Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 11:49 PM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

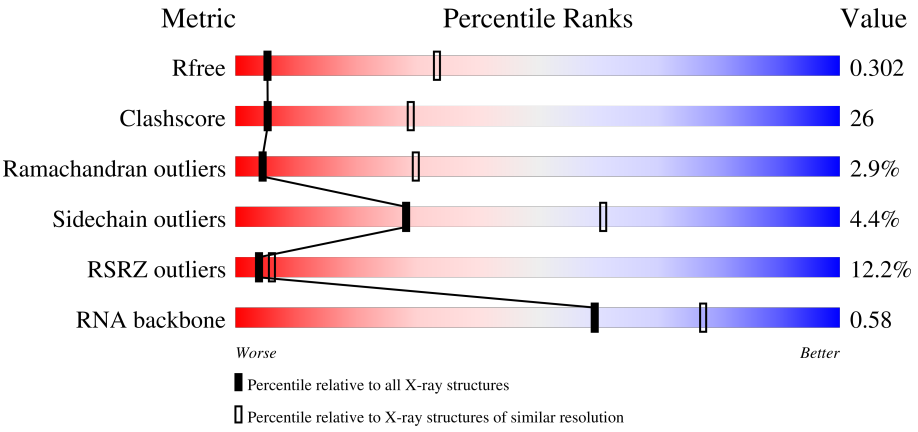
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)

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

Mol	Chain	Length	Quality of chain
1	X	2880	3% 25% 38% 24% • 8%
2	Y	123	2% 33% 50% 14% • •
3	A	274	19% 40% 45% 8% 8%

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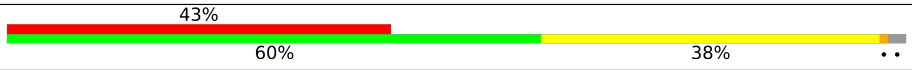
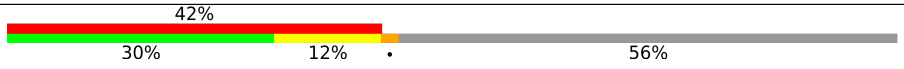
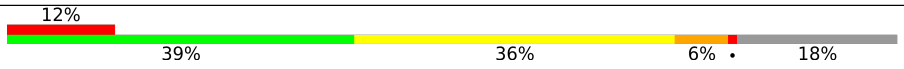
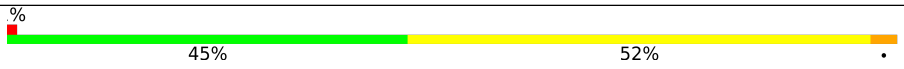
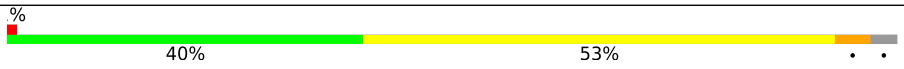
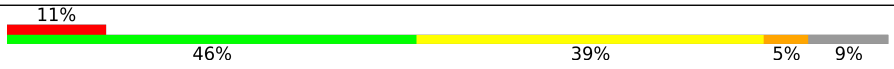
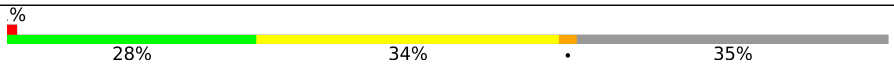
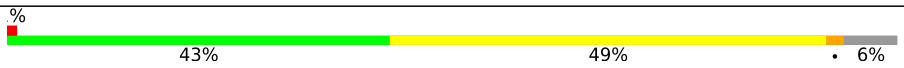
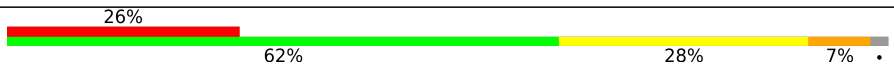
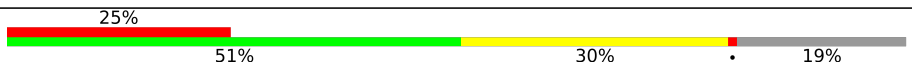
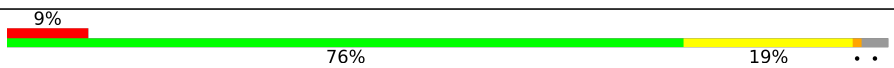
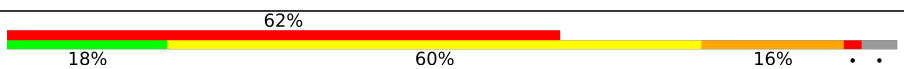
Mol	Chain	Length	Quality of chain
4	B	211	
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	

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Mol	Chain	Length	Quality of chain
29	3	66	79% 36% 44% 9% 11%
30	4	37	89% 62% 35%

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
32	LMA	X	2882	-	-	X	-
33	MG	I	157	-	-	-	X
33	MG	X	2886	-	-	-	X
33	MG	X	2911	-	-	-	X
33	MG	X	2926	-	-	-	X
35	NA	X	2962	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	P			
1	X	2644	56750	25314	10473	18320	2643	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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	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 779	C 476	N 161	O 142	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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			

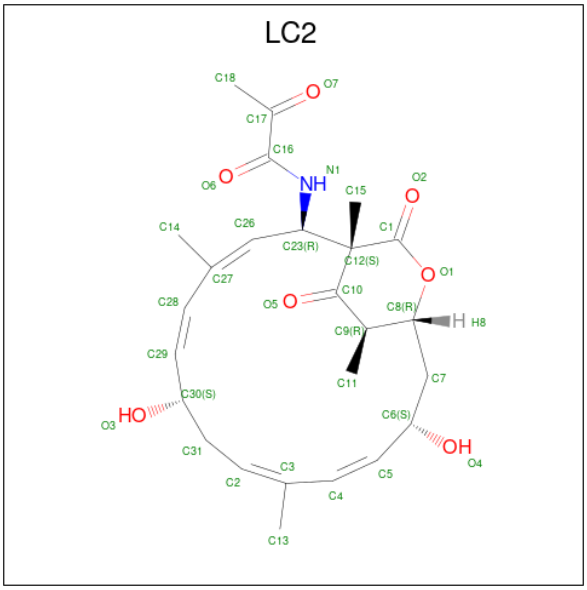
- Molecule 29 is a protein called 50S ribosomal protein L35.

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.

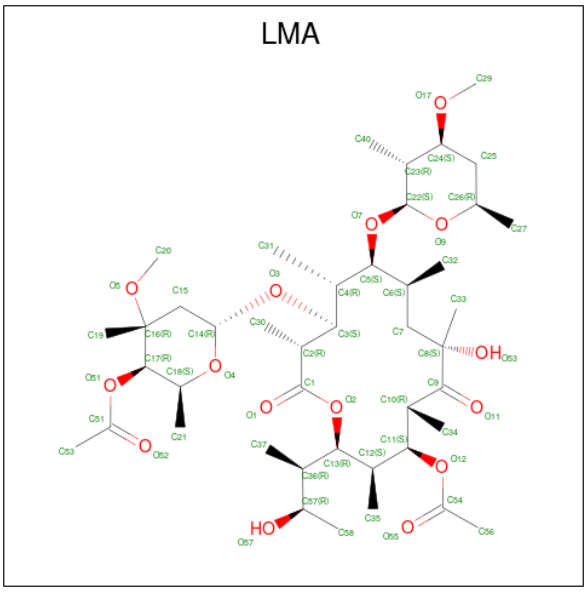
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	37	Total	C	N	O	S	0	0	0
			297	179	66	47	5			

- Molecule 31 is N-[(1S,2R,3E,5E,7S,9E,11E,13S,15R,19R)-7,13-dihydroxy-1,4,10,19-tetramethyl-17,18-dioxo-16-oxabicyclo[13.2.2]nonadeca-3,5,9,11-tetraen-2-yl]-2-oxopropanamide (three-letter code: LC2) (formula: $C_{25}H_{33}NO_7$).



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: $C_{43}H_{74}O_{15}$).



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

- 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).

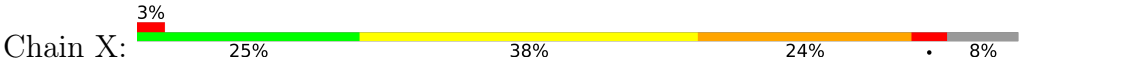
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	X	5	Total Na 5 5	0	0

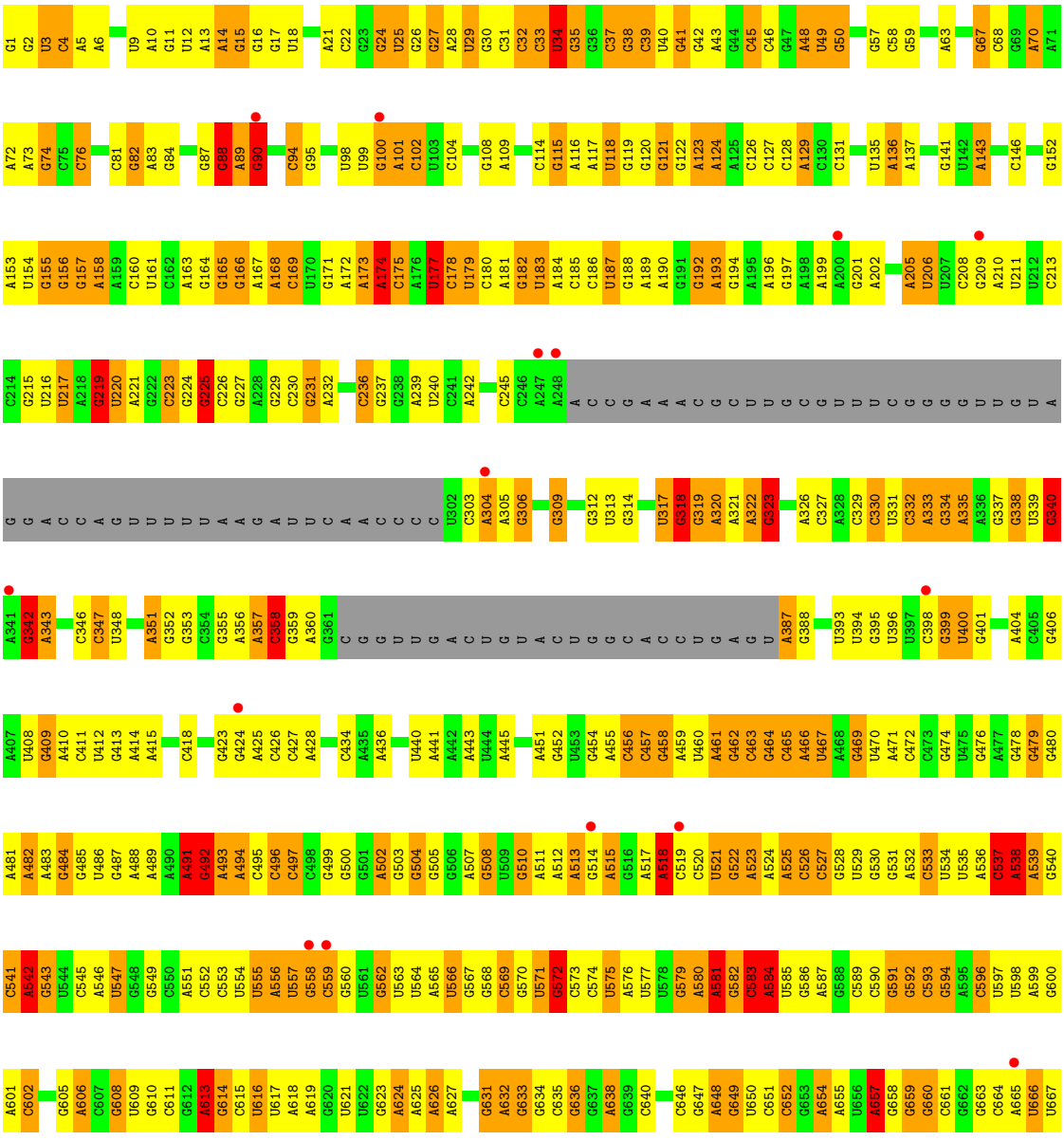
3 Residue-property plots (i)

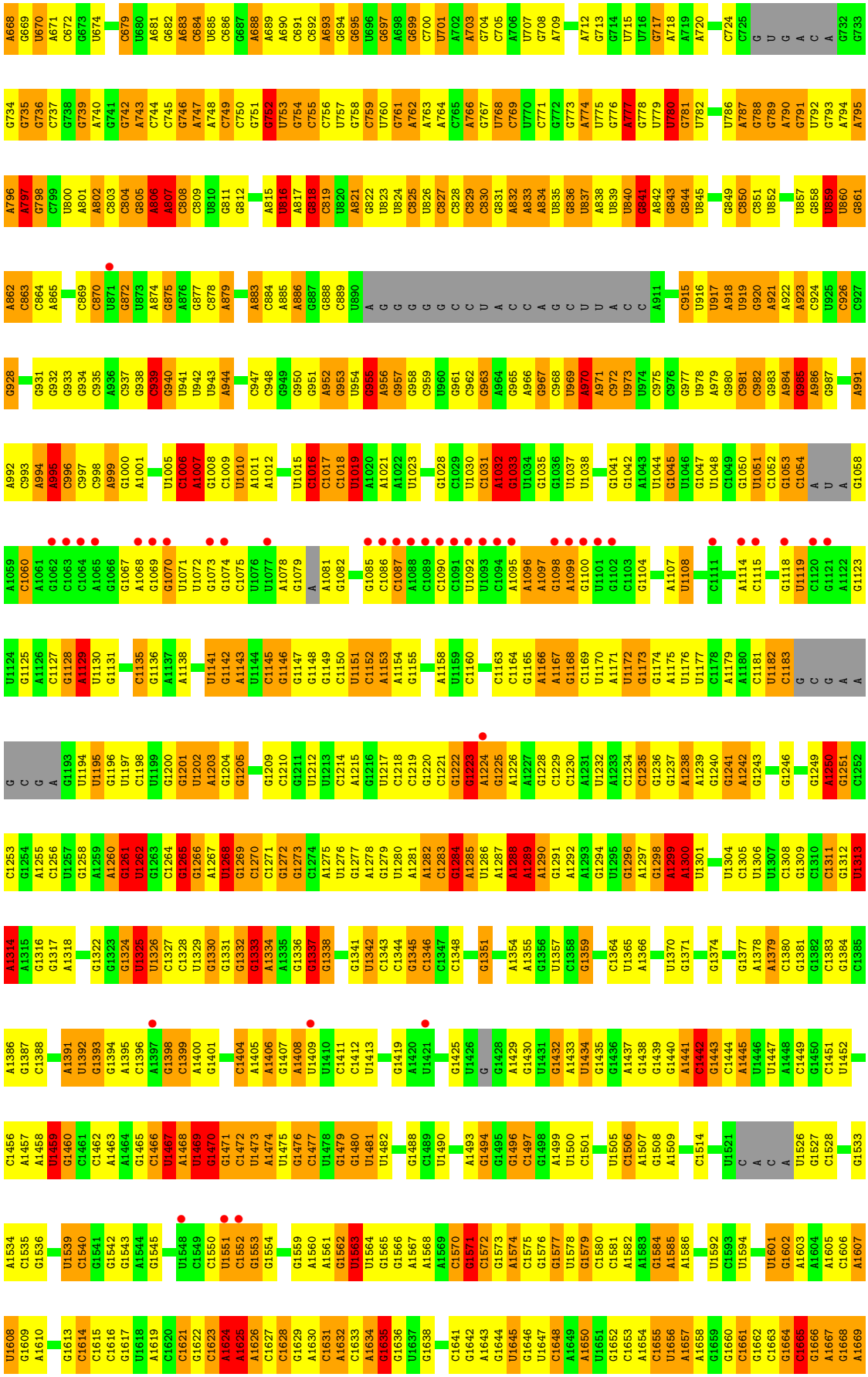
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

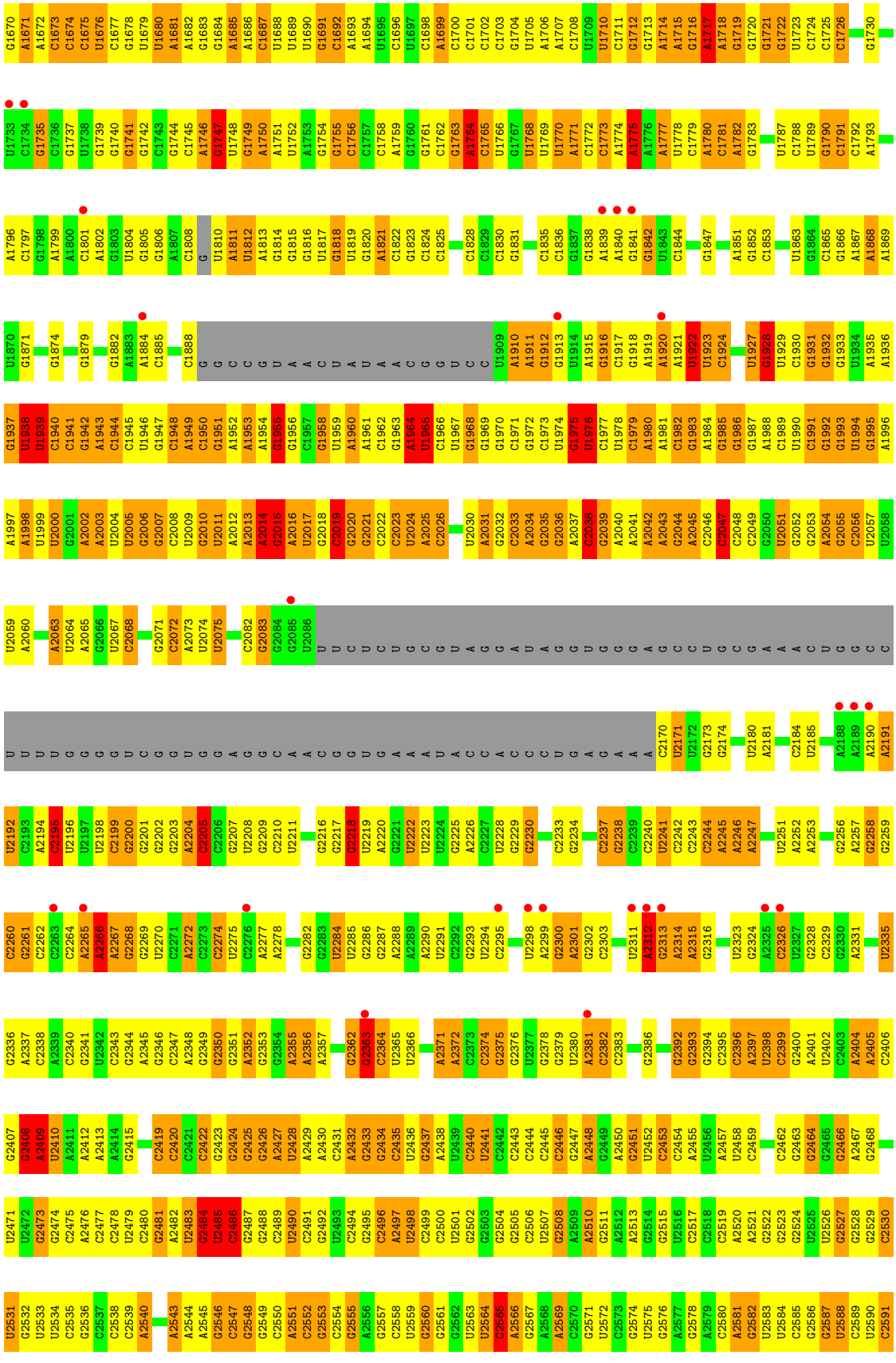
- Molecule 1: RIBOSOMAL 23S RNA

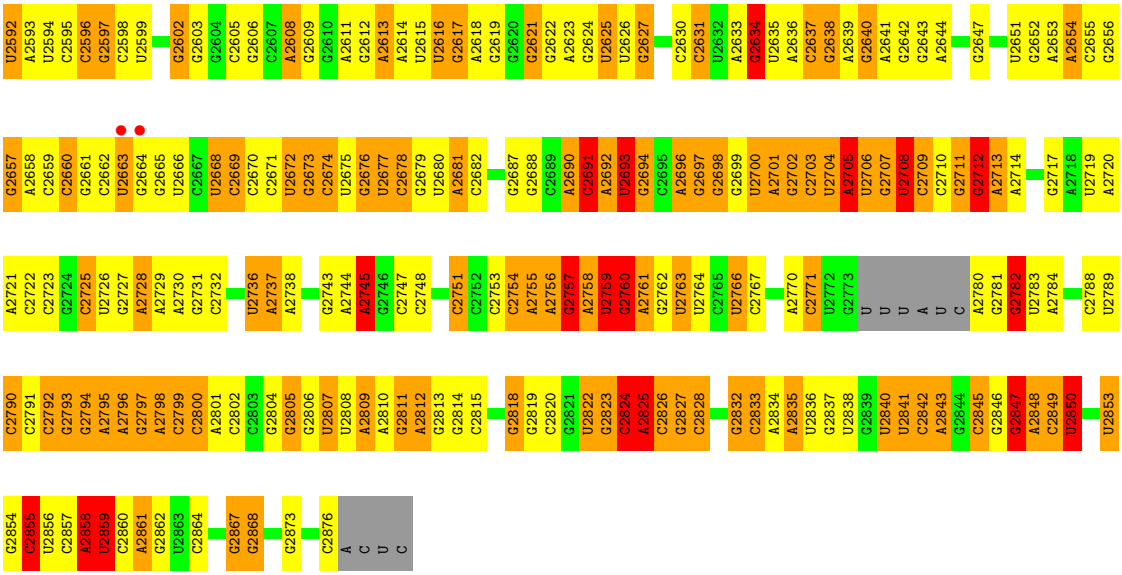
Chain X:





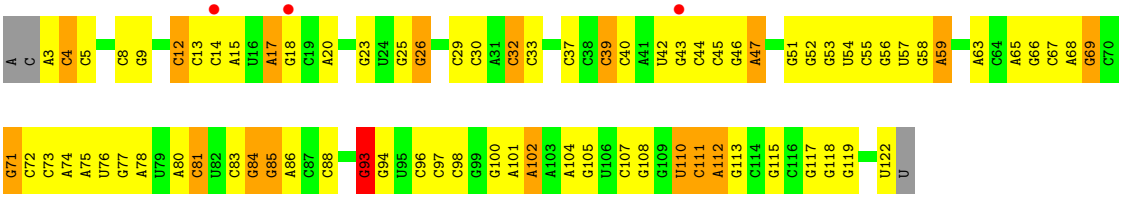






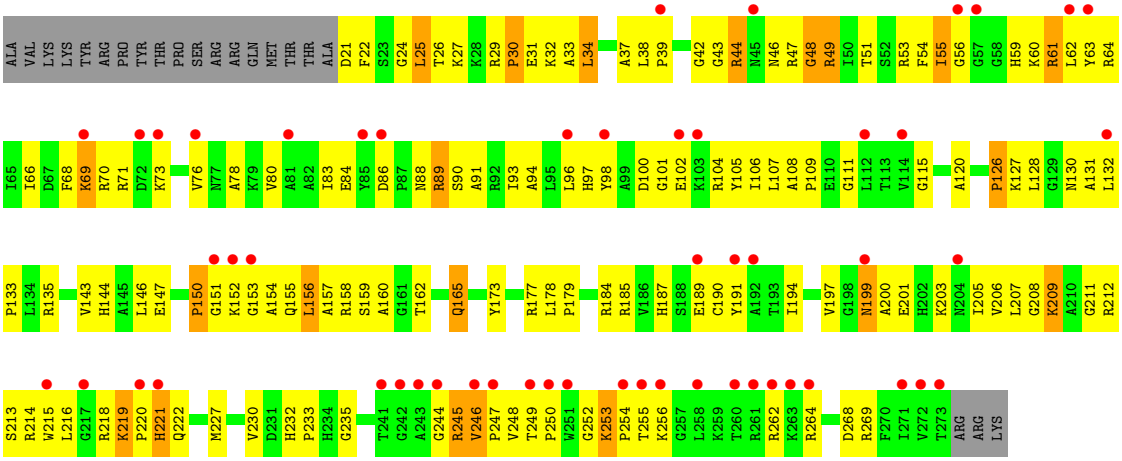
• Molecule 2: 5S ribosomal RNA

Chain Y:



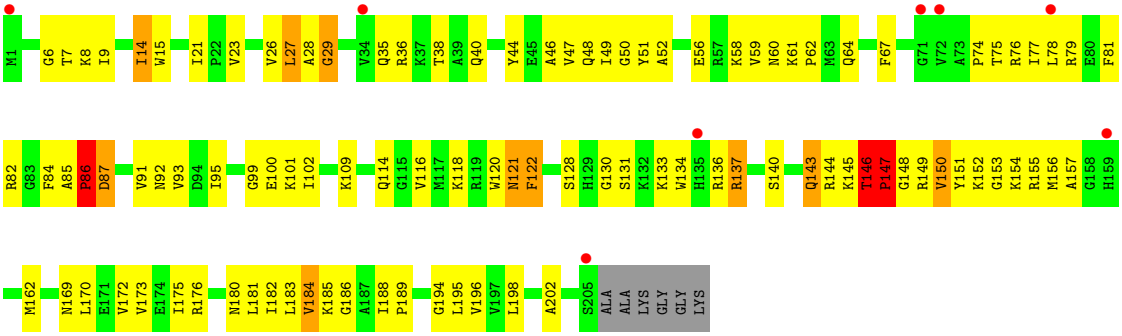
• Molecule 3: 50S ribosomal protein L2

Chain A:



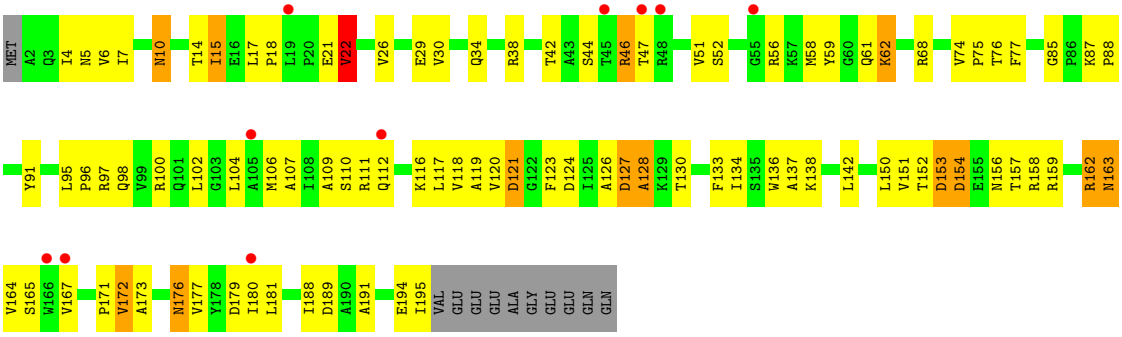
• Molecule 4: 50S ribosomal protein L3

Chain B:



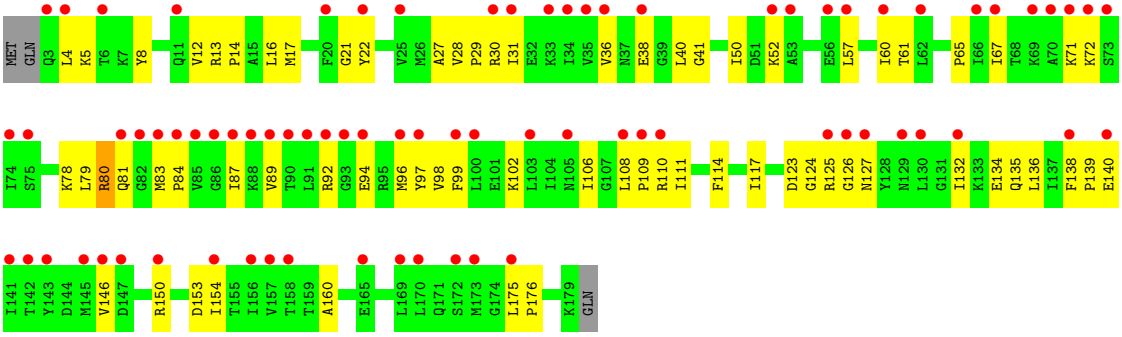
• Molecule 5: 50S ribosomal protein L4

Chain C:



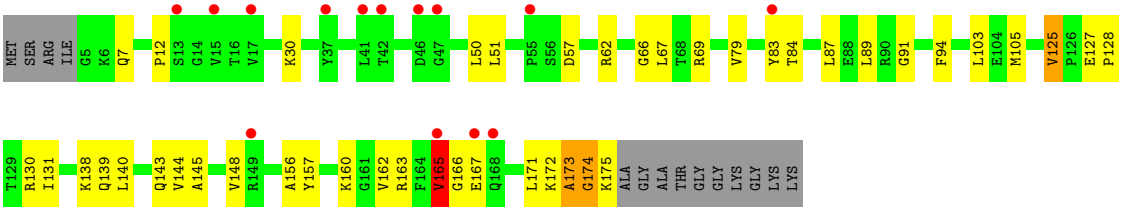
• Molecule 6: 50S ribosomal protein L5

Chain D:



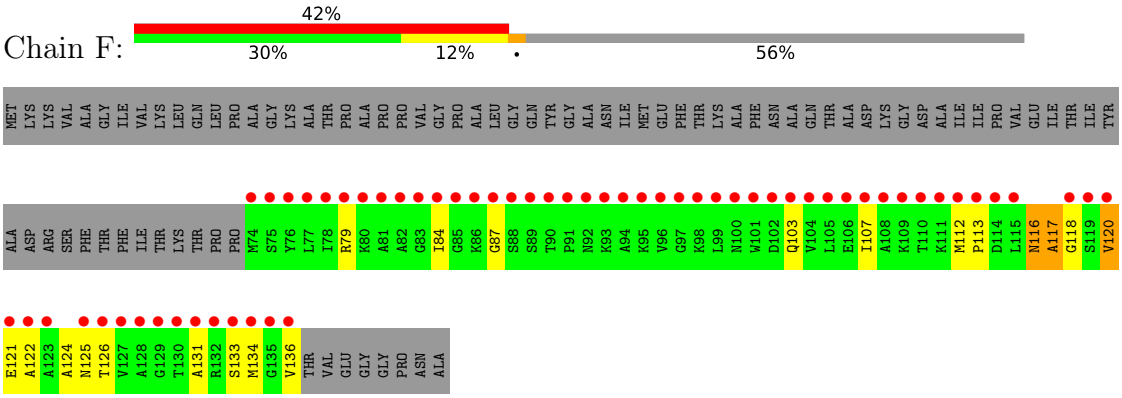
• Molecule 7: 50S ribosomal protein L6

Chain E:



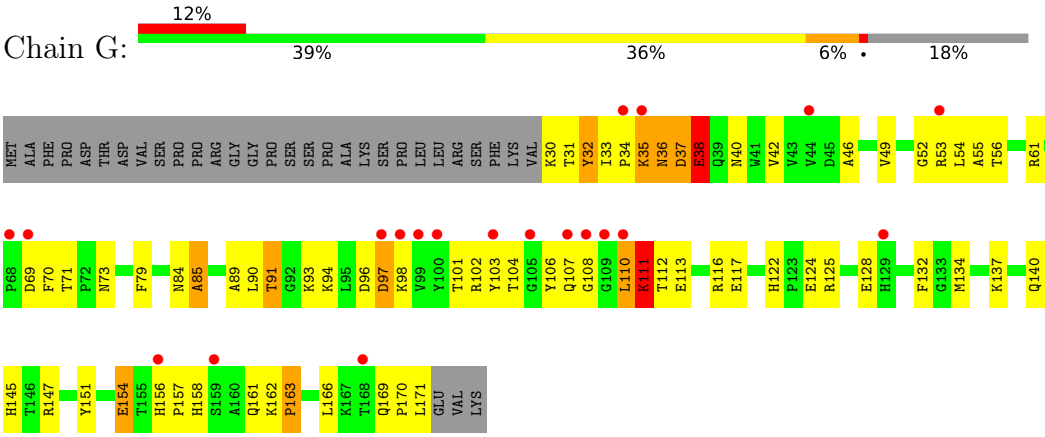
• Molecule 8: 50S ribosomal protein L11

Chain F:



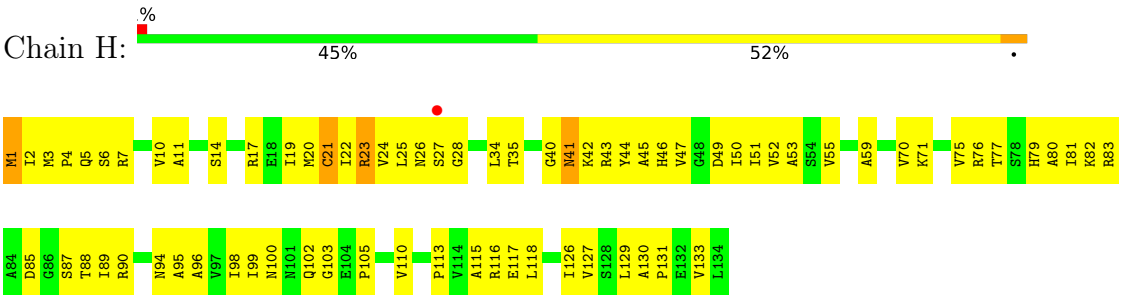
• Molecule 9: 50S ribosomal protein L13

Chain G:



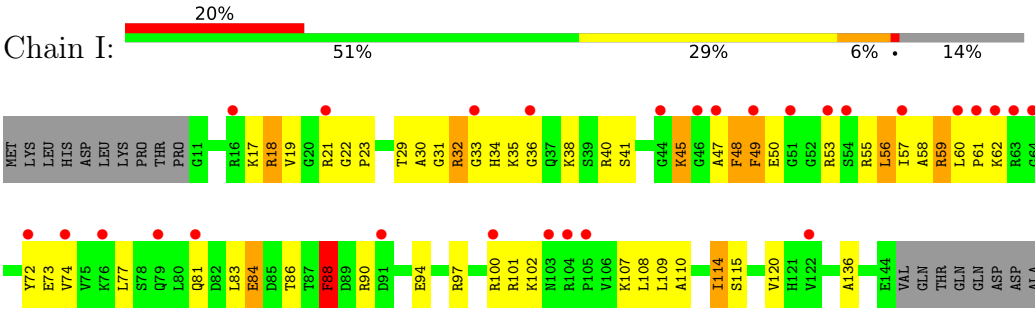
• Molecule 10: 50S ribosomal protein L14

Chain H:

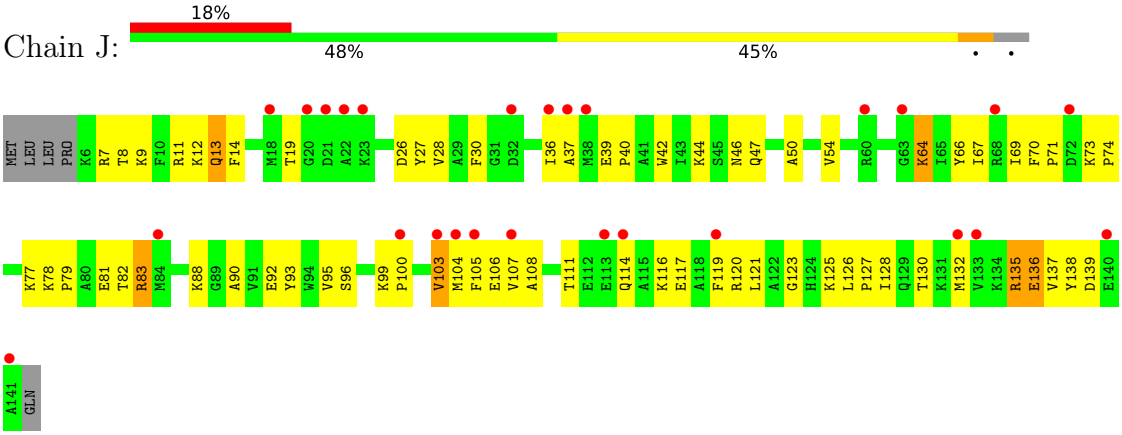


• Molecule 11: 50S ribosomal protein L15

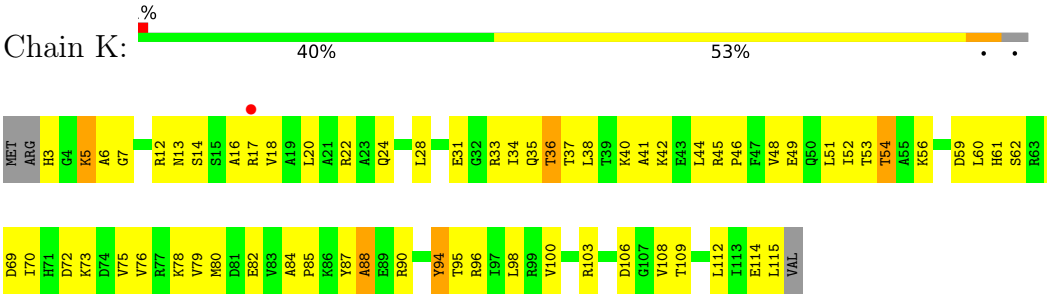
Chain I:



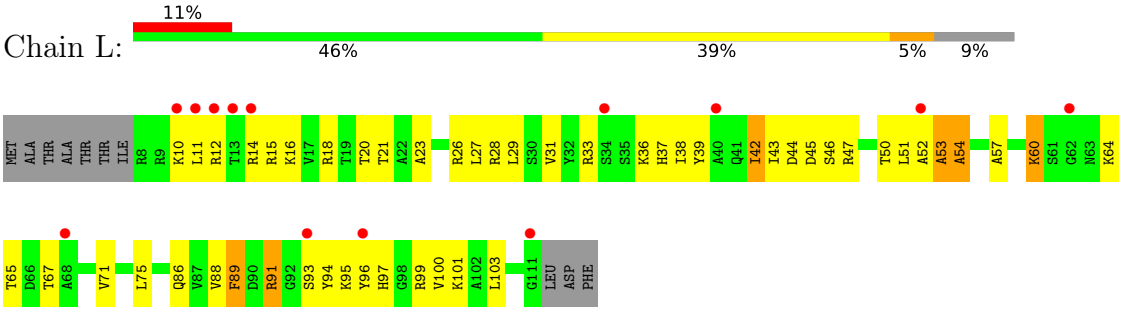
• Molecule 12: 50S ribosomal protein L16



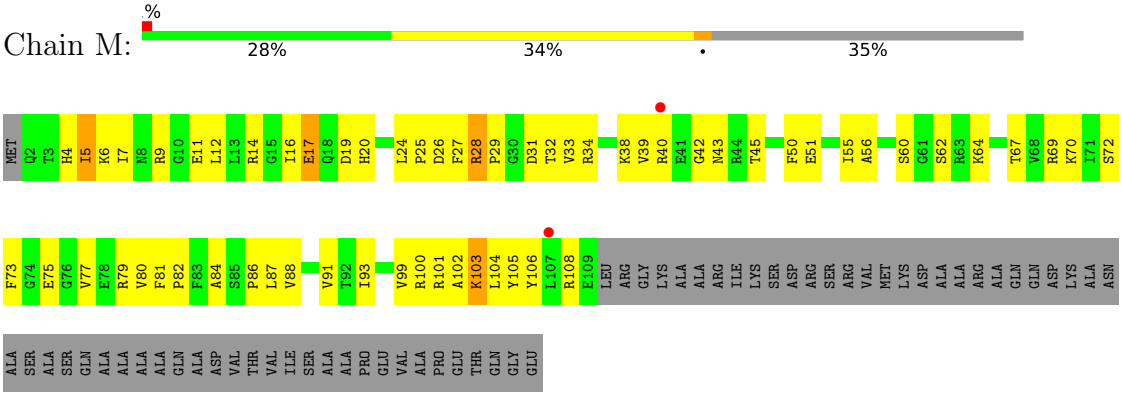
• Molecule 13: 50S ribosomal protein L17



• Molecule 14: 50S ribosomal protein L18

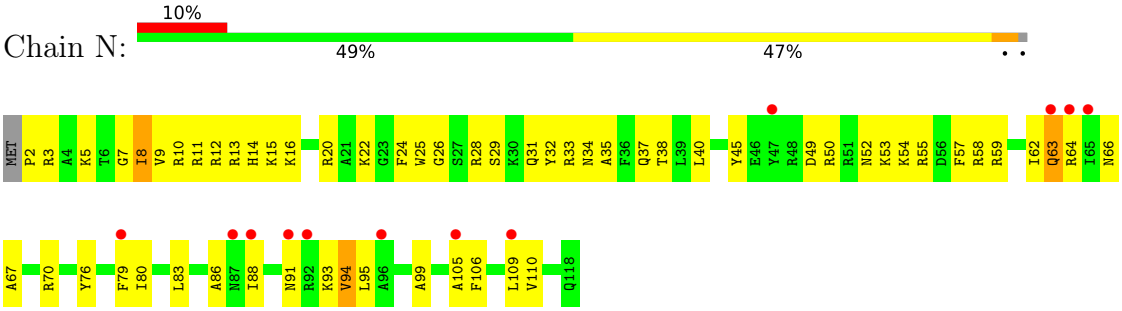


• Molecule 15: 50S ribosomal protein L19



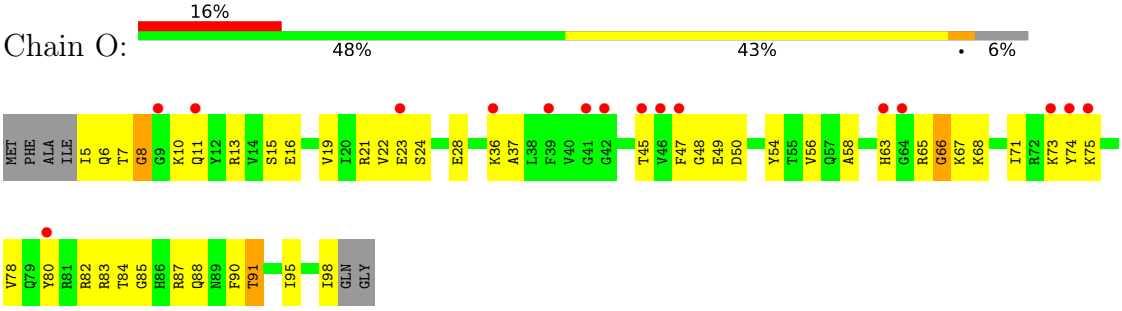
• Molecule 16: 50S ribosomal protein L20

Chain N:



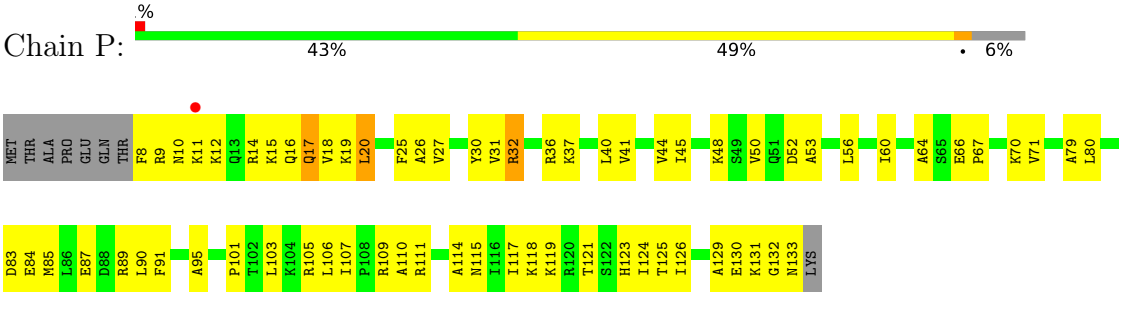
• Molecule 17: 50S ribosomal protein L21

Chain O:



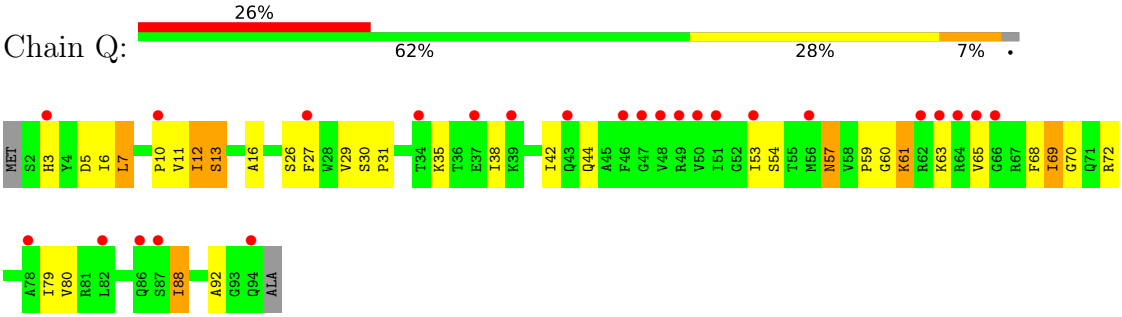
• Molecule 18: 50S ribosomal protein L22

Chain P:



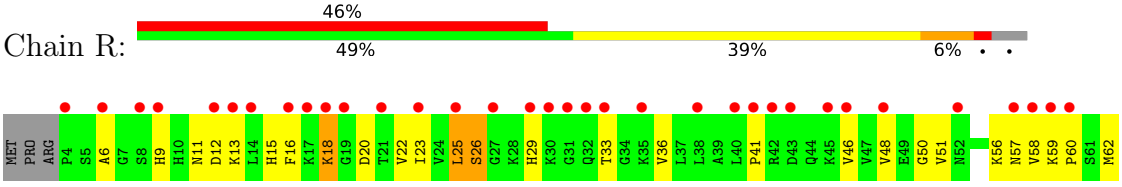
• Molecule 19: 50S ribosomal protein L23

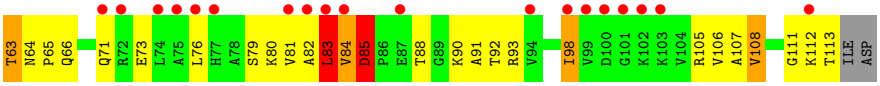
Chain Q:



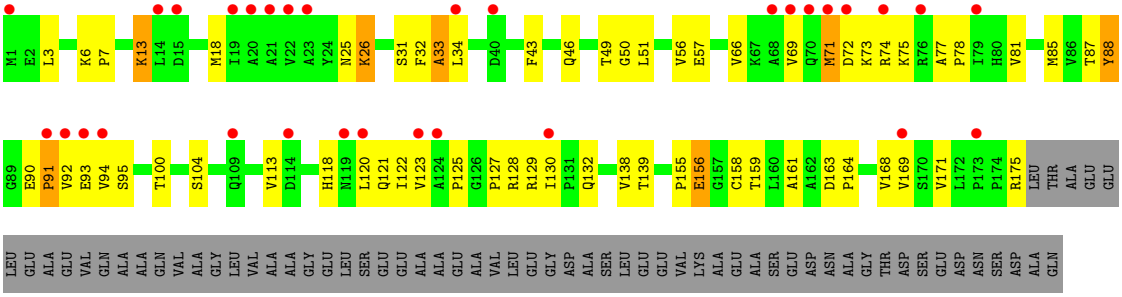
• Molecule 20: 50S ribosomal protein L24

Chain R:

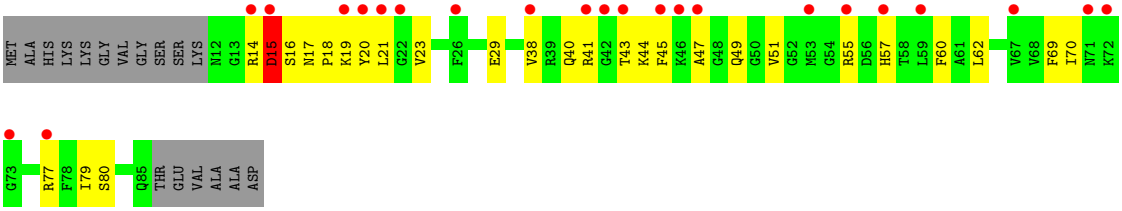




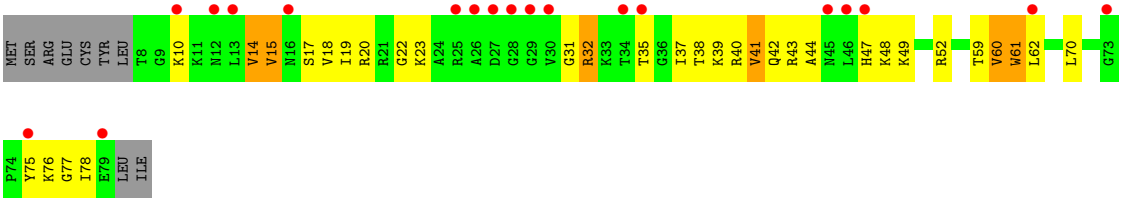
• Molecule 21: 50S ribosomal protein L25



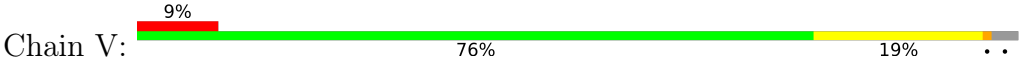
• Molecule 22: 50S ribosomal protein L27

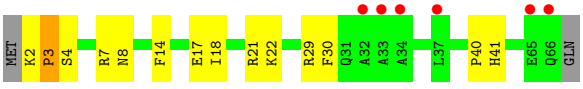


• Molecule 23: 50S ribosomal protein L28

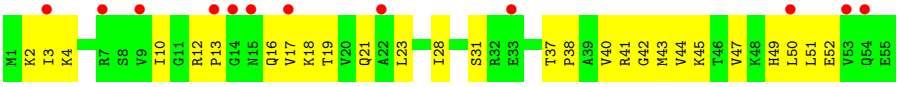


• Molecule 24: 50S ribosomal protein L29

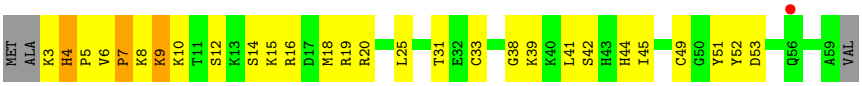




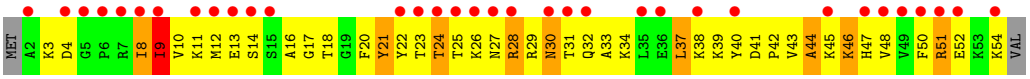
• Molecule 25: 50S ribosomal protein L30



• Molecule 26: 50S ribosomal protein L32

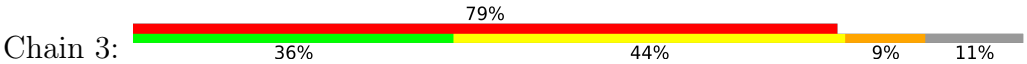


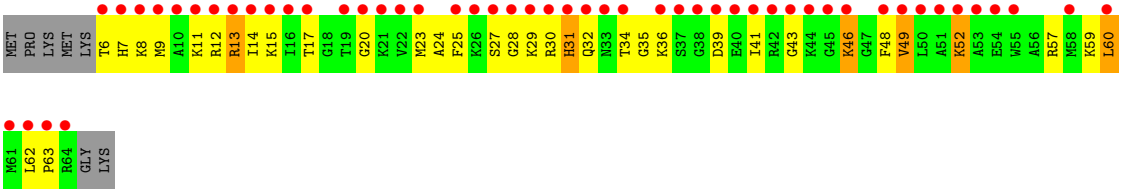
• Molecule 27: 50S ribosomal protein L33



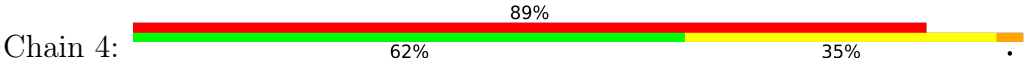
• Molecule 28: 50S ribosomal protein L34

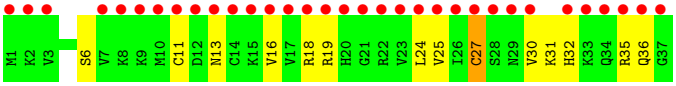
• Molecule 29: 50S ribosomal protein L35





