Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 05:18 am GMT

PDB ID	:	4WFN
Title	:	Crystal structure of the large ribosomal subunit (50S) of Deinococcus radiodurans containing a three residue insertion in L22 in complex with erythromycin
Authors	:	Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.
Deposited on	:	2014-09-16
Resolution	:	3.54 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 (i) 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 (i)) were used in the production of this report:

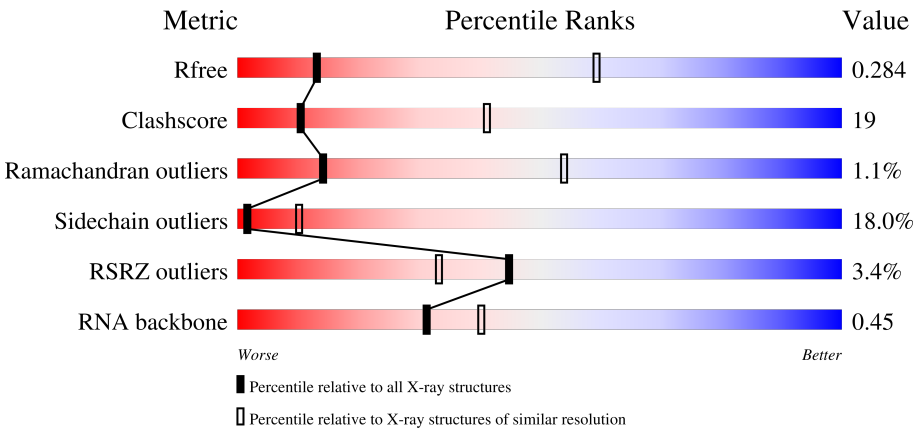
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.54 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	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)
RNA backbone	3102	1003 (4.02-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	275	.% 40% 45% 10% 5%
2	B	211	2% 45% 43% 10% •
3	C	205	4% 42% 44% 8% 5%
4	D	180	6% 48% 46% 5% •

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Mol	Chain	Length	Quality of chain
5	E	185	2%, 52%, 35%, 5%, 8%
6	G	174	5%, 40%, 32%, 10%, 18%
7	H	134	%, 49%, 43%, 7%
8	I	156	3%, 42%, 35%, 9%, 14%
9	J	141	3%, 46%, 39%, 11%
10	K	116	43%, 45%, 9%
11	L	114	5%, 55%, 28%, 8%, 9%
12	M	165	29%, 27%, 9%, 35%
13	N	118	2%, 47%, 44%, 7%
14	O	100	4%, 42%, 45%, 7%, 6%
15	P	137	30%, 50%, 15%, 5%
16	Q	95	%, 52%, 35%, 11%
17	R	115	3%, 38%, 46%, 11%
18	S	237	8%, 51%, 19%, 26%
19	T	91	5%, 41%, 34%, 5%, 19%
20	U	81	5%, 35%, 43%, 11%, 11%
21	V	67	3%, 60%, 31%, 6%
22	W	55	51%, 44%, 5%
23	Z	60	42%, 47%, 5%, 7%
24	1	55	9%, 31%, 47%, 18%
25	2	47	2%, 26%, 53%, 17%
26	3	65	8%, 31%, 49%, 11%, 9%
27	X	2880	3%, 33%, 43%, 15%, 7%
28	Y	124	3%, 42%, 40%, 16%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MG	B	301	-	-	-	X
29	MG	K	202	-	-	-	X

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 84117 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	1987	1235	399	350	3	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	177	1400	892	247	254	7	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L13.

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

- Molecule 7 is a protein called 50S ribosomal protein L14.

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

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	I	134	1011	619	206	186	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L16.

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

- Molecule 10 is a protein called 50S ribosomal protein L17.

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

- Molecule 11 is a protein called 50S ribosomal protein L18.

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

- Molecule 12 is a protein called 50S ribosomal protein L19.

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

- Molecule 13 is a protein called 50S ribosomal protein L20.

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

- Molecule 14 is a protein called 50S ribosomal protein L21.

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

- Molecule 15 is a protein called 50S ribosomal protein L22,50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	P	130	1038	655	205	176	2	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	110	VAL	-	linker	UNP Q9RXJ7
P	111	PRO	-	linker	UNP Q9RXJ7
P	112	ARG	-	linker	UNP Q9RXJ7

- Molecule 16 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	Q	93	726	458	136	130	2	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L24.

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

- Molecule 18 is a protein called 50S ribosomal protein L25.

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

- Molecule 19 is a protein called 50S ribosomal protein L27.

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

- Molecule 20 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
20	U	72	552	341	116	95	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L29.

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

- Molecule 22 is a protein called 50S ribosomal protein L30.

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

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	Z	56	443	272	91	75	5	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	1	53	431	274	80	76	1	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	2	46	383	230	91	60	2	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	3	59	462	290	95	73	4	0	0	0

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
27	X	2680	57533	25663	10626	18564	2680	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

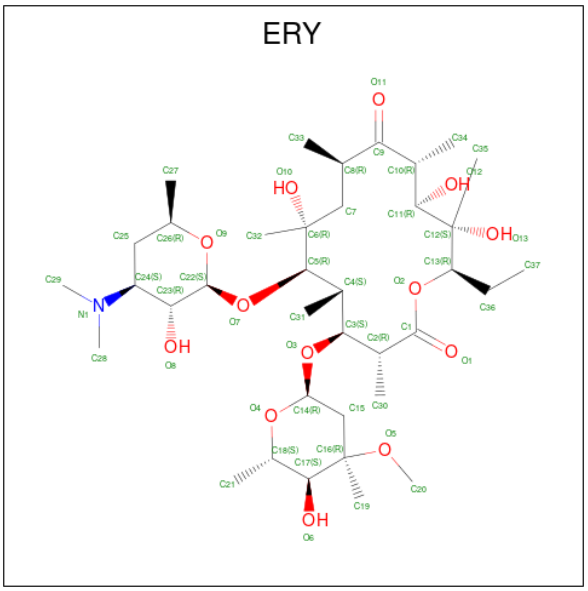
- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
28	Y	122	2601	1161	476	842	122	0	0	0

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
29	A	1	1	1	0	0
29	B	1	1	1	0	0
29	K	2	2	2	0	0
29	M	2	2	2	0	0
29	X	64	64	64	0	0

- Molecule 30 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



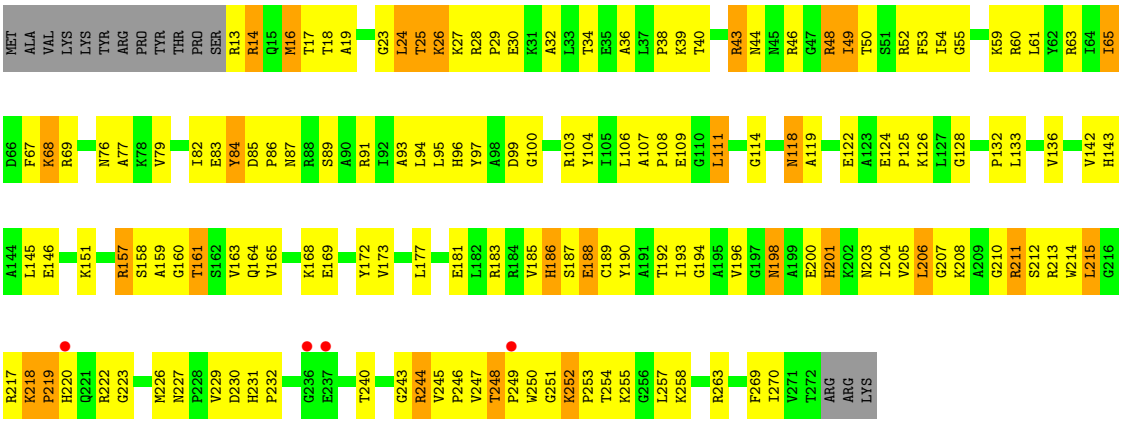
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
30	X	1	51	37	1	13	0	0

3 Residue-property plots (i)

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

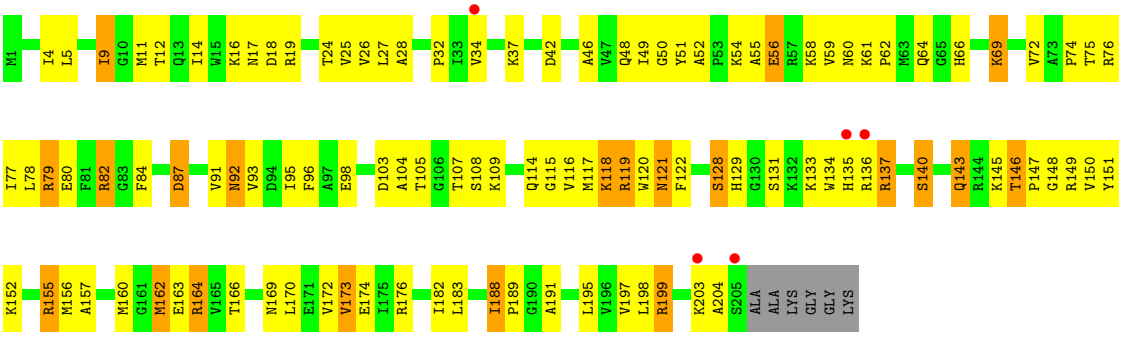
• Molecule 1: 50S ribosomal protein L2

Chain A:



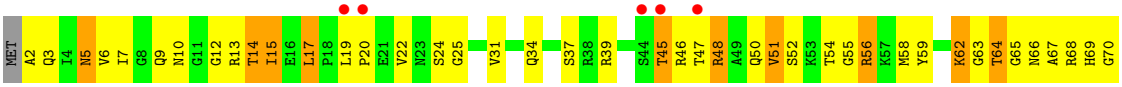
• Molecule 2: 50S ribosomal protein L3

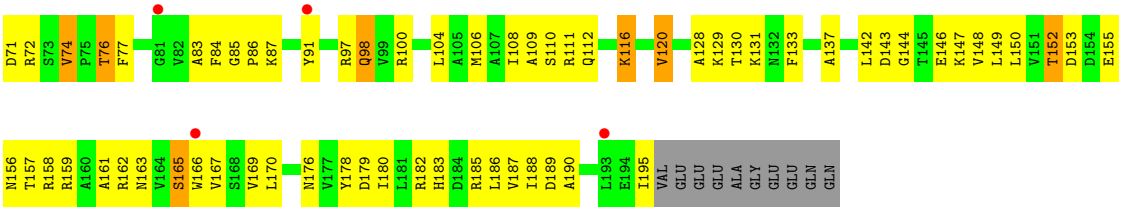
Chain B:



• Molecule 3: 50S ribosomal protein L4

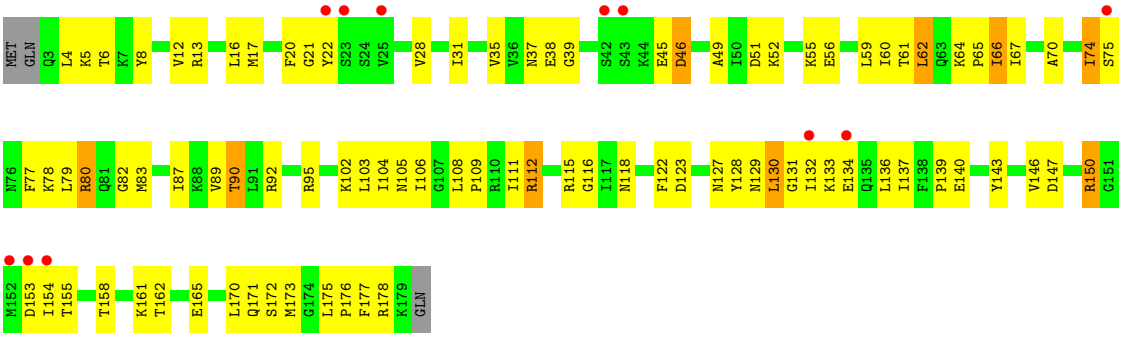
Chain C:





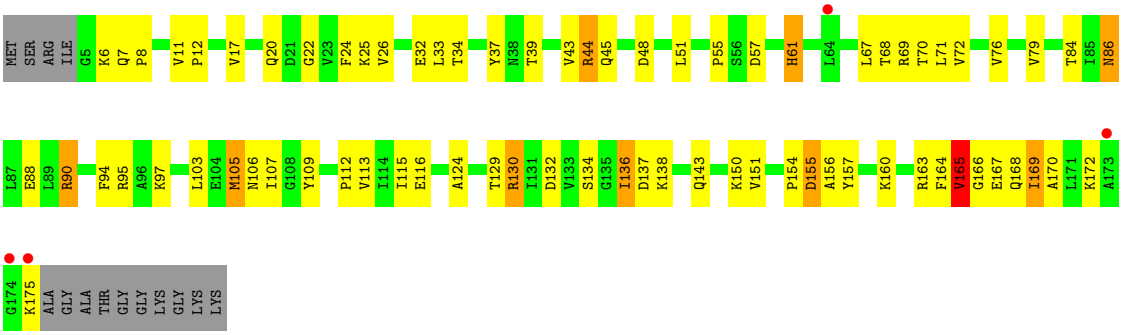
- Molecule 4: 50S ribosomal protein L5

Chain D:



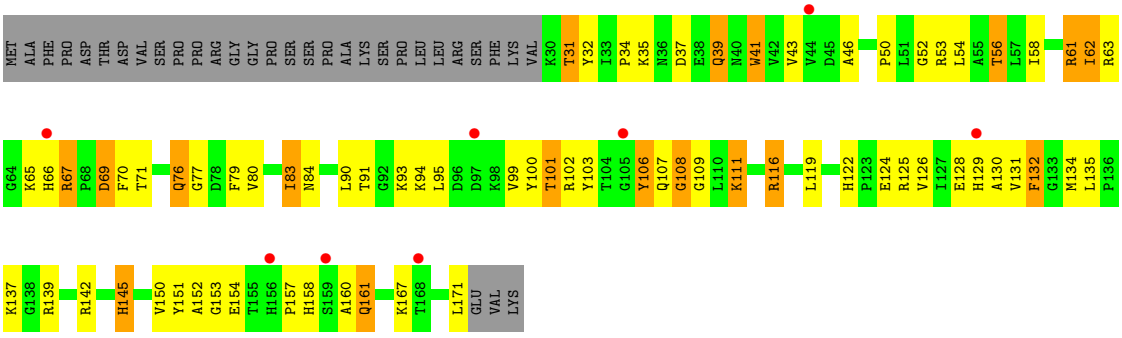
- Molecule 5: 50S ribosomal protein L6

Chain E:



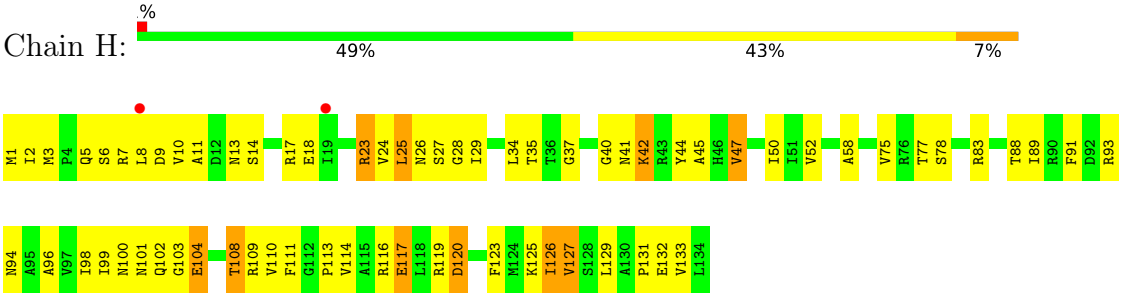
- Molecule 6: 50S ribosomal protein L13

Chain G:



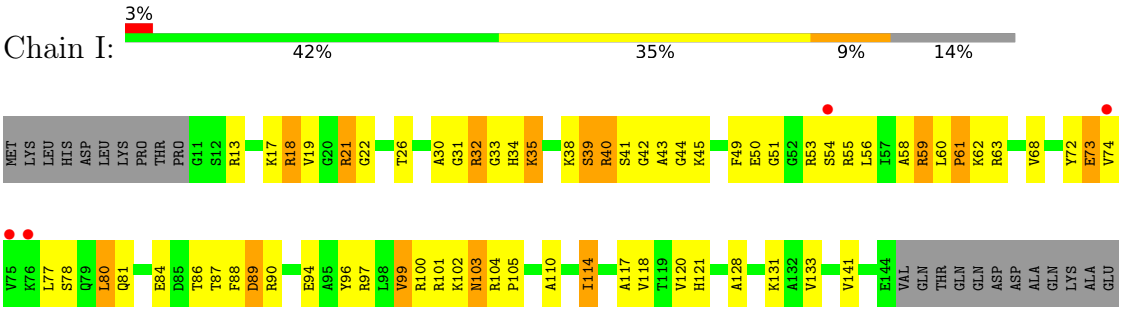
• Molecule 7: 50S ribosomal protein L14

Chain H:



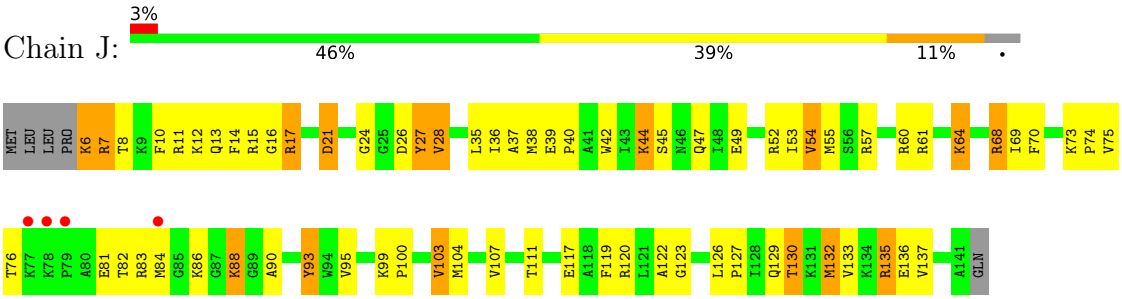
• Molecule 8: 50S ribosomal protein L15

Chain I:



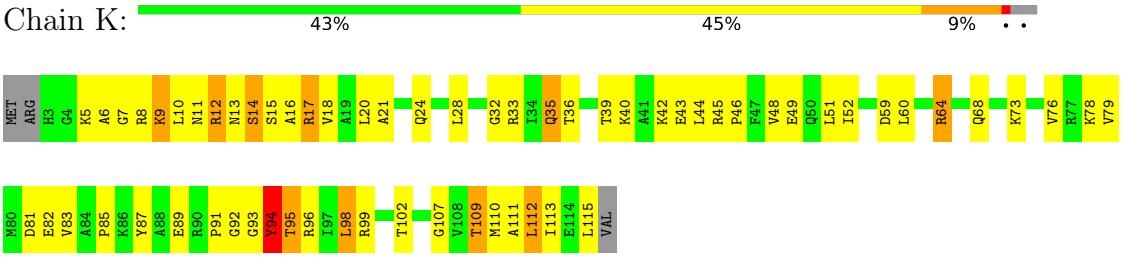
• Molecule 9: 50S ribosomal protein L16

Chain J:



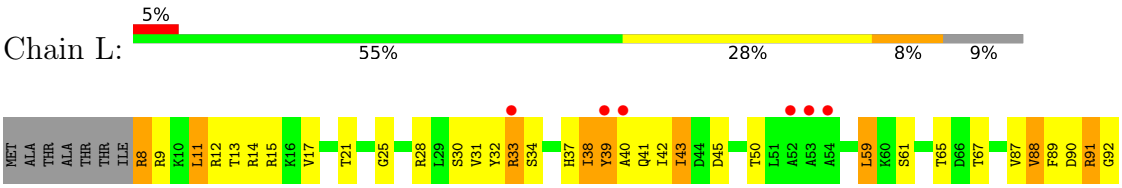
• Molecule 10: 50S ribosomal protein L17

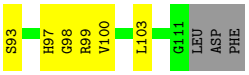
Chain K:



• Molecule 11: 50S ribosomal protein L18

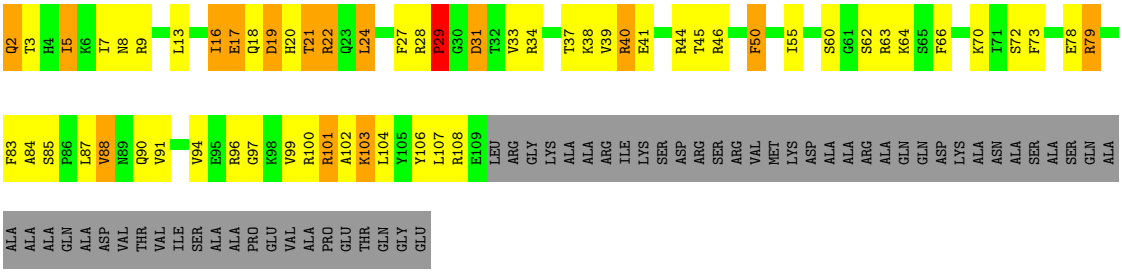
Chain L:





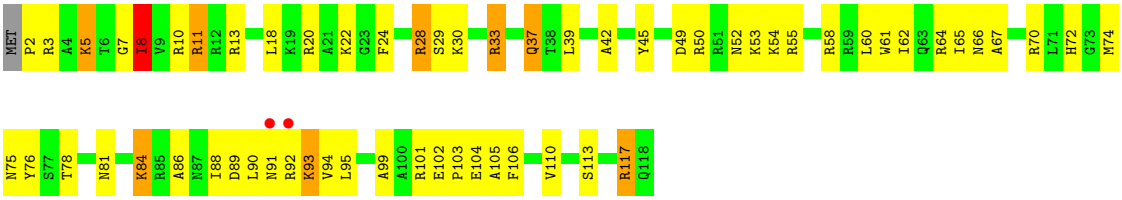
• Molecule 12: 50S ribosomal protein L19

Chain M:



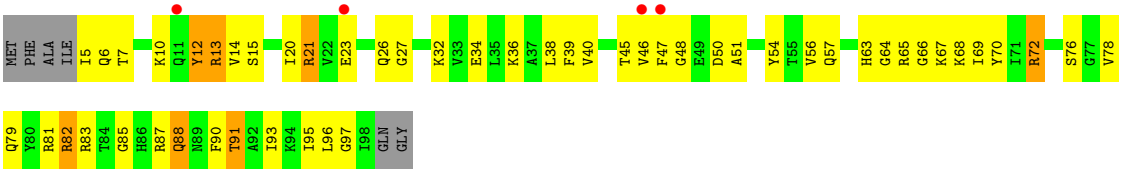
• Molecule 13: 50S ribosomal protein L20

Chain N:



• Molecule 14: 50S ribosomal protein L21

Chain O:

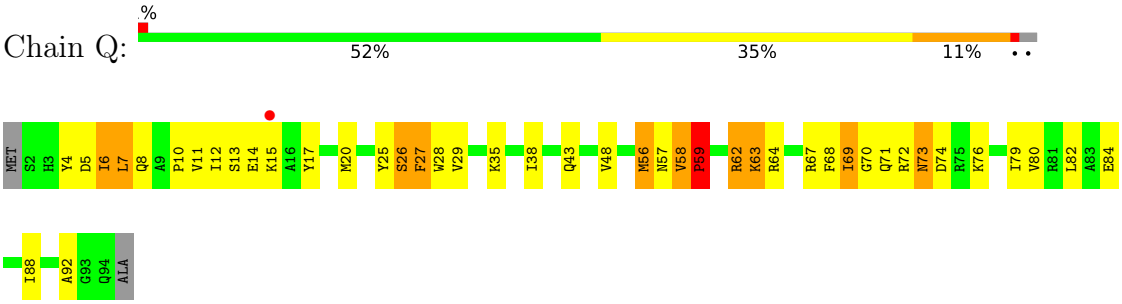


• Molecule 15: 50S ribosomal protein L22,50S ribosomal protein L22

Chain P:

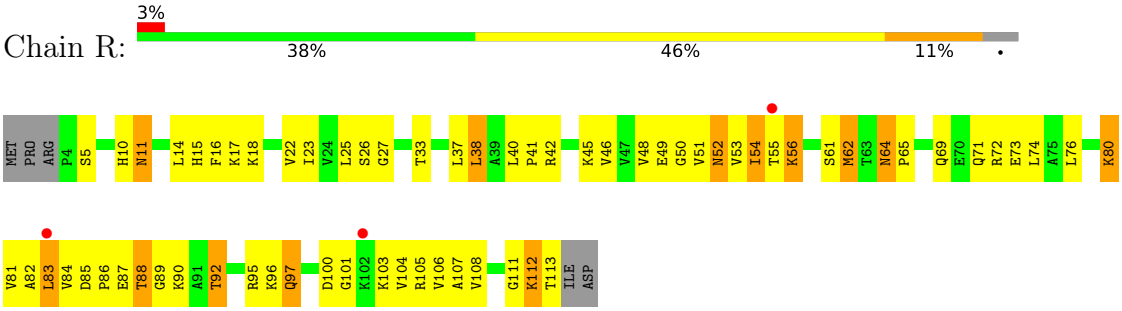
• Molecule 16: 50S ribosomal protein L23

Chain Q:



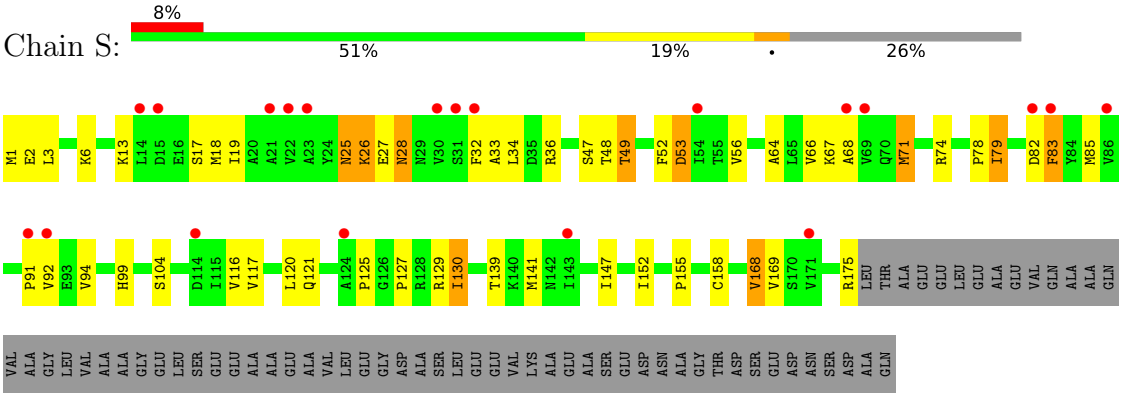
• Molecule 17: 50S ribosomal protein L24

Chain R:



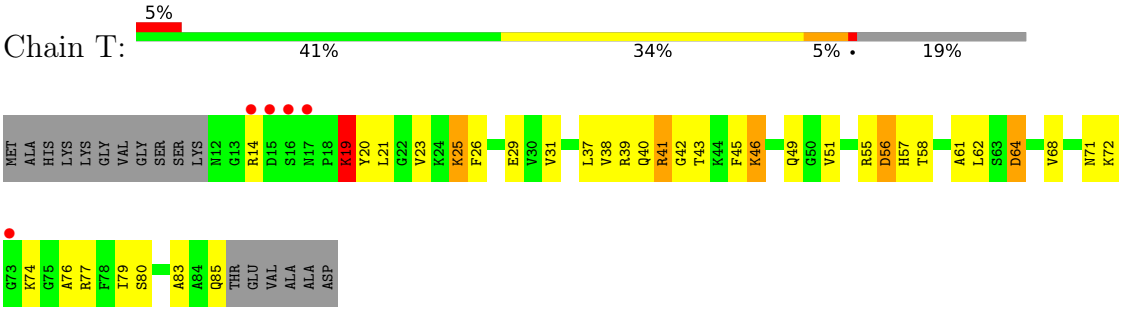
• Molecule 18: 50S ribosomal protein L25

Chain S:



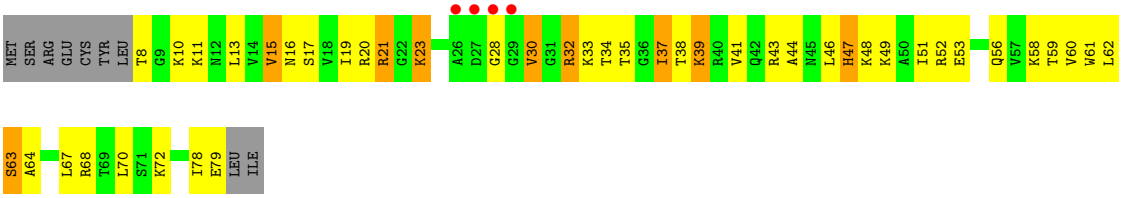
• Molecule 19: 50S ribosomal protein L27

Chain T:



• Molecule 20: 50S ribosomal protein L28

Chain U:

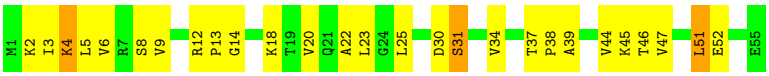


• Molecule 21: 50S ribosomal protein L29

Chain V:

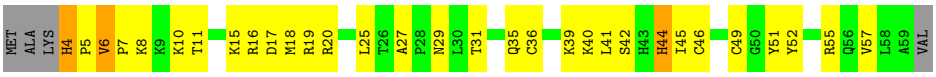
• Molecule 22: 50S ribosomal protein L30

Chain W:



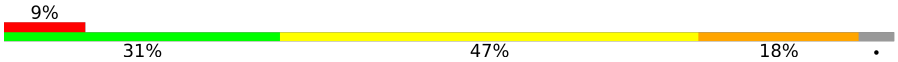
• Molecule 23: 50S ribosomal protein L32

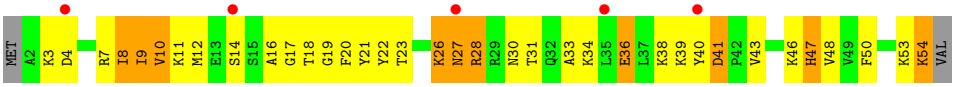
Chain Z:



• Molecule 24: 50S ribosomal protein L33

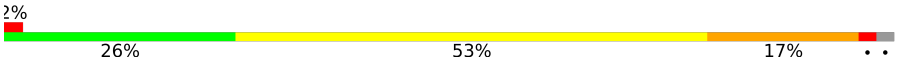
Chain 1:

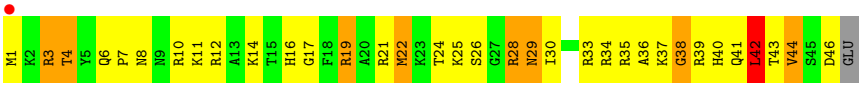




• Molecule 25: 50S ribosomal protein L34

Chain 2:



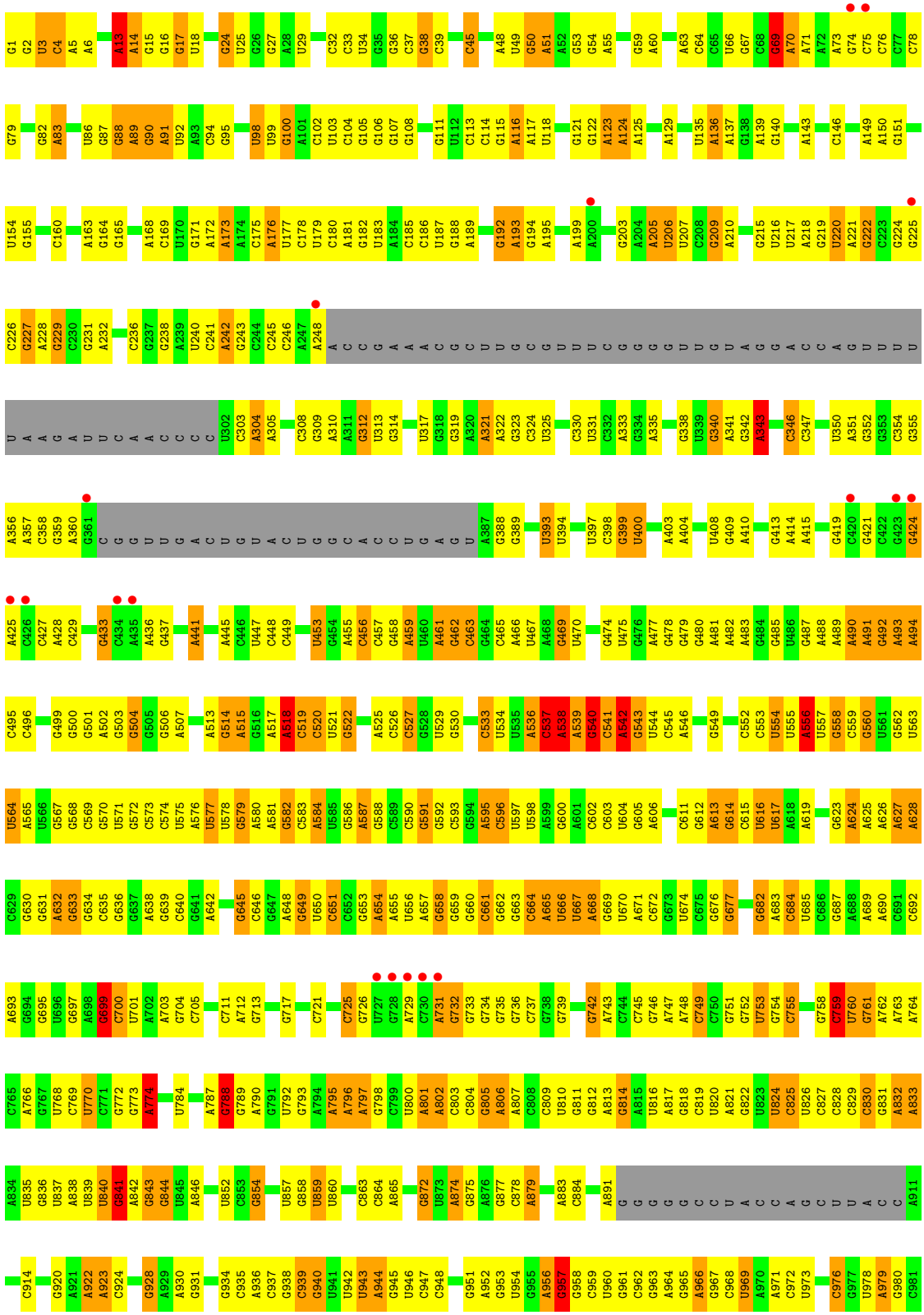


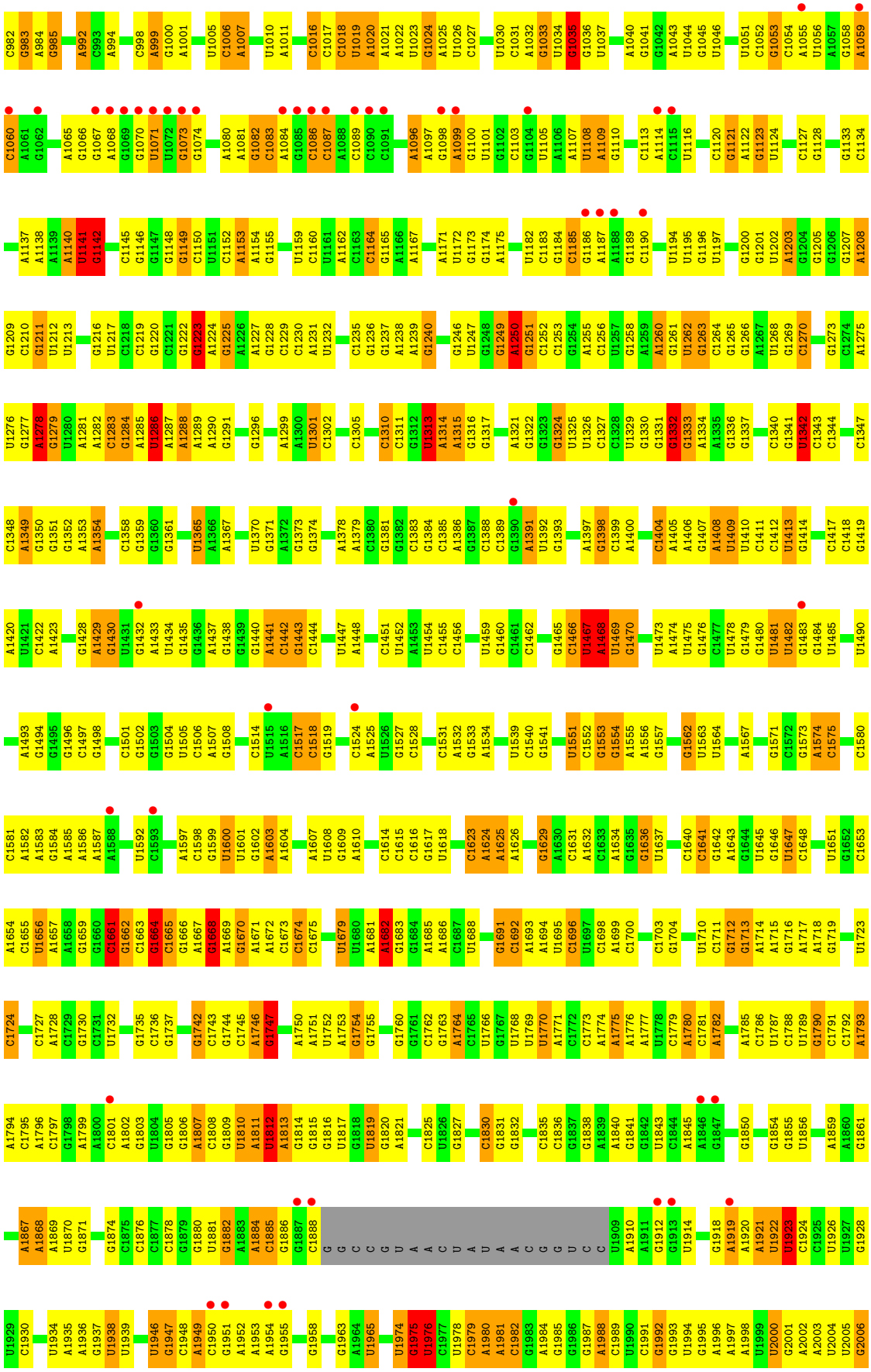
• Molecule 26: 50S ribosomal protein L35

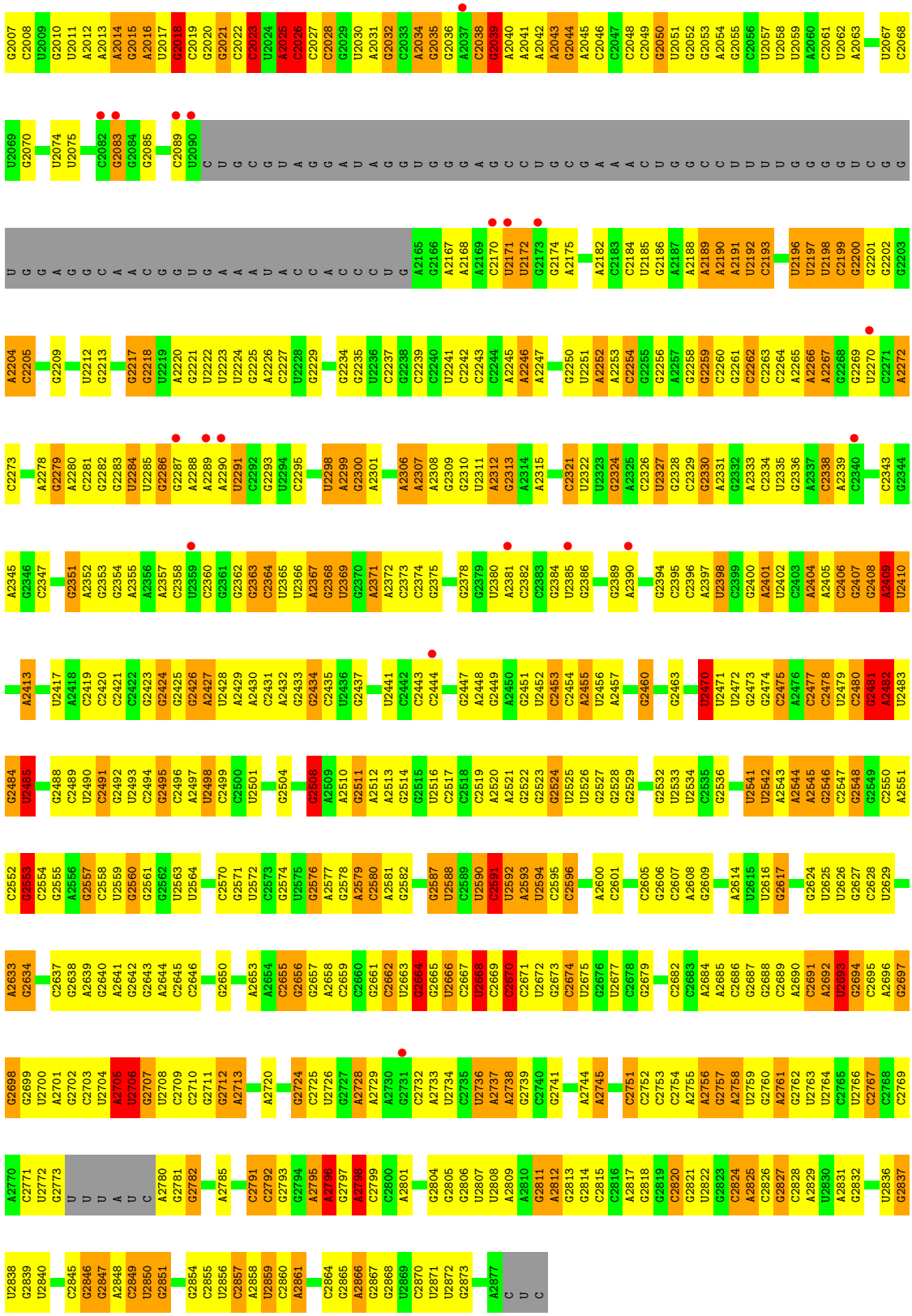
Chain 3:

