Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 05:09 pm GMT

PDB ID	:	5JVH
Title	:	The crystal structure large ribosomal subunit (50S) of Deinococcus radiodurans in complex with evernimicin
Authors	:	Yonath, A.
Deposited on	:	2016-05-11
Resolution	:	3.58 Å(reported)

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

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

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

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

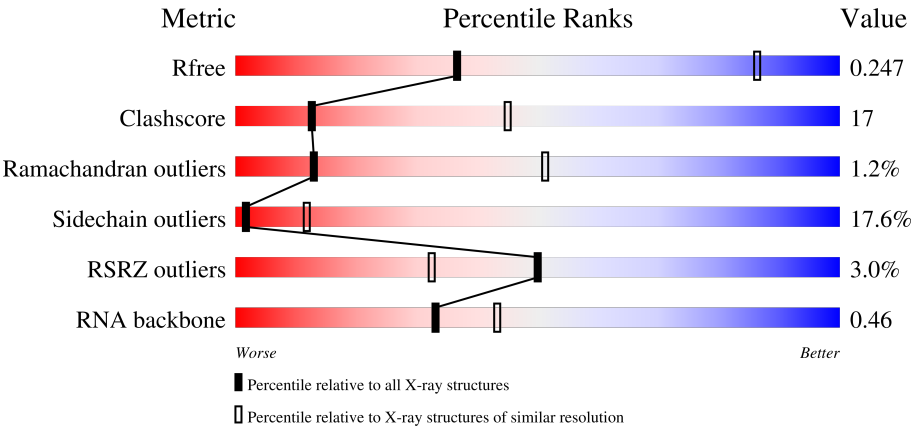
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.58 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	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)
RNA backbone	3102	1008 (4.10-3.00)

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	X	2880	3% 36% 40% 14% • 8%
2	Y	123	2% 46% 41% 11% •
3	A	275	% 40% 45% 9% 6%
4	B	211	53% 38% 6% • •

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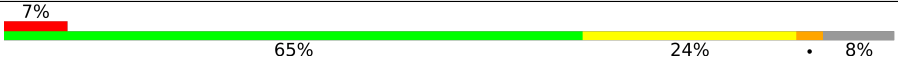
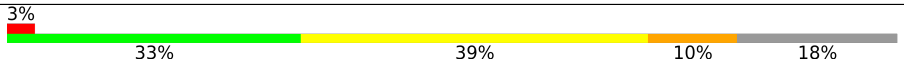
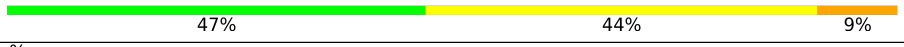
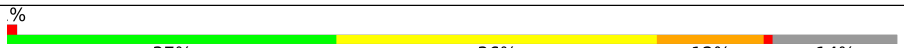
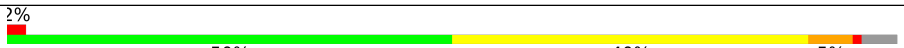
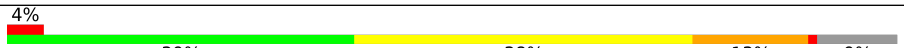
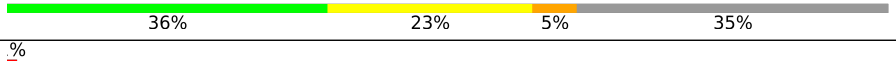
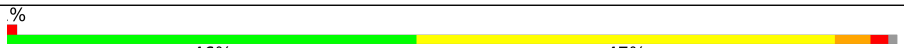
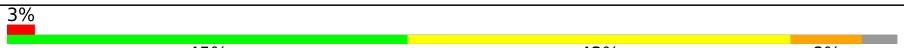
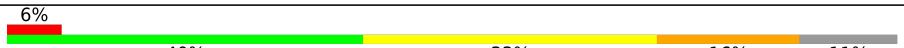
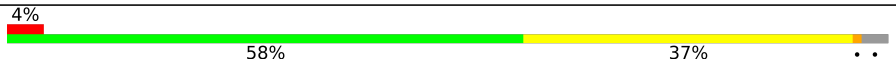
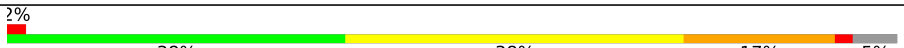
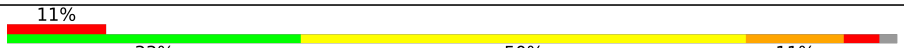
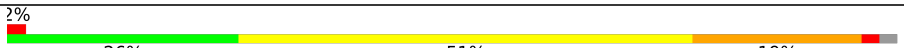
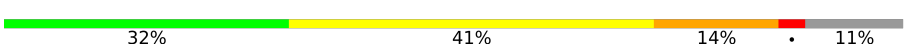
Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	G	174	
9	H	134	
10	I	156	
11	J	141	
12	K	116	
13	L	114	
14	M	166	
15	N	118	
16	O	100	
17	P	134	
18	Q	95	
19	R	115	
20	S	237	
21	T	91	
22	U	81	
23	V	67	
24	W	55	
25	Z	60	
26	1	54	
27	2	47	
28	3	66	

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
30	MG	X	2927	-	-	-	X
30	MG	X	2960	-	-	-	X
30	MG	X	3001	-	-	-	X
30	MG	X	3006	-	-	-	X
30	MG	X	3016	-	-	-	X
30	MG	X	3020	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 83681 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	2658	57052	25450	10532	18413	2657	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	C	conflict	GB 1026245073

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	259	1973	1226	395	349	3	0	0	0

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called 50S ribosomal protein L13.

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

- Molecule 9 is a protein called 50S ribosomal protein L14.

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

- Molecule 10 is a protein called 50S ribosomal protein L15.

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

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1078	690	196	185	7			

- Molecule 12 is a protein called 50S ribosomal protein L17.

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

- Molecule 13 is a protein called 50S ribosomal protein L18.

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

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	108	Total 859	C 537	N 166	O 156	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

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

- Molecule 16 is a protein called 50S ribosomal protein L21.

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

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	127	Total 1014	C 639	N 199	O 174	S 2	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

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

- Molecule 19 is a protein called 50S ribosomal protein L24.

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

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	179	Total	C	N	O	S	0	0	0
			1374	867	240	261	6			

- Molecule 21 is a protein called 50S ribosomal protein L27.

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

- Molecule 22 is a protein called 50S ribosomal protein L28.

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

- Molecule 23 is a protein called 50S ribosomal protein L29.

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

- Molecule 24 is a protein called 50S ribosomal protein L30.

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

- Molecule 25 is a protein called 50S ribosomal protein L32.

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

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	53	Total	C	N	O	S	0	0	0
			427	271	79	76	1			

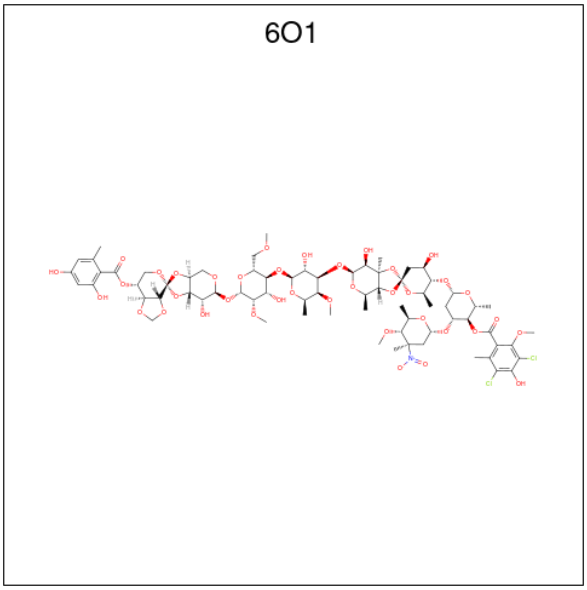
- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- Molecule 29 is Evernimicin (three-letter code: 6O1) (formula: $C_{70}H_{97}Cl_2NO_{38}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	Cl	N	O	0	0
			111	70	2	1	38		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

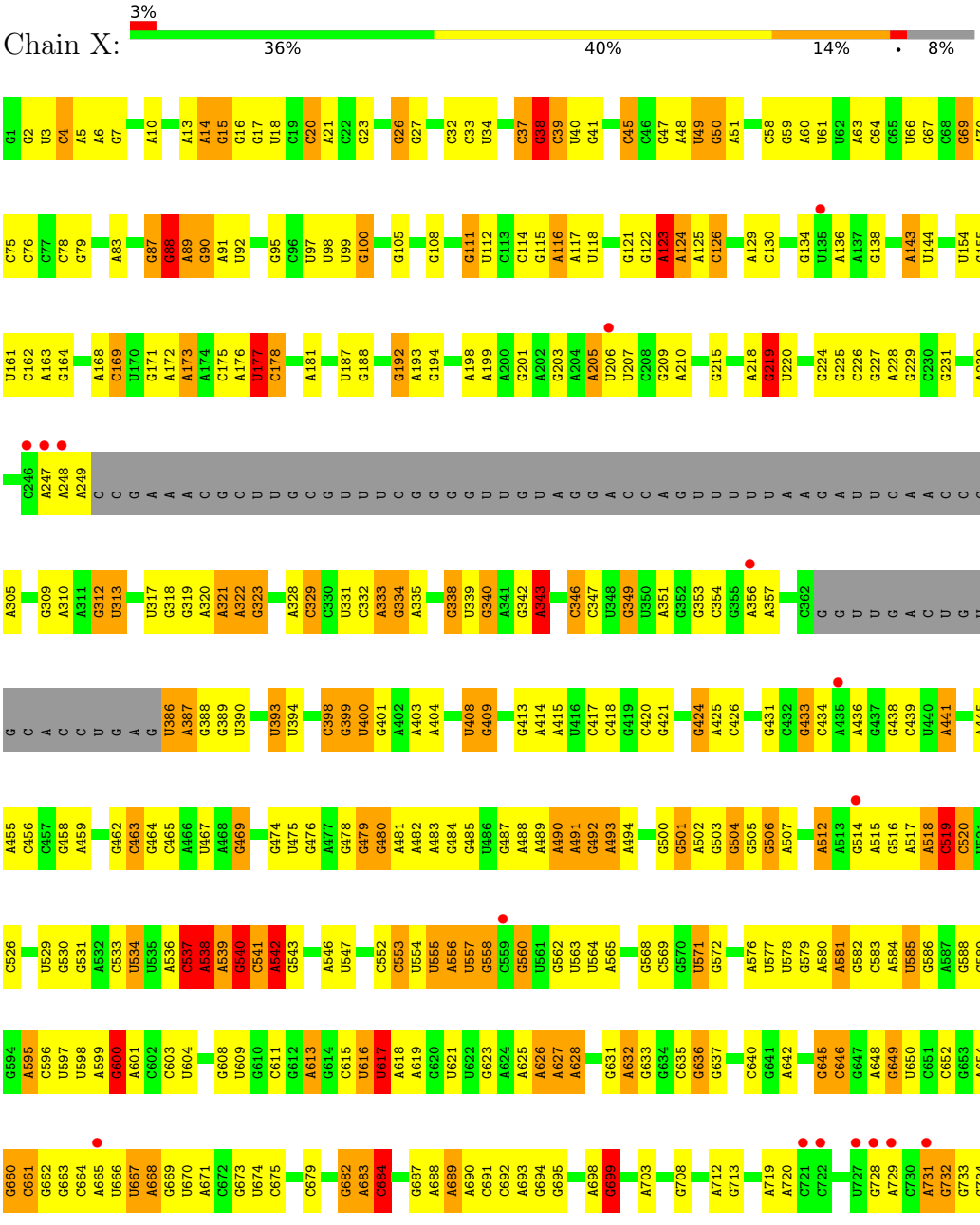
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	119	Total	Mg	0	0
			119	119		
30	Y	1	Total	Mg	0	0
			1	1		
30	K	2	Total	Mg	0	0
			2	2		
30	M	1	Total	Mg	0	0
			1	1		

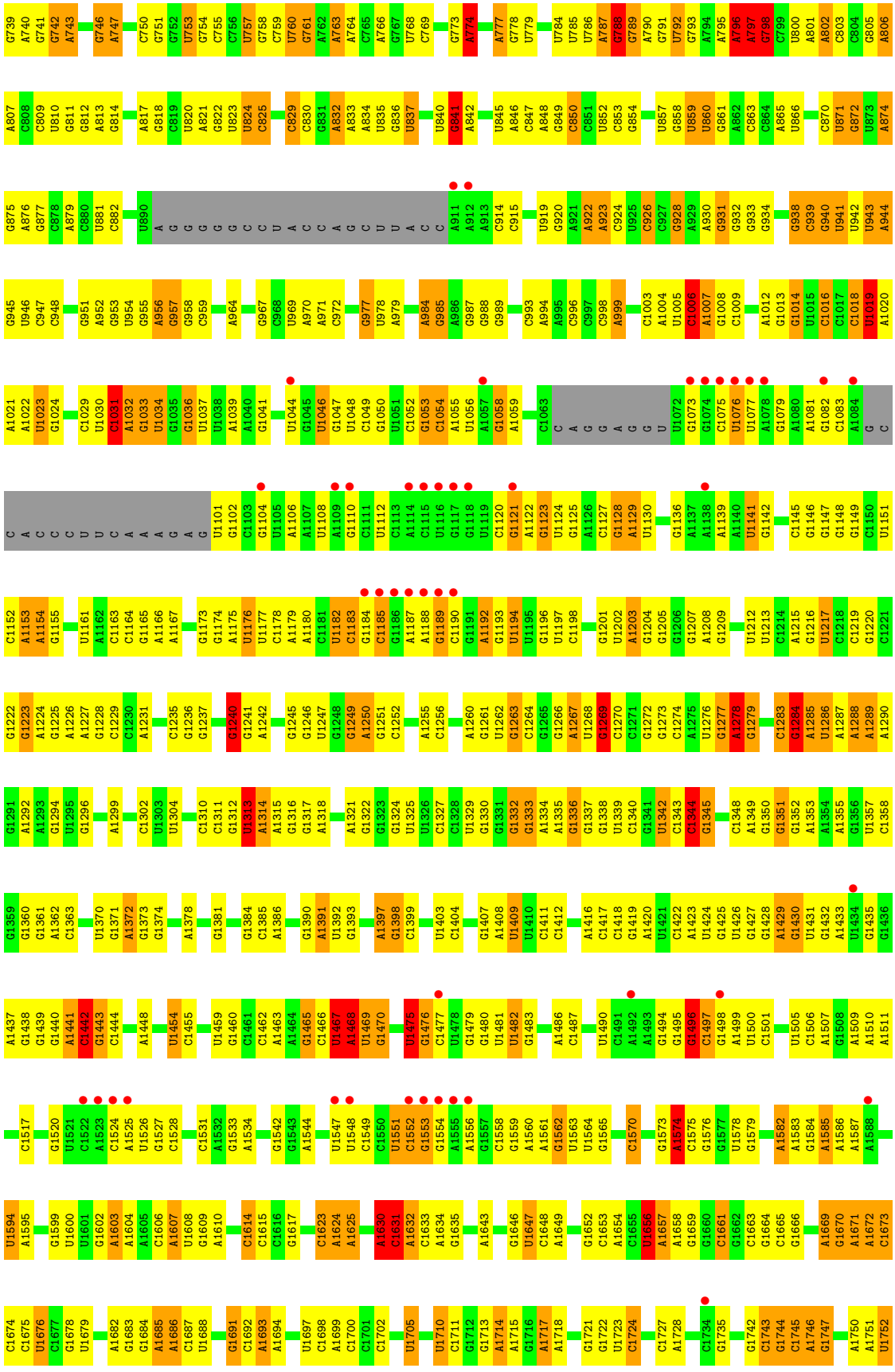
3 Residue-property plots (i)

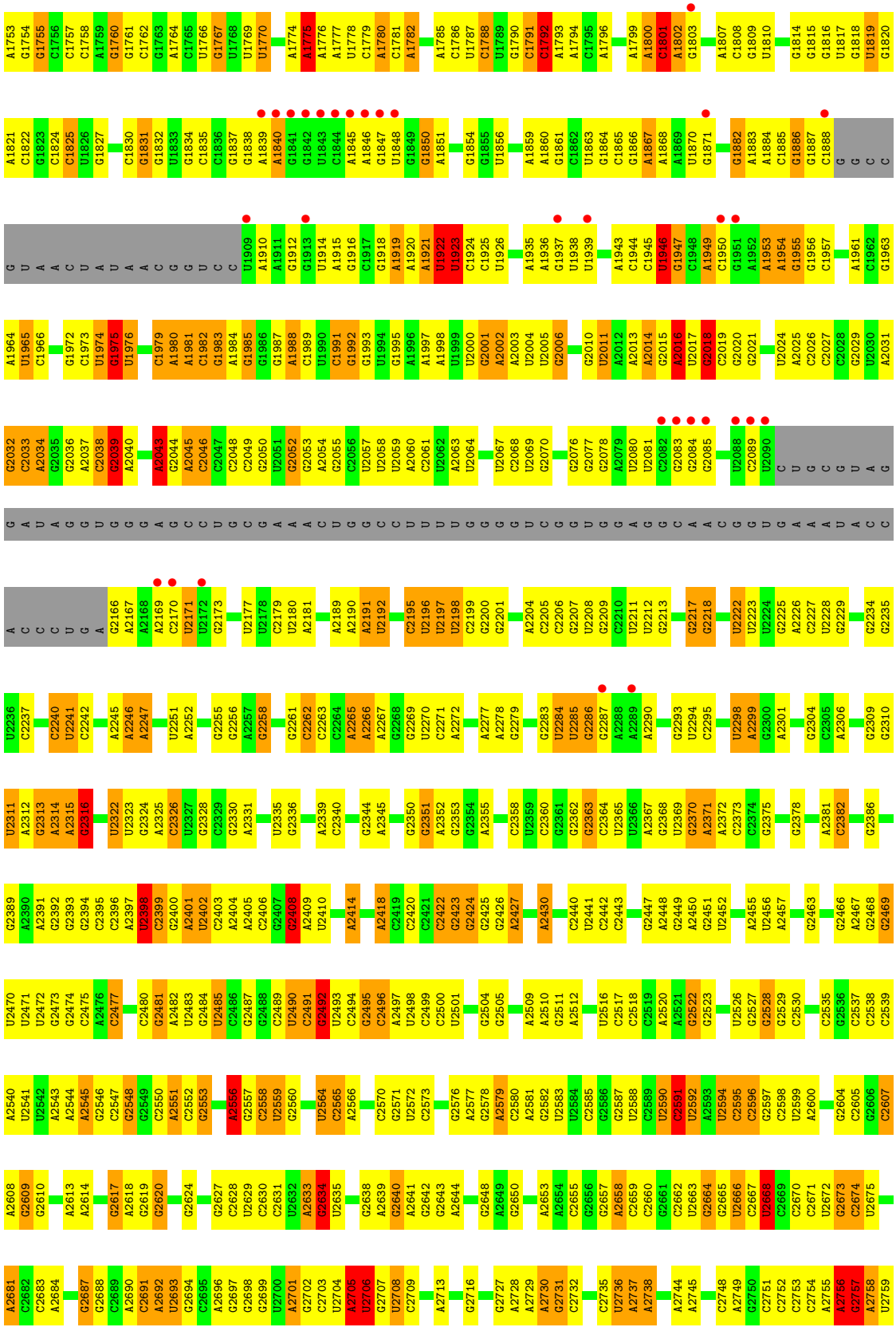
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

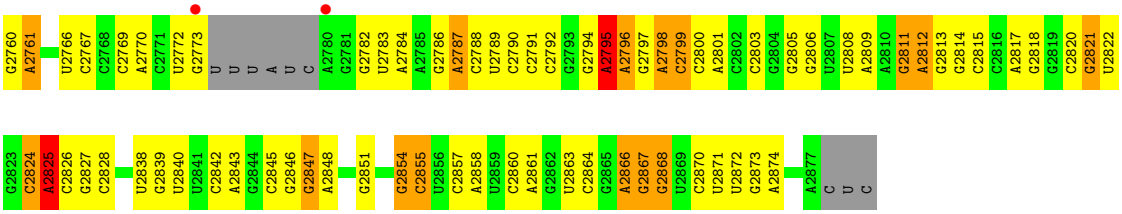
- Molecule 1: 23S ribosomal RNA

Chain X:



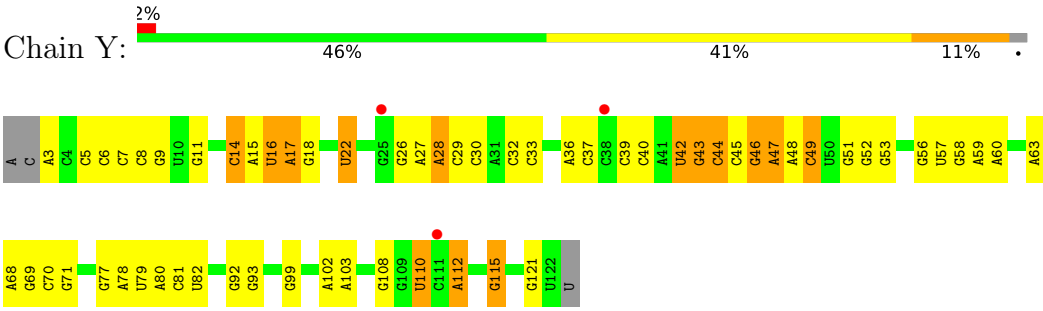






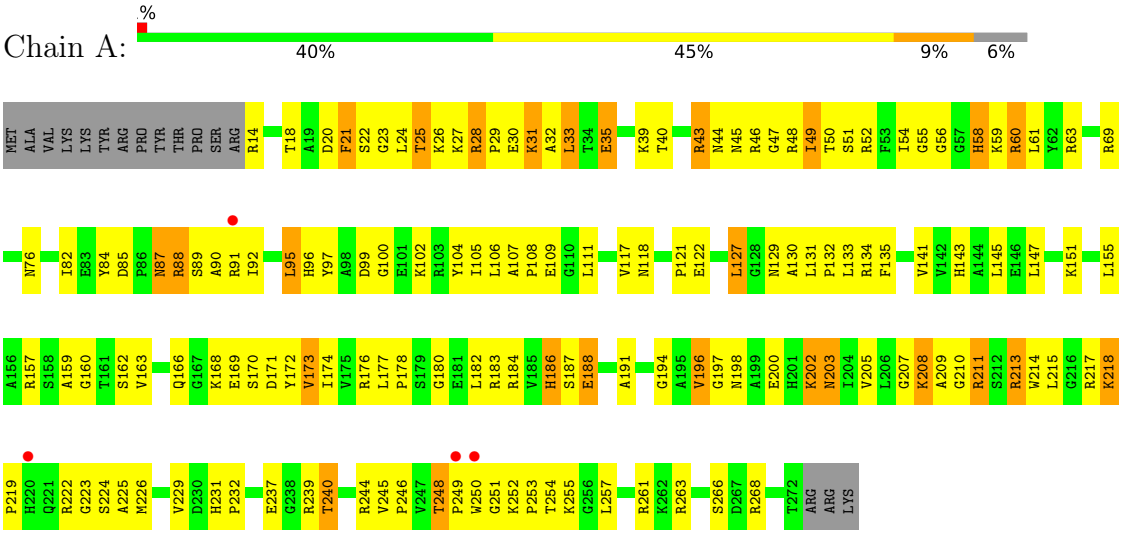
• Molecule 2: 5S ribosomal RNA

Chain Y:



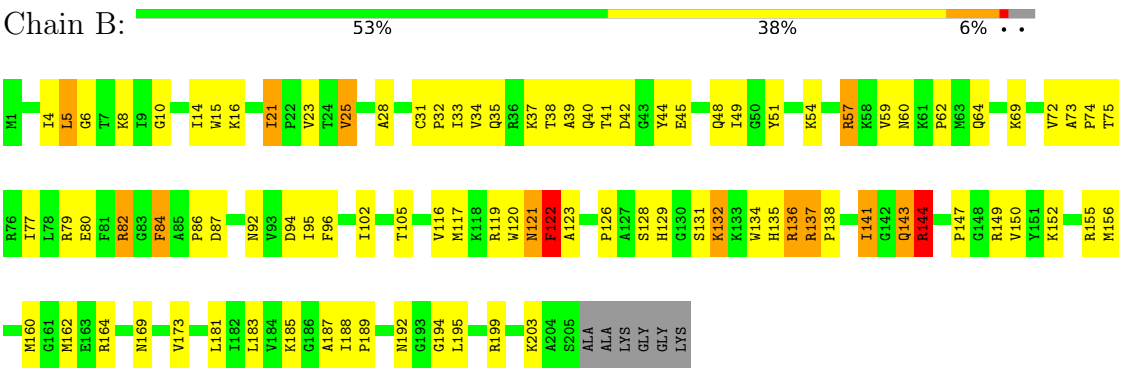
• Molecule 3: 50S ribosomal protein L2

Chain A:



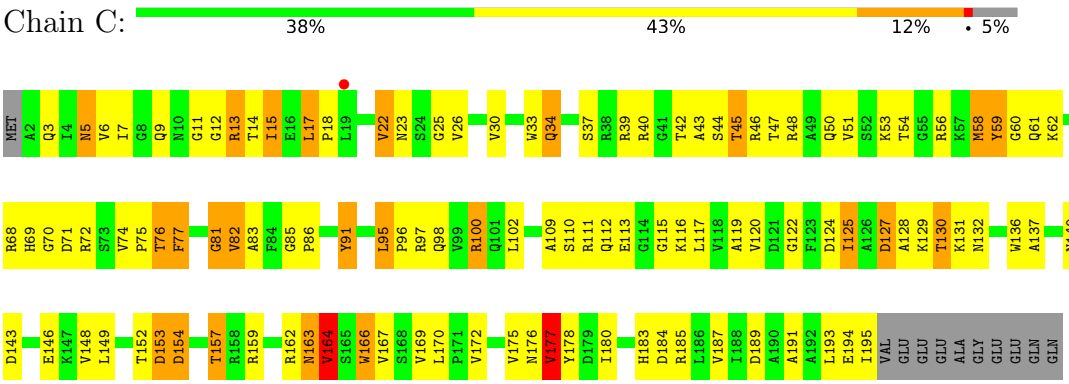
• Molecule 4: 50S ribosomal protein L3

Chain B:



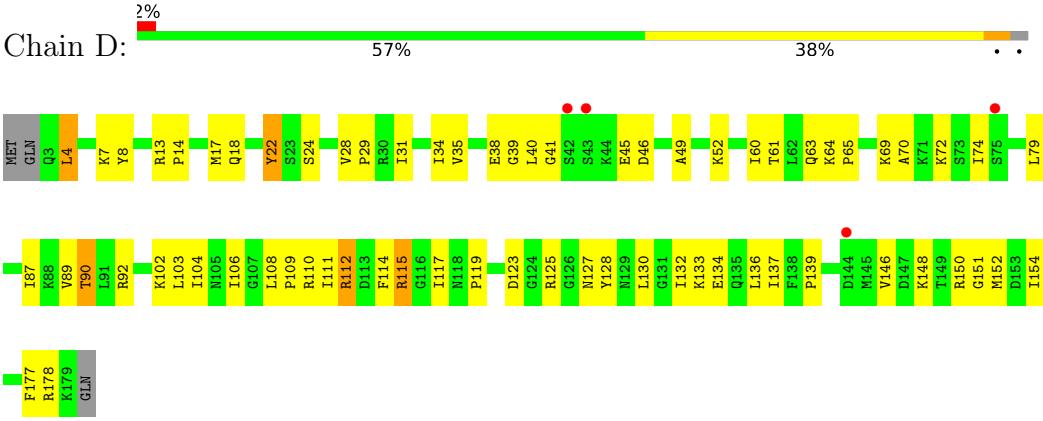
• Molecule 5: 50S ribosomal protein L4

Chain C:



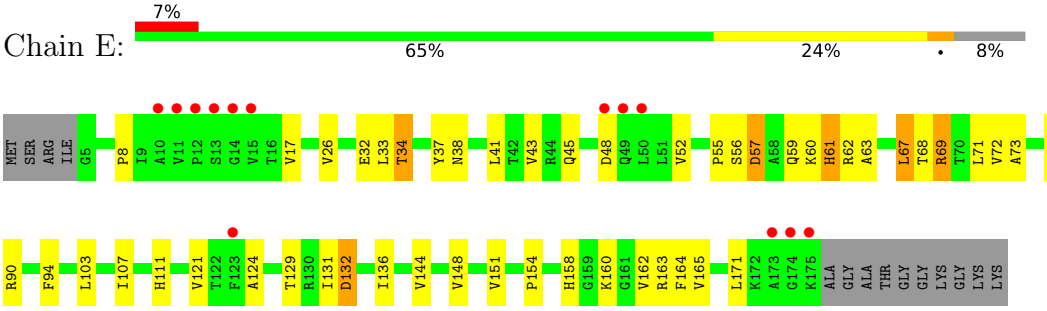
• Molecule 6: 50S ribosomal protein L5

Chain D:



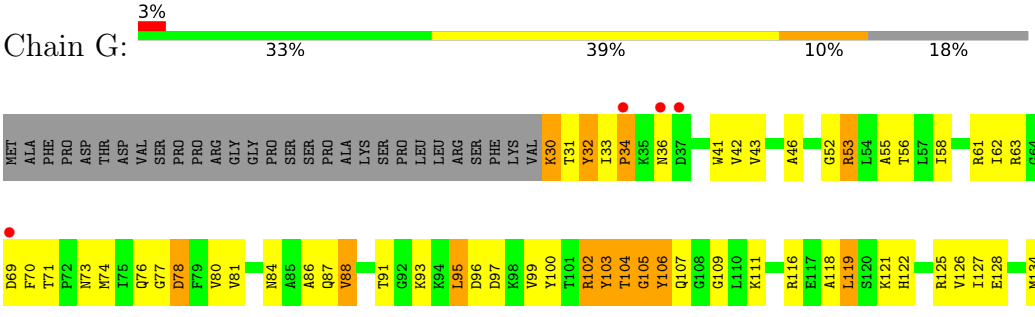
• Molecule 7: 50S ribosomal protein L6

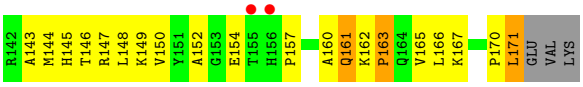
Chain E:



• Molecule 8: 50S ribosomal protein L13

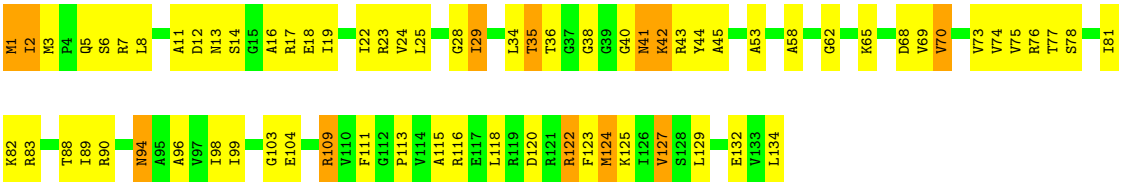
Chain G:





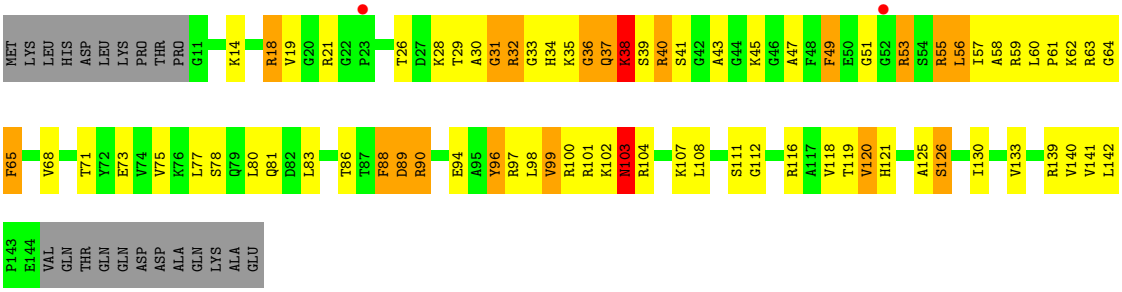
• Molecule 9: 50S ribosomal protein L14

Chain H:



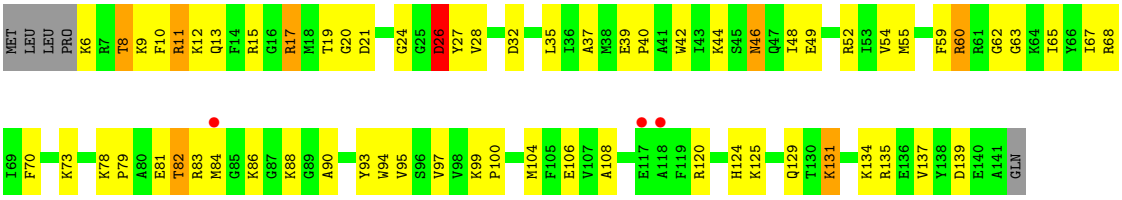
• Molecule 10: 50S ribosomal protein L15

Chain I:



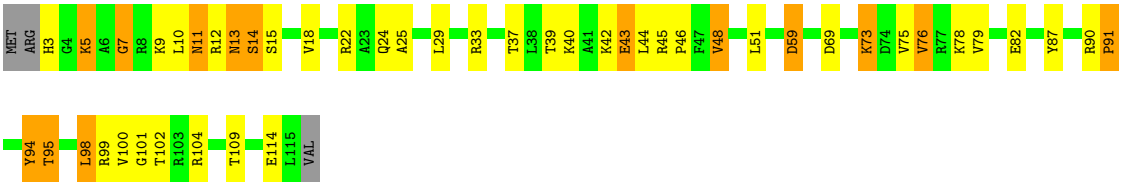
• Molecule 11: 50S ribosomal protein L16

Chain J:



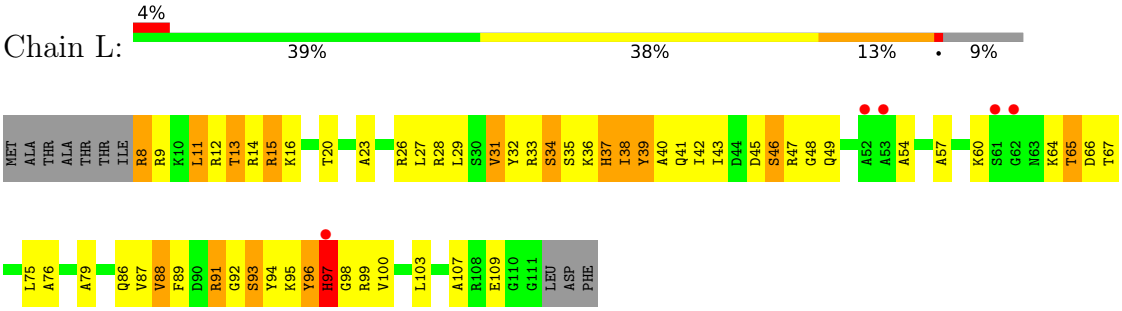
• Molecule 12: 50S ribosomal protein L17

Chain K:



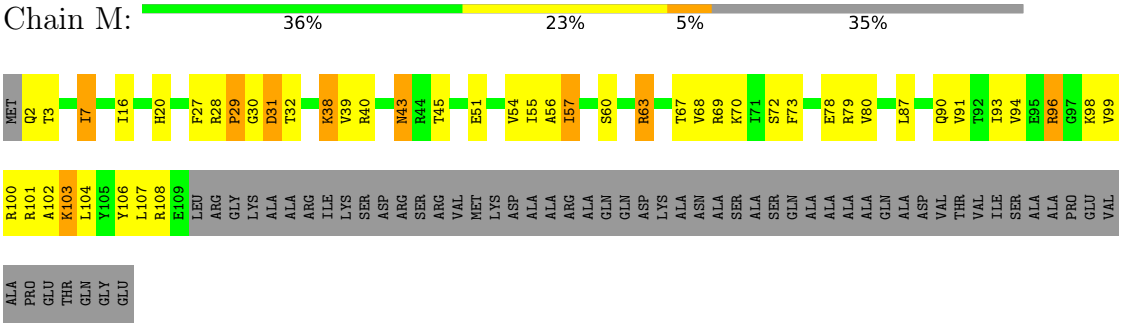
• Molecule 13: 50S ribosomal protein L18

Chain L:



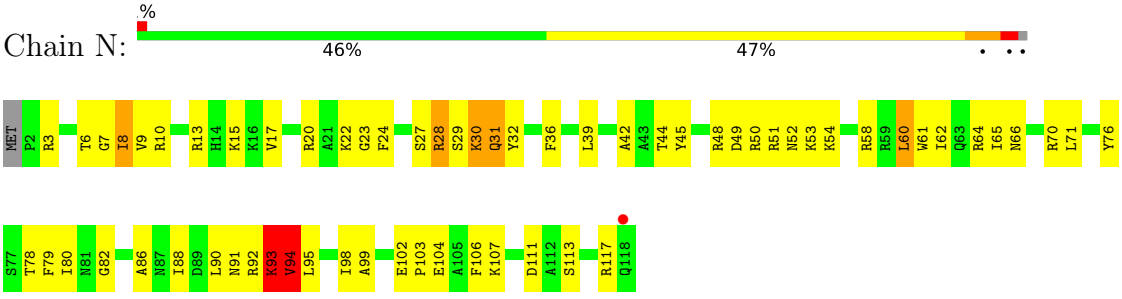
• Molecule 14: 50S ribosomal protein L19

Chain M:



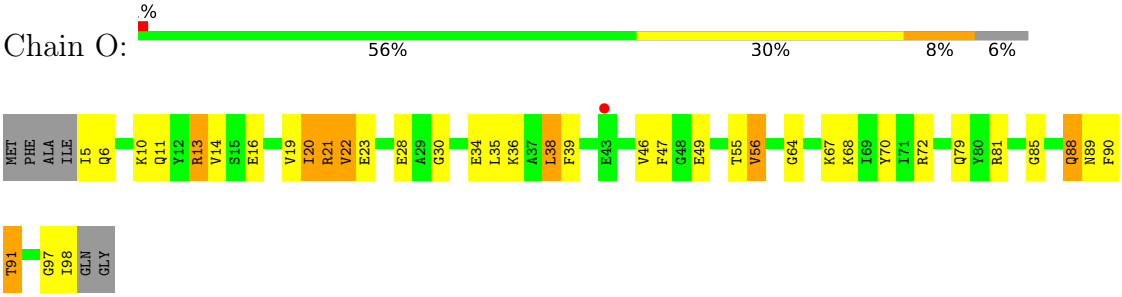
• Molecule 15: 50S ribosomal protein L20

Chain N:



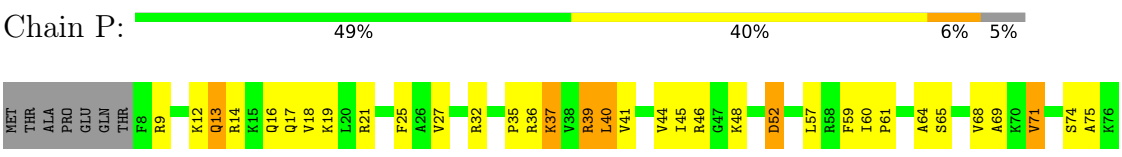
• Molecule 16: 50S ribosomal protein L21

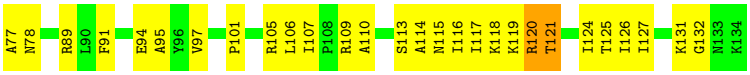
Chain O:



• Molecule 17: 50S ribosomal protein L22

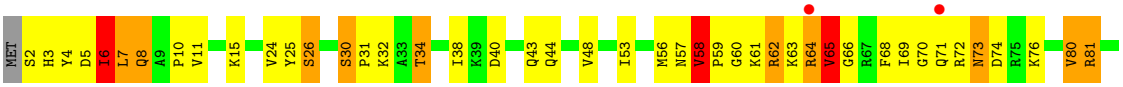
Chain P:

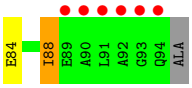




• Molecule 18: 50S ribosomal protein L23

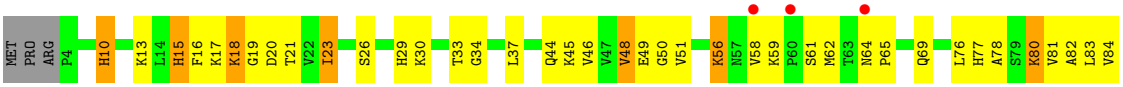
Chain Q:





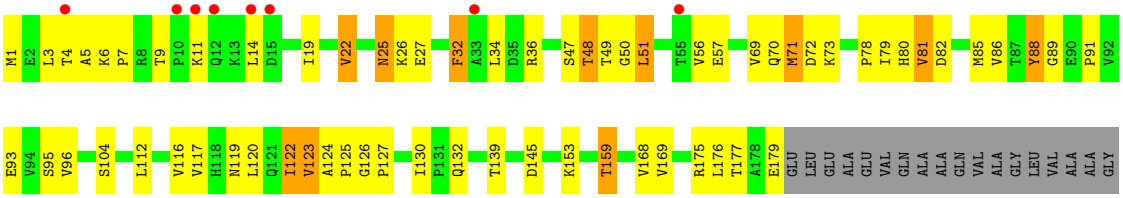
• Molecule 19: 50S ribosomal protein L24

Chain R:



