2.08	0.54
1:X:1607:A:O2'	1:X:1608:U:C6	2.60	0.54
1:X:1928:G:N2	1:X:1929:U:C2	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2497:A:H2'	1:X:2497:A:N3	2.22	0.54
1:X:593:C:N4	1:X:594:G:C6	2.75	0.54
4:B:184:VAL:CG1	4:B:185:LYS:N	2.70	0.54
1:X:2767:C:H1'	4:B:62:PRO:HG3	1.88	0.54
9:G:90:LEU:HD12	9:G:90:LEU:N	2.23	0.54
4:B:15:TRP:CH2	15:M:84:ALA:HB3	2.43	0.54
1:X:1365:U:C2	1:X:1393:G:N2	2.75	0.54
1:X:1668:G:C8	1:X:1668:G:H5''	2.37	0.54
1:X:2371:A:C2'	11:I:59:ARG:HG2	2.38	0.54
1:X:2552:C:OP1	1:X:2553:G:OP1	2.24	0.54
1:X:2659:C:H2'	1:X:2660:C:H6	1.71	0.54
1:X:469:G:H5'	28:2:39:ARG:HB2	1.88	0.54
5:C:26:VAL:HG11	5:C:102:LEU:HD22	1.88	0.54
14:L:33:ARG:HE	14:L:38:ILE:HB	1.73	0.54
15:M:103:LYS:O	15:M:104:LEU:CB	2.51	0.54
20:R:84:VAL:CA	20:R:90:LYS:HE2	2.37	0.54
1:X:1632:A:H4'	1:X:1633:C:OP2	2.06	0.54
1:X:1677:C:H5''	1:X:1677:C:H6	1.71	0.54
1:X:208:C:H41	1:X:209:G:N2	2.05	0.54
1:X:572:G:H5'	1:X:581:A:H4'	1.90	0.54
13:K:87:TYR:CE1	13:K:94:TYR:HB3	2.42	0.54
14:L:51:LEU:HD12	14:L:51:LEU:N	2.23	0.54
18:P:85:MET:HE2	18:P:90:LEU:HD21	1.88	0.54
25:W:47:VAL:CG1	25:W:50:LEU:HD12	2.38	0.54
1:X:1496:G:H4'	1:X:1497:C:OP1	2.08	0.54
1:X:1643:A:N6	1:X:1656:U:H3	2.04	0.54
1:X:2300:G:H3'	1:X:2300:G:N3	2.22	0.54
1:X:2475:C:N4	1:X:2476:A:N6	2.56	0.54
1:X:2791:C:H2'	1:X:2792:C:C6	2.43	0.54
3:A:71:ARG:NH1	3:A:150:PRO:HB3	2.22	0.54
9:G:137:LYS:O	9:G:137:LYS:HG2	2.07	0.54
14:L:38:ILE:HG21	14:L:71:VAL:HG11	1.90	0.54
1:X:1704:G:N2	1:X:1719:G:O6	2.41	0.54
1:X:2722:C:H2'	1:X:2723:C:C6	2.42	0.54
1:X:2867:G:H4'	1:X:2868:G:OP2	2.05	0.54
1:X:652:C:H42	1:X:657:A:H61	1.56	0.54
1:X:821:A:H2'	1:X:822:G:H8	1.71	0.54
1:X:829:C:H2'	1:X:830:C:C6	2.43	0.54
26:Z:3:LYS:O	26:Z:6:VAL:HG23	2.07	0.54
27:1:16:ALA:HB2	27:1:50:PHE:CE1	2.43	0.54
4:B:152:LYS:HB2	9:G:106:TYR:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:51:LEU:CD2	13:K:70:ILE:HD11	2.38	0.54
1:X:1296:G:N2	1:X:1299:A:H8	2.05	0.54
1:X:2364:C:H2'	1:X:2365:U:C6	2.43	0.54
1:X:2394:G:C2	1:X:2395:C:C2	2.96	0.54
1:X:2494:C:OP1	9:G:108:GLY:C	2.44	0.54
1:X:2032:G:N2	1:X:2599:U:N3	2.56	0.54
1:X:749:C:H3'	1:X:749:C:H6	1.72	0.54
3:A:162:THR:H	3:A:197:VAL:HG22	1.73	0.54
4:B:14:ILE:HG23	15:M:20:HIS:CD2	2.43	0.54
5:C:157:THR:CG2	5:C:158:ARG:N	2.70	0.54
7:E:125:VAL:HG13	7:E:127:GLU:O	2.08	0.54
11:I:115:SER:OG	11:I:136:ALA:CB	2.55	0.54
12:J:47:GLN:O	12:J:50:ALA:HB3	2.07	0.54
1:X:2355:A:H61	14:L:91:ARG:CZ	2.21	0.54
15:M:39:VAL:HG12	15:M:45:THR:CB	2.38	0.54
1:X:2392:G:H2'	1:X:2393:G:H8	1.73	0.54
1:X:459:A:C2	1:X:466:A:C8	2.96	0.54
1:X:688:A:H62	1:X:816:U:H3	1.55	0.54
21:S:155:PRO:O	21:S:156:GLU:CB	2.55	0.54
1:X:1141:U:C4	4:B:147:PRO:HG3	2.42	0.54
1:X:1151:U:C5	9:G:91:THR:HG21	2.43	0.54
1:X:2014:A:C5	1:X:2477:C:H1'	2.43	0.54
1:X:572:G:H22	1:X:587:A:H2	1.56	0.54
27:1:8:ILE:CG1	27:1:30:ASN:HD21	2.16	0.53
3:A:43:GLY:N	3:A:44:ARG:NH1	2.56	0.53
6:D:67:ILE:HG21	6:D:84:PRO:HB3	1.90	0.53
1:X:674:U:H1'	11:I:22:GLY:HA2	1.90	0.53
18:P:107:ILE:CG2	18:P:117:ILE:HG12	2.38	0.53
18:P:14:ARG:O	18:P:17:GLN:HG2	2.08	0.53
1:X:1405:A:N6	1:X:1406:A:N6	2.56	0.53
1:X:1438:G:H2'	1:X:1439:G:O4'	2.08	0.53
1:X:1655:C:OP1	1:X:2690:A:H5'	2.07	0.53
1:X:1674:C:H2'	1:X:1675:C:C6	2.43	0.53
1:X:2381:A:O2'	1:X:2382:C:C6	2.61	0.53
1:X:2672:U:H2'	1:X:2673:G:H8	1.73	0.53
1:X:995:A:OP2	1:X:996:C:N4	2.40	0.53
29:3:59:LYS:O	29:3:60:LEU:CB	2.56	0.53
7:E:171:LEU:N	7:E:171:LEU:HD12	2.23	0.53
1:X:2814:G:C4'	13:K:49:GLU:OE2	2.55	0.53
17:O:71:ILE:HB	17:O:84:THR:O	2.07	0.53
18:P:107:ILE:HG21	18:P:117:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:90:LYS:HB2	20:R:108:VAL:HG21	1.90	0.53
1:X:1074:G:H4'	8:F:134:MET:HG3	1.89	0.53
1:X:1680:U:O5'	1:X:1680:U:H6	1.92	0.53
1:X:2557:G:N2	1:X:2558:C:C2	2.77	0.53
1:X:2677:U:H2'	1:X:2678:C:C6	2.43	0.53
1:X:626:A:O2'	5:C:176:ASN:CG	2.46	0.53
2:Y:83:C:C2'	2:Y:84:G:C5'	2.83	0.53
26:Z:8:LYS:C	26:Z:9:LYS:HG3	2.28	0.53
27:1:21:TYR:HD2	27:1:50:PHE:HZ	1.54	0.53
27:1:24:THR:HG21	29:3:35:GLY:HA2	1.90	0.53
3:A:211:GLY:C	3:A:213:SER:H	2.12	0.53
3:A:26:THR:HG22	3:A:27:LYS:H	1.58	0.53
12:J:106:GLU:CD	12:J:106:GLU:N	2.62	0.53
18:P:101:PRO:O	18:P:121:THR:CG2	2.56	0.53
20:R:90:LYS:HD2	20:R:108:VAL:CG2	2.39	0.53
22:T:43:THR:O	22:T:43:THR:HG22	2.07	0.53
1:X:16:G:C2	1:X:535:U:O2	2.62	0.53
1:X:172:A:C8	1:X:174:A:OP1	2.61	0.53
1:X:224:G:N2	1:X:229:G:C6	2.77	0.53
1:X:2378:G:H1'	27:1:22:TYR:HH	1.68	0.53
1:X:2800:C:C2'	1:X:2801:A:H5'	2.38	0.53
1:X:2045:A:C5	32:X:2882:LMA:H27A	2.40	0.53
1:X:427:C:H2'	1:X:428:A:C8	2.44	0.53
1:X:684:C:O2'	1:X:685:U:H5'	2.08	0.53
9:G:46:ALA:HB3	9:G:85:ALA:HB2	1.91	0.53
10:H:10:VAL:HG23	10:H:17:ARG:O	2.08	0.53
10:H:46:HIS:O	10:H:49:ASP:HB2	2.09	0.53
4:B:176:ARG:NH2	15:M:19:ASP:OD2	2.41	0.53
16:N:93:LYS:HZ3	17:O:10:LYS:HE2	1.69	0.53
1:X:1683:G:H4'	10:H:6:SER:OG	2.08	0.53
1:X:1681:A:N6	1:X:1979:C:N4	2.46	0.53
1:X:2395:C:C2'	1:X:2396:C:H5'	2.38	0.53
1:X:2429:A:N6	1:X:2430:A:N6	2.57	0.53
1:X:318:G:O2'	1:X:319:G:C8	2.61	0.53
1:X:2350:G:O2'	27:1:46:LYS:HB3	2.07	0.53
29:3:13:ARG:HD2	29:3:25:PHE:HD1	1.72	0.53
4:B:122:PHE:CZ	4:B:155:ARG:HB2	2.42	0.53
5:C:128:ALA:O	5:C:130:THR:N	2.39	0.53
13:K:80:MET:HA	13:K:80:MET:HE2	1.89	0.53
21:S:87:THR:O	21:S:88:TYR:CB	2.55	0.53
1:X:1006:C:OP2	16:N:54:LYS:NZ	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:131:C:C2	1:X:141:G:N2	2.77	0.53
1:X:1975:G:O2'	1:X:1980:A:N6	2.38	0.53
1:X:2238:G:N7	1:X:2406:C:N4	2.57	0.53
1:X:2496:C:C5	1:X:2521:A:C8	2.97	0.53
1:X:28:A:H1'	1:X:523:A:C2	2.44	0.53
1:X:562:G:C6	1:X:563:U:N3	2.76	0.53
1:X:660:G:H5'	29:3:48:PHE:CZ	2.44	0.53
3:A:160:ALA:CB	3:A:199:ASN:CB	2.87	0.53
3:A:70:ARG:HD3	3:A:120:ALA:HB2	1.90	0.53
11:I:58:ALA:O	11:I:59:ARG:HB2	2.07	0.53
12:J:92:GLU:CG	12:J:93:TYR:CD2	2.86	0.53
1:X:131:C:O2	1:X:141:G:N2	2.42	0.53
1:X:1405:A:H62	1:X:1406:A:N6	2.07	0.53
1:X:1720:G:H2'	1:X:1721:G:C8	2.43	0.53
1:X:1822:C:N4	1:X:1958:G:H1	2.02	0.53
1:X:1928:G:C2	1:X:1929:U:C2	2.96	0.53
1:X:219:G:H2'	1:X:220:U:OP2	2.08	0.53
1:X:1135:C:H1'	30:4:36:GLN:OE1	2.08	0.53
3:A:127:LYS:HB2	3:A:130:ASN:ND2	2.23	0.53
5:C:117:LEU:HD23	5:C:118:VAL:N	2.24	0.53
2:Y:45:C:H2'	6:D:92:ARG:CZ	2.39	0.53
7:E:50:LEU:HD23	7:E:51:LEU:N	2.24	0.53
1:X:1687:C:H2'	1:X:1688:U:O4'	2.09	0.53
1:X:496:C:C2'	1:X:497:C:H5'	2.38	0.53
7:E:140:LEU:O	7:E:144:VAL:HG23	2.08	0.53
12:J:78:LYS:HE2	12:J:81:GLU:HA	1.91	0.53
1:X:1282:A:H2	1:X:1338:G:N2	2.06	0.53
1:X:1391:A:C4	1:X:1393:G:C8	2.97	0.53
1:X:2045:A:N6	32:X:2882:LMA:C27	2.70	0.53
1:X:2624:G:C3'	1:X:2625:U:H5'	2.39	0.53
1:X:537:C:H1'	1:X:538:A:C6	2.44	0.53
27:1:31:THR:O	27:1:32:GLN:C	2.47	0.53
27:1:42:PRO:O	27:1:43:VAL:C	2.46	0.53
29:3:62:LEU:HB3	29:3:63:PRO:HD3	1.90	0.53
1:X:331:U:C2'	5:C:162:ARG:HH12	2.22	0.53
6:D:108:LEU:HB2	6:D:109:PRO:HD3	1.91	0.53
10:H:127:VAL:O	10:H:130:ALA:HB3	2.08	0.53
11:I:73:GLU:HG3	11:I:101:ARG:HG3	1.89	0.53
1:X:2698:G:H5''	15:M:105:TYR:CD2	2.44	0.53
1:X:1324:G:C2'	19:Q:72:ARG:HH22	2.21	0.53
21:S:6:LYS:HB2	21:S:31:SER:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1174:G:H2'	1:X:1175:A:H8	1.74	0.53
1:X:1391:A:C8	1:X:1393:G:C5	2.95	0.53
1:X:1392:U:H5''	1:X:1393:G:OP2	2.07	0.53
1:X:2616:U:H2'	1:X:2617:G:O4'	2.08	0.53
1:X:41:G:H2'	1:X:42:G:C8	2.44	0.53
2:Y:107:C:H2'	2:Y:108:G:O4'	2.09	0.53
3:A:109:PRO:HB3	3:A:144:HIS:HE1	1.73	0.53
5:C:164:VAL:HG23	5:C:165:SER:N	2.18	0.53
7:E:145:ALA:O	7:E:148:VAL:HB	2.09	0.53
9:G:103:TYR:CE2	9:G:111:LYS:HB2	2.43	0.53
1:X:827:C:OP1	17:O:83:ARG:N	2.42	0.53
18:P:32:ARG:CA	18:P:32:ARG:NE	2.61	0.53
1:X:1242:A:H2'	1:X:1243:G:C8	2.44	0.53
1:X:127:C:H2'	1:X:128:C:C6	2.44	0.53
1:X:415:A:H61	1:X:436:A:H61	1.57	0.53
1:X:695:G:N2	1:X:809:C:C2	2.77	0.53
1:X:693:A:C6	1:X:811:G:C2	2.97	0.53
2:Y:39:C:H5'	2:Y:40:C:OP2	2.09	0.53
1:X:795:A:N1	3:A:227:MET:HE3	2.23	0.52
3:A:71:ARG:NH1	3:A:151:GLY:N	2.57	0.52
1:X:756:C:OP1	4:B:130:GLY:HA3	2.09	0.52
16:N:25:TRP:CE3	16:N:26:GLY:HA3	2.43	0.52
22:T:40:GLN:HE21	22:T:57:HIS:HB3	1.74	0.52
1:X:2284:U:C2	6:D:153:ASP:HB2	2.44	0.52
1:X:2698:G:H5''	15:M:105:TYR:HD2	1.73	0.52
1:X:543:G:H5'	16:N:24:PHE:CE1	2.43	0.52
1:X:794:A:H5'	3:A:219:LYS:NZ	2.23	0.52
1:X:821:A:H2'	1:X:822:G:C8	2.44	0.52
3:A:245:ARG:HA	3:A:253:LYS:HZ1	1.74	0.52
1:X:679:C:H4'	11:I:49:PHE:CE1	2.45	0.52
13:K:33:ARG:O	13:K:34:ILE:HG22	2.09	0.52
18:P:8:PHE:O	18:P:9:ARG:HB2	2.09	0.52
19:Q:7:LEU:HD22	24:V:29:ARG:HH12	1.75	0.52
24:V:4:SER:HB3	24:V:7:ARG:HH21	1.74	0.52
1:X:1050:G:C2'	1:X:1051:U:H5'	2.39	0.52
1:X:1223:G:H4'	1:X:1224:A:O5'	2.02	0.52
1:X:1982:C:H1'	1:X:2666:U:H1'	1.91	0.52
1:X:2323:U:O2'	27:1:38:LYS:HB3	2.09	0.52
1:X:2371:A:H1'	11:I:59:ARG:CG	2.39	0.52
1:X:681:A:C8	1:X:681:A:H5''	2.44	0.52
27:1:29:ARG:HA	27:1:33:ALA:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:9:ASN:HA	28:2:12:ARG:HB3	1.91	0.52
3:A:55:ILE:N	3:A:55:ILE:HD13	2.23	0.52
6:D:17:MET:HG3	6:D:22:TYR:HB2	1.91	0.52
7:E:174:GLY:C	7:E:175:LYS:HG2	2.29	0.52
7:E:83:TYR:CZ	7:E:138:LYS:HD2	2.44	0.52
15:M:102:ALA:O	15:M:103:LYS:CD	2.56	0.52
25:W:3:ILE:HD11	25:W:44:VAL:CG2	2.39	0.52
1:X:1393:G:O2'	1:X:1394:G:H5'	2.09	0.52
1:X:177:U:O2'	1:X:178:C:O4'	2.26	0.52
1:X:793:G:N3	1:X:798:G:C6	2.77	0.52
1:X:845:U:OP1	11:I:41:SER:OG	2.27	0.52
7:E:87:LEU:HB2	7:E:131:ILE:HB	1.90	0.52
1:X:1069:G:N3	8:F:116:ASN:ND2	2.57	0.52
9:G:67:ARG:HB2	9:G:70:PHE:CD1	2.45	0.52
10:H:88:THR:HB	15:M:80:VAL:HB	1.91	0.52
14:L:36:LYS:NZ	14:L:65:THR:HG22	2.24	0.52
1:X:2201:G:H2'	1:X:2202:G:C8	2.45	0.52
1:X:2857:C:C5'	13:K:96:ARG:HB2	2.40	0.52
1:X:333:A:C5'	5:C:162:ARG:HG2	2.40	0.52
1:X:542:A:H2'	16:N:28:ARG:HE	1.75	0.52
11:I:62:LYS:CD	29:3:13:ARG:N	2.73	0.52
3:A:157:ALA:HB1	3:A:162:THR:HB	1.90	0.52
8:F:121:GLU:O	8:F:125:ASN:N	2.40	0.52
18:P:110:ALA:O	18:P:111:ARG:HB2	2.09	0.52
1:X:2013:A:H4'	1:X:2014:A:C8	2.43	0.52
1:X:2841:U:HO2'	1:X:2842:C:P	2.31	0.52
2:Y:84:G:C2'	2:Y:85:G:O5'	2.58	0.52
3:A:160:ALA:HB1	3:A:199:ASN:CB	2.39	0.52
9:G:132:PHE:CD2	9:G:145:HIS:CG	2.88	0.52
11:I:73:GLU:CG	11:I:101:ARG:HG3	2.39	0.52
2:Y:40:C:O4'	14:L:97:HIS:CE1	2.62	0.52
19:Q:7:LEU:N	19:Q:7:LEU:HD13	2.24	0.52
1:X:1720:G:H2'	1:X:1721:G:H8	1.74	0.52
1:X:1918:G:C4	1:X:1945:C:N4	2.78	0.52
1:X:2340:C:H2'	1:X:2341:G:O4'	2.09	0.52
1:X:2429:A:N1	1:X:2430:A:C6	2.78	0.52
32:X:2882:LMA:H35	32:X:2882:LMA:H37B	1.91	0.52
1:X:33:C:O2	1:X:466:A:C2	2.61	0.52
6:D:123:ASP:OD1	6:D:123:ASP:C	2.47	0.52
11:I:18:ARG:CG	11:I:21:ARG:CG	2.87	0.52
15:M:27:PHE:CG	15:M:27:PHE:O	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1313:U:H4'	1:X:1314:A:C5'	2.40	0.52
1:X:1680:U:O2'	1:X:1681:A:O5'	2.28	0.52
1:X:2032:G:N2	1:X:2599:U:C2	2.78	0.52
1:X:2485:U:H2'	1:X:2486:C:C5	2.44	0.52
1:X:2712:G:H3'	1:X:2713:A:C5'	2.40	0.52
1:X:2790:C:N4	1:X:2806:G:H1	2.06	0.52
1:X:537:C:O2	1:X:538:A:C2	2.63	0.52
1:X:879:A:C2'	1:X:879:A:N3	2.69	0.52
1:X:2000:U:O2'	26:Z:9:LYS:HA	2.09	0.52
3:A:219:LYS:CD	3:A:219:LYS:C	2.76	0.52
9:G:35:LYS:CB	9:G:37:ASP:H	2.23	0.52
16:N:40:LEU:HB3	17:O:74:TYR:CZ	2.45	0.52
21:S:120:LEU:HD23	21:S:120:LEU:C	2.30	0.52
1:X:1972:G:C6	1:X:1973:C:N3	2.78	0.52
1:X:2505:G:N1	1:X:2517:C:O2	2.43	0.52
1:X:2805:G:O2'	1:X:2858:A:N1	2.33	0.52
1:X:965:G:O5'	1:X:965:G:H8	1.92	0.52
11:I:57:ILE:HG23	29:3:12:ARG:CZ	2.40	0.52
6:D:4:LEU:CG	6:D:5:LYS:H	2.12	0.52
1:X:2357:A:H1'	14:L:88:VAL:HG13	1.92	0.52
1:X:1391:A:C6	1:X:1393:G:C5	2.96	0.52
1:X:1819:U:O2'	1:X:1820:G:H5'	2.10	0.52
1:X:1919:A:H1'	1:X:1923:U:N3	2.24	0.52
1:X:2696:A:H2'	1:X:2697:G:H8	1.74	0.52
1:X:2824:C:O2	1:X:2843:A:C8	2.63	0.52
1:X:700:C:C5	1:X:701:U:C4	2.98	0.52
1:X:983:G:H3'	1:X:984:A:C5'	2.40	0.52
3:A:30:PRO:HB2	3:A:31:GLU:OE1	2.10	0.52
16:N:62:ILE:HG23	16:N:76:TYR:CE1	2.44	0.52
22:T:18:PRO:O	22:T:19:LYS:CG	2.58	0.52
1:X:1447:U:O2	1:X:1577:G:C2	2.63	0.52
1:X:1930:C:O2	1:X:1943:A:H2	1.92	0.52
1:X:2222:U:O2	1:X:2413:A:C2	2.63	0.52
1:X:2432:A:H2'	1:X:2433:G:C8	2.45	0.52
1:X:2624:G:H3'	1:X:2625:U:H5'	1.92	0.52
1:X:2825:A:OP2	1:X:2843:A:C4	2.63	0.52
27:1:9:ILE:CD1	27:1:26:LYS:HD2	2.39	0.51
3:A:31:GLU:HB2	3:A:83:ILE:O	2.09	0.51
10:H:28:GLY:O	10:H:35:THR:N	2.42	0.51
10:H:5:GLN:O	10:H:5:GLN:HG3	2.11	0.51
12:J:99:LYS:CD	12:J:100:PRO:HD2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:54:VAL:CG2	12:J:125:LYS:NZ	2.73	0.51
1:X:1457:A:C2	1:X:1565:G:C2	2.98	0.51
1:X:2404:A:H4'	1:X:2405:A:OP2	2.10	0.51
1:X:2466:G:O2'	1:X:2467:A:H5'	2.10	0.51
1:X:883:A:C2	1:X:920:G:C6	2.98	0.51
3:A:66:ILE:HG23	3:A:66:ILE:O	2.11	0.51
5:C:156:ASN:O	5:C:159:ARG:HB3	2.10	0.51
15:M:27:PHE:CD1	15:M:27:PHE:O	2.63	0.51
18:P:85:MET:HE3	18:P:130:GLU:HG3	1.93	0.51
21:S:69:VAL:HG22	21:S:81:VAL:HG13	1.93	0.51
1:X:1332:G:C6	1:X:1333:G:O6	2.63	0.51
1:X:962:C:H2'	1:X:963:G:H8	1.75	0.51
1:X:978:U:H2'	1:X:979:A:C8	2.45	0.51
3:A:71:ARG:HH12	3:A:150:PRO:HB3	1.76	0.51
3:A:160:ALA:HA	3:A:199:ASN:CB	2.40	0.51
6:D:13:ARG:HG3	6:D:28:VAL:HG21	1.93	0.51
1:X:1073:G:N2	8:F:133:SER:HB3	2.21	0.51
1:X:1182:U:O2'	1:X:1183:C:H5''	2.10	0.51
1:X:1425:G:C2	1:X:1607:A:N6	2.78	0.51
1:X:1693:A:C6	1:X:1694:A:C6	2.97	0.51
1:X:2505:G:C2	1:X:2517:C:O2	2.63	0.51
1:X:2529:G:C2	1:X:2538:C:O2	2.64	0.51
1:X:1937:G:N3	1:X:2530:C:H5'	2.25	0.51
2:Y:84:G:H2'	2:Y:85:G:C8	2.44	0.51
4:B:21:ILE:HG21	4:B:173:VAL:HG21	1.92	0.51
10:H:21:CYS:HA	10:H:53:ALA:HB2	1.92	0.51
12:J:121:LEU:C	12:J:123:GLY:H	2.13	0.51
15:M:24:LEU:HB3	15:M:25:PRO:HD2	1.91	0.51
16:N:99:ALA:HB2	16:N:106:PHE:CD1	2.45	0.51
1:X:1291:G:H5''	13:K:34:ILE:HD12	1.92	0.51
1:X:1692:C:H2'	1:X:1693:A:O4'	2.10	0.51
1:X:1915:A:H62	1:X:1951:G:H21	1.56	0.51
1:X:1673:C:H42	1:X:1987:G:H1	1.58	0.51
1:X:2217:G:H2'	1:X:2217:G:N3	2.26	0.51
1:X:2238:G:C8	1:X:2406:C:C4	2.99	0.51
1:X:2791:C:C2	1:X:2806:G:N2	2.79	0.51
1:X:321:A:O2'	1:X:322:A:H2'	2.10	0.51
1:X:5:A:C2	1:X:2873:G:C2	2.98	0.51
1:X:817:A:OP1	11:I:45:LYS:CG	2.57	0.51
1:X:1692:C:N3	4:B:128:SER:O	2.43	0.51
9:G:67:ARG:HB3	9:G:70:PHE:CA	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:7:GLY:O	16:N:8:ILE:HG12	2.10	0.51
18:P:50:VAL:O	18:P:53:ALA:HB3	2.10	0.51
19:Q:63:LYS:HD3	19:Q:69:ILE:HA	1.93	0.51
1:X:1194:U:O2'	1:X:1195:U:C6	2.55	0.51
1:X:2606:G:N2	1:X:2757:G:C4	2.79	0.51
1:X:2757:G:OP2	1:X:2761:A:O2'	2.25	0.51
1:X:695:G:N2	1:X:809:C:O2	2.43	0.51
1:X:693:A:C2	1:X:811:G:C2	2.98	0.51
3:A:199:ASN:O	3:A:200:ALA:C	2.47	0.51
4:B:15:TRP:CD1	15:M:86:PRO:HD3	2.45	0.51
1:X:2848:A:C2	13:K:7:GLY:N	2.78	0.51
14:L:37:HIS:CE1	14:L:57:ALA:HB2	2.46	0.51
21:S:13:LYS:HE2	21:S:33:ALA:HB1	1.85	0.51
1:X:119:G:H2'	1:X:120:G:H8	1.76	0.51
1:X:1344:C:N4	1:X:1346:C:O2	2.44	0.51
1:X:2335:U:O2	1:X:2341:G:C2	2.63	0.51
1:X:2819:G:C2	1:X:2820:C:C2	2.99	0.51
1:X:2824:C:C4'	1:X:2825:A:OP2	2.58	0.51
1:X:331:U:O2'	5:C:162:ARG:NH1	2.43	0.51
4:B:84:PHE:CG	4:B:84:PHE:O	2.61	0.51
4:B:85:ALA:N	4:B:86:PRO:HD2	2.26	0.51
5:C:124:ASP:CG	5:C:136:TRP:CD1	2.84	0.51
9:G:132:PHE:CD2	9:G:145:HIS:CD2	2.97	0.51
10:H:110:VAL:HG23	10:H:129:LEU:HB2	1.92	0.51
14:L:37:HIS:CG	14:L:37:HIS:O	2.64	0.51
15:M:103:LYS:HG3	15:M:105:TYR:CE2	2.46	0.51
1:X:1128:G:H3'	1:X:1129:A:C5'	2.40	0.51
1:X:1982:C:H2'	1:X:1983:G:H8	1.76	0.51
1:X:1277:G:N2	1:X:1997:A:C8	2.79	0.51
1:X:2073:A:H61	1:X:2208:U:H3	1.58	0.51
1:X:2653:A:O2'	10:H:41:ASN:HB2	2.11	0.51
1:X:313:U:H2'	1:X:314:G:H8	1.75	0.51
1:X:886:A:H4'	12:J:66:TYR:CE2	2.46	0.51
1:X:334:G:H3'	5:C:162:ARG:HD3	1.92	0.51
6:D:78:LYS:C	6:D:79:LEU:HD12	2.31	0.51
9:G:61:ARG:NH2	9:G:61:ARG:HB3	2.26	0.51
10:H:110:VAL:HG23	10:H:129:LEU:HB3	1.93	0.51
10:H:27:SER:HB3	10:H:50:ILE:H	1.75	0.51
14:L:51:LEU:CD1	14:L:51:LEU:N	2.74	0.51
18:P:45:ILE:HA	18:P:48:LYS:HD3	1.92	0.51
19:Q:68:PHE:C	19:Q:69:ILE:HG13	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:17:GLU:O	24:V:21:ARG:HD3	2.11	0.51
1:X:2531:U:C2	1:X:2533:U:H5''	2.46	0.51
1:X:2571:G:C2	1:X:2582:G:N1	2.79	0.51
1:X:2795:A:O4'	13:K:5:LYS:HE3	2.10	0.51
1:X:2818:G:H2'	1:X:2819:G:H8	1.75	0.51
2:Y:51:G:H2'	2:Y:52:G:C8	2.45	0.51
6:D:5:LYS:O	6:D:8:TYR:HB3	2.11	0.51
11:I:115:SER:OG	11:I:136:ALA:HB1	2.11	0.51
13:K:98:LEU:HB2	13:K:112:LEU:HB2	1.93	0.51
20:R:23:ILE:HD11	20:R:81:VAL:HB	1.92	0.51
25:W:37:THR:O	25:W:41:ARG:HG3	2.11	0.51
1:X:1033:G:H2'	9:G:97:ASP:OD1	2.11	0.51
1:X:1223:G:H5'	1:X:1225:G:O4'	2.11	0.51
1:X:1337:G:H1'	1:X:1632:A:N6	2.26	0.51
1:X:1399:C:H2'	1:X:1400:A:C8	2.46	0.51
1:X:1473:U:O2	1:X:1474:A:N6	2.44	0.51
1:X:1605:A:C5	1:X:1606:C:N4	2.78	0.51
1:X:2266:A:N6	1:X:2323:U:H3	2.09	0.51
1:X:2463:G:H5''	12:J:46:ASN:HD22	1.75	0.51
1:X:2555:G:H3'	1:X:2555:G:N3	2.25	0.51
1:X:331:U:H1'	5:C:162:ARG:NH1	2.17	0.51
1:X:2592:U:H2'	26:Z:5:PRO:CG	2.41	0.51
27:1:38:LYS:CD	27:1:40:TYR:HE1	2.24	0.51
5:C:14:THR:C	5:C:15:ILE:HG13	2.29	0.51
6:D:16:LEU:HD13	6:D:22:TYR:HE2	1.75	0.51
10:H:24:VAL:HG12	10:H:42:LYS:HG2	1.93	0.51
1:X:1311:C:C2	1:X:1660:G:N2	2.79	0.51
1:X:1701:C:N3	1:X:1722:G:C2	2.79	0.51
1:X:1739:G:H2'	1:X:1740:G:C8	2.46	0.51
1:X:1777:A:N3	1:X:1921:A:C6	2.78	0.51
1:X:542:A:H2	1:X:2004:U:HO2'	1.57	0.51
1:X:2427:A:H5'	1:X:2428:U:OP2	2.10	0.51
31:X:2881:LC2:C28	31:X:2881:LC2:C3	2.79	0.51
1:X:313:U:H2'	1:X:314:G:C8	2.45	0.51
1:X:538:A:O2'	1:X:539:A:H5''	2.11	0.51
1:X:647:G:O2'	1:X:649:G:H4'	2.10	0.51
1:X:693:A:H2'	1:X:694:G:H8	1.76	0.51
1:X:583:C:N3	4:B:145:LYS:NZ	2.59	0.50
4:B:61:LYS:N	4:B:62:PRO:CD	2.74	0.50
9:G:70:PHE:HB2	16:N:64:ARG:NE	2.23	0.50
16:N:91:ASN:O	16:N:93:LYS:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1073:G:H21	8:F:133:SER:CB	2.21	0.50
1:X:617:U:H5	1:X:632:A:C2	2.28	0.50
1:X:748:A:N7	1:X:749:C:C4	2.79	0.50
11:I:62:LYS:HD2	29:3:13:ARG:CA	2.41	0.50
12:J:13:GLN:NE2	12:J:90:ALA:HB1	2.26	0.50
21:S:3:LEU:HD11	21:S:33:ALA:H	1.76	0.50
25:W:13:PRO:O	25:W:17:VAL:HG23	2.12	0.50
1:X:1811:A:H4'	1:X:1812:U:C5'	2.41	0.50
1:X:2194:A:H3'	1:X:2195:C:H5''	1.93	0.50
1:X:45:C:OP2	1:X:192:G:C2'	2.56	0.50
1:X:860:U:O2	1:X:860:U:C3'	2.59	0.50
11:I:56:LEU:HD11	29:3:52:LYS:HD2	1.93	0.50
1:X:1920:A:C5	1:X:1922:U:O2	2.64	0.50
1:X:2427:A:OP1	1:X:2477:C:OP2	2.29	0.50
1:X:2487:G:HO2'	1:X:2533:U:HO2'	1.56	0.50
1:X:2664:G:H8	1:X:2664:G:H5''	1.76	0.50
1:X:2709:C:O2'	4:B:186:GLY:HA3	2.11	0.50
1:X:2711:G:OP1	4:B:169:ASN:CB	2.60	0.50
1:X:517:A:C5'	1:X:518:A:H5'	2.39	0.50
1:X:671:A:C6	1:X:672:C:C4	2.99	0.50
1:X:693:A:N1	1:X:811:G:C2	2.80	0.50
2:Y:84:G:C2	2:Y:98:C:C2	2.99	0.50
5:C:180:ILE:HG23	5:C:181:LEU:N	2.27	0.50
1:X:884:C:OP1	12:J:9:LYS:HG3	2.12	0.50
1:X:782:U:O2	1:X:1392:U:H1'	2.11	0.50
1:X:1496:G:H1'	1:X:1497:C:O5'	2.10	0.50
1:X:2796:A:H2'	1:X:2797:G:C8	2.47	0.50
1:X:2806:G:O2'	1:X:2859:U:OP1	2.18	0.50
1:X:540:G:N7	1:X:2005:U:H5''	2.26	0.50
1:X:791:G:C2	1:X:800:U:C2	2.99	0.50
2:Y:23:G:C2	2:Y:65:A:C2	3.00	0.50
30:4:24:LEU:HD23	30:4:35:ARG:CZ	2.42	0.50
7:E:165:VAL:HG12	7:E:166:GLY:H	1.77	0.50
10:H:115:ALA:HB3	10:H:118:LEU:HD13	1.91	0.50
13:K:84:ALA:N	13:K:85:PRO:CD	2.75	0.50
10:H:89:ILE:HG23	15:M:79:ARG:HD3	1.93	0.50
1:X:29:U:H4'	16:N:11:ARG:HH22	1.75	0.50
1:X:827:C:OP1	17:O:82:ARG:HA	2.11	0.50
1:X:100:G:H4'	1:X:101:A:OP1	2.12	0.50
1:X:1182:U:H1'	1:X:1183:C:O5'	2.11	0.50
1:X:1949:A:H1'	1:X:2572:U:C5'	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2016:A:O2'	1:X:2018:G:OP2	2.29	0.50
1:X:2261:G:C2	1:X:2404:A:C5	2.99	0.50
1:X:2641:A:H2'	1:X:2642:G:H5'	1.94	0.50
1:X:2819:G:C5	1:X:2820:C:C4	3.00	0.50
26:Z:12:SER:HB2	26:Z:15:LYS:H	1.76	0.50
27:1:29:ARG:HA	27:1:33:ALA:HB2	1.93	0.50
3:A:207:LEU:CA	3:A:212:ARG:NH1	2.71	0.50
4:B:9:ILE:HD11	4:B:27:LEU:CB	2.37	0.50
10:H:116:ARG:NH1	15:M:38:LYS:CE	2.71	0.50
12:J:135:ARG:NH2	21:S:118:HIS:CD2	2.78	0.50
16:N:94:VAL:O	16:N:94:VAL:HG12	2.11	0.50
1:X:1265:G:O2'	1:X:1266:G:N9	2.45	0.50
1:X:1985:G:H3'	1:X:1985:G:C8	2.46	0.50
1:X:2005:U:O4'	1:X:2005:U:OP2	2.30	0.50
1:X:2314:A:O2'	1:X:2315:A:C8	2.65	0.50
1:X:2825:A:H2	13:K:61:HIS:CG	2.28	0.50
1:X:331:U:C2'	5:C:162:ARG:NH1	2.75	0.50
1:X:756:C:OP1	4:B:130:GLY:CA	2.60	0.50
3:A:178:LEU:HB3	3:A:179:PRO:HD2	1.93	0.50
1:X:2554:C:O2'	4:B:140:SER:HB2	2.12	0.50
9:G:107:GLN:HA	9:G:110:LEU:HD12	1.94	0.50
10:H:7:ARG:HA	10:H:20:MET:HA	1.93	0.50
21:S:73:LYS:O	21:S:74:ARG:HB2	2.12	0.50
1:X:1021:A:OP1	16:N:66:ASN:ND2	2.44	0.50
1:X:175:C:O5'	1:X:175:C:H6	1.95	0.50
1:X:2199:C:C2'	1:X:2200:G:H5'	2.41	0.50
1:X:789:G:N2	1:X:2220:A:OP1	2.45	0.50
1:X:2671:C:N3	1:X:2698:G:N2	2.60	0.50
1:X:538:A:H3'	9:G:142:ARG:NH1	2.27	0.50
1:X:584:A:OP2	1:X:2038:C:H5	1.95	0.50
1:X:617:U:C5	1:X:631:G:H8	2.30	0.50
1:X:793:G:H1'	1:X:798:G:H22	1.76	0.50
15:M:26:ASP:O	15:M:26:ASP:OD2	2.30	0.50
1:X:1322:G:H4'	28:2:7:PRO:CB	2.41	0.50
1:X:2780:A:H2'	1:X:2781:G:C8	2.47	0.50
4:B:85:ALA:O	4:B:86:PRO:O	2.29	0.50
6:D:134:GLU:HG2	6:D:136:LEU:H	1.76	0.50
12:J:54:VAL:HG21	12:J:125:LYS:NZ	2.26	0.50
18:P:85:MET:CE	18:P:90:LEU:HD21	2.42	0.50
1:X:1289:A:N1	1:X:1290:A:C6	2.79	0.50
1:X:1601:U:H4'	1:X:1602:G:OP2	2.07	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2378:G:C2	1:X:2397:A:C2	3.00	0.50
1:X:2814:G:H4'	13:K:49:GLU:OE2	2.12	0.50
1:X:611:C:O2'	1:X:615:C:OP1	2.21	0.50
1:X:780:U:O2'	1:X:781:G:O5'	2.30	0.50
1:X:938:G:O2'	1:X:939:C:C5'	2.59	0.50
1:X:980:G:C6	1:X:981:C:N3	2.80	0.50
29:3:13:ARG:HD2	29:3:25:PHE:N	2.28	0.49
29:3:29:LYS:HE3	29:3:34:THR:CB	2.42	0.49
5:C:123:PHE:CD2	5:C:123:PHE:C	2.85	0.49
9:G:132:PHE:HB2	9:G:145:HIS:NE2	2.26	0.49
9:G:36:ASN:O	9:G:38:GLU:O	2.30	0.49
13:K:54:THR:HG22	13:K:66:VAL:HG23	1.94	0.49
16:N:13:ARG:O	16:N:16:LYS:HB2	2.12	0.49
18:P:107:ILE:CG2	18:P:107:ILE:O	2.60	0.49
23:U:49:LYS:HA	23:U:62:LEU:H	1.76	0.49
1:X:1096:A:O4'	1:X:1097:A:OP1	2.30	0.49
1:X:1164:C:H2'	1:X:1165:G:O4'	2.11	0.49
1:X:1399:C:H2'	1:X:1400:A:H8	1.77	0.49
1:X:1542:G:H22	1:X:1562:G:H1	1.58	0.49
1:X:2571:G:C5	1:X:2572:U:C4	3.00	0.49
1:X:2793:G:C2	1:X:2804:G:C2	2.99	0.49
1:X:608:G:C2	1:X:609:U:C2	3.00	0.49
1:X:640:C:H4'	1:X:660:G:H21	1.75	0.49
1:X:693:A:C5	1:X:811:G:N2	2.80	0.49
27:1:9:ILE:C	27:1:10:VAL:HG23	2.32	0.49
3:A:220:PRO:O	3:A:221:HIS:O	2.29	0.49
8:F:116:ASN:OD1	8:F:117:ALA:CA	2.60	0.49
9:G:93:LYS:N	9:G:93:LYS:CD	2.74	0.49
11:I:18:ARG:HG3	11:I:21:ARG:CB	2.41	0.49
12:J:54:VAL:CG2	12:J:125:LYS:HZ2	2.25	0.49
13:K:94:TYR:CE1	13:K:115:LEU:O	2.65	0.49
14:L:36:LYS:HE2	14:L:65:THR:HG22	1.94	0.49
10:H:116:ARG:CD	15:M:38:LYS:HE3	2.42	0.49
1:X:1993:G:OP1	18:P:37:LYS:HE3	2.12	0.49
1:X:1069:G:H2'	1:X:1070:G:H5''	1.94	0.49
1:X:1096:A:C4'	1:X:1097:A:OP1	2.60	0.49
1:X:1224:A:H5'	18:P:10:ASN:HD22	1.76	0.49
1:X:1979:C:OP1	1:X:1979:C:O4'	2.30	0.49
1:X:2040:A:O5'	1:X:2040:A:C8	2.60	0.49
1:X:2038:C:H2'	1:X:2483:U:C4'	2.41	0.49
1:X:2510:A:N6	1:X:2511:G:C6	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:861:G:H2'	1:X:862:A:H5'	1.94	0.49
1:X:998:C:N4	1:X:999:A:C5	2.81	0.49
29:3:13:ARG:HB2	29:3:25:PHE:HD1	1.78	0.49
5:C:22:VAL:CG1	5:C:110:SER:OG	2.56	0.49
1:X:2663:U:C2'	10:H:88:THR:HG21	2.39	0.49
18:P:91:PHE:CE1	18:P:131:LYS:HA	2.47	0.49
1:X:1747:G:O4'	1:X:1747:G:OP2	2.29	0.49
1:X:2451:G:C5	1:X:2454:C:N4	2.81	0.49
1:X:2671:C:H1'	1:X:2822:U:H1'	1.93	0.49
1:X:332:C:H2'	1:X:351:A:O2'	2.13	0.49
1:X:460:U:N3	1:X:592:G:H1'	2.27	0.49
1:X:615:C:H41	11:I:100:ARG:NH1	2.11	0.49
1:X:796:A:H2	1:X:1769:U:HO2'	1.58	0.49
27:1:11:LYS:N	27:1:11:LYS:HD2	2.27	0.49
11:I:60:LEU:HG	29:3:13:ARG:HD3	1.95	0.49
3:A:49:ARG:HH11	3:A:49:ARG:HB3	1.77	0.49
3:A:86:ASP:HB2	3:A:93:ILE:HD12	1.94	0.49
6:D:111:ILE:HB	6:D:114:PHE:HB2	1.93	0.49
6:D:67:ILE:CG2	6:D:84:PRO:HB3	2.42	0.49
2:Y:51:G:OP1	14:L:99:ARG:HG2	2.12	0.49
19:Q:11:VAL:HG11	19:Q:16:ALA:HB2	1.94	0.49
20:R:107:ALA:HB1	20:R:111:GLY:HA2	1.95	0.49
1:X:1072:U:H4'	1:X:1081:A:O2'	2.12	0.49
1:X:1466:C:C2'	1:X:1467:U:O4'	2.60	0.49
1:X:1607:A:O2'	1:X:1608:U:O5'	2.30	0.49
1:X:579:G:H2'	1:X:2013:A:N6	2.28	0.49
1:X:564:U:H2'	1:X:565:A:C8	2.47	0.49
1:X:615:C:HO2'	1:X:670:U:C2'	2.21	0.49
1:X:917:U:O2	12:J:30:PHE:HZ	1.95	0.49
3:A:207:LEU:CA	3:A:212:ARG:HH11	2.24	0.49
10:H:75:VAL:CG1	10:H:118:LEU:HD21	2.14	0.49
13:K:33:ARG:C	13:K:34:ILE:CG2	2.81	0.49
14:L:12:ARG:O	14:L:16:LYS:HG3	2.13	0.49
1:X:2356:A:H2	14:L:91:ARG:HH22	1.59	0.49
2:Y:39:C:C2	14:L:97:HIS:NE2	2.79	0.49
20:R:92:THR:HG22	20:R:108:VAL:CG2	2.43	0.49
1:X:1010:U:O2'	1:X:1011:A:H5'	2.12	0.49
1:X:1118:G:C2'	1:X:1119:U:H5'	2.42	0.49
1:X:123:A:OP1	1:X:123:A:O4'	2.30	0.49
1:X:1261:G:H4'	1:X:1262:U:OP2	2.12	0.49
1:X:1401:G:H1	1:X:1412:C:H42	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1968:G:H2'	1:X:1969:G:C8	2.46	0.49
1:X:1978:U:C2	1:X:1979:C:H5	2.31	0.49
1:X:221:A:C2	1:X:232:A:C4	3.01	0.49
1:X:2404:A:OP2	1:X:2406:C:H5'	2.12	0.49
1:X:303:C:N3	1:X:360:A:H2	2.11	0.49
9:G:102:ARG:C	9:G:103:TYR:HD1	2.15	0.49
1:X:1300:A:H5'	13:K:103:ARG:HD2	1.95	0.49
16:N:11:ARG:HB3	16:N:15:LYS:NZ	2.27	0.49
16:N:93:LYS:O	16:N:94:VAL:HB	2.12	0.49
20:R:106:VAL:HG23	20:R:113:THR:HG21	1.94	0.49
1:X:1545:G:C6	1:X:1559:G:N2	2.80	0.49
1:X:1623:C:N4	1:X:1638:G:OP2	2.45	0.49
1:X:1676:U:C2'	1:X:1677:C:O5'	2.58	0.49
1:X:1704:G:C2	1:X:1719:G:C6	3.01	0.49
1:X:171:G:O2'	1:X:172:A:H5'	2.12	0.49
1:X:1812:U:O2	1:X:1812:U:H3'	2.12	0.49
1:X:2191:A:H5''	1:X:2192:U:H5	1.78	0.49
1:X:2429:A:C6	1:X:2430:A:C6	3.01	0.49
1:X:2625:U:OP2	1:X:2712:G:O2'	2.28	0.49
3:A:25:LEU:CB	3:A:206:VAL:H	2.26	0.49
1:X:2728:A:H4'	7:E:66:GLY:HA3	1.94	0.49
12:J:136:GLU:O	12:J:136:GLU:CG	2.58	0.49
1:X:2475:C:OP1	12:J:83:ARG:HB3	2.13	0.49
15:M:24:LEU:HD11	15:M:34:ARG:NH2	2.27	0.49
15:M:50:PHE:CZ	15:M:70:LYS:HB3	2.48	0.49
18:P:19:LYS:O	18:P:20:LEU:CB	2.60	0.49
20:R:85:ASP:O	20:R:85:ASP:OD1	2.30	0.49
1:X:1609:G:H2'	1:X:1610:A:O4'	2.11	0.49
1:X:1823:G:C4	1:X:1958:G:N2	2.81	0.49
1:X:1976:U:H4'	4:B:128:SER:HB3	1.94	0.49
1:X:2011:U:H2'	1:X:2012:A:C8	2.48	0.49
1:X:2496:C:C5	1:X:2521:A:N7	2.81	0.49
1:X:2548:G:C2'	1:X:2549:G:H5'	2.43	0.49
1:X:463:C:C2	1:X:465:C:C5	3.00	0.49
1:X:553:C:H42	1:X:559:C:H41	1.61	0.49
1:X:877:G:H21	1:X:879:A:H61	1.61	0.49
2:Y:25:G:H2'	2:Y:26:G:C5	2.47	0.49
3:A:66:ILE:HG21	3:A:68:PHE:HZ	1.65	0.49
5:C:7:ILE:HB	5:C:120:VAL:O	2.12	0.49
6:D:52:LYS:HZ2	6:D:150:ARG:HB2	1.78	0.49
2:Y:33:C:H5''	6:D:30:ARG:HH22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:70:VAL:HG22	10:H:71:LYS:N	2.27	0.49
12:J:137:VAL:C	12:J:138:TYR:CD2	2.86	0.49
22:T:69:PHE:C	22:T:70:ILE:HG13	2.33	0.49
1:X:76:C:C2	1:X:108:G:C2	3.00	0.49
1:X:1704:G:C2	1:X:1719:G:O6	2.66	0.49
1:X:1720:G:O2'	1:X:1721:G:H5'	2.13	0.49
1:X:1991:C:H2'	1:X:1992:G:C8	2.46	0.49
1:X:2016:A:O4'	1:X:2016:A:OP2	2.30	0.49
1:X:2592:U:H2'	26:Z:5:PRO:CB	2.43	0.49
1:X:789:G:C2	1:X:2220:A:OP1	2.65	0.49
1:X:888:G:N2	1:X:915:C:C2	2.80	0.49
2:Y:117:G:H2'	2:Y:118:G:C8	2.48	0.49
2:Y:83:C:C2'	2:Y:84:G:O5'	2.60	0.49
3:A:25:LEU:CB	3:A:206:VAL:CG2	2.90	0.49
3:A:97:HIS:CE1	3:A:101:GLY:CA	2.96	0.49
9:G:103:TYR:HB3	9:G:107:GLN:CG	2.39	0.49
16:N:76:TYR:CZ	16:N:80:ILE:HG13	2.47	0.49
18:P:14:ARG:HA	18:P:17:GLN:HG2	1.95	0.49
24:V:2:LYS:O	24:V:3:PRO:O	2.30	0.49
1:X:1015:U:O5'	1:X:1015:U:H6	1.95	0.49
1:X:1299:A:H1'	1:X:1301:U:OP2	2.13	0.49
1:X:2013:A:H5''	1:X:2014:A:OP1	2.12	0.49
1:X:2598:C:OP1	4:B:152:LYS:HE2	2.13	0.49
1:X:861:G:C2'	1:X:862:A:H5'	2.43	0.49
3:A:25:LEU:CB	3:A:206:VAL:HG22	2.43	0.49
4:B:60:ASN:HB3	4:B:62:PRO:HD2	1.95	0.49
10:H:26:ASN:O	10:H:26:ASN:CG	2.47	0.49
1:X:2795:A:C4'	13:K:5:LYS:HE3	2.42	0.49
13:K:80:MET:CA	13:K:80:MET:CE	2.89	0.49
1:X:2275:U:C4	14:L:10:LYS:HE2	2.48	0.49
16:N:52:ASN:HB2	16:N:55:ARG:HH21	1.78	0.49
17:O:10:LYS:O	17:O:11:GLN:HB2	2.12	0.49
17:O:23:GLU:O	17:O:24:SER:CB	2.60	0.49
18:P:85:MET:CE	18:P:130:GLU:HG3	2.43	0.49
20:R:62:MET:O	20:R:63:THR:OG1	2.30	0.49
1:X:1391:A:O4'	1:X:1392:U:OP1	2.30	0.49
1:X:2401:A:H62	29:3:32:GLN:NE2	2.11	0.49
1:X:2404:A:H1'	1:X:2405:A:OP2	2.13	0.49
1:X:681:A:C5	1:X:683:A:N7	2.80	0.49
1:X:708:G:C2	1:X:781:G:C2	3.01	0.49
1:X:775:U:H4'	1:X:776:G:N3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:959:C:OP1	1:X:973:U:OP1	2.30	0.49
1:X:982:C:H4'	1:X:994:A:O2'	2.12	0.49
1:X:958:G:O2'	1:X:995:A:C2	2.61	0.49
2:Y:67:C:C2'	2:Y:68:A:H5'	2.43	0.49
2:Y:84:G:O2'	2:Y:85:G:O5'	2.30	0.49
1:X:1817:U:H5'	3:A:253:LYS:HD3	1.94	0.48
3:A:76:VAL:HG11	3:A:100:ASP:OD2	2.13	0.48
4:B:102:ILE:HD11	4:B:184:VAL:HG22	1.94	0.48
4:B:47:VAL:HB	4:B:84:PHE:HD2	1.76	0.48
1:X:2291:U:OP1	6:D:71:LYS:HD2	2.12	0.48
9:G:70:PHE:HB3	16:N:64:ARG:CG	2.43	0.48
19:Q:60:GLY:O	19:Q:61:LYS:O	2.30	0.48
1:X:1819:U:C2'	1:X:1820:G:H5'	2.43	0.48
1:X:2595:C:H2'	1:X:2596:C:O4'	2.13	0.48
32:X:2882:LMA:C54	32:X:2882:LMA:C34	2.91	0.48
27:1:10:VAL:HG12	27:1:11:LYS:N	2.28	0.48
11:I:77:LEU:HB2	11:I:110:ALA:HA	1.95	0.48
16:N:66:ASN:ND2	16:N:70:ARG:HH12	2.12	0.48
16:N:40:LEU:HB3	17:O:74:TYR:CE2	2.47	0.48
18:P:80:LEU:HD11	18:P:87:GLU:HB3	1.95	0.48
1:X:2720:A:N6	1:X:2721:A:N1	2.60	0.48
1:X:32:C:H6	1:X:32:C:O5'	1.96	0.48
1:X:395:G:C2	1:X:406:G:C2	3.01	0.48
1:X:594:G:N2	1:X:1269:G:C6	2.80	0.48
1:X:955:G:N3	1:X:955:G:H5''	2.27	0.48
2:Y:85:G:C6	2:Y:86:A:C6	3.01	0.48
3:A:55:ILE:N	3:A:55:ILE:HD12	2.28	0.48
5:C:17:LEU:N	5:C:17:LEU:HD12	2.28	0.48
6:D:132:ILE:HG13	6:D:154:ILE:HD13	1.96	0.48
10:H:11:ALA:O	10:H:110:VAL:HG13	2.13	0.48
16:N:79:PHE:HE2	16:N:95:LEU:HD21	1.78	0.48
1:X:1526:U:H2'	1:X:1527:G:O4'	2.13	0.48
1:X:1676:U:O2	1:X:2692:A:H2	1.96	0.48
1:X:581:A:H2'	1:X:582:G:O4'	2.13	0.48
1:X:700:C:OP1	28:2:6:GLN:HG3	2.14	0.48
1:X:780:U:O2'	1:X:781:G:O4'	2.30	0.48
1:X:817:A:H2'	1:X:819:C:N3	2.28	0.48
1:X:863:C:O2'	25:W:19:THR:OG1	2.09	0.48
29:3:6:THR:O	29:3:9:MET:HB3	2.14	0.48
3:A:106:ILE:HG22	3:A:107:LEU:N	2.28	0.48
3:A:90:SER:O	3:A:199:ASN:CG	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:91:VAL:HB	4:B:93:VAL:HG12	1.95	0.48
9:G:141:GLY:O	9:G:144:MET:N	2.46	0.48
14:L:36:LYS:CE	14:L:65:THR:HG22	2.44	0.48
1:X:1017:C:H2'	1:X:1018:C:H6	1.78	0.48
1:X:1282:A:C2	1:X:1338:G:N2	2.81	0.48
1:X:1327:C:N4	1:X:1351:G:H1	2.07	0.48
1:X:1609:G:O2'	1:X:1610:A:H5'	2.12	0.48
1:X:2581:A:OP2	1:X:2582:G:OP2	2.32	0.48
1:X:2592:U:H2'	26:Z:5:PRO:HG2	1.94	0.48
1:X:2762:G:C2	1:X:2763:U:C2	3.02	0.48
1:X:2840:U:O4	1:X:2841:U:O4	2.30	0.48
1:X:496:C:H2'	1:X:497:C:H5'	1.95	0.48
27:1:9:ILE:HD11	27:1:26:LYS:HD2	1.94	0.48
3:A:55:ILE:N	3:A:218:ARG:HB3	2.29	0.48
4:B:120:TRP:CB	4:B:122:PHE:CE2	2.97	0.48
4:B:35:GLN:HB3	4:B:48:GLN:OE1	2.14	0.48
11:I:88:PHE:HD2	11:I:90:ARG:HE	1.62	0.48
15:M:60:SER:HA	15:M:64:LYS:HB2	1.96	0.48
17:O:13:ARG:HD3	17:O:16:GLU:HB2	1.94	0.48
19:Q:7:LEU:CD1	19:Q:7:LEU:H	2.26	0.48
20:R:11:ASN:O	20:R:12:ASP:CB	2.60	0.48
20:R:73:GLU:HA	20:R:73:GLU:OE1	2.12	0.48
24:V:18:ILE:HG22	24:V:22:LYS:HE2	1.94	0.48
1:X:1840:A:H2'	1:X:1841:G:O4'	2.13	0.48
1:X:1948:C:C6	1:X:1949:A:N7	2.81	0.48
1:X:2453:C:H5'	1:X:2454:C:OP2	2.14	0.48
1:X:2745:A:H3'	1:X:2745:A:N3	2.28	0.48
1:X:681:A:C8	1:X:681:A:C3'	2.97	0.48
1:X:746:G:H22	1:X:747:A:N6	2.11	0.48
3:A:132:LEU:HD21	3:A:194:ILE:HD11	1.96	0.48
3:A:66:ILE:CD1	3:A:89:ARG:CZ	2.92	0.48
6:D:40:LEU:HD23	6:D:40:LEU:C	2.34	0.48
11:I:34:HIS:O	11:I:35:LYS:HD3	2.13	0.48
9:G:66:HIS:O	16:N:67:ALA:HB1	2.14	0.48
24:V:7:ARG:HD2	24:V:7:ARG:C	2.34	0.48
25:W:23:LEU:HD21	25:W:43:MET:HB3	1.95	0.48
1:X:1975:G:C1'	1:X:1976:U:OP2	2.62	0.48
1:X:1386:A:H5''	1:X:2191:A:H62	1.77	0.48
1:X:33:C:H4'	1:X:34:U:OP2	2.13	0.48