• Molecule 30: 50S ribosomal protein L36





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.72 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.257 , 0.301 0.262 , 0.302	Depositor DCC
R_{free} test set	2649 reflections (1.01%)	wwPDB-VP
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]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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:H56B	32:X:2882:LMA:C34	1.75	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:13:LYS:HE3	21:S:33:ALA:HB1	1.22	1.13
27:1:41:ASP:OD2	27:1:46:LYS:HD2	1.48	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:H28	31:X:2881:LC2:C2	1.76	1.09
1:X:2426:G:H3'	1:X:2479:U:OP2	1.50	1.09
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.32	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:H	3:A:44:ARG:HD2	1.15	1.07
9:G:35:LYS:HG3	9:G:37:ASP:OD2	1.55	1.07
3:A:22:PHE:O	3:A:209:LYS:HG3	1.52	1.07
6:D:38:GLU:HB3	6:D:87:ILE:HB	1.35	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:H29B	32:X:2882:LMA:H40	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:1142:G:H1'	9:G:103:TYR:CE2	1.94	1.03
1:X:2427:A:N6	11:I:40:ARG:HH22	1.48	1.03
1:X:2663:U:O2'	10:H:88:THR:HG21	1.58	1.02
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:763:A:H2'	1:X:764:A:H5"	1.39	1.02
31:X:2881:LC2:O6	31:X:2881:LC2:H14B	1.58	1.02
11:I:18:ARG:CB	11:I:21:ARG:HB2	1.88	1.02
1:X:2427:A:H61	11:I:40:ARG:NH2	1.54	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:160:ALA:HB2	3:A:199:ASN:ND2	1.72	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
1:X:577:U:H5'	1:X:956:A:N6	1.77	0.99
31:X:2881:LC2:H28	31:X:2881:LC2:C3	1.91	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
1:X:971:A:H61	12:J:83:ARG:HH22	0.99	0.99
4:B:133:LYS:HG3	4:B:137:ARG:HD3	1.43	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
1:X:334:G:H2'	5:C:162:ARG:HE	1.25	0.98
9:G:70:PHE:CG	16:N:64:ARG:HG2	1.99	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:309:G:P	20:R:93:ARG:HB3	2.04	0.96
1:X:1142:G:H21	9:G:101:THR:HG21	0.79	0.96
1:X:2378:G:H1'	27:1:22:TYR:OH	1.66	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:635:C:H2'	1:X:636:G:H5"	1.49	0.94
1:X:2781:G:H2'	1:X:2782:G:H5"	1.49	0.94
1:X:824:U:H2'	11:I:30:ALA:CA	1.97	0.94
20:R:18:LYS:H	20:R:18:LYS:HD3	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
1:X:699:G:H8	28:2:11:LYS:HG2	1.17	0.94
1:X:2264:C:H5	27:1:28:ARG:CZ	1.81	0.94
3:A:61:ARG:HD3	3:A:88:ASN:OD1	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:18:ARG:CG	11:I:21:ARG:HB2	1.98	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
32:X:2882:LMA:H12	32:X:2882:LMA:C56	1.99	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
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
1:X:1092:U:H4'	8:F:122:ALA:CB	1.98	0.92
1:X:1173:G:H4'	17:O:22:VAL:HG22	1.52	0.92
16:N:7:GLY:O	16:N:9:VAL:HG23	1.70	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
2:Y:83:C:H2'	2:Y:84:G:H5'	1.51	0.90
10:H:75:VAL:HG12	10:H:118:LEU:CD2	2.02	0.90
1:X:2671:C:OP1	1:X:2846:G:H4'	1.71	0.90
3:A:66:ILE:HG21	3:A:89:ARG:HH22	1.37	0.90
1:X:2204:A:H4'	1:X:2205:C:O5'	1.70	0.90
3:A:71:ARG:HH12	3:A:150:PRO:CA	1.85	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
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
20:R:48:VAL:HG12	20:R:50:GLY:H	1.37	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
1:X:546:A:H4'	16:N:57:PHE:HZ	1.37	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
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:NE	18:P:32:ARG:HA	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
1:X:2349:G:H21	27:1:46:LYS:NZ	1.71	0.88
9:G:53:ARG:HD3	9:G:171:LEU:HD12	1.52	0.88
1:X:748:A:H8	1:X:748:A:H5"	1.38	0.88
1:X:1391:A:C8	1:X:1393:G:C6	2.61	0.88
32:X:2882:LMA:H56A	32:X:2882:LMA:H57	1.53	0.88
10:H:19:ILE:O	10:H:19:ILE:HG13	1.71	0.88
11:I:62:LYS:HD3	29:3:12:ARG:HA	1.56	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: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
1:X:1810:U:H5	3:A:158:ARG:HD2	1.38	0.86
10:H:23:ARG:NH2	10:H:23:ARG:HB3	1.90	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
1:X:2500:C:H6	1:X:2500:C:O5'	1.58	0.86
15:M:33:VAL:HG22	15:M:51:GLU:CB	2.05	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
1:X:1692:C:C2	4:B:128:SER:O	2.28	0.85
3:A:150:PRO:HD3	3:A:190:CYS:SG	2.16	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
1:X:879:A:H2'	1:X:879:A:N3	1.91	0.84
32:X:2882:LMA:O53	32:X:2882:LMA:H32	1.76	0.84
11:I:31:GLY:HA3	11:I:34:HIS:HB2	1.59	0.84
1:X:525:A:H2'	1:X:526:C:H5'	1.60	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
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
1:X:2366:U:H1'	22:T:41:ARG:NH1	1.93	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:2264:C:C5	27:1:28:ARG:NH1	2.46	0.83
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: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:154:LYS:HE3	4:B:156:MET:SD	2.18	0.83
1:X:1296:G:H22	1:X:1299:A:H5"	1.43	0.83
4:B:136:ARG:HG2	4:B:137:ARG:N	1.92	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:OP2	1:X:2005:U:H6	1.61	0.83
2:Y:83:C:H2'	2:Y:84:G:C5'	2.08	0.83
18:P:41:VAL:O	18:P:44:VAL:CG2	2.27	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)
1:X:590:C:OP1	16:N:31:GLN:HB3	1.77	0.83
1:X:2621:G:OP1	9:G:110:LEU:HD13	1.79	0.83
5:C:162:ARG:CG	5:C:162:ARG:HH11	1.92	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:HH11	3:A:49:ARG:H	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: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:1288:A:C8	13:K:16:ALA:HB2	2.14	0.82
1:X:6:A:H1'	9:G:162:LYS:CG	2.09	0.82
1:X:822:G:O2'	1:X:823:U:H5'	1.79	0.82
15:M:103:LYS:O	15:M:104:LEU:HB2	1.78	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
1:X:27:G:N2	1:X:522:G:H1'	1.94	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:317:U:H2'	1:X:318:G:H5'	1.61	0.82
12:J:42:TRP:HB3	12:J:95:VAL:HG11	1.61	0.82
27:1:41:ASP:HB2	27:1:46:LYS:HA	1.59	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
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
14:L:26:ARG:HD3	14:L:86:GLN:HB3	1.61	0.81
1:X:1437:A:H2'	1:X:1438:G:H8	1.46	0.81
1:X:2350:G:O2'	27:1:46:LYS:CB	2.28	0.81
1:X:763:A:C2'	1:X:764:A:H5"	2.11	0.81
9:G:94:LYS:HG2	9:G:117:GLU:HB2	1.60	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:759:C:OP1	1:X:759:C:H4'	1.80	0.81
1:X:971:A:N6	12:J:83:ARG:HH22	1.78	0.81
3:A:209:LYS:HA	3:A:209:LYS:HE3	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:HD3	3:A:69:LYS:H	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
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
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:759:C:H2'	32:X:2882:LMA:H58A	1.63	0.80
1:X:2045:A:C6	32:X:2882:LMA:C27	2.61	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:123:A:C5'	28:2:19:ARG:HH21	1.93	0.80
1:X:1441:A:H1'	1:X:1442:C:OP2	1.81	0.80
1:X:1816:G:OP1	3:A:53:ARG:HD3	1.80	0.80
29:3:8:LYS:HD2	29:3:11:LYS:HE3	1.61	0.80
1:X:1696:C:O5'	1:X:1696:C:H6	1.65	0.80
31:X:2881:LC2:O6	31:X:2881:LC2:C14	2.30	0.80
9:G:70:PHE:HB2	16:N:64:ARG:HE	1.47	0.80
17:O:80:TYR:CG	17:O:80:TYR:O	2.34	0.80
1:X:1391:A:C4'	1:X:1392:U:OP1	2.30	0.80
3:A:84:GLU:OE2	3:A:105:TYR:CE2	2.34	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
1:X:1981:A:H4'	1:X:2704:U:O2'	1.82	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: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
1:X:1630:A:N1	18:P:114:ALA:HB2	1.98	0.79
32:X:2882:LMA:C34	32:X:2882:LMA:C56	2.60	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
18:P:89:ARG:HG2	18:P:131:LYS:H	1.47	0.79
1:X:1391:A:N7	1:X:1393:G:C5	2.47	0.79
27:1:28:ARG:CB	27:1:30:ASN:OD1	2.20	0.79
1:X:331:U:C1'	5:C:162:ARG:HH12	1.96	0.79
1:X:1691:G:N1	1:X:1972:G:O6	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:938:G:O2'	1:X:939:C:H5'	1.82	0.78
1:X:2045:A:N6	32:X:2882:LMA:H27A	1.97	0.78
31:X:2881:LC2:H14B	31:X:2881:LC2:C16	2.12	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
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
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
17:O:65:ARG:HE	17:O:87:ARG:HD2	1.48	0.78
1:X:1173:G:H2'	1:X:1174:G:H8	1.48	0.78
1:X:2264:C:C5	27:1:28:ARG:CZ	2.66	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:1264:C:O2'	1:X:1265:G:H5"	1.82	0.78
6:D:72:LYS:HA	6:D:81:GLN:O	1.83	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:1391:A:H4'	1:X:1392:U:OP1	1.84	0.78
1:X:1673:C:H5"	4:B:136:ARG:HD3	1.65	0.78
1:X:27:G:H22	1:X:522:G:H1'	1.49	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:587:A:OP1	1:X:1268:U:O2'	2.03	0.77
3:A:33:ALA:HB3	3:A:84:GLU:CD	2.05	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
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:1668:G:N2	1:X:1990:U:C2	2.53	0.77
4:B:14:ILE:HD12	4:B:23:VAL:HG21	1.65	0.77
4:B:136:ARG:HG2	4:B:137:ARG:H	1.49	0.77
1:X:822:G:C2'	1:X:823:U:H5'	2.15	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
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
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
3:A:49:ARG:HH11	3:A:49:ARG:N	1.81	0.77
3:A:71:ARG:NH2	3:A:190:CYS:HA	2.00	0.77
3:A:102:GLU:OE2	3:A:104:ARG:NE	2.18	0.77
29:3:13:ARG:HG3	29:3:24:ALA:HA	1.66	0.77
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:1073:G:H21	8:F:133:SER:HB3	1.49	0.76
3:A:232:HIS:CD2	3:A:233:PRO:HD2	2.20	0.76
5:C:118:VAL:HG12	5:C:188:ILE:HB	1.67	0.76
5:C:162:ARG:HH11	5:C:162:ARG:HB3	1.51	0.76
27:1:26:LYS:HG2	27:1:28:ARG:NH2	2.00	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:791:G:C2	1:X:800:U:O2	2.38	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:1336:G:OP1	18:P:119:LYS:NZ	2.15	0.76
1:X:1668:G:H5"	1:X:1668:G:H8	1.50	0.76
5:C:126:ALA:O	5:C:127:ASP:HB2	1.84	0.76
1:X:1682:A:H8	1:X:1682:A:O5'	1.69	0.76
1:X:2000:U:H4'	26:Z:8:LYS:O	1.86	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: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
6:D:60:ILE:HG13	6:D:61:THR:HG23	1.67	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
1:X:2855:C:O2'	13:K:90:ARG:NH1	2.19	0.75
11:I:31:GLY:CA	11:I:34:HIS:HB2	2.17	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
4:B:154:LYS:HE3	4:B:156:MET:CG	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
17:O:22:VAL:HA	17:O:91:THR:HG22	1.67	0.75
26:Z:4:HIS:HB2	26:Z:5:PRO:CD	2.17	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
3:A:219:LYS:HD2	3:A:219:LYS:C	2.05	0.75
16:N:28:ARG:HD3	16:N:38:THR:OG1	1.87	0.75
1:X:1289:A:C2	1:X:1290:A:C5	2.74	0.75
3:A:27:LYS:HE2	3:A:205:ILE:HD11	1.65	0.75
5:C:162:ARG:HH11	5:C:162:ARG:HG3	1.51	0.75
1:X:596:C:OP2	11:I:29:THR:HG22	1.86	0.75
1:X:1141:U:C4	4:B:147:PRO:HD3	2.22	0.75
32:X:2882:LMA:H56B	32:X:2882:LMA:H34B	1.66	0.75
1:X:817:A:H2'	1:X:819:C:C4	2.22	0.74
3:A:30:PRO:C	3:A:31:GLU:OE1	2.26	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:797:A:O2'	1:X:798:G:C8	2.40	0.74
1:X:863:C:HO2'	25:W:19:THR:HG1	1.26	0.74
1:X:824:U:H3'	11:I:30:ALA:HA	1.69	0.74
1:X:2426:G:C3'	1:X:2479:U:OP2	2.33	0.74
10:H:100:ASN:OD1	10:H:102:GLN:N	2.12	0.74
18:P:60:ILE:O	18:P:60:ILE:HG22	1.85	0.74
21:S:155:PRO:HG2	21:S:158:CYS:SG	2.27	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
1:X:679:C:H5"	11:I:49:PHE:CD1	2.23	0.74
3:A:55:ILE:O	3:A:55:ILE:HG22	1.88	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
1:X:748:A:H5"	1:X:748:A:C8	2.23	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
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:37:C:H1'	5:C:44:SER:OG	1.88	0.74
1:X:309:G:OP1	20:R:93:ARG:C	2.26	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:102:GLU:OE2	3:A:104:ARG:CZ	2.36	0.74
1:X:1050:G:H1	1:X:1127:C:H42	1.33	0.74
1:X:1107:A:H3'	1:X:1108:U:H5"	1.70	0.74
1:X:2272:A:P	14:L:18:ARG:HH12	2.10	0.74
9:G:103:TYR:HB3	9:G:107:GLN:HG2	1.70	0.74
23:U:32:ARG:H	23:U:32:ARG:NE	1.86	0.74
1:X:337:G:O2'	20:R:9:HIS:ND1	2.20	0.74
5:C:162:ARG:HH11	5:C:162:ARG:CB	2.01	0.74
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
7:E:127:GLU:HG2	7:E:128:PRO:HD2	1.70	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
1:X:824:U:H2'	11:I:30:ALA:N	2.03	0.73
1:X:2063:A:H5'	23:U:38:THR:HB	1.69	0.73
11:I:18:ARG:HG2	11:I:21:ARG:HD3	1.70	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
3:A:160:ALA:CB	3:A:199:ASN:ND2	2.51	0.73
1:X:321:A:C2	1:X:323:G:H1'	2.23	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
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
1:X:1289:A:C2	1:X:1290:A:C4	2.77	0.72
17:O:73:LYS:HB2	17:O:82:ARG:HB2	1.71	0.72
1:X:626:A:HO2'	5:C:176:ASN:CG	1.92	0.72
1:X:2840:U:C4	1:X:2841:U:C5	2.77	0.72
5:C:158:ARG:HE	5:C:171:PRO:HA	1.53	0.72
1:X:2064:U:P	23:U:39:LYS:HG2	2.29	0.72
6:D:150:ARG:HA	6:D:150:ARG:HH11	1.53	0.72
1:X:517:A:H5"	1:X:518:A:H5'	1.70	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: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
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:1780:A:H5"	3:A:222:GLN:OE1	1.88	0.72
1:X:1817:U:H4'	3:A:253:LYS:CE	2.20	0.72
3:A:247:PRO:HG2	3:A:249:THR:O	1.89	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
1:X:1007:A:O3'	16:N:93:LYS:HB3	1.88	0.72
3:A:184:ARG:HB3	3:A:184:ARG:NH1	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
27:1:8:ILE:HA	27:1:29:ARG:HH21	1.54	0.72
1:X:654:A:H3'	1:X:654:A:N3	2.05	0.72
1:X:525:A:C2'	1:X:526:C:H5'	2.20	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
8:F:120:VAL:HG12	8:F:121:GLU:N	2.05	0.72
3:A:26:THR:CG2	3:A:27:LYS:H	2.03	0.72
1:X:334:G:H2'	5:C:162:ARG:NE	2.02	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
29:3:59:LYS:O	29:3:60:LEU:HB2	1.90	0.71
1:X:542:A:H8	16:N:28:ARG:HH21	1.37	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: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
3:A:22:PHE:O	3:A:209:LYS:CG	2.35	0.71
1:X:1437:A:H2'	1:X:1438:G:C8	2.24	0.71
1:X:1469:U:H5	13:K:64:ARG:HH21	1.36	0.71
1:X:1949:A:H1'	1:X:2572:U:H5'	1.72	0.71
12:J:27:TYR:O	12:J:28:VAL:CG2	2.39	0.71
13:K:54:THR:HG22	13:K:66:VAL:CG2	2.20	0.71
1:X:6:A:H1'	9:G:162:LYS:HG3	1.71	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
1:X:1391:A:N7	1:X:1393:G:O6	2.17	0.71
1:X:2040:A:H8	1:X:2040:A:O5'	1.73	0.71
27:1:14:SER:HB2	27:1:22:TYR:CA	2.14	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
1:X:755:C:H2'	1:X:756:C:C6	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:798:G:O2'	1:X:1770:U:C5'	2.39	0.71
1:X:1045:G:H5'	30:4:18:ARG:HG3	1.73	0.71
4:B:84:PHE:O	4:B:84:PHE:CD2	2.44	0.71
29:3:9:MET:HE2	29:3:12:ARG:HH12	1.55	0.71
6:D:123:ASP:OD1	6:D:125:ARG:N	2.23	0.71
1:X:703:A:O2'	1:X:793:G:OP1	2.09	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
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
26:Z:52:TYR:O	26:Z:53:ASP:HB2	1.90	0.70
27:1:8:ILE:C	27:1:9:ILE:HG23	2.11	0.70
1:X:1404:C:H5'	1:X:1405:A:OP2	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
3:A:55:ILE:CD1	3:A:55:ILE:N	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:1290:A:OP1	13:K:40:LYS:NZ	2.24	0.70
1:X:2265:A:H61	27:1:25:THR:HG21	1.57	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
14:L:37:HIS:CD2	14:L:39:TYR:CE1	2.79	0.70
1:X:1333:G:H22	1:X:1344:C:N4	1.88	0.70
20:R:91:ALA:O	20:R:108:VAL:HG22	1.91	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
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
10:H:113:PRO:HD3	15:M:73:PHE:HB2	1.73	0.70
11:I:18:ARG:HG3	11:I:21:ARG:HG3	1.73	0.70
1:X:6:A:H1'	9:G:162:LYS:HG2	1.71	0.70
1:X:2692:A:H5"	1:X:2693:U:OP2	1.92	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
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
1:X:2044:G:OP1	5:C:62:LYS:HG3	1.91	0.69
5:C:7:ILE:O	5:C:120:VAL:O	2.09	0.69
1:X:116:A:OP1	28:2:22:MET:SD	2.50	0.69
1:X:755:C:H2'	1:X:756:C:H6	1.57	0.69
1:X:1391:A:C5	1:X:1393:G:N7	2.60	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:555:U:H3'	1:X:556:A:H8	1.56	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
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
3:A:69:LYS:H	3:A:69:LYS:CD	2.06	0.69
29:3:9:MET:HG2	29:3:59:LYS:O	1.92	0.69
1:X:797:A:C5	3:A:230:VAL:HG21	2.27	0.69
20:R:59:LYS:O	20:R:65:PRO:HB3	1.93	0.69
1:X:123:A:H5'	28:2:19:ARG:HH21	1.53	0.69
1:X:797:A:C2	3:A:230:VAL:HG11	2.28	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
6:D:36:VAL:HB	6:D:89:VAL:HB	1.75	0.69
1:X:919:U:OP1	12:J:26:ASP:CG	2.31	0.69
1:X:2012:A:C2	1:X:2016:A:C5	2.80	0.69
16:N:93:LYS:HD2	16:N:93:LYS:O	1.93	0.69
1:X:2045:A:N6	32:X:2882:LMA:H32B	2.08	0.68
1:X:2590:U:H1'	32:X:2882:LMA:H37B	1.74	0.68
3:A:70:ARG:NH2	3:A:106:ILE:HG21	2.07	0.68
1:X:1327:C:H42	1:X:1351:G:H1	1.40	0.68
4:B:60:ASN:O	4:B:64:GLN:HG3	1.94	0.68
4:B:116:VAL:H	4:B:136:ARG:HE	1.41	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: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
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:457:C:O2'	1:X:458:G:H5'	1.94	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:X:2882:LMA:C56	32:X:2882:LMA:C12	2.70	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
1:X:1628:C:H5'	28:2:7:PRO:HG2	1.76	0.68
1:X:1686:A:O2'	1:X:2528:G:OP1	2.11	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
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
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
27:1:21:TYR:C	27:1:21:TYR:CD2	2.67	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
20:R:90:LYS:HD2	20:R:108:VAL:HG21	1.75	0.68
1:X:1444:C:H42	1:X:1579:G:H1	1.42	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:334:G:H4'	1:X:335:A:O5'	1.94	0.68
12:J:64:LYS:HD3	12:J:108:ALA:O	1.93	0.68
1:X:663:G:H3'	1:X:664:C:H5"	1.76	0.68
1:X:2222:U:H2'	1:X:2223:U:C6	2.29	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:526:C:O2'	1:X:527:C:H5'	1.94	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
14:L:67:THR:O	14:L:71:VAL:HG12	1.93	0.67
9:G:158:HIS:HA	9:G:161:GLN:HG3	1.76	0.67
1:X:2571:G:C2	1:X:2582:G:C2	2.82	0.67
14:L:60:LYS:NZ	14:L:64:LYS:HE2	2.09	0.67
1:X:2692:A:C5'	1:X:2693:U:OP2	2.43	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:167:A:OP2	1:X:182:G:N2	2.27	0.67
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.28	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:2238:G:C8	1:X:2406:C:N4	2.63	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:L:37:HIS:CD2	14:L:39:TYR:CZ	2.82	0.67
26:Z:4:HIS:CB	26:Z:5:PRO:CD	2.73	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
3:A:43:GLY:H	3:A:44:ARG:NH1	1.92	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:1404:C:C4	1:X:1406:A:C8	2.82	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
27:1:21:TYR:CD2	27:1:50:PHE:HZ	2.13	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
1:X:239:A:H5"	1:X:621:U:H5'	1.76	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:759:C:C2	32:X:2882:LMA:H37	2.29	0.66
1:X:1224:A:H5'	18:P:10:ASN:ND2	2.10	0.66
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:87:THR:HB	21:S:91:PRO:HB3	1.76	0.66
21:S:128:ARG:HG3	21:S:129:ARG:HG3	1.77	0.66
1:X:589:C:H4'	16:N:31:GLN:NE2	2.10	0.66
1:X:1265:G:O4'	16:N:33:ARG:CD	2.44	0.66
2:Y:83:C:C2'	2:Y:84:G:H5'	2.26	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
18:P:40:LEU:HB3	26:Z:25:LEU:HD13	1.77	0.66
1:X:33:C:O2	1:X:466:A:H2	1.78	0.66
1:X:114:C:O2'	1:X:124:A:N3	2.27	0.66
1:X:851:C:O2	1:X:952:A:C2	2.48	0.66
1:X:1614:C:H5"	19:Q:35:LYS:HB3	1.78	0.66
5:C:163:ASN:C	5:C:163:ASN:HD22	1.99	0.66
21:S:25:ASN:HB3	21:S:85:MET:HB2	1.77	0.66
1:X:1773:C:N3	1:X:2565:C:N4	2.43	0.66
1:X:1774:A:C2	1:X:2566:A:C5	2.84	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
2:Y:84:G:N1	2:Y:98:C:C2	2.64	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
1:X:48:A:H8	1:X:50:G:H21	1.43	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
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: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
1:X:227:G:OP2	29:3:8:LYS:HG2	1.96	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:2464:G:H4'	12:J:125:LYS:O	1.95	0.65
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:1948:C:C5	1:X:1949:A:N7	2.65	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:797:A:O2'	1:X:798:G:N7	2.29	0.65
3:A:54:PHE:HB2	3:A:55:ILE:HD13	1.78	0.65
1:X:834:A:C2'	1:X:957:G:OP2	2.45	0.65
1:X:2668:U:O2	1:X:2693:U:O5'	2.14	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:923:A:C5	12:J:12:LYS:HE2	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1445:A:C2	1:X:1579:G:C2	2.84	0.65
8:F:116:ASN:OD1	8:F:117:ALA:N	2.30	0.65
10:H:26:ASN:O	10:H:26:ASN:ND2	2.30	0.65
15:M:56:ALA:HB3	15:M:67:THR:N	2.12	0.65
1:X:764:A:H8	1:X:764:A:O5'	1.80	0.65
1:X:1607:A:N3	1:X:1608:U:O4'	2.30	0.65
3:A:66:ILE:HD12	3:A:89:ARG:CZ	2.27	0.65
3:A:211:GLY:HA2	3:A:214:ARG:HG2	1.78	0.65
5:C:151:VAL:HG12	5:C:173:ALA:HA	1.78	0.65
12:J:136:GLU:HG2	12:J:136:GLU:O	1.95	0.65
16:N:25:TRP:CE3	16:N:26:GLY:CA	2.80	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
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:HD23	21:S:51:LEU:H	1.61	0.65
1:X:2005:U:OP2	1:X:2005:U:C6	2.47	0.65
1:X:2501:U:H5"	1:X:2501:U:H6	1.60	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
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
1:X:1991:C:H2'	1:X:1992:G:H8	1.63	0.64
5:C:152:THR:CG2	5:C:157:THR:HG21	2.27	0.64
1:X:317:U:C2'	1:X:318:G:H5'	2.27	0.64
1:X:1704:G:N2	1:X:1719:G:C6	2.65	0.64
1:X:1974:U:H3'	1:X:1974:U:C6	2.32	0.64
1:X:2045:A:N6	32:X:2882:LMA:C32	2.60	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
27:1:26:LYS:HG2	27:1:28:ARG:HH21	1.60	0.64
1:X:818:G:N2	1:X:842:A:OP1	2.30	0.64
1:X:1074:G:H1	1:X:1086:C:N4	1.96	0.64
32:X:2882:LMA:H56A	32:X:2882:LMA:C12	2.22	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:493:A:H4'	20:R:56:LYS:HE3	1.80	0.64
1:X:1685:A:N6	1:X:1974:U:C2	2.48	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:2398:U:OP2	29:3:41:ILE:HG21	1.98	0.64
6:D:22:TYR:CD2	6:D:28:VAL:HG22	2.32	0.64
1:X:223:C:N4	29:3:7:HIS:HB3	2.12	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
1:X:1333:G:H22	1:X:1344:C:H41	1.43	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
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:333:A:H5'	5:C:162:ARG:HG2	1.80	0.64
1:X:1238:A:H5'	17:O:85:GLY:N	2.10	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: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
1:X:512:A:H4'	18:P:15:LYS:HB3	1.79	0.64
1:X:596:C:N4	11:I:36:GLY:HA3	2.12	0.64
1:X:1676:U:H2'	1:X:1677:C:O5'	1.97	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
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
29:3:29:LYS:HE3	29:3:34:THR:HB	1.80	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
1:X:2046:C:C5	1:X:2047:C:C4	2.85	0.64
4:B:6:GLY:HA2	4:B:51:TYR:CE1	2.32	0.64
1:X:993:C:H5"	1:X:994:A:OP2	1.98	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
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
11:I:57:ILE:HG23	29:3:12:ARG:NH1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:73:LYS:O	13:K:76:VAL:HG12	1.97	0.64
1:X:2036:G:OP1	4:B:144:ARG:HG3	1.97	0.63
1:X:2663:U:O4	1:X:2664:G:C6	2.51	0.63
1:X:2663:U:C5'	15:M:80:VAL:HG11	2.28	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:O5'	1:X:2502:G:H8	1.79	0.63
4:B:120:TRP:CD1	4:B:155:ARG:HB3	2.33	0.63
1:X:122:G:H2'	1:X:123:A:H5"	1.79	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
1:X:1391:A:C6	1:X:1393:G:C4	2.86	0.63
4:B:150:VAL:HG21	4:B:154:LYS:HE2	1.79	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
1:X:590:C:H2'	1:X:591:G:C8	2.33	0.63
1:X:764:A:O4'	18:P:111:ARG:HA	1.99	0.63
1:X:998:C:N4	1:X:999:A:C6	2.66	0.63
1:X:2796:A:H5"	4:B:162:MET:CE	2.28	0.63
3:A:33:ALA:HB3	3:A:84:GLU:OE1	1.97	0.63
23:U:60:VAL:HG23	23:U:61:TRP:N	2.13	0.63
28:2:8:ASN:OD1	28:2:10:ARG:HG2	1.99	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
15:M:17:GLU:HG3	15:M:62:SER:HB2	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:1681:A:C2	1:X:2706:U:H1'	2.33	0.63
1:X:2257:A:N6	22:T:15:ASP:CG	2.51	0.63
1:X:2272:A:C5'	14:L:15:ARG:HH21	2.08	0.63
1:X:2478:C:O5'	1:X:2478:C:C6	2.44	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
4:B:100:GLU:O	4:B:172:VAL:HG23	1.99	0.63
10:H:23:ARG:HB3	10:H:23:ARG:HH21	1.63	0.63
15:M:9:ARG:HA	15:M:12:LEU:HD12	1.80	0.63
1:X:819:C:OP2	11:I:41:SER:HB3	1.98	0.63
1:X:2660:C:C2	1:X:2704:U:O4	2.52	0.63
16:N:66:ASN:CB	16:N:76:TYR:HB2	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O5'	1:X:2500:C:C6	2.47	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
27:1:43:VAL:O	27:1:44:ALA:HB2	1.99	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
1:X:486:U:C2	1:X:492:G:N2	2.67	0.62
1:X:2013:A:H4'	1:X:2014:A:H8	1.63	0.62
4:B:182:ILE:C	4:B:183:LEU:HD23	2.19	0.62
1:X:966:A:N6	1:X:967:G:C6	2.68	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:166:G:H21	1:X:184:A:H62	1.44	0.62
1:X:959:C:H1'	1:X:995:A:C2	2.35	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:1938:U:H4'	1:X:1939:U:OP2	1.96	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
28:2:1:MET:O	28:2:2:LYS:C	2.36	0.62
1:X:717:G:N3	1:X:739:G:C2	2.67	0.62
1:X:1164:C:H5'	16:N:76:TYR:HE2	1.63	0.62
4:B:152:LYS:HB2	9:G:106:TYR:HB3	1.80	0.62
5:C:162:ARG:HD2	5:C:162:ARG:C	2.20	0.62
11:I:18:ARG:HG3	11:I:21:ARG:CG	2.28	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
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
29:3:49:VAL:HG11	29:3:52:LYS:HD3	1.82	0.62
1:X:699:G:O6	28:2:12:ARG:CA	2.39	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
1:X:2201:G:H2'	1:X:2202:G:H8	1.64	0.62
1:X:2264:C:OP2	27:1:28:ARG:NH1	2.33	0.62
1:X:2710:C:O2'	1:X:2711:G:H5'	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:X:2882:LMA:C56	32:X:2882:LMA:H34B	2.27	0.62
3:A:49:ARG:HB3	3:A:49:ARG:CZ	2.30	0.62
9:G:162:LYS:N	9:G:163:PRO:CD	2.63	0.62
20:R:23:ILE:C	20:R:23:ILE:HD12	2.20	0.62
1:X:1291:G:C5'	13:K:34:ILE:HD12	2.29	0.62
1:X:1392:U:O5'	1:X:1392:U:H6	1.82	0.62
11:I:60:LEU:HD21	29:3:13:ARG:HG2	1.80	0.62
27:1:41:ASP:CG	27:1:46:LYS:HD2	2.18	0.62
1:X:67:G:N2	1:X:73:A:N3	2.48	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:872:G:H22	1:X:928:G:H2'	1.65	0.62
1:X:2430:A:OP1	1:X:2476:A:N6	2.30	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: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
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
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: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
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:1147:G:H2'	1:X:1148:G:C8	2.36	0.61
29:3:60:LEU:HD12	29:3:63:PRO:HG2	1.82	0.61
1:X:798:G:O2'	1:X:1770:U:H5'	1.99	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
4:B:154:LYS:CE	4:B:156:MET:SD	2.88	0.61
1:X:192:G:H4'	1:X:193:A:OP1	1.99	0.61
1:X:1179:A:C2	1:X:1196:G:C2	2.88	0.61
1:X:1671:A:H8	1:X:1671:A:H5"	1.65	0.61
1:X:2349:G:H21	27:1:46:LYS:HZ2	1.44	0.61
12:J:81:GLU:HG2	12:J:82:THR:HG23	1.82	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:N	26:Z:3:LYS:HD3	2.16	0.61
1:X:94:C:H1'	24:V:40:PRO:HG2	1.83	0.61
1:X:592:G:OP2	16:N:10:ARG:HD2	2.00	0.61
1:X:2429:A:C6	1:X:2430:A:N6	2.69	0.61
15:M:32:THR:HG23	15:M:93:ILE:CD1	2.31	0.61
26:Z:52:TYR:O	26:Z:53:ASP:CB	2.48	0.61
1:X:123:A:H5'	28:2:19:ARG:NE	2.16	0.61
1:X:303:C:H2'	1:X:304:A:H5"	1.82	0.61
1:X:1774:A:C2	1:X:2566:A:C4	2.89	0.61
1:X:2257:A:H62	22:T:15:ASP:CG	2.03	0.61
2:Y:85:G:O6	2:Y:86:A:C6	2.53	0.61
3:A:66:ILE:CD1	3:A:107:LEU:HG	2.30	0.61
3:A:69:LYS:HD3	3:A:69:LYS:N	2.14	0.61
12:J:81:GLU:O	12:J:82:THR:OG1	2.19	0.61
1:X:224:G:C2	1:X:229:G:C6	2.88	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: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:1817:U:O4'	3:A:253:LYS:CD	2.49	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: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
1:X:1508:G:H5'	1:X:1509:A:H5"	1.82	0.60
1:X:1755:G:C6	1:X:1972:G:C2	2.89	0.60
1:X:1817:U:O4'	3:A:253:LYS:HD2	2.00	0.60
1:X:2006:G:N2	1:X:2024:U:C2	2.69	0.60
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:762:A:H2	1:X:766:A:O2'	1.77	0.60
1:X:1683:G:O2'	1:X:1684:G:H5'	2.01	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:494:A:C8	1:X:495:C:C5	2.88	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
16:N:40:LEU:HD22	17:O:74:TYR:CD1	2.35	0.60
1:X:749:C:H3'	1:X:749:C:C6	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:71:ARG:HH12	3:A:150:PRO:CB	2.13	0.60
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:HH21	10:H:23:ARG:CB	2.15	0.60
11:I:18:ARG:HB2	11:I:21:ARG:CB	2.17	0.60
1:X:1223:G:C4'	1:X:1224:A:OP2	2.50	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:615:C:H4'	1:X:669:G:N2	2.16	0.60
3:A:147:GLU:HB2	3:A:190:CYS:HB3	1.84	0.60
19:Q:7:LEU:C	19:Q:7:LEU:CD2	2.69	0.60
1:X:304:A:H62	1:X:356:A:N6	1.98	0.60
1:X:795:A:N1	3:A:227:MET:CE	2.64	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
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:749:C:C6	1:X:749:C:C3'	2.85	0.60
1:X:1625:A:H1'	1:X:1632:A:H1'	1.84	0.60
1:X:1674:C:OP1	4:B:136:ARG:O	2.20	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
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:1656:U:H2'	1:X:1657:A:C5'	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2720:A:C6	1:X:2721:A:C6	2.89	0.60
3:A:159:SER:O	3:A:197:VAL:HG21	2.02	0.60
10:H:19:ILE:O	10:H:19:ILE:CG1	2.49	0.60
25:W:38:PRO:HA	25:W:41:ARG:HD2	1.83	0.60
28:2:25:LYS:HE2	28:2:25:LYS:HA	1.83	0.60
1:X:583:C:O2	4:B:145:LYS:NZ	2.35	0.59
1:X:1407:G:O6	1:X:1408:A:N6	2.34	0.59
1:X:2464:G:C4'	12:J:125:LYS:O	2.50	0.59
1:X:2663:U:O2'	10:H:88:THR:CG2	2.43	0.59
3:A:232:HIS:CG	3:A:233:PRO:HD2	2.37	0.59
5:C:177:VAL:O	5:C:180:ILE:HG22	2.01	0.59
14:L:36:LYS:HE3	14:L:64:LYS:O	2.02	0.59
29:3:13:ARG:NE	29:3:25:PHE:H	1.99	0.59
1:X:487:G:H4'	1:X:512:A:N1	2.17	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
2:Y:83:C:H2'	2:Y:84:G:O5'	2.02	0.59
3:A:59:HIS:C	3:A:61:ARG:H	2.05	0.59
1:X:693:A:C4	1:X:811:G:N2	2.70	0.59
1:X:793:G:C2	1:X:798:G:O6	2.55	0.59
1:X:1277:G:OP1	26:Z:19:ARG:NH2	2.35	0.59
1:X:1407:G:H4'	1:X:1619:A:H4'	1.83	0.59
1:X:1466:C:H42	1:X:1476:G:H1	1.51	0.59
1:X:2841:U:H1'	1:X:2843:A:O4'	2.03	0.59
25:W:2:LYS:HE2	25:W:31:SER:HB2	1.84	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
1:X:2760:G:N1	9:G:128:GLU:OE2	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
10:H:110:VAL:HG23	10:H:129:LEU:CB	2.32	0.59
1:X:123:A:C5'	28:2:19:ARG:HE	2.16	0.59
1:X:583:C:O2	4:B:145:LYS:CE	2.51	0.59
1:X:1817:U:H4'	3:A:253:LYS:CD	2.31	0.59
1:X:2824:C:O4'	1:X:2843:A:C6	2.55	0.59
4:B:6:GLY:CA	4:B:27:LEU:O	2.50	0.59
10:H:51:ILE:O	10:H:51:ILE:HG13	2.03	0.59
29:3:46:LYS:HA	29:3:46:LYS:HE3	1.83	0.59
1:X:824:U:H2'	11:I:30:ALA:H	1.66	0.59
1:X:1432:G:O6	1:X:1594:U:H5"	2.03	0.59
1:X:2349:G:N2	27:1:46:LYS:NZ	2.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:583:C:C2	4:B:145:LYS:NZ	2.71	0.59
1:X:709:A:C2	1:X:780:U:C2	2.90	0.59
1:X:1764:A:C2'	1:X:1765:C:H5'	2.33	0.59
1:X:2064:U:C5'	23:U:41:VAL:HG11	2.28	0.59
11:I:57:ILE:O	29:3:12:ARG:CD	2.51	0.59
12:J:42:TRP:HB3	12:J:95:VAL:CG1	2.33	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
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: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
3:A:109:PRO:HB3	3:A:144:HIS:CE1	2.38	0.59
4:B:181:LEU:HD21	15:M:12:LEU:HD22	1.85	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
21:S:71:MET:N	21:S:71:MET:SD	2.74	0.59
1:X:460:U:C4	1:X:592:G:H1'	2.37	0.59
1:X:1042:G:H5'	30:4:6:SER:HG	1.68	0.59
32:X:2882:LMA:H34B	32:X:2882:LMA:C54	2.33	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
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
5:C:7:ILE:HG12	5:C:119:ALA:HB1	1.85	0.58
5:C:194:GLU:HG2	5:C:195:ILE:HG23	1.83	0.58
16:N:20:ARG:NH1	17:O:83:ARG:HH22	2.00	0.58
1:X:681:A:H5"	1:X:681:A:H8	1.68	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: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:1234:C:O2	1:X:1242:A:C2	2.56	0.58
32:X:2882:LMA:H29B	32:X:2882:LMA:C40	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:458:G:H4'	1:X:459:A:H5'	1.84	0.58
1:X:795:A:C6	3:A:227:MET:HE3	2.38	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:2825:A:OP2	1:X:2843:A:N3	2.36	0.58
1:X:2841:U:C1'	1:X:2843:A:O4'	2.51	0.58
2:Y:84:G:O2'	2:Y:85:G:C5'	2.51	0.58
3:A:146:LEU:HD23	3:A:156:LEU:HD12	1.85	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:165:G:H1	1:X:185:C:H42	1.51	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
1:X:1202:U:O2	1:X:1202:U:H2'	2.04	0.58
1:X:1717:A:H2'	1:X:1718:A:H5'	1.86	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
26:Z:16:ARG:HD3	26:Z:20:ARG:CZ	2.34	0.58
27:1:39:LYS:O	27:1:39:LYS:HD3	2.03	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
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
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
27:1:21:TYR:CD2	27:1:50:PHE:CZ	2.91	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
1:X:839:U:H5"	1:X:2408:G:OP2	2.03	0.58
1:X:2447:G:HO2'	1:X:2448:A:H8	1.50	0.58
1:X:2805:G:H5"	4:B:58:LYS:NZ	2.18	0.58
3:A:71:ARG:HH22	3:A:190:CYS:HA	1.65	0.58
9:G:70:PHE:HB3	16:N:64:ARG:HG2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:Q:7:LEU:HD22	19:Q:7:LEU:O	2.04	0.58
27:1:21:TYR:C	27:1:21:TYR:HD2	2.07	0.58
1:X:99:U:H3'	1:X:100:G:H5"	1.86	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
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
3:A:160:ALA:CA	3:A:199:ASN:CG	2.71	0.58
3:A:209:LYS:HA	3:A:209:LYS:CE	2.32	0.58
10:H:116:ARG:CZ	15:M:38:LYS:HE2	2.33	0.58
12:J:71:PRO:CA	12:J:96:SER:HB2	2.32	0.58
1:X:67:G:N2	1:X:73:A:C4	2.72	0.58
1:X:658:G:H2'	1:X:659:G:H8	1.69	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:77:THR:HA	10:H:94:ASN:OD1	2.03	0.58
10:H:100:ASN:OD1	10:H:100:ASN:C	2.41	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:521:U:O4	1:X:522:G:N2	2.37	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
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:342:G:H4'	1:X:343:A:OP2	2.03	0.57
1:X:1270:C:H4'	5:C:77:PHE:CE2	2.39	0.57
1:X:2533:U:C4	1:X:2534:U:O4	2.56	0.57
3:A:89:ARG:HG2	3:A:91:ALA:HB3	1.85	0.57
4:B:183:LEU:HD23	4:B:183:LEU:N	2.18	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
26:Z:14:SER:O	26:Z:18:MET:HG3	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
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:500:G:N7	18:P:70:LYS:NZ	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:860:U:O2	1:X:860:U:C2'	2.50	0.57
1:X:1817:U:H4'	3:A:253:LYS:HE2	1.86	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
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:872:G:N2	1:X:928:G:H2'	2.18	0.57
1:X:923:A:C6	12:J:12:LYS:HD3	2.40	0.57
1:X:1393:G:H1'	1:X:1585:A:H61	1.68	0.57
1:X:1673:C:H5"	4:B:136:ARG:HB3	1.85	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:2848:A:H2	13:K:7:GLY:H	1.53	0.57
5:C:162:ARG:HG3	5:C:162:ARG:NH1	2.14	0.57
1:X:334:G:H21	5:C:162:ARG:NH2	2.01	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
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
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:29:U:H4'	16:N:11:ARG:HH12	1.68	0.57
1:X:88:G:H3'	1:X:89:A:H5"	1.87	0.57
1:X:168:A:H2'	1:X:169:C:C6	2.40	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:2639:A:H2'	1:X:2640:G:O4'	2.05	0.57
20:R:62:MET:O	20:R:63:THR:CB	2.53	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
1:X:2717:G:H1	1:X:2747:C:H42	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:33:CYS:HB2	26:Z:38:GLY:O	2.05	0.57
27:1:40:TYR:HB2	27:1:50:PHE:CD2	2.39	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
1:X:94:C:O2'	24:V:40:PRO:HD2	2.05	0.57
1:X:631:G:H2'	1:X:631:G:N3	2.19	0.57
1:X:2055:G:O2'	1:X:2056:C:H5'	2.04	0.57
25:W:4:LYS:HG3	25:W:52:GLU:HB3	1.86	0.57
1:X:331:U:O2	5:C:162:ARG:NH2	2.38	0.57
1:X:521:U:C2'	1:X:522:G:H5'	2.35	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
10:H:116:ARG:HD2	15:M:38:LYS:CE	2.34	0.57
30:4:31:LYS:H	30:4:31:LYS:HD2	1.70	0.57
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
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
2:Y:66:G:C6	2:Y:67:C:N3	2.73	0.56
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:605:G:H2'	1:X:606:A:C8	2.39	0.56
