



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:06 PM GMT

PDB ID : 4U67  
Title : Crystal structure of the large ribosomal subunit (50S) of *Deinococcus radiodurans* containing a three residue insertion in L22  
Authors : Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.  
Deposited on : 2014-07-28  
Resolution : 3.65 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

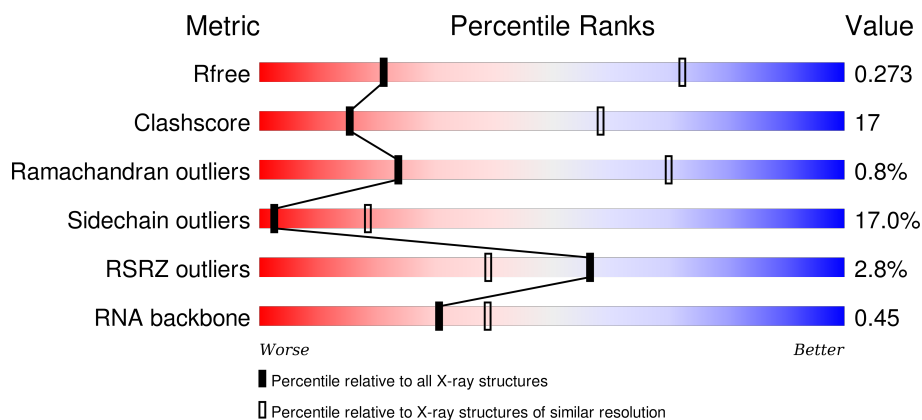
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 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))
$R_{free}$	91344	1010 (3.82-3.50)
Clashscore	102246	1125 (3.82-3.50)
Ramachandran outliers	100387	1079 (3.82-3.50)
Sidechain outliers	100360	1078 (3.82-3.50)
RSRZ outliers	91569	1017 (3.82-3.50)
RNA backbone	2183	1066 (4.52-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div>5%</div> <div>45%</div> <div>39%</div> <div>11%</div> <div>5%</div> </div>
2	B	211	<div> <div>51%</div> <div>40%</div> <div>7%</div> <div>.</div> </div>
3	C	205	<div> <div>5%</div> <div>39%</div> <div>46%</div> <div>10%</div> <div>5%</div> </div>
4	D	180	<div> <div>13%</div> <div>53%</div> <div>41%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	185	
6	G	174	
7	H	134	
8	I	156	
9	J	141	
10	K	116	
11	L	114	
12	M	166	
13	N	118	
14	O	100	
15	P	137	
16	Q	95	
17	R	114	
18	S	237	
19	T	91	
20	U	81	
21	V	67	
22	W	55	
23	Z	60	
24	1	55	
25	2	47	
26	3	66	
27	X	2880	
28	Y	123	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MG	K	201	-	-	-	X
29	MG	X	2901	-	-	-	X
29	MG	X	2902	-	-	-	X
29	MG	X	2905	-	-	-	X
29	MG	X	2907	-	-	-	X
29	MG	X	2909	-	-	-	X
29	MG	X	2910	-	-	-	X
29	MG	X	2912	-	-	-	X
29	MG	X	2913	-	-	-	X
29	MG	X	2917	-	-	-	X
29	MG	X	2919	-	-	-	X
29	MG	X	2920	-	-	-	X
29	MG	X	2921	-	-	-	X
29	MG	X	2922	-	-	-	X
29	MG	X	2924	-	-	-	X
29	MG	X	2926	-	-	-	X
29	MG	X	2928	-	-	-	X
29	MG	X	2929	-	-	-	X
29	MG	X	2931	-	-	-	X
29	MG	X	2934	-	-	-	X
29	MG	X	2936	-	-	-	X
29	MG	X	2939	-	-	-	X
29	MG	X	2940	-	-	-	X
29	MG	X	2943	-	-	-	X
29	MG	X	2944	-	-	-	X
29	MG	X	2947	-	-	-	X

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 83768 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 27 is a RNA chain called 23s RNA.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	X	2667	Total	C	N	O	P	0	0	0
			57254	25538	10574	18475	2667			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 28 is a RNA chain called 5s RNA.

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

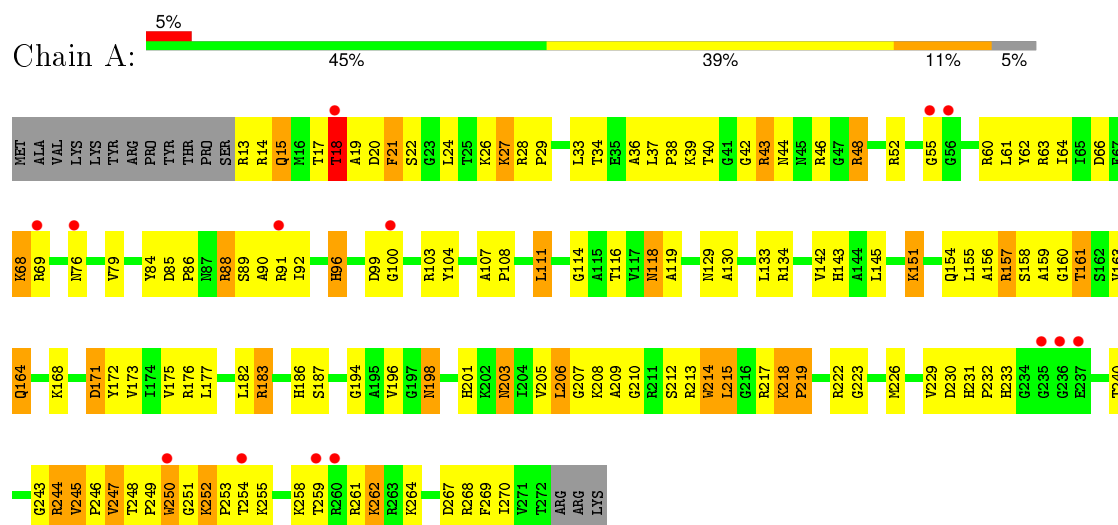
- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	X	50	Total	Mg	0	0
			50	50		
29	K	1	Total	Mg	0	0
			1	1		

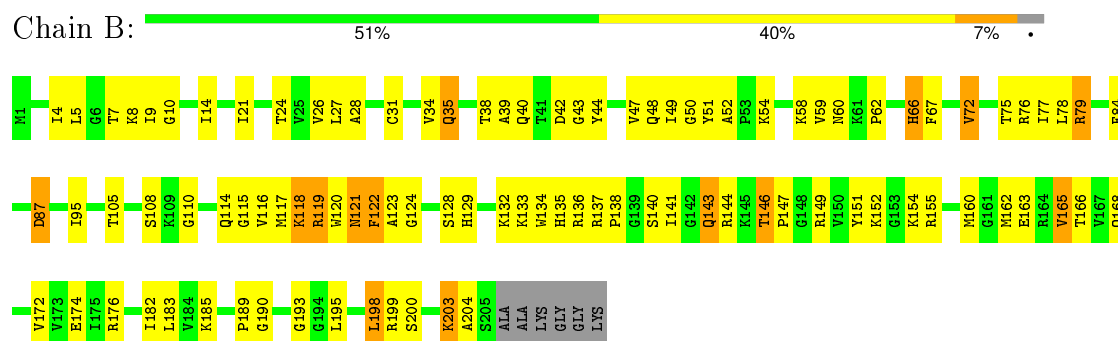
### 3 Residue-property plots

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

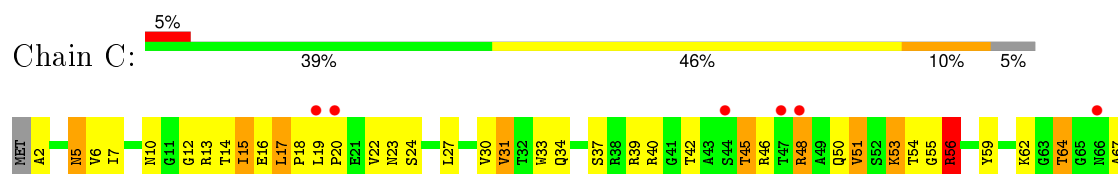
#### • Molecule 1: 50S ribosomal protein L2

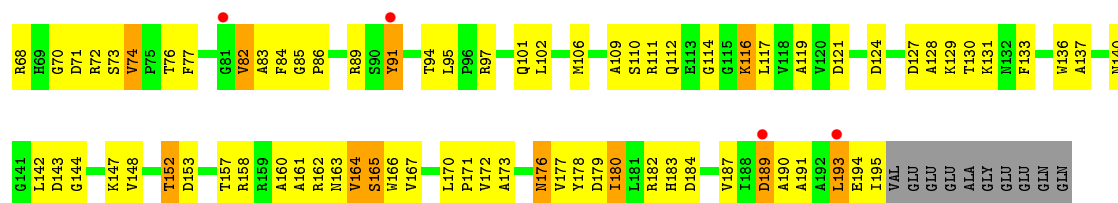


#### • Molecule 2: 50S ribosomal protein L3

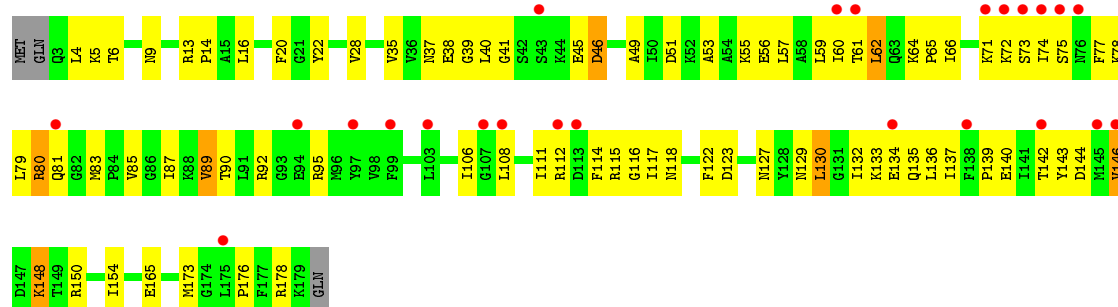


#### • Molecule 3: 50S ribosomal protein L4

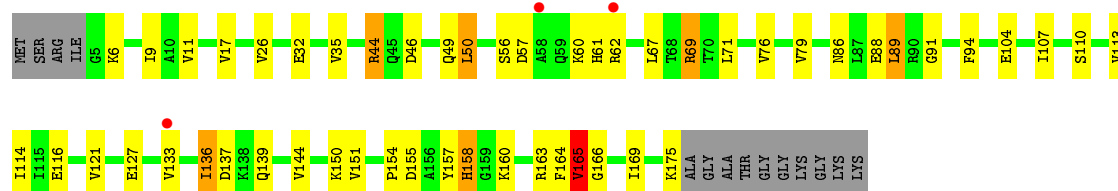




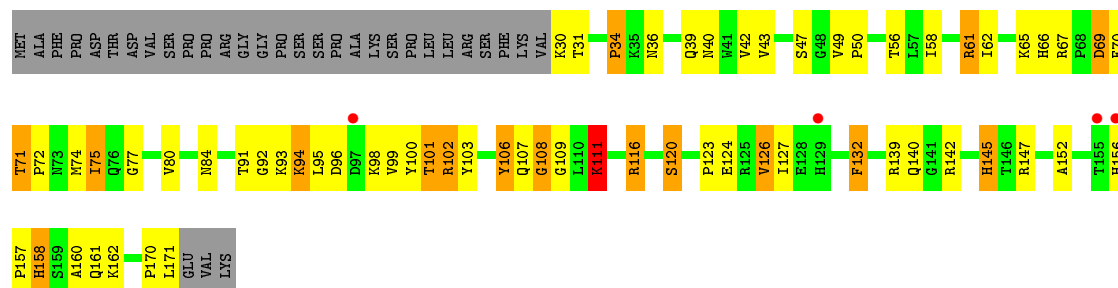
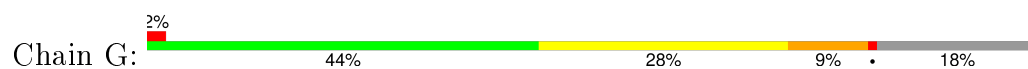
• Molecule 4: 50S ribosomal protein L5



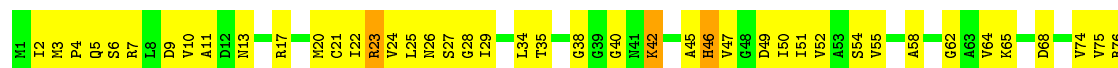
• Molecule 5: 50S ribosomal protein L6



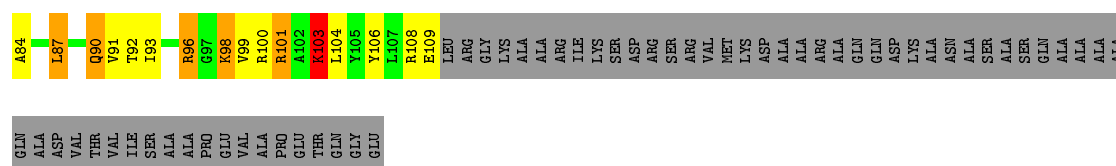
• Molecule 6: 50S ribosomal protein L13



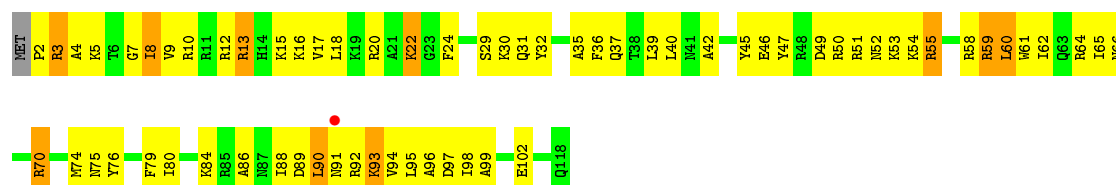
• Molecule 7: 50S ribosomal protein L14



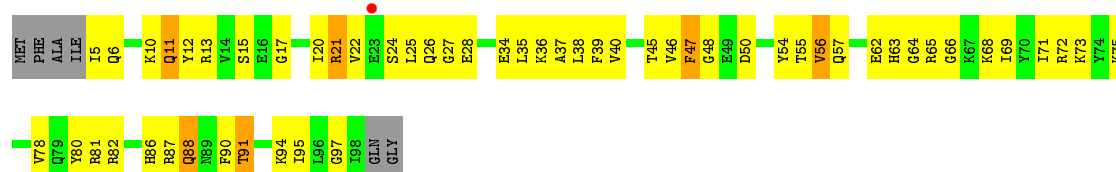
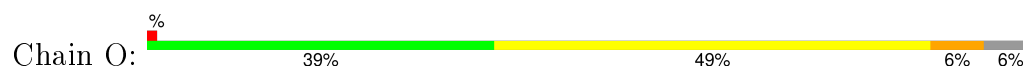




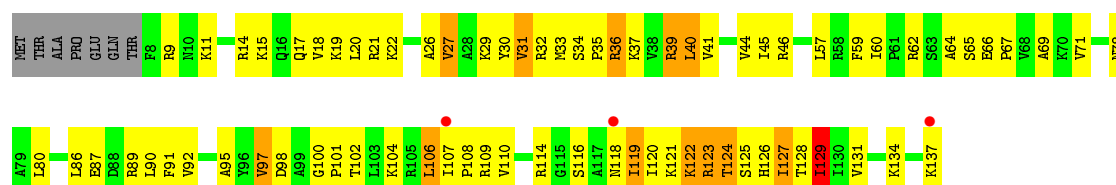
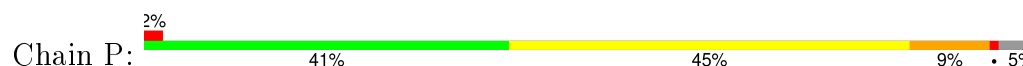
- Molecule 13: 50S ribosomal protein L20



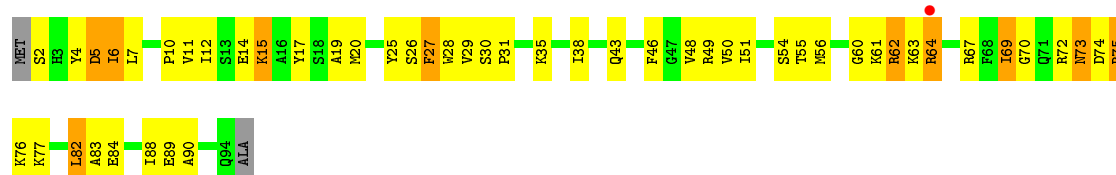
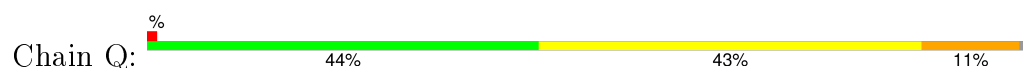
- Molecule 14: 50S ribosomal protein L21



- Molecule 15: 50S ribosomal protein L22

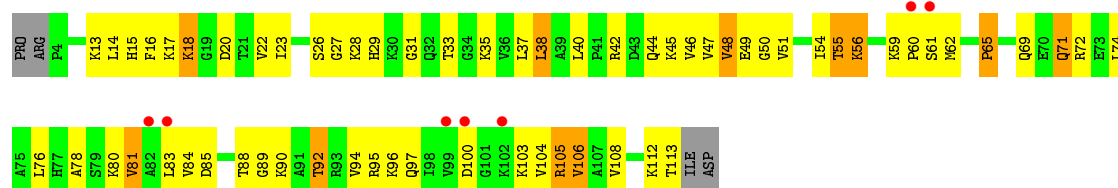


- Molecule 16: 50S ribosomal protein L23

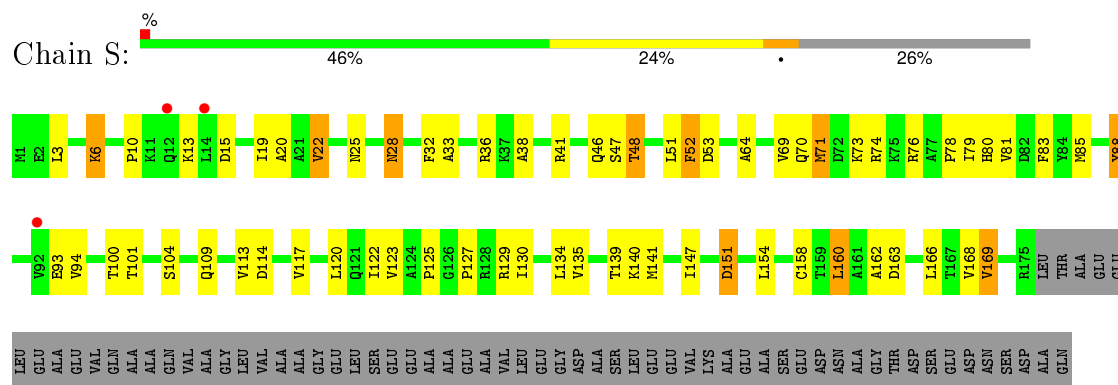


- Molecule 17: 50S ribosomal protein L24

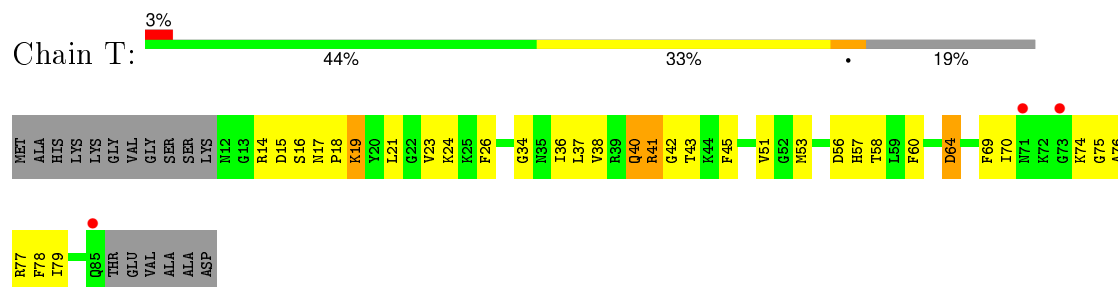




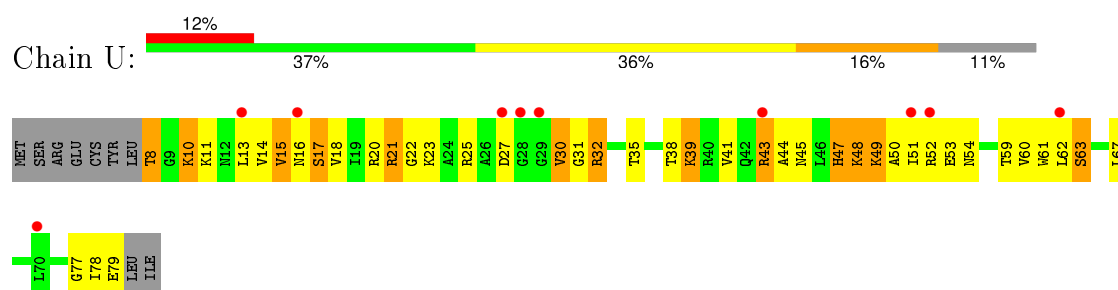
• Molecule 18: 50S ribosomal protein L25



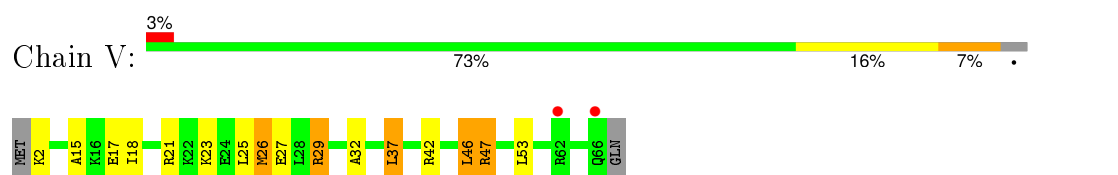
• Molecule 19: 50S ribosomal protein L27



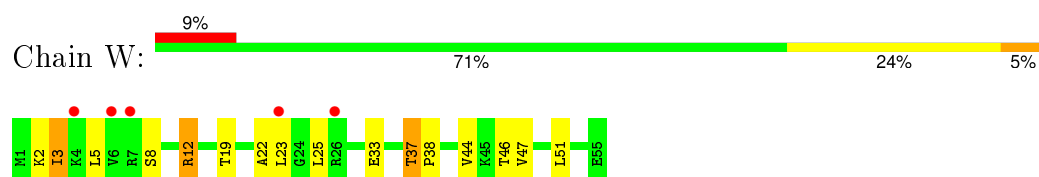
• Molecule 20: 50S ribosomal protein L28



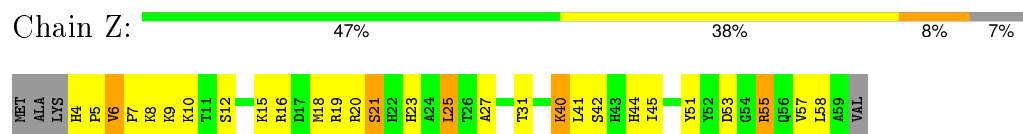
• Molecule 21: 50S ribosomal protein L29



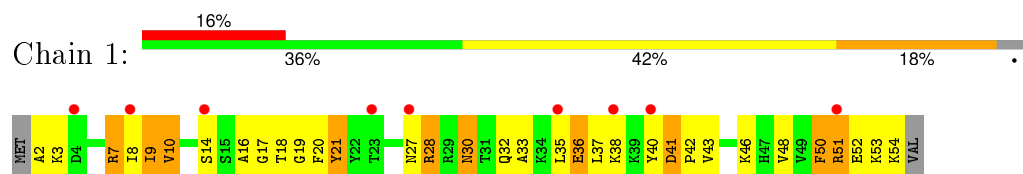
• Molecule 22: 50S ribosomal protein L30



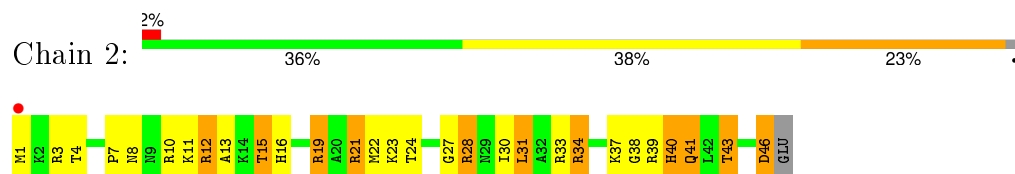
- Molecule 23: 50S ribosomal protein L32



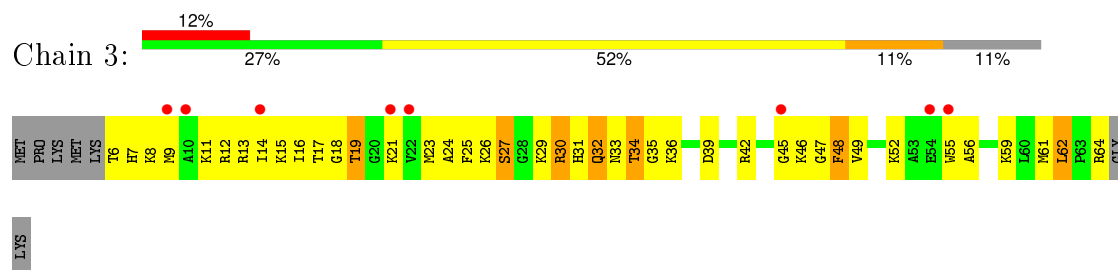
- Molecule 24: 50S ribosomal protein L33



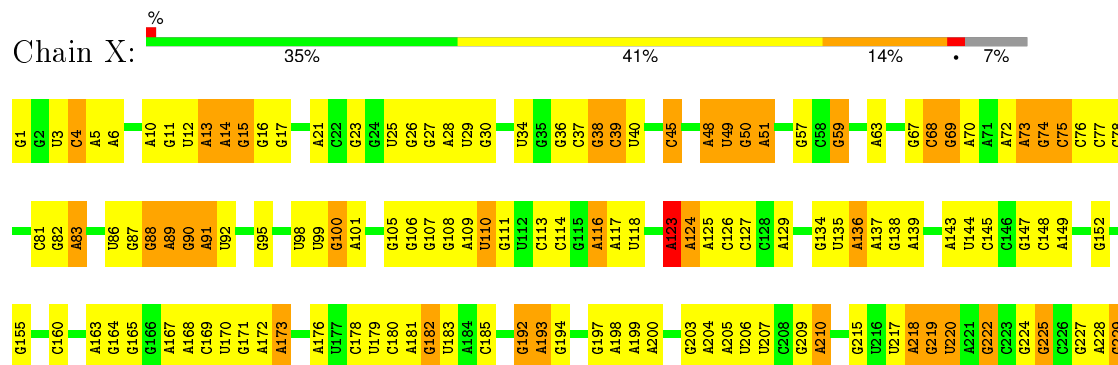
- Molecule 25: 50S ribosomal protein L34



- Molecule 26: 50S ribosomal protein L35



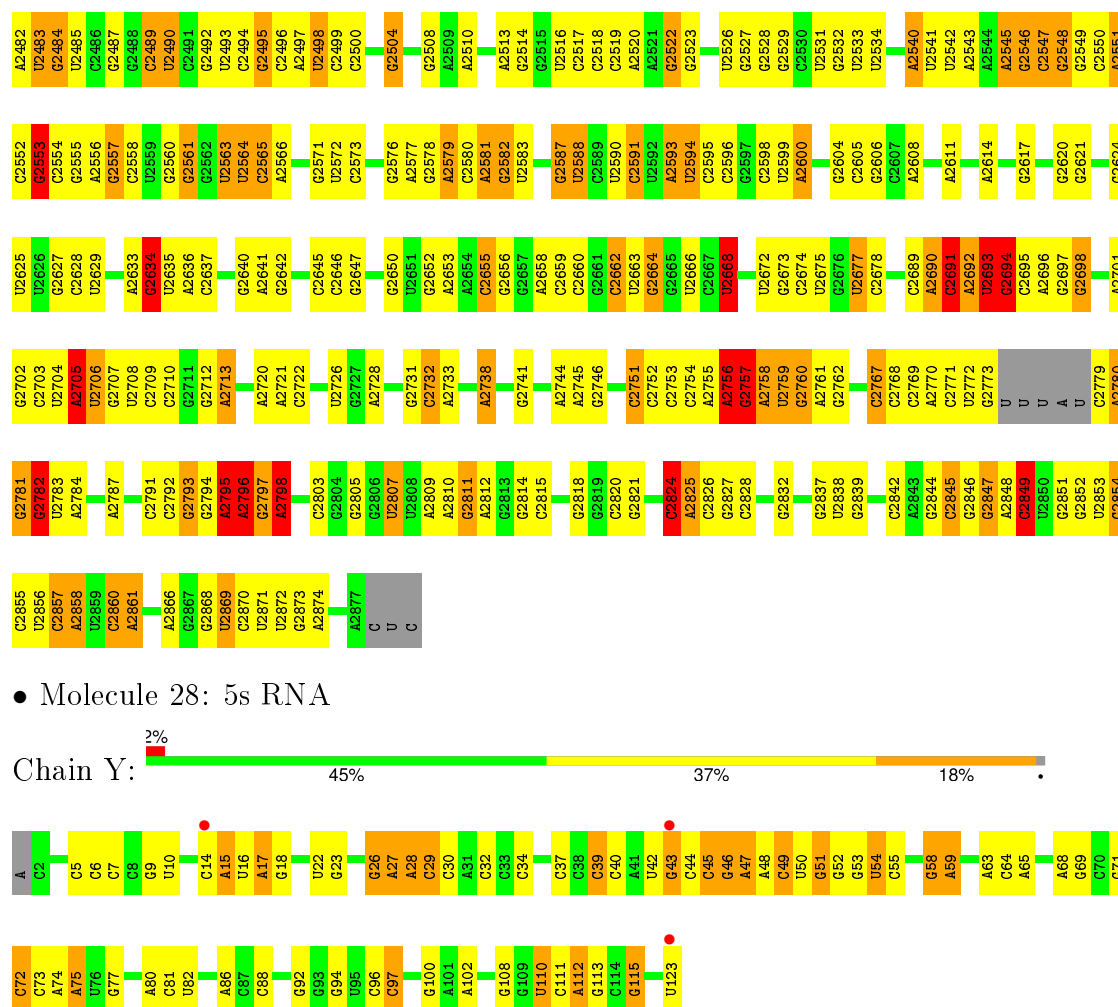
- Molecule 27: 23s RNA











## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.72Å 412.59Å 696.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.65 49.45 – 3.63	Depositor EDS
% Data completeness (in resolution range)	95.9 (19.99-3.65) 95.2 (49.45-3.63)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.226 , 0.270 0.231 , 0.273	Depositor DCC
$R_{free}$ test set	12953 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	108.4	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 17.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 261123 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	83768	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	A	0.44	0/2025	0.71	1/2726 (0.0%)
2	B	0.53	0/1567	0.78	0/2105
3	C	0.45	0/1504	0.70	1/2036 (0.0%)
4	D	0.28	0/1419	0.51	0/1903
5	E	0.30	0/1308	0.51	0/1771
6	G	0.49	0/1138	0.75	1/1539 (0.1%)
7	H	0.53	0/1007	0.75	0/1352
8	I	0.47	0/1022	0.73	0/1366
9	J	0.47	0/1113	0.74	0/1486
10	K	0.61	0/886	0.84	1/1188 (0.1%)
11	L	0.32	0/785	0.59	0/1048
12	M	0.57	0/884	0.86	1/1186 (0.1%)
13	N	0.46	0/994	0.66	0/1323
14	O	0.40	0/750	0.72	0/1000
15	P	0.54	0/1052	0.79	0/1409
16	Q	0.42	0/737	0.70	1/988 (0.1%)
17	R	0.43	0/835	0.73	0/1121
18	S	0.30	0/1370	0.56	0/1862
19	T	0.41	0/563	0.63	0/747
20	U	0.41	0/556	0.66	0/741
21	V	0.34	0/529	0.54	0/704
22	W	0.35	0/426	0.58	0/568
23	Z	0.51	0/455	0.78	0/611
24	1	0.47	0/438	0.71	0/583
25	2	0.43	0/387	0.75	1/509 (0.2%)
26	3	0.49	0/468	0.86	1/614 (0.2%)
27	X	0.59	3/64113 (0.0%)	1.17	296/99999 (0.3%)
28	Y	0.40	0/2907	0.94	2/4529 (0.0%)
All	All	0.55	3/91238 (0.0%)	1.07	306/137014 (0.2%)

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
1	A	0	1
2	B	0	2
6	G	0	4
7	H	0	1
8	I	0	2
10	K	0	1
17	R	0	2
20	U	0	1
26	3	0	1
All	All	0	15

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X	1	G	OP3-P	-10.66	1.48	1.61
27	X	774	A	N7-C5	-6.22	1.35	1.39
27	X	542	A	N9-C4	-5.92	1.34	1.37