1:X:585:U:O2'	1:X:2481:G:C6	2.66	0.48
1:X:594:G:C2	1:X:1269:G:C6	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:958:G:N2	1:X:982:C:C2	2.81	0.48
26:Z:8:LYS:O	26:Z:9:LYS:HG3	2.14	0.48
27:1:37:LEU:HA	27:1:51:ARG:HA	1.96	0.48
1:X:795:A:N1	3:A:227:MET:HE2	2.28	0.48
10:H:3:MET:O	10:H:6:SER:CB	2.62	0.48
10:H:52:VAL:HG12	10:H:53:ALA:N	2.27	0.48
15:M:17:GLU:HG3	15:M:62:SER:CB	2.42	0.48
1:X:1608:U:C5	1:X:1609:G:N7	2.81	0.48
1:X:2180:U:C5	1:X:2203:G:C6	3.01	0.48
1:X:2426:G:O2'	1:X:2427:A:OP2	2.30	0.48
1:X:2665:G:N2	1:X:2704:U:O2	2.46	0.48
1:X:537:C:H5	1:X:2759:U:H2'	1.76	0.48
1:X:537:C:O2	1:X:537:C:H2'	2.14	0.48
1:X:736:G:H2'	1:X:737:C:O4'	2.13	0.48
2:Y:58:G:H5''	2:Y:59:A:OP1	2.14	0.48
2:Y:84:G:N2	2:Y:98:C:H1'	2.28	0.48
1:X:2349:G:N2	27:1:46:LYS:HZ2	2.09	0.48
4:B:7:THR:HG1	4:B:51:TYR:HH	1.60	0.48
14:L:21:THR:HG22	14:L:45:ASP:O	2.13	0.48
17:O:80:TYR:CE2	17:O:82:ARG:HG2	2.49	0.48
1:X:118:U:C2	1:X:143:A:C6	3.02	0.48
1:X:482:A:C2'	1:X:483:A:H5'	2.43	0.48
1:X:954:U:OP2	11:I:38:LYS:HG2	2.13	0.48
3:A:71:ARG:CG	3:A:191:TYR:CE1	2.96	0.48
3:A:44:ARG:CD	3:A:44:ARG:H	2.01	0.48
4:B:49:ILE:HG21	4:B:81:PHE:HE2	1.79	0.48
5:C:130:THR:O	5:C:133:PHE:HB3	2.13	0.48
7:E:174:GLY:C	7:E:175:LYS:CG	2.81	0.48
9:G:49:VAL:HG12	9:G:54:LEU:HB2	1.95	0.48
12:J:7:ARG:C	12:J:70:PHE:HZ	2.17	0.48
1:X:2814:G:O4'	13:K:49:GLU:OE2	2.31	0.48
23:U:10:LYS:NZ	23:U:77:GLY:HA3	2.28	0.48
23:U:22:GLY:HA3	23:U:39:LYS:HD2	1.95	0.48
1:X:1545:G:N1	1:X:1559:G:C2	2.82	0.48
1:X:1693:A:N6	1:X:1694:A:C6	2.82	0.48
1:X:171:G:C2	1:X:179:U:O2	2.67	0.48
1:X:1910:A:C6	1:X:1911:A:N1	2.82	0.48
1:X:1982:C:C2'	1:X:1983:G:H5'	2.43	0.48
1:X:2203:G:H4'	1:X:2205:C:N3	2.29	0.48
1:X:2551:A:P	4:B:146:THR:HG1	2.36	0.48
1:X:2593:A:O2'	1:X:2594:U:OP2	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2626:U:H6	1:X:2626:U:O5'	1.96	0.48
1:X:2754:C:N4	1:X:2755:A:C6	2.82	0.48
1:X:2800:C:H2'	1:X:2801:A:H5'	1.96	0.48
27:1:38:LYS:HD3	27:1:40:TYR:HE1	1.78	0.48
3:A:71:ARG:NH1	3:A:151:GLY:H	2.12	0.48
3:A:216:LEU:N	3:A:216:LEU:HD12	2.29	0.48
9:G:35:LYS:HB2	9:G:37:ASP:H	1.78	0.48
12:J:137:VAL:O	12:J:138:TYR:CG	2.67	0.48
1:X:1387:G:C5	1:X:1388:C:C4	3.02	0.48
1:X:2587:G:H8	1:X:2587:G:O5'	1.96	0.48
1:X:2613:A:H2'	1:X:2614:A:C8	2.49	0.48
1:X:859:U:O2'	1:X:860:U:C2	2.64	0.48
1:X:861:G:C6	1:X:943:U:O2	2.67	0.48
2:Y:84:G:H2'	2:Y:85:G:H8	1.79	0.48
27:1:8:ILE:C	27:1:9:ILE:CG2	2.81	0.47
11:I:62:LYS:HZ3	29:3:12:ARG:C	2.16	0.47
1:X:2399:C:H5	29:3:31:HIS:O	1.97	0.47
3:A:220:PRO:O	3:A:221:HIS:C	2.53	0.47
4:B:50:GLY:HA2	4:B:77:ILE:O	2.13	0.47
12:J:99:LYS:HG3	12:J:100:PRO:HD2	1.96	0.47
15:M:34:ARG:HH11	15:M:88:VAL:CG2	2.23	0.47
21:S:94:VAL:HG23	21:S:125:PRO:HG3	1.96	0.47
1:X:1444:C:N4	1:X:1579:G:H1	2.09	0.47
1:X:1871:G:N3	1:X:1871:G:H3'	2.29	0.47
1:X:542:A:N6	1:X:2003:A:N3	2.61	0.47
1:X:2440:C:C5	1:X:2441:U:C5	3.02	0.47
1:X:2634:G:O2'	1:X:2635:U:C5	2.62	0.47
1:X:525:A:C8	1:X:526:C:C5	3.02	0.47
1:X:959:C:C1'	1:X:995:A:C2	2.96	0.47
28:2:15:THR:C	28:2:17:GLY:H	2.17	0.47
1:X:2400:G:N7	29:3:32:GLN:HB3	2.30	0.47
1:X:1261:G:C5	16:N:3:ARG:HB2	2.49	0.47
21:S:122:ILE:HB	21:S:159:THR:O	2.14	0.47
24:V:2:LYS:N	24:V:3:PRO:HD3	2.29	0.47
1:X:1441:A:C8	1:X:1442:C:C5	3.02	0.47
1:X:2191:A:H5''	1:X:2192:U:C5	2.49	0.47
1:X:2658:A:C2	1:X:2709:C:N3	2.82	0.47
1:X:2728:A:C2	1:X:2737:A:C6	3.03	0.47
1:X:2042:A:N1	32:X:2882:LMA:H29A	2.29	0.47
1:X:334:G:H4'	1:X:335:A:C5'	2.45	0.47
1:X:532:A:C6	1:X:533:C:N3	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:580:A:H1'	1:X:582:G:C8	2.49	0.47
1:X:589:C:H4'	16:N:31:GLN:HE22	1.79	0.47
1:X:793:G:H1'	1:X:798:G:N2	2.29	0.47
27:1:17:GLY:O	27:1:18:THR:HB	2.13	0.47
1:X:1042:G:H5'	30:4:6:SER:OG	2.14	0.47
4:B:136:ARG:HH21	4:B:157:ALA:HB2	1.79	0.47
5:C:6:VAL:HG12	5:C:7:ILE:CD1	2.43	0.47
13:K:36:THR:HG23	13:K:37:THR:O	2.14	0.47
13:K:52:ILE:HG13	13:K:53:THR:N	2.28	0.47
14:L:38:ILE:HD12	14:L:39:TYR:H	1.78	0.47
22:T:44:LYS:O	22:T:77:ARG:HB2	2.13	0.47
1:X:1407:G:C6	1:X:1408:A:N6	2.82	0.47
1:X:2315:A:H1'	1:X:2364:C:O4'	2.15	0.47
1:X:2376:G:C2	1:X:2399:C:O2	2.68	0.47
1:X:2819:G:H2'	1:X:2820:C:H6	1.79	0.47
1:X:469:G:H2'	28:2:39:ARG:O	2.13	0.47
1:X:681:A:C8	1:X:681:A:H3'	2.50	0.47
1:X:921:A:N6	1:X:924:C:O2	2.47	0.47
1:X:942:U:H2'	1:X:943:U:O4'	2.15	0.47
2:Y:71:G:C6	2:Y:72:C:C2	3.03	0.47
3:A:70:ARG:NH1	3:A:131:ALA:HB2	2.29	0.47
1:X:1796:A:H1'	3:A:51:THR:HG23	1.97	0.47
10:H:25:LEU:HD11	10:H:52:VAL:HG23	1.96	0.47
11:I:56:LEU:CD1	29:3:52:LYS:HD2	2.44	0.47
17:O:36:LYS:HE2	17:O:56:VAL:HG13	1.96	0.47
18:P:11:LYS:HA	18:P:14:ARG:NH1	2.29	0.47
1:X:1018:C:H3'	1:X:1019:U:H5''	1.96	0.47
1:X:1656:U:O2'	1:X:1657:A:H5''	2.14	0.47
1:X:173:A:O2'	1:X:2051:U:C5	2.67	0.47
1:X:1763:G:H2'	1:X:1764:A:H5'	1.97	0.47
1:X:2294:U:H4'	6:D:127:ASN:HD21	1.79	0.47
1:X:2539:C:N4	1:X:2540:A:N6	2.63	0.47
1:X:2791:C:O2'	1:X:2792:C:H5'	2.14	0.47
1:X:40:U:H2'	1:X:41:G:O4'	2.14	0.47
2:Y:9:G:C2	2:Y:117:G:C2	3.02	0.47
27:1:43:VAL:HG23	27:1:43:VAL:O	2.14	0.47
3:A:24:GLY:O	3:A:208:GLY:HA2	2.15	0.47
5:C:95:LEU:HD23	5:C:96:PRO:N	2.30	0.47
6:D:94:GLU:O	6:D:98:VAL:HG23	2.14	0.47
12:J:27:TYR:C	12:J:28:VAL:CG2	2.82	0.47
13:K:35:GLN:O	13:K:35:GLN:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:42:ILE:HG22	14:L:53:ALA:H	1.79	0.47
16:N:93:LYS:CE	17:O:5:ILE:HG21	2.45	0.47
1:X:410:A:OP1	23:U:47:HIS:CE1	2.68	0.47
1:X:1681:A:H3'	1:X:1682:A:C8	2.50	0.47
1:X:1986:G:H2'	1:X:1987:G:O5'	2.14	0.47
1:X:2046:C:C5	1:X:2047:C:N4	2.82	0.47
1:X:623:G:H2'	1:X:624:A:H5''	1.94	0.47
1:X:793:G:C2	1:X:798:G:C6	3.03	0.47
1:X:993:C:C5'	1:X:994:A:OP2	2.62	0.47
1:X:123:A:H5'	28:2:19:ARG:HE	1.79	0.47
11:I:60:LEU:HG	29:3:13:ARG:CD	2.44	0.47
3:A:150:PRO:HD3	3:A:187:HIS:NE2	2.29	0.47
13:K:87:TYR:CE1	13:K:94:TYR:CB	2.98	0.47
16:N:86:ALA:C	16:N:88:ILE:H	2.16	0.47
19:Q:35:LYS:HA	19:Q:38:ILE:CG2	2.43	0.47
20:R:80:LYS:O	20:R:80:LYS:HG3	2.14	0.47
23:U:39:LYS:HB3	23:U:41:VAL:HG13	1.96	0.47
23:U:75:TYR:O	23:U:76:LYS:HB2	2.15	0.47
1:X:980:G:H5''	25:W:12:ARG:O	2.15	0.47
1:X:1050:G:H2'	1:X:1051:U:H5'	1.96	0.47
1:X:1550:C:O2'	1:X:1551:U:H5''	2.15	0.47
1:X:977:G:H1'	1:X:2246:A:H62	1.80	0.47
1:X:451:A:H2'	1:X:452:G:C8	2.50	0.47
1:X:616:U:H2'	1:X:617:U:O4'	2.15	0.47
1:X:830:C:H2'	1:X:831:G:O4'	2.15	0.47
7:E:69:ARG:HD3	7:E:69:ARG:C	2.34	0.47
9:G:38:GLU:OE2	9:G:40:ASN:HB2	2.14	0.47
9:G:94:LYS:HB2	9:G:94:LYS:HE3	1.80	0.47
17:O:22:VAL:CA	17:O:91:THR:HG22	2.41	0.47
21:S:95:SER:HA	21:S:121:GLN:HA	1.97	0.47
24:V:7:ARG:HD2	24:V:8:ASN:N	2.29	0.47
1:X:1681:A:OP1	1:X:1682:A:OP2	2.33	0.47
1:X:1685:A:C4'	1:X:1686:A:C2	2.97	0.47
1:X:1780:A:OP1	3:A:222:GLN:OE1	2.32	0.47
1:X:182:G:C2'	1:X:183:U:OP2	2.61	0.47
1:X:216:U:H2'	1:X:217:U:O4'	2.15	0.47
1:X:2672:U:O2'	1:X:2673:G:H5'	2.14	0.47
1:X:2825:A:C6	1:X:2826:C:N3	2.83	0.47
1:X:2855:C:O5'	1:X:2855:C:H6	1.98	0.47
1:X:553:C:H42	1:X:559:C:N4	2.12	0.47
1:X:523:A:H2	1:X:591:G:H4'	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:968:C:OP1	12:J:78:LYS:HB2	2.14	0.47
2:Y:104:A:N6	2:Y:105:G:C6	2.83	0.47
27:1:3:LYS:HG2	27:1:4:ASP:N	2.30	0.47
1:X:2597:G:O2'	4:B:149:ARG:HB2	2.15	0.47
6:D:22:TYR:CZ	6:D:29:PRO:HD3	2.50	0.47
9:G:70:PHE:CD1	16:N:64:ARG:HA	2.49	0.47
21:S:130:ILE:HD12	21:S:130:ILE:N	2.29	0.47
21:S:25:ASN:OD1	21:S:26:LYS:HG2	2.15	0.47
1:X:2258:G:O6	22:T:15:ASP:CG	2.53	0.47
22:T:51:VAL:HG21	22:T:79:ILE:O	2.15	0.47
1:X:1128:G:C3'	1:X:1129:A:H5''	2.45	0.47
1:X:163:A:H2'	1:X:164:G:H8	1.80	0.47
1:X:1851:A:H2'	1:X:1852:G:O4'	2.14	0.47
1:X:2447:G:O2'	1:X:2448:A:C8	2.67	0.47
1:X:2571:G:C6	1:X:2572:U:N3	2.83	0.47
1:X:2571:G:N1	1:X:2582:G:C6	2.83	0.47
1:X:668:A:O2'	1:X:669:G:O4'	2.31	0.47
1:X:801:A:OP1	1:X:804:C:N4	2.47	0.47
1:X:94:C:H1'	24:V:40:PRO:CD	2.45	0.47
26:Z:33:CYS:CB	26:Z:38:GLY:O	2.63	0.47
12:J:117:GLU:O	12:J:121:LEU:HG	2.14	0.47
14:L:39:TYR:O	14:L:54:ALA:C	2.54	0.47
15:M:72:SER:HG	15:M:73:PHE:HD1	1.62	0.47
16:N:50:ARG:O	16:N:53:LYS:HG2	2.15	0.47
20:R:85:ASP:C	20:R:85:ASP:OD1	2.52	0.47
1:X:1141:U:C4	4:B:147:PRO:CD	2.95	0.47
1:X:161:U:H4'	1:X:194:G:N2	2.25	0.47
1:X:2006:G:N2	1:X:2024:U:O2	2.48	0.47
1:X:2063:A:H4'	23:U:39:LYS:HA	1.97	0.47
1:X:2277:A:N6	1:X:2278:A:C2	2.83	0.47
1:X:2394:G:C6	1:X:2395:C:C4	3.03	0.47
1:X:2051:U:H3	1:X:2409:A:H62	1.63	0.47
1:X:2046:C:O2	1:X:2430:A:N1	2.48	0.47
1:X:510:G:N2	1:X:513:A:C8	2.83	0.47
1:X:555:U:H5'	1:X:556:A:N7	2.29	0.47
1:X:709:A:C2	1:X:780:U:O2	2.68	0.47
28:2:15:THR:O	28:2:16:HIS:CB	2.62	0.47
9:G:132:PHE:CD2	9:G:145:HIS:HB2	2.48	0.47
20:R:85:ASP:H	20:R:90:LYS:HD3	1.80	0.47
1:X:1407:G:H3'	1:X:1407:G:N3	2.29	0.47
1:X:2044:G:OP1	5:C:62:LYS:CG	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2299:A:H3'	1:X:2299:A:N3	2.29	0.47
1:X:2671:C:O2'	1:X:2672:U:H5'	2.15	0.47
1:X:596:C:OP2	11:I:29:THR:HG21	2.15	0.47
1:X:579:G:C4'	1:X:994:A:C2	2.98	0.47
3:A:147:GLU:HG2	3:A:154:ALA:CA	2.44	0.47
8:F:79:ARG:HA	8:F:84:ILE:HB	1.97	0.47
10:H:81:ILE:O	10:H:81:ILE:HG23	2.14	0.47
19:Q:12:ILE:N	19:Q:12:ILE:HD13	2.29	0.47
1:X:1225:G:O6	18:P:12:LYS:HB2	2.15	0.47
1:X:1324:G:C4'	1:X:1325:U:OP1	2.60	0.47
1:X:1730:G:C2	1:X:1737:G:C2	3.02	0.47
32:X:2882:LMA:O57	18:P:111:ARG:NH2	2.48	0.47
1:X:757:U:H4'	1:X:1675:C:O3'	2.15	0.47
1:X:791:G:H2'	1:X:792:U:O4'	2.15	0.47
1:X:1998:A:H2	26:Z:5:PRO:O	1.98	0.47
11:I:81:GLN:HB3	11:I:114:ILE:HG23	1.97	0.46
15:M:24:LEU:HD11	15:M:34:ARG:HH22	1.80	0.46
18:P:103:LEU:HB2	18:P:119:LYS:HB2	1.97	0.46
20:R:11:ASN:HD22	20:R:13:LYS:HZ3	1.63	0.46
20:R:11:ASN:HD22	20:R:13:LYS:NZ	2.13	0.46
1:X:1790:G:H5''	3:A:262:ARG:HH21	1.79	0.46
1:X:1817:U:O4'	3:A:253:LYS:HD3	2.14	0.46
1:X:2676:G:N1	1:X:2690:A:C2	2.83	0.46
1:X:2707:G:O2'	1:X:2708:U:O5'	2.31	0.46
1:X:2430:A:C6	31:X:2881:LC2:C15	2.98	0.46
1:X:521:U:C3'	1:X:522:G:H5'	2.45	0.46
1:X:615:C:H4'	1:X:669:G:H21	1.78	0.46
1:X:832:A:H2'	1:X:833:A:O4'	2.14	0.46
4:B:7:THR:HG23	4:B:194:GLY:O	2.15	0.46
9:G:103:TYR:N	9:G:103:TYR:CD1	2.82	0.46
15:M:34:ARG:HE	15:M:91:VAL:HG22	1.80	0.46
1:X:514:G:C6	18:P:20:LEU:HD22	2.50	0.46
1:X:1480:G:C2	1:X:1481:U:O2	2.68	0.46
1:X:314:G:C2	1:X:326:A:C2	3.03	0.46
1:X:584:A:OP2	1:X:2038:C:C5	2.68	0.46
1:X:608:G:C6	1:X:609:U:C4	3.03	0.46
1:X:793:G:N1	1:X:795:A:C2	2.83	0.46
2:Y:3:A:H61	2:Y:122:U:H3	1.64	0.46
26:Z:49:CYS:SG	26:Z:51:TYR:HD1	2.39	0.46
11:I:62:LYS:HZ2	29:3:15:LYS:HE2	1.81	0.46
4:B:114:GLN:HB3	4:B:118:LYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:57:LEU:HD23	6:D:60:ILE:HD11	1.96	0.46
10:H:116:ARG:C	10:H:118:LEU:N	2.67	0.46
14:L:89:PHE:HB3	14:L:91:ARG:HH21	1.81	0.46
17:O:6:GLN:O	17:O:7:THR:OG1	2.30	0.46
23:U:32:ARG:N	23:U:32:ARG:HE	2.13	0.46
1:X:1289:A:H2'	1:X:1290:A:C8	2.50	0.46
1:X:540:G:C6	1:X:2005:U:C5'	2.98	0.46
1:X:26:G:C6	1:X:27:G:N1	2.84	0.46
1:X:330:C:H2'	1:X:331:U:O4'	2.16	0.46
1:X:333:A:H5''	5:C:162:ARG:HG3	1.98	0.46
1:X:412:U:H2'	1:X:413:G:O4'	2.15	0.46
1:X:41:G:H2'	1:X:42:G:H8	1.81	0.46
1:X:791:G:N2	1:X:800:U:O2	2.48	0.46
3:A:244:GLY:H	3:A:245:ARG:NH1	2.13	0.46
1:X:1674:C:OP1	4:B:134:TRP:O	2.33	0.46
12:J:27:TYR:HB2	12:J:137:VAL:HG21	1.91	0.46
21:S:69:VAL:HG13	21:S:81:VAL:HG22	1.96	0.46
1:X:1336:G:O6	1:X:1337:G:C6	2.68	0.46
1:X:1960:A:H2'	1:X:1961:A:O4'	2.16	0.46
1:X:2053:G:N2	1:X:2054:A:N3	2.63	0.46
1:X:2191:A:C5'	1:X:2192:U:H5	2.29	0.46
1:X:2350:G:C6	1:X:2351:G:C5	3.03	0.46
1:X:2860:C:H2'	1:X:2861:A:O4'	2.15	0.46
4:B:92:ASN:OD1	4:B:92:ASN:N	2.46	0.46
5:C:104:LEU:HA	5:C:107:ALA:HB3	1.98	0.46
5:C:119:ALA:H	5:C:189:ASP:HA	1.81	0.46
5:C:46:ARG:HD2	5:C:51:VAL:HG23	1.97	0.46
12:J:13:GLN:HG2	12:J:14:PHE:CD2	2.51	0.46
14:L:33:ARG:NH2	14:L:103:LEU:HD12	2.31	0.46
4:B:183:LEU:HD21	15:M:16:ILE:HD13	1.98	0.46
23:U:14:VAL:O	23:U:15:VAL:CG2	2.63	0.46
1:X:1058:G:H5''	1:X:1058:G:H8	1.81	0.46
1:X:115:G:C6	1:X:117:A:N6	2.84	0.46
1:X:1336:G:C2	1:X:1346:C:H1'	2.50	0.46
1:X:2374:C:N4	1:X:2400:G:H1	2.14	0.46
1:X:2502:G:C2	1:X:2745:A:N6	2.83	0.46
1:X:2606:G:N2	1:X:2757:G:N3	2.64	0.46
1:X:748:A:C5	1:X:749:C:C2	3.04	0.46
2:Y:3:A:H2'	2:Y:4:C:H5'	1.97	0.46
2:Y:75:A:C6	2:Y:76:U:C2	3.03	0.46
6:D:13:ARG:HG2	6:D:17:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:162:LYS:N	9:G:163:PRO:HD2	2.29	0.46
12:J:99:LYS:HD2	12:J:100:PRO:HD2	1.98	0.46
13:K:62:SER:O	13:K:66:VAL:HG23	2.15	0.46
4:B:9:ILE:CG2	15:M:9:ARG:HB2	2.46	0.46
1:X:1202:U:C2'	1:X:1202:U:O2	2.62	0.46
1:X:1686:A:N6	1:X:1977:C:O2	2.48	0.46
1:X:2033:C:N4	1:X:2034:A:N1	2.63	0.46
1:X:2350:G:C6	1:X:2351:G:N7	2.84	0.46
1:X:2379:G:H2'	1:X:2380:U:O4'	2.15	0.46
1:X:2548:G:O2'	1:X:2549:G:H5'	2.16	0.46
1:X:478:G:H2'	1:X:479:G:C8	2.51	0.46
1:X:830:C:O5'	1:X:830:C:H6	1.98	0.46
1:X:89:A:H4'	1:X:90:G:H5''	1.97	0.46
1:X:577:U:C5'	1:X:956:A:H61	2.24	0.46
1:X:986:A:C2	1:X:1001:A:C8	3.03	0.46
15:M:81:PHE:HA	15:M:82:PRO:HD2	1.74	0.46
1:X:1171:A:H1'	17:O:6:GLN:OE1	2.15	0.46
21:S:49:THR:OG1	21:S:132:GLN:HA	2.15	0.46
22:T:47:ALA:HB1	22:T:51:VAL:O	2.16	0.46
1:X:118:U:H5''	1:X:120:G:OP2	2.15	0.46
1:X:1217:U:O2'	1:X:1218:C:H5'	2.15	0.46
1:X:1371:G:C8	1:X:1384:G:O6	2.69	0.46
1:X:2002:A:H62	26:Z:9:LYS:NZ	2.14	0.46
1:X:2563:U:H6	1:X:2563:U:O5'	1.97	0.46
1:X:2701:A:H2'	1:X:2702:G:O4'	2.15	0.46
1:X:28:A:H2'	1:X:29:U:O4'	2.16	0.46
1:X:746:G:N7	1:X:774:A:C6	2.84	0.46
1:X:790:A:N7	1:X:806:A:H2	2.14	0.46
1:X:995:A:P	1:X:996:C:H5	2.39	0.46
1:X:2035:G:O2'	4:B:148:GLY:HA2	2.16	0.46
10:H:34:LEU:HA	10:H:34:LEU:HD23	1.65	0.46
13:K:60:LEU:O	13:K:64:ARG:HG3	2.15	0.46
15:M:39:VAL:CG1	15:M:45:THR:OG1	2.57	0.46
16:N:105:ALA:HA	17:O:45:THR:HG21	1.98	0.46
17:O:67:LYS:HD2	17:O:68:LYS:N	2.31	0.46
1:X:1099:A:O3'	1:X:1100:G:H8	1.99	0.46
1:X:1677:C:C2	1:X:1984:A:C2	3.03	0.46
1:X:2427:A:H62	11:I:40:ARG:NH2	1.77	0.46
1:X:2547:C:H6	1:X:2547:C:H3'	1.81	0.46
1:X:2824:C:O4'	1:X:2843:A:C5	2.68	0.46
1:X:396:U:H3	1:X:404:A:H61	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:478:G:C4	1:X:479:G:C8	3.04	0.46
1:X:539:A:C6	1:X:2006:G:C4	3.04	0.46
1:X:543:G:H5'	16:N:24:PHE:CD1	2.51	0.46
1:X:862:A:O2'	25:W:18:LYS:HB3	2.16	0.46
1:X:919:U:OP1	12:J:26:ASP:OD1	2.34	0.46
1:X:1810:U:N3	3:A:155:GLN:HB3	2.31	0.46
4:B:49:ILE:O	4:B:78:LEU:HA	2.16	0.46
9:G:55:ALA:HB1	9:G:134:MET:HE1	1.97	0.46
10:H:3:MET:O	10:H:6:SER:HB3	2.16	0.46
17:O:68:LYS:HB2	17:O:87:ARG:HH21	1.81	0.46
1:X:1631:C:H5	1:X:1633:C:C4	2.34	0.46
1:X:1682:A:O5'	1:X:1682:A:C8	2.59	0.46
1:X:2445:C:N4	1:X:2446:C:N4	2.64	0.46
1:X:24:G:C2	1:X:25:U:C2	3.04	0.46
1:X:2521:A:H61	1:X:2546:G:N2	2.14	0.46
1:X:2528:G:O2'	1:X:2529:G:H5'	2.15	0.46
1:X:2625:U:O4	1:X:2654:A:C2	2.68	0.46
1:X:26:G:C5	1:X:27:G:C6	3.04	0.46
1:X:347:C:H2'	1:X:348:U:C6	2.50	0.46
1:X:352:G:H2'	1:X:353:G:C8	2.51	0.46
1:X:514:G:H2'	1:X:514:G:N3	2.30	0.46
1:X:699:G:H4'	1:X:700:C:OP2	2.16	0.46
1:X:84:G:H5'	20:R:41:PRO:HD3	1.97	0.46
3:A:97:HIS:HE1	3:A:101:GLY:CA	2.28	0.46
13:K:45:ARG:O	13:K:48:VAL:HG12	2.16	0.46
13:K:54:THR:CG2	13:K:66:VAL:CG2	2.93	0.46
16:N:109:LEU:HD23	17:O:47:PHE:CE2	2.51	0.46
19:Q:57:ASN:N	19:Q:57:ASN:OD1	2.49	0.46
20:R:11:ASN:HB3	20:R:13:LYS:HZ3	1.80	0.46
1:X:865:A:H5'	25:W:42:GLY:HA3	1.97	0.46
1:X:1392:U:C6	1:X:1392:U:O5'	2.67	0.46
1:X:1696:C:C6	1:X:1696:C:O5'	2.56	0.46
1:X:1978:U:C2	1:X:1979:C:C5	3.03	0.46
1:X:577:U:H2'	1:X:579:G:OP2	2.15	0.46
1:X:573:C:H5	1:X:582:G:OP1	1.98	0.46
1:X:623:G:C3'	1:X:624:A:H5''	2.46	0.46
1:X:708:G:N3	1:X:781:G:C2	2.84	0.46
1:X:834:A:C8	1:X:834:A:H3'	2.51	0.46
1:X:935:C:H4'	22:T:29:GLU:HG2	1.97	0.46
2:Y:112:A:H2'	2:Y:113:G:O4'	2.16	0.46
28:2:10:ARG:HE	28:2:10:ARG:N	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:182:ILE:O	4:B:182:ILE:CG2	2.64	0.45
6:D:12:VAL:O	6:D:16:LEU:HG	2.16	0.45
6:D:31:ILE:HG22	6:D:96:MET:SD	2.56	0.45
13:K:52:ILE:CG1	13:K:53:THR:N	2.79	0.45
16:N:54:LYS:O	16:N:58:ARG:HG3	2.16	0.45
18:P:83:ASP:O	18:P:84:GLU:C	2.54	0.45
21:S:155:PRO:HG3	21:S:158:CYS:SG	2.56	0.45
21:S:92:VAL:HG22	21:S:93:GLU:N	2.30	0.45
1:X:1973:C:H6	1:X:1973:C:O5'	1.99	0.45
1:X:2350:G:N1	1:X:2351:G:C5	2.84	0.45
1:X:2671:C:C5'	1:X:2845:C:O2	2.64	0.45
1:X:224:G:H4'	1:X:399:G:C5	2.51	0.45
1:X:551:A:C2	1:X:562:G:C2	3.05	0.45
3:A:73:LYS:HE2	3:A:98:TYR:HD2	1.82	0.45
4:B:136:ARG:O	4:B:137:ARG:HB3	2.16	0.45
5:C:157:THR:HG23	5:C:158:ARG:N	2.30	0.45
6:D:4:LEU:HD23	6:D:97:TYR:HB3	1.97	0.45
10:H:23:ARG:CZ	10:H:23:ARG:HB3	2.43	0.45
15:M:75:GLU:O	15:M:77:VAL:HG23	2.14	0.45
18:P:17:GLN:HG3	18:P:18:VAL:HG23	1.97	0.45
1:X:1379:A:H2'	1:X:1380:C:O4'	2.16	0.45
1:X:1911:A:H2'	1:X:1912:G:O4'	2.17	0.45
1:X:2274:C:H5	14:L:14:ARG:HH12	1.63	0.45
1:X:2274:C:OP2	14:L:11:LEU:CD2	2.63	0.45
1:X:802:A:C2	28:2:3:ARG:NH1	2.85	0.45
1:X:836:G:H2'	1:X:837:U:C6	2.51	0.45
2:Y:118:G:O2'	2:Y:119:G:H5'	2.16	0.45
1:X:1141:U:N3	4:B:147:PRO:HG3	2.31	0.45
4:B:21:ILE:HG22	4:B:23:VAL:HG13	1.98	0.45
5:C:7:ILE:C	5:C:120:VAL:O	2.54	0.45
1:X:2275:U:C4	14:L:10:LYS:HD3	2.51	0.45
20:R:83:LEU:HD22	20:R:113:THR:HB	1.98	0.45
23:U:49:LYS:HD3	23:U:61:TRP:CE2	2.51	0.45
1:X:1097:A:H5''	1:X:1097:A:N3	2.32	0.45
1:X:1172:U:H2'	1:X:1173:G:C8	2.50	0.45
1:X:1975:G:N2	1:X:1979:C:O2'	2.49	0.45
1:X:2270:U:O2'	1:X:2353:G:H1'	2.16	0.45
1:X:1477:C:O2'	1:X:2681:A:H1'	2.15	0.45
1:X:2671:C:H1'	1:X:2822:U:O2'	2.16	0.45
1:X:2840:U:N3	1:X:2841:U:C5	2.84	0.45
1:X:504:G:H4'	18:P:27:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:537:C:C5	1:X:2759:U:C2'	2.99	0.45
1:X:749:C:C3'	1:X:749:C:H6	2.28	0.45
1:X:811:G:OP2	5:C:56:ARG:HG2	2.17	0.45
1:X:818:G:H1'	1:X:844:G:O2'	2.17	0.45
1:X:831:G:N2	1:X:1204:G:C6	2.84	0.45
2:Y:30:C:H42	2:Y:58:G:H1	1.63	0.45
2:Y:32:C:H2'	2:Y:33:C:O4'	2.15	0.45
2:Y:85:G:N2	2:Y:97:C:C2	2.84	0.45
30:4:31:LYS:N	30:4:31:LYS:HD2	2.31	0.45
1:X:797:A:C6	3:A:230:VAL:HG21	2.52	0.45
4:B:182:ILE:O	4:B:182:ILE:HG23	2.15	0.45
11:I:57:ILE:HD12	29:3:9:MET:HE2	1.97	0.45
25:W:40:VAL:O	25:W:43:MET:HB2	2.17	0.45
1:X:1047:G:N3	1:X:1131:G:C2	2.85	0.45
1:X:1683:G:N2	1:X:1978:U:H3	2.13	0.45
1:X:1687:C:H6	1:X:1687:C:O5'	1.99	0.45
1:X:2198:U:C4	1:X:2199:C:C2	3.04	0.45
1:X:759:C:N3	32:X:2882:LMA:H37	2.31	0.45
1:X:493:A:H1'	1:X:508:G:N2	2.30	0.45
1:X:611:C:H4'	5:C:98:GLN:NE2	2.32	0.45
1:X:759:C:C4	1:X:2590:U:H4'	2.51	0.45
1:X:693:A:C2	1:X:811:G:N3	2.84	0.45
3:A:109:PRO:HA	3:A:197:VAL:HA	1.98	0.45
3:A:160:ALA:HA	3:A:199:ASN:HB2	1.98	0.45
10:H:19:ILE:HG22	10:H:55:VAL:HA	1.99	0.45
14:L:96:TYR:OH	14:L:101:LYS:HG3	2.17	0.45
15:M:6:LYS:HD2	15:M:6:LYS:N	2.31	0.45
21:S:72:ASP:HB3	21:S:77:ALA:O	2.17	0.45
1:X:1469:U:H5''	1:X:1470:G:C8	2.51	0.45
1:X:2614:A:N1	1:X:2615:U:O2	2.50	0.45
1:X:2663:U:O2'	10:H:80:ALA:HB1	2.17	0.45
1:X:2827:G:C6	1:X:2828:C:N3	2.85	0.45
1:X:746:G:N2	1:X:747:A:H62	2.13	0.45
1:X:775:U:C4'	1:X:776:G:N3	2.79	0.45
1:X:845:U:C5	1:X:955:G:C6	3.05	0.45
2:Y:110:U:H2'	2:Y:111:C:H5''	1.98	0.45
3:A:126:PRO:HA	3:A:194:ILE:HG13	1.97	0.45
4:B:27:LEU:HD23	4:B:180:ASN:O	2.17	0.45
12:J:116:LYS:O	12:J:120:ARG:HB2	2.17	0.45
16:N:86:ALA:C	16:N:88:ILE:N	2.70	0.45
1:X:94:C:H1'	24:V:40:PRO:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1696:C:O2	1:X:1972:G:N2	2.45	0.45
1:X:1982:C:O2	1:X:2666:U:O2'	2.27	0.45
1:X:2372:A:O4'	11:I:59:ARG:HA	2.16	0.45
1:X:2847:G:C2	1:X:2848:A:N6	2.84	0.45
1:X:568:G:H2'	1:X:569:C:O4'	2.16	0.45
1:X:574:C:H42	1:X:584:A:N6	2.14	0.45
1:X:648:A:H4'	1:X:649:G:C5'	2.43	0.45
1:X:73:A:H5''	1:X:74:G:O4'	2.16	0.45
27:1:43:VAL:O	27:1:44:ALA:CB	2.62	0.45
3:A:245:ARG:HA	3:A:253:LYS:NZ	2.31	0.45
4:B:162:MET:HG3	4:B:162:MET:O	2.17	0.45
5:C:162:ARG:CG	5:C:162:ARG:NH1	2.62	0.45
6:D:36:VAL:HG22	6:D:154:ILE:HG13	1.98	0.45
13:K:33:ARG:O	13:K:34:ILE:CG2	2.65	0.45
14:L:28:ARG:O	14:L:28:ARG:HG3	2.15	0.45
2:Y:52:G:P	14:L:65:THR:HB	2.57	0.45
16:N:24:PHE:HB2	16:N:29:SER:HB3	1.99	0.45
25:W:41:ARG:HB3	25:W:45:LYS:NZ	2.31	0.45
1:X:1493:A:H2'	1:X:1494:G:O4'	2.16	0.45
1:X:2074:U:C4	1:X:2075:U:C4	3.04	0.45
1:X:2269:G:H2'	1:X:2270:U:O4'	2.17	0.45
1:X:2490:U:C4	1:X:2491:C:C4	3.04	0.45
1:X:521:U:O4	1:X:522:G:C2	2.70	0.45
1:X:5:A:O2'	1:X:6:A:H5'	2.16	0.45
1:X:610:G:N2	1:X:616:U:OP1	2.49	0.45
1:X:697:G:C2	1:X:787:A:C2	3.05	0.45
1:X:830:C:O2'	1:X:852:U:H5''	2.17	0.45
4:B:131:SER:O	4:B:134:TRP:CD1	2.69	0.45
4:B:133:LYS:CG	4:B:137:ARG:HD3	2.31	0.45
7:E:30:LYS:HB2	7:E:79:VAL:HA	1.97	0.45
1:X:1226:A:N1	1:X:1250:A:H1'	2.32	0.45
1:X:1715:A:C8	1:X:1717:A:O4'	2.69	0.45
1:X:2046:C:C2'	1:X:2047:C:H5'	2.47	0.45
1:X:843:G:O4'	1:X:2427:A:H2	2.00	0.45
1:X:2754:C:C4	1:X:2755:A:C5	3.05	0.45
1:X:758:G:C2'	1:X:759:C:OP1	2.65	0.45
1:X:334:G:H1'	5:C:164:VAL:HG13	1.98	0.45
12:J:126:LEU:HA	12:J:127:PRO:HD3	1.70	0.45
12:J:36:ILE:HG12	12:J:103:VAL:HG23	1.99	0.45
13:K:12:ARG:HH22	13:K:20:LEU:HD22	1.81	0.45
16:N:8:ILE:O	16:N:12:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:92:THR:HA	20:R:107:ALA:O	2.17	0.45
21:S:72:ASP:O	21:S:75:LYS:O	2.34	0.45
23:U:20:ARG:HD3	23:U:43:ARG:HH22	1.81	0.45
1:X:1272:G:H2'	1:X:1273:G:C8	2.52	0.45
1:X:1701:C:H42	1:X:1721:G:H1	1.64	0.45
1:X:171:G:H2'	1:X:172:A:C8	2.51	0.45
1:X:540:G:C6	1:X:2005:U:H5''	2.52	0.45
1:X:2251:U:H5''	1:X:2252:A:OP1	2.17	0.45
1:X:27:G:C2	1:X:522:G:H1'	2.51	0.45
26:Z:45:ILE:HG12	26:Z:52:TYR:HB2	1.99	0.45
27:1:9:ILE:O	27:1:10:VAL:CG2	2.65	0.45
27:1:42:PRO:HD3	27:1:48:VAL:HG21	1.99	0.45
5:C:158:ARG:O	5:C:159:ARG:C	2.55	0.45
6:D:80:ARG:NE	6:D:80:ARG:H	2.15	0.45
11:I:114:ILE:O	11:I:114:ILE:HG23	2.17	0.45
12:J:36:ILE:HG12	12:J:103:VAL:CG2	2.46	0.45
13:K:31:GLU:HA	13:K:31:GLU:OE1	2.17	0.45
18:P:27:VAL:HG23	18:P:124:ILE:O	2.17	0.45
25:W:16:GLN:HB3	25:W:47:VAL:HG12	1.99	0.45
1:X:1441:A:C1'	1:X:1442:C:OP2	2.57	0.45
1:X:1456:C:C2	1:X:1566:G:N2	2.85	0.45
1:X:2053:G:C2	1:X:2054:A:C4	3.05	0.45
1:X:2783:U:O2'	1:X:2784:A:H5'	2.16	0.45
1:X:557:U:H4'	1:X:558:G:O4'	2.17	0.45
1:X:753:U:H2'	1:X:754:G:C8	2.52	0.45
1:X:759:C:H2'	32:X:2882:LMA:C58	2.42	0.45
1:X:969:U:H4'	1:X:970:A:O5'	2.17	0.45
2:Y:67:C:H2'	2:Y:68:A:H5'	1.98	0.45
2:Y:73:C:N4	2:Y:74:A:C6	2.85	0.45
13:K:28:LEU:O	13:K:28:LEU:HD23	2.17	0.44
14:L:37:HIS:NE2	14:L:39:TYR:OH	2.49	0.44
15:M:55:ILE:HG22	15:M:104:LEU:HB2	2.00	0.44
15:M:39:VAL:CG1	15:M:45:THR:HG23	2.46	0.44
16:N:20:ARG:HH12	17:O:83:ARG:NH2	2.13	0.44
17:O:67:LYS:HD2	17:O:68:LYS:H	1.82	0.44
1:X:512:A:H5'	18:P:16:GLN:HB3	1.99	0.44
21:S:3:LEU:HD21	21:S:32:PHE:CG	2.52	0.44
21:S:73:LYS:C	21:S:75:LYS:H	2.19	0.44
21:S:77:ALA:HA	21:S:78:PRO:HD3	1.74	0.44
1:X:2670:C:H2'	1:X:2671:C:C6	2.52	0.44
1:X:2664:G:N2	1:X:2705:A:N7	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:688:A:O2'	1:X:2422:C:H4'	2.16	0.44
1:X:832:A:C2	1:X:1203:A:C2	3.05	0.44
3:A:66:ILE:HD12	3:A:89:ARG:NH2	2.32	0.44
4:B:26:VAL:O	4:B:182:ILE:HG22	2.16	0.44
6:D:40:LEU:HD11	6:D:50:ILE:HA	1.99	0.44
9:G:124:GLU:CD	9:G:124:GLU:H	2.21	0.44
16:N:53:LYS:O	16:N:57:PHE:HD1	2.00	0.44
16:N:3:ARG:HH12	16:N:5:LYS:HG2	1.81	0.44
17:O:19:VAL:HG13	17:O:90:PHE:CD1	2.52	0.44
20:R:57:ASN:OD1	20:R:59:LYS:HE2	2.17	0.44
1:X:337:G:HO2'	20:R:9:HIS:HD1	1.38	0.44
21:S:175:ARG:O	21:S:175:ARG:HG2	2.16	0.44
1:X:101:A:H2'	1:X:102:C:O4'	2.17	0.44
1:X:1195:U:H2'	1:X:1196:G:C8	2.52	0.44
1:X:555:U:C4	1:X:1243:G:N2	2.86	0.44
1:X:135:U:H5''	1:X:136:A:OP1	2.17	0.44
1:X:13:A:N3	1:X:15:G:C6	2.85	0.44
1:X:1841:G:C2'	1:X:1842:G:H5'	2.46	0.44
1:X:1982:C:H2'	1:X:1983:G:C8	2.53	0.44
1:X:2046:C:H2'	1:X:2047:C:H5'	1.99	0.44
1:X:2082:C:H2'	1:X:2083:G:H5'	1.99	0.44
1:X:2727:G:C2	1:X:2736:U:C5	3.04	0.44
1:X:469:G:H5''	28:2:39:ARG:H	1.82	0.44
1:X:617:U:C5	1:X:631:G:C8	3.05	0.44
1:X:67:G:N2	1:X:73:A:C2	2.86	0.44
1:X:923:A:N6	12:J:12:LYS:HD3	2.31	0.44
26:Z:3:LYS:O	26:Z:4:HIS:C	2.55	0.44
4:B:52:ALA:O	4:B:76:ARG:N	2.51	0.44
9:G:122:HIS:HB3	9:G:125:ARG:HG2	1.99	0.44
11:I:32:ARG:HH22	17:O:82:ARG:HE	1.65	0.44
20:R:11:ASN:ND2	20:R:13:LYS:NZ	2.66	0.44
21:S:155:PRO:CG	21:S:158:CYS:HB2	2.46	0.44
24:V:4:SER:HB3	24:V:7:ARG:NH2	2.33	0.44
25:W:16:GLN:HB3	25:W:47:VAL:CG1	2.47	0.44
1:X:1677:C:C3'	1:X:1677:C:C6	3.01	0.44
1:X:2018:G:H3'	1:X:2019:C:H5'	2.00	0.44
1:X:2030:U:H2'	1:X:2031:A:H8	1.81	0.44
1:X:2295:C:H1'	6:D:125:ARG:NH1	2.32	0.44
1:X:306:G:C6	1:X:355:G:C2	3.06	0.44
1:X:48:A:N6	1:X:154:U:H5	2.14	0.44
1:X:623:G:H3'	1:X:624:A:H5''	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:760:U:C5	1:X:2592:U:C5	3.05	0.44
1:X:834:A:H2'	1:X:957:G:O5'	2.18	0.44
1:X:838:A:C2	1:X:839:U:C2	3.05	0.44
1:X:849:G:C5	1:X:850:C:C4	3.05	0.44
2:Y:8:C:O2'	2:Y:9:G:H5'	2.18	0.44
1:X:1836:C:H5'	3:A:255:THR:O	2.18	0.44
1:X:2599:U:H5''	4:B:153:GLY:HA2	2.00	0.44
8:F:131:ALA:HB1	8:F:136:VAL:HB	2.00	0.44
11:I:101:ARG:O	11:I:102:LYS:HB2	2.17	0.44
12:J:11:ARG:HA	12:J:11:ARG:HD3	1.84	0.44
19:Q:10:PRO:HD3	24:V:30:PHE:HD2	1.75	0.44
23:U:23:LYS:HB2	23:U:35:THR:HG23	1.98	0.44
1:X:1168:G:O2'	25:W:28:ILE:HD11	2.17	0.44
1:X:1265:G:C6	16:N:37:GLN:HB2	2.52	0.44
1:X:1564:U:H2'	1:X:1565:G:C8	2.52	0.44
1:X:1704:G:H1'	1:X:1719:G:N2	2.32	0.44
1:X:1851:A:C2	1:X:1867:A:C4	3.05	0.44
1:X:1971:C:O2'	1:X:1972:G:H5'	2.17	0.44
1:X:2400:G:O6	29:3:32:GLN:CG	2.63	0.44
1:X:2670:C:H4'	1:X:2846:G:O2'	2.17	0.44
1:X:827:C:OP2	11:I:32:ARG:CZ	2.66	0.44
2:Y:66:G:C5	2:Y:67:C:C4	3.06	0.44
29:3:49:VAL:HG21	29:3:52:LYS:HE2	1.99	0.44
3:A:34:LEU:HD12	3:A:34:LEU:C	2.38	0.44
1:X:2554:C:O2'	4:B:140:SER:CB	2.66	0.44
5:C:180:ILE:CG2	5:C:181:LEU:N	2.80	0.44
9:G:53:ARG:CD	9:G:171:LEU:HD12	2.35	0.44
12:J:42:TRP:CB	12:J:95:VAL:HG11	2.41	0.44
9:G:70:PHE:HE1	16:N:67:ALA:HB3	1.82	0.44
20:R:98:ILE:HD11	20:R:105:ARG:HD2	1.99	0.44
1:X:1235:C:C2	1:X:1241:G:N2	2.86	0.44
1:X:1242:A:H2'	1:X:1243:G:H8	1.81	0.44
1:X:2046:C:C4	1:X:2047:C:C4	3.04	0.44
1:X:224:G:C2	1:X:229:G:N1	2.86	0.44
1:X:2426:G:O2'	1:X:2427:A:P	2.76	0.44
1:X:2827:G:N2	1:X:2840:U:O2	2.45	0.44
1:X:484:G:O2'	1:X:485:G:H5'	2.18	0.44
1:X:777:A:OP2	3:A:215:TRP:CH2	2.70	0.44
1:X:81:C:C4	1:X:82:G:C6	3.06	0.44
27:1:16:ALA:HB2	27:1:50:PHE:CD1	2.53	0.44
29:3:13:ARG:HD2	29:3:25:PHE:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:93:VAL:C	4:B:95:ILE:N	2.71	0.44
6:D:106:ILE:HG23	6:D:110:ARG:HD2	1.98	0.44
9:G:35:LYS:HG2	9:G:69:ASP:OD1	2.17	0.44
13:K:84:ALA:N	13:K:85:PRO:HD2	2.33	0.44
13:K:49:GLU:OE1	13:K:95:THR:HG22	2.18	0.44
16:N:14:HIS:CD2	16:N:32:TYR:CZ	3.06	0.44
1:X:1265:G:C4'	16:N:33:ARG:HD3	2.48	0.44
16:N:76:TYR:CE2	16:N:80:ILE:HG13	2.53	0.44
17:O:48:GLY:O	17:O:50:ASP:N	2.49	0.44
1:X:1283:C:H5''	1:X:1284:G:O5'	2.18	0.44
1:X:1782:A:C2'	1:X:1783:G:H5'	2.47	0.44
1:X:2074:U:H3'	1:X:2075:U:H5''	1.99	0.44
1:X:2274:C:O5'	1:X:2274:C:H6	2.00	0.44
1:X:2451:G:C4	1:X:2454:C:N4	2.86	0.44
1:X:2696:A:H2'	1:X:2697:G:C8	2.50	0.44
1:X:575:U:H2'	1:X:576:A:O4'	2.18	0.44
1:X:575:U:H4'	1:X:822:G:OP2	2.18	0.44
1:X:614:G:C5	1:X:615:C:C5	3.05	0.44
1:X:764:A:C8	1:X:764:A:H3'	2.52	0.44
2:Y:12:C:C5	2:Y:13:C:C4	3.06	0.44
27:1:3:LYS:HG2	27:1:4:ASP:H	1.82	0.44
29:3:12:ARG:O	29:3:14:ILE:N	2.38	0.44
3:A:21:ASP:C	3:A:22:PHE:CD2	2.90	0.44
4:B:46:ALA:HA	4:B:81:PHE:O	2.18	0.44
9:G:61:ARG:HG2	9:G:65:LYS:HD2	2.00	0.44
23:U:60:VAL:CG2	23:U:61:TRP:N	2.80	0.44
1:X:2240:C:O2'	1:X:2241:U:H5'	2.17	0.44
1:X:2526:U:H2'	1:X:2527:G:H8	1.83	0.44
1:X:2543:A:C2	1:X:2626:U:H4'	2.52	0.44
1:X:2595:C:C6	1:X:2595:C:C3'	3.01	0.44
1:X:2691:C:OP1	1:X:2694:G:H4'	2.17	0.44
1:X:860:U:H2'	1:X:860:U:O2	2.17	0.44
29:3:34:THR:OG1	29:3:35:GLY:N	2.51	0.44
3:A:184:ARG:HB3	3:A:184:ARG:HH11	1.79	0.44
13:K:28:LEU:C	13:K:28:LEU:HD23	2.38	0.44
13:K:24:GLN:HB3	13:K:44:LEU:HD22	2.00	0.44
13:K:72:ASP:HB3	13:K:75:VAL:CG2	2.47	0.44
14:L:20:THR:HG21	14:L:23:ALA:HB3	1.99	0.44
14:L:29:LEU:HD23	14:L:89:PHE:CE1	2.53	0.44
14:L:45:ASP:OD2	14:L:46:SER:N	2.51	0.44
1:X:1070:G:N3	8:F:126:THR:HG23	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:182:G:H2'	1:X:183:U:OP2	2.18	0.44
1:X:225:G:N7	1:X:227:G:N3	2.65	0.44
1:X:2496:C:C4	1:X:2521:A:C5	3.05	0.44
1:X:2547:C:C3'	1:X:2547:C:C6	3.01	0.44
1:X:2569:A:C2	1:X:2584:U:O2	2.70	0.44
1:X:26:G:C6	1:X:27:G:C6	3.05	0.44
1:X:2:G:O2'	1:X:3:U:H5'	2.17	0.44
1:X:454:G:H21	5:C:42:THR:HB	1.82	0.44
1:X:3:U:O2'	1:X:4:C:O5'	2.30	0.44
1:X:566:U:H2'	1:X:567:G:C8	2.53	0.44
1:X:649:G:N1	1:X:660:G:N1	2.65	0.44
27:1:21:TYR:HE2	27:1:23:THR:OG1	2.01	0.44
3:A:246:VAL:C	3:A:253:LYS:HE3	2.38	0.44
7:E:91:GLY:HA3	7:E:94:PHE:CD2	2.53	0.44
9:G:32:TYR:HD1	9:G:33:ILE:H	1.66	0.44
10:H:24:VAL:HG12	10:H:42:LYS:CG	2.48	0.44
12:J:92:GLU:OE1	12:J:92:GLU:HA	2.18	0.44
13:K:108:VAL:HG12	13:K:109:THR:O	2.17	0.44
14:L:31:VAL:HG23	14:L:38:ILE:HD13	2.00	0.44
23:U:52:ARG:HG3	23:U:62:LEU:HD22	1.99	0.44
1:X:1329:U:H2'	1:X:1330:G:C8	2.52	0.44
1:X:163:A:H2'	1:X:164:G:C8	2.52	0.44
1:X:187:U:H6	1:X:187:U:O5'	2.00	0.44
1:X:2225:G:H1	1:X:2237:C:H42	1.65	0.44
1:X:2500:C:OP2	1:X:2500:C:H5	2.01	0.44
1:X:2543:A:OP1	1:X:2627:G:H4'	2.18	0.44
1:X:2754:C:C4	1:X:2755:A:N7	2.86	0.44
1:X:651:C:H2'	1:X:652:C:H5'	1.99	0.44
1:X:953:G:H2'	1:X:954:U:O4'	2.18	0.44
1:X:962:C:H2'	1:X:963:G:C8	2.52	0.44
2:Y:51:G:H2'	2:Y:52:G:H8	1.82	0.44
3:A:126:PRO:HG3	3:A:132:LEU:HD11	2.00	0.43
1:X:1790:G:O2'	3:A:184:ARG:HD3	2.18	0.43
4:B:146:THR:CB	4:B:147:PRO:HD2	2.41	0.43
4:B:99:GLY:H	4:B:172:VAL:HB	1.82	0.43
5:C:4:ILE:HG13	5:C:4:ILE:O	2.18	0.43
7:E:89:LEU:HD23	7:E:162:VAL:HG22	1.98	0.43
9:G:132:PHE:HD2	9:G:145:HIS:CB	2.30	0.43
14:L:52:ALA:O	14:L:53:ALA:O	2.35	0.43
17:O:65:ARG:O	17:O:66:GLY:O	2.35	0.43
19:Q:11:VAL:HG23	19:Q:27:PHE:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:12:ILE:O	19:Q:13:SER:CB	2.64	0.43
1:X:1006:C:H4'	1:X:1007:A:OP1	2.15	0.43
1:X:1030:U:O2	1:X:1155:G:N2	2.51	0.43
1:X:1096:A:HO2'	1:X:1097:A:C5'	2.30	0.43
1:X:1222:G:N1	1:X:1251:G:C6	2.86	0.43
1:X:1332:G:C5	1:X:1333:G:C6	3.06	0.43
1:X:1469:U:H5'	1:X:1470:G:OP2	2.18	0.43
1:X:1508:G:C5'	1:X:1509:A:H5''	2.48	0.43
1:X:1726:C:C2	1:X:1741:G:N2	2.86	0.43
1:X:1931:G:O2'	1:X:1932:G:H5'	2.18	0.43
1:X:2583:U:O2'	1:X:2584:U:H5'	2.17	0.43
1:X:2637:C:N4	1:X:2638:G:C6	2.86	0.43
1:X:2671:C:N3	1:X:2698:G:C2	2.86	0.43
1:X:2745:A:C3'	1:X:2745:A:N3	2.81	0.43
1:X:494:A:C8	1:X:495:C:C6	3.06	0.43
1:X:540:G:C5	1:X:2005:U:C5'	3.00	0.43
1:X:959:C:H1'	1:X:995:A:N3	2.32	0.43
1:X:958:G:C2	1:X:982:C:N3	2.86	0.43
2:Y:80:A:H2'	2:Y:81:C:O4'	2.17	0.43
3:A:184:ARG:CZ	3:A:184:ARG:HB3	2.49	0.43
3:A:47:ARG:HD3	3:A:48:GLY:N	2.33	0.43
4:B:28:ALA:O	4:B:29:GLY:O	2.36	0.43
6:D:61:THR:HG22	6:D:99:PHE:CD1	2.54	0.43
12:J:111:THR:OG1	12:J:114:GLN:HG2	2.18	0.43
14:L:60:LYS:HZ3	14:L:64:LYS:CE	2.30	0.43
19:Q:30:SER:HA	19:Q:31:PRO:HD3	1.85	0.43
23:U:10:LYS:HZ3	23:U:77:GLY:HA3	1.82	0.43
1:X:1030:U:H3	1:X:1153:A:H62	1.67	0.43
1:X:1265:G:O2'	1:X:1266:G:C4	2.71	0.43
1:X:219:G:C2'	1:X:220:U:OP2	2.66	0.43
1:X:2394:G:C6	1:X:2395:C:N3	2.87	0.43
1:X:2840:U:O2'	1:X:2841:U:OP1	2.30	0.43
1:X:337:G:HO2'	1:X:338:G:H5'	1.83	0.43
1:X:472:C:H6	1:X:472:C:O5'	2.01	0.43
1:X:482:A:H2'	1:X:483:A:O4'	2.18	0.43
1:X:589:C:H4'	16:N:31:GLN:CD	2.38	0.43
1:X:807:A:C2	1:X:808:C:C2	3.06	0.43
26:Z:42:SER:O	26:Z:44:HIS:CD2	2.72	0.43
27:1:11:LYS:N	27:1:11:LYS:CD	2.81	0.43
1:X:2722:C:P	30:4:35:ARG:NH1	2.91	0.43
3:A:47:ARG:HD3	3:A:47:ARG:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:117:ILE:HD12	6:D:175:LEU:HD11	2.00	0.43
6:D:4:LEU:CG	6:D:5:LYS:N	2.78	0.43
1:X:2291:U:P	6:D:71:LYS:HD2	2.59	0.43