1:X:760:U:C4	1:X:2592:U:C5	2.92	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
3:A:151:GLY:C	3:A:153:GLY:H	2.06	0.56
9:G:31:THR:HB	16:N:64:ARG:HH22	1.68	0.56
11:I:62:LYS:NZ	29:3:15:LYS:HE2	2.20	0.56
13:K:80:MET:HE2	13:K:80:MET:CA	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:40:TYR:H	27:1:50:PHE:CB	2.19	0.56
1:X:408:U:H2'	1:X:409:G:C8	2.41	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
1:X:1573:G:H3'	1:X:1574:A:H5"	1.87	0.56
1:X:1650:A:N6	1:X:1652:G:C2	2.73	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
5:C:120:VAL:O	5:C:121:ASP:CB	2.52	0.56
6:D:22:TYR:OH	6:D:29:PRO:CD	2.52	0.56
6:D:126:GLY:O	6:D:160:ALA:HB3	2.05	0.56
25:W:3:ILE:HD11	25:W:44:VAL:HG22	1.86	0.56
30:4:19:ARG:NH1	30:4:24:LEU:HD22	2.20	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:2848:A:H2	13:K:6:ALA:HB1	1.70	0.56
1:X:2857:C:H5'	13:K:96:ARG:HB2	1.87	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: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
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
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
1:X:208:C:N4	1:X:209:G:N2	2.53	0.56
1:X:693:A:H2'	1:X:694:G:C8	2.41	0.56
1:X:1164:C:H5'	16:N:76:TYR:CE2	2.39	0.56
1:X:2002:A:H62	26:Z:9:LYS:HZ2	1.53	0.56
1:X:2595:C:O5'	1:X:2595:C:H6	1.88	0.56
1:X:2825:A:O4'	1:X:2843:A:C2	2.55	0.56
11:I:45:LYS:HD3	11:I:48:PHE:CZ	2.40	0.56
29:3:13:ARG:HG3	29:3:13:ARG:O	2.05	0.56
1:X:955:G:C5'	1:X:955:G:N3	2.69	0.56
1:X:2657:G:H1	1:X:2709:C:H42	1.54	0.56
1:X:2669:C:OP2	13:K:14:SER:HB2	2.05	0.56
32:X:2882:LMA:O53	32:X:2882:LMA:C32	2.50	0.56
3:A:66:ILE:HG23	3:A:68:PHE:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:4:19:ARG:HH11	30:4:24:LEU:HD22	1.70	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
1:X:1166:A:H5"	16:N:55:ARG:HD3	1.88	0.56
1:X:1790:G:H5"	3:A:262:ARG:NH2	2.21	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
5:C:162:ARG:HB3	5:C:162:ARG:NH1	2.17	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: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
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
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:538:A:H2'	1:X:538:A:N3	2.20	0.56
1:X:1261:G:O2'	16:N:3:ARG:HA	2.05	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
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
20:R:16:PHE:HB3	20:R:82:ALA:HB1	1.88	0.56
20:R:23:ILE:HG22	20:R:33:THR:HB	1.87	0.56
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
1:X:1142:G:C4	9:G:103:TYR:CD2	2.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:79:PHE:CE2	9:G:147:ARG:HG2	2.40	0.55
9:G:103:TYR:CD2	9:G:111:LYS:HB2	2.41	0.55
13:K:87:TYR:CD1	13:K:90:ARG:HD2	2.41	0.55
18:P:85:MET:HE1	18:P:129:ALA:HA	1.88	0.55
18:P:101:PRO:O	18:P:121:THR:HG23	2.06	0.55
1:X:396:U:C4	1:X:398:C:C5	2.94	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
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
29:3:9:MET:HE2	29:3:12:ARG:NH1	2.21	0.55
1:X:48:A:H4'	1:X:49:U:C5'	2.35	0.55
1:X:487:G:H21	1:X:491:A:H62	1.52	0.55
1:X:599:A:C2	1:X:681:A:C2	2.93	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
2:Y:45:C:H2'	6:D:92:ARG:NE	2.21	0.55
3:A:160:ALA:HA	3:A:199:ASN:OD1	2.06	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
27:1:9:ILE:HD12	27:1:26:LYS:CG	2.36	0.55
1:X:1605:A:C6	1:X:1606:C:N4	2.73	0.55
1:X:2371:A:HO2'	11:I:59:ARG:HG2	1.72	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
18:P:30:TYR:H	18:P:123:HIS:CE1	2.24	0.55
29:3:13:ARG:HB2	29:3:25:PHE:CD1	2.42	0.55
1:X:332:C:H5"	1:X:333:A:OP2	2.06	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
1:X:2707:G:N7	1:X:2708:U:C4	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:760:U:C4	1:X:2592:U:C4	2.94	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
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:303:C:H42	1:X:359:G:H1	1.54	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
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
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
1:X:201:G:H2'	1:X:202:A:C8	2.42	0.55
1:X:525:A:N7	1:X:526:C:C4	2.75	0.55
1:X:1989:C:O2'	1:X:2798:A:C2'	2.55	0.55
1:X:2045:A:C5	32:X:2882:LMA:C27	2.90	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:236:C:H1'	1:X:632:A:O2'	2.07	0.55
1:X:869:C:O5'	1:X:869:C:H6	1.90	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:2612:G:C2	1:X:2766:U:O2	2.59	0.55
2:Y:17:A:H1'	2:Y:112:A:C8	2.42	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: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
1:X:1145:C:C6	1:X:1147:G:OP2	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1265:G:H1	16:N:37:GLN:HB2	1.72	0.55
1:X:1645:U:O2	1:X:2677:U:H4'	2.07	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
19:Q:7:LEU:HD13	19:Q:7:LEU:H	1.71	0.55
1:X:17:G:C2	1:X:534:U:O2	2.60	0.54
1:X:121:G:H2'	1:X:122:G:O4'	2.07	0.54
1:X:177:U:O4	1:X:225:G:C2	2.60	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
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:2020:G:H2'	1:X:2021:G:C8	2.42	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
27:1:12:MET:CG	27:1:27:ASN:OD1	2.50	0.54
1:X:832:A:C4	1:X:1203:A:C2	2.95	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
9:G:30:LYS:HG2	9:G:30:LYS:O	2.06	0.54
10:H:76:ARG:O	10:H:95:ALA:N	2.38	0.54
12:J:27:TYR:O	12:J:28:VAL:HG22	2.07	0.54
12:J:135:ARG:O	12:J:136:GLU:CB	2.54	0.54
20:R:90:LYS:HZ1	20:R:113:THR:HG22	1.71	0.54
1:X:593:C:N4	1:X:594:G:C6	2.75	0.54
1:X:825:C:H6	11:I:30:ALA:HB1	1.73	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
1:X:2497:A:H2'	1:X:2497:A:N3	2.22	0.54
1:X:2659:C:H5'	4:B:189:PRO:HA	1.89	0.54
4:B:184:VAL:HG13	4:B:185:LYS:N	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:23:ARG:NH2	10:H:23:ARG:CB	2.66	0.54
21:S:13:LYS:HE2	21:S:33:ALA:CB	2.38	0.54
1:X:1365:U:C2	1:X:1393:G:N2	2.75	0.54
1:X:1668:G:H5"	1:X:1668:G:C8	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:2767:C:H1'	4:B:62:PRO:HG3	1.88	0.54
4:B:15:TRP:CH2	15:M:84:ALA:HB3	2.43	0.54
4:B:184:VAL:CG1	4:B:185:LYS:N	2.70	0.54
9:G:90:LEU:HD12	9:G:90:LEU:N	2.23	0.54
1:X:208:C:H41	1:X:209:G:N2	2.05	0.54
1:X:469:G:H5'	28:2:39:ARG:HB2	1.88	0.54
1:X:572:G:H5'	1:X:581:A:H4'	1.90	0.54
1:X:1632:A:H4'	1:X:1633:C:OP2	2.06	0.54
1:X:1677:C:H6	1:X:1677:C:H5"	1.71	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: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
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: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
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
3:A:71:ARG:NH1	3:A:150:PRO:HB3	2.22	0.54
9:G:137:LYS:HG2	9:G:137:LYS:O	2.07	0.54
14:L:38:ILE:HG21	14:L:71:VAL:HG11	1.90	0.54
26:Z:3:LYS:O	26:Z:6:VAL:HG23	2.07	0.54
1:X:749:C:H3'	1:X:749:C:H6	1.72	0.54
1:X:1296:G:N2	1:X:1299:A:H8	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2032:G:N2	1:X:2599:U:N3	2.56	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
4:B:152:LYS:HB2	9:G:106:TYR:CB	2.38	0.54
13:K:51:LEU:CD2	13:K:70:ILE:HD11	2.38	0.54
27:1:16:ALA:HB2	27:1:50:PHE:CE1	2.43	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
1:X:2355:A:H61	14:L:91:ARG:CZ	2.21	0.54
1:X:2392:G:H2'	1:X:2393:G:H8	1.73	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
15:M:39:VAL:HG12	15:M:45:THR:CB	2.38	0.54
1:X:572:G:H22	1:X:587:A:H2	1.56	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
21:S:155:PRO:O	21:S:156:GLU:CB	2.55	0.54
1:X:674:U:H1'	11:I:22:GLY:HA2	1.90	0.53
1:X:995:A:OP2	1:X:996:C:N4	2.40	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
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
18:P:14:ARG:O	18:P:17:GLN:HG2	2.08	0.53
18:P:107:ILE:CG2	18:P:117:ILE:HG12	2.38	0.53
27:1:8:ILE:CG1	27:1:30:ASN:HD21	2.16	0.53
1:X:626:A:O2'	5:C:176:ASN:CG	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2814:G:C4'	13:K:49:GLU:OE2	2.55	0.53
2:Y:83:C:C2'	2:Y:84:G:C5'	2.83	0.53
7:E:171:LEU:N	7:E:171:LEU:HD12	2.23	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
20:R:90:LYS:HB2	20:R:108:VAL:HG21	1.90	0.53
26:Z:8:LYS:C	26:Z:9:LYS:HG3	2.28	0.53
29:3:59:LYS:O	29:3:60:LEU:CB	2.56	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: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
1:X:2045:A:C5	32:X:2882:LMA:H27A	2.40	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
3:A:26:THR:HG22	3:A:27:LYS:H	1.58	0.53
3:A:211:GLY:C	3:A:213:SER:H	2.12	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:HG22	22:T:43:THR:O	2.07	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
1:X:318:G:O2'	1:X:319:G:C8	2.61	0.53
1:X:1681:A:N6	1:X:1979:C:N4	2.46	0.53
1:X:1683:G:H4'	10:H:6:SER:OG	2.08	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
4:B:176:ARG:NH2	15:M:19:ASP:OD2	2.41	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
16:N:93:LYS:HZ3	17:O:10:LYS:HE2	1.69	0.53
1:X:28:A:H1'	1:X:523:A:C2	2.44	0.53
1:X:131:C:C2	1:X:141:G:N2	2.77	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
1:X:1006:C:OP2	16:N:54:LYS:NZ	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2350:G:O2'	27:1:46:LYS:HB3	2.07	0.53
1:X:2496:C:C5	1:X:2521:A:C8	2.97	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:HE2	13:K:80:MET:HA	1.89	0.53
21:S:87:THR:O	21:S:88:TYR:CB	2.55	0.53
29:3:13:ARG:HD2	29:3:25:PHE:HD1	1.72	0.53
1:X:131:C:O2	1:X:141:G:N2	2.42	0.53
1:X:219:G:H2'	1:X:220:U:OP2	2.08	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
3:A:70:ARG:HD3	3:A:120:ALA:HB2	1.90	0.53
3:A:160:ALA:CB	3:A:199:ASN:CB	2.87	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:496:C:C2'	1:X:497:C:H5'	2.38	0.53
1:X:1135:C:H1'	30:4:36:GLN:OE1	2.08	0.53
1:X:1687:C:H2'	1:X:1688:U:O4'	2.09	0.53
2:Y:45:C:H2'	6:D:92:ARG:CZ	2.39	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
7:E:50:LEU:HD23	7:E:51:LEU:N	2.24	0.53
1:X:537:C:H1'	1:X:538:A:C6	2.44	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
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:41:G:H2'	1:X:42:G:C8	2.44	0.53
1:X:331:U:C2'	5:C:162:ARG:HH12	2.22	0.53
1:X:1174:G:H2'	1:X:1175:A:H8	1.74	0.53
1:X:1324:G:C2'	19:Q:72:ARG:HH22	2.21	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:2698:G:H5"	15:M:105:TYR:CD2	2.44	0.53
2:Y:107:C:H2'	2:Y:108:G:O4'	2.09	0.53
6:D:108:LEU:HB2	6:D:109:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
21:S:6:LYS:HB2	21:S:31:SER:O	2.08	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: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:693:A:C6	1:X:811:G:C2	2.97	0.53
1:X:695:G:N2	1:X:809:C:C2	2.77	0.53
1:X:827:C:OP1	17:O:83:ARG:N	2.42	0.53
1:X:1242:A:H2'	1:X:1243:G:C8	2.44	0.53
2:Y:39:C:H5'	2:Y:40:C:OP2	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
18:P:32:ARG:NE	18:P:32:ARG:CA	2.61	0.53
1:X:543:G:H5'	16:N:24:PHE:CE1	2.43	0.52
1:X:756:C:OP1	4:B:130:GLY:HA3	2.09	0.52
1:X:794:A:H5'	3:A:219:LYS:NZ	2.23	0.52
1:X:795:A:N1	3:A:227:MET:HE3	2.23	0.52
1:X:821:A:H2'	1:X:822:G:C8	2.44	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
3:A:71:ARG:NH1	3:A:151:GLY:N	2.57	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:679:C:H4'	11:I:49:PHE:CE1	2.45	0.52
1:X:681:A:H5"	1:X:681:A:C8	2.44	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
3:A:245:ARG:HA	3:A:253:LYS:HZ1	1.74	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:177:U:O2'	1:X:178:C:O4'	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:X:1393:G:O2'	1:X:1394:G:H5'	2.09	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:83:TYR:CZ	7:E:138:LYS:HD2	2.44	0.52
7:E:174:GLY:C	7:E:175:LYS:HG2	2.29	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
27:1:29:ARG:HA	27:1:33:ALA:CB	2.40	0.52
28:2:9:ASN:HA	28:2:12:ARG:HB3	1.91	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
1:X:1069:G:N3	8:F:116:ASN:ND2	2.57	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
7:E:87:LEU:HB2	7:E:131:ILE:HB	1.90	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: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: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
11:I:62:LYS:CD	29:3:13:ARG:N	2.73	0.52
18:P:110:ALA:O	18:P:111:ARG:HB2	2.09	0.52
1:X:33:C:O2	1:X:466:A:C2	2.61	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:H37B	32:X:2882:LMA:H35	1.91	0.52
2:Y:40:C:O4'	14:L:97:HIS:CE1	2.62	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
19:Q:7:LEU:HD13	19:Q:7:LEU:N	2.24	0.52
1:X:537:C:O2	1:X:538:A:C2	2.63	0.52
1:X:879:A:N3	1:X:879:A:C2'	2.69	0.52
1:X:1313:U:H4'	1:X:1314:A:C5'	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1680:U:O2'	1:X:1681:A:O5'	2.28	0.52
1:X:2000:U:O2'	26:Z:9:LYS:HA	2.09	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
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
1:X:965:G:H8	1:X:965:G:O5'	1.92	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
3:A:219:LYS:C	3:A:219:LYS:CD	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: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
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:2357:A:H1'	14:L:88:VAL:HG13	1.92	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
6:D:4:LEU:CG	6:D:5:LYS:H	2.12	0.52
11:I:57:ILE:HG23	29:3:12:ARG:CZ	2.40	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
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:883:A:C2	1:X:920:G:C6	2.98	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
3:A:31:GLU:HB2	3:A:83:ILE:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:5:GLN:HG3	10:H:5:GLN:O	2.11	0.51
10:H:28:GLY:O	10:H:35:THR:N	2.42	0.51
12:J:54:VAL:CG2	12:J:125:LYS:NZ	2.73	0.51
12:J:99:LYS:CD	12:J:100:PRO:HD2	2.39	0.51
27:1:9:ILE:CD1	27:1:26:LYS:HD2	2.39	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
1:X:1332:G:C6	1:X:1333:G:O6	2.63	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:O	15:M:27:PHE:CD1	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: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:1937:G:N3	1:X:2530:C:H5'	2.25	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
2:Y:84:G:H2'	2:Y:85:G:C8	2.44	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:5:A:C2	1:X:2873:G:C2	2.98	0.51
1:X:321:A:O2'	1:X:322:A:H2'	2.10	0.51
1:X:817:A:OP1	11:I:45:LYS:CG	2.57	0.51
1:X:1291:G:H5"	13:K:34:ILE:HD12	1.92	0.51
1:X:1673:C:H42	1:X:1987:G:H1	1.58	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: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
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:693:A:C2	1:X:811:G:C2	2.98	0.51
1:X:695:G:N2	1:X:809:C:O2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1194:U:O2'	1:X:1195:U:C6	2.55	0.51
1:X:1692:C:N3	4:B:128:SER:O	2.43	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
9:G:67:ARG:HB3	9:G:70:PHE:CA	2.26	0.51
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:119:G:H2'	1:X:120:G:H8	1.76	0.51
1:X:331:U:O2'	5:C:162:ARG:NH1	2.43	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:2848:A:C2	13:K:7:GLY:N	2.78	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
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: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:1128:G:H3'	1:X:1129:A:C5'	2.40	0.51
1:X:1277:G:N2	1:X:1997:A:C8	2.79	0.51
1:X:1982:C:H2'	1:X:1983:G:H8	1.76	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
4:B:84:PHE:O	4:B:84:PHE:CG	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:O	14:L:37:HIS:CG	2.64	0.51
15:M:103:LYS:HG3	15:M:105:TYR:CE2	2.46	0.51
1:X:334:G:H3'	5:C:162:ARG:HD3	1.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:27:SER:HB3	10:H:50:ILE:H	1.75	0.51
10:H:110:VAL:HG23	10:H:129:LEU:HB3	1.93	0.51
14:L:51:LEU:N	14:L:51:LEU:CD1	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
24:V:17:GLU:O	24:V:21:ARG:HD3	2.11	0.51
1:X:331:U:H1'	5:C:162:ARG:NH1	2.17	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:2592:U:H2'	26:Z:5:PRO:CG	2.41	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: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:542:A:H2	1:X:2004:U:HO2'	1.57	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: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:2427:A:H5'	1:X:2428:U:OP2	2.10	0.51
31:X:2881:LC2:C3	31:X:2881:LC2:C28	2.79	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
27:1:38:LYS:CD	27:1:40:TYR:HE1	2.24	0.51
1:X:583:C:N3	4:B:145:LYS:NZ	2.59	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
1:X:1073:G:H21	8:F:133:SER:CB	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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
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:H5"	1:X:2664:G:H8	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
2:Y:84:G:C2	2:Y:98:C:C2	2.99	0.50
11:I:56:LEU:HD11	29:3:52:LYS:HD2	1.93	0.50
1:X:540:G:N7	1:X:2005:U:H5"	2.26	0.50
1:X:782:U:O2	1:X:1392:U:H1'	2.11	0.50
1:X:791:G:C2	1:X:800:U:C2	2.99	0.50
1:X:884:C:OP1	12:J:9:LYS:HG3	2.12	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
2:Y:23:G:C2	2:Y:65:A:C2	3.00	0.50
5:C:180:ILE:HG23	5:C:181:LEU:N	2.27	0.50
1:X:29:U:H4'	16:N:11:ARG:HH22	1.75	0.50
1:X:100:G:H4'	1:X:101:A:OP1	2.12	0.50
1:X:827:C:OP1	17:O:82:ARG:HA	2.11	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
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
7:E:165:VAL:HG12	7:E:166:GLY:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:89:ILE:HG23	15:M:79:ARG:HD3	1.93	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
26:Z:12:SER:HB2	26:Z:15:LYS:H	1.76	0.50
30:4:24:LEU:HD23	30:4:35:ARG:CZ	2.42	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
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:OP2	1:X:2005:U:O4'	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
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
27:1:29:ARG:HA	27:1:33:ALA:HB2	1.93	0.50
1:X:175:C:H6	1:X:175:C:O5'	1.95	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:789:G:N2	1:X:2220:A:OP1	2.45	0.50
1:X:793:G:H1'	1:X:798:G:H22	1.76	0.50
1:X:1021:A:OP1	16:N:66:ASN:ND2	2.44	0.50
1:X:2199:C:C2'	1:X:2200:G:H5'	2.41	0.50
1:X:2554:C:O2'	4:B:140:SER:HB2	2.12	0.50
1:X:2671:C:N3	1:X:2698:G:N2	2.60	0.50
3:A:178:LEU:HB3	3:A:179:PRO:HD2	1.93	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: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
15:M:26:ASP:O	15:M:26:ASP:OD2	2.30	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
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
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: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
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
5:C:123:PHE:C	5:C:123:PHE:CD2	2.85	0.49
9:G:36:ASN:O	9:G:38:GLU:O	2.30	0.49
9:G:132:PHE:HB2	9:G:145:HIS:NE2	2.26	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:O	18:P:107:ILE:CG2	2.60	0.49
23:U:49:LYS:HA	23:U:62:LEU:H	1.76	0.49
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
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
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:O4'	1:X:1979:C:OP1	2.30	0.49
1:X:1993:G:OP1	18:P:37:LYS:HE3	2.12	0.49
1:X:2038:C:H2'	1:X:2483:U:C4'	2.41	0.49
1:X:2040:A:O5'	1:X:2040:A:C8	2.60	0.49
1:X:2510:A:N6	1:X:2511:G:C6	2.80	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
10:H:116:ARG:CD	15:M:38:LYS:HE3	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:36:LYS:HE2	14:L:65:THR:HG22	1.94	0.49
27:1:9:ILE:C	27:1:10:VAL:HG23	2.32	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
1:X:1747:G:OP2	1:X:1747:G:O4'	2.29	0.49
1:X:2451:G:C5	1:X:2454:C:N4	2.81	0.49
1:X:2663:U:C2'	10:H:88:THR:HG21	2.39	0.49
1:X:2671:C:H1'	1:X:2822:U:H1'	1.93	0.49
5:C:22:VAL:CG1	5:C:110:SER:OG	2.56	0.49
18:P:91:PHE:CE1	18:P:131:LYS:HA	2.47	0.49
29:3:13:ARG:HB2	29:3:25:PHE:HD1	1.78	0.49
1:X:564:U:H2'	1:X:565:A:C8	2.47	0.49
1:X:579:G:H2'	1:X:2013:A:N6	2.28	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
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
2:Y:51:G:OP1	14:L:99:ARG:HG2	2.12	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:67:ILE:CG2	6:D:84:PRO:HB3	2.42	0.49
6:D:111:ILE:HB	6:D:114:PHE:HB2	1.93	0.49
11:I:60:LEU:HG	29:3:13:ARG:HD3	1.95	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
27:1:11:LYS:N	27:1:11:LYS:HD2	2.27	0.49
1:X:123:A:O4'	1:X:123:A:OP1	2.30	0.49
1:X:221:A:C2	1:X:232:A:C4	3.01	0.49
1:X:303:C:N3	1:X:360:A:H2	2.11	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: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
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:2356:A:H2	14:L:91:ARG:HH22	1.59	0.49
1:X:2404:A:OP2	1:X:2406:C:H5'	2.12	0.49
2:Y:39:C:C2	14:L:97:HIS:NE2	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
20:R:92:THR:HG22	20:R:108:VAL:CG2	2.43	0.49
1:X:171:G:O2'	1:X:172:A:H5'	2.12	0.49
1:X:1300:A:H5'	13:K:103:ARG:HD2	1.95	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: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
9:G:102:ARG:C	9:G:103:TYR:HD1	2.15	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: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
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:2475:C:OP1	12:J:83:ARG:HB3	2.13	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:2728:A:H4'	7:E:66:GLY:HA3	1.94	0.49
2:Y:25:G:H2'	2:Y:26:G:C5	2.47	0.49
3:A:25:LEU:CB	3:A:206:VAL:H	2.26	0.49
12:J:136:GLU:O	12:J:136:GLU:CG	2.58	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:OD1	20:R:85:ASP:O	2.30	0.49
1:X:76:C:C2	1:X:108:G:C2	3.00	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
1:X:1704:G:C2	1:X:1719:G:O6	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:Y:33:C:H5"	6:D:30:ARG:HH22	1.77	0.49
2:Y:83:C:C2'	2:Y:84:G:O5'	2.60	0.49
2:Y:117:G:H2'	2:Y:118:G:C8	2.48	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
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:861:G:C2'	1:X:862:A:H5'	2.43	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
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: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
1:X:958:G:O2'	1:X:995:A:C2	2.61	0.49
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:1391:A:O4'	1:X:1392:U:OP1	2.30	0.49
1:X:2275:U:C4	14:L:10:LYS:HE2	2.48	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:2795:A:C4'	13:K:5:LYS:HE3	2.42	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
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
13:K:80:MET:CA	13:K:80:MET:CE	2.89	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1817:U:H5'	3:A:253:LYS:HD3	1.94	0.48
1:X:1819:U:C2'	1:X:1820:G:H5'	2.43	0.48
1:X:2291:U:OP1	6:D:71:LYS:HD2	2.12	0.48
1:X:2595:C:H2'	1:X:2596:C:O4'	2.13	0.48
32:X:2882:LMA:C34	32:X:2882:LMA:C54	2.91	0.48
3:A:76:VAL:HG11	3:A:100:ASP:OD2	2.13	0.48
4:B:47:VAL:HB	4:B:84:PHE:HD2	1.76	0.48
4:B:102:ILE:HD11	4:B:184:VAL:HG22	1.94	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:32:C:O5'	1:X:32:C:H6	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
1:X:2720:A:N6	1:X:2721:A:N1	2.60	0.48
2:Y:85:G:C6	2:Y:86:A:C6	3.01	0.48
11:I:77:LEU:HB2	11:I:110:ALA:HA	1.95	0.48
16:N:40:LEU:HB3	17:O:74:TYR:CE2	2.47	0.48
16:N:66:ASN:ND2	16:N:70:ARG:HH12	2.12	0.48
18:P:80:LEU:HD11	18:P:87:GLU:HB3	1.95	0.48
27:1:10:VAL:HG12	27:1:11:LYS:N	2.28	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
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
3:A:55:ILE:N	3:A:55:ILE:HD12	2.28	0.48
5:C:17:LEU:HD12	5:C:17:LEU:N	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:496:C:H2'	1:X:497:C:H5'	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:90:SER:O	3:A:199:ASN:CG	2.50	0.48
3:A:106:ILE:HG22	3:A:107:LEU:N	2.28	0.48
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
29:3:6:THR:O	29:3:9:MET:HB3	2.14	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
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
3:A:55:ILE:N	3:A:218:ARG:HB3	2.29	0.48
4:B:35:GLN:HB3	4:B:48:GLN:OE1	2.14	0.48
4:B:120:TRP:CB	4:B:122:PHE:CE2	2.97	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:H	19:Q:7:LEU:CD1	2.26	0.48
20:R:11:ASN:O	20:R:12:ASP:CB	2.60	0.48
20:R:73:GLU:OE1	20:R:73:GLU:HA	2.12	0.48
24:V:18:ILE:HG22	24:V:22:LYS:HE2	1.94	0.48
27:1:9:ILE:HD11	27:1:26:LYS:HD2	1.94	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
1:X:958:G:N2	1:X:982:C:C2	2.81	0.48
1:X:1386:A:H5"	1:X:2191:A:H62	1.77	0.48
1:X:1975:G:C1'	1:X:1976:U:OP2	2.62	0.48
3:A:66:ILE:CD1	3:A:89:ARG:CZ	2.92	0.48
3:A:132:LEU:HD21	3:A:194:ILE:HD11	1.96	0.48
6:D:40:LEU:HD23	6:D:40:LEU:C	2.34	0.48
9:G:66:HIS:O	16:N:67:ALA:HB1	2.14	0.48
11:I:34:HIS:O	11:I:35:LYS:HD3	2.13	0.48
24:V:7:ARG:HD2	24:V:7:ARG:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:23:LEU:HD21	25:W:43:MET:HB3	1.95	0.48
26:Z:8:LYS:O	26:Z:9:LYS:HG3	2.14	0.48
1:X:537:C:O2	1:X:537:C:H2'	2.14	0.48
1:X:537:C:H5	1:X:2759:U:H2'	1.76	0.48
1:X:736:G:H2'	1:X:737:C:O4'	2.13	0.48
1:X:795:A:N1	3:A:227:MET:HE2	2.28	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
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
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
27:1:37:LEU:HA	27:1:51:ARG:HA	1.96	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
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:171:G:C2	1:X:179:U:O2	2.67	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: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
1:X:2626:U:O5'	1:X:2626:U:H6	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
1:X:2814:G:O4'	13:K:49:GLU:OE2	2.31	0.48
3:A:44:ARG:H	3:A:44:ARG:CD	2.01	0.48
3:A:71:ARG:CG	3:A:191:TYR:CE1	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:7:ARG:C	12:J:70:PHE:HZ	2.17	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: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
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
2:Y:84:G:H2'	2:Y:85:G:H8	1.79	0.48
3:A:71:ARG:NH1	3:A:151:GLY:H	2.12	0.48
3:A:216:LEU:HD12	3:A:216:LEU:N	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
27:1:38:LYS:HD3	27:1:40:TYR:HE1	1.78	0.48
1:X:525:A:C8	1:X:526:C:C5	3.02	0.47
1:X:542:A:N6	1:X:2003:A:N3	2.61	0.47
1:X:959:C:C1'	1:X:995:A:C2	2.96	0.47
1:X:1444:C:N4	1:X:1579:G:H1	2.09	0.47
1:X:1871:G:H3'	1:X:1871:G:N3	2.29	0.47
1:X:2399:C:H5	29:3:31:HIS:O	1.97	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
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
11:I:62:LYS:HZ3	29:3:12:ARG:C	2.16	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
27:1:8:ILE:C	27:1:9:ILE:CG2	2.81	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
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
1:X:1261:G:C5	16:N:3:ARG:HB2	2.49	0.47
1:X:1441:A:C8	1:X:1442:C:C5	3.02	0.47
1:X:2042:A:N1	32:X:2882:LMA:H29A	2.29	0.47
1:X:2191:A:H5"	1:X:2192:U:C5	2.49	0.47
1:X:2400:G:N7	29:3:32:GLN:HB3	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
28:2:15:THR:C	28:2:17:GLY:H	2.17	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
1:X:1042:G:H5'	30:4:6:SER:OG	2.14	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
2:Y:71:G:C6	2:Y:72:C:C2	3.03	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
27:1:17:GLY:O	27:1:18:THR:HB	2.13	0.47
1:X:40:U:H2'	1:X:41:G:O4'	2.14	0.47
1:X:173:A:O2'	1:X:2051:U:C5	2.67	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:1763:G:H2'	1:X:1764:A:H5'	1.97	0.47
1:X:1796:A:H1'	3:A:51:THR:HG23	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
2:Y:9:G:C2	2:Y:117:G:C2	3.02	0.47
3:A:70:ARG:NH1	3:A:131:ALA:HB2	2.29	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:410:A:OP1	23:U:47:HIS:CE1	2.68	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2046:C:C5	1:X:2047:C:N4	2.82	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
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
27:1:43:VAL:O	27:1:43:VAL:HG23	2.14	0.47
1:X:123:A:H5'	28:2:19:ARG:HE	1.79	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
1:X:977:G:H1'	1:X:2246:A:H62	1.80	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
3:A:150:PRO:HD3	3:A:187:HIS:NE2	2.29	0.47
11:I:60:LEU:HG	29:3:13:ARG:CD	2.44	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:94:C:H1'	24:V:40:PRO:CD	2.45	0.47
1:X:163:A:H2'	1:X:164:G:H8	1.80	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:523:A:H2	1:X:591:G:H4'	1.80	0.47
1:X:553:C:H42	1:X:559:C:N4	2.12	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:968:C:OP1	12:J:78:LYS:HB2	2.14	0.47
1:X:1128:G:C3'	1:X:1129:A:H5"	2.45	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:1851:A:H2'	1:X:1852:G:O4'	2.14	0.47
1:X:2258:G:O6	22:T:15:ASP:CG	2.53	0.47
1:X:2447:G:O2'	1:X:2448:A:C8	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2597:G:O2'	4:B:149:ARG:HB2	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
2:Y:104:A:N6	2:Y:105:G:C6	2.83	0.47
6:D:22:TYR:CZ	6:D:29:PRO:HD3	2.50	0.47
7:E:69:ARG:C	7:E:69:ARG:HD3	2.34	0.47
9:G:38:GLU:OE2	9:G:40:ASN:HB2	2.14	0.47
9:G:70:PHE:CD1	16:N:64:ARG:HA	2.49	0.47
9:G:94:LYS:HE3	9:G:94:LYS:HB2	1.80	0.47
17:O:22:VAL:CA	17:O:91:THR:HG22	2.41	0.47
21:S:25:ASN:OD1	21:S:26:LYS:HG2	2.15	0.47
21:S:95:SER:HA	21:S:121:GLN:HA	1.97	0.47
21:S:130:ILE:N	21:S:130:ILE:HD12	2.29	0.47
22:T:51:VAL:HG21	22:T:79:ILE:O	2.15	0.47
24:V:7:ARG:HD2	24:V:8:ASN:N	2.29	0.47
26:Z:33:CYS:CB	26:Z:38:GLY:O	2.63	0.47
27:1:3:LYS:HG2	27:1:4:ASP:N	2.30	0.47
1:X:161:U:H4'	1:X:194:G:N2	2.25	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
1:X:1141:U:C4	4:B:147:PRO:CD	2.95	0.47
1:X:2006:G:N2	1:X:2024:U:O2	2.48	0.47
1:X:2046:C:O2	1:X:2430:A:N1	2.48	0.47
1:X:2051:U:H3	1:X:2409:A:H62	1.63	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
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:OD1	20:R:85:ASP:C	2.52	0.47
1:X:579:G:C4'	1:X:994:A:C2	2.98	0.47
1:X:596:C:OP2	11:I:29:THR:HG21	2.15	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
1:X:2299:A:H3'	1:X:2299:A:N3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2671:C:O2'	1:X:2672:U:H5'	2.15	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
28:2:15:THR:O	28:2:16:HIS:CB	2.62	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: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
1:X:1998:A:H2	26:Z:5:PRO:O	1.98	0.47
32:X:2882:LMA:O57	18:P:111:ARG:NH2	2.48	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:HG23	10:H:81:ILE:O	2.14	0.47
19:Q:12:ILE:HD13	19:Q:12:ILE:N	2.29	0.47
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
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:2430:A:C6	31:X:2881:LC2:C15	2.98	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
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:314:G:C2	1:X:326:A:C2	3.03	0.46
1:X:514:G:C6	18:P:20:LEU:HD22	2.50	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
1:X:1480:G:C2	1:X:1481:U:O2	2.68	0.46
2:Y:3:A:H61	2:Y:122:U:H3	1.64	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
26:Z:49:CYS:SG	26:Z:51:TYR:HD1	2.39	0.46
1:X:26:G:C6	1:X:27:G:N1	2.84	0.46
1:X:41:G:H2'	1:X:42:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:540:G:C6	1:X:2005:U:C5'	2.98	0.46
1:X:791:G:N2	1:X:800:U:O2	2.48	0.46
1:X:1289:A:H2'	1:X:1290:A:C8	2.50	0.46
4:B:114:GLN:HB3	4:B:118:LYS:HB3	1.97	0.46
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
11:I:62:LYS:HZ2	29:3:15:LYS:HE2	1.81	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:1336:G:O6	1:X:1337:G:C6	2.68	0.46
1:X:1674:C:OP1	4:B:134:TRP:O	2.33	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
3:A:244:GLY:H	3:A:245:ARG:NH1	2.13	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:115:G:C6	1:X:117:A:N6	2.84	0.46
1:X:748:A:C5	1:X:749:C:C2	3.04	0.46
1:X:1058:G:H8	1:X:1058:G:H5"	1.81	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
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
4:B:92:ASN:OD1	4:B:92:ASN:N	2.46	0.46
4:B:183:LEU:HD21	15:M:16:ILE:HD13	1.98	0.46
5:C:46:ARG:HD2	5:C:51:VAL:HG23	1.97	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
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
23:U:14:VAL:O	23:U:15:VAL:CG2	2.63	0.46
1:X:89:A:H4'	1:X:90:G:H5"	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:478:G:H2'	1:X:479:G:C8	2.51	0.46
1:X:577:U:C5'	1:X:956:A:H61	2.24	0.46
1:X:830:C:O5'	1:X:830:C:H6	1.98	0.46
1:X:986:A:C2	1:X:1001:A:C8	3.03	0.46
1:X:1202:U:O2	1:X:1202:U:C2'	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
4:B:9:ILE:CG2	15:M:9:ARG:HB2	2.46	0.46
6:D:13:ARG:HG2	6:D:17:MET:HE1	1.98	0.46
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
1:X:28:A:H2'	1:X:29:U:O4'	2.16	0.46
1:X:118:U:H5"	1:X:120:G:OP2	2.15	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:1171:A:H1'	17:O:6:GLN:OE1	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
15:M:81:PHE:HA	15:M:82:PRO:HD2	1.74	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:396:U:H3	1:X:404:A:H61	1.63	0.46
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: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:2035:G:O2'	4:B:148:GLY:HA2	2.16	0.46
1:X:2427:A:H62	11:I:40:ARG:NH2	1.77	0.46
1:X:2547:C:H3'	1:X:2547:C:H6	1.81	0.46
1:X:2824:C:O4'	1:X:2843:A:C5	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:34:LEU:HD23	10:H:34:LEU:HA	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:24:G:C2	1:X:25:U:C2	3.04	0.46
1:X:26:G:C5	1:X:27:G:C6	3.04	0.46
1:X:84:G:H5'	20:R:41:PRO:HD3	1.97	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: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:1810:U:N3	3:A:155:GLN:HB3	2.31	0.46
1:X:2445:C:N4	1:X:2446:C:N4	2.64	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
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:573:C:H5	1:X:582:G:OP1	1.98	0.46
1:X:577:U:H2'	1:X:579:G:OP2	2.15	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:865:A:H5'	25:W:42:GLY:HA3	1.97	0.46
1:X:935:C:H4'	22:T:29:GLU:HG2	1.97	0.46
1:X:1392:U:O5'	1:X:1392:U:C6	2.67	0.46
1:X:1696:C:O5'	1:X:1696:C:C6	2.56	0.46
1:X:1978:U:C2	1:X:1979:C:C5	3.03	0.46
2:Y:112:A:H2'	2:Y:113:G:O4'	2.16	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:OD1	19:Q:57:ASN:N	2.49	0.46
20:R:11:ASN:HB3	20:R:13:LYS:HZ3	1.80	0.46
1:X:224:G:H4'	1:X:399:G:C5	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:551:A:C2	1:X:562:G:C2	3.05	0.45
1:X:1973:C:O5'	1:X:1973:C:H6	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
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:92:VAL:HG22	21:S:93:GLU:N	2.30	0.45
21:S:155:PRO:HG3	21:S:158:CYS:SG	2.56	0.45
28:2:10:ARG:HE	28:2:10:ARG:N	2.13	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
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:OP2	14:L:11:LEU:CD2	2.63	0.45
1:X:2274:C:H5	14:L:14:ARG:HH12	1.63	0.45
2:Y:118:G:O2'	2:Y:119:G:H5'	2.16	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:HB3	10:H:23:ARG:CZ	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:504:G:H4'	18:P:27:VAL:HG13	1.98	0.45
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
1:X:1097:A:H5"	1:X:1097:A:N3	2.32	0.45
1:X:1141:U:N3	4:B:147:PRO:HG3	2.31	0.45
1:X:1172:U:H2'	1:X:1173:G:C8	2.50	0.45
1:X:1477:C:O2'	1:X:2681:A:H1'	2.15	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:2275:U:C4	14:L:10:LYS:HD3	2.51	0.45
1:X:2671:C:H1'	1:X:2822:U:O2'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2840:U:N3	1:X:2841:U:C5	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
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
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: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:693:A:C2	1:X:811:G:N3	2.84	0.45
1:X:759:C:N3	32:X:2882:LMA:H37	2.31	0.45
1:X:759:C:C4	1:X:2590:U:H4'	2.51	0.45
1:X:797:A:C6	3:A:230:VAL:HG21	2.52	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:O5'	1:X:1687:C:H6	1.99	0.45
1:X:2198:U:C4	1:X:2199:C:C2	3.04	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
30:4:31:LYS:HD2	30:4:31:LYS:N	2.31	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
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
2:Y:110:U:H2'	2:Y:111:C:H5"	1.98	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:N	15:M:6:LYS:HD2	2.31	0.45
21:S:72:ASP:HB3	21:S:77:ALA:O	2.17	0.45
1:X:73:A:H5"	1:X:74:G:O4'	2.16	0.45
1:X:94:C:H1'	24:V:40:PRO:CG	2.47	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