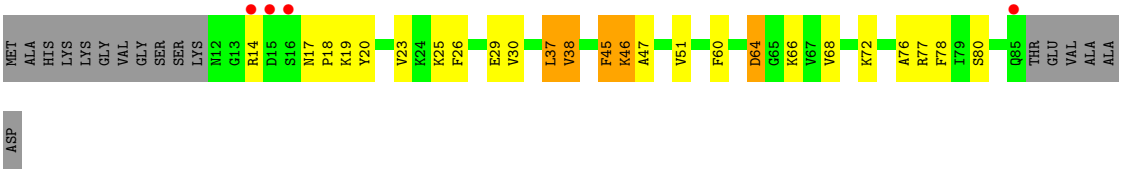
• Molecule 20: 50S ribosomal protein L25

Chain S:



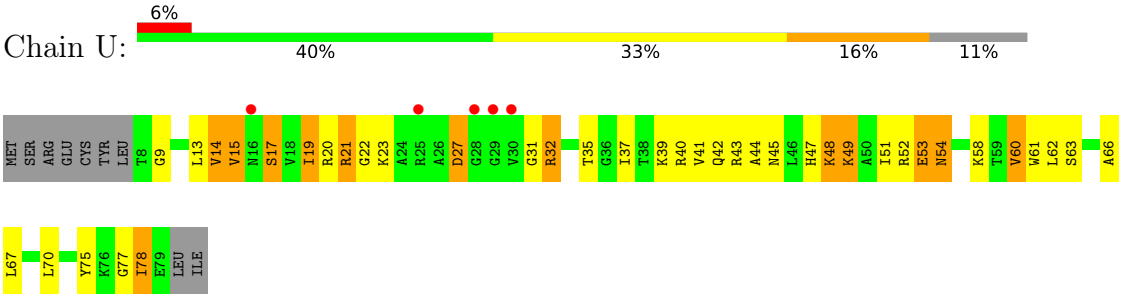
• Molecule 21: 50S ribosomal protein L27

Chain T:



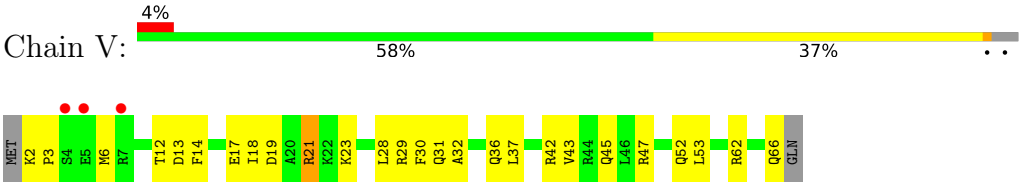
• Molecule 22: 50S ribosomal protein L28

Chain U:



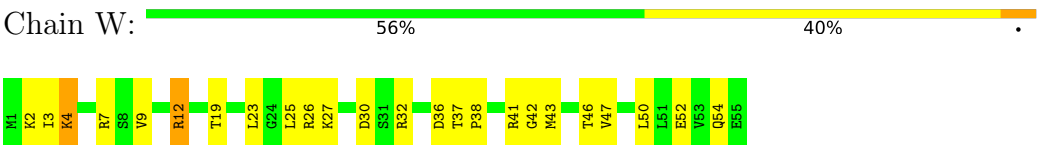
• Molecule 23: 50S ribosomal protein L29

Chain V:



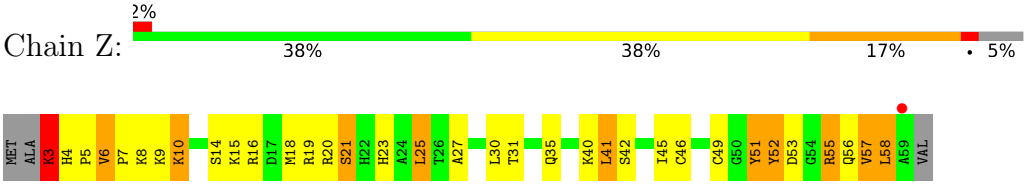
• Molecule 24: 50S ribosomal protein L30

Chain W:



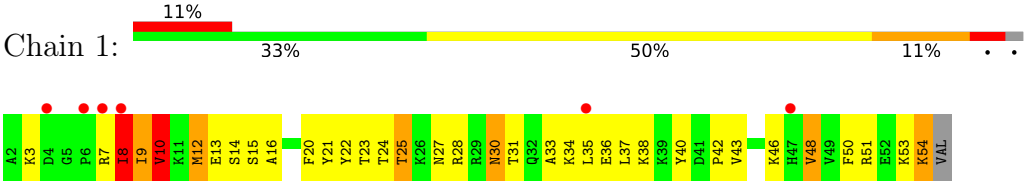
• Molecule 25: 50S ribosomal protein L32

Chain Z:



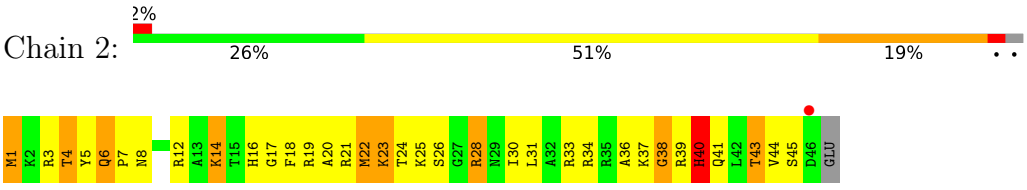
• Molecule 26: 50S ribosomal protein L33

Chain 1:



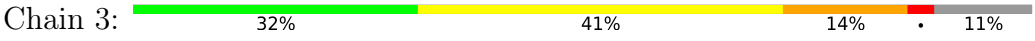
• Molecule 27: 50S ribosomal protein L34

Chain 2:



• Molecule 28: 50S ribosomal protein L35

Chain 3:




MET
PRO
LYS
MET
LYS
T6
H7
K8
M9
A10
K11
R12
R13
I14
K15
T19
V22
M23
A24
F25
K26
S27
G28
K29
R30
H31
Q32
N33
T34
G35
K36
S37
G38
R42
G43
K44
G45
K46
G47
F48
V49
L50
A51
K52
A53
A56
K59
L60
M61
R64
GLY
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	169.47Å 407.38Å 692.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.58 29.84 – 3.57	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.84-3.58) 94.2 (29.84-3.57)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 3.56Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.247 0.204 , 0.247	Depositor DCC
R_{free} test set	13397 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	112.0	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	83681	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6O1, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	X	0.69	20/63887 (0.0%)	1.25	500/99650 (0.5%)
2	Y	0.41	0/2863	0.93	0/4461
3	A	0.49	0/2011	0.79	4/2708 (0.1%)
4	B	0.58	0/1567	0.85	0/2105
5	C	0.49	0/1504	0.77	1/2036 (0.0%)
6	D	0.30	0/1419	0.51	0/1903
7	E	0.30	0/1308	0.54	0/1771
8	G	0.51	0/1138	0.81	1/1539 (0.1%)
9	H	0.56	0/1007	0.74	0/1352
10	I	0.61	0/1022	0.93	3/1366 (0.2%)
11	J	0.48	0/1101	0.71	0/1472
12	K	0.67	0/886	0.89	2/1188 (0.2%)
13	L	0.39	0/785	0.69	0/1048
14	M	0.67	1/872 (0.1%)	0.91	2/1172 (0.2%)
15	N	0.52	0/994	0.77	0/1323
16	O	0.46	0/750	0.81	2/1000 (0.2%)
17	P	0.58	0/1027	0.71	0/1373
18	Q	0.49	0/737	0.82	2/988 (0.2%)
19	R	0.45	0/835	0.75	0/1121
20	S	0.31	0/1399	0.57	0/1902
21	T	0.45	0/563	0.75	0/747
22	U	0.46	0/556	0.73	0/741
23	V	0.34	0/529	0.52	0/704
24	W	0.43	0/426	0.67	0/568
25	Z	0.56	0/464	0.77	0/622
26	1	0.55	0/434	0.83	0/579
27	2	0.58	0/387	1.04	2/509 (0.4%)
28	3	0.59	0/468	0.98	2/614 (0.3%)
All	All	0.63	21/90939 (0.0%)	1.14	521/136562 (0.4%)

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
3	A	0	1
4	B	0	1
5	C	0	2
8	G	0	4
10	I	0	5
11	J	0	1
13	L	0	1
15	N	0	2
19	R	0	1
25	Z	0	1
27	2	0	3
28	3	0	2
All	All	0	24

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	774	A	C5-C4	7.18	1.43	1.38
1	X	542	A	N9-C4	-7.12	1.33	1.37
14	M	29	PRO	CA-C	6.60	1.66	1.52
1	X	540	G	C2-N3	6.49	1.38	1.32
1	X	2548	G	C6-O6	6.47	1.29	1.24
1	X	1278	A	N3-C4	-6.36	1.31	1.34
1	X	774	A	N7-C5	-6.11	1.35	1.39
1	X	1278	A	C6-N1	-5.86	1.31	1.35
1	X	540	G	N9-C4	5.80	1.42	1.38
1	X	1688	U	C2-N3	5.72	1.41	1.37
1	X	1333	G	N9-C4	-5.69	1.33	1.38
1	X	542	A	N3-C4	-5.66	1.31	1.34
1	X	512	A	N9-C4	-5.66	1.34	1.37
1	X	2795	A	N9-C4	5.46	1.41	1.37
1	X	1981	A	N3-C4	-5.45	1.31	1.34
1	X	2591	C	N1-C2	5.35	1.45	1.40
1	X	1672	A	N7-C5	-5.30	1.36	1.39
1	X	796	A	N9-C4	-5.19	1.34	1.37
1	X	1278	A	N9-C4	-5.18	1.34	1.37
1	X	1630	A	N7-C5	-5.13	1.36	1.39
1	X	2701	A	N9-C4	-5.07	1.34	1.37

All (521) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	774	A	N7-C8-N9	14.67	121.13	113.80
1	X	774	A	C8-N9-C4	-14.58	99.97	105.80
1	X	542	A	C2-N3-C4	-13.70	103.75	110.60
1	X	1333	G	N3-C4-N9	-12.51	118.49	126.00
1	X	2018	G	C4-C5-N7	11.72	115.49	110.80
1	X	537	C	N3-C2-O2	-11.52	113.84	121.90
1	X	540	G	N3-C4-C5	-11.45	122.88	128.60
1	X	1670	G	C8-N9-C4	11.16	110.86	106.40
1	X	1468	A	C8-N9-C4	-11.14	101.35	105.80
1	X	2548	G	C5-C6-N1	-10.99	106.00	111.50
1	X	542	A	N1-C2-N3	10.98	134.79	129.30
1	X	2705	A	N7-C8-N9	10.86	119.23	113.80
1	X	1333	G	N3-C4-C5	10.86	134.03	128.60
1	X	1278	A	C2-N3-C4	-10.68	105.26	110.60
1	X	774	A	C6-C5-N7	-10.52	124.94	132.30
1	X	346	C	C6-N1-C2	-10.48	116.11	120.30
1	X	540	G	N3-C2-N2	10.39	127.18	119.90
1	X	661	C	C6-N1-C2	-10.33	116.17	120.30
1	X	2018	G	O4'-C1'-N9	10.29	116.43	108.20
1	X	540	G	N1-C6-O6	-10.23	113.76	119.90
1	X	540	G	C5-C6-N1	10.10	116.55	111.50
1	X	774	A	C5-N7-C8	-9.75	99.03	103.90
1	X	1670	G	N9-C4-C5	-9.68	101.53	105.40
1	X	2033	C	C6-N1-C2	-9.62	116.45	120.30
1	X	2705	A	C8-N9-C4	-9.54	101.98	105.80
1	X	540	G	N1-C2-N2	-9.47	107.68	116.20
1	X	2690	A	C2-N3-C4	-9.33	105.93	110.60
1	X	1630	A	N1-C6-N6	9.31	124.19	118.60
1	X	2018	G	C5-N7-C8	-9.27	99.67	104.30
1	X	309	G	C4-C5-N7	9.15	114.46	110.80
1	X	2705	A	C2-N3-C4	-9.14	106.03	110.60
1	X	1333	G	C2-N3-C4	-9.11	107.34	111.90
1	X	2591	C	N1-C2-O2	9.10	124.36	118.90
1	X	537	C	C6-N1-C2	-9.01	116.69	120.30
1	X	2018	G	O5'-P-OP2	-9.00	97.60	105.70
1	X	2705	A	C5-N7-C8	-8.91	99.44	103.90
1	X	1770	U	C5-C6-N1	-8.87	118.26	122.70
1	X	699	G	C5-N7-C8	-8.76	99.92	104.30
1	X	479	G	N1-C6-O6	8.74	125.15	119.90
1	X	1278	A	N1-C2-N3	8.70	133.65	129.30
1	X	540	G	N3-C4-N9	8.68	131.21	126.00
1	X	1975	G	O5'-P-OP1	-8.65	97.91	105.70
1	X	538	A	C2-N3-C4	8.65	114.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1278	A	O5'-P-OP1	-8.58	97.98	105.70
1	X	1631	C	C2-N1-C1'	8.48	128.12	118.80
1	X	2045	A	N1-C6-N6	8.40	123.64	118.60
1	X	2820	C	C6-N1-C2	8.40	123.66	120.30
1	X	2246	A	N1-C6-N6	-8.39	113.57	118.60
1	X	2820	C	N3-C4-C5	8.37	125.25	121.90
1	X	774	A	C2-N3-C4	-8.35	106.42	110.60
1	X	2485	U	C2-N1-C1'	8.32	127.69	117.70
1	X	309	G	C5-N7-C8	-8.20	100.20	104.30
12	K	10	LEU	CA-CB-CG	8.17	134.08	115.30
1	X	1631	C	C5-C6-N1	8.14	125.07	121.00
1	X	1468	A	N1-C6-N6	-8.08	113.75	118.60
1	X	1746	A	N1-C2-N3	8.06	133.33	129.30
1	X	177	U	C5-C4-O4	-8.06	121.06	125.90
1	X	1630	A	C6-C5-N7	-8.05	126.67	132.30
1	X	2668	U	O5'-P-OP1	-8.03	98.48	105.70
1	X	1663	C	N1-C2-O2	8.01	123.70	118.90
1	X	1669	A	N1-C6-N6	7.98	123.39	118.60
1	X	699	G	C4-C5-N7	7.95	113.98	110.80
1	X	479	G	C5-C6-O6	-7.86	123.88	128.60
1	X	123	A	C8-N9-C4	7.86	108.94	105.80
1	X	1336	G	C4-C5-N7	7.85	113.94	110.80
1	X	774	A	N1-C6-N6	7.84	123.31	118.60
1	X	1336	G	N9-C4-C5	-7.80	102.28	105.40
1	X	343	A	C8-N9-C4	-7.72	102.71	105.80
1	X	841	G	N7-C8-N9	7.70	116.95	113.10
1	X	2553	G	N3-C4-C5	7.70	132.45	128.60
10	I	51	GLY	N-CA-C	7.64	132.20	113.10
1	X	774	A	C4-C5-C6	7.60	120.80	117.00
1	X	2490	U	N3-C2-O2	-7.46	116.98	122.20
1	X	542	A	C5-N7-C8	-7.45	100.17	103.90
1	X	2705	A	P-O3'-C3'	7.41	128.59	119.70
1	X	540	G	O4'-C1'-N9	7.41	114.12	108.20
28	3	60	LEU	CA-CB-CG	7.39	132.31	115.30
1	X	1770	U	C2-N1-C1'	-7.39	108.83	117.70
1	X	2820	C	C5-C6-N1	-7.38	117.31	121.00
1	X	537	C	N1-C2-O2	7.38	123.33	118.90
1	X	1992	G	C8-N9-C4	7.35	109.34	106.40
1	X	2018	G	N3-C4-C5	7.33	132.26	128.60
14	M	28	ARG	N-CA-C	-7.28	91.34	111.00
1	X	2018	G	C5-C6-O6	-7.27	124.24	128.60
1	X	689	A	C2-N3-C4	-7.27	106.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2815	C	C6-N1-C2	7.26	123.20	120.30
1	X	343	A	N7-C8-N9	7.23	117.42	113.80
1	X	522	G	N1-C6-O6	7.23	124.24	119.90
1	X	1688	U	N3-C4-C5	-7.22	110.27	114.60
1	X	522	G	C5-C6-O6	-7.22	124.27	128.60
1	X	2596	C	C6-N1-C2	7.22	123.19	120.30
1	X	2687	G	C8-N9-C4	7.19	109.28	106.40
1	X	2658	A	C8-N9-C4	7.18	108.67	105.80
1	X	540	G	C8-N9-C4	-7.18	103.53	106.40
1	X	774	A	C4-C5-N7	7.11	114.25	110.70
1	X	787	A	C2-N3-C4	-7.09	107.06	110.60
1	X	841	G	C5-N7-C8	-7.07	100.77	104.30
1	X	841	G	C8-N9-C4	-7.06	103.58	106.40
1	X	1006	C	N3-C2-O2	-7.03	116.98	121.90
1	X	617	U	N3-C2-O2	-7.00	117.30	122.20
1	X	540	G	C6-N1-C2	-7.00	120.90	125.10
1	X	462	G	C8-N9-C4	6.99	109.20	106.40
1	X	540	G	C2-N3-C4	6.96	115.38	111.90
1	X	542	A	C5-C6-N1	-6.95	114.22	117.70
1	X	1993	G	N1-C6-O6	6.94	124.06	119.90
1	X	1285	A	C2-N3-C4	-6.93	107.13	110.60
1	X	1277	G	N1-C6-O6	-6.92	115.75	119.90
1	X	88	G	C8-N9-C4	-6.92	103.63	106.40
1	X	542	A	N1-C6-N6	6.89	122.74	118.60
1	X	757	U	OP2-P-O3'	6.87	120.32	105.20
1	X	1338	G	N3-C4-N9	6.87	130.12	126.00
1	X	2553	G	N3-C4-N9	-6.87	121.88	126.00
1	X	923	A	C2-N3-C4	6.86	114.03	110.60
1	X	26	G	C8-N9-C4	-6.86	103.66	106.40
1	X	1975	G	N1-C6-O6	-6.86	115.78	119.90
1	X	1631	C	C4-C5-C6	-6.86	113.97	117.40
1	X	1630	A	C5-N7-C8	-6.85	100.47	103.90
1	X	2399	C	C6-N1-C2	6.81	123.02	120.30
1	X	1006	C	N1-C2-O2	6.81	122.98	118.90
1	X	1679	U	C5-C6-N1	-6.81	119.30	122.70
1	X	519	C	C6-N1-C2	-6.79	117.58	120.30
1	X	746	G	N3-C4-C5	-6.77	125.22	128.60
1	X	522	G	C4-C5-N7	6.74	113.50	110.80
1	X	955	G	C8-N9-C1'	-6.74	118.23	127.00
1	X	699	G	C2-N3-C4	-6.73	108.54	111.90
1	X	699	G	N7-C8-N9	6.73	116.46	113.10
1	X	2607	C	N3-C2-O2	-6.67	117.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	774	A	C5-C6-N1	-6.67	114.36	117.70
1	X	2423	G	O5'-P-OP2	-6.66	99.70	105.70
1	X	2547	C	N3-C4-C5	6.66	124.56	121.90
1	X	1333	G	C8-N9-C4	-6.63	103.75	106.40
1	X	1631	C	C6-N1-C1'	-6.62	112.85	120.80
1	X	1693	A	C8-N9-C4	-6.62	103.15	105.80
16	O	38	LEU	CA-CB-CG	6.60	130.48	115.30
1	X	413	G	C8-N9-C4	-6.59	103.76	106.40
1	X	2757	G	N1-C6-O6	6.58	123.85	119.90
1	X	542	A	C6-C5-N7	-6.58	127.70	132.30
1	X	661	C	N3-C4-C5	-6.56	119.28	121.90
1	X	540	G	P-O3'-C3'	6.56	127.57	119.70
1	X	1333	G	C5-N7-C8	-6.56	101.02	104.30
1	X	1304	U	C5-C6-N1	-6.56	119.42	122.70
1	X	763	A	N1-C6-N6	-6.55	114.67	118.60
1	X	837	U	C5-C6-N1	-6.53	119.44	122.70
1	X	1475	U	P-O3'-C3'	6.50	127.50	119.70
1	X	955	G	N3-C4-N9	6.50	129.90	126.00
1	X	2371	A	C4-C5-C6	6.47	120.23	117.00
1	X	1468	A	N7-C8-N9	6.45	117.02	113.80
1	X	309	G	C5-C6-O6	-6.45	124.73	128.60
1	X	2398	U	C6-N1-C2	-6.45	117.13	121.00
1	X	1688	U	N3-C4-O4	6.42	123.89	119.40
1	X	1647	U	N3-C4-C5	-6.41	110.75	114.60
16	O	30	GLY	N-CA-C	-6.41	97.07	113.10
1	X	689	A	O4'-C1'-N9	6.40	113.32	108.20
1	X	617	U	C4-C5-C6	6.39	123.54	119.70
1	X	955	G	C4-N9-C1'	6.39	134.81	126.50
1	X	1983	G	C8-N9-C4	6.38	108.95	106.40
1	X	1991	C	C5-C6-N1	-6.38	117.81	121.00
1	X	1985	G	C2-N3-C4	-6.37	108.71	111.90
1	X	1724	C	C6-N1-C2	6.37	122.85	120.30
1	X	1631	C	N1-C2-O2	6.37	122.72	118.90
1	X	1468	A	C5-C6-N1	6.36	120.88	117.70
1	X	2560	G	C8-N9-C4	-6.34	103.86	106.40
1	X	985	G	C4-C5-N7	6.34	113.34	110.80
1	X	309	G	N1-C6-O6	6.34	123.70	119.90
1	X	1746	A	C2-N3-C4	-6.33	107.44	110.60
1	X	2398	U	N3-C4-C5	-6.31	110.81	114.60
1	X	2485	U	C6-N1-C1'	-6.31	112.37	121.20
1	X	1141	U	C5-C6-N1	-6.30	119.55	122.70
1	X	993	C	N1-C2-O2	6.30	122.68	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1770	U	N1-C2-N3	6.30	118.68	114.90
1	X	1770	U	C5-C4-O4	6.30	129.68	125.90
1	X	1975	G	P-O3'-C3'	6.29	127.25	119.70
1	X	689	A	N1-C6-N6	6.29	122.37	118.60
1	X	88	G	N7-C8-N9	6.27	116.23	113.10
5	C	81	GLY	N-CA-C	-6.26	97.44	113.10
1	X	1647	U	N1-C2-O2	-6.25	118.42	122.80
1	X	860	U	C2-N1-C1'	6.25	125.20	117.70
1	X	1391	A	P-O3'-C3'	6.25	127.19	119.70
1	X	2820	C	C2-N3-C4	-6.24	116.78	119.90
1	X	746	G	N3-C4-N9	6.24	129.74	126.00
1	X	346	C	N3-C4-C5	-6.23	119.41	121.90
1	X	2553	G	C5-N7-C8	-6.23	101.18	104.30
1	X	2242	C	N3-C2-O2	-6.23	117.54	121.90
1	X	1974	U	O5'-P-OP2	-6.23	100.10	105.70
1	X	2705	A	C6-C5-N7	-6.22	127.94	132.30
1	X	1745	C	N1-C2-O2	-6.21	115.18	118.90
1	X	2655	C	C5-C6-N1	-6.21	117.90	121.00
1	X	2495	G	C5-C6-N1	6.20	114.60	111.50
1	X	2371	A	N7-C8-N9	6.20	116.90	113.80
1	X	746	G	C4-N9-C1'	6.20	134.56	126.50
1	X	1975	G	C8-N9-C4	-6.19	103.92	106.40
3	A	35	GLU	N-CA-C	6.18	127.69	111.00
1	X	1019	U	P-O3'-C3'	6.17	127.10	119.70
1	X	1664	G	N3-C4-C5	6.17	131.68	128.60
1	X	2624	G	C4-C5-N7	6.16	113.27	110.80
1	X	1923	U	P-O3'-C3'	6.15	127.08	119.70
1	X	796	A	C2-N3-C4	-6.15	107.52	110.60
1	X	2045	A	C5-C6-N6	-6.14	118.79	123.70
1	X	393	U	N3-C4-C5	-6.14	110.92	114.60
1	X	2541	U	N3-C2-O2	-6.14	117.90	122.20
12	K	7	GLY	N-CA-C	6.14	128.44	113.10
1	X	632	A	C2-N3-C4	-6.13	107.54	110.60
1	X	853	C	C6-N1-C2	6.13	122.75	120.30
1	X	2001	G	N1-C6-O6	-6.13	116.22	119.90
1	X	2854	G	N7-C8-N9	6.12	116.16	113.10
1	X	1630	A	C4-C5-N7	6.12	113.76	110.70
1	X	2698	G	OP1-P-O3'	6.11	118.65	105.20
1	X	2668	U	N3-C4-O4	-6.11	115.12	119.40
1	X	2371	A	C6-C5-N7	-6.11	128.03	132.30
1	X	661	C	C5-C6-N1	6.11	124.05	121.00
1	X	689	A	C5-N7-C8	-6.11	100.85	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1770	U	C6-N1-C1'	6.08	129.72	121.20
14	M	30	GLY	N-CA-C	-6.08	97.89	113.10
1	X	1775	A	C6-N1-C2	-6.08	114.95	118.60
1	X	1981	A	N1-C2-N3	6.07	132.34	129.30
1	X	742	G	N3-C4-N9	6.05	129.63	126.00
1	X	1683	G	O4'-C1'-N9	6.05	113.04	108.20
1	X	2559	U	O5'-P-OP1	-6.04	100.26	105.70
1	X	2043	A	OP2-P-O3'	6.03	118.47	105.20
1	X	1656	U	C5-C6-N1	-6.03	119.69	122.70
1	X	1991	C	N3-C4-C5	6.01	124.30	121.90
1	X	806	A	C8-N9-C4	6.00	108.20	105.80
1	X	2825	A	N1-C6-N6	6.00	122.20	118.60
1	X	1705	U	C2-N1-C1'	-6.00	110.50	117.70
1	X	2045	A	C6-C5-N7	-5.99	128.10	132.30
1	X	1304	U	C6-N1-C2	5.99	124.59	121.00
1	X	2496	C	C5-C4-N4	-5.99	116.01	120.20
1	X	123	A	N7-C8-N9	-5.96	110.82	113.80
1	X	2681	A	N1-C6-N6	5.96	122.18	118.60
1	X	2578	G	C4-N9-C1'	5.96	134.25	126.50
1	X	2668	U	C2-N1-C1'	-5.96	110.55	117.70
1	X	2490	U	N1-C2-N3	5.96	118.47	114.90
1	X	2705	A	N1-C2-N3	5.95	132.27	129.30
1	X	1570	C	N1-C2-O2	5.94	122.47	118.90
1	X	2002	A	N1-C6-N6	5.94	122.17	118.60
1	X	1975	G	N3-C4-C5	-5.94	125.63	128.60
1	X	1801	C	O5'-P-OP1	-5.93	100.36	105.70
1	X	660	G	N3-C4-N9	-5.93	122.44	126.00
1	X	699	G	C6-C5-N7	-5.92	126.85	130.40
1	X	2805	G	N3-C4-N9	5.91	129.54	126.00
1	X	1946	U	C2-N1-C1'	5.90	124.78	117.70
1	X	2634	G	O4'-C1'-N9	5.90	112.92	108.20
1	X	1278	A	O4'-C1'-N9	5.89	112.91	108.20
1	X	689	A	C6-C5-N7	-5.88	128.18	132.30
1	X	2655	C	C6-N1-C2	5.88	122.65	120.30
1	X	2668	U	C5-C4-O4	5.88	129.43	125.90
1	X	2548	G	C4-C5-N7	-5.87	108.45	110.80
1	X	797	A	P-O3'-C3'	5.86	126.73	119.70
1	X	177	U	N3-C4-O4	5.84	123.49	119.40
1	X	2258	G	C4-N9-C1'	-5.84	118.91	126.50
1	X	956	A	N1-C6-N6	5.84	122.10	118.60
1	X	955	G	C6-C5-N7	-5.83	126.90	130.40
1	X	1982	C	C5-C6-N1	-5.83	118.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2799	C	C6-N1-C2	-5.82	117.97	120.30
1	X	1670	G	N3-C2-N2	5.82	123.97	119.90
1	X	1669	A	C5-C6-N6	-5.82	119.05	123.70
1	X	1019	U	OP2-P-O3'	5.81	117.98	105.20
10	I	47	ALA	N-CA-C	5.79	126.64	111.00
1	X	219	G	P-O3'-C3'	5.78	126.64	119.70
1	X	1688	U	C2-N3-C4	5.78	130.47	127.00
1	X	2854	G	C4-N9-C1'	5.77	134.00	126.50
1	X	1468	A	N9-C4-C5	5.77	108.11	105.80
1	X	1666	G	C4-N9-C1'	-5.77	119.00	126.50
1	X	1283	C	N1-C2-O2	-5.75	115.45	118.90
1	X	798	G	N3-C4-C5	-5.75	125.72	128.60
1	X	581	A	O5'-P-OP1	-5.73	100.54	105.70
1	X	1702	C	C6-N1-C2	5.73	122.59	120.30
1	X	699	G	O4'-C1'-N9	-5.73	103.62	108.20
1	X	177	U	O4'-C1'-N1	5.72	112.78	108.20
1	X	788	G	P-O3'-C3'	5.72	126.57	119.70
1	X	1630	A	N7-C8-N9	5.72	116.66	113.80
1	X	699	G	N3-C4-C5	5.71	131.46	128.60
1	X	2812	A	C8-N9-C4	-5.71	103.52	105.80
1	X	850	C	C6-N1-C2	-5.71	118.02	120.30
1	X	1760	G	O5'-P-OP2	-5.70	100.57	105.70
1	X	2558	C	N3-C4-C5	5.70	124.18	121.90
1	X	1336	G	C5-C6-O6	-5.70	125.18	128.60
1	X	2591	C	C5-C6-N1	5.69	123.85	121.00
1	X	2039	G	C8-N9-C4	-5.69	104.12	106.40
1	X	2578	G	C8-N9-C1'	-5.68	119.61	127.00
1	X	2228	U	C6-N1-C2	-5.67	117.59	121.00
3	A	33	LEU	CA-CB-CG	5.67	128.35	115.30
1	X	2705	A	C4-C5-N7	5.66	113.53	110.70
1	X	2495	G	C6-N1-C2	-5.66	121.71	125.10
1	X	1335	A	C8-N9-C4	5.65	108.06	105.80
1	X	1468	A	N3-C4-C5	-5.65	122.84	126.80
1	X	2854	G	C4-C5-N7	5.65	113.06	110.80
1	X	571	U	C5-C6-N1	-5.65	119.88	122.70
1	X	1318	A	C8-N9-C4	5.65	108.06	105.80
1	X	1981	A	C6-N1-C2	-5.65	115.21	118.60
1	X	2673	G	C4-C5-N7	5.65	113.06	110.80
1	X	1454	U	N3-C4-O4	5.65	123.35	119.40
1	X	1688	U	C5-C6-N1	5.64	125.52	122.70
1	X	1780	A	N1-C6-N6	5.64	121.99	118.60
1	X	1982	C	C2-N3-C4	-5.63	117.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1975	G	O4'-C1'-N9	-5.63	103.69	108.20
1	X	1663	C	N3-C2-O2	-5.63	117.96	121.90
1	X	169	C	C6-N1-C2	5.63	122.55	120.30
1	X	2018	G	N1-C6-O6	5.63	123.28	119.90
1	X	2371	A	C8-N9-C4	-5.62	103.55	105.80
1	X	660	G	N3-C4-C5	5.62	131.41	128.60
1	X	1991	C	C6-N1-C2	5.62	122.55	120.30
1	X	2587	G	C5-C6-O6	-5.62	125.23	128.60
1	X	2756	A	P-O3'-C3'	5.61	126.43	119.70
1	X	177	U	P-O3'-C3'	5.61	126.43	119.70
1	X	1279	G	C8-N9-C4	5.61	108.64	106.40
1	X	1292	A	O5'-P-OP2	-5.61	100.65	105.70
3	A	21	PHE	N-CA-C	5.61	126.14	111.00
1	X	542	A	C4-C5-N7	5.61	113.50	110.70
1	X	1312	G	C5-N7-C8	-5.60	101.50	104.30
1	X	1333	G	N7-C8-N9	5.59	115.90	113.10
1	X	796	A	C5-N7-C8	-5.59	101.10	103.90
1	X	984	A	N1-C6-N6	5.59	121.95	118.60
1	X	309	G	N7-C8-N9	5.59	115.89	113.10
1	X	742	G	C4-N9-C1'	5.59	133.76	126.50
1	X	1991	C	C2-N3-C4	-5.59	117.11	119.90
1	X	1752	U	N1-C2-O2	-5.58	118.89	122.80
1	X	1939	U	N3-C2-O2	-5.58	118.29	122.20
1	X	1278	A	C5-C6-N1	-5.58	114.91	117.70
1	X	1647	U	C6-N1-C1'	5.58	129.00	121.20
1	X	874	A	C8-N9-C4	-5.57	103.57	105.80
1	X	1630	A	C5-C6-N1	-5.57	114.91	117.70
1	X	1939	U	N1-C2-O2	5.57	126.70	122.80
1	X	2825	A	N9-C4-C5	-5.57	103.57	105.80
1	X	338	G	C8-N9-C4	-5.56	104.17	106.40
1	X	1286	U	N3-C2-O2	-5.56	118.31	122.20
1	X	2490	U	C5-C4-O4	5.55	129.23	125.90
1	X	2590	U	N3-C2-O2	-5.55	118.31	122.20
1	X	2033	C	N3-C2-O2	-5.55	118.02	121.90
1	X	1269	G	C5-C6-O6	-5.55	125.27	128.60
1	X	2667	C	N1-C2-O2	5.54	122.22	118.90
1	X	747	A	N1-C6-N6	5.54	121.92	118.60
1	X	2252	A	C2-N3-C4	5.54	113.37	110.60
1	X	479	G	C4-C5-N7	5.53	113.01	110.80
1	X	1974	U	OP2-P-O3'	5.53	117.36	105.20
27	2	40	HIS	N-CA-C	-5.52	96.09	111.00
1	X	646	C	C6-N1-C2	-5.52	118.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1344	C	N1-C2-O2	5.52	122.21	118.90
1	X	504	G	C4-C5-N7	5.51	113.01	110.80
1	X	985	G	C5-N7-C8	-5.51	101.54	104.30
1	X	1664	G	C8-N9-C4	5.51	108.60	106.40
1	X	1304	U	C2-N3-C4	-5.51	123.69	127.00
1	X	742	G	C8-N9-C1'	-5.50	119.85	127.00
1	X	2528	G	C8-N9-C1'	-5.50	119.85	127.00
1	X	2550	C	C6-N1-C2	-5.50	118.10	120.30
1	X	1241	G	N3-C4-C5	-5.49	125.86	128.60
1	X	2240	C	N3-C2-O2	-5.49	118.06	121.90
1	X	2018	G	N9-C4-C5	-5.49	103.20	105.40
1	X	1467	U	C6-N1-C2	5.49	124.29	121.00
1	X	393	U	C6-N1-C2	-5.48	117.71	121.00
1	X	520	C	C6-N1-C2	-5.48	118.11	120.30
1	X	817	A	O4'-C1'-N9	5.48	112.58	108.20
1	X	1792	C	P-O3'-C3'	5.48	126.27	119.70
1	X	504	G	N1-C6-O6	5.47	123.19	119.90
1	X	2673	G	N1-C6-O6	5.47	123.19	119.90
1	X	2756	A	C8-N9-C4	-5.47	103.61	105.80
1	X	1269	G	C4-C5-N7	5.47	112.99	110.80
1	X	789	G	C4-N9-C1'	5.47	133.61	126.50
1	X	1468	A	C6-N1-C2	-5.47	115.32	118.60
1	X	2258	G	O4'-C1'-N9	5.46	112.57	108.20
18	Q	59	PRO	N-CA-C	5.45	126.28	112.10
1	X	841	G	C4-C5-N7	5.45	112.98	110.80
1	X	1670	G	C8-N9-C1'	-5.45	119.92	127.00
1	X	1946	U	N1-C2-O2	5.45	126.61	122.80
10	I	56	LEU	N-CA-C	5.45	125.70	111.00
1	X	1031	C	P-O3'-C3'	5.44	126.23	119.70
1	X	1979	C	N1-C2-O2	5.44	122.16	118.90
1	X	2749	A	N1-C6-N6	5.44	121.86	118.60
1	X	1705	U	C5-C4-O4	5.43	129.16	125.90
1	X	931	G	C8-N9-C4	5.43	108.57	106.40
1	X	2867	G	C4-C5-N7	5.42	112.97	110.80
1	X	1332	G	N1-C6-O6	5.41	123.15	119.90
1	X	1669	A	C6-C5-N7	-5.41	128.51	132.30
1	X	1632	A	C4-C5-C6	5.40	119.70	117.00
1	X	480	G	C5-C6-O6	-5.40	125.36	128.60
1	X	2617	G	N1-C6-O6	-5.40	116.66	119.90
1	X	957	G	N3-C4-C5	-5.40	125.90	128.60
1	X	1292	A	N1-C6-N6	-5.39	115.36	118.60
1	X	2854	G	C6-C5-N7	-5.39	127.17	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1676	U	O5'-P-OP2	-5.38	100.86	105.70
1	X	1302	C	C6-N1-C2	5.38	122.45	120.30
1	X	684	C	N1-C2-O2	-5.38	115.67	118.90
1	X	2016	A	N1-C6-N6	5.38	121.83	118.60
1	X	2857	C	C6-N1-C2	-5.38	118.15	120.30
1	X	537	C	C5-C4-N4	5.37	123.96	120.20
1	X	2414	A	O5'-P-OP1	-5.37	100.87	105.70
1	X	742	G	N1-C2-N2	-5.37	111.37	116.20
1	X	2027	C	C2-N1-C1'	5.36	124.70	118.80
1	X	2495	G	N3-C4-N9	5.36	129.22	126.00
1	X	2655	C	C2-N3-C4	-5.36	117.22	119.90
1	X	1313	U	P-O3'-C3'	5.36	126.13	119.70
1	X	2242	C	C6-N1-C2	-5.35	118.16	120.30
1	X	788	G	C5-C6-N1	5.35	114.17	111.50
1	X	20	C	C5-C4-N4	-5.34	116.47	120.20
1	X	1285	A	C5-C6-N1	-5.33	115.03	117.70
1	X	526	C	N3-C4-C5	5.33	124.03	121.90
1	X	2553	G	C4-C5-N7	5.32	112.93	110.80
1	X	585	U	N3-C4-O4	5.32	123.12	119.40
1	X	985	G	N7-C8-N9	5.32	115.76	113.10
1	X	2579	A	C8-N9-C4	5.32	107.93	105.80
1	X	2668	U	N1-C2-O2	-5.32	119.08	122.80
1	X	2821	G	C2-N3-C4	-5.32	109.24	111.90
1	X	1670	G	N7-C8-N9	-5.31	110.44	113.10
18	Q	58	VAL	C-N-CD	-5.31	108.92	120.60
1	X	746	G	C8-N9-C1'	-5.30	120.11	127.00
1	X	1975	G	C5-C6-O6	5.30	131.78	128.60
1	X	2620	G	C8-N9-C4	5.30	108.52	106.40
1	X	2418	A	N1-C6-N6	5.30	121.78	118.60
1	X	1312	G	C4-C5-N7	5.30	112.92	110.80
1	X	2634	G	C4-N9-C1'	-5.29	119.62	126.50
1	X	1975	G	N9-C4-C5	5.29	107.52	105.40
1	X	829	C	C5-C6-N1	-5.29	118.36	121.00
1	X	2607	C	N1-C2-O2	5.29	122.07	118.90
1	X	1770	U	C4-C5-C6	5.28	122.87	119.70
1	X	1980	A	OP1-P-OP2	5.28	127.51	119.60
1	X	2246	A	N9-C4-C5	5.27	107.91	105.80
1	X	2757	G	C8-N9-C4	5.27	108.51	106.40
1	X	2854	G	C5-N7-C8	-5.27	101.67	104.30
1	X	2673	G	C5-C6-O6	-5.27	125.44	128.60
1	X	1339	U	OP2-P-O3'	5.27	116.78	105.20
1	X	2382	C	C6-N1-C2	-5.26	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2570	C	N3-C2-O2	-5.26	118.22	121.90
1	X	538	A	N3-C4-C5	-5.26	123.12	126.80
1	X	1288	A	OP1-P-O3'	5.26	116.76	105.20
1	X	2228	U	N3-C4-C5	-5.25	111.45	114.60
28	3	37	SER	N-CA-C	5.25	125.18	111.00
1	X	1630	A	P-O3'-C3'	5.25	126.00	119.70
1	X	1983	G	N7-C8-N9	-5.25	110.48	113.10
1	X	2556	A	C8-N9-C4	-5.25	103.70	105.80
1	X	540	G	N7-C8-N9	5.24	115.72	113.10
1	X	689	A	C4-C5-N7	5.24	113.32	110.70
1	X	1746	A	N9-C4-C5	5.24	107.89	105.80
1	X	2674	C	C6-N1-C2	5.23	122.39	120.30
1	X	1203	A	OP1-P-O3'	5.23	116.71	105.20
1	X	2323	U	C5-C4-O4	5.23	129.04	125.90
1	X	1285	A	N1-C6-N6	5.22	121.73	118.60
1	X	1770	U	O4'-C1'-N1	5.22	112.38	108.20
1	X	38	G	C4-N9-C1'	5.22	133.29	126.50
1	X	2560	G	N7-C8-N9	5.22	115.71	113.10
1	X	2489	C	C6-N1-C2	-5.22	118.21	120.30
1	X	1217	U	C5-C6-N1	-5.22	120.09	122.70
1	X	583	C	C5-C6-N1	5.22	123.61	121.00
1	X	2487	G	N1-C6-O6	5.22	123.03	119.90
1	X	1285	A	C8-N9-C4	5.21	107.88	105.80
1	X	1744	G	N1-C6-O6	-5.20	116.78	119.90
1	X	522	G	N9-C4-C5	-5.20	103.32	105.40
1	X	1333	G	N9-C4-C5	5.20	107.48	105.40
1	X	1975	G	C2'-C3'-O3'	5.19	122.01	113.70
1	X	2624	G	C5-N7-C8	-5.19	101.70	104.30
1	X	1240	G	N3-C4-N9	5.19	129.11	126.00
1	X	1679	U	C2-N3-C4	-5.18	123.89	127.00
1	X	1284	G	N1-C6-O6	5.18	123.01	119.90
1	X	1496	G	OP1-P-O3'	5.17	116.58	105.20
1	X	2039	G	C6-N1-C2	-5.17	122.00	125.10
1	X	522	G	C5-N7-C8	-5.17	101.72	104.30
1	X	2756	A	N9-C4-C5	5.16	107.86	105.80
1	X	850	C	N3-C4-C5	-5.16	119.84	121.90
1	X	49	U	P-O3'-C3'	5.15	125.88	119.70
1	X	928	G	C5-C6-O6	-5.15	125.51	128.60
1	X	1630	A	C4-C5-C6	5.15	119.58	117.00
1	X	1574	A	O5'-P-OP1	5.15	116.88	110.70
1	X	1647	U	C5-C4-O4	5.14	128.99	125.90
1	X	537	C	N1-C2-N3	5.14	122.80	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	462	G	N7-C8-N9	-5.14	110.53	113.10
1	X	2706	U	O5'-P-OP2	-5.14	101.08	105.70
1	X	1012	A	N1-C6-N6	5.13	121.68	118.60
1	X	2371	A	N1-C6-N6	5.13	121.68	118.60
1	X	2430	A	C2-N3-C4	-5.13	108.03	110.60
1	X	977	G	C8-N9-C4	5.13	108.45	106.40
1	X	1336	G	C6-C5-N7	-5.12	127.33	130.40
3	A	24	LEU	N-CA-C	5.12	124.83	111.00
1	X	522	G	C6-C5-N7	-5.12	127.33	130.40
1	X	2658	A	N7-C8-N9	-5.12	111.24	113.80
1	X	689	A	N7-C8-N9	5.11	116.36	113.80
1	X	1292	A	C5-C6-N1	5.11	120.26	117.70
1	X	1278	A	C8-N9-C4	-5.11	103.75	105.80
1	X	2540	A	O4'-C1'-N9	5.11	112.29	108.20
1	X	2708	U	N3-C4-C5	5.11	117.67	114.60
1	X	699	G	N1-C6-O6	5.11	122.96	119.90
1	X	1336	G	C8-N9-C4	5.10	108.44	106.40
1	X	2050	G	N1-C6-O6	5.10	122.96	119.90
8	G	95	LEU	CA-CB-CG	5.10	127.02	115.30
1	X	636	G	N1-C6-O6	5.09	122.95	119.90
1	X	2705	A	C5-C6-N1	-5.08	115.16	117.70
1	X	1285	A	N3-C4-C5	5.08	130.36	126.80
1	X	2491	C	O5'-P-OP1	-5.08	101.13	105.70
1	X	833	A	N1-C6-N6	5.08	121.65	118.60
1	X	1705	U	C6-N1-C1'	5.08	128.31	121.20
1	X	2674	C	N3-C2-O2	5.07	125.45	121.90
1	X	1338	G	N3-C4-C5	-5.07	126.06	128.60
1	X	2316	G	N3-C4-N9	5.07	129.04	126.00
1	X	2489	C	N3-C4-C5	-5.07	119.87	121.90
1	X	1442	C	N1-C2-O2	5.06	121.94	118.90
1	X	2408	G	N3-C4-C5	-5.06	126.07	128.60
1	X	2039	G	N1-C2-N3	5.06	126.94	123.90
1	X	2687	G	N7-C8-N9	-5.06	110.57	113.10
1	X	632	A	N1-C2-N3	5.06	131.83	129.30
1	X	1397	A	N1-C6-N6	5.06	121.63	118.60
1	X	1241	G	N3-C4-N9	5.05	129.03	126.00
1	X	1333	G	C8-N9-C1'	5.05	133.57	127.00
1	X	553	C	C2-N1-C1'	5.04	124.35	118.80
1	X	2558	C	N3-C4-N4	-5.04	114.47	118.00
1	X	2371	A	C5-C6-N1	-5.04	115.18	117.70
1	X	1993	G	C6-C5-N7	-5.04	127.38	130.40
1	X	2495	G	N3-C4-C5	-5.04	126.08	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1467	U	O4'-C1'-N1	-5.03	104.17	108.20
1	X	1294	G	N1-C6-O6	5.03	122.92	119.90
1	X	329	C	C6-N1-C2	-5.03	118.29	120.30
1	X	2037	A	C2-N3-C4	-5.03	108.08	110.60
1	X	1673	C	C6-N1-C2	5.03	122.31	120.30
1	X	2492	G	N3-C4-C5	-5.03	126.09	128.60
27	2	38	GLY	N-CA-C	-5.03	100.54	113.10
1	X	1336	G	N3-C2-N2	5.02	123.42	119.90
1	X	1672	A	OP2-P-O3'	5.02	116.25	105.20
1	X	1922	U	N3-C2-O2	-5.02	118.69	122.20
1	X	787	A	N1-C2-N3	5.02	131.81	129.30
1	X	600	G	P-O3'-C3'	5.01	125.71	119.70
1	X	636	G	C6-C5-N7	-5.01	127.39	130.40
1	X	841	G	C6-C5-N7	-5.01	127.39	130.40
1	X	957	G	N1-C6-O6	-5.00	116.90	119.90
1	X	742	G	N3-C4-C5	-5.00	126.10	128.60