• Molecule 27: 23S ribosomal RNA

Chain X: 3% 33% 43% 15% • 7%

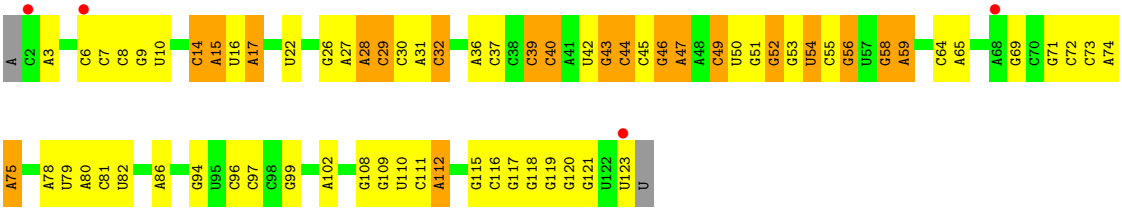






• Molecule 28: 5S ribosomal RNA

Chain Y:


A
C2
A3
C6
C7
C8
G9
U10
C14
A15
U16
A17
U22
G26
A27
A28
C29
C30
A31
C32
A36
C37
C38
C39
C40
A41
U42
G43
C44
C45
G46
A47
A48
C49
U50
G51
G52
G53
U54
C55
G56
U57
G58
A59
C64
A65
A68
G69
C70
G71
C72
C73
A74

A75
A78
U79
A80
C81
U82
A86
G94
U95
C96
C97
C98
G99
A102
G108
G109
U110
C111
A112
G115
C116
G117
G118
G119
G120
G121
U122
U123
U

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	170.09Å 411.59Å 695.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.54 49.53 – 3.52	Depositor EDS
% Data completeness (in resolution range)	90.4 (19.99-3.54) 89.6 (49.53-3.52)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.234 , 0.282 0.235 , 0.284	Depositor DCC
R_{free} test set	13533 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	100.0	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 14.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	84117	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ERY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.43	0/2025	0.70	0/2726
2	B	0.55	0/1567	0.76	0/2105
3	C	0.47	0/1504	0.72	1/2036 (0.0%)
4	D	0.29	0/1419	0.52	0/1903
5	E	0.29	0/1308	0.51	0/1771
6	G	0.47	0/1138	0.78	1/1539 (0.1%)
7	H	0.61	0/1007	0.80	0/1352
8	I	0.46	0/1022	0.76	0/1366
9	J	0.52	0/1113	0.75	0/1486
10	K	0.67	0/886	0.90	1/1188 (0.1%)
11	L	0.32	0/785	0.60	0/1048
12	M	0.61	0/884	0.87	1/1186 (0.1%)
13	N	0.45	0/994	0.68	0/1323
14	O	0.44	0/750	0.74	1/1000 (0.1%)
15	P	0.58	0/1052	0.79	1/1409 (0.1%)
16	Q	0.42	0/737	0.67	1/988 (0.1%)
17	R	0.45	0/835	0.72	0/1121
18	S	0.30	0/1370	0.53	0/1862
19	T	0.44	0/563	0.70	0/747
20	U	0.41	0/556	0.69	0/741
21	V	0.31	0/529	0.51	0/704
22	W	0.36	0/426	0.61	0/568
23	Z	0.52	0/455	0.87	0/611
24	1	0.47	0/438	0.74	0/583
25	2	0.46	0/387	0.79	1/509 (0.2%)
26	3	0.53	0/468	0.85	0/614
27	X	0.63	3/64429 (0.0%)	1.22	424/100499 (0.4%)
28	Y	0.40	0/2907	0.96	1/4529 (0.0%)
All	All	0.58	3/91554 (0.0%)	1.11	433/137514 (0.3%)

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
2	B	0	1
6	G	0	1
7	H	0	1
8	I	0	3
10	K	0	2
16	Q	0	1
17	R	0	1
19	T	0	1
20	U	0	1
23	Z	0	1
25	2	0	1
26	3	0	1
All	All	0	15

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X	1	G	OP3-P	-10.37	1.48	1.61
27	X	1981	A	N3-C4	-5.23	1.31	1.34
27	X	774	A	N3-C4	5.08	1.37	1.34

All (433) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	1468	A	C8-N9-C4	-12.74	100.70	105.80
27	X	1746	A	O5'-P-OP1	-12.19	94.73	105.70
27	X	1670	G	C8-N9-C4	11.14	110.86	106.40
27	X	537	C	C6-N1-C2	-10.97	115.91	120.30
27	X	774	A	N7-C8-N9	10.55	119.08	113.80
27	X	2018	G	O5'-P-OP2	-9.92	96.77	105.70
27	X	774	A	C8-N9-C4	-9.89	101.84	105.80
27	X	2544	A	O5'-P-OP1	-9.88	96.80	105.70
27	X	1468	A	N7-C8-N9	9.40	118.50	113.80
27	X	522	G	N1-C6-O6	9.20	125.42	119.90
27	X	2705	A	C5-N7-C8	-9.11	99.35	103.90
27	X	2489	C	C6-N1-C2	-8.98	116.71	120.30
27	X	2478	C	C5-C6-N1	8.96	125.48	121.00
27	X	2705	A	N7-C8-N9	8.93	118.26	113.80
27	X	2815	C	C6-N1-C2	8.84	123.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	1333	G	N3-C4-N9	-8.82	120.71	126.00
27	X	2478	C	C6-N1-C2	-8.79	116.78	120.30
27	X	2488	G	N1-C6-O6	-8.78	114.63	119.90
27	X	2018	G	O4'-C1'-N9	8.78	115.22	108.20
27	X	1668	G	N1-C6-O6	8.74	125.14	119.90
27	X	2018	G	C4-C5-N7	8.71	114.28	110.80
27	X	2705	A	N1-C6-N6	8.61	123.76	118.60
27	X	1670	G	N9-C4-C5	-8.59	101.97	105.40
27	X	538	A	C2-N3-C4	8.56	114.88	110.60
27	X	2542	U	C5-C4-O4	8.55	131.03	125.90
27	X	661	C	C6-N1-C2	-8.55	116.88	120.30
27	X	1812	U	C2-N1-C1'	8.54	127.95	117.70
27	X	2470	U	N1-C2-O2	8.33	128.63	122.80
27	X	2542	U	N1-C2-N3	8.32	119.89	114.90
27	X	2470	U	C2-N1-C1'	8.28	127.64	117.70
27	X	1992	G	C8-N9-C4	8.26	109.70	106.40
27	X	2693	U	C2-N1-C1'	-8.25	107.80	117.70
27	X	542	A	C2-N3-C4	-8.21	106.50	110.60
27	X	2495	G	N3-C4-C5	-7.82	124.69	128.60
27	X	2025	A	C8-N9-C4	-7.74	102.70	105.80
27	X	957	G	N1-C6-O6	-7.72	115.27	119.90
27	X	1467	U	C4-C5-C6	-7.72	115.07	119.70
6	G	106	TYR	N-CA-C	-7.69	90.24	111.00
27	X	774	A	C5-N7-C8	-7.69	100.06	103.90
27	X	2018	G	C5-N7-C8	-7.66	100.47	104.30
27	X	2553	G	N3-C4-C5	7.65	132.43	128.60
27	X	2548	G	C5-C6-N1	-7.56	107.72	111.50
27	X	2687	G	C8-N9-C4	7.53	109.41	106.40
27	X	2705	A	C4-C5-N7	7.49	114.44	110.70
27	X	1664	G	C4-N9-C1'	-7.43	116.83	126.50
27	X	928	G	C5-C6-O6	-7.43	124.14	128.60
27	X	343	A	C8-N9-C4	-7.42	102.83	105.80
27	X	2799	C	C6-N1-C2	-7.41	117.34	120.30
27	X	522	G	C6-C5-N7	-7.41	125.96	130.40
27	X	2690	A	C2-N3-C4	-7.41	106.90	110.60
27	X	1333	G	N3-C4-C5	7.38	132.29	128.60
27	X	860	U	C2-N1-C1'	7.33	126.50	117.70
27	X	2329	C	C5-C6-N1	7.32	124.66	121.00
27	X	774	A	C6-C5-N7	-7.27	127.21	132.30
27	X	2488	G	C5-C6-N1	7.26	115.13	111.50
27	X	1208	A	C8-N9-C4	-7.23	102.91	105.80
27	X	540	G	O4'-C1'-N9	7.23	113.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	2857	C	C6-N1-C2	-7.21	117.42	120.30
27	X	527	C	C6-N1-C2	-7.20	117.42	120.30
27	X	2591	C	C6-N1-C2	-7.19	117.42	120.30
27	X	1989	C	C5-C6-N1	7.18	124.59	121.00
27	X	2470	U	C6-N1-C1'	-7.13	111.22	121.20
27	X	2845	C	N3-C4-C5	-7.12	119.05	121.90
27	X	1283	C	N1-C2-O2	-7.11	114.63	118.90
27	X	2705	A	C2-N3-C4	-7.11	107.05	110.60
27	X	343	A	N7-C8-N9	7.09	117.35	113.80
27	X	1682	A	N1-C6-N6	7.08	122.85	118.60
27	X	462	G	C5-C6-N1	-6.96	108.02	111.50
27	X	1468	A	C2-N3-C4	6.95	114.08	110.60
10	K	92	GLY	N-CA-C	-6.94	95.74	113.10
27	X	2485	U	C2-N1-C1'	6.94	126.03	117.70
27	X	983	G	C8-N9-C4	-6.93	103.63	106.40
27	X	1270	C	C6-N1-C2	-6.92	117.53	120.30
27	X	841	G	C8-N9-C4	-6.91	103.64	106.40
27	X	774	A	N1-C6-N6	6.91	122.74	118.60
27	X	796	A	C2-N3-C4	-6.90	107.15	110.60
27	X	1724	C	C6-N1-C2	6.88	123.05	120.30
27	X	579	G	C4-C5-N7	-6.88	108.05	110.80
27	X	1468	A	C5-C6-N1	6.83	121.11	117.70
27	X	1993	G	N1-C6-O6	6.83	124.00	119.90
27	X	1235	C	C6-N1-C2	6.82	123.03	120.30
14	O	38	LEU	CA-CB-CG	6.81	130.97	115.30
27	X	1253	C	C6-N1-C2	-6.79	117.58	120.30
27	X	661	C	C5-C6-N1	6.77	124.39	121.00
27	X	1979	C	N3-C2-O2	-6.77	117.16	121.90
27	X	2815	C	C5-C6-N1	-6.76	117.62	121.00
27	X	2592	U	N3-C4-O4	6.75	124.12	119.40
27	X	2371	A	N7-C8-N9	6.72	117.16	113.80
27	X	2706	U	O5'-P-OP2	-6.72	99.65	105.70
27	X	796	A	C5-C6-N1	-6.70	114.35	117.70
27	X	1982	C	C2-N3-C4	-6.69	116.55	119.90
27	X	2553	G	N3-C4-N9	-6.69	121.98	126.00
27	X	2668	U	N1-C2-N3	6.69	118.92	114.90
27	X	1208	A	N7-C8-N9	6.69	117.15	113.80
27	X	759	C	C6-N1-C2	6.68	122.97	120.30
27	X	816	U	N3-C2-O2	-6.68	117.53	122.20
25	2	38	GLY	N-CA-C	-6.67	96.42	113.10
27	X	2845	C	C6-N1-C2	-6.65	117.64	120.30
27	X	2478	C	C2-N1-C1'	6.63	126.09	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	1682	A	C4-C5-C6	6.63	120.31	117.00
27	X	2607	C	N1-C2-O2	6.62	122.87	118.90
27	X	2434	G	C4-N9-C1'	6.62	135.11	126.50
27	X	1332	G	N1-C6-O6	6.57	123.84	119.90
27	X	2488	G	N3-C4-C5	-6.52	125.34	128.60
27	X	2508	G	N1-C6-O6	6.52	123.81	119.90
27	X	1288	A	O4'-C1'-N9	6.51	113.41	108.20
27	X	957	G	N3-C4-C5	-6.50	125.35	128.60
27	X	1481	U	C2-N1-C1'	-6.49	109.91	117.70
27	X	2542	U	C6-N1-C2	-6.49	117.10	121.00
27	X	1716	G	N1-C6-O6	-6.48	116.01	119.90
27	X	538	A	N1-C2-N3	-6.48	126.06	129.30
27	X	522	G	C5-C6-O6	-6.47	124.72	128.60
27	X	2404	A	P-O3'-C3'	6.46	127.46	119.70
27	X	537	C	N3-C2-O2	-6.41	117.41	121.90
27	X	774	A	C4-C5-N7	6.41	113.91	110.70
27	X	1664	G	C8-N9-C1'	6.41	135.33	127.00
27	X	1812	U	C5-C6-N1	6.40	125.90	122.70
27	X	2705	A	C6-C5-N7	-6.38	127.84	132.30
27	X	699	G	C4-C5-N7	6.38	113.35	110.80
27	X	2670	C	C6-N1-C2	-6.38	117.75	120.30
27	X	522	G	N9-C4-C5	-6.37	102.85	105.40
27	X	2705	A	C8-N9-C4	-6.35	103.26	105.80
27	X	1467	U	C5-C6-N1	6.33	125.86	122.70
27	X	1682	A	C6-C5-N7	-6.32	127.88	132.30
27	X	1481	U	N1-C2-O2	-6.31	118.38	122.80
27	X	2541	U	N3-C2-O2	-6.29	117.80	122.20
27	X	2542	U	N3-C2-O2	-6.26	117.82	122.20
27	X	1975	G	P-O3'-C3'	6.25	127.20	119.70
27	X	1812	U	C6-N1-C1'	-6.23	112.48	121.20
27	X	522	G	C4-C5-N7	6.20	113.28	110.80
27	X	2697	G	C2-N3-C4	6.20	115.00	111.90
27	X	2421	C	C6-N1-C2	-6.19	117.82	120.30
27	X	29	U	N3-C4-O4	6.17	123.72	119.40
27	X	556	A	N1-C6-N6	6.16	122.30	118.60
27	X	928	G	C4-C5-N7	6.16	113.26	110.80
27	X	2587	G	C5-C6-O6	-6.16	124.91	128.60
27	X	346	C	C6-N1-C2	-6.15	117.84	120.30
27	X	1466	C	C6-N1-C2	-6.14	117.84	120.30
27	X	24	G	O4'-C1'-N9	6.14	113.11	108.20
27	X	1250	A	P-O3'-C3'	6.12	127.04	119.70
27	X	923	A	C2-N3-C4	6.11	113.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	2508	G	C4-C5-N7	6.11	113.24	110.80
27	X	968	C	C2-N1-C1'	6.10	125.51	118.80
27	X	1674	C	N1-C2-O2	6.10	122.56	118.90
27	X	2795	A	N1-C6-N6	-6.10	114.94	118.60
27	X	841	G	N7-C8-N9	6.10	116.15	113.10
27	X	843	G	C5-C6-O6	-6.10	124.94	128.60
27	X	2767	C	C6-N1-C2	-6.08	117.87	120.30
27	X	2799	C	N1-C2-O2	-6.07	115.26	118.90
27	X	816	U	C6-N1-C2	-6.07	117.36	121.00
27	X	928	G	N9-C4-C5	-6.07	102.97	105.40
27	X	1984	A	C2-N3-C4	-6.07	107.57	110.60
27	X	1305	C	C6-N1-C2	6.05	122.72	120.30
27	X	617	U	N3-C2-O2	-6.04	117.97	122.20
27	X	538	A	C5-C6-N1	6.02	120.71	117.70
27	X	1747	G	C8-N9-C4	-6.02	103.99	106.40
27	X	2867	G	N3-C4-C5	6.01	131.61	128.60
27	X	1668	G	C6-C5-N7	-6.01	126.79	130.40
27	X	1988	A	N1-C6-N6	6.01	122.21	118.60
27	X	2034	A	N1-C6-N6	-6.01	115.00	118.60
27	X	1812	U	N1-C2-O2	6.01	127.00	122.80
27	X	2279	G	N1-C6-O6	6.01	123.50	119.90
27	X	1333	G	C2-N3-C4	-6.00	108.90	111.90
27	X	2668	U	C5-C4-O4	5.99	129.50	125.90
27	X	2638	G	N3-C4-C5	5.99	131.60	128.60
27	X	2410	U	C6-N1-C2	-5.97	117.42	121.00
27	X	2398	U	C6-N1-C2	-5.97	117.42	121.00
27	X	2854	G	C4-C5-N7	5.96	113.19	110.80
27	X	2669	C	N3-C2-O2	-5.96	117.73	121.90
27	X	2806	G	N1-C6-O6	5.96	123.48	119.90
27	X	699	G	C5-N7-C8	-5.96	101.32	104.30
27	X	699	G	N1-C6-O6	5.96	123.47	119.90
27	X	2019	C	C6-N1-C2	-5.96	117.92	120.30
27	X	540	G	N1-C6-O6	-5.95	116.33	119.90
27	X	1286	U	O5'-P-OP1	-5.94	100.36	105.70
27	X	2705	A	P-O3'-C3'	5.93	126.81	119.70
27	X	1975	G	N3-C4-C5	-5.92	125.64	128.60
27	X	2799	C	N1-C2-N3	5.91	123.34	119.20
27	X	2812	A	C8-N9-C4	-5.90	103.44	105.80
27	X	2485	U	C5-C6-N1	5.89	125.65	122.70
27	X	1141	U	P-O3'-C3'	5.88	126.75	119.70
27	X	2478	C	N3-C4-N4	5.88	122.11	118.00
27	X	684	C	N3-C4-C5	-5.87	119.55	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	1674	C	N3-C4-C5	5.87	124.25	121.90
27	X	2495	G	C2-N3-C4	5.87	114.84	111.90
27	X	985	G	C8-N9-C4	-5.86	104.06	106.40
27	X	1481	U	N3-C2-O2	5.86	126.30	122.20
27	X	2049	C	C6-N1-C2	-5.85	117.96	120.30
27	X	1324	G	O4'-C1'-N9	5.83	112.86	108.20
27	X	536	A	N1-C6-N6	5.83	122.10	118.60
27	X	2021	G	C6-C5-N7	-5.82	126.91	130.40
27	X	2409	A	P-O3'-C3'	5.82	126.68	119.70
27	X	1636	G	C8-N9-C4	5.81	108.72	106.40
27	X	1647	U	N3-C4-C5	-5.81	111.11	114.60
27	X	1770	U	C5-C6-N1	-5.81	119.79	122.70
27	X	1979	C	N1-C2-O2	5.81	122.39	118.90
27	X	2508	G	C6-C5-N7	-5.81	126.92	130.40
27	X	699	G	C6-C5-N7	-5.80	126.92	130.40
27	X	1712	G	C4-N9-C1'	5.80	134.04	126.50
27	X	538	A	P-O3'-C3'	5.79	126.65	119.70
27	X	2827	G	N3-C4-N9	5.79	129.47	126.00
27	X	2488	G	C2-N3-C4	5.78	114.79	111.90
27	X	2638	G	N3-C4-N9	-5.78	122.53	126.00
27	X	479	G	N1-C6-O6	5.78	123.37	119.90
27	X	1691	G	N9-C4-C5	-5.78	103.09	105.40
27	X	1142	G	N3-C4-C5	-5.78	125.71	128.60
27	X	1982	C	C5-C6-N1	-5.78	118.11	121.00
27	X	2846	G	C8-N9-C4	5.77	108.71	106.40
12	M	17	GLU	N-CA-C	-5.77	95.43	111.00
27	X	1992	G	N7-C8-N9	-5.77	110.22	113.10
27	X	579	G	C5-C6-O6	5.76	132.06	128.60
27	X	2034	A	C8-N9-C4	-5.76	103.50	105.80
27	X	1315	A	N1-C6-N6	-5.76	115.14	118.60
27	X	2508	G	C5-C6-O6	-5.75	125.15	128.60
27	X	661	C	C2-N1-C1'	5.74	125.11	118.80
27	X	1693	A	C8-N9-C4	-5.71	103.51	105.80
27	X	1712	G	C6-C5-N7	-5.71	126.97	130.40
27	X	2563	U	C2-N1-C1'	5.71	124.55	117.70
27	X	700	C	C6-N1-C2	-5.70	118.02	120.30
27	X	841	G	C5-N7-C8	-5.69	101.46	104.30
27	X	2576	G	N1-C6-O6	5.68	123.31	119.90
27	X	2854	G	C5-N7-C8	-5.68	101.46	104.30
27	X	1934	U	C6-N1-C2	-5.68	117.59	121.00
27	X	2859	U	O5'-P-OP1	-5.68	100.59	105.70
27	X	1746	A	C8-N9-C4	-5.67	103.53	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	2434	G	N3-C4-C5	-5.67	125.76	128.60
27	X	2655	C	C6-N1-C2	5.67	122.57	120.30
27	X	2634	G	O4'-C1'-N9	5.66	112.73	108.20
27	X	29	U	C5-C4-O4	-5.66	122.51	125.90
27	X	1691	G	C5-C6-O6	-5.65	125.21	128.60
27	X	2409	A	OP1-P-O3'	5.64	117.62	105.20
27	X	2587	G	C6-C5-N7	-5.64	127.01	130.40
27	X	684	C	C6-N1-C2	-5.64	118.04	120.30
27	X	2495	G	C5-C6-N1	5.63	114.32	111.50
27	X	2491	C	C6-N1-C2	-5.62	118.05	120.30
27	X	2587	G	N1-C6-O6	5.62	123.27	119.90
27	X	2813	G	C8-N9-C4	5.61	108.65	106.40
27	X	841	G	N3-C4-N9	-5.61	122.63	126.00
27	X	533	C	C2-N1-C1'	-5.61	112.63	118.80
27	X	1712	G	N3-C4-N9	5.61	129.36	126.00
27	X	2806	G	C6-C5-N7	-5.61	127.04	130.40
27	X	2656	G	OP2-P-O3'	5.60	117.52	105.20
27	X	617	U	C4-C5-C6	5.59	123.06	119.70
27	X	822	G	N3-C4-C5	-5.59	125.80	128.60
27	X	2371	A	C8-N9-C4	-5.59	103.56	105.80
27	X	1981	A	N1-C2-N3	5.59	132.10	129.30
27	X	2426	G	OP1-P-O3'	5.59	117.50	105.20
27	X	689	A	O4'-C1'-N9	5.59	112.67	108.20
27	X	1994	U	C5-C6-N1	5.58	125.49	122.70
27	X	2580	C	N1-C2-O2	-5.58	115.55	118.90
27	X	860	U	N1-C2-O2	5.57	126.70	122.80
27	X	2796	A	O5'-P-OP2	-5.57	100.69	105.70
27	X	2806	G	C5-C6-O6	-5.57	125.26	128.60
27	X	1670	G	N7-C8-N9	-5.57	110.31	113.10
27	X	1770	U	C4-C5-C6	5.57	123.04	119.70
27	X	2693	U	C6-N1-C1'	5.53	128.95	121.20
27	X	1692	C	C4-C5-C6	5.53	120.16	117.40
27	X	1713	G	N1-C6-O6	-5.52	116.59	119.90
27	X	2437	G	C8-N9-C4	-5.52	104.19	106.40
27	X	2664	G	N3-C2-N2	-5.51	116.05	119.90
27	X	542	A	N1-C2-N3	5.50	132.05	129.30
27	X	2475	C	C6-N1-C2	-5.50	118.10	120.30
27	X	522	G	C8-N9-C1'	-5.49	119.86	127.00
27	X	2481	G	C8-N9-C4	-5.49	104.20	106.40
28	Y	32	C	C6-N1-C2	-5.49	118.10	120.30
27	X	2398	U	N3-C4-C5	-5.49	111.31	114.60
27	X	1770	U	O4'-C1'-N1	5.49	112.59	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	1780	A	N1-C6-N6	5.48	121.89	118.60
27	X	1982	C	N3-C4-C5	5.48	124.09	121.90
27	X	1208	A	C5-N7-C8	-5.48	101.16	103.90
27	X	1629	G	OP1-P-O3'	5.47	117.24	105.20
27	X	2796	A	N1-C6-N6	-5.47	115.32	118.60
27	X	2812	A	N7-C8-N9	5.46	116.53	113.80
27	X	2579	A	C8-N9-C4	5.46	107.98	105.80
27	X	788	G	P-O3'-C3'	5.46	126.25	119.70
27	X	1664	G	O5'-P-OP1	-5.46	100.79	105.70
27	X	2254	C	C6-N1-C2	-5.46	118.12	120.30
27	X	2382	C	C6-N1-C2	-5.46	118.12	120.30
27	X	2025	A	N9-C4-C5	5.45	107.98	105.80
27	X	1770	U	C5-C4-O4	5.45	129.17	125.90
27	X	1661	C	N3-C2-O2	-5.45	118.08	121.90
27	X	2669	C	N3-C4-C5	-5.45	119.72	121.90
27	X	1691	G	C4-C5-N7	5.45	112.98	110.80
27	X	2607	C	N3-C2-O2	-5.44	118.09	121.90
27	X	577	U	C6-N1-C2	-5.43	117.74	121.00
27	X	928	G	N1-C6-O6	5.43	123.16	119.90
27	X	2798	A	N9-C4-C5	-5.42	103.63	105.80
27	X	1923	U	P-O3'-C3'	5.42	126.21	119.70
27	X	2548	G	C4-C5-N7	-5.42	108.63	110.80
27	X	1240	G	C8-N9-C4	5.42	108.57	106.40
27	X	755	C	O5'-P-OP1	-5.41	100.83	105.70
27	X	2756	A	P-O3'-C3'	5.41	126.20	119.70
27	X	2674	C	N3-C4-N4	5.41	121.79	118.00
27	X	2706	U	C5-C6-N1	5.41	125.40	122.70
27	X	2018	G	N3-C4-C5	5.40	131.30	128.60
27	X	1682	A	C8-N9-C4	-5.39	103.64	105.80
27	X	1664	G	N3-C4-C5	5.39	131.30	128.60
27	X	2820	C	N3-C4-C5	5.39	124.06	121.90
27	X	2246	A	N1-C6-N6	-5.39	115.37	118.60
27	X	2854	G	N7-C8-N9	5.39	115.80	113.10
27	X	2837	G	C8-N9-C4	5.39	108.55	106.40
27	X	2490	U	N3-C2-O2	-5.38	118.43	122.20
27	X	519	C	C6-N1-C2	-5.38	118.15	120.30
27	X	338	G	C8-N9-C4	-5.37	104.25	106.40
27	X	2561	G	C5-C6-N1	5.37	114.19	111.50
27	X	1696	C	N1-C2-O2	-5.36	115.68	118.90
27	X	1468	A	N3-C4-C5	-5.36	123.05	126.80
27	X	2694	G	OP2-P-O3'	5.34	116.94	105.20
27	X	2019	C	C2-N1-C1'	5.34	124.67	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	2023	C	C6-N1-C2	5.34	122.43	120.30
27	X	2019	C	C5-C6-N1	5.33	123.67	121.00
27	X	1657	A	C2-N3-C4	-5.33	107.93	110.60
27	X	2032	G	N3-C4-N9	5.33	129.20	126.00
27	X	2279	G	C6-C5-N7	-5.33	127.20	130.40
27	X	2025	A	N1-C6-N6	-5.32	115.41	118.60
27	X	2434	G	C8-N9-C1'	-5.32	120.08	127.00
27	X	774	A	C2-N3-C4	-5.32	107.94	110.60
27	X	1246	G	N1-C6-O6	-5.32	116.71	119.90
27	X	2470	U	N3-C2-O2	-5.32	118.48	122.20
27	X	1164	C	C6-N1-C2	-5.30	118.18	120.30
27	X	1934	U	N3-C4-O4	5.29	123.11	119.40
27	X	540	G	C8-N9-C4	-5.29	104.28	106.40
27	X	596	C	N3-C4-C5	-5.28	119.79	121.90
27	X	1742	G	N3-C4-N9	5.28	129.17	126.00
27	X	1746	A	N1-C6-N6	-5.28	115.43	118.60
27	X	1313	U	P-O3'-C3'	5.28	126.03	119.70
27	X	1679	U	N3-C2-O2	-5.28	118.50	122.20
27	X	2021	G	N1-C6-O6	5.28	123.07	119.90
27	X	2751	C	N3-C4-C5	5.28	124.01	121.90
27	X	699	G	N7-C8-N9	5.27	115.73	113.10
27	X	2693	U	N3-C4-O4	-5.26	115.72	119.40
27	X	1976	U	N3-C4-O4	-5.25	115.72	119.40
27	X	1747	G	N3-C4-C5	-5.25	125.98	128.60
27	X	833	A	C5-C6-N6	-5.24	119.50	123.70
27	X	1934	U	N3-C4-C5	-5.24	111.45	114.60
27	X	2831	A	C4-C5-C6	-5.24	114.38	117.00
27	X	1310	C	N3-C4-C5	5.24	124.00	121.90
27	X	2321	C	C6-N1-C2	-5.23	118.21	120.30
27	X	923	A	C8-N9-C4	-5.23	103.71	105.80
27	X	2239	C	C6-N1-C2	-5.22	118.21	120.30
27	X	2524	G	C4-C5-N7	5.22	112.89	110.80
27	X	1713	G	C4-C5-N7	-5.21	108.71	110.80
27	X	1993	G	C4-C5-N7	5.21	112.89	110.80
27	X	1278	A	O5'-P-OP2	-5.21	101.01	105.70
27	X	844	G	OP2-P-O3'	5.20	116.65	105.20
27	X	2662	C	C6-N1-C2	-5.20	118.22	120.30
27	X	2791	C	C6-N1-C2	5.20	122.38	120.30
27	X	2712	G	N1-C2-N2	-5.20	111.52	116.20
27	X	742	G	C4-N9-C1'	5.20	133.26	126.50
3	C	56	ARG	N-CA-C	5.20	125.03	111.00
27	X	2560	G	O4'-C1'-N9	5.20	112.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	1288	A	N7-C8-N9	5.19	116.40	113.80
27	X	1391	A	P-O3'-C3'	5.19	125.93	119.70
27	X	2524	G	C5-C6-O6	-5.19	125.49	128.60
27	X	1647	U	C6-N1-C2	-5.19	117.89	121.00
27	X	1342	U	O5'-P-OP2	-5.18	101.03	105.70
27	X	2541	U	N1-C2-O2	5.18	126.43	122.80
27	X	874	A	C8-N9-C4	-5.18	103.73	105.80
27	X	2638	G	N3-C2-N2	-5.18	116.27	119.90
27	X	2827	G	N3-C4-C5	-5.18	126.01	128.60
27	X	2338	C	C6-N1-C2	-5.18	118.23	120.30
27	X	2485	U	N1-C2-O2	5.18	126.42	122.80
27	X	24	G	C4-N9-C1'	-5.17	119.78	126.50
27	X	833	A	C4-C5-N7	5.17	113.28	110.70
27	X	1223	G	C6-C5-N7	-5.17	127.30	130.40
27	X	2590	U	C2-N1-C1'	5.17	123.90	117.70
27	X	1885	C	N1-C2-O2	5.16	122.00	118.90
27	X	1712	G	C8-N9-C1'	-5.16	120.29	127.00
27	X	2815	C	N3-C4-C5	5.16	123.96	121.90
27	X	522	G	N3-C4-N9	5.16	129.09	126.00
27	X	2057	U	C6-N1-C2	-5.15	117.91	121.00
27	X	1141	U	N3-C2-O2	-5.15	118.59	122.20
27	X	1694	A	C5-N7-C8	-5.15	101.33	103.90
27	X	1623	C	N1-C2-O2	5.14	121.99	118.90
27	X	2050	G	N9-C4-C5	-5.14	103.34	105.40
27	X	1934	U	C5-C6-N1	5.14	125.27	122.70
27	X	2592	U	N3-C4-C5	-5.14	111.52	114.60
27	X	1326	U	C2-N1-C1'	5.13	123.86	117.70
27	X	593	C	C6-N1-C2	-5.13	118.25	120.30
27	X	2857	C	N3-C4-C5	-5.13	119.85	121.90
27	X	461	A	O5'-P-OP1	-5.13	101.08	105.70
27	X	1625	A	P-O3'-C3'	5.13	125.86	119.70
27	X	1232	U	N1-C2-O2	-5.13	119.21	122.80
27	X	1035	G	N3-C4-C5	-5.12	126.04	128.60
27	X	2410	U	C5-C6-N1	5.12	125.26	122.70
27	X	1992	G	N9-C4-C5	-5.12	103.35	105.40
27	X	2000	U	N3-C2-O2	5.12	125.79	122.20
27	X	2495	G	C6-N1-C2	-5.12	122.03	125.10
27	X	1211	G	N3-C4-N9	5.12	129.07	126.00
27	X	1142	G	C2-N3-C4	5.12	114.46	111.90
27	X	2668	U	N1-C2-O2	-5.12	119.22	122.80
27	X	13	A	OP2-P-O3'	5.12	116.45	105.20
27	X	985	G	N7-C8-N9	5.11	115.66	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	1223	G	C4-N9-C1'	5.11	133.14	126.50
27	X	1975	G	C4-N9-C1'	5.11	133.14	126.50
27	X	2690	A	N1-C6-N6	5.11	121.67	118.60
27	X	968	C	N1-C2-O2	5.10	121.96	118.90
27	X	1222	G	N3-C4-N9	5.10	129.06	126.00
27	X	2576	G	C6-C5-N7	-5.10	127.34	130.40
27	X	2039	G	C8-N9-C4	-5.09	104.36	106.40
27	X	2850	U	O5'-P-OP1	-5.08	101.13	105.70
27	X	537	C	P-O3'-C3'	5.08	125.80	119.70
27	X	518	A	C8-N9-C4	-5.08	103.77	105.80
27	X	1315	A	N1-C2-N3	5.08	131.84	129.30
27	X	2050	G	N1-C6-O6	5.08	122.95	119.90
27	X	2482	A	OP1-P-OP2	-5.07	112.00	119.60
27	X	2837	G	C6-C5-N7	5.07	133.44	130.40
27	X	236	C	C6-N1-C2	-5.07	118.27	120.30
27	X	479	G	C5-C6-O6	-5.06	125.56	128.60
27	X	1662	G	N3-C4-N9	5.06	129.04	126.00
27	X	1141	U	C2-N1-C1'	5.06	123.77	117.70
27	X	558	G	C4-N9-C1'	5.05	133.06	126.50
15	P	120	ILE	N-CA-C	5.04	124.62	111.00
27	X	2795	A	P-O3'-C3'	5.04	125.75	119.70
16	Q	7	LEU	CA-CB-CG	5.04	126.89	115.30
27	X	2026	C	N1-C2-O2	5.03	121.92	118.90
27	X	536	A	C5-C6-N6	-5.03	119.68	123.70
27	X	1467	U	N1-C2-N3	-5.03	111.89	114.90
27	X	1683	G	N3-C4-N9	-5.03	122.98	126.00
27	X	2371	A	C5-N7-C8	-5.03	101.39	103.90
27	X	2596	C	C6-N1-C2	5.03	122.31	120.30
27	X	69	G	C4-N9-C1'	5.02	133.03	126.50
27	X	854	G	N1-C6-O6	5.02	122.91	119.90
27	X	1240	G	N9-C4-C5	-5.02	103.39	105.40
27	X	2792	C	C6-N1-C2	5.02	122.31	120.30
27	X	2682	C	C2-N1-C1'	5.02	124.32	118.80
27	X	2693	U	C5-C6-N1	-5.02	120.19	122.70
27	X	1315	A	C5-C6-N6	5.01	127.71	123.70
27	X	2472	U	O5'-P-OP1	-5.01	101.19	105.70
27	X	770	U	C6-N1-C2	-5.01	118.00	121.00
27	X	1682	A	N7-C8-N9	5.01	116.30	113.80
27	X	1618	U	N3-C4-C5	-5.00	111.60	114.60
27	X	2687	G	N7-C8-N9	-5.00	110.60	113.10