All (306) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1468	A	C8-N9-C4	-15.21	99.72	105.80
27	X	774	A	C8-N9-C4	-13.39	100.45	105.80
27	X	774	A	N7-C8-N9	11.68	119.64	113.80
27	X	1333	G	N3-C4-N9	-11.32	119.21	126.00
27	X	1468	A	N7-C8-N9	11.23	119.41	113.80
27	X	537	C	N3-C2-O2	-11.07	114.15	121.90
27	X	540	G	N1-C6-O6	-10.87	113.38	119.90
27	X	1979	C	N3-C2-O2	-9.89	114.98	121.90
27	X	1670	G	C8-N9-C4	9.81	110.32	106.40
27	X	1746	A	O5'-P-OP1	-9.75	96.92	105.70
27	X	1467	U	C4-C5-C6	-9.45	114.03	119.70
27	X	537	C	N1-C2-O2	9.36	124.52	118.90
27	X	1333	G	N3-C4-C5	9.30	133.25	128.60
27	X	1975	G	N3-C4-C5	-9.15	124.03	128.60
27	X	1979	C	N1-C2-O2	8.60	124.06	118.90
27	X	540	G	C5-C6-O6	8.57	133.74	128.60
27	X	2548	G	C5-C6-N1	-8.51	107.25	111.50
27	X	1288	A	O4'-C1'-N9	8.36	114.89	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1670	G	N9-C4-C5	-8.34	102.06	105.40
27	X	2767	C	C6-N1-C2	-8.22	117.01	120.30
27	X	2705	A	N7-C8-N9	8.08	117.84	113.80
27	X	700	C	C6-N1-C2	-8.01	117.10	120.30
27	X	2018	G	C4-C5-N7	7.83	113.93	110.80
27	X	1682	A	N1-C6-N6	7.68	123.21	118.60
27	X	2018	G	O4'-C1'-N9	7.51	114.21	108.20
27	X	1724	C	C6-N1-C2	7.49	123.30	120.30
27	X	2705	A	C5-N7-C8	-7.47	100.17	103.90
27	X	1647	U	N3-C4-C5	-7.44	110.14	114.60
27	X	2634	G	O4'-C1'-N9	7.44	114.15	108.20
27	X	2857	C	C6-N1-C2	-7.42	117.33	120.30
27	X	2845	C	C6-N1-C2	-7.38	117.35	120.30
27	X	1975	G	N3-C4-N9	7.31	130.39	126.00
27	X	774	A	C5-N7-C8	-7.30	100.25	103.90
27	X	955	G	N3-C4-N9	7.26	130.36	126.00
27	X	1467	U	C5-C6-N1	7.22	126.31	122.70
27	X	1979	C	C6-N1-C2	-7.22	117.41	120.30
27	X	2547	C	C6-N1-C2	-7.19	117.42	120.30
27	X	1975	G	N1-C6-O6	-7.12	115.63	119.90
27	X	2470	U	C2-N1-C1'	7.11	126.23	117.70
27	X	661	C	C6-N1-C2	-7.09	117.46	120.30
27	X	2757	G	C8-N9-C4	7.06	109.22	106.40
27	X	2815	C	C6-N1-C2	6.99	123.10	120.30
27	X	2033	C	C6-N1-C2	-6.99	117.50	120.30
27	X	579	G	C4-C5-N7	-6.93	108.03	110.80
27	X	1975	G	P-O3'-C3'	6.85	127.92	119.70
27	X	538	A	C2-N3-C4	6.83	114.02	110.60
27	X	774	A	C6-C5-N7	-6.83	127.52	132.30
27	X	1280	U	O5'-P-OP2	-6.83	99.56	105.70
27	X	2041	A	N1-C6-N6	6.81	122.69	118.60
27	X	2470	U	N1-C2-O2	6.81	127.57	122.80
27	X	2478	C	C6-N1-C2	-6.81	117.58	120.30
27	X	1141	U	P-O3'-C3'	6.77	127.83	119.70
27	X	2798	A	N1-C6-N6	6.74	122.64	118.60
27	X	2547	C	C2-N1-C1'	6.73	126.20	118.80
27	X	1674	C	N3-C4-C5	6.71	124.58	121.90
27	X	2690	A	C2-N3-C4	-6.69	107.25	110.60
27	X	1674	C	N1-C2-O2	6.64	122.88	118.90
27	X	1278	A	C2-N3-C4	-6.64	107.28	110.60
27	X	1468	A	N9-C4-C5	6.62	108.45	105.80
27	X	2228	U	C6-N1-C2	-6.61	117.04	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	540	G	C8-N9-C4	-6.60	103.76	106.40
27	X	2032	G	N3-C4-N9	6.58	129.95	126.00
27	X	2489	C	C6-N1-C2	-6.56	117.68	120.30
27	X	646	C	C6-N1-C2	-6.53	117.69	120.30
27	X	1668	G	N1-C6-O6	6.50	123.80	119.90
27	X	1305	C	C6-N1-C2	6.49	122.90	120.30
27	X	413	G	O4'-C1'-N9	6.48	113.38	108.20
27	X	742	G	C4-N9-C1'	6.47	134.91	126.50
27	X	1992	G	C8-N9-C4	6.46	108.98	106.40
27	X	2705	A	N1-C6-N6	6.40	122.44	118.60
27	X	1627	C	C6-N1-C2	-6.40	117.74	120.30
27	X	955	G	C8-N9-C1'	-6.37	118.72	127.00
27	X	1979	C	C2-N1-C1'	6.36	125.80	118.80
27	X	413	G	N3-C4-C5	-6.36	125.42	128.60
27	X	742	G	N3-C4-N9	6.35	129.81	126.00
27	X	2705	A	P-O3'-C3'	6.35	127.32	119.70
27	X	938	G	N3-C4-C5	-6.34	125.43	128.60
27	X	742	G	N3-C4-C5	-6.34	125.43	128.60
27	X	2404	A	P-O3'-C3'	6.33	127.30	119.70
27	X	853	C	C6-N1-C2	6.33	122.83	120.30
27	X	1770	U	C5-C6-N1	-6.32	119.54	122.70
27	X	2495	G	C8-N9-C4	-6.31	103.88	106.40
27	X	2329	C	C5-C6-N1	6.31	124.15	121.00
27	X	2023	C	C6-N1-C2	6.29	122.82	120.30
27	X	346	C	C6-N1-C2	-6.29	117.78	120.30
27	X	1647	U	N3-C4-O4	6.28	123.80	119.40
27	X	985	G	C8-N9-C4	-6.26	103.90	106.40
27	X	2427	A	N1-C6-N6	6.26	122.36	118.60
27	X	2478	C	C5-C6-N1	6.25	124.13	121.00
27	X	2015	G	C4-C5-C6	-6.25	115.05	118.80
27	X	1633	C	C2-N1-C1'	-6.24	111.94	118.80
27	X	2664	G	N3-C2-N2	-6.24	115.53	119.90
27	X	2540	A	O4'-C1'-N9	6.24	113.19	108.20
27	X	542	A	C2-N3-C4	-6.22	107.49	110.60
27	X	2691	C	O5'-P-OP2	-6.22	100.10	105.70
27	X	955	G	C4-N9-C1'	6.19	134.55	126.50
27	X	2705	A	C2-N3-C4	-6.17	107.52	110.60
27	X	462	G	C8-N9-C4	6.14	108.86	106.40
27	X	579	G	N3-C4-C5	-6.13	125.54	128.60
27	X	2579	A	C8-N9-C4	6.12	108.25	105.80
27	X	928	G	C5-C6-O6	-6.12	124.93	128.60
27	X	2479	U	C5-C6-N1	6.10	125.75	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	2490	U	N3-C2-O2	-6.10	117.93	122.20
27	X	1326	U	N3-C2-O2	-6.09	117.94	122.20
27	X	2798	A	N9-C4-C5	-6.09	103.36	105.80
27	X	2647	G	N3-C4-C5	6.07	131.63	128.60
27	X	699	G	N3-C4-C5	6.06	131.63	128.60
27	X	343	A	N7-C8-N9	6.04	116.82	113.80
27	X	2470	U	N3-C2-O2	-6.02	117.99	122.20
27	X	1664	G	O5'-P-OP1	-6.01	100.29	105.70
27	X	1031	C	P-O3'-C3'	6.01	126.91	119.70
27	X	1206	G	C5-C6-N1	-6.00	108.50	111.50
27	X	955	G	N3-C4-C5	-5.99	125.60	128.60
27	X	2228	U	N3-C4-C5	-5.99	111.01	114.60
27	X	1326	U	C2-N1-C1'	5.98	124.87	117.70
27	X	2018	G	C4-N9-C1'	5.96	134.25	126.50
27	X	1681	A	O5'-P-OP1	-5.96	100.34	105.70
6	G	106	TYR	N-CA-C	-5.95	94.93	111.00
27	X	2495	G	N3-C4-C5	-5.92	125.64	128.60
27	X	2795	A	P-O3'-C3'	5.91	126.79	119.70
27	X	1919	A	C2-N3-C4	-5.91	107.65	110.60
27	X	2701	A	C2-N3-C4	-5.89	107.65	110.60
10	K	92	GLY	N-CA-C	-5.88	98.39	113.10
27	X	617	U	N3-C2-O2	-5.88	118.08	122.20
27	X	1315	A	N1-C6-N6	-5.88	115.07	118.60
27	X	1923	U	P-O3'-C3'	5.86	126.73	119.70
27	X	2647	G	N3-C4-N9	-5.83	122.50	126.00
27	X	556	A	N1-C6-N6	5.83	122.10	118.60
27	X	1682	A	C4-C5-C6	5.83	119.91	117.00
27	X	2647	G	C4-N9-C1'	-5.83	118.93	126.50
27	X	540	G	N9-C4-C5	5.82	107.73	105.40
27	X	2018	G	C5-N7-C8	-5.81	101.39	104.30
27	X	1391	A	P-O3'-C3'	5.80	126.66	119.70
27	X	2796	A	N1-C6-N6	-5.79	115.13	118.60
27	X	334	G	P-O3'-C3'	5.78	126.64	119.70
27	X	1682	A	C6-C5-N7	-5.78	128.25	132.30
12	M	103	LYS	N-CA-C	5.78	126.59	111.00
27	X	1240	G	N1-C6-O6	5.77	123.36	119.90
27	X	1332	G	N1-C6-O6	5.77	123.36	119.90
27	X	1469	U	N3-C2-O2	-5.75	118.17	122.20
27	X	2677	U	C5-C4-O4	5.75	129.35	125.90
27	X	2553	G	N3-C4-N9	-5.74	122.56	126.00
27	X	742	G	C8-N9-C1'	-5.74	119.54	127.00
27	X	1468	A	N1-C6-N6	-5.73	115.16	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	577	U	N3-C4-C5	-5.72	111.17	114.60
27	X	635	C	C6-N1-C2	-5.71	118.02	120.30
27	X	1670	G	N3-C2-N2	5.70	123.89	119.90
27	X	413	G	C2-N3-C4	5.70	114.75	111.90
27	X	2490	U	C6-N1-C2	-5.70	117.58	121.00
27	X	16	G	C8-N9-C4	5.69	108.67	106.40
27	X	2018	G	C6-C5-N7	-5.68	126.99	130.40
27	X	2499	C	C5-C6-N1	5.67	123.83	121.00
27	X	957	G	N3-C4-C5	-5.67	125.77	128.60
27	X	661	C	C5-C6-N1	5.66	123.83	121.00
27	X	522	G	O4'-C1'-N9	5.65	112.72	108.20
27	X	1278	A	C5-C6-N6	5.64	128.21	123.70
27	X	2371	A	N7-C8-N9	5.64	116.62	113.80
27	X	1467	U	N1-C2-N3	-5.62	111.53	114.90
27	X	774	A	C2-N3-C4	-5.61	107.79	110.60
27	X	1982	C	C5-C6-N1	-5.61	118.19	121.00
27	X	2849	C	N3-C2-O2	-5.61	117.97	121.90
27	X	1466	C	C6-N1-C2	-5.61	118.06	120.30
27	X	2015	G	C4-N9-C1'	-5.61	119.21	126.50
27	X	1469	U	O4'-C1'-N1	5.60	112.68	108.20
27	X	2553	G	N3-C4-C5	5.60	131.40	128.60
27	X	1266	G	N3-C4-N9	-5.60	122.64	126.00
27	X	2793	G	C8-N9-C4	5.60	108.64	106.40
27	X	594	G	N1-C6-O6	-5.59	116.54	119.90
27	X	393	U	N3-C4-O4	5.59	123.31	119.40
27	X	2553	G	N1-C6-O6	5.59	123.25	119.90
27	X	2705	A	C8-N9-C4	-5.55	103.58	105.80
27	X	1973	C	C6-N1-C2	-5.55	118.08	120.30
27	X	1996	A	C8-N9-C4	5.55	108.02	105.80
27	X	2705	A	C6-C5-N7	-5.55	128.42	132.30
27	X	2662	C	C6-N1-C2	-5.54	118.08	120.30
27	X	617	U	C4-C5-C6	5.54	123.02	119.70
27	X	1677	C	O5'-P-OP2	-5.53	100.72	105.70
27	X	2371	A	C8-N9-C4	-5.53	103.59	105.80
27	X	816	U	N3-C2-O2	-5.53	118.33	122.20
27	X	2039	G	C8-N9-C4	-5.52	104.19	106.40
27	X	2705	A	C4-C5-N7	5.52	113.46	110.70
27	X	2036	G	N1-C6-O6	5.51	123.21	119.90
27	X	537	C	C6-N1-C2	-5.51	118.10	120.30
27	X	1683	G	C8-N9-C1'	5.51	134.16	127.00
27	X	343	A	O5'-P-OP1	-5.51	100.74	105.70
27	X	1975	G	N1-C2-N2	-5.50	111.25	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	2553	G	N3-C2-N2	-5.50	116.05	119.90
27	X	938	G	N3-C4-N9	5.50	129.30	126.00
27	X	1661	C	N3-C2-O2	-5.50	118.05	121.90
27	X	2797	G	N3-C4-N9	5.49	129.29	126.00
27	X	559	C	C6-N1-C2	-5.49	118.10	120.30
27	X	2757	G	N7-C8-N9	-5.49	110.36	113.10
27	X	236	C	C6-N1-C2	-5.48	118.11	120.30
27	X	434	C	P-O3'-C3'	5.47	126.27	119.70
27	X	2018	G	C8-N9-C1'	-5.47	119.89	127.00
27	X	1286	U	N3-C2-O2	-5.45	118.38	122.20
27	X	2634	G	C4-N9-C1'	-5.45	119.42	126.50
27	X	393	U	N3-C4-C5	-5.45	111.33	114.60
27	X	955	G	O4'-C1'-N9	5.44	112.56	108.20
27	X	2541	U	N3-C2-O2	-5.44	118.39	122.20
27	X	579	G	C5-C6-O6	5.44	131.86	128.60
27	X	1333	G	C2-N3-C4	-5.44	109.18	111.90
27	X	2751	C	C6-N1-C2	5.43	122.47	120.30
27	X	2668	U	C5-C4-O4	5.41	129.15	125.90
27	X	2693	U	C2-N1-C1'	-5.40	111.22	117.70
27	X	2015	G	C8-N9-C1'	5.38	133.99	127.00
27	X	2793	G	N7-C8-N9	-5.38	110.41	113.10
27	X	1674	C	N3-C2-O2	-5.37	118.14	121.90
27	X	2049	C	C6-N1-C2	-5.37	118.15	120.30
27	X	2547	C	C5-C6-N1	5.37	123.68	121.00
27	X	1333	G	N9-C4-C5	5.36	107.55	105.40
27	X	1468	A	N3-C4-C5	-5.35	123.06	126.80
16	Q	61	LYS	N-CA-C	5.35	125.44	111.00
27	X	985	G	N7-C8-N9	5.34	115.77	113.10
27	X	1712	G	C4-N9-C1'	5.32	133.42	126.50
27	X	1326	U	N1-C2-O2	5.32	126.53	122.80
27	X	2422	C	C6-N1-C2	-5.32	118.17	120.30
27	X	1812	U	C2-N1-C1'	5.32	124.08	117.70
27	X	841	G	N7-C8-N9	5.32	115.76	113.10
27	X	1647	U	C6-N1-C2	-5.32	117.81	121.00
27	X	1950	C	C6-N1-C2	-5.31	118.17	120.30
27	X	1975	G	C4-N9-C1'	5.31	133.40	126.50
27	X	1982	C	C2-N3-C4	-5.31	117.25	119.90
27	X	2694	G	OP2-P-O3'	5.31	116.88	105.20
27	X	2702	G	C8-N9-C1'	-5.30	120.10	127.00
27	X	2547	C	N3-C2-O2	-5.30	118.19	121.90
27	X	2018	G	O5'-P-OP2	-5.30	100.93	105.70
27	X	2427	A	C6-C5-N7	-5.29	128.60	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	788	G	P-O3'-C3'	5.29	126.04	119.70
27	X	343	A	C8-N9-C4	-5.29	103.69	105.80
27	X	2655	C	C6-N1-C2	5.29	122.41	120.30
27	X	1266	G	C8-N9-C1'	5.28	133.86	127.00
27	X	2782	G	N1-C6-O6	5.27	123.06	119.90
27	X	1668	G	C4-C5-N7	5.27	112.91	110.80
27	X	522	G	N1-C6-O6	-5.26	116.74	119.90
27	X	2797	G	C4-N9-C1'	5.26	133.33	126.50
27	X	798	G	O5'-P-OP1	-5.23	100.99	105.70
27	X	2664	G	C4-N9-C1'	-5.23	119.71	126.50
27	X	413	G	N1-C6-O6	-5.23	116.76	119.90
27	X	1745	C	O5'-P-OP2	-5.22	101.00	105.70
27	X	1934	U	C6-N1-C2	-5.21	117.88	121.00
27	X	757	U	N1-C2-N3	5.20	118.02	114.90
27	X	1313	U	P-O3'-C3'	5.20	125.94	119.70
27	X	1240	G	C8-N9-C1'	-5.19	120.26	127.00
27	X	1683	G	N3-C4-N9	-5.18	122.89	126.00
27	X	841	G	C8-N9-C4	-5.17	104.33	106.40
25	2	38	GLY	N-CA-C	-5.16	100.19	113.10
27	X	1992	G	N7-C8-N9	-5.16	110.52	113.10
27	X	1716	G	C8-N9-C4	-5.16	104.34	106.40
27	X	2587	G	C6-C5-N7	-5.16	127.31	130.40
27	X	2432	A	N1-C2-N3	-5.15	126.73	129.30
27	X	2018	G	N9-C1'-C2'	5.13	120.67	114.00
27	X	580	A	N1-C6-N6	5.13	121.68	118.60
27	X	542	A	N1-C6-N6	5.13	121.68	118.60
27	X	843	G	C5-C6-O6	-5.13	125.52	128.60
27	X	2590	U	C2-N1-C1'	5.13	123.85	117.70
27	X	462	G	C5-C6-N1	-5.12	108.94	111.50
27	X	1574	A	O5'-P-OP1	5.12	116.84	110.70
27	X	2015	G	C5-N7-C8	-5.12	101.74	104.30
27	X	2756	A	P-O3'-C3'	5.12	125.84	119.70
27	X	1240	G	C6-C5-N7	-5.11	127.33	130.40
27	X	537	C	C2-N1-C1'	5.11	124.42	118.80
27	X	1668	G	C6-C5-N7	-5.11	127.33	130.40
28	Y	39	C	C2-N1-C1'	5.11	124.42	118.80
27	X	2251	U	N3-C4-C5	5.11	117.66	114.60
27	X	2702	G	C4-N9-C1'	5.11	133.14	126.50
27	X	2018	G	N7-C8-N9	5.10	115.65	113.10
27	X	985	G	C5-N7-C8	-5.10	101.75	104.30
27	X	1991	C	N3-C4-C5	5.09	123.94	121.90
27	X	1315	A	C5-C6-N6	5.09	127.77	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	123	A	P-O3'-C3'	5.08	125.80	119.70
27	X	2600	A	N1-C6-N6	-5.08	115.55	118.60
27	X	1633	C	N1-C2-O2	-5.08	115.85	118.90
27	X	2854	G	C4-C5-N7	5.08	112.83	110.80
27	X	1747	G	C2-N3-C4	5.08	114.44	111.90
27	X	1663	C	OP1-P-O3'	5.08	116.37	105.20
27	X	1467	U	N3-C4-C5	5.07	117.64	114.60
27	X	2470	U	C6-N1-C1'	-5.07	114.10	121.20
27	X	2563	U	C2-N1-C1'	5.07	123.79	117.70
27	X	2495	G	C6-N1-C2	-5.07	122.06	125.10
27	X	2490	U	OP1-P-O3'	5.06	116.33	105.20
27	X	993	C	N1-C2-O2	5.05	121.93	118.90
26	3	24	ALA	N-CA-C	-5.05	97.36	111.00
27	X	1270	C	N3-C4-C5	-5.05	119.88	121.90
27	X	1965	U	C2-N1-C1'	5.05	123.76	117.70
27	X	1278	A	N1-C2-N3	5.05	131.82	129.30
27	X	2705	A	C5-C6-N1	-5.05	115.17	117.70
27	X	1663	C	N1-C2-O2	5.05	121.93	118.90
27	X	2565	C	OP1-P-O3'	5.05	116.30	105.20
27	X	1247	U	N3-C2-O2	-5.04	118.67	122.20
27	X	1664	G	N3-C4-C5	5.03	131.12	128.60
27	X	1685	A	N1-C6-N6	-5.03	115.58	118.60
27	X	1469	U	C5-C4-O4	5.03	128.92	125.90
28	Y	88	C	N1-C2-O2	5.03	121.92	118.90
27	X	1634	A	N1-C6-N6	-5.03	115.58	118.60
27	X	413	G	N3-C4-N9	5.02	129.01	126.00
27	X	542	A	N3-C4-C5	5.02	130.31	126.80
27	X	823	U	C2-N1-C1'	5.02	123.72	117.70
27	X	2647	G	C8-N9-C1'	5.02	133.53	127.00
1	A	18	THR	N-CA-C	5.02	124.54	111.00
27	X	1337	G	O4'-C1'-N9	5.02	112.21	108.20
27	X	1683	G	O4'-C1'-N9	5.01	112.21	108.20
27	X	2824	C	P-O3'-C3'	5.01	125.71	119.70
27	X	2590	U	C6-N1-C2	-5.01	118.00	121.00
3	C	56	ARG	N-CA-C	5.00	124.51	111.00
27	X	2045	A	C8-N9-C4	-5.00	103.80	105.80