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	2	4	THR	Peptide
27	2	40	HIS	Peptide
27	2	6	GLN	Peptide
28	3	37	SER	Peptide
28	3	44	LYS	Peptide
3	A	58	HIS	Peptide
4	B	122	PHE	Peptide
5	C	176	ASN	Peptide
5	C	66	ASN	Peptide
8	G	105	GLY	Peptide
8	G	109	GLY	Peptide
8	G	111	LYS	Peptide
8	G	34	PRO	Peptide
10	I	31	GLY	Peptide
10	I	36	GLY	Peptide
10	I	38	LYS	Peptide
10	I	53	ARG	Peptide
10	I	55	ARG	Peptide
11	J	26	ASP	Peptide
13	L	97	HIS	Peptide
15	N	93	LYS	Peptide

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Mol	Chain	Res	Type	Group
15	N	94	VAL	Peptide
19	R	64	ASN	Peptide
25	Z	3	LYS	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	X	57052	0	28750	1265	0
2	Y	2561	0	1306	59	0
3	A	1973	0	2034	131	0
4	B	1539	0	1600	81	0
5	C	1481	0	1504	97	0
6	D	1400	0	1481	60	0
7	E	1286	0	1336	31	0
8	G	1114	0	1144	83	0
9	H	997	0	1046	55	0
10	I	1011	0	1047	76	0
11	J	1078	0	1103	47	0
12	K	878	0	930	34	0
13	L	779	0	820	49	0
14	M	859	0	872	35	0
15	N	978	0	1020	66	0
16	O	741	0	756	34	0
17	P	1014	0	1096	49	0
18	Q	726	0	753	29	0
19	R	825	0	881	57	0
20	S	1374	0	1401	44	0
21	T	556	0	579	24	0
22	U	552	0	604	42	0
23	V	525	0	546	14	0
24	W	424	0	470	16	0
25	Z	452	0	457	34	0
26	1	427	0	445	35	0
27	2	383	0	414	37	0
28	3	462	0	506	36	0
29	X	111	0	0	2	0
30	K	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	M	1	0	0	0	0
30	X	119	0	0	0	0
30	Y	1	0	0	0	0
All	All	83681	0	54901	2278	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 17.