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	2	42	LEU	Peptide
26	3	45	GLY	Peptide
2	B	146	THR	Peptide
6	G	108	GLY	Peptide
7	H	26	ASN	Peptide
8	I	35	LYS	Peptide
8	I	40	ARG	Peptide
8	I	99	VAL	Peptide
10	K	93	GLY	Peptide
10	K	94	TYR	Peptide
16	Q	59	PRO	Peptide
17	R	64	ASN	Peptide
19	T	19	LYS	Peptide
20	U	30	VAL	Peptide
23	Z	4	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1987	0	2056	145	0
2	B	1539	0	1600	109	0
3	C	1481	0	1504	99	0
4	D	1400	0	1481	55	0
5	E	1286	0	1336	54	0
6	G	1114	0	1144	73	0
7	H	997	0	1046	56	0
8	I	1011	0	1047	72	0
9	J	1090	0	1125	64	0
10	K	878	0	930	45	0
11	L	779	0	820	36	0
12	M	871	0	894	61	0
13	N	978	0	1020	52	0
14	O	741	0	756	51	0
15	P	1038	0	1125	85	0
16	Q	726	0	753	32	0
17	R	825	0	881	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	S	1345	0	1372	37	0
19	T	556	0	579	30	0
20	U	552	0	604	35	0
21	V	525	0	546	19	0
22	W	424	0	470	16	0
23	Z	443	0	444	26	0
24	1	431	0	456	29	0
25	2	383	0	414	26	0
26	3	462	0	506	53	0
27	X	57533	0	28987	1344	0
28	Y	2601	0	1327	62	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	K	2	0	0	0	0
29	M	2	0	0	0	0
29	X	64	0	0	0	0
30	X	51	0	67	9	0
All	All	84117	0	55290	2467	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (2467) 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)
2:B:116:VAL:HG22	2:B:136:ARG:HG3	1.32	1.11
23:Z:19:ARG:NH2	27:X:1277:G:OP1	1.90	1.04
13:N:66:ASN:HB3	13:N:76:TYR:HB2	1.46	0.97
27:X:854:G:H1	27:X:948:C:H42	1.04	0.96
7:H:40:GLY:HA3	27:X:2545:A:H61	1.29	0.95
8:I:21:ARG:HE	8:I:22:GLY:H	1.08	0.95
6:G:109:GLY:HA2	6:G:111:LYS:HE3	1.46	0.95
27:X:517:A:H5"	27:X:518:A:H5'	1.50	0.94
1:A:250:TRP:O	1:A:255:LYS:NZ	2.01	0.93
27:X:2447:G:HO2'	27:X:2448:A:H8	1.07	0.92
9:J:82:THR:HA	27:X:2474:G:H5"	1.53	0.90
27:X:4:C:H42	27:X:2873:G:H1	1.17	0.89
1:A:55:GLY:H	1:A:217:ARG:HB2	1.38	0.88
27:X:571:U:HO2'	27:X:581:A:H8	1.21	0.87
10:K:60:LEU:HG	10:K:64:ARG:HD2	1.55	0.86
27:X:2281:C:H42	27:X:2293:G:H1	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:38:THR:HB	27:X:2063:A:H5'	1.58	0.85
15:P:80:LEU:HD11	15:P:87:GLU:HB3	1.58	0.85
8:I:21:ARG:HE	8:I:22:GLY:N	1.75	0.85
24:1:41:ASP:HB2	24:1:46:LYS:HE3	1.56	0.85
27:X:538:A:H62	27:X:2026:C:H5'	1.40	0.84
27:X:832:A:OP2	27:X:1201:G:N2	2.10	0.84
1:A:218:LYS:NZ	1:A:219:PRO:O	2.10	0.84
27:X:2016:A:O2'	27:X:2018:G:OP2	1.95	0.84
27:X:833:A:N3	27:X:954:U:O2'	2.10	0.83
27:X:2225:G:H2'	27:X:2226:A:H8	1.41	0.83
9:J:83:ARG:HH22	27:X:971:A:H61	1.22	0.83
27:X:2757:G:H5"	27:X:2758:A:H5'	1.60	0.83
26:3:13:ARG:HE	26:3:25:PHE:H	1.27	0.83
15:P:100:GLY:HA3	15:P:124:THR:HA	1.58	0.83
2:B:14:ILE:HG12	12:M:20:HIS:HD2	1.43	0.82
27:X:2811:G:H2'	27:X:2812:A:C8	2.13	0.82
2:B:146:THR:HG1	27:X:2550:C:HO2'	1.19	0.82
1:A:252:LYS:H	1:A:252:LYS:HZ2	1.28	0.81
14:O:12:TYR:HB3	14:O:40:VAL:H	1.45	0.81
27:X:649:G:H22	27:X:661:C:H1'	1.45	0.81
22:W:8:SER:HB2	27:X:999:A:H5"	1.62	0.81
27:X:1173:G:H2'	27:X:1174:G:H8	1.46	0.80
6:G:37:ASP:O	6:G:39:GLN:NE2	2.15	0.79
27:X:841:G:H2'	27:X:842:A:C8	2.16	0.79
27:X:2259:G:H4'	27:X:2306:A:H5'	1.65	0.79
27:X:415:A:H61	27:X:436:A:H61	1.30	0.79
15:P:99:ALA:HB2	27:X:24:G:O2'	1.83	0.78
2:B:82:ARG:NH2	27:X:2617:G:OP2	2.16	0.78
26:3:26:LYS:HD3	26:3:28:GLY:H	1.45	0.78
9:J:17:ARG:NH1	27:X:966:A:OP2	2.17	0.78
15:P:30:TYR:H	15:P:126:HIS:HD2	1.32	0.78
14:O:57:GLN:H	14:O:97:GLY:HA3	1.47	0.78
27:X:538:A:O2'	27:X:539:A:O5'	2.00	0.78
2:B:51:TYR:HE2	12:M:3:THR:HG21	1.49	0.77
18:S:125:PRO:O	18:S:129:ARG:NH1	2.18	0.77
1:A:157:ARG:NH1	27:X:1810:U:OP2	2.17	0.77
9:J:100:PRO:HB2	18:S:74:ARG:HG2	1.67	0.77
7:H:23:ARG:NH1	27:X:2526:U:O2	2.17	0.77
27:X:2796:A:H2'	27:X:2797:G:C8	2.19	0.77
27:X:89:A:H4'	27:X:90:G:H5'	1.68	0.76
27:X:1856:U:OP1	27:X:2389:G:O2'	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:ASN:HD21	3:C:167:VAL:H	1.31	0.76
27:X:215:G:H21	27:X:632:A:H8	1.30	0.76
27:X:1882:G:N2	27:X:1885:C:H41	1.83	0.76
20:U:21:ARG:HD3	20:U:23:LYS:HG2	1.66	0.76
3:C:162:ARG:NH1	3:C:162:ARG:O	2.19	0.76
27:X:1329:U:H2'	27:X:1330:G:H8	1.49	0.76
27:X:2002:A:N6	27:X:2018:G:O6	2.19	0.76
1:A:14:ARG:HG3	1:A:24:LEU:HG	1.68	0.76
8:I:40:ARG:NH2	27:X:820:U:OP1	2.18	0.76
2:B:176:ARG:HH21	12:M:16:ILE:HG23	1.51	0.75
3:C:161:ALA:HB1	3:C:167:VAL:HG21	1.69	0.75
27:X:2543:A:H5'	27:X:2627:G:H4'	1.66	0.75
27:X:2761:A:H5"	27:X:2762:G:H5'	1.67	0.75
1:A:243:GLY:C	1:A:244:ARG:HE	1.89	0.75
1:A:24:LEU:HB2	1:A:205:VAL:HG22	1.68	0.75
15:P:45:ILE:HD11	15:P:57:LEU:HD11	1.68	0.75
27:X:965:G:O2'	27:X:2253:A:N1	2.20	0.75
3:C:137:ALA:HB1	3:C:142:LEU:HB2	1.68	0.75
1:A:210:GLY:HA2	1:A:213:ARG:HG2	1.69	0.75
16:Q:14:GLU:OE2	27:X:1405:A:N6	2.18	0.75
17:R:56:LYS:HB3	17:R:69:GLN:HG2	1.69	0.75
24:1:27:ASN:ND2	24:1:36:GLU:OE1	2.20	0.75
27:X:1327:C:H42	27:X:1351:G:H1	1.32	0.75
26:3:32:GLN:HB3	27:X:2400:G:N7	2.02	0.75
27:X:27:G:N2	27:X:522:G:H1'	2.02	0.75
27:X:2225:G:H2'	27:X:2226:A:C8	2.20	0.75
27:X:2796:A:H2'	27:X:2797:G:H8	1.50	0.74
11:L:90:ASP:OD2	11:L:91:ARG:N	2.20	0.74
1:A:91:ARG:HB2	1:A:107:ALA:HB3	1.69	0.74
15:P:30:TYR:H	15:P:126:HIS:CD2	2.05	0.74
2:B:91:VAL:HB	2:B:93:VAL:HG12	1.70	0.74
27:X:1278:A:H2	27:X:1997:A:H62	1.35	0.74
27:X:1673:C:H2'	27:X:1674:C:H6	1.52	0.74
27:X:591:G:H3'	27:X:592:G:H8	1.51	0.74
27:X:1922:U:H3'	27:X:1923:U:H5'	1.70	0.74
6:G:34:PRO:HB3	6:G:71:THR:HG21	1.69	0.74
9:J:117:GLU:OE1	9:J:120:ARG:NH1	2.21	0.74
12:M:60:SER:HA	12:M:64:LYS:HB2	1.69	0.74
27:X:2757:G:OP2	27:X:2761:A:O2'	2.06	0.74
22:W:5:LEU:HB2	22:W:25:LEU:HD13	1.68	0.74
25:2:19:ARG:HG2	27:X:123:A:H5'	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:465:C:O2'	27:X:483:A:N6	2.21	0.74
27:X:2820:C:H2'	27:X:2821:G:H8	1.52	0.73
11:L:65:THR:OG1	28:Y:52:G:OP1	2.06	0.73
27:X:1337:G:N2	27:X:1343:C:O2	2.20	0.73
2:B:137:ARG:NH2	27:X:2034:A:OP1	2.19	0.73
27:X:854:G:N2	27:X:948:C:N3	2.32	0.73
2:B:9:ILE:HD11	2:B:27:LEU:HB2	1.70	0.73
27:X:872:G:O2'	27:X:928:G:O6	2.07	0.73
2:B:128:SER:HB3	27:X:1976:U:H4'	1.71	0.73
12:M:100:ARG:HD2	27:X:1744:G:OP1	1.89	0.73
27:X:115:G:OP2	27:X:117:A:O2'	2.07	0.73
27:X:613:A:N6	27:X:668:A:O2'	2.22	0.73
4:D:116:GLY:HA2	4:D:176:PRO:HB2	1.71	0.73
15:P:35:PRO:HD3	15:P:124:THR:OG1	1.89	0.73
27:X:1963:G:O2'	27:X:1965:U:OP2	2.07	0.73
27:X:2708:U:H2'	27:X:2709:C:C6	2.23	0.73
17:R:17:LYS:NZ	27:X:83:A:OP2	2.16	0.72
27:X:2484:G:H22	30:X:2902:ERY:H191	1.54	0.72
17:R:105:ARG:HH22	17:R:113:THR:H	1.37	0.72
27:X:313:U:H2'	27:X:314:G:H8	1.54	0.72
1:A:63:ARG:HH21	1:A:86:PRO:HD2	1.55	0.72
2:B:152:LYS:HB3	6:G:106:TYR:HB2	1.71	0.72
16:Q:35:LYS:NZ	27:X:1615:C:OP2	2.23	0.72
27:X:1399:C:OP2	27:X:1409:U:N3	2.21	0.72
27:X:2324:G:HO2'	27:X:2360:C:HO2'	1.35	0.72
14:O:68:LYS:NZ	27:X:1238:A:OP1	2.18	0.72
23:Z:16:ARG:NH1	23:Z:17:ASP:OD2	2.22	0.72
27:X:1744:G:N2	27:X:1747:G:OP2	2.18	0.72
24:1:28:ARG:NH1	27:X:2264:C:OP2	2.22	0.72
27:X:1643:A:H61	27:X:1656:U:H3	1.38	0.72
1:A:54:ILE:HA	1:A:217:ARG:H	1.55	0.71
27:X:168:A:H2'	27:X:169:C:C6	2.24	0.71
27:X:209:G:N2	27:X:433:G:OP1	2.22	0.71
3:C:6:VAL:HG13	3:C:7:ILE:HG12	1.72	0.71
14:O:66:GLY:O	14:O:87:ARG:NH2	2.23	0.71
27:X:1030:U:H3	27:X:1153:A:H62	1.38	0.71
16:Q:64:ARG:NH2	27:X:1348:C:O2'	2.22	0.71
26:3:30:ARG:HE	26:3:31:HIS:CE1	2.09	0.71
27:X:2048:C:O2	27:X:2428:U:N3	2.20	0.71
9:J:16:GLY:HA2	9:J:17:ARG:HH11	1.55	0.71
27:X:2020:G:H2'	27:X:2021:G:C8	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:O	1:A:252:LYS:NZ	2.20	0.71
27:X:1551:U:OP2	27:X:1553:G:N2	2.24	0.71
3:C:149:LEU:HD11	3:C:170:LEU:HB2	1.73	0.71
8:I:38:LYS:NZ	27:X:954:U:OP2	2.20	0.71
22:W:25:LEU:HD22	22:W:30:ASP:HB3	1.73	0.71
27:X:2354:G:N2	27:X:2357:A:OP2	2.22	0.71
8:I:31:GLY:O	8:I:32:ARG:NH2	2.23	0.71
27:X:1466:C:H2'	27:X:1467:U:O4'	1.91	0.71
6:G:116:ARG:HA	6:G:119:LEU:HD23	1.73	0.70
8:I:18:ARG:NH2	8:I:18:ARG:O	2.23	0.70
27:X:1845:A:N3	27:X:2212:U:O2'	2.24	0.70
28:Y:51:G:H2'	28:Y:52:G:H8	1.56	0.70
6:G:100:TYR:HB2	6:G:116:ARG:NH1	2.06	0.70
27:X:1361:G:H1	27:X:1614:C:H42	1.39	0.70
7:H:28:GLY:HA3	7:H:35:THR:OG1	1.91	0.70
8:I:17:LYS:HG3	8:I:19:VAL:H	1.57	0.70
24:1:41:ASP:OD1	24:1:41:ASP:N	2.24	0.70
5:E:33:LEU:HD21	5:E:136:ILE:HB	1.73	0.70
26:3:13:ARG:NE	26:3:25:PHE:H	1.89	0.70
1:A:96:HIS:NE2	27:X:1517:C:O2'	2.21	0.69
27:X:113:C:HO2'	27:X:125:A:HO2'	1.40	0.69
27:X:538:A:HO2'	27:X:539:A:P	2.15	0.69
27:X:661:C:H2'	27:X:662:G:C8	2.27	0.69
5:E:124:ALA:HB3	5:E:132:ASP:HB3	1.73	0.69
10:K:24:GLN:HB3	10:K:44:LEU:HD22	1.74	0.69
27:X:27:G:H22	27:X:522:G:H1'	1.58	0.69
27:X:2241:U:H2'	27:X:2242:C:H6	1.56	0.69
1:A:231:HIS:CD2	1:A:232:PRO:HD2	2.26	0.69
1:A:249:PRO:HD3	27:X:2218:G:H5'	1.73	0.69
27:X:793:G:H21	27:X:796:A:H62	1.38	0.69
27:X:2237:C:O2'	27:X:2406:C:OP2	2.11	0.69
12:M:31:ASP:HB2	12:M:94:VAL:HB	1.75	0.69
14:O:23:GLU:HB2	14:O:91:THR:HG21	1.75	0.69
27:X:953:G:O2'	27:X:1203:A:N3	2.24	0.69
6:G:106:TYR:CD2	6:G:108:GLY:HA2	2.28	0.68
27:X:1030:U:O2	27:X:1155:G:N2	2.26	0.68
27:X:1082:G:O6	27:X:1103:C:N4	2.26	0.68
27:X:2617:G:H1	27:X:2755:A:H2'	1.58	0.68
27:X:224:G:OP2	27:X:226:C:N4	2.26	0.68
27:X:105:G:H21	27:X:357:A:H61	1.42	0.68
11:L:28:ARG:NH1	11:L:90:ASP:OD1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1342:U:H5"	27:X:1343:C:H5	1.57	0.68
4:D:66:ILE:HD11	28:Y:43:G:H3'	1.75	0.68
19:T:41:ARG:HH12	27:X:2366:U:H1'	1.59	0.68
21:V:48:ARG:NH2	27:X:76:C:OP1	2.27	0.68
6:G:50:PRO:HG2	6:G:53:ARG:HB2	1.76	0.68
1:A:55:GLY:N	1:A:217:ARG:HB2	2.07	0.68
8:I:51:GLY:HA3	26:3:59:LYS:HE3	1.74	0.68
9:J:61:ARG:HH11	18:S:175:ARG:HB2	1.58	0.68
11:L:39:TYR:OH	28:Y:118:G:N3	2.27	0.68
25:2:33:ARG:NE	27:X:478:G:OP1	2.25	0.68
26:3:19:THR:OG1	27:X:661:C:OP1	2.12	0.67
27:X:226:C:OP2	27:X:2373:C:O2'	2.12	0.67
27:X:2200:G:H2'	27:X:2201:G:C8	2.29	0.67
2:B:78:LEU:O	2:B:79:ARG:NE	2.27	0.67
3:C:48:ARG:NH1	3:C:51:VAL:HG13	2.09	0.67
9:J:81:GLU:HG2	9:J:82:THR:HG23	1.76	0.67
27:X:1573:G:O6	27:X:1574:A:N6	2.27	0.67
3:C:111:ARG:NH1	3:C:180:ILE:O	2.27	0.67
10:K:12:ARG:HD3	10:K:16:ALA:HB1	1.77	0.67
2:B:26:VAL:HB	2:B:182:ILE:HG23	1.77	0.67
8:I:56:LEU:HB3	26:3:52:LYS:HZ1	1.60	0.67
15:P:28:ALA:HB2	15:P:71:VAL:HG21	1.76	0.67
27:X:1202:U:H2'	27:X:1203:A:H8	1.60	0.67
27:X:760:U:O2'	27:X:761:G:OP2	2.12	0.67
27:X:2672:U:H2'	27:X:2673:G:H8	1.60	0.67
4:D:115:ARG:HH22	4:D:178:ARG:HH12	1.43	0.67
7:H:40:GLY:HA3	27:X:2545:A:N6	2.08	0.67
23:Z:36:CYS:SG	23:Z:49:CYS:N	2.67	0.67
27:X:203:G:O2'	27:X:205:A:N1	2.23	0.67
27:X:2040:A:H2'	27:X:2041:A:C8	2.29	0.67
3:C:59:TYR:OH	3:C:67:ALA:HB1	1.93	0.67
15:P:99:ALA:HB1	27:X:25:U:H5'	1.76	0.67
4:D:62:LEU:O	4:D:95:ARG:NH1	2.28	0.66
10:K:28:LEU:HD21	10:K:115:LEU:HG	1.78	0.66
14:O:10:LYS:HG3	14:O:13:ARG:HH22	1.60	0.66
18:S:47:SER:OG	18:S:48:THR:N	2.18	0.66
27:X:1287:A:N1	27:X:1661:C:O2'	2.26	0.66
9:J:38:MET:HB2	9:J:129:GLN:HB2	1.76	0.66
27:X:1278:A:N6	27:X:1996:A:H5"	2.10	0.66
25:2:16:HIS:HB3	25:2:43:THR:HG21	1.77	0.66
27:X:18:U:O2'	27:X:563:U:OP1	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:571:U:O2'	27:X:581:A:H8	1.77	0.66
27:X:617:U:H5	27:X:632:A:C2	2.12	0.66
27:X:1173:G:H2'	27:X:1174:G:C8	2.30	0.66
23:Z:31:THR:OG1	27:X:2861:A:O2'	2.12	0.66
27:X:854:G:H1	27:X:948:C:N4	1.86	0.66
27:X:1850:G:O2'	27:X:1867:A:N6	2.29	0.66
3:C:46:ARG:HB3	3:C:51:VAL:HB	1.77	0.66
12:M:101:ARG:NH2	27:X:1745:C:OP1	2.29	0.66
17:R:61:SER:HA	17:R:65:PRO:HG3	1.77	0.66
27:X:2298:U:O2	27:X:2299:A:N6	2.28	0.66
2:B:77:ILE:HD13	2:B:195:LEU:HD22	1.77	0.66
27:X:1089:C:O2'	27:X:1099:A:OP1	2.10	0.66
27:X:2324:G:N3	27:X:2360:C:H2'	2.10	0.66
6:G:122:HIS:HB3	6:G:125:ARG:HB2	1.78	0.66
27:X:2284:U:H5'	27:X:2286:G:H1	1.59	0.66
3:C:83:ALA:HB3	27:X:595:A:H5'	1.77	0.65
7:H:13:ASN:HD21	7:H:109:ARG:HG2	1.61	0.65
17:R:84:VAL:HG11	17:R:90:LYS:H	1.59	0.65
27:X:1283:C:H5"	27:X:1284:G:H5'	1.78	0.65
28:Y:46:G:N3	28:Y:49:C:N4	2.44	0.65
1:A:183:ARG:NH1	27:X:1790:G:O2'	2.29	0.65
6:G:103:TYR:CG	6:G:111:LYS:HB2	2.31	0.65
9:J:36:ILE:HG12	9:J:103:VAL:HA	1.78	0.65
27:X:1329:U:H2'	27:X:1330:G:C8	2.30	0.65
6:G:130:ALA:O	27:X:1148:G:O2'	2.14	0.65
7:H:13:ASN:ND2	7:H:109:ARG:HG2	2.11	0.65
19:T:74:LYS:HA	19:T:77:ARG:HG3	1.77	0.65
1:A:52:ARG:HD3	27:X:1816:G:OP1	1.96	0.65
6:G:61:ARG:HH12	6:G:66:HIS:H	1.45	0.65
13:N:93:LYS:HE2	14:O:10:LYS:HD3	1.76	0.65
27:X:1109:A:H3'	27:X:1110:G:H8	1.62	0.65
27:X:1466:C:H42	27:X:1476:G:H1	1.45	0.65
27:X:2015:G:OP2	27:X:2433:G:O2'	2.09	0.65
27:X:578:U:O2'	27:X:994:A:N1	2.26	0.65
27:X:1562:G:H5'	27:X:1563:U:H5'	1.78	0.65
2:B:140:SER:HB3	27:X:2554:C:O2'	1.96	0.65
7:H:1:MET:HE2	27:X:1682:A:H1'	1.78	0.65
23:Z:6:VAL:HG22	23:Z:7:PRO:HD2	1.79	0.65
27:X:840:U:H4'	27:X:841:G:C2	2.32	0.65
27:X:1082:G:O2'	27:X:1100:G:OP2	2.14	0.65
2:B:76:ARG:NH2	27:X:2804:G:O3'	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:56:LYS:HD2	27:X:494:A:C8	2.31	0.65
27:X:219:G:HO2'	27:X:231:G:H1	1.44	0.65
27:X:87:G:H2'	27:X:88:G:H5"	1.77	0.65
3:C:163:ASN:ND2	3:C:167:VAL:H	1.95	0.65
15:P:105:ARG:NE	15:P:105:ARG:O	2.29	0.65
27:X:545:C:H2'	27:X:546:A:C8	2.32	0.65
27:X:812:G:H3'	27:X:813:A:H2'	1.79	0.65
27:X:1067:G:H5"	27:X:1068:A:H5'	1.77	0.65
27:X:308:C:O2	27:X:352:G:N2	2.23	0.65
27:X:403:A:H4'	27:X:404:A:H5'	1.79	0.65
3:C:9:GLN:HG2	3:C:120:VAL:HG21	1.79	0.64
6:G:132:PHE:CZ	6:G:145:HIS:HB2	2.32	0.64
27:X:1225:G:O2'	27:X:1250:A:N6	2.30	0.64
27:X:1742:G:HO2'	27:X:2836:U:HO2'	1.43	0.64
8:I:40:ARG:NH1	27:X:576:A:O3'	2.30	0.64
10:K:87:TYR:HE1	10:K:94:TYR:HD1	1.46	0.64
11:L:38:ILE:HD11	11:L:40:ALA:HB2	1.77	0.64
19:T:40:GLN:NE2	19:T:42:GLY:O	2.30	0.64
27:X:304:A:N6	27:X:356:A:N7	2.44	0.64
27:X:1373:G:H22	27:X:2192:U:H3	1.45	0.64
27:X:2432:A:H61	27:X:2479:U:H3	1.45	0.64
2:B:16:LYS:HD3	2:B:173:VAL:HG12	1.80	0.64
5:E:94:PHE:HB3	5:E:107:ILE:HG22	1.80	0.64
20:U:47:HIS:ND1	27:X:410:A:OP1	2.30	0.64
27:X:759:C:H5"	27:X:761:G:H1'	1.79	0.64
27:X:800:U:H5"	27:X:801:A:H5'	1.79	0.64
2:B:5:LEU:HD11	2:B:79:ARG:HB2	1.79	0.64
27:X:1225:G:H2'	27:X:1249:G:N2	2.12	0.64
4:D:92:ARG:CZ	28:Y:47:A:H1'	2.27	0.64
7:H:104:GLU:OE2	7:H:125:LYS:NZ	2.31	0.64
10:K:68:GLN:NE2	27:X:2686:C:O3'	2.28	0.64
10:K:102:THR:HA	10:K:109:THR:HA	1.80	0.64
27:X:542:A:OP1	27:X:570:G:N2	2.29	0.64
27:X:1017:C:H2'	27:X:1018:C:H6	1.60	0.64
9:J:84:MET:HG2	27:X:2229:G:H5'	1.80	0.64
17:R:90:LYS:HG3	17:R:108:VAL:HG21	1.79	0.64
27:X:1504:G:N2	27:X:1517:C:O2	2.31	0.64
9:J:15:ARG:HD3	9:J:74:PRO:HD2	1.79	0.64
12:M:103:LYS:HG2	27:X:2698:G:H4'	1.79	0.64
27:X:1882:G:H21	27:X:1885:C:H41	1.45	0.64
3:C:2:ALA:HA	3:C:13:ARG:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:5:A:H2'	27:X:6:A:C8	2.33	0.64
27:X:2811:G:H2'	27:X:2812:A:H8	1.58	0.64
2:B:14:ILE:HG12	12:M:20:HIS:CD2	2.29	0.63
5:E:8:PRO:HD2	5:E:69:ARG:HH11	1.62	0.63
6:G:70:PHE:HB3	13:N:64:ARG:HG2	1.78	0.63
2:B:92:ASN:HA	2:B:95:ILE:HB	1.78	0.63
5:E:90:ARG:HH21	5:E:163:ARG:HD2	1.64	0.63
16:Q:48:VAL:HG21	16:Q:82:LEU:HD13	1.79	0.63
27:X:619:A:N6	27:X:630:G:O2'	2.31	0.63
27:X:874:A:H2'	27:X:875:G:O4'	1.99	0.63
14:O:5:ILE:HG23	14:O:13:ARG:NH1	2.13	0.63
16:Q:88:ILE:HG13	16:Q:92:ALA:HB2	1.80	0.63
1:A:159:ALA:HB3	27:X:1812:U:H3'	1.80	0.63
1:A:254:THR:OG1	27:X:1835:C:O2'	2.15	0.63
3:C:58:MET:HG2	3:C:59:TYR:CD1	2.33	0.63
27:X:1827:G:H1	27:X:1888:C:H42	1.45	0.63
7:H:123:PHE:HB3	7:H:126:ILE:HG13	1.80	0.63
26:3:17:THR:HG22	26:3:21:LYS:H	1.62	0.63
27:X:584:A:OP2	27:X:2038:C:N4	2.31	0.63
27:X:826:U:H2'	27:X:827:C:C6	2.33	0.63
27:X:1422:C:H2'	27:X:1423:A:H8	1.63	0.63
27:X:1030:U:H2'	27:X:1032:A:H2	1.63	0.63
27:X:2039:G:C2	27:X:2040:A:C8	2.87	0.63
27:X:646:C:O2'	27:X:650:U:OP1	2.17	0.63
27:X:748:A:H5'	27:X:749:C:OP2	1.99	0.63
14:O:21:ARG:HH22	27:X:1005:U:H1'	1.64	0.62
19:T:51:VAL:HG21	19:T:79:ILE:HG22	1.80	0.62
27:X:160:C:O2'	27:X:445:A:N3	2.28	0.62
27:X:1502:G:H22	27:X:1518:C:H42	1.46	0.62
27:X:1554:G:H2'	27:X:1555:A:H8	1.64	0.62
28:Y:27:A:O2'	28:Y:28:A:O5'	2.17	0.62
4:D:16:LEU:O	4:D:20:PHE:N	2.27	0.62
6:G:119:LEU:HD12	6:G:122:HIS:HB2	1.80	0.62
8:I:61:PRO:HB2	26:3:30:ARG:HD3	1.80	0.62
15:P:70:LYS:NZ	27:X:500:G:O6	2.31	0.62
18:S:91:PRO:HD3	18:S:127:PRO:HD3	1.80	0.62
27:X:661:C:H2'	27:X:662:G:H8	1.62	0.62
28:Y:42:U:O2'	28:Y:47:A:N6	2.32	0.62
1:A:46:ARG:NE	27:X:1383:C:OP1	2.32	0.62
2:B:51:TYR:CE2	12:M:3:THR:HG21	2.33	0.62
8:I:59:ARG:HB2	27:X:2371:A:H8	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:725:C:O2	27:X:732:G:N2	2.26	0.62
27:X:2200:G:H2'	27:X:2201:G:H8	1.63	0.62
8:I:59:ARG:HB2	27:X:2371:A:C8	2.34	0.62
15:P:57:LEU:HD13	15:P:69:ALA:HA	1.82	0.62
27:X:772:G:H2'	27:X:773:G:H8	1.65	0.62
27:X:2679:G:H1	27:X:2686:C:H42	1.48	0.62
4:D:39:GLY:O	4:D:150:ARG:NH2	2.33	0.62
6:G:157:PRO:O	6:G:161:GLN:NE2	2.32	0.62
7:H:25:LEU:HD21	7:H:52:VAL:HG23	1.81	0.62
27:X:313:U:H2'	27:X:314:G:C8	2.35	0.62
27:X:1919:A:N6	27:X:1946:U:H3	1.97	0.62
5:E:45:GLN:NE2	5:E:48:ASP:O	2.32	0.62
27:X:588:G:O2'	27:X:2002:A:OP1	2.14	0.62
2:B:115:GLY:HA2	2:B:136:ARG:HD2	1.81	0.62
17:R:22:VAL:HG22	17:R:82:ALA:HA	1.81	0.62
27:X:1361:G:H1	27:X:1614:C:N4	1.97	0.62
8:I:102:LYS:O	8:I:104:ARG:N	2.32	0.62
20:U:53:GLU:HB3	20:U:58:LYS:H	1.65	0.62
23:Z:51:TYR:CE1	23:Z:55:ARG:HB2	2.35	0.62
19:T:41:ARG:NH2	27:X:2366:U:O2'	2.25	0.61
27:X:2617:G:N1	27:X:2755:A:H2'	2.15	0.61
4:D:4:LEU:HG	4:D:5:LYS:H	1.66	0.61
10:K:6:ALA:HB1	27:X:2848:A:H2	1.63	0.61
13:N:66:ASN:ND2	27:X:1021:A:OP1	2.33	0.61
27:X:2417:U:O2'	27:X:2419:C:OP1	2.16	0.61
1:A:252:LYS:H	1:A:252:LYS:NZ	1.97	0.61
4:D:106:ILE:HG21	4:D:139:PRO:HB3	1.81	0.61
5:E:86:ASN:HB2	5:E:165:VAL:HG13	1.82	0.61
15:P:25:PHE:HD1	15:P:130:ILE:HD11	1.66	0.61
27:X:605:G:H2'	27:X:606:A:H8	1.66	0.61
27:X:1140:A:O2'	27:X:2494:C:O2'	2.15	0.61
28:Y:78:A:H2'	28:Y:79:U:O4'	2.01	0.61
7:H:13:ASN:OD1	7:H:108:THR:N	2.32	0.61
12:M:18:GLN:HA	12:M:21:THR:HB	1.82	0.61
13:N:50:ARG:HA	13:N:53:LYS:HE2	1.83	0.61
27:X:1440:G:H5"	27:X:1441:A:H2'	1.83	0.61
27:X:2191:A:OP1	27:X:2193:C:N4	2.32	0.61
2:B:189:PRO:HA	27:X:2659:C:H5'	1.82	0.61
12:M:17:GLU:HG3	12:M:62:SER:H	1.65	0.61
14:O:36:LYS:HB2	14:O:51:ALA:HB1	1.82	0.61
27:X:165:G:H1	27:X:185:C:H42	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:ARG:HB3	27:X:1673:C:H5"	1.81	0.61
12:M:66:PHE:HB3	12:M:83:PHE:HE1	1.66	0.61
22:W:4:LYS:HG3	22:W:52:GLU:HB3	1.83	0.61
25:2:7:PRO:HB2	27:X:1322:G:H4'	1.81	0.61
27:X:1070:G:H5"	27:X:1071:U:H2'	1.82	0.61
1:A:246:PRO:HD3	1:A:252:LYS:HE3	1.82	0.61
6:G:35:LYS:N	6:G:69:ASP:OD2	2.34	0.61
13:N:5:LYS:HG2	13:N:7:GLY:H	1.64	0.61
20:U:51:ILE:HG23	20:U:59:THR:HA	1.82	0.61
21:V:15:ALA:HA	21:V:18:ILE:HD12	1.83	0.61
27:X:540:G:HO2'	27:X:542:A:H2	1.48	0.61
27:X:1514:C:H4'	27:X:1592:U:O2'	2.01	0.61
27:X:635:C:O2'	27:X:670:U:OP1	2.17	0.61
2:B:174:GLU:HB3	2:B:183:LEU:HD12	1.82	0.61
17:R:42:ARG:NH2	27:X:86:U:OP2	2.33	0.61
27:X:810:U:H2'	27:X:811:G:O4'	2.01	0.61
7:H:99:ILE:HD12	7:H:103:GLY:HA2	1.83	0.60
11:L:28:ARG:NH2	28:Y:10:U:O3'	2.34	0.60
20:U:49:LYS:HD3	20:U:61:TRP:CE2	2.36	0.60
27:X:2820:C:H2'	27:X:2821:G:C8	2.36	0.60
3:C:15:ILE:HD11	3:C:195:ILE:H	1.66	0.60
27:X:2591:C:H2'	27:X:2592:U:H5	1.65	0.60
7:H:47:VAL:HG23	7:H:77:THR:HG23	1.83	0.60
8:I:81:GLN:HB3	8:I:114:ILE:HG23	1.84	0.60
11:L:50:THR:N	28:Y:116:C:O2'	2.33	0.60
20:U:52:ARG:HD2	20:U:79:GLU:HA	1.82	0.60
27:X:1073:G:H22	27:X:1087:C:H42	1.48	0.60
27:X:1301:U:O2'	27:X:1664:G:N2	2.34	0.60
27:X:2191:A:H5"	27:X:2192:U:H5	1.66	0.60
8:I:62:LYS:HB3	26:3:12:ARG:HA	1.83	0.60
18:S:117:VAL:HB	18:S:168:VAL:HG22	1.82	0.60
27:X:2591:C:H2'	27:X:2592:U:C5	2.35	0.60
1:A:252:LYS:HZ2	1:A:252:LYS:N	1.99	0.60
4:D:45:GLU:OE1	4:D:78:LYS:NZ	2.30	0.60
5:E:103:LEU:HD23	5:E:115:ILE:HD12	1.83	0.60
13:N:13:ARG:NH1	27:X:1264:C:H5"	2.17	0.60
27:X:482:A:H2'	27:X:483:A:O4'	2.02	0.60
27:X:623:G:C2	27:X:624:A:H1'	2.37	0.60
2:B:169:ASN:HD21	2:B:204:ALA:HB2	1.66	0.60
15:P:118:ASN:HA	27:X:1996:A:O2'	2.01	0.60
16:Q:13:SER:OG	16:Q:14:GLU:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:28:ASN:OD1	18:S:28:ASN:N	2.34	0.60
27:X:1430:G:H1	27:X:1598:C:H42	1.50	0.60
28:Y:3:A:N6	28:Y:121:G:O6	2.34	0.60
1:A:68:LYS:HD3	1:A:68:LYS:H	1.67	0.60
2:B:52:ALA:O	2:B:76:ARG:N	2.25	0.60
3:C:71:ASP:OD1	3:C:72:ARG:N	2.34	0.60
7:H:11:ALA:O	7:H:111:PHE:N	2.30	0.60
9:J:6:LYS:HB3	9:J:45:SER:HB2	1.84	0.60
18:S:26:LYS:HG3	18:S:27:GLU:HG3	1.83	0.60
27:X:663:G:H3'	27:X:664:C:H5"	1.84	0.60
3:C:48:ARG:HB2	3:C:50:GLN:HB3	1.82	0.60
7:H:9:ASP:O	7:H:96:ALA:N	2.34	0.60
27:X:615:C:O2	27:X:670:U:O2'	2.17	0.60
27:X:1451:C:H2'	27:X:1452:U:H6	1.67	0.60
2:B:105:THR:HB	2:B:166:THR:HG23	1.84	0.60
3:C:158:ARG:HB3	3:C:169:VAL:HG11	1.83	0.60
4:D:133:LYS:HE2	27:X:2284:U:H4'	1.83	0.60
6:G:62:ILE:O	6:G:77:GLY:HA3	2.02	0.60
26:3:17:THR:HG23	26:3:19:THR:H	1.67	0.60
27:X:2707:G:H2'	27:X:2708:U:C6	2.36	0.60
1:A:63:ARG:HE	1:A:85:ASP:HB3	1.67	0.60
12:M:3:THR:HG22	12:M:5:ILE:HG13	1.84	0.60
12:M:27:PHE:HA	12:M:96:ARG:NH2	2.16	0.60
27:X:13:A:O2'	27:X:15:G:N7	2.35	0.60
27:X:1350:G:H2'	27:X:1351:G:H8	1.66	0.60
27:X:2767:C:HO2'	27:X:2785:A:HO2'	1.49	0.60
10:K:10:LEU:HD11	10:K:17:ARG:HE	1.66	0.59
18:S:71:MET:HA	18:S:78:PRO:HA	1.84	0.59
27:X:1777:A:H1'	27:X:1921:A:N6	2.17	0.59
27:X:2330:G:H21	27:X:2345:A:H62	1.50	0.59
4:D:171:GLN:HE21	4:D:177:PHE:HE1	1.49	0.59
27:X:242:A:N6	27:X:441:A:N7	2.50	0.59
27:X:1997:A:H2'	27:X:1998:A:C8	2.37	0.59
27:X:2279:G:N2	27:X:2295:C:O2	2.33	0.59
4:D:70:ALA:HB3	4:D:82:GLY:HA2	1.83	0.59
4:D:112:ARG:NH2	4:D:134:GLU:OE2	2.35	0.59
13:N:93:LYS:HE3	14:O:6:GLN:HG3	1.84	0.59
14:O:85:GLY:O	27:X:1237:G:H4'	2.02	0.59
28:Y:7:C:O2'	28:Y:29:C:O2	2.14	0.59
1:A:163:VAL:HG22	1:A:177:LEU:HA	1.84	0.59
2:B:136:ARG:HD3	27:X:1673:C:H5'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:26:THR:OG1	27:X:676:G:OP1	2.15	0.59
13:N:20:ARG:HD2	13:N:39:LEU:HD13	1.84	0.59
27:X:2174:G:H2'	27:X:2175:A:H8	1.68	0.59
2:B:56:GLU:HG2	2:B:74:PRO:HG3	1.83	0.59
8:I:30:ALA:CA	27:X:824:U:H2'	2.33	0.59
25:2:3:ARG:O	25:2:6:GLN:NE2	2.30	0.59
27:X:721:C:H42	27:X:736:G:H1	1.51	0.59
1:A:168:LYS:HD3	1:A:173:VAL:HG22	1.83	0.59
2:B:60:ASN:HB3	2:B:62:PRO:HD2	1.85	0.59
5:E:22:GLY:HA3	5:E:39:THR:HG22	1.85	0.59
7:H:2:ILE:HD12	7:H:8:LEU:HD21	1.85	0.59
14:O:70:TYR:OH	27:X:1236:G:O6	2.21	0.59
27:X:1563:U:H2'	27:X:1564:U:C6	2.38	0.59
27:X:2837:G:H2'	27:X:2838:U:H6	1.67	0.59
5:E:107:ILE:HD11	5:E:151:VAL:HG12	1.85	0.59
17:R:107:ALA:HB2	17:R:111:GLY:HA2	1.83	0.59
27:X:711:C:O2'	27:X:747:A:N6	2.36	0.59
27:X:2283:G:H1	27:X:2291:U:H3	1.51	0.59
27:X:1141:U:H6	27:X:1141:U:O5'	1.86	0.59
27:X:1479:G:H2'	27:X:1480:G:C8	2.38	0.59
2:B:128:SER:OG	27:X:1976:U:O3'	2.21	0.59
16:Q:26:SER:HB3	16:Q:79:ILE:HG12	1.85	0.59
24:1:14:SER:HB2	24:1:23:THR:H	1.68	0.59
27:X:1937:G:O2'	27:X:1939:U:O4	2.14	0.59
27:X:2849:C:H2'	27:X:2850:U:H6	1.68	0.59
1:A:172:TYR:HA	1:A:186:HIS:HA	1.84	0.59
2:B:121:ASN:O	2:B:122:PHE:HB2	2.03	0.59
13:N:49:ASP:HA	13:N:52:ASN:HB2	1.85	0.59
3:C:48:ARG:NE	3:C:51:VAL:HG22	2.18	0.58
3:C:68:ARG:NH1	27:X:687:G:H1'	2.18	0.58
10:K:79:VAL:HA	10:K:83:VAL:HB	1.85	0.58
15:P:30:TYR:O	15:P:123:ARG:NE	2.27	0.58
27:X:2201:G:H2'	27:X:2202:G:H8	1.68	0.58
2:B:5:LEU:HD22	2:B:195:LEU:HD11	1.85	0.58
27:X:139:A:H2'	27:X:140:G:H8	1.68	0.58
27:X:1854:G:H2'	27:X:1855:G:H8	1.69	0.58
27:X:2522:G:H2'	27:X:2523:G:C8	2.38	0.58
2:B:76:ARG:HH22	27:X:2805:G:P	2.25	0.58
2:B:128:SER:CB	27:X:1976:U:H4'	2.34	0.58
2:B:133:LYS:HG3	2:B:137:ARG:HB3	1.85	0.58
10:K:10:LEU:HD23	10:K:13:ASN:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:24:PHE:CE1	27:X:543:G:H5'	2.38	0.58
17:R:26:SER:OG	17:R:27:GLY:N	2.34	0.58
1:A:245:VAL:HB	1:A:249:PRO:HA	1.85	0.58
4:D:122:PHE:HA	27:X:2282:G:H4'	1.85	0.58
20:U:51:ILE:HG12	20:U:59:THR:HB	1.84	0.58
27:X:154:U:H3'	27:X:155:G:H8	1.68	0.58
27:X:1785:A:H2'	27:X:1786:C:H6	1.66	0.58
1:A:16:MET:SD	1:A:17:THR:N	2.74	0.58
17:R:84:VAL:HG21	17:R:89:GLY:HA2	1.85	0.58
27:X:500:G:C2	27:X:501:G:H1'	2.39	0.58
27:X:1210:C:H2'	27:X:1211:G:H8	1.68	0.58
27:X:1468:A:H8	27:X:1468:A:O5'	1.87	0.58
1:A:76:ASN:ND2	1:A:118:ASN:OD1	2.37	0.58
6:G:61:ARG:NH1	6:G:65:LYS:HB3	2.19	0.58
7:H:75:VAL:HG22	7:H:96:ALA:HA	1.84	0.58
9:J:61:ARG:HB3	18:S:175:ARG:H	1.69	0.58
10:K:68:GLN:HG2	27:X:2686:C:O2'	2.04	0.58
27:X:312:G:HO2'	27:X:313:U:H6	1.52	0.58
27:X:1554:G:H2'	27:X:1555:A:C8	2.38	0.58
27:X:2245:A:H4'	27:X:2246:A:N3	2.18	0.58
1:A:252:LYS:HZ2	1:A:253:PRO:HD2	1.67	0.58
27:X:1019:U:O2'	27:X:1020:A:O5'	2.19	0.58
27:X:1140:A:HO2'	27:X:2494:C:HO2'	1.42	0.58
27:X:1501:C:H42	27:X:1519:G:H1	1.50	0.58
4:D:64:LYS:O	28:Y:44:C:O2'	2.20	0.58
27:X:1919:A:H2	27:X:1926:U:H3	1.52	0.58
2:B:176:ARG:HH21	12:M:16:ILE:CG2	2.17	0.58
6:G:84:ASN:O	6:G:152:ALA:HA	2.03	0.58
6:G:103:TYR:CD2	6:G:111:LYS:HB2	2.39	0.58
13:N:37:GLN:HB3	27:X:1265:G:H1	1.69	0.58
27:X:712:A:H2'	27:X:713:G:O4'	2.04	0.58
12:M:7:ILE:HD12	12:M:8:ASN:H	1.68	0.58
27:X:70:A:H4'	27:X:71:A:H5"	1.85	0.58
27:X:163:A:H2'	27:X:164:G:C8	2.39	0.58
27:X:670:U:H2'	27:X:671:A:C8	2.38	0.58
27:X:2006:G:H5'	27:X:2596:C:H4'	1.85	0.58
19:T:68:VAL:HB	19:T:80:SER:HB2	1.86	0.57
19:T:72:LYS:HD3	28:Y:14:C:H5"	1.85	0.57
27:X:222:G:O2'	27:X:397:U:O2	2.18	0.57
27:X:1699:A:H61	27:X:1723:U:H3	1.52	0.57
27:X:2492:G:C2	27:X:2493:U:C2	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:176:ASN:HB3	3:C:179:ASP:H	1.68	0.57
8:I:73:GLU:HG3	8:I:101:ARG:HG3	1.84	0.57
15:P:95:ALA:HB2	15:P:129:ILE:HG23	1.86	0.57
26:3:15:LYS:O	26:3:23:MET:N	2.35	0.57
27:X:1443:G:H2'	27:X:1444:C:C6	2.39	0.57
27:X:1454:U:H2'	27:X:1455:C:C6	2.40	0.57
2:B:143:GLN:O	27:X:2035:G:H4'	2.03	0.57
6:G:69:ASP:H	6:G:76:GLN:HE22	1.51	0.57
9:J:15:ARG:HH21	9:J:73:LYS:HZ2	1.51	0.57
27:X:2594:U:H2'	27:X:2595:C:H6	1.69	0.57
3:C:69:HIS:HE2	27:X:1270:C:P	2.27	0.57
4:D:60:ILE:HG13	4:D:61:THR:HG23	1.86	0.57
5:E:6:LYS:HB2	5:E:69:ARG:HG3	1.85	0.57
11:L:32:TYR:CZ	11:L:34:SER:HB3	2.39	0.57
18:S:3:LEU:HD23	18:S:56:VAL:HG13	1.86	0.57
27:X:346:C:H2'	27:X:347:C:C6	2.40	0.57
28:Y:17:A:H1'	28:Y:112:A:C8	2.39	0.57
1:A:158:SER:OG	1:A:159:ALA:N	2.35	0.57
19:T:74:LYS:C	19:T:76:ALA:H	2.07	0.57
27:X:303:C:H3'	27:X:304:A:H5"	1.86	0.57
27:X:1310:C:H2'	27:X:1311:C:C6	2.39	0.57
27:X:1342:U:H5"	27:X:1343:C:C5	2.37	0.57
13:N:78:THR:HG23	13:N:117:ARG:CZ	2.34	0.57
13:N:105:ALA:HB2	14:O:45:THR:HG21	1.86	0.57
27:X:1422:C:H2'	27:X:1423:A:C8	2.38	0.57
27:X:2528:G:H2'	27:X:2529:G:H8	1.69	0.57
27:X:2570:C:H2'	27:X:2571:G:C8	2.40	0.57
17:R:92:THR:O	17:R:92:THR:OG1	2.21	0.57
27:X:554:U:H5"	27:X:556:A:C2	2.39	0.57
27:X:751:G:H2'	27:X:752:G:C8	2.40	0.57
27:X:1185:C:H2'	27:X:1186:G:H2'	1.85	0.57
27:X:1373:G:N2	27:X:2192:U:H3	2.03	0.57
27:X:2493:U:H2'	27:X:2494:C:C6	2.40	0.57
6:G:132:PHE:HZ	6:G:142:ARG:HA	1.70	0.57
9:J:81:GLU:HB2	27:X:2473:G:O2'	2.05	0.57
10:K:32:GLY:HA2	10:K:115:LEU:HD12	1.86	0.57
22:W:3:ILE:HD11	22:W:44:VAL:HG11	1.86	0.57
24:1:16:ALA:HB2	24:1:50:PHE:CZ	2.40	0.57
27:X:772:G:H2'	27:X:773:G:C8	2.40	0.57
27:X:859:U:H3	27:X:944:A:N6	2.03	0.57
27:X:992:A:N1	27:X:2010:G:O2'	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1645:U:H2'	27:X:1646:G:C8	2.40	0.57
27:X:2590:U:H1'	30:X:2902:ERY:H361	1.85	0.57
1:A:223:GLY:HA2	1:A:226:MET:HG3	1.87	0.57
1:A:252:LYS:O	27:X:1787:U:O2'	2.22	0.57
2:B:136:ARG:HB3	27:X:1673:C:C5'	2.34	0.57
10:K:76:VAL:HA	10:K:79:VAL:HG12	1.87	0.57
10:K:87:TYR:CE1	10:K:94:TYR:HD1	2.23	0.57
18:S:64:ALA:HB2	18:S:85:MET:HG2	1.86	0.57
27:X:82:G:H1	27:X:100:G:HO2'	1.52	0.57
27:X:436:A:H5"	27:X:437:G:H5"	1.85	0.57
27:X:638:A:H4'	27:X:639:G:H5'	1.86	0.57
1:A:89:SER:C	1:A:198:ASN:HD21	2.08	0.56
8:I:30:ALA:HA	27:X:824:U:H2'	1.87	0.56
27:X:1333:G:N7	27:X:1342:U:H5'	2.20	0.56
27:X:1455:C:H2'	27:X:1456:C:H6	1.70	0.56
27:X:1774:A:H5'	27:X:2587:G:H4'	1.87	0.56
27:X:1982:C:H5"	27:X:2703:C:O2'	2.05	0.56
9:J:26:ASP:OD1	9:J:27:TYR:N	2.38	0.56
12:M:17:GLU:OE2	12:M:63:ARG:NH2	2.31	0.56
13:N:13:ARG:HH12	27:X:1264:C:H5"	1.70	0.56
27:X:1033:G:H22	27:X:1153:A:H2	1.53	0.56
27:X:2025:A:H5"	27:X:2026:C:OP2	2.05	0.56
27:X:2085:G:H22	27:X:2171:U:H1'	1.69	0.56
27:X:2222:U:H2'	27:X:2223:U:C6	2.39	0.56
27:X:2336:G:N2	27:X:2339:A:OP2	2.38	0.56
9:J:86:LYS:O	9:J:88:LYS:HE3	2.05	0.56
27:X:540:G:C6	27:X:2005:U:H5"	2.40	0.56
27:X:726:G:H21	27:X:731:A:H2	1.53	0.56
27:X:1017:C:H2'	27:X:1018:C:C6	2.40	0.56
27:X:1830:C:N4	27:X:1882:G:OP2	2.39	0.56
27:X:2708:U:H2'	27:X:2709:C:H6	1.70	0.56
27:X:2736:U:H1'	27:X:2737:A:H5"	1.87	0.56
27:X:2763:U:H2'	27:X:2764:U:H6	1.70	0.56
4:D:13:ARG:HG3	4:D:28:VAL:HG11	1.87	0.56
9:J:26:ASP:H	9:J:103:VAL:HG12	1.70	0.56
12:M:22:ARG:HB2	12:M:84:ALA:HB2	1.87	0.56
19:T:21:LEU:HD11	19:T:41:ARG:HG2	1.87	0.56
20:U:63:SER:O	20:U:67:LEU:N	2.38	0.56
27:X:1327:C:N4	27:X:1351:G:H1	2.02	0.56
1:A:43:ARG:NH1	27:X:704:G:O2'	2.39	0.56
2:B:87:ASP:OD2	2:B:87:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:22:ARG:NH1	12:M:83:PHE:O	2.39	0.56
27:X:705:C:O2'	27:X:1367:A:O2'	2.21	0.56
27:X:1674:C:H2'	27:X:1675:C:C6	2.41	0.56
27:X:2431:C:H2'	27:X:2432:A:C8	2.40	0.56
27:X:2871:U:H2'	27:X:2872:U:C6	2.40	0.56
15:P:117:ALA:HB3	27:X:1997:A:H5"	1.87	0.56
15:P:117:ALA:O	15:P:118:ASN:ND2	2.38	0.56
27:X:2174:G:H2'	27:X:2175:A:C8	2.41	0.56
2:B:176:ARG:NH2	12:M:16:ILE:HG23	2.18	0.56
3:C:54:THR:HG21	3:C:72:ARG:HB2	1.88	0.56
10:K:7:GLY:N	27:X:2848:A:N3	2.52	0.56
13:N:104:GLU:N	13:N:104:GLU:OE2	2.37	0.56
17:R:54:ILE:HG12	17:R:71:GLN:HG3	1.86	0.56
27:X:597:U:H2'	27:X:598:U:C6	2.41	0.56
27:X:1467:U:C6	27:X:1468:A:H5'	2.41	0.56
27:X:2492:G:H2'	27:X:2493:U:C6	2.40	0.56
12:M:28:ARG:HB2	12:M:29:PRO:HD3	1.87	0.56
27:X:75:C:H2'	27:X:76:C:C6	2.41	0.56
27:X:1174:G:H2'	27:X:1175:A:H8	1.71	0.56
15:P:44:VAL:HG11	23:Z:27:ALA:HB2	1.86	0.56
24:1:9:ILE:HA	24:1:28:ARG:HA	1.87	0.56
24:1:12:MET:HB2	24:1:27:ASN:ND2	2.21	0.56
27:X:388:G:H2'	27:X:389:G:C8	2.41	0.56
27:X:1501:C:H2'	27:X:1502:G:O4'	2.06	0.56
28:Y:51:G:H2'	28:Y:52:G:C8	2.38	0.56
1:A:43:ARG:HH21	1:A:55:GLY:HA2	1.71	0.55
7:H:117:GLU:O	7:H:120:ASP:HB2	2.05	0.55
21:V:23:LYS:O	21:V:27:GLU:HG2	2.06	0.55
2:B:143:GLN:NE2	2:B:151:TYR:OH	2.39	0.55
3:C:144:GLY:HA3	3:C:166:TRP:CD1	2.42	0.55
3:C:152:THR:OG1	3:C:153:ASP:O	2.22	0.55
13:N:58:ARG:O	13:N:62:ILE:HG13	2.07	0.55
25:2:39:ARG:O	27:X:469:G:H3'	2.07	0.55
27:X:1795:C:H2'	27:X:1796:A:H8	1.71	0.55
6:G:132:PHE:CZ	6:G:142:ARG:HA	2.41	0.55
23:Z:42:SER:O	23:Z:44:HIS:HD2	1.88	0.55
17:R:16:PHE:CZ	17:R:46:VAL:HG22	2.42	0.55
25:2:1:MET:HB3	25:2:3:ARG:HH12	1.71	0.55
27:X:388:G:H2'	27:X:389:G:H8	1.72	0.55
27:X:533:C:O2	27:X:563:U:O2'	2.23	0.55
27:X:1918:G:H1'	27:X:1947:G:N2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:30:ASN:ND2	27:X:2264:C:OP2	2.40	0.55
1:A:28:ARG:HD2	27:X:1583:A:N6	2.22	0.55
6:G:151:TYR:CE1	6:G:160:ALA:HB3	2.41	0.55
17:R:83:LEU:HD13	17:R:113:THR:HB	1.87	0.55
18:S:3:LEU:HB3	18:S:56:VAL:HA	1.88	0.55
27:X:1336:G:H2'	27:X:1337:G:H5'	1.88	0.55
27:X:1348:C:H2'	27:X:1349:A:C8	2.41	0.55
2:B:4:ILE:HD13	2:B:28:ALA:HB1	1.88	0.55
15:P:90:LEU:HD22	15:P:131:VAL:HG12	1.88	0.55
17:R:11:ASN:O	17:R:11:ASN:ND2	2.36	0.55
27:X:542:A:O2'	27:X:543:G:OP1	2.25	0.55
27:X:1825:C:O2'	27:X:1952:A:N1	2.33	0.55
1:A:48:ARG:H	1:A:48:ARG:HD2	1.72	0.55
2:B:146:THR:OG1	27:X:2550:C:O2'	2.00	0.55
15:P:27:VAL:HG13	27:X:504:G:H4'	1.88	0.55
27:X:2828:C:H2'	27:X:2829:A:H8	1.71	0.55
28:Y:39:C:N4	28:Y:51:G:O4'	2.40	0.55
3:C:48:ARG:HB2	3:C:50:GLN:H	1.72	0.55
4:D:123:ASP:HB3	4:D:127:ASN:H	1.71	0.55
10:K:96:ARG:NE	27:X:2857:C:OP1	2.39	0.55
15:P:47:GLY:H	15:P:92:VAL:HG23	1.71	0.55
27:X:1480:G:C2	27:X:1481:U:O2	2.59	0.55
13:N:54:LYS:NZ	27:X:1006:C:OP2	2.40	0.55
14:O:12:TYR:HD2	14:O:40:VAL:HB	1.72	0.55
18:S:168:VAL:HG12	18:S:169:VAL:HG23	1.89	0.55
27:X:2594:U:H2'	27:X:2595:C:C6	2.42	0.55
27:X:2856:U:H2'	27:X:2857:C:C6	2.41	0.55
1:A:60:ARG:HD3	1:A:86:PRO:HB2	1.89	0.54
11:L:8:ARG:HG3	11:L:9:ARG:H	1.71	0.54
14:O:83:ARG:NH2	27:X:1239:A:OP1	2.40	0.54
19:T:40:GLN:HE22	19:T:43:THR:HA	1.71	0.54
27:X:2235:G:N2	27:X:2254:C:C4	2.75	0.54
27:X:2860:C:H2'	27:X:2861:A:O4'	2.07	0.54
2:B:104:ALA:HB3	2:B:170:LEU:HD12	1.88	0.54
2:B:118:LYS:HG2	2:B:160:MET:SD	2.48	0.54
3:C:66:ASN:HA	27:X:1268:U:H2'	1.89	0.54
4:D:74:ILE:HA	4:D:79:LEU:HB3	1.89	0.54
4:D:130:LEU:HD13	4:D:131:GLY:H	1.71	0.54
27:X:188:G:H2'	27:X:189:A:C8	2.43	0.54
27:X:228:A:C5	27:X:229:G:H1'	2.42	0.54
27:X:1412:C:O2'	27:X:1413:U:O5'	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1454:U:H3	27:X:1567:A:H61	1.53	0.54
28:Y:58:G:H4'	28:Y:59:A:O5'	2.07	0.54
1:A:44:ASN:HB3	1:A:49:ILE:HA	1.89	0.54
5:E:86:ASN:HB3	5:E:130:ARG:HH21	1.72	0.54
13:N:93:LYS:HB3	27:X:1007:A:H4'	1.89	0.54
27:X:540:G:N1	27:X:2005:U:OP1	2.40	0.54
27:X:946:U:H2'	27:X:947:C:H6	1.72	0.54
27:X:1279:G:O2'	27:X:1995:G:O6	2.11	0.54
27:X:1919:A:H2	27:X:1926:U:N3	2.04	0.54
1:A:93:ALA:HB2	1:A:107:ALA:HB2	1.88	0.54
1:A:146:GLU:HB2	1:A:189:CYS:HB3	1.88	0.54
3:C:65:GLY:HA3	27:X:2042:A:H5"	1.90	0.54
3:C:129:LYS:C	3:C:131:LYS:H	2.11	0.54
23:Z:51:TYR:CE1	23:Z:55:ARG:HD3	2.43	0.54
27:X:2384:G:N2	27:X:2390:A:N7	2.56	0.54
1:A:27:LYS:HZ3	1:A:29:PRO:HB3	1.72	0.54
12:M:29:PRO:HB3	12:M:99:VAL:HG12	1.90	0.54
15:P:13:GLN:O	15:P:17:GLN:HG2	2.07	0.54
27:X:219:G:N2	27:X:231:G:H2'	2.23	0.54
27:X:627:A:H2'	27:X:628:A:C8	2.43	0.54
27:X:825:C:H5"	27:X:1263:G:O2'	2.07	0.54
27:X:1673:C:H2'	27:X:1674:C:C6	2.38	0.54
27:X:1785:A:H2'	27:X:1786:C:C6	2.42	0.54
28:Y:27:A:N6	28:Y:56:G:OP2	2.41	0.54
11:L:32:TYR:CE2	28:Y:9:G:H5'	2.43	0.54
15:P:116:SER:OG	15:P:117:ALA:N	2.40	0.54
27:X:317:U:O2'	27:X:1224:A:N7	2.40	0.54
27:X:963:G:H1	27:X:976:C:H42	1.56	0.54
27:X:1141:U:O2	27:X:2008:C:H5"	2.08	0.54
27:X:1787:U:H2'	27:X:1788:C:C6	2.43	0.54
27:X:1827:G:H1'	27:X:1914:U:C2	2.43	0.54
27:X:1991:C:H2'	27:X:1992:G:H8	1.72	0.54
2:B:62:PRO:O	27:X:2766:U:O2'	2.22	0.54
4:D:17:MET:HA	4:D:21:GLY:H	1.72	0.54
25:2:12:ARG:NH2	25:2:46:ASP:O	2.36	0.54
27:X:490:A:H1'	27:X:491:A:H5'	1.89	0.54
27:X:653:G:H2'	27:X:654:A:H5"	1.89	0.54
27:X:838:A:H4'	27:X:2407:G:C5	2.42	0.54
27:X:1790:G:H5'	27:X:1811:A:N6	2.23	0.54
27:X:2054:A:H2'	27:X:2055:G:H8	1.71	0.54
3:C:48:ARG:HD2	3:C:50:GLN:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:5:ILE:HG23	14:O:13:ARG:HH12	1.73	0.54
15:P:19:LYS:NZ	27:X:507:A:OP2	2.23	0.54
25:2:26:SER:O	25:2:30:ILE:HG13	2.08	0.54
27:X:343:A:H1'	27:X:346:C:H41	1.73	0.54
27:X:684:C:H2'	27:X:685:U:C6	2.42	0.54
27:X:2705:A:H1'	27:X:2706:U:H2'	1.89	0.54
5:E:44:ARG:HH22	5:E:51:LEU:HB3	1.72	0.54
15:P:97:VAL:HG22	15:P:127:ILE:HA	1.90	0.54
27:X:1484:G:H2'	27:X:1485:U:C6	2.43	0.54
27:X:2791:C:O2'	27:X:2792:C:H5'	2.08	0.54
1:A:61:LEU:HG	27:X:1584:G:H5"	1.90	0.54
3:C:74:VAL:HG23	3:C:76:THR:H	1.72	0.54
24:1:33:ALA:O	24:1:34:LYS:HD2	2.08	0.54
27:X:774:A:H8	27:X:774:A:O5'	1.90	0.54
27:X:805:G:O2'	27:X:2419:C:N3	2.35	0.54
27:X:946:U:H2'	27:X:947:C:C6	2.43	0.54
27:X:1296:G:H22	27:X:1299:A:H5'	1.73	0.54
27:X:1974:U:H2'	27:X:1975:G:H5"	1.90	0.54
27:X:2707:G:H2'	27:X:2708:U:H6	1.72	0.54
3:C:48:ARG:O	3:C:51:VAL:HG23	2.07	0.53
3:C:67:ALA:HB2	15:P:112:ARG:HH22	1.73	0.53
8:I:62:LYS:H	26:3:12:ARG:HG3	1.72	0.53
13:N:93:LYS:HB3	27:X:1007:A:O3'	2.08	0.53
17:R:56:LYS:HD3	17:R:69:GLN:HE21	1.73	0.53
27:X:171:G:H2'	27:X:172:A:O4'	2.08	0.53
27:X:455:A:H2	27:X:1258:G:N3	2.06	0.53
27:X:2378:G:H1	27:X:2396:C:H42	1.56	0.53
27:X:2555:G:N2	27:X:2555:G:OP2	2.41	0.53
5:E:160:LYS:HZ1	27:X:2637:C:H5'	1.72	0.53
20:U:21:ARG:HH12	27:X:400:U:H2'	1.74	0.53
2:B:118:LYS:NZ	27:X:2704:U:OP1	2.24	0.53
3:C:50:GLN:HE22	3:C:56:ARG:HH12	1.56	0.53
25:2:19:ARG:HG2	27:X:123:A:C5'	2.36	0.53
27:X:1374:G:N2	27:X:1384:G:H1'	2.23	0.53
27:X:2241:U:H2'	27:X:2242:C:C6	2.38	0.53
4:D:75:SER:H	4:D:79:LEU:HD12	1.73	0.53
10:K:14:SER:HB3	27:X:2693:U:OP1	2.08	0.53
10:K:40:LYS:NZ	27:X:1290:A:OP1	2.42	0.53
25:2:41:GLN:NE2	27:X:470:U:OP1	2.36	0.53
27:X:75:C:H2'	27:X:76:C:H6	1.73	0.53
27:X:1854:G:H2'	27:X:1855:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2374:C:H42	27:X:2400:G:H1	1.56	0.53
27:X:2572:U:H3	27:X:2579:A:H61	1.57	0.53
8:I:89:ASP:HB2	8:I:120:VAL:HG13	1.90	0.53
17:R:52:ASN:HA	17:R:74:LEU:H	1.72	0.53
18:S:68:ALA:HB3	18:S:82:ASP:HB2	1.91	0.53
27:X:605:G:H2'	27:X:606:A:C8	2.44	0.53
27:X:978:U:H2'	27:X:979:A:C8	2.43	0.53
27:X:1714:A:OP2	27:X:1715:A:O2'	2.26	0.53
1:A:50:THR:HG21	27:X:1805:G:N3	2.24	0.53
3:C:106:MET:O	3:C:110:SER:OG	2.19	0.53
3:C:148:VAL:HB	3:C:167:VAL:HG12	1.91	0.53
5:E:155:ASP:OD1	5:E:155:ASP:N	2.36	0.53
10:K:81:ASP:O	10:K:85:PRO:HG2	2.09	0.53
13:N:84:LYS:HB2	13:N:92:ARG:HH12	1.74	0.53
17:R:26:SER:HB2	27:X:321:A:H5"	1.90	0.53
18:S:6:LYS:HD3	18:S:32:PHE:HD2	1.73	0.53