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	3	27	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	18	THR	Peptide
2	B	122	PHE	Peptide
2	B	146	THR	Peptide
6	G	108	GLY	Peptide
6	G	111	LYS	Peptide
6	G	120	SER	Peptide
6	G	34	PRO	Peptide
7	H	26	ASN	Peptide
8	I	35	LYS	Peptide
8	I	40	ARG	Peptide
10	K	93	GLY	Peptide
17	R	60	PRO	Peptide
17	R	65	PRO	Peptide
20	U	30	VAL	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1987	0	2056	130	0
2	B	1539	0	1600	101	0
3	C	1481	0	1504	101	0
4	D	1400	0	1481	62	0
5	E	1286	0	1336	35	0
6	G	1114	0	1144	63	0
7	H	997	0	1046	63	0
8	I	1011	0	1047	54	0
9	J	1090	0	1125	56	0
10	K	878	0	930	37	0
11	L	779	0	820	40	0
12	M	871	0	894	49	0
13	N	978	0	1020	72	0
14	O	741	0	756	46	0
15	P	1038	0	1125	78	0
16	Q	726	0	753	35	0
17	R	825	0	881	51	0
18	S	1345	0	1372	41	0
19	T	556	0	579	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	U	552	0	604	29	0
21	V	525	0	546	14	0
22	W	424	0	470	15	0
23	Z	443	0	444	27	0
24	1	431	0	456	30	0
25	2	383	0	414	27	0
26	3	462	0	506	52	0
27	X	57254	0	28850	1328	0
28	Y	2601	0	1327	54	0
29	K	1	0	0	0	0
29	X	50	0	0	0	0
All	All	83768	0	55086	2361	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 (2361) 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:A:55:GLY:H	1:A:217:ARG:HB2	1.20	1.04
2:B:136:ARG:HB3	27:X:1673:C:H5'	1.36	1.04
27:X:571:U:HO2'	27:X:581:A:H8	1.12	0.98
27:X:517:A:H5''	27:X:518:A:H5'	1.45	0.95
2:B:116:VAL:HG22	2:B:136:ARG:HG3	1.49	0.95
3:C:163:ASN:HD21	3:C:167:VAL:H	1.15	0.93
23:Z:19:ARG:NH2	27:X:1277:G:OP1	2.02	0.91
27:X:1542:G:H22	27:X:1562:G:H1	1.12	0.91
2:B:133:LYS:HB2	2:B:137:ARG:HG2	1.55	0.89
7:H:25:LEU:HD11	7:H:52:VAL:HG23	1.53	0.89
27:X:833:A:N3	27:X:954:U:O2'	2.05	0.89
1:A:252:LYS:HZ2	1:A:252:LYS:H	1.20	0.86
25:2:12:ARG:HG2	27:X:699:G:H1	1.40	0.85
13:N:5:LYS:HG3	13:N:7:GLY:H	1.39	0.84
8:I:38:LYS:NZ	27:X:954:U:OP2	2.10	0.84
8:I:62:LYS:HB3	26:3:12:ARG:HA	1.57	0.84
1:A:250:TRP:O	1:A:255:LYS:NZ	2.09	0.84
27:X:2757:G:H5''	27:X:2758:A:H5'	1.58	0.82
27:X:2510:A:H61	27:X:2641:A:H61	1.28	0.82
1:A:43:ARG:NH1	27:X:705:C:OP1	2.13	0.82
3:C:46:ARG:NH1	27:X:463:C:OP1	2.13	0.82
27:X:854:G:H1	27:X:948:C:H42	1.26	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1850:G:O2'	27:X:1867:A:N6	2.14	0.81
6:G:74:MET:HA	6:G:140:GLN:HE22	1.45	0.81
27:X:1202:U:H2'	27:X:1203:A:H8	1.45	0.81
27:X:1562:G:H5'	27:X:1563:U:H5'	1.62	0.80
27:X:320:A:N3	27:X:340:G:O2'	2.13	0.80
14:O:57:GLN:H	14:O:97:GLY:HA3	1.44	0.80
27:X:123:A:O2'	27:X:124:A:OP1	1.99	0.80
25:2:19:ARG:HG2	27:X:123:A:H5''	1.63	0.80
6:G:34:PRO:HB3	6:G:69:ASP:HB3	1.64	0.79
20:U:8:THR:HA	20:U:14:VAL:HG21	1.61	0.79
27:X:538:A:O2'	27:X:539:A:O5'	1.99	0.79
15:P:122:LYS:NZ	27:X:1279:G:O6	2.13	0.79
12:M:41:GLU:HG3	12:M:46:ARG:HD2	1.63	0.79
20:U:50:ALA:HB3	20:U:62:LEU:HB2	1.65	0.79
27:X:1030:U:H3	27:X:1153:A:H62	1.27	0.79
2:B:118:LYS:NZ	27:X:2704:U:OP1	2.14	0.79
27:X:841:G:H2'	27:X:842:A:C8	2.18	0.79
22:W:5:LEU:HB2	22:W:25:LEU:HD13	1.63	0.79
1:A:28:ARG:HD3	27:X:1583:A:H62	1.46	0.79
3:C:161:ALA:HB1	3:C:167:VAL:HG21	1.63	0.78
27:X:1963:G:O2'	27:X:1965:U:OP2	2.00	0.78
27:X:2551:A:H5'	27:X:2553:G:H4'	1.64	0.78
2:B:189:PRO:HA	27:X:2659:C:H5'	1.63	0.78
13:N:66:ASN:HB3	13:N:76:TYR:HB2	1.65	0.78
2:B:174:GLU:HB3	2:B:183:LEU:HD12	1.66	0.78
22:W:8:SER:HB2	27:X:999:A:H5''	1.65	0.78
15:P:97:VAL:HG13	15:P:125:SER:HB2	1.65	0.78
2:B:137:ARG:NH2	27:X:2034:A:OP1	2.17	0.77
18:S:47:SER:OG	18:S:48:THR:N	2.17	0.77
27:X:2016:A:O2'	27:X:2018:G:OP2	2.01	0.77
7:H:40:GLY:HA3	27:X:2545:A:H61	1.47	0.77
2:B:10:GLY:HA3	12:M:13:LEU:HD21	1.66	0.77
25:2:34:ARG:HD2	25:2:40:HIS:HB3	1.65	0.77
1:A:79:VAL:HB	1:A:114:GLY:H	1.48	0.77
17:R:56:LYS:HB3	17:R:69:GLN:HG2	1.66	0.77
27:X:864:C:O2	27:X:940:G:N2	2.18	0.77
3:C:5:ASN:N	3:C:5:ASN:OD1	2.18	0.77
1:A:17:THR:O	1:A:19:ALA:HA	1.83	0.77
27:X:2447:G:HO2'	27:X:2448:A:H8	1.34	0.76
1:A:244:ARG:HH12	27:X:1834:G:H1'	1.50	0.76
27:X:2557:G:OP1	27:X:2593:A:N6	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:HE	1:A:27:LYS:HB3	1.49	0.75
7:H:62:GLY:O	7:H:65:LYS:NZ	2.12	0.75
27:X:2327:U:O4	27:X:2361:G:N2	2.19	0.75
23:Z:4:HIS:O	27:X:2039:G:N2	2.18	0.75
7:H:123:PHE:HB3	7:H:126:ILE:HG13	1.68	0.74
27:X:2818:G:H1	27:X:2849:C:H42	1.35	0.74
12:M:34:ARG:NH2	12:M:90:GLN:O	2.16	0.74
27:X:1856:U:OP1	27:X:2389:G:O2'	2.05	0.74
4:D:62:LEU:O	4:D:95:ARG:NH1	2.20	0.74
3:C:74:VAL:HG23	3:C:76:THR:H	1.50	0.74
4:D:75:SER:H	4:D:79:LEU:HD13	1.50	0.74
15:P:124:THR:HG21	15:P:126:HIS:CD2	2.23	0.74
3:C:162:ARG:O	3:C:162:ARG:NH1	2.19	0.74
15:P:34:SER:OG	15:P:122:LYS:NZ	2.20	0.74
27:X:793:G:H21	27:X:796:A:H62	1.34	0.74
4:D:116:GLY:HA2	4:D:176:PRO:HB2	1.70	0.74
27:X:421:G:H22	27:X:433:G:H1'	1.51	0.74
3:C:68:ARG:HH12	27:X:2043:A:H62	1.33	0.74
23:Z:9:LYS:NZ	27:X:2001:G:OP1	2.19	0.74
27:X:2543:A:OP1	27:X:2627:G:O2'	2.04	0.74
8:I:41:SER:HB2	27:X:844:G:H5''	1.69	0.74
27:X:872:G:O2'	27:X:928:G:O6	2.06	0.74
26:3:42:ARG:NE	27:X:2328:G:OP1	2.21	0.73
27:X:1465:G:H22	27:X:1476:G:H1	1.37	0.73
26:3:32:GLN:NE2	27:X:2371:A:OP2	2.16	0.73
6:G:157:PRO:O	6:G:161:GLN:NE2	2.20	0.73
27:X:304:A:N7	27:X:356:A:N6	2.36	0.73
6:G:140:GLN:HG3	27:X:567:G:H5'	1.71	0.72
27:X:2451:G:O2'	27:X:2457:A:N6	2.22	0.72
27:X:649:G:H22	27:X:661:C:H1'	1.53	0.72
24:1:30:ASN:ND2	27:X:2264:C:OP2	2.22	0.72
4:D:115:ARG:HD2	4:D:178:ARG:HH22	1.53	0.72
27:X:412:U:H2'	27:X:413:G:H5'	1.69	0.72
27:X:1466:C:H2'	27:X:1467:U:O4'	1.89	0.72
3:C:136:TRP:O	3:C:140:ASN:ND2	2.23	0.72
27:X:203:G:O2'	27:X:205:A:N1	2.22	0.72
27:X:200:A:HO2'	27:X:433:G:HO2'	1.37	0.72
27:X:168:A:H2'	27:X:169:C:C6	2.25	0.72
27:X:2811:G:H2'	27:X:2812:A:C8	2.25	0.72
26:3:13:ARG:HE	26:3:25:PHE:H	1.37	0.71
3:C:162:ARG:HE	27:X:333:A:H5''	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:7:C:O2'	28:Y:29:C:O2	2.07	0.71
27:X:1412:C:O2'	27:X:1413:U:O5'	2.07	0.71
27:X:825:C:HO2'	27:X:1239:A:HO2'	1.37	0.71
4:D:123:ASP:HB3	4:D:127:ASN:H	1.55	0.71
2:B:50:GLY:HA3	2:B:75:THR:HG21	1.72	0.71
3:C:83:ALA:HB3	27:X:595:A:H5'	1.72	0.71
27:X:1223:G:H5'	27:X:1225:G:O4'	1.91	0.71
27:X:215:G:H21	27:X:632:A:H8	1.37	0.71
5:E:160:LYS:HZ1	27:X:2637:C:H5'	1.56	0.71
1:A:233:HIS:NE2	1:A:245:VAL:O	2.24	0.71
26:3:52:LYS:NZ	27:X:2338:C:O2'	2.17	0.71
24:1:28:ARG:NH1	27:X:2264:C:OP2	2.24	0.71
12:M:100:ARG:HD2	27:X:1744:G:OP1	1.90	0.71
27:X:1073:G:H22	27:X:1087:C:H42	1.39	0.71
27:X:2081:U:H3	27:X:2174:G:H1	1.39	0.71
27:X:552:C:H2'	27:X:553:C:H5''	1.71	0.70
15:P:35:PRO:HA	15:P:125:SER:HB3	1.73	0.70
1:A:89:SER:O	1:A:198:ASN:ND2	2.22	0.70
13:N:84:LYS:HB2	13:N:92:ARG:HH22	1.56	0.70
4:D:78:LYS:HG2	4:D:80:ARG:HH11	1.57	0.70
16:Q:31:PRO:HA	16:Q:76:LYS:HD3	1.73	0.70
7:H:3:MET:HE1	27:X:1683:G:H21	1.54	0.70
27:X:689:A:H8	27:X:2052:G:H21	1.40	0.70
19:T:51:VAL:HG21	19:T:79:ILE:HG22	1.74	0.70
1:A:52:ARG:HD3	27:X:1816:G:OP1	1.91	0.70
1:A:143:HIS:ND1	1:A:194:GLY:O	2.22	0.70
1:A:24:LEU:HB2	1:A:205:VAL:HG22	1.74	0.70
27:X:1109:A:H3'	27:X:1110:G:H8	1.55	0.70
27:X:1398:G:O2'	27:X:1399:C:O4'	2.10	0.70
8:I:40:ARG:NH2	27:X:820:U:OP1	2.25	0.70
11:L:38:ILE:HD11	11:L:40:ALA:HB2	1.74	0.69
6:G:103:TYR:CG	6:G:111:LYS:HB2	2.27	0.69
18:S:93:GLU:HG2	18:S:123:VAL:HG13	1.74	0.69
15:P:27:VAL:HG13	27:X:504:G:H4'	1.74	0.69
27:X:2371:A:H2	27:X:2403:C:H42	1.39	0.69
3:C:54:THR:HG21	3:C:72:ARG:HB3	1.74	0.69
1:A:244:ARG:O	1:A:252:LYS:NZ	2.23	0.69
27:X:2757:G:OP2	27:X:2761:A:O2'	2.07	0.69
24:1:42:PRO:O	24:1:46:LYS:NZ	2.25	0.69
16:Q:43:GLN:HE21	16:Q:50:VAL:H	1.38	0.69
1:A:158:SER:HB2	27:X:1810:U:H5''	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2796:A:H2'	27:X:2797:G:H8	1.56	0.69
27:X:2605:C:H2'	27:X:2606:G:H8	1.58	0.69
12:M:104:LEU:HA	12:M:106:TYR:CE2	2.27	0.69
1:A:157:ARG:NH1	27:X:1810:U:OP2	2.25	0.69
8:I:65:PHE:HB2	27:X:2394:G:H4'	1.72	0.69
3:C:45:THR:OG1	3:C:86:PRO:O	2.10	0.69
8:I:94:GLU:OE1	8:I:97:ARG:NH1	2.25	0.69
3:C:176:ASN:HB3	3:C:179:ASP:HB2	1.73	0.69
4:D:133:LYS:HD3	27:X:2284:U:H4'	1.74	0.69
18:S:125:PRO:O	18:S:129:ARG:NH1	2.25	0.69
3:C:144:GLY:HA3	3:C:166:TRP:CD1	2.27	0.69
27:X:1336:G:H2'	27:X:1337:G:H5'	1.74	0.69
27:X:1975:G:H22	27:X:1979:C:H6	1.40	0.69
27:X:1769:U:H2'	27:X:1775:A:H62	1.57	0.69
27:X:2378:G:H1	27:X:2396:C:H42	1.40	0.69
26:3:46:LYS:HD2	27:X:659:G:H1'	1.75	0.68
25:2:39:ARG:O	25:2:41:GLN:NE2	2.26	0.68
15:P:104:LYS:HZ2	15:P:104:LYS:HA	1.58	0.68
27:X:1533:G:H2'	27:X:1534:A:H8	1.56	0.68
27:X:1733:U:OP2	27:X:1735:G:N2	2.25	0.68
17:R:105:ARG:NH2	17:R:106:VAL:O	2.26	0.68
25:2:7:PRO:HB2	27:X:1322:G:H4'	1.76	0.68
1:A:252:LYS:N	1:A:252:LYS:HZ2	1.92	0.68
27:X:2199:C:H2'	27:X:2200:G:H8	1.58	0.68
2:B:140:SER:HB3	27:X:2554:C:O2'	1.93	0.68
28:Y:26:G:N2	28:Y:30:C:N3	2.42	0.68
2:B:26:VAL:HG11	2:B:198:LEU:HD21	1.76	0.68
27:X:588:G:O2'	27:X:2002:A:OP1	2.12	0.68
17:R:61:SER:HA	17:R:65:PRO:HB3	1.75	0.68
12:M:32:THR:O	12:M:51:GLU:HA	1.94	0.68
27:X:2298:U:O2	27:X:2299:A:N6	2.26	0.68
27:X:661:C:H2'	27:X:662:G:H8	1.58	0.68
2:B:34:VAL:HG12	2:B:72:VAL:HG21	1.76	0.68
3:C:48:ARG:HB2	3:C:51:VAL:HG22	1.75	0.68
27:X:1065:A:H2'	27:X:1066:G:H8	1.58	0.68
1:A:48:ARG:H	1:A:48:ARG:HD2	1.58	0.68
13:N:13:ARG:NH2	27:X:1264:C:OP1	2.27	0.68
27:X:812:G:H3'	27:X:813:A:H2'	1.75	0.68
22:W:3:ILE:HD11	22:W:44:VAL:HG11	1.76	0.68
27:X:537:C:H1'	27:X:538:A:C6	2.28	0.67
1:A:28:ARG:HD3	27:X:1583:A:N6	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:132:PHE:CZ	6:G:145:HIS:HB2	2.30	0.67
2:B:48:GLN:NE2	27:X:2614:A:O2'	2.27	0.67
8:I:53:ARG:HD2	8:I:54:SER:HB3	1.75	0.67
10:K:79:VAL:HA	10:K:83:VAL:HB	1.76	0.67
6:G:58:ILE:HG12	6:G:80:VAL:HG11	1.76	0.67
3:C:137:ALA:HB1	3:C:142:LEU:HB2	1.76	0.67
6:G:43:VAL:HG21	6:G:158:HIS:HE1	1.59	0.67
14:O:38:LEU:HD23	14:O:47:PHE:HA	1.77	0.67
27:X:2546:G:H2'	27:X:2547:C:C6	2.30	0.67
4:D:16:LEU:O	4:D:20:PHE:N	2.28	0.67
1:A:68:LYS:H	1:A:68:LYS:HD3	1.60	0.67
3:C:45:THR:HG21	3:C:85:GLY:HA3	1.77	0.67
3:C:59:TYR:OH	3:C:67:ALA:HB3	1.95	0.67
4:D:64:LYS:O	28:Y:44:C:O2'	2.12	0.67
15:P:71:VAL:HG12	15:P:129:ILE:HD12	1.76	0.67
1:A:158:SER:O	1:A:196:VAL:HG21	1.95	0.67
24:1:27:ASN:ND2	24:1:36:GLU:OE2	2.28	0.66
28:Y:64:C:H2'	28:Y:65:A:H8	1.58	0.66
27:X:1882:G:H21	27:X:1885:C:N4	1.94	0.66
27:X:712:A:H2'	27:X:713:G:O4'	1.96	0.66
4:D:60:ILE:HG13	4:D:61:THR:HG23	1.78	0.66
20:U:31:GLY:H	20:U:32:ARG:NH1	1.93	0.66
19:T:23:VAL:HG13	19:T:38:VAL:HG22	1.78	0.66
27:X:820:U:H2'	27:X:821:A:H8	1.59	0.66
13:N:37:GLN:HG3	27:X:1265:G:H1	1.58	0.66
16:Q:2:SER:N	16:Q:5:ASP:OD2	2.28	0.66
1:A:218:LYS:NZ	1:A:219:PRO:O	2.20	0.66
16:Q:60:GLY:HA3	16:Q:72:ARG:HA	1.77	0.66
2:B:108:SER:HB3	2:B:163:GLU:H	1.61	0.66
6:G:34:PRO:HB3	6:G:69:ASP:CB	2.26	0.66
18:S:19:ILE:HD11	18:S:36:ARG:HD3	1.78	0.66
27:X:1350:G:H2'	27:X:1351:G:H8	1.60	0.66
23:Z:31:THR:OG1	27:X:2861:A:O2'	2.11	0.66
27:X:1059:A:O2'	27:X:1060:C:OP1	2.12	0.66
27:X:1573:G:O6	27:X:1574:A:N6	2.29	0.66
25:2:34:ARG:NH2	27:X:477:A:OP1	2.29	0.65
24:1:41:ASP:HB2	24:1:46:LYS:HD3	1.77	0.65
27:X:832:A:OP2	27:X:1201:G:N2	2.25	0.65
1:A:229:VAL:HG21	27:X:797:A:C5	2.31	0.65
2:B:5:LEU:HD23	2:B:195:LEU:HD11	1.77	0.65
15:P:57:LEU:HD13	15:P:69:ALA:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:95:LEU:HD12	13:N:98:ILE:HD12	1.77	0.65
27:X:1678:G:H1	27:X:1982:C:H42	1.43	0.65
8:I:53:ARG:HH21	8:I:54:SER:HB3	1.60	0.65
17:R:59:LYS:HD2	17:R:62:MET:HB2	1.78	0.65
27:X:318:G:N2	27:X:321:A:OP2	2.29	0.65
27:X:800:U:H5''	27:X:801:A:H5'	1.78	0.65
3:C:119:ALA:HB3	3:C:189:ASP:HA	1.77	0.65
17:R:55:THR:HG23	17:R:72:ARG:HD3	1.78	0.65
21:V:32:ALA:HA	21:V:37:LEU:HD22	1.78	0.65
20:U:38:THR:HB	27:X:2063:A:H5'	1.77	0.65
4:D:117:ILE:HG13	4:D:176:PRO:HG2	1.77	0.65
7:H:113:PRO:HD3	12:M:73:PHE:HB2	1.77	0.65
27:X:664:C:H5'	27:X:666:U:H5''	1.79	0.65
4:D:132:ILE:HG13	4:D:154:ILE:HD13	1.79	0.65
2:B:152:LYS:HB2	6:G:106:TYR:HB2	1.79	0.65
1:A:172:TYR:HA	1:A:186:HIS:HA	1.78	0.65
27:X:1919:A:H62	27:X:1946:U:H3	1.45	0.65
1:A:88:ARG:NH2	27:X:1809:G:OP1	2.30	0.65
1:A:251:GLY:HA3	1:A:255:LYS:NZ	2.12	0.65
13:N:66:ASN:O	13:N:70:ARG:NH1	2.29	0.65
24:1:41:ASP:HB2	24:1:46:LYS:HB3	1.78	0.65
12:M:51:GLU:H	12:M:70:LYS:NZ	1.94	0.65
27:X:2237:C:O2'	27:X:2406:C:OP2	2.15	0.65
27:X:2492:G:H2'	27:X:2493:U:C6	2.32	0.64
2:B:9:ILE:HD11	2:B:27:LEU:HB2	1.79	0.64
27:X:1033:G:H22	27:X:1153:A:H2	1.45	0.64
2:B:128:SER:HB3	27:X:1976:U:H4'	1.77	0.64
27:X:1919:A:H2	27:X:1926:U:N3	1.95	0.64
10:K:6:ALA:HB1	27:X:2848:A:H2	1.62	0.64
27:X:1141:U:O2'	27:X:1142:G:O5'	2.15	0.64
27:X:573:C:O2'	27:X:1266:G:O6	2.14	0.64
27:X:1283:C:H5''	27:X:1284:G:H5'	1.79	0.64
11:L:88:VAL:HG11	27:X:2357:A:H1'	1.79	0.64
15:P:36:ARG:HG2	27:X:1279:G:N7	2.12	0.64
27:X:1079:G:N2	27:X:1106:A:O2'	2.29	0.64
8:I:90:ARG:HA	8:I:121:HIS:HB2	1.80	0.64
27:X:145:C:O2	27:X:152:G:N2	2.28	0.64
10:K:10:LEU:HD11	10:K:17:ARG:HD3	1.80	0.64
27:X:1329:U:H2'	27:X:1330:G:H8	1.61	0.64
27:X:218:A:H5'	27:X:220:U:H1'	1.79	0.64
27:X:1843:U:H3	27:X:1874:G:H1	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:23:ILE:HG22	17:R:33:THR:HB	1.80	0.64
27:X:1465:G:N2	27:X:1466:C:N3	2.45	0.64
19:T:70:ILE:HB	19:T:78:PHE:HB2	1.80	0.64
4:D:51:ASP:HB3	4:D:55:LYS:HE2	1.81	0.63
27:X:492:G:H1'	27:X:516:G:N2	2.13	0.63
27:X:590:C:H2'	27:X:591:G:H8	1.63	0.63
27:X:2605:C:H2'	27:X:2606:G:C8	2.33	0.63
27:X:748:A:H5'	27:X:749:C:OP2	1.99	0.63
28:Y:40:C:O2	28:Y:50:U:O2'	2.16	0.63
23:Z:41:LEU:HD12	23:Z:42:SER:H	1.63	0.63
27:X:82:G:H1	27:X:100:G:HO2'	1.46	0.63
6:G:70:PHE:HB3	13:N:64:ARG:HG2	1.79	0.63
27:X:1089:C:O2'	27:X:1099:A:OP1	2.17	0.63
18:S:154:LEU:HD11	18:S:160:LEU:HG	1.79	0.63
27:X:2672:U:H2'	27:X:2673:G:H8	1.62	0.63
28:Y:27:A:O2'	28:Y:28:A:O5'	2.14	0.63
27:X:759:C:H5''	27:X:761:G:H1'	1.79	0.63
27:X:1561:A:O2'	27:X:1562:G:O4'	2.13	0.63
13:N:31:GLN:NE2	27:X:589:C:H4'	2.12	0.63
6:G:100:TYR:HB2	6:G:116:ARG:NH1	2.14	0.63
27:X:1488:G:HO2'	27:X:1489:C:H5	1.46	0.63
27:X:661:C:H2'	27:X:662:G:C8	2.33	0.63
27:X:617:U:H5	27:X:632:A:C2	2.16	0.63
3:C:117:LEU:HD22	3:C:187:VAL:HG13	1.81	0.63
27:X:1923:U:OP1	27:X:2582:G:N2	2.31	0.63
18:S:71:MET:N	18:S:71:MET:SD	2.66	0.63
27:X:1468:A:H8	27:X:1468:A:P	2.21	0.63
27:X:2336:G:N2	27:X:2339:A:OP2	2.31	0.63
18:S:51:LEU:HB2	18:S:64:ALA:O	1.99	0.63
15:P:118:ASN:HD21	15:P:120:ILE:HB	1.64	0.63
27:X:1845:A:N3	27:X:2212:U:O2'	2.30	0.63
27:X:1058:G:H2'	27:X:1121:G:H22	1.64	0.63
6:G:106:TYR:CD2	6:G:108:GLY:HA2	2.33	0.63
27:X:313:U:H2'	27:X:314:G:H8	1.64	0.63
26:3:32:GLN:HB3	27:X:2400:G:N7	2.14	0.62
2:B:110:GLY:O	10:K:3:HIS:HD2	1.81	0.62
23:Z:31:THR:HG1	27:X:2861:A:HO2'	1.47	0.62
15:P:11:LYS:HG2	15:P:14:ARG:HH12	1.62	0.62
16:Q:63:LYS:HE2	16:Q:69:ILE:HA	1.79	0.62
27:X:1017:C:H2'	27:X:1018:C:H6	1.64	0.62
26:3:25:PHE:CD2	26:3:46:LYS:HA	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1769:U:H2'	27:X:1775:A:N6	2.15	0.62
2:B:176:ARG:NH2	12:M:16:ILE:HG23	2.14	0.62
7:H:89:ILE:HG23	12:M:79:ARG:HD3	1.80	0.62
27:X:590:C:H2'	27:X:591:G:C8	2.34	0.62
3:C:53:LYS:H	3:C:53:LYS:HE2	1.62	0.62
27:X:1349:A:H2'	27:X:1350:G:C8	2.35	0.62
27:X:619:A:N6	27:X:630:G:O2'	2.33	0.62
27:X:469:G:N2	27:X:480:G:H2'	2.14	0.62
27:X:754:G:H2'	27:X:755:C:H6	1.63	0.62
27:X:403:A:H4'	27:X:404:A:H5'	1.81	0.62
27:X:222:G:O2'	27:X:397:U:O2	2.16	0.62
27:X:1007:A:H2'	27:X:1008:G:H8	1.64	0.62
1:A:252:LYS:NZ	1:A:252:LYS:H	1.96	0.62
27:X:854:G:H1	27:X:948:C:N4	1.95	0.62
1:A:48:ARG:HD3	27:X:1797:C:H4'	1.81	0.62
1:A:145:LEU:HB3	1:A:155:LEU:HB2	1.80	0.62
27:X:2020:G:H2'	27:X:2021:G:C8	2.34	0.62
27:X:2085:G:N2	27:X:2171:U:O2'	2.32	0.62
1:A:254:THR:OG1	27:X:1835:C:O2'	2.16	0.62
8:I:42:GLY:HA2	8:I:45:LYS:HE3	1.82	0.62
18:S:162:ALA:HB1	18:S:166:LEU:HD13	1.82	0.62
27:X:1373:G:H22	27:X:2192:U:H3	1.47	0.62
26:3:39:ASP:OD1	27:X:2329:C:N4	2.33	0.62
27:X:1065:A:H2'	27:X:1066:G:C8	2.35	0.62
27:X:437:G:H2'	27:X:438:G:H8	1.63	0.62
2:B:117:MET:HA	2:B:121:ASN:O	2.00	0.62
3:C:112:GLN:HA	3:C:116:LYS:HE2	1.82	0.62
1:A:164:GLN:HG3	1:A:176:ARG:HB3	1.82	0.62
27:X:1937:G:O2'	27:X:1939:U:O4	2.13	0.62
27:X:1235:C:H42	27:X:1240:G:H1	1.46	0.62
1:A:43:ARG:HD3	1:A:55:GLY:HA2	1.81	0.61
15:P:97:VAL:CG1	15:P:125:SER:HB2	2.30	0.61
27:X:2447:G:O2'	27:X:2448:A:H8	1.82	0.61
7:H:47:VAL:HG11	7:H:115:ALA:HB3	1.81	0.61
24:1:30:ASN:N	24:1:30:ASN:OD1	2.32	0.61
6:G:132:PHE:CE2	6:G:145:HIS:HB2	2.35	0.61
2:B:9:ILE:HD13	12:M:12:LEU:HD13	1.82	0.61
27:X:1991:C:H2'	27:X:1992:G:H8	1.66	0.61
27:X:2174:G:H2'	27:X:2175:A:H8	1.63	0.61
27:X:2796:A:H2'	27:X:2797:G:C8	2.35	0.61
15:P:17:GLN:HG3	15:P:18:VAL:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:THR:HG21	27:X:38:G:H21	1.63	0.61
17:R:54:ILE:HD13	17:R:71:GLN:HA	1.81	0.61
11:L:16:LYS:HE3	11:L:28:ARG:HH12	1.66	0.61
8:I:18:ARG:HH12	27:X:609:U:H4'	1.65	0.61
27:X:2174:G:H2'	27:X:2175:A:C8	2.36	0.61
27:X:469:G:H22	27:X:480:G:H2'	1.65	0.61
1:A:158:SER:OG	1:A:159:ALA:N	2.26	0.61
27:X:1399:C:H2'	27:X:1400:A:H8	1.66	0.61
27:X:1448:A:H61	27:X:1574:A:H61	1.47	0.61
3:C:6:VAL:HG12	3:C:7:ILE:HG12	1.83	0.61
27:X:587:A:OP1	27:X:1268:U:O2'	2.13	0.61
7:H:6:SER:HB2	27:X:1683:G:O3'	2.00	0.61
27:X:2286:G:O6	27:X:2287:G:N2	2.33	0.61
3:C:111:ARG:NH1	3:C:180:ILE:O	2.33	0.61
1:A:258:LYS:HD3	1:A:264:LYS:HZ1	1.64	0.61
15:P:39:ARG:HB2	15:P:39:ARG:HH11	1.66	0.61
8:I:53:ARG:HD2	8:I:54:SER:H	1.65	0.61
27:X:1222:G:O2'	27:X:1250:A:N6	2.34	0.61
19:T:40:GLN:HE22	19:T:43:THR:HA	1.65	0.61
3:C:53:LYS:NZ	27:X:463:C:O3'	2.33	0.61
27:X:1030:U:H2'	27:X:1032:A:H2	1.65	0.61
9:J:83:ARG:HH22	27:X:971:A:H61	1.47	0.61
27:X:825:C:O2'	27:X:1239:A:O2'	2.13	0.61
27:X:2546:G:H2'	27:X:2547:C:H6	1.64	0.61
2:B:146:THR:HG1	27:X:2550:C:HO2'	1.48	0.61
9:J:67:ILE:HG12	9:J:105:PHE:HD1	1.66	0.60
20:U:51:ILE:HG23	20:U:59:THR:HA	1.82	0.60
3:C:33:TRP:NE1	3:C:95:LEU:HB2	2.16	0.60
15:P:33:MET:SD	15:P:37:LYS:NZ	2.74	0.60
5:E:154:PRO:HA	5:E:160:LYS:O	2.00	0.60
6:G:67:ARG:HH21	6:G:72:PRO:HA	1.65	0.60
27:X:163:A:H2'	27:X:164:G:C8	2.36	0.60
23:Z:55:ARG:HH21	23:Z:58:LEU:HA	1.66	0.60
12:M:29:PRO:HB2	12:M:99:VAL:HG11	1.82	0.60
27:X:2660:C:H42	27:X:2705:A:H2	1.48	0.60
2:B:35:GLN:HG3	2:B:66:HIS:HE1	1.66	0.60
26:3:14:ILE:HD11	26:3:56:ALA:HB1	1.83	0.60
25:2:33:ARG:NE	27:X:478:G:OP1	2.31	0.60
17:R:38:LEU:H	17:R:47:VAL:HB	1.65	0.60
27:X:2516:U:H2'	27:X:2517:C:C6	2.36	0.60
1:A:96:HIS:CE1	27:X:1517:C:H4'	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1988:A:H5'	27:X:1989:C:OP2	2.01	0.60
27:X:1542:G:N2	27:X:1562:G:H1	1.91	0.60
7:H:23:ARG:NH1	27:X:2526:U:O2	2.27	0.60
1:A:91:ARG:HB2	1:A:107:ALA:HB3	1.82	0.60
2:B:143:GLN:O	27:X:2035:G:H4'	2.00	0.60
16:Q:29:VAL:HG21	16:Q:38:ILE:HD11	1.82	0.60
27:X:1117:G:H2'	27:X:1118:G:H8	1.65	0.60
27:X:1859:A:H2'	27:X:1860:A:H8	1.67	0.60
3:C:173:ALA:HB1	3:C:193:LEU:HD13	1.83	0.60
3:C:33:TRP:CD1	3:C:95:LEU:HB2	2.36	0.60
18:S:28:ASN:OD1	18:S:28:ASN:N	2.29	0.60
25:2:12:ARG:HG2	27:X:699:G:N1	2.14	0.60
12:M:51:GLU:H	12:M:70:LYS:HZ1	1.48	0.60
24:1:2:ALA:N	27:X:2369:U:OP2	2.34	0.60
27:X:582:G:O2'	27:X:583:C:H3'	2.01	0.60
26:3:25:PHE:HA	26:3:47:GLY:H	1.67	0.60
27:X:2634:G:O2'	27:X:2635:U:OP2	2.20	0.60
27:X:2417:U:O2'	27:X:2419:C:OP1	2.19	0.60
27:X:116:A:N3	27:X:155:G:H1'	2.17	0.60
14:O:22:VAL:HG13	27:X:1173:G:H4'	1.84	0.60
27:X:1643:A:H61	27:X:1656:U:H3	1.50	0.60
27:X:2311:U:O2'	27:X:2315:A:N7	2.34	0.60
27:X:2234:G:H2'	27:X:2235:G:O4'	2.01	0.60
8:I:56:LEU:HD23	8:I:59:ARG:HH21	1.65	0.60
6:G:107:GLN:HB3	27:X:1142:G:H5'	1.83	0.60
19:T:23:VAL:HA	19:T:38:VAL:HG13	1.84	0.60
6:G:84:ASN:O	6:G:152:ALA:HA	2.00	0.60
27:X:1699:A:H61	27:X:1723:U:H3	1.48	0.60
27:X:1455:C:H2'	27:X:1456:C:H6	1.67	0.60
27:X:1836:C:H42	27:X:1879:G:H1	1.48	0.59
1:A:161:THR:H	1:A:196:VAL:HG22	1.66	0.59
27:X:836:G:H2'	27:X:837:U:H6	1.67	0.59
8:I:59:ARG:HB2	27:X:2371:A:H8	1.67	0.59
9:J:44:LYS:HB2	9:J:47:GLN:HG3	1.84	0.59
15:P:59:PHE:HE1	23:Z:40:LYS:HA	1.66	0.59
1:A:159:ALA:HA	1:A:198:ASN:CG	2.23	0.59
20:U:39:LYS:HA	27:X:2063:A:H4'	1.84	0.59
3:C:106:MET:O	3:C:110:SER:OG	2.14	0.59
1:A:108:PRO:HB3	1:A:143:HIS:CE1	2.37	0.59
27:X:1371:G:O2'	27:X:1386:A:N6	2.35	0.59
27:X:627:A:H2'	27:X:628:A:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2845:C:H2'	27:X:2846:G:H5'	1.85	0.59
1:A:37:LEU:HD12	27:X:1808:C:H41	1.67	0.59
26:3:13:ARG:HE	26:3:25:PHE:N	2.00	0.59
15:P:118:ASN:ND2	27:X:1996:A:OP1	2.35	0.59
27:X:82:G:O2'	27:X:100:G:N2	2.34	0.59
27:X:2270:U:O2'	27:X:2353:G:N3	2.35	0.59
1:A:108:PRO:HB3	1:A:143:HIS:HE1	1.68	0.59
4:D:4:LEU:HG	4:D:5:LYS:H	1.67	0.59
15:P:87:GLU:HA	15:P:90:LEU:HG	1.84	0.59
3:C:53:LYS:HE3	27:X:464:G:H8	1.67	0.59
1:A:88:ARG:HD2	1:A:92:ILE:HD11	1.84	0.59
27:X:752:G:N2	27:X:753:U:O4	2.31	0.59
6:G:93:LYS:HD2	6:G:96:ASP:HB2	1.85	0.59
27:X:2708:U:H2'	27:X:2709:C:C6	2.38	0.59
7:H:99:ILE:HD12	7:H:103:GLY:HA2	1.85	0.59
21:V:15:ALA:HA	21:V:18:ILE:HD12	1.84	0.59
27:X:2014:A:C6	27:X:2477:C:H1'	2.38	0.59
10:K:3:HIS:NE2	27:X:2797:G:OP2	2.35	0.59
27:X:90:G:H3'	27:X:91:A:H8	1.68	0.59
13:N:66:ASN:CB	13:N:76:TYR:HB2	2.32	0.59
27:X:2329:C:H2'	27:X:2330:G:O4'	2.03	0.59
22:W:37:THR:HG22	22:W:38:PRO:HD2	1.84	0.59
17:R:37:LEU:HD11	17:R:49:GLU:HG3	1.84	0.59
27:X:1383:C:H3'	27:X:1384:G:H8	1.68	0.59
27:X:670:U:H2'	27:X:671:A:C8	2.38	0.59
20:U:17:SER:HB2	20:U:44:ALA:HA	1.84	0.59
9:J:70:PHE:CE2	27:X:884:C:H4'	2.38	0.59
27:X:540:G:C5	27:X:2005:U:H5''	2.37	0.58
14:O:10:LYS:NZ	14:O:13:ARG:HH12	2.01	0.58
27:X:1554:G:H2'	27:X:1555:A:H8	1.68	0.58
21:V:26:MET:HA	21:V:29:ARG:HE	1.66	0.58
27:X:2431:C:H2'	27:X:2432:A:C8	2.37	0.58
22:W:23:LEU:HD11	22:W:44:VAL:HG22	1.83	0.58
6:G:116:ARG:HE	6:G:126:VAL:HG22	1.68	0.58
27:X:163:A:H2'	27:X:164:G:H8	1.67	0.58
1:A:37:LEU:HD22	1:A:38:PRO:HD2	1.84	0.58
1:A:231:HIS:CD2	1:A:232:PRO:HD2	2.38	0.58
15:P:35:PRO:HG3	15:P:123:ARG:HD3	1.84	0.58
27:X:874:A:H2'	27:X:875:G:O4'	2.03	0.58
27:X:1811:A:H4'	27:X:1812:U:O5'	2.03	0.58
1:A:46:ARG:NE	27:X:1383:C:OP1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2691:C:O2'	27:X:2693:U:H5'	2.04	0.58
25:2:28:ARG:HH11	25:2:31:LEU:HG	1.68	0.58
6:G:124:GLU:N	6:G:124:GLU:OE1	2.36	0.58
27:X:1223:G:H4'	27:X:1224:A:H5''	1.85	0.58
10:K:24:GLN:HB3	10:K:44:LEU:HD22	1.86	0.58
15:P:89:ARG:HE	15:P:137:LYS:HE3	1.68	0.58
9:J:39:GLU:HG2	28:Y:92:G:H22	1.68	0.58
1:A:252:LYS:HD2	1:A:253:PRO:HD3	1.86	0.58
27:X:2560:G:OP2	27:X:2560:G:N2	2.34	0.58
27:X:571:U:O2'	27:X:581:A:H8	1.82	0.58
27:X:840:U:H4'	27:X:841:G:C2	2.38	0.58
27:X:421:G:N2	27:X:433:G:H1'	2.19	0.58
27:X:26:G:H1'	27:X:525:A:H61	1.68	0.58
27:X:1437:A:H2'	27:X:1438:G:C8	2.39	0.58
18:S:41:ARG:NH1	27:X:1052:C:OP1	2.36	0.58
6:G:56:THR:HG21	27:X:1016:C:O2'	2.04	0.58
17:R:22:VAL:HG11	17:R:80:LYS:HE3	1.85	0.58
17:R:84:VAL:HG21	17:R:89:GLY:HA2	1.85	0.58
2:B:116:VAL:H	2:B:136:ARG:HG3	1.68	0.58
6:G:109:GLY:H	6:G:111:LYS:HG3	1.68	0.58
10:K:5:LYS:HD2	27:X:2795:A:H4'	1.85	0.58
28:Y:96:C:H2'	28:Y:97:C:H6	1.69	0.58
14:O:78:VAL:HG22	27:X:1202:U:H5'	1.86	0.58
27:X:2494:C:H42	27:X:2548:G:H1	1.50	0.58
27:X:1329:U:H2'	27:X:1330:G:C8	2.37	0.58
27:X:2284:U:H2'	27:X:2285:U:H5''	1.85	0.58
27:X:2772:U:H1'	27:X:2781:G:N2	2.19	0.58
27:X:784:U:H2'	27:X:785:U:C6	2.39	0.58
27:X:160:C:O2'	27:X:445:A:N3	2.32	0.57
11:L:48:GLY:O	28:Y:115:G:N2	2.31	0.57
25:2:27:GLY:HA2	25:2:30:ILE:HD12	1.86	0.57
5:E:150:LYS:NZ	27:X:2741:G:H21	2.01	0.57
27:X:2807:U:H5''	27:X:2807:U:H6	1.69	0.57
3:C:163:ASN:ND2	3:C:167:VAL:H	1.94	0.57
15:P:29:LYS:HA	15:P:126:HIS:CD2	2.39	0.57
2:B:203:LYS:NZ	2:B:204:ALA:H	2.02	0.57
4:D:60:ILE:HG22	4:D:140:GLU:HB2	1.84	0.57
27:X:2318:U:H4'	28:Y:43:G:N2	2.19	0.57
27:X:1103:C:H42	27:X:1110:G:H1	1.51	0.57
9:J:100:PRO:HB2	18:S:74:ARG:HG2	1.84	0.57
3:C:89:ARG:HD2	27:X:599:A:OP1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1479:G:H2'	27:X:1480:G:C8	2.39	0.57
26:3:25:PHE:CG	26:3:46:LYS:HA	2.39	0.57
5:E:157:TYR:CZ	27:X:2510:A:H5''	2.39	0.57
27:X:28:A:H1'	27:X:523:A:C2	2.38	0.57
7:H:124:MET:O	7:H:127:VAL:HG12	2.05	0.57
27:X:1727:C:H2'	27:X:1728:A:C8	2.40	0.57
15:P:36:ARG:NH2	27:X:1279:G:O5'	2.38	0.57
27:X:474:G:N2	27:X:477:A:OP2	2.32	0.57
16:Q:35:LYS:HE2	16:Q:55:THR:HG22	1.87	0.57
2:B:119:ARG:HG2	2:B:120:TRP:CD1	2.40	0.57
1:A:99:ASP:OD1	27:X:1506:C:H2'	2.04	0.57
26:3:34:THR:OG1	26:3:35:GLY:N	2.36	0.57
27:X:558:G:H4'	27:X:559:C:C4	2.39	0.57
19:T:74:LYS:C	19:T:76:ALA:H	2.07	0.57
15:P:27:VAL:HA	15:P:128:THR:HA	1.86	0.57
27:X:1399:C:H2'	27:X:1400:A:C8	2.40	0.57
2:B:146:THR:OG1	27:X:2550:C:O2'	2.19	0.57
27:X:2262:C:H2'	27:X:2263:C:O4'	2.05	0.57
27:X:2263:C:O2'	27:X:2267:A:N6	2.37	0.57
27:X:90:G:H3'	27:X:91:A:C8	2.40	0.57
9:J:73:LYS:H	9:J:94:TRP:HD1	1.53	0.57
6:G:31:THR:OG1	27:X:1006:C:O2	2.18	0.57
27:X:2201:G:H2'	27:X:2202:G:H8	1.70	0.57
27:X:1468:A:H8	27:X:1468:A:O5'	1.87	0.57
27:X:2212:U:H2'	27:X:2213:G:C8	2.40	0.57
27:X:48:A:H4'	27:X:49:U:O5'	2.05	0.57
27:X:1223:G:H5''	27:X:1224:A:H3'	1.85	0.57
6:G:67:ARG:HD3	6:G:70:PHE:HA	1.86	0.57
2:B:14:ILE:HG12	12:M:20:HIS:CD2	2.39	0.57
27:X:774:A:H8	27:X:774:A:O5'	1.88	0.57
4:D:92:ARG:NH2	28:Y:45:C:O2	2.38	0.57
20:U:48:LYS:HG3	20:U:49:LYS:N	2.18	0.57
27:X:1348:C:H2'	27:X:1349:A:C8	2.40	0.57
27:X:2283:G:H22	27:X:2291:U:H3	1.53	0.57
9:J:131:LYS:HD2	18:S:76:ARG:HH21	1.70	0.57
27:X:138:G:H2'	27:X:139:A:H8	1.70	0.57
3:C:162:ARG:HE	27:X:333:A:C5'	2.18	0.56
26:3:19:THR:OG1	27:X:661:C:OP1	2.22	0.56
24:1:41:ASP:N	24:1:41:ASP:OD1	2.38	0.56
27:X:1539:U:H2'	27:X:1540:C:C6	2.39	0.56
11:L:8:ARG:HG3	11:L:9:ARG:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2442:C:H2'	27:X:2443:C:H6	1.70	0.56
27:X:500:G:C2	27:X:501:G:H1'	2.40	0.56
27:X:1782:A:N6	27:X:1820:G:O2'	2.38	0.56
20:U:52:ARG:HB3	20:U:79:GLU:HA	1.87	0.56
27:X:555:U:OP2	27:X:556:A:O2'	2.13	0.56
27:X:1039:A:N6	27:X:1136:G:H2'	2.20	0.56
27:X:1279:G:O2'	27:X:1995:G:O6	2.16	0.56
13:N:66:ASN:HB2	13:N:70:ARG:HH12	1.70	0.56
2:B:35:GLN:HG3	2:B:66:HIS:CE1	2.41	0.56
6:G:170:PRO:O	6:G:171:LEU:HB2	2.05	0.56
27:X:1286:U:O2	27:X:1985:G:O2'	2.23	0.56
17:R:15:HIS:CE1	17:R:16:PHE:HD2	2.23	0.56
2:B:4:ILE:HD13	2:B:28:ALA:HB1	1.87	0.56
1:A:13:ARG:CZ	1:A:27:LYS:HD3	2.35	0.56
7:H:76:ARG:NH1	7:H:113:PRO:O	2.38	0.56
26:3:30:ARG:HB2	27:X:2372:A:OP1	2.05	0.56
4:D:66:ILE:HD12	28:Y:43:G:H5''	1.86	0.56
2:B:154:LYS:HG3	2:B:155:ARG:N	2.19	0.56
27:X:135:U:H2'	27:X:136:A:C8	2.41	0.56
4:D:13:ARG:NH1	4:D:14:PRO:HG3	2.21	0.56
27:X:2555:G:H5'	27:X:2558:C:H41	1.70	0.56
24:1:16:ALA:HB2	24:1:50:PHE:CE1	2.40	0.56
15:P:59:PHE:CE1	23:Z:40:LYS:HA	2.40	0.56
20:U:17:SER:OG	20:U:45:ASN:N	2.39	0.56
28:Y:58:G:H4'	28:Y:59:A:O5'	2.03	0.56
27:X:197:G:N3	27:X:210:A:H2	2.03	0.56
27:X:2557:G:H2'	27:X:2558:C:C6	2.40	0.56
27:X:2818:G:H1	27:X:2849:C:N4	2.02	0.56
13:N:93:LYS:HB3	27:X:1007:A:O3'	2.05	0.56
14:O:15:SER:HA	14:O:95:ILE:O	2.06	0.56
27:X:1725:C:H42	27:X:1741:G:H1	1.52	0.56
27:X:1645:U:H2'	27:X:1646:G:C8	2.41	0.56
3:C:163:ASN:HD22	3:C:165:SER:N	2.04	0.56
27:X:939:C:H3'	27:X:940:G:O4'	2.06	0.56
27:X:1982:C:H5''	27:X:2703:C:O2'	2.05	0.56
9:J:83:ARG:NH2	27:X:970:A:H62	2.03	0.56
27:X:89:A:O2'	27:X:91:A:N6	2.39	0.56
27:X:1554:G:H2'	27:X:1555:A:C8	2.41	0.56
25:2:22:MET:HA	25:2:28:ARG:HG2	1.86	0.56
17:R:17:LYS:HG3	27:X:83:A:H5''	1.87	0.56
27:X:1451:C:H1'	27:X:1532:A:H2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1272:G:H2'	27:X:1273:G:C8	2.41	0.56
27:X:398:C:H42	27:X:424:G:H1	1.54	0.56
9:J:78:LYS:HA	9:J:88:LYS:HZ1	1.70	0.56
1:A:60:ARG:HD3	1:A:86:PRO:HB2	1.87	0.56
27:X:796:A:H8	27:X:797:A:H4'	1.70	0.56
27:X:224:G:H4'	27:X:399:G:C5	2.40	0.56
9:J:17:ARG:HB2	27:X:969:U:C4	2.41	0.56
2:B:165:VAL:HG12	2:B:189:PRO:HG3	1.87	0.56
27:X:1348:C:H2'	27:X:1349:A:H8	1.71	0.56
1:A:88:ARG:HG2	1:A:90:ALA:HB3	1.88	0.56
27:X:492:G:H1'	27:X:516:G:H21	1.71	0.56
27:X:89:A:H4'	27:X:90:G:H5'	1.88	0.56
27:X:2772:U:H2'	27:X:2773:G:C8	2.41	0.56
27:X:1827:G:H1'	27:X:1914:U:C2	2.41	0.56
26:3:6:THR:N	26:3:59:LYS:O	2.39	0.56
1:A:246:PRO:HD2	1:A:251:GLY:HA2	1.86	0.55
3:C:71:ASP:OD1	3:C:72:ARG:N	2.35	0.55
24:1:27:ASN:HD21	24:1:33:ALA:HB1	1.70	0.55
28:Y:64:C:H2'	28:Y:65:A:C8	2.41	0.55
27:X:616:U:O2'	27:X:671:A:H4'	2.06	0.55
26:3:15:LYS:O	26:3:23:MET:N	2.31	0.55
2:B:31:CYS:HB3	2:B:49:ILE:HD12	1.88	0.55
27:X:69:G:H1'	27:X:72:A:H1'	1.88	0.55
6:G:43:VAL:HG21	6:G:158:HIS:CE1	2.39	0.55
27:X:1705:U:O2	27:X:1717:A:H5'	2.07	0.55
16:Q:49:ARG:NH2	27:X:1612:U:OP1	2.38	0.55
20:U:13:LEU:HD11	20:U:16:ASN:HD22	1.71	0.55
1:A:183:ARG:NH2	27:X:1791:C:OP2	2.39	0.55
16:Q:56:MET:HG2	27:X:1354:A:H4'	1.88	0.55
5:E:104:GLU:HG2	5:E:114:ILE:HG22	1.87	0.55
27:X:649:G:H2'	27:X:650:U:H6	1.71	0.55
27:X:2672:U:H2'	27:X:2673:G:C8	2.39	0.55
3:C:34:GLN:NE2	27:X:627:A:OP1	2.36	0.55
1:A:231:HIS:CD2	1:A:247:VAL:HA	2.41	0.55
12:M:27:PHE:HA	12:M:96:ARG:NH2	2.22	0.55
1:A:210:GLY:HA2	1:A:213:ARG:HG2	1.89	0.55
27:X:1762:C:H2'	27:X:1763:G:C8	2.42	0.55
27:X:75:C:H2'	27:X:76:C:C6	2.41	0.55
13:N:58:ARG:NH1	27:X:1166:A:OP2	2.39	0.55
27:X:938:G:O2'	27:X:939:C:H5''	2.07	0.55
27:X:826:U:H2'	27:X:827:C:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:758:G:H2'	27:X:759:C:H5'	1.88	0.55
13:N:93:LYS:HE3	14:O:6:GLN:HG3	1.88	0.55
15:P:41:VAL:HG11	15:P:65:SER:HA	1.89	0.55
19:T:21:LEU:HD11	19:T:41:ARG:HD2	1.89	0.55
27:X:876:A:H2	27:X:926:C:H41	1.53	0.55
19:T:40:GLN:NE2	19:T:42:GLY:O	2.40	0.55
27:X:2245:A:H4'	27:X:2246:A:N3	2.22	0.55
28:Y:22:U:H2'	28:Y:23:G:C8	2.42	0.55
6:G:95:LEU:HD23	6:G:95:LEU:H	1.72	0.55
27:X:2081:U:O2	27:X:2174:G:N2	2.36	0.55
17:R:105:ARG:HH12	17:R:113:THR:H	1.55	0.55
3:C:59:TYR:CD1	3:C:64:THR:HG21	2.42	0.55
4:D:65:PRO:HA	4:D:89:VAL:HG13	1.89	0.55
27:X:718:A:H2'	27:X:719:A:H8	1.71	0.55
27:X:2241:U:H2'	27:X:2242:C:C6	2.42	0.55
2:B:141:ILE:HD11	27:X:2034:A:O4'	2.07	0.55
15:P:27:VAL:HB	15:P:128:THR:HG22	1.89	0.55
15:P:11:LYS:NZ	27:X:1247:U:OP2	2.23	0.55
6:G:126:VAL:HG12	6:G:127:ILE:HD12	1.88	0.55
3:C:133:PHE:CE1	3:C:161:ALA:HB2	2.42	0.54
27:X:1479:G:H2'	27:X:1480:G:H8	1.72	0.54
15:P:35:PRO:HG3	15:P:123:ARG:HH11	1.72	0.54
27:X:2335:U:H2'	27:X:2336:G:C8	2.42	0.54
27:X:2191:A:OP1	27:X:2193:C:N4	2.39	0.54
10:K:39:THR:HG21	27:X:1668:G:H5'	1.88	0.54
27:X:1296:G:N2	27:X:1299:A:H5'	2.23	0.54
27:X:1654:A:H4'	27:X:2690:A:O2'	2.07	0.54
8:I:26:THR:OG1	27:X:676:G:OP1	2.16	0.54
18:S:3:LEU:HD13	18:S:33:ALA:H	1.70	0.54
12:M:109:GLU:OE2	12:M:109:GLU:N	2.40	0.54
27:X:580:A:H4'	27:X:581:A:OP1	2.07	0.54
6:G:109:GLY:HA2	6:G:111:LYS:HE3	1.89	0.54
24:I:42:PRO:HG3	24:I:50:PHE:HE1	1.73	0.54
2:B:162:MET:SD	27:X:2796:A:H4'	2.47	0.54
27:X:2345:A:H2'	27:X:2346:G:O4'	2.08	0.54
27:X:833:A:H1'	27:X:954:U:H1'	1.90	0.54
6:G:109:GLY:HA2	6:G:111:LYS:CE	2.37	0.54
27:X:312:G:HO2'	27:X:313:U:H6	1.54	0.54
27:X:1174:G:H2'	27:X:1175:A:H8	1.73	0.54
21:V:26:MET:HA	21:V:29:ARG:NE	2.23	0.54
10:K:14:SER:HB3	27:X:2693:U:OP1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:138:G:H2'	27:X:139:A:C8	2.42	0.54
27:X:781:G:N2	27:X:1392:U:O2'	2.39	0.54
13:N:10:ARG:HG3	27:X:1264:C:OP1	2.06	0.54
2:B:143:GLN:NE2	2:B:143:GLN:H	2.05	0.54
27:X:652:C:O2'	27:X:2329:C:OP1	2.17	0.54
27:X:718:A:H2'	27:X:719:A:C8	2.42	0.54
23:Z:16:ARG:HD3	23:Z:20:ARG:NH1	2.22	0.54
27:X:2281:C:H42	27:X:2293:G:H1	1.55	0.54
3:C:46:ARG:HD2	3:C:51:VAL:HB	1.90	0.54
27:X:2663:U:H3	27:X:2705:A:H62	1.55	0.54
27:X:1086:C:H3'	27:X:1087:C:H5''	1.89	0.54
27:X:1974:U:H2'	27:X:1975:G:H5''	1.89	0.54
9:J:17:ARG:NH1	27:X:969:U:O4'	2.41	0.54
27:X:1793:A:H2'	27:X:1794:A:C8	2.43	0.54
16:Q:28:TRP:CE3	16:Q:75:ARG:HD2	2.42	0.54
3:C:152:THR:OG1	3:C:153:ASP:O	2.19	0.54
27:X:2053:G:H2'	27:X:2054:A:C8	2.43	0.54
7:H:27:SER:HA	7:H:50:ILE:HD12	1.89	0.54
26:3:13:ARG:NH2	26:3:25:PHE:HB2	2.23	0.54
3:C:6:VAL:H	3:C:119:ALA:HA	1.72	0.54
27:X:1859:A:H2'	27:X:1860:A:C8	2.42	0.54
27:X:26:G:C6	27:X:27:G:N1	2.76	0.54
27:X:2781:G:H2'	27:X:2782:G:H5''	1.90	0.54
4:D:134:GLU:HG2	4:D:136:LEU:H	1.73	0.54
17:R:51:VAL:HG12	17:R:74:LEU:HD23	1.89	0.54
2:B:136:ARG:HB3	27:X:1673:C:C5'	2.26	0.54
27:X:646:C:O2'	27:X:650:U:OP1	2.26	0.54
20:U:78:ILE:HG12	20:U:79:GLU:H	1.71	0.54
16:Q:28:TRP:CZ3	16:Q:77:LYS:HB2	2.43	0.54
6:G:120:SER:HA	6:G:123:PRO:HG3	1.90	0.54
11:L:104:ALA:O	11:L:108:ARG:HB2	2.07	0.54
28:Y:5:C:H2'	28:Y:6:C:O4'	2.07	0.54
19:T:64:ASP:N	19:T:64:ASP:OD1	2.41	0.54
4:D:78:LYS:HG2	4:D:80:ARG:NH1	2.22	0.54
27:X:1973:C:H2'	27:X:1974:U:C6	2.43	0.54
27:X:754:G:H2'	27:X:755:C:C6	2.41	0.54
6:G:71:THR:O	6:G:71:THR:OG1	2.23	0.54
27:X:2199:C:O2'	27:X:2200:G:H5'	2.08	0.54
14:O:68:LYS:HA	14:O:87:ARG:HG2	1.89	0.54
3:C:128:ALA:HB1	3:C:160:ALA:HA	1.90	0.54
9:J:12:LYS:HD3	27:X:923:A:N7	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:VAL:HB	3:C:167:VAL:HG12	1.90	0.54
27:X:1816:G:H2'	27:X:1817:U:H6	1.73	0.54
10:K:10:LEU:HG	10:K:17:ARG:HB3	1.90	0.54
4:D:51:ASP:O	4:D:55:LYS:HG2	2.08	0.54
18:S:3:LEU:HB2	18:S:33:ALA:O	2.07	0.54
16:Q:15:LYS:NZ	16:Q:19:ALA:HB2	2.23	0.54
27:X:1204:G:H2'	27:X:1205:G:H8	1.72	0.54
13:N:39:LEU:HA	13:N:42:ALA:HB3	1.90	0.54
3:C:163:ASN:HD21	3:C:167:VAL:N	1.95	0.53
27:X:953:G:O2'	27:X:1203:A:N3	2.34	0.53
8:I:56:LEU:HB3	26:3:52:LYS:HZ2	1.73	0.53
7:H:131:PRO:HB3	12:M:73:PHE:CE2	2.43	0.53
27:X:2235:G:N2	27:X:2254:C:C4	2.76	0.53
19:T:21:LEU:HD21	19:T:41:ARG:NH1	2.23	0.53
7:H:34:LEU:HD13	7:H:50:ILE:HD13	1.90	0.53
10:K:81:ASP:O	10:K:85:PRO:HG2	2.08	0.53
13:N:49:ASP:HA	13:N:52:ASN:HB2	1.90	0.53
7:H:42:LYS:HD2	27:X:2653:A:H4'	1.90	0.53
27:X:788:G:H4'	27:X:789:G:O5'	2.08	0.53
17:R:95:ARG:HH21	27:X:308:C:H4'	1.72	0.53
2:B:78:LEU:O	2:B:79:ARG:NE	2.36	0.53
18:S:122:ILE:HG22	18:S:160:LEU:HA	1.90	0.53
9:J:83:ARG:HH12	27:X:971:A:H61	1.56	0.53
3:C:10:ASN:HD21	3:C:13:ARG:NH1	2.06	0.53
27:X:2200:G:H2'	27:X:2201:G:C8	2.44	0.53
21:V:26:MET:HB2	21:V:29:ARG:HH21	1.74	0.53
9:J:76:THR:HA	9:J:89:GLY:O	2.07	0.53
15:P:40:LEU:HD13	23:Z:25:LEU:HD13	1.91	0.53
27:X:859:U:O2'	27:X:860:U:O5'	2.27	0.53
27:X:684:C:H2'	27:X:685:U:C6	2.42	0.53
1:A:26:LYS:HE3	1:A:28:ARG:HH21	1.73	0.53
27:X:2040:A:H2'	27:X:2041:A:C8	2.43	0.53
7:H:123:PHE:HB3	7:H:126:ILE:CG1	2.36	0.53
27:X:2598:C:O2'	27:X:2599:U:H5'	2.08	0.53
17:R:22:VAL:HG11	17:R:80:LYS:HB2	1.91	0.53
6:G:102:ARG:HH21	27:X:2620:G:P	2.31	0.53
27:X:1349:A:H2'	27:X:1350:G:H8	1.72	0.53
27:X:2054:A:H2'	27:X:2055:G:H8	1.74	0.53
10:K:43:GLU:O	10:K:46:PRO:HD2	2.09	0.53
6:G:162:LYS:HE3	27:X:5:A:H1'	1.90	0.53
27:X:978:U:H2'	27:X:979:A:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:61:ARG:HA	6:G:61:ARG:HE	1.74	0.53
4:D:39:GLY:O	4:D:150:ARG:NH2	2.38	0.53
27:X:2604:G:H2'	27:X:2605:C:C6	2.43	0.53
27:X:2351:G:H1	27:X:2360:C:H42	1.57	0.53
27:X:330:C:H2'	27:X:331:U:O4'	2.08	0.53
27:X:2041:A:O5'	27:X:2041:A:H8	1.92	0.53
4:D:74:ILE:HG23	4:D:79:LEU:HB2	1.91	0.53
27:X:1422:C:H2'	27:X:1423:A:C8	2.44	0.53
27:X:2581:A:H2'	27:X:2582:G:H4'	1.91	0.53
13:N:93:LYS:HE2	14:O:10:LYS:HD3	1.90	0.53
5:E:139:GLN:NE2	27:X:2726:U:O2'	2.40	0.53
27:X:2860:C:H2'	27:X:2861:A:O4'	2.08	0.53
27:X:1454:U:H2'	27:X:1455:C:C6	2.44	0.53
8:I:28:LYS:NZ	27:X:596:C:O2'	2.39	0.53
18:S:6:LYS:HD2	18:S:32:PHE:HA	1.91	0.53