All (2278) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:356:A:HO2'	1:X:357:A:H8	1.10	0.99
8:G:100:TYR:HB2	8:G:116:ARG:HE	1.25	0.96
10:I:56:LEU:H	10:I:59:ARG:HD3	1.30	0.94
1:X:1277:G:OP1	25:Z:19:ARG:NH2	2.01	0.93
1:X:1264:C:H5"	15:N:13:ARG:HH12	1.34	0.93
15:N:66:ASN:HB3	15:N:76:TYR:HB2	1.48	0.92
1:X:608:G:H1'	10:I:21:ARG:HG3	1.52	0.91
1:X:971:A:H61	11:J:83:ARG:HH22	1.16	0.89
1:X:177:U:O2'	1:X:178:C:O5'	1.90	0.88
1:X:2598:C:OP1	4:B:152:LYS:NZ	2.07	0.87
1:X:1030:U:H3	1:X:1153:A:H62	1.23	0.87
1:X:2016:A:O2'	1:X:2018:G:OP2	1.94	0.85
26:1:12:MET:SD	26:1:13:GLU:N	2.50	0.85
1:X:796:A:H8	1:X:797:A:H4'	1.40	0.85
1:X:640:C:H4'	1:X:660:G:H21	1.40	0.85
4:B:77:ILE:HD13	4:B:195:LEU:HD22	1.59	0.85
1:X:538:A:O2'	1:X:539:A:O5'	1.95	0.84
1:X:1882:G:H21	1:X:1885:C:H41	1.26	0.83
17:P:45:ILE:HD11	17:P:57:LEU:HD11	1.58	0.83
1:X:1562:G:H5'	1:X:1563:U:H5'	1.61	0.82
1:X:824:U:H2'	10:I:30:ALA:HA	1.59	0.82
1:X:1322:G:H4'	27:2:7:PRO:HB2	1.61	0.82
1:X:2039:G:N2	25:Z:4:HIS:O	2.12	0.82
1:X:2757:G:H5"	1:X:2758:A:H5'	1.60	0.82
19:R:84:VAL:HG11	19:R:90:LYS:H	1.44	0.82
15:N:95:LEU:HA	15:N:98:ILE:HD13	1.62	0.81
16:O:5:ILE:HG23	16:O:10:LYS:HZ2	1.45	0.81
10:I:41:SER:OG	10:I:45:LYS:NZ	2.12	0.81
1:X:332:C:O2	5:C:159:ARG:NH2	2.14	0.81
1:X:2653:A:O2'	9:H:41:ASN:ND2	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:145:LEU:HB3	3:A:155:LEU:HB2	1.62	0.81
1:X:339:U:H4'	19:R:77:HIS:CD2	2.16	0.80
1:X:339:U:H4'	19:R:77:HIS:HD2	1.45	0.80
1:X:2218:G:H5'	3:A:249:PRO:HD3	1.62	0.80
1:X:2796:A:OP2	12:K:3:HIS:NE2	2.15	0.79
1:X:215:G:H21	1:X:632:A:H8	1.27	0.79
19:R:80:LYS:NZ	19:R:81:VAL:O	2.13	0.79
8:G:73:ASN:O	8:G:140:GLN:NE2	2.16	0.78
1:X:2638:G:OP1	7:E:158:HIS:NE2	2.17	0.78
28:3:37:SER:OG	28:3:38:GLY:N	2.16	0.78
4:B:194:GLY:HA2	14:M:2:GLN:HB3	1.65	0.78
6:D:13:ARG:HG3	6:D:28:VAL:HG21	1.63	0.78
7:E:56:SER:HG	7:E:61:HIS:HD1	1.26	0.78
1:X:596:C:N3	10:I:37:GLN:NE2	2.32	0.78
4:B:143:GLN:HB2	4:B:147:PRO:HG3	1.65	0.78
1:X:841:G:H2'	1:X:842:A:C8	2.19	0.78
1:X:1007:A:H4'	15:N:93:LYS:HZ3	1.49	0.77
1:X:89:A:O2'	1:X:91:A:N6	2.18	0.77
13:L:26:ARG:NH1	13:L:86:GLN:O	2.17	0.77
1:X:2237:C:O2'	1:X:2406:C:OP2	2.00	0.77
13:L:11:LEU:HD12	13:L:93:SER:HB3	1.65	0.77
1:X:1278:A:H2	1:X:1997:A:H62	1.32	0.77
1:X:1337:G:OP2	17:P:105:ARG:NH1	2.18	0.77
1:X:2660:C:H42	1:X:2705:A:H2	1.31	0.76
9:H:88:THR:HB	14:M:80:VAL:HB	1.67	0.76
1:X:923:A:N7	11:J:12:LYS:HG2	1.99	0.76
1:X:1617:G:OP2	18:Q:57:ASN:ND2	2.18	0.76
1:X:1834:G:O2'	3:A:244:ARG:NH2	2.19	0.76
3:A:246:PRO:HD2	3:A:251:GLY:H	1.49	0.76
9:H:29:ILE:HG21	9:H:122:ARG:HB2	1.68	0.76
10:I:33:GLY:HA2	16:O:79:GLN:HG3	1.68	0.76
19:R:59:LYS:HB3	19:R:62:MET:HB2	1.68	0.76
3:A:172:TYR:HA	3:A:186:HIS:HA	1.68	0.76
9:H:124:MET:HA	9:H:127:VAL:HB	1.68	0.75
2:Y:46:G:N3	2:Y:49:C:N4	2.34	0.75
8:G:31:THR:HG22	15:N:61:TRP:CH2	2.22	0.75
8:G:67:ARG:HB2	8:G:70:PHE:HA	1.69	0.75
16:O:34:GLU:HB2	16:O:56:VAL:HG23	1.69	0.75
1:X:2672:U:H2'	1:X:2673:G:H8	1.50	0.75
1:X:1373:G:H22	1:X:2192:U:H3	1.35	0.74
1:X:2474:G:H5"	11:J:82:THR:HA	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:101:PRO:O	17:P:121:THR:OG1	2.05	0.74
1:X:989:G:HO2'	1:X:1013:G:HO2'	1.29	0.74
2:Y:42:U:O2'	2:Y:47:A:N6	2.20	0.74
2:Y:57:U:HO2'	6:D:24:SER:HG	1.32	0.74
12:K:24:GLN:HB3	12:K:44:LEU:HD22	1.69	0.74
1:X:2043:A:H62	5:C:68:ARG:HH12	1.36	0.74
15:N:92:ARG:HB3	15:N:95:LEU:HD22	1.69	0.74
1:X:1348:C:OP2	18:Q:62:ARG:NH1	2.21	0.74
24:W:2:LYS:HB3	24:W:54:GLN:HB3	1.69	0.74
1:X:1222:G:O2'	1:X:1250:A:N6	2.21	0.74
20:S:69:VAL:HG13	20:S:81:VAL:HG22	1.70	0.73
1:X:954:U:OP2	10:I:38:LYS:NZ	2.17	0.73
3:A:205:VAL:HG12	3:A:207:GLY:H	1.50	0.73
9:H:76:ARG:NH1	9:H:113:PRO:O	2.20	0.73
3:A:108:PRO:HA	3:A:196:VAL:HA	1.71	0.73
1:X:1769:U:H2'	1:X:1775:A:H62	1.53	0.73
1:X:2551:A:H5"	1:X:2553:G:H4'	1.68	0.73
3:A:250:TRP:O	3:A:255:LYS:NZ	2.19	0.73
1:X:1283:C:H5"	1:X:1284:G:H5'	1.71	0.72
1:X:2059:U:OP2	1:X:2217:G:N2	2.20	0.72
1:X:2556:A:H5"	1:X:2557:G:H5'	1.71	0.72
19:R:37:LEU:HD11	19:R:49:GLU:HG3	1.71	0.72
1:X:492:G:O2'	1:X:517:A:N6	2.22	0.72
1:X:2170:C:H3'	1:X:2171:U:H5"	1.70	0.72
4:B:60:ASN:HB3	4:B:62:PRO:HD2	1.70	0.72
9:H:70:VAL:HG21	9:H:98:ILE:HG23	1.72	0.72
22:U:19:ILE:HA	22:U:42:GLN:HA	1.72	0.72
2:Y:27:A:N6	2:Y:56:G:OP2	2.23	0.72
1:X:168:A:H2'	1:X:169:C:C6	2.25	0.71
1:X:558:G:H8	1:X:560:G:C8	2.08	0.71
1:X:2450:A:N3	29:X:2901:6O1:O30	2.23	0.71
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.71	0.71
3:A:45:ASN:OD1	3:A:46:ARG:NH1	2.22	0.71
9:H:113:PRO:HD3	14:M:73:PHE:HB2	1.72	0.71
1:X:1264:C:H5"	15:N:13:ARG:NH1	2.05	0.71
20:S:47:SER:OG	20:S:48:THR:N	2.20	0.71
1:X:2545:A:H61	9:H:40:GLY:HA3	1.56	0.71
1:X:2716:G:H1	1:X:2748:C:H42	1.39	0.71
16:O:11:GLN:HE22	16:O:38:LEU:HB3	1.55	0.71
1:X:89:A:H4'	1:X:90:G:H5'	1.73	0.71
1:X:160:C:O2'	1:X:445:A:N3	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:349:G:OP1	19:R:13:LYS:NZ	2.20	0.71
5:C:54:THR:HG21	5:C:72:ARG:HB2	1.72	0.71
12:K:29:LEU:HD13	12:K:79:VAL:HG11	1.73	0.71
21:T:23:VAL:HG13	21:T:38:VAL:HG23	1.71	0.71
22:U:31:GLY:HA2	22:U:32:ARG:HH11	1.56	0.71
1:X:408:U:H2'	1:X:409:G:C8	2.26	0.71
1:X:1079:G:N2	1:X:1106:A:O2'	2.24	0.71
1:X:1333:G:N2	1:X:1344:C:H41	1.88	0.70
1:X:2516:U:H2'	1:X:2517:C:C6	2.26	0.70
8:G:157:PRO:O	8:G:161:GLN:NE2	2.24	0.70
15:N:88:ILE:HG12	16:O:49:GLU:HB2	1.71	0.70
12:K:13:ASN:OD1	12:K:14:SER:N	2.24	0.70
22:U:27:ASP:HB3	22:U:32:ARG:HA	1.73	0.70
18:Q:62:ARG:O	18:Q:70:GLY:HA3	1.90	0.70
1:X:346:C:H2'	1:X:347:C:H6	1.55	0.70
1:X:2634:G:O2'	1:X:2635:U:OP2	2.09	0.70
3:A:168:LYS:HB3	3:A:173:VAL:HG13	1.73	0.70
1:X:242:A:N6	1:X:441:A:OP2	2.24	0.70
1:X:1007:A:H2'	1:X:1008:G:H8	1.55	0.70
1:X:1551:U:OP2	1:X:1553:G:N2	2.24	0.70
1:X:1922:U:OP1	1:X:2583:U:O2'	2.08	0.70
1:X:2029:G:OP1	25:Z:15:LYS:NZ	2.16	0.69
20:S:93:GLU:HG3	20:S:123:VAL:HG23	1.74	0.69
1:X:304:A:N6	1:X:356:A:N7	2.39	0.69
6:D:38:GLU:HB3	6:D:87:ILE:HB	1.73	0.69
1:X:2400:G:N7	28:3:32:GLN:HB3	2.07	0.69
1:X:797:A:C5	3:A:229:VAL:HG21	2.27	0.69
2:Y:30:C:OP1	13:L:37:HIS:ND1	2.25	0.69
28:3:14:ILE:HD13	28:3:56:ALA:HB1	1.74	0.69
3:A:218:LYS:NZ	3:A:219:PRO:O	2.25	0.69
4:B:122:PHE:HE2	4:B:138:PRO:HB3	1.58	0.69
5:C:163:ASN:HB3	5:C:166:TRP:HB2	1.73	0.69
1:X:588:G:O2'	1:X:2002:A:OP1	2.07	0.69
1:X:1422:C:H2'	1:X:1423:A:H8	1.58	0.69
10:I:18:ARG:HB3	10:I:21:ARG:HB2	1.74	0.69
1:X:854:G:H1	1:X:948:C:H42	1.39	0.69
8:G:149:LYS:NZ	8:G:160:ALA:O	2.26	0.69
17:P:25:PHE:HD1	17:P:127:ILE:HD11	1.58	0.69
1:X:1329:U:H2'	1:X:1330:G:H8	1.58	0.68
1:X:1386:A:OP1	1:X:2191:A:N6	2.25	0.68
1:X:1810:U:OP2	3:A:157:ARG:NH1	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1542:G:H22	1:X:1562:G:H1	1.39	0.68
17:P:25:PHE:HA	17:P:127:ILE:HG12	1.74	0.68
20:S:25:ASN:HB3	20:S:85:MET:HB2	1.74	0.68
22:U:53:GLU:HB3	22:U:58:LYS:H	1.57	0.68
1:X:1296:G:H22	1:X:1299:A:H5'	1.58	0.68
13:L:15:ARG:HA	13:L:15:ARG:HH11	1.58	0.68
1:X:863:C:HO2'	24:W:19:THR:HG1	1.38	0.68
1:X:1124:U:H2'	1:X:1125:G:H8	1.58	0.68
22:U:54:ASN:HA	22:U:78:ILE:HG22	1.75	0.68
3:A:14:ARG:HH11	3:A:27:LYS:HB3	1.59	0.68
9:H:75:VAL:HG12	9:H:118:LEU:HD21	1.76	0.68
1:X:673:G:N3	10:I:21:ARG:NH2	2.41	0.68
20:S:3:LEU:HD13	20:S:32:PHE:HB3	1.75	0.68
3:A:245:VAL:HA	3:A:251:GLY:HA2	1.75	0.68
7:E:8:PRO:O	7:E:69:ARG:NH1	2.26	0.68
13:L:8:ARG:HG3	13:L:9:ARG:H	1.59	0.68
1:X:203:G:O2'	1:X:205:A:N6	2.26	0.68
1:X:2838:U:H2'	1:X:2839:G:H8	1.58	0.68
1:X:2551:A:C8	4:B:144:ARG:HG2	2.29	0.68
1:X:2659:C:H5'	4:B:189:PRO:HA	1.77	0.68
26:1:30:ASN:HD22	26:1:31:THR:H	1.41	0.67
1:X:2672:U:H2'	1:X:2673:G:C8	2.29	0.67
1:X:2786:G:H5"	4:B:60:ASN:HD22	1.59	0.67
1:X:346:C:H2'	1:X:347:C:C6	2.28	0.67
1:X:1054:C:H42	1:X:1123:G:H1	1.40	0.67
1:X:1850:G:O2'	1:X:1867:A:N6	2.27	0.67
1:X:2663:U:H3	1:X:2705:A:H62	1.39	0.67
8:G:41:TRP:HZ3	8:G:149:LYS:HD2	1.58	0.67
2:Y:52:G:OP1	13:L:65:THR:OG1	2.11	0.67
1:X:646:C:O2'	1:X:650:U:OP1	2.09	0.67
1:X:1678:G:H1	1:X:1982:C:H42	1.42	0.67
1:X:1684:G:O2'	1:X:1974:U:O4	2.11	0.67
1:X:1882:G:N2	1:X:1885:C:H41	1.93	0.67
1:X:64:C:OP1	18:Q:71:GLN:HB2	1.95	0.67
1:X:492:G:H1'	1:X:516:G:N2	2.10	0.67
1:X:1800:A:H4'	1:X:1801:C:OP1	1.95	0.67
10:I:18:ARG:O	10:I:18:ARG:NH2	2.27	0.67
10:I:56:LEU:HB3	28:3:52:LYS:NZ	2.09	0.67
13:L:76:ALA:HB2	13:L:107:ALA:HA	1.75	0.67
1:X:504:G:H4'	17:P:27:VAL:HG12	1.76	0.67
1:X:791:G:H5"	3:A:48:ARG:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:812:G:H3'	1:X:813:A:H2'	1.75	0.67
1:X:1340:C:O3'	12:K:104:ARG:NH2	2.28	0.67
1:X:1429:A:H1'	1:X:1603:A:C6	2.30	0.67
1:X:2372:A:H62	1:X:2401:A:H62	1.43	0.67
3:A:176:ARG:HH11	3:A:180:GLY:HA2	1.60	0.67
18:Q:63:LYS:HE3	18:Q:65:VAL:HA	1.77	0.67
1:X:712:A:H2'	1:X:713:G:O4'	1.94	0.66
1:X:953:G:O2'	1:X:1203:A:N3	2.27	0.66
6:D:72:LYS:HA	6:D:81:GLN:HA	1.77	0.66
6:D:119:PRO:HD3	6:D:178:ARG:HG3	1.77	0.66
1:X:746:G:N7	1:X:774:A:C6	2.63	0.66
2:Y:115:G:N2	13:L:48:GLY:O	2.28	0.66
5:C:136:TRP:O	5:C:140:ASN:ND2	2.27	0.66
3:A:244:ARG:HD2	3:A:253:PRO:HD3	1.78	0.66
2:Y:27:A:O2'	2:Y:28:A:O5'	2.12	0.66
5:C:129:LYS:O	5:C:131:LYS:N	2.28	0.66
13:L:54:ALA:H	13:L:75:LEU:HD13	1.60	0.66
1:X:1264:C:OP1	15:N:13:ARG:NH1	2.29	0.66
1:X:920:G:H21	11:J:11:ARG:HH22	1.44	0.66
25:Z:6:VAL:HG22	25:Z:7:PRO:HD2	1.77	0.66
1:X:761:G:H5"	17:P:110:ALA:HB2	1.78	0.66
1:X:1431:U:H4'	1:X:1604:A:H4'	1.78	0.66
4:B:131:SER:O	4:B:134:TRP:NE1	2.26	0.66
22:U:21:ARG:HA	22:U:39:LYS:HB2	1.77	0.66
1:X:88:G:H3'	1:X:89:A:H5"	1.78	0.66
1:X:83:A:H3'	19:R:17:LYS:HG2	1.78	0.65
1:X:1332:G:O2'	1:X:1333:G:H5'	1.96	0.65
1:X:1675:C:H2'	1:X:1676:U:C6	2.30	0.65
15:N:24:PHE:HB2	15:N:29:SER:HB3	1.77	0.65
22:U:48:LYS:HE2	22:U:49:LYS:H	1.61	0.65
1:X:318:G:N2	1:X:321:A:OP2	2.28	0.65
11:J:21:ASP:HA	11:J:99:LYS:HE2	1.79	0.65
13:L:26:ARG:HH11	13:L:88:VAL:HG22	1.61	0.65
1:X:595:A:H5'	5:C:83:ALA:HB3	1.79	0.65
1:X:814:G:OP2	5:C:56:ARG:NH2	2.29	0.65
1:X:2064:U:H5'	22:U:41:VAL:HG21	1.78	0.65
5:C:3:GLN:H	5:C:12:GLY:HA3	1.62	0.65
8:G:100:TYR:CB	8:G:116:ARG:HE	2.06	0.65
1:X:786:U:H4'	3:A:47:GLY:HA2	1.78	0.65
3:A:43:ARG:HB3	3:A:54:ILE:HG13	1.78	0.65
21:T:26:PHE:N	21:T:29:GLU:OE1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:11:GLY:O	5:C:13:ARG:NH1	2.30	0.65
10:I:80:LEU:O	10:I:116:ARG:NH2	2.30	0.65
3:A:56:GLY:H	3:A:217:ARG:HB2	1.60	0.65
15:N:61:TRP:CE2	15:N:94:VAL:HG22	2.32	0.65
1:X:540:G:C5	1:X:2005:U:H5"	2.32	0.65
1:X:1184:G:H3'	1:X:1185:C:H5"	1.79	0.65
5:C:95:LEU:O	5:C:100:ARG:NH2	2.30	0.65
1:X:679:C:H5"	10:I:49:PHE:HB3	1.77	0.65
21:T:45:PHE:HB3	21:T:77:ARG:HB2	1.79	0.65
1:X:1270:C:H5'	5:C:69:HIS:CE1	2.32	0.65
26:1:35:LEU:HA	26:1:53:LYS:HD2	1.78	0.65
1:X:692:C:H2'	1:X:693:A:H8	1.61	0.64
1:X:1342:U:H5"	1:X:1343:C:H5	1.62	0.64
10:I:88:PHE:HE1	10:I:118:VAL:HA	1.62	0.64
1:X:2481:G:H5'	1:X:2482:A:H5"	1.79	0.64
1:X:87:G:H2'	1:X:88:G:H5"	1.79	0.64
10:I:81:GLN:HG2	10:I:116:ARG:HB3	1.78	0.64
13:L:33:ARG:HH11	13:L:38:ILE:HG21	1.62	0.64
3:A:143:HIS:ND1	3:A:194:GLY:O	2.27	0.64
1:X:332:C:HO2'	1:X:351:A:HO2'	1.42	0.64
1:X:1443:G:H2'	1:X:1444:C:C6	2.33	0.64
19:R:84:VAL:HG21	19:R:89:GLY:HA2	1.78	0.64
1:X:2556:A:H1'	25:Z:4:HIS:HB3	1.79	0.64
1:X:2838:U:H2'	1:X:2839:G:C8	2.33	0.64
13:L:27:LEU:HB2	13:L:87:VAL:HG22	1.79	0.64
11:J:78:LYS:HD2	11:J:81:GLU:HA	1.80	0.64
1:X:1345:G:N7	1:X:1625:A:O2'	2.26	0.64
1:X:2766:U:OP1	4:B:69:LYS:NZ	2.28	0.64
3:A:203:ASN:OD1	3:A:203:ASN:N	2.28	0.64
1:X:1685:A:O2'	1:X:1691:G:N7	2.28	0.64
1:X:2811:G:H2'	1:X:2812:A:C8	2.32	0.64
6:D:60:ILE:HG13	6:D:61:THR:HG23	1.79	0.64
8:G:84:ASN:O	8:G:152:ALA:HA	1.97	0.64
19:R:97:GLN:HB3	19:R:101:GLY:HA2	1.80	0.64
1:X:1674:C:H2'	1:X:1675:C:C6	2.33	0.63
1:X:1744:G:N2	1:X:1747:G:OP2	2.30	0.63
1:X:1296:G:N2	1:X:1299:A:H5'	2.13	0.63
1:X:1746:A:H2	1:X:2696:A:HO2'	1.47	0.63
22:U:47:HIS:ND1	22:U:48:LYS:O	2.32	0.63
1:X:1007:A:H1'	16:O:6:GLN:HG3	1.80	0.63
1:X:1791:C:OP1	3:A:261:ARG:NH2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2371:A:C8	10:I:59:ARG:HG2	2.33	0.63
1:X:946:U:H2'	1:X:947:C:C6	2.33	0.63
22:U:21:ARG:HE	22:U:40:ARG:HG2	1.64	0.63
1:X:2324:G:N3	1:X:2360:C:H2'	2.14	0.63
2:Y:7:C:O2'	2:Y:29:C:O2	2.16	0.63
10:I:62:LYS:HD3	10:I:63:ARG:H	1.64	0.63
19:R:81:VAL:HG12	19:R:82:ALA:H	1.64	0.63
1:X:796:A:C8	1:X:797:A:H4'	2.28	0.63
1:X:2222:U:H2'	1:X:2223:U:C6	2.34	0.63
1:X:2796:A:H2'	1:X:2797:G:H8	1.64	0.63
1:X:876:A:H2	1:X:926:C:H41	1.46	0.63
7:E:103:LEU:HD21	7:E:131:ILE:HD13	1.80	0.63
16:O:56:VAL:HG12	16:O:97:GLY:HA3	1.79	0.63
26:1:51:ARG:NH2	26:1:53:LYS:O	2.32	0.63
1:X:1003:C:H2'	1:X:1004:A:H8	1.63	0.63
1:X:1223:G:H5'	1:X:1225:G:O4'	1.98	0.63
1:X:649:G:C6	1:X:662:G:N2	2.67	0.62
1:X:938:G:H4'	1:X:939:C:H5'	1.81	0.62
1:X:2240:C:N4	21:T:14:ARG:O	2.32	0.62
8:G:61:ARG:NH1	8:G:66:HIS:H	1.97	0.62
25:Z:18:MET:O	25:Z:21:SER:HB3	1.98	0.62
1:X:830:C:O2'	1:X:852:U:OP1	2.17	0.62
3:A:25:THR:HG23	3:A:211:ARG:HH12	1.65	0.62
4:B:37:LYS:NZ	4:B:80:GLU:OE2	2.29	0.62
4:B:117:MET:HA	4:B:121:ASN:O	1.99	0.62
19:R:16:PHE:HZ	19:R:46:VAL:HG21	1.64	0.62
19:R:48:VAL:HG13	19:R:50:GLY:H	1.64	0.62
1:X:824:U:C2'	10:I:30:ALA:HA	2.30	0.62
2:Y:11:G:OP2	13:L:16:LYS:NZ	2.26	0.62
20:S:51:LEU:HD23	20:S:51:LEU:H	1.64	0.62
5:C:39:ARG:HH21	5:C:91:TYR:HB2	1.64	0.62
6:D:74:ILE:HA	6:D:79:LEU:HB3	1.81	0.62
1:X:564:U:H2'	1:X:565:A:C8	2.34	0.62
16:O:5:ILE:HG23	16:O:10:LYS:NZ	2.14	0.62
1:X:824:U:H2'	10:I:30:ALA:CA	2.27	0.62
3:A:96:HIS:HE1	3:A:100:GLY:HA2	1.65	0.62
29:X:2901:6O1:O57	29:X:2901:6O1:O52	2.15	0.62
20:S:50:GLY:HA2	20:S:130:ILE:HD12	1.82	0.62
1:X:172:A:H61	1:X:175:C:H3'	1.65	0.62
1:X:403:A:H4'	1:X:404:A:H5'	1.82	0.62
1:X:2579:A:H2'	1:X:2580:C:C6	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2693:U:OP1	12:K:14:SER:HB3	2.00	0.61
8:G:103:TYR:C	8:G:107:GLN:HG3	2.21	0.61
10:I:56:LEU:HD22	28:3:52:LYS:HZ2	1.65	0.61
21:T:64:ASP:OD1	21:T:64:ASP:N	2.32	0.61
5:C:149:LEU:HD11	5:C:170:LEU:HB2	1.83	0.61
1:X:825:C:H5"	10:I:30:ALA:HB1	1.82	0.61
1:X:1052:C:N4	1:X:1053:G:N7	2.48	0.61
1:X:2372:A:H62	1:X:2401:A:N6	1.99	0.61
4:B:35:GLN:HB3	4:B:48:GLN:HB3	1.82	0.61
22:U:19:ILE:HG22	22:U:42:GLN:HG3	1.82	0.61
22:U:52:ARG:HG3	22:U:62:LEU:HD22	1.81	0.61
3:A:184:ARG:HD2	3:A:266:SER:HA	1.82	0.61
14:M:31:ASP:N	14:M:31:ASP:OD1	2.31	0.61
1:X:872:G:O2'	1:X:928:G:O6	2.17	0.61
1:X:1584:G:H5"	3:A:61:LEU:HG	1.82	0.61
11:J:49:GLU:OE2	11:J:52:ARG:NH2	2.34	0.61
20:S:104:SER:HA	20:S:139:THR:HA	1.81	0.61
2:Y:9:G:H5'	13:L:32:TYR:CE2	2.35	0.61
13:L:40:ALA:HB2	13:L:103:LEU:HD11	1.82	0.61
22:U:47:HIS:CG	22:U:48:LYS:H	2.19	0.61
1:X:171:G:H2'	1:X:172:A:O4'	2.00	0.61
1:X:517:A:H5"	1:X:518:A:H5'	1.83	0.61
1:X:1279:G:O2'	1:X:1995:G:O6	2.12	0.61
27:2:41:GLN:HA	27:2:41:GLN:NE2	2.14	0.61
1:X:943:U:O2'	1:X:944:A:O4'	2.10	0.61
1:X:1008:G:OP1	15:N:93:LYS:HB2	2.01	0.61
1:X:1182:U:H3	1:X:1192:A:H61	1.48	0.61
6:D:46:ASP:HB2	6:D:49:ALA:HB3	1.83	0.61
13:L:89:PHE:O	13:L:91:ARG:NH2	2.33	0.61
26:1:25:THR:O	26:1:27:ASN:ND2	2.34	0.61
28:3:26:LYS:HE2	28:3:43:GLY:HA3	1.81	0.61
1:X:2696:A:O2'	1:X:2697:G:H5'	2.01	0.60
8:G:70:PHE:HB3	15:N:64:ARG:HG2	1.83	0.60
20:S:9:THR:HG22	20:S:11:LYS:H	1.65	0.60
1:X:1250:A:OP1	1:X:1250:A:H4'	1.99	0.60
1:X:1468:A:C8	1:X:1468:A:H5"	2.36	0.60
8:G:31:THR:HG22	15:N:61:TRP:HH2	1.65	0.60
12:K:33:ARG:HG3	12:K:114:GLU:HB3	1.83	0.60
22:U:63:SER:O	22:U:67:LEU:N	2.33	0.60
25:Z:35:GLN:HG3	25:Z:51:TYR:CD2	2.36	0.60
1:X:1279:G:O5'	17:P:36:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:603:C:H2'	1:X:604:U:C6	2.36	0.60
1:X:2873:G:H2'	1:X:2874:A:C8	2.35	0.60
8:G:119:LEU:HD13	8:G:122:HIS:CE1	2.36	0.60
1:X:537:C:O2'	1:X:538:A:C4	2.54	0.60
1:X:2466:G:H2'	1:X:2467:A:H8	1.65	0.60
20:S:70:GLN:HB2	20:S:80:HIS:HB3	1.82	0.60
1:X:1196:G:H2'	1:X:1197:U:O4'	2.01	0.60
1:X:1313:U:H4'	1:X:1314:A:H5"	1.84	0.60
1:X:1915:A:H3'	1:X:1916:G:H8	1.66	0.60
1:X:2335:U:H4'	21:T:20:TYR:CD2	2.37	0.60
22:U:22:GLY:HA3	22:U:39:LYS:NZ	2.15	0.60
26:1:28:ARG:HB2	26:1:30:ASN:OD1	2.02	0.60
17:P:14:ARG:HA	17:P:17:GLN:HG2	1.82	0.60
1:X:37:C:O2	5:C:44:SER:OG	2.19	0.60
1:X:806:A:OP2	1:X:2054:A:O2'	2.20	0.60
1:X:2757:G:OP2	1:X:2761:A:O2'	2.19	0.60
2:Y:52:G:OP2	13:L:65:THR:HG21	2.02	0.60
2:Y:57:U:O2'	6:D:24:SER:OG	2.17	0.60
8:G:84:ASN:HD22	8:G:87:GLN:HG3	1.66	0.60
9:H:12:ASP:OD1	9:H:14:SER:OG	2.14	0.60
1:X:478:G:OP1	27:2:33:ARG:HD2	2.01	0.60
26:1:14:SER:HB2	26:1:22:TYR:HA	1.84	0.60
1:X:863:C:O2'	24:W:19:THR:OG1	2.13	0.60
10:I:32:ARG:HD2	10:I:32:ARG:O	2.02	0.60
18:Q:61:LYS:H	18:Q:72:ARG:HA	1.66	0.60
24:W:38:PRO:HD3	24:W:41:ARG:HH21	1.66	0.60
1:X:415:A:H61	1:X:436:A:H61	1.50	0.59
1:X:627:A:H2'	1:X:628:A:C8	2.36	0.59
5:C:76:THR:O	5:C:76:THR:OG1	2.15	0.59
9:H:28:GLY:O	9:H:35:THR:N	2.29	0.59
12:K:87:TYR:HE1	12:K:94:TYR:HD1	1.49	0.59
1:X:636:G:H5'	1:X:637:G:OP2	2.01	0.59
1:X:1422:C:H2'	1:X:1423:A:C8	2.38	0.59
1:X:1643:A:H61	1:X:1656:U:H3	1.49	0.59
1:X:2245:A:H4'	1:X:2246:A:C2	2.37	0.59
6:D:74:ILE:HG12	6:D:80:ARG:HA	1.83	0.59
26:1:30:ASN:ND2	26:1:31:THR:H	1.99	0.59
3:A:133:LEU:HB2	3:A:187:SER:HA	1.84	0.59
14:M:56:ALA:HB3	14:M:67:THR:HB	1.84	0.59
24:W:23:LEU:HD21	24:W:43:MET:HB3	1.84	0.59
1:X:1333:G:N7	1:X:1342:U:H5'	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:8:TYR:HH	6:D:31:ILE:H	1.50	0.59
6:D:8:TYR:OH	6:D:31:ILE:N	2.29	0.59
1:X:48:A:H61	1:X:154:U:H2'	1.67	0.59
1:X:417:C:H4'	1:X:418:C:H5'	1.83	0.59
1:X:1058:G:O2'	1:X:1122:A:N6	2.36	0.59
1:X:1154:A:H8	1:X:1154:A:OP1	1.85	0.59
1:X:1673:C:OP1	4:B:136:ARG:HG2	2.02	0.59
1:X:2038:C:H5'	1:X:2039:G:H5"	1.84	0.59
2:Y:17:A:H1'	2:Y:112:A:C8	2.37	0.59
2:Y:22:U:O2'	2:Y:66:G:N2	2.36	0.59
6:D:13:ARG:HA	6:D:28:VAL:HG11	1.85	0.59
1:X:742:G:C6	3:A:208:LYS:HB3	2.37	0.59
1:X:1963:G:O2'	1:X:1965:U:OP2	2.20	0.59
6:D:167:ARG:HG3	6:D:177:PHE:CZ	2.38	0.59
26:1:35:LEU:HD13	26:1:37:LEU:HD12	1.83	0.59
3:A:170:SER:OG	3:A:171:ASP:N	2.35	0.59
4:B:5:LEU:HD13	4:B:51:TYR:HB2	1.84	0.59
4:B:122:PHE:CE2	4:B:138:PRO:HB3	2.36	0.59
1:X:2226:A:H2'	1:X:2227:C:C6	2.37	0.59
6:D:132:ILE:HG13	6:D:154:ILE:HD13	1.85	0.59
1:X:1983:G:HO2'	1:X:2668:U:H6	1.51	0.59
3:A:14:ARG:HD2	3:A:27:LYS:HB3	1.84	0.59
9:H:77:THR:HA	9:H:94:ASN:HB3	1.84	0.59
27:2:1:MET:HG3	27:2:3:ARG:NH1	2.18	0.59
1:X:1179:A:H2'	1:X:1180:A:C8	2.37	0.58
1:X:2285:U:O4'	6:D:150:ARG:NH1	2.36	0.58
1:X:1225:G:H2'	1:X:1249:G:H22	1.68	0.58
1:X:2298:U:O2	1:X:2299:A:N6	2.36	0.58
1:X:2491:C:OP1	4:B:123:ALA:HB2	2.03	0.58
1:X:2607:C:H1'	1:X:2761:A:H2'	1.85	0.58
2:Y:9:G:H21	13:L:41:GLN:HE22	1.49	0.58
9:H:23:ARG:HG2	9:H:25:LEU:HD23	1.84	0.58
1:X:492:G:H1'	1:X:516:G:H21	1.67	0.58
1:X:1839:A:HO2'	1:X:1840:A:H8	1.49	0.58
3:A:60:ARG:HD3	3:A:87:ASN:HD22	1.68	0.58
1:X:1212:U:H2'	1:X:1213:U:C6	2.38	0.58
1:X:1745:C:O2	1:X:2697:G:H4'	2.04	0.58
1:X:2634:G:O2'	1:X:2643:G:N1	2.36	0.58
9:H:41:ASN:HD22	9:H:42:LYS:H	1.52	0.58
21:T:18:PRO:O	21:T:19:LYS:HG2	2.02	0.58
1:X:691:C:H2'	1:X:692:C:C6	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1582:A:OP1	3:A:211:ARG:NH1	2.35	0.58
1:X:1594:U:H2'	1:X:1595:A:H8	1.68	0.58
1:X:2262:C:O2	1:X:2304:G:N2	2.26	0.58
1:X:178:C:O5'	22:U:40:ARG:NH2	2.36	0.58
1:X:834:A:H5'	1:X:835:U:C6	2.39	0.58
1:X:930:A:N3	2:Y:82:U:O2'	2.33	0.58
1:X:1264:C:OP1	15:N:10:ARG:HG3	2.02	0.58
1:X:1268:U:H2'	5:C:66:ASN:HA	1.85	0.58
1:X:1332:G:C6	1:X:1333:G:N1	2.71	0.58
1:X:1047:G:H1	1:X:1130:U:H3	1.52	0.58
1:X:1770:U:H5	1:X:1775:A:N7	2.01	0.58
21:T:25:LYS:HB2	21:T:37:LEU:HA	1.86	0.58
1:X:774:A:H8	1:X:774:A:O5'	1.86	0.58
1:X:1261:G:C4	15:N:3:ARG:HG2	2.39	0.58
1:X:1350:G:H2'	1:X:1351:G:H8	1.69	0.58
1:X:2494:C:H42	1:X:2548:G:H1	1.50	0.58
4:B:92:ASN:HA	4:B:95:ILE:HB	1.84	0.58
11:J:48:ILE:O	11:J:52:ARG:N	2.26	0.58
1:X:537:C:H1'	1:X:538:A:C6	2.39	0.58
1:X:1586:A:H2'	1:X:1587:A:C8	2.39	0.58
26:1:8:ILE:HG12	26:1:9:ILE:HG23	1.86	0.58
1:X:1919:A:H2	1:X:1926:U:H3	1.51	0.58
1:X:1922:U:H3'	1:X:1923:U:H5'	1.84	0.58
3:A:182:LEU:HB2	3:A:268:ARG:O	2.04	0.58
6:D:60:ILE:O	6:D:102:LYS:NZ	2.31	0.58
15:N:78:THR:HG23	15:N:117:ARG:CZ	2.34	0.58
1:X:2594:U:C6	25:Z:7:PRO:HA	2.39	0.57
3:A:231:HIS:CD2	3:A:232:PRO:HD2	2.38	0.57
6:D:134:GLU:HG2	6:D:136:LEU:H	1.69	0.57
18:Q:10:PRO:HD3	23:V:30:PHE:CD2	2.38	0.57
19:R:92:THR:HA	19:R:108:VAL:HG22	1.85	0.57
26:1:46:LYS:O	26:1:48:VAL:HG12	2.04	0.57
1:X:753:U:H2'	1:X:754:G:C8	2.39	0.57
1:X:2212:U:H2'	1:X:2213:G:C8	2.39	0.57
1:X:2772:U:H2'	1:X:2773:G:C8	2.38	0.57
6:D:70:ALA:HB3	6:D:82:GLY:HA2	1.86	0.57
10:I:81:GLN:HA	10:I:116:ARG:HD2	1.86	0.57
20:S:117:VAL:HG22	20:S:168:VAL:HA	1.86	0.57
1:X:636:G:O2'	1:X:669:G:H4'	2.03	0.57
1:X:487:G:H4'	1:X:512:A:N1	2.18	0.57
1:X:829:C:H2'	1:X:830:C:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2234:G:H2'	1:X:2235:G:O4'	2.04	0.57
1:X:2269:G:H22	1:X:2322:U:H1'	1.70	0.57
2:Y:44:C:O2'	6:D:64:LYS:O	2.18	0.57
4:B:38:THR:HB	4:B:41:THR:HG23	1.86	0.57
6:D:111:ILE:HG12	6:D:137:ILE:HD12	1.87	0.57
10:I:90:ARG:HA	10:I:121:HIS:H	1.69	0.57
14:M:78:GLU:OE1	14:M:108:ARG:NH2	2.35	0.57
15:N:66:ASN:ND2	15:N:70:ARG:HH12	2.01	0.57
8:G:31:THR:OG1	8:G:32:TYR:N	2.37	0.57
1:X:1974:U:O2'	1:X:1975:G:H5'	2.04	0.57
1:X:2398:U:H5'	26:1:24:THR:HG21	1.86	0.57
1:X:2708:U:H2'	1:X:2709:C:C6	2.39	0.57
8:G:122:HIS:ND1	8:G:122:HIS:O	2.38	0.57
1:X:408:U:H2'	1:X:409:G:H8	1.67	0.57
1:X:1886:G:H2'	1:X:1887:G:H8	1.69	0.57
1:X:398:C:H42	1:X:424:G:H1	1.52	0.57
3:A:246:PRO:HD2	3:A:251:GLY:N	2.19	0.57
4:B:120:TRP:CD1	4:B:155:ARG:HB3	2.40	0.57
9:H:109:ARG:HA	9:H:129:LEU:HD13	1.86	0.57
26:1:13:GLU:HG2	26:1:24:THR:HA	1.86	0.57
9:H:19:ILE:O	9:H:19:ILE:HG13	2.05	0.57
15:N:17:VAL:HG21	15:N:32:TYR:HE1	1.69	0.57
1:X:1030:U:H3	1:X:1153:A:N6	1.98	0.57
1:X:1336:G:O6	1:X:1337:G:C6	2.58	0.57
1:X:2006:G:H5'	1:X:2596:C:H4'	1.86	0.57
1:X:2795:A:N3	1:X:2795:A:H2'	2.18	0.57
14:M:104:LEU:HD23	14:M:106:TYR:CE2	2.40	0.57
1:X:143:A:H2'	1:X:144:U:C6	2.39	0.56
1:X:394:U:OP2	22:U:21:ARG:NH2	2.38	0.56
1:X:1333:G:N2	1:X:1344:C:N4	2.52	0.56
1:X:2034:A:H4'	4:B:141:ILE:HG12	1.85	0.56
19:R:16:PHE:CZ	19:R:46:VAL:HG21	2.40	0.56
28:3:29:LYS:NZ	28:3:36:LYS:O	2.36	0.56
1:X:16:G:H2'	1:X:17:G:H8	1.69	0.56
1:X:1443:G:H2'	1:X:1444:C:H6	1.68	0.56
2:Y:7:C:H2'	2:Y:8:C:H6	1.70	0.56
1:X:1046:U:H5'	7:E:59:GLN:HG2	1.87	0.56
1:X:1321:A:H5'	1:X:1322:G:OP2	2.05	0.56
1:X:1834:G:H2'	1:X:1835:C:C6	2.41	0.56
1:X:1976:U:C5'	4:B:128:SER:HB3	2.35	0.56
1:X:2020:G:H2'	1:X:2021:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:14:ILE:HG12	14:M:20:HIS:CD2	2.39	0.56
5:C:152:THR:OG1	5:C:153:ASP:N	2.39	0.56
9:H:2:ILE:HD12	9:H:8:LEU:HD21	1.87	0.56
1:X:1831:G:H2'	1:X:1832:G:H8	1.71	0.56
1:X:2313:G:C2	13:L:13:THR:HG22	2.41	0.56
1:X:2372:A:N6	1:X:2401:A:H62	2.02	0.56
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.88	0.56
4:B:39:ALA:HB2	4:B:45:GLU:HG2	1.87	0.56
1:X:2225:G:H2'	1:X:2226:A:H8	1.68	0.56
19:R:26:SER:O	19:R:30:LYS:HB2	2.05	0.56
20:S:3:LEU:HD23	20:S:56:VAL:HG13	1.87	0.56
1:X:693:A:H2'	1:X:694:G:C8	2.40	0.56
1:X:1223:G:H4'	1:X:1224:A:H5"	1.87	0.56
1:X:1448:A:H61	1:X:1574:A:H61	1.53	0.56
1:X:1883:A:H1'	1:X:1953:A:H2'	1.88	0.56
1:X:1919:A:H62	1:X:1946:U:H3	1.53	0.56
15:N:20:ARG:NH1	16:O:72:ARG:HD2	2.21	0.56
1:X:568:G:N2	15:N:49:ASP:OD1	2.38	0.56
1:X:1183:C:N4	1:X:1189:G:O6	2.39	0.56
1:X:1360:G:N2	1:X:1615:C:O2	2.34	0.56
2:Y:59:A:H5'	2:Y:60:A:OP2	2.05	0.56
1:X:682:G:H3'	1:X:683:A:H5"	1.88	0.56
1:X:708:G:OP1	1:X:1393:G:O2'	2.24	0.56
1:X:1792:C:OP1	3:A:263:ARG:NH2	2.39	0.56
1:X:2272:A:OP2	13:L:15:ARG:NH2	2.39	0.56
1:X:2797:G:OP2	12:K:3:HIS:NE2	2.38	0.56
1:X:539:A:OP1	1:X:539:A:H4'	2.06	0.56
1:X:1727:C:H2'	1:X:1728:A:C8	2.40	0.56
1:X:2352:A:H2'	1:X:2353:G:C8	2.41	0.56
4:B:8:LYS:HG2	4:B:192:ASN:HA	1.88	0.56
5:C:127:ASP:OD2	5:C:129:LYS:NZ	2.39	0.56
10:I:88:PHE:HB3	10:I:90:ARG:NH2	2.21	0.56
19:R:23:ILE:HG23	19:R:33:THR:HB	1.87	0.56
20:S:72:ASP:HB2	20:S:79:ILE:HD13	1.88	0.56
1:X:854:G:H1	1:X:948:C:N4	2.02	0.55
1:X:1250:A:H2'	1:X:1251:G:O4'	2.06	0.55
1:X:1919:A:H1'	1:X:1923:U:C2	2.41	0.55
6:D:130:LEU:HD13	6:D:132:ILE:HD11	1.88	0.55
9:H:116:ARG:CZ	14:M:38:LYS:HD3	2.36	0.55
11:J:55:MET:HB3	11:J:65:ILE:HD11	1.88	0.55
13:L:31:VAL:HA	13:L:40:ALA:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:27:G:N2	1:X:522:G:H1'	2.21	0.55
1:X:832:A:OP2	1:X:1201:G:N2	2.34	0.55
1:X:953:G:H5"	10:I:38:LYS:HA	1.88	0.55
1:X:2226:A:H2'	1:X:2227:C:H6	1.71	0.55
8:G:141:GLY:O	8:G:144:MET:N	2.39	0.55
9:H:89:ILE:HG23	14:M:79:ARG:HD3	1.89	0.55
1:X:642:A:O2'	10:I:65:PHE:HB2	2.06	0.55
1:X:954:U:P	10:I:38:LYS:HZ3	2.28	0.55
1:X:1482:U:H2'	1:X:1483:G:H8	1.72	0.55
18:Q:73:ASN:N	18:Q:73:ASN:OD1	2.39	0.55
26:1:38:LYS:HD2	26:1:40:TYR:HE1	1.71	0.55
1:X:542:A:C2	1:X:2004:U:H2'	2.41	0.55
1:X:617:U:H5	1:X:632:A:C2	2.24	0.55
1:X:1482:U:H2'	1:X:1483:G:C8	2.41	0.55
1:X:2526:U:H2'	1:X:2527:G:H8	1.71	0.55
1:X:2705:A:H1'	1:X:2706:U:H2'	1.89	0.55
8:G:140:GLN:O	8:G:144:MET:HG3	2.07	0.55
2:Y:44:C:N3	6:D:90:THR:OG1	2.40	0.55
8:G:41:TRP:CZ3	8:G:149:LYS:HD2	2.41	0.55
1:X:2708:U:H2'	1:X:2709:C:H6	1.71	0.55
2:Y:45:C:O2	6:D:92:ARG:NH2	2.40	0.55
7:E:37:TYR:CZ	7:E:72:VAL:HG22	2.42	0.55
8:G:61:ARG:HH12	8:G:66:HIS:HB2	1.72	0.55
10:I:32:ARG:HH12	10:I:34:HIS:HE1	1.55	0.55
17:P:57:LEU:HD13	17:P:69:ALA:HB2	1.88	0.55
18:Q:34:THR:O	18:Q:38:ILE:HG12	2.06	0.55
1:X:75:C:H2'	1:X:76:C:H6	1.70	0.55
1:X:603:C:H4'	28:3:61:MET:HG2	1.88	0.55
1:X:787:A:H2	1:X:800:U:HO2'	1.53	0.55
1:X:2195:C:H5'	1:X:2196:U:OP1	2.07	0.55
8:G:103:TYR:HB3	8:G:107:GLN:CG	2.37	0.55
17:P:95:ALA:HB2	17:P:126:ILE:HG13	1.89	0.55
22:U:54:ASN:CG	22:U:78:ILE:H	2.10	0.55
1:X:2469:G:H8	1:X:2469:G:OP2	1.89	0.55
2:Y:39:C:H5'	2:Y:40:C:OP2	2.08	0.55
6:D:4:LEU:HD11	6:D:7:LYS:HB2	1.88	0.55
1:X:219:G:N2	1:X:231:G:H2'	2.22	0.54
1:X:617:U:C5	1:X:632:A:C2	2.96	0.54
1:X:793:G:H21	1:X:796:A:H62	1.54	0.54
1:X:1630:A:O2'	1:X:1631:C:OP1	2.24	0.54
1:X:1785:A:H2'	1:X:1786:C:C6	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1809:G:H3'	3:A:157:ARG:HH12	1.71	0.54
5:C:58:MET:HG2	5:C:70:GLY:O	2.07	0.54
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.88	0.54
7:E:154:PRO:HA	7:E:160:LYS:O	2.07	0.54
14:M:43:ASN:OD1	14:M:43:ASN:N	2.39	0.54
1:X:2674:C:H2'	1:X:2675:U:H6	1.73	0.54
1:X:2756:A:H3'	1:X:2756:A:OP1	2.07	0.54
2:Y:46:G:H1'	2:Y:49:C:H41	1.72	0.54
3:A:168:LYS:HA	3:A:173:VAL:HA	1.89	0.54
8:G:67:ARG:HG3	8:G:70:PHE:CD1	2.42	0.54
19:R:56:LYS:HA	19:R:69:GLN:HG2	1.88	0.54
1:X:224:G:H4'	1:X:399:G:C5	2.43	0.54
1:X:834:A:H5'	1:X:835:U:H6	1.72	0.54
1:X:1005:U:H1'	16:O:21:ARG:HH22	1.72	0.54
1:X:1288:A:H4'	1:X:1289:A:OP1	2.06	0.54
1:X:1547:U:H3	1:X:1556:A:H61	1.55	0.54
1:X:1973:C:H2'	1:X:1974:U:O4'	2.07	0.54
1:X:2753:C:H5"	4:B:164:ARG:HG2	1.88	0.54
2:Y:51:G:H2'	2:Y:52:G:H8	1.73	0.54
10:I:34:HIS:O	10:I:35:LYS:HD3	2.07	0.54
10:I:89:ASP:HB2	10:I:120:VAL:HG12	1.88	0.54
20:S:116:VAL:HG12	20:S:117:VAL:HG13	1.90	0.54
1:X:14:A:H5"	1:X:15:G:OP2	2.06	0.54
1:X:20:C:H2'	1:X:21:A:H8	1.72	0.54
1:X:319:G:N7	17:P:12:LYS:NZ	2.54	0.54
1:X:1687:C:O2	4:B:129:HIS:HE1	1.90	0.54
2:Y:40:C:H5'	13:L:97:HIS:CE1	2.43	0.54
6:D:103:LEU:HG	6:D:108:LEU:HG	1.89	0.54
1:X:320:A:N3	1:X:340:G:O2'	2.37	0.54
1:X:475:U:O3'	27:2:12:ARG:NH2	2.41	0.54
1:X:2368:G:H5"	1:X:2369:U:H5'	1.89	0.54
1:X:2522:G:H2'	1:X:2523:G:C8	2.42	0.54
1:X:2572:U:H2'	1:X:2573:C:H6	1.71	0.54
2:Y:7:C:H2'	2:Y:8:C:C6	2.43	0.54
1:X:1261:G:C5	15:N:3:ARG:HG2	2.42	0.54
1:X:2528:G:H2'	1:X:2529:G:H8	1.73	0.54
9:H:28:GLY:HA3	9:H:34:LEU:HD22	1.88	0.54
16:O:89:ASN:OD1	16:O:89:ASN:N	2.40	0.54
17:P:40:LEU:HB3	25:Z:25:LEU:HD22	1.90	0.54
18:Q:6:ILE:HA	18:Q:30:SER:OG	2.07	0.54
1:X:847:C:H2'	1:X:848:A:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1329:U:H2'	1:X:1330:G:C8	2.40	0.54
1:X:2466:G:H2'	1:X:2467:A:C8	2.41	0.54
1:X:2597:G:H21	4:B:150:VAL:HG21	1.73	0.54
1:X:2736:U:H1'	1:X:2737:A:H5"	1.88	0.54
11:J:99:LYS:HE3	11:J:100:PRO:HD2	1.90	0.54
12:K:39:THR:O	12:K:42:LYS:N	2.41	0.54
1:X:530:G:H2'	1:X:531:G:H8	1.72	0.54
1:X:613:A:H8	1:X:636:G:H21	1.54	0.54
1:X:758:G:H2'	1:X:759:C:H5'	1.90	0.54
1:X:1782:A:O2'	3:A:207:GLY:O	2.18	0.54
1:X:1845:A:N6	1:X:1871:G:O2'	2.41	0.54
1:X:1856:U:OP1	1:X:2389:G:O2'	2.21	0.54
3:A:43:ARG:HB3	3:A:54:ILE:O	2.08	0.54
17:P:39:ARG:HD2	17:P:97:VAL:HB	1.90	0.54
19:R:92:THR:OG1	19:R:92:THR:O	2.17	0.54
20:S:25:ASN:H	20:S:25:ASN:HD22	1.56	0.54
24:W:12:ARG:HG2	24:W:12:ARG:HH11	1.72	0.54
1:X:1991:C:H2'	1:X:1992:G:H8	1.73	0.54
1:X:2043:A:H62	5:C:68:ARG:NH1	2.04	0.54
1:X:2729:A:N1	1:X:2730:A:N6	2.56	0.54
3:A:134:ARG:HG3	3:A:135:PHE:CD2	2.43	0.54
17:P:37:LYS:HZ3	17:P:64:ALA:H	1.56	0.54
18:Q:11:VAL:HB	18:Q:26:SER:HB2	1.90	0.54
28:3:6:THR:HG23	28:3:8:LYS:H	1.73	0.54
1:X:1121:G:H2'	1:X:1122:A:H8	1.72	0.54
1:X:2293:G:H5'	6:D:35:VAL:HG11	1.89	0.54
1:X:2579:A:H2'	1:X:2580:C:H6	1.71	0.54
1:X:2767:C:H1'	4:B:62:PRO:HG3	1.89	0.54
7:E:43:VAL:HA	7:E:52:VAL:HG22	1.90	0.54
9:H:16:ALA:HB3	9:H:98:ILE:HD11	1.90	0.54
1:X:177:U:H1'	1:X:178:C:OP1	2.08	0.53
1:X:1496:G:H4'	1:X:1497:C:OP1	2.07	0.53
1:X:2195:C:H2'	1:X:2196:U:C5	2.44	0.53
1:X:2806:G:OP1	4:B:57:ARG:NH1	2.41	0.53
3:A:44:ASN:HA	3:A:49:ILE:HA	1.90	0.53
3:A:160:GLY:N	3:A:196:VAL:O	2.41	0.53
13:L:46:SER:OG	13:L:47:ARG:N	2.38	0.53
1:X:388:G:H2'	1:X:389:G:H8	1.73	0.53
1:X:852:U:H1'	1:X:1205:G:H1'	1.91	0.53
1:X:1816:G:OP1	3:A:52:ARG:HD3	2.07	0.53
1:X:1820:G:OP2	3:A:239:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2591:C:O2'	1:X:2592:U:OP1	2.25	0.53
3:A:209:ALA:C	3:A:211:ARG:H	2.11	0.53
1:X:611:C:O2	1:X:615:C:H4'	2.09	0.53
1:X:667:U:O2'	1:X:668:A:H8	1.91	0.53
1:X:691:C:H2'	1:X:692:C:H6	1.71	0.53
13:L:95:LYS:HG3	13:L:96:TYR:H	1.73	0.53
21:T:46:LYS:NZ	21:T:76:ALA:HA	2.24	0.53
21:T:46:LYS:HB2	21:T:78:PHE:CE2	2.43	0.53
1:X:492:G:OP2	19:R:56:LYS:HG2	2.09	0.53
1:X:1744:G:OP1	14:M:100:ARG:HD2	2.08	0.53
1:X:608:G:H2'	1:X:609:U:H6	1.73	0.53
1:X:1385:C:H2'	1:X:1386:A:O4'	2.09	0.53
1:X:1674:C:H2'	1:X:1675:C:H6	1.74	0.53
1:X:1693:A:H2'	1:X:1694:A:O4'	2.08	0.53
1:X:2526:U:H2'	1:X:2527:G:C8	2.44	0.53
11:J:32:ASP:H	11:J:108:ALA:HB2	1.74	0.53
14:M:29:PRO:HB2	14:M:99:VAL:HG11	1.91	0.53
14:M:103:LYS:O	14:M:104:LEU:HB2	2.08	0.53
1:X:742:G:H2'	1:X:1766:U:H1'	1.90	0.53
1:X:1777:A:H1'	1:X:1921:A:N6	2.24	0.53
1:X:1884:A:O2'	3:A:244:ARG:HD3	2.08	0.53
1:X:2043:A:H1'	1:X:2481:G:H1'	1.89	0.53
4:B:33:ILE:HD11	4:B:86:PRO:HB2	1.91	0.53
8:G:67:ARG:CB	8:G:70:PHE:HA	2.38	0.53
12:K:90:ARG:HD2	12:K:94:TYR:HB2	1.90	0.53
22:U:49:LYS:HD3	22:U:61:TRP:CE2	2.44	0.53
28:3:13:ARG:HG3	28:3:14:ILE:HG13	1.90	0.53
1:X:1046:U:H4'	7:E:60:LYS:HE2	1.91	0.53
1:X:1517:C:H4'	3:A:96:HIS:NE2	2.24	0.53
1:X:2245:A:H4'	1:X:2246:A:N3	2.24	0.53
1:X:70:A:H4'	1:X:71:A:H5"	1.90	0.53
1:X:1059:A:H2	1:X:1123:G:H21	1.55	0.53
1:X:1184:G:O6	1:X:1190:C:N4	2.41	0.53
1:X:1479:G:H2'	1:X:1480:G:C8	2.44	0.53
3:A:246:PRO:HG2	3:A:248:THR:O	2.09	0.53
5:C:125:ILE:HG12	5:C:157:THR:HA	1.91	0.53
5:C:154:ASP:HB3	5:C:157:THR:HB	1.91	0.53
6:D:80:ARG:HD3	6:D:83:MET:HB2	1.91	0.53
13:L:32:TYR:HB3	13:L:39:TYR:HB2	1.89	0.53
19:R:16:PHE:HE2	19:R:80:LYS:HZ3	1.57	0.53
28:3:52:LYS:O	28:3:56:ALA:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1692:C:N3	4:B:128:SER:OG	2.39	0.53
1:X:2054:A:H2'	1:X:2055:G:H8	1.73	0.53
3:A:111:LEU:HD23	3:A:127:LEU:HD13	1.91	0.53
26:1:9:ILE:O	26:1:10:VAL:HB	2.08	0.53
1:X:99:U:H3'	1:X:100:G:H5'	1.91	0.53
1:X:857:U:H2'	1:X:858:G:O4'	2.09	0.53
1:X:1177:U:H2'	1:X:1178:C:O4'	2.09	0.53
1:X:1418:C:H2'	1:X:1419:G:C8	2.44	0.53
12:K:100:VAL:HG12	12:K:101:GLY:N	2.24	0.53
14:M:29:PRO:HA	14:M:54:VAL:HG13	1.91	0.53
1:X:1342:U:H5"	1:X:1343:C:C5	2.43	0.52
1:X:1816:G:H21	3:A:252:LYS:HG3	1.73	0.52
1:X:1819:U:H2'	1:X:1820:G:O4'	2.08	0.52
1:X:863:C:H42	1:X:940:G:H1	1.57	0.52
1:X:2639:A:H2'	1:X:2640:G:O4'	2.09	0.52
10:I:77:LEU:HD12	10:I:108:LEU:HD11	1.92	0.52
16:O:19:VAL:HG13	16:O:90:PHE:CD1	2.44	0.52
27:2:26:SER:O	27:2:30:ILE:HG13	2.09	0.52
1:X:1204:G:H2'	1:X:1205:G:C8	2.45	0.52
1:X:1781:C:H4'	3:A:209:ALA:HB2	1.90	0.52
1:X:2440:C:H2'	1:X:2441:U:C6	2.44	0.52
5:C:76:THR:O	5:C:77:PHE:HD1	1.92	0.52
8:G:103:TYR:HB3	8:G:107:GLN:HG2	1.91	0.52
9:H:29:ILE:HD13	9:H:123:PHE:CE1	2.44	0.52
10:I:62:LYS:CB	28:3:12:ARG:HA	2.39	0.52
19:R:84:VAL:CG1	19:R:90:LYS:H	2.17	0.52
24:W:46:THR:HG22	24:W:47:VAL:HG13	1.91	0.52
1:X:469:G:N2	1:X:480:G:H2'	2.25	0.52
1:X:1870:U:P	1:X:1871:G:H22	2.32	0.52
3:A:186:HIS:HB2	3:A:188:GLU:HG2	1.92	0.52
5:C:6:VAL:HG12	5:C:7:ILE:HG12	1.91	0.52
14:M:70:LYS:HE2	14:M:72:SER:HB3	1.90	0.52
1:X:394:U:OP1	22:U:19:ILE:HG12	2.10	0.52
1:X:503:G:H2'	1:X:504:G:O4'	2.10	0.52
1:X:692:C:H2'	1:X:693:A:C8	2.43	0.52
1:X:2855:C:H1'	12:K:91:PRO:HB2	1.92	0.52
5:C:112:GLN:HA	5:C:112:GLN:OE1	2.08	0.52
10:I:62:LYS:HD3	10:I:63:ARG:N	2.24	0.52
1:X:502:A:H2'	1:X:503:G:O4'	2.10	0.52
1:X:1223:G:H5"	1:X:1224:A:H3'	1.92	0.52
1:X:1454:U:H2'	1:X:1455:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:78:SER:HB3	10:I:112:GLY:HA3	1.92	0.52
11:J:42:TRP:CD1	11:J:97:VAL:HG12	2.44	0.52
13:L:75:LEU:O	13:L:79:ALA:N	2.42	0.52
18:Q:7:LEU:H	18:Q:7:LEU:HD22	1.75	0.52
19:R:105:ARG:NH2	19:R:111:GLY:O	2.42	0.52
22:U:17:SER:OG	22:U:45:ASN:N	2.42	0.52
1:X:47:G:N2	1:X:154:U:OP2	2.29	0.52
1:X:761:G:H2'	1:X:763:A:N7	2.25	0.52
1:X:940:G:H4'	24:W:37:THR:HG21	1.92	0.52
1:X:1673:C:H5"	4:B:136:ARG:HB3	1.91	0.52
1:X:2441:U:H1'	1:X:2470:U:O4	2.09	0.52
1:X:2824:C:H4'	1:X:2825:A:O5'	2.10	0.52
2:Y:9:G:H5'	13:L:32:TYR:CZ	2.45	0.52
8:G:46:ALA:HB1	8:G:88:VAL:HG23	1.92	0.52
9:H:83:ARG:HG2	14:M:40:ARG:NH2	2.24	0.52
15:N:66:ASN:HB3	15:N:76:TYR:CB	2.33	0.52
23:V:32:ALA:HB2	23:V:37:LEU:HD13	1.92	0.52
1:X:580:A:H4'	1:X:581:A:OP1	2.10	0.52
1:X:615:C:H41	10:I:100:ARG:NH1	2.07	0.52
1:X:2078:G:H1	1:X:2177:U:H3	1.57	0.52
1:X:2668:U:P	1:X:2699:G:H22	2.33	0.52
9:H:73:VAL:HG21	9:H:123:PHE:CE2	2.44	0.52
22:U:15:VAL:HA	22:U:45:ASN:O	2.10	0.52
1:X:538:A:H2'	1:X:538:A:N3	2.24	0.52
1:X:1004:A:H1'	16:O:88:GLN:HG3	1.92	0.52
1:X:1558:C:H2'	1:X:1559:G:O4'	2.10	0.52
1:X:2451:G:H22	1:X:2456:U:H5'	1.74	0.52
1:X:2716:G:H1	1:X:2748:C:N4	2.07	0.52
5:C:47:THR:HA	5:C:82:VAL:HG13	1.90	0.52
13:L:37:HIS:HD2	13:L:57:ALA:HA	1.75	0.52
1:X:1787:U:H2'	1:X:1788:C:C6	2.44	0.52
5:C:26:VAL:HG11	5:C:102:LEU:HD22	1.91	0.52
6:D:65:PRO:HA	6:D:89:VAL:HG22	1.92	0.52
9:H:99:ILE:HD12	9:H:103:GLY:HA2	1.91	0.52
15:N:58:ARG:O	15:N:62:ILE:HG13	2.10	0.52
15:N:86:ALA:HB1	15:N:88:ILE:HB	1.92	0.52
20:S:19:ILE:HD11	20:S:36:ARG:HG3	1.91	0.52
26:1:12:MET:HG3	26:1:54:LYS:HB3	1.92	0.52
1:X:1225:G:HO2'	1:X:1226:A:H8	1.59	0.51
1:X:2269:G:N2	1:X:2322:U:H1'	2.24	0.51
9:H:73:VAL:HG21	9:H:123:PHE:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:29:HIS:NE2	19:R:51:VAL:HG13	2.25	0.51
20:S:7:PRO:HB2	20:S:9:THR:H	1.74	0.51
1:X:1033:G:H4'	1:X:1034:U:H5'	1.92	0.51
1:X:1128:G:H3'	1:X:1129:A:H5"	1.93	0.51
2:Y:16:U:O2'	2:Y:17:A:OP2	2.28	0.51
19:R:33:THR:OG1	19:R:34:GLY:N	2.43	0.51
1:X:608:G:H2'	1:X:609:U:C6	2.45	0.51
1:X:1825:C:O2	1:X:1955:G:N2	2.35	0.51
5:C:45:THR:HG23	5:C:47:THR:H	1.74	0.51
7:E:17:VAL:HG13	7:E:26:VAL:HG22	1.91	0.51
7:E:41:LEU:HD22	7:E:68:THR:HG21	1.93	0.51
8:G:68:PRO:HD2	8:G:76:GLN:HB3	1.91	0.51
19:R:77:HIS:CG	19:R:78:ALA:H	2.29	0.51
1:X:346:C:C6	1:X:347:C:H5	2.29	0.51
1:X:967:G:N2	1:X:971:A:OP2	2.43	0.51
1:X:1429:A:H1'	1:X:1603:A:C5	2.46	0.51
1:X:2692:A:H5"	1:X:2693:U:OP2	2.10	0.51
6:D:110:ARG:O	6:D:111:ILE:HG13	2.10	0.51
24:W:4:LYS:HG2	24:W:52:GLU:HB3	1.92	0.51
26:1:30:ASN:HD22	26:1:31:THR:HG23	1.75	0.51
1:X:224:G:OP2	1:X:226:C:N4	2.42	0.51
1:X:977:G:H1'	1:X:2246:A:H62	1.75	0.51
1:X:1599:G:C2	1:X:1600:U:H1'	2.45	0.51
1:X:1714:A:O2'	1:X:1961:A:OP1	2.23	0.51
1:X:1886:G:H2'	1:X:1887:G:C8	2.45	0.51
8:G:33:ILE:HB	8:G:34:PRO:HD2	1.92	0.51
17:P:35:PRO:HD3	17:P:121:THR:O	2.10	0.51
1:X:334:G:C8	5:C:164:VAL:HG13	2.46	0.51
1:X:845:U:OP1	10:I:41:SER:HB3	2.11	0.51
1:X:1686:A:H5"	1:X:1687:C:OP2	2.10	0.51
1:X:1769:U:H2'	1:X:1775:A:N6	2.24	0.51
4:B:102:ILE:N	4:B:169:ASN:O	2.43	0.51
14:M:60:SER:HB3	14:M:63:ARG:HH12	1.75	0.51
15:N:7:GLY:O	15:N:8:ILE:HG12	2.11	0.51
15:N:39:LEU:HA	15:N:42:ALA:HB3	1.93	0.51
20:S:6:LYS:HE2	20:S:56:VAL:HG11	1.93	0.51
25:Z:4:HIS:HB2	25:Z:5:PRO:HD3	1.92	0.51
1:X:617:U:H5	1:X:632:A:H2	1.58	0.51
1:X:938:G:O2'	1:X:939:C:O5'	2.28	0.51
1:X:1101:U:H2'	1:X:1102:G:C8	2.45	0.51
1:X:1724:C:N3	1:X:1747:G:C6	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2766:U:O2'	4:B:62:PRO:O	2.24	0.51
5:C:119:ALA:HB3	5:C:189:ASP:HA	1.92	0.51
1:X:542:A:H5'	15:N:28:ARG:HH21	1.74	0.51
1:X:1770:U:C2	1:X:1774:A:N7	2.79	0.51
1:X:2043:A:N3	1:X:2481:G:C4	2.79	0.51
1:X:2371:A:H8	10:I:59:ARG:HG2	1.76	0.51
1:X:2594:U:H2'	1:X:2595:C:H6	1.75	0.51
1:X:836:G:H2'	1:X:837:U:H6	1.76	0.51
1:X:1846:A:H2'	1:X:1847:G:O4'	2.11	0.51
1:X:2270:U:H2'	1:X:2271:C:C6	2.46	0.51
4:B:41:THR:OG1	4:B:42:ASP:N	2.41	0.51
8:G:96:ASP:HB3	8:G:97:ASP:OD1	2.10	0.51
8:G:128:GLU:HG3	8:G:150:VAL:HG21	1.93	0.51
9:H:13:ASN:HD21	9:H:109:ARG:HG2	1.75	0.51
1:X:455:A:H1'	1:X:1215:A:O4'	2.11	0.51
1:X:590:C:H2'	1:X:591:G:H8	1.76	0.51
1:X:1173:G:H5"	16:O:22:VAL:HG22	1.93	0.51
1:X:1348:C:H2'	1:X:1349:A:H8	1.76	0.51
1:X:1469:U:H5'	1:X:1470:G:OP2	2.11	0.51
3:A:88:ARG:HG3	3:A:90:ALA:HB3	1.93	0.51
17:P:59:PHE:CD1	25:Z:41:LEU:HD22	2.45	0.51
26:1:8:ILE:O	26:1:9:ILE:HG12	2.11	0.51
1:X:1486:A:H2'	1:X:1487:C:C6	2.46	0.50
3:A:108:PRO:HB3	3:A:143:HIS:CE1	2.46	0.50
5:C:153:ASP:OD1	5:C:172:VAL:HA	2.11	0.50
10:I:94:GLU:HA	10:I:97:ARG:NE	2.25	0.50
20:S:88:TYR:O	20:S:127:PRO:HB3	2.11	0.50
28:3:22:VAL:HG21	28:3:53:ALA:HA	1.92	0.50
1:X:50:G:H4'	1:X:51:A:H5'	1.93	0.50
1:X:558:G:OP2	1:X:558:G:N2	2.42	0.50
1:X:1048:U:H3	1:X:1129:A:H61	1.59	0.50
1:X:1919:A:H1'	1:X:1923:U:N3	2.25	0.50
1:X:2372:A:H5"	10:I:61:PRO:HB3	1.92	0.50
1:X:2474:G:H5"	11:J:82:THR:CA	2.40	0.50
1:X:2640:G:H2'	1:X:2641:A:C8	2.46	0.50
6:D:34:ILE:HD12	6:D:156:ILE:HG12	1.92	0.50
1:X:740:A:C6	1:X:741:G:C6	2.99	0.50
1:X:875:G:H2'	1:X:876:A:O4'	2.11	0.50
1:X:1935:A:N3	1:X:2539:C:O2'	2.38	0.50
1:X:2283:G:O2'	6:D:130:LEU:O	2.28	0.50
1:X:2558:C:H2'	1:X:2559:U:O4'	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:33:LEU:HD22	7:E:136:ILE:HG22	1.92	0.50
1:X:399:G:H5'	1:X:401:G:H22	1.75	0.50
1:X:489:A:O3'	19:R:45:LYS:NZ	2.44	0.50
1:X:754:G:H2'	1:X:755:C:H6	1.77	0.50
1:X:1573:G:H3'	1:X:1574:A:H5"	1.92	0.50
1:X:1997:A:H2'	1:X:1998:A:C8	2.47	0.50
1:X:2620:G:P	8:G:102:ARG:HH21	2.34	0.50
1:X:2705:A:C8	1:X:2706:U:H2'	2.47	0.50
5:C:47:THR:OG1	5:C:85:GLY:N	2.38	0.50
6:D:63:GLN:NE2	6:D:90:THR:O	2.24	0.50
8:G:67:ARG:HB2	8:G:76:GLN:NE2	2.26	0.50
20:S:91:PRO:HG2	20:S:125:PRO:HD2	1.93	0.50
26:1:14:SER:HB3	26:1:50:PHE:CD2	2.47	0.50
27:2:34:ARG:HG2	27:2:40:HIS:HD2	1.75	0.50
27:2:36:ALA:C	27:2:38:GLY:H	2.15	0.50
1:X:719:A:H2'	1:X:720:A:O4'	2.12	0.50
1:X:1850:G:H1'	1:X:1867:A:H62	1.77	0.50
10:I:88:PHE:HB3	10:I:90:ARG:CZ	2.41	0.50
12:K:11:ASN:ND2	12:K:11:ASN:H	2.07	0.50
1:X:761:G:C8	1:X:763:A:C8	2.99	0.50
1:X:877:G:H1	1:X:924:C:H42	1.58	0.50
1:X:1441:A:H4'	1:X:1442:C:O5'	2.12	0.50
1:X:1578:U:H2'	1:X:1579:G:H8	1.77	0.50
1:X:1870:U:O5'	1:X:1871:G:N2	2.45	0.50
15:N:90:LEU:O	15:N:92:ARG:HG3	2.11	0.50
1:X:409:G:H1'	22:U:45:ASN:ND2	2.27	0.50
1:X:734:G:H2'	1:X:735:G:H8	1.76	0.50
1:X:1427:G:N1	1:X:1603:A:OP1	2.45	0.50
1:X:2262:C:H2'	1:X:2263:C:O4'	2.11	0.50
1:X:2627:G:O2'	9:H:38:GLY:HA2	2.12	0.50
10:I:86:THR:OG1	10:I:116:ARG:NE	2.45	0.50
15:N:49:ASP:HA	15:N:52:ASN:HB2	1.92	0.50
17:P:97:VAL:HG22	17:P:124:ILE:HG23	1.94	0.50
18:Q:2:SER:OG	18:Q:3:HIS:N	2.45	0.50
19:R:90:LYS:HG3	19:R:108:VAL:HG21	1.93	0.50
28:3:34:THR:OG1	28:3:35:GLY:N	2.43	0.50
1:X:123:A:H1'	27:2:14:LYS:HD3	1.93	0.50
1:X:919:U:O3'	11:J:24:GLY:HA3	2.12	0.50
1:X:1614:C:H2'	1:X:1615:C:H6	1.77	0.50
3:A:244:ARG:HG2	3:A:244:ARG:O	2.12	0.50
17:P:52:ASP:OD1	17:P:52:ASP:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:56:GLN:OE1	25:Z:56:GLN:N	2.45	0.50
1:X:615:C:O2	1:X:670:U:O2'	2.30	0.50
1:X:971:A:H61	11:J:83:ARG:NH2	1.98	0.50
1:X:1235:C:H42	1:X:1240:G:H1	1.60	0.50
1:X:1481:U:O2'	1:X:1562:G:H1'	2.12	0.50
14:M:102:ALA:C	14:M:103:LYS:HD2	2.32	0.50
1:X:332:C:H5"	1:X:333:A:OP2	2.12	0.49
1:X:399:G:H5'	1:X:401:G:N2	2.28	0.49
1:X:542:A:H8	15:N:28:ARG:NH2	2.10	0.49
1:X:542:A:C5'	15:N:28:ARG:HH21	2.26	0.49
1:X:825:C:H1'	1:X:1263:G:C2	2.46	0.49
1:X:1949:A:H1'	1:X:2572:U:H5'	1.93	0.49
1:X:2036:G:H5'	4:B:144:ARG:O	2.12	0.49
9:H:70:VAL:CG2	9:H:98:ILE:HG23	2.38	0.49
1:X:558:G:H8	1:X:560:G:N7	2.10	0.49
1:X:667:U:H2'	1:X:668:A:H5"	1.94	0.49
1:X:922:A:N7	1:X:923:A:C6	2.80	0.49
1:X:1223:G:N2	1:X:1249:G:O2'	2.45	0.49
2:Y:42:U:HO2'	2:Y:47:A:N6	2.10	0.49
5:C:53:LYS:O	5:C:54:THR:OG1	2.23	0.49
10:I:18:ARG:HB3	10:I:21:ARG:CB	2.42	0.49
11:J:44:LYS:HA	11:J:95:VAL:HG12	1.92	0.49
24:W:25:LEU:HD23	24:W:30:ASP:HB3	1.94	0.49
27:2:22:MET:HA	27:2:28:ARG:HD3	1.94	0.49
1:X:592:G:O5'	15:N:10:ARG:NH1	2.45	0.49
1:X:1236:G:O6	16:O:70:TYR:OH	2.29	0.49
1:X:1390:G:H8	1:X:1390:G:O5'	1.95	0.49
1:X:1750:A:C8	1:X:2675:U:H1'	2.47	0.49
1:X:2498:U:C5	1:X:2520:A:C6	3.00	0.49
1:X:2854:G:H4'	1:X:2855:C:OP1	2.12	0.49
5:C:47:THR:OG1	5:C:82:VAL:HG22	2.12	0.49
15:N:82:GLY:HA3	15:N:113:SER:OG	2.12	0.49
19:R:15:HIS:N	19:R:15:HIS:CD2	2.81	0.49
1:X:1006:C:N3	8:G:31:THR:HG23	2.26	0.49
1:X:2335:U:H2'	1:X:2336:G:C8	2.48	0.49
5:C:5:ASN:ND2	5:C:9:GLN:HG3	2.27	0.49
9:H:83:ARG:HH12	14:M:38:LYS:HE2	1.77	0.49
17:P:35:PRO:O	17:P:39:ARG:HD3	2.12	0.49
27:2:41:GLN:HA	27:2:41:GLN:HE21	1.76	0.49
1:X:420:C:H2'	1:X:421:G:C8	2.47	0.49
1:X:946:U:H2'	1:X:947:C:H6	1.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1034:U:OP2	1:X:1036:G:O2'	2.31	0.49
1:X:1468:A:C8	1:X:1468:A:OP2	2.66	0.49
1:X:1827:G:H1'	1:X:1914:U:C2	2.48	0.49
1:X:2018:G:H4'	1:X:2019:C:OP2	2.13	0.49
1:X:2314:A:O2'	1:X:2316:G:N7	2.32	0.49
6:D:115:ARG:HH22	6:D:178:ARG:HH12	1.59	0.49
8:G:78:ASP:OD1	8:G:78:ASP:N	2.45	0.49
22:U:60:VAL:O	22:U:61:TRP:HD1	1.95	0.49
27:2:38:GLY:O	27:2:40:HIS:N	2.45	0.49
1:X:585:U:H4'	1:X:2481:G:C8	2.48	0.49
1:X:746:G:C8	1:X:774:A:N1	2.80	0.49
1:X:871:U:O2	1:X:2247:A:H2'	2.12	0.49
1:X:1816:G:H2'	1:X:1817:U:C6	2.48	0.49
1:X:1918:G:H1'	1:X:1947:G:N2	2.28	0.49
1:X:2311:U:O2'	1:X:2315:A:N7	2.45	0.49
1:X:2500:C:H2'	1:X:2501:U:C6	2.47	0.49
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.95	0.49
1:X:386:U:H5'	1:X:436:A:N3	2.27	0.49
1:X:426:C:O2'	1:X:1863:U:O2'	2.16	0.49
1:X:518:A:O2'	1:X:519:C:OP1	2.28	0.49
1:X:667:U:HO2'	1:X:668:A:H8	1.60	0.49
1:X:1834:G:H2'	1:X:1835:C:H6	1.77	0.49
1:X:2084:G:H2'	1:X:2085:G:C8	2.47	0.49
8:G:58:ILE:HG12	8:G:80:VAL:HG11	1.95	0.49
14:M:104:LEU:HA	14:M:106:TYR:CE2	2.48	0.49
25:Z:57:VAL:HG12	25:Z:58:LEU:HD23	1.95	0.49
27:2:1:MET:HE2	27:2:3:ARG:HH12	1.77	0.49
1:X:635:C:O2'	1:X:670:U:OP1	2.29	0.49
1:X:645:G:H2'	1:X:646:C:C6	2.47	0.49
1:X:687:G:H4'	5:C:68:ARG:O	2.13	0.49
1:X:1675:C:H2'	1:X:1676:U:H6	1.76	0.49
1:X:1974:U:C2'	1:X:1975:G:H5'	2.42	0.49
1:X:2206:C:H2'	1:X:2207:G:O4'	2.12	0.49
8:G:43:VAL:HB	8:G:167:LYS:HG2	1.94	0.49
1:X:227:G:OP2	28:3:8:LYS:HG2	2.13	0.49
1:X:493:A:H4'	19:R:56:LYS:HG3	1.95	0.49
1:X:1004:A:OP1	15:N:50:ARG:NH1	2.41	0.49
1:X:1023:U:C4	8:G:53:ARG:HG3	2.47	0.49
1:X:1742:G:H2'	1:X:1743:C:C6	2.47	0.49
1:X:1746:A:C2	1:X:2696:A:H1'	2.47	0.49
1:X:1779:C:H2'	1:X:1780:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2598:C:O2'	1:X:2599:U:H5'	2.12	0.49
3:A:76:ASN:HA	3:A:118:ASN:HA	1.94	0.49
5:C:22:VAL:HG22	5:C:110:SER:HA	1.94	0.49
10:I:56:LEU:HB3	28:3:52:LYS:HZ2	1.76	0.49
11:J:60:ARG:HA	11:J:60:ARG:HE	1.77	0.49
23:V:2:LYS:HB2	23:V:3:PRO:HD3	1.95	0.49
1:X:58:C:H1'	1:X:72:A:H2'	1.93	0.49
1:X:870:C:H5"	21:T:77:ARG:HH22	1.78	0.49
1:X:1225:G:O6	17:P:12:LYS:HB2	2.12	0.49
1:X:1272:G:H2'	1:X:1273:G:C8	2.48	0.49
1:X:1350:G:H2'	1:X:1351:G:C8	2.46	0.49
1:X:1448:A:N6	1:X:1574:A:H61	2.11	0.49
1:X:1578:U:H2'	1:X:1579:G:C8	2.48	0.49
1:X:1791:C:OP2	3:A:183:ARG:NH1	2.44	0.49
1:X:2326:C:OP1	1:X:2326:C:H4'	2.13	0.49
1:X:2572:U:H2'	1:X:2573:C:C6	2.47	0.49
5:C:128:ALA:O	5:C:130:THR:N	2.38	0.49
12:K:73:LYS:O	12:K:76:VAL:HG12	2.13	0.49
13:L:33:ARG:NH1	13:L:38:ILE:HG21	2.28	0.49
20:S:80:HIS:NE2	20:S:82:ASP:OD2	2.43	0.49
1:X:38:G:O2'	1:X:39:C:O5'	2.23	0.48
1:X:89:A:H4'	1:X:90:G:C5'	2.40	0.48
1:X:321:A:C6	1:X:323:G:C4	3.01	0.48
1:X:591:G:C6	1:X:592:G:C6	3.00	0.48
1:X:1468:A:OP2	1:X:1468:A:H8	1.96	0.48
1:X:2516:U:H2'	1:X:2517:C:H6	1.75	0.48
2:Y:3:A:N6	2:Y:121:G:O6	2.46	0.48
8:G:62:ILE:O	8:G:77:GLY:HA3	2.13	0.48
8:G:71:THR:N	8:G:76:GLN:HE22	2.10	0.48
22:U:17:SER:HB2	22:U:44:ALA:HA	1.95	0.48
1:X:5:A:H2'	1:X:6:A:C8	2.48	0.48
1:X:40:U:H2'	1:X:41:G:C8	2.48	0.48
1:X:70:A:H5"	1:X:71:A:H2'	1.95	0.48
1:X:121:G:H2'	1:X:122:G:O4'	2.13	0.48
1:X:590:C:H2'	1:X:591:G:C8	2.48	0.48
1:X:865:A:H5'	24:W:42:GLY:HA3	1.94	0.48
1:X:977:G:C1'	1:X:2246:A:H62	2.26	0.48
1:X:1699:A:H61	1:X:1723:U:H3	1.61	0.48
1:X:2211:U:OP1	22:U:43:ARG:NH1	2.22	0.48
1:X:2225:G:H2'	1:X:2226:A:C8	2.47	0.48
1:X:2619:G:OP1	8:G:125:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2796:A:H4'	4:B:162:MET:SD	2.53	0.48
4:B:16:LYS:H	4:B:21:ILE:HD11	1.78	0.48
16:O:10:LYS:HE2	16:O:13:ARG:NH2	2.27	0.48
17:P:71:VAL:HG13	17:P:126:ILE:HG22	1.95	0.48
22:U:23:LYS:HB2	22:U:35:THR:HG23	1.94	0.48
1:X:318:G:N1	1:X:321:A:OP2	2.45	0.48
1:X:577:U:H2'	1:X:579:G:OP2	2.12	0.48
1:X:596:C:C4	1:X:684:C:C2	3.02	0.48
1:X:824:U:H2'	10:I:30:ALA:N	2.29	0.48
1:X:1269:G:N3	1:X:1269:G:H2'	2.28	0.48
1:X:2240:C:C2'	1:X:2241:U:H5'	2.43	0.48
1:X:2370:G:O6	1:X:2406:C:H1'	2.13	0.48
1:X:2596:C:H2'	1:X:2597:G:H8	1.77	0.48
4:B:119:ARG:HA	4:B:160:MET:SD	2.53	0.48
5:C:26:VAL:O	5:C:30:VAL:HG23	2.12	0.48
14:M:32:THR:O	14:M:51:GLU:HA	2.13	0.48
1:X:1466:C:H2'	1:X:1467:U:C1'	2.43	0.48
1:X:1510:A:H2'	1:X:1511:A:O4'	2.13	0.48
1:X:1630:A:OP1	1:X:1633:C:N4	2.40	0.48
1:X:1982:C:O2	1:X:2666:U:O2'	2.29	0.48
1:X:2031:A:H2'	1:X:2032:G:O4'	2.13	0.48
1:X:2571:G:C6	1:X:2572:U:N3	2.82	0.48
11:J:11:ARG:NE	11:J:15:ARG:HH12	2.11	0.48
20:S:3:LEU:HD22	20:S:32:PHE:CD2	2.48	0.48
23:V:31:GLN:O	23:V:36:GLN:HB3	2.12	0.48
1:X:154:U:H3'	1:X:155:G:H8	1.78	0.48
1:X:331:U:H2'	5:C:130:THR:HG21	1.93	0.48
1:X:343:A:O2'	1:X:346:C:N4	2.42	0.48
1:X:540:G:C6	1:X:2005:U:H5"	2.48	0.48
1:X:1075:C:H2'	1:X:1076:U:O4'	2.13	0.48
1:X:1678:G:H1	1:X:1982:C:N4	2.07	0.48
1:X:2200:G:H2'	1:X:2201:G:C8	2.47	0.48
1:X:2691:C:O2'	1:X:2693:U:H5'	2.14	0.48
5:C:47:THR:HG1	5:C:85:GLY:H	1.58	0.48
6:D:13:ARG:O	6:D:17:MET:HG3	2.13	0.48
7:E:121:VAL:HG11	7:E:144:VAL:HG21	1.95	0.48
9:H:62:GLY:O	9:H:65:LYS:NZ	2.36	0.48
11:J:15:ARG:HD3	11:J:73:LYS:HE3	1.96	0.48
16:O:11:GLN:HA	16:O:38:LEU:O	2.13	0.48
25:Z:16:ARG:HD3	25:Z:20:ARG:CZ	2.44	0.48
1:X:1023:U:O4	8:G:56:THR:OG1	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1029:C:H42	1:X:1155:G:H1	1.62	0.48
1:X:1151:U:O4	8:G:93:LYS:HE3	2.14	0.48
1:X:1310:C:H2'	1:X:1311:C:H6	1.79	0.48
1:X:1705:U:O2	1:X:1717:A:H5'	2.13	0.48
1:X:2670:C:H2'	1:X:2671:C:H6	1.79	0.48
1:X:2751:C:H2'	1:X:2752:C:C6	2.48	0.48
1:X:2787:A:H2'	1:X:2788:C:H6	1.78	0.48
3:A:14:ARG:NH1	3:A:27:LYS:O	2.47	0.48
26:1:37:LEU:HD23	26:1:51:ARG:HA	1.96	0.48
1:X:438:G:H2'	1:X:439:C:C6	2.49	0.48
1:X:507:A:OP2	17:P:19:LYS:NZ	2.36	0.48
1:X:546:A:H2'	1:X:547:U:C6	2.48	0.48
1:X:810:U:H2'	1:X:811:G:O4'	2.12	0.48
1:X:1603:A:H8	1:X:1603:A:OP2	1.96	0.48
1:X:2738:A:C5	7:E:67:LEU:HD11	2.49	0.48
6:D:17:MET:HG2	6:D:22:TYR:HB2	1.94	0.48
7:E:67:LEU:O	7:E:71:LEU:HG	2.13	0.48
9:H:13:ASN:ND2	9:H:109:ARG:HG2	2.29	0.48
15:N:76:TYR:CZ	15:N:80:ILE:HG13	2.48	0.48
22:U:32:ARG:HE	22:U:32:ARG:N	2.10	0.48
1:X:303:C:H3'	1:X:304:A:H5"	1.95	0.48
1:X:542:A:H2	1:X:2004:U:H2'	1.78	0.48
1:X:649:G:C5	1:X:650:U:C5	3.01	0.48
1:X:688:A:H4'	5:C:61:GLN:OE1	2.12	0.48
1:X:736:G:H2'	1:X:737:C:O4'	2.13	0.48
1:X:1148:G:O2'	8:G:134:MET:HG3	2.13	0.48
1:X:1269:G:O3'	5:C:69:HIS:CE1	2.67	0.48
1:X:1276:U:O4'	25:Z:10:LYS:HG3	2.13	0.48
1:X:1398:G:O2'	1:X:1399:C:O4'	2.21	0.48
1:X:1426:U:H2'	1:X:1427:G:O4'	2.14	0.48
1:X:1563:U:H2'	1:X:1564:U:C6	2.48	0.48
1:X:1984:A:H2'	1:X:1985:G:O4'	2.14	0.48
5:C:71:ASP:OD1	5:C:72:ARG:N	2.44	0.48
5:C:117:LEU:HB3	5:C:187:VAL:HA	1.94	0.48
19:R:18:LYS:HE2	19:R:19:GLY:N	2.28	0.48
1:X:115:G:OP2	1:X:117:A:O2'	2.32	0.48
1:X:227:G:C6	1:X:228:A:C6	3.02	0.48
1:X:401:G:OP1	22:U:35:THR:HB	2.13	0.48
1:X:536:A:N6	1:X:2605:C:H4'	2.28	0.48
1:X:1202:U:H2'	1:X:1203:A:H8	1.78	0.48
1:X:1442:C:O2'	1:X:1585:A:OP2	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1782:A:N3	3:A:208:LYS:HE2	2.29	0.48
1:X:1816:G:H2'	1:X:1817:U:H6	1.78	0.48
1:X:1816:G:N2	3:A:252:LYS:HG3	2.28	0.48
1:X:2370:G:C6	1:X:2406:C:H1'	2.49	0.48
2:Y:63:A:H2'	2:Y:64:C:H6	1.79	0.48
6:D:14:PRO:HA	6:D:17:MET:HB2	1.96	0.48
11:J:42:TRP:HB3	11:J:95:VAL:HG11	1.95	0.48
20:S:168:VAL:HG12	20:S:169:VAL:HG23	1.95	0.48
28:3:15:LYS:HB2	28:3:23:MET:HB2	1.96	0.48
1:X:69:G:H1'	1:X:72:A:H1'	1.95	0.48
1:X:240:U:H2'	1:X:241:C:O4'	2.14	0.48
1:X:613:A:N6	1:X:668:A:O4'	2.46	0.48
1:X:809:C:H2'	1:X:810:U:C6	2.49	0.48