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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
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:5:A:O2'	1:X:6:A:H5'	2.16	0.45
1:X:521:U:O4	1:X:522:G:C2	2.70	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
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
2:Y:52:G:P	14:L:65:THR:HB	2.57	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
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
27:1:43:VAL:O	27:1:44:ALA:CB	2.62	0.45
1:X:758:G:C2'	1:X:759:C:OP1	2.65	0.45
1:X:843:G:O4'	1:X:2427:A:H2	2.00	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:2754:C:C4	1:X:2755:A:C5	3.05	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:27:G:C2	1:X:522:G:H1'	2.51	0.45
1:X:171:G:H2'	1:X:172:A:C8	2.51	0.45
1:X:334:G:H1'	5:C:164:VAL:HG13	1.98	0.45
1:X:540:G:C6	1:X:2005:U:H5"	2.52	0.45
1:X:1272:G:H2'	1:X:1273:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1701:C:H42	1:X:1721:G:H1	1.64	0.45
1:X:2251:U:H5"	1:X:2252:A:OP1	2.17	0.45
12:J:36:ILE:HG12	12:J:103:VAL:HG23	1.99	0.45
12:J:126:LEU:HA	12:J:127:PRO:HD3	1.70	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
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
26:Z:45:ILE:HG12	26:Z:52:TYR:HB2	1.99	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
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
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
5:C:158:ARG:O	5:C:159:ARG:C	2.55	0.45
6:D:80:ARG:H	6:D:80:ARG:NE	2.15	0.45
11:I:114:ILE:HG23	11:I:114:ILE:O	2.17	0.45
12:J:36:ILE:HG12	12:J:103:VAL:CG2	2.46	0.45
13:K:31:GLU:OE1	13:K:31:GLU:HA	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
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
1:X:512:A:H5'	18:P:16:GLN:HB3	1.99	0.44
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
1:X:2664:G:N2	1:X:2705:A:N7	2.56	0.44
1:X:2670:C:H2'	1:X:2671:C:C6	2.52	0.44
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:39:VAL:CG1	15:M:45:THR:HG23	2.46	0.44
15:M:55:ILE:HG22	15:M:104:LEU:HB2	2.00	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
21:S:3:LEU:HD21	21:S:32:PHE:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:13:A:N3	1:X:15:G:C6	2.85	0.44
1:X:67:G:N2	1:X:73:A:C2	2.86	0.44
1:X:101:A:H2'	1:X:102:C:O4'	2.17	0.44
1:X:135:U:H5"	1:X:136:A:OP1	2.17	0.44
1:X:337:G:HO2'	20:R:9:HIS:HD1	1.38	0.44
1:X:469:G:H5"	28:2:39:ARG:H	1.82	0.44
1:X:555:U:C4	1:X:1243:G:N2	2.86	0.44
1:X:617:U:C5	1:X:631:G:C8	3.05	0.44
1:X:923:A:N6	12:J:12:LYS:HD3	2.31	0.44
1:X:1195:U:H2'	1:X:1196:G:C8	2.52	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
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:3:ARG:HH12	16:N:5:LYS:HG2	1.81	0.44
16:N:53:LYS:O	16:N:57:PHE:HD1	2.00	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
21:S:175:ARG:O	21:S:175:ARG:HG2	2.16	0.44
26:Z:3:LYS:O	26:Z:4:HIS:C	2.55	0.44
1:X:48:A:N6	1:X:154:U:H5	2.14	0.44
1:X:306:G:C6	1:X:355:G:C2	3.06	0.44
1:X:623:G:H3'	1:X:624:A:H5"	1.98	0.44
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
1:X:1677:C:C6	1:X:1677:C:C3'	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
2:Y:8:C:O2'	2:Y:9:G:H5'	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:827:C:OP2	11:I:32:ARG:CZ	2.66	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:1836:C:H5'	3:A:255:THR:O	2.18	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:2599:U:H5"	4:B:153:GLY:HA2	2.00	0.44
1:X:2670:C:H4'	1:X:2846:G:O2'	2.17	0.44
2:Y:66:G:C5	2:Y:67:C:C4	3.06	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:HD3	12:J:11:ARG:HA	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:81:C:C4	1:X:82:G:C6	3.06	0.44
1:X:224:G:C2	1:X:229:G:N1	2.86	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: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:2426:G:O2'	1:X:2427:A:P	2.76	0.44
1:X:2554:C:O2'	4:B:140:SER:CB	2.66	0.44
1:X:2827:G:N2	1:X:2840:U:O2	2.45	0.44
3:A:34:LEU:C	3:A:34:LEU:HD12	2.38	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
9:G:70:PHE:HE1	16:N:67:ALA:HB3	1.82	0.44
12:J:42:TRP:CB	12:J:95:VAL:HG11	2.41	0.44
20:R:98:ILE:HD11	20:R:105:ARG:HD2	1.99	0.44
29:3:49:VAL:HG21	29:3:52:LYS:HE2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:X:1265:G:C4'	16:N:33:ARG:HD3	2.48	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
2:Y:12:C:C5	2:Y:13:C:C4	3.06	0.44
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:49:GLU:OE1	13:K:95:THR:HG22	2.18	0.44
13:K:84:ALA:N	13:K:85:PRO:HD2	2.33	0.44
16:N:14:HIS:CD2	16:N:32:TYR:CZ	3.06	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
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
1:X:860:U:O2	1:X:860:U:H2'	2.17	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:C3'	1:X:2595:C:C6	3.01	0.44
1:X:2691:C:OP1	1:X:2694:G:H4'	2.17	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
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
1:X:2:G:O2'	1:X:3:U:H5'	2.17	0.44
1:X:3:U:O2'	1:X:4:C:O5'	2.30	0.44
1:X:26:G:C6	1:X:27:G:C6	3.05	0.44
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:454:G:H21	5:C:42:THR:HB	1.82	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
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: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
3:A:184:ARG:HB3	3:A:184:ARG:HH11	1.79	0.44
13:K:24:GLN:HB3	13:K:44:LEU:HD22	2.00	0.44
13:K:28:LEU:HD23	13:K:28:LEU:C	2.38	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
29:3:34:THR:OG1	29:3:35:GLY:N	2.51	0.44
1:X:163:A:H2'	1:X:164:G:C8	2.52	0.44
1:X:187:U:O5'	1:X:187:U:H6	2.00	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
1:X:1329:U:H2'	1:X:1330:G:C8	2.52	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
2:Y:51:G:H2'	2:Y:52:G:H8	1.82	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
27:1:21:TYR:HE2	27:1:23:THR:OG1	2.01	0.44
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:958:G:C2	1:X:982:C:N3	2.86	0.43
1:X:959:C:H1'	1:X:995:A:N3	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1790:G:O2’	3:A:184:ARG:HD3	2.18	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:N3	1:X:2745:A:C3’	2.81	0.43
2:Y:80:A:H2’	2:Y:81:C:O4’	2.17	0.43
3:A:126:PRO:HG3	3:A:132:LEU:HD11	2.00	0.43
4:B:99:GLY:H	4:B:172:VAL:HB	1.82	0.43
4:B:146:THR:CB	4:B:147:PRO:HD2	2.41	0.43
5:C:4:ILE:O	5:C:4:ILE:HG13	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
19:Q:12:ILE:O	19:Q:13:SER:CB	2.64	0.43
1:X:219:G:C2’	1:X:220:U:OP2	2.66	0.43
1:X:337:G:HO2’	1:X:338:G:H5’	1.83	0.43
1:X:472:C:O5’	1:X:472:C:H6	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
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: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
3:A:47:ARG:HD3	3:A:48:GLY:N	2.33	0.43
3:A:184:ARG:HB3	3:A:184:ARG:CZ	2.49	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
26:Z:42:SER:O	26:Z:44:HIS:CD2	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:919:U:H2'	1:X:920:G:C8	2.54	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:2291:U:P	6:D:71:LYS:HD2	2.59	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:H3'	1:X:2547:C:C6	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: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
6:D:4:LEU:CG	6:D:5:LYS:N	2.78	0.43
6:D:117:ILE:HD12	6:D:175:LEU:HD11	2.00	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
27:1:11:LYS:N	27:1:11:LYS:CD	2.81	0.43
1:X:123:A:C2'	1:X:124:A:OP1	2.66	0.43
1:X:547:U:H1'	9:G:73:ASN:HD21	1.83	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
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:2400:G:OP1	27:1:4:ASP:CG	2.57	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
2:Y:54:U:H2'	2:Y:55:C:O4'	2.18	0.43
6:D:17:MET:N	6:D:17:MET:SD	2.92	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:239:A:H2'	1:X:240:U:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:699:G:C2	28:2:5:TYR:HE1	2.17	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
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:2818:G:H2'	1:X:2819:G:C8	2.53	0.43
2:Y:93:G:H2'	2:Y:94:G:O4'	2.18	0.43
3:A:34:LEU:CG	3:A:34:LEU:O	2.66	0.43
4:B:36:ARG:NH1	4:B:86:PRO:O	2.52	0.43
4:B:77:ILE:HD13	4:B:195:LEU:HD22	2.00	0.43
4:B:183:LEU:HD11	15:M:16:ILE:HG21	2.00	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:CD1	19:Q:88:ILE:O	2.66	0.43
29:3:28:GLY:C	29:3:29:LYS:HG2	2.39	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:212:ARG:O	3:A:212:ARG:HG3	2.17	0.43
4:B:26:VAL:HG11	4:B:196:VAL:HG21	2.00	0.43
4:B:101:LYS:HA	4:B:170:LEU:O	2.18	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
27:1:45:LYS:C	27:1:46:LYS:HG2	2.39	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
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:1999:U:O2	26:Z:7:PRO:HG2	2.18	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:170:LEU:HD13	4:B:184:VAL:HG11	2.00	0.43
5:C:74:VAL:HG23	5:C:74:VAL:O	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:63:HIS:CE1	17:O:91:THR:HB	2.54	0.43
17:O:80:TYR:O	17:O:80:TYR:CD1	2.70	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
26:Z:41:LEU:O	26:Z:44:HIS:HB2	2.19	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
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:1686:A:O3'	1:X:2528:G:H5'	2.19	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: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
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: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:576:A:H4'	1:X:821:A:OP1	2.19	0.43
1:X:742:G:O6	1:X:1765:C:N3	2.52	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
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
3:A:43:GLY:N	3:A:44:ARG:HH11	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:94:C:H1'	24:V:40:PRO:HD2	2.00	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
1:X:1261:G:OP1	16:N:2:PRO:HD2	2.19	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:1996:A:OP1	18:P:118:LYS:HB2	2.18	0.43
1:X:2024:U:H2'	1:X:2025:A:C8	2.54	0.43
1:X:2475:C:OP1	12:J:83:ARG:CB	2.67	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
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
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
17:O:11:GLN:NE2	17:O:11:GLN:HA	2.33	0.43
20:R:64:ASN:N	20:R:65:PRO:HD3	2.34	0.43
27:1:42:PRO:HD3	27:1:48:VAL:CG2	2.49	0.43
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
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:2038:C:N4	1:X:2479:U:H1'	2.34	0.42
1:X:2071:G:C2	1:X:2072:C:C2	3.07	0.42
1:X:2795:A:H3'	1:X:2795:A:N3	2.34	0.42
3:A:61:ARG:HH22	3:A:216:LEU:HG	1.83	0.42
3:A:268:ASP:C	3:A:268:ASP:OD1	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	12:J:67:ILE:HG22	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
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:29:U:C4'	16:N:11:ARG:HH22	2.31	0.42
1:X:995:A:P	1:X:996:C:C5	3.13	0.42
1:X:1075:C:H5"	8:F:87:GLY:HA3	2.01	0.42
1:X:1326:U:O2	1:X:1326:U:H3'	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:1935:A:C2	10:H:22:ILE:HG23	2.54	0.42
1:X:1996:A:O2'	18:P:115:ASN:ND2	2.50	0.42
2:Y:117:G:H2'	2:Y:118:G:H8	1.84	0.42
3:A:55:ILE:HD12	3:A:55:ILE:H	1.83	0.42
3:A:151:GLY:O	3:A:153:GLY:N	2.52	0.42
15:M:69:ARG:CZ	15:M:108:ARG:HA	2.49	0.42
16:N:83:LEU:HD12	16:N:83:LEU:N	2.34	0.42
23:U:17:SER:HB2	23:U:44:ALA:HA	1.99	0.42
1:X:45:C:C2	1:X:157:G:N2	2.87	0.42
1:X:221:A:C2	1:X:232:A:C5	3.07	0.42
1:X:426:C:H4'	1:X:1863:U:O2'	2.19	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: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:2002:A:N6	26:Z:9:LYS:HZ2	2.18	0.42
1:X:2012:A:C2	1:X:2016:A:C6	3.06	0.42
1:X:2594:U:O2	1:X:2594:U:C2'	2.61	0.42
1:X:2657:G:N2	1:X:2710:C:O2	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:7:THR:O	17:O:8:GLY:O	2.37	0.42
17:O:65:ARG:HE	17:O:87:ARG:CD	2.24	0.42
21:S:100:THR:HG23	21:S:138:VAL:HG21	2.00	0.42
1:X:188:G:C6	1:X:189:A:C6	3.06	0.42
1:X:224:G:H4'	1:X:399:G:C4	2.54	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:C8	1:X:764:A:C3'	3.02	0.42
1:X:941:U:H2'	1:X:942:U:O4'	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: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: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
3:A:151:GLY:C	3:A:153:GLY:N	2.71	0.42
4:B:67:PHE:CZ	4:B:75:THR:CG2	3.01	0.42
4:B:154:LYS:HE3	4:B:156:MET:HG3	1.99	0.42
9:G:103:TYR:CG	9:G:111:LYS:HB2	2.55	0.42
9:G:104:THR:O	9:G:107:GLN:NE2	2.52	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:171:G:C2	1:X:179:U:C2	3.06	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:H6	1:X:616:U:H5"	1.84	0.42
1:X:797:A:N1	3:A:230:VAL:HG11	2.33	0.42
1:X:1219:C:O5'	1:X:1219:C:H6	2.02	0.42
1:X:1466:C:H2'	1:X:1467:U:O4'	2.19	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2622:G:H1	1:X:2751:C:H42	1.68	0.42
1:X:2799:C:O5'	1:X:2799:C:H6	2.02	0.42
31:X:2881:LC2:H5	31:X:2881:LC2:H13	1.73	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:HD13	18:P:117:ILE:HA	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
27:1:45:LYS:O	27:1:46:LYS:CB	2.67	0.42
1:X:459:A:N7	1:X:484:G:C5	2.88	0.42
1:X:463:C:P	5:C:46:ARG:HG2	2.60	0.42
1:X:798:G:O2'	1:X:1770:U:H5"	2.19	0.42
1:X:1282:A:H61	1:X:1994:U:H3	1.68	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:1992:G:H1'	13:K:106:ASP:O	2.18	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
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:HD12	4:B:198:LEU:N	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
14:L:43:ILE:N	14:L:43:ILE:HD12	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
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
1:X:155:G:H2'	1:X:156:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:613:A:C6	1:X:668:A:H1'	2.54	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: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
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
3:A:93:ILE:CG2	3:A:105:TYR:HB3	2.50	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
28:2:12:ARG:O	28:2:15:THR:O	2.37	0.42
30:4:16:VAL:HG22	30:4:25:VAL:HG22	2.01	0.42
1:X:13:A:C2	1:X:15:G:N1	2.88	0.42
1:X:180:C:C4	1:X:181:A:C5	3.08	0.42
1:X:492:G:H2'	1:X:517:A:N1	2.35	0.42
1:X:504:G:O2'	18:P:26:ALA:HA	2.20	0.42
1:X:574:C:H4'	1:X:1266:G:O6	2.19	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
1:X:1128:G:H2'	1:X:1129:A:H5"	2.02	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: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:H8	1:X:1632:A:OP1	2.03	0.42
1:X:1768:U:O5'	1:X:1768:U:H6	2.03	0.42
1:X:2438:A:N6	1:X:2473:G:C2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:46:GLN:HB3	21:S:50:GLY:HA3	2.00	0.42
21:S:129:ARG:HH22	21:S:156:GLU:CD	2.09	0.42
27:1:14:SER:H	27:1:22:TYR:HD2	1.68	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
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:1691:G:C6	1:X:1972:G:O6	2.73	0.42
1:X:1836:C:N4	1:X:1879:G:H1	2.17	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:2737:A:N1	7:E:67:LEU:HD12	2.35	0.42
4:B:44:TYR:HB2	4:B:82:ARG:NH1	2.31	0.42
17:O:21:ARG:O	17:O:91:THR:HG22	2.18	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:CD	28:2:10:ARG:H	2.33	0.42
1:X:178:C:H2'	1:X:179:U:C6	2.55	0.42
1:X:205:A:H2'	1:X:206:U:H5'	2.01	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:750:C:C4'	1:X:779:U:O2'	2.68	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1967:U:H2'	1:X:1968:G:C8	2.54	0.42
1:X:2244:C:C4	1:X:2245:A:C5	3.08	0.42
1:X:2350:G:C2'	27:1:46:LYS:HG3	2.48	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
2:Y:26:G:H21	2:Y:29:C:N4	2.18	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:33:ARG:NH1	14:L:99:ARG:O	2.53	0.42
14:L:89:PHE:HZ	14:L:103:LEU:CD2	2.17	0.42
23:U:70:LEU:O	23:U:70:LEU:HD23	2.20	0.42
27:1:25:THR:HG22	27:1:27:ASN:ND2	2.35	0.42
1:X:658:G:H2'	1:X:659:G:C8	2.51	0.41
1:X:857:U:O5'	1:X:857:U:H6	2.02	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:O5'	1:X:1348:C:H6	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
1:X:1745:C:OP1	15:M:101:ARG:NH2	2.52	0.41
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:2344:G:H4'	22:T:60:PHE:CE1	2.54	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:93:SER:C	14:L:94:TYR:CD2	2.92	0.41
21:S:43:PHE:HE1	21:S:66:VAL:HG11	1.85	0.41
27:1:9:ILE:C	27:1:10:VAL:CG2	2.88	0.41
28:2:42:LEU:H	28:2:42:LEU:HD12	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
1:X:461:A:N7	1:X:462:G:N7	2.68	0.41
1:X:463:C:OP2	5:C:46:ARG:HG2	2.19	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:752:G:OP1	1:X:1775:A:N1	2.53	0.41
1:X:755:C:H4'	1:X:1692:C:O2'	2.20	0.41
1:X:800:U:C5	1:X:804:C:N3	2.88	0.41
1:X:1048:U:H3	1:X:1129:A:H61	1.66	0.41
1:X:1468:A:P	1:X:1468:A:H8	2.42	0.41
1:X:1635:G:O2'	28:2:1:MET:HG2	2.20	0.41
1:X:1684:G:H22	1:X:1977:C:N4	2.17	0.41
1:X:1997:A:H5'	18:P:115:ASN:CG	2.41	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
3:A:49:ARG:HH11	3:A:49:ARG:CB	2.33	0.41
5:C:163:ASN:OD1	5:C:167:VAL:HG22	2.20	0.41
15:M:60:SER:CA	15:M:64:LYS:HB2	2.49	0.41
22:T:62:LEU:N	22:T:62:LEU:HD22	2.35	0.41
1:X:215:G:H4'	1:X:618:A:O2'	2.20	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:825:C:C6	11:I:30:ALA:HB1	2.54	0.41
1:X:879:A:C2	1:X:926:C:H5"	2.55	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
1:X:1955:G:H2'	1:X:1956:G:C8	2.55	0.41
1:X:2500:C:H4'	1:X:2544:A:C4'	2.50	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
12:J:119:PHE:HD1	12:J:132:MET:SD	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:13:ASN:OD1	13:K:16:ALA:CB	2.69	0.41
16:N:24:PHE:O	16:N:29:SER:HB3	2.19	0.41
16:N:28:ARG:O	16:N:35:ALA:CB	2.67	0.41
18:P:48:LYS:HB2	18:P:48:LYS:HE3	1.69	0.41
21:S:6:LYS:N	21:S:7:PRO:HD3	2.35	0.41
30:4:19:ARG:HD2	30:4:24:LEU:HD22	2.03	0.41
1:X:455:A:H2	1:X:1258:G:N3	2.19	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:705:C:H4'	3:A:42:GLY:O	2.20	0.41
1:X:834:A:H2'	1:X:957:G:P	2.60	0.41
1:X:938:G:H2'	1:X:939:C:OP2	2.21	0.41
1:X:1265:G:H4'	16:N:33:ARG:HD3	2.02	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
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
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
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:13:A:C2	1:X:15:G:C6	3.08	0.41
1:X:95:G:H4'	24:V:41:HIS:CE1	2.55	0.41
1:X:104:C:O5'	1:X:104:C:H6	2.03	0.41
1:X:306:G:N2	1:X:355:G:H1'	2.35	0.41
1:X:320:A:N3	1:X:340:G:O2'	2.53	0.41
1:X:594:G:N7	1:X:1264:C:N4	2.69	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2598:C:H4'	4:B:151:TYR:O	2.19	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
3:A:133:PRO:HB2	3:A:135:ARG:HG2	2.03	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
26:Z:4:HIS:HB2	26:Z:5:PRO:HD2	1.98	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
1:X:984:A:C8	1:X:1202:U:C2	3.08	0.41
1:X:1142:G:N9	9:G:103:TYR:HD2	2.17	0.41
1:X:1175:A:C2	1:X:1176:U:C2	3.09	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:H5"	1:X:1671:A:C8	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:O5'	1:X:2665:G:C8	2.74	0.41
31:X:2881:LC2:H14	31:X:2881:LC2:H29	1.73	0.41
3:A:46:ASN:ND2	3:A:47:ARG:N	2.68	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
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
10:H:116:ARG:O	10:H:117:GLU:C	2.58	0.41
10:H:126:ILE:HG23	10:H:126:ILE:HD12	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
26:Z:31:THR:O	26:Z:39:LYS:HA	2.20	0.41
27:1:43:VAL:O	27:1:43:VAL:CG2	2.69	0.41
1:X:230:C:C2'	1:X:231:G:H5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:459:A:N6	1:X:484:G:H1'	2.36	0.41
1:X:547:U:H6	1:X:547:U:O5'	2.04	0.41
1:X:579:G:H2'	1:X:2013:A:C6	2.56	0.41
1:X:985:G:C8	1:X:1200:G:N2	2.89	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: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: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:H6	1:X:2853:U:O5'	2.04	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:OE1	11:I:73:GLU:N	2.53	0.41
14:L:60:LYS:HZ2	14:L:64:LYS:HE2	1.85	0.41
15:M:80:VAL:O	15:M:80:VAL:HG12	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
28:2:1:MET:CE	28:2:3:ARG:CZ	2.98	0.41
28:2:15:THR:O	28:2:16:HIS:HB2	2.21	0.41
1:X:152:G:O2'	1:X:153:A:H5'	2.21	0.41
1:X:1118:G:H2'	1:X:1119:U:H5'	2.03	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
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:39:C:H2'	1:X:40:U:C6	2.56	0.41
1:X:42:G:H2'	1:X:43:A:O4'	2.20	0.41
1:X:223:C:H42	29:3:7:HIS:HB3	1.82	0.41
1:X:469:G:C2'	28:2:39:ARG:O	2.69	0.41
1:X:538:A:C4'	1:X:539:A:OP1	2.69	0.41
1:X:573:C:C5	1:X:574:C:C5	3.09	0.41
1:X:752:G:OP1	1:X:1775:A:C2	2.74	0.41
1:X:795:A:C2	3:A:227:MET:HE2	2.55	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:C6	1:X:997:C:C3'	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1218:C:H2'	1:X:1219:C:C6	2.55	0.41
1:X:1341:G:N2	1:X:1664:G:N1	2.69	0.41
1:X:1386:A:H5"	1:X:2191:A:N6	2.35	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:1818:G:C6	1:X:1819:U:N3	2.89	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:2040:A:C8	1:X:2040:A:H3'	2.55	0.41
1:X:2051:U:O2	1:X:2051:U:H2'	2.20	0.41
1:X:2222:U:O2	1:X:2413:A:H2	2.02	0.41
1:X:2241:U:C6	1:X:2241:U:H3'	2.55	0.41
1:X:2258:G:O6	22:T:15:ASP:CB	2.69	0.41
1:X:2419:C:H6	1:X:2419:C:O5'	2.04	0.41
1:X:2429:A:H2'	1:X:2430:A:C8	2.55	0.41
1:X:2580:C:HO2'	1:X:2581:A:P	2.44	0.41
2:Y:32:C:H1'	2:Y:59:A:H61	1.86	0.41
2:Y:59:A:H1'	6:D:27:ALA:HB2	2.03	0.41
3:A:178:LEU:HD11	3:A:184:ARG:HG3	2.02	0.41
3:A:201:GLU:HG3	3:A:203:LYS:HB3	2.03	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
5:C:191:ALA:HA	5:C:194:GLU:HB3	2.02	0.41
6:D:80:ARG:NE	6:D:80:ARG:N	2.69	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
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
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
20:R:18:LYS:CD	20:R:18:LYS:N	2.79	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
1:X:1:G:H2'	1:X:2:G:C8	2.56	0.41
1:X:196:A:N6	1:X:197:G:C6	2.89	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:851:C:C2	1:X:952:A:C6	3.09	0.41
1:X:919:U:O2'	1:X:920:G:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:943:U:O2'	1:X:944:A:O4'	2.37	0.41
1:X:977:G:C1'	1:X:2246:A:H62	2.34	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: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:C51	32:X:2882:LMA:H21A	2.51	0.41
2:Y:66:G:H2'	2:Y:67:C:O4'	2.20	0.41
4:B:188:ILE:HA	4:B:189:PRO:HD3	1.81	0.41
5:C:102:LEU:HD23	5:C:102:LEU:C	2.39	0.41
7:E:105:MET:HA	7:E:105:MET:CE	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
12:J:8:THR:N	12:J:70:PHE:HZ	2.18	0.41
12:J:135:ARG:O	12:J:136:GLU:HB2	2.20	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
29:3:49:VAL:HG21	29:3:52:LYS:CE	2.51	0.41
1:X:333:A:C5'	5:C:162:ARG:CG	2.99	0.40
1:X:626:A:H4'	5:C:176:ASN:OD1	2.21	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: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
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
29:3:36:LYS:N	29:3:36:LYS:HD3	2.36	0.40
30:4:13:ASN:HB2	30:4:27:CYS:SG	2.61	0.40
1:X:119:G:H2'	1:X:120:G:C8	2.54	0.40
1:X:182:G:O2'	1:X:183:U:C5	2.74	0.40
1:X:688:A:H4'	5:C:61:GLN:HG2	2.03	0.40
1:X:754:G:C6	1:X:755:C:N4	2.90	0.40
1:X:1196:G:H2'	1:X:1197:U:O4'	2.21	0.40
1:X:1865:C:H2'	1:X:1866:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2814:G:C1'	13:K:49:GLU:OE2	2.70	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
9:G:116:ARG:HD2	9:G:116:ARG:HA	1.88	0.40
20:R:11:ASN:O	20:R:12:ASP:HB3	2.21	0.40
1:X:29:U:C5'	16:N:11:ARG:HH12	2.34	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
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:1628:C:C5'	28:2:7:PRO:HG2	2.49	0.40
1:X:1673:C:H5"	4:B:136:ARG:CD	2.43	0.40
1:X:1817:U:C5'	3:A:253:LYS:HD3	2.51	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
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:N	9:G:90:LEU:CD1	2.85	0.40
12:J:107:VAL:HG22	12:J:119:PHE:CZ	2.56	0.40
20:R:65:PRO:O	20:R:66:GLN:C	2.57	0.40
25:W:10:ILE:H	25:W:10:ILE:HG13	1.62	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:94:C:HO2'	24:V:40:PRO:HD2	1.86	0.40
1:X:486:U:O2	1:X:492:G:N2	2.54	0.40
1:X:583:C:N4	1:X:2017:U:OP1	2.51	0.40
1:X:965:G:O6	1:X:966:A:C6	2.74	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:1811:A:H2'	3:A:179:PRO:HG2	2.03	0.40
1:X:1928:G:N1	1:X:1929:U:N3	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2395:C:H2'	1:X:2396:C:H5'	2.03	0.40
1:X:2502:G:O5'	1:X:2502:G:C8	2.68	0.40
1:X:2506:C:H5"	30:4:30:VAL:HB	2.04	0.40
1:X:2671:C:N4	1:X:2698:G:H1	2.20	0.40
2:Y:33:C:H42	2:Y:53:G:H1	1.69	0.40
5:C:29:GLU:HG2	5:C:95:LEU:HD11	2.03	0.40
5:C:134:ILE:HG22	5:C:138:LYS:HE3	2.02	0.40
6:D:52:LYS:C	6:D:52:LYS:HD3	2.42	0.40
6:D:123:ASP:OD1	6:D:124:GLY:N	2.54	0.40
9:G:46:ALA:CB	9:G:54:LEU:HD21	2.52	0.40
10:H:4:PRO:O	10:H:5:GLN:HB3	2.22	0.40
10:H:129:LEU:HD23	10:H:129:LEU:HA	1.73	0.40
12:J:54:VAL:HG23	12:J:125:LYS:HZ2	1.86	0.40
12:J:88:LYS:NZ	12:J:88:LYS:HB2	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
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:309:G:OP1	20:R:93:ARG:CA	2.69	0.40
1:X:497:C:C6	1:X:497:C:H3'	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
1:X:1098:G:O6	1:X:1100:G:C2	2.74	0.40
1:X:1275:A:N3	26:Z:10:LYS:HE2	2.35	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
2:Y:4:C:H2'	2:Y:5:C:C6	2.57	0.40
2:Y:77:G:H2'	2:Y:78:A:O4'	2.21	0.40
3:A:160:ALA:CA	3:A:199:ASN:CB	3.00	0.40
6:D:22:TYR:CZ	6:D:29:PRO:CD	3.05	0.40
6:D:135:GLN:HA	6:D:138:PHE:CE1	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:83:LEU:HD22	20:R:113:THR:CB	2.51	0.40
28:2:12:ARG:HE	28:2:43:THR:HG22	1.86	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	251/274 (92%)	207 (82%)	36 (14%)	8 (3%)	4 28
4	B	203/211 (96%)	174 (86%)	22 (11%)	7 (3%)	3 27
5	C	192/205 (94%)	153 (80%)	30 (16%)	9 (5%)	2 19
6	D	175/180 (97%)	146 (83%)	27 (15%)	2 (1%)	14 50
7	E	169/185 (91%)	147 (87%)	18 (11%)	4 (2%)	6 34
8	F	61/144 (42%)	51 (84%)	9 (15%)	1 (2%)	9 42
9	G	140/174 (80%)	118 (84%)	18 (13%)	4 (3%)	4 30
10	H	132/134 (98%)	115 (87%)	17 (13%)	0	100 100
11	I	132/156 (85%)	96 (73%)	29 (22%)	7 (5%)	2 16
12	J	134/141 (95%)	107 (80%)	25 (19%)	2 (2%)	10 43
13	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	17 54
14	L	102/114 (90%)	81 (79%)	20 (20%)	1 (1%)	15 52
15	M	106/166 (64%)	94 (89%)	9 (8%)	3 (3%)	5 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	N	115/118 (98%)	106 (92%)	7 (6%)	2 (2%)	9 40
17	O	92/100 (92%)	77 (84%)	12 (13%)	3 (3%)	4 27
18	P	124/134 (92%)	109 (88%)	13 (10%)	2 (2%)	9 42
19	Q	91/95 (96%)	66 (72%)	20 (22%)	5 (6%)	2 16
20	R	108/115 (94%)	82 (76%)	20 (18%)	6 (6%)	2 15
21	S	173/237 (73%)	140 (81%)	28 (16%)	5 (3%)	4 30
22	T	72/91 (79%)	57 (79%)	12 (17%)	3 (4%)	3 22
23	U	70/81 (86%)	44 (63%)	21 (30%)	5 (7%)	1 11
24	V	63/67 (94%)	58 (92%)	4 (6%)	1 (2%)	9 42
25	W	53/55 (96%)	49 (92%)	4 (8%)	0	100 100
26	Z	55/60 (92%)	42 (76%)	12 (22%)	1 (2%)	8 39
27	1	51/55 (93%)	31 (61%)	15 (29%)	5 (10%)	0 6
28	2	44/47 (94%)	37 (84%)	7 (16%)	0	100 100
29	3	57/66 (86%)	37 (65%)	18 (32%)	2 (4%)	3 26
30	4	35/37 (95%)	31 (89%)	4 (11%)	0	100 100
All	All	3111/3558 (87%)	2556 (82%)	466 (15%)	89 (3%)	4 30