27:X:305:A:H5'	27:X:306:G:OP2	2.09	0.53
1:A:108:PRO:HG2	1:A:111:LEU:HD12	1.91	0.52
27:X:1872:A:H2'	27:X:1873:A:C8	2.44	0.52
11:L:33:ARG:HH21	11:L:103:LEU:HD12	1.72	0.52
27:X:2198:U:C2	27:X:2199:C:H1'	2.44	0.52
27:X:116:A:OP2	27:X:117:A:H2'	2.10	0.52
3:C:2:ALA:HA	3:C:13:ARG:HD2	1.91	0.52
27:X:2484:G:HO2'	27:X:2485:U:H6	1.56	0.52
27:X:1840:A:H2'	27:X:1841:G:O4'	2.09	0.52
27:X:1030:U:H3	27:X:1153:A:N6	2.04	0.52
23:Z:4:HIS:HB3	23:Z:5:PRO:HD3	1.91	0.52
4:D:79:LEU:HD11	27:X:2289:A:C2	2.44	0.52
11:L:15:ARG:HA	11:L:15:ARG:HH11	1.74	0.52
27:X:2222:U:H2'	27:X:2223:U:C6	2.44	0.52
27:X:2873:G:H2'	27:X:2874:A:C8	2.44	0.52
2:B:121:ASN:O	2:B:122:PHE:HB2	2.09	0.52
9:J:78:LYS:HA	9:J:88:LYS:NZ	2.25	0.52
12:M:27:PHE:HA	12:M:96:ARG:HH22	1.74	0.52
27:X:2056:C:HO2'	27:X:2577:A:HO2'	1.55	0.52
27:X:346:C:H6	27:X:347:C:H5	1.56	0.52
22:W:47:VAL:HG23	22:W:51:LEU:HD11	1.91	0.52
5:E:94:PHE:HB3	5:E:107:ILE:HG22	1.91	0.52
27:X:1675:C:H2'	27:X:1676:U:C6	2.43	0.52
27:X:1212:U:H2'	27:X:1213:U:C6	2.44	0.52
2:B:115:GLY:HA2	2:B:136:ARG:HD2	1.92	0.52
27:X:1835:C:H2'	27:X:1836:C:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2557:G:H2'	27:X:2558:C:H6	1.73	0.52
3:C:45:THR:HG22	3:C:82:VAL:HG21	1.91	0.52
3:C:34:GLN:O	3:C:37:SER:OG	2.14	0.52
5:E:150:LYS:HZ3	27:X:2741:G:H21	1.58	0.52
9:J:78:LYS:NZ	27:X:2438:A:N3	2.57	0.52
18:S:10:PRO:HB2	18:S:13:LYS:HD2	1.92	0.52
27:X:1943:A:H5'	27:X:1944:C:OP2	2.09	0.52
11:L:65:THR:OG1	28:Y:52:G:OP1	2.28	0.52
9:J:72:ASP:N	9:J:72:ASP:OD2	2.42	0.52
27:X:1481:U:O2'	27:X:1562:G:O2'	2.17	0.52
6:G:160:ALA:HB3	6:G:161:GLN:HE21	1.75	0.52
3:C:109:ALA:HA	3:C:112:GLN:HG2	1.91	0.52
27:X:717:G:H1'	27:X:739:G:N2	2.25	0.52
27:X:242:A:N6	27:X:440:U:O2'	2.42	0.52
27:X:1429:A:H1'	27:X:1603:A:C6	2.45	0.52
27:X:537:C:C5	27:X:2759:U:H2'	2.44	0.52
25:2:19:ARG:HG3	25:2:23:LYS:HE3	1.92	0.52
26:3:52:LYS:HZ1	27:X:2339:A:H5'	1.74	0.52
27:X:1211:G:N2	27:X:1262:U:O2	2.33	0.52
27:X:1342:U:H5''	27:X:1343:C:H5	1.74	0.52
27:X:1816:G:H2'	27:X:1817:U:C6	2.45	0.52
3:C:54:THR:HG22	3:C:55:GLY:O	2.10	0.52
17:R:84:VAL:CG1	17:R:90:LYS:H	2.23	0.52
3:C:2:ALA:N	3:C:12:GLY:O	2.42	0.52
10:K:12:ARG:NH2	10:K:20:LEU:HD13	2.24	0.52
8:I:35:LYS:NZ	27:X:575:U:H5''	2.25	0.52
27:X:692:C:H2'	27:X:693:A:C8	2.45	0.52
1:A:13:ARG:NE	1:A:27:LYS:HD3	2.24	0.52
27:X:2543:A:H5'	27:X:2627:G:H4'	1.92	0.52
8:I:53:ARG:HD2	8:I:54:SER:N	2.25	0.52
9:J:99:LYS:HG3	9:J:100:PRO:HD2	1.92	0.52
25:2:8:ASN:HB3	25:2:11:LYS:HB3	1.91	0.52
1:A:66:ASP:OD2	1:A:103:ARG:NH1	2.43	0.52
3:C:163:ASN:HA	27:X:334:G:O2'	2.10	0.52
27:X:125:A:H5''	27:X:126:C:O4'	2.10	0.52
14:O:22:VAL:HA	14:O:91:THR:HG23	1.92	0.52
27:X:2241:U:H2'	27:X:2242:C:H6	1.75	0.52
27:X:1674:C:H2'	27:X:1675:C:C6	2.45	0.52
3:C:56:ARG:NE	27:X:814:G:OP2	2.43	0.52
27:X:624:A:O5'	27:X:626:A:N6	2.43	0.52
18:S:140:LYS:HE3	18:S:147:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:ILE:HB	4:D:114:PHE:HB2	1.92	0.52
27:X:2640:G:H2'	27:X:2641:A:C8	2.44	0.51
8:I:30:ALA:N	27:X:824:U:H2'	2.25	0.51
6:G:103:TYR:HB3	6:G:107:GLN:HE21	1.75	0.51
24:1:14:SER:OG	24:1:52:GLU:HG2	2.10	0.51
1:A:42:GLY:C	1:A:43:ARG:HE	2.13	0.51
27:X:518:A:H4'	27:X:519:C:OP2	2.10	0.51
24:1:38:LYS:HD2	27:X:2265:A:C6	2.44	0.51
27:X:1991:C:H2'	27:X:1992:G:C8	2.45	0.51
9:J:21:ASP:C	9:J:99:LYS:HG2	2.31	0.51
27:X:746:G:N7	27:X:774:A:C6	2.78	0.51
27:X:227:G:C6	27:X:228:A:C6	2.98	0.51
27:X:455:A:H2	27:X:1258:G:N3	2.09	0.51
15:P:66:GLU:HB3	15:P:67:PRO:HD3	1.92	0.51
19:T:60:PHE:CZ	27:X:2344:G:H4'	2.45	0.51
9:J:24:GLY:HA3	27:X:920:G:P	2.50	0.51
7:H:100:ASN:HD21	7:H:104:GLU:HG3	1.74	0.51
27:X:1751:A:H2'	27:X:1752:U:C6	2.46	0.51
13:N:24:PHE:O	13:N:29:SER:HB3	2.11	0.51
27:X:1865:C:H2'	27:X:1866:G:H8	1.75	0.51
27:X:2167:A:H2'	27:X:2168:A:C8	2.45	0.51
27:X:2039:G:C2	27:X:2040:A:C8	2.98	0.51
27:X:650:U:H2'	27:X:651:C:C6	2.45	0.51
12:M:100:ARG:NH1	27:X:2824:C:OP2	2.44	0.51
22:W:3:ILE:HG21	22:W:23:LEU:HD13	1.92	0.51
27:X:2484:G:O2'	27:X:2485:U:H6	1.93	0.51
27:X:165:G:H1	27:X:185:C:H42	1.57	0.51
27:X:2621:G:H1	27:X:2752:C:H42	1.58	0.51
27:X:1301:U:O2'	27:X:1664:G:N2	2.43	0.51
6:G:139:ARG:HG2	6:G:142:ARG:HH12	1.75	0.51
15:P:14:ARG:HA	15:P:17:GLN:HG2	1.92	0.51
27:X:542:A:OP1	27:X:570:G:N2	2.38	0.51
1:A:61:LEU:HG	27:X:1584:G:H5''	1.93	0.51
17:R:13:LYS:NZ	27:X:349:G:OP1	2.22	0.51
3:C:176:ASN:ND2	3:C:178:TYR:HB3	2.26	0.51
27:X:2284:U:H5''	27:X:2286:G:H22	1.75	0.51
9:J:137:VAL:HG21	18:S:71:MET:HG3	1.93	0.51
7:H:17:ARG:H	7:H:58:ALA:HA	1.76	0.51
27:X:930:A:C2	28:Y:82:U:H4'	2.46	0.51
16:Q:62:ARG:O	16:Q:70:GLY:HA2	2.11	0.51
3:C:19:LEU:HA	3:C:20:PRO:C	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:58:ARG:O	13:N:62:ILE:HG13	2.10	0.51
27:X:2516:U:H2'	27:X:2517:C:H6	1.74	0.51
27:X:1656:U:C2'	27:X:1657:A:H5''	2.41	0.51
27:X:1777:A:H1'	27:X:1921:A:N6	2.25	0.51
27:X:1831:G:H2'	27:X:1832:G:H8	1.76	0.51
17:R:97:GLN:HB2	17:R:100:ASP:O	2.10	0.51
27:X:828:C:H42	27:X:1206:G:H1	1.57	0.51
11:L:79:ALA:HB1	11:L:84:ILE:HB	1.91	0.51
2:B:54:LYS:HD3	2:B:59:VAL:HG22	1.92	0.51
24:I:40:TYR:HB2	24:I:50:PHE:HB2	1.92	0.51
6:G:132:PHE:HZ	6:G:142:ARG:HA	1.75	0.51
27:X:746:G:N7	27:X:774:A:C5	2.79	0.51
18:S:20:ALA:O	18:S:80:HIS:ND1	2.43	0.51
27:X:77:C:H42	27:X:106:G:H1	1.59	0.51
1:A:133:LEU:HB2	1:A:187:SER:HA	1.93	0.51
3:C:163:ASN:HD22	3:C:165:SER:H	1.58	0.51
1:A:250:TRP:HA	1:A:250:TRP:CE3	2.46	0.51
15:P:108:PRO:HD3	15:P:119:ILE:HG21	1.92	0.51
27:X:1678:G:H1	27:X:1982:C:N4	2.09	0.51
11:L:16:LYS:HE2	28:Y:10:U:H5''	1.92	0.51
8:I:101:ARG:HG3	27:X:637:G:N1	2.26	0.51
27:X:451:A:H2'	27:X:452:G:C8	2.46	0.51
27:X:768:U:H2'	27:X:769:C:O4'	2.11	0.51
20:U:47:HIS:HE1	27:X:409:G:H4'	1.74	0.51
27:X:218:A:H61	27:X:232:A:H5''	1.76	0.51
4:D:56:GLU:HA	4:D:59:LEU:HD12	1.93	0.51
27:X:1313:U:H4'	27:X:1314:A:H5'	1.93	0.51
27:X:1692:C:H5	27:X:1693:A:C5	2.28	0.51
2:B:136:ARG:HH12	27:X:2033:C:H5''	1.75	0.51
27:X:2372:A:H62	27:X:2401:A:N6	2.09	0.51
10:K:82:GLU:O	10:K:85:PRO:HD2	2.11	0.51
18:S:168:VAL:HG12	18:S:169:VAL:HG12	1.93	0.51
27:X:2751:C:H2'	27:X:2752:C:C6	2.46	0.51
5:E:57:ASP:HB3	5:E:62:ARG:HE	1.76	0.51
18:S:104:SER:HA	18:S:139:THR:HA	1.92	0.51
28:Y:17:A:H1'	28:Y:112:A:N7	2.26	0.51
13:N:3:ARG:HB2	27:X:1261:G:C5	2.46	0.51
20:U:20:ARG:O	20:U:43:ARG:NH2	2.44	0.51
2:B:136:ARG:HG2	2:B:137:ARG:N	2.25	0.50
22:W:3:ILE:HG12	22:W:44:VAL:HG21	1.93	0.50
27:X:876:A:H2'	27:X:877:G:C8	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1149:G:O2'	27:X:1154:A:N1	2.41	0.50
27:X:87:G:H2'	27:X:88:G:H5''	1.93	0.50
27:X:1672:A:C6	27:X:1673:C:C2	3.00	0.50
25:2:12:ARG:HG2	27:X:699:G:H22	1.75	0.50
27:X:537:C:O2'	27:X:538:A:O5'	2.29	0.50
15:P:29:LYS:HA	15:P:126:HIS:HD2	1.75	0.50
9:J:75:VAL:O	9:J:92:GLU:HB3	2.10	0.50
27:X:1698:C:O2'	27:X:1753:A:N3	2.31	0.50
27:X:674:U:H2'	27:X:675:C:O4'	2.11	0.50
2:B:116:VAL:HG22	2:B:136:ARG:CG	2.31	0.50
1:A:246:PRO:HD3	1:A:252:LYS:HE3	1.94	0.50
2:B:189:PRO:HA	27:X:2659:C:C5'	2.38	0.50
27:X:1923:U:P	27:X:2582:G:H21	2.33	0.50
27:X:1532:A:O2'	27:X:1572:C:O2'	2.25	0.50
28:Y:16:U:O2'	28:Y:110:U:O2	2.30	0.50
27:X:2500:C:H42	27:X:2523:G:H1	1.58	0.50
2:B:193:GLY:O	12:M:2:GLN:N	2.44	0.50
27:X:1501:C:H2'	27:X:1502:G:O4'	2.11	0.50
8:I:62:LYS:NZ	26:3:13:ARG:HH11	2.09	0.50
27:X:2761:A:H5''	27:X:2762:G:H5'	1.92	0.50
2:B:203:LYS:HE3	27:X:2713:A:H61	1.77	0.50
11:L:8:ARG:CG	11:L:9:ARG:H	2.24	0.50
16:Q:54:SER:HB2	27:X:1354:A:H1'	1.92	0.50
27:X:1422:C:H2'	27:X:1423:A:H8	1.76	0.50
27:X:2655:C:O2	27:X:2712:G:N2	2.41	0.50
16:Q:73:ASN:OD1	16:Q:73:ASN:N	2.44	0.50
27:X:591:G:H1	27:X:1271:C:H42	1.57	0.50
18:S:117:VAL:HG22	18:S:168:VAL:HA	1.93	0.50
27:X:1949:A:O2'	27:X:2572:U:H5'	2.11	0.50
25:2:4:THR:O	27:X:700:C:H5'	2.12	0.50
9:J:6:LYS:HG3	9:J:45:SER:HB2	1.93	0.50
27:X:2309:G:H2'	27:X:2310:G:O4'	2.11	0.50
7:H:28:GLY:HA3	7:H:35:THR:OG1	2.10	0.50
14:O:36:LYS:NZ	14:O:54:TYR:HB3	2.27	0.50
14:O:36:LYS:HE3	14:O:56:VAL:HG22	1.93	0.50
27:X:114:C:O2'	27:X:124:A:N3	2.38	0.50
1:A:171:ASP:O	1:A:186:HIS:HB2	2.12	0.50
12:M:9:ARG:HA	12:M:12:LEU:HB2	1.94	0.50
3:C:111:ARG:NH1	3:C:183:HIS:O	2.45	0.50
28:Y:17:A:H1'	28:Y:112:A:C5	2.47	0.50
9:J:26:ASP:OD1	9:J:27:TYR:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:LYS:C	3:C:131:LYS:H	2.14	0.50
4:D:53:ALA:HB3	4:D:87:ILE:HD12	1.93	0.50
27:X:2528:G:H2'	27:X:2529:G:H8	1.76	0.50
27:X:2645:C:H3'	27:X:2646:C:H6	1.76	0.50
27:X:2328:G:O6	27:X:2361:G:N2	2.37	0.50
8:I:41:SER:OG	8:I:41:SER:O	2.25	0.50
24:1:21:TYR:HB3	24:1:50:PHE:HZ	1.75	0.50
11:L:8:ARG:HE	11:L:9:ARG:HG3	1.77	0.50
27:X:1806:G:H5''	27:X:1807:A:H2'	1.94	0.50
14:O:17:GLY:HA2	14:O:94:LYS:HA	1.92	0.50
7:H:64:VAL:HG22	7:H:106:ARG:NH2	2.27	0.50
27:X:393:U:H2'	27:X:394:U:C6	2.46	0.50
27:X:1846:A:H62	27:X:1871:G:H8	1.60	0.50
27:X:1202:U:H2'	27:X:1203:A:C8	2.35	0.50
4:D:74:ILE:HA	4:D:79:LEU:HB2	1.93	0.50
27:X:1103:C:H2'	27:X:1104:G:H8	1.77	0.50
27:X:1103:C:N4	27:X:1110:G:H1	2.10	0.50
2:B:122:PHE:CE1	2:B:138:PRO:HB3	2.47	0.50
27:X:1656:U:H2'	27:X:1657:A:H5''	1.94	0.50
3:C:128:ALA:C	3:C:130:THR:H	2.15	0.50
5:E:9:ILE:HA	5:E:69:ARG:HH11	1.77	0.50
17:R:42:ARG:NH2	27:X:86:U:OP2	2.45	0.50
5:E:76:VAL:HA	5:E:79:VAL:HG22	1.93	0.50
27:X:1050:G:N2	27:X:1051:U:O4	2.44	0.50
27:X:1982:C:H4'	27:X:2703:C:O2	2.12	0.50
27:X:2820:C:H2'	27:X:2821:G:H8	1.77	0.50
27:X:2318:U:H4'	28:Y:43:G:H22	1.75	0.50
17:R:74:LEU:HG	17:R:76:LEU:HD21	1.94	0.50
27:X:1070:G:H5''	27:X:1071:U:H2'	1.94	0.50
26:3:17:THR:OG1	26:3:18:GLY:N	2.45	0.50
27:X:1098:G:C5	27:X:1100:G:H1'	2.46	0.50
1:A:28:ARG:NH1	27:X:1583:A:N7	2.59	0.49
15:P:37:LYS:CE	15:P:64:ALA:HB2	2.42	0.49
27:X:2581:A:H8	27:X:2582:G:O4'	1.95	0.49
27:X:4:C:H42	27:X:2873:G:H1	1.60	0.49
20:U:20:ARG:HB3	20:U:43:ARG:NH2	2.27	0.49
27:X:2617:G:H1	27:X:2755:A:H2'	1.77	0.49
27:X:965:G:O2'	27:X:2253:A:N1	2.39	0.49
11:L:61:SER:O	11:L:61:SER:OG	2.25	0.49
27:X:659:G:H2'	27:X:660:G:C8	2.46	0.49
27:X:854:G:H2'	27:X:855:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:113:C:HO2'	27:X:125:A:HO2'	1.59	0.49
16:Q:48:VAL:HG11	16:Q:82:LEU:HD13	1.93	0.49
1:A:207:GLY:O	27:X:1782:A:O2'	2.25	0.49
7:H:109:ARG:HA	7:H:129:LEU:HD22	1.94	0.49
27:X:1235:C:N4	27:X:1240:G:H1	2.10	0.49
17:R:22:VAL:HG13	17:R:81:VAL:H	1.77	0.49
28:Y:58:G:O2'	28:Y:59:A:H5''	2.12	0.49
9:J:48:ILE:HD12	9:J:71:PRO:HD3	1.95	0.49
27:X:1159:U:H2'	27:X:1160:C:H6	1.77	0.49
27:X:1107:A:H3'	27:X:1108:U:H5''	1.94	0.49
23:Z:7:PRO:HA	27:X:2594:U:C6	2.47	0.49
1:A:182:LEU:HD12	1:A:269:PHE:HB2	1.93	0.49
27:X:2422:C:H2'	27:X:2423:G:H8	1.77	0.49
5:E:136:ILE:HD12	5:E:137:ASP:H	1.77	0.49
27:X:2757:G:H1'	27:X:2759:U:H5	1.77	0.49
27:X:854:G:H2'	27:X:855:G:H8	1.77	0.49
15:P:124:THR:OG1	15:P:126:HIS:N	2.29	0.49
28:Y:27:A:HO2'	28:Y:28:A:P	2.36	0.49
9:J:21:ASP:OD1	9:J:21:ASP:N	2.45	0.49
17:R:84:VAL:HG11	17:R:90:LYS:H	1.77	0.49
9:J:77:LYS:HD3	9:J:92:GLU:OE2	2.12	0.49
27:X:2006:G:H5'	27:X:2596:C:H4'	1.94	0.49
27:X:2513:A:C2	27:X:2514:G:H1'	2.46	0.49
10:K:87:TYR:OH	10:K:115:LEU:HD22	2.12	0.49
1:A:160:GLY:HA3	27:X:1812:U:N3	2.27	0.49
12:M:50:PHE:CE1	12:M:79:ARG:HG3	2.47	0.49
17:R:55:THR:OG1	17:R:72:ARG:NH1	2.46	0.49
26:3:62:LEU:HD23	27:X:219:G:H5'	1.95	0.49
15:P:80:LEU:HD11	15:P:87:GLU:HB3	1.94	0.49
27:X:1431:U:H4'	27:X:1604:A:H4'	1.95	0.49
27:X:1818:G:H2'	27:X:1819:U:H6	1.78	0.49
1:A:203:ASN:N	1:A:203:ASN:OD1	2.45	0.49
27:X:2549:G:H2'	27:X:2550:C:O4'	2.12	0.49
27:X:321:A:C6	27:X:323:G:C4	3.01	0.49
27:X:217:U:H3'	27:X:218:A:H2'	1.93	0.49
27:X:218:A:N6	27:X:232:A:H5''	2.28	0.49
27:X:2085:G:N1	27:X:2171:U:O2	2.45	0.49
27:X:2594:U:H2'	27:X:2595:C:H6	1.77	0.49
27:X:1449:C:N4	27:X:1450:G:O6	2.45	0.49
16:Q:46:PHE:CD2	16:Q:88:ILE:HB	2.47	0.49
27:X:1310:C:H2'	27:X:1311:C:H6	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:72:ASP:HB3	10:K:75:VAL:HG23	1.94	0.49
11:L:85:LYS:HE3	11:L:86:GLN:NE2	2.27	0.49
18:S:151:ASP:OD2	18:S:151:ASP:N	2.44	0.49
3:C:77:PHE:CD2	27:X:1270:C:H4'	2.48	0.49
27:X:693:A:H2'	27:X:694:G:C8	2.47	0.49
5:E:9:ILE:O	5:E:49:GLN:HB3	2.12	0.49
27:X:2856:U:H2'	27:X:2857:C:H6	1.78	0.49
27:X:1854:G:H2'	27:X:1855:G:H8	1.78	0.49
3:C:158:ARG:CZ	3:C:171:PRO:HB3	2.43	0.49
3:C:24:SER:HA	3:C:27:LEU:HD22	1.94	0.49
13:N:7:GLY:O	13:N:8:ILE:HG12	2.12	0.49
10:K:6:ALA:HB1	27:X:2848:A:C2	2.46	0.49
1:A:156:ALA:HB2	1:A:163:VAL:HG23	1.93	0.49
6:G:103:TYR:CD1	6:G:111:LYS:HB2	2.47	0.49
1:A:100:GLY:O	27:X:1516:A:O2'	2.26	0.49
11:L:15:ARG:O	11:L:18:ARG:HB3	2.13	0.49
13:N:4:ALA:HB2	27:X:1213:U:H1'	1.95	0.49
27:X:930:A:N3	28:Y:82:U:H4'	2.27	0.49
2:B:62:PRO:HG3	27:X:2767:C:H1'	1.93	0.49
28:Y:73:C:H2'	28:Y:74:A:O4'	2.12	0.49
27:X:946:U:H2'	27:X:947:C:H6	1.78	0.49
27:X:2705:A:C8	27:X:2706:U:H2'	2.48	0.49
4:D:65:PRO:HB3	4:D:89:VAL:HG22	1.94	0.49
3:C:17:LEU:HD23	3:C:112:GLN:HG3	1.94	0.49
17:R:95:ARG:HE	27:X:308:C:H5''	1.78	0.49
27:X:635:C:O2'	27:X:670:U:OP1	2.27	0.49
27:X:540:G:C6	27:X:2005:U:H5''	2.48	0.49
27:X:1451:C:H2'	27:X:1452:U:C6	2.48	0.49
9:J:26:ASP:H	9:J:103:VAL:HG12	1.78	0.49
4:D:122:PHE:HA	27:X:2282:G:H4'	1.95	0.49
27:X:1183:C:H2'	27:X:1184:G:H8	1.78	0.49
2:B:168:GLN:O	27:X:2710:C:O2'	2.24	0.49
27:X:966:A:H5''	27:X:967:G:OP2	2.13	0.49
6:G:36:ASN:N	6:G:36:ASN:OD1	2.42	0.49
1:A:43:ARG:N	1:A:43:ARG:HE	2.11	0.49
27:X:2758:A:O2'	27:X:2760:G:O2'	2.31	0.49
27:X:649:G:C8	27:X:650:U:H5	2.31	0.49
10:K:76:VAL:HA	10:K:79:VAL:HG12	1.95	0.49
27:X:1484:G:O6	27:X:1538:A:N6	2.46	0.49
27:X:399:G:H5'	27:X:401:G:H22	1.78	0.49
27:X:1660:G:H2'	27:X:1661:C:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:69:VAL:HG22	18:S:81:VAL:HG22	1.94	0.49
27:X:2677:U:H2'	27:X:2678:C:C6	2.48	0.49
27:X:57:G:H1	27:X:68:C:H42	1.59	0.49
27:X:1766:U:H2'	27:X:1767:G:O4'	2.13	0.49
27:X:1987:G:C5	27:X:1988:A:C8	3.01	0.49
27:X:1988:A:H5''	27:X:1989:C:H5	1.77	0.49
17:R:56:LYS:HD2	27:X:494:A:C8	2.47	0.49
27:X:303:C:H2'	27:X:304:A:H5''	1.95	0.49
27:X:2007:G:C2	27:X:2023:C:C2	3.00	0.49
7:H:47:VAL:HA	7:H:74:VAL:HG12	1.95	0.49
2:B:154:LYS:HG3	2:B:155:ARG:H	1.77	0.49
14:O:35:LEU:HA	14:O:55:THR:HG22	1.95	0.49
27:X:2837:G:H2'	27:X:2838:U:H6	1.76	0.49
26:3:26:LYS:HB2	26:3:45:GLY:H	1.78	0.49
15:P:118:ASN:ND2	15:P:120:ILE:HB	2.28	0.48
2:B:144:ARG:HD3	27:X:2551:A:C8	2.48	0.48
1:A:159:ALA:HA	1:A:198:ASN:OD1	2.13	0.48
27:X:2167:A:H2'	27:X:2168:A:H8	1.78	0.48
27:X:1787:U:H2'	27:X:1788:C:C6	2.47	0.48
27:X:388:G:H2'	27:X:389:G:H8	1.78	0.48
7:H:21:CYS:SG	7:H:22:ILE:N	2.86	0.48
27:X:2663:U:H3	27:X:2705:A:N6	2.11	0.48
1:A:159:ALA:HB3	27:X:1813:A:OP1	2.13	0.48
27:X:1586:A:H2'	27:X:1587:A:C8	2.48	0.48
4:D:71:LYS:N	27:X:2291:U:OP1	2.47	0.48
27:X:2837:G:H2'	27:X:2838:U:C6	2.48	0.48
14:O:24:SER:OG	14:O:25:LEU:N	2.45	0.48
27:X:405:C:H2'	27:X:406:G:C8	2.48	0.48
2:B:87:ASP:OD2	2:B:87:ASP:N	2.45	0.48
27:X:2827:G:H2'	27:X:2828:C:O4'	2.13	0.48
27:X:1563:U:H2'	27:X:1564:U:C6	2.47	0.48
27:X:2811:G:H2'	27:X:2812:A:H8	1.74	0.48
27:X:2284:U:H5''	27:X:2286:G:N2	2.28	0.48
27:X:1350:G:H2'	27:X:1351:G:C8	2.45	0.48
7:H:76:ARG:O	7:H:94:ASN:HA	2.13	0.48
25:2:33:ARG:HH21	27:X:478:G:P	2.36	0.48
27:X:838:A:H4'	27:X:2407:G:C5	2.49	0.48
16:Q:10:PRO:HA	16:Q:27:PHE:HB3	1.95	0.48
27:X:29:U:H6	27:X:29:U:O5'	1.97	0.48
27:X:810:U:H2'	27:X:811:G:O4'	2.13	0.48
27:X:1655:C:H5''	27:X:2689:C:O2'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:43:THR:HA	25:2:46:ASP:HB2	1.96	0.48
27:X:1326:U:H4'	27:X:1345:G:H4'	1.96	0.48
1:A:251:GLY:HA3	1:A:255:LYS:HZ1	1.76	0.48
25:2:21:ARG:NH2	27:X:476:G:O3'	2.46	0.48
2:B:35:GLN:HB2	2:B:48:GLN:OE1	2.13	0.48
27:X:1008:G:H1	27:X:1169:C:H42	1.61	0.48
8:I:101:ARG:HG3	27:X:637:G:H1	1.78	0.48
27:X:2058:U:C4	27:X:2217:G:C6	3.02	0.48
27:X:1031:C:H5''	27:X:1032:A:N3	2.29	0.48
23:Z:10:LYS:HE2	27:X:1275:A:N3	2.29	0.48
12:M:34:ARG:NH2	12:M:35:VAL:O	2.26	0.48
27:X:231:G:H4'	27:X:397:U:H5''	1.95	0.48
9:J:83:ARG:HH12	27:X:971:A:N6	2.12	0.48
27:X:838:A:H2'	27:X:839:U:O4'	2.14	0.48
27:X:540:G:N1	27:X:2005:U:OP1	2.46	0.48
27:X:1135:C:H2'	27:X:1136:G:O4'	2.12	0.48
27:X:1441:A:H4'	27:X:1442:C:O5'	2.13	0.48
27:X:2185:U:H2'	27:X:2186:G:C8	2.49	0.48
26:3:16:ILE:HD12	26:3:64:ARG:HE	1.78	0.48
27:X:1514:C:H4'	27:X:1592:U:O2'	2.13	0.48
1:A:55:GLY:N	1:A:217:ARG:HB2	2.05	0.48
7:H:40:GLY:HA3	27:X:2545:A:N6	2.23	0.48
1:A:143:HIS:HB2	1:A:156:ALA:O	2.14	0.48
2:B:5:LEU:HD12	2:B:49:ILE:HD11	1.96	0.48
17:R:59:LYS:HD2	17:R:62:MET:CB	2.41	0.48
27:X:48:A:H4'	27:X:49:U:C5'	2.43	0.48
11:L:8:ARG:HH21	11:L:9:ARG:NE	2.12	0.48
17:R:45:LYS:HA	17:R:76:LEU:O	2.13	0.48
27:X:1342:U:H5''	27:X:1343:C:C5	2.48	0.48
27:X:1072:U:H4'	27:X:1081:A:O2'	2.13	0.48
15:P:106:LEU:O	15:P:109:ARG:HD2	2.14	0.48
18:S:46:GLN:HE22	18:S:52:PHE:HB2	1.78	0.48
27:X:1316:G:H5'	27:X:1659:G:H21	1.78	0.48
6:G:62:ILE:O	6:G:77:GLY:HA3	2.13	0.48
24:1:9:ILE:O	24:1:10:VAL:HB	2.14	0.48
27:X:1060:C:H1'	27:X:1124:U:O2'	2.13	0.48
27:X:1495:G:H5'	27:X:1574:A:H2	1.77	0.48
28:Y:46:G:N3	28:Y:49:C:N4	2.62	0.48
26:3:29:LYS:HD2	26:3:33:ASN:O	2.13	0.48
13:N:47:TYR:CE2	14:O:73:LYS:HE2	2.47	0.48
12:M:2:GLN:HG3	12:M:3:THR:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:90:ARG:HH12	12:M:108:ARG:NH2	2.11	0.48
23:Z:8:LYS:HE2	27:X:2039:G:O2'	2.14	0.48
5:E:160:LYS:NZ	27:X:2636:A:O3'	2.47	0.48
6:G:101:THR:HG23	6:G:103:TYR:CE1	2.49	0.48
4:D:57:LEU:O	4:D:61:THR:OG1	2.30	0.48
27:X:1059:A:HO2'	27:X:1060:C:P	2.34	0.48
27:X:492:G:HO2'	27:X:493:A:P	2.37	0.48
27:X:246:C:H1'	27:X:437:G:N2	2.28	0.48
19:T:74:LYS:O	19:T:76:ALA:N	2.42	0.48
7:H:28:GLY:O	7:H:35:THR:HG23	2.13	0.48
27:X:1935:A:C6	27:X:1936:A:N1	2.82	0.48
8:I:62:LYS:HZ1	26:3:13:ARG:HH11	1.61	0.48
28:Y:80:A:H2'	28:Y:81:C:O4'	2.14	0.48
13:N:37:GLN:NE2	27:X:1265:G:H22	2.12	0.48
7:H:75:VAL:HG22	7:H:96:ALA:HA	1.96	0.48
27:X:2437:G:H21	27:X:2438:A:H61	1.62	0.48
4:D:35:VAL:HG11	27:X:2293:G:H5'	1.95	0.48
11:L:65:THR:HG21	28:Y:52:G:OP2	2.13	0.48
8:I:75:VAL:O	8:I:108:LEU:HD12	2.14	0.48
12:M:103:LYS:N	12:M:103:LYS:HD2	2.28	0.48
3:C:70:GLY:H	27:X:687:G:H5''	1.78	0.48
2:B:165:VAL:HG11	27:X:2658:A:H4'	1.95	0.48
27:X:587:A:H8	27:X:587:A:OP2	1.97	0.48
15:P:78:ASN:HD21	27:X:504:G:H21	1.61	0.48
13:N:13:ARG:NH1	27:X:1264:C:H5''	2.29	0.48
27:X:1924:C:C4	27:X:1925:C:C4	3.02	0.48
27:X:1919:A:N6	27:X:1946:U:H3	2.10	0.48
9:J:83:ARG:NH2	27:X:971:A:H61	2.11	0.48
27:X:2437:G:H21	27:X:2438:A:N6	2.12	0.48
27:X:1098:G:N2	27:X:1114:A:H1'	2.29	0.48
20:U:63:SER:O	20:U:67:LEU:N	2.47	0.48
27:X:73:A:H5''	27:X:74:G:O4'	2.13	0.48
27:X:1947:G:O2'	27:X:1950:C:OP1	2.28	0.48
2:B:116:VAL:HG13	2:B:136:ARG:HE	1.78	0.47
13:N:7:GLY:O	13:N:9:VAL:HG23	2.14	0.47
27:X:820:U:H2'	27:X:821:A:C8	2.45	0.47
9:J:83:ARG:HH22	27:X:971:A:N6	2.11	0.47
27:X:1332:G:C6	27:X:1333:G:N1	2.82	0.47
21:V:47:ARG:HH22	27:X:59:G:P	2.37	0.47
4:D:106:ILE:HG21	4:D:139:PRO:HB3	1.95	0.47
14:O:75:LYS:HB2	14:O:80:TYR:HD1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2498:U:C5	27:X:2520:A:C6	3.02	0.47
27:X:1686:A:H5''	27:X:1687:C:OP2	2.13	0.47
6:G:75:ILE:HB	6:G:147:ARG:HH12	1.77	0.47
27:X:1141:U:O5'	27:X:1141:U:H6	1.97	0.47
15:P:95:ALA:HB2	15:P:129:ILE:HG23	1.95	0.47
27:X:1573:G:H3'	27:X:1574:A:H5''	1.95	0.47
18:S:71:MET:HA	18:S:78:PRO:HA	1.96	0.47
9:J:70:PHE:CD2	27:X:884:C:H4'	2.49	0.47
2:B:14:ILE:HG12	12:M:20:HIS:HD2	1.77	0.47
20:U:48:LYS:HD2	27:X:2074:U:H1'	1.96	0.47
27:X:2442:C:H2'	27:X:2443:C:C6	2.48	0.47
9:J:6:LYS:O	9:J:71:PRO:HG2	2.14	0.47
7:H:64:VAL:HG22	7:H:106:ARG:HH21	1.80	0.47
5:E:88:GLU:HB3	5:E:163:ARG:HG3	1.96	0.47
21:V:23:LYS:O	21:V:27:GLU:HG2	2.14	0.47
22:W:22:ALA:HA	27:X:942:U:O2'	2.13	0.47
27:X:2625:U:O5'	27:X:2625:U:H6	1.97	0.47
27:X:841:G:H2'	27:X:842:A:N7	2.28	0.47
26:3:19:THR:HB	26:3:21:LYS:HG3	1.96	0.47
10:K:29:LEU:HD13	10:K:79:VAL:HB	1.96	0.47
27:X:725:C:H2'	27:X:726:G:C8	2.50	0.47
27:X:219:G:N2	27:X:231:G:H2'	2.29	0.47
15:P:80:LEU:HD21	15:P:87:GLU:HB3	1.97	0.47
27:X:2487:G:C2	27:X:2561:G:C6	3.02	0.47
12:M:27:PHE:HB3	12:M:93:ILE:HD12	1.95	0.47
27:X:1204:G:H2'	27:X:1205:G:C8	2.48	0.47
27:X:692:C:H2'	27:X:693:A:H8	1.79	0.47
8:I:62:LYS:HG3	26:3:13:ARG:HG2	1.95	0.47
28:Y:32:C:H1'	28:Y:59:A:H61	1.79	0.47
27:X:502:A:H2'	27:X:503:G:O4'	2.13	0.47
27:X:203:G:H2'	27:X:204:A:C8	2.49	0.47
1:A:142:VAL:HA	1:A:194:GLY:H	1.78	0.47
1:A:38:PRO:HB3	27:X:1586:A:H5'	1.96	0.47
3:C:27:LEU:O	3:C:31:VAL:HG22	2.13	0.47
27:X:1316:G:N2	27:X:1317:G:H1'	2.30	0.47
28:Y:53:G:H2'	28:Y:54:U:H5''	1.97	0.47
27:X:1021:A:N3	27:X:1164:C:H1'	2.29	0.47
27:X:1774:A:H5'	27:X:2587:G:H4'	1.95	0.47
27:X:126:C:N4	27:X:127:C:H41	2.12	0.47
27:X:2662:C:H2'	27:X:2663:U:H6	1.79	0.47
24:1:9:ILE:HA	24:1:28:ARG:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:GLY:O	10:K:3:HIS:CD2	2.65	0.47
27:X:1495:G:H5'	27:X:1574:A:C2	2.48	0.47
27:X:82:G:N2	27:X:100:G:H1'	2.29	0.47
27:X:346:C:H2'	27:X:347:C:C5	2.49	0.47
20:U:20:ARG:HB3	20:U:43:ARG:CZ	2.44	0.47
27:X:998:C:O2'	27:X:1011:A:N3	2.35	0.47
27:X:1478:U:H2'	27:X:1479:G:C8	2.50	0.47
27:X:824:U:O2	27:X:1263:G:H3'	2.15	0.47
16:Q:35:LYS:HB2	27:X:1614:C:H5''	1.97	0.47
27:X:2298:U:H1'	27:X:2299:A:C6	2.48	0.47
14:O:39:PHE:HE2	14:O:46:VAL:HB	1.79	0.47
1:A:209:ALA:HB2	27:X:1781:C:O2'	2.15	0.47
7:H:13:ASN:HD21	7:H:109:ARG:H	1.63	0.47
4:D:55:LYS:O	4:D:59:LEU:HG	2.14	0.47
7:H:47:VAL:HG11	7:H:115:ALA:CB	2.44	0.47
28:Y:96:C:H2'	28:Y:97:C:C6	2.48	0.47
27:X:557:U:H1'	27:X:558:G:C5	2.49	0.47
13:N:54:LYS:NZ	27:X:1006:C:OP2	2.47	0.47
2:B:14:ILE:HA	12:M:20:HIS:HD2	1.79	0.47
27:X:774:A:C8	27:X:774:A:O5'	2.68	0.47
27:X:398:C:N4	27:X:424:G:H1	2.12	0.47
13:N:45:TYR:HH	27:X:570:G:HO2'	1.61	0.47
27:X:1211:G:H2'	27:X:1212:U:H6	1.80	0.47
27:X:1436:G:N2	27:X:1514:C:H1'	2.30	0.47
16:Q:20:MET:HG3	16:Q:25:TYR:HE1	1.80	0.47
27:X:1376:C:O2'	27:X:1800:A:H1'	2.15	0.47
27:X:1621:C:H2'	27:X:1622:G:O4'	2.14	0.47
9:J:53:ILE:O	9:J:57:ARG:HG2	2.14	0.47
17:R:26:SER:OG	17:R:27:GLY:N	2.45	0.47
27:X:1193:G:H2'	27:X:1194:U:C6	2.49	0.47
27:X:302:U:O4	27:X:360:A:N6	2.48	0.47
2:B:38:THR:HG22	2:B:40:GLN:H	1.78	0.47
27:X:1785:A:H2'	27:X:1786:C:C6	2.50	0.47
5:E:17:VAL:HG22	5:E:26:VAL:HG13	1.96	0.47
27:X:2579:A:H2'	27:X:2580:C:C6	2.50	0.47
27:X:936:A:H2'	27:X:937:C:O4'	2.14	0.47
27:X:498:C:N4	27:X:499:G:O6	2.48	0.47
10:K:92:GLY:O	27:X:2855:C:H1'	2.14	0.47
1:A:13:ARG:NE	1:A:27:LYS:HB3	2.24	0.47
3:C:77:PHE:CE2	27:X:1270:C:H4'	2.49	0.47
6:G:70:PHE:O	13:N:64:ARG:NE	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:LYS:HD2	2:B:203:LYS:HA	1.49	0.47
26:3:34:THR:HG23	27:X:2399:C:OP2	2.15	0.47
27:X:554:U:H5''	27:X:556:A:C2	2.50	0.47
26:3:16:ILE:HD12	26:3:64:ARG:HG2	1.97	0.47
27:X:2194:A:H2'	27:X:2195:C:O4'	2.14	0.47
24:1:51:ARG:NH1	24:1:53:LYS:HB3	2.29	0.47
12:M:101:ARG:HH21	12:M:101:ARG:HG2	1.80	0.47
27:X:793:G:N2	27:X:796:A:H62	2.09	0.47
27:X:825:C:H5''	27:X:1263:G:O2'	2.14	0.47
27:X:1770:U:H5	27:X:1775:A:N7	2.13	0.47
7:H:11:ALA:N	7:H:96:ALA:O	2.39	0.47
27:X:437:G:H2'	27:X:438:G:C8	2.47	0.47
27:X:2707:G:H2'	27:X:2708:U:C6	2.50	0.47
20:U:15:VAL:HA	20:U:45:ASN:O	2.14	0.47
27:X:228:A:C5	27:X:229:G:H1'	2.50	0.47
8:I:51:GLY:HA3	26:3:59:LYS:HE3	1.97	0.47
27:X:1714:A:OP2	27:X:1715:A:O2'	2.25	0.47
27:X:105:G:H21	27:X:357:A:H61	1.63	0.47
10:K:49:GLU:O	10:K:52:ILE:HG12	2.15	0.47
14:O:71:ILE:HD13	27:X:1003:C:H4'	1.96	0.47
5:E:56:SER:OG	5:E:61:HIS:NE2	2.48	0.47
4:D:148:LYS:H	4:D:148:LYS:HD3	1.80	0.47
1:A:243:GLY:C	1:A:244:ARG:HE	2.19	0.47
23:Z:10:LYS:HG3	27:X:1276:U:H1'	1.96	0.47
10:K:73:LYS:HA	10:K:76:VAL:HG12	1.97	0.47
27:X:732:G:H2'	27:X:733:G:C8	2.49	0.47
27:X:2010:G:C6	27:X:2011:U:C4	3.03	0.47
27:X:1174:G:C2	27:X:1175:A:C5	3.03	0.47
27:X:773:G:H2'	27:X:774:A:H5'	1.97	0.47
8:I:32:ARG:HH12	14:O:82:ARG:HH21	1.63	0.47
27:X:5:A:H2'	27:X:6:A:C8	2.49	0.47
5:E:67:LEU:O	5:E:71:LEU:HG	2.15	0.47
18:S:141:MET:SD	18:S:147:ILE:HG12	2.55	0.47
4:D:37:ASN:ND2	4:D:87:ILE:O	2.48	0.47
2:B:124:GLY:HA2	2:B:135:HIS:O	2.15	0.47
17:R:48:VAL:HG13	17:R:50:GLY:H	1.79	0.47
2:B:52:ALA:O	2:B:76:ARG:N	2.31	0.47
13:N:8:ILE:O	13:N:12:ARG:HG3	2.15	0.46
27:X:476:G:H2'	27:X:477:A:C8	2.49	0.46
1:A:27:LYS:HE2	1:A:29:PRO:HD3	1.97	0.46
8:I:58:ALA:O	8:I:59:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:552:C:C2'	27:X:553:C:H5''	2.43	0.46
27:X:2200:G:H2'	27:X:2201:G:H8	1.79	0.46
27:X:2494:C:O2	27:X:2549:G:C2	2.68	0.46
27:X:992:A:N1	27:X:2010:G:O2'	2.37	0.46
27:X:346:C:H2'	27:X:347:C:C6	2.50	0.46
27:X:2645:C:H3'	27:X:2646:C:C6	2.50	0.46
2:B:133:LYS:O	2:B:134:TRP:HD1	1.98	0.46
1:A:157:ARG:HH11	1:A:157:ARG:HB2	1.80	0.46
1:A:218:LYS:HB2	1:A:218:LYS:HE2	1.44	0.46
27:X:2844:G:H2'	27:X:2845:C:O4'	2.15	0.46
27:X:2691:C:H2'	27:X:2694:G:H5''	1.97	0.46
14:O:72:ARG:HA	14:O:82:ARG:O	2.15	0.46
9:J:77:LYS:H	9:J:89:GLY:HA3	1.79	0.46
4:D:135:GLN:N	4:D:150:ARG:O	2.48	0.46
1:A:182:LEU:HB2	1:A:268:ARG:O	2.14	0.46
12:M:55:ILE:O	12:M:103:LYS:O	2.33	0.46
27:X:1256:C:H2'	27:X:1257:U:C6	2.50	0.46
27:X:170:U:O3'	27:X:816:U:H4'	2.15	0.46
1:A:118:ASN:HD22	1:A:119:ALA:H	1.63	0.46
15:P:26:ALA:O	15:P:128:THR:HA	2.15	0.46
2:B:9:ILE:CD1	2:B:27:LEU:HB2	2.44	0.46
27:X:1018:C:C5	27:X:1019:U:H5	2.33	0.46
27:X:26:G:H1'	27:X:525:A:N6	2.30	0.46
2:B:21:ILE:HD12	2:B:185:LYS:HD2	1.96	0.46
16:Q:15:LYS:HD2	16:Q:15:LYS:HA	1.62	0.46
27:X:2223:U:H2'	27:X:2224:U:O4'	2.15	0.46
10:K:87:TYR:HE1	10:K:94:TYR:HD1	1.63	0.46
12:M:103:LYS:HG2	27:X:2698:G:H4'	1.95	0.46
3:C:15:ILE:HD11	3:C:195:ILE:HA	1.98	0.46
27:X:1427:G:O6	27:X:1428:G:N2	2.36	0.46
7:H:7:ARG:HA	7:H:20:MET:HA	1.97	0.46
27:X:1156:U:H2'	27:X:1157:G:H8	1.81	0.46
27:X:2825:A:C2	27:X:2826:C:C2	3.03	0.46
27:X:2732:C:H2'	27:X:2733:A:O4'	2.15	0.46
17:R:14:LEU:HA	17:R:14:LEU:HD23	1.62	0.46
27:X:2478:C:N4	27:X:2479:U:C4	2.84	0.46
27:X:2555:G:OP1	27:X:2555:G:H3'	2.16	0.46
27:X:1398:G:O2'	27:X:1399:C:O5'	2.33	0.46
17:R:105:ARG:NH1	17:R:113:THR:H	2.14	0.46
23:Z:51:TYR:CE2	23:Z:55:ARG:HB2	2.50	0.46
27:X:555:U:O2'	27:X:1234:C:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1777:A:C4	27:X:1921:A:C6	3.04	0.46
8:I:73:GLU:OE2	8:I:101:ARG:HB2	2.16	0.46
4:D:72:LYS:HA	4:D:81:GLN:HA	1.97	0.46
6:G:65:LYS:HE3	6:G:66:HIS:CE1	2.49	0.46
27:X:1418:C:H2'	27:X:1419:G:C8	2.49	0.46
27:X:2230:G:OP2	27:X:2230:G:H8	1.98	0.46
25:2:13:ALA:HB1	27:X:123:A:H1'	1.97	0.46
12:M:13:LEU:HD12	12:M:13:LEU:HA	1.60	0.46
10:K:3:HIS:CD2	10:K:5:LYS:NZ	2.83	0.46
2:B:34:VAL:HG21	2:B:78:LEU:HD22	1.97	0.46
27:X:1451:C:H2'	27:X:1452:U:H6	1.80	0.46
14:O:73:LYS:HB2	14:O:82:ARG:HB2	1.98	0.46
27:X:1212:U:H2'	27:X:1213:U:H6	1.80	0.46
27:X:624:A:H4'	27:X:626:A:N7	2.30	0.46
9:J:68:ARG:CZ	9:J:103:VAL:HG11	2.46	0.46
27:X:1355:A:N1	27:X:1358:C:C2	2.83	0.46
27:X:192:G:H4'	27:X:193:A:H4'	1.98	0.46
21:V:25:LEU:HD12	21:V:25:LEU:HA	1.63	0.46
27:X:1467:U:H3'	27:X:1467:U:H6	1.80	0.46
6:G:103:TYR:CD2	27:X:1142:G:N3	2.83	0.46
27:X:2199:C:H2'	27:X:2200:G:C8	2.46	0.46
27:X:2299:A:H5''	27:X:2300:G:OP1	2.16	0.46
27:X:2522:G:H2'	27:X:2523:G:C8	2.51	0.46
24:1:3:LYS:NZ	24:1:7:ARG:HH11	2.14	0.46
27:X:721:C:H42	27:X:736:G:H1	1.64	0.46
5:E:86:ASN:HB2	5:E:165:VAL:HG22	1.98	0.46
7:H:55:VAL:HG23	7:H:68:ASP:O	2.16	0.46
27:X:650:U:H2'	27:X:651:C:H6	1.80	0.46
2:B:5:LEU:HD11	2:B:79:ARG:HB3	1.97	0.46
27:X:591:G:H1	27:X:1271:C:N4	2.14	0.46
27:X:618:A:H2'	27:X:619:A:C8	2.50	0.46
14:O:10:LYS:NZ	14:O:13:ARG:HH22	2.12	0.46
27:X:597:U:O4	27:X:683:A:H1'	2.16	0.46
5:E:163:ARG:NH2	5:E:169:ILE:HB	2.31	0.46
27:X:2453:C:H5''	27:X:2454:C:OP2	2.16	0.46
3:C:40:ARG:NH2	27:X:39:C:O2	2.49	0.46
2:B:136:ARG:HH22	27:X:2033:C:H4'	1.81	0.46
27:X:1834:G:H2'	27:X:1835:C:C6	2.50	0.46
15:P:78:ASN:HD21	27:X:504:G:N2	2.14	0.46
16:Q:55:THR:OG1	16:Q:76:LYS:HE3	2.15	0.46
27:X:1872:A:N1	27:X:2213:G:H1'	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2372:A:H62	27:X:2401:A:H61	1.64	0.46
9:J:82:THR:HG22	27:X:2475:C:OP2	2.15	0.46
27:X:1455:C:H2'	27:X:1456:C:C6	2.49	0.46
27:X:627:A:H2'	27:X:628:A:H8	1.78	0.46
17:R:16:PHE:CZ	17:R:46:VAL:HG22	2.51	0.46
27:X:1081:A:N7	27:X:1108:U:H4'	2.31	0.46
27:X:2656:G:H1	27:X:2710:C:H42	1.64	0.46
27:X:1922:U:H5	27:X:1950:C:HO2'	1.63	0.46
4:D:22:TYR:OH	4:D:165:GLU:OE1	2.30	0.46
14:O:86:HIS:NE2	14:O:88:GLN:HB2	2.31	0.46
13:N:2:PRO:HA	27:X:457:C:OP1	2.15	0.46
11:L:91:ARG:NH2	27:X:2355:A:H61	2.14	0.46
15:P:21:ARG:NH2	27:X:507:A:OP1	2.49	0.46
23:Z:15:LYS:HA	23:Z:15:LYS:HD2	1.64	0.46
17:R:103:LYS:HB3	17:R:103:LYS:HE2	1.76	0.46
9:J:117:GLU:HA	9:J:120:ARG:HB2	1.97	0.46
15:P:31:VAL:O	15:P:124:THR:HA	2.15	0.46
3:C:162:ARG:HG3	27:X:333:A:OP1	2.16	0.46
19:T:37:LEU:HD23	19:T:79:ILE:HG21	1.98	0.46
15:P:114:ARG:HD2	27:X:760:U:O2	2.16	0.46
2:B:203:LYS:HZ3	2:B:204:ALA:H	1.63	0.46
27:X:2245:A:H4'	27:X:2246:A:C2	2.51	0.46
16:Q:20:MET:HG3	16:Q:25:TYR:CE1	2.51	0.46
27:X:105:G:N2	27:X:357:A:H61	2.14	0.46
15:P:30:TYR:CE1	15:P:101:PRO:HG3	2.51	0.46
1:A:39:LYS:HB2	1:A:62:TYR:HB2	1.98	0.46
18:S:134:LEU:HA	18:S:134:LEU:HD12	1.81	0.46
2:B:114:GLN:HG3	2:B:160:MET:SD	2.55	0.46
27:X:1073:G:H1	27:X:1087:C:H42	1.64	0.46
28:Y:39:C:H5'	28:Y:40:C:OP2	2.16	0.46
27:X:1174:G:H2'	27:X:1175:A:C8	2.49	0.46
27:X:27:G:O2'	27:X:28:A:OP2	2.28	0.46
27:X:788:G:H5'	27:X:790:A:C1'	2.45	0.46
27:X:788:G:H5'	27:X:790:A:H1'	1.98	0.46
13:N:22:LYS:C	13:N:24:PHE:H	2.18	0.46
27:X:408:U:H2'	27:X:409:G:C8	2.51	0.46
14:O:40:VAL:HA	14:O:45:THR:HG22	1.97	0.46
27:X:179:U:H2'	27:X:180:C:O4'	2.16	0.46
27:X:485:G:C6	27:X:520:C:N4	2.83	0.46
27:X:2427:A:H3'	27:X:2428:U:H2'	1.97	0.46
27:X:1795:C:H2'	27:X:1796:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:12:U:H5	27:X:536:A:H62	1.64	0.45
27:X:1468:A:OP2	27:X:1468:A:C8	2.69	0.45
27:X:2055:G:C6	27:X:2056:C:C4	3.04	0.45
8:I:31:GLY:O	8:I:32:ARG:HG3	2.16	0.45
18:S:147:ILE:HB	18:S:169:VAL:HG13	1.97	0.45
7:H:80:ALA:HB2	7:H:90:ARG:HD3	1.98	0.45
27:X:849:G:C5	27:X:850:C:C4	3.04	0.45
15:P:104:LYS:NZ	15:P:119:ILE:HG22	2.31	0.45
12:M:50:PHE:CE2	12:M:70:LYS:HB3	2.50	0.45
27:X:1283:C:H5''	27:X:1284:G:C5'	2.46	0.45
6:G:67:ARG:CG	6:G:70:PHE:HA	2.47	0.45
27:X:540:G:H21	27:X:2004:U:H1'	1.81	0.45
27:X:877:G:H1	27:X:924:C:H42	1.62	0.45
27:X:1793:A:OP2	27:X:1806:G:N1	2.49	0.45
1:A:208:LYS:HD3	1:A:208:LYS:HA	1.60	0.45
27:X:1802:A:H2'	27:X:1803:G:O4'	2.16	0.45
4:D:46:ASP:HB2	4:D:49:ALA:H	1.81	0.45
14:O:20:ILE:HG12	14:O:21:ARG:N	2.31	0.45
2:B:133:LYS:C	2:B:134:TRP:CD1	2.90	0.45
15:P:33:MET:O	15:P:123:ARG:O	2.34	0.45
27:X:825:C:H5''	27:X:1263:G:HO2'	1.80	0.45
27:X:824:U:H1'	27:X:1264:C:O4'	2.16	0.45
10:K:66:VAL:HG12	10:K:76:VAL:HG23	1.98	0.45
1:A:218:LYS:HA	1:A:219:PRO:HD3	1.58	0.45
1:A:210:GLY:HA2	1:A:213:ARG:CG	2.46	0.45
3:C:128:ALA:O	3:C:130:THR:N	2.49	0.45
7:H:17:ARG:HG3	7:H:58:ALA:HA	1.98	0.45
12:M:69:ARG:HG3	12:M:78:GLU:HG2	1.98	0.45
27:X:706:A:H2'	27:X:707:U:O4'	2.16	0.45
27:X:1433:A:OP2	27:X:1593:C:N4	2.45	0.45
27:X:2178:U:H2'	27:X:2179:C:C6	2.51	0.45
24:1:36:GLU:HB3	24:1:52:GLU:HB2	1.97	0.45
27:X:1925:C:OP2	27:X:1926:U:O2'	2.29	0.45
27:X:490:A:H1'	27:X:491:A:H5''	1.98	0.45
26:3:29:LYS:HE3	26:3:34:THR:HB	1.98	0.45
20:U:49:LYS:HB2	20:U:61:TRP:NE1	2.31	0.45
27:X:2572:U:H2'	27:X:2573:C:C6	2.51	0.45
27:X:612:G:HO2'	27:X:614:G:HO2'	1.64	0.45
10:K:102:THR:HA	10:K:109:THR:HA	1.99	0.45
27:X:2268:G:H5'	27:X:2363:G:O2'	2.16	0.45
5:E:155:ASP:OD2	5:E:158:HIS:N	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:100:TYR:HB2	6:G:116:ARG:CZ	2.46	0.45
18:S:74:ARG:HH22	28:Y:94:G:H5''	1.81	0.45
27:X:225:G:N7	27:X:227:G:H1'	2.30	0.45
27:X:224:G:H4'	27:X:399:G:C6	2.51	0.45
26:3:23:MET:HG2	26:3:48:PHE:CE2	2.51	0.45
23:Z:6:VAL:HG22	23:Z:7:PRO:HD2	1.97	0.45
1:A:223:GLY:O	1:A:226:MET:N	2.37	0.45
8:I:56:LEU:CB	26:3:52:LYS:HZ2	2.29	0.45
13:N:91:ASN:HB3	13:N:95:LEU:HD13	1.99	0.45
27:X:2170:C:H3'	27:X:2171:U:H5''	1.98	0.45
3:C:42:THR:HG21	27:X:38:G:N2	2.30	0.45
27:X:2053:G:C2	27:X:2054:A:C4	3.05	0.45
12:M:37:THR:HG22	12:M:87:LEU:HD22	1.99	0.45
27:X:1781:C:H2'	27:X:1782:A:C5	2.51	0.45
27:X:836:G:H2'	27:X:837:U:C6	2.51	0.45
18:S:22:VAL:HG21	28:Y:77:G:H1'	1.99	0.45
27:X:1750:A:H4'	27:X:2695:C:O4'	2.17	0.45
15:P:32:ARG:HB3	15:P:32:ARG:CZ	2.47	0.45
2:B:39:ALA:HA	2:B:43:GLY:H	1.82	0.45
27:X:1407:G:O6	27:X:1408:A:N6	2.50	0.45
3:C:74:VAL:HG22	3:C:77:PHE:HD1	1.81	0.45
24:1:42:PRO:O	24:1:46:LYS:HG2	2.16	0.45
24:1:46:LYS:O	24:1:48:VAL:HG13	2.16	0.45
12:M:16:ILE:H	12:M:16:ILE:HD12	1.81	0.45
27:X:2191:A:H5''	27:X:2192:U:H5	1.82	0.45
3:C:18:PRO:HD2	3:C:109:ALA:HB2	1.99	0.45
27:X:597:U:H5''	27:X:598:U:OP2	2.17	0.45
10:K:49:GLU:OE1	10:K:95:THR:HG22	2.16	0.45
3:C:97:ARG:O	3:C:101:GLN:HG2	2.17	0.45
27:X:1561:A:O2'	27:X:1562:G:OP2	2.34	0.45
13:N:66:ASN:HD22	13:N:70:ARG:NH2	2.14	0.45
27:X:588:G:N2	27:X:1275:A:C4	2.84	0.45
27:X:2791:C:O2	27:X:2858:A:O2'	2.30	0.45
1:A:163:VAL:HG22	1:A:177:LEU:HA	1.99	0.45
27:X:1142:G:O6	27:X:2023:C:H1'	2.17	0.45
17:R:23:ILE:HD12	17:R:31:GLY:HA2	1.97	0.45
9:J:15:ARG:HG2	9:J:73:LYS:HZ2	1.82	0.45
20:U:49:LYS:HB2	20:U:61:TRP:CD1	2.52	0.45
2:B:133:LYS:HB2	2:B:137:ARG:CG	2.38	0.45
27:X:2494:C:N4	27:X:2548:G:H1	2.12	0.45
13:N:89:ASP:HB3	13:N:91:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1468:A:C8	27:X:1468:A:P	3.05	0.45
13:N:93:LYS:HB3	27:X:1007:A:H4'	1.99	0.45
27:X:1725:C:N4	27:X:1741:G:H1	2.15	0.45
27:X:2056:C:O2'	27:X:2577:A:O2'	2.32	0.45
27:X:828:C:N4	27:X:1206:G:H1	2.15	0.45
5:E:110:SER:HB2	27:X:2646:C:O2	2.17	0.45
27:X:1011:A:N7	27:X:1165:G:N2	2.65	0.45
1:A:76:ASN:ND2	1:A:118:ASN:OD1	2.43	0.45
27:X:564:U:H2'	27:X:565:A:C8	2.51	0.45
9:J:64:LYS:HD2	9:J:108:ALA:O	2.16	0.45
27:X:2674:C:H2'	27:X:2675:U:C6	2.52	0.45
27:X:584:A:OP2	27:X:2038:C:N4	2.50	0.45
27:X:873:U:H1'	27:X:2247:A:H5''	1.99	0.45
27:X:2433:G:C4	27:X:2434:G:C8	3.05	0.45
1:A:43:ARG:HD2	27:X:704:G:O3'	2.17	0.44
12:M:34:ARG:HH12	12:M:91:VAL:CA	2.30	0.44
27:X:2424:G:O2'	27:X:2425:G:H5'	2.17	0.44
27:X:1141:U:O2	27:X:2008:C:H5''	2.16	0.44
24:1:41:ASP:HB2	24:1:46:LYS:CB	2.46	0.44
27:X:2312:A:H4'	27:X:2313:G:O5'	2.16	0.44
27:X:1124:U:H2'	27:X:1125:G:C8	2.52	0.44
27:X:760:U:H4'	27:X:761:G:H5''	1.99	0.44
27:X:837:U:H2'	27:X:838:A:C8	2.52	0.44
27:X:91:A:H2'	27:X:92:U:C6	2.52	0.44
9:J:37:ALA:O	9:J:100:PRO:HA	2.17	0.44
17:R:92:THR:HA	17:R:108:VAL:HG22	1.98	0.44
13:N:47:TYR:CE1	13:N:51:ARG:HD3	2.52	0.44
4:D:46:ASP:HB2	4:D:49:ALA:HB3	1.99	0.44
23:Z:18:MET:O	23:Z:21:SER:HB3	2.16	0.44
27:X:1671:A:H1'	27:X:2798:A:OP2	2.17	0.44
3:C:30:VAL:HG11	3:C:177:VAL:HG21	1.99	0.44
7:H:82:LYS:HE3	7:H:82:LYS:HB2	1.87	0.44
27:X:2477:C:O2'	27:X:2478:C:H5'	2.18	0.44
3:C:53:LYS:HZ1	27:X:464:G:P	2.40	0.44
28:Y:39:C:N4	28:Y:51:G:O4'	2.51	0.44
3:C:111:ARG:O	3:C:116:LYS:HG3	2.17	0.44
27:X:1174:G:N2	27:X:1175:A:C4	2.85	0.44
27:X:923:A:N3	27:X:2243:C:H1'	2.31	0.44
27:X:794:A:H2	27:X:1767:G:N3	2.15	0.44
27:X:2696:A:H2'	27:X:2697:G:H8	1.82	0.44
27:X:577:U:H2'	27:X:579:G:OP2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:32:TYR:O	13:N:35:ALA:N	2.50	0.44
19:T:36:ILE:HD12	19:T:58:THR:HG21	1.99	0.44
27:X:517:A:H1'	27:X:519:C:N3	2.31	0.44
1:A:26:LYS:HE3	1:A:28:ARG:NH2	2.31	0.44