1:X:1163:C:H2'	1:X:1164:C:H6	1.78	0.48
1:X:1337:G:N2	1:X:1344:C:C2	2.82	0.48
1:X:2551:A:N7	4:B:144:ARG:HG2	2.28	0.48
1:X:2674:C:H2'	1:X:2675:U:C6	2.49	0.48
1:X:2784:A:C6	1:X:2866:A:C8	3.02	0.48
1:X:2821:G:H2'	1:X:2822:U:O4'	2.14	0.48
1:X:2825:A:N7	1:X:2843:A:O2'	2.36	0.48
3:A:208:LYS:O	3:A:211:ARG:HB3	2.14	0.48
5:C:149:LEU:HB2	5:C:183:HIS:ND1	2.29	0.48
11:J:131:LYS:HB2	11:J:131:LYS:NZ	2.28	0.48
13:L:60:LYS:HD2	13:L:60:LYS:HA	1.58	0.48
15:N:49:ASP:O	15:N:53:LYS:HG2	2.14	0.48
15:N:92:ARG:O	15:N:93:LYS:HD3	2.12	0.48
16:O:5:ILE:N	16:O:10:LYS:HD3	2.28	0.48
1:X:469:G:H5'	27:2:39:ARG:O	2.14	0.47
1:X:785:U:H2'	1:X:786:U:H6	1.78	0.47
1:X:1003:C:H2'	1:X:1004:A:C8	2.46	0.47
1:X:1024:G:N2	1:X:1161:U:O2	2.47	0.47
1:X:1054:C:N4	1:X:1123:G:H1	2.10	0.47
1:X:1653:C:H2'	1:X:1654:A:C8	2.49	0.47
1:X:2060:A:H2'	1:X:2061:C:H6	1.78	0.47
1:X:2378:G:H1	1:X:2396:C:H42	1.61	0.47
12:K:3:HIS:HB3	12:K:5:LYS:HD2	1.96	0.47
16:O:11:GLN:HB2	16:O:13:ARG:HH21	1.78	0.47
18:Q:31:PRO:HA	18:Q:76:LYS:CB	2.44	0.47
21:T:17:ASN:HA	21:T:18:PRO:HD3	1.64	0.47
23:V:42:ARG:NH1	23:V:45:GLN:OE1	2.47	0.47
26:1:13:GLU:O	26:1:14:SER:OG	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:824:U:H2'	10:I:30:ALA:H	1.78	0.47
1:X:2492:G:H2'	1:X:2493:U:C6	2.48	0.47
1:X:2798:A:C5	1:X:2799:C:C5	3.02	0.47
4:B:4:ILE:HG22	4:B:96:PHE:HE1	1.79	0.47
8:G:81:VAL:HG21	8:G:161:GLN:HG2	1.96	0.47
12:K:11:ASN:O	12:K:12:ARG:HG2	2.13	0.47
15:N:79:PHE:HE2	15:N:95:LEU:HD21	1.79	0.47
19:R:10:HIS:HD2	19:R:44:GLN:NE2	2.12	0.47
1:X:125:A:H5"	1:X:126:C:O4'	2.14	0.47
1:X:1357:U:H4'	1:X:1397:A:C6	2.49	0.47
1:X:1988:A:H5"	1:X:1989:C:OP2	2.14	0.47
1:X:2614:A:O2'	4:B:48:GLN:NE2	2.47	0.47
4:B:38:THR:HG22	4:B:40:GLN:H	1.79	0.47
7:E:56:SER:OG	7:E:61:HIS:ND1	2.26	0.47
11:J:82:THR:HG23	11:J:84:MET:H	1.79	0.47
17:P:94:GLU:HG3	17:P:127:ILE:HB	1.96	0.47
18:Q:31:PRO:HA	18:Q:76:LYS:HB2	1.97	0.47
1:X:557:U:O4	1:X:560:G:N2	2.47	0.47
1:X:1348:C:H2'	1:X:1349:A:C8	2.49	0.47
1:X:1854:G:H1	1:X:1863:U:H3	1.62	0.47
1:X:1976:U:H5"	4:B:128:SER:HB3	1.96	0.47
1:X:2382:C:N4	1:X:2393:G:H1	2.11	0.47
1:X:2477:C:H5'	1:X:2477:C:H6	1.79	0.47
3:A:96:HIS:HB2	3:A:102:LYS:NZ	2.29	0.47
3:A:198:ASN:O	3:A:198:ASN:ND2	2.48	0.47
5:C:43:ALA:HB3	5:C:86:PRO:HB2	1.96	0.47
21:T:38:VAL:HG21	21:T:45:PHE:CE1	2.50	0.47
1:X:830:C:O2'	1:X:852:U:H5"	2.15	0.47
1:X:1779:C:H2'	1:X:1780:A:H8	1.78	0.47
1:X:1884:A:OP2	3:A:252:LYS:HE3	2.14	0.47
1:X:2826:C:H2'	1:X:2827:G:O4'	2.15	0.47
1:X:2860:C:H2'	1:X:2861:A:O4'	2.14	0.47
1:X:2871:U:H2'	1:X:2872:U:C6	2.49	0.47
5:C:3:GLN:HB2	5:C:116:LYS:HZ2	1.79	0.47
5:C:58:MET:HE2	5:C:59:TYR:HB2	1.97	0.47
8:G:162:LYS:N	8:G:163:PRO:HD2	2.30	0.47
11:J:137:VAL:HG11	20:S:71:MET:SD	2.55	0.47
19:R:59:LYS:HD2	19:R:62:MET:HG3	1.96	0.47
20:S:25:ASN:OD1	20:S:27:GLU:HB2	2.14	0.47
20:S:122:ILE:HB	20:S:123:VAL:H	1.58	0.47
1:X:87:G:C2'	1:X:88:G:H5"	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:485:G:C6	1:X:520:C:N4	2.83	0.47
1:X:788:G:C4	1:X:807:A:C8	3.02	0.47
1:X:792:U:OP1	3:A:48:ARG:HA	2.14	0.47
1:X:1260:A:C6	1:X:1262:U:C2	3.02	0.47
1:X:1283:C:H5"	1:X:1284:G:C5'	2.44	0.47
1:X:1348:C:H4'	18:Q:64:ARG:HH12	1.79	0.47
1:X:1399:C:OP2	1:X:1409:U:N3	2.46	0.47
1:X:1494:G:H2'	1:X:1495:G:H8	1.78	0.47
1:X:1746:A:H2	1:X:2696:A:H1'	1.80	0.47
1:X:1785:A:H2'	1:X:1786:C:H6	1.79	0.47
4:B:188:ILE:HG12	4:B:189:PRO:HD2	1.96	0.47
5:C:18:PRO:HD2	5:C:109:ALA:HB2	1.96	0.47
5:C:25:GLY:HA3	10:I:18:ARG:NH1	2.30	0.47
11:J:8:THR:HG23	11:J:70:PHE:HE2	1.79	0.47
11:J:46:ASN:C	11:J:48:ILE:H	2.17	0.47
13:L:27:LEU:C	13:L:87:VAL:HG13	2.35	0.47
17:P:59:PHE:CG	25:Z:30:LEU:HD21	2.50	0.47
18:Q:53:ILE:HD13	18:Q:80:VAL:HG13	1.97	0.47
22:U:31:GLY:HA2	22:U:32:ARG:HE	1.80	0.47
1:X:105:G:H21	1:X:357:A:H61	1.62	0.47
1:X:239:A:H5"	1:X:621:U:H5'	1.96	0.47
1:X:340:G:O4'	1:X:488:A:H1'	2.15	0.47
1:X:474:G:N2	1:X:476:G:H3'	2.30	0.47
1:X:597:U:H2'	1:X:598:U:C6	2.49	0.47
1:X:652:C:H42	1:X:657:A:H61	1.63	0.47
1:X:836:G:H2'	1:X:837:U:C6	2.49	0.47
1:X:865:A:H2'	1:X:866:U:C6	2.50	0.47
1:X:875:G:O2'	2:Y:80:A:N3	2.47	0.47
1:X:1330:G:O6	1:X:1349:A:N6	2.48	0.47
1:X:1349:A:H2'	1:X:1350:G:H8	1.79	0.47
1:X:1437:A:H2'	1:X:1438:G:C8	2.49	0.47
1:X:2067:U:H2'	1:X:2068:C:C6	2.49	0.47
1:X:2084:G:H1	1:X:2171:U:H3	1.62	0.47
1:X:2258:G:O6	21:T:14:ARG:HG3	2.15	0.47
2:Y:36:A:N6	2:Y:46:G:H2'	2.29	0.47
3:A:108:PRO:HG2	3:A:111:LEU:HB2	1.95	0.47
3:A:246:PRO:CD	3:A:251:GLY:H	2.21	0.47
4:B:37:LYS:HD2	4:B:42:ASP:OD1	2.14	0.47
4:B:96:PHE:CD2	4:B:102:ILE:HG21	2.48	0.47
5:C:5:ASN:N	5:C:5:ASN:OD1	2.47	0.47
8:G:55:ALA:C	8:G:134:MET:HE1	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:116:ARG:NH1	8:G:126:VAL:HG13	2.29	0.47
9:H:17:ARG:H	9:H:58:ALA:HA	1.78	0.47
10:I:102:LYS:C	10:I:104:ARG:H	2.18	0.47
10:I:107:LYS:HG3	10:I:125:ALA:HA	1.96	0.47
11:J:137:VAL:HG21	20:S:71:MET:SD	2.54	0.47
12:K:98:LEU:HD13	12:K:98:LEU:HA	1.60	0.47
14:M:55:ILE:O	14:M:103:LYS:O	2.32	0.47
15:N:45:TYR:O	15:N:49:ASP:HB2	2.15	0.47
19:R:29:HIS:CG	19:R:51:VAL:HG22	2.50	0.47
19:R:45:LYS:HA	19:R:76:LEU:O	2.15	0.47
21:T:38:VAL:HG21	21:T:45:PHE:CZ	2.49	0.47
1:X:37:C:O2'	5:C:44:SER:HB3	2.15	0.47
1:X:768:U:H2'	1:X:769:C:O4'	2.15	0.47
1:X:876:A:O2'	1:X:877:G:H5'	2.14	0.47
1:X:1219:C:H2'	1:X:1220:G:O4'	2.14	0.47
1:X:1631:C:H2'	1:X:1631:C:O2	2.15	0.47
1:X:1850:G:HO2'	1:X:1851:A:H8	1.61	0.47
1:X:1975:G:O2'	1:X:1976:U:OP2	2.24	0.47
1:X:2171:U:H4'	1:X:2171:U:OP1	2.15	0.47
1:X:2284:U:H3'	1:X:2286:G:N2	2.29	0.47
1:X:2537:C:H2'	1:X:2538:C:O4'	2.14	0.47
2:Y:80:A:H2'	2:Y:81:C:O4'	2.15	0.47
4:B:84:PHE:O	4:B:86:PRO:HD3	2.14	0.47
7:E:94:PHE:HB3	7:E:107:ILE:HG22	1.95	0.47
8:G:55:ALA:HB1	8:G:134:MET:HE1	1.97	0.47
13:L:33:ARG:NH2	13:L:103:LEU:HB2	2.29	0.47
16:O:39:PHE:HE2	16:O:46:VAL:HB	1.78	0.47
19:R:15:HIS:CD2	19:R:15:HIS:H	2.33	0.47
1:X:17:G:H2'	1:X:18:U:C6	2.50	0.47
1:X:39:C:H1'	5:C:42:THR:HG21	1.96	0.47
1:X:187:U:H2'	1:X:188:G:C8	2.50	0.47
1:X:321:A:N6	1:X:323:G:N3	2.63	0.47
1:X:353:G:H2'	1:X:354:C:C6	2.50	0.47
1:X:469:G:H3'	27:2:39:ARG:O	2.14	0.47
1:X:1669:A:OP1	12:K:9:LYS:HE2	2.15	0.47
1:X:1757:C:O2'	1:X:1758:C:H5'	2.15	0.47
1:X:2817:A:H2'	1:X:2818:G:O4'	2.15	0.47
8:G:63:ARG:HA	8:G:144:MET:HE1	1.97	0.47
28:3:26:LYS:HG2	28:3:43:GLY:O	2.15	0.47
1:X:825:C:H5"	10:I:30:ALA:CB	2.45	0.47
1:X:2367:A:N7	1:X:2368:G:C6	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2660:C:C2	1:X:2704:U:O4	2.68	0.47
1:X:2769:C:H1'	1:X:2866:A:H2	1.79	0.47
3:A:163:VAL:HG22	3:A:177:LEU:HA	1.97	0.47
5:C:112:GLN:HE22	5:C:116:LYS:HZ2	1.62	0.47
11:J:62:GLY:N	11:J:63:GLY:HA2	2.30	0.47
19:R:61:SER:HA	19:R:65:PRO:HG3	1.97	0.47
20:S:3:LEU:HB3	20:S:56:VAL:HA	1.96	0.47
25:Z:40:LYS:HD3	25:Z:46:CYS:HB2	1.97	0.47
1:X:757:U:H2'	1:X:758:G:O4'	2.14	0.46
4:B:183:LEU:HD21	14:M:16:ILE:HG12	1.97	0.46
6:D:111:ILE:HG22	6:D:114:PHE:HB2	1.96	0.46
14:M:57:ILE:H	14:M:57:ILE:HD12	1.81	0.46
22:U:20:ARG:HE	22:U:20:ARG:HB2	1.47	0.46
1:X:494:A:O4'	19:R:56:LYS:HB2	2.14	0.46
1:X:956:A:C4	1:X:2427:A:C2	3.03	0.46
1:X:2265:A:OP1	26:1:31:THR:OG1	2.21	0.46
3:A:63:ARG:HG3	3:A:85:ASP:OD1	2.15	0.46
3:A:188:GLU:HG2	3:A:188:GLU:H	1.42	0.46
8:G:65:LYS:NZ	15:N:70:ARG:HD2	2.30	0.46
20:S:95:SER:HB3	20:S:119:ASN:HB3	1.97	0.46
23:V:62:ARG:O	23:V:66:GLN:N	2.45	0.46
1:X:32:C:O2'	1:X:33:C:H5'	2.16	0.46
1:X:538:A:HO2'	1:X:539:A:P	2.34	0.46
1:X:811:G:OP2	5:C:56:ARG:HG2	2.15	0.46
1:X:1584:G:H4'	3:A:59:LYS:HG3	1.97	0.46
1:X:1673:C:H2'	1:X:1674:C:H6	1.80	0.46
1:X:1802:A:H2'	1:X:1803:G:O4'	2.15	0.46
1:X:1827:G:H1	1:X:1888:C:H42	1.63	0.46
1:X:2394:G:C2	1:X:2395:C:C2	3.03	0.46
1:X:2629:U:H2'	1:X:2630:C:H6	1.81	0.46
2:Y:51:G:OP1	13:L:99:ARG:N	2.41	0.46
3:A:91:ARG:O	3:A:107:ALA:N	2.33	0.46
3:A:245:VAL:HB	3:A:249:PRO:HA	1.97	0.46
6:D:104:ILE:HG12	6:D:108:LEU:HD12	1.98	0.46
11:J:54:VAL:HG21	11:J:125:LYS:HE3	1.97	0.46
15:N:102:GLU:HA	15:N:103:PRO:HD3	1.69	0.46
21:T:47:ALA:HB1	21:T:51:VAL:HB	1.96	0.46
1:X:224:G:H4'	1:X:399:G:C6	2.50	0.46
1:X:623:G:H21	1:X:626:A:H2	1.61	0.46
1:X:1609:G:H2'	1:X:1610:A:O4'	2.16	0.46
1:X:1761:G:C5	1:X:1762:C:C5	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:14:C:H4'	2:Y:17:A:H62	1.79	0.46
4:B:14:ILE:HA	14:M:20:HIS:CD2	2.49	0.46
6:D:112:ARG:CZ	6:D:137:ILE:HG22	2.46	0.46
7:E:34:THR:O	7:E:34:THR:OG1	2.34	0.46
11:J:79:PRO:CD	11:J:88:LYS:HD2	2.45	0.46
22:U:20:ARG:HD2	22:U:43:ARG:NE	2.30	0.46
9:H:134:LEU:HA	9:H:134:LEU:HD23	1.78	0.46
11:J:20:GLY:O	11:J:99:LYS:HG2	2.16	0.46
15:N:66:ASN:HD22	15:N:70:ARG:HH12	1.63	0.46
18:Q:4:TYR:CE2	23:V:23:LYS:HB2	2.51	0.46
19:R:81:VAL:HG12	19:R:82:ALA:N	2.30	0.46
1:X:670:U:H2'	1:X:671:A:C8	2.50	0.46
1:X:753:U:H2'	1:X:754:G:H8	1.80	0.46
1:X:1046:U:C5'	7:E:59:GLN:HG2	2.45	0.46
1:X:1925:C:H2'	1:X:1926:U:C5	2.50	0.46
1:X:2309:G:H2'	1:X:2310:G:O4'	2.15	0.46
1:X:2663:U:H3	1:X:2705:A:N6	2.09	0.46
1:X:2707:G:H2'	1:X:2708:U:C6	2.50	0.46
2:Y:46:G:H1'	2:Y:49:C:N4	2.31	0.46
3:A:117:VAL:HG13	3:A:129:ASN:HD22	1.80	0.46
4:B:188:ILE:HG12	4:B:189:PRO:CD	2.46	0.46
6:D:133:LYS:O	6:D:151:GLY:HA3	2.15	0.46
9:H:2:ILE:HB	9:H:45:ALA:HB3	1.97	0.46
17:P:44:VAL:HG21	25:Z:27:ALA:HB2	1.98	0.46
19:R:18:LYS:H	19:R:18:LYS:HD3	1.79	0.46
19:R:61:SER:HA	19:R:65:PRO:HB3	1.97	0.46
27:2:28:ARG:HD2	27:2:28:ARG:HA	1.75	0.46
1:X:388:G:H2'	1:X:389:G:C8	2.51	0.46
1:X:529:U:H2'	1:X:530:G:H8	1.80	0.46
1:X:568:G:H2'	1:X:569:C:O4'	2.16	0.46
1:X:1004:A:N3	16:O:88:GLN:NE2	2.63	0.46
1:X:1104:G:H1'	1:X:1110:G:N2	2.31	0.46
1:X:1231:A:C2	1:X:1245:G:C2	3.04	0.46
1:X:1349:A:H2'	1:X:1350:G:C8	2.50	0.46
1:X:2272:A:P	13:L:15:ARG:HH21	2.38	0.46
3:A:244:ARG:NH1	3:A:253:PRO:HG3	2.31	0.46
7:E:90:ARG:CZ	7:E:163:ARG:HD2	2.46	0.46
8:G:140:GLN:O	8:G:143:ALA:HB3	2.15	0.46
26:1:42:PRO:HG3	26:1:50:PHE:CE1	2.51	0.46
1:X:20:C:H2'	1:X:21:A:C8	2.50	0.46
1:X:162:C:H2'	1:X:163:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:742:G:C5	3:A:208:LYS:HB3	2.50	0.46
1:X:1361:G:H2'	1:X:1362:A:C8	2.51	0.46
1:X:1606:C:N4	1:X:1607:A:H62	2.14	0.46
1:X:2057:U:H2'	1:X:2058:U:C6	2.51	0.46
1:X:2363:G:OP2	1:X:2363:G:H8	1.99	0.46
1:X:2474:G:H2'	1:X:2475:C:O4'	2.16	0.46
2:Y:16:U:HO2'	2:Y:17:A:P	2.39	0.46
2:Y:70:C:H2'	2:Y:71:G:O4'	2.15	0.46
2:Y:77:G:H1'	20:S:22:VAL:HG21	1.97	0.46
3:A:218:LYS:HA	3:A:218:LYS:HD2	1.60	0.46
8:G:42:VAL:HA	8:G:166:LEU:O	2.16	0.46
8:G:170:PRO:O	8:G:171:LEU:HB2	2.15	0.46
13:L:15:ARG:HA	13:L:15:ARG:HD3	1.70	0.46
16:O:36:LYS:NZ	16:O:56:VAL:HG13	2.31	0.46
16:O:67:LYS:HG3	16:O:68:LYS:N	2.30	0.46
27:2:18:PHE:H	27:2:44:VAL:CG2	2.29	0.46
1:X:464:G:H2'	1:X:465:C:C6	2.51	0.46
1:X:627:A:H2'	1:X:628:A:H8	1.78	0.46
1:X:1583:A:H2	3:A:31:LYS:HE2	1.80	0.46
1:X:1845:A:N3	1:X:2212:U:O2'	2.43	0.46
1:X:1987:G:C5	1:X:1988:A:C8	3.04	0.46
1:X:2448:A:H2'	1:X:2449:G:O4'	2.16	0.46
1:X:2845:C:C4	1:X:2846:G:N7	2.84	0.46
9:H:23:ARG:HG3	9:H:24:VAL:N	2.31	0.46
13:L:8:ARG:HG3	13:L:9:ARG:N	2.30	0.46
1:X:18:U:O2'	15:N:23:GLY:HA2	2.16	0.46
1:X:334:G:OP1	1:X:349:G:N2	2.47	0.46
1:X:1439:G:H2'	1:X:1440:G:C8	2.51	0.46
1:X:1494:G:C4	1:X:1495:G:C8	3.04	0.46
1:X:1710:U:H5"	1:X:1711:C:H5	1.81	0.46
1:X:2039:G:C2	1:X:2040:A:C8	3.04	0.46
1:X:2200:G:H2'	1:X:2201:G:H8	1.80	0.46
1:X:2707:G:H2'	1:X:2708:U:H6	1.81	0.46
1:X:2796:A:H2'	1:X:2797:G:C8	2.47	0.46
2:Y:78:A:H2'	2:Y:79:U:O4'	2.16	0.46
9:H:29:ILE:CG2	9:H:122:ARG:HB2	2.44	0.46
13:L:20:THR:HG21	13:L:23:ALA:HB3	1.97	0.46
15:N:62:ILE:HG23	15:N:76:TYR:CE1	2.51	0.46
17:P:89:ARG:HD3	17:P:132:GLY:HA2	1.98	0.46
18:Q:66:GLY:HA3	18:Q:68:PHE:CD2	2.51	0.46
27:2:1:MET:HG3	27:2:3:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:21:ARG:HE	27:2:43:THR:HG21	1.81	0.46
1:X:78:C:O2'	1:X:357:A:N3	2.46	0.45
1:X:562:G:C6	1:X:563:U:C4	3.04	0.45
1:X:732:G:H2'	1:X:733:G:C8	2.51	0.45
1:X:750:C:H2'	1:X:751:G:H5'	1.98	0.45
1:X:849:G:C5	1:X:850:C:C4	3.04	0.45
1:X:1407:G:C6	1:X:1408:A:N6	2.84	0.45
1:X:2197:U:H5'	1:X:2198:U:OP1	2.16	0.45
1:X:2447:G:OP1	11:J:120:ARG:NH2	2.49	0.45
6:D:112:ARG:N	6:D:112:ARG:HD2	2.31	0.45
9:H:11:ALA:O	9:H:111:PHE:N	2.41	0.45
1:X:746:G:C8	1:X:774:A:C6	3.04	0.45
1:X:938:G:H2'	1:X:940:G:N7	2.32	0.45
1:X:1008:G:H5'	15:N:93:LYS:HG3	1.98	0.45
1:X:1459:U:O2	1:X:1475:U:H5"	2.15	0.45
1:X:1715:A:C8	1:X:1717:A:O4'	2.70	0.45
1:X:1981:A:O2'	1:X:2704:U:O2'	2.23	0.45
1:X:2229:G:C6	11:J:83:ARG:HG2	2.52	0.45
1:X:2468:G:C6	1:X:2469:G:C6	3.05	0.45
1:X:2495:G:O2'	1:X:2496:C:H5'	2.16	0.45
3:A:222:ARG:HH11	3:A:225:ALA:HB2	1.81	0.45
7:E:45:GLN:NE2	7:E:48:ASP:O	2.48	0.45
7:E:69:ARG:HH21	7:E:73:ALA:HB2	1.81	0.45
8:G:66:HIS:CD2	15:N:71:LEU:HD13	2.51	0.45
25:Z:58:LEU:HG	25:Z:58:LEU:O	2.16	0.45
1:X:66:U:H2'	1:X:67:G:H8	1.82	0.45
1:X:1745:C:C5	1:X:1746:A:C5	3.04	0.45
1:X:2262:C:OP1	26:1:7:ARG:NH1	2.48	0.45
1:X:2422:C:H2'	1:X:2423:G:H8	1.81	0.45
1:X:2594:U:N1	25:Z:7:PRO:HA	2.31	0.45
2:Y:27:A:HO2'	2:Y:28:A:P	2.38	0.45
9:H:3:MET:O	9:H:6:SER:HB3	2.16	0.45
10:I:75:VAL:HG22	10:I:99:VAL:HG21	1.97	0.45
11:J:6:LYS:HE2	11:J:6:LYS:HB3	1.69	0.45
19:R:96:LYS:O	19:R:104:VAL:HA	2.16	0.45
28:3:13:ARG:HD2	28:3:24:ALA:HA	1.98	0.45
1:X:400:U:H4'	1:X:401:G:O5'	2.16	0.45
1:X:764:A:C6	1:X:802:A:C5	3.04	0.45
1:X:1121:G:H2'	1:X:1122:A:C8	2.52	0.45
1:X:1164:C:H2'	1:X:1165:G:O4'	2.17	0.45
1:X:1781:C:OP1	3:A:219:PRO:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1922:U:H5"	1:X:1922:U:O2	2.16	0.45
1:X:2058:U:H2'	1:X:2217:G:N2	2.32	0.45
1:X:2401:A:N3	1:X:2401:A:H2'	2.31	0.45
1:X:2442:C:H2'	1:X:2443:C:C6	2.52	0.45
1:X:2662:C:H2'	1:X:2663:U:C6	2.52	0.45
3:A:96:HIS:NE2	3:A:97:TYR:O	2.49	0.45
3:A:169:GLU:N	3:A:172:TYR:O	2.34	0.45
3:A:169:GLU:OE2	3:A:184:ARG:NH1	2.49	0.45
5:C:191:ALA:HA	5:C:194:GLU:HB2	1.99	0.45
9:H:29:ILE:HB	9:H:123:PHE:HE1	1.81	0.45
12:K:25:ALA:HB1	12:K:48:VAL:HG23	1.99	0.45
17:P:89:ARG:HG2	17:P:131:LYS:H	1.81	0.45
18:Q:8:GLN:O	23:V:29:ARG:HD2	2.16	0.45
25:Z:51:TYR:CE1	25:Z:55:ARG:HG2	2.52	0.45
1:X:824:U:H1'	1:X:1264:C:O4'	2.15	0.45
1:X:1374:G:N2	1:X:1384:G:H1'	2.31	0.45
4:B:5:LEU:H	4:B:5:LEU:HD12	1.80	0.45
4:B:32:PRO:O	4:B:49:ILE:HA	2.17	0.45
27:2:4:THR:O	27:2:4:THR:OG1	2.34	0.45
1:X:88:G:C3'	1:X:89:A:H5"	2.45	0.45
1:X:969:U:O4'	11:J:17:ARG:NH1	2.50	0.45
1:X:999:A:OP1	24:W:7:ARG:HD3	2.16	0.45
1:X:1007:A:H2'	1:X:1008:G:C8	2.44	0.45
1:X:1008:G:C2	1:X:1009:C:C5	3.05	0.45
1:X:1227:A:H4'	1:X:1252:C:H4'	1.98	0.45
1:X:1462:C:H2'	1:X:1463:A:C8	2.52	0.45
1:X:1935:A:C6	1:X:1936:A:N1	2.85	0.45
1:X:2255:G:H2'	1:X:2256:G:H8	1.82	0.45
1:X:2576:G:C6	1:X:2577:A:N6	2.84	0.45
3:A:96:HIS:CE1	3:A:100:GLY:HA2	2.47	0.45
7:E:57:ASP:HB3	7:E:62:ARG:HH11	1.82	0.45
13:L:97:HIS:HB3	13:L:98:GLY:H	1.60	0.45
17:P:114:ALA:O	17:P:115:ASN:ND2	2.43	0.45
26:1:28:ARG:O	26:1:33:ALA:HB2	2.17	0.45
1:X:111:G:H8	1:X:111:G:OP2	2.00	0.45
1:X:177:U:O2'	1:X:178:C:O4'	2.35	0.45
1:X:746:G:N7	1:X:774:A:C5	2.85	0.45
1:X:1050:G:H1	1:X:1127:C:H42	1.64	0.45
1:X:1330:G:C6	1:X:1349:A:C6	3.05	0.45
1:X:2014:A:C6	1:X:2477:C:H1'	2.52	0.45
1:X:2067:U:H2'	1:X:2068:C:H6	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2309:G:N2	1:X:2365:U:C2	2.85	0.45
1:X:2371:A:C4	1:X:2408:G:C6	3.05	0.45
4:B:137:ARG:HG3	4:B:138:PRO:HD2	1.99	0.45
5:C:97:ARG:O	5:C:100:ARG:HG2	2.15	0.45
10:I:31:GLY:HA2	10:I:34:HIS:HB2	1.99	0.45
11:J:124:HIS:CD2	11:J:124:HIS:H	2.34	0.45
15:N:92:ARG:CA	15:N:95:LEU:HB2	2.46	0.45
17:P:35:PRO:HB2	17:P:39:ARG:NH1	2.32	0.45
17:P:75:ALA:HB2	17:P:126:ILE:HG23	1.98	0.45
27:2:17:GLY:O	27:2:21:ARG:HG2	2.17	0.45
28:3:29:LYS:HD2	28:3:33:ASN:O	2.17	0.45
1:X:750:C:C2'	1:X:751:G:H5'	2.47	0.45
1:X:1189:G:H2'	1:X:1190:C:C6	2.51	0.45
1:X:1652:G:H2'	1:X:1653:C:H6	1.82	0.45
1:X:1818:G:OP1	3:A:224:SER:OG	2.27	0.45
1:X:1949:A:H1'	1:X:2572:U:C5'	2.47	0.45
1:X:2033:C:H1'	4:B:156:MET:CE	2.47	0.45
1:X:2727:G:O6	1:X:2735:C:H5"	2.17	0.45
3:A:85:ASP:CG	3:A:92:ILE:HD12	2.37	0.45
3:A:89:SER:O	3:A:159:ALA:HB2	2.17	0.45
3:A:143:HIS:CD2	3:A:196:VAL:HG13	2.52	0.45
3:A:200:GLU:HG3	3:A:202:LYS:HG3	1.97	0.45
10:I:32:ARG:HH22	10:I:34:HIS:CE1	2.34	0.45
11:J:35:LEU:HD12	11:J:131:LYS:O	2.17	0.45
27:2:1:MET:HG3	27:2:3:ARG:CZ	2.46	0.45
28:3:11:LYS:HD2	28:3:11:LYS:N	2.32	0.45
1:X:469:G:H22	1:X:480:G:H2'	1.82	0.45
1:X:481:A:C6	1:X:482:A:C6	3.05	0.45
1:X:603:C:H2'	1:X:604:U:H6	1.82	0.45
1:X:920:G:P	11:J:24:GLY:HA3	2.57	0.45
1:X:938:G:O2'	1:X:939:C:P	2.75	0.45
1:X:978:U:H2'	1:X:979:A:C8	2.52	0.45
1:X:2340:C:O5'	28:3:27:SER:OG	2.35	0.45
1:X:2579:A:O2'	1:X:2580:C:H5'	2.16	0.45
1:X:2754:C:H2'	1:X:2755:A:O4'	2.17	0.45
1:X:2827:G:H2'	1:X:2828:C:O4'	2.17	0.45
7:E:107:ILE:HD11	7:E:151:VAL:HG12	1.99	0.45
8:G:97:ASP:O	8:G:99:VAL:HG23	2.16	0.45
11:J:46:ASN:HA	11:J:49:GLU:HB2	1.99	0.45
1:X:389:G:H2'	1:X:390:U:C6	2.52	0.45
1:X:481:A:N3	1:X:481:A:H2'	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:576:A:H4'	1:X:821:A:OP1	2.16	0.45
1:X:1398:G:O2'	1:X:1399:C:O5'	2.34	0.45
1:X:1517:C:H4'	3:A:96:HIS:CE1	2.52	0.45
1:X:1692:C:N4	1:X:1976:U:O4'	2.49	0.45
1:X:2662:C:H2'	1:X:2663:U:H6	1.81	0.45
1:X:2691:C:O2'	1:X:2692:A:P	2.75	0.45
2:Y:5:C:H2'	2:Y:6:C:O4'	2.16	0.45
8:G:88:VAL:HG21	8:G:127:ILE:HD11	1.99	0.45
13:L:8:ARG:HB2	13:L:8:ARG:CZ	2.46	0.45
13:L:35:SER:OG	13:L:36:LYS:N	2.50	0.45
14:M:32:THR:HG22	14:M:93:ILE:HA	1.99	0.45
16:O:36:LYS:HZ1	16:O:56:VAL:HG13	1.82	0.45
18:Q:6:ILE:HG22	18:Q:7:LEU:HD13	1.99	0.45
20:S:153:LYS:HA	20:S:153:LYS:HD3	1.79	0.45
21:T:66:LYS:HB3	21:T:66:LYS:HE2	1.78	0.45
1:X:854:G:N2	1:X:948:C:N3	2.58	0.44
1:X:1287:A:N1	1:X:1661:C:O2'	2.34	0.44
1:X:1479:G:H2'	1:X:1480:G:H8	1.81	0.44
1:X:1552:C:O2	1:X:1553:G:N2	2.50	0.44
1:X:1778:U:H2'	1:X:1779:C:H6	1.82	0.44
1:X:1786:C:O2	3:A:252:LYS:HD2	2.17	0.44
1:X:2344:G:H4'	21:T:60:PHE:CE1	2.52	0.44
1:X:2398:U:H4'	26:1:13:GLU:OE1	2.17	0.44
1:X:2543:A:C6	1:X:2544:A:N1	2.85	0.44
2:Y:64:C:H2'	2:Y:65:A:H8	1.82	0.44
3:A:31:LYS:HE3	3:A:32:ALA:H	1.82	0.44
5:C:177:VAL:HB	5:C:178:TYR:H	1.59	0.44
8:G:67:ARG:HD3	8:G:70:PHE:HA	1.99	0.44
8:G:84:ASN:C	8:G:86:ALA:H	2.20	0.44
8:G:118:ALA:O	8:G:121:LYS:HB3	2.17	0.44
9:H:75:VAL:HG22	9:H:96:ALA:HA	1.98	0.44
9:H:83:ARG:HG2	14:M:40:ARG:HH22	1.83	0.44
12:K:75:VAL:O	12:K:79:VAL:HG13	2.17	0.44
13:L:11:LEU:HA	13:L:14:ARG:NH1	2.32	0.44
13:L:27:LEU:HD13	13:L:87:VAL:HG22	1.99	0.44
18:Q:60:GLY:HA3	18:Q:73:ASN:H	1.81	0.44
19:R:84:VAL:HG11	19:R:90:LYS:N	2.23	0.44
22:U:42:GLN:OE1	22:U:42:GLN:N	2.51	0.44
1:X:353:G:H2'	1:X:354:C:H6	1.82	0.44
1:X:596:C:N4	10:I:36:GLY:HA3	2.32	0.44
1:X:934:G:H1'	21:T:26:PHE:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1032:A:H62	1:X:1151:U:H3	1.65	0.44
1:X:1658:A:H2'	1:X:1659:G:O4'	2.17	0.44
1:X:2339:A:P	28:3:49:VAL:HG11	2.57	0.44
1:X:2396:C:H2'	1:X:2397:A:O4'	2.17	0.44
1:X:2526:U:C4	1:X:2545:A:N7	2.85	0.44
1:X:2630:C:H2'	1:X:2631:C:C6	2.52	0.44
2:Y:63:A:H2'	2:Y:64:C:C6	2.53	0.44
3:A:121:PRO:HA	3:A:132:PRO:HD2	1.98	0.44
6:D:106:ILE:HG21	6:D:139:PRO:HB3	1.99	0.44
11:J:37:ALA:O	11:J:100:PRO:HA	2.17	0.44
11:J:39:GLU:HA	11:J:40:PRO:HD3	1.86	0.44
14:M:107:LEU:HD23	14:M:107:LEU:HA	1.73	0.44
17:P:106:LEU:HD23	17:P:106:LEU:O	2.17	0.44
1:X:75:C:H2'	1:X:76:C:C6	2.52	0.44
1:X:321:A:N1	1:X:323:G:H1'	2.32	0.44
1:X:1212:U:H2'	1:X:1213:U:H6	1.81	0.44
1:X:1353:A:H2'	18:Q:56:MET:SD	2.57	0.44
1:X:1430:G:H2'	1:X:1431:U:C6	2.52	0.44
1:X:1713:G:C5	1:X:1714:A:C8	3.06	0.44
1:X:2024:U:H2'	1:X:2025:A:O4'	2.18	0.44
1:X:2701:A:H2'	1:X:2702:G:O4'	2.16	0.44
1:X:2848:A:N3	12:K:7:GLY:N	2.61	0.44
2:Y:11:G:OP1	13:L:28:ARG:NH1	2.50	0.44
5:C:129:LYS:C	5:C:131:LYS:H	2.16	0.44
12:K:59:ASP:OD2	12:K:59:ASP:N	2.51	0.44
13:L:88:VAL:HG12	13:L:89:PHE:H	1.82	0.44
25:Z:41:LEU:HD13	25:Z:41:LEU:HA	1.70	0.44
28:3:30:ARG:HB3	28:3:31:HIS:ND1	2.33	0.44
1:X:433:G:N2	1:X:434:C:H1'	2.32	0.44
1:X:490:A:H1'	1:X:491:A:H5"	2.00	0.44
1:X:836:G:C5	1:X:837:U:C5	3.05	0.44
1:X:1727:C:H2'	1:X:1728:A:H8	1.81	0.44
1:X:1847:G:H2'	1:X:1848:U:C6	2.52	0.44
1:X:1919:A:OP2	1:X:1944:C:N4	2.46	0.44
1:X:2633:A:N1	1:X:2644:A:H5"	2.32	0.44
3:A:23:GLY:HA3	3:A:205:VAL:HG11	1.99	0.44
3:A:39:LYS:HD2	3:A:39:LYS:HA	1.66	0.44
4:B:173:VAL:HG23	4:B:185:LYS:HB2	1.98	0.44
5:C:122:GLY:O	5:C:125:ILE:HB	2.18	0.44
8:G:104:THR:OG1	8:G:105:GLY:N	2.48	0.44
12:K:43:GLU:O	12:K:46:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:50:ARG:HA	15:N:53:LYS:HD3	1.99	0.44
20:S:36:ARG:HH21	20:S:78:PRO:HD2	1.83	0.44
1:X:593:C:OP2	15:N:6:THR:OG1	2.36	0.44
1:X:2010:G:C6	1:X:2011:U:C4	3.06	0.44
1:X:2529:G:C6	1:X:2530:C:C4	3.06	0.44
1:X:2630:C:H2'	1:X:2631:C:H6	1.83	0.44
2:Y:51:G:H2'	2:Y:52:G:C8	2.53	0.44
2:Y:52:G:C2	2:Y:53:G:C8	3.06	0.44
6:D:128:TYR:HB3	6:D:156:ILE:HB	1.98	0.44
8:G:141:GLY:O	8:G:145:HIS:HD2	2.00	0.44
15:N:27:SER:HB2	15:N:31:GLN:HG3	1.98	0.44
15:N:60:LEU:O	15:N:64:ARG:HG3	2.17	0.44
17:P:45:ILE:HD11	17:P:57:LEU:CD1	2.40	0.44
1:X:452:G:H2'	1:X:453:U:O4'	2.17	0.44
1:X:1316:G:N2	1:X:1317:G:H1'	2.33	0.44
1:X:1919:A:H2	1:X:1926:U:N3	2.15	0.44
1:X:1998:A:N3	25:Z:6:VAL:HG23	2.32	0.44
1:X:2261:G:H5"	1:X:2262:C:O4'	2.17	0.44
1:X:2545:A:H61	9:H:40:GLY:CA	2.28	0.44
1:X:2595:C:H5"	1:X:2596:C:OP2	2.17	0.44
1:X:2736:U:H4'	1:X:2737:A:OP1	2.18	0.44
5:C:60:GLY:C	5:C:62:LYS:H	2.21	0.44
7:E:68:THR:O	7:E:72:VAL:HG23	2.18	0.44
8:G:52:GLY:O	8:G:55:ALA:HB3	2.18	0.44
15:N:61:TRP:O	15:N:65:ILE:HG12	2.17	0.44
16:O:20:ILE:HG13	16:O:21:ARG:N	2.27	0.44
1:X:21:A:C6	1:X:530:G:C6	3.05	0.44
1:X:530:G:H2'	1:X:531:G:C8	2.51	0.44
1:X:703:A:O2'	1:X:793:G:OP1	2.36	0.44
1:X:1018:C:OP2	1:X:1019:U:O2'	2.15	0.44
1:X:1041:G:OP2	11:J:129:GLN:NE2	2.50	0.44
1:X:1430:G:H2'	1:X:1431:U:H6	1.83	0.44
1:X:1594:U:H2'	1:X:1595:A:C8	2.52	0.44
1:X:2265:A:H61	26:1:25:THR:HG21	1.83	0.44
1:X:2285:U:H2'	1:X:2286:G:H5'	1.98	0.44
6:D:108:LEU:HD22	6:D:117:ILE:HD11	1.99	0.44
7:E:61:HIS:C	7:E:63:ALA:H	2.21	0.44
14:M:27:PHE:HA	14:M:96:ARG:NH2	2.33	0.44
19:R:23:ILE:O	19:R:80:LYS:HB2	2.17	0.44
20:S:70:GLN:CB	20:S:80:HIS:HB3	2.48	0.44
20:S:96:VAL:O	20:S:119:ASN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:54:ASN:HD21	22:U:77:GLY:HA2	1.82	0.44
1:X:66:U:H2'	1:X:67:G:C8	2.52	0.44
1:X:187:U:H2'	1:X:188:G:H8	1.82	0.44
1:X:386:U:H5'	1:X:436:A:C2	2.52	0.44
1:X:1775:A:H4'	1:X:1776:A:O5'	2.18	0.44
1:X:2418:A:N1	1:X:2564:U:O2'	2.48	0.44
1:X:2839:G:H2'	1:X:2840:U:C6	2.53	0.44
3:A:29:PRO:HB2	3:A:30:GLU:CD	2.38	0.44
4:B:59:VAL:HG12	4:B:64:GLN:HG3	1.99	0.44
9:H:1:MET:HB2	9:H:44:TYR:HB3	1.98	0.44
9:H:83:ARG:HD2	9:H:89:ILE:HD11	1.99	0.44
23:V:21:ARG:NH1	23:V:53:LEU:HD11	2.33	0.44
1:X:178:C:P	22:U:40:ARG:CZ	3.06	0.44
1:X:312:G:HO2'	1:X:313:U:H6	1.64	0.44
1:X:778:G:H2'	1:X:779:U:H6	1.83	0.44
1:X:998:C:H2'	1:X:999:A:O4'	2.18	0.44
1:X:1175:A:C2	1:X:1176:U:C2	3.06	0.44
1:X:1193:G:H2'	1:X:1194:U:C6	2.53	0.44
1:X:1652:G:H2'	1:X:1653:C:C6	2.53	0.44
1:X:1966:C:H4'	1:X:2585:C:H4'	2.00	0.44
1:X:2399:C:H41	28:3:31:HIS:HB2	1.82	0.44
1:X:2491:C:H2'	1:X:2492:G:O4'	2.18	0.44
1:X:2610:G:N2	1:X:2767:C:O2	2.44	0.44
17:P:13:GLN:O	17:P:16:GLN:HG2	2.18	0.44
17:P:41:VAL:O	17:P:44:VAL:HG12	2.18	0.44
18:Q:25:TYR:CZ	18:Q:88:ILE:HG23	2.53	0.44
1:X:14:A:C6	1:X:536:A:C2	3.06	0.43
1:X:504:G:H4'	17:P:27:VAL:CG1	2.47	0.43
1:X:518:A:HO2'	1:X:519:C:P	2.40	0.43
1:X:556:A:O2'	1:X:557:U:OP2	2.32	0.43
1:X:661:C:O2	1:X:662:G:N2	2.51	0.43
1:X:2010:G:H1	1:X:2019:C:H42	1.66	0.43
1:X:2295:C:O2'	6:D:125:ARG:NH2	2.50	0.43
1:X:2609:G:H2'	1:X:2610:G:C8	2.52	0.43
1:X:2812:A:H2'	1:X:2813:G:C8	2.53	0.43
2:Y:16:U:O2'	2:Y:110:U:O2	2.36	0.43
4:B:14:ILE:HG12	14:M:20:HIS:NE2	2.32	0.43
5:C:17:LEU:HD12	5:C:17:LEU:HA	1.73	0.43
5:C:50:GLN:NE2	5:C:56:ARG:HH12	2.16	0.43
11:J:13:GLN:HE21	11:J:90:ALA:HB1	1.82	0.43
15:N:92:ARG:HB3	15:N:95:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:35:LEU:HD23	16:O:55:THR:HG22	1.98	0.43
17:P:60:ILE:HA	17:P:61:PRO:HD3	1.45	0.43
26:1:9:ILE:HG22	26:1:30:ASN:OD1	2.17	0.43
26:1:14:SER:HB2	26:1:23:THR:H	1.82	0.43
1:X:463:C:P	5:C:46:ARG:HG2	2.59	0.43
1:X:540:G:N1	1:X:2005:U:OP1	2.51	0.43
1:X:814:G:OP1	5:C:50:GLN:HB2	2.17	0.43
1:X:1635:G:O2'	27:2:1:MET:HB2	2.17	0.43
1:X:2069:U:H2'	1:X:2070:G:C8	2.52	0.43
1:X:2222:U:H2'	1:X:2223:U:H6	1.80	0.43
1:X:2787:A:H2'	1:X:2788:C:C6	2.53	0.43
2:Y:14:C:O5'	21:T:72:LYS:NZ	2.51	0.43
4:B:38:THR:HB	4:B:41:THR:H	1.83	0.43
5:C:45:THR:HB	5:C:86:PRO:O	2.17	0.43
8:G:36:ASN:HB3	8:G:74:MET:HG3	2.00	0.43
10:I:62:LYS:HB3	28:3:12:ARG:HA	2.00	0.43
13:L:89:PHE:HZ	13:L:100:VAL:HG22	1.83	0.43
25:Z:19:ARG:O	25:Z:21:SER:N	2.51	0.43
1:X:1216:G:C6	1:X:1217:U:C4	3.06	0.43
1:X:1228:G:C6	1:X:1229:C:C4	3.05	0.43
1:X:1672:A:C6	1:X:1673:C:C2	3.06	0.43
1:X:1721:G:H2'	1:X:1722:G:O4'	2.18	0.43
1:X:2758:A:HO2'	1:X:2760:G:HO2'	1.57	0.43
4:B:122:PHE:HE2	4:B:138:PRO:CB	2.30	0.43
10:I:103:ASN:O	10:I:103:ASN:ND2	2.52	0.43
14:M:87:LEU:HD23	14:M:87:LEU:HA	1.61	0.43
1:X:5:A:O2'	8:G:162:LYS:HE3	2.18	0.43
1:X:662:G:H2'	1:X:663:G:O4'	2.19	0.43
1:X:2077:G:N2	1:X:2179:C:H1'	2.33	0.43
1:X:2169:A:H2'	1:X:2170:C:C6	2.53	0.43
1:X:2504:G:C2	1:X:2518:C:C2	3.07	0.43
1:X:2657:G:H2'	1:X:2658:A:O4'	2.18	0.43
3:A:186:HIS:CD2	3:A:186:HIS:H	2.34	0.43
4:B:10:GLY:O	4:B:25:VAL:HG23	2.19	0.43
5:C:97:ARG:HA	5:C:100:ARG:HD3	1.99	0.43
5:C:111:ARG:O	5:C:115:GLY:O	2.37	0.43
6:D:14:PRO:O	6:D:18:GLN:HG2	2.17	0.43
8:G:67:ARG:HD3	8:G:70:PHE:C	2.39	0.43
8:G:84:ASN:HD21	8:G:154:GLU:HG2	1.84	0.43
9:H:115:ALA:O	9:H:118:LEU:HB2	2.19	0.43
17:P:17:GLN:HG3	17:P:18:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:21:ARG:HD2	27:2:30:ILE:HD12	2.00	0.43
27:2:24:THR:OG1	27:2:25:LYS:N	2.51	0.43
28:3:24:ALA:N	28:3:47:GLY:O	2.37	0.43
1:X:26:G:H1'	1:X:524:A:N6	2.33	0.43
1:X:125:A:H5"	1:X:126:C:C1'	2.49	0.43
1:X:328:A:H2'	1:X:329:C:C6	2.53	0.43
1:X:1507:A:O4'	3:A:99:ASP:HB3	2.18	0.43
1:X:2424:G:O2'	1:X:2425:G:H5'	2.18	0.43
1:X:2576:G:C6	1:X:2577:A:C6	3.07	0.43
1:X:2751:C:H2'	1:X:2752:C:H6	1.84	0.43
3:A:217:ARG:HG2	3:A:218:LYS:HB2	2.00	0.43
10:I:73:GLU:OE2	10:I:104:ARG:HB2	2.18	0.43
12:K:45:ARG:HD3	12:K:95:THR:HG22	2.01	0.43
16:O:64:GLY:HA3	16:O:90:PHE:CZ	2.54	0.43
17:P:45:ILE:HG21	17:P:45:ILE:HD13	1.77	0.43
22:U:63:SER:HB2	22:U:66:ALA:H	1.84	0.43
1:X:393:U:H2'	1:X:394:U:C6	2.53	0.43
1:X:494:A:H5"	19:R:58:VAL:HG22	2.00	0.43
1:X:518:A:H5"	1:X:518:A:N3	2.34	0.43
1:X:608:G:H1'	10:I:21:ARG:CG	2.36	0.43
1:X:661:C:OP1	28:3:19:THR:OG1	2.20	0.43
1:X:1586:A:C6	1:X:1587:A:C6	3.07	0.43
1:X:1693:A:C2	1:X:1976:U:H5'	2.53	0.43
1:X:1699:A:C2	1:X:1700:C:C2	3.07	0.43
1:X:1944:C:H2'	1:X:1945:C:O4'	2.18	0.43
1:X:2788:C:H2'	1:X:2789:U:H6	1.84	0.43
8:G:67:ARG:HD3	8:G:70:PHE:O	2.18	0.43
8:G:67:ARG:CG	8:G:70:PHE:HA	2.49	0.43
8:G:106:TYR:HD1	8:G:106:TYR:HA	1.50	0.43
13:L:47:ARG:C	13:L:49:GLN:H	2.20	0.43
19:R:108:VAL:HB	19:R:109:ALA:H	1.66	0.43
26:1:9:ILE:HG13	26:1:10:VAL:N	2.34	0.43
26:1:42:PRO:HG3	26:1:50:PHE:HE1	1.82	0.43
28:3:13:ARG:HH12	28:3:49:VAL:CG2	2.32	0.43
1:X:116:A:N3	1:X:155:G:H1'	2.34	0.43
1:X:694:G:H2'	1:X:695:G:O4'	2.18	0.43
1:X:1746:A:H2	1:X:2696:A:O2'	2.00	0.43
1:X:2528:G:C2	1:X:2529:G:N7	2.87	0.43
3:A:177:LEU:HB3	3:A:178:PRO:HD2	2.00	0.43
4:B:79:ARG:HA	4:B:79:ARG:HD3	1.71	0.43
5:C:3:GLN:HB2	5:C:116:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:76:VAL:HA	7:E:79:VAL:HG22	2.00	0.43
8:G:71:THR:N	8:G:76:GLN:NE2	2.67	0.43
24:W:7:ARG:HB2	24:W:50:LEU:HA	1.99	0.43
28:3:9:MET:SD	28:3:59:LYS:HG3	2.58	0.43
1:X:618:A:H2'	1:X:619:A:C8	2.54	0.43
1:X:861:G:N3	1:X:944:A:H1'	2.34	0.43
1:X:874:A:H2'	1:X:875:G:O4'	2.18	0.43
1:X:914:C:H2'	1:X:915:C:C6	2.54	0.43
1:X:1954:A:H1'	3:A:240:THR:HA	2.01	0.43
1:X:2033:C:H2'	1:X:2034:A:O4'	2.19	0.43
1:X:2048:C:H2'	1:X:2049:C:C6	2.54	0.43
1:X:2271:C:H2'	1:X:2272:A:C8	2.53	0.43
3:A:56:GLY:N	3:A:217:ARG:HB2	2.29	0.43
3:A:223:GLY:HA2	3:A:226:MET:HG3	2.01	0.43
5:C:102:LEU:O	5:C:102:LEU:HD23	2.18	0.43
10:I:43:ALA:O	10:I:45:LYS:HG2	2.17	0.43
11:J:26:ASP:HB2	11:J:68:ARG:HH22	1.84	0.43
15:N:36:PHE:O	15:N:39:LEU:HB2	2.18	0.43
23:V:2:LYS:HB3	23:V:52:GLN:HE22	1.84	0.43
1:X:589:C:H2'	1:X:590:C:C6	2.54	0.43
1:X:687:G:H21	5:C:68:ARG:NH2	2.15	0.43
1:X:699:G:C6	27:2:12:ARG:HA	2.53	0.43
1:X:764:A:C6	1:X:802:A:C6	3.06	0.43
1:X:824:U:C4	10:I:29:THR:HB	2.53	0.43
1:X:1031:C:O2'	1:X:1032:A:OP2	2.33	0.43
1:X:1174:G:H2'	1:X:1175:A:H8	1.84	0.43
1:X:1198:C:OP1	24:W:26:ARG:NH1	2.52	0.43
1:X:1371:G:O2'	1:X:1386:A:N6	2.47	0.43
1:X:1419:G:H2'	1:X:1420:A:C8	2.54	0.43
1:X:1646:G:C5	1:X:1647:U:N3	2.87	0.43
1:X:2442:C:H2'	1:X:2443:C:H6	1.84	0.43
1:X:2681:A:OP1	12:K:73:LYS:NZ	2.52	0.43
1:X:2687:G:H2'	1:X:2688:G:H8	1.83	0.43
4:B:44:TYR:HB2	4:B:82:ARG:NH1	2.34	0.43
19:R:29:HIS:CE1	19:R:51:VAL:HA	2.54	0.43
1:X:589:C:H4'	15:N:31:GLN:NE2	2.34	0.43
1:X:599:A:O2'	1:X:600:G:H5'	2.19	0.43
1:X:1278:A:H2	1:X:1997:A:N6	2.08	0.43
1:X:1495:G:OP1	1:X:1576:G:O2'	2.28	0.43
1:X:1751:A:H2'	1:X:1752:U:C6	2.53	0.43
1:X:1774:A:C2	1:X:2566:A:C5	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2000:U:H4'	25:Z:8:LYS:O	2.18	0.43
1:X:2304:G:P	1:X:2304:G:H8	2.41	0.43
4:B:59:VAL:CG1	4:B:64:GLN:HG3	2.49	0.43
6:D:130:LEU:HA	6:D:130:LEU:HD23	1.80	0.43
8:G:103:TYR:HB3	8:G:107:GLN:HG3	2.01	0.43
16:O:23:GLU:HG3	16:O:91:THR:OG1	2.19	0.43
19:R:23:ILE:HD11	19:R:84:VAL:HG21	2.01	0.43
19:R:77:HIS:CG	19:R:78:ALA:N	2.87	0.43
26:1:16:ALA:HB2	26:1:50:PHE:HA	2.01	0.43
27:2:36:ALA:C	27:2:38:GLY:N	2.73	0.43
1:X:79:G:HO2'	1:X:356:A:H2	1.65	0.42
1:X:661:C:C2	1:X:662:G:N1	2.87	0.42
1:X:689:A:H1'	1:X:2422:C:H1'	2.01	0.42
1:X:760:U:C4	1:X:2592:U:C4	3.06	0.42
1:X:1246:G:C5	1:X:1247:U:C5	3.07	0.42
1:X:1351:G:H2'	1:X:1352:G:C8	2.54	0.42
1:X:1407:G:O6	1:X:1408:A:N6	2.52	0.42
1:X:1583:A:C2	3:A:31:LYS:HE2	2.54	0.42
1:X:2863:U:H2'	1:X:2864:C:O4'	2.18	0.42
3:A:166:GLN:HB2	3:A:174:ILE:HB	2.00	0.42
3:A:250:TRP:N	3:A:250:TRP:CD1	2.87	0.42
4:B:21:ILE:H	4:B:21:ILE:HG12	1.60	0.42
4:B:31:CYS:HA	4:B:32:PRO:HD3	1.79	0.42
4:B:59:VAL:HG21	4:B:74:PRO:HB3	2.01	0.42
5:C:54:THR:CG2	5:C:72:ARG:HB2	2.46	0.42
10:I:14:LYS:HD2	10:I:14:LYS:HA	1.90	0.42
10:I:119:THR:HG22	10:I:139:ARG:HB3	2.01	0.42
19:R:97:GLN:CB	19:R:101:GLY:HA2	2.49	0.42
1:X:123:A:O5'	27:2:19:ARG:HG2	2.19	0.42
1:X:555:U:H3'	1:X:556:A:H8	1.84	0.42
1:X:1370:U:H2'	1:X:1371:G:C8	2.54	0.42
1:X:1544:A:C4	1:X:1560:A:C6	3.08	0.42
1:X:1647:U:H6	1:X:1649:A:OP2	2.02	0.42
1:X:1710:U:H5"	1:X:1711:C:C5	2.54	0.42
1:X:1810:U:H2'	3:A:157:ARG:HD3	2.01	0.42
1:X:2006:G:H4'	1:X:2596:C:O3'	2.19	0.42
1:X:2052:G:C2	1:X:2053:G:C8	3.08	0.42
1:X:2371:A:H2	1:X:2403:C:H42	1.67	0.42
3:A:31:LYS:HA	3:A:31:LYS:HD2	1.72	0.42
10:I:57:ILE:N	10:I:58:ALA:O	2.52	0.42
1:X:500:G:C2	1:X:501:G:H1'	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:571:U:C2	1:X:581:A:C8	3.07	0.42
1:X:699:G:C2	27:2:12:ARG:HB2	2.55	0.42
1:X:733:G:H2'	1:X:734:G:H8	1.84	0.42
1:X:1466:C:H2'	1:X:1467:U:H1'	1.99	0.42
1:X:1777:A:C4	1:X:1921:A:C6	3.07	0.42
1:X:1859:A:H2'	1:X:1860:A:C8	2.54	0.42
6:D:17:MET:HG2	6:D:22:TYR:CB	2.49	0.42
8:G:67:ARG:O	8:G:70:PHE:CG	2.72	0.42
9:H:68:ASP:O	9:H:70:VAL:HG12	2.19	0.42
10:I:60:LEU:HA	10:I:61:PRO:HD3	1.85	0.42
22:U:27:ASP:OD2	22:U:32:ARG:HG3	2.19	0.42
26:1:8:ILE:HD13	26:1:8:ILE:H	1.84	0.42
1:X:320:A:H1'	1:X:340:G:N3	2.33	0.42
1:X:524:A:H2'	1:X:525:A:O4'	2.19	0.42
1:X:859:U:O2'	1:X:860:U:O5'	2.30	0.42
1:X:954:U:OP2	10:I:38:LYS:HG2	2.20	0.42
1:X:1429:A:H2'	1:X:1429:A:N3	2.34	0.42
1:X:1548:U:H2'	1:X:1549:C:C6	2.54	0.42
1:X:1630:A:N6	17:P:113:SER:O	2.48	0.42
1:X:1698:C:O2	1:X:1753:A:H2'	2.19	0.42
1:X:1982:C:H5"	1:X:2703:C:O2'	2.19	0.42
1:X:1991:C:H2'	1:X:1992:G:C8	2.53	0.42
1:X:2046:C:O2	1:X:2430:A:C2	2.72	0.42
1:X:2328:G:OP2	28:3:42:ARG:HG3	2.18	0.42
1:X:2350:G:C2	1:X:2351:G:C5	3.07	0.42
1:X:2664:G:C2'	1:X:2665:G:H5'	2.49	0.42
1:X:2800:C:H3'	1:X:2801:A:H8	1.85	0.42
4:B:96:PHE:CE2	4:B:102:ILE:HG21	2.54	0.42
4:B:149:ARG:HG3	4:B:150:VAL:N	2.34	0.42
5:C:74:VAL:HG23	5:C:76:THR:H	1.83	0.42
5:C:187:VAL:HG12	5:C:189:ASP:HB2	2.02	0.42
1:X:114:C:O2'	1:X:124:A:N3	2.45	0.42
1:X:491:A:N3	1:X:491:A:H2'	2.34	0.42
1:X:552:C:H2'	1:X:553:C:H5"	2.02	0.42
1:X:1013:G:C5	1:X:1014:G:C8	3.07	0.42
1:X:1164:C:H2'	1:X:1165:G:C8	2.53	0.42
1:X:1349:A:H5'	18:Q:64:ARG:NH2	2.35	0.42
1:X:1766:U:H2'	1:X:1767:G:O4'	2.19	0.42
1:X:1956:G:C6	1:X:1957:C:N4	2.87	0.42
1:X:2039:G:H22	25:Z:4:HIS:HA	1.85	0.42
1:X:2505:G:N1	1:X:2517:C:C2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:58:G:H4'	2:Y:59:A:C5'	2.49	0.42
3:A:109:GLU:OE1	3:A:197:GLY:HA3	2.19	0.42
8:G:65:LYS:HZ3	15:N:70:ARG:HD2	1.85	0.42
17:P:35:PRO:HD2	17:P:120:ARG:HB2	2.00	0.42
18:Q:57:ASN:O	18:Q:58:VAL:HG23	2.19	0.42
19:R:107:ALA:HB2	19:R:111:GLY:HA3	2.02	0.42
20:S:4:THR:HA	20:S:57:GLU:HG3	2.02	0.42
1:X:346:C:H5"	19:R:91:ALA:HB2	2.02	0.42
1:X:507:A:P	17:P:21:ARG:HE	2.42	0.42
1:X:538:A:N3	1:X:538:A:C2'	2.82	0.42
1:X:540:G:C2	1:X:2005:U:OP1	2.73	0.42
1:X:699:G:N2	27:2:12:ARG:HB2	2.35	0.42
1:X:753:U:O4'	1:X:1964:A:C4	2.73	0.42
1:X:1102:G:N2	1:X:1112:U:H1'	2.35	0.42
1:X:1187:A:H2'	1:X:1188:A:C8	2.55	0.42
1:X:1416:A:H2'	1:X:1417:C:C6	2.55	0.42
1:X:1755:G:C6	1:X:1972:G:C2	3.08	0.42
1:X:2054:A:H2'	1:X:2055:G:C8	2.54	0.42
1:X:2691:C:O2'	1:X:2692:A:OP2	2.31	0.42
1:X:2861:A:O2'	25:Z:31:THR:HG23	2.19	0.42
6:D:80:ARG:HD3	6:D:83:MET:CB	2.49	0.42
6:D:119:PRO:HB2	6:D:167:ARG:HH22	1.83	0.42
10:I:62:LYS:HB2	28:3:12:ARG:HA	2.02	0.42
10:I:133:VAL:HG11	10:I:140:VAL:HG23	2.01	0.42
11:J:19:THR:HG23	11:J:99:LYS:HD3	2.01	0.42
22:U:9:GLY:H	22:U:14:VAL:HG21	1.85	0.42
24:W:27:LYS:HE2	24:W:27:LYS:HB3	1.83	0.42
1:X:175:C:H5'	1:X:2223:U:OP1	2.18	0.42
1:X:585:U:H2'	1:X:586:G:C8	2.55	0.42
1:X:615:C:H1'	1:X:670:U:H1'	2.00	0.42
1:X:731:A:H2'	1:X:732:G:H4'	2.02	0.42
1:X:777:A:H5'	3:A:210:GLY:HA3	2.01	0.42
1:X:820:U:P	10:I:40:ARG:NH2	2.93	0.42
1:X:1336:G:H2'	1:X:1337:G:H5'	2.00	0.42
1:X:1480:G:N3	1:X:1561:A:H2	2.18	0.42
1:X:2284:U:P	1:X:2286:G:H22	2.42	0.42
1:X:2293:G:H2'	1:X:2294:U:C6	2.54	0.42
1:X:2796:A:C4	1:X:2797:G:C8	3.07	0.42
5:C:59:TYR:HE1	5:C:67:ALA:HA	1.85	0.42
9:H:7:ARG:HD3	9:H:18:GLU:OE2	2.19	0.42
11:J:83:ARG:HD3	11:J:83:ARG:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:14:VAL:N	16:O:16:GLU:OE2	2.53	0.42
25:Z:52:TYR:HB3	25:Z:56:GLN:NE2	2.34	0.42
1:X:60:A:C6	1:X:61:U:C4	3.08	0.42
1:X:2266:A:HO2'	1:X:2267:A:P	2.43	0.42
1:X:2284:U:H3	6:D:39:GLY:HA3	1.84	0.42
1:X:2355:A:H8	1:X:2355:A:OP1	2.03	0.42
1:X:2471:U:H2'	1:X:2472:U:C6	2.55	0.42
1:X:2604:G:H2'	1:X:2605:C:C6	2.55	0.42
1:X:2729:A:C6	1:X:2730:A:N6	2.88	0.42
3:A:30:GLU:HB2	3:A:82:ILE:O	2.20	0.42
3:A:69:ARG:NH1	3:A:130:ALA:HB2	2.35	0.42
4:B:132:LYS:HB2	4:B:132:LYS:HE3	1.71	0.42
5:C:125:ILE:HD12	5:C:125:ILE:HA	1.87	0.42
9:H:104:GLU:HG3	9:H:125:LYS:HG3	2.02	0.42
10:I:96:TYR:HD2	10:I:96:TYR:HA	1.65	0.42
13:L:12:ARG:HG3	13:L:92:GLY:HA2	2.02	0.42
1:X:674:U:H2'	1:X:675:C:O4'	2.20	0.42
1:X:788:G:C5	1:X:807:A:C8	3.08	0.42
1:X:1147:G:H2'	1:X:1148:G:C8	2.55	0.42
1:X:2080:U:H2'	1:X:2081:U:C6	2.55	0.42
2:Y:33:C:H1'	2:Y:56:G:N2	2.35	0.42
2:Y:103:A:O5'	2:Y:103:A:H8	2.03	0.42
3:A:130:ALA:HA	3:A:191:ALA:O	2.19	0.42
8:G:34:PRO:HA	8:G:69:ASP:CB	2.49	0.42
9:H:22:ILE:H	9:H:53:ALA:HA	1.84	0.42
19:R:95:ARG:HB2	19:R:104:VAL:HB	2.02	0.42
20:S:71:MET:HB2	20:S:78:PRO:HA	2.01	0.42
20:S:89:GLY:O	20:S:126:GLY:HA2	2.20	0.42
20:S:123:VAL:HG13	20:S:124:ALA:HB3	2.01	0.42
1:X:88:G:OP2	1:X:89:A:H3'	2.20	0.42
1:X:161:U:H1'	1:X:194:G:O2'	2.20	0.42
1:X:333:A:H5'	1:X:351:A:H1'	2.01	0.42
1:X:984:A:O4'	1:X:1202:U:C6	2.73	0.42
1:X:1005:U:H3'	15:N:54:LYS:HE3	2.02	0.42
1:X:1745:C:H5	1:X:1746:A:C5	2.37	0.42
2:Y:92:G:N7	2:Y:93:G:H1'	2.35	0.42
9:H:132:GLU:HB2	14:M:73:PHE:CE1	2.54	0.42
15:N:107:LYS:HE3	15:N:111:ASP:OD2	2.20	0.42
19:R:48:VAL:HG12	19:R:51:VAL:H	1.85	0.42
27:2:25:LYS:HA	27:2:25:LYS:HD3	1.72	0.42
1:X:617:U:H3'	1:X:617:U:O2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:673:G:H21	10:I:21:ARG:HG2	1.84	0.41
1:X:876:A:H2	1:X:926:C:N4	2.16	0.41
1:X:987:G:C2	1:X:988:G:C8	3.08	0.41
1:X:1794:A:O2'	3:A:257:LEU:HD12	2.20	0.41
1:X:1796:A:N3	3:A:50:THR:HB	2.35	0.41
1:X:1865:C:H2'	1:X:1866:G:O4'	2.20	0.41
1:X:2019:C:O2'	1:X:2020:G:H5'	2.20	0.41
5:C:23:ASN:ND2	5:C:26:VAL:HG23	2.34	0.41
5:C:33:TRP:CZ3	5:C:34:GLN:HG2	2.55	0.41
5:C:50:GLN:OE1	5:C:56:ARG:NH1	2.53	0.41
7:E:55:PRO:HB2	7:E:61:HIS:CE1	2.55	0.41
10:I:126:SER:O	10:I:130:ILE:HG13	2.19	0.41
11:J:93:TYR:CE1	11:J:95:VAL:HG13	2.55	0.41
12:K:15:SER:O	12:K:18:VAL:HB	2.20	0.41
12:K:73:LYS:HE2	12:K:73:LYS:HB3	1.86	0.41
22:U:31:GLY:HA2	22:U:32:ARG:NH1	2.30	0.41
1:X:741:G:O2'	1:X:743:A:H8	2.03	0.41
1:X:1269:G:O3'	5:C:69:HIS:HE1	2.03	0.41
1:X:1290:A:OP1	12:K:40:LYS:NZ	2.53	0.41
1:X:1314:A:O2'	1:X:1315:A:H3'	2.19	0.41
1:X:1476:G:C6	1:X:1477:C:C4	3.08	0.41
1:X:2490:U:H2'	1:X:2491:C:C6	2.55	0.41
1:X:2495:G:C6	1:X:2496:C:N4	2.88	0.41
3:A:50:THR:OG1	3:A:51:SER:N	2.53	0.41
4:B:102:ILE:O	4:B:102:ILE:HG13	2.19	0.41
5:C:47:THR:HA	5:C:82:VAL:H	1.85	0.41
5:C:146:GLU:HG3	5:C:185:ARG:HH22	1.84	0.41
8:G:34:PRO:HA	8:G:69:ASP:CG	2.41	0.41
8:G:103:TYR:CE1	8:G:107:GLN:O	2.73	0.41
20:S:49:THR:HB	20:S:132:GLN:HA	2.02	0.41
28:3:26:LYS:CE	28:3:43:GLY:HA3	2.46	0.41
1:X:129:A:H2'	1:X:130:C:C6	2.56	0.41
1:X:649:G:N1	1:X:660:G:N1	2.68	0.41
1:X:732:G:H2'	1:X:733:G:H8	1.86	0.41
1:X:1216:G:C5	1:X:1217:U:C5	3.08	0.41
1:X:1332:G:C2	1:X:1333:G:C2	3.09	0.41
1:X:1499:A:H2'	1:X:1500:U:C6	2.55	0.41
1:X:1509:A:H8	1:X:1510:A:N7	2.18	0.41
1:X:1656:U:C2'	1:X:1657:A:H5"	2.50	0.41
1:X:1837:G:H2'	1:X:1838:G:C8	2.55	0.41
1:X:2277:A:H2'	1:X:2278:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2394:G:H4'	10:I:64:GLY:O	2.21	0.41
1:X:2394:G:C6	1:X:2395:C:C4	3.09	0.41
1:X:2659:C:H1'	4:B:187:ALA:HB1	2.02	0.41
3:A:31:LYS:NZ	3:A:84:TYR:H	2.19	0.41
27:2:20:ALA:HA	27:2:23:LYS:HD2	2.03	0.41
1:X:13:A:N3	1:X:15:G:C6	2.87	0.41
1:X:14:A:C5	1:X:536:A:C2	3.08	0.41
1:X:616:U:O2'	1:X:671:A:H4'	2.19	0.41
1:X:1016:C:C2	1:X:1154:A:C5	3.08	0.41
1:X:1329:U:C2	1:X:1330:G:C8	3.09	0.41
1:X:1355:A:N1	1:X:1358:C:C2	2.88	0.41
1:X:1408:A:C6	1:X:1411:C:C2	3.08	0.41
1:X:1448:A:H61	1:X:1574:A:N6	2.18	0.41
1:X:1497:C:H42	1:X:1527:G:H1	1.69	0.41
1:X:1682:A:O2'	9:H:1:MET:N	2.50	0.41
1:X:1788:C:H5'	3:A:254:THR:HA	2.01	0.41
1:X:2628:C:O3'	9:H:35:THR:HG21	2.20	0.41
3:A:25:THR:CG2	3:A:211:ARG:HH12	2.31	0.41
4:B:6:GLY:HA3	4:B:28:ALA:HA	2.02	0.41
4:B:25:VAL:HG12	4:B:181:LEU:HD22	2.01	0.41
4:B:126:PRO:HG2	4:B:131:SER:HB3	2.01	0.41
5:C:13:ARG:H	5:C:13:ARG:HD2	1.85	0.41
5:C:95:LEU:HD23	5:C:96:PRO:HD2	2.03	0.41
5:C:124:ASP:OD1	5:C:136:TRP:NE1	2.49	0.41
8:G:70:PHE:CA	8:G:76:GLN:HE22	2.33	0.41
10:I:31:GLY:O	10:I:32:ARG:HG3	2.20	0.41
12:K:22:ARG:HG2	12:K:69:ASP:HB3	2.03	0.41
12:K:78:LYS:O	12:K:82:GLU:HB2	2.20	0.41
12:K:99:ARG:HG2	12:K:99:ARG:HH11	1.86	0.41
15:N:91:ASN:O	15:N:93:LYS:HB3	2.20	0.41
1:X:91:A:H2'	1:X:92:U:C6	2.56	0.41
1:X:539:A:C2	1:X:2006:G:C8	3.09	0.41
1:X:958:G:H2'	1:X:959:C:C6	2.55	0.41
1:X:1776:A:C8	1:X:1778:U:C5	3.08	0.41
1:X:2208:U:H2'	1:X:2209:G:C8	2.56	0.41
1:X:2331:A:C4	1:X:2345:A:C2	3.08	0.41
1:X:2509:A:H2'	1:X:2510:A:H5"	2.02	0.41
1:X:2702:G:H2'	1:X:2703:C:O4'	2.20	0.41
3:A:32:ALA:O	3:A:33:LEU:HB3	2.20	0.41
5:C:15:ILE:HD11	5:C:195:ILE:H	1.84	0.41
6:D:41:GLY:HA2	6:D:45:GLU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:79:LEU:HD23	6:D:79:LEU:HA	1.86	0.41
16:O:11:GLN:CB	16:O:13:ARG:HH21	2.34	0.41
17:P:57:LEU:HD13	17:P:69:ALA:CB	2.49	0.41
20:S:25:ASN:H	20:S:25:ASN:ND2	2.16	0.41
25:Z:3:LYS:HA	25:Z:3:LYS:HD2	1.63	0.41
1:X:463:C:OP2	5:C:46:ARG:HG2	2.20	0.41
1:X:474:G:C6	1:X:478:G:O6	2.74	0.41
1:X:738:G:C6	1:X:739:G:N1	2.89	0.41
1:X:787:A:H2	1:X:800:U:O2'	2.02	0.41
1:X:792:U:P	3:A:48:ARG:HA	2.61	0.41
1:X:797:A:HO2'	1:X:798:G:P	2.44	0.41
1:X:945:G:C4	1:X:946:U:C5	3.09	0.41
1:X:951:G:N3	1:X:1205:G:H4'	2.35	0.41
1:X:1313:U:H4'	1:X:1314:A:C5'	2.51	0.41
1:X:1412:C:OP1	18:Q:81:ARG:NH1	2.54	0.41
1:X:1623:C:H4'	1:X:1624:A:O5'	2.21	0.41
1:X:2039:G:H2'	1:X:2039:G:N3	2.36	0.41
1:X:2402:U:OP2	26:1:3:LYS:HG3	2.20	0.41
1:X:2450:A:N6	1:X:2451:G:C2	2.89	0.41
3:A:55:GLY:C	3:A:217:ARG:HD3	2.40	0.41
6:D:52:LYS:HD2	6:D:148:LYS:HE2	2.02	0.41
12:K:76:VAL:O	12:K:79:VAL:HG22	2.20	0.41
15:N:44:THR:O	15:N:48:ARG:HG3	2.21	0.41
18:Q:43:GLN:HG2	18:Q:48:VAL:O	2.20	0.41
21:T:19:LYS:O	21:T:20:TYR:CG	2.73	0.41
28:3:6:THR:HG23	28:3:8:LYS:N	2.35	0.41
1:X:1372:A:H2'	1:X:1373:G:O4'	2.21	0.41
1:X:1583:A:H2'	3:A:84:TYR:HE1	1.85	0.41
1:X:1685:A:H5"	9:H:5:GLN:HG2	2.02	0.41
1:X:2324:G:H4'	1:X:2325:A:H5"	2.03	0.41
1:X:2391:A:H2'	1:X:2392:G:H8	1.85	0.41
1:X:2511:G:H2'	1:X:2512:A:O4'	2.21	0.41
1:X:2564:U:H4'	1:X:2565:C:OP2	2.18	0.41
16:O:23:GLU:HB2	16:O:91:THR:HG21	2.02	0.41
17:P:44:VAL:O	17:P:48:LYS:HD3	2.19	0.41
17:P:59:PHE:CZ	25:Z:40:LYS:HA	2.55	0.41
19:R:100:ASP:OD1	19:R:102:LYS:HB3	2.20	0.41
21:T:25:LYS:HA	21:T:25:LYS:HD3	1.88	0.41
21:T:45:PHE:CD1	21:T:45:PHE:N	2.87	0.41
23:V:6:MET:HB3	23:V:6:MET:HE2	1.73	0.41
1:X:26:G:C6	1:X:27:G:N1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:226:C:OP2	1:X:2373:C:O2'	2.38	0.41
1:X:1235:C:N4	1:X:1240:G:H1	2.19	0.41
1:X:1781:C:H4'	3:A:209:ALA:CB	2.50	0.41
1:X:2279:G:N2	1:X:2295:C:O2	2.33	0.41
1:X:2631:C:C2	1:X:2648:G:C2	3.09	0.41
1:X:2791:C:O2'	1:X:2792:C:H5'	2.21	0.41
1:X:2870:C:H2'	1:X:2871:U:C6	2.56	0.41
2:Y:48:A:H2'	2:Y:49:C:O4'	2.20	0.41
5:C:75:PRO:HA	5:C:81:GLY:O	2.19	0.41
6:D:28:VAL:HA	6:D:29:PRO:HD3	1.96	0.41
9:H:28:GLY:O	9:H:34:LEU:HA	2.20	0.41
15:N:86:ALA:C	15:N:88:ILE:N	2.74	0.41
17:P:117:ILE:HD13	17:P:117:ILE:HA	1.63	0.41
1:X:45:C:OP2	1:X:192:G:H2'	2.21	0.41
1:X:158:A:H2'	1:X:159:A:C8	2.55	0.41
1:X:538:A:C2	1:X:2025:A:C6	3.09	0.41
1:X:699:G:N1	27:2:12:ARG:HB2	2.35	0.41
1:X:822:G:C6	1:X:823:U:C4	3.09	0.41
1:X:870:C:C2'	1:X:871:U:H5'	2.51	0.41
1:X:881:U:C4	1:X:882:C:N4	2.89	0.41
1:X:1007:A:H4'	15:N:93:LYS:NZ	2.29	0.41
1:X:1237:G:O3'	16:O:85:GLY:HA3	2.21	0.41
1:X:1255:A:H2'	1:X:1256:C:H6	1.86	0.41
1:X:1270:C:H4'	5:C:77:PHE:CE1	2.56	0.41
1:X:1418:C:H2'	1:X:1419:G:H8	1.85	0.41
1:X:1469:U:H5"	1:X:1470:G:N7	2.35	0.41
1:X:1533:G:H2'	1:X:1534:A:H8	1.85	0.41
1:X:1564:U:H2'	1:X:1565:G:H8	1.86	0.41
1:X:1742:G:H2'	1:X:1743:C:H6	1.86	0.41
1:X:2262:C:C2	1:X:2368:G:C2	3.09	0.41
1:X:2310:G:H2'	1:X:2311:U:O4'	2.20	0.41
1:X:2557:G:N2	1:X:2558:C:C2	2.89	0.41
1:X:2790:C:H42	1:X:2806:G:H1	1.66	0.41
1:X:2847:G:C2	1:X:2848:A:N6	2.88	0.41
2:Y:53:G:C5'	13:L:64:LYS:HG3	2.51	0.41
5:C:34:GLN:O	5:C:37:SER:OG	2.34	0.41
5:C:62:LYS:HD3	5:C:62:LYS:HA	1.87	0.41
6:D:123:ASP:HB3	6:D:127:ASN:H	1.85	0.41
8:G:62:ILE:HG21	8:G:135:LEU:HD11	2.02	0.41
8:G:128:GLU:HG2	8:G:148:LEU:HD23	2.03	0.41
8:G:154:GLU:C	8:G:157:PRO:HD2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:31:GLY:O	10:I:32:ARG:NH2	2.54	0.41
14:M:7:ILE:HD12	14:M:7:ILE:HA	1.88	0.41
14:M:90:GLN:OE1	14:M:91:VAL:N	2.42	0.41
18:Q:66:GLY:HA3	18:Q:68:PHE:CE2	2.56	0.41
19:R:103:LYS:HE2	19:R:103:LYS:HB3	1.92	0.41
20:S:3:LEU:HD11	20:S:5:ALA:O	2.21	0.41
20:S:89:GLY:HA2	20:S:127:PRO:HB3	2.03	0.41
20:S:123:VAL:HG12	20:S:159:THR:H	1.86	0.41
23:V:13:ASP:O	23:V:17:GLU:HG2	2.21	0.41
24:W:4:LYS:HE3	24:W:52:GLU:HB3	2.03	0.41
25:Z:45:ILE:HD11	25:Z:56:GLN:HG2	2.02	0.41
1:X:506:G:C6	1:X:507:A:C4	3.09	0.41
1:X:533:C:H2'	1:X:534:U:O4'	2.21	0.41
1:X:540:G:H4'	1:X:541:C:OP1	2.21	0.41
1:X:661:C:C2	1:X:662:G:C2	3.09	0.41
1:X:699:G:N2	27:2:7:PRO:O	2.53	0.41
1:X:941:U:H2'	1:X:942:U:O4'	2.21	0.41
1:X:1039:A:N6	1:X:1136:G:H2'	2.36	0.41
1:X:1179:A:H2'	1:X:1180:A:H8	1.85	0.41
1:X:1500:U:H2'	1:X:1501:C:C6	2.56	0.41
1:X:1814:G:H2'	1:X:1815:G:H8	1.86	0.41
1:X:2794:G:C2	1:X:2803:C:C2	3.09	0.41
2:Y:43:G:H1	6:D:69:LYS:HZ1	1.68	0.41
6:D:106:ILE:O	6:D:109:PRO:HD2	2.20	0.41
7:E:94:PHE:CB	7:E:107:ILE:HG22	2.50	0.41
8:G:93:LYS:HA	8:G:93:LYS:HD3	1.80	0.41
10:I:77:LEU:HB2	10:I:111:SER:H	1.85	0.41
23:V:43:VAL:O	23:V:47:ARG:HG2	2.21	0.41
25:Z:14:SER:O	25:Z:18:MET:HB2	2.21	0.41
26:1:34:LYS:HG3	26:1:35:LEU:H	1.85	0.41
28:3:13:ARG:HB2	28:3:23:MET:O	2.21	0.41
1:X:163:A:H2'	1:X:164:G:H8	1.87	0.40
1:X:312:G:C4	1:X:313:U:C5	3.10	0.40
1:X:580:A:C8	1:X:2013:A:N6	2.89	0.40
1:X:1204:G:H2'	1:X:1205:G:H8	1.84	0.40
1:X:1500:U:H3	1:X:1520:G:H1	1.69	0.40
1:X:1669:A:N7	1:X:1670:G:C6	2.89	0.40
1:X:2867:G:H4'	1:X:2868:G:O4'	2.22	0.40
3:A:95:LEU:HG	3:A:105:ILE:HD12	2.02	0.40
7:E:124:ALA:HB3	7:E:132:ASP:HB2	2.02	0.40
7:E:148:VAL:HG12	7:E:162:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:99:ALA:HB2	15:N:106:PHE:CD1	2.56	0.40
21:T:23:VAL:HA	21:T:38:VAL:HG23	2.03	0.40
22:U:47:HIS:CG	22:U:48:LYS:N	2.89	0.40
22:U:51:ILE:O	22:U:52:ARG:NH2	2.37	0.40
27:2:37:LYS:HG2	27:2:37:LYS:O	2.21	0.40
1:X:322:A:H62	1:X:339:U:H2'	1.86	0.40
1:X:698:A:H5"	1:X:801:A:H62	1.85	0.40
1:X:734:G:H2'	1:X:735:G:C8	2.56	0.40
1:X:841:G:N2	1:X:2225:G:O2'	2.46	0.40
1:X:1273:G:H2'	1:X:1274:C:O4'	2.21	0.40
1:X:2001:G:C6	1:X:2002:A:C6	3.08	0.40
1:X:2043:A:C2	1:X:2481:G:C5	3.09	0.40
1:X:2422:C:H2'	1:X:2423:G:C8	2.56	0.40
1:X:2482:A:H4'	1:X:2483:U:OP1	2.20	0.40
1:X:2658:A:H2'	1:X:2659:C:O4'	2.20	0.40
4:B:122:PHE:HB3	4:B:123:ALA:H	1.64	0.40
8:G:30:LYS:O	8:G:31:THR:OG1	2.26	0.40
8:G:100:TYR:CD2	8:G:119:LEU:HD12	2.55	0.40
11:J:73:LYS:H	11:J:94:TRP:HD1	1.69	0.40
15:N:104:GLU:N	15:N:104:GLU:OE2	2.54	0.40
16:O:68:LYS:HE3	16:O:70:TYR:CZ	2.56	0.40
17:P:68:VAL:HG22	17:P:124:ILE:HG21	2.02	0.40
22:U:13:LEU:O	22:U:14:VAL:HG13	2.22	0.40
23:V:14:PHE:O	23:V:18:ILE:HG13	2.21	0.40
25:Z:8:LYS:O	25:Z:9:LYS:HD2	2.21	0.40
1:X:317:U:H2'	1:X:318:G:O4'	2.22	0.40
1:X:478:G:H2'	1:X:479:G:O4'	2.20	0.40
1:X:932:G:H2'	1:X:933:G:H8	1.86	0.40
1:X:1915:A:N1	1:X:1956:G:H1'	2.36	0.40
1:X:2166:G:H2'	1:X:2167:A:C8	2.57	0.40
1:X:2340:C:P	28:3:27:SER:HG	2.44	0.40
1:X:2594:U:C2	1:X:2595:C:C5	3.08	0.40
3:A:176:ARG:NH1	3:A:180:GLY:HA2	2.31	0.40
4:B:54:LYS:HD3	4:B:59:VAL:HG22	2.03	0.40
15:N:30:LYS:HA	15:N:30:LYS:HD2	1.82	0.40
16:O:36:LYS:HE2	16:O:56:VAL:HG22	2.03	0.40
19:R:10:HIS:ND1	19:R:10:HIS:N	2.69	0.40
20:S:71:MET:CB	20:S:78:PRO:HA	2.52	0.40
1:X:3:U:O2'	1:X:4:C:P	2.80	0.40
1:X:173:A:H2'	1:X:173:A:N3	2.36	0.40
1:X:505:G:O2'	17:P:78:ASN:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:625:A:H4'	1:X:626:A:OP1	2.21	0.40
1:X:1424:U:H2'	1:X:1425:G:C8	2.57	0.40
1:X:1643:A:N6	1:X:1656:U:H3	2.18	0.40
1:X:1671:A:H1'	1:X:2798:A:H5'	2.02	0.40
1:X:1697:U:N3	1:X:1755:G:OP2	2.55	0.40
1:X:2039:G:N2	1:X:2040:A:N9	2.70	0.40
1:X:2060:A:H2'	1:X:2061:C:C6	2.57	0.40
1:X:2597:G:O2'	4:B:149:ARG:HB2	2.21	0.40
1:X:2617:G:O2'	1:X:2755:A:N1	2.50	0.40
1:X:2730:A:O2'	1:X:2731:G:N2	2.54	0.40
2:Y:44:C:OP2	6:D:64:LYS:NZ	2.48	0.40
5:C:112:GLN:HE22	5:C:116:LYS:NZ	2.20	0.40
10:I:73:GLU:OE2	10:I:101:ARG:HB2	2.21	0.40
13:L:34:SER:HB3	13:L:35:SER:H	1.77	0.40
27:2:36:ALA:O	27:2:38:GLY:N	2.54	0.40
1:X:387:A:H2'	1:X:387:A:N3	2.36	0.40
1:X:475:U:O2'	27:2:16:HIS:NE2	2.50	0.40
1:X:540:G:O2'	1:X:542:A:C2	2.63	0.40
1:X:787:A:C2	1:X:800:U:O2'	2.74	0.40
1:X:861:G:N2	1:X:943:U:H1'	2.36	0.40
1:X:977:G:H5'	1:X:2251:U:O2	2.22	0.40
1:X:1208:A:H2'	1:X:1209:G:O4'	2.21	0.40
1:X:1267:A:H5"	1:X:1268:U:H5"	2.03	0.40
1:X:1327:C:H42	1:X:1351:G:H1	1.69	0.40
1:X:1465:G:N3	1:X:1466:C:O2	2.54	0.40
1:X:1919:A:N6	1:X:1946:U:N3	2.69	0.40
1:X:2691:C:H2'	1:X:2694:G:H5"	2.03	0.40
1:X:2728:A:C6	1:X:2729:A:C6	3.10	0.40
1:X:2867:G:O5'	1:X:2867:G:H8	2.04	0.40
3:A:28:ARG:HA	3:A:29:PRO:HD3	1.85	0.40
5:C:154:ASP:O	5:C:157:THR:N	2.54	0.40
12:K:45:ARG:HD3	12:K:95:THR:CG2	2.51	0.40
17:P:74:SER:HA	17:P:77:ALA:HB3	2.04	0.40
25:Z:3:LYS:O	25:Z:4:HIS:C	2.60	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
3	A	257/275 (94%)	219 (85%)	37 (14%)	1 (0%)	34 71
4	B	203/211 (96%)	183 (90%)	15 (7%)	5 (2%)	5 36
5	C	192/205 (94%)	161 (84%)	25 (13%)	6 (3%)	4 32
6	D	175/180 (97%)	151 (86%)	24 (14%)	0	100 100
7	E	169/185 (91%)	155 (92%)	13 (8%)	1 (1%)	25 64
8	G	140/174 (80%)	124 (89%)	15 (11%)	1 (1%)	22 62
9	H	132/134 (98%)	123 (93%)	8 (6%)	1 (1%)	19 59
10	I	132/156 (85%)	98 (74%)	30 (23%)	4 (3%)	4 33
11	J	134/141 (95%)	117 (87%)	16 (12%)	1 (1%)	22 62
12	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	17 57
13	L	102/114 (90%)	80 (78%)	22 (22%)	0	100 100
14	M	106/166 (64%)	100 (94%)	6 (6%)	0	100 100
15	N	115/118 (98%)	100 (87%)	13 (11%)	2 (2%)	9 44
16	O	92/100 (92%)	83 (90%)	9 (10%)	0	100 100
17	P	125/134 (93%)	121 (97%)	4 (3%)	0	100 100
18	Q	91/95 (96%)	69 (76%)	19 (21%)	3 (3%)	4 31
19	R	108/115 (94%)	80 (74%)	28 (26%)	0	100 100
20	S	177/237 (75%)	150 (85%)	25 (14%)	2 (1%)	14 53
21	T	72/91 (79%)	63 (88%)	9 (12%)	0	100 100
22	U	70/81 (86%)	51 (73%)	17 (24%)	2 (3%)	4 33
23	V	63/67 (94%)	58 (92%)	5 (8%)	0	100 100
24	W	53/55 (96%)	49 (92%)	4 (8%)	0	100 100
25	Z	55/60 (92%)	45 (82%)	10 (18%)	0	100 100
26	1	51/54 (94%)	36 (71%)	12 (24%)	3 (6%)	1 18
27	2	44/47 (94%)	37 (84%)	5 (11%)	2 (4%)	2 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	3	57/66 (86%)	44 (77%)	11 (19%)	2 (4%)	3 30
All	All	3026/3377 (90%)	2598 (86%)	391 (13%)	37 (1%)	13 51