26:3:15:LYS:HZ3	26:3:60:LEU:HD11	1.73	0.53
27:X:538:A:H62	27:X:2026:C:C5'	2.16	0.53
28:Y:16:U:H1'	28:Y:109:G:H21	1.74	0.53
6:G:132:PHE:CE2	6:G:145:HIS:HB2	2.44	0.53
15:P:122:LYS:HB3	15:P:124:THR:HG23	1.90	0.53
27:X:542:A:H62	27:X:2002:A:H2	1.55	0.53
27:X:746:G:OP2	27:X:774:A:N6	2.32	0.53
27:X:1184:G:H1	27:X:1190:C:H42	1.57	0.53
1:A:25:THR:HG22	1:A:26:LYS:H	1.74	0.53
1:A:28:ARG:HD3	1:A:84:TYR:HB3	1.90	0.53
3:C:112:GLN:HE22	3:C:116:LYS:HG3	1.73	0.53
9:J:44:LYS:HA	9:J:95:VAL:HG12	1.91	0.53
11:L:91:ARG:HG2	11:L:92:GLY:O	2.08	0.53
12:M:63:ARG:HD3	27:X:2661:G:H4'	1.90	0.53
27:X:746:G:N7	27:X:774:A:C5	2.76	0.53
27:X:2870:C:H2'	27:X:2871:U:C6	2.44	0.53
1:A:186:HIS:HB2	1:A:188:GLU:HG2	1.91	0.53
27:X:5:A:H2'	27:X:6:A:H8	1.71	0.53
27:X:2083:G:H1	27:X:2172:U:H3	1.56	0.53
27:X:2633:A:N1	27:X:2644:A:H5"	2.23	0.53
28:Y:7:C:H2'	28:Y:8:C:H6	1.74	0.53
1:A:108:PRO:HB3	1:A:143:HIS:CE1	2.45	0.52
1:A:254:THR:HG1	27:X:1835:C:HO2'	1.56	0.52
5:E:7:GLN:N	5:E:7:GLN:OE1	2.42	0.52
6:G:100:TYR:HB2	6:G:116:ARG:HH11	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:24:GLY:O	15:P:130:ILE:HA	2.09	0.52
27:X:754:G:H2'	27:X:755:C:H6	1.74	0.52
27:X:1348:C:H2'	27:X:1349:A:H8	1.73	0.52
13:N:39:LEU:HA	13:N:42:ALA:HB3	1.92	0.52
24:1:7:ARG:NH2	27:X:2262:C:OP1	2.42	0.52
27:X:88:G:H3'	27:X:89:A:H5"	1.91	0.52
27:X:2245:A:H4'	27:X:2246:A:C2	2.44	0.52
1:A:91:ARG:NH1	1:A:109:GLU:OE1	2.43	0.52
9:J:83:ARG:HH22	27:X:971:A:N6	1.99	0.52
21:V:7:ARG:HB2	21:V:60:LEU:HD11	1.91	0.52
21:V:28:LEU:HD21	21:V:42:ARG:HG2	1.91	0.52
26:3:6:THR:OG1	26:3:7:HIS:N	2.42	0.52
27:X:90:G:H3'	27:X:91:A:C8	2.45	0.52
27:X:732:G:H2'	27:X:733:G:H8	1.74	0.52
27:X:872:G:OP2	27:X:872:G:H8	1.91	0.52
27:X:1250:A:H5'	27:X:1250:A:H8	1.73	0.52
27:X:1744:G:N2	27:X:1746:A:H3'	2.25	0.52
27:X:2837:G:H2'	27:X:2838:U:C6	2.45	0.52
27:X:2856:U:H2'	27:X:2857:C:H6	1.74	0.52
1:A:108:PRO:HB3	1:A:143:HIS:HE1	1.75	0.52
15:P:104:LYS:HE2	15:P:119:ILE:HD12	1.90	0.52
18:S:74:ARG:HH22	28:Y:94:G:H5"	1.75	0.52
27:X:1333:G:N2	27:X:1344:C:H41	2.08	0.52
27:X:1556:A:H2'	27:X:1557:G:H8	1.74	0.52
27:X:2014:A:C6	27:X:2477:C:H1'	2.44	0.52
1:A:212:SER:O	1:A:215:LEU:HD12	2.10	0.52
1:A:227:ASN:ND2	27:X:797:A:H5"	2.24	0.52
11:L:89:PHE:O	11:L:91:ARG:NH2	2.43	0.52
17:R:51:VAL:HG12	17:R:74:LEU:HD21	1.91	0.52
19:T:23:VAL:HB	19:T:26:PHE:HE2	1.74	0.52
19:T:64:ASP:OD1	19:T:64:ASP:N	2.41	0.52
27:X:2062:U:H2'	27:X:2063:A:C8	2.45	0.52
28:Y:64:C:H2'	28:Y:65:A:H8	1.75	0.52
2:B:120:TRP:CD2	2:B:155:ARG:HD2	2.44	0.52
5:E:76:VAL:HA	5:E:79:VAL:HG22	1.91	0.52
10:K:45:ARG:HD3	10:K:95:THR:HG22	1.91	0.52
16:Q:71:GLN:NE2	27:X:64:C:OP1	2.42	0.52
28:Y:36:A:H61	28:Y:46:G:H2'	1.74	0.52
1:A:48:ARG:HB2	27:X:792:U:P	2.49	0.52
2:B:55:ALA:HB3	2:B:58:LYS:HD2	1.92	0.52
9:J:15:ARG:NH2	9:J:73:LYS:HZ2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:5:ILE:HD12	12:M:5:ILE:H	1.75	0.52
15:P:31:VAL:N	15:P:125:SER:OG	2.43	0.52
20:U:48:LYS:HE3	27:X:2074:U:H1'	1.92	0.52
27:X:447:U:O2'	27:X:449:C:N4	2.42	0.52
27:X:1350:G:H2'	27:X:1351:G:C8	2.45	0.52
27:X:2306:A:O2'	27:X:2307:A:O4'	2.26	0.52
7:H:44:TYR:OH	27:X:1978:U:O2	2.28	0.52
16:Q:29:VAL:HG21	16:Q:38:ILE:HD11	1.91	0.52
27:X:1441:A:H4'	27:X:1442:C:O5'	2.10	0.52
27:X:1762:C:H2'	27:X:1763:G:C8	2.45	0.52
27:X:2335:U:H2'	27:X:2336:G:C8	2.45	0.52
1:A:49:ILE:HD11	1:A:52:ARG:HA	1.92	0.52
1:A:94:LEU:HD12	1:A:95:LEU:H	1.75	0.52
5:E:67:LEU:HD21	27:X:2738:A:C4	2.45	0.52
8:I:55:ARG:HH21	27:X:846:A:H4'	1.74	0.52
9:J:15:ARG:HH21	9:J:73:LYS:NZ	2.07	0.52
12:M:29:PRO:HG2	12:M:97:GLY:H	1.75	0.52
14:O:36:LYS:HE2	14:O:56:VAL:HB	1.92	0.52
20:U:39:LYS:HA	27:X:2063:A:H4'	1.92	0.52
27:X:1655:C:H5"	27:X:2689:C:O2'	2.10	0.52
27:X:2309:G:H2'	27:X:2310:G:O4'	2.10	0.52
1:A:43:ARG:O	27:X:1805:G:O2'	2.28	0.52
3:C:187:VAL:HG12	3:C:189:ASP:HB2	1.92	0.52
7:H:116:ARG:NH2	12:M:41:GLU:OE2	2.35	0.52
16:Q:17:TYR:HA	16:Q:20:MET:HB2	1.92	0.52
27:X:188:G:H2'	27:X:189:A:H8	1.73	0.52
27:X:1316:G:H5'	27:X:1659:G:H21	1.75	0.52
27:X:2299:A:H4'	27:X:2300:G:O5'	2.09	0.52
2:B:52:ALA:HB3	2:B:76:ARG:HB2	1.91	0.51
3:C:34:GLN:O	3:C:37:SER:OG	2.19	0.51
6:G:43:VAL:HG21	6:G:158:HIS:HE1	1.75	0.51
7:H:42:LYS:HA	27:X:2653:A:O3'	2.10	0.51
8:I:35:LYS:NZ	27:X:575:U:H5"	2.25	0.51
14:O:36:LYS:NZ	14:O:54:TYR:HB3	2.25	0.51
25:2:34:ARG:HD3	25:2:37:LYS:HD2	1.92	0.51
27:X:1573:G:O5'	27:X:1574:A:H5"	2.10	0.51
27:X:1662:G:H5"	27:X:1663:C:H5'	1.92	0.51
27:X:2234:G:H2'	27:X:2235:G:O4'	2.10	0.51
11:L:91:ARG:NH2	27:X:2355:A:H61	2.08	0.51
12:M:55:ILE:O	12:M:103:LYS:O	2.28	0.51
15:P:50:VAL:HG23	15:P:91:PHE:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:103:LEU:HB2	15:P:121:LYS:O	2.10	0.51
16:Q:62:ARG:O	16:Q:70:GLY:HA2	2.09	0.51
26:3:20:GLY:O	26:3:57:ARG:NH1	2.43	0.51
27:X:185:C:H2'	27:X:186:C:H6	1.74	0.51
27:X:1296:G:N2	27:X:1299:A:H5'	2.25	0.51
28:Y:96:C:H2'	28:Y:97:C:H6	1.76	0.51
7:H:129:LEU:O	7:H:131:PRO:HD3	2.11	0.51
9:J:15:ARG:HE	9:J:73:LYS:HZ2	1.58	0.51
20:U:61:TRP:O	20:U:62:LEU:HD12	2.10	0.51
26:3:62:LEU:HD13	27:X:603:C:H5"	1.91	0.51
27:X:939:C:OP2	27:X:940:G:H8	1.94	0.51
27:X:2007:G:C2	27:X:2023:C:C2	2.98	0.51
27:X:2451:G:O2'	27:X:2457:A:N6	2.42	0.51
4:D:102:LYS:NZ	4:D:140:GLU:OE2	2.33	0.51
18:S:17:SER:HB2	18:S:36:ARG:HB3	1.93	0.51
27:X:503:G:H2'	27:X:504:G:O4'	2.10	0.51
27:X:2171:U:H2'	27:X:2172:U:C5	2.46	0.51
27:X:2826:C:H2'	27:X:2827:G:O4'	2.11	0.51
5:E:24:PHE:HB2	5:E:37:TYR:CD1	2.45	0.51
6:G:58:ILE:HG12	6:G:80:VAL:HG11	1.93	0.51
15:P:36:ARG:HD3	27:X:1279:G:N7	2.26	0.51
27:X:2:G:O2'	27:X:3:U:H5'	2.10	0.51
27:X:636:G:O2'	27:X:669:G:H4'	2.10	0.51
27:X:746:G:C8	27:X:774:A:C6	2.98	0.51
27:X:2824:C:H4'	27:X:2825:A:O5'	2.10	0.51
2:B:54:LYS:HD3	2:B:59:VAL:HG22	1.92	0.51
4:D:46:ASP:HB2	4:D:49:ALA:H	1.75	0.51
6:G:61:ARG:HH22	6:G:65:LYS:H	1.59	0.51
14:O:12:TYR:CD2	14:O:40:VAL:HB	2.46	0.51
17:R:100:ASP:HB3	17:R:103:LYS:HB2	1.93	0.51
23:Z:4:HIS:HB2	23:Z:5:PRO:HD3	1.93	0.51
27:X:3:U:O2'	27:X:4:C:O5'	2.26	0.51
7:H:27:SER:HB2	7:H:50:ILE:HB	1.93	0.51
9:J:86:LYS:NZ	27:X:2256:G:OP2	2.29	0.51
12:M:50:PHE:HE2	12:M:70:LYS:HB2	1.76	0.51
27:X:474:G:N2	27:X:477:A:OP2	2.38	0.51
27:X:1316:G:N2	27:X:1317:G:H1'	2.26	0.51
27:X:1599:G:C2	27:X:1600:U:H1'	2.46	0.51
27:X:2250:G:H2'	27:X:2251:U:C6	2.45	0.51
3:C:39:ARG:HG3	27:X:455:A:C8	2.46	0.51
19:T:26:PHE:HD1	27:X:934:G:H1'	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:40:PRO:HD2	27:X:94:C:H1'	1.92	0.51
23:Z:35:GLN:HG3	23:Z:51:TYR:HB3	1.91	0.51
27:X:959:C:H42	27:X:980:G:H1	1.59	0.51
27:X:1692:C:N4	27:X:1976:U:O4'	2.44	0.51
27:X:2167:A:H2	27:X:2168:A:H62	1.59	0.51
3:C:48:ARG:CZ	3:C:51:VAL:HG13	2.41	0.51
3:C:67:ALA:HB2	15:P:112:ARG:HH12	1.76	0.51
5:E:109:TYR:HD2	27:X:2646:C:H1'	1.75	0.51
5:E:154:PRO:HA	5:E:160:LYS:O	2.10	0.51
6:G:67:ARG:CG	6:G:70:PHE:HA	2.41	0.51
27:X:577:U:O5'	27:X:956:A:N6	2.44	0.51
27:X:796:A:C8	27:X:797:A:H4'	2.45	0.51
3:C:25:GLY:HA3	8:I:18:ARG:NH1	2.26	0.51
3:C:58:MET:HG2	3:C:59:TYR:HD1	1.76	0.51
15:P:36:ARG:NH2	27:X:1279:G:O5'	2.44	0.51
20:U:20:ARG:HB2	20:U:43:ARG:HD2	1.92	0.51
27:X:1443:G:H2'	27:X:1444:C:H6	1.75	0.51
3:C:162:ARG:HH21	27:X:333:A:H2'	1.76	0.50
11:L:15:ARG:HH21	27:X:2272:A:P	2.34	0.50
15:P:119:ILE:HG13	15:P:120:ILE:H	1.76	0.50
18:S:25:ASN:HD22	18:S:85:MET:HB2	1.75	0.50
27:X:541:C:H4'	27:X:542:A:H5"	1.92	0.50
2:B:117:MET:HA	2:B:121:ASN:O	2.11	0.50
3:C:149:LEU:HD23	3:C:180:ILE:HG22	1.92	0.50
5:E:136:ILE:HD12	5:E:137:ASP:H	1.76	0.50
6:G:101:THR:HG23	6:G:103:TYR:CE1	2.46	0.50
16:Q:56:MET:HG2	27:X:1354:A:H4'	1.93	0.50
17:R:15:HIS:CE1	17:R:80:LYS:HE2	2.45	0.50
18:S:13:LYS:HA	18:S:18:MET:HB2	1.93	0.50
25:2:17:GLY:O	25:2:21:ARG:HG2	2.11	0.50
27:X:493:A:H5"	27:X:494:A:OP1	2.10	0.50
27:X:943:U:H2'	27:X:944:A:C8	2.46	0.50
27:X:1539:U:H2'	27:X:1540:C:C6	2.45	0.50
6:G:53:ARG:NH2	27:X:1150:C:O3'	2.43	0.50
8:I:90:ARG:HG2	8:I:121:HIS:CE1	2.47	0.50
11:L:30:SER:HB2	11:L:43:ILE:HD11	1.93	0.50
15:P:35:PRO:HD3	15:P:124:THR:CB	2.41	0.50
19:T:39:ARG:NH2	27:X:2334:C:O2	2.44	0.50
26:3:6:THR:N	26:3:9:MET:HG2	2.26	0.50
27:X:116:A:N3	27:X:155:G:H1'	2.26	0.50
27:X:1843:U:H3	27:X:1874:G:H1	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1870:U:H3'	27:X:1871:G:H21	1.77	0.50
27:X:2020:G:H2'	27:X:2021:G:H8	1.76	0.50
27:X:2380:U:H3	27:X:2394:G:H1	1.58	0.50
27:X:2664:G:H2'	27:X:2665:G:H8	1.74	0.50
2:B:11:MET:HG2	2:B:24:THR:OG1	2.10	0.50
6:G:84:ASN:HD21	6:G:154:GLU:HG2	1.74	0.50
7:H:10:VAL:HA	7:H:96:ALA:O	2.11	0.50
8:I:35:LYS:HZ2	27:X:575:U:H5"	1.75	0.50
9:J:68:ARG:CZ	9:J:103:VAL:HG11	2.42	0.50
15:P:134:LYS:HG3	15:P:136:ASN:H	1.75	0.50
19:T:23:VAL:HG13	19:T:38:VAL:HG22	1.92	0.50
27:X:633:G:H2'	27:X:634:G:H8	1.77	0.50
1:A:63:ARG:O	1:A:65:ILE:HG22	2.12	0.50
10:K:35:GLN:HB3	10:K:112:LEU:HD23	1.94	0.50
27:X:163:A:H2'	27:X:164:G:H8	1.76	0.50
27:X:461:A:C4	27:X:462:G:C8	2.99	0.50
27:X:700:C:H2'	27:X:701:U:O4'	2.11	0.50
27:X:1332:G:O2'	27:X:1333:G:H5'	2.11	0.50
27:X:1770:U:H5	27:X:1775:A:N7	2.10	0.50
27:X:1867:A:O2'	27:X:1868:A:H8	1.95	0.50
27:X:2067:U:H2'	27:X:2068:C:C6	2.47	0.50
27:X:2674:C:H2'	27:X:2675:U:C6	2.46	0.50
6:G:106:TYR:CE2	6:G:108:GLY:HA2	2.47	0.50
9:J:44:LYS:HB2	9:J:47:GLN:NE2	2.26	0.50
15:P:28:ALA:HB2	15:P:71:VAL:CG2	2.42	0.50
21:V:42:ARG:O	21:V:46:LEU:HG	2.11	0.50
22:W:20:VAL:HG23	22:W:47:VAL:HG11	1.94	0.50
26:3:30:ARG:HE	26:3:31:HIS:HE1	1.57	0.50
27:X:2270:U:O2'	27:X:2353:G:N3	2.43	0.50
1:A:244:ARG:HD2	27:X:1884:A:O2'	2.11	0.50
4:D:170:LEU:HB2	4:D:175:LEU:HD22	1.92	0.50
14:O:64:GLY:HA3	14:O:90:PHE:CZ	2.46	0.50
27:X:358:C:H2'	27:X:359:G:O4'	2.11	0.50
27:X:857:U:H2'	27:X:858:G:O4'	2.11	0.50
3:C:163:ASN:HD21	3:C:167:VAL:N	2.03	0.50
6:G:125:ARG:HD2	6:G:129:HIS:CE1	2.45	0.50
8:I:38:LYS:HE3	8:I:41:SER:OG	2.12	0.50
11:L:32:TYR:CE1	11:L:34:SER:HB3	2.46	0.50
12:M:85:SER:O	12:M:88:VAL:N	2.42	0.50
15:P:66:GLU:HB3	15:P:67:PRO:HD3	1.93	0.50
21:V:5:GLU:HA	21:V:7:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:806:A:OP2	27:X:806:A:H8	1.94	0.50
27:X:1001:A:H1'	27:X:1167:A:N3	2.26	0.50
27:X:1399:C:H2'	27:X:1400:A:H8	1.77	0.50
27:X:2482:A:H4'	27:X:2483:U:OP1	2.10	0.50
27:X:2828:C:H2'	27:X:2829:A:C8	2.47	0.50
1:A:161:THR:H	1:A:196:VAL:HG23	1.76	0.50
2:B:115:GLY:CA	2:B:136:ARG:HD2	2.42	0.50
3:C:146:GLU:OE2	3:C:185:ARG:NH2	2.45	0.50
15:P:21:ARG:HG3	15:P:22:LYS:H	1.77	0.50
20:U:51:ILE:O	20:U:52:ARG:HD3	2.11	0.50
26:3:11:LYS:H	26:3:11:LYS:HD2	1.77	0.50
27:X:121:G:H2'	27:X:122:G:O4'	2.12	0.50
27:X:958:G:H2'	27:X:959:C:H6	1.77	0.50
27:X:1059:A:O2'	27:X:1060:C:OP1	2.26	0.50
27:X:1098:G:N2	27:X:1114:A:H1'	2.27	0.50
27:X:1148:G:H5"	27:X:1149:G:OP2	2.11	0.50
27:X:1481:U:O2'	27:X:1562:G:O2'	2.18	0.50
27:X:2557:G:H2'	27:X:2558:C:H6	1.77	0.50
27:X:2628:C:H2'	27:X:2629:U:H6	1.77	0.50
28:Y:43:G:H5'	28:Y:44:C:H5"	1.94	0.50
1:A:169:GLU:N	1:A:172:TYR:O	2.36	0.49
10:K:39:THR:O	10:K:42:LYS:N	2.45	0.49
17:R:105:ARG:NH2	17:R:111:GLY:O	2.43	0.49
27:X:820:U:H2'	27:X:821:A:H8	1.76	0.49
27:X:1060:C:O2	27:X:1124:U:H4'	2.12	0.49
27:X:1383:C:H3'	27:X:1384:G:H8	1.76	0.49
27:X:2528:G:H2'	27:X:2529:G:C8	2.47	0.49
1:A:132:PRO:HD3	1:A:190:TYR:CE2	2.47	0.49
1:A:160:GLY:HA3	27:X:1812:U:C4	2.47	0.49
1:A:244:ARG:HD3	27:X:1885:C:O4'	2.12	0.49
3:C:14:THR:HG22	3:C:15:ILE:H	1.77	0.49
6:G:103:TYR:HD2	27:X:1142:G:O4'	1.94	0.49
15:P:102:THR:HA	15:P:123:ARG:H	1.76	0.49
27:X:1665:C:H42	27:X:1992:G:H1	1.59	0.49
1:A:145:LEU:HD21	1:A:185:VAL:HG11	1.93	0.49
1:A:169:GLU:HB3	1:A:172:TYR:HB2	1.94	0.49
4:D:111:ILE:HG23	4:D:137:ILE:HG21	1.94	0.49
16:Q:63:LYS:HD3	16:Q:69:ILE:H	1.78	0.49
22:W:2:LYS:HZ1	22:W:31:SER:HB2	1.76	0.49
27:X:50:G:O2'	27:X:51:A:OP2	2.30	0.49
27:X:116:A:OP2	27:X:117:A:H2'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:520:C:H2'	27:X:521:U:O4'	2.13	0.49
27:X:705:C:HO2'	27:X:1367:A:HO2'	1.52	0.49
27:X:1310:C:H2'	27:X:1311:C:H6	1.76	0.49
27:X:1938:U:H5	27:X:2536:G:N2	2.10	0.49
28:Y:6:C:H2'	28:Y:7:C:C6	2.47	0.49
3:C:56:ARG:NE	27:X:814:G:OP2	2.45	0.49
6:G:103:TYR:O	6:G:107:GLN:NE2	2.46	0.49
9:J:21:ASP:C	9:J:99:LYS:HG2	2.33	0.49
15:P:41:VAL:HG21	15:P:64:ALA:HB3	1.94	0.49
16:Q:15:LYS:HG2	27:X:1404:C:O2	2.13	0.49
16:Q:73:ASN:N	16:Q:73:ASN:OD1	2.44	0.49
24:1:8:ILE:HG12	24:1:9:ILE:HG23	1.93	0.49
27:X:562:G:H2'	27:X:563:U:O4'	2.12	0.49
27:X:1035:G:C6	27:X:1036:G:C6	3.00	0.49
27:X:1277:G:H2'	27:X:1997:A:N6	2.28	0.49
27:X:1313:U:H4'	27:X:1314:A:H5'	1.93	0.49
27:X:1482:U:HO2'	27:X:1483:G:H8	1.60	0.49
27:X:1703:C:H2'	27:X:1704:G:O4'	2.12	0.49
27:X:2324:G:O2'	27:X:2360:C:O2'	2.13	0.49
27:X:2484:G:N2	30:X:2902:ERY:H191	2.26	0.49
1:A:226:MET:HB3	1:A:230:ASP:HB2	1.93	0.49
2:B:50:GLY:HA3	2:B:75:THR:HG21	1.93	0.49
3:C:3:GLN:N	3:C:12:GLY:O	2.30	0.49
4:D:37:ASN:ND2	27:X:2291:U:O2'	2.39	0.49
10:K:6:ALA:HB1	27:X:2848:A:C2	2.47	0.49
13:N:20:ARG:NH1	14:O:83:ARG:HH11	2.11	0.49
14:O:10:LYS:HE3	14:O:13:ARG:HH22	1.77	0.49
17:R:45:LYS:HA	17:R:76:LEU:O	2.12	0.49
23:Z:44:HIS:N	23:Z:44:HIS:CD2	2.80	0.49
27:X:1255:A:H2'	27:X:1256:C:C6	2.48	0.49
27:X:1640:C:H2'	27:X:1641:C:H6	1.78	0.49
27:X:1790:G:H5'	27:X:1811:A:H62	1.77	0.49
27:X:1922:U:H1'	27:X:2571:G:O4'	2.12	0.49
27:X:2189:A:H3'	27:X:2190:A:H5"	1.93	0.49
27:X:2457:A:C8	27:X:2508:G:C5	3.01	0.49
27:X:2520:A:H2	27:X:2745:A:H61	1.58	0.49
27:X:2557:G:H2'	27:X:2558:C:C6	2.47	0.49
27:X:2839:G:H2'	27:X:2840:U:C6	2.48	0.49
28:Y:58:G:O2'	28:Y:59:A:H5"	2.13	0.49
1:A:48:ARG:HD3	27:X:1797:C:H4'	1.94	0.49
8:I:72:TYR:CE2	8:I:105:PRO:HG2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:27:PHE:HA	12:M:96:ARG:HH22	1.78	0.49
17:R:37:LEU:HD11	17:R:49:GLU:HG2	1.95	0.49
27:X:32:C:O2'	27:X:33:C:H5'	2.13	0.49
27:X:828:C:H2'	27:X:829:C:C6	2.47	0.49
27:X:1787:U:H2'	27:X:1788:C:H6	1.75	0.49
27:X:1979:C:H4'	27:X:1980:A:OP1	2.13	0.49
27:X:2053:G:H2'	27:X:2054:A:C8	2.48	0.49
28:Y:73:C:H2'	28:Y:74:A:O4'	2.13	0.49
1:A:38:PRO:HA	1:A:61:LEU:HD22	1.93	0.49
1:A:252:LYS:H	1:A:252:LYS:CE	2.26	0.49
2:B:37:LYS:HB2	2:B:46:ALA:HB3	1.95	0.49
3:C:111:ARG:NH1	3:C:183:HIS:O	2.45	0.49
7:H:10:VAL:HG23	7:H:17:ARG:O	2.12	0.49
24:1:9:ILE:HB	24:1:27:ASN:O	2.13	0.49
24:1:38:LYS:HE2	24:1:40:TYR:HE1	1.78	0.49
27:X:2226:A:H2'	27:X:2227:C:C6	2.47	0.49
27:X:2605:C:H2'	27:X:2606:G:H8	1.76	0.49
1:A:161:THR:O	1:A:196:VAL:HG22	2.13	0.49
2:B:104:ALA:HB1	2:B:188:ILE:HD11	1.93	0.49
3:C:128:ALA:C	3:C:130:THR:H	2.16	0.49
8:I:42:GLY:N	8:I:45:LYS:HE3	2.27	0.49
17:R:84:VAL:HG11	17:R:89:GLY:HA2	1.95	0.49
18:S:155:PRO:HG2	18:S:158:CYS:SG	2.53	0.49
26:3:42:ARG:NE	27:X:2328:G:OP1	2.46	0.49
27:X:104:C:H2'	27:X:105:G:H8	1.78	0.49
27:X:346:C:C6	27:X:347:C:H5	2.30	0.49
27:X:538:A:N6	27:X:2025:A:H3'	2.28	0.49
27:X:960:U:H2'	27:X:961:G:C8	2.47	0.49
27:X:1184:G:H3'	27:X:1185:C:H5"	1.95	0.49
27:X:1699:A:H2'	27:X:1700:C:C6	2.48	0.49
27:X:2198:U:C2	27:X:2199:C:H1'	2.48	0.49
27:X:2553:G:N1	27:X:2554:C:O2	2.45	0.49
1:A:143:HIS:ND1	1:A:194:GLY:O	2.35	0.49
1:A:206:LEU:HD23	1:A:211:ARG:HD2	1.94	0.49
4:D:56:GLU:HA	4:D:59:LEU:HD12	1.95	0.49
5:E:24:PHE:HB2	5:E:37:TYR:HD1	1.76	0.49
10:K:12:ARG:HG2	10:K:12:ARG:HH11	1.78	0.49
17:R:62:MET:O	17:R:65:PRO:HA	2.12	0.49
26:3:14:ILE:HG23	26:3:60:LEU:HD22	1.95	0.49
26:3:30:ARG:HB3	26:3:31:HIS:ND1	2.28	0.49
27:X:1672:A:C6	27:X:1673:C:C2	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2427:A:HO2'	27:X:2428:U:H5	1.61	0.49
4:D:38:GLU:HB3	4:D:87:ILE:HB	1.95	0.49
7:H:28:GLY:O	7:H:35:THR:HG23	2.13	0.49
9:J:16:GLY:C	9:J:17:ARG:HD3	2.33	0.49
27:X:830:C:O2'	27:X:852:U:H5"	2.13	0.49
27:X:1802:A:H2'	27:X:1803:G:O4'	2.13	0.49
28:Y:15:A:O2'	28:Y:16:U:H5"	2.12	0.49
28:Y:39:C:H5'	28:Y:40:C:OP2	2.12	0.49
2:B:136:ARG:HG2	2:B:137:ARG:N	2.27	0.48
6:G:67:ARG:HG2	6:G:70:PHE:HA	1.95	0.48
6:G:69:ASP:H	6:G:76:GLN:NE2	2.10	0.48
11:L:32:TYR:O	11:L:38:ILE:HA	2.13	0.48
12:M:104:LEU:HA	12:M:106:TYR:CE2	2.47	0.48
17:R:86:PRO:HG2	17:R:90:LYS:HE2	1.95	0.48
27:X:1351:G:H2'	27:X:1352:G:C8	2.48	0.48
27:X:2543:A:C2	27:X:2626:U:H4'	2.47	0.48
28:Y:96:C:H2'	28:Y:97:C:C6	2.47	0.48
2:B:145:LYS:HB2	27:X:2551:A:N7	2.29	0.48
8:I:33:GLY:HA2	14:O:79:GLN:HG3	1.95	0.48
13:N:66:ASN:HB2	13:N:70:ARG:NH1	2.28	0.48
14:O:85:GLY:N	27:X:1238:A:H5'	2.27	0.48
15:P:41:VAL:HG11	15:P:65:SER:HA	1.95	0.48
27:X:836:G:H2'	27:X:837:U:H6	1.78	0.48
27:X:2204:A:H4'	27:X:2205:C:O5'	2.13	0.48
27:X:2261:G:H5"	27:X:2262:C:O4'	2.14	0.48
1:A:251:GLY:HA3	1:A:255:LYS:NZ	2.27	0.48
2:B:203:LYS:HG2	27:X:2713:A:H61	1.78	0.48
3:C:163:ASN:HD21	3:C:166:TRP:HB2	1.78	0.48
6:G:43:VAL:HG12	6:G:167:LYS:HE3	1.96	0.48
12:M:102:ALA:C	12:M:103:LYS:HD2	2.33	0.48
18:S:104:SER:HA	18:S:139:THR:HA	1.95	0.48
19:T:41:ARG:HD2	19:T:41:ARG:HA	1.52	0.48
27:X:38:G:H1	27:X:453:U:H3	1.61	0.48
27:X:346:C:H2'	27:X:347:C:C5	2.48	0.48
27:X:514:G:H4'	27:X:515:A:OP2	2.11	0.48
27:X:543:G:C5	27:X:544:U:C4	3.02	0.48
27:X:558:G:C8	27:X:560:G:C8	3.01	0.48
27:X:1283:C:H5"	27:X:1284:G:C5'	2.42	0.48
27:X:2532:G:C2	27:X:2533:U:H1'	2.47	0.48
4:D:80:ARG:NE	4:D:83:MET:SD	2.81	0.48
11:L:21:THR:O	11:L:25:GLY:N	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:30:ASN:OD1	24:1:31:THR:N	2.47	0.48
26:3:26:LYS:NZ	26:3:28:GLY:HA3	2.28	0.48
27:X:165:G:H1	27:X:185:C:N4	2.11	0.48
27:X:736:G:H2'	27:X:737:C:O4'	2.14	0.48
27:X:2040:A:H2'	27:X:2041:A:H8	1.73	0.48
27:X:2278:A:H2'	27:X:2279:G:C8	2.47	0.48
27:X:2407:G:H5"	27:X:2408:G:O5'	2.12	0.48
27:X:2498:U:C5	27:X:2520:A:C6	3.01	0.48
27:X:2655:C:O2	27:X:2712:G:N2	2.38	0.48
1:A:30:GLU:HB2	1:A:82:ILE:O	2.14	0.48
2:B:128:SER:HB2	2:B:129:HIS:ND1	2.29	0.48
2:B:172:VAL:HG22	2:B:182:ILE:HD11	1.96	0.48
3:C:182:ARG:NH1	3:C:183:HIS:HE1	2.10	0.48
9:J:99:LYS:HG3	9:J:100:PRO:HD2	1.94	0.48
16:Q:62:ARG:NH1	16:Q:73:ASN:HD21	2.11	0.48
26:3:58:MET:HA	26:3:61:MET:HB2	1.94	0.48
27:X:224:G:H4'	27:X:399:G:C5	2.48	0.48
27:X:459:A:H4'	27:X:461:A:N7	2.28	0.48
27:X:1019:U:HO2'	27:X:1020:A:P	2.35	0.48
27:X:1437:A:H2'	27:X:1438:G:C8	2.47	0.48
27:X:1623:C:H4'	27:X:1624:A:O5'	2.13	0.48
28:Y:7:C:H2'	28:Y:8:C:C6	2.49	0.48
3:C:104:LEU:O	3:C:108:ILE:HG13	2.12	0.48
5:E:37:TYR:CZ	5:E:72:VAL:HG22	2.48	0.48
5:E:143:GLN:NE2	27:X:2724:G:H21	2.12	0.48
6:G:56:THR:HA	6:G:134:MET:HE1	1.96	0.48
7:H:14:SER:OG	7:H:98:ILE:HD12	2.13	0.48
16:Q:28:TRP:HZ3	16:Q:58:VAL:HG21	1.78	0.48
27:X:936:A:H2'	27:X:937:C:O4'	2.13	0.48
3:C:62:LYS:HD2	27:X:2044:G:OP1	2.13	0.48
9:J:57:ARG:NE	27:X:2448:A:O2'	2.38	0.48
15:P:39:ARG:HD2	15:P:97:VAL:HB	1.94	0.48
20:U:20:ARG:N	20:U:41:VAL:O	2.38	0.48
20:U:20:ARG:HH21	20:U:43:ARG:HG2	1.79	0.48
27:X:537:C:O2'	27:X:538:A:C4	2.66	0.48
27:X:764:A:H2	27:X:802:A:HO2'	1.59	0.48
27:X:1653:C:H2'	27:X:1654:A:C8	2.49	0.48
27:X:1815:G:H2'	27:X:1816:G:H8	1.79	0.48
27:X:2013:A:H4'	27:X:2014:A:C8	2.49	0.48
8:I:94:GLU:HA	8:I:97:ARG:NE	2.28	0.48
10:K:82:GLU:O	10:K:85:PRO:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:58:VAL:HA	16:Q:59:PRO:HD2	1.61	0.48
17:R:61:SER:HA	17:R:65:PRO:CG	2.42	0.48
24:1:28:ARG:HB2	24:1:30:ASN:ND2	2.28	0.48
27:X:492:G:H2'	27:X:517:A:N1	2.29	0.48
27:X:603:C:H2'	27:X:604:U:H6	1.79	0.48
27:X:1333:G:N2	27:X:1344:C:N4	2.61	0.48
27:X:1404:C:C2	27:X:1406:A:N7	2.81	0.48
27:X:1451:C:H2'	27:X:1452:U:C6	2.47	0.48
27:X:1586:A:H2'	27:X:1587:A:C8	2.49	0.48
27:X:2199:C:H2'	27:X:2200:G:H8	1.79	0.48
27:X:2590:U:C1'	30:X:2902:ERY:H361	2.44	0.48
27:X:2657:G:H2'	27:X:2658:A:O4'	2.14	0.48
3:C:72:ARG:CZ	3:C:77:PHE:HE2	2.27	0.48
4:D:134:GLU:HG2	4:D:136:LEU:H	1.79	0.48
5:E:24:PHE:CD1	5:E:37:TYR:HB2	2.49	0.48
5:E:165:VAL:HB	5:E:166:GLY:H	1.46	0.48
6:G:137:LYS:HD2	27:X:2022:C:OP2	2.14	0.48
13:N:74:MET:HE1	13:N:113:SER:HB3	1.95	0.48
15:P:70:LYS:HE2	27:X:499:G:O2'	2.14	0.48
27:X:568:G:H2'	27:X:569:C:O4'	2.14	0.48
27:X:732:G:H2'	27:X:733:G:C8	2.48	0.48
27:X:2260:C:O2'	27:X:2261:G:H5'	2.14	0.48
1:A:200:GLU:HB2	1:A:203:ASN:ND2	2.29	0.48
1:A:206:LEU:HA	1:A:211:ARG:HH11	1.79	0.48
5:E:143:GLN:HG2	27:X:2725:C:H1'	1.95	0.48
23:Z:7:PRO:HA	27:X:2594:U:C6	2.49	0.48
27:X:227:G:C6	27:X:228:A:C6	3.01	0.48
27:X:2190:A:H61	27:X:2196:U:H3	1.60	0.48
1:A:212:SER:OG	1:A:213:ARG:N	2.48	0.47
3:C:62:LYS:HE2	3:C:63:GLY:N	2.29	0.47
8:I:31:GLY:HA3	8:I:34:HIS:ND1	2.29	0.47
8:I:38:LYS:HG3	27:X:954:U:OP2	2.14	0.47
13:N:81:ASN:HD22	13:N:117:ARG:HH12	1.61	0.47
24:1:36:GLU:HG3	24:1:53:LYS:HA	1.96	0.47
27:X:114:C:O2'	27:X:124:A:N3	2.43	0.47
27:X:773:G:H2'	27:X:774:A:H5'	1.95	0.47
27:X:824:U:O2	27:X:1263:G:H3'	2.14	0.47
27:X:1107:A:H3'	27:X:1108:U:H5"	1.96	0.47
27:X:1417:C:H2'	27:X:1418:C:H6	1.78	0.47
2:B:108:SER:HB3	2:B:163:GLU:H	1.79	0.47
8:I:38:LYS:HG3	27:X:954:U:P	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:28:VAL:HG11	9:J:135:ARG:HB3	1.95	0.47
18:S:67:LYS:NZ	18:S:92:VAL:HG21	2.28	0.47
27:X:66:U:H2'	27:X:67:G:C8	2.49	0.47
30:X:2902:ERY:H312	30:X:2902:ERY:H2	1.63	0.47
1:A:97:TYR:HE2	1:A:103:ARG:HB2	1.79	0.47
7:H:11:ALA:N	7:H:96:ALA:O	2.37	0.47
8:I:62:LYS:HB3	26:3:13:ARG:H	1.77	0.47
16:Q:59:PRO:HA	16:Q:74:ASP:OD1	2.15	0.47
19:T:56:ASP:OD1	27:X:2343:C:H4'	2.15	0.47
19:T:83:ALA:HB1	19:T:85:GLN:HE21	1.79	0.47
21:V:46:LEU:O	21:V:50:VAL:HG23	2.14	0.47
27:X:1074:G:H1	27:X:1086:C:N4	2.12	0.47
27:X:1636:G:H2'	27:X:1637:U:C6	2.49	0.47
27:X:1655:C:H4'	27:X:2689:C:O2	2.14	0.47
27:X:1672:A:H3'	27:X:1673:C:C6	2.49	0.47
27:X:2542:U:O2	27:X:2544:A:H8	1.98	0.47
2:B:136:ARG:HH21	2:B:157:ALA:H	1.62	0.47
8:I:128:ALA:HA	8:I:131:LYS:HB3	1.95	0.47
9:J:16:GLY:HA2	9:J:17:ARG:NH1	2.25	0.47
9:J:70:PHE:C	9:J:70:PHE:CD2	2.87	0.47
21:V:54:ASN:HB3	27:X:71:A:C5	2.49	0.47
27:X:91:A:H2'	27:X:92:U:C6	2.49	0.47
27:X:333:A:H5'	27:X:351:A:H1'	1.95	0.47
27:X:760:U:OP1	27:X:2591:C:H1'	2.15	0.47
27:X:1052:C:N4	27:X:1053:G:N7	2.63	0.47
27:X:1171:A:H2'	27:X:1172:U:C6	2.49	0.47
27:X:2184:C:H2'	27:X:2185:U:O4'	2.14	0.47
27:X:2258:G:C2	27:X:2259:G:C8	3.02	0.47
27:X:2691:C:O2'	27:X:2693:U:H5'	2.13	0.47
27:X:2701:A:C2	27:X:2848:A:C4	3.03	0.47
4:D:4:LEU:C	4:D:6:THR:H	2.18	0.47
23:Z:45:ILE:HD13	23:Z:57:VAL:HG23	1.96	0.47
27:X:525:A:N1	27:X:1273:G:O2'	2.40	0.47
27:X:540:G:C5	27:X:2005:U:H5"	2.49	0.47
27:X:2363:G:H3'	27:X:2365:U:OP1	2.14	0.47
4:D:31:ILE:HA	4:D:158:THR:HA	1.97	0.47
4:D:153:ASP:OD1	27:X:2283:G:O2'	2.28	0.47
8:I:56:LEU:CB	26:3:52:LYS:HZ1	2.25	0.47
15:P:21:ARG:HH21	27:X:506:G:H5'	1.79	0.47
15:P:122:LYS:HB3	15:P:124:THR:CG2	2.45	0.47
27:X:552:C:H2'	27:X:553:C:H5"	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:682:G:H3'	27:X:683:A:C8	2.50	0.47
27:X:1468:A:H8	27:X:1468:A:P	2.38	0.47
27:X:1750:A:H4'	27:X:2695:C:O4'	2.14	0.47
27:X:2363:G:HO2'	27:X:2364:C:P	2.37	0.47
27:X:2368:G:H5"	27:X:2369:U:H5'	1.97	0.47
27:X:2576:G:C6	27:X:2577:A:C6	3.03	0.47
1:A:79:VAL:HB	1:A:114:GLY:H	1.80	0.47
7:H:23:ARG:HD2	7:H:24:VAL:O	2.15	0.47
7:H:110:VAL:HB	7:H:129:LEU:HB3	1.97	0.47
10:K:60:LEU:HD11	10:K:64:ARG:HH11	1.80	0.47
15:P:47:GLY:H	15:P:92:VAL:CG2	2.27	0.47
17:R:62:MET:H	17:R:65:PRO:HA	1.79	0.47
27:X:136:A:H2'	27:X:137:A:O4'	2.15	0.47
27:X:469:G:N2	27:X:480:G:H2'	2.30	0.47
27:X:536:A:N6	27:X:2605:C:H4'	2.30	0.47
27:X:582:G:O2'	27:X:583:C:H3'	2.14	0.47
27:X:742:G:H2'	27:X:1766:U:H1'	1.96	0.47
27:X:1164:C:H2'	27:X:1165:G:O4'	2.15	0.47
27:X:1353:A:H4'	27:X:1407:G:H1'	1.95	0.47
27:X:1419:G:H2'	27:X:1420:A:C8	2.50	0.47
27:X:1673:C:C2	27:X:1674:C:C5	3.02	0.47
27:X:1779:C:O5'	27:X:1779:C:H6	1.97	0.47
27:X:2512:A:OP1	27:X:2644:A:O2'	2.26	0.47
27:X:2524:G:C6	27:X:2525:U:C4	3.02	0.47
27:X:2670:C:H5'	27:X:2847:G:H5"	1.97	0.47
27:X:2684:A:H2'	27:X:2685:A:O4'	2.14	0.47
1:A:181:GLU:HG3	1:A:270:ILE:HA	1.95	0.47
2:B:32:PRO:O	2:B:49:ILE:HA	2.15	0.47
5:E:138:LYS:HG2	27:X:2726:U:H5"	1.97	0.47
11:L:8:ARG:HE	11:L:9:ARG:HG2	1.79	0.47
11:L:59:LEU:HD23	11:L:61:SER:HB3	1.97	0.47
15:P:34:SER:O	15:P:37:LYS:HB3	2.15	0.47
16:Q:57:ASN:HD21	16:Q:76:LYS:HE3	1.80	0.47
27:X:343:A:H1'	27:X:346:C:N4	2.29	0.47
27:X:835:U:H2'	27:X:836:G:C8	2.50	0.47
27:X:1332:G:C6	27:X:1333:G:N1	2.82	0.47
27:X:1838:G:N2	27:X:1878:C:N3	2.63	0.47
27:X:2280:A:H2'	27:X:2281:C:C6	2.49	0.47
28:Y:16:U:O2'	28:Y:110:U:H1'	2.15	0.47
1:A:38:PRO:HG3	27:X:1586:A:H5'	1.97	0.47
3:C:54:THR:HG22	3:C:55:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:33:ARG:HH21	11:L:103:LEU:HD12	1.79	0.47
17:R:22:VAL:HG13	17:R:81:VAL:O	2.15	0.47
19:T:46:LYS:HE3	19:T:76:ALA:HA	1.96	0.47
26:3:23:MET:HB3	26:3:25:PHE:CE2	2.49	0.47
26:3:30:ARG:HB2	27:X:2372:A:OP1	2.15	0.47
27:X:393:U:H2'	27:X:394:U:C6	2.49	0.47
27:X:640:C:H1'	27:X:650:U:H1'	1.97	0.47
27:X:1727:C:H2'	27:X:1728:A:C8	2.50	0.47
27:X:1813:A:H5"	27:X:1814:G:OP2	2.15	0.47
1:A:118:ASN:HD22	1:A:119:ALA:N	2.12	0.47
3:C:129:LYS:O	3:C:131:LYS:N	2.47	0.47
6:G:151:TYR:HE1	6:G:161:GLN:HE21	1.63	0.47
9:J:28:VAL:HG21	9:J:135:ARG:HB3	1.97	0.47
14:O:88:GLN:HE21	14:O:88:GLN:HB3	1.48	0.47
15:P:9:ARG:HD2	15:P:13:GLN:HG3	1.96	0.47
18:S:1:MET:N	18:S:53:ASP:O	2.42	0.47
20:U:64:ALA:O	20:U:67:LEU:HB3	2.15	0.47
23:Z:42:SER:O	23:Z:44:HIS:CD2	2.67	0.47
27:X:203:G:H21	27:X:205:A:H62	1.63	0.47
27:X:649:G:C5	27:X:650:U:C5	3.02	0.47
27:X:879:A:H2'	27:X:879:A:N3	2.30	0.47
27:X:1643:A:N6	27:X:1656:U:H3	2.08	0.47
27:X:2266:A:H5"	27:X:2267:A:OP1	2.15	0.47
27:X:2781:G:H2'	27:X:2782:G:H5"	1.96	0.47
28:Y:53:G:N3	28:Y:53:G:H2'	2.29	0.47
1:A:159:ALA:HA	1:A:198:ASN:CG	2.35	0.46
4:D:103:LEU:HG	4:D:108:LEU:HG	1.97	0.46
6:G:83:ILE:HG22	6:G:153:GLY:O	2.15	0.46
7:H:29:ILE:HB	7:H:34:LEU:HD23	1.96	0.46
7:H:132:GLU:HB2	12:M:73:PHE:CE1	2.49	0.46
8:I:102:LYS:C	8:I:104:ARG:H	2.17	0.46
9:J:21:ASP:OD1	9:J:21:ASP:N	2.36	0.46
11:L:11:LEU:HD21	27:X:2273:C:H5"	1.97	0.46
15:P:45:ILE:O	15:P:48:LYS:HG2	2.15	0.46
26:3:6:THR:N	26:3:59:LYS:HB3	2.30	0.46
27:X:1301:U:C2	27:X:1340:C:O2	2.68	0.46
27:X:1448:A:H61	27:X:1574:A:H61	1.61	0.46
27:X:1467:U:H3'	27:X:1467:U:H6	1.80	0.46
27:X:2170:C:H3'	27:X:2171:U:H5"	1.97	0.46
1:A:18:THR:HG22	1:A:19:ALA:H	1.79	0.46
1:A:133:LEU:HB3	1:A:173:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:LEU:HA	3:C:20:PRO:C	2.34	0.46
5:E:84:THR:HG22	5:E:134:SER:OG	2.15	0.46
8:I:31:GLY:O	8:I:32:ARG:HD2	2.15	0.46
10:K:13:ASN:OD1	10:K:15:SER:N	2.43	0.46
10:K:78:LYS:O	10:K:83:VAL:HG23	2.15	0.46
12:M:99:VAL:HG21	12:M:104:LEU:HD11	1.97	0.46
27:X:179:U:H2'	27:X:180:C:O4'	2.15	0.46
27:X:218:A:H61	27:X:232:A:H5"	1.80	0.46
27:X:522:G:OP1	27:X:1247:U:O2'	2.23	0.46
27:X:540:G:O2'	27:X:542:A:H2	1.97	0.46
27:X:687:G:N2	27:X:2423:G:O3'	2.48	0.46
27:X:747:A:H2'	27:X:748:A:O4'	2.14	0.46
27:X:758:G:H2'	27:X:759:C:H5'	1.98	0.46
27:X:1141:U:O2'	27:X:1142:G:O5'	2.23	0.46
27:X:1407:G:C6	27:X:1408:A:C6	3.03	0.46
27:X:1781:C:H2'	27:X:1782:A:C5	2.50	0.46
27:X:1919:A:C6	27:X:1928:G:C4	3.03	0.46
27:X:2312:A:H4'	27:X:2313:G:O5'	2.15	0.46
1:A:25:THR:HG22	1:A:26:LYS:N	2.30	0.46
1:A:222:ARG:HD3	27:X:1820:G:O6	2.16	0.46
2:B:162:MET:SD	27:X:2796:A:H4'	2.55	0.46
3:C:5:ASN:N	3:C:5:ASN:OD1	2.48	0.46
5:E:68:THR:O	5:E:72:VAL:HG23	2.15	0.46
5:E:150:LYS:HZ1	27:X:2724:G:H1'	1.81	0.46
7:H:5:GLN:HG2	27:X:1685:A:H5"	1.97	0.46
9:J:37:ALA:O	9:J:100:PRO:HA	2.14	0.46
12:M:22:ARG:HH22	12:M:24:LEU:HD23	1.80	0.46
12:M:90:GLN:OE1	12:M:90:GLN:N	2.34	0.46
16:Q:8:GLN:O	21:V:29:ARG:HG2	2.15	0.46
26:3:6:THR:N	26:3:59:LYS:HD3	2.31	0.46
27:X:1388:C:H2'	27:X:1389:C:C6	2.50	0.46
27:X:1840:A:H2'	27:X:1841:G:O4'	2.15	0.46
27:X:2020:G:C6	27:X:2021:G:C6	3.03	0.46
6:G:31:THR:HG21	13:N:61:TRP:HE1	1.81	0.46
9:J:6:LYS:HE2	9:J:6:LYS:HB2	1.57	0.46
15:P:28:ALA:O	15:P:126:HIS:HA	2.16	0.46
27:X:835:U:H2'	27:X:836:G:H8	1.80	0.46
27:X:962:C:H2'	27:X:963:G:H8	1.81	0.46
27:X:1159:U:H2'	27:X:1160:C:C6	2.51	0.46
27:X:1975:G:H22	27:X:1979:C:H6	1.63	0.46
27:X:2026:C:H2'	27:X:2027:C:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2226:A:H2'	27:X:2227:C:H6	1.81	0.46
27:X:2605:C:H2'	27:X:2606:G:C8	2.50	0.46
7:H:2:ILE:HG22	7:H:6:SER:HB3	1.98	0.46
13:N:74:MET:SD	13:N:110:VAL:HG13	2.55	0.46
14:O:5:ILE:N	14:O:10:LYS:HE2	2.30	0.46
14:O:20:ILE:HG22	14:O:21:ARG:H	1.80	0.46
14:O:68:LYS:HA	14:O:87:ARG:HG2	1.97	0.46
17:R:40:LEU:HB2	17:R:45:LYS:HB2	1.98	0.46
18:S:94:VAL:O	18:S:121:GLN:HA	2.15	0.46
19:T:74:LYS:HG2	19:T:77:ARG:NE	2.30	0.46
27:X:89:A:H4'	27:X:90:G:C5'	2.42	0.46
27:X:104:C:H2'	27:X:105:G:C8	2.50	0.46
27:X:571:U:C2	27:X:581:A:C8	3.03	0.46
27:X:769:C:C4	27:X:770:U:C4	3.03	0.46
27:X:958:G:H2'	27:X:959:C:C6	2.51	0.46
27:X:2030:U:H2'	27:X:2031:A:H8	1.81	0.46
27:X:2406:C:H5"	27:X:2407:G:OP1	2.15	0.46
27:X:2425:G:C2	27:X:2480:C:C4	3.03	0.46
3:C:46:ARG:HD3	27:X:463:C:OP1	2.15	0.46
8:I:118:VAL:HG23	8:I:133:VAL:HG13	1.98	0.46
9:J:37:ALA:HB2	9:J:104:MET:SD	2.55	0.46
14:O:15:SER:N	14:O:95:ILE:O	2.49	0.46
18:S:19:ILE:HG23	18:S:79:ILE:O	2.16	0.46
19:T:25:LYS:HD3	19:T:31:VAL:HG12	1.98	0.46
22:W:12:ARG:HG2	22:W:12:ARG:HH11	1.81	0.46
27:X:54:G:O2'	27:X:125:A:N1	2.43	0.46
27:X:817:A:H2'	27:X:819:C:C4	2.50	0.46
27:X:824:U:H1'	27:X:1264:C:O4'	2.15	0.46
27:X:1018:C:H5"	27:X:1019:U:H5"	1.98	0.46
27:X:1030:U:H2'	27:X:1032:A:C2	2.48	0.46
27:X:1040:A:C8	27:X:1041:G:C8	3.04	0.46
27:X:1073:G:OP2	27:X:1073:G:H8	1.99	0.46
27:X:1806:G:H5"	27:X:1807:A:H2'	1.97	0.46
27:X:2197:U:H2'	27:X:2198:U:C5	2.51	0.46
27:X:2485:U:O2	27:X:2485:U:H2'	2.15	0.46
27:X:2522:G:H2'	27:X:2523:G:H8	1.79	0.46
27:X:2692:A:H5"	27:X:2693:U:OP2	2.16	0.46
2:B:98:GLU:HA	2:B:172:VAL:HG12	1.97	0.46
3:C:58:MET:HB2	3:C:70:GLY:O	2.16	0.46
5:E:90:ARG:HB3	5:E:160:LYS:HA	1.97	0.46
5:E:169:ILE:HD13	5:E:170:ALA:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:28:LEU:HD12	10:K:113:ILE:HG23	1.96	0.46
12:M:31:ASP:OD2	12:M:31:ASP:N	2.49	0.46
15:P:89:ARG:HB3	15:P:133:GLU:HB3	1.97	0.46
15:P:105:ARG:HG3	15:P:107:ILE:HB	1.97	0.46
25:2:21:ARG:O	25:2:28:ARG:HD3	2.16	0.46
27:X:308:C:H2'	27:X:309:G:O4'	2.15	0.46
27:X:603:C:H2'	27:X:604:U:C6	2.51	0.46
27:X:1412:C:H6	27:X:1412:C:H2'	1.61	0.46
27:X:2051:U:H3	27:X:2409:A:H62	1.63	0.46
2:B:129:HIS:CD2	27:X:1692:C:C2	3.03	0.46
4:D:22:TYR:OH	4:D:165:GLU:OE1	2.34	0.46
6:G:94:LYS:HE3	6:G:95:LEU:HG	1.98	0.46
7:H:132:GLU:HB2	12:M:73:PHE:HE1	1.80	0.46
26:3:29:LYS:HD2	26:3:33:ASN:O	2.16	0.46
27:X:82:G:N1	27:X:100:G:O2'	2.42	0.46
27:X:839:U:H5"	27:X:2408:G:P	2.56	0.46
27:X:1681:A:C2	27:X:2706:U:C2	3.04	0.46
27:X:2516:U:H2'	27:X:2517:C:C6	2.51	0.46
27:X:2546:G:H2'	27:X:2547:C:C6	2.51	0.46
27:X:2696:A:O2'	27:X:2697:G:H5'	2.15	0.46
27:X:2753:C:H2'	27:X:2754:C:H6	1.81	0.46
1:A:201:HIS:HA	1:A:204:ILE:HD12	1.97	0.46
3:C:59:TYR:CD2	3:C:64:THR:HG21	2.51	0.46
13:N:24:PHE:HB3	13:N:28:ARG:HB2	1.97	0.46
15:P:97:VAL:HG13	15:P:125:SER:O	2.16	0.46
16:Q:11:VAL:HG23	16:Q:27:PHE:HA	1.97	0.46
26:3:13:ARG:HG3	26:3:13:ARG:O	2.16	0.46
27:X:312:G:C4	27:X:313:U:C5	3.04	0.46
27:X:330:C:H2'	27:X:331:U:O4'	2.16	0.46
27:X:1096:A:H5"	27:X:1116:U:H4'	1.98	0.46
27:X:1223:G:H5'	27:X:1225:G:O4'	2.16	0.46
27:X:1770:U:C5	27:X:1775:A:N7	2.84	0.46
27:X:2309:G:H1	27:X:2364:C:H42	1.63	0.46
27:X:2453:C:H5'	27:X:2454:C:OP2	2.16	0.46
27:X:2526:U:H2'	27:X:2527:G:C8	2.50	0.46
1:A:252:LYS:NZ	1:A:253:PRO:HD2	2.31	0.46
2:B:37:LYS:NZ	2:B:80:GLU:OE2	2.42	0.46
3:C:34:GLN:NE2	3:C:176:ASN:OD1	2.49	0.46
12:M:16:ILE:H	12:M:16:ILE:HD12	1.81	0.46
27:X:650:U:H2'	27:X:651:C:C6	2.51	0.46
27:X:820:U:H2'	27:X:821:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1981:A:O3'	27:X:2704:U:H4'	2.15	0.46
27:X:1998:A:O5'	27:X:1998:A:H8	1.99	0.46
27:X:2372:A:H62	27:X:2401:A:N6	2.14	0.46
27:X:2434:G:H2'	27:X:2435:C:C6	2.51	0.46
2:B:164:ARG:HD2	27:X:2753:C:H5"	1.98	0.45
10:K:89:GLU:O	10:K:91:PRO:HD3	2.15	0.45
12:M:104:LEU:HD23	12:M:106:TYR:CZ	2.51	0.45
27:X:658:G:H2'	27:X:659:G:H8	1.81	0.45
27:X:666:U:H2'	27:X:667:U:H5"	1.98	0.45
27:X:746:G:N7	27:X:774:A:C6	2.85	0.45
27:X:787:A:H2	27:X:800:U:HO2'	1.63	0.45
27:X:825:C:H5"	27:X:1263:G:HO2'	1.81	0.45
27:X:939:C:OP2	27:X:940:G:C8	2.70	0.45
27:X:984:A:O4'	27:X:1202:U:C6	2.69	0.45
27:X:1478:U:H2'	27:X:1479:G:C8	2.51	0.45
27:X:1782:A:N6	27:X:1820:G:O2'	2.49	0.45
27:X:1793:A:H2'	27:X:1794:A:C8	2.51	0.45
27:X:2048:C:H1'	27:X:2428:U:H3	1.81	0.45
28:Y:16:U:H4'	28:Y:72:C:O2	2.16	0.45
1:A:252:LYS:HD3	27:X:1817:U:O4'	2.16	0.45
2:B:52:ALA:HB2	12:M:3:THR:HG23	1.98	0.45
7:H:91:PHE:N	7:H:91:PHE:CD1	2.84	0.45
13:N:8:ILE:HG22	13:N:11:ARG:NH2	2.31	0.45
16:Q:10:PRO:HA	16:Q:27:PHE:HB3	1.98	0.45
27:X:88:G:C3'	27:X:89:A:H5"	2.47	0.45
27:X:982:C:H2'	27:X:983:G:O4'	2.16	0.45
27:X:2736:U:H4'	27:X:2737:A:OP1	2.17	0.45
27:X:2797:G:H2'	27:X:2798:A:H5"	1.99	0.45
27:X:2849:C:H2'	27:X:2850:U:C6	2.51	0.45
2:B:9:ILE:HD11	2:B:27:LEU:CB	2.43	0.45
5:E:150:LYS:NZ	27:X:2741:G:H21	2.13	0.45
8:I:59:ARG:CB	27:X:2371:A:H8	2.30	0.45
8:I:94:GLU:HA	8:I:97:ARG:HG3	1.97	0.45
9:J:82:THR:HA	27:X:2474:G:C5'	2.34	0.45
15:P:99:ALA:CB	27:X:25:U:H5'	2.43	0.45
15:P:104:LYS:HG3	15:P:106:LEU:H	1.82	0.45
16:Q:68:PHE:O	16:Q:70:GLY:N	2.42	0.45
24:1:39:LYS:NZ	24:1:47:HIS:HA	2.31	0.45
25:2:38:GLY:HA3	27:X:469:G:H8	1.82	0.45
27:X:115:G:P	27:X:117:A:HO2'	2.40	0.45
27:X:324:C:H2'	27:X:325:U:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1230:C:H2'	27:X:1231:A:C8	2.52	0.45
27:X:1763:G:H2'	27:X:1764:A:H4'	1.97	0.45
27:X:2477:C:O2'	27:X:2478:C:H5'	2.15	0.45
27:X:2640:G:H2'	27:X:2641:A:C8	2.51	0.45
1:A:206:LEU:HD22	1:A:211:ARG:HB3	1.98	0.45
2:B:69:LYS:HE2	2:B:69:LYS:HB3	1.80	0.45
3:C:133:PHE:CE1	3:C:161:ALA:HB2	2.51	0.45
5:E:44:ARG:NH2	5:E:51:LEU:HB3	2.32	0.45
9:J:13:GLN:HG3	9:J:14:PHE:CD1	2.51	0.45
12:M:50:PHE:CE2	12:M:70:LYS:HB2	2.52	0.45
13:N:45:TYR:HH	27:X:570:G:HO2'	1.64	0.45
27:X:577:U:H2'	27:X:579:G:OP2	2.17	0.45
27:X:768:U:C4	27:X:769:C:C4	3.05	0.45
27:X:2044:G:C8	27:X:2482:A:C8	3.04	0.45
27:X:2590:U:C5	30:X:2902:ERY:H312	2.51	0.45
27:X:2645:C:H3'	27:X:2646:C:H6	1.82	0.45
27:X:2674:C:H2'	27:X:2675:U:H6	1.81	0.45
28:Y:43:G:OP1	28:Y:45:C:N4	2.40	0.45
2:B:152:LYS:HB3	6:G:106:TYR:CB	2.44	0.45
7:H:24:VAL:HG22	7:H:45:ALA:HB2	1.97	0.45
8:I:56:LEU:HD21	8:I:59:ARG:HH21	1.82	0.45
9:J:42:TRP:CZ2	27:X:969:U:H5	2.35	0.45
17:R:105:ARG:HH22	17:R:112:LYS:HA	1.82	0.45
26:3:14:ILE:HD11	26:3:56:ALA:HB1	1.98	0.45
27:X:90:G:H3'	27:X:91:A:H8	1.80	0.45
27:X:172:A:H5"	27:X:173:A:OP2	2.17	0.45
27:X:1083:C:H42	27:X:1103:C:N4	2.15	0.45
27:X:1225:G:H2'	27:X:1249:G:H22	1.81	0.45
27:X:1724:C:N3	27:X:1747:G:C6	2.85	0.45
27:X:1751:A:H2'	27:X:1752:U:C6	2.51	0.45
27:X:2499:C:C4	27:X:2546:G:C8	3.04	0.45
27:X:2519:C:O2	27:X:2720:A:H2	2.00	0.45
1:A:43:ARG:NH1	1:A:43:ARG:H	2.14	0.45
1:A:208:LYS:HD3	27:X:1782:A:H1'	1.99	0.45
1:A:231:HIS:CG	1:A:232:PRO:HD2	2.52	0.45
9:J:76:THR:HB	9:J:88:LYS:O	2.17	0.45
10:K:43:GLU:O	10:K:46:PRO:HD2	2.17	0.45
13:N:64:ARG:O	13:N:67:ALA:HB3	2.16	0.45
20:U:46:LEU:O	27:X:2209:G:O2'	2.28	0.45
25:2:25:LYS:HD3	25:2:25:LYS:HA	1.74	0.45
26:3:52:LYS:O	26:3:56:ALA:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:16:G:H2'	27:X:17:G:H8	1.80	0.45
27:X:725:C:H2'	27:X:726:G:C8	2.52	0.45
27:X:1223:G:N2	27:X:1249:G:O2'	2.49	0.45
27:X:1646:G:C5	27:X:1647:U:C5	3.04	0.45
27:X:1736:C:H2'	27:X:1737:G:C8	2.52	0.45
27:X:2220:A:H2'	27:X:2221:G:H8	1.81	0.45
27:X:2306:A:O2'	27:X:2307:A:O5'	2.34	0.45
27:X:2579:A:H2'	27:X:2580:C:H6	1.81	0.45
28:Y:71:G:C6	28:Y:72:C:C4	3.05	0.45
2:B:145:LYS:HB2	27:X:2551:A:C8	2.51	0.45
4:D:129:ASN:ND2	27:X:2282:G:O2'	2.49	0.45
24:1:16:ALA:HB2	24:1:50:PHE:CE1	2.51	0.45
27:X:36:G:N3	27:X:462:G:O2'	2.50	0.45
3:C:65:GLY:O	15:P:112:ARG:NH2	2.50	0.45
5:E:25:LYS:HG3	5:E:34:THR:HG22	1.98	0.45
7:H:23:ARG:HH11	27:X:2541:U:H1'	1.82	0.45
10:K:98:LEU:O	10:K:111:ALA:HB1	2.17	0.45
20:U:78:ILE:HG12	20:U:79:GLU:H	1.81	0.45
21:V:15:ALA:O	21:V:18:ILE:HB	2.17	0.45
22:W:14:GLY:O	22:W:18:LYS:HG2	2.17	0.45
26:3:62:LEU:HD12	26:3:62:LEU:HA	1.86	0.45
27:X:186:C:H2'	27:X:187:U:O4'	2.17	0.45
27:X:231:G:H4'	27:X:397:U:H5"	1.99	0.45
27:X:242:A:C8	27:X:441:A:N6	2.84	0.45
27:X:346:C:H2'	27:X:347:C:H6	1.80	0.45
27:X:587:A:OP1	27:X:1268:U:O2'	2.26	0.45
27:X:742:G:N2	27:X:1766:U:O4'	2.50	0.45
27:X:809:C:H2'	27:X:810:U:C6	2.52	0.45
27:X:828:C:H2'	27:X:829:C:H6	1.82	0.45
27:X:838:A:H2'	27:X:839:U:O4'	2.17	0.45
27:X:1098:G:C5	27:X:1100:G:H1'	2.51	0.45
27:X:1286:U:O2	27:X:1985:G:O2'	2.35	0.45
27:X:1982:C:OP1	27:X:2704:U:H5'	2.16	0.45
27:X:2368:G:H5"	27:X:2369:U:C5'	2.47	0.45
27:X:2513:A:C2	27:X:2514:G:H1'	2.50	0.45
27:X:2668:U:OP2	27:X:2847:G:N2	2.36	0.45
27:X:2859:U:C5	27:X:2860:C:C2	3.05	0.45
1:A:107:ALA:HA	1:A:108:PRO:HD2	1.82	0.45
6:G:124:GLU:O	6:G:128:GLU:HG2	2.17	0.45
9:J:15:ARG:NE	9:J:73:LYS:HZ2	2.15	0.45