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	194/215 (90%)	180 (93%)	14 (7%)	14 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	B	155/157 (99%)	147 (95%)	8 (5%)	23 55
5	C	154/163 (94%)	146 (95%)	8 (5%)	23 55
6	D	152/156 (97%)	151 (99%)	1 (1%)	84 93
7	E	136/144 (94%)	135 (99%)	1 (1%)	84 93
8	F	46/107 (43%)	46 (100%)	0	100 100
9	G	118/146 (81%)	111 (94%)	7 (6%)	19 52
10	H	103/103 (100%)	100 (97%)	3 (3%)	42 71
11	I	100/121 (83%)	93 (93%)	7 (7%)	15 46
12	J	110/115 (96%)	106 (96%)	4 (4%)	35 66
13	K	90/93 (97%)	85 (94%)	5 (6%)	21 53
14	L	74/82 (90%)	70 (95%)	4 (5%)	22 54
15	M	94/134 (70%)	90 (96%)	4 (4%)	29 61
16	N	96/97 (99%)	94 (98%)	2 (2%)	53 78
17	O	75/79 (95%)	73 (97%)	2 (3%)	44 73
18	P	108/115 (94%)	107 (99%)	1 (1%)	78 91
19	Q	73/76 (96%)	69 (94%)	4 (6%)	21 53
20	R	91/96 (95%)	83 (91%)	8 (9%)	10 36
21	S	149/192 (78%)	146 (98%)	3 (2%)	55 79
22	T	55/67 (82%)	54 (98%)	1 (2%)	59 81
23	U	54/66 (82%)	51 (94%)	3 (6%)	21 53
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%)	55 79
27	1	46/48 (96%)	36 (78%)	10 (22%)	1 4
28	2	39/40 (98%)	34 (87%)	5 (13%)	4 20
29	3	46/52 (88%)	41 (89%)	5 (11%)	6 27
30	4	35/35 (100%)	35 (100%)	0	100 100
All	All	2545/2855 (89%)	2434 (96%)	111 (4%)	28 61