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	94	VAL
18	Q	6	ILE
5	C	177	VAL
20	S	122	ILE
26	1	9	ILE
26	1	10	VAL
4	B	136	ARG
11	J	82	THR
22	U	60	VAL
27	2	5	TYR
3	A	21	PHE
4	B	144	ARG
5	C	130	THR
7	E	165	VAL
10	I	103	ASN
12	K	91	PRO
18	Q	69	ILE
22	U	15	VAL
4	B	121	ASN
5	C	113	GLU
5	C	164	VAL
10	I	38	LYS
27	2	8	ASN
4	B	137	ARG
9	H	42	LYS
18	Q	65	VAL
28	3	13	ARG
28	3	61	MET
8	G	163	PRO
4	B	73	ALA
5	C	15	ILE
15	N	8	ILE
26	1	8	ILE
5	C	22	VAL
10	I	19	VAL
10	I	68	VAL

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Mol	Chain	Res	Type
20	S	81	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
3	A	200/216 (93%)	160 (80%)	40 (20%)	1 8
4	B	155/157 (99%)	132 (85%)	23 (15%)	3 20
5	C	154/163 (94%)	117 (76%)	37 (24%)	0 5
6	D	153/156 (98%)	144 (94%)	9 (6%)	19 54
7	E	136/144 (94%)	124 (91%)	12 (9%)	10 40
8	G	118/146 (81%)	100 (85%)	18 (15%)	2 19
9	H	103/103 (100%)	83 (81%)	20 (19%)	1 9
10	I	101/121 (84%)	77 (76%)	24 (24%)	0 5
11	J	108/115 (94%)	89 (82%)	19 (18%)	2 12
12	K	90/93 (97%)	74 (82%)	16 (18%)	2 11
13	L	74/82 (90%)	50 (68%)	24 (32%)	0 2
14	M	92/134 (69%)	76 (83%)	16 (17%)	2 12
15	N	96/97 (99%)	87 (91%)	9 (9%)	8 38
16	O	75/79 (95%)	64 (85%)	11 (15%)	3 20
17	P	109/115 (95%)	90 (83%)	19 (17%)	2 12
18	Q	75/76 (99%)	53 (71%)	22 (29%)	0 3
19	R	91/96 (95%)	77 (85%)	14 (15%)	2 18
20	S	152/192 (79%)	130 (86%)	22 (14%)	3 20
21	T	55/67 (82%)	47 (86%)	8 (14%)	3 20
22	U	57/66 (86%)	43 (75%)	14 (25%)	0 5
23	V	53/55 (96%)	49 (92%)	4 (8%)	13 45
24	W	48/48 (100%)	42 (88%)	6 (12%)	4 25
25	Z	51/53 (96%)	36 (71%)	15 (29%)	0 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	1	45/47 (96%)	33 (73%)	12 (27%)	0 3
27	2	39/40 (98%)	29 (74%)	10 (26%)	0 4
28	3	46/52 (88%)	34 (74%)	12 (26%)	0 4
All	All	2476/2713 (91%)	2040 (82%)	436 (18%)	2 12