2:B:67:PHE:HE1	2:B:78:LEU:HD21	1.81	0.44
27:X:2495:G:N2	27:X:2548:G:H1'	2.33	0.44
27:X:2495:G:C5	27:X:2496:C:C4	3.06	0.44
27:X:313:U:H2'	27:X:314:G:C8	2.48	0.44
1:A:164:GLN:HB2	1:A:164:GLN:HE21	1.57	0.44
27:X:1250:A:H4'	27:X:1250:A:OP1	2.18	0.44
19:T:40:GLN:NE2	19:T:57:HIS:O	2.47	0.44
25:2:24:THR:HG23	25:2:27:GLY:H	1.81	0.44
22:W:46:THR:HG22	22:W:47:VAL:HG13	1.99	0.44
16:Q:46:PHE:HD2	16:Q:88:ILE:HB	1.83	0.44
11:L:72:GLY:HA2	11:L:107:ALA:HB2	1.98	0.44
27:X:571:U:C2	27:X:581:A:C8	3.05	0.44
1:A:161:THR:H	1:A:196:VAL:CG2	2.30	0.44
19:T:45:PHE:CE2	19:T:77:ARG:HD3	2.53	0.44
28:Y:63:A:H2'	28:Y:64:C:C6	2.53	0.44
7:H:75:VAL:HG12	7:H:118:LEU:HD11	1.99	0.44
10:K:17:ARG:HE	10:K:18:VAL:HG23	1.82	0.44
9:J:77:LYS:HD3	9:J:92:GLU:CD	2.38	0.44
27:X:1332:G:O2'	27:X:1333:G:H5'	2.17	0.44
5:E:6:LYS:HB2	5:E:6:LYS:HE2	1.84	0.44
15:P:62:ARG:HD3	27:X:1993:G:OP1	2.18	0.44
1:A:36:ALA:HB1	1:A:63:ARG:HA	2.00	0.44
7:H:2:ILE:HG12	7:H:45:ALA:O	2.17	0.44
1:A:254:THR:O	27:X:1836:C:H5'	2.16	0.44
27:X:2432:A:O2'	27:X:2551:A:H1'	2.16	0.44
13:N:66:ASN:HB2	13:N:70:ARG:NH1	2.33	0.44
7:H:38:GLY:HA2	27:X:2627:G:O2'	2.18	0.44
27:X:1351:G:C2	27:X:1352:G:C4	3.06	0.44
27:X:799:C:H2'	27:X:800:U:O4'	2.18	0.44
14:O:63:HIS:CD2	14:O:91:THR:HB	2.52	0.44
11:L:15:ARG:HA	11:L:15:ARG:HD3	1.63	0.44
1:A:151:LYS:N	27:X:2186:G:O2'	2.50	0.44
5:E:165:VAL:HB	5:E:166:GLY:H	1.55	0.44
8:I:95:ALA:HA	8:I:100:ARG:HB3	2.00	0.44
27:X:831:G:H5'	27:X:852:U:OP1	2.17	0.44
22:W:12:ARG:HG2	22:W:12:ARG:HH11	1.83	0.44
11:L:60:LYS:H	11:L:60:LYS:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1779:C:O5'	27:X:1779:C:H6	2.01	0.44
15:P:34:SER:HG	15:P:122:LYS:NZ	2.16	0.44
27:X:1856:U:H2'	27:X:1857:G:C8	2.53	0.44
27:X:1573:G:O5'	27:X:1574:A:H5''	2.18	0.44
7:H:9:ASP:HB2	7:H:95:ALA:HB2	1.99	0.44
27:X:876:A:H2	27:X:926:C:N4	2.16	0.44
27:X:683:A:H4'	27:X:684:C:H5''	2.00	0.44
27:X:1333:G:N7	27:X:1342:U:H5'	2.32	0.44
27:X:2168:A:H2'	27:X:2169:A:O4'	2.17	0.44
27:X:1430:G:H2'	27:X:1431:U:C6	2.52	0.44
13:N:86:ALA:C	13:N:88:ILE:N	2.71	0.44
27:X:172:A:H5''	27:X:173:A:OP2	2.18	0.44
27:X:1551:U:OP2	27:X:1553:G:N2	2.50	0.44
27:X:461:A:C4	27:X:462:G:C8	3.06	0.44
27:X:1357:U:H4'	27:X:1397:A:C6	2.52	0.44
27:X:2756:A:H3'	27:X:2756:A:OP1	2.18	0.44
2:B:140:SER:HA	27:X:2035:G:OP1	2.18	0.44
28:Y:39:C:H5''	28:Y:40:C:C5	2.52	0.44
27:X:1939:U:H1'	27:X:2531:U:OP1	2.17	0.44
27:X:2260:C:O2'	27:X:2261:G:H5'	2.17	0.44
17:R:29:HIS:CD2	17:R:51:VAL:HG13	2.52	0.44
13:N:20:ARG:HD2	13:N:39:LEU:HD22	1.99	0.44
5:E:6:LYS:O	5:E:69:ARG:HG3	2.17	0.44
27:X:1724:C:C2	27:X:1747:G:C6	3.06	0.44
15:P:116:SER:HB3	27:X:1997:A:H4'	1.99	0.44
27:X:2031:A:H2'	27:X:2032:G:O4'	2.18	0.44
27:X:1026:U:H2'	27:X:1027:C:C6	2.52	0.44
27:X:70:A:OP2	27:X:111:G:H4'	2.18	0.44
5:E:11:VAL:HG21	5:E:50:LEU:HB2	1.99	0.44
17:R:40:LEU:HD23	17:R:40:LEU:HA	1.68	0.44
27:X:334:G:OP1	27:X:349:G:N2	2.50	0.44
27:X:1030:U:O2	27:X:1155:G:N2	2.51	0.44
27:X:433:G:N2	27:X:434:C:O2	2.50	0.44
2:B:9:ILE:HG23	12:M:9:ARG:HB2	1.99	0.44
27:X:1117:G:H2'	27:X:1118:G:C8	2.50	0.44
27:X:2261:G:H21	27:X:2369:U:H3	1.65	0.44
27:X:2241:U:H4'	27:X:2307:A:H2	1.83	0.44
27:X:388:G:H2'	27:X:389:G:C8	2.53	0.44
16:Q:17:TYR:HA	16:Q:20:MET:HE2	2.00	0.44
27:X:1800:A:C6	27:X:1802:A:C6	3.06	0.44
27:X:1724:C:C2	27:X:1747:G:C5	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1608:U:H2'	27:X:1609:G:C8	2.53	0.44
16:Q:51:ILE:HD11	16:Q:83:ALA:HA	1.99	0.44
12:M:31:ASP:N	12:M:31:ASP:OD2	2.51	0.44
27:X:148:C:H2'	27:X:149:A:O4'	2.18	0.44
2:B:95:ILE:HA	2:B:95:ILE:HD13	1.80	0.44
1:A:244:ARG:HG2	27:X:1885:C:H5'	1.99	0.44
27:X:2551:A:H5'	27:X:2553:G:C4'	2.41	0.44
1:A:229:VAL:HG21	27:X:797:A:N7	2.33	0.44
27:X:875:G:N2	27:X:928:G:H1'	2.33	0.44
3:C:54:THR:HB	3:C:73:SER:HB3	2.00	0.44
28:Y:63:A:H2'	28:Y:64:C:H6	1.82	0.44
15:P:45:ILE:HD11	15:P:57:LEU:CG	2.48	0.44
27:X:1454:U:H3	27:X:1567:A:H61	1.66	0.44
13:N:2:PRO:HD3	27:X:456:C:P	2.58	0.44
27:X:1550:C:H4'	27:X:1551:U:H5	1.82	0.44
27:X:861:G:C4	27:X:862:A:C8	3.06	0.44
3:C:147:LYS:HB2	3:C:184:ASP:HB2	2.00	0.44
27:X:1867:A:O2'	27:X:1868:A:H8	2.01	0.43
15:P:118:ASN:ND2	27:X:1995:G:O3'	2.51	0.43
24:1:9:ILE:HG13	24:1:10:VAL:N	2.33	0.43
27:X:991:A:H62	27:X:992:A:N6	2.15	0.43
27:X:1303:U:H2'	27:X:1304:U:C6	2.52	0.43
17:R:80:LYS:HE3	17:R:80:LYS:HB2	1.79	0.43
27:X:543:G:C5	27:X:544:U:C4	3.05	0.43
4:D:122:PHE:HD1	4:D:129:ASN:H	1.64	0.43
27:X:2563:U:HO2'	27:X:2564:U:H6	1.63	0.43
27:X:2301:A:H2'	27:X:2302:G:O4'	2.18	0.43
27:X:957:G:H1	27:X:982:C:H42	1.65	0.43
27:X:1200:G:H2'	27:X:1201:G:O4'	2.17	0.43
27:X:946:U:H2'	27:X:947:C:C6	2.52	0.43
27:X:640:C:H1'	27:X:650:U:H1'	2.00	0.43
27:X:2811:G:C5	27:X:2858:A:C6	3.06	0.43
27:X:1684:G:H1	27:X:1974:U:H3'	1.83	0.43
20:U:22:GLY:N	20:U:39:LYS:HB2	2.33	0.43
16:Q:63:LYS:HG3	16:Q:64:ARG:N	2.31	0.43
17:R:95:ARG:HB2	17:R:104:VAL:HB	2.00	0.43
27:X:1374:G:N2	27:X:1384:G:H1'	2.32	0.43
27:X:500:G:H2'	27:X:501:G:O4'	2.18	0.43
3:C:84:PHE:HB3	27:X:597:U:O2'	2.17	0.43
27:X:2483:U:H2'	27:X:2484:G:H5'	2.00	0.43
27:X:346:C:C6	27:X:347:C:H5	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:90:ARG:NH1	12:M:78:GLU:OE1	2.51	0.43
27:X:2579:A:H2'	27:X:2580:C:H6	1.83	0.43
17:R:20:ASP:HB3	17:R:83:LEU:HG	2.00	0.43
1:A:267:ASP:HB3	1:A:270:ILE:HG22	2.00	0.43
27:X:2869:U:H2'	27:X:2870:C:C6	2.53	0.43
27:X:2277:A:H2'	27:X:2278:A:O4'	2.18	0.43
27:X:944:A:H2'	27:X:945:G:H8	1.82	0.43
27:X:98:U:H4'	27:X:99:U:H5''	2.01	0.43
27:X:1681:A:C2	27:X:2706:U:C2	3.06	0.43
27:X:494:A:C8	27:X:495:C:C5	3.07	0.43
8:I:59:ARG:CB	27:X:2371:A:H8	2.30	0.43
11:L:32:TYR:O	11:L:38:ILE:HA	2.17	0.43
27:X:1773:C:H1'	27:X:2588:U:H5'	2.01	0.43
17:R:35:LYS:HE3	17:R:37:LEU:HD21	2.00	0.43
27:X:2691:C:HO2'	27:X:2692:A:P	2.40	0.43
9:J:39:GLU:HB3	9:J:128:ILE:CG2	2.48	0.43
27:X:1039:A:H2'	27:X:1040:A:C8	2.53	0.43
9:J:17:ARG:HB2	27:X:969:U:C5	2.53	0.43
5:E:67:LEU:HD21	27:X:2738:A:C4	2.53	0.43
27:X:439:C:H2'	27:X:440:U:O4'	2.18	0.43
27:X:624:A:H4'	27:X:626:A:H62	1.84	0.43
27:X:1552:C:O2	27:X:1553:G:N2	2.51	0.43
27:X:1679:U:O2	27:X:2666:U:H5''	2.18	0.43
27:X:1001:A:H1'	27:X:1167:A:N3	2.32	0.43
1:A:20:ASP:HB3	1:A:21:PHE:CE2	2.53	0.43
20:U:10:LYS:NZ	20:U:11:LYS:HG3	2.33	0.43
27:X:2078:G:H1	27:X:2177:U:H3	1.66	0.43
27:X:324:C:H2'	27:X:325:U:O4'	2.18	0.43
27:X:1346:C:H6	27:X:1346:C:O5'	2.01	0.43
25:2:3:ARG:HD3	25:2:3:ARG:HA	1.49	0.43
27:X:2015:G:N1	27:X:2551:A:C8	2.87	0.43
27:X:2526:U:H2'	27:X:2527:G:H8	1.83	0.43
11:L:33:ARG:NH2	11:L:38:ILE:HG21	2.33	0.43
18:S:19:ILE:HG12	18:S:36:ARG:HB2	2.01	0.43
13:N:95:LEU:HA	13:N:98:ILE:HD12	2.01	0.43
7:H:129:LEU:O	7:H:131:PRO:HD3	2.18	0.43
6:G:70:PHE:HB3	13:N:64:ARG:CG	2.48	0.43
27:X:1040:A:C8	27:X:1041:G:C8	3.07	0.43
27:X:923:A:N6	27:X:2256:G:HO2'	2.16	0.43
27:X:682:G:H3'	27:X:683:A:C8	2.53	0.43
27:X:2324:G:N3	27:X:2360:C:H2'	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:339:U:O4	27:X:343:A:H8	2.01	0.43
5:E:91:GLY:HA3	5:E:94:PHE:CD2	2.53	0.43
27:X:1333:G:N2	27:X:1344:C:N4	2.65	0.43
27:X:2571:G:H2'	27:X:2572:U:O4'	2.18	0.43
3:C:170:LEU:HA	3:C:170:LEU:HD12	1.84	0.43
11:L:64:LYS:HG3	28:Y:53:G:H5"	1.99	0.43
27:X:987:G:C2	27:X:988:G:C8	3.07	0.43
27:X:1002:C:H2'	27:X:1003:C:H6	1.84	0.43
27:X:958:G:H2'	27:X:959:C:C6	2.54	0.43
12:M:28:ARG:H	12:M:28:ARG:HG2	1.61	0.43
7:H:23:ARG:NH1	7:H:40:GLY:O	2.51	0.43
27:X:503:G:H2'	27:X:504:G:O4'	2.18	0.43
8:I:94:GLU:HG2	8:I:94:GLU:H	1.39	0.43
27:X:1066:G:H2'	27:X:1067:G:O4'	2.18	0.43
14:O:38:LEU:HD22	14:O:39:PHE:H	1.83	0.43
9:J:137:VAL:HG11	18:S:71:MET:SD	2.58	0.43
3:C:94:THR:OG1	27:X:618:A:OP1	2.27	0.43
14:O:10:LYS:HZ1	14:O:13:ARG:HH12	1.66	0.43
27:X:50:G:H4'	27:X:51:A:O5'	2.18	0.43
9:J:39:GLU:HA	9:J:40:PRO:HD3	1.75	0.43
17:R:17:LYS:HG2	17:R:18:LYS:HD3	1.99	0.43
14:O:65:ARG:HE	14:O:87:ARG:HD3	1.84	0.43
27:X:681:A:H2'	27:X:683:A:H62	1.82	0.43
27:X:1429:A:N6	27:X:1600:U:H4'	2.33	0.43
13:N:3:ARG:HB2	27:X:1261:G:C8	2.53	0.43
8:I:75:VAL:HG22	8:I:99:VAL:HG11	2.00	0.43
15:P:19:LYS:NZ	27:X:507:A:OP2	2.30	0.43
21:V:42:ARG:HG3	21:V:46:LEU:HD12	2.01	0.43
27:X:1179:A:H2'	27:X:1180:A:C8	2.53	0.43
16:Q:14:GLU:OE2	27:X:1405:A:N6	2.45	0.43
27:X:2026:C:H2'	27:X:2027:C:H6	1.84	0.43
27:X:933:G:H2'	27:X:934:G:H8	1.82	0.43
27:X:1395:A:H2'	27:X:1396:C:H6	1.84	0.43
27:X:770:U:C4	27:X:771:C:C5	3.06	0.43
14:O:48:GLY:C	14:O:50:ASP:H	2.22	0.43
27:X:411:C:OP1	27:X:2073:A:O2'	2.32	0.43
1:A:222:ARG:HB2	1:A:222:ARG:HE	1.61	0.43
2:B:144:ARG:HH11	27:X:2551:A:H2'	1.84	0.43
8:I:56:LEU:HD22	26:3:52:LYS:HZ2	1.84	0.43
27:X:617:U:C5	27:X:632:A:N1	2.87	0.43
19:T:69:PHE:CZ	19:T:79:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:SER:HB3	27:X:2554:C:HO2'	1.83	0.43
6:G:106:TYR:CE2	6:G:108:GLY:HA2	2.54	0.43
27:X:2354:G:N2	27:X:2357:A:OP2	2.52	0.43
3:C:112:GLN:NE2	3:C:116:LYS:HG2	2.34	0.43
9:J:83:ARG:HD3	9:J:83:ARG:HA	1.66	0.43
9:J:82:THR:HB	9:J:83:ARG:H	1.33	0.43
27:X:2820:C:H2'	27:X:2821:G:C8	2.53	0.43
17:R:90:LYS:HE3	17:R:108:VAL:HB	2.00	0.43
17:R:18:LYS:HD2	27:X:83:A:H3'	2.00	0.43
27:X:2252:A:H2'	27:X:2253:A:C8	2.54	0.43
27:X:2838:U:H2'	27:X:2839:G:H8	1.83	0.43
27:X:638:A:H4'	27:X:639:G:H5'	2.00	0.43
27:X:2065:A:H3'	27:X:2066:G:H8	1.84	0.43
27:X:2519:C:O2'	27:X:2720:A:N3	2.40	0.43
27:X:1882:G:H21	27:X:1885:C:H41	1.63	0.43
27:X:796:A:C8	27:X:797:A:H4'	2.53	0.43
3:C:68:ARG:NH1	27:X:2043:A:H62	2.08	0.43
27:X:1336:G:C2'	27:X:1337:G:H5'	2.46	0.43
13:N:37:GLN:HE21	27:X:1265:G:H22	1.67	0.43
11:L:28:ARG:O	11:L:43:ILE:HD12	2.19	0.43
19:T:40:GLN:NE2	19:T:43:THR:HA	2.32	0.43
20:U:78:ILE:HG12	20:U:79:GLU:N	2.33	0.43
17:R:38:LEU:HD23	17:R:38:LEU:HA	1.74	0.43
27:X:1674:C:H2'	27:X:1675:C:H6	1.83	0.43
14:O:36:LYS:HZ2	14:O:55:THR:N	2.16	0.43
27:X:2563:U:O2'	27:X:2564:U:H5'	2.18	0.43
12:M:17:GLU:HG3	12:M:62:SER:H	1.84	0.43
27:X:1217:U:H2'	27:X:1218:C:C6	2.53	0.43
3:C:16:GLU:H	3:C:16:GLU:HG3	1.59	0.43
27:X:1987:G:C6	27:X:1988:A:C4	3.06	0.43
27:X:1361:G:H1	27:X:1614:C:H42	1.66	0.43
11:L:32:TYR:CG	28:Y:9:G:H4'	2.54	0.43
27:X:318:G:N1	27:X:321:A:OP2	2.52	0.43
27:X:2492:G:C2	27:X:2493:U:C2	3.07	0.43
21:V:26:MET:HA	21:V:29:ARG:HB2	2.01	0.43
9:J:40:PRO:HB3	9:J:99:LYS:HD2	1.99	0.43
27:X:746:G:C8	27:X:774:A:C6	3.06	0.43
9:J:88:LYS:NZ	27:X:968:C:OP2	2.51	0.43
27:X:1663:C:H5"	27:X:1664:G:H5"	2.01	0.43
27:X:45:C:OP2	27:X:192:G:H2'	2.18	0.43
27:X:2434:G:C6	27:X:2435:C:N4	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2519:C:O2	27:X:2720:A:H2	2.01	0.43
27:X:2810:A:N6	27:X:2853:U:H2'	2.33	0.43
27:X:2768:C:O2'	27:X:2784:A:N3	2.44	0.43
1:A:252:LYS:HG2	27:X:1816:G:O2'	2.18	0.43
15:P:127:ILE:HG22	15:P:128:THR:N	2.34	0.43
11:L:32:TYR:CE2	28:Y:9:G:H5'	2.54	0.43
27:X:2201:G:H2'	27:X:2202:G:C8	2.53	0.43
27:X:492:G:O2'	27:X:493:A:P	2.77	0.43
2:B:14:ILE:O	2:B:21:ILE:N	2.46	0.43
4:D:130:LEU:O	27:X:2283:G:O2'	2.33	0.43
27:X:554:U:H5''	27:X:556:A:N3	2.34	0.43
27:X:2056:C:O2'	27:X:2057:U:H5'	2.19	0.43
13:N:24:PHE:CE1	27:X:543:G:H5'	2.54	0.43
27:X:2668:U:OP2	27:X:2847:G:N2	2.43	0.43
11:L:29:LEU:HA	11:L:42:ILE:HD13	2.01	0.43
27:X:2266:A:H62	27:X:2323:U:H3	1.65	0.43
19:T:34:GLY:HA3	27:X:2332:G:H1'	2.00	0.43
27:X:1054:C:N4	27:X:1055:A:N1	2.67	0.43
27:X:938:G:C2'	27:X:939:C:H5''	2.48	0.43
27:X:1361:G:H1	27:X:1614:C:N4	2.17	0.43
6:G:132:PHE:CZ	6:G:142:ARG:HA	2.53	0.43
21:V:32:ALA:HB2	21:V:37:LEU:HD13	2.01	0.43
27:X:1184:G:H3'	27:X:1185:C:H5''	2.00	0.43
27:X:533:C:O2	27:X:563:U:O2'	2.36	0.43
11:L:45:ASP:N	11:L:45:ASP:OD1	2.31	0.43
27:X:539:A:H4'	27:X:539:A:OP1	2.18	0.42
15:P:100:GLY:HA2	27:X:25:U:H5'	2.00	0.42
3:C:74:VAL:HG23	3:C:76:THR:N	2.24	0.42
15:P:31:VAL:N	15:P:124:THR:HB	2.34	0.42
27:X:2394:G:C2	27:X:2395:C:C2	3.07	0.42
27:X:2370:G:O6	27:X:2406:C:H1'	2.19	0.42
2:B:7:THR:O	2:B:9:ILE:HG13	2.18	0.42
10:K:10:LEU:HD21	10:K:17:ARG:HG2	2.01	0.42
27:X:513:A:C6	27:X:515:A:C6	3.07	0.42
12:M:98:LYS:HE3	12:M:99:VAL:N	2.34	0.42
27:X:1715:A:C8	27:X:1717:A:O4'	2.72	0.42
7:H:34:LEU:HG	7:H:101:ASN:O	2.19	0.42
27:X:306:G:N2	27:X:355:G:H1'	2.34	0.42
27:X:1693:A:H2'	27:X:1694:A:O4'	2.18	0.42
18:S:104:SER:OG	18:S:113:VAL:HG21	2.18	0.42
1:A:226:MET:HB3	1:A:230:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:GLY:HA2	4:D:45:GLU:HB2	2.00	0.42
1:A:173:VAL:HG12	1:A:175:VAL:HG13	2.01	0.42
1:A:214:TRP:CD1	27:X:1582:A:C8	3.07	0.42
23:Z:45:ILE:HG21	23:Z:57:VAL:HG23	2.01	0.42
15:P:123:ARG:H	15:P:123:ARG:CD	2.32	0.42
4:D:75:SER:OG	27:X:2289:A:H1'	2.20	0.42
13:N:13:ARG:CZ	27:X:1264:C:H5"	2.49	0.42
2:B:77:ILE:HD13	2:B:195:LEU:HD22	2.01	0.42
11:L:16:LYS:HE3	11:L:28:ARG:NH1	2.32	0.42
27:X:1250:A:H2'	27:X:1251:G:O4'	2.18	0.42
27:X:2228:U:H4'	27:X:2254:C:C5	2.54	0.42
16:Q:28:TRP:CD2	16:Q:75:ARG:HD2	2.53	0.42
16:Q:11:VAL:HG21	16:Q:77:LYS:HE3	2.00	0.42
27:X:2057:U:O3'	27:X:2576:G:O2'	2.36	0.42
27:X:3:U:HO2'	27:X:4:C:H6	1.63	0.42
27:X:2572:U:H2'	27:X:2573:C:H6	1.84	0.42
27:X:563:U:H2'	27:X:564:U:O4'	2.19	0.42
20:U:21:ARG:NH2	20:U:23:LYS:HB3	2.34	0.42
28:Y:71:G:C6	28:Y:72:C:C4	3.07	0.42
5:E:60:LYS:H	5:E:60:LYS:HG2	1.68	0.42
13:N:62:ILE:HG23	13:N:76:TYR:CE1	2.55	0.42
27:X:310:A:N1	27:X:333:A:O2'	2.45	0.42
27:X:2043:A:O4'	27:X:2481:G:H1'	2.18	0.42
13:N:13:ARG:NH2	27:X:1264:C:H5"	2.34	0.42
11:L:13:THR:HG22	27:X:2313:G:C2	2.54	0.42
27:X:1780:A:H2'	27:X:1781:C:C6	2.54	0.42
27:X:762:A:H2	27:X:766:A:HO2'	1.65	0.42
3:C:170:LEU:HA	3:C:171:PRO:HD3	1.74	0.42
27:X:742:G:H2'	27:X:1766:U:H1'	2.00	0.42
13:N:17:VAL:HG21	13:N:32:TYR:HE1	1.84	0.42
27:X:1724:C:N3	27:X:1747:G:C6	2.88	0.42
27:X:1703:C:H2'	27:X:1704:G:O4'	2.20	0.42
27:X:2377:U:H3	27:X:2397:A:H61	1.68	0.42
18:S:101:THR:HG21	18:S:135:VAL:HG13	2.00	0.42
7:H:46:HIS:CD2	7:H:49:ASP:OD2	2.72	0.42
26:3:12:ARG:HG2	26:3:13:ARG:N	2.35	0.42
15:P:122:LYS:H	15:P:122:LYS:HG3	1.39	0.42
15:P:39:ARG:CZ	15:P:97:VAL:HG12	2.49	0.42
27:X:661:C:C2	27:X:662:G:N7	2.88	0.42
27:X:2792:C:H2'	27:X:2793:G:O4'	2.19	0.42
7:H:75:VAL:HG23	7:H:76:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:83:ARG:NH1	27:X:971:A:H61	2.17	0.42
25:2:33:ARG:O	25:2:37:LYS:HG3	2.19	0.42
27:X:1827:G:H1	27:X:1888:C:H42	1.67	0.42
26:3:15:LYS:HD3	26:3:15:LYS:HA	1.62	0.42
27:X:1332:G:C2	27:X:1333:G:C2	3.07	0.42
3:C:171:PRO:HB2	3:C:172:VAL:HG23	2.01	0.42
27:X:29:U:H2'	27:X:30:G:H8	1.83	0.42
27:X:78:C:O2'	27:X:357:A:N3	2.45	0.42
2:B:39:ALA:HA	2:B:44:TYR:N	2.34	0.42
27:X:2078:G:H2'	27:X:2079:A:C8	2.55	0.42
27:X:656:U:H4'	27:X:657:A:C8	2.54	0.42
16:Q:89:GLU:HB3	16:Q:90:ALA:H	1.57	0.42
1:A:69:ARG:CZ	1:A:130:ALA:HB2	2.49	0.42
26:3:36:LYS:HD2	26:3:36:LYS:HA	1.80	0.42
6:G:30:LYS:HB2	6:G:30:LYS:NZ	2.34	0.42
3:C:163:ASN:ND2	3:C:166:TRP:N	2.66	0.42
8:I:38:LYS:HG2	27:X:954:U:OP2	2.19	0.42
27:X:947:C:H2'	27:X:948:C:C6	2.54	0.42
27:X:2848:A:O2'	27:X:2849:C:H5'	2.18	0.42
2:B:152:LYS:NZ	27:X:2598:C:OP1	2.34	0.42
25:2:28:ARG:HA	25:2:31:LEU:HB2	2.02	0.42
13:N:51:ARG:H	13:N:51:ARG:HG2	1.73	0.42
27:X:242:A:C8	27:X:441:A:N6	2.87	0.42
27:X:1692:C:C5	27:X:1693:A:C4	3.07	0.42
27:X:2528:G:H2'	27:X:2529:G:C8	2.53	0.42
27:X:405:C:H2'	27:X:406:G:H8	1.84	0.42
27:X:1774:A:C6	27:X:2566:A:C2	3.08	0.42
13:N:2:PRO:HD3	27:X:456:C:O5'	2.19	0.42
27:X:13:A:N3	27:X:15:G:C6	2.88	0.42
14:O:64:GLY:HA3	14:O:90:PHE:CZ	2.54	0.42
27:X:1469:U:H5'	27:X:1470:G:OP2	2.20	0.42
5:E:121:VAL:HG11	5:E:144:VAL:HG21	2.02	0.42
27:X:1480:G:H2'	27:X:1481:U:O4'	2.19	0.42
4:D:79:LEU:HD11	27:X:2289:A:H2	1.82	0.42
27:X:167:A:C6	27:X:168:A:C6	3.08	0.42
1:A:107:ALA:HA	1:A:108:PRO:HD2	1.74	0.42
14:O:11:GLN:HE21	14:O:12:TYR:N	2.17	0.42
2:B:122:PHE:HB3	2:B:123:ALA:H	1.53	0.42
9:J:17:ARG:HD3	27:X:969:U:C2	2.54	0.42
5:E:139:GLN:HG2	27:X:2726:U:H4'	2.02	0.42
27:X:343:A:H1'	27:X:346:C:N4	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:ASN:HB3	4:D:122:PHE:HZ	1.84	0.42
25:2:16:HIS:O	25:2:43:THR:OG1	2.24	0.42
14:O:88:GLN:HB3	14:O:88:GLN:HE21	1.68	0.42
27:X:171:G:H2'	27:X:172:A:O4'	2.20	0.42
27:X:2721:A:H2'	27:X:2722:C:O4'	2.19	0.42
27:X:21:A:C6	27:X:530:G:C6	3.08	0.42
27:X:1378:A:H5'	27:X:1379:A:OP2	2.19	0.42
27:X:2226:A:H2'	27:X:2227:C:C6	2.54	0.42
27:X:2746:G:N3	27:X:2746:G:H2'	2.35	0.42
27:X:488:A:OP1	27:X:488:A:H8	2.02	0.42
27:X:1964:A:H5''	27:X:1965:U:OP2	2.20	0.42
27:X:1574:A:H2'	27:X:1575:C:H5''	2.01	0.42
15:P:45:ILE:HD11	15:P:57:LEU:HG	2.02	0.42
10:K:18:VAL:HG12	10:K:19:ALA:N	2.35	0.42
27:X:514:G:H4'	27:X:515:A:OP2	2.20	0.42
7:H:47:VAL:HB	7:H:117:GLU:OE1	2.19	0.42
27:X:1451:C:H1'	27:X:1532:A:C2	2.53	0.42
1:A:261:ARG:NH2	27:X:1791:C:OP1	2.52	0.42
27:X:1332:G:C5	27:X:1333:G:C6	3.07	0.42
26:3:61:MET:O	26:3:64:ARG:HG3	2.20	0.42
5:E:44:ARG:NH2	5:E:46:ASP:HB2	2.35	0.42
27:X:2441:U:H6	27:X:2441:U:O5'	2.02	0.42
27:X:2526:U:H2'	27:X:2527:G:C8	2.54	0.42
9:J:120:ARG:NH2	27:X:2447:G:OP1	2.52	0.42
27:X:1467:U:H3'	27:X:1467:U:C6	2.55	0.42
24:1:38:LYS:HE2	24:1:40:TYR:HE1	1.85	0.42
27:X:2794:G:O2'	27:X:2795:A:H5''	2.20	0.42
27:X:1731:C:N3	27:X:1735:G:N1	2.68	0.42
27:X:1124:U:H2'	27:X:1125:G:H8	1.85	0.42
7:H:9:ASP:O	7:H:96:ALA:N	2.50	0.42
13:N:31:GLN:HB3	27:X:590:C:OP1	2.20	0.42
27:X:758:G:C2'	27:X:759:C:H5'	2.49	0.42
14:O:10:LYS:HZ3	14:O:11:GLN:HB2	1.85	0.42
27:X:1386:A:OP1	27:X:2191:A:N6	2.42	0.42
27:X:478:G:H2'	27:X:479:G:O4'	2.20	0.42
28:Y:54:U:C4	28:Y:55:C:C4	3.08	0.42
2:B:38:THR:O	2:B:42:ASP:HB2	2.19	0.42
8:I:17:LYS:HE3	27:X:1257:U:OP1	2.20	0.42
1:A:18:THR:HG21	1:A:20:ASP:OD2	2.20	0.42
20:U:54:ASN:OD1	20:U:77:GLY:HA2	2.19	0.42
3:C:191:ALA:HA	3:C:194:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:15:ASP:O	19:T:16:SER:OG	2.34	0.42
27:X:568:G:H2'	27:X:569:C:O4'	2.20	0.42
3:C:164:VAL:HG13	27:X:335:A:OP1	2.19	0.42
27:X:1073:G:N2	27:X:1087:C:H42	2.12	0.42
24:1:38:LYS:HD2	27:X:2265:A:N6	2.34	0.42
13:N:61:TRP:O	13:N:65:ILE:HG13	2.19	0.42
7:H:76:ARG:HB3	7:H:91:PHE:HD1	1.85	0.42
11:L:16:LYS:NZ	11:L:90:ASP:OD2	2.26	0.42
3:C:33:TRP:CE2	3:C:95:LEU:HB2	2.55	0.42
4:D:4:LEU:C	4:D:6:THR:H	2.24	0.42
2:B:155:ARG:HG3	2:B:155:ARG:HH11	1.84	0.42
27:X:1713:G:C6	27:X:1714:A:C5	3.08	0.42
27:X:1675:C:H2'	27:X:1676:U:H6	1.84	0.42
27:X:1935:A:C5	27:X:1936:A:N1	2.88	0.42
10:K:63:ARG:HD3	27:X:1469:U:O2	2.20	0.42
17:R:44:GLN:HE21	17:R:78:ALA:HB2	1.84	0.42
27:X:2504:G:C2	27:X:2518:C:C2	3.08	0.42
27:X:1776:A:C8	27:X:1778:U:C5	3.08	0.42
13:N:15:LYS:NZ	27:X:1230:C:OP1	2.44	0.42
8:I:55:ARG:H	8:I:55:ARG:HG2	1.69	0.42
27:X:580:A:C8	27:X:2013:A:N6	2.88	0.42
27:X:486:U:H4'	27:X:519:C:H2'	2.01	0.42
26:3:13:ARG:O	26:3:13:ARG:HG3	2.20	0.42
26:3:13:ARG:CZ	26:3:25:PHE:HB2	2.50	0.42
27:X:537:C:O2'	27:X:538:A:C4	2.62	0.42
26:3:49:VAL:HG13	27:X:2339:A:OP1	2.20	0.42
27:X:304:A:C6	27:X:359:G:C2	3.08	0.42
8:I:93:LEU:O	8:I:97:ARG:HG3	2.20	0.42
22:W:23:LEU:HD23	22:W:23:LEU:HA	1.85	0.42
15:P:14:ARG:NE	27:X:514:G:O6	2.51	0.42
27:X:513:A:C6	27:X:516:G:C6	3.08	0.42
27:X:314:G:H2'	27:X:315:G:H8	1.84	0.42
27:X:2010:G:H1'	27:X:2020:G:N2	2.34	0.42
27:X:2270:U:H2'	27:X:2271:C:C6	2.55	0.42
18:S:73:LYS:O	18:S:74:ARG:HB2	2.20	0.42
27:X:1539:U:H2'	27:X:1540:C:H6	1.84	0.42
13:N:20:ARG:HH22	14:O:72:ARG:HD3	1.85	0.42
27:X:1312:G:H5'	27:X:1314:A:O4'	2.20	0.42
27:X:988:G:N3	27:X:1012:A:H2	2.18	0.42
15:P:32:ARG:HG3	27:X:1335:A:OP1	2.20	0.42
27:X:1625:A:H1'	27:X:1632:A:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:4:PRO:HD3	7:H:24:VAL:HG23	2.02	0.42
27:X:1402:G:H2'	27:X:1403:U:O4'	2.20	0.42
7:H:134:LEU:HA	7:H:134:LEU:HD23	1.72	0.42
27:X:1152:C:H4'	27:X:1153:A:OP2	2.20	0.41
15:P:27:VAL:HG23	15:P:126:HIS:O	2.19	0.41
27:X:875:G:O2'	28:Y:80:A:N3	2.53	0.41
16:Q:43:GLN:HG2	16:Q:48:VAL:O	2.20	0.41
28:Y:46:G:H21	28:Y:50:U:H1'	1.85	0.41
27:X:2262:C:C2	27:X:2368:G:C2	3.08	0.41
15:P:90:LEU:HD22	15:P:131:VAL:HG12	2.02	0.41
27:X:1948:C:H3'	27:X:1949:A:H8	1.84	0.41
27:X:1310:C:C2	27:X:1311:C:C5	3.08	0.41
3:C:23:ASN:O	3:C:27:LEU:HD13	2.20	0.41
27:X:456:C:H2'	27:X:457:C:H6	1.84	0.41
27:X:2871:U:H2'	27:X:2872:U:C6	2.54	0.41
27:X:1469:U:H5''	27:X:1470:G:C8	2.55	0.41
27:X:2387:U:H2'	27:X:2388:G:C8	2.55	0.41
27:X:1544:A:C4	27:X:1560:A:C6	3.08	0.41
27:X:1852:G:H2'	27:X:1853:C:C6	2.54	0.41
6:G:49:VAL:HG12	6:G:50:PRO:O	2.20	0.41
7:H:5:GLN:HG2	27:X:1685:A:H5''	2.01	0.41
14:O:26:GLN:HG2	14:O:27:GLY:N	2.34	0.41
27:X:2533:U:H2'	27:X:2534:U:C6	2.55	0.41
10:K:99:ARG:HG2	10:K:99:ARG:HH11	1.84	0.41
27:X:1481:U:H4'	27:X:1562:G:H21	1.85	0.41
1:A:251:GLY:HA3	1:A:255:LYS:CE	2.50	0.41
27:X:537:C:O2	27:X:537:C:H2'	2.19	0.41
27:X:2791:C:O2'	27:X:2792:C:H5'	2.19	0.41
22:W:3:ILE:HA	22:W:3:ILE:HD12	1.64	0.41
14:O:39:PHE:CE2	14:O:46:VAL:HB	2.55	0.41
1:A:219:PRO:HG2	27:X:1782:A:OP1	2.19	0.41
28:Y:48:A:C6	28:Y:49:C:C5	3.07	0.41
6:G:67:ARG:CD	6:G:70:PHE:HA	2.50	0.41
13:N:59:ARG:NH1	27:X:1019:U:H1'	2.35	0.41
14:O:11:GLN:H	14:O:37:ALA:HB3	1.84	0.41
14:O:5:ILE:N	14:O:10:LYS:HE3	2.36	0.41
27:X:670:U:H2'	27:X:671:A:H8	1.84	0.41
27:X:224:G:C2	27:X:229:G:C6	3.08	0.41
26:3:23:MET:HA	26:3:48:PHE:CD2	2.55	0.41
3:C:84:PHE:CE1	27:X:596:C:H5''	2.54	0.41
27:X:343:A:O2'	27:X:346:C:N4	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:46:GLU:HG3	27:X:544:U:H4'	2.02	0.41
16:Q:4:TYR:CD2	21:V:23:LYS:HB2	2.54	0.41
27:X:36:G:N3	27:X:462:G:O2'	2.52	0.41
27:X:1997:A:H2'	27:X:1998:A:C8	2.55	0.41
4:D:40:LEU:HD23	4:D:41:GLY:N	2.36	0.41
15:P:44:VAL:HG11	23:Z:27:ALA:HB2	2.01	0.41
27:X:1824:C:N4	27:X:1825:C:C4	2.88	0.41
27:X:1281:A:H2'	27:X:1282:A:O4'	2.20	0.41
11:L:31:VAL:HG11	11:L:89:PHE:CZ	2.55	0.41
27:X:1672:A:H3'	27:X:1673:C:H6	1.85	0.41
4:D:77:PHE:O	4:D:79:LEU:HD12	2.20	0.41
13:N:13:ARG:O	13:N:16:LYS:HB2	2.20	0.41
27:X:1682:A:H2'	27:X:1683:G:O4'	2.21	0.41
27:X:836:G:C4	27:X:837:U:C5	3.08	0.41
27:X:1303:U:H2'	27:X:1304:U:H6	1.84	0.41
27:X:1039:A:H61	27:X:1136:G:H2'	1.85	0.41
27:X:1740:G:H2'	27:X:1741:G:H8	1.84	0.41
8:I:49:PHE:HE2	27:X:229:G:OP1	2.03	0.41
13:N:39:LEU:O	14:O:72:ARG:NH2	2.33	0.41
13:N:45:TYR:O	13:N:49:ASP:HB2	2.19	0.41
19:T:60:PHE:CE1	27:X:2344:G:H4'	2.55	0.41
18:S:22:VAL:O	18:S:83:PHE:HB2	2.19	0.41
27:X:10:A:H2'	27:X:11:G:O4'	2.20	0.41
24:I:35:LEU:HB3	24:I:37:LEU:HG	2.02	0.41
1:A:249:PRO:HD3	27:X:2218:G:H5'	2.02	0.41
9:J:34:GLY:HA2	9:J:106:GLU:HA	2.02	0.41
15:P:22:LYS:N	27:X:506:G:OP1	2.52	0.41
19:T:24:LYS:HD3	19:T:24:LYS:HA	1.84	0.41
27:X:2660:C:C2	27:X:2704:U:O4	2.74	0.41
13:N:76:TYR:CZ	13:N:80:ILE:HG13	2.56	0.41
15:P:31:VAL:HG21	15:P:127:ILE:HD13	2.02	0.41
27:X:825:C:H1'	27:X:1263:G:N2	2.35	0.41
27:X:1975:G:O2'	27:X:1976:U:OP2	2.29	0.41
27:X:1322:G:H21	27:X:1627:C:H5'	1.86	0.41
4:D:16:LEU:HD12	4:D:28:VAL:HG13	2.01	0.41
3:C:7:ILE:HB	3:C:121:ASP:HB2	2.01	0.41
27:X:1925:C:C4	27:X:1926:U:N3	2.88	0.41
1:A:85:ASP:HB2	1:A:92:ILE:HD12	2.01	0.41
27:X:1330:G:C4	27:X:1331:G:C8	3.09	0.41
17:R:96:LYS:O	17:R:104:VAL:HA	2.19	0.41
27:X:307:C:C2'	27:X:308:C:H5'	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:859:U:O2'	27:X:860:U:O2	2.31	0.41
28:Y:34:C:H1'	28:Y:54:U:O4	2.20	0.41
4:D:83:MET:O	4:D:85:VAL:N	2.53	0.41
21:V:17:GLU:HB3	21:V:53:LEU:HD11	2.02	0.41
27:X:658:G:H2'	27:X:659:G:C8	2.55	0.41
2:B:51:TYR:N	2:B:75:THR:OG1	2.53	0.41
27:X:1734:C:H5'	27:X:1735:G:OP2	2.20	0.41
4:D:64:LYS:HG2	4:D:65:PRO:O	2.21	0.41
3:C:189:ASP:HB3	3:C:190:ALA:H	1.63	0.41
27:X:490:A:HO2'	27:X:492:G:H8	1.64	0.41
14:O:10:LYS:HZ2	14:O:13:ARG:HH12	1.67	0.41
27:X:246:C:H1'	27:X:437:G:H22	1.85	0.41
27:X:1643:A:N6	27:X:1656:U:H3	2.17	0.41
15:P:89:ARG:HG2	15:P:134:LYS:H	1.85	0.41
27:X:1210:C:C2	27:X:1211:G:C8	3.08	0.41
7:H:100:ASN:ND2	7:H:104:GLU:HG3	2.36	0.41
27:X:1128:G:H2'	27:X:1129:A:H5''	2.03	0.41
27:X:2856:U:H2'	27:X:2857:C:C6	2.55	0.41
5:E:133:VAL:HG11	5:E:144:VAL:HG11	2.02	0.41
15:P:46:ARG:HA	15:P:92:VAL:HG11	2.03	0.41
6:G:91:THR:HB	6:G:92:GLY:H	1.76	0.41
22:W:2:LYS:HD3	22:W:33:GLU:OE1	2.20	0.41
27:X:1623:C:H5''	27:X:1624:A:H5'	2.02	0.41
13:N:96:ALA:O	13:N:99:ALA:N	2.53	0.41
27:X:832:A:C5	27:X:833:A:C8	3.09	0.41
27:X:648:A:H2	27:X:649:G:H21	1.68	0.41
1:A:161:THR:HG21	27:X:1811:A:H3'	2.02	0.41
13:N:90:LEU:HD23	13:N:92:ARG:HG3	2.02	0.41
6:G:103:TYR:CD2	27:X:1142:G:O4'	2.73	0.41
27:X:2062:U:H2'	27:X:2063:A:C8	2.55	0.41
18:S:64:ALA:HB2	18:S:85:MET:HG2	2.02	0.41
14:O:62:GLU:HG2	14:O:63:HIS:N	2.36	0.41
11:L:15:ARG:HH21	27:X:2272:A:P	2.43	0.41
5:E:107:ILE:HD11	5:E:151:VAL:HG12	2.02	0.41
27:X:717:G:H1'	27:X:739:G:H22	1.83	0.41
27:X:1333:G:N2	27:X:1344:C:H41	2.19	0.41
27:X:930:A:H4'	28:Y:100:G:N3	2.36	0.41
11:L:64:LYS:HD3	11:L:64:LYS:HA	1.89	0.41
24:1:51:ARG:HH11	24:1:51:ARG:HB2	1.86	0.41
27:X:1255:A:H2'	27:X:1256:C:C6	2.55	0.41
27:X:13:A:H1'	27:X:14:A:N7	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1958:G:H2'	27:X:1959:U:C6	2.55	0.41
8:I:71:THR:O	8:I:104:ARG:HB3	2.20	0.41
8:I:129:ALA:O	8:I:133:VAL:HG23	2.21	0.41
5:E:89:LEU:HD23	5:E:89:LEU:HA	1.89	0.41
20:U:25:ARG:HD3	20:U:25:ARG:HA	1.79	0.41
27:X:587:A:H2'	27:X:588:G:H5''	2.03	0.41
7:H:23:ARG:HE	27:X:2540:A:H2	1.69	0.41
27:X:825:C:H2'	27:X:826:U:H6	1.86	0.41
15:P:104:LYS:HZ3	15:P:119:ILE:HG22	1.85	0.41
27:X:321:A:N6	27:X:323:G:N3	2.68	0.41
27:X:144:U:H2'	27:X:145:C:H6	1.85	0.41
16:Q:63:LYS:HB2	16:Q:69:ILE:HA	2.02	0.41
17:R:94:VAL:HA	27:X:309:G:OP1	2.20	0.41
18:S:38:ALA:HA	18:S:41:ARG:HB3	2.03	0.41
4:D:38:GLU:HB3	4:D:87:ILE:HB	2.02	0.41
25:2:16:HIS:HB3	25:2:43:THR:OG1	2.21	0.41
6:G:75:ILE:HB	6:G:147:ARG:NH1	2.36	0.41
27:X:39:C:H2'	27:X:40:U:C6	2.55	0.41
13:N:17:VAL:HG11	13:N:36:PHE:HB2	2.02	0.41
2:B:105:THR:HG22	2:B:166:THR:OG1	2.21	0.41
27:X:2250:G:H2'	27:X:2251:U:C6	2.56	0.41
1:A:262:LYS:H	1:A:262:LYS:HE2	1.86	0.41
27:X:669:G:OP2	27:X:669:G:H8	2.04	0.41
1:A:252:LYS:HZ3	1:A:253:PRO:HD2	1.86	0.41
27:X:537:C:H1'	27:X:538:A:C5	2.55	0.41
6:G:69:ASP:C	6:G:71:THR:HG22	2.41	0.41
27:X:1965:U:H2'	27:X:1966:C:C6	2.54	0.41
27:X:2039:G:H2'	27:X:2039:G:N3	2.36	0.41
26:3:30:ARG:HH21	26:3:31:HIS:CD2	2.39	0.41
20:U:51:ILE:H	20:U:52:ARG:NH2	2.18	0.41
23:Z:51:TYR:CD2	23:Z:55:ARG:HB2	2.55	0.41
27:X:676:G:C6	27:X:677:G:C5	3.09	0.41
4:D:108:LEU:HA	4:D:111:ILE:HD11	2.03	0.41
7:H:10:VAL:HG23	7:H:17:ARG:O	2.21	0.41
27:X:1693:A:N6	27:X:1694:A:C6	2.88	0.41
27:X:1287:A:N3	27:X:1310:C:H1'	2.36	0.41
27:X:1655:C:H4'	27:X:2689:C:O2	2.20	0.41
11:L:31:VAL:HG21	11:L:100:VAL:HG23	2.02	0.41
10:K:36:THR:HG23	10:K:37:THR:O	2.21	0.41
27:X:545:C:H2'	27:X:546:A:C8	2.55	0.41
8:I:84:GLU:HB3	8:I:85:ASP:H	1.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:1640:C:H2'	27:X:1641:C:H6	1.86	0.41
27:X:829:C:H2'	27:X:830:C:O4'	2.21	0.41
27:X:1578:U:H2'	27:X:1579:G:C8	2.56	0.41
27:X:1035:G:C6	27:X:1036:G:C6	3.09	0.41
7:H:116:ARG:HD3	12:M:40:ARG:HB2	2.02	0.41
3:C:39:ARG:HH21	3:C:91:TYR:CB	2.33	0.41
1:A:206:LEU:HA	1:A:206:LEU:HD23	1.94	0.41
8:I:62:LYS:HG3	8:I:62:LYS:HZ2	1.70	0.41
27:X:538:A:N3	27:X:2025:A:C6	2.89	0.41
4:D:123:ASP:OD2	4:D:127:ASN:HB2	2.20	0.41
27:X:820:U:H1'	27:X:2424:G:OP1	2.20	0.41
27:X:1327:C:H42	27:X:1351:G:H1	1.67	0.41
2:B:151:TYR:HD1	6:G:106:TYR:CE1	2.38	0.41
27:X:2492:G:H2'	27:X:2493:U:H6	1.81	0.41
15:P:15:LYS:HG3	27:X:514:G:C2	2.55	0.41
27:X:313:U:C2	27:X:314:G:C8	3.09	0.41
27:X:753:U:H2'	27:X:754:G:C8	2.56	0.41
3:C:114:GLY:O	3:C:116:LYS:HE3	2.20	0.41
27:X:309:G:N2	27:X:352:G:O6	2.54	0.41
19:T:74:LYS:C	19:T:76:ALA:N	2.74	0.41
4:D:92:ARG:CZ	28:Y:47:A:H1'	2.51	0.41
27:X:1537:U:H2'	27:X:1538:A:O4'	2.21	0.41
27:X:1538:A:H2'	27:X:1539:U:O4'	2.20	0.41
27:X:1984:A:H2'	27:X:1985:G:O4'	2.21	0.41
27:X:1763:G:H2'	27:X:1764:A:H4'	2.02	0.41
27:X:3:U:O2'	27:X:4:C:P	2.79	0.41
27:X:106:G:C2	27:X:107:G:C5	3.09	0.41
20:U:41:VAL:HG23	20:U:43:ARG:HD2	2.02	0.41
25:2:15:THR:O	25:2:16:HIS:HB2	2.21	0.41
8:I:108:LEU:O	8:I:109:LEU:HD23	2.21	0.41
27:X:2870:C:H2'	27:X:2871:U:C6	2.56	0.41
11:L:96:TYR:HA	11:L:100:VAL:HG13	2.03	0.41
27:X:2489:C:C4	27:X:2490:U:C5	3.09	0.41
27:X:182:G:HO2'	27:X:183:U:P	2.43	0.41
22:W:19:THR:OG1	27:X:863:C:O2'	2.05	0.41
10:K:88:ALA:C	10:K:90:ARG:H	2.24	0.41
13:N:50:ARG:HA	13:N:53:LYS:HE3	2.03	0.41
27:X:1672:A:H3'	27:X:1673:C:C6	2.55	0.41
12:M:34:ARG:HA	12:M:34:ARG:NH1	2.36	0.41
27:X:1225:G:H2'	27:X:1249:G:H22	1.85	0.41
27:X:762:A:H4'	27:X:1284:G:N3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:72:PRO:HG2	13:N:60:LEU:HG	2.03	0.41
27:X:2304:G:P	27:X:2304:G:H8	2.44	0.41
27:X:1705:U:O4'	27:X:1718:A:N6	2.54	0.41
7:H:27:SER:HB2	7:H:50:ILE:H	1.84	0.41
14:O:66:GLY:O	14:O:87:ARG:NE	2.48	0.41
27:X:389:G:H2'	27:X:390:U:C6	2.56	0.41
27:X:109:A:C6	27:X:110:U:C4	3.09	0.41
8:I:16:ARG:HG2	8:I:17:LYS:H	1.85	0.41
27:X:2434:G:H2'	27:X:2435:C:C6	2.56	0.41
27:X:933:G:H2'	27:X:934:G:C8	2.56	0.41
27:X:521:U:H5	27:X:522:G:C5	2.38	0.41
27:X:1804:U:H2'	27:X:1805:G:H8	1.86	0.41
2:B:147:PRO:HB2	2:B:149:ARG:HG2	2.03	0.41
12:M:22:ARG:H	12:M:84:ALA:HB2	1.85	0.41
27:X:2779:C:O2'	27:X:2780:A:O4'	2.37	0.41
4:D:142:THR:HG22	4:D:143:TYR:H	1.85	0.41
27:X:2628:C:H2'	27:X:2629:U:H6	1.86	0.41
27:X:235:C:H2'	27:X:236:C:O4'	2.21	0.41
9:J:23:LYS:HB3	9:J:23:LYS:HE2	1.95	0.41
3:C:102:LEU:HD23	3:C:102:LEU:O	2.21	0.41
26:3:8:LYS:HE2	26:3:12:ARG:NH2	2.35	0.40
27:X:659:G:H2'	27:X:660:G:O4'	2.21	0.40
27:X:114:C:OP1	27:X:126:C:N4	2.53	0.40
15:P:100:GLY:C	15:P:123:ARG:HB2	2.42	0.40
15:P:18:VAL:HG12	15:P:20:LEU:H	1.86	0.40
27:X:492:G:O2'	27:X:493:A:O5'	2.35	0.40
27:X:2821:G:C6	27:X:2846:G:C6	3.09	0.40
27:X:877:G:O2'	27:X:878:C:H5'	2.20	0.40
17:R:28:LYS:HG2	17:R:29:HIS:H	1.87	0.40
28:Y:15:A:O2'	28:Y:16:U:H5''	2.21	0.40
27:X:1287:A:H2	27:X:1661:C:O2	2.03	0.40
27:X:67:G:N2	27:X:73:A:C4	2.90	0.40
19:T:36:ILE:HD11	27:X:2343:C:O2	2.21	0.40
12:M:31:ASP:HA	12:M:52:GLY:O	2.22	0.40
19:T:26:PHE:CD1	27:X:934:G:H1'	2.56	0.40
2:B:8:LYS:HE2	2:B:190:GLY:O	2.21	0.40
27:X:1171:A:H2'	27:X:1172:U:C6	2.56	0.40
18:S:88:TYR:C	18:S:127:PRO:HG2	2.41	0.40
11:L:27:LEU:HB2	11:L:87:VAL:HG12	2.04	0.40
8:I:57:ILE:HD12	26:3:9:MET:SD	2.61	0.40
28:Y:75:A:H4'	28:Y:75:A:OP1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:2380:U:H3	27:X:2394:G:H1	1.70	0.40
4:D:16:LEU:HD22	4:D:20:PHE:CE1	2.56	0.40
13:N:65:ILE:CD1	13:N:95:LEU:HB3	2.51	0.40
27:X:2329:C:N4	27:X:2330:G:C6	2.89	0.40
3:C:17:LEU:HD12	3:C:17:LEU:HA	1.93	0.40
27:X:75:C:H2'	27:X:76:C:H6	1.82	0.40
7:H:29:ILE:HA	7:H:34:LEU:HA	2.03	0.40
14:O:82:ARG:HD3	14:O:82:ARG:HA	1.67	0.40
27:X:1211:G:H2'	27:X:1212:U:C6	2.55	0.40
7:H:104:GLU:HB3	7:H:125:LYS:HD2	2.03	0.40
27:X:1652:G:N2	27:X:1752:U:O2	2.44	0.40
28:Y:17:A:H1'	28:Y:112:A:C8	2.56	0.40
27:X:2355:A:H8	27:X:2355:A:OP1	2.04	0.40
27:X:2753:C:O2'	27:X:2754:C:H5'	2.21	0.40
10:K:100:VAL:HG23	10:K:112:LEU:HG	2.03	0.40
26:3:27:SER:OG	27:X:2340:C:OP1	2.27	0.40
1:A:168:LYS:HE2	1:A:168:LYS:HB2	1.84	0.40
4:D:144:ASP:OD1	4:D:144:ASP:N	2.54	0.40
27:X:1224:A:H4'	27:X:1225:G:OP2	2.21	0.40
6:G:111:LYS:O	6:G:111:LYS:HD2	2.21	0.40
27:X:536:A:N6	27:X:2605:C:H4'	2.36	0.40
2:B:129:HIS:HE1	27:X:1976:U:O2'	2.04	0.40
27:X:759:C:O2'	27:X:2591:C:H5'	2.22	0.40
27:X:81:C:H5''	27:X:307:C:H5'	2.03	0.40
8:I:63:ARG:HD2	26:3:30:ARG:NH1	2.37	0.40
1:A:100:GLY:HA2	27:X:1517:C:H1'	2.03	0.40
27:X:2652:G:H2'	27:X:2653:A:H8	1.86	0.40
25:2:15:THR:OG1	25:2:16:HIS:N	2.53	0.40
27:X:1325:U:H4'	27:X:1326:U:O5'	2.22	0.40
27:X:1011:A:C8	27:X:1165:G:N2	2.90	0.40
27:X:1164:C:H2'	27:X:1165:G:O4'	2.22	0.40
27:X:565:A:O5'	27:X:565:A:H8	2.04	0.40
1:A:44:ASN:HA	27:X:1805:G:O2'	2.21	0.40
27:X:644:A:N3	27:X:2382:C:H4'	2.36	0.40
1:A:212:SER:O	1:A:215:LEU:HD12	2.21	0.40
27:X:822:G:H2'	27:X:823:U:H6	1.86	0.40
19:T:17:ASN:HA	19:T:18:PRO:HD3	1.79	0.40
2:B:58:LYS:HE3	27:X:2805:G:OP1	2.21	0.40
27:X:2013:A:H4'	27:X:2014:A:C8	2.56	0.40
27:X:1885:C:N3	27:X:1886:G:H1'	2.36	0.40
8:I:62:LYS:HB2	26:3:13:ARG:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:34:ARG:HH12	12:M:91:VAL:HA	1.86	0.40
19:T:45:PHE:CE2	19:T:69:PHE:HE2	2.39	0.40
8:I:94:GLU:CD	8:I:97:ARG:HH11	2.23	0.40
27:X:2299:A:N6	27:X:2312:A:O2'	2.55	0.40
11:L:26:ARG:NH1	27:X:2357:A:H4'	2.37	0.40
23:Z:42:SER:O	23:Z:44:HIS:HD2	2.03	0.40
27:X:1226:A:N1	27:X:1250:A:H1'	2.35	0.40
27:X:836:G:N2	27:X:847:C:O2	2.54	0.40
23:Z:12:SER:OG	27:X:2004:U:OP1	2.23	0.40
2:B:119:ARG:HG2	2:B:120:TRP:NE1	2.36	0.40
23:Z:25:LEU:HD12	23:Z:25:LEU:HA	1.86	0.40
1:A:208:LYS:HB3	27:X:742:G:O6	2.22	0.40
27:X:193:A:C2	27:X:194:G:H1'	2.57	0.40
8:I:76:LYS:HB2	8:I:79:GLN:HG2	2.03	0.40
24:1:17:GLY:O	24:1:19:GLY:N	2.52	0.40
27:X:2189:A:H8	27:X:2189:A:O5'	2.03	0.40
6:G:94:LYS:HB3	6:G:94:LYS:HE3	1.54	0.40
27:X:200:A:O2'	27:X:421:G:N2	2.55	0.40
1:A:15:GLN:O	1:A:24:LEU:HA	2.21	0.40
27:X:2794:G:C2	27:X:2803:C:N3	2.90	0.40
2:B:128:SER:O	2:B:128:SER:OG	2.39	0.40
26:3:62:LEU:HD12	26:3:62:LEU:HA	1.90	0.40
23:Z:51:TYR:CE1	23:Z:55:ARG:HG3	2.57	0.40
27:X:1173:G:H2'	27:X:1174:G:H8	1.86	0.40
27:X:540:G:N2	27:X:2004:U:H1'	2.37	0.40
27:X:2560:G:H4'	27:X:2561:G:C8	2.57	0.40
27:X:773:G:C2'	27:X:774:A:H5'	2.52	0.40
27:X:1712:G:N2	27:X:1713:G:C8	2.89	0.40
13:N:52:ASN:HA	13:N:55:ARG:HG3	2.03	0.40
27:X:165:G:N2	27:X:185:C:N3	2.54	0.40
27:X:1698:C:O2	27:X:1753:A:H2'	2.21	0.40
7:H:28:GLY:C	7:H:35:THR:H	2.25	0.40
1:A:151:LYS:HA	1:A:151:LYS:HD2	1.92	0.40
27:X:2186:G:H2'	27:X:2187:A:C8	2.56	0.40
16:Q:4:TYR:CE2	21:V:23:LYS:HB2	2.57	0.40
27:X:1671:A:C1'	27:X:2798:A:H5'	2.51	0.40
19:T:53:MET:HA	19:T:58:THR:O	2.21	0.40
13:N:74:MET:SD	13:N:79:PHE:HD1	2.45	0.40
15:P:98:ASP:CG	27:X:23:G:H21	2.25	0.40
27:X:428:A:H2'	27:X:429:C:C6	2.56	0.40
2:B:172:VAL:HG22	2:B:182:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:98:LEU:O	10:K:111:ALA:HB1	2.22	0.40
27:X:1967:U:H2'	27:X:1968:G:H8	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/275 (94%)	223 (86%)	34 (13%)	1 (0%)	39	80
2	B	203/211 (96%)	182 (90%)	20 (10%)	1 (0%)	34	77
3	C	192/205 (94%)	165 (86%)	25 (13%)	2 (1%)	19	66
4	D	175/180 (97%)	153 (87%)	21 (12%)	1 (1%)	30	74
5	E	169/185 (91%)	155 (92%)	13 (8%)	1 (1%)	30	74
6	G	140/174 (80%)	126 (90%)	14 (10%)	0	100	100
7	H	132/134 (98%)	123 (93%)	8 (6%)	1 (1%)	24	70
8	I	132/156 (85%)	101 (76%)	28 (21%)	3 (2%)	8	52
9	J	134/141 (95%)	115 (86%)	19 (14%)	0	100	100
10	K	111/116 (96%)	102 (92%)	9 (8%)	0	100	100
11	L	102/114 (90%)	86 (84%)	16 (16%)	0	100	100
12	M	106/166 (64%)	101 (95%)	5 (5%)	0	100	100
13	N	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	11	57
14	O	92/100 (92%)	81 (88%)	11 (12%)	0	100	100
15	P	128/137 (93%)	109 (85%)	17 (13%)	2 (2%)	12	58
16	Q	91/95 (96%)	78 (86%)	11 (12%)	2 (2%)	8	52
17	R	108/114 (95%)	86 (80%)	22 (20%)	0	100	100
18	S	173/237 (73%)	152 (88%)	21 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	T	72/91 (79%)	61 (85%)	9 (12%)	2 (3%)	6	47
20	U	70/81 (86%)	52 (74%)	14 (20%)	4 (6%)	2	28
21	V	63/67 (94%)	59 (94%)	4 (6%)	0	100	100
22	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
23	Z	54/60 (90%)	48 (89%)	6 (11%)	0	100	100
24	1	51/55 (93%)	37 (72%)	11 (22%)	3 (6%)	2	27
25	2	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
26	3	57/66 (86%)	46 (81%)	11 (19%)	0	100	100
All	All	3025/3380 (90%)	2633 (87%)	367 (12%)	25 (1%)	24	70