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

Sometimes 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%)	73 (2%)
2	Y	119/123 (96%)	22 (18%)	0
All	All	2749/3003 (91%)	492 (17%)	73 (2%)

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

All (73) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	33	C
1	X	38	G
1	X	48	A
1	X	173	A
1	X	182	G
1	X	192	G
1	X	334	G
1	X	342	G
1	X	466	A
1	X	538	A
1	X	583	C
1	X	631	G
1	X	682	G
1	X	777	A
1	X	780	U
1	X	788	G
1	X	789	G
1	X	795	A
1	X	802	A
1	X	803	C
1	X	843	G
1	X	969	U
1	X	995	A
1	X	1006	C
1	X	1031	C
1	X	1053	G
1	X	1096	A
1	X	1141	U
1	X	1182	U
1	X	1223	G

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Mol	Chain	Res	Type
1	X	1261	G
1	X	1299	A
1	X	1313	U
1	X	1324	G
1	X	1337	G
1	X	1338	G
1	X	1391	A
1	X	1441	A
1	X	1442	C
1	X	1459	U
1	X	1496	G
1	X	1601	U
1	X	1607	A
1	X	1623	C
1	X	1634	A
1	X	1691	G
1	X	1749	G
1	X	1750	A
1	X	1790	G
1	X	1811	A
1	X	1923	U
1	X	1938	U
1	X	1975	G
1	X	2005	U
1	X	2015	G
1	X	2044	G
1	X	2204	A
1	X	2245	A
1	X	2312	A
1	X	2404	A
1	X	2409	A
1	X	2426	G
1	X	2427	A
1	X	2485	U
1	X	2581	A
1	X	2705	A
1	X	2708	U
1	X	2736	U
1	X	2756	A
1	X	2824	C
1	X	2841	U
1	X	2842	C

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Mol	Chain	Res	Type
1	X	2867	G

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 monosaccharides 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	-	29,34,34	1.82	6 (20%)	26,49,49	1.18	2 (7%)
32	LMA	X	2882	-	58,60,60	4.94	27 (46%)	75,90,90	1.30	6 (8%)

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	-	-	5/33/61/61	0/0/2/2
32	LMA	X	2882	-	-	23/80/115/115	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	-19.81	1.10	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2882	LMA	C2-C1	-16.96	1.13	1.51
32	X	2882	LMA	O53-C8	-10.28	1.25	1.43
32	X	2882	LMA	O2-C13	8.48	1.57	1.44
32	X	2882	LMA	C35-C12	-8.25	1.36	1.53
32	X	2882	LMA	C33-C8	-7.33	1.41	1.52
32	X	2882	LMA	C7-C6	-7.27	1.43	1.54
32	X	2882	LMA	C19-C16	-6.13	1.38	1.52
32	X	2882	LMA	C32-C6	-6.04	1.38	1.53
32	X	2882	LMA	C8-C9	-5.89	1.41	1.54
31	X	2881	LC2	C31-C2	-5.70	1.39	1.50
32	X	2882	LMA	C16-C17	-5.29	1.41	1.53
32	X	2882	LMA	O5-C16	-5.25	1.33	1.44
32	X	2882	LMA	C40-C23	-4.82	1.43	1.53
32	X	2882	LMA	O55-C54	4.80	1.38	1.20
32	X	2882	LMA	C6-C5	4.53	1.61	1.53
32	X	2882	LMA	O52-C51	4.43	1.37	1.20
32	X	2882	LMA	O51-C17	-4.21	1.37	1.45
32	X	2882	LMA	O2-C1	3.77	1.43	1.34
32	X	2882	LMA	C2-C3	3.73	1.63	1.55
32	X	2882	LMA	C12-C13	-3.70	1.44	1.54
32	X	2882	LMA	O17-C24	3.16	1.51	1.43
31	X	2881	LC2	C4-C5	3.03	1.39	1.32
31	X	2881	LC2	C4-C3	-3.02	1.39	1.45
31	X	2881	LC2	C28-C29	3.02	1.39	1.32
31	X	2881	LC2	C28-C27	-2.99	1.39	1.45
32	X	2882	LMA	O3-C3	2.74	1.51	1.43
32	X	2882	LMA	O4-C18	2.24	1.49	1.44
32	X	2882	LMA	C4-C5	2.17	1.59	1.54
32	X	2882	LMA	C15-C16	2.15	1.57	1.52
32	X	2882	LMA	O12-C54	2.08	1.39	1.35
31	X	2881	LC2	C2-C3	2.03	1.39	1.33
32	X	2882	LMA	O7-C5	2.02	1.49	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	X	2882	LMA	O12-C54-C56	4.58	119.51	111.09
32	X	2882	LMA	O51-C51-C53	4.53	119.42	111.09
32	X	2882	LMA	O7-C5-C4	3.89	112.91	108.22
32	X	2882	LMA	C3-C2-C1	-2.75	104.39	110.01
32	X	2882	LMA	C25-C24-C23	-2.46	106.52	113.08
31	X	2881	LC2	C6-C5-C4	-2.25	119.94	125.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	X	2881	LC2	C30-C29-C28	-2.18	120.10	125.19
32	X	2882	LMA	O12-C11-C10	2.01	111.10	107.55

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	X	2881	LC2	C12-C23-C26-C27
32	X	2882	LMA	C3-C4-C5-C6
32	X	2882	LMA	C3-C4-C5-O7
32	X	2882	LMA	C31-C4-C5-C6
32	X	2882	LMA	C12-C11-O12-C54
32	X	2882	LMA	O55-C54-O12-C11
32	X	2882	LMA	C12-C13-C36-C57
32	X	2882	LMA	C23-C24-O17-C29
32	X	2882	LMA	C13-C36-C57-O57
32	X	2882	LMA	C13-C36-C57-C58
32	X	2882	LMA	C37-C36-C57-O57
32	X	2882	LMA	C37-C36-C57-C58
32	X	2882	LMA	O52-C51-O51-C17
32	X	2882	LMA	C53-C51-O51-C17
32	X	2882	LMA	C56-C54-O12-C11
32	X	2882	LMA	C31-C4-C5-O7
32	X	2882	LMA	O2-C13-C36-C57
32	X	2882	LMA	C10-C11-O12-C54
31	X	2881	LC2	C4-C5-C6-O4
31	X	2881	LC2	C4-C5-C6-C7
31	X	2881	LC2	C28-C29-C30-C31
32	X	2882	LMA	C6-C7-C8-C9
32	X	2882	LMA	O2-C13-C36-C37
32	X	2882	LMA	O9-C22-O7-C5
32	X	2882	LMA	C12-C13-C36-C37
32	X	2882	LMA	C6-C7-C8-C33
31	X	2881	LC2	N1-C23-C26-C27
32	X	2882	LMA	C6-C7-C8-O53

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

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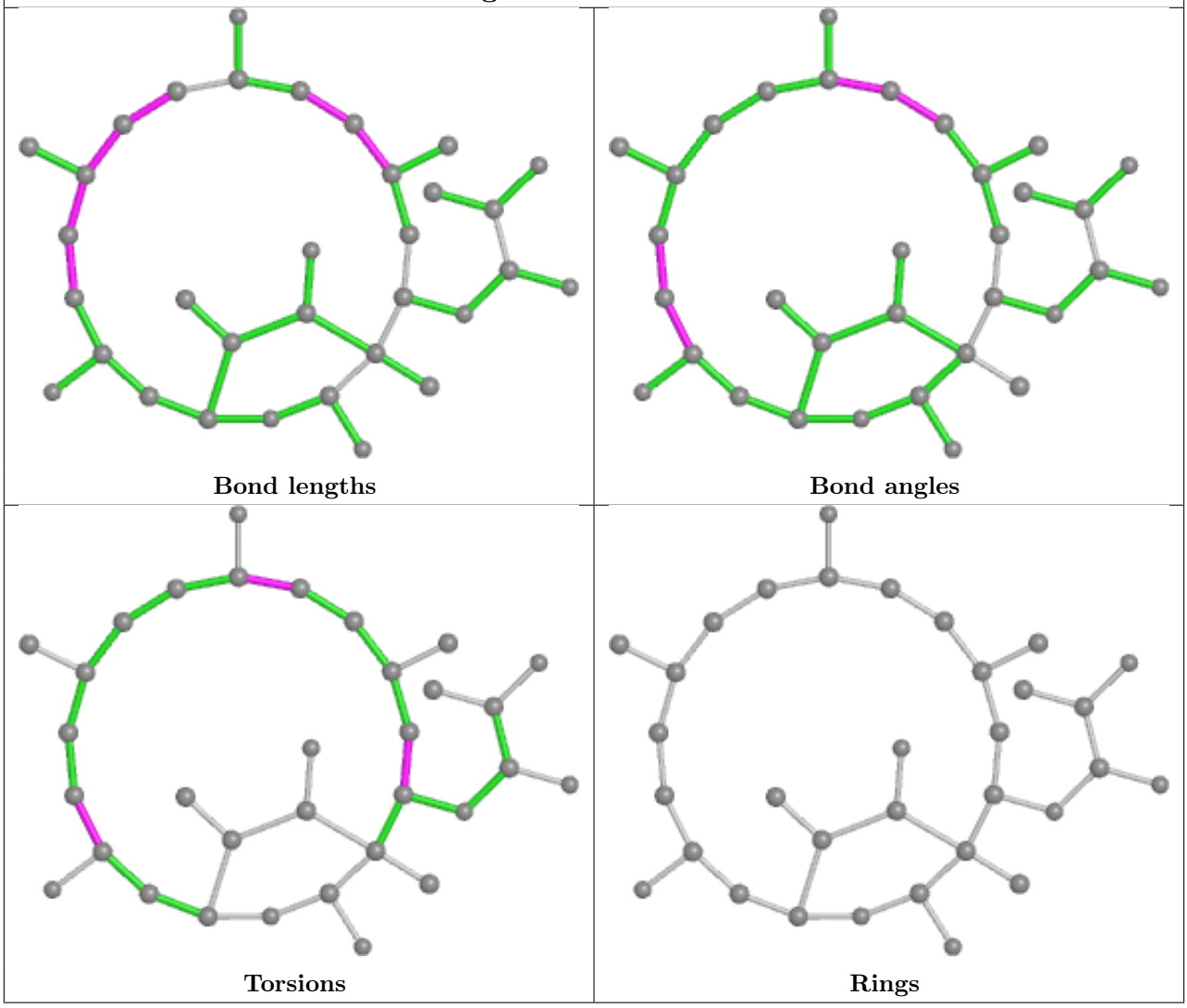
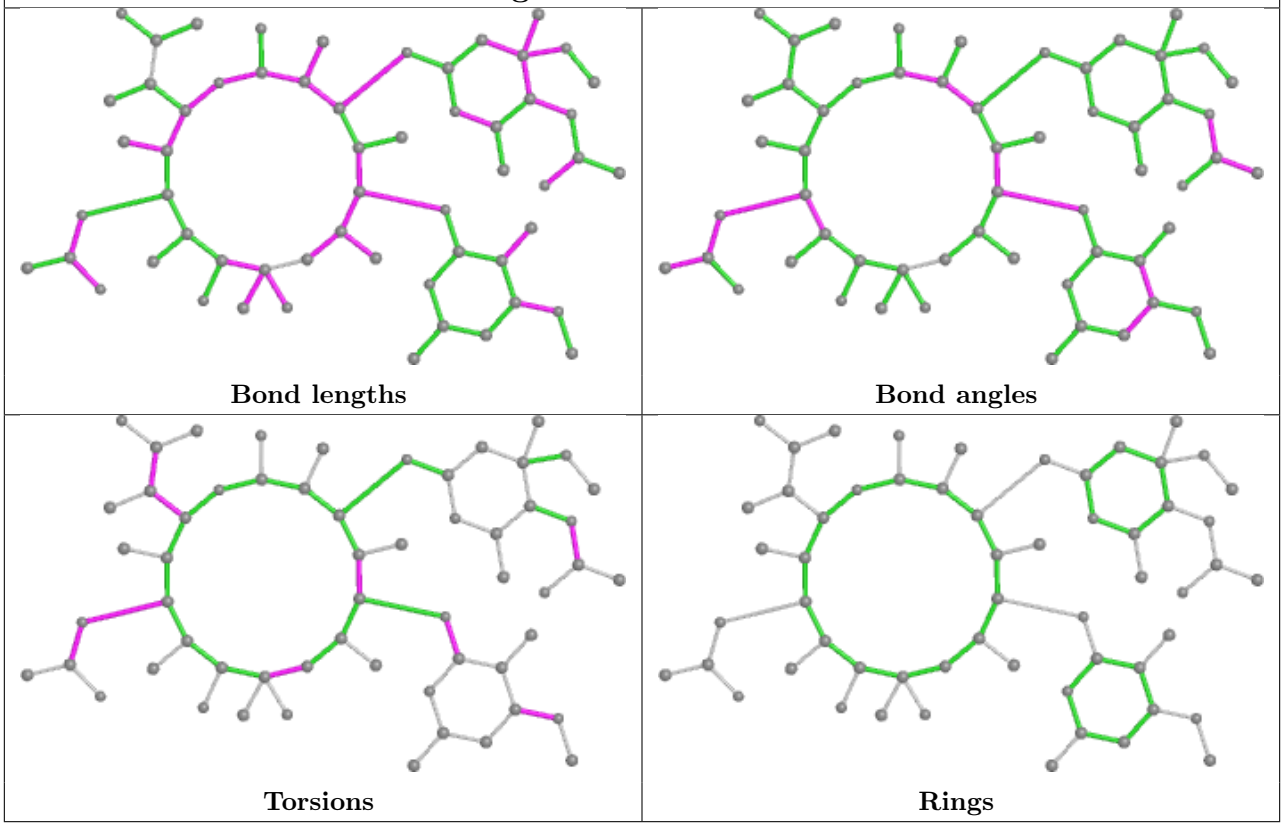
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2882	LMA	43	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand LC2 X 2881



Ligand LMA X 2882



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	X	2644/2880 (91%)	0.10	83 (3%) 49 47	44, 115, 240, 575	0
2	Y	120/123 (97%)	-0.13	3 (2%) 57 54	108, 183, 252, 342	0
3	A	253/274 (92%)	1.01	53 (20%) 1 1	66, 158, 225, 423	0
4	B	205/211 (97%)	0.25	8 (3%) 39 38	35, 85, 159, 249	0
5	C	194/205 (94%)	0.03	10 (5%) 27 27	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%) 11 14	87, 183, 269, 354	0
8	F	63/144 (43%)	5.03	60 (95%) 0 0	208, 334, 476, 516	0
9	G	142/174 (81%)	0.65	21 (14%) 2 3	73, 126, 257, 421	0
10	H	134/134 (100%)	-0.20	1 (0%) 87 85	39, 71, 135, 248	0
11	I	134/156 (85%)	0.89	31 (23%) 0 0	75, 168, 261, 375	0
12	J	136/141 (96%)	0.93	26 (19%) 1 1	76, 135, 223, 388	0
13	K	113/116 (97%)	0.01	1 (0%) 84 81	32, 61, 101, 128	0
14	L	104/114 (91%)	0.36	13 (12%) 3 6	134, 193, 300, 325	0
15	M	108/166 (65%)	-0.06	2 (1%) 66 64	32, 73, 138, 298	0
16	N	117/118 (99%)	0.47	12 (10%) 6 9	57, 116, 177, 328	0
17	O	94/100 (94%)	0.72	16 (17%) 1 2	82, 145, 271, 322	0
18	P	126/134 (94%)	-0.19	1 (0%) 86 82	33, 84, 149, 226	0
19	Q	93/95 (97%)	1.34	25 (26%) 0 0	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	31 (17%) 1 2	130, 202, 285, 326	0
22	T	74/91 (81%)	1.54	23 (31%) 0 0	112, 141, 201, 284	0
23	U	72/81 (88%)	1.55	19 (26%) 0 0	119, 188, 304, 349	0
24	V	65/67 (97%)	0.39	6 (9%) 9 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%) 0 1	97, 126, 181, 194	0
26	Z	57/60 (95%)	-0.23	1 (1%) 68 65	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%)	0.68	5 (10%) 5 8	72, 123, 258, 308	0
29	3	59/66 (89%)	4.22	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%) 4 6	32, 131, 276, 575	0

All (726) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	28	GLY	23.8
8	F	113	PRO	15.2
30	4	28	SER	14.4
30	4	1	MET	13.8
30	4	24	LEU	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
8	F	94	ALA	11.6
30	4	17	VAL	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	9.8
20	R	100	ASP	9.6
30	4	21	GLY	9.5
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	8.9
6	D	82	GLY	8.8
29	3	37	SER	8.7
27	1	27	ASN	8.4
29	3	33	ASN	8.3
30	4	36	GLN	8.3
8	F	90	THR	8.2

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Mol	Chain	Res	Type	RSRZ
27	1	23	THR	8.2
29	3	7	HIS	8.1
8	F	95	LYS	8.1
8	F	136	VAL	8.1
30	4	26	ILE	8.0
24	V	66	GLN	8.0
12	J	141	ALA	8.0
29	3	63	PRO	8.0
3	A	251	TRP	7.9
8	F	78	ILE	7.9
3	A	255	THR	7.9
8	F	127	VAL	7.8
30	4	2	LYS	7.8
8	F	125	ASN	7.7
30	4	12	ASP	7.7
30	4	13	ASN	7.5
27	1	6	PRO	7.5
8	F	77	LEU	7.5
29	3	38	GLY	7.5
29	3	20	GLY	7.4
29	3	16	ILE	7.3
27	1	47	HIS	7.2
3	A	250	PRO	7.2
30	4	3	VAL	7.1
29	3	9	MET	7.0
29	3	60	LEU	6.9
1	X	2190	A	6.8
20	R	83	LEU	6.7
30	4	33	LYS	6.6
8	F	112	MET	6.6
12	J	133	VAL	6.6
30	4	10	MET	6.5
22	T	73	GLY	6.5
30	4	37	GLY	6.5
3	A	220	PRO	6.5
12	J	21	ASP	6.4
6	D	67	ILE	6.4
30	4	11	CYS	6.4
30	4	35	ARG	6.4
6	D	11	GLN	6.4
6	D	34	ILE	6.3
30	4	20	HIS	6.3

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Mol	Chain	Res	Type	RSRZ
3	A	152	LYS	6.3
23	U	27	ASP	6.3
8	F	89	SER	6.2
8	F	84	ILE	6.2
20	R	82	ALA	6.2
1	X	1089	C	6.2
27	1	35	LEU	6.1
6	D	85	VAL	6.1
27	1	13	GLU	6.1
30	4	9	LYS	6.0
30	4	22	ARG	6.0
1	X	1086	C	6.0
27	1	24	THR	5.9
11	I	61	PRO	5.9
30	4	14	CYS	5.8
17	O	41	GLY	5.8
20	R	77	HIS	5.8
29	3	40	GLU	5.8
1	X	1114	A	5.7
27	1	40	TYR	5.7
29	3	28	GLY	5.7
20	R	112	LYS	5.7
6	D	93	GLY	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
30	4	27	CYS	5.7
29	3	27	SER	5.6
27	1	31	THR	5.6
3	A	57	GLY	5.5
8	F	109	LYS	5.5
6	D	74	ILE	5.5
7	E	37	TYR	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
8	F	93	LYS	5.3
21	S	94	VAL	5.3
8	F	105	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
21	S	74	ARG	5.2
8	F	104	VAL	5.2
21	S	68	ALA	5.2
6	D	86	GLY	5.2
6	D	81	GLN	5.2
19	Q	27	PHE	5.2
23	U	47	HIS	5.2
8	F	98	LYS	5.1
27	1	14	SER	5.1
2	Y	43	G	5.1
29	3	29	LYS	5.1
27	1	32	GLN	5.1
20	R	81	VAL	5.0
22	T	71	ASN	5.0
22	T	72	LYS	5.0
20	R	46	VAL	5.0
20	R	4	PRO	5.0
29	3	17	THR	5.0
8	F	102	ASP	4.9
23	U	29	GLY	4.9
29	3	8	LYS	4.9
3	A	243	ALA	4.9
9	G	97	ASP	4.9
6	D	169	LEU	4.9
3	A	242	GLY	4.9
29	3	55	TRP	4.9
28	2	40	HIS	4.9
6	D	91	LEU	4.9
6	D	105	ASN	4.9
1	X	1115	C	4.9
11	I	60	LEU	4.9
8	F	128	ALA	4.8
6	D	140	GLU	4.8
1	X	1734	C	4.8
3	A	204	ASN	4.8
1	X	871	U	4.8
14	L	52	ALA	4.8
3	A	73	LYS	4.7
1	X	665	A	4.7
6	D	127	ASN	4.7
16	N	105	ALA	4.7
8	F	91	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	X	1063	C	4.7
8	F	130	THR	4.7
20	R	74	LEU	4.7
23	U	62	LEU	4.7
29	3	54	GLU	4.7
29	3	45	GLY	4.7
9	G	68	PRO	4.7
6	D	138	PHE	4.7
20	R	52	ASN	4.7
19	Q	48	VAL	4.6
20	R	75	ALA	4.6
17	O	74	TYR	4.6
25	W	14	GLY	4.6
6	D	89	VAL	4.6
29	3	21	LYS	4.6
29	3	12	ARG	4.6
27	1	51	ARG	4.5
17	O	64	GLY	4.5
22	T	47	ALA	4.5
24	V	33	ALA	4.5
29	3	61	MET	4.5
9	G	34	PRO	4.5
29	3	31	HIS	4.5
1	X	1098	G	4.5
29	3	41	ILE	4.5
20	R	12	ASP	4.5
29	3	46	LYS	4.5
11	I	54	SER	4.5
30	4	32	HIS	4.5
1	X	1095	A	4.5
6	D	36	VAL	4.4
14	L	12	ARG	4.4
19	Q	64	ARG	4.4
29	3	23	MET	4.4
20	R	99	VAL	4.4
6	D	156	ILE	4.4
3	A	256	LYS	4.4
12	J	60	ARG	4.4
6	D	3	GLN	4.4
30	4	19	ARG	4.4
1	X	1085	G	4.3
9	G	156	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
27	1	12	MET	4.3
6	D	88	LYS	4.3
29	3	30	ARG	4.3
8	F	87	GLY	4.3
19	Q	62	ARG	4.3
8	F	106	GLU	4.3
27	1	25	THR	4.2
1	X	1087	C	4.2
14	L	14	ARG	4.2
30	4	23	VAL	4.2
7	E	168	GLN	4.2
12	J	20	GLY	4.2
6	D	69	LYS	4.2
8	F	80	LYS	4.2
19	Q	49	ARG	4.2
29	3	13	ARG	4.2
1	X	424	G	4.1
3	A	260	THR	4.1
19	Q	50	VAL	4.1
22	T	15	ASP	4.1
9	G	107	GLN	4.1
8	F	133	SER	4.1
20	R	9	HIS	4.1
19	Q	39	LYS	4.0
20	R	57	ASN	4.0
8	F	123	ALA	4.0
6	D	141	ILE	4.0
27	1	2	ALA	4.0
23	U	75	TYR	4.0
8	F	81	ALA	4.0
20	R	6	ALA	4.0
3	A	254	PRO	4.0
1	X	1088	A	4.0
6	D	99	PHE	4.0
6	D	126	GLY	4.0
29	3	53	ALA	4.0
28	2	38	GLY	3.9
3	A	192	ALA	3.9
6	D	35	VAL	3.9
7	E	41	LEU	3.9
9	G	109	GLY	3.9
6	D	145	MET	3.9