11:L:88:VAL:HG11	27:X:2357:A:H1'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:120:ILE:HG12	27:X:1996:A:OP1	2.17	0.45
17:R:38:LEU:HD22	17:R:40:LEU:HG	1.99	0.45
17:R:105:ARG:HH22	17:R:113:THR:N	2.10	0.45
26:3:7:HIS:NE2	27:X:220:U:OP2	2.47	0.45
27:X:658:G:H1'	27:X:2330:G:OP1	2.17	0.45
27:X:659:G:H2'	27:X:660:G:C8	2.51	0.45
27:X:1418:C:H2'	27:X:1419:G:C8	2.52	0.45
27:X:1987:G:C6	27:X:1988:A:C4	3.05	0.45
27:X:2579:A:H2'	27:X:2580:C:C6	2.52	0.45
27:X:2656:G:H1	27:X:2710:C:H42	1.63	0.45
27:X:2706:U:OP1	27:X:2706:U:C6	2.70	0.45
27:X:2738:A:H2'	27:X:2739:G:O4'	2.17	0.45
2:B:95:ILE:HD13	2:B:95:ILE:HA	1.82	0.45
2:B:109:LYS:NZ	27:X:2703:C:OP2	2.50	0.45
3:C:17:LEU:HG	3:C:109:ALA:HB2	1.99	0.45
5:E:109:TYR:CD2	27:X:2646:C:H1'	2.51	0.45
14:O:83:ARG:HG2	27:X:1238:A:H4'	1.99	0.45
19:T:29:GLU:HG2	27:X:935:C:H1'	1.98	0.45
24:1:9:ILE:HG13	24:1:10:VAL:N	2.32	0.45
27:X:513:A:H5"	27:X:514:G:H5'	1.99	0.45
27:X:699:G:H5"	27:X:699:G:H8	1.82	0.45
27:X:2034:A:H2	27:X:2035:G:O6	1.99	0.45
27:X:2792:C:C2	27:X:2805:G:C2	3.05	0.45
27:X:2796:A:O2'	27:X:2801:A:N1	2.46	0.45
2:B:115:GLY:O	2:B:119:ARG:HB2	2.17	0.44
2:B:152:LYS:CB	6:G:106:TYR:HB2	2.45	0.44
6:G:94:LYS:HB3	6:G:94:LYS:HE2	1.48	0.44
8:I:22:GLY:HA3	27:X:674:U:O2'	2.17	0.44
13:N:93:LYS:H	13:N:93:LYS:HG3	1.49	0.44
20:U:37:ILE:HD12	27:X:177:U:O2'	2.17	0.44
20:U:49:LYS:HB2	20:U:61:TRP:HA	1.99	0.44
22:W:12:ARG:HA	22:W:13:PRO:HD3	1.83	0.44
25:2:36:ALA:C	25:2:38:GLY:H	2.21	0.44
27:X:577:U:O2'	27:X:579:G:N7	2.42	0.44
27:X:613:A:N7	27:X:668:A:H1'	2.31	0.44
27:X:649:G:C8	27:X:650:U:H5	2.35	0.44
27:X:1121:G:H2'	27:X:1122:A:C8	2.52	0.44
27:X:1468:A:C8	27:X:1468:A:OP2	2.69	0.44
27:X:2053:G:C2	27:X:2054:A:C4	3.05	0.44
27:X:2269:G:N2	27:X:2322:U:H1'	2.32	0.44
27:X:2495:G:C6	27:X:2548:G:C2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2864:C:H2'	27:X:2865:G:C8	2.52	0.44
28:Y:56:G:H8	28:Y:56:G:O5'	2.00	0.44
28:Y:80:A:H2'	28:Y:81:C:O4'	2.17	0.44
1:A:32:ALA:HB3	1:A:83:GLU:CD	2.38	0.44
1:A:142:VAL:HG12	1:A:193:ILE:HA	1.98	0.44
2:B:134:TRP:HB2	2:B:135:HIS:CD2	2.52	0.44
4:D:115:ARG:HH22	4:D:178:ARG:NH1	2.12	0.44
7:H:116:ARG:CZ	12:M:38:LYS:HD2	2.47	0.44
8:I:100:ARG:NH1	27:X:614:G:N7	2.64	0.44
15:P:11:LYS:HD2	27:X:1225:G:N7	2.32	0.44
16:Q:10:PRO:HD3	21:V:30:PHE:CD2	2.52	0.44
17:R:14:LEU:HD21	17:R:41:PRO:HA	1.99	0.44
17:R:23:ILE:HG22	17:R:33:THR:HB	1.98	0.44
17:R:105:ARG:NH2	17:R:112:LYS:HA	2.32	0.44
27:X:205:A:H2'	27:X:206:U:H5'	1.99	0.44
27:X:495:C:H2'	27:X:496:C:C6	2.52	0.44
27:X:1210:C:C2	27:X:1211:G:C8	3.05	0.44
27:X:1329:U:O2'	27:X:1330:G:H5'	2.17	0.44
27:X:2058:U:C4	27:X:2217:G:C6	3.05	0.44
27:X:2451:G:H22	27:X:2456:U:H5"	1.81	0.44
27:X:2728:A:H2'	27:X:2729:A:C8	2.51	0.44
1:A:24:LEU:HB3	1:A:25:THR:H	1.61	0.44
1:A:99:ASP:HB3	27:X:1507:A:O4'	2.17	0.44
8:I:54:SER:HB3	8:I:55:ARG:HE	1.82	0.44
11:L:88:VAL:HG12	11:L:89:PHE:H	1.82	0.44
11:L:91:ARG:HH22	27:X:2355:A:H61	1.66	0.44
13:N:60:LEU:O	13:N:64:ARG:HG3	2.17	0.44
13:N:75:ASN:H	13:N:78:THR:HB	1.83	0.44
20:U:46:LEU:C	20:U:47:HIS:CG	2.90	0.44
27:X:354:C:H2'	27:X:355:G:H8	1.82	0.44
27:X:588:G:C2	27:X:1275:A:C4	3.05	0.44
27:X:748:A:H5"	27:X:749:C:C5	2.52	0.44
27:X:2044:G:N2	27:X:2046:C:C2	2.85	0.44
27:X:2372:A:H62	27:X:2401:A:H61	1.65	0.44
27:X:2406:C:H5'	27:X:2408:G:H5'	1.99	0.44
28:Y:39:C:H5"	28:Y:40:C:C5	2.53	0.44
1:A:16:MET:HE1	1:A:24:LEU:H	1.83	0.44
1:A:246:PRO:HG2	1:A:248:THR:O	2.18	0.44
3:C:39:ARG:HE	3:C:91:TYR:HD2	1.65	0.44
3:C:47:THR:N	3:C:51:VAL:HG21	2.32	0.44
5:E:156:ALA:O	5:E:172:LYS:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:160:LYS:NZ	27:X:2637:C:H5'	2.32	0.44
8:I:73:GLU:N	8:I:73:GLU:OE2	2.50	0.44
16:Q:72:ARG:NH2	27:X:1324:G:O2'	2.51	0.44
18:S:3:LEU:HD11	18:S:33:ALA:H	1.81	0.44
23:Z:51:TYR:CD1	23:Z:55:ARG:HD3	2.53	0.44
27:X:1482:U:OP2	27:X:1562:G:O2'	2.35	0.44
27:X:1686:A:O3'	27:X:2528:G:H5'	2.17	0.44
27:X:2510:A:C2'	27:X:2511:G:H5'	2.48	0.44
1:A:208:LYS:O	1:A:211:ARG:HB2	2.18	0.44
5:E:88:GLU:HG3	5:E:130:ARG:HG2	1.99	0.44
6:G:134:MET:HG3	27:X:1148:G:O2'	2.17	0.44
6:G:151:TYR:HB2	6:G:157:PRO:HB3	1.99	0.44
7:H:8:LEU:HD22	7:H:94:ASN:HB3	2.00	0.44
12:M:22:ARG:NH1	12:M:22:ARG:HB3	2.32	0.44
15:P:39:ARG:NH2	27:X:527:C:O2'	2.47	0.44
23:Z:4:HIS:HB3	27:X:2039:G:H22	1.83	0.44
27:X:98:U:H4'	27:X:99:U:H5"	1.99	0.44
27:X:494:A:N7	27:X:507:A:H2	2.16	0.44
27:X:763:A:H2'	27:X:764:A:H5"	1.98	0.44
27:X:1329:U:C2	27:X:1330:G:N7	2.85	0.44
27:X:1816:G:H2'	27:X:1817:U:H6	1.83	0.44
27:X:1882:G:N2	27:X:1885:C:N4	2.60	0.44
27:X:2495:G:O2'	27:X:2496:C:H5'	2.18	0.44
2:B:61:LYS:HB3	2:B:62:PRO:HD3	1.99	0.44
2:B:105:THR:CG2	2:B:197:VAL:HB	2.48	0.44
2:B:116:VAL:CG2	2:B:136:ARG:HG3	2.23	0.44
6:G:62:ILE:HG13	6:G:80:VAL:HG23	2.00	0.44
19:T:20:TYR:CD2	27:X:2335:U:H4'	2.52	0.44
19:T:26:PHE:CD1	27:X:934:G:H1'	2.53	0.44
26:3:57:ARG:O	26:3:61:MET:N	2.50	0.44
27:X:245:C:H42	27:X:437:G:H1	1.64	0.44
27:X:748:A:H3'	27:X:749:C:C6	2.52	0.44
27:X:1065:A:H2'	27:X:1066:G:H8	1.83	0.44
27:X:2058:U:H1'	27:X:2576:G:H21	1.81	0.44
27:X:2251:U:H5"	27:X:2252:A:OP1	2.18	0.44
27:X:2351:G:C2	27:X:2352:A:C5	3.06	0.44
3:C:112:GLN:NE2	3:C:116:LYS:HD2	2.33	0.44
6:G:35:LYS:HD3	6:G:35:LYS:HA	1.44	0.44
7:H:17:ARG:H	7:H:58:ALA:HA	1.82	0.44
7:H:83:ARG:HD2	7:H:89:ILE:HD11	2.00	0.44
8:I:38:LYS:HG2	8:I:40:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:49:GLU:O	10:K:52:ILE:HG12	2.18	0.44
12:M:78:GLU:OE2	12:M:108:ARG:NE	2.48	0.44
16:Q:35:LYS:HB2	27:X:1614:C:H5"	2.00	0.44
23:Z:16:ARG:HD3	23:Z:20:ARG:CZ	2.48	0.44
27:X:448:C:H2'	27:X:449:C:O4'	2.18	0.44
27:X:580:A:H4'	27:X:581:A:OP1	2.17	0.44
27:X:840:U:H4'	27:X:841:G:N2	2.32	0.44
27:X:1296:G:N2	27:X:1299:A:C8	2.85	0.44
27:X:1935:A:C6	27:X:1936:A:N1	2.85	0.44
27:X:2528:G:C2	27:X:2529:G:N7	2.85	0.44
27:X:2578:G:N2	27:X:2579:A:C4	2.86	0.44
1:A:59:LYS:HG3	1:A:59:LYS:O	2.18	0.44
3:C:112:GLN:HE22	3:C:116:LYS:HD2	1.83	0.44
3:C:176:ASN:ND2	3:C:178:TYR:HB3	2.32	0.44
15:P:44:VAL:O	15:P:48:LYS:HD3	2.18	0.44
18:S:66:VAL:HG22	18:S:83:PHE:CE2	2.53	0.44
22:W:18:LYS:HB2	27:X:863:C:H4'	1.99	0.44
27:X:586:G:C6	27:X:587:A:N6	2.86	0.44
27:X:616:U:O2'	27:X:671:A:H4'	2.18	0.44
27:X:753:U:H2'	27:X:754:G:C8	2.52	0.44
27:X:1679:U:O2	27:X:2666:U:H5"	2.18	0.44
27:X:1773:C:H1'	27:X:2588:U:C5'	2.48	0.44
27:X:1777:A:C4	27:X:1921:A:C6	3.06	0.44
27:X:1795:C:H2'	27:X:1796:A:C8	2.52	0.44
27:X:1810:U:HO2'	27:X:1811:A:P	2.40	0.44
27:X:2474:G:H2'	27:X:2475:C:O4'	2.18	0.44
27:X:2493:U:H2'	27:X:2494:C:H6	1.81	0.44
27:X:2634:G:O2'	27:X:2643:G:O6	2.28	0.44
5:E:17:VAL:HG13	5:E:26:VAL:HG22	1.98	0.44
5:E:55:PRO:HD2	5:E:61:HIS:CD2	2.53	0.44
6:G:158:HIS:HA	6:G:161:GLN:HE22	1.83	0.44
15:P:27:VAL:CG1	27:X:504:G:H4'	2.48	0.44
15:P:29:LYS:HB3	15:P:30:TYR:CD2	2.52	0.44
27:X:14:A:N6	27:X:15:G:C2	2.86	0.44
27:X:226:C:H4'	27:X:227:G:O5'	2.18	0.44
27:X:796:A:H8	27:X:797:A:H4'	1.82	0.44
27:X:1359:G:C6	27:X:1617:G:C6	3.06	0.44
27:X:1597:A:H2'	27:X:1598:C:C6	2.52	0.44
27:X:1698:C:O2'	27:X:1753:A:N3	2.42	0.44
27:X:2198:U:N3	27:X:2199:C:H1'	2.32	0.44
27:X:2201:G:H2'	27:X:2202:G:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HB2	1:A:187:SER:HA	2.00	0.43
1:A:222:ARG:HG3	27:X:1780:A:OP1	2.17	0.43
2:B:120:TRP:CE3	2:B:155:ARG:HD2	2.53	0.43
9:J:35:LEU:HD11	9:J:130:THR:HB	2.00	0.43
9:J:54:VAL:O	9:J:57:ARG:HB2	2.18	0.43
11:L:32:TYR:CZ	28:Y:9:G:H5'	2.53	0.43
17:R:97:GLN:NE2	17:R:101:GLY:HA2	2.33	0.43
27:X:500:G:H2'	27:X:501:G:O4'	2.18	0.43
27:X:748:A:H3'	27:X:749:C:H6	1.83	0.43
27:X:957:G:H2'	27:X:958:G:H8	1.83	0.43
27:X:1026:U:H2'	27:X:1027:C:C6	2.53	0.43
27:X:1043:A:H2	27:X:1133:G:H22	1.65	0.43
27:X:1098:G:H22	27:X:1114:A:H1'	1.82	0.43
27:X:1580:C:H2'	27:X:1581:C:C6	2.53	0.43
27:X:1670:G:H5'	27:X:2797:G:N2	2.33	0.43
27:X:1835:C:H2'	27:X:1836:C:C6	2.52	0.43
27:X:2670:C:H2'	27:X:2671:C:H6	1.83	0.43
2:B:95:ILE:HG22	2:B:96:PHE:CD1	2.53	0.43
2:B:122:PHE:CE1	27:X:2491:C:H4'	2.53	0.43
4:D:12:VAL:HG22	4:D:172:SER:HB2	2.00	0.43
8:I:56:LEU:HD22	26:3:52:LYS:HZ1	1.83	0.43
8:I:80:LEU:HD21	8:I:89:ASP:OD2	2.18	0.43
27:X:649:G:H2'	27:X:650:U:H6	1.84	0.43
27:X:773:G:C2'	27:X:774:A:H5'	2.48	0.43
27:X:1141:U:HO2'	27:X:1142:G:P	2.39	0.43
27:X:1219:C:H2'	27:X:1220:G:O4'	2.18	0.43
27:X:1399:C:H2'	27:X:1400:A:C8	2.53	0.43
27:X:2041:A:H61	30:X:2902:ERY:H282	1.83	0.43
27:X:2307:A:H2'	27:X:2308:A:C8	2.53	0.43
27:X:2310:G:N2	27:X:2364:C:C4	2.86	0.43
28:Y:64:C:H2'	28:Y:65:A:C8	2.52	0.43
1:A:108:PRO:HG2	1:A:111:LEU:HD12	2.00	0.43
1:A:254:THR:O	27:X:1836:C:H5'	2.19	0.43
8:I:63:ARG:HD3	26:3:30:ARG:HH22	1.82	0.43
11:L:8:ARG:HB2	11:L:8:ARG:CZ	2.48	0.43
12:M:103:LYS:O	12:M:104:LEU:HB2	2.18	0.43
13:N:81:ASN:ND2	27:X:1162:A:H4'	2.33	0.43
14:O:32:LYS:HA	14:O:32:LYS:HD3	1.77	0.43
14:O:39:PHE:CE2	14:O:46:VAL:HB	2.53	0.43
17:R:48:VAL:HG13	17:R:50:GLY:H	1.83	0.43
27:X:1336:G:O6	27:X:1337:G:C6	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1573:G:H3'	27:X:1574:A:H5"	2.00	0.43
27:X:1880:G:C6	27:X:1881:U:C4	3.06	0.43
27:X:2555:G:OP1	27:X:2555:G:H3'	2.19	0.43
2:B:34:VAL:HG11	2:B:78:LEU:HD21	2.00	0.43
10:K:107:GLY:HA3	27:X:1992:G:H1'	2.00	0.43
21:V:41:HIS:CD2	27:X:95:G:H4'	2.52	0.43
26:3:15:LYS:HZ3	26:3:60:LEU:HD21	1.84	0.43
27:X:485:G:C6	27:X:520:C:N4	2.86	0.43
27:X:1255:A:H2'	27:X:1256:C:H6	1.82	0.43
27:X:1712:G:H3'	27:X:1712:G:N3	2.34	0.43
27:X:1974:U:O5'	27:X:1974:U:H6	2.01	0.43
27:X:2017:U:H2'	27:X:2018:G:H5"	2.00	0.43
27:X:2048:C:H1'	27:X:2428:U:N3	2.33	0.43
27:X:2470:U:H2'	27:X:2470:U:O2	2.17	0.43
27:X:2511:G:C6	27:X:2512:A:C5	3.07	0.43
28:Y:27:A:N6	28:Y:55:C:H5"	2.34	0.43
28:Y:30:C:H2'	28:Y:31:A:C8	2.53	0.43
8:I:59:ARG:HA	27:X:2371:A:H8	1.81	0.43
18:S:125:PRO:HA	18:S:158:CYS:SG	2.58	0.43
22:W:39:ALA:O	27:X:864:C:O2'	2.37	0.43
23:Z:10:LYS:HG3	27:X:1276:U:O4'	2.18	0.43
24:1:3:LYS:HB3	24:1:3:LYS:HE2	1.83	0.43
27:X:529:U:H2'	27:X:530:G:H8	1.83	0.43
27:X:611:C:N4	27:X:612:G:C5	2.86	0.43
27:X:754:G:H2'	27:X:755:C:C6	2.53	0.43
27:X:859:U:H3	27:X:944:A:H61	1.66	0.43
27:X:956:A:C4	27:X:2427:A:C2	3.06	0.43
27:X:1493:A:H2'	27:X:1494:G:O4'	2.19	0.43
27:X:2027:C:C2'	27:X:2028:C:H5'	2.48	0.43
27:X:2451:G:H2'	27:X:2454:C:H42	1.83	0.43
1:A:63:ARG:HH22	27:X:1584:G:P	2.42	0.43
1:A:258:LYS:HG3	27:X:1790:G:OP1	2.18	0.43
2:B:54:LYS:HB3	2:B:74:PRO:HB2	2.00	0.43
4:D:52:LYS:HE3	4:D:147:ASP:HB2	2.01	0.43
4:D:66:ILE:HD12	28:Y:44:C:C6	2.54	0.43
5:E:103:LEU:HD21	5:E:105:MET:HG3	1.99	0.43
6:G:46:ALA:HB2	6:G:54:LEU:HD22	2.00	0.43
7:H:104:GLU:HB3	7:H:125:LYS:HD2	1.99	0.43
11:L:32:TYR:CG	28:Y:9:G:H4'	2.54	0.43
12:M:101:ARG:HG2	12:M:101:ARG:HH21	1.84	0.43
14:O:15:SER:OG	14:O:96:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:48:GLY:C	14:O:50:ASP:H	2.22	0.43
18:S:130:ILE:H	18:S:130:ILE:HD12	1.84	0.43
20:U:48:LYS:HE2	20:U:48:LYS:HB2	1.76	0.43
25:2:8:ASN:HB3	25:2:11:LYS:HB3	2.00	0.43
25:2:42:LEU:H	25:2:42:LEU:HD12	1.83	0.43
27:X:240:U:H2'	27:X:241:C:O4'	2.19	0.43
27:X:617:U:C5	27:X:632:A:N1	2.87	0.43
27:X:632:A:C2	27:X:633:G:C4	3.07	0.43
27:X:1574:A:H2'	27:X:1575:C:H5"	2.00	0.43
27:X:2224:U:H5"	27:X:2225:G:H5'	2.00	0.43
1:A:188:GLU:HG2	1:A:188:GLU:H	1.46	0.43
15:P:60:ILE:HA	15:P:61:PRO:HD3	1.67	0.43
19:T:57:HIS:CD2	19:T:57:HIS:N	2.87	0.43
24:1:54:LYS:HE2	24:1:54:LYS:HB2	1.76	0.43
26:3:25:PHE:CG	26:3:46:LYS:HA	2.54	0.43
27:X:734:G:C2	27:X:735:G:C8	3.07	0.43
27:X:1398:G:O2'	27:X:1399:C:O5'	2.36	0.43
27:X:1949:A:O2'	27:X:2572:U:H5'	2.18	0.43
27:X:2234:G:C6	27:X:2235:G:C4	3.06	0.43
27:X:2367:A:N7	27:X:2368:G:C5	2.87	0.43
1:A:91:ARG:NH1	1:A:109:GLU:HA	2.34	0.43
1:A:248:THR:HG22	1:A:249:PRO:HD2	2.01	0.43
7:H:7:ARG:HB3	7:H:18:GLU:OE2	2.18	0.43
11:L:33:ARG:HH11	11:L:99:ARG:HD2	1.84	0.43
12:M:104:LEU:HD23	12:M:106:TYR:CE2	2.54	0.43
15:P:109:ARG:HD2	15:P:109:ARG:O	2.19	0.43
18:S:49:THR:OG1	18:S:49:THR:O	2.37	0.43
27:X:187:U:H2'	27:X:188:G:C8	2.54	0.43
27:X:883:A:H2'	27:X:884:C:O4'	2.19	0.43
27:X:1408:A:C6	27:X:1411:C:C2	3.07	0.43
27:X:1429:A:N6	27:X:1600:U:H4'	2.33	0.43
27:X:1769:U:H2'	27:X:1775:A:H62	1.83	0.43
27:X:2262:C:C2	27:X:2368:G:C2	3.06	0.43
1:A:24:LEU:HD22	1:A:205:VAL:HG13	2.00	0.43
1:A:124:GLU:HA	1:A:125:PRO:HD3	1.80	0.43
8:I:17:LYS:HB3	8:I:17:LYS:HE2	1.81	0.43
8:I:42:GLY:H	8:I:45:LYS:HE3	1.84	0.43
8:I:77:LEU:HB2	8:I:110:ALA:HA	2.01	0.43
9:J:136:GLU:OE1	9:J:137:VAL:HB	2.19	0.43
15:P:9:ARG:HB3	15:P:10:ASN:H	1.46	0.43
15:P:99:ALA:O	15:P:124:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:6:VAL:HG13	23:Z:7:PRO:O	2.19	0.43
24:1:9:ILE:O	24:1:10:VAL:HB	2.17	0.43
27:X:17:G:H1	27:X:533:C:H42	1.66	0.43
27:X:78:C:H2'	27:X:79:G:H8	1.84	0.43
27:X:172:A:H61	27:X:175:C:H3'	1.84	0.43
27:X:194:G:H3'	27:X:195:A:H8	1.84	0.43
27:X:1154:A:H8	27:X:1154:A:OP1	2.01	0.43
27:X:1370:U:H2'	27:X:1371:G:C8	2.53	0.43
27:X:1845:A:N1	27:X:2070:G:H1'	2.34	0.43
27:X:2574:G:N1	27:X:2578:G:C6	2.86	0.43
1:A:39:LYS:HE2	1:A:87:ASN:HD21	1.84	0.43
1:A:87:ASN:O	27:X:1809:G:H5"	2.19	0.43
4:D:51:ASP:O	4:D:55:LYS:HG2	2.18	0.43
6:G:71:THR:HG22	6:G:76:GLN:OE1	2.17	0.43
9:J:15:ARG:HE	9:J:73:LYS:NZ	2.17	0.43
9:J:126:LEU:HA	9:J:127:PRO:HD3	1.86	0.43
12:M:38:LYS:HE2	12:M:38:LYS:HB3	1.78	0.43
13:N:20:ARG:HH22	14:O:72:ARG:HD3	1.83	0.43
13:N:101:ARG:O	13:N:103:PRO:HD3	2.18	0.43
19:T:40:GLN:HE21	19:T:57:HIS:HB3	1.84	0.43
23:Z:40:LYS:HD3	23:Z:46:CYS:HB2	1.99	0.43
26:3:9:MET:N	26:3:9:MET:SD	2.92	0.43
26:3:13:ARG:HD2	26:3:24:ALA:HA	2.01	0.43
27:X:1196:G:H2'	27:X:1197:U:O4'	2.19	0.43
1:A:218:LYS:HD2	1:A:219:PRO:HD2	2.00	0.42
3:C:46:ARG:HD2	3:C:51:VAL:HG11	2.01	0.42
4:D:65:PRO:HA	4:D:89:VAL:HG22	2.00	0.42
4:D:104:ILE:HD13	4:D:173:MET:HB3	2.01	0.42
5:E:175:LYS:HD3	5:E:175:LYS:HA	1.74	0.42
7:H:3:MET:O	7:H:6:SER:HB3	2.19	0.42
9:J:61:ARG:NH1	18:S:175:ARG:HD3	2.34	0.42
18:S:141:MET:SD	18:S:147:ILE:HG12	2.59	0.42
20:U:17:SER:CB	20:U:44:ALA:HA	2.49	0.42
22:W:46:THR:HG22	22:W:47:VAL:HG13	2.01	0.42
26:3:23:MET:HB3	26:3:25:PHE:HE2	1.82	0.42
27:X:69:G:H5"	27:X:111:G:H1'	2.01	0.42
27:X:149:A:H2'	27:X:150:A:C8	2.54	0.42
27:X:1281:A:H2'	27:X:1282:A:O4'	2.19	0.42
27:X:2044:G:H2'	27:X:2480:C:O2'	2.19	0.42
27:X:2331:A:C4	27:X:2345:A:C2	3.06	0.42
3:C:97:ARG:HA	3:C:100:ARG:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:157:TYR:CZ	27:X:2510:A:H5'	2.53	0.42
9:J:40:PRO:HB3	9:J:99:LYS:HD2	2.00	0.42
10:K:20:LEU:HD23	10:K:21:ALA:N	2.35	0.42
12:M:104:LEU:HD22	12:M:107:LEU:HD11	2.01	0.42
13:N:24:PHE:O	13:N:29:SER:HB3	2.19	0.42
13:N:65:ILE:HD13	13:N:95:LEU:HD22	2.01	0.42
13:N:81:ASN:CG	27:X:1162:A:H4'	2.39	0.42
14:O:39:PHE:HE2	14:O:46:VAL:HB	1.84	0.42
14:O:72:ARG:HA	14:O:82:ARG:O	2.18	0.42
20:U:15:VAL:HG23	20:U:16:ASN:H	1.83	0.42
20:U:20:ARG:HD3	20:U:43:ARG:HD2	2.01	0.42
27:X:565:A:H8	27:X:565:A:O5'	2.02	0.42
27:X:745:C:H2'	27:X:746:G:O4'	2.19	0.42
27:X:820:U:H1'	27:X:2424:G:OP1	2.19	0.42
27:X:1260:A:C6	27:X:1262:U:C2	3.07	0.42
27:X:1330:G:H2'	27:X:1331:G:O4'	2.19	0.42
27:X:2559:U:C2'	27:X:2560:G:H5'	2.49	0.42
1:A:133:LEU:HD23	1:A:133:LEU:HA	1.91	0.42
1:A:183:ARG:NH2	1:A:263:ARG:HB3	2.34	0.42
1:A:210:GLY:HA2	1:A:213:ARG:CG	2.45	0.42
5:E:106:ASN:HD22	5:E:112:PRO:HB3	1.84	0.42
7:H:109:ARG:HA	7:H:129:LEU:HD22	2.00	0.42
7:H:129:LEU:HD23	7:H:129:LEU:HA	1.74	0.42
11:L:39:TYR:OH	28:Y:117:G:N2	2.52	0.42
14:O:26:GLN:HG2	14:O:27:GLY:N	2.34	0.42
14:O:85:GLY:H	27:X:1238:A:H5'	1.84	0.42
17:R:25:LEU:H	17:R:80:LYS:HA	1.83	0.42
20:U:68:ARG:O	20:U:72:LYS:HG2	2.19	0.42
24:1:8:ILE:HD13	24:1:8:ILE:H	1.85	0.42
27:X:105:G:C2	27:X:106:G:C8	3.07	0.42
27:X:475:U:C2	27:X:801:A:C6	3.07	0.42
27:X:488:A:H8	27:X:488:A:OP1	2.02	0.42
27:X:725:C:H2'	27:X:726:G:H8	1.84	0.42
27:X:764:A:C2	27:X:802:A:C4	3.07	0.42
27:X:795:A:OP2	27:X:1768:U:O2'	2.26	0.42
27:X:877:G:H1	27:X:924:C:H42	1.67	0.42
27:X:1032:A:O2'	27:X:1134:C:H5"	2.19	0.42
27:X:1466:C:N4	27:X:1476:G:H1	2.16	0.42
27:X:1603:A:H2'	27:X:1604:A:H8	1.84	0.42
27:X:1742:G:C2	27:X:1743:C:C4	3.07	0.42
27:X:1832:G:H1	27:X:1885:C:H42	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2011:U:H2'	27:X:2012:A:C8	2.54	0.42
27:X:2221:G:H22	27:X:2413:A:H2	1.67	0.42
27:X:2328:G:H1	27:X:2347:C:H42	1.66	0.42
1:A:16:MET:HE1	1:A:23:GLY:HA2	2.01	0.42
2:B:147:PRO:HD3	27:X:1141:U:C5	2.54	0.42
4:D:4:LEU:CG	4:D:5:LYS:H	2.27	0.42
4:D:90:THR:OG1	28:Y:44:C:N3	2.42	0.42
15:P:73:ASN:O	15:P:77:ALA:N	2.42	0.42
15:P:119:ILE:HG13	15:P:120:ILE:N	2.35	0.42
25:2:44:VAL:HG11	27:X:124:A:OP1	2.19	0.42
27:X:930:A:C2	28:Y:82:U:H4'	2.55	0.42
27:X:1227:A:H4'	27:X:1252:C:H4'	2.02	0.42
27:X:1469:U:H5'	27:X:1470:G:OP2	2.20	0.42
27:X:2780:A:H2'	27:X:2780:A:N3	2.35	0.42
28:Y:39:C:N4	28:Y:50:U:O2'	2.53	0.42
28:Y:42:U:O2'	28:Y:45:C:N4	2.53	0.42
2:B:131:SER:C	2:B:134:TRP:HE1	2.19	0.42
3:C:156:ASN:HA	3:C:159:ARG:HH21	1.84	0.42
4:D:118:ASN:HB3	4:D:122:PHE:HZ	1.85	0.42
6:G:119:LEU:HA	6:G:119:LEU:HD13	1.64	0.42
8:I:90:ARG:HA	8:I:121:HIS:CG	2.54	0.42
9:J:53:ILE:O	9:J:57:ARG:HG2	2.20	0.42
10:K:60:LEU:CG	10:K:64:ARG:HD2	2.36	0.42
14:O:6:GLN:HB2	14:O:7:THR:H	1.66	0.42
15:P:64:ALA:O	15:P:67:PRO:HD2	2.20	0.42
16:Q:43:GLN:HG2	16:Q:48:VAL:O	2.20	0.42
17:R:52:ASN:HB2	17:R:73:GLU:HA	2.01	0.42
27:X:14:A:C5	27:X:536:A:C2	3.07	0.42
27:X:54:G:H2'	27:X:55:A:H8	1.83	0.42
27:X:398:C:N4	27:X:424:G:H1	2.18	0.42
27:X:564:U:H2'	27:X:565:A:C8	2.54	0.42
27:X:748:A:H5"	27:X:749:C:H5	1.84	0.42
27:X:1086:C:H2'	27:X:1087:C:H5"	2.01	0.42
27:X:2284:U:H5'	27:X:2286:G:N1	2.32	0.42
27:X:2432:A:O2'	27:X:2551:A:H1'	2.19	0.42
27:X:2817:A:H2'	27:X:2818:G:O4'	2.19	0.42
2:B:5:LEU:CD2	2:B:195:LEU:HD11	2.49	0.42
3:C:48:ARG:H	3:C:48:ARG:HG3	1.45	0.42
3:C:128:ALA:O	3:C:130:THR:N	2.51	0.42
4:D:105:ASN:O	4:D:109:PRO:HG2	2.19	0.42
4:D:161:LYS:HG3	4:D:162:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:103:TYR:CD2	27:X:1142:G:O4'	2.73	0.42
8:I:17:LYS:HG3	8:I:19:VAL:N	2.31	0.42
9:J:123:GLY:HA2	9:J:126:LEU:HD12	2.01	0.42
14:O:26:GLN:HG3	14:O:63:HIS:HD2	1.85	0.42
15:P:109:ARG:H	15:P:109:ARG:HG3	1.64	0.42
17:R:52:ASN:HB2	17:R:72:ARG:O	2.20	0.42
20:U:68:ARG:NH1	27:X:413:G:N7	2.67	0.42
22:W:38:PRO:HB2	27:X:865:A:O2'	2.20	0.42
27:X:340:G:O4'	27:X:488:A:H1'	2.20	0.42
27:X:427:C:H2'	27:X:428:A:C8	2.54	0.42
27:X:788:G:C4	27:X:807:A:C8	3.08	0.42
27:X:802:A:H8	27:X:802:A:OP2	2.02	0.42
27:X:1016:C:C2	27:X:1154:A:C5	3.07	0.42
27:X:1437:A:H2'	27:X:1438:G:H8	1.85	0.42
27:X:1562:G:H8	27:X:1562:G:OP2	2.03	0.42
27:X:2424:G:O2'	27:X:2425:G:H5'	2.19	0.42
1:A:94:LEU:HD12	1:A:95:LEU:N	2.35	0.42
1:A:96:HIS:HE1	1:A:100:GLY:HA2	1.84	0.42
1:A:207:GLY:O	27:X:1782:A:O2'	2.35	0.42
10:K:39:THR:OG1	27:X:1668:G:H5'	2.20	0.42
12:M:19:ASP:OD2	12:M:19:ASP:N	2.33	0.42
13:N:89:ASP:HB3	13:N:91:ASN:HB2	2.02	0.42
14:O:6:GLN:HG2	27:X:1007:A:O2'	2.19	0.42
14:O:10:LYS:HE3	14:O:13:ARG:NH2	2.35	0.42
14:O:82:ARG:HA	14:O:82:ARG:HD3	1.56	0.42
17:R:15:HIS:HE1	17:R:80:LYS:HE2	1.84	0.42
24:1:17:GLY:O	24:1:19:GLY:N	2.51	0.42
27:X:102:C:C4	27:X:103:U:C4	3.08	0.42
27:X:590:C:H2'	27:X:591:G:H8	1.84	0.42
27:X:964:A:H2'	27:X:965:G:O4'	2.19	0.42
27:X:1454:U:H2'	27:X:1455:C:H6	1.83	0.42
27:X:2327:U:O5'	27:X:2327:U:H6	2.03	0.42
2:B:103:ASP:O	2:B:199:ARG:HG3	2.20	0.42
3:C:45:THR:HG21	3:C:85:GLY:HA3	2.00	0.42
5:E:130:ARG:CZ	5:E:130:ARG:HB3	2.49	0.42
6:G:43:VAL:HG21	6:G:158:HIS:CE1	2.53	0.42
11:L:97:HIS:CG	11:L:98:GLY:N	2.85	0.42
13:N:72:HIS:CD2	13:N:110:VAL:HG21	2.55	0.42
14:O:64:GLY:HA3	14:O:90:PHE:CE1	2.54	0.42
16:Q:4:TYR:HB3	21:V:26:MET:HE2	2.02	0.42
24:1:8:ILE:O	24:1:9:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:3:ARG:HA	25:2:3:ARG:HD3	1.51	0.42
27:X:459:A:N1	27:X:466:A:O2'	2.45	0.42
27:X:591:G:H3'	27:X:592:G:C8	2.42	0.42
27:X:1730:G:N2	27:X:1736:C:O2	2.51	0.42
27:X:1812:U:O2	27:X:1812:U:H2'	2.20	0.42
27:X:2043:A:O4'	27:X:2481:G:H1'	2.20	0.42
27:X:2263:C:O2'	27:X:2267:A:N6	2.53	0.42
27:X:2696:A:H2'	27:X:2697:G:H8	1.84	0.42
1:A:67:PHE:CE2	1:A:106:LEU:HD11	2.54	0.42
2:B:133:LYS:C	2:B:134:TRP:CD1	2.93	0.42
2:B:195:LEU:HB3	12:M:2:GLN:HE21	1.84	0.42
9:J:64:LYS:O	9:J:107:VAL:HA	2.19	0.42
14:O:78:VAL:HG22	27:X:1202:U:H5'	2.02	0.42
16:Q:64:ARG:HH21	27:X:1349:A:H5'	1.84	0.42
27:X:459:A:O4'	27:X:461:A:N6	2.53	0.42
27:X:485:G:C5	27:X:520:C:N4	2.88	0.42
27:X:615:C:H1'	27:X:670:U:H1'	2.00	0.42
27:X:762:A:H4'	27:X:1284:G:N3	2.34	0.42
27:X:797:A:N7	27:X:805:G:C4	2.88	0.42
27:X:1484:G:H2'	27:X:1485:U:H6	1.85	0.42
27:X:1505:U:H1'	27:X:1506:C:C5	2.55	0.42
27:X:1810:U:O2'	27:X:1811:A:O5'	2.36	0.42
28:Y:58:G:H5"	28:Y:59:A:OP1	2.20	0.42
3:C:176:ASN:HD22	3:C:178:TYR:HB3	1.85	0.42
5:E:44:ARG:HH22	5:E:51:LEU:HD23	1.85	0.42
6:G:116:ARG:HE	6:G:126:VAL:HG13	1.85	0.42
8:I:84:GLU:OE2	8:I:87:THR:OG1	2.30	0.42
9:J:119:PHE:CD1	9:J:132:MET:HB2	2.55	0.42
13:N:10:ARG:HG3	27:X:1264:C:OP1	2.19	0.42
25:2:4:THR:O	27:X:700:C:H5'	2.19	0.42
27:X:48:A:H61	27:X:154:U:H2'	1.85	0.42
27:X:1212:U:H2'	27:X:1213:U:C6	2.55	0.42
27:X:2321:C:O2'	27:X:2353:G:H5"	2.20	0.42
1:A:69:ARG:NH1	1:A:128:GLY:O	2.40	0.41
1:A:118:ASN:HD22	1:A:119:ALA:H	1.68	0.41
2:B:17:ASN:HB3	2:B:18:ASP:H	1.57	0.41
2:B:48:GLN:NE2	27:X:2614:A:O2'	2.53	0.41
12:M:44:ARG:NH2	12:M:46:ARG:HE	2.18	0.41
18:S:79:ILE:HD11	28:Y:78:A:O2'	2.19	0.41
20:U:49:LYS:HB3	20:U:61:TRP:CE3	2.55	0.41
25:2:24:THR:OG1	25:2:25:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:25:LYS:O	25:2:29:ASN:HB2	2.20	0.41
27:X:502:A:H2'	27:X:503:G:O4'	2.19	0.41
27:X:742:G:C2	27:X:1766:U:C6	3.08	0.41
27:X:753:U:H2'	27:X:754:G:H8	1.85	0.41
27:X:1788:C:C4	27:X:1789:U:C4	3.07	0.41
27:X:2048:C:H1'	27:X:2428:U:C2	2.55	0.41
27:X:2189:A:H61	27:X:2190:A:N6	2.18	0.41
27:X:2338:C:H2'	27:X:2339:A:C8	2.55	0.41
27:X:2553:G:C2	27:X:2554:C:O2	2.73	0.41
28:Y:75:A:OP1	28:Y:75:A:H4'	2.19	0.41
1:A:133:LEU:HD23	1:A:136:VAL:HG21	2.01	0.41
3:C:10:ASN:OD1	3:C:13:ARG:NH1	2.53	0.41
6:G:116:ARG:HD2	6:G:119:LEU:HG	2.02	0.41
7:H:101:ASN:N	7:H:101:ASN:HD22	2.18	0.41
9:J:12:LYS:HD3	27:X:923:A:N7	2.34	0.41
9:J:75:VAL:HG21	9:J:93:TYR:HE1	1.86	0.41
13:N:66:ASN:HB2	13:N:70:ARG:HH11	1.85	0.41
15:P:35:PRO:O	15:P:39:ARG:HD3	2.20	0.41
17:R:96:LYS:O	17:R:104:VAL:HA	2.20	0.41
22:W:22:ALA:HA	27:X:942:U:O2'	2.20	0.41
26:3:50:LEU:HD23	26:3:53:ALA:CB	2.50	0.41
27:X:627:A:C6	27:X:628:A:C6	3.08	0.41
27:X:837:U:H2'	27:X:838:A:C8	2.54	0.41
27:X:1137:A:H4'	27:X:1138:A:O5'	2.19	0.41
27:X:1615:C:H2'	27:X:1616:C:C6	2.55	0.41
27:X:1793:A:N1	27:X:1814:G:H1'	2.35	0.41
27:X:2188:A:H2'	27:X:2189:A:N7	2.36	0.41
2:B:136:ARG:O	2:B:137:ARG:C	2.59	0.41
3:C:162:ARG:NH2	27:X:331:U:O2'	2.54	0.41
3:C:178:TYR:OH	27:X:1216:G:O2'	2.32	0.41
3:C:180:ILE:HG22	3:C:186:LEU:HD13	2.03	0.41
4:D:102:LYS:O	4:D:106:ILE:HB	2.21	0.41
5:E:11:VAL:HA	5:E:12:PRO:HD2	1.95	0.41
8:I:44:GLY:HA2	27:X:684:C:H5	1.84	0.41
8:I:86:THR:HG21	8:I:117:ALA:O	2.20	0.41
12:M:8:ASN:HA	27:X:2851:G:O5'	2.21	0.41
14:O:93:ILE:HG13	14:O:95:ILE:HD11	2.02	0.41
17:R:84:VAL:HB	17:R:88:THR:O	2.20	0.41
24:1:28:ARG:O	24:1:33:ALA:HB2	2.20	0.41
27:X:182:G:HO2'	27:X:183:U:P	2.44	0.41
27:X:1030:U:C4	27:X:1031:C:H5	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1447:U:HO2'	27:X:1448:A:H8	1.69	0.41
27:X:2499:C:N3	27:X:2546:G:C8	2.88	0.41
27:X:2578:G:C2	27:X:2579:A:C4	3.08	0.41
27:X:2705:A:H8	27:X:2706:U:O2'	2.03	0.41
28:Y:53:G:H2'	28:Y:54:U:H5"	2.02	0.41
1:A:49:ILE:HG22	27:X:792:U:OP1	2.20	0.41
1:A:257:LEU:HB3	27:X:1794:A:O3'	2.21	0.41
4:D:79:LEU:HD23	4:D:79:LEU:HA	1.92	0.41
9:J:49:GLU:OE2	9:J:52:ARG:NH2	2.54	0.41
10:K:28:LEU:CD2	10:K:115:LEU:HG	2.49	0.41
10:K:73:LYS:HA	10:K:76:VAL:HG12	2.03	0.41
17:R:40:LEU:HA	17:R:41:PRO:HD2	1.95	0.41
23:Z:36:CYS:HB3	23:Z:49:CYS:HB3	1.94	0.41
27:X:640:C:H5"	27:X:660:G:O2'	2.20	0.41
27:X:671:A:H2'	27:X:672:C:O4'	2.20	0.41
27:X:1228:G:C6	27:X:1229:C:C4	3.08	0.41
27:X:1841:G:H1	27:X:1876:C:H42	1.68	0.41
27:X:2046:C:O2	27:X:2430:A:C2	2.74	0.41
27:X:2283:G:H2'	27:X:2283:G:N3	2.35	0.41
27:X:2447:G:O2'	27:X:2448:A:H8	1.85	0.41
27:X:2705:A:O2'	27:X:2706:U:O5'	2.33	0.41
1:A:157:ARG:HB2	1:A:157:ARG:HH11	1.85	0.41
5:E:86:ASN:O	5:E:165:VAL:HG22	2.20	0.41
5:E:95:ARG:HH22	5:E:97:LYS:HD3	1.86	0.41
6:G:67:ARG:HH11	6:G:67:ARG:HB2	1.86	0.41
7:H:37:GLY:O	27:X:2542:U:H5"	2.20	0.41
8:I:62:LYS:HB3	26:3:13:ARG:N	2.35	0.41
8:I:62:LYS:HG3	8:I:63:ARG:N	2.35	0.41
8:I:74:VAL:HG11	27:X:638:A:C8	2.56	0.41
9:J:14:PHE:HE1	9:J:90:ALA:HA	1.86	0.41
11:L:14:ARG:HE	11:L:14:ARG:HB2	1.50	0.41
13:N:99:ALA:HB2	13:N:106:PHE:CE1	2.56	0.41
19:T:23:VAL:HB	19:T:26:PHE:CE2	2.54	0.41
19:T:37:LEU:HD11	19:T:61:ALA:HB2	2.03	0.41
23:Z:15:LYS:O	23:Z:18:MET:HB3	2.19	0.41
27:X:525:A:C8	27:X:526:C:C6	3.09	0.41
27:X:726:G:H1'	27:X:731:A:H61	1.86	0.41
27:X:1010:U:O2'	27:X:1011:A:H5'	2.20	0.41
27:X:1024:G:H2'	27:X:1025:A:C8	2.55	0.41
27:X:1278:A:H2	27:X:1997:A:N6	2.09	0.41
27:X:1462:C:C2	27:X:1480:G:N2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1642:G:O5'	27:X:1642:G:H8	2.03	0.41
27:X:2667:C:N4	27:X:2700:U:OP2	2.41	0.41
1:A:124:GLU:O	1:A:126:LYS:N	2.52	0.41
2:B:5:LEU:HD21	2:B:79:ARG:CG	2.50	0.41
2:B:62:PRO:HG3	27:X:2767:C:H1'	2.01	0.41
3:C:152:THR:OG1	3:C:153:ASP:N	2.53	0.41
4:D:132:ILE:HG13	4:D:154:ILE:HD13	2.03	0.41
6:G:134:MET:HE3	6:G:134:MET:HB3	1.58	0.41
8:I:33:GLY:CA	14:O:79:GLN:HG3	2.49	0.41
11:L:12:ARG:HG3	11:L:13:THR:N	2.35	0.41
15:P:27:VAL:HG23	15:P:128:THR:HG22	2.02	0.41
15:P:72:LEU:HA	15:P:129:ILE:HD12	2.01	0.41
16:Q:64:ARG:NH1	27:X:1348:C:H4'	2.35	0.41
21:V:41:HIS:ND1	27:X:94:C:O2'	2.33	0.41
27:X:176:A:H2	27:X:2061:C:HO2'	1.65	0.41
27:X:645:G:H2'	27:X:646:C:C6	2.55	0.41
27:X:828:C:C2	27:X:1207:G:C2	3.08	0.41
27:X:1031:C:OP1	27:X:1045:G:N2	2.30	0.41
27:X:2557:G:OP1	27:X:2593:A:N6	2.53	0.41
27:X:2733:A:H2'	27:X:2734:U:O4'	2.20	0.41
30:X:2902:ERY:H71	30:X:2902:ERY:H4	1.92	0.41
1:A:44:ASN:CB	1:A:49:ILE:HA	2.51	0.41
1:A:77:ALA:HB2	1:A:97:TYR:CD1	2.56	0.41
1:A:89:SER:O	1:A:198:ASN:ND2	2.46	0.41
3:C:48:ARG:C	3:C:50:GLN:N	2.74	0.41
3:C:98:GLN:HE21	3:C:98:GLN:HB3	1.56	0.41
6:G:41:TRP:CZ3	6:G:79:PHE:CG	3.09	0.41
8:I:30:ALA:N	27:X:824:U:H2'	2.35	0.41
8:I:58:ALA:HA	26:3:12:ARG:NH1	2.35	0.41
9:J:39:GLU:HA	9:J:40:PRO:HD3	1.79	0.41
12:M:9:ARG:O	12:M:13:LEU:HB2	2.21	0.41
15:P:119:ILE:O	15:P:120:ILE:HG12	2.21	0.41
27:X:665:A:N7	27:X:666:U:H1'	2.36	0.41
27:X:754:G:C2	27:X:755:C:C4	3.08	0.41
27:X:922:A:N7	27:X:923:A:C6	2.89	0.41
27:X:944:A:C2	27:X:945:G:C8	3.09	0.41
27:X:1398:G:O2'	27:X:1399:C:O4'	2.25	0.41
27:X:2042:A:C6	27:X:2482:A:C2	3.08	0.41
27:X:2510:A:H2'	27:X:2511:G:H5'	2.02	0.41
27:X:2522:G:H2'	27:X:2523:G:O4'	2.21	0.41
27:X:2679:G:H1	27:X:2686:C:N4	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2751:C:H2'	27:X:2752:C:C6	2.55	0.41
1:A:27:LYS:HZ3	1:A:29:PRO:CB	2.33	0.41
3:C:68:ARG:HH12	27:X:687:G:H1'	1.83	0.41
7:H:2:ILE:HG12	7:H:45:ALA:O	2.21	0.41
7:H:100:ASN:OD1	7:H:100:ASN:C	2.59	0.41
8:I:99:VAL:O	8:I:101:ARG:HG2	2.21	0.41
11:L:15:ARG:HA	11:L:15:ARG:HD3	1.57	0.41
11:L:39:TYR:HD2	11:L:41:GLN:HG3	1.86	0.41
14:O:23:GLU:CB	14:O:91:THR:HG21	2.48	0.41
14:O:65:ARG:NH2	27:X:1237:G:OP2	2.53	0.41
15:P:41:VAL:O	15:P:44:VAL:HG22	2.21	0.41
17:R:85:ASP:O	17:R:87:GLU:N	2.46	0.41
19:T:45:PHE:HE2	19:T:77:ARG:CZ	2.33	0.41
21:V:2:LYS:HE3	21:V:2:LYS:HB2	1.90	0.41
21:V:43:VAL:O	21:V:47:ARG:HG2	2.21	0.41
27:X:457:C:O2'	27:X:458:G:H5'	2.21	0.41
27:X:998:C:O2	27:X:1011:A:H2	2.04	0.41
27:X:1533:G:H2'	27:X:1534:A:H8	1.85	0.41
27:X:2050:G:C6	27:X:2423:G:C6	3.09	0.41
27:X:2394:G:C2	27:X:2395:C:C2	3.08	0.41
27:X:2663:U:H3	27:X:2705:A:H62	1.66	0.41
1:A:36:ALA:CB	1:A:63:ARG:HA	2.50	0.41
1:A:69:ARG:NH2	1:A:192:THR:OG1	2.54	0.41
2:B:9:ILE:HG13	2:B:25:VAL:O	2.21	0.41
2:B:59:VAL:CG1	2:B:64:GLN:HG3	2.51	0.41
4:D:77:PHE:HB2	27:X:2289:A:N1	2.36	0.41
6:G:62:ILE:HG22	6:G:135:LEU:HD21	2.02	0.41
6:G:111:LYS:HG2	27:X:1142:G:H5"	2.01	0.41
7:H:113:PRO:HD3	12:M:73:PHE:HB2	2.03	0.41
8:I:41:SER:HB2	27:X:844:G:O3'	2.21	0.41
9:J:55:MET:HG3	9:J:122:ALA:HB2	2.03	0.41
10:K:12:ARG:HG2	10:K:12:ARG:NH1	2.36	0.41
11:L:42:ILE:HD13	11:L:42:ILE:HA	1.90	0.41
13:N:33:ARG:H	13:N:33:ARG:HG2	1.46	0.41
13:N:72:HIS:HD2	13:N:110:VAL:HG21	1.86	0.41
13:N:86:ALA:C	13:N:88:ILE:N	2.73	0.41
15:P:113:ALA:HB1	15:P:114:ARG:HD2	2.02	0.41
17:R:56:LYS:HD3	17:R:69:GLN:NE2	2.35	0.41
19:T:56:ASP:OD1	19:T:58:THR:OG1	2.34	0.41
20:U:51:ILE:HG23	20:U:59:THR:HG22	2.03	0.41
27:X:216:U:H2'	27:X:217:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:224:G:H4'	27:X:399:G:C6	2.56	0.41
27:X:242:A:N6	27:X:441:A:C8	2.89	0.41
27:X:474:G:C6	27:X:478:G:O6	2.74	0.41
27:X:481:A:H3'	27:X:482:A:C8	2.56	0.41
27:X:487:G:N2	27:X:489:A:H3'	2.35	0.41
27:X:534:U:P	27:X:549:G:H21	2.43	0.41
27:X:717:G:N3	27:X:739:G:C2	2.89	0.41
27:X:1250:A:H5'	27:X:1250:A:C8	2.54	0.41
27:X:1365:U:O2'	27:X:1586:A:N3	2.43	0.41
27:X:1385:C:H2'	27:X:1386:A:O4'	2.21	0.41
27:X:1609:G:H2'	27:X:1610:A:O4'	2.21	0.41
27:X:1779:C:H2'	27:X:1780:A:C8	2.56	0.41
27:X:1816:G:H2'	27:X:1817:U:C6	2.56	0.41
27:X:1869:A:H2'	27:X:1870:U:O4'	2.21	0.41
27:X:1991:C:H2'	27:X:1992:G:C8	2.53	0.41
27:X:2185:U:H2'	27:X:2186:G:C8	2.56	0.41
27:X:2355:A:H8	27:X:2355:A:OP1	2.04	0.41
27:X:2432:A:N6	27:X:2479:U:H3	2.15	0.41
27:X:2443:C:H2'	27:X:2444:C:H6	1.86	0.41
27:X:2501:U:O2'	27:X:2626:U:OP1	2.32	0.41
27:X:2579:A:O2'	27:X:2580:C:H5'	2.21	0.41
27:X:2702:G:H2'	27:X:2703:C:O4'	2.21	0.41
27:X:2772:U:H2'	27:X:2773:G:C8	2.56	0.41
27:X:2838:U:H2'	27:X:2839:G:H8	1.86	0.41
3:C:65:GLY:CA	27:X:2042:A:H5"	2.50	0.41
6:G:56:THR:HG21	27:X:1016:C:O2'	2.21	0.41
7:H:116:ARG:HD3	12:M:40:ARG:HB2	2.03	0.41
7:H:127:VAL:HG22	7:H:133:VAL:HG21	2.03	0.41
9:J:24:GLY:HA3	27:X:920:G:P	2.61	0.41
24:1:10:VAL:HG22	24:1:11:LYS:N	2.36	0.41
27:X:215:G:H1'	27:X:619:A:H1'	2.03	0.41
27:X:617:U:H5	27:X:632:A:N1	2.19	0.41
27:X:830:C:H3'	27:X:831:G:H8	1.86	0.41
27:X:923:A:N3	27:X:2243:C:H1'	2.36	0.41
27:X:1123:G:C6	27:X:1124:U:N3	2.89	0.41
27:X:1417:C:H2'	27:X:1418:C:C6	2.56	0.41
27:X:1717:A:H5'	27:X:1718:A:OP2	2.20	0.41
27:X:2712:G:H3'	27:X:2713:A:O4'	2.21	0.41
28:Y:32:C:H6	28:Y:32:C:O5'	2.03	0.41
2:B:148:GLY:HA3	27:X:2036:G:C4'	2.51	0.40
3:C:17:LEU:HD12	3:C:17:LEU:HA	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:SER:HB3	3:C:166:TRP:CE3	2.56	0.40
10:K:96:ARG:HB2	27:X:2857:C:H5'	2.03	0.40
12:M:101:ARG:HH22	27:X:1745:C:P	2.43	0.40
17:R:14:LEU:HD23	17:R:14:LEU:HA	1.85	0.40
20:U:28:GLY:HA3	20:U:32:ARG:HG2	2.03	0.40
23:Z:52:TYR:CE1	27:X:2859:U:N3	2.88	0.40
25:2:35:ARG:NH1	27:X:53:G:H1'	2.36	0.40
27:X:877:G:C6	27:X:878:C:N4	2.89	0.40
27:X:1671:A:O4'	27:X:2798:A:H5'	2.21	0.40
27:X:1754:G:OP1	27:X:1754:G:H4'	2.21	0.40
27:X:2220:A:H2'	27:X:2221:G:C8	2.56	0.40
27:X:2288:A:C5	27:X:2289:A:N7	2.89	0.40
27:X:2616:U:H5"	27:X:2617:G:OP2	2.21	0.40
3:C:163:ASN:ND2	3:C:166:TRP:HB2	2.36	0.40
3:C:189:ASP:HB3	3:C:190:ALA:H	1.65	0.40
4:D:35:VAL:HB	4:D:155:THR:OG1	2.21	0.40
6:G:52:GLY:HA3	27:X:1150:C:H5'	2.04	0.40
6:G:139:ARG:HB2	27:X:567:G:OP1	2.21	0.40
7:H:88:THR:O	12:M:79:ARG:HG2	2.22	0.40
8:I:56:LEU:HD22	26:3:52:LYS:NZ	2.37	0.40
9:J:26:ASP:OD1	9:J:28:VAL:N	2.52	0.40
13:N:2:PRO:HD3	27:X:456:C:O5'	2.22	0.40
13:N:52:ASN:O	13:N:55:ARG:N	2.55	0.40
15:P:125:SER:OG	15:P:126:HIS:N	2.53	0.40
18:S:1:MET:HB3	18:S:2:GLU:H	1.70	0.40
18:S:152:ILE:HD11	18:S:168:VAL:HB	2.03	0.40
20:U:10:LYS:HD3	20:U:11:LYS:N	2.37	0.40
20:U:33:LYS:HD3	20:U:33:LYS:HA	1.72	0.40
22:W:47:VAL:HG23	22:W:51:LEU:HD21	2.03	0.40
26:3:15:LYS:HA	26:3:15:LYS:HD3	1.70	0.40
27:X:350:U:H6	27:X:350:U:O5'	2.04	0.40
27:X:825:C:C6	27:X:1263:G:C5	3.10	0.40
27:X:951:G:N3	27:X:1205:G:H4'	2.35	0.40
27:X:1251:G:O2'	27:X:1252:C:H5'	2.21	0.40
27:X:1531:C:H5'	27:X:1532:A:OP1	2.21	0.40
27:X:1882:G:N2	27:X:1886:G:C6	2.89	0.40
27:X:2609:G:H21	27:X:2866:A:H1'	1.85	0.40
28:Y:31:A:N3	28:Y:58:G:N2	2.69	0.40
2:B:37:LYS:HD2	2:B:42:ASP:OD1	2.22	0.40
3:C:84:PHE:CD2	27:X:597:U:H1'	2.57	0.40
3:C:86:PRO:C	3:C:87:LYS:HD2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LYS:O	3:C:185:ARG:N	2.50	0.40
8:I:43:ALA:HB1	27:X:684:C:H41	1.85	0.40
15:P:30:TYR:HB3	15:P:123:ARG:CZ	2.51	0.40
26:3:32:GLN:H	26:3:32:GLN:HG3	1.67	0.40
27:X:45:C:OP2	27:X:192:G:H2'	2.21	0.40
27:X:312:G:O2'	27:X:313:U:H6	2.03	0.40
27:X:494:A:C8	27:X:495:C:C5	3.09	0.40
27:X:538:A:N3	27:X:2025:A:C6	2.89	0.40
27:X:676:G:C6	27:X:677:G:C5	3.10	0.40
27:X:1026:U:H2'	27:X:1027:C:H6	1.86	0.40
27:X:1080:A:N7	27:X:1084:A:N6	2.69	0.40
27:X:1742:G:H2'	27:X:1743:C:C6	2.56	0.40
27:X:1850:G:C1'	27:X:1867:A:H62	2.35	0.40
27:X:2013:A:H4'	27:X:2014:A:H8	1.87	0.40
27:X:2262:C:H2'	27:X:2263:C:O4'	2.21	0.40
27:X:2455:A:N3	27:X:2460:G:N1	2.62	0.40
28:Y:36:A:N6	28:Y:46:G:H2'	2.36	0.40
1:A:222:ARG:NH2	27:X:1819:U:OP2	2.53	0.40
2:B:109:LYS:HE2	2:B:191:ALA:HB2	2.02	0.40
2:B:136:ARG:CZ	2:B:157:ALA:HB2	2.51	0.40
5:E:67:LEU:O	5:E:71:LEU:HG	2.22	0.40
5:E:143:GLN:HE21	27:X:2724:G:H21	1.69	0.40
6:G:111:LYS:HE2	27:X:1142:G:H5"	2.03	0.40
7:H:3:MET:HG2	7:H:44:TYR:CE1	2.57	0.40
8:I:56:LEU:HD21	8:I:59:ARG:NH2	2.35	0.40
10:K:36:THR:OG1	27:X:1291:G:OP1	2.16	0.40
12:M:103:LYS:HD2	12:M:103:LYS:N	2.36	0.40
13:N:13:ARG:NH2	27:X:1264:C:OP1	2.53	0.40
15:P:51:GLN:HE22	23:Z:39:LYS:NZ	2.20	0.40
16:Q:20:MET:HG3	16:Q:25:TYR:CD1	2.57	0.40
20:U:53:GLU:HB2	20:U:56:GLN:O	2.21	0.40
24:1:11:LYS:HE3	24:1:26:LYS:HD3	2.03	0.40
25:2:19:ARG:O	25:2:22:MET:HB3	2.22	0.40
26:3:25:PHE:CD2	26:3:25:PHE:N	2.88	0.40
27:X:192:G:H4'	27:X:193:A:H4'	2.04	0.40
27:X:573:C:H2'	27:X:574:C:O4'	2.21	0.40
27:X:600:G:C6	27:X:602:C:C4	3.09	0.40
27:X:692:C:H2'	27:X:693:A:C8	2.56	0.40
27:X:836:G:C4	27:X:837:U:C5	3.10	0.40
27:X:1354:A:H2'	27:X:1410:U:O2	2.21	0.40
27:X:1473:U:O2	27:X:1474:A:N6	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1773:C:H2'	27:X:2587:G:O2'	2.22	0.40
27:X:2030:U:H2'	27:X:2031:A:C8	2.57	0.40
27:X:2281:C:N4	27:X:2293:G:H1	2.04	0.40
27:X:2533:U:H2'	27:X:2534:U:C6	2.56	0.40
27:X:2609:G:N3	27:X:2866:A:O2'	2.53	0.40
27:X:2827:G:C6	27:X:2828:C:N3	2.90	0.40
28:Y:119:G:C6	28:Y:120:G:C5	3.10	0.40
2:B:114:GLN:C	27:X:1672:A:H4'	2.42	0.40
2:B:147:PRO:HB2	2:B:149:ARG:HG2	2.03	0.40
6:G:131:VAL:O	6:G:134:MET:N	2.41	0.40
9:J:6:LYS:HB2	9:J:7:ARG:H	1.68	0.40
10:K:9:LYS:HE2	27:X:1669:A:OP1	2.22	0.40
10:K:45:ARG:O	10:K:49:GLU:HG3	2.21	0.40
15:P:12:LYS:HA	15:P:15:LYS:HB2	2.04	0.40
15:P:31:VAL:O	15:P:125:SER:HB3	2.21	0.40
17:R:14:LEU:HD13	17:R:16:PHE:CZ	2.57	0.40
18:S:116:VAL:N	18:S:168:VAL:O	2.49	0.40
21:V:18:ILE:HG23	21:V:22:LYS:HE2	2.04	0.40
23:Z:8:LYS:O	27:X:2000:U:H4'	2.21	0.40
27:X:354:C:H2'	27:X:355:G:C8	2.55	0.40
27:X:759:C:C2	30:X:2902:ERY:H371	2.56	0.40
27:X:1174:G:N2	27:X:1175:A:C5	2.89	0.40
27:X:1413:U:H2'	27:X:1414:G:H8	1.87	0.40
27:X:1662:G:O5'	27:X:1662:G:H8	2.04	0.40
27:X:1695:U:H2'	27:X:1696:C:O4'	2.21	0.40
27:X:2212:U:H2'	27:X:2213:G:C8	2.56	0.40
27:X:2528:G:C2	27:X:2529:G:C5	3.09	0.40
27:X:2662:C:C4	27:X:2663:U:C5	3.10	0.40
27:X:2698:G:H2'	27:X:2699:G:O4'	2.21	0.40
27:X:2763:U:H2'	27:X:2764:U:C6	2.51	0.40
27:X:2821:G:H2'	27:X:2822:U:O4'	2.20	0.40
27:X:2825:A:N3	27:X:2825:A:H2'	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/275 (94%)	221 (86%)	34 (13%)	3 (1%)	13	52
2	B	203/211 (96%)	178 (88%)	24 (12%)	1 (0%)	29	68
3	C	192/205 (94%)	164 (85%)	26 (14%)	2 (1%)	15	55
4	D	175/180 (97%)	155 (89%)	19 (11%)	1 (1%)	25	65
5	E	169/185 (91%)	157 (93%)	11 (6%)	1 (1%)	25	65
6	G	140/174 (80%)	127 (91%)	13 (9%)	0	100	100
7	H	132/134 (98%)	120 (91%)	11 (8%)	1 (1%)	19	60
8	I	132/156 (85%)	102 (77%)	26 (20%)	4 (3%)	4	33
9	J	134/141 (95%)	113 (84%)	21 (16%)	0	100	100
10	K	111/116 (96%)	102 (92%)	8 (7%)	1 (1%)	17	58
11	L	102/114 (90%)	86 (84%)	16 (16%)	0	100	100
12	M	106/165 (64%)	99 (93%)	6 (6%)	1 (1%)	17	58
13	N	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	9	45
14	O	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
15	P	128/137 (93%)	109 (85%)	15 (12%)	4 (3%)	4	32
16	Q	91/95 (96%)	76 (84%)	12 (13%)	3 (3%)	4	31
17	R	108/115 (94%)	91 (84%)	16 (15%)	1 (1%)	17	58
18	S	173/237 (73%)	154 (89%)	19 (11%)	0	100	100
19	T	72/91 (79%)	62 (86%)	9 (12%)	1 (1%)	11	48
20	U	70/81 (86%)	52 (74%)	14 (20%)	4 (6%)	1	18
21	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
22	W	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
23	Z	54/60 (90%)	48 (89%)	6 (11%)	0	100	100
24	1	51/55 (93%)	38 (74%)	10 (20%)	3 (6%)	1	17
25	2	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
26	3	57/65 (88%)	46 (81%)	10 (18%)	1 (2%)	8	43
All	All	3025/3379 (90%)	2632 (87%)	359 (12%)	34 (1%)	14	54