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	6	ILE
13	N	94	VAL
15	P	127	ILE
24	1	9	ILE
24	1	10	VAL
16	Q	69	ILE
19	T	19	LYS
20	U	60	VAL
2	B	121	ASN
4	D	146	VAL
5	E	165	VAL
8	I	53	ARG
20	U	15	VAL
20	U	39	LYS
1	A	219	PRO
7	H	42	LYS
24	1	18	THR
15	P	129	ILE
3	C	15	ILE
13	N	8	ILE
20	U	30	VAL
19	T	75	GLY
3	C	22	VAL
8	I	19	VAL
8	I	68	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/216 (94%)	158 (78%)	44 (22%)	1	9
2	B	155/157 (99%)	137 (88%)	18 (12%)	7	37
3	C	154/163 (94%)	126 (82%)	28 (18%)	2	15
4	D	153/156 (98%)	140 (92%)	13 (8%)	13	53
5	E	136/144 (94%)	122 (90%)	14 (10%)	9	43
6	G	118/146 (81%)	98 (83%)	20 (17%)	2	18
7	H	103/103 (100%)	88 (85%)	15 (15%)	4	27
8	I	101/121 (84%)	83 (82%)	18 (18%)	2	16
9	J	110/115 (96%)	86 (78%)	24 (22%)	1	9
10	K	90/93 (97%)	75 (83%)	15 (17%)	3	19
11	L	74/82 (90%)	53 (72%)	21 (28%)	0	4
12	M	94/134 (70%)	71 (76%)	23 (24%)	1	7
13	N	96/97 (99%)	81 (84%)	15 (16%)	3	23
14	O	75/79 (95%)	65 (87%)	10 (13%)	5	31
15	P	112/118 (95%)	92 (82%)	20 (18%)	2	16
16	Q	75/76 (99%)	59 (79%)	16 (21%)	1	10
17	R	91/95 (96%)	78 (86%)	13 (14%)	4	28
18	S	149/192 (78%)	126 (85%)	23 (15%)	3	24
19	T	55/67 (82%)	49 (89%)	6 (11%)	8	41
20	U	57/66 (86%)	43 (75%)	14 (25%)	1	7
21	V	53/55 (96%)	46 (87%)	7 (13%)	5	31
22	W	48/48 (100%)	45 (94%)	3 (6%)	22	65
23	Z	50/53 (94%)	43 (86%)	7 (14%)	4	29
24	1	46/48 (96%)	33 (72%)	13 (28%)	0	4
25	2	39/40 (98%)	26 (67%)	13 (33%)	0	2
26	3	46/52 (88%)	37 (80%)	9 (20%)	1	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2482/2716 (91%)	2060 (83%)	422 (17%)	2 18