All (436) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	18	THR
3	A	20	ASP
3	A	22	SER
3	A	25	THR
3	A	26	LYS
3	A	28	ARG
3	A	31	LYS
3	A	35	GLU
3	A	40	THR
3	A	43	ARG
3	A	49	ILE
3	A	58	HIS
3	A	60	ARG
3	A	87	ASN
3	A	88	ARG
3	A	95	LEU
3	A	104	TYR
3	A	106	LEU
3	A	122	GLU
3	A	127	LEU
3	A	131	LEU
3	A	141	VAL
3	A	147	LEU
3	A	151	LYS
3	A	162	SER
3	A	173	VAL
3	A	186	HIS
3	A	188	GLU
3	A	196	VAL
3	A	202	LYS
3	A	203	ASN
3	A	208	LYS
3	A	211	ARG

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Mol	Chain	Res	Type
3	A	213	ARG
3	A	214	TRP
3	A	215	LEU
3	A	218	LYS
3	A	237	GLU
3	A	240	THR
3	A	248	THR
4	B	5	LEU
4	B	15	TRP
4	B	21	ILE
4	B	23	VAL
4	B	25	VAL
4	B	34	VAL
4	B	57	ARG
4	B	72	VAL
4	B	75	THR
4	B	82	ARG
4	B	84	PHE
4	B	87	ASP
4	B	94	ASP
4	B	105	THR
4	B	116	VAL
4	B	122	PHE
4	B	132	LYS
4	B	135	HIS
4	B	141	ILE
4	B	143	GLN
4	B	144	ARG
4	B	199	ARG
4	B	203	LYS
5	C	5	ASN
5	C	13	ARG
5	C	14	THR
5	C	17	LEU
5	C	34	GLN
5	C	40	ARG
5	C	45	THR
5	C	58	MET
5	C	59	TYR
5	C	66	ASN
5	C	76	THR
5	C	77	PHE

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Mol	Chain	Res	Type
5	C	82	VAL
5	C	91	TYR
5	C	95	LEU
5	C	98	GLN
5	C	100	ARG
5	C	120	VAL
5	C	125	ILE
5	C	127	ASP
5	C	132	ASN
5	C	143	ASP
5	C	148	VAL
5	C	153	ASP
5	C	154	ASP
5	C	157	THR
5	C	162	ARG
5	C	163	ASN
5	C	164	VAL
5	C	166	TRP
5	C	167	VAL
5	C	169	VAL
5	C	175	VAL
5	C	177	VAL
5	C	180	ILE
5	C	184	ASP
5	C	193	LEU
6	D	4	LEU
6	D	22	TYR
6	D	40	LEU
6	D	80	ARG
6	D	90	THR
6	D	112	ARG
6	D	115	ARG
6	D	146	VAL
6	D	152	MET
7	E	32	GLU
7	E	34	THR
7	E	38	ASN
7	E	57	ASP
7	E	61	HIS
7	E	67	LEU
7	E	69	ARG
7	E	111	HIS

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Mol	Chain	Res	Type
7	E	129	THR
7	E	132	ASP
7	E	164	PHE
7	E	171	LEU
8	G	30	LYS
8	G	32	TYR
8	G	53	ARG
8	G	65	LYS
8	G	78	ASP
8	G	88	VAL
8	G	91	THR
8	G	95	LEU
8	G	102	ARG
8	G	103	TYR
8	G	104	THR
8	G	106	TYR
8	G	119	LEU
8	G	146	THR
8	G	147	ARG
8	G	161	GLN
8	G	165	VAL
8	G	171	LEU
9	H	1	MET
9	H	2	ILE
9	H	29	ILE
9	H	35	THR
9	H	36	THR
9	H	41	ASN
9	H	43	ARG
9	H	69	VAL
9	H	70	VAL
9	H	74	VAL
9	H	78	SER
9	H	81	ILE
9	H	82	LYS
9	H	90	ARG
9	H	94	ASN
9	H	109	ARG
9	H	120	ASP
9	H	122	ARG
9	H	124	MET
9	H	127	VAL

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Mol	Chain	Res	Type
10	I	18	ARG
10	I	26	THR
10	I	28	LYS
10	I	32	ARG
10	I	37	GLN
10	I	39	SER
10	I	40	ARG
10	I	49	PHE
10	I	53	ARG
10	I	55	ARG
10	I	65	PHE
10	I	71	THR
10	I	83	LEU
10	I	88	PHE
10	I	89	ASP
10	I	90	ARG
10	I	96	TYR
10	I	98	LEU
10	I	99	VAL
10	I	103	ASN
10	I	120	VAL
10	I	126	SER
10	I	141	VAL
10	I	142	LEU
11	J	8	THR
11	J	9	LYS
11	J	10	PHE
11	J	11	ARG
11	J	17	ARG
11	J	26	ASP
11	J	27	TYR
11	J	28	VAL
11	J	46	ASN
11	J	59	PHE
11	J	60	ARG
11	J	67	ILE
11	J	86	LYS
11	J	104	MET
11	J	106	GLU
11	J	131	LYS
11	J	134	LYS
11	J	135	ARG

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Mol	Chain	Res	Type
11	J	139	ASP
12	K	5	LYS
12	K	11	ASN
12	K	13	ASN
12	K	14	SER
12	K	37	THR
12	K	43	GLU
12	K	48	VAL
12	K	51	LEU
12	K	59	ASP
12	K	73	LYS
12	K	76	VAL
12	K	94	TYR
12	K	95	THR
12	K	98	LEU
12	K	102	THR
12	K	109	THR
13	L	8	ARG
13	L	11	LEU
13	L	13	THR
13	L	15	ARG
13	L	29	LEU
13	L	31	VAL
13	L	34	SER
13	L	37	HIS
13	L	38	ILE
13	L	39	TYR
13	L	42	ILE
13	L	43	ILE
13	L	45	ASP
13	L	46	SER
13	L	65	THR
13	L	66	ASP
13	L	67	THR
13	L	88	VAL
13	L	91	ARG
13	L	93	SER
13	L	94	TYR
13	L	96	TYR
13	L	97	HIS
13	L	109	GLU
14	M	3	THR

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Mol	Chain	Res	Type
14	M	7	ILE
14	M	31	ASP
14	M	38	LYS
14	M	39	VAL
14	M	43	ASN
14	M	45	THR
14	M	57	ILE
14	M	63	ARG
14	M	68	VAL
14	M	69	ARG
14	M	94	VAL
14	M	96	ARG
14	M	98	LYS
14	M	101	ARG
14	M	103	LYS
15	N	9	VAL
15	N	15	LYS
15	N	22	LYS
15	N	28	ARG
15	N	30	LYS
15	N	31	GLN
15	N	51	ARG
15	N	60	LEU
15	N	93	LYS
16	O	13	ARG
16	O	20	ILE
16	O	21	ARG
16	O	22	VAL
16	O	28	GLU
16	O	47	PHE
16	O	56	VAL
16	O	81	ARG
16	O	88	GLN
16	O	91	THR
16	O	98	ILE
17	P	9	ARG
17	P	13	GLN
17	P	32	ARG
17	P	37	LYS
17	P	39	ARG
17	P	40	LEU
17	P	46	ARG

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Mol	Chain	Res	Type
17	P	52	ASP
17	P	65	SER
17	P	71	VAL
17	P	91	PHE
17	P	107	ILE
17	P	109	ARG
17	P	116	ILE
17	P	118	LYS
17	P	119	LYS
17	P	120	ARG
17	P	121	THR
17	P	125	THR
18	Q	5	ASP
18	Q	6	ILE
18	Q	7	LEU
18	Q	8	GLN
18	Q	15	LYS
18	Q	24	VAL
18	Q	26	SER
18	Q	30	SER
18	Q	32	LYS
18	Q	34	THR
18	Q	40	ASP
18	Q	44	GLN
18	Q	58	VAL
18	Q	62	ARG
18	Q	64	ARG
18	Q	65	VAL
18	Q	73	ASN
18	Q	74	ASP
18	Q	80	VAL
18	Q	81	ARG
18	Q	84	GLU
18	Q	88	ILE
19	R	10	HIS
19	R	15	HIS
19	R	18	LYS
19	R	20	ASP
19	R	21	THR
19	R	23	ILE
19	R	48	VAL
19	R	56	LYS

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Mol	Chain	Res	Type
19	R	80	LYS
19	R	83	LEU
19	R	94	VAL
19	R	95	ARG
19	R	97	GLN
19	R	110	SER
20	S	1	MET
20	S	14	LEU
20	S	22	VAL
20	S	25	ASN
20	S	26	LYS
20	S	32	PHE
20	S	34	LEU
20	S	48	THR
20	S	51	LEU
20	S	71	MET
20	S	73	LYS
20	S	86	VAL
20	S	88	TYR
20	S	112	LEU
20	S	120	LEU
20	S	123	VAL
20	S	145	ASP
20	S	159	THR
20	S	175	ARG
20	S	176	LEU
20	S	177	THR
20	S	179	GLU
21	T	30	VAL
21	T	37	LEU
21	T	38	VAL
21	T	45	PHE
21	T	46	LYS
21	T	64	ASP
21	T	68	VAL
21	T	80	SER
22	U	14	VAL
22	U	17	SER
22	U	19	ILE
22	U	21	ARG
22	U	27	ASP
22	U	32	ARG

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Mol	Chain	Res	Type
22	U	37	ILE
22	U	48	LYS
22	U	49	LYS
22	U	53	GLU
22	U	54	ASN
22	U	70	LEU
22	U	75	TYR
22	U	78	ILE
23	V	12	THR
23	V	19	ASP
23	V	21	ARG
23	V	28	LEU
24	W	3	ILE
24	W	4	LYS
24	W	9	VAL
24	W	12	ARG
24	W	32	ARG
24	W	36	ASP
25	Z	3	LYS
25	Z	6	VAL
25	Z	10	LYS
25	Z	21	SER
25	Z	23	HIS
25	Z	25	LEU
25	Z	41	LEU
25	Z	42	SER
25	Z	49	CYS
25	Z	51	TYR
25	Z	52	TYR
25	Z	53	ASP
25	Z	55	ARG
25	Z	57	VAL
25	Z	58	LEU
26	1	8	ILE
26	1	10	VAL
26	1	12	MET
26	1	15	SER
26	1	20	PHE
26	1	21	TYR
26	1	25	THR
26	1	30	ASN
26	1	36	GLU

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Mol	Chain	Res	Type
26	1	43	VAL
26	1	48	VAL
26	1	54	LYS
27	2	1	MET
27	2	6	GLN
27	2	14	LYS
27	2	22	MET
27	2	23	LYS
27	2	28	ARG
27	2	31	LEU
27	2	40	HIS
27	2	43	THR
27	2	45	SER
28	3	6	THR
28	3	7	HIS
28	3	13	ARG
28	3	22	VAL
28	3	31	HIS
28	3	34	THR
28	3	44	LYS
28	3	46	LYS
28	3	49	VAL
28	3	50	LEU
28	3	52	LYS
28	3	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	87	ASN
3	A	129	ASN
3	A	198	ASN
4	B	48	GLN
4	B	60	ASN
4	B	129	HIS
5	C	101	GLN
5	C	112	GLN
5	C	163	ASN
6	D	118	ASN
6	D	135	GLN
7	E	20	GLN
7	E	38	ASN

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Mol	Chain	Res	Type
7	E	74	ASN
8	G	76	GLN
8	G	84	ASN
8	G	140	GLN
8	G	145	HIS
8	G	158	HIS
9	H	41	ASN
10	I	34	HIS
10	I	103	ASN
11	J	47	GLN
11	J	58	HIS
11	J	124	HIS
12	K	11	ASN
12	K	35	GLN
13	L	41	GLN
13	L	97	HIS
15	N	66	ASN
16	O	6	GLN
16	O	11	GLN
16	O	79	GLN
19	R	10	HIS
19	R	44	GLN
19	R	77	HIS
20	S	25	ASN
20	S	46	GLN
20	S	146	HIS
22	U	45	ASN
23	V	52	GLN
24	W	49	HIS
24	W	54	GLN
25	Z	44	HIS
26	1	30	ASN
27	2	6	GLN
27	2	29	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2650/2880 (92%)	580 (21%)	49 (1%)
2	Y	119/123 (96%)	23 (19%)	1 (0%)
All	All	2769/3003 (92%)	603 (21%)	50 (1%)