9:G:154:GLU:O	9:G:157:PRO:HD2	2.18	0.43
13:K:78:LYS:O	13:K:82:GLU:HB2	2.17	0.43
1:X:1017:C:H2'	1:X:1018:C:C6	2.53	0.43
1:X:1473:U:O2	1:X:1474:A:C6	2.72	0.43
1:X:1571:G:C2	1:X:1572:C:C2	3.06	0.43
1:X:1699:A:H61	1:X:1723:U:H3	1.67	0.43
1:X:1820:G:H4'	1:X:1821:A:OP1	2.17	0.43
1:X:1974:U:H6	1:X:1974:U:C3'	2.22	0.43
1:X:2067:U:H2'	1:X:2068:C:C6	2.53	0.43
1:X:2345:A:N6	1:X:2346:G:C2	2.87	0.43
1:X:2351:G:O2'	1:X:2352:A:H5'	2.17	0.43
1:X:2547:C:C6	1:X:2547:C:H3'	2.53	0.43
1:X:2615:U:OP1	4:B:79:ARG:HA	2.18	0.43
1:X:2630:C:C2'	1:X:2631:C:H5'	2.48	0.43
1:X:600:G:H2'	1:X:601:A:OP1	2.17	0.43
1:X:775:U:C5'	1:X:776:G:N3	2.80	0.43
1:X:833:A:N3	1:X:954:U:O2'	2.45	0.43
1:X:919:U:H2'	1:X:920:G:C8	2.54	0.43
1:X:2400:G:OP1	27:1:4:ASP:CG	2.57	0.43
6:D:17:MET:N	6:D:17:MET:SD	2.92	0.43
1:X:547:U:H1'	9:G:73:ASN:HD21	1.83	0.43
10:H:22:ILE:CG1	10:H:53:ALA:HA	2.47	0.43
20:R:83:LEU:O	20:R:90:LYS:CE	2.64	0.43
22:T:18:PRO:C	22:T:19:LYS:CG	2.86	0.43
1:X:123:A:C2'	1:X:124:A:OP1	2.66	0.43
1:X:1298:G:C6	1:X:1342:U:C5	3.07	0.43
1:X:1377:G:H21	1:X:1380:C:H5	1.66	0.43
1:X:1437:A:C2	1:X:1592:U:O2	2.71	0.43
1:X:1941:C:O2'	1:X:1942:G:H5'	2.18	0.43
1:X:2434:G:C6	1:X:2435:C:N4	2.87	0.43
1:X:2653:A:N6	1:X:2654:A:C6	2.87	0.43
1:X:2659:C:O3'	4:B:8:LYS:NZ	2.51	0.43
1:X:2717:G:H1	1:X:2747:C:N4	2.14	0.43
1:X:559:C:H2'	1:X:560:G:O4'	2.18	0.43
1:X:750:C:H5'	1:X:779:U:O2'	2.17	0.43
1:X:923:A:C5	12:J:12:LYS:CE	3.01	0.43
2:Y:54:U:H2'	2:Y:55:C:O4'	2.18	0.43
1:X:699:G:C2	28:2:5:TYR:HE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:28:GLY:C	29:3:29:LYS:HG2	2.39	0.43
3:A:34:LEU:O	3:A:34:LEU:CG	2.66	0.43
4:B:183:LEU:HD11	15:M:16:ILE:HG21	2.00	0.43
4:B:77:ILE:HD13	4:B:195:LEU:HD22	2.00	0.43
4:B:36:ARG:NH1	4:B:86:PRO:O	2.52	0.43
5:C:74:VAL:HG23	5:C:76:THR:OG1	2.18	0.43
10:H:47:VAL:HG22	10:H:77:THR:HG23	1.99	0.43
13:K:34:ILE:O	13:K:34:ILE:HG13	2.18	0.43
13:K:48:VAL:O	13:K:52:ILE:HG23	2.19	0.43
19:Q:88:ILE:O	19:Q:88:ILE:CD1	2.66	0.43
1:X:1847:G:N1	1:X:1871:G:H8	2.17	0.43
1:X:2043:A:O4'	1:X:2481:G:O4'	2.35	0.43
1:X:239:A:H2'	1:X:240:U:O4'	2.18	0.43
1:X:2818:G:H2'	1:X:2819:G:C8	2.53	0.43
1:X:957:G:H2'	1:X:958:G:C8	2.53	0.43
1:X:987:G:H4'	1:X:1167:A:H62	1.84	0.43
2:Y:93:G:H2'	2:Y:94:G:O4'	2.18	0.43
27:1:45:LYS:C	27:1:46:LYS:HG2	2.39	0.43
3:A:212:ARG:O	3:A:212:ARG:HG3	2.17	0.43
4:B:101:LYS:HA	4:B:170:LEU:O	2.18	0.43
4:B:26:VAL:HG11	4:B:196:VAL:HG21	2.00	0.43
6:D:16:LEU:HB3	6:D:22:TYR:CE2	2.54	0.43
6:D:98:VAL:O	6:D:102:LYS:HG3	2.19	0.43
7:E:83:TYR:CE1	7:E:138:LYS:HB2	2.53	0.43
1:X:1095:A:N6	1:X:1096:A:H62	2.16	0.43
1:X:1152:C:H3'	1:X:1153:A:H5''	2.00	0.43
1:X:1445:A:C2	1:X:1579:G:N3	2.87	0.43
1:X:2363:G:OP2	22:T:55:ARG:HD2	2.18	0.43
1:X:2424:G:O2'	1:X:2425:G:H5'	2.18	0.43
1:X:2805:G:H5''	4:B:58:LYS:HZ1	1.83	0.43
2:Y:56:G:H2'	2:Y:57:U:O4'	2.18	0.43
3:A:185:ARG:HH21	3:A:269:ARG:HH11	1.65	0.43
4:B:120:TRP:O	4:B:121:ASN:C	2.56	0.43
4:B:170:LEU:HD13	4:B:184:VAL:HG11	2.00	0.43
5:C:74:VAL:O	5:C:74:VAL:HG23	2.16	0.43
7:E:163:ARG:HB2	7:E:167:GLU:HB2	2.00	0.43
8:F:120:VAL:HG12	8:F:121:GLU:H	1.80	0.43
10:H:99:ILE:HD12	10:H:103:GLY:HA2	2.01	0.43
11:I:62:LYS:HD3	29:3:11:LYS:C	2.39	0.43
14:L:37:HIS:CD2	14:L:39:TYR:OH	2.71	0.43
17:O:80:TYR:CD1	17:O:80:TYR:O	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:63:HIS:CE1	17:O:91:THR:HB	2.54	0.43
19:Q:35:LYS:HD3	19:Q:53:ILE:HG23	1.99	0.43
20:R:16:PHE:HB3	20:R:82:ALA:CB	2.48	0.43
20:R:46:VAL:HG12	20:R:48:VAL:HG23	2.00	0.43
1:X:1008:G:C2	1:X:1170:U:C2	3.07	0.43
1:X:1447:U:H1'	1:X:1577:G:N2	2.34	0.43
1:X:2501:U:H5'	1:X:2502:G:OP2	2.19	0.43
1:X:2691:C:H2'	1:X:2694:G:H5''	2.01	0.43
1:X:511:A:H2'	1:X:512:A:O4'	2.19	0.43
1:X:870:C:O2	1:X:933:G:N2	2.52	0.43
1:X:939:C:OP2	1:X:940:G:C8	2.72	0.43
26:Z:41:LEU:O	26:Z:44:HIS:HB2	2.19	0.43
1:X:1999:U:O2	26:Z:7:PRO:HG2	2.18	0.43
5:C:7:ILE:HG22	5:C:121:ASP:HB3	1.99	0.43
9:G:96:ASP:O	9:G:98:LYS:N	2.51	0.43
11:I:115:SER:OG	11:I:136:ALA:HB2	2.18	0.43
13:K:22:ARG:HD3	13:K:69:ASP:HA	2.01	0.43
19:Q:26:SER:HB3	19:Q:79:ILE:HG12	2.01	0.43
1:X:1204:G:H2'	1:X:1205:G:C8	2.53	0.43
1:X:1585:A:N1	1:X:1586:A:C2	2.87	0.43
1:X:1790:G:C6	1:X:1811:A:C5	3.07	0.43
1:X:2010:G:H1	1:X:2019:C:H42	1.66	0.43
1:X:1686:A:O3'	1:X:2528:G:H5'	2.19	0.43
1:X:2551:A:OP2	1:X:2551:A:H8	2.02	0.43
1:X:2725:C:H2'	1:X:2726:U:C6	2.54	0.43
1:X:562:G:H2'	1:X:563:U:O4'	2.18	0.43
1:X:638:A:C8	11:I:74:VAL:HG11	2.54	0.43
3:A:43:GLY:N	3:A:44:ARG:HH11	2.17	0.43
7:E:171:LEU:N	7:E:171:LEU:CD1	2.81	0.43
8:F:103:GLN:O	8:F:107:ILE:HG13	2.19	0.43
10:H:43:ARG:HG3	10:H:44:TYR:CD2	2.54	0.43
11:I:57:ILE:HD12	29:3:9:MET:CE	2.49	0.43
13:K:36:THR:CG2	13:K:41:ALA:HB2	2.48	0.43
15:M:26:ASP:O	15:M:26:ASP:CG	2.57	0.43
19:Q:5:ASP:O	19:Q:6:ILE:HB	2.18	0.43
1:X:1016:C:O2'	9:G:56:THR:HG21	2.19	0.43
1:X:1750:A:C8	1:X:1750:A:H5'	2.54	0.43
1:X:2475:C:N4	1:X:2476:A:C6	2.87	0.43
1:X:2580:C:O2'	1:X:2581:A:OP2	2.32	0.43
1:X:2663:U:C1'	10:H:88:THR:HG21	2.48	0.43
1:X:2767:C:H6	1:X:2767:C:O5'	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2823:G:H3'	15:M:100:ARG:O	2.19	0.43
31:X:2881:LC2:H9	31:X:2881:LC2:H6	1.77	0.43
1:X:463:C:O2	1:X:465:C:N4	2.51	0.43
1:X:505:G:H5'	18:P:25:PHE:HD2	1.84	0.43
1:X:575:U:H2'	1:X:576:A:C8	2.53	0.43
1:X:742:G:O6	1:X:1765:C:N3	2.52	0.43
1:X:576:A:H4'	1:X:821:A:OP1	2.19	0.43
27:1:42:PRO:HD3	27:1:48:VAL:CG2	2.49	0.43
3:A:97:HIS:HE1	3:A:101:GLY:HA2	1.81	0.43
3:A:187:HIS:CD2	3:A:189:GLU:HB2	2.54	0.43
3:A:232:HIS:CD2	3:A:248:VAL:HA	2.54	0.43
3:A:252:GLY:HA3	3:A:256:LYS:NZ	2.34	0.43
6:D:38:GLU:HB3	6:D:87:ILE:CB	2.26	0.43
9:G:93:LYS:HB3	9:G:96:ASP:O	2.18	0.43
1:X:2475:C:OP1	12:J:83:ARG:CB	2.67	0.43
13:K:33:ARG:C	13:K:34:ILE:HG23	2.38	0.43
14:L:95:LYS:HB3	14:L:95:LYS:NZ	2.32	0.43
1:X:1261:G:OP1	16:N:2:PRO:HD2	2.19	0.43
17:O:11:GLN:HA	17:O:11:GLN:NE2	2.33	0.43
1:X:1996:A:OP1	18:P:118:LYS:HB2	2.18	0.43
20:R:64:ASN:N	20:R:65:PRO:HD3	2.34	0.43
1:X:94:C:H1'	24:V:40:PRO:HD2	2.00	0.43
1:X:1665:C:H2'	1:X:1666:G:C8	2.53	0.43
1:X:1745:C:H2'	1:X:1746:A:O5'	2.18	0.43
1:X:1935:A:C6	1:X:1936:A:N1	2.87	0.43
1:X:1939:U:C5	1:X:1940:C:C4	3.06	0.43
1:X:2024:U:H2'	1:X:2025:A:C8	2.54	0.43
1:X:2507:U:HO2'	1:X:2508:G:H8	1.67	0.43
1:X:2590:U:C1'	32:X:2882:LMA:H37B	2.46	0.43
1:X:851:C:C2	1:X:952:A:C2	3.06	0.43
1:X:870:C:C2	1:X:933:G:N2	2.87	0.43
3:A:268:ASP:OD1	3:A:268:ASP:C	2.57	0.42
3:A:61:ARG:HH22	3:A:216:LEU:HG	1.83	0.42
4:B:26:VAL:HG13	4:B:196:VAL:HG21	1.99	0.42
8:F:121:GLU:O	8:F:124:ALA:HB3	2.18	0.42
9:G:169:GLN:NE2	9:G:171:LEU:C	2.73	0.42
11:I:45:LYS:HE2	11:I:47:ALA:HB3	1.99	0.42
11:I:53:ARG:O	11:I:58:ALA:HB3	2.19	0.42
12:J:67:ILE:HG22	12:J:67:ILE:O	2.19	0.42
13:K:5:LYS:HB3	13:K:5:LYS:HE2	1.73	0.42
15:M:79:ARG:HB3	15:M:81:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:45:TYR:O	16:N:49:ASP:OD1	2.37	0.42
20:R:83:LEU:C	20:R:90:LYS:HE2	2.39	0.42
1:X:1238:A:OP1	17:O:68:LYS:NZ	2.46	0.42
1:X:1370:U:H2'	1:X:1371:G:O4'	2.18	0.42
1:X:2071:G:C2	1:X:2072:C:C2	3.07	0.42
1:X:2038:C:N4	1:X:2479:U:H1'	2.34	0.42
1:X:2795:A:H3'	1:X:2795:A:N3	2.34	0.42
1:X:538:A:O2'	1:X:539:A:C5'	2.67	0.42
1:X:617:U:C6	1:X:631:G:H8	2.37	0.42
1:X:961:G:C5	1:X:962:C:C4	3.07	0.42
3:A:151:GLY:O	3:A:153:GLY:N	2.52	0.42
3:A:55:ILE:HD12	3:A:55:ILE:H	1.83	0.42
1:X:1075:C:H5''	8:F:87:GLY:HA3	2.01	0.42
1:X:1935:A:C2	10:H:22:ILE:HG23	2.54	0.42
15:M:69:ARG:CZ	15:M:108:ARG:HA	2.49	0.42
1:X:29:U:C4'	16:N:11:ARG:HH22	2.31	0.42
16:N:83:LEU:N	16:N:83:LEU:HD12	2.34	0.42
23:U:17:SER:HB2	23:U:44:ALA:HA	1.99	0.42
1:X:1326:U:H3'	1:X:1326:U:O2	2.19	0.42
1:X:1790:G:H4'	1:X:1791:C:OP1	2.17	0.42
1:X:1868:A:H2'	1:X:1869:A:O4'	2.19	0.42
1:X:1882:G:H21	1:X:1885:C:N4	2.16	0.42
1:X:1996:A:O2'	18:P:115:ASN:ND2	2.50	0.42
1:X:995:A:P	1:X:996:C:C5	3.13	0.42
2:Y:117:G:H2'	2:Y:118:G:H8	1.84	0.42
5:C:51:VAL:HG23	5:C:52:SER:N	2.34	0.42
11:I:61:PRO:HD3	29:3:27:SER:HB3	2.01	0.42
12:J:39:GLU:HB3	12:J:128:ILE:CG2	2.49	0.42
15:M:34:ARG:NH1	15:M:88:VAL:CG2	2.70	0.42
17:O:65:ARG:HE	17:O:87:ARG:CD	2.24	0.42
17:O:7:THR:O	17:O:8:GLY:O	2.37	0.42
21:S:100:THR:HG23	21:S:138:VAL:HG21	2.00	0.42
1:X:943:U:H4'	25:W:21:GLN:NE2	2.34	0.42
1:X:1179:A:C2	1:X:1196:G:N2	2.87	0.42
1:X:1374:G:N2	1:X:1384:G:H1'	2.34	0.42
1:X:1393:G:H2'	1:X:1394:G:C8	2.54	0.42
1:X:1404:C:N4	1:X:1406:A:C8	2.87	0.42
1:X:426:C:H4'	1:X:1863:U:O2'	2.19	0.42
1:X:2012:A:C2	1:X:2016:A:C6	3.06	0.42
1:X:221:A:C2	1:X:232:A:C5	3.07	0.42
1:X:2594:U:C2'	1:X:2594:U:O2	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2657:G:N2	1:X:2710:C:O2	2.53	0.42
1:X:45:C:C2	1:X:157:G:N2	2.87	0.42
1:X:476:G:H4'	28:2:16:HIS:ND1	2.33	0.42
1:X:668:A:H2'	1:X:669:G:O4'	2.20	0.42
1:X:2002:A:N6	26:Z:9:LYS:HZ2	2.18	0.42
3:A:151:GLY:C	3:A:153:GLY:N	2.71	0.42
4:B:154:LYS:HE3	4:B:156:MET:HG3	1.99	0.42
4:B:67:PHE:CZ	4:B:75:THR:CG2	3.01	0.42
9:G:104:THR:O	9:G:107:GLN:NE2	2.52	0.42
9:G:103:TYR:CG	9:G:111:LYS:HB2	2.55	0.42
14:L:60:LYS:NZ	14:L:64:LYS:CE	2.81	0.42
16:N:88:ILE:O	17:O:48:GLY:HA3	2.20	0.42
1:X:1052:C:H42	1:X:1125:G:H1	1.65	0.42
1:X:1283:C:H42	1:X:1993:G:H1	1.68	0.42
1:X:1683:G:O2'	10:H:6:SER:HB2	2.20	0.42
1:X:188:G:C6	1:X:189:A:C6	3.06	0.42
1:X:1987:G:C6	1:X:1988:A:C5	3.07	0.42
1:X:2013:A:C5'	1:X:2014:A:OP1	2.66	0.42
1:X:224:G:H4'	1:X:399:G:C4	2.54	0.42
1:X:2636:A:C2	1:X:2644:A:C4	3.07	0.42
1:X:2690:A:N6	1:X:2694:G:C4	2.88	0.42
1:X:2813:G:O2'	13:K:46:PRO:HB3	2.18	0.42
1:X:2825:A:OP2	1:X:2843:A:C2	2.71	0.42
1:X:635:C:C3'	1:X:636:G:H5''	2.50	0.42
1:X:701:U:H5'	1:X:1771:A:C2	2.55	0.42
1:X:734:G:H2'	1:X:735:G:C8	2.54	0.42
1:X:764:A:C3'	1:X:764:A:C8	3.02	0.42
1:X:941:U:H2'	1:X:942:U:O4'	2.20	0.42
27:1:45:LYS:O	27:1:46:LYS:CB	2.67	0.42
6:D:135:GLN:HA	6:D:138:PHE:HE1	1.84	0.42
9:G:103:TYR:CZ	9:G:111:LYS:HB2	2.55	0.42
10:H:130:ALA:HA	10:H:131:PRO:HD3	1.96	0.42
11:I:55:ARG:C	11:I:57:ILE:H	2.19	0.42
12:J:69:ILE:HD13	12:J:104:MET:HB3	2.01	0.42
18:P:117:ILE:HA	18:P:117:ILE:HD13	1.80	0.42
20:R:84:VAL:O	20:R:84:VAL:HG23	2.18	0.42
21:S:163:ASP:HA	21:S:164:PRO:HD3	1.88	0.42
22:T:21:LEU:HD11	22:T:41:ARG:HG2	2.02	0.42
23:U:31:GLY:HA2	23:U:32:ARG:NH1	2.34	0.42
1:X:1219:C:H6	1:X:1219:C:O5'	2.02	0.42
1:X:1466:C:H2'	1:X:1467:U:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1500:U:H2'	1:X:1501:C:C6	2.54	0.42
1:X:1552:C:H4'	1:X:1553:G:O4'	2.20	0.42
1:X:1666:G:H2'	1:X:1667:A:C8	2.55	0.42
1:X:171:G:C2	1:X:179:U:C2	3.06	0.42
1:X:1910:A:N6	1:X:1911:A:N1	2.68	0.42
1:X:1923:U:O2'	1:X:1924:C:OP2	2.36	0.42
1:X:2622:G:H1	1:X:2751:C:H42	1.68	0.42
1:X:2799:C:H6	1:X:2799:C:O5'	2.02	0.42
31:X:2881:LC2:H5	31:X:2881:LC2:H13	1.73	0.42
1:X:464:G:H2'	1:X:465:C:C6	2.54	0.42
1:X:571:U:HO2'	1:X:581:A:H5'	1.84	0.42
1:X:611:C:O2	1:X:615:C:H5''	2.19	0.42
1:X:616:U:H5''	1:X:616:U:H6	1.84	0.42
1:X:797:A:N1	3:A:230:VAL:HG11	2.33	0.42
29:3:13:ARG:O	29:3:13:ARG:CG	2.67	0.42
29:3:57:ARG:C	29:3:59:LYS:H	2.23	0.42
3:A:108:ALA:HA	3:A:109:PRO:HD2	1.82	0.42
3:A:162:THR:H	3:A:197:VAL:CG2	2.32	0.42
4:B:198:LEU:N	4:B:198:LEU:HD12	2.33	0.42
9:G:141:GLY:O	9:G:142:ARG:C	2.55	0.42
10:H:24:VAL:HG11	10:H:42:LYS:HG3	2.01	0.42
11:I:94:GLU:HA	11:I:97:ARG:HE	1.84	0.42
1:X:1992:G:H1'	13:K:106:ASP:O	2.18	0.42
14:L:43:ILE:HD12	14:L:43:ILE:N	2.34	0.42
18:P:133:ASN:OD1	18:P:133:ASN:N	2.52	0.42
20:R:48:VAL:C	20:R:50:GLY:H	2.23	0.42
1:X:1336:G:C6	1:X:1337:G:C5	3.08	0.42
1:X:1344:C:C4	1:X:1346:C:C2	3.08	0.42
1:X:1386:A:H2'	1:X:1387:G:O4'	2.20	0.42
1:X:1939:U:H5	1:X:1940:C:C4	2.37	0.42
1:X:1978:U:H3'	1:X:1979:C:H5''	2.01	0.42
1:X:1282:A:H61	1:X:1994:U:H3	1.68	0.42
1:X:2277:A:H2'	1:X:2278:A:O4'	2.20	0.42
1:X:2392:G:H2'	1:X:2393:G:C8	2.54	0.42
1:X:2436:U:O2'	1:X:2437:G:H5'	2.20	0.42
1:X:2445:C:C4	1:X:2446:C:N4	2.87	0.42
1:X:2507:U:H5''	30:4:31:LYS:HE3	2.02	0.42
1:X:463:C:P	5:C:46:ARG:HG2	2.60	0.42
1:X:459:A:N7	1:X:484:G:C5	2.88	0.42
1:X:798:G:O2'	1:X:1770:U:H5''	2.19	0.42
28:2:12:ARG:O	28:2:15:THR:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:16:VAL:HG22	30:4:25:VAL:HG22	2.01	0.42
3:A:93:ILE:CG2	3:A:105:TYR:HB3	2.50	0.42
3:A:26:THR:HG23	3:A:27:LYS:H	1.82	0.42
3:A:37:ALA:CB	3:A:64:ARG:HG2	2.50	0.42
3:A:70:ARG:HH21	3:A:106:ILE:HD13	1.84	0.42
5:C:17:LEU:HA	5:C:18:PRO:HD3	1.76	0.42
5:C:21:GLU:C	5:C:22:VAL:CG2	2.87	0.42
5:C:97:ARG:HA	5:C:100:ARG:HE	1.84	0.42
9:G:156:HIS:N	9:G:157:PRO:CD	2.82	0.42
12:J:39:GLU:HA	12:J:40:PRO:HD3	1.69	0.42
20:R:25:LEU:O	20:R:26:SER:OG	2.30	0.42
20:R:85:ASP:HB3	20:R:90:LYS:HZ2	1.85	0.42
21:S:43:PHE:CE1	21:S:66:VAL:HG11	2.55	0.42
1:X:1177:U:C2	1:X:1198:C:O2	2.73	0.42
1:X:1271:C:H2'	1:X:1272:G:C8	2.54	0.42
1:X:1469:U:H5	13:K:64:ARG:NH2	2.08	0.42
1:X:1469:U:H5'	1:X:1470:G:P	2.59	0.42
1:X:155:G:H2'	1:X:156:G:C8	2.55	0.42
1:X:1814:G:H2'	1:X:1815:G:H8	1.85	0.42
1:X:1915:A:H2'	1:X:1916:G:O4'	2.19	0.42
1:X:1937:G:N3	1:X:2530:C:C5'	2.82	0.42
1:X:1948:C:N4	1:X:1949:A:N6	2.68	0.42
1:X:2867:G:H4'	1:X:2868:G:O5'	2.19	0.42
1:X:613:A:C6	1:X:668:A:H1'	2.54	0.42
27:1:14:SER:H	27:1:22:TYR:HD2	1.68	0.42
3:A:30:PRO:O	3:A:31:GLU:HB2	2.19	0.42
4:B:121:ASN:O	4:B:122:PHE:CG	2.72	0.42
5:C:58:MET:HG2	5:C:59:TYR:N	2.34	0.42
9:G:84:ASN:O	9:G:151:TYR:O	2.38	0.42
13:K:94:TYR:CZ	13:K:115:LEU:O	2.72	0.42
21:S:129:ARG:HH22	21:S:156:GLU:CD	2.09	0.42
21:S:46:GLN:HB3	21:S:50:GLY:HA3	2.00	0.42
1:X:1128:G:H2'	1:X:1129:A:H5''	2.02	0.42
1:X:574:C:H4'	1:X:1266:G:O6	2.19	0.42
1:X:1354:A:O3'	19:Q:54:SER:HB2	2.20	0.42
1:X:1391:A:C1'	1:X:1392:U:P	3.08	0.42
1:X:13:A:C2	1:X:15:G:N1	2.88	0.42
1:X:1404:C:C4	1:X:1406:A:H8	2.33	0.42
1:X:1470:G:O2'	1:X:1471:G:H5'	2.20	0.42
1:X:1632:A:OP1	1:X:1632:A:H8	2.03	0.42
1:X:1768:U:O5'	1:X:1768:U:H6	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:180:C:C4	1:X:181:A:C5	3.08	0.42
1:X:2438:A:N6	1:X:2473:G:C2	2.88	0.42
1:X:2510:A:H61	1:X:2641:A:H61	1.66	0.42
1:X:2657:G:H1	1:X:2709:C:N4	2.15	0.42
1:X:2788:C:O2'	1:X:2789:U:H5'	2.19	0.42
1:X:504:G:O2'	18:P:26:ALA:HA	2.20	0.42
1:X:492:G:H2'	1:X:517:A:N1	2.35	0.42
1:X:646:C:O2'	1:X:650:U:H5''	2.19	0.42
1:X:649:G:N2	1:X:660:G:C2	2.88	0.42
1:X:681:A:C5	1:X:683:A:C8	3.08	0.42
1:X:923:A:C5	12:J:12:LYS:HD3	2.54	0.42
27:1:14:SER:HA	27:1:52:GLU:HA	2.01	0.42
27:1:45:LYS:O	27:1:46:LYS:HG2	2.20	0.42
28:2:10:ARG:H	28:2:10:ARG:CD	2.33	0.42
4:B:44:TYR:HB2	4:B:82:ARG:NH1	2.31	0.42
1:X:2737:A:N1	7:E:67:LEU:HD12	2.35	0.42
17:O:21:ARG:O	17:O:91:THR:HG22	2.18	0.42
1:X:1081:A:H62	1:X:1107:A:H2'	1.83	0.42
1:X:1344:C:C4	1:X:1346:C:N3	2.88	0.42
1:X:1836:C:N4	1:X:1879:G:H1	2.17	0.42
1:X:1691:G:C6	1:X:1972:G:O6	2.73	0.42
1:X:2245:A:C2	1:X:2251:U:C5	3.08	0.42
1:X:2256:G:O3'	12:J:14:PHE:CD2	2.73	0.42
1:X:2371:A:H1'	11:I:59:ARG:HG2	2.01	0.42
1:X:2375:G:H2'	1:X:2376:G:H8	1.85	0.42
1:X:2590:U:H1'	32:X:2882:LMA:C37	2.48	0.42
1:X:2641:A:C2'	1:X:2642:G:H5'	2.49	0.42
1:X:2658:A:H2	1:X:2709:C:N3	2.17	0.42
1:X:495:C:H2'	1:X:496:C:C6	2.55	0.42
1:X:794:A:H5'	3:A:219:LYS:HZ3	1.84	0.42
27:1:25:THR:HG22	27:1:27:ASN:ND2	2.35	0.42
1:X:2350:G:C2'	27:1:46:LYS:HG3	2.48	0.42
3:A:71:ARG:HG2	3:A:191:TYR:HE1	1.82	0.42
4:B:61:LYS:N	4:B:62:PRO:HD2	2.35	0.42
6:D:80:ARG:CD	6:D:83:MET:HB3	2.44	0.42
10:H:1:MET:H2	10:H:79:HIS:HB2	1.83	0.42
11:I:83:LEU:C	11:I:84:GLU:HG2	2.40	0.42
13:K:84:ALA:HB3	13:K:85:PRO:CD	2.41	0.42
14:L:89:PHE:HZ	14:L:103:LEU:CD2	2.17	0.42
14:L:33:ARG:NH1	14:L:99:ARG:O	2.53	0.42
23:U:70:LEU:HD23	23:U:70:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1068:A:H2'	1:X:1069:G:C8	2.55	0.42
1:X:1288:A:C8	13:K:16:ALA:CB	2.94	0.42
1:X:1329:U:O2'	1:X:1330:G:H5'	2.20	0.42
1:X:1365:U:C2	1:X:1393:G:C2	3.07	0.42
1:X:1533:G:H2'	1:X:1534:A:C8	2.54	0.42
1:X:178:C:H2'	1:X:179:U:C6	2.55	0.42
1:X:1967:U:H2'	1:X:1968:G:C8	2.54	0.42
1:X:205:A:H2'	1:X:206:U:H5'	2.01	0.42
1:X:2244:C:C4	1:X:2245:A:C5	3.08	0.42
1:X:2404:A:C4'	1:X:2405:A:OP2	2.68	0.42
1:X:2419:C:H2'	1:X:2420:C:O5'	2.20	0.42
1:X:2674:C:O2'	1:X:2675:U:H5'	2.20	0.42
1:X:2832:G:N2	1:X:2835:A:OP2	2.47	0.42
32:X:2882:LMA:HO57	18:P:111:ARG:NH2	2.17	0.42
1:X:611:C:O2	1:X:615:C:C5'	2.68	0.42
1:X:632:A:H2'	1:X:633:G:H5'	2.02	0.42
1:X:671:A:C5	1:X:672:C:C4	3.08	0.42
1:X:707:U:OP1	3:A:60:LYS:HE3	2.20	0.42
1:X:758:G:O2'	1:X:759:C:OP1	2.28	0.42
1:X:768:U:C4	1:X:769:C:C4	3.08	0.42
1:X:750:C:C4'	1:X:779:U:O2'	2.68	0.42
2:Y:26:G:H21	2:Y:29:C:N4	2.18	0.42
27:1:9:ILE:C	27:1:10:VAL:CG2	2.88	0.41
28:2:42:LEU:HD12	28:2:42:LEU:H	1.85	0.41
29:3:9:MET:CE	29:3:59:LYS:HB2	2.50	0.41
30:4:24:LEU:HD12	30:4:24:LEU:N	2.35	0.41
3:A:90:SER:O	3:A:199:ASN:OD1	2.37	0.41
4:B:84:PHE:CE1	4:B:86:PRO:CB	3.00	0.41
5:C:34:GLN:OE1	5:C:176:ASN:ND2	2.52	0.41
7:E:94:PHE:CE2	7:E:160:LYS:HD3	2.55	0.41
10:H:133:VAL:HG12	15:M:38:LYS:NZ	2.35	0.41
14:L:93:SER:C	14:L:94:TYR:CD2	2.92	0.41
1:X:1745:C:OP1	15:M:101:ARG:NH2	2.52	0.41
21:S:43:PHE:HE1	21:S:66:VAL:HG11	1.85	0.41
1:X:2344:G:H4'	22:T:60:PHE:CE1	2.54	0.41
1:X:985:G:N2	1:X:1000:G:H1'	2.35	0.41
1:X:1200:G:C6	1:X:1201:G:C4	3.08	0.41
1:X:1299:A:C4'	1:X:1300:A:OP1	2.68	0.41
1:X:1348:C:H6	1:X:1348:C:O5'	2.03	0.41
1:X:1473:U:O2'	1:X:1474:A:P	2.77	0.41
1:X:1499:A:H2'	1:X:1500:U:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1790:G:C6	1:X:1811:A:N7	2.88	0.41
1:X:1944:C:H2'	1:X:1945:C:O4'	2.19	0.41
1:X:2727:G:N2	1:X:2736:U:C5	2.88	0.41
1:X:2826:C:H2'	1:X:2827:G:O4'	2.19	0.41
1:X:658:G:H2'	1:X:659:G:C8	2.51	0.41
1:X:857:U:H6	1:X:857:U:O5'	2.02	0.41
3:A:49:ARG:CB	3:A:49:ARG:HH11	2.33	0.41
5:C:163:ASN:OD1	5:C:167:VAL:HG22	2.20	0.41
1:X:463:C:OP2	5:C:46:ARG:HG2	2.19	0.41
15:M:60:SER:CA	15:M:64:LYS:HB2	2.49	0.41
1:X:1997:A:H5'	18:P:115:ASN:CG	2.41	0.41
22:T:62:LEU:N	22:T:62:LEU:HD22	2.35	0.41
1:X:1048:U:H3	1:X:1129:A:H61	1.66	0.41
1:X:1468:A:H8	1:X:1468:A:P	2.42	0.41
1:X:1635:G:O2'	28:2:1:MET:HG2	2.20	0.41
1:X:755:C:H4'	1:X:1692:C:O2'	2.20	0.41
1:X:752:G:OP1	1:X:1775:A:N1	2.53	0.41
1:X:1684:G:H22	1:X:1977:C:N4	2.17	0.41
1:X:2047:C:H2'	1:X:2048:C:C6	2.56	0.41
1:X:2059:U:H5	1:X:2575:U:O2	2.02	0.41
1:X:2703:C:P	4:B:109:LYS:HZ2	2.43	0.41
1:X:2793:G:N3	1:X:2804:G:C2	2.88	0.41
1:X:461:A:N7	1:X:462:G:N7	2.68	0.41
1:X:514:G:H4'	1:X:515:A:OP2	2.20	0.41
1:X:572:G:C2	1:X:573:C:C2	3.08	0.41
1:X:800:U:C5	1:X:804:C:N3	2.88	0.41
30:4:19:ARG:HD2	30:4:24:LEU:HD22	2.03	0.41
6:D:4:LEU:O	6:D:5:LYS:HB3	2.20	0.41
11:I:22:GLY:HA2	11:I:23:PRO:HD2	1.92	0.41
1:X:825:C:C6	11:I:30:ALA:HB1	2.54	0.41
12:J:119:PHE:HD1	12:J:132:MET:SD	2.43	0.41
13:K:13:ASN:OD1	13:K:16:ALA:CB	2.69	0.41
16:N:28:ARG:O	16:N:35:ALA:CB	2.67	0.41
16:N:24:PHE:O	16:N:29:SER:HB3	2.19	0.41
18:P:48:LYS:HE3	18:P:48:LYS:HB2	1.69	0.41
21:S:6:LYS:N	21:S:7:PRO:HD3	2.35	0.41
1:X:1071:U:H3	1:X:1099:A:H8	1.69	0.41
1:X:1174:G:H2'	1:X:1175:A:C8	2.54	0.41
1:X:1479:G:H2'	1:X:1480:G:C8	2.54	0.41
1:X:1574:A:C2	1:X:1576:G:H1'	2.54	0.41
1:X:1790:G:C4'	1:X:1791:C:O5'	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1955:G:H2'	1:X:1956:G:C8	2.55	0.41
1:X:215:G:H4'	1:X:618:A:O2'	2.20	0.41
1:X:2500:C:H4'	1:X:2544:A:C4'	2.50	0.41
1:X:387:A:C2'	1:X:388:G:H5'	2.50	0.41
1:X:635:C:O2'	1:X:670:U:H5''	2.20	0.41
1:X:879:A:C2	1:X:926:C:H5''	2.55	0.41
28:2:39:ARG:O	28:2:40:HIS:CG	2.73	0.41
29:3:14:ILE:O	29:3:14:ILE:HG12	2.19	0.41
1:X:705:C:H4'	3:A:42:GLY:O	2.20	0.41
10:H:27:SER:HB3	10:H:49:ASP:HA	2.02	0.41
12:J:99:LYS:CG	12:J:100:PRO:HD2	2.51	0.41
13:K:59:ASP:O	13:K:60:LEU:C	2.56	0.41
15:M:11:GLU:HG3	15:M:14:ARG:HH11	1.86	0.41
1:X:1265:G:H4'	16:N:33:ARG:HD3	2.02	0.41
16:N:63:GLN:O	16:N:66:ASN:OD1	2.39	0.41
18:P:95:ALA:HB2	18:P:126:ILE:HD13	2.03	0.41
22:T:17:ASN:HA	22:T:18:PRO:HD3	1.97	0.41
22:T:49:GLN:O	22:T:80:SER:HA	2.20	0.41
1:X:455:A:H2	1:X:1258:G:N3	2.19	0.41
1:X:1539:U:H2'	1:X:1540:C:C6	2.55	0.41
1:X:1634:A:H1'	1:X:1635:G:OP1	2.20	0.41
1:X:2003:A:C6	1:X:2005:U:C2	3.08	0.41
1:X:2170:C:C3'	1:X:2171:U:H5''	2.29	0.41
1:X:2654:A:H5'	10:H:41:ASN:HB3	2.01	0.41
1:X:494:A:N7	1:X:495:C:C5	2.88	0.41
1:X:546:A:H2'	1:X:547:U:C6	2.55	0.41
1:X:938:G:H2'	1:X:939:C:OP2	2.21	0.41
1:X:834:A:H2'	1:X:957:G:P	2.60	0.41
3:A:133:PRO:HB2	3:A:135:ARG:HG2	2.03	0.41
1:X:2598:C:H4'	4:B:151:TYR:O	2.19	0.41
5:C:7:ILE:CG1	5:C:119:ALA:HB1	2.49	0.41
10:H:76:ARG:O	10:H:94:ASN:CA	2.65	0.41
10:H:76:ARG:HB2	10:H:95:ALA:HB3	2.02	0.41
17:O:10:LYS:HG3	17:O:11:GLN:HG2	2.02	0.41
19:Q:26:SER:CB	19:Q:79:ILE:HG12	2.50	0.41
23:U:48:LYS:HG2	23:U:49:LYS:H	1.83	0.41
1:X:95:G:H4'	24:V:41:HIS:CE1	2.55	0.41
1:X:104:C:H6	1:X:104:C:O5'	2.03	0.41
1:X:1095:A:C3'	1:X:1096:A:H5''	2.51	0.41
1:X:1129:A:C6	1:X:1130:U:N3	2.88	0.41
1:X:594:G:N7	1:X:1264:C:N4	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:13:A:C2	1:X:15:G:C6	3.08	0.41
1:X:1405:A:N6	1:X:1406:A:H61	2.18	0.41
1:X:1488:G:C2	1:X:1536:G:C2	3.08	0.41
1:X:2344:G:H4'	22:T:60:PHE:CZ	2.55	0.41
1:X:2450:A:N6	1:X:2451:G:C2	2.89	0.41
1:X:2674:C:H2'	1:X:2675:U:C6	2.56	0.41
1:X:2728:A:C2	1:X:2737:A:C5	3.08	0.41
1:X:2841:U:O2'	1:X:2842:C:OP2	2.30	0.41
1:X:320:A:N3	1:X:340:G:O2'	2.53	0.41
1:X:306:G:N2	1:X:355:G:H1'	2.35	0.41
1:X:734:G:H2'	1:X:735:G:H8	1.85	0.41
1:X:761:G:OP1	1:X:2591:C:N4	2.53	0.41
1:X:869:C:O2	1:X:934:G:C2	2.73	0.41
26:Z:4:HIS:HB2	26:Z:5:PRO:HD2	1.98	0.41
27:1:43:VAL:CG2	27:1:43:VAL:O	2.69	0.41
3:A:84:GLU:CD	3:A:105:TYR:HE2	2.20	0.41
3:A:212:ARG:O	3:A:212:ARG:CG	2.68	0.41
3:A:46:ASN:ND2	3:A:47:ARG:N	2.68	0.41
4:B:120:TRP:O	4:B:122:PHE:CD2	2.68	0.41
5:C:102:LEU:HD21	5:C:106:MET:CE	2.51	0.41
1:X:1142:G:N9	9:G:103:TYR:HD2	2.17	0.41
10:H:116:ARG:O	10:H:117:GLU:C	2.58	0.41
10:H:126:ILE:HD12	10:H:126:ILE:HG23	1.51	0.41
20:R:63:THR:O	20:R:64:ASN:C	2.58	0.41
21:S:56:VAL:HG12	21:S:57:GLU:N	2.35	0.41
1:X:1175:A:C2	1:X:1176:U:C2	3.09	0.41
1:X:984:A:C8	1:X:1202:U:C2	3.08	0.41
1:X:1434:U:H5''	1:X:1435:G:OP2	2.20	0.41
1:X:1506:C:H2'	1:X:1507:A:H5'	2.03	0.41
1:X:1671:A:C8	1:X:1671:A:H5''	2.52	0.41
1:X:2173:G:H2'	1:X:2174:G:C8	2.56	0.41
1:X:2200:G:H2'	1:X:2201:G:H8	1.85	0.41
1:X:2404:A:C8	1:X:2406:C:O2	2.74	0.41
1:X:2560:G:C6	1:X:2589:C:C2	3.09	0.41
1:X:2665:G:C8	1:X:2665:G:O5'	2.74	0.41
31:X:2881:LC2:H29	31:X:2881:LC2:H14	1.73	0.41
1:X:591:G:C6	1:X:592:G:C6	3.08	0.41
1:X:788:G:O2'	1:X:789:G:P	2.79	0.41
1:X:824:U:C5	11:I:29:THR:HB	2.56	0.41
26:Z:31:THR:O	26:Z:39:LYS:HA	2.20	0.41
28:2:15:THR:O	28:2:16:HIS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:1:MET:CE	28:2:3:ARG:CZ	2.98	0.41
3:A:111:GLY:HA3	3:A:128:LEU:HD13	2.03	0.41
3:A:143:VAL:HG12	3:A:194:ILE:HA	2.02	0.41
11:I:73:GLU:N	11:I:73:GLU:OE1	2.53	0.41
14:L:60:LYS:HZ2	14:L:64:LYS:HE2	1.85	0.41
15:M:80:VAL:HG12	15:M:80:VAL:O	2.20	0.41
17:O:48:GLY:O	17:O:49:GLU:HB2	2.20	0.41
18:P:89:ARG:CG	18:P:131:LYS:HB3	2.49	0.41
19:Q:69:ILE:CD1	19:Q:70:GLY:N	2.83	0.41
21:S:168:VAL:HG12	21:S:169:VAL:HG13	2.01	0.41
1:X:1005:U:OP1	16:N:53:LYS:NZ	2.50	0.41
1:X:1142:G:N2	1:X:1143:A:N3	2.69	0.41
1:X:985:G:C8	1:X:1200:G:N2	2.89	0.41
1:X:1226:A:C4	1:X:1250:A:N3	2.88	0.41
1:X:1987:G:C5	1:X:1988:A:C8	3.08	0.41
1:X:230:C:C2'	1:X:231:G:H5'	2.50	0.41
1:X:2535:C:C5	1:X:2536:G:C5	3.09	0.41
1:X:2571:G:N1	1:X:2582:G:N1	2.69	0.41
1:X:2853:U:O5'	1:X:2853:U:H6	2.04	0.41
1:X:459:A:N6	1:X:484:G:H1'	2.36	0.41
1:X:547:U:O5'	1:X:547:U:H6	2.04	0.41
1:X:579:G:H2'	1:X:2013:A:C6	2.56	0.41
6:D:150:ARG:HA	6:D:150:ARG:NH1	2.30	0.41
17:O:10:LYS:HZ3	17:O:37:ALA:HB3	1.82	0.41
17:O:54:TYR:HD2	17:O:98:ILE:HG21	1.85	0.41
1:X:1118:G:H2'	1:X:1119:U:H5'	2.03	0.41
1:X:152:G:O2'	1:X:153:A:H5'	2.21	0.41
1:X:1739:G:H2'	1:X:1740:G:H8	1.85	0.41
1:X:1983:G:C2'	1:X:1984:A:H5'	2.50	0.41
1:X:2184:C:C4	1:X:2185:U:C4	3.08	0.41
27:1:31:THR:O	27:1:33:ALA:N	2.54	0.41
28:2:21:ARG:HD2	28:2:30:ILE:HD12	2.03	0.41
29:3:30:ARG:HE	29:3:31:HIS:CE1	2.39	0.41
30:4:11:CYS:HG	30:4:32:HIS:CE1	2.39	0.41
3:A:178:LEU:HD11	3:A:184:ARG:HG3	2.02	0.41
5:C:191:ALA:HA	5:C:194:GLU:HB3	2.02	0.41
7:E:156:ALA:O	7:E:157:TYR:CD1	2.73	0.41
13:K:72:ASP:CG	13:K:75:VAL:HG23	2.42	0.41
18:P:52:ASP:O	18:P:56:LEU:HG	2.21	0.41
19:Q:3:HIS:CG	19:Q:44:GLN:HB2	2.56	0.41
1:X:2258:G:O6	22:T:15:ASP:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1341:G:N2	1:X:1664:G:N1	2.69	0.41
1:X:1923:U:H4'	1:X:1924:C:O5'	2.20	0.41
1:X:2038:C:H2'	1:X:2483:U:C5'	2.51	0.41
1:X:223:C:H42	29:3:7:HIS:HB3	1.82	0.41
1:X:2241:U:C6	1:X:2241:U:H3'	2.55	0.41
1:X:2222:U:O2	1:X:2413:A:H2	2.02	0.41
1:X:2429:A:H2'	1:X:2430:A:C8	2.55	0.41
1:X:42:G:H2'	1:X:43:A:O4'	2.20	0.41
1:X:538:A:C4'	1:X:539:A:OP1	2.69	0.41
2:Y:59:A:H1'	6:D:27:ALA:HB2	2.03	0.41
1:X:469:G:C2'	28:2:39:ARG:O	2.69	0.41
3:A:201:GLU:HG3	3:A:203:LYS:HB3	2.03	0.41
1:X:795:A:C2	3:A:227:MET:HE2	2.55	0.41
4:B:26:VAL:CG1	4:B:196:VAL:CG2	2.95	0.41
5:C:14:THR:O	5:C:15:ILE:CB	2.69	0.41
6:D:80:ARG:NE	6:D:80:ARG:N	2.69	0.41
13:K:80:MET:HB2	13:K:80:MET:HE3	1.34	0.41
16:N:88:ILE:HG23	17:O:48:GLY:O	2.20	0.41
20:R:18:LYS:CD	20:R:18:LYS:N	2.79	0.41
1:X:1218:C:H2'	1:X:1219:C:C6	2.55	0.41
1:X:1391:A:C2	1:X:1393:G:C8	3.09	0.41
1:X:1774:A:OP1	1:X:1775:A:OP2	2.39	0.41
1:X:752:G:OP1	1:X:1775:A:C2	2.74	0.41
1:X:1818:G:C6	1:X:1819:U:N3	2.89	0.41
1:X:2040:A:C8	1:X:2040:A:H3'	2.55	0.41
1:X:2051:U:H2'	1:X:2051:U:O2	2.20	0.41
1:X:1386:A:H5''	1:X:2191:A:N6	2.35	0.41
1:X:2419:C:H6	1:X:2419:C:O5'	2.04	0.41
1:X:2580:C:HO2'	1:X:2581:A:P	2.44	0.41
1:X:39:C:H2'	1:X:40:U:C6	2.56	0.41
1:X:573:C:C5	1:X:574:C:C5	3.09	0.41
1:X:919:U:H2'	1:X:920:G:H8	1.86	0.41
1:X:980:G:C2	1:X:981:C:C2	3.09	0.41
1:X:997:C:C3'	1:X:997:C:C6	3.04	0.41
2:Y:32:C:H1'	2:Y:59:A:H61	1.86	0.41
29:3:49:VAL:HG21	29:3:52:LYS:CE	2.51	0.41
4:B:188:ILE:HA	4:B:189:PRO:HD3	1.81	0.41
5:C:102:LEU:C	5:C:102:LEU:HD23	2.39	0.41
7:E:105:MET:CE	7:E:105:MET:HA	2.51	0.41
11:I:57:ILE:O	29:3:12:ARG:NE	2.54	0.41
11:I:62:LYS:HD3	29:3:12:ARG:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:135:ARG:O	12:J:136:GLU:HB2	2.20	0.41
12:J:8:THR:N	12:J:70:PHE:HZ	2.18	0.41
20:R:92:THR:CB	20:R:107:ALA:O	2.69	0.41
23:U:19:ILE:HG22	23:U:42:GLN:CG	2.50	0.41
1:X:1008:G:N2	1:X:1170:U:H1'	2.36	0.41
1:X:1230:C:OP1	16:N:15:LYS:HD3	2.21	0.41
1:X:1289:A:C2	1:X:1290:A:C6	3.09	0.41
1:X:1462:C:O2'	1:X:1463:A:H5'	2.21	0.41
1:X:1623:C:H4'	1:X:1624:A:OP2	2.13	0.41
1:X:1755:G:O2'	1:X:1756:C:H5'	2.21	0.41
1:X:1787:U:H2'	1:X:1788:C:C6	2.56	0.41
1:X:196:A:N6	1:X:197:G:C6	2.89	0.41
1:X:2064:U:C5	1:X:2216:G:C2	3.09	0.41
1:X:2806:G:H4'	1:X:2858:A:C6	2.56	0.41
32:X:2882:LMA:H21A	32:X:2882:LMA:C51	2.51	0.41
1:X:1:G:H2'	1:X:2:G:C8	2.56	0.41
1:X:748:A:N7	1:X:749:C:C2	2.88	0.41
1:X:841:G:C2'	1:X:841:G:N3	2.83	0.41
1:X:919:U:O2'	1:X:920:G:H5'	2.20	0.41
1:X:943:U:O2'	1:X:944:A:O4'	2.37	0.41
1:X:851:C:C2	1:X:952:A:C6	3.09	0.41
1:X:977:G:C1'	1:X:2246:A:H62	2.34	0.41
2:Y:66:G:H2'	2:Y:67:C:O4'	2.20	0.41
29:3:36:LYS:HD3	29:3:36:LYS:N	2.36	0.40
30:4:13:ASN:HB2	30:4:27:CYS:SG	2.61	0.40
1:X:626:A:H4'	5:C:176:ASN:OD1	2.21	0.40
9:G:140:GLN:HG2	9:G:144:MET:HE3	2.04	0.40
21:S:104:SER:HA	21:S:139:THR:HA	2.02	0.40
23:U:49:LYS:HB2	23:U:61:TRP:HA	2.03	0.40
1:X:1948:C:C4	1:X:1949:A:N7	2.89	0.40
1:X:2004:U:P	26:Z:12:SER:OG	2.79	0.40
1:X:2581:A:C2'	1:X:2582:G:O5'	2.69	0.40
1:X:333:A:C5'	5:C:162:ARG:CG	2.99	0.40
1:X:874:A:H2'	1:X:875:G:O4'	2.20	0.40
1:X:916:U:C4	1:X:917:U:C4	3.09	0.40
1:X:688:A:H4'	5:C:61:GLN:HG2	2.03	0.40
9:G:116:ARG:HD2	9:G:116:ARG:HA	1.88	0.40
1:X:2814:G:C1'	13:K:49:GLU:OE2	2.70	0.40
20:R:11:ASN:O	20:R:12:ASP:HB3	2.21	0.40
1:X:1196:G:H2'	1:X:1197:U:O4'	2.21	0.40
1:X:119:G:H2'	1:X:120:G:C8	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:182:G:O2'	1:X:183:U:C5	2.74	0.40
1:X:1865:C:H2'	1:X:1866:G:O4'	2.21	0.40
1:X:2670:C:O4'	1:X:2847:G:C6	2.75	0.40
1:X:2713:A:O2'	1:X:2714:A:H5'	2.21	0.40
1:X:2833:C:H2'	1:X:2834:A:O4'	2.22	0.40
32:X:2882:LMA:H4	32:X:2882:LMA:H7	1.88	0.40
1:X:754:G:C6	1:X:755:C:N4	2.90	0.40
1:X:1628:C:C5'	28:2:7:PRO:HG2	2.49	0.40
29:3:15:LYS:HB2	29:3:23:MET:HG3	2.04	0.40
29:3:41:ILE:C	29:3:43:GLY:H	2.22	0.40
1:X:1817:U:C5'	3:A:253:LYS:HD3	2.51	0.40
3:A:66:ILE:CD1	3:A:89:ARG:NH2	2.83	0.40
5:C:74:VAL:HB	5:C:75:PRO:HD2	2.03	0.40
5:C:87:LYS:HA	5:C:88:PRO:HD3	1.78	0.40
9:G:90:LEU:CD1	9:G:90:LEU:N	2.85	0.40
12:J:107:VAL:HG22	12:J:119:PHE:CZ	2.56	0.40
1:X:29:U:C5'	16:N:11:ARG:HH12	2.34	0.40
20:R:65:PRO:O	20:R:66:GLN:C	2.57	0.40
25:W:10:ILE:HG13	25:W:10:ILE:H	1.62	0.40
1:X:1096:A:C1'	1:X:1097:A:OP1	2.69	0.40
1:X:1142:G:N3	9:G:103:TYR:CE2	2.89	0.40
1:X:1673:C:H5''	4:B:136:ARG:CD	2.43	0.40
1:X:1920:A:C5	1:X:1922:U:C2	3.09	0.40
1:X:2425:G:C6	1:X:2480:C:H2'	2.56	0.40
1:X:2526:U:H2'	1:X:2527:G:C8	2.55	0.40
1:X:2555:G:N3	1:X:2555:G:C3'	2.84	0.40
1:X:2719:U:C5	1:X:2743:G:C6	3.09	0.40
1:X:29:U:H6	1:X:29:U:O5'	2.04	0.40
1:X:526:C:O2'	1:X:527:C:C5'	2.67	0.40
1:X:931:G:H2'	1:X:932:G:O4'	2.21	0.40
27:1:8:ILE:CG1	27:1:30:ASN:ND2	2.68	0.40
27:1:40:TYR:H	27:1:50:PHE:HB3	1.85	0.40
1:X:2506:C:H5''	30:4:30:VAL:HB	2.04	0.40
1:X:1811:A:H2'	3:A:179:PRO:HG2	2.03	0.40
5:C:134:ILE:HG22	5:C:138:LYS:HE3	2.02	0.40
5:C:29:GLU:HG2	5:C:95:LEU:HD11	2.03	0.40
6:D:123:ASP:OD1	6:D:124:GLY:N	2.54	0.40
6:D:52:LYS:C	6:D:52:LYS:HD3	2.42	0.40
9:G:46:ALA:CB	9:G:54:LEU:HD21	2.52	0.40
10:H:129:LEU:HA	10:H:129:LEU:HD23	1.73	0.40
10:H:4:PRO:O	10:H:5:GLN:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:54:VAL:HG23	12:J:125:LYS:HZ2	1.86	0.40
12:J:88:LYS:HB2	12:J:88:LYS:NZ	2.36	0.40
14:L:14:ARG:O	14:L:18:ARG:HB2	2.22	0.40
16:N:93:LYS:HE2	17:O:10:LYS:HE3	2.03	0.40
1:X:94:C:HO2'	24:V:40:PRO:HD2	1.86	0.40
1:X:1166:A:H2'	1:X:1167:A:H5''	2.03	0.40
1:X:1567:A:H2'	1:X:1568:A:O4'	2.20	0.40
1:X:1741:G:O2'	1:X:1742:G:H5'	2.21	0.40
1:X:1928:G:N1	1:X:1929:U:N3	2.70	0.40
1:X:583:C:N4	1:X:2017:U:OP1	2.51	0.40
1:X:2260:C:O2'	1:X:2261:G:H5'	2.22	0.40
1:X:2337:A:H2'	1:X:2338:C:O4'	2.22	0.40
1:X:2395:C:H2'	1:X:2396:C:H5'	2.03	0.40
1:X:2502:G:C8	1:X:2502:G:O5'	2.68	0.40
1:X:2671:C:N4	1:X:2698:G:H1	2.20	0.40
1:X:486:U:O2	1:X:492:G:N2	2.54	0.40
1:X:965:G:O6	1:X:966:A:C6	2.74	0.40
2:Y:33:C:H42	2:Y:53:G:H1	1.69	0.40
28:2:12:ARG:HE	28:2:43:THR:HG22	1.86	0.40
3:A:160:ALA:CA	3:A:199:ASN:CB	3.00	0.40
6:D:135:GLN:HA	6:D:138:PHE:CE1	2.57	0.40
6:D:22:TYR:CZ	6:D:29:PRO:CD	3.05	0.40
13:K:20:LEU:HA	13:K:20:LEU:HD12	1.87	0.40
16:N:35:ALA:O	16:N:38:THR:HB	2.22	0.40
20:R:83:LEU:HD22	20:R:113:THR:CB	2.51	0.40
1:X:1098:G:O6	1:X:1100:G:C2	2.74	0.40
1:X:1364:C:O2	1:X:1394:G:C2	2.75	0.40
1:X:1621:C:O4'	1:X:1626:A:C6	2.75	0.40
1:X:1688:U:C2	1:X:1690:U:OP2	2.74	0.40
1:X:1724:C:C4	1:X:1747:G:O6	2.75	0.40
1:X:1763:G:C2'	1:X:1764:A:H5'	2.51	0.40
1:X:1947:G:O6	1:X:1950:C:N4	2.54	0.40
1:X:2462:C:H2'	1:X:2463:G:O4'	2.22	0.40
1:X:2571:G:N2	1:X:2582:G:C4	2.90	0.40
1:X:309:G:OP1	20:R:93:ARG:CA	2.69	0.40
1:X:497:C:H3'	1:X:497:C:C6	2.57	0.40
1:X:513:A:OP1	1:X:514:G:N2	2.55	0.40
1:X:640:C:C4'	1:X:660:G:H21	2.34	0.40
1:X:742:G:O2'	1:X:776:G:H4'	2.22	0.40
1:X:830:C:HO2'	1:X:831:G:H5'	1.87	0.40
2:Y:4:C:H2'	2:Y:5:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:77:G:H2'	2:Y:78:A:O4'	2.21	0.40
1:X:1275:A:N3	26:Z:10:LYS:HE2	2.35	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1552:C:O2	15:M:43:ASN:ND2[8_455]	0.99	1.21
1:X:1552:C:O2	15:M:43:ASN:CG[8_455]	1.93	0.27
1:X:1552:C:C2	15:M:43:ASN:ND2[8_455]	2.03	0.17