All (422) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	15	GLN
1	A	21	PHE
1	A	22	SER
1	A	27	LYS
1	A	33	LEU
1	A	34	THR
1	A	40	THR
1	A	43	ARG
1	A	48	ARG
1	A	64	ILE
1	A	68	LYS
1	A	84	TYR
1	A	88	ARG
1	A	96	HIS
1	A	104	TYR
1	A	111	LEU
1	A	116	THR
1	A	118	ASN
1	A	129	ASN
1	A	134	ARG
1	A	151	LYS
1	A	154	GLN
1	A	157	ARG
1	A	161	THR
1	A	164	GLN
1	A	171	ASP
1	A	183	ARG
1	A	198	ASN
1	A	201	HIS
1	A	203	ASN
1	A	206	LEU
1	A	214	TRP
1	A	215	LEU
1	A	218	LYS
1	A	240	THR
1	A	244	ARG

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Mol	Chain	Res	Type
1	A	245	VAL
1	A	247	VAL
1	A	248	THR
1	A	250	TRP
1	A	252	LYS
1	A	259	THR
1	A	262	LYS
2	B	24	THR
2	B	35	GLN
2	B	47	VAL
2	B	60	ASN
2	B	66	HIS
2	B	72	VAL
2	B	79	ARG
2	B	84	PHE
2	B	87	ASP
2	B	118	LYS
2	B	119	ARG
2	B	132	LYS
2	B	143	GLN
2	B	165	VAL
2	B	198	LEU
2	B	199	ARG
2	B	200	SER
2	B	203	LYS
3	C	5	ASN
3	C	14	THR
3	C	17	LEU
3	C	31	VAL
3	C	45	THR
3	C	48	ARG
3	C	50	GLN
3	C	51	VAL
3	C	53	LYS
3	C	56	ARG
3	C	62	LYS
3	C	64	THR
3	C	74	VAL
3	C	82	VAL
3	C	91	TYR
3	C	116	LYS
3	C	124	ASP