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	P	120	ILE
16	Q	6	ILE
16	Q	69	ILE
1	A	24	LEU
1	A	25	THR
13	N	94	VAL
16	Q	59	PRO
24	1	9	ILE
24	1	10	VAL
15	P	125	SER
20	U	60	VAL
5	E	165	VAL
7	H	42	LYS
8	I	39	SER
8	I	103	ASN
15	P	119	ILE
20	U	15	VAL
20	U	39	LYS
10	K	18	VAL
15	P	99	ALA
19	T	19	LYS
24	1	18	THR
2	B	121	ASN
4	D	8	TYR
13	N	8	ILE
17	R	80	LYS
26	3	37	SER
1	A	219	PRO
3	C	15	ILE
12	M	29	PRO
20	U	30	VAL
3	C	22	VAL
8	I	61	PRO
8	I	68	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	202/216 (94%)	163 (81%)	39 (19%)	1 8
2	B	155/157 (99%)	127 (82%)	28 (18%)	1 10
3	C	154/163 (94%)	131 (85%)	23 (15%)	3 19
4	D	153/156 (98%)	140 (92%)	13 (8%)	10 40
5	E	136/144 (94%)	115 (85%)	21 (15%)	2 18
6	G	118/146 (81%)	93 (79%)	25 (21%)	1 6
7	H	103/103 (100%)	88 (85%)	15 (15%)	3 19
8	I	101/121 (84%)	82 (81%)	19 (19%)	1 9
9	J	110/115 (96%)	87 (79%)	23 (21%)	1 7
10	K	90/93 (97%)	70 (78%)	20 (22%)	1 5
11	L	74/82 (90%)	57 (77%)	17 (23%)	1 5
12	M	94/133 (71%)	71 (76%)	23 (24%)	0 4
13	N	96/97 (99%)	81 (84%)	15 (16%)	2 17
14	O	75/79 (95%)	61 (81%)	14 (19%)	1 9
15	P	112/118 (95%)	87 (78%)	25 (22%)	1 5
16	Q	75/76 (99%)	61 (81%)	14 (19%)	1 9
17	R	91/96 (95%)	72 (79%)	19 (21%)	1 7
18	S	149/192 (78%)	135 (91%)	14 (9%)	8 37
19	T	55/67 (82%)	44 (80%)	11 (20%)	1 8
20	U	57/66 (86%)	45 (79%)	12 (21%)	1 7
21	V	53/55 (96%)	46 (87%)	7 (13%)	4 23
22	W	48/48 (100%)	39 (81%)	9 (19%)	1 9
23	Z	50/53 (94%)	44 (88%)	6 (12%)	5 27
24	1	46/48 (96%)	32 (70%)	14 (30%)	0 3
25	2	39/40 (98%)	28 (72%)	11 (28%)	0 3
26	3	46/51 (90%)	36 (78%)	10 (22%)	1 6
All	All	2482/2715 (91%)	2035 (82%)	447 (18%)	1 10