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
3	A	251/274 (92%)	207 (82%)	36 (14%)	8 (3%)	5	35
4	B	203/211 (96%)	174 (86%)	22 (11%)	7 (3%)	4	34
5	C	192/205 (94%)	153 (80%)	30 (16%)	9 (5%)	3	25
6	D	175/180 (97%)	146 (83%)	27 (15%)	2 (1%)	17	58
7	E	169/185 (91%)	147 (87%)	18 (11%)	4 (2%)	7	42
8	F	61/144 (42%)	51 (84%)	9 (15%)	1 (2%)	11	50
9	G	140/174 (80%)	118 (84%)	18 (13%)	4 (3%)	5	37
10	H	132/134 (98%)	115 (87%)	17 (13%)	0	100	100
11	I	132/156 (85%)	96 (73%)	29 (22%)	7 (5%)	2	21
12	J	134/141 (95%)	107 (80%)	25 (19%)	2 (2%)	12	51
13	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	20	63
14	L	102/114 (90%)	81 (79%)	20 (20%)	1 (1%)	18	60
15	M	106/166 (64%)	94 (89%)	9 (8%)	3 (3%)	6	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	N	115/118 (98%)	106 (92%)	7 (6%)	2 (2%)	11	49
17	O	92/100 (92%)	77 (84%)	12 (13%)	3 (3%)	4	34
18	P	124/134 (92%)	109 (88%)	13 (10%)	2 (2%)	11	50
19	Q	91/95 (96%)	66 (72%)	20 (22%)	5 (6%)	2	20
20	R	108/115 (94%)	82 (76%)	20 (18%)	6 (6%)	2	20
21	S	173/237 (73%)	140 (81%)	28 (16%)	5 (3%)	5	37
22	T	72/91 (79%)	57 (79%)	12 (17%)	3 (4%)	3	28
23	U	70/81 (86%)	44 (63%)	21 (30%)	5 (7%)	1	14
24	V	63/67 (94%)	58 (92%)	4 (6%)	1 (2%)	11	50
25	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
26	Z	55/60 (92%)	42 (76%)	12 (22%)	1 (2%)	10	47
27	1	51/55 (93%)	31 (61%)	15 (29%)	5 (10%)	1	8
28	2	44/47 (94%)	37 (84%)	7 (16%)	0	100	100
29	3	57/66 (86%)	37 (65%)	18 (32%)	2 (4%)	4	33
30	4	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	3111/3558 (87%)	2556 (82%)	466 (15%)	89 (3%)	5	37