All (603) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	4	C
1	X	7	G
1	X	10	A
1	X	14	A
1	X	15	G
1	X	23	G
1	X	34	U
1	X	37	C
1	X	39	C
1	X	45	C
1	X	49	U
1	X	50	G
1	X	59	G
1	X	63	A
1	X	69	G
1	X	73	A
1	X	74	G
1	X	87	G
1	X	88	G
1	X	89	A
1	X	90	G
1	X	95	G
1	X	97	U
1	X	98	U
1	X	100	G
1	X	108	G
1	X	111	G
1	X	112	U
1	X	116	A
1	X	118	U
1	X	123	A
1	X	124	A
1	X	126	C
1	X	134	G
1	X	136	A
1	X	138	G
1	X	143	A
1	X	158	A
1	X	173	A
1	X	176	A
1	X	177	U

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Mol	Chain	Res	Type
1	X	178	C
1	X	181	A
1	X	192	G
1	X	193	A
1	X	198	A
1	X	199	A
1	X	201	G
1	X	205	A
1	X	206	U
1	X	207	U
1	X	209	G
1	X	210	A
1	X	218	A
1	X	219	G
1	X	220	U
1	X	225	G
1	X	229	G
1	X	241	C
1	X	242	A
1	X	243	G
1	X	247	A
1	X	248	A
1	X	249	A
1	X	302	U
1	X	303	C
1	X	304	A
1	X	305	A
1	X	310	A
1	X	312	G
1	X	313	U
1	X	321	A
1	X	322	A
1	X	323	G
1	X	333	A
1	X	334	G
1	X	335	A
1	X	338	G
1	X	340	G
1	X	342	G
1	X	343	A
1	X	349	G
1	X	387	A

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Mol	Chain	Res	Type
1	X	398	C
1	X	399	G
1	X	400	U
1	X	408	U
1	X	409	G
1	X	414	A
1	X	424	G
1	X	425	A
1	X	431	G
1	X	433	G
1	X	441	A
1	X	456	C
1	X	459	A
1	X	463	C
1	X	467	U
1	X	469	G
1	X	483	A
1	X	484	G
1	X	491	A
1	X	492	G
1	X	493	A
1	X	501	G
1	X	506	G
1	X	514	G
1	X	515	A
1	X	518	A
1	X	519	C
1	X	534	U
1	X	537	C
1	X	538	A
1	X	539	A
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	556	A
1	X	557	U
1	X	558	G
1	X	560	G
1	X	572	G
1	X	578	U

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Mol	Chain	Res	Type
1	X	582	G
1	X	584	A
1	X	591	G
1	X	595	A
1	X	601	A
1	X	613	A
1	X	616	U
1	X	617	U
1	X	626	A
1	X	627	A
1	X	628	A
1	X	631	G
1	X	633	G
1	X	645	G
1	X	648	A
1	X	649	G
1	X	654	A
1	X	655	A
1	X	656	U
1	X	657	A
1	X	664	C
1	X	665	A
1	X	666	U
1	X	667	U
1	X	668	A
1	X	682	G
1	X	683	A
1	X	684	C
1	X	690	A
1	X	699	G
1	X	728	G
1	X	729	A
1	X	731	A
1	X	732	G
1	X	743	A
1	X	747	A
1	X	753	U
1	X	760	U
1	X	761	G
1	X	766	A
1	X	773	G
1	X	774	A

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Mol	Chain	Res	Type
1	X	777	A
1	X	784	U
1	X	788	G
1	X	789	G
1	X	790	A
1	X	792	U
1	X	795	A
1	X	796	A
1	X	797	A
1	X	798	G
1	X	802	A
1	X	803	C
1	X	805	G
1	X	818	G
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	846	A
1	X	859	U
1	X	871	U
1	X	872	G
1	X	879	A
1	X	922	A
1	X	926	C
1	X	931	G
1	X	939	C
1	X	940	G
1	X	941	U
1	X	943	U
1	X	944	A
1	X	952	A
1	X	957	G
1	X	964	A
1	X	970	A
1	X	972	C
1	X	985	G
1	X	994	A
1	X	996	C
1	X	999	A
1	X	1006	C
1	X	1007	A

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Mol	Chain	Res	Type
1	X	1014	G
1	X	1016	C
1	X	1018	C
1	X	1020	A
1	X	1021	A
1	X	1022	A
1	X	1023	U
1	X	1031	C
1	X	1032	A
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1044	U
1	X	1046	U
1	X	1049	C
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1058	G
1	X	1073	G
1	X	1076	U
1	X	1077	U
1	X	1081	A
1	X	1082	G
1	X	1083	C
1	X	1108	U
1	X	1120	C
1	X	1121	G
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1139	A
1	X	1141	U
1	X	1142	G
1	X	1145	C
1	X	1146	G
1	X	1149	G
1	X	1152	C
1	X	1153	A
1	X	1154	A
1	X	1166	A

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Mol	Chain	Res	Type
1	X	1167	A
1	X	1176	U
1	X	1183	C
1	X	1185	C
1	X	1189	G
1	X	1192	A
1	X	1194	U
1	X	1207	G
1	X	1240	G
1	X	1242	A
1	X	1249	G
1	X	1250	A
1	X	1263	G
1	X	1266	G
1	X	1267	A
1	X	1269	G
1	X	1278	A
1	X	1284	G
1	X	1285	A
1	X	1286	U
1	X	1289	A
1	X	1313	U
1	X	1314	A
1	X	1324	G
1	X	1325	U
1	X	1334	A
1	X	1342	U
1	X	1344	C
1	X	1345	G
1	X	1351	G
1	X	1363	C
1	X	1372	A
1	X	1378	A
1	X	1381	G
1	X	1391	A
1	X	1392	U
1	X	1398	G
1	X	1403	U
1	X	1404	C
1	X	1409	U
1	X	1428	G
1	X	1429	A

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Mol	Chain	Res	Type
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1435	G
1	X	1442	C
1	X	1443	G
1	X	1460	G
1	X	1465	G
1	X	1467	U
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1475	U
1	X	1476	G
1	X	1482	U
1	X	1490	U
1	X	1497	C
1	X	1498	G
1	X	1505	U
1	X	1506	C
1	X	1524	C
1	X	1525	A
1	X	1526	U
1	X	1528	C
1	X	1531	C
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1570	C
1	X	1574	A
1	X	1575	C
1	X	1582	A
1	X	1585	A
1	X	1594	U
1	X	1602	G
1	X	1603	A
1	X	1608	U
1	X	1614	C
1	X	1623	C
1	X	1624	A

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Mol	Chain	Res	Type
1	X	1625	A
1	X	1630	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1648	C
1	X	1656	U
1	X	1657	A
1	X	1661	C
1	X	1665	C
1	X	1671	A
1	X	1685	A
1	X	1686	A
1	X	1691	G
1	X	1710	U
1	X	1714	A
1	X	1717	A
1	X	1718	A
1	X	1735	G
1	X	1743	C
1	X	1747	G
1	X	1754	G
1	X	1755	G
1	X	1760	G
1	X	1764	A
1	X	1767	G
1	X	1775	A
1	X	1782	A
1	X	1788	C
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1799	A
1	X	1801	C
1	X	1802	A
1	X	1807	A
1	X	1808	C
1	X	1819	U
1	X	1821	A
1	X	1822	C
1	X	1824	C

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Mol	Chain	Res	Type
1	X	1825	C
1	X	1830	C
1	X	1831	G
1	X	1840	A
1	X	1850	G
1	X	1861	G
1	X	1864	G
1	X	1867	A
1	X	1868	A
1	X	1882	G
1	X	1886	G
1	X	1910	A
1	X	1912	G
1	X	1919	A
1	X	1920	A
1	X	1921	A
1	X	1922	U
1	X	1923	U
1	X	1924	C
1	X	1937	G
1	X	1938	U
1	X	1943	A
1	X	1946	U
1	X	1947	G
1	X	1949	A
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1965	U
1	X	1975	G
1	X	1976	U
1	X	1979	C
1	X	1980	A
1	X	1988	A
1	X	2003	A
1	X	2006	G
1	X	2011	U
1	X	2014	A
1	X	2015	G
1	X	2016	A
1	X	2017	U

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Mol	Chain	Res	Type
1	X	2018	G
1	X	2026	C
1	X	2032	G
1	X	2034	A
1	X	2038	C
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2063	A
1	X	2076	G
1	X	2083	G
1	X	2089	C
1	X	2171	U
1	X	2173	G
1	X	2180	U
1	X	2181	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2192	U
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2198	U
1	X	2199	C
1	X	2204	A
1	X	2205	C
1	X	2217	G
1	X	2218	G
1	X	2222	U
1	X	2241	U
1	X	2247	A
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G

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Mol	Chain	Res	Type
1	X	2290	A
1	X	2298	U
1	X	2299	A
1	X	2301	A
1	X	2306	A
1	X	2311	U
1	X	2313	G
1	X	2314	A
1	X	2315	A
1	X	2316	G
1	X	2322	U
1	X	2326	C
1	X	2330	G
1	X	2351	G
1	X	2358	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2370	G
1	X	2375	G
1	X	2381	A
1	X	2386	G
1	X	2398	U
1	X	2401	A
1	X	2402	U
1	X	2404	A
1	X	2405	A
1	X	2408	G
1	X	2410	U
1	X	2414	A
1	X	2420	C
1	X	2422	C
1	X	2424	G
1	X	2426	G
1	X	2427	A
1	X	2452	U
1	X	2455	A
1	X	2457	A
1	X	2463	G
1	X	2469	G
1	X	2473	G
1	X	2477	C

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Mol	Chain	Res	Type
1	X	2480	C
1	X	2481	G
1	X	2484	G
1	X	2485	U
1	X	2492	G
1	X	2497	A
1	X	2499	C
1	X	2522	G
1	X	2535	C
1	X	2545	A
1	X	2546	G
1	X	2551	A
1	X	2552	C
1	X	2556	A
1	X	2564	U
1	X	2565	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2590	U
1	X	2591	C
1	X	2592	U
1	X	2594	U
1	X	2595	C
1	X	2600	A
1	X	2608	A
1	X	2609	G
1	X	2613	A
1	X	2618	A
1	X	2633	A
1	X	2634	G
1	X	2640	G
1	X	2642	G
1	X	2650	G
1	X	2664	G
1	X	2666	U
1	X	2668	U
1	X	2683	C
1	X	2684	A
1	X	2691	C
1	X	2692	A
1	X	2693	U

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Mol	Chain	Res	Type
1	X	2705	A
1	X	2706	U
1	X	2713	A
1	X	2730	A
1	X	2731	G
1	X	2732	C
1	X	2737	A
1	X	2738	A
1	X	2744	A
1	X	2745	A
1	X	2757	G
1	X	2758	A
1	X	2759	U
1	X	2761	A
1	X	2770	A
1	X	2782	G
1	X	2783	U
1	X	2787	A
1	X	2795	A
1	X	2796	A
1	X	2798	A
1	X	2808	U
1	X	2809	A
1	X	2811	G
1	X	2814	G
1	X	2824	C
1	X	2825	A
1	X	2842	C
1	X	2847	G
1	X	2851	G
1	X	2855	C
1	X	2858	A
1	X	2866	A
1	X	2868	G
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	22	U
2	Y	26	G
2	Y	28	A
2	Y	32	C

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Mol	Chain	Res	Type
2	Y	37	C
2	Y	42	U
2	Y	43	G
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	49	C
2	Y	68	A
2	Y	69	G
2	Y	99	G
2	Y	102	A
2	Y	108	G
2	Y	110	U
2	Y	112	A
2	Y	115	G

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	38	G
1	X	49	U
1	X	177	U
1	X	219	G
1	X	334	G
1	X	386	U
1	X	458	G
1	X	490	A
1	X	518	A
1	X	540	G
1	X	557	U
1	X	600	G
1	X	683	A
1	X	788	G
1	X	789	G
1	X	797	A
1	X	824	U
1	X	938	G
1	X	1019	U
1	X	1031	C
1	X	1053	G
1	X	1055	A
1	X	1182	U

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Mol	Chain	Res	Type
1	X	1223	G
1	X	1313	U
1	X	1391	A
1	X	1441	A
1	X	1475	U
1	X	1496	G
1	X	1607	A
1	X	1630	A
1	X	1792	C
1	X	1800	A
1	X	1923	U
1	X	1975	G
1	X	2015	G
1	X	2016	A
1	X	2043	A
1	X	2190	A
1	X	2204	A
1	X	2312	A
1	X	2409	A
1	X	2485	U
1	X	2564	U
1	X	2591	C
1	X	2705	A
1	X	2736	U
1	X	2756	A
1	X	2824	C
2	Y	16	U

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 124 ligands modelled in this entry, 123 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	$\#\|Z\| > 2$
29	6O1	X	2901	-	117,123,123	1.60	14 (11%)	155,191,191	1.86	27 (17%)

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
29	6O1	X	2901	-	-	10/50/234/234	0/13/13/13

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	2901	6O1	O71-N65	6.73	1.36	1.22
29	X	2901	6O1	C08-C05	-5.84	1.39	1.51
29	X	2901	6O1	O53-C49	5.39	1.45	1.40
29	X	2901	6O1	C62-C61	-5.28	1.40	1.51
29	X	2901	6O1	C04-C09	-4.34	1.40	1.50
29	X	2901	6O1	C56-C55	-3.82	1.41	1.50
29	X	2901	6O1	O51-C54	3.45	1.47	1.41
29	X	2901	6O1	C22-C23	3.30	1.55	1.53
29	X	2901	6O1	O20-C16	2.89	1.44	1.41
29	X	2901	6O1	C51-C50	-2.85	1.48	1.53
29	X	2901	6O1	O25-C16	2.66	1.46	1.41
29	X	2901	6O1	O50-C54	2.63	1.45	1.41
29	X	2901	6O1	C65-N65	-2.55	1.47	1.52
29	X	2901	6O1	O26-C22	2.25	1.47	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	2901	6O1	O50-C50-C51	-10.43	97.90	106.63
29	X	2901	6O1	O51-C51-C50	-6.40	98.11	106.41
29	X	2901	6O1	C44-O44-C36	-5.12	105.27	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	2901	6O1	C36-C37-C38	-4.77	102.16	110.38
29	X	2901	6O1	C01-C06-C05	-4.45	119.97	122.79
29	X	2901	6O1	C06-C01-C02	4.40	122.20	117.81
29	X	2901	6O1	C29-O33-C33	-3.69	107.33	113.67
29	X	2901	6O1	O25-C25-C24	-3.15	98.32	104.14
29	X	2901	6O1	C29-C30-C31	-3.11	104.61	110.07
29	X	2901	6O1	C03-C02-CL1	3.02	123.84	118.90
29	X	2901	6O1	O47-C47-C46	-2.99	98.50	103.49
29	X	2901	6O1	C15-C14-C13	-2.95	108.91	113.41
29	X	2901	6O1	C13-O13-C09	-2.86	112.64	117.21
29	X	2901	6O1	C16-O20-C20	-2.86	109.56	112.16
29	X	2901	6O1	C30-C31-C32	-2.79	105.28	111.66
29	X	2901	6O1	C48-C47-C46	-2.53	107.37	112.49
29	X	2901	6O1	C28-C26-C25	-2.51	108.52	113.52
29	X	2901	6O1	O53-C49-O47	2.43	114.45	109.91
29	X	2901	6O1	C69-O66-C66	-2.33	110.42	114.44
29	X	2901	6O1	C01-C02-C03	-2.32	117.25	120.63
29	X	2901	6O1	C53-O53-C49	-2.24	110.07	111.59
29	X	2901	6O1	C34-O32-C32	-2.23	108.67	114.52
29	X	2901	6O1	O31-C31-C32	2.23	113.14	107.48
29	X	2901	6O1	C10-O19-C19	-2.19	110.22	114.66
29	X	2901	6O1	O20-C20-C21	2.13	108.50	105.85
29	X	2901	6O1	C42-C40-C39	-2.13	108.06	113.33
29	X	2901	6O1	O57-C57-C56	-2.12	117.17	121.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	2901	6O1	O67-C63-O12-C12
29	X	2901	6O1	O33-C29-O39-C39
29	X	2901	6O1	O40-C36-O44-C44
29	X	2901	6O1	C37-C36-O44-C44
29	X	2901	6O1	O55-C55-C56-C61
29	X	2901	6O1	O52-C55-C56-C61
29	X	2901	6O1	O55-C55-C56-C57
29	X	2901	6O1	C30-C31-O31-C22
29	X	2901	6O1	O52-C55-C56-C57
29	X	2901	6O1	C32-C31-O31-C22

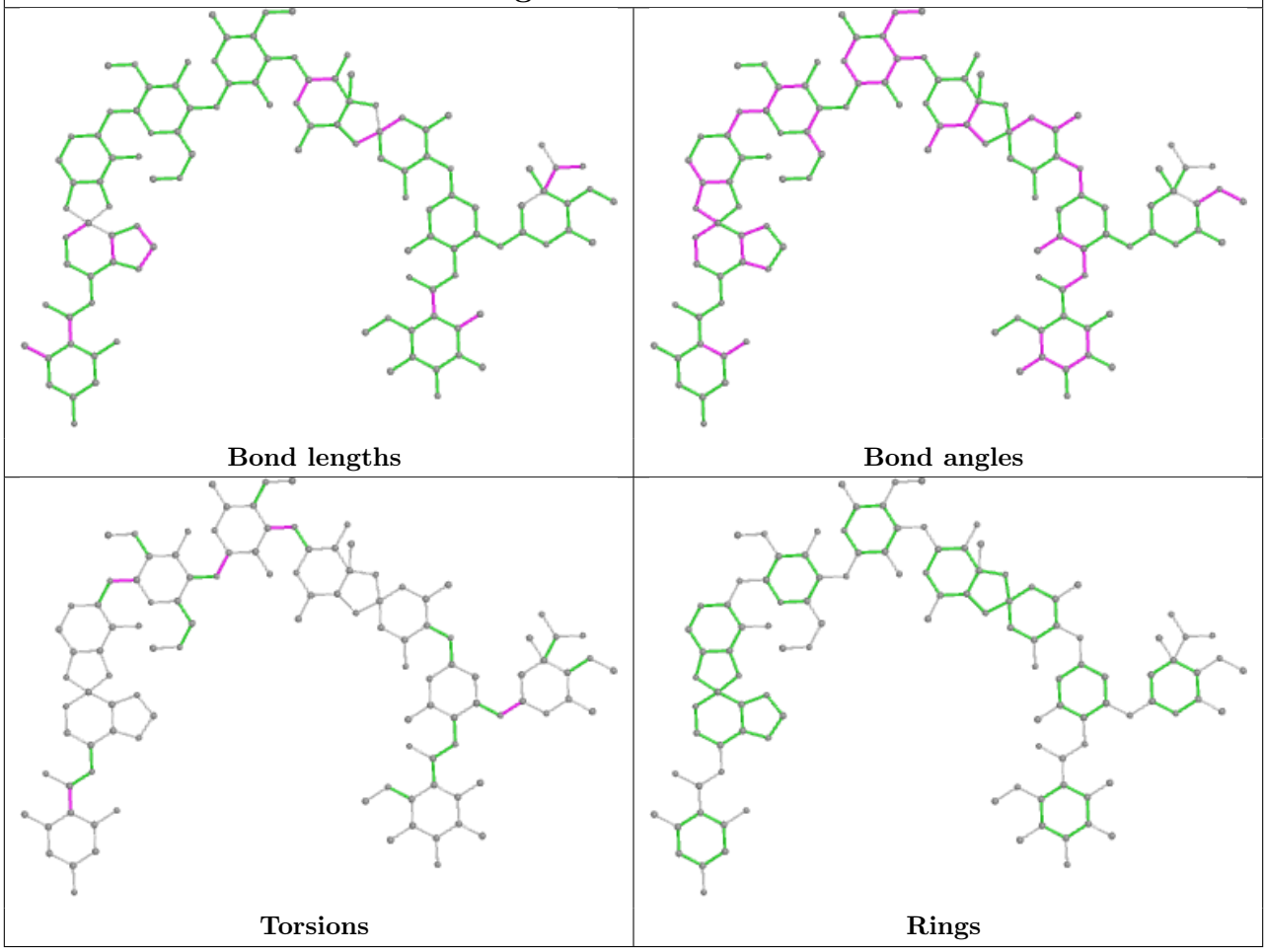
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	2901	6O1	2	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 6O1 X 2901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	X	2658/2880 (92%)	-0.12	95 (3%) 42 27	30, 77, 204, 337	0
2	Y	120/123 (97%)	-0.07	3 (2%) 57 39	80, 150, 187, 207	0
3	A	259/275 (94%)	-0.19	4 (1%) 73 58	50, 105, 160, 212	0
4	B	205/211 (97%)	-0.49	0 100 100	30, 51, 113, 199	0
5	C	194/205 (94%)	-0.38	1 (0%) 91 82	35, 103, 180, 254	0
6	D	177/180 (98%)	-0.14	4 (2%) 60 42	128, 183, 249, 280	0
7	E	171/185 (92%)	-0.08	13 (7%) 13 7	70, 142, 203, 254	0
8	G	142/174 (81%)	-0.12	6 (4%) 36 22	38, 78, 188, 245	0
9	H	134/134 (100%)	-0.43	0 100 100	40, 55, 108, 175	0
10	I	134/156 (85%)	-0.10	2 (1%) 73 58	50, 120, 191, 236	0
11	J	136/141 (96%)	-0.04	3 (2%) 62 43	65, 106, 170, 225	0
12	K	113/116 (97%)	-0.54	0 100 100	30, 37, 91, 200	0
13	L	104/114 (91%)	0.01	5 (4%) 30 18	120, 154, 189, 241	0
14	M	108/166 (65%)	-0.66	0 100 100	37, 50, 117, 169	0
15	N	117/118 (99%)	-0.47	1 (0%) 84 71	42, 82, 136, 279	0
16	O	94/100 (94%)	-0.37	1 (1%) 80 66	48, 101, 170, 216	0
17	P	127/134 (94%)	-0.53	0 100 100	34, 53, 105, 192	0
18	Q	93/95 (97%)	-0.28	8 (8%) 10 6	49, 88, 174, 215	0
19	R	110/115 (95%)	-0.28	4 (3%) 42 27	62, 117, 213, 259	0
20	S	179/237 (75%)	-0.10	8 (4%) 33 19	97, 158, 213, 289	0
21	T	74/91 (81%)	-0.09	4 (5%) 25 14	67, 104, 157, 206	0
22	U	72/81 (88%)	0.10	5 (6%) 16 9	70, 125, 187, 215	0
23	V	65/67 (97%)	-0.23	3 (4%) 32 19	83, 125, 197, 216	0
24	W	55/55 (100%)	-0.61	0 100 100	68, 90, 135, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Z	57/60 (95%)	-0.28	1 (1%) 68 51	32, 43, 104, 182	0
26	1	53/54 (98%)	0.36	6 (11%) 5 3	101, 129, 224, 259	0
27	2	46/47 (97%)	-0.29	1 (2%) 62 43	44, 59, 103, 162	0
28	3	59/66 (89%)	0.04	0 100 100	72, 100, 161, 239	0
All	All	5856/6380 (91%)	-0.19	178 (3%) 50 32	30, 91, 201, 337	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	1523	A	15.5
6	D	43	SER	8.1
22	U	29	GLY	6.4
1	X	1522	C	6.2
1	X	1073	G	5.9
11	J	84	MET	5.8
1	X	1553	G	5.6
1	X	2780	A	5.4
1	X	1186	G	5.3
1	X	1187	A	5.2
8	G	156	HIS	5.2
1	X	1115	C	5.2
1	X	514	G	5.1
1	X	1117	G	5.0
1	X	1552	C	4.9
18	Q	64	ARG	4.9
1	X	1109	A	4.8
1	X	1074	G	4.8
1	X	248	A	4.8
1	X	1188	A	4.8
1	X	2287	G	4.5
1	X	731	A	4.5
1	X	1524	C	4.5
6	D	42	SER	4.4
20	S	15	ASP	4.4
1	X	1845	A	4.4
7	E	13	SER	4.3
1	X	1525	A	4.2
19	R	60	PRO	4.2
23	V	4	SER	4.0
1	X	911	A	4.0
20	S	14	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
21	T	16	SER	3.8
20	S	11	LYS	3.8
19	R	58	VAL	3.7
3	A	249	PRO	3.6
1	X	1734	C	3.6
1	X	1121	G	3.6
1	X	1951	G	3.6
1	X	1076	U	3.6
1	X	728	G	3.5
1	X	1044	U	3.5
1	X	1077	U	3.5
1	X	1841	G	3.5
1	X	1078	A	3.5
13	L	97	HIS	3.5
2	Y	25	G	3.4
1	X	1114	A	3.4
22	U	30	VAL	3.4
7	E	174	GLY	3.4
1	X	2083	G	3.3
18	Q	92	ALA	3.3
1	X	1909	U	3.3
22	U	28	GLY	3.3
25	Z	59	ALA	3.3
8	G	155	THR	3.3
1	X	1110	G	3.2
7	E	12	PRO	3.2
1	X	1913	G	3.2
7	E	10	ALA	3.2
1	X	1075	C	3.2
13	L	62	GLY	3.2
1	X	727	U	3.1
1	X	1842	G	3.1
5	C	19	LEU	3.1
6	D	144	ASP	3.1
1	X	435	A	3.1
1	X	1588	A	3.1
1	X	1847	G	3.1
1	X	665	A	3.1
18	Q	90	ALA	3.0
1	X	1871	G	3.0
3	A	250	TRP	3.0
1	X	1554	G	3.0

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Mol	Chain	Res	Type	RSRZ
1	X	1189	G	3.0
1	X	1548	U	3.0
1	X	1185	C	3.0
1	X	206	U	3.0
20	S	4	THR	2.9
7	E	123	PHE	2.9
1	X	1848	U	2.8
1	X	1844	C	2.8
1	X	1556	A	2.8
19	R	99	VAL	2.8
1	X	1843	U	2.8
8	G	69	ASP	2.8
16	O	43	GLU	2.8
13	L	61	SER	2.8
1	X	1184	G	2.8
1	X	2773	G	2.8
1	X	2088	U	2.8
1	X	2084	G	2.7
1	X	2082	C	2.7
13	L	53	ALA	2.7
1	X	1477	C	2.7
1	X	1803	G	2.7
1	X	2085	G	2.7
1	X	1116	U	2.7
18	Q	93	GLY	2.7
1	X	2169	A	2.7
26	1	47	HIS	2.7
1	X	729	A	2.7
22	U	25	ARG	2.6
1	X	1084	A	2.6
21	T	85	GLN	2.6
1	X	1434	U	2.6
13	L	52	ALA	2.6
1	X	2170	C	2.6
1	X	1104	G	2.6
1	X	1498	G	2.6
1	X	1937	G	2.6
26	1	4	ASP	2.6
23	V	5	GLU	2.5
1	X	1082	G	2.5
6	D	75	SER	2.5
26	1	6	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
18	Q	71	GLN	2.5
19	R	64	ASN	2.4
18	Q	91	LEU	2.4
21	T	14	ARG	2.4
7	E	50	LEU	2.4
26	1	8	ILE	2.4
26	1	35	LEU	2.4
3	A	220	HIS	2.4
10	I	23	PRO	2.4
20	S	33	ALA	2.4
10	I	52	GLY	2.4
15	N	118	GLN	2.4
18	Q	94	GLN	2.4
3	A	91	ARG	2.4
7	E	175	LYS	2.3
1	X	1138	A	2.3
1	X	1555	A	2.3
7	E	173	ALA	2.3
1	X	1939	U	2.3
18	Q	89	GLU	2.3
1	X	356	A	2.3
1	X	2089	C	2.3
2	Y	38	C	2.3
8	G	37	ASP	2.3
20	S	10	PRO	2.3
21	T	15	ASP	2.3
1	X	2289	A	2.3
23	V	7	ARG	2.3
27	2	46	ASP	2.3
20	S	12	GLN	2.3
1	X	1492	A	2.3
1	X	1888	C	2.3
1	X	1547	U	2.3
7	E	11	VAL	2.3
1	X	1846	A	2.2
26	1	7	ARG	2.2
1	X	1950	C	2.2
1	X	912	A	2.2
1	X	721	C	2.2
7	E	49	GLN	2.2
7	E	15	VAL	2.2
1	X	1840	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	246	C	2.2
2	Y	111	C	2.2
1	X	2172	U	2.2
1	X	1118	G	2.2
1	X	2090	U	2.1
8	G	36	ASN	2.1
11	J	117	GLU	2.1
1	X	722	C	2.1
1	X	1190	C	2.1
7	E	14	GLY	2.1
7	E	48	ASP	2.1
11	J	118	ALA	2.1
8	G	34	PRO	2.1
20	S	55	THR	2.1
1	X	1057	A	2.0
1	X	559	C	2.0
1	X	135	U	2.0
1	X	1839	A	2.0
1	X	247	A	2.0
22	U	16	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3020	1/1	0.53	1.58	64,64,64,64	0
30	MG	X	3016	1/1	0.71	1.26	74,74,74,74	0
30	MG	X	3012	1/1	0.73	0.39	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3006	1/1	0.74	0.50	34,34,34,34	0
30	MG	X	2927	1/1	0.79	0.54	57,57,57,57	0
30	MG	X	2960	1/1	0.79	0.89	34,34,34,34	0
30	MG	X	2999	1/1	0.80	0.77	74,74,74,74	0
30	MG	X	3001	1/1	0.80	1.62	86,86,86,86	0
30	MG	X	2916	1/1	0.81	1.06	51,51,51,51	0
30	MG	X	3019	1/1	0.83	1.06	46,46,46,46	0
30	MG	K	201	1/1	0.83	0.70	31,31,31,31	0
30	MG	X	2974	1/1	0.87	0.84	30,30,30,30	0
30	MG	X	2935	1/1	0.88	2.22	41,41,41,41	0
30	MG	X	2933	1/1	0.88	1.35	38,38,38,38	0
30	MG	X	3017	1/1	0.88	0.77	52,52,52,52	0
30	MG	X	2979	1/1	0.89	0.29	46,46,46,46	0
30	MG	X	2982	1/1	0.89	0.86	31,31,31,31	0
30	MG	X	3007	1/1	0.89	0.50	40,40,40,40	0
30	MG	X	2975	1/1	0.89	1.36	49,49,49,49	0
30	MG	X	3015	1/1	0.89	0.55	98,98,98,98	0
30	MG	X	2992	1/1	0.90	1.04	34,34,34,34	0
30	MG	X	2907	1/1	0.90	1.25	49,49,49,49	0
30	MG	X	2967	1/1	0.90	0.37	55,55,55,55	0
30	MG	X	2928	1/1	0.91	0.17	41,41,41,41	0
29	6O1	X	2901	111/111	0.91	0.39	106,116,136,139	0
30	MG	X	2913	1/1	0.91	0.63	36,36,36,36	0
30	MG	X	2940	1/1	0.91	0.41	34,34,34,34	0
30	MG	X	2942	1/1	0.91	0.25	31,31,31,31	0
30	MG	X	2904	1/1	0.91	1.01	32,32,32,32	0
30	MG	X	2964	1/1	0.91	0.53	60,60,60,60	0
30	MG	X	2906	1/1	0.91	0.88	42,42,42,42	0
30	MG	X	2972	1/1	0.92	0.63	36,36,36,36	0
30	MG	X	2981	1/1	0.92	0.61	99,99,99,99	0
30	MG	X	2925	1/1	0.92	0.53	43,43,43,43	0
30	MG	X	2971	1/1	0.92	0.61	33,33,33,33	0
30	MG	X	2978	1/1	0.92	0.42	49,49,49,49	0
30	MG	M	201	1/1	0.92	1.58	35,35,35,35	0
30	MG	X	2937	1/1	0.93	0.73	32,32,32,32	0
30	MG	X	2987	1/1	0.93	0.46	43,43,43,43	0
30	MG	X	2945	1/1	0.93	1.20	55,55,55,55	0
30	MG	X	2995	1/1	0.93	0.82	83,83,83,83	0
30	MG	X	2947	1/1	0.94	1.18	52,52,52,52	0
30	MG	X	2938	1/1	0.94	0.33	36,36,36,36	0
30	MG	X	2976	1/1	0.94	0.49	53,53,53,53	0
30	MG	X	2902	1/1	0.94	1.16	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3008	1/1	0.94	0.62	39,39,39,39	0
30	MG	X	3011	1/1	0.94	0.34	58,58,58,58	0
30	MG	X	2909	1/1	0.94	0.72	36,36,36,36	0
30	MG	X	2968	1/1	0.94	0.26	35,35,35,35	0
30	MG	X	2970	1/1	0.94	1.02	63,63,63,63	0
30	MG	X	2944	1/1	0.94	0.88	37,37,37,37	0
30	MG	X	2917	1/1	0.94	0.21	33,33,33,33	0
30	MG	X	2994	1/1	0.94	0.37	77,77,77,77	0
30	MG	X	2973	1/1	0.94	0.35	52,52,52,52	0
30	MG	X	2998	1/1	0.94	0.22	35,35,35,35	0
30	MG	X	2943	1/1	0.95	0.29	33,33,33,33	0
30	MG	X	2932	1/1	0.95	0.32	53,53,53,53	0
30	MG	X	2910	1/1	0.95	0.62	34,34,34,34	0
30	MG	X	2988	1/1	0.95	0.65	55,55,55,55	0
30	MG	X	2920	1/1	0.95	0.74	34,34,34,34	0
30	MG	X	2956	1/1	0.95	0.57	32,32,32,32	0
30	MG	X	2922	1/1	0.95	0.44	35,35,35,35	0
30	MG	X	2912	1/1	0.95	0.46	34,34,34,34	0
30	MG	X	2908	1/1	0.95	0.67	34,34,34,34	0
30	MG	X	2903	1/1	0.95	0.61	37,37,37,37	0
30	MG	X	3002	1/1	0.95	0.31	44,44,44,44	0
30	MG	K	202	1/1	0.95	0.19	31,31,31,31	0
30	MG	X	3003	1/1	0.95	0.88	63,63,63,63	0
30	MG	X	2958	1/1	0.96	0.86	38,38,38,38	0
30	MG	X	2959	1/1	0.96	0.69	54,54,54,54	0
30	MG	X	2977	1/1	0.96	1.03	78,78,78,78	0
30	MG	X	2939	1/1	0.96	0.61	30,30,30,30	0
30	MG	X	3004	1/1	0.96	0.30	54,54,54,54	0
30	MG	X	3005	1/1	0.96	0.92	66,66,66,66	0
30	MG	X	2961	1/1	0.96	0.68	68,68,68,68	0
30	MG	X	2931	1/1	0.96	0.58	32,32,32,32	0
30	MG	X	2914	1/1	0.96	0.46	43,43,43,43	0
30	MG	X	2986	1/1	0.96	0.47	46,46,46,46	0
30	MG	X	2949	1/1	0.96	0.36	32,32,32,32	0
30	MG	X	2950	1/1	0.96	0.52	36,36,36,36	0
30	MG	X	2989	1/1	0.96	0.67	56,56,56,56	0
30	MG	X	2990	1/1	0.96	0.64	39,39,39,39	0
30	MG	X	3018	1/1	0.96	0.28	32,32,32,32	0
30	MG	X	2991	1/1	0.96	0.69	72,72,72,72	0
30	MG	X	2951	1/1	0.96	0.22	35,35,35,35	0
30	MG	Y	201	1/1	0.96	0.90	77,77,77,77	0
30	MG	X	2955	1/1	0.96	0.39	31,31,31,31	0

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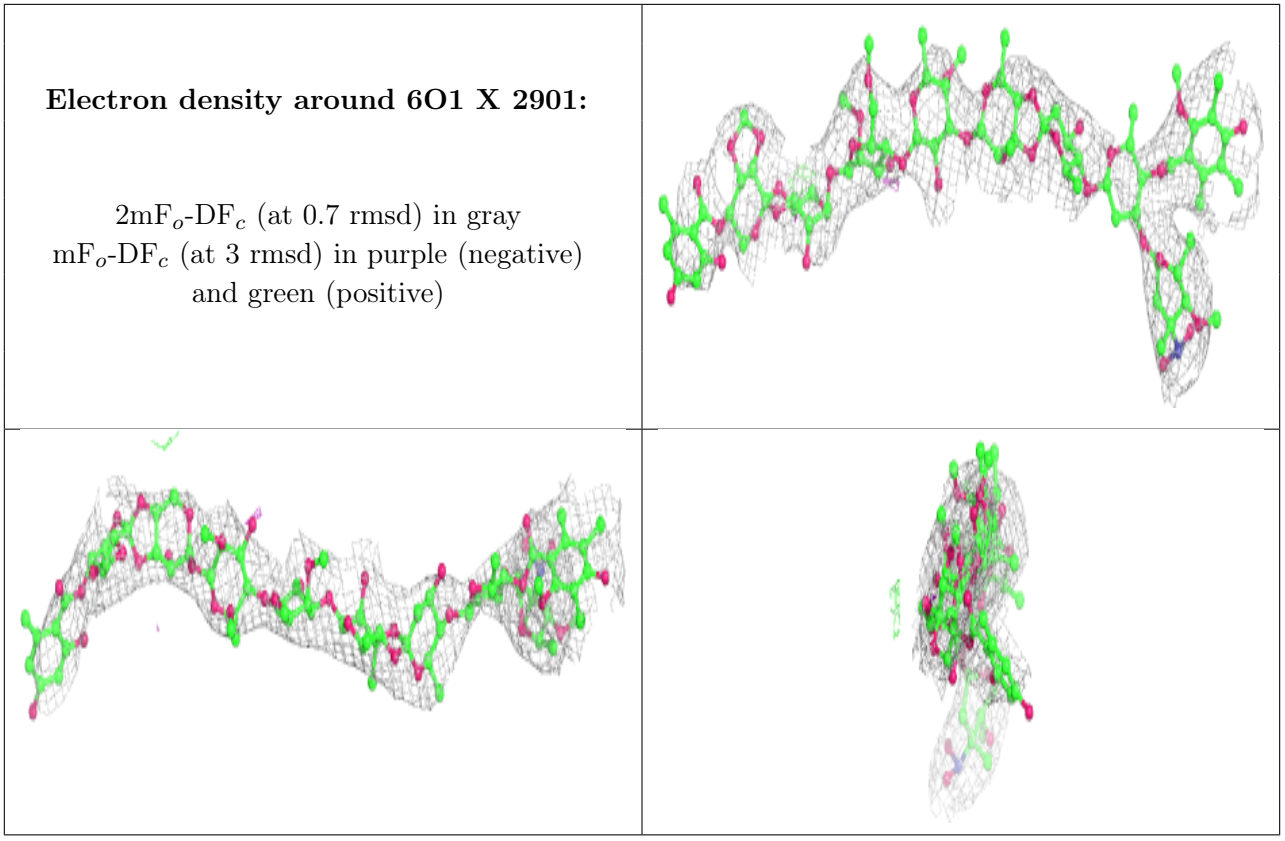
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	2921	1/1	0.96	0.98	37,37,37,37	0
30	MG	X	2957	1/1	0.96	0.33	42,42,42,42	0
30	MG	X	2926	1/1	0.97	0.32	32,32,32,32	0
30	MG	X	2911	1/1	0.97	0.66	46,46,46,46	0
30	MG	X	3014	1/1	0.97	0.28	43,43,43,43	0
30	MG	X	2984	1/1	0.97	0.57	49,49,49,49	0
30	MG	X	2905	1/1	0.97	0.82	30,30,30,30	0
30	MG	X	2952	1/1	0.97	1.27	54,54,54,54	0
30	MG	X	2953	1/1	0.97	0.29	38,38,38,38	0
30	MG	X	2965	1/1	0.97	0.48	40,40,40,40	0
30	MG	X	2930	1/1	0.97	0.64	46,46,46,46	0
30	MG	X	2941	1/1	0.97	0.43	55,55,55,55	0
30	MG	X	2948	1/1	0.97	0.26	30,30,30,30	0
30	MG	X	2980	1/1	0.97	0.44	49,49,49,49	0
30	MG	X	3010	1/1	0.97	0.27	41,41,41,41	0
30	MG	X	2946	1/1	0.98	0.43	34,34,34,34	0
30	MG	X	2966	1/1	0.98	0.34	37,37,37,37	0
30	MG	X	2919	1/1	0.98	0.31	33,33,33,33	0
30	MG	X	2993	1/1	0.98	0.42	44,44,44,44	0
30	MG	X	2923	1/1	0.98	0.39	30,30,30,30	0
30	MG	X	3013	1/1	0.98	0.49	47,47,47,47	0
30	MG	X	2934	1/1	0.98	0.81	39,39,39,39	0
30	MG	X	2996	1/1	0.98	0.19	43,43,43,43	0
30	MG	X	2929	1/1	0.98	0.73	39,39,39,39	0
30	MG	X	2983	1/1	0.98	0.30	63,63,63,63	0
30	MG	X	3000	1/1	0.98	0.28	39,39,39,39	0
30	MG	X	2936	1/1	0.98	0.47	53,53,53,53	0
30	MG	X	2985	1/1	0.98	0.28	55,55,55,55	0
30	MG	X	2915	1/1	0.98	0.36	36,36,36,36	0
30	MG	X	2962	1/1	0.98	0.20	41,41,41,41	0
30	MG	X	2963	1/1	0.98	0.67	71,71,71,71	0
30	MG	X	2918	1/1	0.98	0.47	45,45,45,45	0
30	MG	X	2997	1/1	0.99	0.35	38,38,38,38	0
30	MG	X	2924	1/1	0.99	0.39	30,30,30,30	0
30	MG	X	2954	1/1	0.99	0.56	41,41,41,41	0
30	MG	X	2969	1/1	0.99	0.64	43,43,43,43	0
30	MG	X	3009	1/1	0.99	0.33	41,41,41,41	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 6O1 X 2901:

$2mF_o$-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.