All (447) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	14	ARG
1	A	16	MET

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Mol	Chain	Res	Type
1	A	26	LYS
1	A	34	THR
1	A	40	THR
1	A	43	ARG
1	A	48	ARG
1	A	49	ILE
1	A	53	PHE
1	A	65	ILE
1	A	68	LYS
1	A	84	TYR
1	A	104	TYR
1	A	111	LEU
1	A	118	ASN
1	A	122	GLU
1	A	151	LYS
1	A	157	ARG
1	A	161	THR
1	A	164	GLN
1	A	165	VAL
1	A	186	HIS
1	A	188	GLU
1	A	198	ASN
1	A	201	HIS
1	A	206	LEU
1	A	211	ARG
1	A	214	TRP
1	A	215	LEU
1	A	218	LYS
1	A	220	HIS
1	A	229	VAL
1	A	240	THR
1	A	244	ARG
1	A	247	VAL
1	A	248	THR
1	A	252	LYS
1	A	269	PHE
2	B	9	ILE
2	B	12	THR
2	B	19	ARG
2	B	56	GLU
2	B	66	HIS
2	B	69	LYS

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Mol	Chain	Res	Type
2	B	72	VAL
2	B	79	ARG
2	B	82	ARG
2	B	84	PHE
2	B	87	ASP
2	B	92	ASN
2	B	107	THR
2	B	118	LYS
2	B	119	ARG
2	B	128	SER
2	B	137	ARG
2	B	140	SER
2	B	143	GLN
2	B	150	VAL
2	B	155	ARG
2	B	156	MET
2	B	162	MET
2	B	164	ARG
2	B	173	VAL
2	B	188	ILE
2	B	198	LEU
2	B	199	ARG
3	C	5	ASN
3	C	14	THR
3	C	17	LEU
3	C	24	SER
3	C	31	VAL
3	C	45	THR
3	C	48	ARG
3	C	51	VAL
3	C	52	SER
3	C	62	LYS
3	C	64	THR
3	C	74	VAL
3	C	76	THR
3	C	98	GLN
3	C	116	LYS
3	C	120	VAL
3	C	143	ASP
3	C	150	LEU
3	C	152	THR
3	C	155	GLU

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Mol	Chain	Res	Type
3	C	157	THR
3	C	165	SER
3	C	188	ILE
4	D	46	ASP
4	D	62	LEU
4	D	66	ILE
4	D	67	ILE
4	D	74	ILE
4	D	80	ARG
4	D	90	THR
4	D	112	ARG
4	D	128	TYR
4	D	130	LEU
4	D	143	TYR
4	D	146	VAL
4	D	150	ARG
5	E	20	GLN
5	E	32	GLU
5	E	43	VAL
5	E	44	ARG
5	E	57	ASP
5	E	61	HIS
5	E	70	THR
5	E	86	ASN
5	E	90	ARG
5	E	105	MET
5	E	113	VAL
5	E	116	GLU
5	E	129	THR
5	E	130	ARG
5	E	136	ILE
5	E	155	ASP
5	E	164	PHE
5	E	165	VAL
5	E	167	GLU
5	E	168	GLN
5	E	169	ILE
6	G	31	THR
6	G	32	TYR
6	G	39	GLN
6	G	41	TRP
6	G	56	THR

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Mol	Chain	Res	Type
6	G	61	ARG
6	G	62	ILE
6	G	63	ARG
6	G	67	ARG
6	G	69	ASP
6	G	76	GLN
6	G	83	ILE
6	G	90	LEU
6	G	91	THR
6	G	93	LYS
6	G	99	VAL
6	G	101	THR
6	G	102	ARG
6	G	111	LYS
6	G	116	ARG
6	G	132	PHE
6	G	145	HIS
6	G	150	VAL
6	G	161	GLN
6	G	171	LEU
7	H	23	ARG
7	H	25	LEU
7	H	41	ASN
7	H	47	VAL
7	H	78	SER
7	H	93	ARG
7	H	102	GLN
7	H	104	GLU
7	H	108	THR
7	H	114	VAL
7	H	117	GLU
7	H	119	ARG
7	H	120	ASP
7	H	126	ILE
7	H	127	VAL
8	I	13	ARG
8	I	18	ARG
8	I	21	ARG
8	I	32	ARG
8	I	39	SER
8	I	49	PHE
8	I	50	GLU

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Mol	Chain	Res	Type
8	I	53	ARG
8	I	59	ARG
8	I	60	LEU
8	I	73	GLU
8	I	78	SER
8	I	80	LEU
8	I	88	PHE
8	I	89	ASP
8	I	96	TYR
8	I	103	ASN
8	I	114	ILE
8	I	141	VAL
9	J	6	LYS
9	J	7	ARG
9	J	8	THR
9	J	10	PHE
9	J	11	ARG
9	J	17	ARG
9	J	21	ASP
9	J	27	TYR
9	J	28	VAL
9	J	44	LYS
9	J	54	VAL
9	J	60	ARG
9	J	64	LYS
9	J	68	ARG
9	J	69	ILE
9	J	88	LYS
9	J	93	TYR
9	J	103	VAL
9	J	111	THR
9	J	130	THR
9	J	132	MET
9	J	133	VAL
9	J	135	ARG
10	K	5	LYS
10	K	8	ARG
10	K	9	LYS
10	K	11	ASN
10	K	12	ARG
10	K	14	SER
10	K	17	ARG

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Mol	Chain	Res	Type
10	K	33	ARG
10	K	35	GLN
10	K	48	VAL
10	K	51	LEU
10	K	59	ASP
10	K	64	ARG
10	K	94	TYR
10	K	95	THR
10	K	98	LEU
10	K	99	ARG
10	K	109	THR
10	K	110	MET
10	K	112	LEU
11	L	8	ARG
11	L	11	LEU
11	L	17	VAL
11	L	31	VAL
11	L	33	ARG
11	L	37	HIS
11	L	38	ILE
11	L	39	TYR
11	L	43	ILE
11	L	45	ASP
11	L	59	LEU
11	L	67	THR
11	L	87	VAL
11	L	88	VAL
11	L	91	ARG
11	L	93	SER
11	L	100	VAL
12	M	2	GLN
12	M	5	ILE
12	M	16	ILE
12	M	19	ASP
12	M	21	THR
12	M	22	ARG
12	M	24	LEU
12	M	29	PRO
12	M	31	ASP
12	M	33	VAL
12	M	34	ARG
12	M	37	THR

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Mol	Chain	Res	Type
12	M	39	VAL
12	M	40	ARG
12	M	45	THR
12	M	50	PHE
12	M	72	SER
12	M	79	ARG
12	M	87	LEU
12	M	88	VAL
12	M	91	VAL
12	M	101	ARG
12	M	103	LYS
13	N	3	ARG
13	N	5	LYS
13	N	8	ILE
13	N	11	ARG
13	N	18	LEU
13	N	22	LYS
13	N	28	ARG
13	N	30	LYS
13	N	33	ARG
13	N	37	GLN
13	N	84	LYS
13	N	90	LEU
13	N	93	LYS
13	N	102	GLU
13	N	117	ARG
14	O	12	TYR
14	O	13	ARG
14	O	14	VAL
14	O	21	ARG
14	O	34	GLU
14	O	47	PHE
14	O	67	LYS
14	O	69	ILE
14	O	72	ARG
14	O	76	SER
14	O	81	ARG
14	O	82	ARG
14	O	88	GLN
14	O	91	THR
15	P	9	ARG
15	P	12	LYS

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Mol	Chain	Res	Type
15	P	20	LEU
15	P	21	ARG
15	P	32	ARG
15	P	39	ARG
15	P	43	ASP
15	P	48	LYS
15	P	86	LEU
15	P	88	ASP
15	P	91	PHE
15	P	92	VAL
15	P	93	LYS
15	P	96	TYR
15	P	98	ASP
15	P	102	THR
15	P	103	LEU
15	P	104	LYS
15	P	105	ARG
15	P	106	LEU
15	P	109	ARG
15	P	114	ARG
15	P	122	LYS
15	P	128	THR
15	P	131	VAL
16	Q	5	ASP
16	Q	6	ILE
16	Q	7	LEU
16	Q	12	ILE
16	Q	26	SER
16	Q	27	PHE
16	Q	56	MET
16	Q	58	VAL
16	Q	62	ARG
16	Q	63	LYS
16	Q	67	ARG
16	Q	73	ASN
16	Q	80	VAL
16	Q	84	GLU
17	R	5	SER
17	R	10	HIS
17	R	11	ASN
17	R	18	LYS
17	R	38	LEU