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	221	HIS
4	B	86	PRO
4	B	122	PHE
4	B	137	ARG
4	B	147	PRO
5	C	154	ASP
7	E	12	PRO
12	J	13	GLN
12	J	136	GLU
15	M	29	PRO
16	N	94	VAL
20	R	83	LEU
21	S	91	PRO
21	S	156	GLU
23	U	15	VAL
23	U	60	VAL
24	V	3	PRO

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Mol	Chain	Res	Type
27	1	9	ILE
27	1	44	ALA
29	3	60	LEU
3	A	30	PRO
3	A	89	ARG
5	C	15	ILE
5	C	121	ASP
6	D	21	GLY
14	L	53	ALA
15	M	17	GLU
17	O	8	GLY
18	P	132	GLY
19	Q	13	SER
19	Q	59	PRO
19	Q	61	LYS
19	Q	69	ILE
20	R	63	THR
21	S	26	LYS
21	S	88	TYR
22	T	16	SER
3	A	25	LEU
3	A	235	GLY
5	C	10	ASN
5	C	127	ASP
11	I	56	LEU
11	I	84	GLU
13	K	100	VAL
18	P	20	LEU
22	T	15	ASP
22	T	20	TYR
27	1	24	THR
27	1	34	LYS
27	1	46	LYS
3	A	152	LYS
4	B	29	GLY
4	B	202	ALA
5	C	22	VAL
5	C	128	ALA
7	E	165	VAL
7	E	173	ALA
8	F	120	VAL
9	G	67	ARG