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Mol	Chain	Res	Type	RSRZ
6	D	94	GLU	3.9
17	O	39	PHE	3.9
29	3	22	VAL	3.9
27	1	50	PHE	3.9
29	3	6	THR	3.9
29	3	11	LYS	3.9
3	A	114	VAL	3.9
1	X	248	A	3.9
8	F	120	VAL	3.9
20	R	35	LYS	3.9
27	1	26	LYS	3.9
8	F	129	GLY	3.9
8	F	132	ARG	3.9
20	R	76	LEU	3.8
12	J	114	GLN	3.8
20	R	43	ASP	3.8
29	3	48	PHE	3.8
3	A	56	GLY	3.8
22	T	43	THR	3.8
20	R	25	LEU	3.8
22	T	20	TYR	3.8
6	D	154	ILE	3.8
22	T	59	LEU	3.8
22	T	55	ARG	3.8
8	F	88	SER	3.8
29	3	44	LYS	3.7
25	W	13	PRO	3.7
12	J	103	VAL	3.7
27	1	45	LYS	3.7
21	S	15	ASP	3.7
20	R	41	PRO	3.7
21	S	34	LEU	3.6
5	C	45	THR	3.6
27	1	15	SER	3.6
20	R	38	LEU	3.6
20	R	87	GLU	3.6
22	T	22	GLY	3.6
21	S	70	GLN	3.6
29	3	36	LYS	3.6
16	N	87	ASN	3.6
1	X	1074	G	3.6
8	F	126	THR	3.6

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Mol	Chain	Res	Type	RSRZ
23	U	13	LEU	3.6
11	I	74	VAL	3.6
8	F	101	TRP	3.6
3	A	271	ILE	3.6
8	F	134	MET	3.6
1	X	2326	C	3.6
23	U	46	LEU	3.6
1	X	1069	G	3.6
19	Q	65	VAL	3.6
8	F	131	ALA	3.6
8	F	79	ARG	3.5
6	D	31	ILE	3.5
21	S	91	PRO	3.5
1	X	1552	C	3.5
1	X	90	G	3.5
6	D	108	LEU	3.5
12	J	22	ALA	3.5
20	R	101	GLY	3.5
21	S	123	VAL	3.5
8	F	74	MET	3.5
3	A	221	HIS	3.5
19	Q	3	HIS	3.5
21	S	71	MET	3.5
1	X	1733	U	3.5
29	3	26	LYS	3.5
20	R	58	VAL	3.5
1	X	1101	U	3.5
2	Y	14	C	3.5
6	D	66	ILE	3.5
3	A	246	VAL	3.5
20	R	13	LYS	3.5
27	1	11	LYS	3.5
27	1	5	GLY	3.5
14	L	11	LEU	3.4
8	F	108	ALA	3.4
21	S	79	ILE	3.4
6	D	20	PHE	3.4
6	D	175	LEU	3.4
17	O	47	PHE	3.4
1	X	558	G	3.4
22	T	45	PHE	3.4
1	X	1068	A	3.4

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Mol	Chain	Res	Type	RSRZ
3	A	81	ALA	3.4
1	X	1091	C	3.4
22	T	38	VAL	3.4
19	Q	47	GLY	3.4
6	D	146	VAL	3.4
8	F	86	LYS	3.4
11	I	63	ARG	3.4
12	J	68	ARG	3.4
27	1	38	LYS	3.4
1	X	1099	A	3.3
11	I	62	LYS	3.3
11	I	100	ARG	3.3
20	R	60	PRO	3.3
1	X	1077	U	3.3
6	D	60	ILE	3.3
30	4	30	VAL	3.3
20	R	29	HIS	3.3
20	R	33	THR	3.3
20	R	94	VAL	3.3
27	1	8	ILE	3.3
27	1	52	GLU	3.3
23	U	12	ASN	3.3
21	S	114	ASP	3.3
4	B	205	SER	3.2
7	E	167	GLU	3.2
12	J	140	GLU	3.2
21	S	14	LEU	3.2
1	X	100	G	3.2
8	F	96	VAL	3.2
6	D	53	ALA	3.2
29	3	42	ARG	3.2
8	F	82	ALA	3.2
27	1	22	TYR	3.2
22	T	41	ARG	3.2
6	D	147	ASP	3.2
28	2	41	GLN	3.2
22	T	46	LYS	3.2
9	G	100	TYR	3.2
6	D	84	PRO	3.2
21	S	76	ARG	3.1
1	X	1064	C	3.1
17	O	23	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
6	D	173	MET	3.1
22	T	53	MET	3.1
1	X	1120	C	3.1
21	S	23	ALA	3.1
3	A	103	LYS	3.1
1	X	1090	C	3.1
12	J	32	ASP	3.1
20	R	103	LYS	3.1
24	V	37	LEU	3.1
21	S	109	GLN	3.1
3	A	244	GLY	3.1
20	R	14	LEU	3.1
7	E	47	GLY	3.1
17	O	11	GLN	3.1
29	3	39	ASP	3.0
21	S	93	GLU	3.0
21	S	19	ILE	3.0
29	3	32	GLN	3.0
17	O	36	LYS	3.0
20	R	30	LYS	3.0
1	X	2313	G	3.0
3	A	72	ASP	3.0
14	L	34	SER	3.0
21	S	1	MET	3.0
30	4	8	LYS	3.0
20	R	21	THR	3.0
27	1	48	VAL	3.0
6	D	170	LEU	3.0
23	U	45	ASN	3.0
3	A	153	GLY	2.9
6	D	165	GLU	3.0
12	J	37	ALA	2.9
25	W	9	VAL	2.9
1	X	1062	G	2.9
6	D	6	THR	2.9
6	D	90	THR	2.9
29	3	49	VAL	2.9
8	F	97	GLY	2.9
25	W	53	VAL	2.9
17	O	80	TYR	2.9
24	V	32	ALA	2.9
3	A	45	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
6	D	73	SER	2.9
4	B	34	VAL	2.9
1	X	398	C	2.9
20	R	17	LYS	2.9
21	S	40	ASP	2.9
3	A	247	PRO	2.9
9	G	159	SER	2.9
8	F	83	GLY	2.9
20	R	16	PHE	2.9
6	D	71	LYS	2.9
1	X	304	A	2.9
3	A	76	VAL	2.9
8	F	119	SER	2.9
8	F	121	GLU	2.9
6	D	157	VAL	2.8
25	W	17	VAL	2.8
1	X	341	A	2.8
6	D	62	LEU	2.8
6	D	150	ARG	2.8
19	Q	43	GLN	2.8
29	3	15	LYS	2.8
23	U	25	ARG	2.8
25	W	7	ARG	2.8
8	F	103	GLN	2.8
11	I	66	ASN	2.8
11	I	44	GLY	2.8
9	G	99	VAL	2.8
20	R	42	ARG	2.8
1	X	1070	G	2.8
19	Q	56	MET	2.8
1	X	2188	A	2.8
3	A	102	GLU	2.8
11	I	103	ASN	2.8
9	G	67	ARG	2.8
29	3	51	ALA	2.8
1	X	2664	G	2.8
4	B	72	VAL	2.8
20	R	23	ILE	2.8
12	J	23	LYS	2.8
1	X	1397	A	2.8
20	R	98	ILE	2.8
6	D	75	SER	2.8

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Mol	Chain	Res	Type	RSRZ
8	F	75	SER	2.8
14	L	93	SER	2.8
6	D	142	THR	2.8
5	C	166	TRP	2.8
11	I	53	ARG	2.8
17	O	42	GLY	2.8
21	S	119	ASN	2.8
1	X	2276	C	2.8
12	J	132	MET	2.7
6	D	92	ARG	2.7
16	N	88	ILE	2.7
20	R	71	GLN	2.7
1	X	514	G	2.7
1	X	1102	G	2.7
1	X	2298	U	2.7
6	D	56	GLU	2.7
12	J	36	ILE	2.7
24	V	65	GLU	2.7
29	3	43	GLY	2.7
29	3	50	LEU	2.7
11	I	57	ILE	2.7
8	F	118	GLY	2.7
20	R	18	LYS	2.7
11	I	79	GLN	2.7
3	A	86	ASP	2.7
1	X	519	C	2.7
19	Q	10	PRO	2.7
23	U	34	THR	2.6
12	J	84	MET	2.6
19	Q	66	GLY	2.6
16	N	92	ARG	2.6
19	Q	78	ALA	2.6
23	U	16	ASN	2.6
1	X	1092	U	2.6
20	R	59	LYS	2.6
6	D	132	ILE	2.6
12	J	119	PHE	2.6
11	I	36	GLY	2.6
6	D	97	TYR	2.6
16	N	65	ILE	2.6
21	S	124	ALA	2.6
4	B	78	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
19	Q	63	LYS	2.6
3	A	151	GLY	2.6
7	E	15	VAL	2.6
7	E	17	VAL	2.6
11	I	67	ASN	2.6
3	A	272	VAL	2.6
1	X	2312	A	2.6
6	D	72	LYS	2.6
11	I	76	LYS	2.6
3	A	261	ARG	2.6
20	R	48	VAL	2.6
6	D	125	ARG	2.6
12	J	113	GLU	2.6
14	L	13	THR	2.6
5	C	48	ARG	2.6
11	I	21	ARG	2.6
22	T	67	VAL	2.6
20	R	72	ARG	2.6
19	Q	46	PHE	2.6
19	Q	86	GLN	2.6
27	1	4	ASP	2.6
27	1	36	GLU	2.6
17	O	46	VAL	2.6
9	G	110	LEU	2.6
21	S	120	LEU	2.6
23	U	79	GLU	2.6
29	3	52	LYS	2.6
16	N	79	PHE	2.5
1	X	2325	A	2.5
9	G	53	ARG	2.5
20	R	19	GLY	2.5
29	3	62	LEU	2.5
6	D	158	THR	2.5
12	J	105	PHE	2.5
25	W	3	ILE	2.5
4	B	159	HIS	2.5
8	F	122	ALA	2.5
11	I	64	GLY	2.5
22	T	26	PHE	2.5
12	J	100	PRO	2.5
19	Q	94	GLN	2.5
5	C	112	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
29	3	19	THR	2.5
1	X	1093	U	2.5
4	B	1	MET	2.5
1	X	1224	A	2.5
19	Q	87	SER	2.5
22	T	57	HIS	2.5
25	W	50	LEU	2.5
3	A	39	PRO	2.5
14	L	10	LYS	2.5
3	A	189	GLU	2.5
5	C	180	ILE	2.5
27	1	30	ASN	2.5
6	D	87	ILE	2.5
19	Q	53	ILE	2.5
27	1	7	ARG	2.5
11	I	33	GLY	2.4
16	N	96	ALA	2.4
3	A	112	LEU	2.4
9	G	108	GLY	2.4
17	O	9	GLY	2.4
1	X	2381	A	2.4
23	U	35	THR	2.4
3	A	96	LEU	2.4
11	I	49	PHE	2.4
11	I	72	TYR	2.4
1	X	1841	G	2.4
1	X	1065	A	2.4
9	G	98	LYS	2.4
12	J	38	MET	2.4
27	1	28	ARG	2.4
11	I	65	PHE	2.4
16	N	63	GLN	2.4
6	D	96	MET	2.4
6	D	130	LEU	2.4
14	L	68	ALA	2.4
4	B	71	GLY	2.4
1	X	2263	C	2.4
1	X	1840	A	2.4
6	D	172	SER	2.4
6	D	30	ARG	2.4
6	D	4	LEU	2.4
8	F	100	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
6	D	33	LYS	2.4
9	G	69	ASP	2.4
14	L	62	GLY	2.4
21	S	72	ASP	2.4
6	D	100	LEU	2.4
1	X	1884	A	2.4
14	L	40	ALA	2.4
8	F	85	GLY	2.4
23	U	26	ALA	2.4
4	B	135	HIS	2.4
19	Q	51	ILE	2.4
5	C	19	LEU	2.4
27	1	49	VAL	2.4
1	X	209	G	2.4
29	3	25	PHE	2.4
5	C	47	THR	2.4
22	T	77	ARG	2.3
5	C	55	GLY	2.3
22	T	42	GLY	2.3
16	N	64	ARG	2.3
1	X	1100	G	2.3
8	F	135	GLY	2.3
12	J	63	GLY	2.3
21	S	169	VAL	2.3
1	X	1548	U	2.3
11	I	51	GLY	2.3
1	X	559	C	2.3
1	X	1111	C	2.3
2	Y	18	G	2.3
10	H	27	SER	2.3
11	I	122	VAL	2.3
21	S	173	PRO	2.3
7	E	55	PRO	2.3
6	D	38	GLU	2.3
11	I	104	ARG	2.3
17	O	75	LYS	2.3
21	S	20	ALA	2.3
11	I	105	PRO	2.3
28	2	34	ARG	2.3
27	1	9	ILE	2.3
1	X	2299	A	2.3
25	W	22	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	1073	G	2.3
6	D	25	VAL	2.3
6	D	129	ASN	2.3
1	X	2189	A	2.3
15	M	107	LEU	2.3
20	R	8	SER	2.3
3	A	191	TYR	2.3
7	E	83	TYR	2.3
14	L	96	TYR	2.3
1	X	1409	U	2.3
29	3	34	THR	2.3
5	C	105	ALA	2.3
9	G	129	HIS	2.3
12	J	107	VAL	2.3
23	U	30	VAL	2.3
7	E	42	THR	2.2
8	F	115	LEU	2.2
1	X	1094	C	2.2
1	X	1421	U	2.2
1	X	1801	C	2.2
3	A	63	TYR	2.2
6	D	70	ALA	2.2
11	I	46	GLY	2.2
11	I	47	ALA	2.2
17	O	63	HIS	2.2
17	O	73	LYS	2.2
9	G	105	GLY	2.2
20	R	32	GLN	2.2
3	A	263	LYS	2.2
1	X	247	A	2.2
1	X	2265	A	2.2
11	I	81	GLN	2.2
22	T	19	LYS	2.2
3	A	264	ARG	2.2
3	A	98	TYR	2.2
23	U	10	LYS	2.2
9	G	44	VAL	2.2
11	I	16	ARG	2.2
3	A	85	TYR	2.2
3	A	273	THR	2.2
12	J	18	MET	2.2
22	T	14	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
29	3	58	MET	2.2
19	Q	37	GLU	2.2
6	D	22	TYR	2.2
11	I	91	ASP	2.2
1	X	2085	G	2.2
1	X	2311	U	2.2
6	D	109	PRO	2.2
3	A	199	ASN	2.2
7	E	13	SER	2.2
16	N	47	TYR	2.2
12	J	104	MET	2.2
15	M	40	ARG	2.2
24	V	34	ALA	2.2
1	X	2663	U	2.2
12	J	72	ASP	2.2
25	W	33	GLU	2.2
29	3	64	ARG	2.1
1	X	2363	G	2.1
5	C	167	VAL	2.1
3	A	241	THR	2.1
19	Q	34	THR	2.1
1	X	1118	G	2.1
26	Z	56	GLN	2.1
22	T	21	LEU	2.1
6	D	110	ARG	2.1
6	D	57	LEU	2.1
7	E	165	VAL	2.1
25	W	15	ASN	2.1
25	W	54	GLN	2.1
3	A	217	GLY	2.1
19	Q	82	LEU	2.1
20	R	27	GLY	2.1
3	A	69	LYS	2.1
20	R	45	LYS	2.1
9	G	103	TYR	2.1
1	X	1121	G	2.1
9	G	35	LYS	2.1
16	N	91	ASN	2.1
3	A	258	LEU	2.1
1	X	1920	A	2.1
6	D	52	LYS	2.1
9	G	168	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	2295	C	2.1
20	R	84	VAL	2.1
20	R	40	LEU	2.1
17	O	45	THR	2.1
21	S	22	VAL	2.1
3	A	249	THR	2.0
28	2	31	LEU	2.0
1	X	200	A	2.0
27	1	54	LYS	2.0
3	A	215	TRP	2.0
13	K	17	ARG	2.0
6	D	143	TYR	2.0
16	N	109	LEU	2.0
21	S	21	ALA	2.0
21	S	130	ILE	2.0
1	X	1551	U	2.0
3	A	62	LEU	2.0
3	A	132	LEU	2.0
14	L	111	GLY	2.0
23	U	73	GLY	2.0
3	A	262	ARG	2.0
7	E	149	ARG	2.0
1	X	1913	G	2.0
1	X	1839	A	2.0
18	P	11	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	X	2911	1/1	0.28	0.63	124,124,124,124	0
33	MG	X	2912	1/1	0.66	0.20	62,62,62,62	0
33	MG	U	82	1/1	0.67	0.38	72,72,72,72	0
33	MG	I	157	1/1	0.74	0.47	67,67,67,67	0
33	MG	X	2917	1/1	0.75	0.32	104,104,104,104	0
33	MG	X	2886	1/1	0.76	1.10	54,54,54,54	0
33	MG	X	2926	1/1	0.79	0.45	67,67,67,67	0
35	NA	X	2962	1/1	0.79	1.12	98,98,98,98	0
33	MG	X	2909	1/1	0.80	0.17	58,58,58,58	0
32	LMA	X	2882	58/58	0.80	0.38	120,120,120,120	0
33	MG	X	2942	1/1	0.81	0.63	77,77,77,77	0
33	MG	X	2902	1/1	0.81	0.17	89,89,89,89	0
33	MG	X	2940	1/1	0.82	0.31	71,71,71,71	0
33	MG	X	2894	1/1	0.82	0.47	65,65,65,65	0
33	MG	X	2948	1/1	0.82	0.85	110,110,110,110	0
34	K	X	2956	1/1	0.83	0.39	146,146,146,146	0
31	LC2	X	2881	33/33	0.83	0.33	49,106,118,122	0
33	MG	X	2931	1/1	0.84	0.68	72,72,72,72	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
35	NA	X	2960	1/1	0.85	0.47	86,86,86,86	0
33	MG	X	2920	1/1	0.85	0.37	100,100,100,100	0
33	MG	X	2915	1/1	0.86	0.57	67,67,67,67	0
33	MG	X	2914	1/1	0.87	0.52	74,74,74,74	0
33	MG	X	2928	1/1	0.87	0.34	29,29,29,29	0
33	MG	X	2885	1/1	0.87	0.47	68,68,68,68	0
33	MG	X	2950	1/1	0.88	0.31	36,36,36,36	0
33	MG	X	2925	1/1	0.88	0.57	80,80,80,80	0
33	MG	X	2904	1/1	0.88	0.43	64,64,64,64	0
33	MG	X	2951	1/1	0.89	0.47	142,142,142,142	0
34	K	X	2957	1/1	0.89	0.57	82,82,82,82	0
33	MG	X	2891	1/1	0.89	0.33	50,50,50,50	0
33	MG	X	2941	1/1	0.89	0.23	71,71,71,71	0
33	MG	X	2916	1/1	0.90	0.20	44,44,44,44	0
33	MG	X	2903	1/1	0.90	0.54	65,65,65,65	0
33	MG	X	2910	1/1	0.90	0.37	44,44,44,44	0
33	MG	X	2895	1/1	0.90	0.29	26,26,26,26	0
33	MG	X	2921	1/1	0.91	0.17	61,61,61,61	0
35	NA	X	2958	1/1	0.91	0.47	48,48,48,48	0
35	NA	X	2959	1/1	0.91	0.25	60,60,60,60	0
33	MG	X	2938	1/1	0.91	0.62	62,62,62,62	0
33	MG	X	2905	1/1	0.91	0.67	50,50,50,50	0
33	MG	X	2901	1/1	0.92	0.39	19,19,19,19	0

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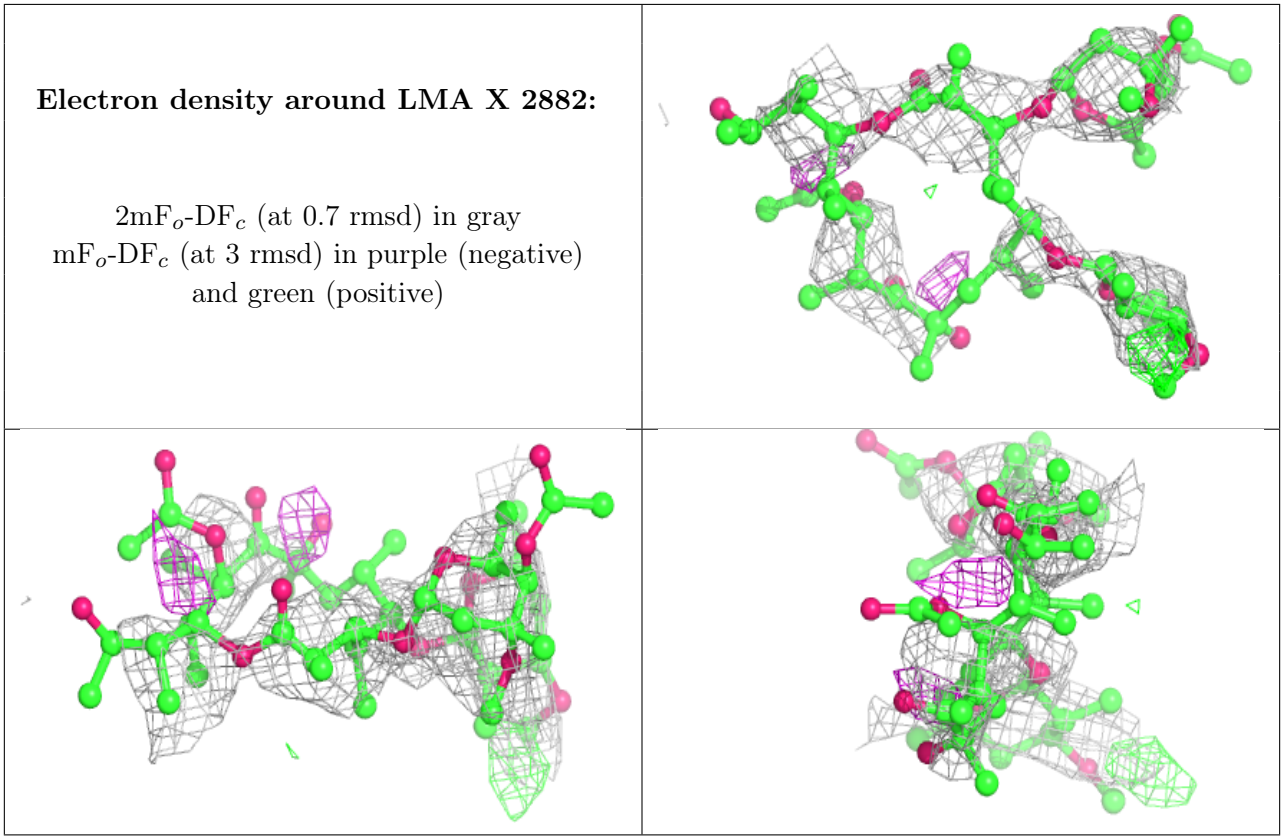
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	X	2908	1/1	0.92	0.67	80,80,80,80	0
33	MG	X	2883	1/1	0.92	0.54	23,23,23,23	0
33	MG	X	2922	1/1	0.92	0.36	53,53,53,53	0
35	NA	X	2961	1/1	0.92	0.43	75,75,75,75	0
33	MG	X	2924	1/1	0.92	0.13	51,51,51,51	0
33	MG	X	2929	1/1	0.93	0.83	61,61,61,61	0
33	MG	X	2884	1/1	0.93	1.00	72,72,72,72	0
33	MG	X	2923	1/1	0.93	0.15	97,97,97,97	0
33	MG	X	2918	1/1	0.93	0.53	84,84,84,84	0
34	K	X	2955	1/1	0.93	0.15	113,113,113,113	0
33	MG	X	2949	1/1	0.93	0.55	83,83,83,83	0
33	MG	X	2900	1/1	0.94	0.64	42,42,42,42	0
33	MG	X	2932	1/1	0.94	0.35	62,62,62,62	0
33	MG	X	2934	1/1	0.94	0.41	56,56,56,56	0
33	MG	X	2946	1/1	0.94	0.16	123,123,123,123	0
33	MG	X	2935	1/1	0.94	0.23	36,36,36,36	0
33	MG	X	2936	1/1	0.94	0.25	55,55,55,55	0
33	MG	X	2937	1/1	0.94	0.38	109,109,109,109	0
33	MG	X	2907	1/1	0.94	0.36	46,46,46,46	0
33	MG	X	2919	1/1	0.94	0.33	65,65,65,65	0
33	MG	X	2933	1/1	0.95	0.37	83,83,83,83	0
33	MG	X	2887	1/1	0.95	0.41	35,35,35,35	0
33	MG	X	2896	1/1	0.95	0.26	24,24,24,24	0
33	MG	X	2892	1/1	0.95	0.30	71,71,71,71	0
33	MG	X	2943	1/1	0.95	0.20	43,43,43,43	0
33	MG	X	2952	1/1	0.95	0.35	59,59,59,59	0
33	MG	X	2927	1/1	0.95	0.74	65,65,65,65	0
33	MG	X	2945	1/1	0.95	0.17	67,67,67,67	0
33	MG	X	2906	1/1	0.96	0.38	52,52,52,52	0
34	K	X	2954	1/1	0.96	0.24	70,70,70,70	0
33	MG	X	2888	1/1	0.96	0.49	51,51,51,51	0
33	MG	X	2890	1/1	0.96	0.40	59,59,59,59	0
33	MG	X	2897	1/1	0.96	0.14	79,79,79,79	0
33	MG	X	2899	1/1	0.97	0.54	41,41,41,41	0
33	MG	X	2913	1/1	0.97	0.40	63,63,63,63	0
33	MG	X	2939	1/1	0.97	0.49	54,54,54,54	0
33	MG	X	2953	1/1	0.97	0.39	53,53,53,53	0
33	MG	X	2930	1/1	0.97	0.21	77,77,77,77	0
33	MG	X	2947	1/1	0.98	0.13	56,56,56,56	0
33	MG	X	2889	1/1	0.98	0.24	61,61,61,61	0
33	MG	X	2898	1/1	0.98	0.39	19,19,19,19	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

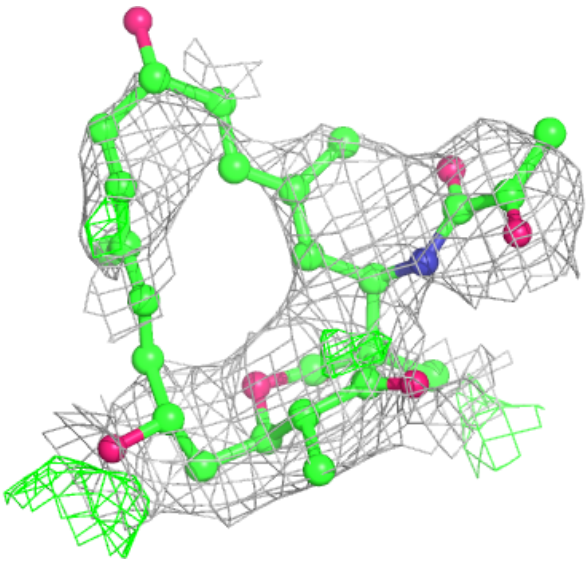
Electron density around LMA X 2882:

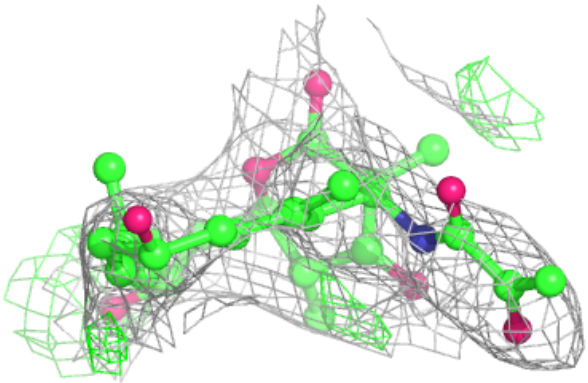
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

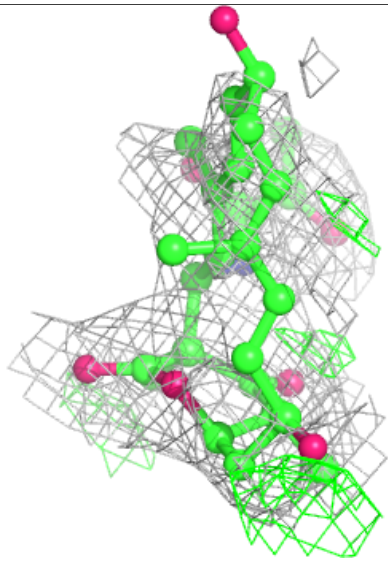


Electron density around LC2 X 2881:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.