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Mol	Chain	Res	Type
17	R	52	ASN
17	R	53	VAL
17	R	54	ILE
17	R	55	THR
17	R	56	LYS
17	R	62	MET
17	R	64	ASN
17	R	83	LEU
17	R	88	THR
17	R	92	THR
17	R	95	ARG
17	R	97	GLN
17	R	106	VAL
17	R	112	LYS
18	S	25	ASN
18	S	26	LYS
18	S	28	ASN
18	S	34	LEU
18	S	49	THR
18	S	52	PHE
18	S	53	ASP
18	S	71	MET
18	S	79	ILE
18	S	83	PHE
18	S	99	HIS
18	S	120	LEU
18	S	130	ILE
18	S	168	VAL
19	T	14	ARG
19	T	19	LYS
19	T	25	LYS
19	T	41	ARG
19	T	46	LYS
19	T	49	GLN
19	T	55	ARG
19	T	56	ASP
19	T	62	LEU
19	T	64	ASP
19	T	71	ASN
20	U	8	THR
20	U	13	LEU
20	U	19	ILE

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Mol	Chain	Res	Type
20	U	21	ARG
20	U	23	LYS
20	U	32	ARG
20	U	34	THR
20	U	35	THR
20	U	37	ILE
20	U	47	HIS
20	U	63	SER
20	U	70	LEU
21	V	7	ARG
21	V	19	ASP
21	V	25	LEU
21	V	26	MET
21	V	29	ARG
21	V	37	LEU
21	V	42	ARG
22	W	4	LYS
22	W	6	VAL
22	W	9	VAL
22	W	23	LEU
22	W	31	SER
22	W	34	VAL
22	W	37	THR
22	W	45	LYS
22	W	51	LEU
23	Z	6	VAL
23	Z	11	THR
23	Z	25	LEU
23	Z	29	ASN
23	Z	41	LEU
23	Z	44	HIS
24	1	4	ASP
24	1	8	ILE
24	1	20	PHE
24	1	21	TYR
24	1	22	TYR
24	1	26	LYS
24	1	27	ASN
24	1	28	ARG
24	1	36	GLU
24	1	41	ASP
24	1	43	VAL

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Mol	Chain	Res	Type
24	1	47	HIS
24	1	48	VAL
24	1	54	LYS
25	2	3	ARG
25	2	4	THR
25	2	10	ARG
25	2	14	LYS
25	2	19	ARG
25	2	22	MET
25	2	28	ARG
25	2	29	ASN
25	2	40	HIS
25	2	42	LEU
25	2	44	VAL
26	3	6	THR
26	3	11	LYS
26	3	19	THR
26	3	31	HIS
26	3	32	GLN
26	3	36	LYS
26	3	39	ASP
26	3	46	LYS
26	3	55	TRP
26	3	57	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	198	ASN
2	B	35	GLN
2	B	48	GLN
2	B	135	HIS
2	B	169	ASN
3	C	34	GLN
3	C	98	GLN
3	C	112	GLN
3	C	163	ASN
4	D	37	ASN
4	D	129	ASN
4	D	135	GLN
4	D	171	GLN

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Mol	Chain	Res	Type
5	E	61	HIS
5	E	65	HIS
5	E	74	ASN
5	E	106	ASN
5	E	168	GLN
6	G	39	GLN
6	G	76	GLN
6	G	84	ASN
6	G	158	HIS
6	G	161	GLN
7	H	101	ASN
8	I	66	ASN
8	I	79	GLN
8	I	103	ASN
9	J	58	HIS
10	K	3	HIS
10	K	11	ASN
11	L	37	HIS
11	L	86	GLN
12	M	2	GLN
12	M	20	HIS
13	N	37	GLN
13	N	41	ASN
13	N	52	ASN
13	N	63	GLN
13	N	72	HIS
13	N	81	ASN
14	O	88	GLN
15	P	16	GLN
15	P	51	GLN
15	P	78	ASN
15	P	81	HIS
15	P	118	ASN
16	Q	44	GLN
16	Q	57	ASN
16	Q	71	GLN
16	Q	73	ASN
16	Q	94	GLN
17	R	10	HIS
17	R	15	HIS
17	R	32	GLN
17	R	69	GLN

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Mol	Chain	Res	Type
17	R	71	GLN
17	R	97	GLN
18	S	118	HIS
19	T	71	ASN
19	T	85	GLN
21	V	10	GLN
22	W	15	ASN
22	W	49	HIS
23	Z	44	HIS
24	1	32	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	2673/2880 (92%)	638 (23%)	40 (1%)
28	Y	121/124 (97%)	29 (23%)	1 (0%)
All	All	2794/3004 (93%)	667 (23%)	41 (1%)

All (667) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	X	3	U
27	X	4	C
27	X	13	A
27	X	14	A
27	X	17	G
27	X	34	U
27	X	37	C
27	X	39	C
27	X	45	C
27	X	49	U
27	X	50	G
27	X	51	A
27	X	59	G
27	X	60	A
27	X	63	A
27	X	69	G
27	X	70	A
27	X	73	A
27	X	74	G
27	X	83	A

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Mol	Chain	Res	Type
27	X	88	G
27	X	89	A
27	X	90	G
27	X	91	A
27	X	98	U
27	X	100	G
27	X	107	G
27	X	108	G
27	X	116	A
27	X	118	U
27	X	123	A
27	X	124	A
27	X	129	A
27	X	135	U
27	X	136	A
27	X	143	A
27	X	146	C
27	X	151	G
27	X	173	A
27	X	176	A
27	X	178	C
27	X	181	A
27	X	192	G
27	X	193	A
27	X	199	A
27	X	205	A
27	X	206	U
27	X	207	U
27	X	209	G
27	X	210	A
27	X	220	U
27	X	221	A
27	X	222	G
27	X	225	G
27	X	227	G
27	X	229	G
27	X	238	G
27	X	242	A
27	X	243	G
27	X	246	C
27	X	248	A
27	X	304	A

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Mol	Chain	Res	Type
27	X	305	A
27	X	310	A
27	X	312	G
27	X	319	G
27	X	321	A
27	X	322	A
27	X	323	G
27	X	335	A
27	X	340	G
27	X	341	A
27	X	342	G
27	X	343	A
27	X	360	A
27	X	393	U
27	X	399	G
27	X	400	U
27	X	408	U
27	X	409	G
27	X	414	A
27	X	419	G
27	X	421	G
27	X	424	G
27	X	425	A
27	X	429	C
27	X	433	G
27	X	441	A
27	X	453	U
27	X	456	C
27	X	459	A
27	X	463	C
27	X	467	U
27	X	469	G
27	X	490	A
27	X	491	A
27	X	492	G
27	X	493	A
27	X	494	A
27	X	504	G
27	X	514	G
27	X	515	A
27	X	518	A
27	X	519	C

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Mol	Chain	Res	Type
27	X	520	C
27	X	537	C
27	X	538	A
27	X	539	A
27	X	540	G
27	X	541	C
27	X	542	A
27	X	543	G
27	X	554	U
27	X	555	U
27	X	556	A
27	X	557	U
27	X	559	C
27	X	560	G
27	X	564	U
27	X	572	G
27	X	582	G
27	X	584	A
27	X	587	A
27	X	591	G
27	X	595	A
27	X	596	C
27	X	613	A
27	X	614	G
27	X	616	U
27	X	624	A
27	X	625	A
27	X	626	A
27	X	627	A
27	X	628	A
27	X	631	G
27	X	632	A
27	X	633	G
27	X	642	A
27	X	645	G
27	X	648	A
27	X	649	G
27	X	651	C
27	X	654	A
27	X	655	A
27	X	656	U
27	X	657	A

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Mol	Chain	Res	Type
27	X	658	G
27	X	664	C
27	X	665	A
27	X	666	U
27	X	667	U
27	X	668	A
27	X	677	G
27	X	682	G
27	X	690	A
27	X	695	G
27	X	697	G
27	X	699	G
27	X	703	A
27	X	725	C
27	X	729	A
27	X	731	A
27	X	732	G
27	X	743	A
27	X	749	C
27	X	753	U
27	X	759	C
27	X	760	U
27	X	761	G
27	X	766	A
27	X	774	A
27	X	784	U
27	X	789	G
27	X	790	A
27	X	795	A
27	X	797	A
27	X	798	G
27	X	801	A
27	X	802	A
27	X	803	C
27	X	804	C
27	X	805	G
27	X	806	A
27	X	814	G
27	X	818	G
27	X	824	U
27	X	825	C
27	X	830	C

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Mol	Chain	Res	Type
27	X	832	A
27	X	840	U
27	X	841	G
27	X	843	G
27	X	859	U
27	X	872	G
27	X	879	A
27	X	891	A
27	X	914	C
27	X	922	A
27	X	931	G
27	X	938	G
27	X	939	C
27	X	940	G
27	X	943	U
27	X	944	A
27	X	952	A
27	X	956	A
27	X	957	G
27	X	966	A
27	X	967	G
27	X	969	U
27	X	972	C
27	X	973	U
27	X	976	C
27	X	979	A
27	X	985	G
27	X	992	A
27	X	999	A
27	X	1000	G
27	X	1006	C
27	X	1007	A
27	X	1016	C
27	X	1018	C
27	X	1019	U
27	X	1020	A
27	X	1022	A
27	X	1023	U
27	X	1024	G
27	X	1033	G
27	X	1034	U
27	X	1035	G

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Mol	Chain	Res	Type
27	X	1037	U
27	X	1044	U
27	X	1046	U
27	X	1051	U
27	X	1054	C
27	X	1055	A
27	X	1056	U
27	X	1058	G
27	X	1060	C
27	X	1071	U
27	X	1073	G
27	X	1081	A
27	X	1082	G
27	X	1083	C
27	X	1086	C
27	X	1087	C
27	X	1096	A
27	X	1097	A
27	X	1099	A
27	X	1101	U
27	X	1105	U
27	X	1108	U
27	X	1109	A
27	X	1113	C
27	X	1120	C
27	X	1121	G
27	X	1123	G
27	X	1127	C
27	X	1128	G
27	X	1140	A
27	X	1142	G
27	X	1145	C
27	X	1146	G
27	X	1149	G
27	X	1152	C
27	X	1153	A
27	X	1183	C
27	X	1185	C
27	X	1187	A
27	X	1189	G
27	X	1194	U
27	X	1195	U

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Mol	Chain	Res	Type
27	X	1200	G
27	X	1203	A
27	X	1208	A
27	X	1209	G
27	X	1217	U
27	X	1223	G
27	X	1225	G
27	X	1240	G
27	X	1249	G
27	X	1250	A
27	X	1251	G
27	X	1260	A
27	X	1261	G
27	X	1262	U
27	X	1263	G
27	X	1266	G
27	X	1269	G
27	X	1278	A
27	X	1279	G
27	X	1284	G
27	X	1285	A
27	X	1286	U
27	X	1288	A
27	X	1289	A
27	X	1301	U
27	X	1302	C
27	X	1313	U
27	X	1314	A
27	X	1315	A
27	X	1321	A
27	X	1325	U
27	X	1332	G
27	X	1334	A
27	X	1341	G
27	X	1342	U
27	X	1347	C
27	X	1349	A
27	X	1354	A
27	X	1358	C
27	X	1365	U
27	X	1378	A
27	X	1379	A

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Mol	Chain	Res	Type
27	X	1381	G
27	X	1391	A
27	X	1392	U
27	X	1393	G
27	X	1397	A
27	X	1398	G
27	X	1404	C
27	X	1408	A
27	X	1409	U
27	X	1413	U
27	X	1428	G
27	X	1429	A
27	X	1430	G
27	X	1432	G
27	X	1433	A
27	X	1434	U
27	X	1435	G
27	X	1441	A
27	X	1442	C
27	X	1443	G
27	X	1459	U
27	X	1460	G
27	X	1465	G
27	X	1467	U
27	X	1468	A
27	X	1469	U
27	X	1470	G
27	X	1475	U
27	X	1482	U
27	X	1490	U
27	X	1497	C
27	X	1498	G
27	X	1508	G
27	X	1517	C
27	X	1518	C
27	X	1524	C
27	X	1525	A
27	X	1527	G
27	X	1528	C
27	X	1541	G
27	X	1551	U
27	X	1552	C

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Mol	Chain	Res	Type
27	X	1553	G
27	X	1554	G
27	X	1562	G
27	X	1571	G
27	X	1574	A
27	X	1575	C
27	X	1582	A
27	X	1585	A
27	X	1600	U
27	X	1601	U
27	X	1602	G
27	X	1603	A
27	X	1608	U
27	X	1624	A
27	X	1625	A
27	X	1626	A
27	X	1629	G
27	X	1631	C
27	X	1632	A
27	X	1634	A
27	X	1641	C
27	X	1648	C
27	X	1651	U
27	X	1656	U
27	X	1661	C
27	X	1664	G
27	X	1665	C
27	X	1666	G
27	X	1667	A
27	X	1668	G
27	X	1682	A
27	X	1688	U
27	X	1691	G
27	X	1710	U
27	X	1711	C
27	X	1713	G
27	X	1719	G
27	X	1732	U
27	X	1735	G
27	X	1747	G
27	X	1754	G
27	X	1755	G

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Mol	Chain	Res	Type
27	X	1760	G
27	X	1764	A
27	X	1771	A
27	X	1775	A
27	X	1776	A
27	X	1782	A
27	X	1790	G
27	X	1791	C
27	X	1792	C
27	X	1793	A
27	X	1799	A
27	X	1801	C
27	X	1807	A
27	X	1808	C
27	X	1811	A
27	X	1812	U
27	X	1813	A
27	X	1819	U
27	X	1821	A
27	X	1830	C
27	X	1831	G
27	X	1859	A
27	X	1861	G
27	X	1867	A
27	X	1868	A
27	X	1882	G
27	X	1884	A
27	X	1910	A
27	X	1912	G
27	X	1919	A
27	X	1920	A
27	X	1921	A
27	X	1922	U
27	X	1923	U
27	X	1924	C
27	X	1930	C
27	X	1938	U
27	X	1946	U
27	X	1947	G
27	X	1948	C
27	X	1949	A
27	X	1950	C

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Mol	Chain	Res	Type
27	X	1951	G
27	X	1953	A
27	X	1954	A
27	X	1955	G
27	X	1958	G
27	X	1965	U
27	X	1974	U
27	X	1976	U
27	X	1980	A
27	X	2001	G
27	X	2003	A
27	X	2004	U
27	X	2006	G
27	X	2014	A
27	X	2015	G
27	X	2016	A
27	X	2018	G
27	X	2023	C
27	X	2025	A
27	X	2026	C
27	X	2028	C
27	X	2032	G
27	X	2035	G
27	X	2038	C
27	X	2039	G
27	X	2043	A
27	X	2044	G
27	X	2045	A
27	X	2052	G
27	X	2059	U
27	X	2075	U
27	X	2083	G
27	X	2089	C
27	X	2171	U
27	X	2172	U
27	X	2182	A
27	X	2189	A
27	X	2190	A
27	X	2191	A
27	X	2192	U
27	X	2193	C
27	X	2196	U

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Mol	Chain	Res	Type
27	X	2197	U
27	X	2198	U
27	X	2199	C
27	X	2200	G
27	X	2204	A
27	X	2205	C
27	X	2217	G
27	X	2218	G
27	X	2247	A
27	X	2252	A
27	X	2259	G
27	X	2262	C
27	X	2265	A
27	X	2266	A
27	X	2267	A
27	X	2272	A
27	X	2284	U
27	X	2285	U
27	X	2286	G
27	X	2287	G
27	X	2290	A
27	X	2291	U
27	X	2298	U
27	X	2299	A
27	X	2300	G
27	X	2301	A
27	X	2306	A
27	X	2307	A
27	X	2311	U
27	X	2312	A
27	X	2313	G
27	X	2315	A
27	X	2324	G
27	X	2326	C
27	X	2327	U
27	X	2330	G
27	X	2333	A
27	X	2351	G
27	X	2358	C
27	X	2362	G
27	X	2364	C
27	X	2367	A

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Mol	Chain	Res	Type
27	X	2368	G
27	X	2369	U
27	X	2375	G
27	X	2381	A
27	X	2385	U
27	X	2386	G
27	X	2397	A
27	X	2398	U
27	X	2401	A
27	X	2402	U
27	X	2404	A
27	X	2405	A
27	X	2406	C
27	X	2407	G
27	X	2408	G
27	X	2410	U
27	X	2413	A
27	X	2420	C
27	X	2424	G
27	X	2426	G
27	X	2427	A
27	X	2429	A
27	X	2441	U
27	X	2449	G
27	X	2452	U
27	X	2453	C
27	X	2455	A
27	X	2460	G
27	X	2463	G
27	X	2470	U
27	X	2471	U
27	X	2477	C
27	X	2480	C
27	X	2481	G
27	X	2482	A
27	X	2484	G
27	X	2485	U
27	X	2497	A
27	X	2498	U
27	X	2504	G
27	X	2508	G
27	X	2511	G

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Mol	Chain	Res	Type
27	X	2521	A
27	X	2545	A
27	X	2546	G
27	X	2552	C
27	X	2553	G
27	X	2557	G
27	X	2564	U
27	X	2581	A
27	X	2582	G
27	X	2588	U
27	X	2591	C
27	X	2593	A
27	X	2594	U
27	X	2600	A
27	X	2601	C
27	X	2608	A
27	X	2617	G
27	X	2624	G
27	X	2625	U
27	X	2633	A
27	X	2639	A
27	X	2642	G
27	X	2650	G
27	X	2664	G
27	X	2666	U
27	X	2668	U
27	X	2670	C
27	X	2677	U
27	X	2688	G
27	X	2691	C
27	X	2692	A
27	X	2693	U
27	X	2694	G
27	X	2698	G
27	X	2706	U
27	X	2707	G
27	X	2711	G
27	X	2713	A
27	X	2724	G
27	X	2728	A
27	X	2732	C
27	X	2737	A

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Mol	Chain	Res	Type
27	X	2738	A
27	X	2744	A
27	X	2745	A
27	X	2757	G
27	X	2758	A
27	X	2759	U
27	X	2760	G
27	X	2761	A
27	X	2769	C
27	X	2771	C
27	X	2782	G
27	X	2793	G
27	X	2795	A
27	X	2796	A
27	X	2798	A
27	X	2807	U
27	X	2808	U
27	X	2809	A
27	X	2811	G
27	X	2814	G
27	X	2825	A
27	X	2832	G
27	X	2847	G
27	X	2849	C
27	X	2851	G
27	X	2855	C
27	X	2858	A
27	X	2861	A
27	X	2866	A
27	X	2868	G
28	Y	14	C
28	Y	15	A
28	Y	17	A
28	Y	22	U
28	Y	26	G
28	Y	28	A
28	Y	29	C
28	Y	37	C
28	Y	39	C
28	Y	40	C
28	Y	43	G
28	Y	44	C

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Mol	Chain	Res	Type
28	Y	46	G
28	Y	47	A
28	Y	49	C
28	Y	52	G
28	Y	54	U
28	Y	56	G
28	Y	59	A
28	Y	69	G
28	Y	75	A
28	Y	86	A
28	Y	99	G
28	Y	102	A
28	Y	108	G
28	Y	111	C
28	Y	112	A
28	Y	115	G
28	Y	123	U

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	X	38	G
27	X	50	G
27	X	537	C
27	X	538	A
27	X	542	A
27	X	557	U
27	X	760	U
27	X	788	G
27	X	789	G
27	X	956	A
27	X	1019	U
27	X	1053	G
27	X	1059	A
27	X	1096	A
27	X	1141	U
27	X	1182	U
27	X	1250	A
27	X	1313	U
27	X	1391	A
27	X	1441	A
27	X	1496	G

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Mol	Chain	Res	Type
27	X	1607	A
27	X	1625	A
27	X	1664	G
27	X	1810	U
27	X	1919	A
27	X	1923	U
27	X	1975	G
27	X	2204	A
27	X	2299	A
27	X	2312	A
27	X	2363	G
27	X	2404	A
27	X	2409	A
27	X	2452	U
27	X	2705	A
27	X	2736	U
27	X	2756	A
27	X	2824	C
27	X	2846	G
28	Y	58	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 71 ligands modelled in this entry, 70 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	ERY	X	2902	-	53,53,53	0.85	1 (1%)	82,82,82	1.29	7 (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
30	ERY	X	2902	-	-	3/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	X	2902	ERY	O2-C13	2.06	1.50	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	X	2902	ERY	O8-C23-C22	-2.50	103.96	110.05
30	X	2902	ERY	C2-C3-C4	-2.46	105.94	113.05
30	X	2902	ERY	C30-C2-C1	-2.30	103.83	109.02
30	X	2902	ERY	C16-C15-C14	-2.20	111.25	115.07
30	X	2902	ERY	C34-C10-C11	-2.16	111.69	114.38
30	X	2902	ERY	C13-O2-C1	-2.15	114.36	118.18
30	X	2902	ERY	O10-C6-C7	2.09	113.80	108.40

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	X	2902	ERY	C15-C14-O3-C3
30	X	2902	ERY	O4-C14-O3-C3
30	X	2902	ERY	C25-C24-N1-C28

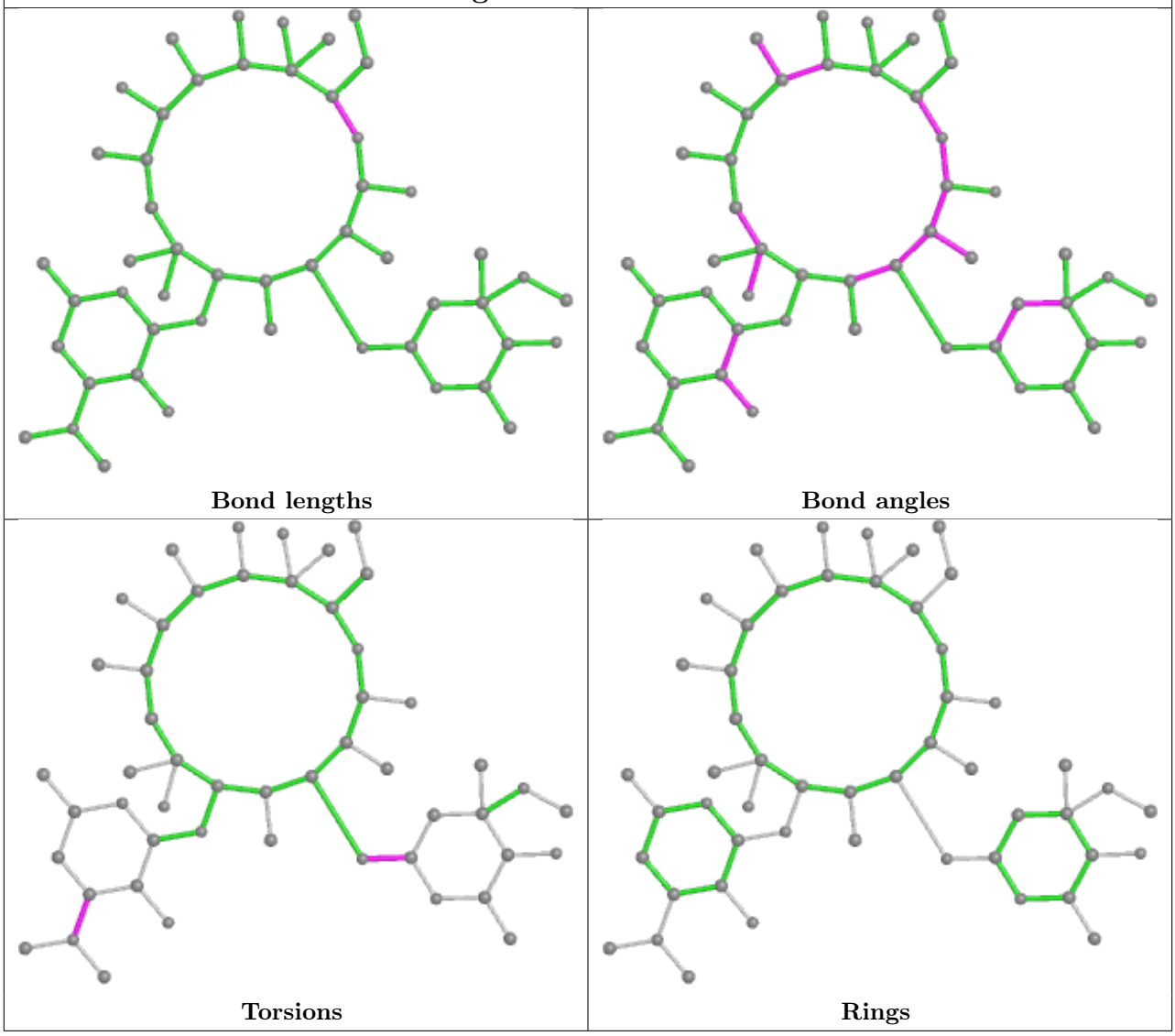
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	X	2902	ERY	9	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 ERY X 2902



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	260/275 (94%)	0.01	4 (1%)	73	61	48, 104, 163, 221	0
2	B	205/211 (97%)	-0.33	5 (2%)	59	45	27, 50, 107, 233	0
3	C	194/205 (94%)	0.02	9 (4%)	32	23	39, 102, 180, 292	0
4	D	177/180 (98%)	0.15	11 (6%)	20	15	114, 175, 232, 282	0
5	E	171/185 (92%)	-0.28	4 (2%)	60	46	57, 131, 192, 243	0
6	G	142/174 (81%)	-0.01	8 (5%)	24	17	38, 77, 160, 339	0
7	H	134/134 (100%)	-0.40	2 (1%)	73	61	33, 45, 87, 135	0
8	I	134/156 (85%)	0.19	4 (2%)	50	37	55, 126, 192, 315	0
9	J	136/141 (96%)	-0.00	4 (2%)	51	38	56, 94, 163, 214	0
10	K	113/116 (97%)	-0.47	0	100	100	27, 32, 67, 100	0
11	L	104/114 (91%)	0.08	6 (5%)	23	16	130, 161, 200, 243	0
12	M	108/165 (65%)	-0.48	0	100	100	30, 43, 95, 242	0
13	N	117/118 (99%)	-0.20	2 (1%)	70	57	41, 76, 133, 232	0
14	O	94/100 (94%)	-0.26	4 (4%)	35	25	52, 94, 178, 204	0
15	P	130/137 (94%)	-0.40	0	100	100	33, 51, 147, 188	0
16	Q	93/95 (97%)	-0.39	1 (1%)	80	69	49, 94, 162, 192	0
17	R	110/115 (95%)	0.02	3 (2%)	54	41	65, 100, 189, 259	0
18	S	175/237 (73%)	0.39	20 (11%)	5	5	93, 144, 224, 285	0
19	T	74/91 (81%)	0.11	5 (6%)	17	13	72, 112, 158, 228	0
20	U	72/81 (88%)	0.37	4 (5%)	24	17	75, 119, 185, 238	0
21	V	65/67 (97%)	-0.26	2 (3%)	49	36	76, 115, 164, 208	0
22	W	55/55 (100%)	0.10	0	100	100	72, 91, 128, 190	0
23	Z	56/60 (93%)	-0.42	0	100	100	32, 40, 80, 152	0
24	1	53/55 (96%)	0.42	5 (9%)	8	6	102, 129, 217, 266	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
25	2	46/47 (97%)	0.11	1 (2%)	62	48	38, 67, 122, 169	0
26	3	59/65 (90%)	0.42	5 (8%)	10	9	80, 100, 172, 278	0
27	X	2680/2880 (93%)	-0.13	84 (3%)	49	36	26, 76, 186, 299	0
28	Y	122/124 (98%)	-0.09	4 (3%)	46	34	74, 153, 190, 332	0
All	All	5879/6383 (92%)	-0.10	197 (3%)	45	33	26, 89, 188, 339	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	S	15	ASP	7.4
27	X	1072	U	7.1
18	S	23	ALA	7.1
18	S	22	VAL	7.0
27	X	731	A	6.6
27	X	1071	U	6.2
4	D	153	ASP	6.0
27	X	1913	G	5.8
28	Y	123	U	5.7
20	U	28	GLY	5.6
27	X	1086	C	5.6
27	X	1073	G	5.5
27	X	1099	A	5.5
3	C	44	SER	5.2
27	X	1060	C	5.2
27	X	1070	G	5.1
4	D	43	SER	5.1
4	D	134	GLU	4.7
20	U	27	ASP	4.6
27	X	1115	C	4.6
18	S	14	LEU	4.6
11	L	52	ALA	4.4
3	C	19	LEU	4.4
20	U	26	ALA	4.4
4	D	23	SER	4.3
27	X	1069	G	4.3
9	J	84	MET	4.3
27	X	1954	A	4.3
24	1	35	LEU	4.1
8	I	75	VAL	4.1
25	2	1	MET	4.0
8	I	74	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
27	X	728	G	4.0
27	X	1188	A	3.9
1	A	236	GLY	3.8
17	R	83	LEU	3.8
27	X	1055	A	3.8
3	C	47	THR	3.8
27	X	2444	C	3.8
6	G	97	ASP	3.6
27	X	1090	C	3.5
11	L	53	ALA	3.5
18	S	68	ALA	3.5
27	X	200	A	3.5
27	X	424	G	3.5
27	X	1068	A	3.5
26	3	38	GLY	3.5
6	G	129	HIS	3.5
27	X	1912	G	3.4
27	X	1085	G	3.4
27	X	727	U	3.4
4	D	22	TYR	3.4
14	O	47	PHE	3.3
14	O	23	GLU	3.3
27	X	2287	G	3.3
27	X	1114	A	3.3
27	X	730	C	3.3
27	X	2082	C	3.2
18	S	83	PHE	3.2
4	D	75	SER	3.2
24	1	27	ASN	3.2
28	Y	68	A	3.2
27	X	75	C	3.1
27	X	1098	G	3.1
11	L	40	ALA	3.1
27	X	1951	G	3.1
4	D	42	SER	3.1
18	S	171	VAL	3.1
27	X	426	C	3.0
17	R	102	LYS	3.0
19	T	16	SER	3.0
5	E	174	GLY	3.0
19	T	15	ASP	3.0
27	X	425	A	3.0

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Mol	Chain	Res	Type	RSRZ
18	S	21	ALA	3.0
27	X	1091	C	3.0
27	X	2171	U	3.0
27	X	2731	G	3.0
18	S	91	PRO	2.9
18	S	92	VAL	2.9
5	E	175	LYS	2.9
27	X	1059	A	2.9
9	J	79	PRO	2.9
18	S	32	PHE	2.9
27	X	1087	C	2.9
19	T	73	GLY	2.9
8	I	54	SER	2.9
1	A	237	GLU	2.9
27	X	2090	U	2.9
27	X	420	C	2.8
27	X	1524	C	2.8
3	C	91	TYR	2.8
27	X	1104	G	2.8
4	D	25	VAL	2.8
4	D	132	ILE	2.8
18	S	30	VAL	2.8
19	T	14	ARG	2.8
2	B	136	ARG	2.8
27	X	1950	C	2.8
18	S	86	VAL	2.7
20	U	29	GLY	2.7
11	L	39	TYR	2.7
18	S	124	ALA	2.7
11	L	33	ARG	2.7
27	X	248	A	2.7
6	G	159	SER	2.7
28	Y	6	C	2.7
27	X	2381	A	2.6
27	X	74	G	2.6
27	X	2089	C	2.6
27	X	1186	G	2.6
26	3	55	TRP	2.6
17	R	55	THR	2.5
2	B	205	SER	2.5
27	X	2359	U	2.5
24	1	40	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
27	X	435	A	2.5
27	X	1187	A	2.5
27	X	1089	C	2.4
27	X	361	G	2.4
27	X	1062	G	2.4
27	X	2270	U	2.4
18	S	82	ASP	2.4
27	X	1067	G	2.4
13	N	91	ASN	2.4
14	O	11	GLN	2.4
4	D	152	MET	2.4
3	C	20	PRO	2.4
3	C	166	TRP	2.4
6	G	168	THR	2.4
27	X	434	C	2.4
27	X	2290	A	2.4
9	J	77	LYS	2.4
18	S	114	ASP	2.4
27	X	2083	G	2.4
21	V	48	ARG	2.4
26	3	37	SER	2.4
1	A	220	HIS	2.4
6	G	156	HIS	2.4
27	X	1846	A	2.4
27	X	225	G	2.3
27	X	2289	A	2.3
27	X	1888	C	2.3
3	C	81	GLY	2.3
9	J	78	LYS	2.3
27	X	1432	G	2.3
27	X	1955	G	2.3
27	X	1190	C	2.3
18	S	54	ILE	2.3
5	E	173	ALA	2.3
27	X	1074	G	2.3
27	X	1483	G	2.3
24	1	14	SER	2.3
7	H	19	ILE	2.3
27	X	2037	A	2.2
28	Y	2	C	2.2
26	3	39	ASP	2.2
27	X	2390	A	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	203	LYS	2.2
11	L	54	ALA	2.2
2	B	34	VAL	2.2
26	3	63	PRO	2.2
8	I	76	LYS	2.2
3	C	45	THR	2.2
27	X	1515	U	2.2
5	E	64	LEU	2.2
27	X	2170	C	2.2
27	X	1847	G	2.2
4	D	154	ILE	2.2
27	X	729	A	2.2
27	X	1887	G	2.2
18	S	69	VAL	2.2
27	X	1919	A	2.1
27	X	1390	G	2.1
3	C	193	LEU	2.1
6	G	66	HIS	2.1
13	N	92	ARG	2.1
27	X	1593	C	2.1
6	G	105	GLY	2.1
2	B	135	HIS	2.1
27	X	1588	A	2.1
18	S	143	ILE	2.1
6	G	44	VAL	2.1
27	X	423	G	2.1
24	1	4	ASP	2.1
19	T	17	ASN	2.1
27	X	1801	C	2.1
27	X	1084	A	2.1
27	X	2340	C	2.0
18	S	31	SER	2.0
7	H	8	LEU	2.0
27	X	2385	U	2.0
1	A	249	PRO	2.0
21	V	52	GLN	2.0
27	X	2173	G	2.0
16	Q	15	LYS	2.0
14	O	46	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MG	K	202	1/1	0.77	0.83	27,27,27,27	0
29	MG	B	301	1/1	0.79	0.78	34,34,34,34	0
29	MG	X	2930	1/1	0.80	0.99	29,29,29,29	0
29	MG	X	2919	1/1	0.82	0.10	62,62,62,62	0
29	MG	X	2958	1/1	0.82	0.48	44,44,44,44	0
29	MG	X	2915	1/1	0.83	0.17	63,63,63,63	0
29	MG	X	2906	1/1	0.85	0.85	28,28,28,28	0
29	MG	X	2933	1/1	0.86	0.65	36,36,36,36	0
29	MG	K	201	1/1	0.86	0.49	27,27,27,27	0
29	MG	X	2931	1/1	0.87	0.57	46,46,46,46	0
29	MG	X	2907	1/1	0.90	0.77	28,28,28,28	0
29	MG	X	2963	1/1	0.90	0.31	56,56,56,56	0
29	MG	X	2925	1/1	0.91	1.04	31,31,31,31	0
29	MG	X	2946	1/1	0.91	0.19	46,46,46,46	0
29	MG	X	2952	1/1	0.91	0.44	29,29,29,29	0
29	MG	X	2917	1/1	0.91	0.86	40,40,40,40	0
29	MG	X	2911	1/1	0.91	0.53	56,56,56,56	0
29	MG	X	2965	1/1	0.91	0.91	43,43,43,43	0
29	MG	X	2960	1/1	0.92	0.32	61,61,61,61	0
29	MG	X	2943	1/1	0.92	0.95	42,42,42,42	0
29	MG	X	2951	1/1	0.92	0.76	32,32,32,32	0
29	MG	X	2957	1/1	0.93	0.85	52,52,52,52	0
29	MG	X	2916	1/1	0.93	0.87	41,41,41,41	0
29	MG	A	301	1/1	0.93	0.39	54,54,54,54	0
29	MG	X	2961	1/1	0.93	1.07	56,56,56,56	0
29	MG	X	2926	1/1	0.93	0.91	44,44,44,44	0
29	MG	X	2964	1/1	0.93	0.90	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MG	X	2939	1/1	0.93	0.60	50,50,50,50	0
29	MG	X	2956	1/1	0.94	0.52	27,27,27,27	0
29	MG	X	2962	1/1	0.94	0.13	69,69,69,69	0
29	MG	X	2901	1/1	0.94	0.39	69,69,69,69	0
29	MG	X	2923	1/1	0.94	0.40	40,40,40,40	0
29	MG	X	2908	1/1	0.94	0.61	32,32,32,32	0
30	ERY	X	2902	51/51	0.94	0.23	31,34,36,36	0
29	MG	X	2904	1/1	0.95	0.56	32,32,32,32	0
29	MG	X	2927	1/1	0.95	0.34	29,29,29,29	0
29	MG	X	2921	1/1	0.95	0.34	28,28,28,28	0
29	MG	X	2950	1/1	0.95	0.40	32,32,32,32	0
29	MG	X	2905	1/1	0.95	0.50	31,31,31,31	0
29	MG	X	2903	1/1	0.95	0.66	30,30,30,30	0
29	MG	X	2934	1/1	0.95	0.25	29,29,29,29	0
29	MG	X	2937	1/1	0.95	0.69	44,44,44,44	0
29	MG	X	2948	1/1	0.96	0.28	34,34,34,34	0
29	MG	X	2936	1/1	0.96	0.65	45,45,45,45	0
29	MG	X	2913	1/1	0.96	0.46	43,43,43,43	0
29	MG	X	2910	1/1	0.96	0.64	56,56,56,56	0
29	MG	X	2920	1/1	0.96	0.46	52,52,52,52	0
29	MG	X	2912	1/1	0.96	0.14	27,27,27,27	0
29	MG	X	2947	1/1	0.96	0.26	34,34,34,34	0
29	MG	X	2955	1/1	0.97	0.48	30,30,30,30	0
29	MG	X	2922	1/1	0.97	0.34	29,29,29,29	0
29	MG	X	2944	1/1	0.97	0.41	35,35,35,35	0
29	MG	X	2945	1/1	0.97	0.14	38,38,38,38	0
29	MG	X	2959	1/1	0.97	0.64	41,41,41,41	0
29	MG	X	2935	1/1	0.97	0.47	34,34,34,34	0
29	MG	M	201	1/1	0.97	0.35	35,35,35,35	0
29	MG	X	2909	1/1	0.97	0.45	28,28,28,28	0
29	MG	M	202	1/1	0.97	0.35	35,35,35,35	0
29	MG	X	2941	1/1	0.97	0.46	38,38,38,38	0
29	MG	X	2942	1/1	0.97	0.66	46,46,46,46	0
29	MG	X	2954	1/1	0.97	0.44	45,45,45,45	0
29	MG	X	2918	1/1	0.98	0.80	43,43,43,43	0
29	MG	X	2940	1/1	0.98	0.36	36,36,36,36	0
29	MG	X	2928	1/1	0.98	0.39	55,55,55,55	0
29	MG	X	2932	1/1	0.98	0.40	37,37,37,37	0
29	MG	X	2949	1/1	0.98	0.44	42,42,42,42	0
29	MG	X	2929	1/1	0.98	0.14	30,30,30,30	0
29	MG	X	2938	1/1	0.98	0.79	31,31,31,31	0
29	MG	X	2924	1/1	0.99	0.22	38,38,38,38	0

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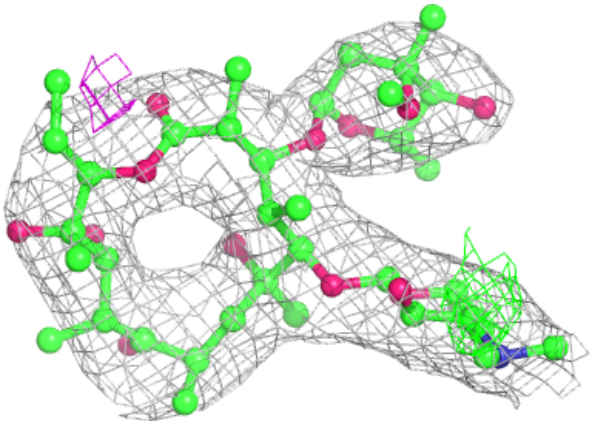
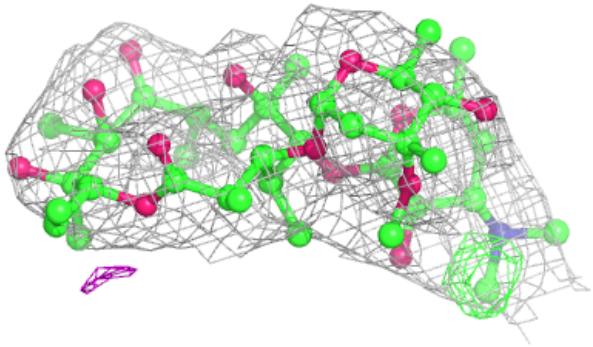
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MG	X	2953	1/1	0.99	0.39	56,56,56,56	0
29	MG	X	2914	1/1	0.99	0.57	27,27,27,27	0

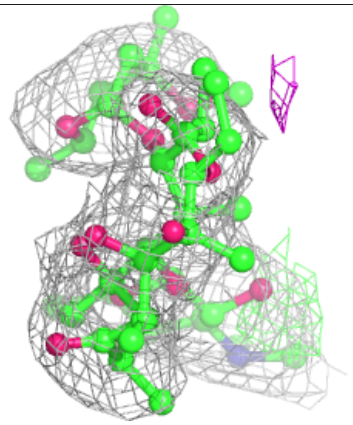
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ERY X 2902:

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 (i)

There are no such residues in this entry.