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Mol	Chain	Res	Type
11	I	86	THR
11	I	88	PHE
15	M	28	ARG
16	N	8	ILE
17	O	66	GLY
19	Q	65	VAL
20	R	6	ALA
3	A	61	ARG
5	C	68	ARG
17	O	15	SER
20	R	26	SER
9	G	97	ASP
21	S	33	ALA
26	Z	7	PRO
29	3	13	ARG
6	D	146	VAL
9	G	163	PRO
20	R	98	ILE
3	A	48	GLY
7	E	7	GLN
9	G	52	GLY
11	I	19	VAL
11	I	68	VAL
20	R	108	VAL
23	U	14	VAL
23	U	18	VAL
5	C	172	VAL
11	I	114	ILE
23	U	41	VAL
4	B	14	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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
3	A	194/215 (90%)	180 (93%)	14 (7%)	17 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	155/157 (99%)	147 (95%)	8 (5%)	27	63
5	C	154/163 (94%)	146 (95%)	8 (5%)	27	63
6	D	152/156 (97%)	151 (99%)	1 (1%)	87	95
7	E	136/144 (94%)	135 (99%)	1 (1%)	87	95
8	F	46/107 (43%)	46 (100%)	0	100	100
9	G	118/146 (81%)	111 (94%)	7 (6%)	23	60
10	H	103/103 (100%)	100 (97%)	3 (3%)	48	79
11	I	100/121 (83%)	93 (93%)	7 (7%)	18	54
12	J	110/115 (96%)	106 (96%)	4 (4%)	40	74
13	K	90/93 (97%)	85 (94%)	5 (6%)	25	61
14	L	74/82 (90%)	70 (95%)	4 (5%)	26	62
15	M	94/134 (70%)	90 (96%)	4 (4%)	33	70
16	N	96/97 (99%)	94 (98%)	2 (2%)	59	84
17	O	75/79 (95%)	73 (97%)	2 (3%)	50	80
18	P	108/115 (94%)	107 (99%)	1 (1%)	82	93
19	Q	73/76 (96%)	69 (94%)	4 (6%)	25	62
20	R	91/96 (95%)	83 (91%)	8 (9%)	12	43
21	S	149/192 (78%)	146 (98%)	3 (2%)	60	84
22	T	55/67 (82%)	54 (98%)	1 (2%)	64	86
23	U	54/66 (82%)	51 (94%)	3 (6%)	25	61
24	V	53/55 (96%)	53 (100%)	0	100	100
25	W	48/48 (100%)	48 (100%)	0	100	100
26	Z	51/53 (96%)	50 (98%)	1 (2%)	60	84
27	1	46/48 (96%)	36 (78%)	10 (22%)	1	5
28	2	39/40 (98%)	34 (87%)	5 (13%)	5	25
29	3	46/52 (88%)	41 (89%)	5 (11%)	7	32
30	4	35/35 (100%)	35 (100%)	0	100	100
All	All	2545/2855 (89%)	2434 (96%)	111 (4%)	33	69