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Mol	Chain	Res	Type
3	C	127	ASP
3	C	143	ASP
3	C	152	THR
3	C	157	THR
3	C	164	VAL
3	C	165	SER
3	C	176	ASN
3	C	180	ILE
3	C	182	ARG
3	C	189	ASP
3	C	193	LEU
4	D	9	ASN
4	D	46	ASP
4	D	62	LEU
4	D	73	SER
4	D	80	ARG
4	D	89	VAL
4	D	90	THR
4	D	112	ARG
4	D	130	LEU
4	D	137	ILE
4	D	146	VAL
4	D	148	LYS
4	D	173	MET
5	E	32	GLU
5	E	35	VAL
5	E	44	ARG
5	E	50	LEU
5	E	69	ARG
5	E	89	LEU
5	E	113	VAL
5	E	116	GLU
5	E	127	GLU
5	E	136	ILE
5	E	158	HIS
5	E	164	PHE
5	E	165	VAL
5	E	175	LYS
6	G	39	GLN
6	G	40	ASN
6	G	42	VAL
6	G	47	SER

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Mol	Chain	Res	Type
6	G	61	ARG
6	G	69	ASP
6	G	71	THR
6	G	75	ILE
6	G	94	LYS
6	G	98	LYS
6	G	99	VAL
6	G	101	THR
6	G	102	ARG
6	G	111	LYS
6	G	116	ARG
6	G	126	VAL
6	G	132	PHE
6	G	145	HIS
6	G	156	HIS
6	G	158	HIS
7	H	23	ARG
7	H	46	HIS
7	H	51	ILE
7	H	54	SER
7	H	81	ILE
7	H	87	SER
7	H	89	ILE
7	H	104	GLU
7	H	108	THR
7	H	109	ARG
7	H	110	VAL
7	H	118	LEU
7	H	119	ARG
7	H	126	ILE
7	H	127	VAL
8	I	26	THR
8	I	32	ARG
8	I	39	SER
8	I	49	PHE
8	I	50	GLU
8	I	54	SER
8	I	55	ARG
8	I	56	LEU
8	I	59	ARG
8	I	60	LEU
8	I	65	PHE

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Mol	Chain	Res	Type
8	I	80	LEU
8	I	88	PHE
8	I	94	GLU
8	I	96	TYR
8	I	114	ILE
8	I	139	ARG
8	I	141	VAL
9	J	8	THR
9	J	9	LYS
9	J	10	PHE
9	J	11	ARG
9	J	15	ARG
9	J	17	ARG
9	J	27	TYR
9	J	28	VAL
9	J	44	LYS
9	J	45	SER
9	J	60	ARG
9	J	77	LYS
9	J	84	MET
9	J	93	TYR
9	J	94	TRP
9	J	103	VAL
9	J	105	PHE
9	J	110	VAL
9	J	111	THR
9	J	113	GLU
9	J	133	VAL
9	J	134	LYS
9	J	135	ARG
9	J	140	GLU
10	K	5	LYS
10	K	8	ARG
10	K	9	LYS
10	K	11	ASN
10	K	12	ARG
10	K	17	ARG
10	K	20	LEU
10	K	37	THR
10	K	45	ARG
10	K	59	ASP
10	K	94	TYR

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Mol	Chain	Res	Type
10	K	95	THR
10	K	98	LEU
10	K	109	THR
10	K	110	MET
11	L	8	ARG
11	L	11	LEU
11	L	12	ARG
11	L	13	THR
11	L	15	ARG
11	L	17	VAL
11	L	18	ARG
11	L	31	VAL
11	L	34	SER
11	L	37	HIS
11	L	38	ILE
11	L	39	TYR
11	L	43	ILE
11	L	45	ASP
11	L	50	THR
11	L	60	LYS
11	L	87	VAL
11	L	90	ASP
11	L	91	ARG
11	L	93	SER
11	L	108	ARG
12	M	3	THR
12	M	6	LYS
12	M	13	LEU
12	M	16	ILE
12	M	19	ASP
12	M	20	HIS
12	M	25	PRO
12	M	28	ARG
12	M	31	ASP
12	M	34	ARG
12	M	38	LYS
12	M	45	THR
12	M	46	ARG
12	M	60	SER
12	M	71	ILE
12	M	83	PHE
12	M	87	LEU

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Mol	Chain	Res	Type
12	M	90	GLN
12	M	92	THR
12	M	96	ARG
12	M	98	LYS
12	M	101	ARG
12	M	103	LYS
13	N	3	ARG
13	N	13	ARG
13	N	18	LEU
13	N	22	LYS
13	N	30	LYS
13	N	40	LEU
13	N	55	ARG
13	N	59	ARG
13	N	60	LEU
13	N	70	ARG
13	N	75	ASN
13	N	90	LEU
13	N	93	LYS
13	N	97	ASP
13	N	102	GLU
14	O	11	GLN
14	O	21	ARG
14	O	28	GLU
14	O	34	GLU
14	O	47	PHE
14	O	56	VAL
14	O	69	ILE
14	O	81	ARG
14	O	88	GLN
14	O	91	THR
15	P	9	ARG
15	P	27	VAL
15	P	31	VAL
15	P	36	ARG
15	P	39	ARG
15	P	40	LEU
15	P	60	ILE
15	P	86	LEU
15	P	91	PHE
15	P	97	VAL
15	P	102	THR

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Mol	Chain	Res	Type
15	P	106	LEU
15	P	107	ILE
15	P	110	VAL
15	P	119	ILE
15	P	121	LYS
15	P	122	LYS
15	P	123	ARG
15	P	124	THR
15	P	129	ILE
16	Q	5	ASP
16	Q	6	ILE
16	Q	7	LEU
16	Q	12	ILE
16	Q	15	LYS
16	Q	26	SER
16	Q	27	PHE
16	Q	30	SER
16	Q	62	ARG
16	Q	64	ARG
16	Q	67	ARG
16	Q	73	ASN
16	Q	74	ASP
16	Q	75	ARG
16	Q	82	LEU
16	Q	84	GLU
17	R	18	LYS
17	R	38	LEU
17	R	48	VAL
17	R	55	THR
17	R	56	LYS
17	R	71	GLN
17	R	81	VAL
17	R	85	ASP
17	R	88	THR
17	R	92	THR
17	R	105	ARG
17	R	106	VAL
17	R	112	LYS
18	S	6	LYS
18	S	15	ASP
18	S	22	VAL
18	S	25	ASN

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Mol	Chain	Res	Type
18	S	28	ASN
18	S	48	THR
18	S	52	PHE
18	S	53	ASP
18	S	70	GLN
18	S	71	MET
18	S	79	ILE
18	S	88	TYR
18	S	94	VAL
18	S	100	THR
18	S	109	GLN
18	S	114	ASP
18	S	120	LEU
18	S	130	ILE
18	S	151	ASP
18	S	158	CYS
18	S	160	LEU
18	S	163	ASP
18	S	169	VAL
19	T	14	ARG
19	T	19	LYS
19	T	40	GLN
19	T	41	ARG
19	T	56	ASP
19	T	64	ASP
20	U	8	THR
20	U	10	LYS
20	U	17	SER
20	U	18	VAL
20	U	21	ARG
20	U	27	ASP
20	U	32	ARG
20	U	35	THR
20	U	43	ARG
20	U	47	HIS
20	U	48	LYS
20	U	49	LYS
20	U	53	GLU
20	U	63	SER
21	V	2	LYS
21	V	21	ARG
21	V	26	MET

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Mol	Chain	Res	Type
21	V	29	ARG
21	V	37	LEU
21	V	46	LEU
21	V	47	ARG
22	W	3	ILE
22	W	12	ARG
22	W	37	THR
23	Z	6	VAL
23	Z	21	SER
23	Z	23	HIS
23	Z	25	LEU
23	Z	40	LYS
23	Z	53	ASP
23	Z	55	ARG
24	1	7	ARG
24	1	8	ILE
24	1	20	PHE
24	1	21	TYR
24	1	28	ARG
24	1	30	ASN
24	1	32	GLN
24	1	36	GLU
24	1	41	ASP
24	1	43	VAL
24	1	50	PHE
24	1	51	ARG
24	1	54	LYS
25	2	1	MET
25	2	10	ARG
25	2	12	ARG
25	2	15	THR
25	2	19	ARG
25	2	21	ARG
25	2	28	ARG
25	2	31	LEU
25	2	34	ARG
25	2	40	HIS
25	2	41	GLN
25	2	43	THR
25	2	46	ASP
26	3	7	HIS
26	3	11	LYS

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Mol	Chain	Res	Type
26	3	19	THR
26	3	30	ARG
26	3	32	GLN
26	3	34	THR
26	3	48	PHE
26	3	55	TRP
26	3	62	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	164	GLN
1	A	166	GLN
2	B	66	HIS
2	B	129	HIS
3	C	10	ASN
3	C	34	GLN
3	C	132	ASN
3	C	156	ASN
3	C	163	ASN
3	C	176	ASN
4	D	37	ASN
4	D	129	ASN
5	E	74	ASN
5	E	139	GLN
6	G	39	GLN
6	G	84	ASN
6	G	107	GLN
6	G	140	GLN
8	I	103	ASN
9	J	58	HIS
9	J	124	HIS
10	K	3	HIS
10	K	24	GLN
12	M	23	GLN
13	N	34	ASN
13	N	37	GLN
13	N	41	ASN
13	N	63	GLN
13	N	66	ASN
14	O	63	HIS

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Mol	Chain	Res	Type
14	O	88	GLN
15	P	16	GLN
15	P	73	ASN
15	P	78	ASN
15	P	81	HIS
15	P	118	ASN
15	P	126	HIS
16	Q	43	GLN
16	Q	57	ASN
17	R	10	HIS
17	R	15	HIS
17	R	29	HIS
17	R	44	GLN
17	R	69	GLN
17	R	71	GLN
18	S	118	HIS
18	S	121	GLN
19	T	17	ASN
20	U	16	ASN
22	W	15	ASN
23	Z	4	HIS
23	Z	35	GLN
23	Z	44	HIS
25	2	6	GLN
25	2	8	ASN
26	3	7	HIS
26	3	33	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	2657/2880 (92%)	611 (22%)	39 (1%)
28	Y	121/123 (98%)	31 (25%)	2 (1%)
All	All	2778/3003 (92%)	642 (23%)	41 (1%)

All (642) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	X	4	C
27	X	13	A
27	X	14	A

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Mol	Chain	Res	Type
27	X	15	G
27	X	17	G
27	X	34	U
27	X	37	C
27	X	39	C
27	X	45	C
27	X	48	A
27	X	49	U
27	X	50	G
27	X	51	A
27	X	59	G
27	X	63	A
27	X	68	C
27	X	69	G
27	X	73	A
27	X	74	G
27	X	75	C
27	X	83	A
27	X	88	G
27	X	89	A
27	X	90	G
27	X	91	A
27	X	95	G
27	X	100	G
27	X	101	A
27	X	108	G
27	X	110	U
27	X	116	A
27	X	118	U
27	X	123	A
27	X	124	A
27	X	129	A
27	X	134	G
27	X	136	A
27	X	137	A
27	X	143	A
27	X	147	G
27	X	173	A
27	X	176	A
27	X	178	C
27	X	181	A
27	X	182	G

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Mol	Chain	Res	Type
27	X	192	G
27	X	193	A
27	X	198	A
27	X	199	A
27	X	206	U
27	X	207	U
27	X	209	G
27	X	210	A
27	X	219	G
27	X	220	U
27	X	222	G
27	X	225	G
27	X	229	G
27	X	241	C
27	X	242	A
27	X	243	G
27	X	304	A
27	X	306	G
27	X	310	A
27	X	312	G
27	X	319	G
27	X	321	A
27	X	323	G
27	X	333	A
27	X	334	G
27	X	335	A
27	X	337	G
27	X	340	G
27	X	342	G
27	X	343	A
27	X	344	G
27	X	360	A
27	X	388	G
27	X	397	U
27	X	398	C
27	X	399	G
27	X	400	U
27	X	408	U
27	X	409	G
27	X	413	G
27	X	414	A
27	X	418	C

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Mol	Chain	Res	Type
27	X	419	G
27	X	421	G
27	X	424	G
27	X	425	A
27	X	435	A
27	X	441	A
27	X	453	U
27	X	456	C
27	X	459	A
27	X	463	C
27	X	467	U
27	X	469	G
27	X	483	A
27	X	484	G
27	X	492	G
27	X	493	A
27	X	500	G
27	X	504	G
27	X	514	G
27	X	515	A
27	X	518	A
27	X	519	C
27	X	520	C
27	X	521	U
27	X	537	C
27	X	538	A
27	X	539	A
27	X	540	G
27	X	541	C
27	X	542	A
27	X	543	G
27	X	554	U
27	X	555	U
27	X	556	A
27	X	557	U
27	X	559	C
27	X	572	G
27	X	582	G
27	X	584	A
27	X	587	A
27	X	591	G
27	X	595	A

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Mol	Chain	Res	Type
27	X	596	C
27	X	597	U
27	X	611	C
27	X	613	A
27	X	614	G
27	X	624	A
27	X	625	A
27	X	626	A
27	X	627	A
27	X	628	A
27	X	631	G
27	X	632	A
27	X	633	G
27	X	636	G
27	X	638	A
27	X	645	G
27	X	648	A
27	X	649	G
27	X	651	C
27	X	654	A
27	X	655	A
27	X	656	U
27	X	657	A
27	X	664	C
27	X	665	A
27	X	666	U
27	X	667	U
27	X	668	A
27	X	669	G
27	X	682	G
27	X	689	A
27	X	690	A
27	X	695	G
27	X	699	G
27	X	712	A
27	X	736	G
27	X	739	G
27	X	743	A
27	X	747	A
27	X	752	G
27	X	753	U
27	X	759	C

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Mol	Chain	Res	Type
27	X	760	U
27	X	766	A
27	X	774	A
27	X	788	G
27	X	789	G
27	X	790	A
27	X	795	A
27	X	797	A
27	X	798	G
27	X	801	A
27	X	802	A
27	X	803	C
27	X	805	G
27	X	806	A
27	X	814	G
27	X	818	G
27	X	824	U
27	X	825	C
27	X	832	A
27	X	840	U
27	X	841	G
27	X	845	U
27	X	846	A
27	X	856	A
27	X	859	U
27	X	872	G
27	X	879	A
27	X	891	A
27	X	922	A
27	X	931	G
27	X	938	G
27	X	939	C
27	X	940	G
27	X	944	A
27	X	952	A
27	X	956	A
27	X	957	G
27	X	964	A
27	X	966	A
27	X	967	G
27	X	972	C
27	X	973	U

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Mol	Chain	Res	Type
27	X	976	C
27	X	979	A
27	X	985	G
27	X	994	A
27	X	996	C
27	X	1006	C
27	X	1007	A
27	X	1014	G
27	X	1016	C
27	X	1019	U
27	X	1021	A
27	X	1023	U
27	X	1028	G
27	X	1032	A
27	X	1033	G
27	X	1034	U
27	X	1037	U
27	X	1044	U
27	X	1051	U
27	X	1054	C
27	X	1056	U
27	X	1057	A
27	X	1058	G
27	X	1060	C
27	X	1066	G
27	X	1068	A
27	X	1077	U
27	X	1079	G
27	X	1082	G
27	X	1083	C
27	X	1086	C
27	X	1087	C
27	X	1090	C
27	X	1097	A
27	X	1099	A
27	X	1108	U
27	X	1109	A
27	X	1123	G
27	X	1129	A
27	X	1130	U
27	X	1133	G
27	X	1139	A

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Mol	Chain	Res	Type
27	X	1142	G
27	X	1143	A
27	X	1144	U
27	X	1145	C
27	X	1146	G
27	X	1152	C
27	X	1153	A
27	X	1166	A
27	X	1183	C
27	X	1185	C
27	X	1192	A
27	X	1208	A
27	X	1209	G
27	X	1226	A
27	X	1247	U
27	X	1249	G
27	X	1250	A
27	X	1256	C
27	X	1266	G
27	X	1268	U
27	X	1269	G
27	X	1278	A
27	X	1284	G
27	X	1285	A
27	X	1288	A
27	X	1289	A
27	X	1301	U
27	X	1313	U
27	X	1314	A
27	X	1322	G
27	X	1325	U
27	X	1334	A
27	X	1336	G
27	X	1342	U
27	X	1354	A
27	X	1372	A
27	X	1378	A
27	X	1381	G
27	X	1391	A
27	X	1392	U
27	X	1397	A
27	X	1398	G

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Mol	Chain	Res	Type
27	X	1399	C
27	X	1404	C
27	X	1409	U
27	X	1413	U
27	X	1425	G
27	X	1428	G
27	X	1429	A
27	X	1430	G
27	X	1433	A
27	X	1434	U
27	X	1435	G
27	X	1442	C
27	X	1443	G
27	X	1459	U
27	X	1460	G
27	X	1465	G
27	X	1466	C
27	X	1468	A
27	X	1469	U
27	X	1470	G
27	X	1471	G
27	X	1475	U
27	X	1482	U
27	X	1490	U
27	X	1497	C
27	X	1498	G
27	X	1522	C
27	X	1523	A
27	X	1524	C
27	X	1525	A
27	X	1528	C
27	X	1531	C
27	X	1545	G
27	X	1551	U
27	X	1552	C
27	X	1553	G
27	X	1554	G
27	X	1562	G
27	X	1564	U
27	X	1570	C
27	X	1571	G
27	X	1574	A

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Mol	Chain	Res	Type
27	X	1575	C
27	X	1582	A
27	X	1585	A
27	X	1594	U
27	X	1601	U
27	X	1602	G
27	X	1603	A
27	X	1608	U
27	X	1624	A
27	X	1626	A
27	X	1629	G
27	X	1632	A
27	X	1634	A
27	X	1648	C
27	X	1651	U
27	X	1656	U
27	X	1657	A
27	X	1661	C
27	X	1665	C
27	X	1674	C
27	X	1680	U
27	X	1682	A
27	X	1686	A
27	X	1688	U
27	X	1691	G
27	X	1710	U
27	X	1713	G
27	X	1717	A
27	X	1718	A
27	X	1735	G
27	X	1747	G
27	X	1749	G
27	X	1755	G
27	X	1760	G
27	X	1764	A
27	X	1767	G
27	X	1770	U
27	X	1775	A
27	X	1782	A
27	X	1790	G
27	X	1791	C
27	X	1792	C

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Mol	Chain	Res	Type
27	X	1793	A
27	X	1799	A
27	X	1801	C
27	X	1802	A
27	X	1807	A
27	X	1808	C
27	X	1812	U
27	X	1813	A
27	X	1819	U
27	X	1821	A
27	X	1825	C
27	X	1831	G
27	X	1846	A
27	X	1861	G
27	X	1867	A
27	X	1868	A
27	X	1874	G
27	X	1882	G
27	X	1886	G
27	X	1887	G
27	X	1888	C
27	X	1910	A
27	X	1912	G
27	X	1919	A
27	X	1920	A
27	X	1921	A
27	X	1922	U
27	X	1923	U
27	X	1924	C
27	X	1938	U
27	X	1943	A
27	X	1944	C
27	X	1945	C
27	X	1946	U
27	X	1948	C
27	X	1949	A
27	X	1950	C
27	X	1953	A
27	X	1954	A
27	X	1955	G
27	X	1965	U
27	X	1970	G

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Mol	Chain	Res	Type
27	X	1974	U
27	X	1976	U
27	X	1980	A
27	X	1999	U
27	X	2003	A
27	X	2004	U
27	X	2006	G
27	X	2014	A
27	X	2015	G
27	X	2016	A
27	X	2018	G
27	X	2023	C
27	X	2026	C
27	X	2032	G
27	X	2038	C
27	X	2039	G
27	X	2043	A
27	X	2044	G
27	X	2045	A
27	X	2052	G
27	X	2075	U
27	X	2076	G
27	X	2083	G
27	X	2089	C
27	X	2171	U
27	X	2181	A
27	X	2189	A
27	X	2190	A
27	X	2191	A
27	X	2192	U
27	X	2195	C
27	X	2196	U
27	X	2197	U
27	X	2198	U
27	X	2199	C
27	X	2200	G
27	X	2204	A
27	X	2205	C
27	X	2217	G
27	X	2218	G
27	X	2222	U
27	X	2225	G

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Mol	Chain	Res	Type
27	X	2247	A
27	X	2262	C
27	X	2265	A
27	X	2266	A
27	X	2268	G
27	X	2284	U
27	X	2285	U
27	X	2286	G
27	X	2287	G
27	X	2290	A
27	X	2294	U
27	X	2298	U
27	X	2300	G
27	X	2301	A
27	X	2305	C
27	X	2306	A
27	X	2311	U
27	X	2312	A
27	X	2313	G
27	X	2315	A
27	X	2324	G
27	X	2326	C
27	X	2329	C
27	X	2330	G
27	X	2333	A
27	X	2351	G
27	X	2358	C
27	X	2361	G
27	X	2362	G
27	X	2364	C
27	X	2369	U
27	X	2371	A
27	X	2375	G
27	X	2381	A
27	X	2386	G
27	X	2387	U
27	X	2398	U
27	X	2401	A
27	X	2402	U
27	X	2404	A
27	X	2405	A
27	X	2406	C

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Mol	Chain	Res	Type
27	X	2408	G
27	X	2410	U
27	X	2413	A
27	X	2420	C
27	X	2424	G
27	X	2427	A
27	X	2429	A
27	X	2449	G
27	X	2452	U
27	X	2453	C
27	X	2455	A
27	X	2457	A
27	X	2458	U
27	X	2463	G
27	X	2471	U
27	X	2477	C
27	X	2479	U
27	X	2480	C
27	X	2481	G
27	X	2482	A
27	X	2483	U
27	X	2484	G
27	X	2497	A
27	X	2498	U
27	X	2504	G
27	X	2508	G
27	X	2522	G
27	X	2532	G
27	X	2542	U
27	X	2545	A
27	X	2546	G
27	X	2551	A
27	X	2552	C
27	X	2553	G
27	X	2556	A
27	X	2557	G
27	X	2561	G
27	X	2564	U
27	X	2565	C
27	X	2578	G
27	X	2581	A
27	X	2582	G

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Mol	Chain	Res	Type
27	X	2583	U
27	X	2588	U
27	X	2591	C
27	X	2593	A
27	X	2594	U
27	X	2600	A
27	X	2608	A
27	X	2611	A
27	X	2624	G
27	X	2633	A
27	X	2634	G
27	X	2642	G
27	X	2650	G
27	X	2664	G
27	X	2668	U
27	X	2691	C
27	X	2692	A
27	X	2693	U
27	X	2694	G
27	X	2698	G
27	X	2706	U
27	X	2713	A
27	X	2728	A
27	X	2731	G
27	X	2732	C
27	X	2738	A
27	X	2744	A
27	X	2745	A
27	X	2757	G
27	X	2758	A
27	X	2759	U
27	X	2760	G
27	X	2769	C
27	X	2770	A
27	X	2771	C
27	X	2780	A
27	X	2781	G
27	X	2782	G
27	X	2783	U
27	X	2787	A
27	X	2795	A
27	X	2796	A

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Mol	Chain	Res	Type
27	X	2798	A
27	X	2807	U
27	X	2809	A
27	X	2811	G
27	X	2814	G
27	X	2824	C
27	X	2825	A
27	X	2832	G
27	X	2842	C
27	X	2847	G
27	X	2849	C
27	X	2851	G
27	X	2852	G
27	X	2854	G
27	X	2858	A
27	X	2860	C
27	X	2861	A
27	X	2866	A
27	X	2868	G
27	X	2869	U
28	Y	14	C
28	Y	15	A
28	Y	17	A
28	Y	18	G
28	Y	26	G
28	Y	28	A
28	Y	29	C
28	Y	37	C
28	Y	42	U
28	Y	43	G
28	Y	45	C
28	Y	46	G
28	Y	47	A
28	Y	49	C
28	Y	51	G
28	Y	54	U
28	Y	59	A
28	Y	68	A
28	Y	69	G
28	Y	72	C
28	Y	75	A
28	Y	86	A

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Mol	Chain	Res	Type
28	Y	97	C
28	Y	102	A
28	Y	108	G
28	Y	110	U
28	Y	111	C
28	Y	112	A
28	Y	113	G
28	Y	115	G
28	Y	123	U

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	X	38	G
27	X	48	A
27	X	50	G
27	X	123	A
27	X	218	A
27	X	219	G
27	X	334	G
27	X	434	C
27	X	458	G
27	X	492	G
27	X	499	G
27	X	537	C
27	X	553	C
27	X	788	G
27	X	789	G
27	X	1031	C
27	X	1053	G
27	X	1059	A
27	X	1141	U
27	X	1182	U
27	X	1225	G
27	X	1313	U
27	X	1391	A
27	X	1398	G
27	X	1441	A
27	X	1496	G
27	X	1607	A
27	X	1811	A
27	X	1923	U

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Mol	Chain	Res	Type
27	X	1975	G
27	X	2190	A
27	X	2228	U
27	X	2299	A
27	X	2312	A
27	X	2404	A
27	X	2409	A
27	X	2705	A
27	X	2756	A
27	X	2824	C
28	Y	27	A
28	Y	58	G

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 51 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	260/275 (94%)	0.05	14 (5%) 29 18	45, 101, 165, 255	0
2	B	205/211 (97%)	-0.53	0 100 100	26, 43, 97, 208	0
3	C	194/205 (94%)	-0.13	10 (5%) 31 19	38, 101, 172, 256	0
4	D	177/180 (98%)	0.37	24 (13%) 4 3	108, 173, 225, 261	0
5	E	171/185 (92%)	-0.26	3 (1%) 71 54	51, 120, 177, 236	0
6	G	142/174 (81%)	-0.13	4 (2%) 56 39	35, 72, 151, 204	0
7	H	134/134 (100%)	-0.42	0 100 100	31, 42, 85, 136	0
8	I	134/156 (85%)	0.42	10 (7%) 17 10	53, 125, 199, 245	0
9	J	136/141 (96%)	-0.01	4 (2%) 55 37	56, 88, 168, 221	0
10	K	113/116 (97%)	-0.58	0 100 100	25, 30, 61, 99	0
11	L	104/114 (91%)	0.62	18 (17%) 2 1	128, 160, 197, 232	0
12	M	108/166 (65%)	-0.49	1 (0%) 85 74	29, 37, 93, 143	0
13	N	117/118 (99%)	-0.37	1 (0%) 85 74	40, 78, 123, 213	0
14	O	94/100 (94%)	-0.24	1 (1%) 82 68	51, 96, 164, 191	0
15	P	130/137 (94%)	-0.35	3 (2%) 64 46	31, 51, 149, 168	0
16	Q	93/95 (97%)	-0.35	1 (1%) 82 68	45, 83, 145, 192	0
17	R	110/114 (96%)	0.17	7 (6%) 23 12	66, 97, 187, 238	0
18	S	175/237 (73%)	-0.26	3 (1%) 73 56	89, 141, 204, 258	0
19	T	74/91 (81%)	0.16	3 (4%) 41 25	70, 110, 148, 231	0
20	U	72/81 (88%)	0.77	10 (13%) 4 3	73, 123, 178, 252	0
21	V	65/67 (97%)	-0.18	2 (3%) 52 35	67, 111, 168, 222	0
22	W	55/55 (100%)	0.32	5 (9%) 11 6	72, 94, 147, 177	0
23	Z	56/60 (93%)	-0.57	0 100 100	30, 36, 87, 100	0
24	1	53/55 (96%)	0.84	9 (16%) 2 2	98, 127, 189, 275	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	2	46/47 (97%)	-0.20	1 (2%) 65 47	39, 69, 102, 127	0
26	3	59/66 (89%)	0.83	8 (13%) 4 3	79, 99, 176, 252	0
27	X	2667/2880 (92%)	-0.54	22 (0%) 87 76	25, 73, 176, 304	0
28	Y	122/123 (99%)	-0.50	3 (2%) 61 43	74, 150, 189, 279	0
All	All	5866/6383 (91%)	-0.30	167 (2%) 56 39	25, 87, 183, 304	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	U	28	GLY	10.8
27	X	1086	C	9.1
27	X	1525	A	5.9
27	X	1734	C	5.8
27	X	1524	C	5.7
27	X	1085	G	5.6
3	C	19	LEU	5.6
11	L	97	HIS	4.9
11	L	52	ALA	4.9
4	D	81	GLN	4.5
17	R	102	LYS	4.5
28	Y	123	U	4.4
4	D	73	SER	4.4
6	G	156	HIS	4.4
17	R	83	LEU	4.3
24	1	35	LEU	4.3
4	D	75	SER	4.2
20	U	27	ASP	4.2
11	L	40	ALA	4.2
24	1	27	ASN	4.2
17	R	60	PRO	4.1
24	1	51	ARG	4.0
27	X	1089	C	3.8
4	D	43	SER	3.8
26	3	10	ALA	3.7
4	D	61	THR	3.6
20	U	16	ASN	3.6
11	L	33	ARG	3.6
1	A	236	GLY	3.6
27	X	248	A	3.5
8	I	52	GLY	3.5
27	X	1037	U	3.5

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Mol	Chain	Res	Type	RSRZ
11	L	54	ALA	3.5
26	3	9	MET	3.5
17	R	61	SER	3.5
4	D	94	GLU	3.5
11	L	53	ALA	3.4
4	D	76	ASN	3.4
21	V	66	GLN	3.3
4	D	72	LYS	3.2
20	U	52	ARG	3.2
24	1	40	TYR	3.2
27	X	1190	C	3.2
11	L	39	TYR	3.2
26	3	54	GLU	3.2
1	A	55	GLY	3.2
27	X	1185	C	3.2
1	A	69	ARG	3.2
22	W	4	LYS	3.2
27	X	1072	U	3.1
28	Y	14	C	3.1
8	I	67	ASN	3.0
11	L	31	VAL	3.0
9	J	84	MET	3.0
27	X	1733	U	3.0
9	J	22	ALA	3.0
6	G	97	ASP	3.0
8	I	53	ARG	3.0
22	W	7	ARG	3.0
4	D	99	PHE	3.0
11	L	89	PHE	3.0
24	1	14	SER	2.9
18	S	92	VAL	2.9
27	X	2090	U	2.9
17	R	99	VAL	2.9
17	R	82	ALA	2.9
16	Q	64	ARG	2.9
3	C	44	SER	2.9
11	L	85	LYS	2.9
20	U	51	ILE	2.9
22	W	6	VAL	2.9
11	L	58	ALA	2.8
26	3	14	ILE	2.8
4	D	138	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	91	TYR	2.8
4	D	74	ILE	2.8
5	E	62	ARG	2.8
1	A	237	GLU	2.8
11	L	96	TYR	2.8
19	T	73	GLY	2.8
9	J	21	ASP	2.7
11	L	62	GLY	2.7
4	D	112	ARG	2.7
4	D	71	LYS	2.7
4	D	113	ASP	2.7
26	3	45	GLY	2.6
8	I	75	VAL	2.6
27	X	1069	G	2.6
24	1	23	THR	2.6
4	D	103	LEU	2.5
19	T	85	GLN	2.5
26	3	55	TRP	2.5
22	W	23	LEU	2.5
26	3	21	LYS	2.5
11	L	51	LEU	2.5
27	X	2381	A	2.5
1	A	18	THR	2.5
8	I	25	GLY	2.5
11	L	61	SER	2.5
24	1	38	LYS	2.5
1	A	259	THR	2.5
22	W	26	ARG	2.5
8	I	31	GLY	2.5
19	T	71	ASN	2.4
27	X	1954	A	2.4
14	O	23	GLU	2.4
11	L	12	ARG	2.4
15	P	137	LYS	2.4
4	D	97	TYR	2.4
1	A	56	GLY	2.4
27	X	361	G	2.4
3	C	47	THR	2.4
4	D	134	GLU	2.3
3	C	193	LEU	2.3
8	I	27	ASP	2.3
1	A	91	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
9	J	100	PRO	2.3
4	D	60	ILE	2.3
18	S	14	LEU	2.3
12	M	40	ARG	2.3
8	I	54	SER	2.3
15	P	107	ILE	2.3
13	N	91	ASN	2.3
4	D	175	LEU	2.3
20	U	70	LEU	2.3
11	L	30	SER	2.3
28	Y	43	G	2.2
1	A	100	GLY	2.2
1	A	254	THR	2.2
4	D	142	THR	2.2
27	X	1087	C	2.2
8	I	100	ARG	2.2
18	S	12	GLN	2.2
3	C	20	PRO	2.2
1	A	76	ASN	2.2
3	C	48	ARG	2.2
1	A	250	TRP	2.2
5	E	133	VAL	2.2
27	X	1084	A	2.2
4	D	145	MET	2.2
3	C	81	GLY	2.1
26	3	22	VAL	2.1
27	X	665	A	2.1
1	A	260	ARG	2.1
24	1	8	ILE	2.1
6	G	129	HIS	2.1
3	C	189	ASP	2.1
6	G	155	THR	2.1
21	V	62	ARG	2.1
8	I	24	GLY	2.1
20	U	43	ARG	2.1
20	U	13	LEU	2.1
20	U	62	LEU	2.1
1	A	235	GLY	2.1
4	D	107	GLY	2.1
4	D	108	LEU	2.1
5	E	58	ALA	2.1
25	2	1	MET	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	66	ASN	2.1
4	D	146	VAL	2.0
11	L	100	VAL	2.0
15	P	118	ASN	2.0
17	R	100	ASP	2.0
27	X	1138	A	2.0
27	X	2089	C	2.0
24	1	4	ASP	2.0
20	U	29	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MG	X	2926	1/1	0.91	0.83	83.37	32,32,32,32	0
29	MG	X	2921	1/1	0.99	0.70	43.54	51,51,51,51	0
29	MG	X	2907	1/1	0.90	1.23	28.02	42,42,42,42	0
29	MG	X	2917	1/1	0.93	1.05	26.93	55,55,55,55	0
29	MG	X	2912	1/1	0.93	0.59	20.49	27,27,27,27	0
29	MG	X	2947	1/1	0.94	0.62	18.49	49,49,49,49	0
29	MG	X	2944	1/1	0.86	1.39	17.81	55,55,55,55	0
29	MG	X	2943	1/1	0.97	0.32	14.87	31,31,31,31	0
29	MG	X	2913	1/1	0.97	0.52	14.45	27,27,27,27	0
29	MG	X	2910	1/1	0.96	0.53	14.23	39,39,39,39	0
29	MG	X	2905	1/1	0.98	0.45	13.28	27,27,27,27	0
29	MG	X	2924	1/1	0.93	0.66	12.66	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MG	X	2902	1/1	0.96	0.55	11.91	33,33,33,33	0
29	MG	X	2931	1/1	0.99	0.39	11.54	25,25,25,25	0
29	MG	X	2934	1/1	0.97	0.44	11.17	42,42,42,42	0
29	MG	X	2919	1/1	0.97	0.50	8.23	59,59,59,59	0
29	MG	K	201	1/1	0.86	0.70	8.22	25,25,25,25	0
29	MG	X	2940	1/1	0.96	0.66	8.15	54,54,54,54	0
29	MG	X	2929	1/1	0.96	0.45	7.53	37,37,37,37	0
29	MG	X	2928	1/1	0.98	0.29	6.92	36,36,36,36	0
29	MG	X	2939	1/1	0.97	0.31	6.08	32,32,32,32	0
29	MG	X	2920	1/1	0.97	0.32	4.47	41,41,41,41	0
29	MG	X	2901	1/1	0.96	0.32	4.34	37,37,37,37	0
29	MG	X	2936	1/1	0.97	0.21	3.46	33,33,33,33	0
29	MG	X	2909	1/1	0.91	0.53	2.90	51,51,51,51	0
29	MG	X	2922	1/1	0.95	0.35	2.27	30,30,30,30	0
29	MG	X	2923	1/1	0.96	0.38	-	33,33,33,33	0
29	MG	X	2903	1/1	0.94	0.60	-	30,30,30,30	0
29	MG	X	2950	1/1	0.92	0.84	-	37,37,37,37	0
29	MG	X	2927	1/1	0.91	0.16	-	69,69,69,69	0
29	MG	X	2908	1/1	0.97	0.49	-	31,31,31,31	0
29	MG	X	2904	1/1	0.92	0.40	-	29,29,29,29	0
29	MG	X	2906	1/1	0.92	0.88	-	27,27,27,27	0
29	MG	X	2916	1/1	0.93	1.10	-	26,26,26,26	0
29	MG	X	2915	1/1	0.93	0.37	-	28,28,28,28	0
29	MG	X	2911	1/1	0.96	0.87	-	40,40,40,40	0
29	MG	X	2938	1/1	0.97	0.40	-	27,27,27,27	0
29	MG	X	2945	1/1	0.97	0.46	-	61,61,61,61	0
29	MG	X	2935	1/1	0.90	0.33	-	74,74,74,74	0
29	MG	X	2930	1/1	0.96	0.45	-	30,30,30,30	0
29	MG	X	2925	1/1	0.98	0.54	-	32,32,32,32	0
29	MG	X	2949	1/1	0.98	0.22	-	32,32,32,32	0
29	MG	X	2937	1/1	0.97	0.38	-	36,36,36,36	0
29	MG	X	2933	1/1	0.95	0.34	-	55,55,55,55	0
29	MG	X	2946	1/1	0.97	0.69	-	27,27,27,27	0
29	MG	X	2914	1/1	0.98	0.55	-	26,26,26,26	0
29	MG	X	2941	1/1	0.86	0.78	-	115,115,115,115	0
29	MG	X	2932	1/1	0.97	0.47	-	39,39,39,39	0
29	MG	X	2948	1/1	0.93	0.23	-	48,48,48,48	0
29	MG	X	2918	1/1	0.99	0.56	-	36,36,36,36	0
29	MG	X	2942	1/1	0.96	0.33	-	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.