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	34	LEU

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Mol	Chain	Res	Type
3	A	44	ARG
3	A	49	ARG
3	A	55	ILE
3	A	69	LYS
3	A	126	PRO
3	A	150	PRO
3	A	156	LEU
3	A	165	GLN
3	A	199	ASN
3	A	209	LYS
3	A	219	LYS
3	A	245	ARG
3	A	246	VAL
4	B	27	LEU
4	B	86	PRO
4	B	87	ASP
4	B	143	GLN
4	B	146	THR
4	B	147	PRO
4	B	150	VAL
4	B	184	VAL
5	C	10	ASN
5	C	22	VAL
5	C	62	LYS
5	C	91	TYR
5	C	153	ASP
5	C	162	ARG
5	C	163	ASN
5	C	176	ASN
6	D	80	ARG
7	E	84	THR
9	G	32	TYR
9	G	37	ASP
9	G	38	GLU
9	G	111	LYS
9	G	112	THR
9	G	113	GLU
9	G	154	GLU
10	H	1	MET
10	H	21	CYS
10	H	23	ARG
11	I	17	LYS

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Mol	Chain	Res	Type
11	I	32	ARG
11	I	45	LYS
11	I	48	PHE
11	I	49	PHE
11	I	59	ARG
11	I	88	PHE
12	J	64	LYS
12	J	103	VAL
12	J	135	ARG
12	J	139	ASP
13	K	3	HIS
13	K	5	LYS
13	K	36	THR
13	K	54	THR
13	K	94	TYR
14	L	42	ILE
14	L	60	LYS
14	L	89	PHE
14	L	91	ARG
15	M	5	ILE
15	M	28	ARG
15	M	31	ASP
15	M	103	LYS
16	N	22	LYS
16	N	63	GLN
17	O	28	GLU
17	O	91	THR
18	P	32	ARG
19	Q	7	LEU
19	Q	12	ILE
19	Q	57	ASN
19	Q	88	ILE
20	R	18	LYS
20	R	25	LEU
20	R	71	GLN
20	R	79	SER
20	R	83	LEU
20	R	84	VAL
20	R	85	ASP
20	R	112	LYS
21	S	13	LYS
21	S	34	LEU

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Mol	Chain	Res	Type
21	S	71	MET
22	T	15	ASP
23	U	32	ARG
23	U	61	TRP
23	U	78	ILE
26	Z	9	LYS
27	1	8	ILE
27	1	9	ILE
27	1	20	PHE
27	1	21	TYR
27	1	28	ARG
27	1	30	ASN
27	1	37	LEU
27	1	47	HIS
27	1	51	ARG
27	1	54	LYS
28	2	5	TYR
28	2	9	ASN
28	2	10	ARG
28	2	12	ARG
28	2	15	THR
29	3	31	HIS
29	3	39	ASP
29	3	46	LYS
29	3	49	VAL
29	3	52	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	97	HIS
3	A	130	ASN
3	A	232	HIS
4	B	129	HIS
5	C	98	GLN
6	D	37	ASN
6	D	127	ASN
7	E	111	HIS
9	G	73	ASN
9	G	169	GLN
10	H	46	HIS
12	J	46	ASN

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Mol	Chain	Res	Type
16	N	37	GLN
18	P	81	HIS
18	P	82	ASN
20	R	11	ASN
21	S	118	HIS
21	S	121	GLN
23	U	47	HIS
24	V	54	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2630/2880 (91%)	470 (17%)	0
2	Y	119/123 (96%)	22 (18%)	0
All	All	2749/3003 (91%)	492 (17%)	0

All (492) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	14	A
1	X	34	U
1	X	35	G
1	X	39	C
1	X	45	C
1	X	49	U
1	X	59	G
1	X	63	A
1	X	68	C
1	X	70	A
1	X	74	G
1	X	76	C
1	X	83	A
1	X	87	G
1	X	88	G
1	X	89	A
1	X	90	G
1	X	98	U
1	X	100	G
1	X	101	A
1	X	118	U

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Mol	Chain	Res	Type
1	X	123	A
1	X	124	A
1	X	129	A
1	X	136	A
1	X	155	G
1	X	158	A
1	X	173	A
1	X	174	A
1	X	177	U
1	X	178	C
1	X	182	G
1	X	183	U
1	X	193	A
1	X	199	A
1	X	205	A
1	X	206	U
1	X	210	A
1	X	219	G
1	X	225	G
1	X	226	C
1	X	242	A
1	X	245	C
1	X	304	A
1	X	305	A
1	X	312	G
1	X	318	G
1	X	323	G
1	X	333	A
1	X	334	G
1	X	335	A
1	X	340	G
1	X	342	G
1	X	343	A
1	X	358	C
1	X	399	G
1	X	400	U
1	X	411	C
1	X	414	A
1	X	418	C
1	X	424	G
1	X	425	A
1	X	441	A

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Mol	Chain	Res	Type
1	X	456	C
1	X	463	C
1	X	467	U
1	X	469	G
1	X	491	A
1	X	492	G
1	X	497	C
1	X	515	A
1	X	518	A
1	X	519	C
1	X	526	C
1	X	537	C
1	X	538	A
1	X	539	A
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	556	A
1	X	557	U
1	X	558	G
1	X	559	C
1	X	572	G
1	X	581	A
1	X	583	C
1	X	584	A
1	X	602	C
1	X	613	A
1	X	614	G
1	X	624	A
1	X	625	A
1	X	626	A
1	X	627	A
1	X	631	G
1	X	632	A
1	X	633	G
1	X	636	G
1	X	648	A
1	X	649	G
1	X	652	C
1	X	654	A
1	X	655	A

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Mol	Chain	Res	Type
1	X	657	A
1	X	665	A
1	X	666	U
1	X	668	A
1	X	682	G
1	X	683	A
1	X	684	C
1	X	699	G
1	X	743	A
1	X	749	C
1	X	752	G
1	X	759	C
1	X	766	A
1	X	774	A
1	X	777	A
1	X	778	G
1	X	781	G
1	X	788	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	796	A
1	X	797	A
1	X	798	G
1	X	802	A
1	X	803	C
1	X	805	G
1	X	806	A
1	X	807	A
1	X	816	U
1	X	818	G
1	X	819	C
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	844	G
1	X	859	U
1	X	860	U
1	X	862	A
1	X	879	A
1	X	919	U

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Mol	Chain	Res	Type
1	X	921	A
1	X	922	A
1	X	926	C
1	X	939	C
1	X	940	G
1	X	944	A
1	X	952	A
1	X	955	G
1	X	956	A
1	X	957	G
1	X	969	U
1	X	970	A
1	X	972	C
1	X	984	A
1	X	985	G
1	X	994	A
1	X	995	A
1	X	996	C
1	X	1006	C
1	X	1007	A
1	X	1016	C
1	X	1019	U
1	X	1023	U
1	X	1032	A
1	X	1033	G
1	X	1037	U
1	X	1044	U
1	X	1051	U
1	X	1054	C
1	X	1060	C
1	X	1070	G
1	X	1078	A
1	X	1079	G
1	X	1082	G
1	X	1087	C
1	X	1090	C
1	X	1097	A
1	X	1098	G
1	X	1099	A
1	X	1108	U
1	X	1115	C
1	X	1119	U

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Mol	Chain	Res	Type
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1141	U
1	X	1142	G
1	X	1143	A
1	X	1145	C
1	X	1146	G
1	X	1152	C
1	X	1153	A
1	X	1167	A
1	X	1168	G
1	X	1183	C
1	X	1195	U
1	X	1220	G
1	X	1223	G
1	X	1224	A
1	X	1250	A
1	X	1262	U
1	X	1265	G
1	X	1266	G
1	X	1268	U
1	X	1269	G
1	X	1279	G
1	X	1284	G
1	X	1285	A
1	X	1288	A
1	X	1289	A
1	X	1299	A
1	X	1300	A
1	X	1313	U
1	X	1314	A
1	X	1325	U
1	X	1326	U
1	X	1331	G
1	X	1333	G
1	X	1334	A
1	X	1342	U
1	X	1359	G
1	X	1378	A
1	X	1381	G
1	X	1391	A

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Mol	Chain	Res	Type
1	X	1392	U
1	X	1393	G
1	X	1398	G
1	X	1413	U
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1434	U
1	X	1440	G
1	X	1442	C
1	X	1443	G
1	X	1460	G
1	X	1465	G
1	X	1467	U
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1473	U
1	X	1475	U
1	X	1476	G
1	X	1482	U
1	X	1490	U
1	X	1497	C
1	X	1506	C
1	X	1528	C
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1563	U
1	X	1570	C
1	X	1571	G
1	X	1574	A
1	X	1575	C
1	X	1582	A
1	X	1585	A
1	X	1601	U
1	X	1602	G
1	X	1608	U
1	X	1624	A
1	X	1625	A

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Mol	Chain	Res	Type
1	X	1626	A
1	X	1632	A
1	X	1635	G
1	X	1648	C
1	X	1657	A
1	X	1665	C
1	X	1668	G
1	X	1669	A
1	X	1681	A
1	X	1685	A
1	X	1689	U
1	X	1691	G
1	X	1692	C
1	X	1710	U
1	X	1712	G
1	X	1714	A
1	X	1716	G
1	X	1717	A
1	X	1735	G
1	X	1746	A
1	X	1747	G
1	X	1749	G
1	X	1750	A
1	X	1754	G
1	X	1755	G
1	X	1764	A
1	X	1765	C
1	X	1772	C
1	X	1775	A
1	X	1782	A
1	X	1790	G
1	X	1791	C
1	X	1793	A
1	X	1801	C
1	X	1802	A
1	X	1808	C
1	X	1812	U
1	X	1825	C
1	X	1831	G
1	X	1842	G
1	X	1868	A
1	X	1884	A

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Mol	Chain	Res	Type
1	X	1910	A
1	X	1920	A
1	X	1922	U
1	X	1923	U
1	X	1924	C
1	X	1927	U
1	X	1928	G
1	X	1939	U
1	X	1946	U
1	X	1949	A
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1964	A
1	X	1965	U
1	X	1975	G
1	X	1976	U
1	X	1979	C
1	X	1980	A
1	X	2005	U
1	X	2006	G
1	X	2014	A
1	X	2015	G
1	X	2016	A
1	X	2017	U
1	X	2019	C
1	X	2026	C
1	X	2038	C
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2047	C
1	X	2052	G
1	X	2057	U
1	X	2075	U
1	X	2083	G
1	X	2171	U
1	X	2181	A
1	X	2190	A
1	X	2191	A

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Mol	Chain	Res	Type
1	X	2192	U
1	X	2195	C
1	X	2196	U
1	X	2199	C
1	X	2200	G
1	X	2205	C
1	X	2218	G
1	X	2230	G
1	X	2238	G
1	X	2242	C
1	X	2246	A
1	X	2247	A
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2272	A
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2298	U
1	X	2300	G
1	X	2301	A
1	X	2313	G
1	X	2316	G
1	X	2324	G
1	X	2326	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2386	G
1	X	2396	C
1	X	2402	U
1	X	2404	A
1	X	2405	A
1	X	2407	G
1	X	2408	G
1	X	2410	U
1	X	2420	C
1	X	2427	A
1	X	2428	U

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Mol	Chain	Res	Type
1	X	2452	U
1	X	2455	A
1	X	2458	U
1	X	2481	G
1	X	2482	A
1	X	2483	U
1	X	2484	G
1	X	2485	U
1	X	2486	C
1	X	2497	A
1	X	2498	U
1	X	2499	C
1	X	2545	A
1	X	2546	G
1	X	2552	C
1	X	2564	U
1	X	2565	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2591	C
1	X	2592	U
1	X	2602	G
1	X	2608	A
1	X	2609	G
1	X	2625	U
1	X	2634	G
1	X	2661	G
1	X	2668	U
1	X	2691	C
1	X	2692	A
1	X	2693	U
1	X	2700	U
1	X	2706	U
1	X	2707	G
1	X	2708	U
1	X	2709	C
1	X	2712	G
1	X	2713	A
1	X	2728	A
1	X	2730	A
1	X	2731	G

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Mol	Chain	Res	Type
1	X	2732	C
1	X	2737	A
1	X	2744	A
1	X	2745	A
1	X	2757	G
1	X	2758	A
1	X	2759	U
1	X	2760	G
1	X	2761	A
1	X	2770	A
1	X	2771	C
1	X	2782	G
1	X	2795	A
1	X	2796	A
1	X	2807	U
1	X	2808	U
1	X	2809	A
1	X	2825	A
1	X	2840	U
1	X	2841	U
1	X	2842	C
1	X	2843	A
1	X	2847	G
1	X	2850	U
1	X	2855	C
1	X	2858	A
1	X	2859	U
1	X	2868	G
2	Y	4	C
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	26	G
2	Y	37	C
2	Y	43	G
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	59	A
2	Y	69	G
2	Y	71	G

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Mol	Chain	Res	Type
2	Y	84	G
2	Y	85	G
2	Y	93	G
2	Y	102	A
2	Y	110	U
2	Y	111	C
2	Y	112	A
2	Y	115	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 84 ligands modelled in this entry, 82 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
31	LC2	X	2881	-	30,34,34	1.80	7 (23%)	25,49,49	1.01	0
32	LMA	X	2882	-	58,60,60	4.73	26 (44%)	72,90,90	1.28	5 (6%)

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
31	LC2	X	2881	-	-	0/31/61/61	0/0/2/2
32	LMA	X	2882	-	-	0/80/115/115	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2882	LMA	C30-C2	-18.98	1.10	1.53
32	X	2882	LMA	C2-C1	-16.27	1.13	1.51
32	X	2882	LMA	O53-C8	-10.12	1.25	1.43
32	X	2882	LMA	C35-C12	-7.78	1.36	1.53
32	X	2882	LMA	C33-C8	-7.68	1.41	1.52
32	X	2882	LMA	C7-C6	-7.05	1.43	1.54
32	X	2882	LMA	C32-C6	-5.84	1.38	1.53
32	X	2882	LMA	C19-C16	-5.79	1.38	1.52
31	X	2881	LC2	C31-C2	-5.48	1.39	1.50
32	X	2882	LMA	C16-C17	-5.21	1.41	1.53
32	X	2882	LMA	O5-C16	-5.07	1.33	1.44
32	X	2882	LMA	C40-C23	-4.55	1.43	1.53
32	X	2882	LMA	O51-C17	-4.10	1.37	1.45
32	X	2882	LMA	C12-C13	-3.46	1.44	1.54
31	X	2881	LC2	C4-C3	-2.98	1.39	1.45
31	X	2881	LC2	C28-C27	-2.94	1.39	1.45
31	X	2881	LC2	O1-C8	-2.01	1.43	1.46
32	X	2882	LMA	C4-C5	2.01	1.59	1.54
32	X	2882	LMA	O12-C54	2.04	1.39	1.35
31	X	2881	LC2	C23-C26	2.04	1.53	1.49
32	X	2882	LMA	C15-C16	2.09	1.57	1.52
32	X	2882	LMA	O7-C5	2.18	1.49	1.43
32	X	2882	LMA	O4-C18	2.22	1.49	1.44
31	X	2881	LC2	C28-C29	2.85	1.39	1.32
31	X	2881	LC2	C4-C5	2.86	1.39	1.32
32	X	2882	LMA	O3-C3	2.96	1.51	1.43
32	X	2882	LMA	O17-C24	3.05	1.51	1.43
32	X	2882	LMA	C2-C3	3.60	1.63	1.55
32	X	2882	LMA	O2-C1	3.78	1.43	1.34
32	X	2882	LMA	O52-C51	4.41	1.37	1.20
32	X	2882	LMA	C6-C5	4.43	1.61	1.53
32	X	2882	LMA	O55-C54	4.78	1.38	1.20
32	X	2882	LMA	O2-C13	8.36	1.57	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2882	LMA	C3-C2-C1	-2.77	104.39	110.07
32	X	2882	LMA	C25-C24-C23	-2.45	106.52	113.33
32	X	2882	LMA	O7-C5-C4	3.96	112.91	108.16
32	X	2882	LMA	O51-C51-C53	4.43	119.42	111.10
32	X	2882	LMA	O12-C54-C56	4.48	119.51	111.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	X	2881	LC2	18	0
32	X	2882	LMA	43	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95th 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	X	2644/2880 (91%)	0.10	83 (3%) 49 43	44, 115, 240, 575	0
2	Y	120/123 (97%)	-0.12	3 (2%) 58 51	108, 183, 252, 342	0
3	A	253/274 (92%)	1.02	53 (20%) 1 1	66, 158, 225, 423	0
4	B	205/211 (97%)	0.25	8 (3%) 40 35	35, 85, 159, 249	0
5	C	194/205 (94%)	0.03	10 (5%) 28 25	61, 142, 250, 381	0
6	D	177/180 (98%)	1.98	77 (43%) 0 0	174, 255, 358, 427	0
7	E	171/185 (92%)	0.32	14 (8%) 12 13	87, 183, 269, 354	0
8	F	63/144 (43%)	5.02	60 (95%) 0 0	208, 334, 476, 516	0
9	G	142/174 (81%)	0.65	21 (14%) 3 4	73, 126, 257, 421	0
10	H	134/134 (100%)	-0.20	1 (0%) 87 83	39, 71, 135, 248	0
11	I	134/156 (85%)	0.89	31 (23%) 1 1	75, 168, 261, 375	0
12	J	136/141 (96%)	0.93	26 (19%) 1 2	76, 135, 223, 388	0
13	K	113/116 (97%)	0.01	1 (0%) 84 78	32, 61, 101, 128	0
14	L	104/114 (91%)	0.35	13 (12%) 4 6	134, 193, 300, 325	0
15	M	108/166 (65%)	-0.06	2 (1%) 67 61	32, 73, 138, 298	0
16	N	117/118 (99%)	0.47	12 (10%) 7 9	57, 116, 177, 328	0
17	O	94/100 (94%)	0.71	16 (17%) 2 2	82, 145, 271, 322	0
18	P	126/134 (94%)	-0.19	0 100 100	33, 84, 149, 226	0
19	Q	93/95 (97%)	1.34	25 (26%) 1 1	86, 134, 245, 329	0
20	R	110/115 (95%)	2.29	53 (48%) 0 0	93, 166, 332, 423	0
21	S	175/237 (73%)	0.79	32 (18%) 1 2	130, 202, 285, 326	0
22	T	74/91 (81%)	1.54	23 (31%) 0 1	112, 141, 201, 284	0
23	U	72/81 (88%)	1.54	19 (26%) 1 1	119, 188, 304, 349	0
24	V	65/67 (97%)	0.40	6 (9%) 10 11	116, 175, 235, 292	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	0.93	12 (21%) 1 1	97, 126, 181, 194	0
26	Z	57/60 (95%)	-0.23	1 (1%) 69 62	44, 79, 182, 234	0
27	1	53/55 (96%)	2.99	34 (64%) 0 0	126, 192, 295, 403	0
28	2	46/47 (97%)	0.67	5 (10%) 6 8	72, 123, 258, 308	0
29	3	59/66 (89%)	4.21	52 (88%) 0 0	139, 213, 356, 435	0
30	4	37/37 (100%)	7.32	33 (89%) 0 0	152, 219, 307, 382	0
All	All	5931/6561 (90%)	0.55	726 (12%) 5 6	32, 131, 276, 575	0

All (726) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	28	GLY	23.5
8	F	113	PRO	15.2
30	4	28	SER	14.4
30	4	24	LEU	13.9
30	4	1	MET	13.8
30	4	15	LYS	12.8
30	4	34	GLN	12.3
30	4	25	VAL	11.7
8	F	110	THR	11.6
30	4	17	VAL	11.6
8	F	94	ALA	11.5
30	4	16	VAL	11.0
30	4	29	ASN	10.4
8	F	111	LYS	10.3
8	F	99	LEU	10.1
30	4	7	VAL	9.7
20	R	100	ASP	9.5
30	4	21	GLY	9.4
8	F	92	ASN	9.2
20	R	102	LYS	9.1
29	3	10	ALA	9.0
8	F	114	ASP	8.9
21	S	92	VAL	8.8
6	D	82	GLY	8.8
29	3	37	SER	8.7
27	1	27	ASN	8.4
30	4	36	GLN	8.4
29	3	33	ASN	8.4
27	1	23	THR	8.3

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Mol	Chain	Res	Type	RSRZ
8	F	90	THR	8.2
29	3	7	HIS	8.1
8	F	136	VAL	8.0
8	F	95	LYS	8.0
12	J	141	ALA	8.0
24	V	66	GLN	8.0
3	A	251	TRP	8.0
30	4	26	ILE	7.9
8	F	78	ILE	7.9
29	3	63	PRO	7.9
3	A	255	THR	7.9
30	4	2	LYS	7.9
8	F	127	VAL	7.8
8	F	125	ASN	7.7
30	4	12	ASP	7.6
8	F	77	LEU	7.5
27	1	6	PRO	7.4
29	3	38	GLY	7.4
30	4	13	ASN	7.4
29	3	20	GLY	7.4
29	3	16	ILE	7.3
3	A	250	PRO	7.3
27	1	47	HIS	7.3
30	4	3	VAL	7.1
29	3	9	MET	6.9
29	3	60	LEU	6.9
1	X	2190	A	6.7
30	4	33	LYS	6.7
12	J	133	VAL	6.6
8	F	112	MET	6.6
20	R	83	LEU	6.6
30	4	37	GLY	6.5
30	4	10	MET	6.5
3	A	220	PRO	6.5
22	T	73	GLY	6.5
12	J	21	ASP	6.5
30	4	11	CYS	6.4
30	4	35	ARG	6.4
6	D	67	ILE	6.4
3	A	152	LYS	6.4
6	D	11	GLN	6.3
6	D	34	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
30	4	20	HIS	6.3
23	U	27	ASP	6.2
8	F	89	SER	6.2
8	F	84	ILE	6.2
20	R	82	ALA	6.2
27	1	13	GLU	6.1
6	D	85	VAL	6.1
1	X	1089	C	6.1
27	1	35	LEU	6.1
27	1	24	THR	6.0
30	4	22	ARG	6.0
30	4	9	LYS	6.0
11	I	61	PRO	5.9
1	X	1086	C	5.9
20	R	77	HIS	5.8
29	3	40	GLU	5.8
29	3	28	GLY	5.8
30	4	14	CYS	5.7
17	O	41	GLY	5.7
6	D	93	GLY	5.7
27	1	40	TYR	5.7
1	X	1114	A	5.7
8	F	76	TYR	5.7
30	4	18	ARG	5.7
29	3	14	ILE	5.7
6	D	83	MET	5.7
7	E	46	ASP	5.7
20	R	112	LYS	5.6
30	4	27	CYS	5.6
29	3	27	SER	5.6
27	1	31	THR	5.6
3	A	57	GLY	5.5
8	F	109	LYS	5.5
7	E	37	TYR	5.5
6	D	74	ILE	5.4
6	D	103	LEU	5.4
8	F	107	ILE	5.4
21	S	69	VAL	5.4
20	R	31	GLY	5.4
21	S	74	ARG	5.3
21	S	94	VAL	5.3
8	F	93	LYS	5.3

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Mol	Chain	Res	Type	RSRZ
21	S	68	ALA	5.2
8	F	104	VAL	5.2
8	F	105	LEU	5.2
6	D	86	GLY	5.2
27	1	14	SER	5.2
23	U	47	HIS	5.1
19	Q	27	PHE	5.1
6	D	81	GLN	5.1
29	3	29	LYS	5.1
2	Y	43	G	5.1
20	R	46	VAL	5.0
8	F	98	LYS	5.0
20	R	81	VAL	5.0
20	R	4	PRO	5.0
22	T	71	ASN	5.0
22	T	72	LYS	5.0
27	1	32	GLN	5.0
29	3	17	THR	5.0
3	A	242	GLY	5.0
23	U	29	GLY	5.0
8	F	128	ALA	4.9
3	A	243	ALA	4.9
29	3	55	TRP	4.9
6	D	91	LEU	4.9
6	D	169	LEU	4.9
9	G	97	ASP	4.9
29	3	8	LYS	4.9
28	2	40	HIS	4.9
11	I	60	LEU	4.9
8	F	102	ASP	4.9
1	X	1115	C	4.8
6	D	140	GLU	4.8
1	X	1734	C	4.8
6	D	105	ASN	4.8
9	G	68	PRO	4.8
3	A	204	ASN	4.8
14	L	52	ALA	4.8
1	X	871	U	4.8
16	N	105	ALA	4.7
8	F	91	PRO	4.7
3	A	73	LYS	4.7
1	X	665	A	4.7

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Mol	Chain	Res	Type	RSRZ
20	R	52	ASN	4.7
23	U	62	LEU	4.7
6	D	127	ASN	4.7
8	F	130	THR	4.7
29	3	54	GLU	4.7
20	R	74	LEU	4.7
1	X	1063	C	4.7
6	D	138	PHE	4.7
20	R	75	ALA	4.7
29	3	45	GLY	4.6
19	Q	48	VAL	4.6
6	D	89	VAL	4.6
17	O	74	TYR	4.6
29	3	21	LYS	4.6
25	W	14	GLY	4.6
29	3	12	ARG	4.6
1	X	1098	G	4.6
24	V	33	ALA	4.5
9	G	34	PRO	4.5
17	O	64	GLY	4.5
22	T	47	ALA	4.5
29	3	61	MET	4.5
20	R	12	ASP	4.5
27	1	51	ARG	4.5
29	3	41	ILE	4.5
29	3	31	HIS	4.5
30	4	32	HIS	4.5
11	I	54	SER	4.5
6	D	36	VAL	4.4
29	3	46	LYS	4.4
14	L	12	ARG	4.4
1	X	1095	A	4.4
29	3	23	MET	4.4
6	D	3	GLN	4.4
19	Q	64	ARG	4.4
30	4	19	ARG	4.4
3	A	256	LYS	4.4
12	J	60	ARG	4.4
6	D	156	ILE	4.4
20	R	99	VAL	4.4
27	1	12	MET	4.4
9	G	156	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	X	1085	G	4.3
30	4	23	VAL	4.3
6	D	88	LYS	4.3
29	3	30	ARG	4.3
1	X	1087	C	4.3
27	1	25	THR	4.3
8	F	87	GLY	4.3
8	F	106	GLU	4.3
19	Q	62	ARG	4.3
12	J	20	GLY	4.2
14	L	14	ARG	4.2
6	D	69	LYS	4.2
19	Q	49	ARG	4.2
7	E	168	GLN	4.2
8	F	80	LYS	4.2
29	3	13	ARG	4.2
3	A	260	THR	4.1
1	X	424	G	4.1
9	G	107	GLN	4.1
20	R	9	HIS	4.1
8	F	133	SER	4.1
22	T	15	ASP	4.1
20	R	57	ASN	4.1
19	Q	50	VAL	4.0
8	F	123	ALA	4.0
19	Q	39	LYS	4.0
20	R	6	ALA	4.0
3	A	192	ALA	4.0
27	1	2	ALA	4.0
6	D	141	ILE	4.0
23	U	75	TYR	4.0
3	A	254	PRO	4.0
1	X	1088	A	4.0
8	F	81	ALA	4.0
6	D	99	PHE	4.0
29	3	53	ALA	4.0
6	D	35	VAL	3.9
6	D	126	GLY	3.9
9	G	109	GLY	3.9
28	2	38	GLY	3.9
6	D	145	MET	3.9
6	D	94	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
7	E	41	LEU	3.9
17	O	39	PHE	3.9
20	R	76	LEU	3.9
29	3	6	THR	3.9
29	3	22	VAL	3.9
27	1	50	PHE	3.9
8	F	120	VAL	3.9
20	R	35	LYS	3.9
29	3	11	LYS	3.9
8	F	129	GLY	3.9
8	F	132	ARG	3.9
12	J	114	GLN	3.9
27	1	26	LYS	3.9
3	A	114	VAL	3.8
1	X	248	A	3.8
3	A	56	GLY	3.8
29	3	48	PHE	3.8
20	R	43	ASP	3.8
20	R	25	LEU	3.8
22	T	59	LEU	3.8
8	F	88	SER	3.8
6	D	154	ILE	3.8
22	T	43	THR	3.8
29	3	44	LYS	3.7
22	T	20	TYR	3.7
22	T	55	ARG	3.7
12	J	103	VAL	3.7
25	W	13	PRO	3.7
27	1	45	LYS	3.7
21	S	15	ASP	3.7
20	R	41	PRO	3.7
21	S	34	LEU	3.7
22	T	22	GLY	3.6
1	X	1074	G	3.6
16	N	87	ASN	3.6
29	3	36	LYS	3.6
5	C	45	THR	3.6
8	F	126	THR	3.6
23	U	13	LEU	3.6
27	1	15	SER	3.6
21	S	70	GLN	3.6
8	F	134	MET	3.6

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Mol	Chain	Res	Type	RSRZ
3	A	271	ILE	3.6
20	R	38	LEU	3.6
20	R	87	GLU	3.6
1	X	2326	C	3.6
11	I	74	VAL	3.6
8	F	131	ALA	3.6
6	D	31	ILE	3.5
12	J	22	ALA	3.5
23	U	46	LEU	3.5
1	X	1069	G	3.5
20	R	58	VAL	3.5
21	S	91	PRO	3.5
1	X	1552	C	3.5
19	Q	3	HIS	3.5
8	F	101	TRP	3.5
19	Q	65	VAL	3.5
3	A	221	HIS	3.5
21	S	123	VAL	3.5
8	F	79	ARG	3.5
21	S	71	MET	3.5
1	X	1733	U	3.5
8	F	74	MET	3.5
14	L	11	LEU	3.5
6	D	108	LEU	3.5
1	X	90	G	3.5
2	Y	14	C	3.5
20	R	13	LYS	3.5
29	3	26	LYS	3.5
6	D	20	PHE	3.5
1	X	1101	U	3.5
6	D	66	ILE	3.5
8	F	108	ALA	3.5
20	R	101	GLY	3.5
27	1	11	LYS	3.5
3	A	246	VAL	3.4
21	S	79	ILE	3.4
1	X	1068	A	3.4
6	D	175	LEU	3.4
27	1	5	GLY	3.4
17	O	47	PHE	3.4
22	T	38	VAL	3.4
1	X	1091	C	3.4

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Mol	Chain	Res	Type	RSRZ
12	J	68	ARG	3.4
19	Q	47	GLY	3.4
8	F	86	LYS	3.4
1	X	558	G	3.4
3	A	81	ALA	3.4
27	1	38	LYS	3.4
22	T	45	PHE	3.4
11	I	63	ARG	3.3
6	D	146	VAL	3.3
11	I	62	LYS	3.3
1	X	1099	A	3.3
20	R	94	VAL	3.3
20	R	60	PRO	3.3
27	1	52	GLU	3.3
21	S	114	ASP	3.3
30	4	30	VAL	3.3
11	I	100	ARG	3.3
12	J	140	GLU	3.3
1	X	1077	U	3.3
20	R	29	HIS	3.3
23	U	12	ASN	3.3
20	R	33	THR	3.3
6	D	60	ILE	3.3
7	E	167	GLU	3.3
27	1	8	ILE	3.2
1	X	100	G	3.2
4	B	205	SER	3.2
21	S	14	LEU	3.2
6	D	53	ALA	3.2
8	F	96	VAL	3.2
29	3	42	ARG	3.2
6	D	147	ASP	3.2
28	2	41	GLN	3.2
6	D	84	PRO	3.2
27	1	22	TYR	3.2
8	F	82	ALA	3.2
9	G	100	TYR	3.2
17	O	23	GLU	3.2
21	S	76	ARG	3.2
22	T	41	ARG	3.2
22	T	46	LYS	3.1
24	V	37	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	X	1064	C	3.1
1	X	1120	C	3.1
6	D	173	MET	3.1
21	S	23	ALA	3.1
3	A	103	LYS	3.1
22	T	53	MET	3.1
12	J	32	ASP	3.1
7	E	47	GLY	3.1
21	S	109	GLN	3.1
20	R	14	LEU	3.1
20	R	103	LYS	3.1
3	A	244	GLY	3.1
17	O	11	GLN	3.1
1	X	1090	C	3.1
17	O	36	LYS	3.0
21	S	19	ILE	3.0
29	3	32	GLN	3.0
29	3	39	ASP	3.0
21	S	93	GLU	3.0
1	X	2313	G	3.0
20	R	30	LYS	3.0
20	R	21	THR	3.0
6	D	170	LEU	3.0
3	A	153	GLY	3.0
27	1	48	VAL	3.0
21	S	1	MET	3.0
25	W	53	VAL	3.0
23	U	45	ASN	3.0
25	W	9	VAL	2.9
6	D	6	THR	2.9
1	X	1062	G	2.9
6	D	90	THR	2.9
30	4	8	LYS	2.9
6	D	165	GLU	2.9
14	L	34	SER	2.9
3	A	76	VAL	2.9
12	J	37	ALA	2.9
1	X	304	A	2.9
4	B	34	VAL	2.9
3	A	45	ASN	2.9
24	V	32	ALA	2.9
3	A	72	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
29	3	49	VAL	2.9
21	S	40	ASP	2.9
9	G	159	SER	2.9
1	X	341	A	2.9
3	A	247	PRO	2.9
25	W	17	VAL	2.9
20	R	16	PHE	2.9
17	O	80	TYR	2.9
6	D	150	ARG	2.9
8	F	119	SER	2.9
29	3	15	LYS	2.9
19	Q	43	GLN	2.9
20	R	17	LYS	2.9
8	F	83	GLY	2.9
1	X	398	C	2.8
6	D	71	LYS	2.8
8	F	121	GLU	2.8
8	F	97	GLY	2.8
6	D	157	VAL	2.8
1	X	2188	A	2.8
25	W	7	ARG	2.8
11	I	103	ASN	2.8
9	G	67	ARG	2.8
9	G	99	VAL	2.8
19	Q	56	MET	2.8
3	A	102	GLU	2.8
1	X	1070	G	2.8
20	R	42	ARG	2.8
6	D	62	LEU	2.8
6	D	73	SER	2.8
8	F	103	GLN	2.8
11	I	66	ASN	2.8
1	X	2664	G	2.8
11	I	44	GLY	2.8
12	J	132	MET	2.8
23	U	25	ARG	2.8
1	X	1397	A	2.8
4	B	72	VAL	2.8
20	R	23	ILE	2.8
8	F	75	SER	2.8
12	J	23	LYS	2.8
14	L	93	SER	2.8

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Mol	Chain	Res	Type	RSRZ
20	R	71	GLN	2.8
11	I	53	ARG	2.8
6	D	92	ARG	2.7
21	S	119	ASN	2.7
29	3	51	ALA	2.7
6	D	142	THR	2.7
20	R	98	ILE	2.7
24	V	65	GLU	2.7
5	C	166	TRP	2.7
1	X	514	G	2.7
1	X	1102	G	2.7
6	D	75	SER	2.7
17	O	42	GLY	2.7
12	J	36	ILE	2.7
16	N	88	ILE	2.7
1	X	2298	U	2.7
6	D	56	GLU	2.7
1	X	2276	C	2.7
11	I	79	GLN	2.7
29	3	43	GLY	2.7
11	I	57	ILE	2.7
3	A	151	GLY	2.7
8	F	118	GLY	2.7
1	X	519	C	2.7
29	3	50	LEU	2.7
19	Q	10	PRO	2.7
23	U	16	ASN	2.7
20	R	59	LYS	2.7
23	U	34	THR	2.7
6	D	132	ILE	2.7
11	I	76	LYS	2.6
20	R	18	LYS	2.6
16	N	92	ARG	2.6
1	X	1092	U	2.6
12	J	119	PHE	2.6
19	Q	78	ALA	2.6
3	A	272	VAL	2.6
11	I	36	GLY	2.6
12	J	84	MET	2.6
4	B	78	LEU	2.6
19	Q	66	GLY	2.6
27	1	4	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
6	D	97	TYR	2.6
21	S	124	ALA	2.6
6	D	125	ARG	2.6
3	A	86	ASP	2.6
16	N	65	ILE	2.6
20	R	48	VAL	2.6
22	T	67	VAL	2.6
19	Q	63	LYS	2.6
11	I	21	ARG	2.6
19	Q	46	PHE	2.6
7	E	17	VAL	2.6
23	U	79	GLU	2.6
1	X	2312	A	2.6
20	R	19	GLY	2.6
3	A	261	ARG	2.6
5	C	48	ARG	2.6
12	J	113	GLU	2.6
6	D	72	LYS	2.6
20	R	72	ARG	2.6
27	1	36	GLU	2.6
7	E	15	VAL	2.6
17	O	46	VAL	2.6
9	G	53	ARG	2.6
14	L	13	THR	2.6
16	N	79	PHE	2.6
9	G	110	LEU	2.6
12	J	105	PHE	2.5
11	I	67	ASN	2.5
6	D	158	THR	2.5
29	3	52	LYS	2.5
1	X	2325	A	2.5
21	S	120	LEU	2.5
4	B	159	HIS	2.5
19	Q	86	GLN	2.5
1	X	1093	U	2.5
25	W	3	ILE	2.5
29	3	62	LEU	2.5
4	B	1	MET	2.5
8	F	122	ALA	2.5
22	T	26	PHE	2.5
12	J	100	PRO	2.5
19	Q	94	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
11	I	64	GLY	2.5
27	1	30	ASN	2.5
1	X	1224	A	2.5
5	C	112	GLN	2.5
3	A	189	GLU	2.5
25	W	50	LEU	2.5
14	L	10	LYS	2.5
19	Q	87	SER	2.5
16	N	96	ALA	2.5
5	C	180	ILE	2.5
6	D	87	ILE	2.5
11	I	33	GLY	2.5
29	3	19	THR	2.5
1	X	1841	G	2.5
22	T	57	HIS	2.5
1	X	1065	A	2.4
9	G	108	GLY	2.4
17	O	9	GLY	2.4
14	L	68	ALA	2.4
4	B	71	GLY	2.4
6	D	4	LEU	2.4
11	I	49	PHE	2.4
27	1	28	ARG	2.4
3	A	39	PRO	2.4
19	Q	53	ILE	2.4
12	J	38	MET	2.4
1	X	2263	C	2.4
23	U	35	THR	2.4
1	X	1840	A	2.4
1	X	2381	A	2.4
9	G	98	LYS	2.4
3	A	96	LEU	2.4
3	A	112	LEU	2.4
6	D	30	ARG	2.4
11	I	72	TYR	2.4
16	N	63	GLN	2.4
6	D	96	MET	2.4
6	D	130	LEU	2.4
9	G	69	ASP	2.4
8	F	85	GLY	2.4
21	S	72	ASP	2.4
27	1	7	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
6	D	33	LYS	2.4
6	D	172	SER	2.4
1	X	1884	A	2.4
8	F	100	ASN	2.4
1	X	1100	G	2.4
11	I	65	PHE	2.4
4	B	135	HIS	2.4
6	D	100	LEU	2.4
1	X	209	G	2.4
29	3	25	PHE	2.4
14	L	40	ALA	2.4
5	C	55	GLY	2.3
11	I	104	ARG	2.3
14	L	62	GLY	2.3
16	N	64	ARG	2.3
10	H	27	SER	2.3
5	C	47	THR	2.3
21	S	169	VAL	2.3
27	1	49	VAL	2.3
6	D	38	GLU	2.3
1	X	1548	U	2.3
22	T	77	ARG	2.3
19	Q	51	ILE	2.3
21	S	173	PRO	2.3
8	F	135	GLY	2.3
11	I	51	GLY	2.3
11	I	122	VAL	2.3
12	J	63	GLY	2.3
29	3	34	THR	2.3
1	X	559	C	2.3
1	X	1111	C	2.3
5	C	19	LEU	2.3
23	U	26	ALA	2.3
22	T	42	GLY	2.3
2	Y	18	G	2.3
21	S	20	ALA	2.3
11	I	105	PRO	2.3
1	X	1073	G	2.3
1	X	2189	A	2.3
5	C	105	ALA	2.3
28	2	34	ARG	2.3
17	O	75	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	1094	C	2.3
7	E	83	TYR	2.3
25	W	22	ALA	2.3
9	G	129	HIS	2.3
3	A	191	TYR	2.3
12	J	107	VAL	2.3
23	U	30	VAL	2.3
1	X	1409	U	2.3
1	X	2299	A	2.3
20	R	8	SER	2.3
6	D	129	ASN	2.2
1	X	1421	U	2.2
1	X	1801	C	2.2
23	U	10	LYS	2.2
27	1	9	ILE	2.2
3	A	63	TYR	2.2
9	G	105	GLY	2.2
15	M	107	LEU	2.2
6	D	25	VAL	2.2
11	I	47	ALA	2.2
14	L	96	TYR	2.2
3	A	264	ARG	2.2
17	O	63	HIS	2.2
1	X	2265	A	2.2
7	E	55	PRO	2.2
6	D	70	ALA	2.2
11	I	91	ASP	2.2
3	A	98	TYR	2.2
3	A	263	LYS	2.2
7	E	42	THR	2.2
17	O	73	LYS	2.2
20	R	32	GLN	2.2
1	X	2085	G	2.2
29	3	58	MET	2.2
9	G	44	VAL	2.2
19	Q	37	GLU	2.2
22	T	19	LYS	2.2
8	F	115	LEU	2.2
1	X	2311	U	2.2
11	I	16	ARG	2.2
12	J	18	MET	2.2
11	I	46	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	273	THR	2.2
6	D	22	TYR	2.2
11	I	81	GLN	2.2
15	M	40	ARG	2.2
12	J	104	MET	2.2
1	X	2663	U	2.2
1	X	247	A	2.2
3	A	199	ASN	2.2
3	A	241	THR	2.2
3	A	85	TYR	2.2
16	N	47	TYR	2.2
7	E	13	SER	2.2
6	D	109	PRO	2.2
25	W	33	GLU	2.2
24	V	34	ALA	2.1
22	T	14	ARG	2.1
1	X	2363	G	2.1
25	W	54	GLN	2.1
5	C	167	VAL	2.1
29	3	64	ARG	2.1
12	J	72	ASP	2.1
19	Q	34	THR	2.1
1	X	1118	G	2.1
6	D	110	ARG	2.1
7	E	165	VAL	2.1
26	Z	56	GLN	2.1
22	T	21	LEU	2.1
27	1	54	LYS	2.1
6	D	57	LEU	2.1
20	R	27	GLY	2.1
3	A	69	LYS	2.1
20	R	45	LYS	2.1
3	A	217	GLY	2.1
3	A	258	LEU	2.1
21	S	22	VAL	2.1
1	X	1121	G	2.1
6	D	52	LYS	2.1
9	G	35	LYS	2.1
9	G	103	TYR	2.1
19	Q	82	LEU	2.1
20	R	40	LEU	2.1
9	G	168	THR	2.1

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Mol	Chain	Res	Type	RSRZ
16	N	91	ASN	2.1
1	X	1920	A	2.1
28	2	31	LEU	2.1
3	A	215	TRP	2.1
1	X	1551	U	2.1
3	A	249	THR	2.1
17	O	45	THR	2.1
25	W	15	ASN	2.1
1	X	2295	C	2.1
21	S	21	ALA	2.0
3	A	132	LEU	2.0
1	X	1913	G	2.0
13	K	17	ARG	2.0
1	X	200	A	2.0
21	S	32	PHE	2.0
6	D	143	TYR	2.0
20	R	84	VAL	2.0
3	A	129	GLY	2.0
7	E	149	ARG	2.0
23	U	73	GLY	2.0
3	A	62	LEU	2.0
16	N	109	LEU	2.0
14	L	111	GLY	2.0
21	S	130	ILE	2.0
1	X	1839	A	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	X	2886	1/1	0.76	1.10	87.98	54,54,54,54	0
33	MG	X	2905	1/1	0.91	0.67	48.48	50,50,50,50	0
33	MG	X	2948	1/1	0.82	0.85	31.00	110,110,110,110	0
33	MG	X	2884	1/1	0.93	1.00	29.68	72,72,72,72	0
33	MG	X	2899	1/1	0.97	0.54	18.00	41,41,41,41	0
33	MG	X	2951	1/1	0.90	0.47	16.96	142,142,142,142	0
33	MG	X	2908	1/1	0.92	0.67	13.37	80,80,80,80	0
33	MG	X	2918	1/1	0.93	0.53	12.82	84,84,84,84	0
33	MG	X	2934	1/1	0.94	0.41	10.34	56,56,56,56	0
35	NA	X	2958	1/1	0.91	0.47	8.93	48,48,48,48	0
33	MG	X	2937	1/1	0.94	0.37	7.97	109,109,109,109	0
35	NA	X	2961	1/1	0.92	0.43	7.91	75,75,75,75	0
33	MG	X	2922	1/1	0.92	0.36	7.88	53,53,53,53	0
32	LMA	X	2882	58/58	0.80	0.38	5.78	120,120,120,120	0
33	MG	X	2891	1/1	0.89	0.33	5.44	50,50,50,50	0
33	MG	X	2887	1/1	0.95	0.41	5.34	35,35,35,35	0
33	MG	X	2950	1/1	0.88	0.31	4.88	36,36,36,36	0
33	MG	X	2900	1/1	0.94	0.64	4.62	42,42,42,42	0
33	MG	X	2901	1/1	0.92	0.39	4.14	19,19,19,19	0
33	MG	X	2932	1/1	0.94	0.35	4.10	62,62,62,62	0
33	MG	X	2926	1/1	0.79	0.45	3.07	67,67,67,67	0
33	MG	X	2919	1/1	0.94	0.33	2.72	65,65,65,65	0
31	LC2	X	2881	33/33	0.83	0.33	2.66	49,106,118,122	0
33	MG	X	2890	1/1	0.96	0.40	2.37	59,59,59,59	0
33	MG	X	2940	1/1	0.82	0.31	2.30	71,71,71,71	0
33	MG	X	2892	1/1	0.95	0.30	2.18	71,71,71,71	0
33	MG	X	2928	1/1	0.87	0.34	1.35	29,29,29,29	0
33	MG	X	2896	1/1	0.95	0.26	0.26	24,24,24,24	0
34	K	X	2954	1/1	0.96	0.24	0.10	70,70,70,70	0
33	MG	X	2916	1/1	0.90	0.20	-0.15	44,44,44,44	0
33	MG	X	2897	1/1	0.96	0.14	-2.87	79,79,79,79	0
33	MG	X	2943	1/1	0.95	0.20	-	43,43,43,43	0
33	MG	X	2917	1/1	0.74	0.32	-	104,104,104,104	0
33	MG	X	2942	1/1	0.81	0.63	-	77,77,77,77	0
33	MG	X	2925	1/1	0.88	0.57	-	80,80,80,80	0
33	MG	X	2883	1/1	0.92	0.54	-	23,23,23,23	0
33	MG	X	2938	1/1	0.91	0.62	-	62,62,62,62	0
33	MG	X	2902	1/1	0.81	0.17	-	89,89,89,89	0
33	MG	X	2893	1/1	0.84	0.42	-	66,66,66,66	0
33	MG	X	2944	1/1	0.85	0.29	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	X	2927	1/1	0.95	0.75	-	65,65,65,65	0
33	MG	X	2911	1/1	0.28	0.64	-	124,124,124,124	0
33	MG	X	2903	1/1	0.90	0.54	-	65,65,65,65	0
33	MG	X	2907	1/1	0.94	0.36	-	46,46,46,46	0
33	MG	X	2894	1/1	0.82	0.47	-	65,65,65,65	0
33	MG	I	157	1/1	0.74	0.47	-	67,67,67,67	0
33	MG	X	2915	1/1	0.87	0.57	-	67,67,67,67	0
33	MG	X	2933	1/1	0.95	0.37	-	83,83,83,83	0
33	MG	X	2904	1/1	0.88	0.43	-	64,64,64,64	0
33	MG	X	2952	1/1	0.95	0.35	-	59,59,59,59	0
34	K	X	2955	1/1	0.93	0.15	-	113,113,113,113	0
33	MG	X	2941	1/1	0.88	0.23	-	71,71,71,71	0
33	MG	X	2920	1/1	0.85	0.37	-	100,100,100,100	0
33	MG	X	2931	1/1	0.84	0.68	-	72,72,72,72	0
33	MG	X	2946	1/1	0.94	0.16	-	123,123,123,123	0
34	K	X	2956	1/1	0.83	0.39	-	146,146,146,146	0
33	MG	X	2935	1/1	0.94	0.23	-	36,36,36,36	0
33	MG	X	2888	1/1	0.96	0.49	-	51,51,51,51	0
33	MG	X	2930	1/1	0.97	0.21	-	77,77,77,77	0
33	MG	X	2895	1/1	0.90	0.29	-	26,26,26,26	0
33	MG	X	2906	1/1	0.97	0.38	-	52,52,52,52	0
33	MG	U	82	1/1	0.67	0.38	-	72,72,72,72	0
33	MG	X	2945	1/1	0.95	0.18	-	67,67,67,67	0
33	MG	X	2949	1/1	0.93	0.56	-	83,83,83,83	0
33	MG	X	2913	1/1	0.97	0.40	-	63,63,63,63	0
33	MG	X	2924	1/1	0.92	0.13	-	51,51,51,51	0
33	MG	X	2885	1/1	0.88	0.47	-	68,68,68,68	0
35	NA	X	2960	1/1	0.85	0.47	-	86,86,86,86	0
35	NA	X	2962	1/1	0.79	1.12	-	98,98,98,98	0
33	MG	X	2912	1/1	0.67	0.20	-	62,62,62,62	0
33	MG	X	2936	1/1	0.94	0.25	-	55,55,55,55	0
33	MG	X	2889	1/1	0.98	0.24	-	61,61,61,61	0
34	K	X	2957	1/1	0.89	0.57	-	82,82,82,82	0
33	MG	X	2947	1/1	0.98	0.13	-	56,56,56,56	0
33	MG	X	2909	1/1	0.80	0.17	-	58,58,58,58	0
33	MG	X	2923	1/1	0.93	0.15	-	97,97,97,97	0
33	MG	X	2910	1/1	0.90	0.37	-	44,44,44,44	0
33	MG	X	2939	1/1	0.97	0.49	-	54,54,54,54	0
35	NA	X	2959	1/1	0.91	0.26	-	60,60,60,60	0
33	MG	X	2898	1/1	0.98	0.39	-	19,19,19,19	0
33	MG	X	2953	1/1	0.97	0.39	-	53,53,53,53	0
33	MG	X	2914	1/1	0.87	0.53	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	X	2929	1/1	0.92	0.83	-	61,61,61,61	0
33	MG	X	2921	1/1	0.91	0.17	-	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.