



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2016 – 12:20 AM GMT

PDB ID : 5DM6
Title : Crystal structure of the 50S ribosomal subunit from *Deinococcus radiodurans*
Authors : Kaminishi, T.; Schedlbauer, A.; Ochoa-Lizarralde, B.; Connell, S.R.; Fucini, P.
Deposited on : 2015-09-08
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 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

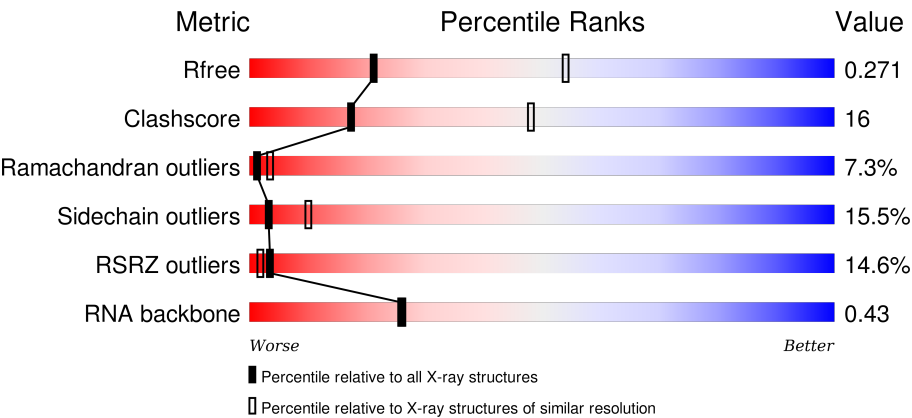
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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

Mol	Chain	Length	Quality of chain
1	0	224	<div><div>89%</div><div><div></div><div>54%</div><div>38%</div><div>8%</div></div></div>
2	A	274	<div><div>11%</div><div><div></div><div>58%</div><div>37%</div><div>5%</div></div></div>
3	B	205	<div><div>3%</div><div><div></div><div>53%</div><div>40%</div><div>7%</div></div></div>
4	C	197	<div><div>8%</div><div><div></div><div>44%</div><div>46%</div><div>10%</div></div></div>

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	171	
7	F	144	
8	G	142	
9	H	134	
10	I	141	
11	J	136	
12	K	113	
13	L	104	
14	M	109	
15	N	117	
16	O	94	
17	P	127	
18	Q	93	
19	R	110	
20	S	175	
21	T	84	
22	U	72	
23	V	66	
24	W	55	
25	Z	57	
26	1	54	
27	2	47	
28	3	65	
29	X	2881	

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Mol	Chain	Length	Quality of chain
30	Y	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6001	-	-	-	X
31	MG	X	6002	-	-	-	X
31	MG	X	6004	-	-	-	X
31	MG	X	6006	-	-	-	X
31	MG	X	6007	-	-	-	X
31	MG	X	6008	-	-	-	X
31	MG	X	6011	-	-	-	X
31	MG	X	6013	-	-	-	X
31	MG	X	6014	-	-	-	X
31	MG	X	6016	-	-	-	X
31	MG	X	6017	-	-	-	X
31	MG	X	6018	-	-	-	X
31	MG	X	6019	-	-	-	X
31	MG	X	6020	-	-	-	X
31	MG	X	6022	-	-	-	X
31	MG	X	6023	-	-	-	X
31	MG	X	6024	-	-	-	X
31	MG	X	6035	-	-	-	X
31	MG	X	6036	-	-	-	X
31	MG	X	6040	-	-	-	X
31	MG	X	6041	-	-	-	X
31	MG	X	6051	-	-	-	X
31	MG	X	6054	-	-	-	X
31	MG	X	6056	-	-	-	X
31	MG	X	6057	-	-	-	X
31	MG	X	6058	-	-	-	X
31	MG	X	6059	-	-	-	X
31	MG	X	6060	-	-	-	X
31	MG	X	6062	-	-	-	X
31	MG	X	6063	-	-	-	X
31	MG	X	6066	-	-	-	X
31	MG	X	6070	-	-	-	X
31	MG	X	6071	-	-	-	X
31	MG	X	6072	-	-	-	X
31	MG	X	6078	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6084	-	-	-	X
31	MG	X	6091	-	-	-	X
31	MG	X	6092	-	-	-	X
31	MG	X	6093	-	-	-	X
31	MG	X	6112	-	-	-	X
31	MG	X	6117	-	-	-	X
31	MG	X	6118	-	-	-	X
31	MG	X	6121	-	-	-	X
31	MG	X	6125	-	-	-	X
31	MG	X	6135	-	-	-	X
31	MG	X	6140	-	-	-	X
31	MG	X	6142	-	-	-	X
31	MG	X	6147	-	-	-	X
31	MG	X	6151	-	-	-	X
31	MG	X	6158	-	-	-	X
31	MG	X	6169	-	-	-	X
31	MG	X	6180	-	-	-	X
31	MG	X	6185	-	-	-	X

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 89337 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 L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	224	Total	C	N	O	S	0	0	0
			1651	1031	302	313	5			

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	274	Total	C	N	O	S	0	0	0
			2107	1313	423	368	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	ARG	conflict	UNP Q9RXJ9
A	25	ALA	THR	conflict	UNP Q9RXJ9
A	270	LEU	ILE	conflict	UNP Q9RXJ9

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	177	Total	C	N	O	S	0	0	0
			1401	892	247	255	7			

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	171	Total	C	N	O	S	0	0	0
			1287	812	237	237	1			

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	144	Total	C	N	O	S	0	0	0
			1048	663	183	197	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	expression tag	UNP Q9RSS7
F	2	ARG	-	expression tag	UNP Q9RSS7
F	3	ARG	-	expression tag	UNP Q9RSS7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1115	704	209	199	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	141	Total	C	N	O		0	0	0
			1068	655	216	197				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1091	696	202	186	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	113	Total	C	N	O	S	0	0	0
			879	541	178	158	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			778	476	159	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	LYS	ARG	conflict	UNP Q9RSL2

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O	0	0	0
			867	540	171	156			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	107	GLY	-	expression tag	UNP Q9RWB4
M	108	LYS	-	expression tag	UNP Q9RWB4
M	109	ALA	-	expression tag	UNP Q9RWB4
M	110	ALA	-	expression tag	UNP Q9RWB4

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	94	Total	C	N	O	0	0	0
			742	465	139	138			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			826	513	160	152	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	0
			1346	849	236	255	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	84	Total	C	N	O	S	0	0	0
			626	393	122	110	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	72	Total	C	N	O	0	0	0
			553	341	116	96			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	67	ILE	LEU	conflict	UNP Q9RRG8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	66	Total	C	N	O	S	0	0	0
			534	327	107	97	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			453	278	93	77	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	54	Total	C	N	O	S	0	0	0
			404	256	73	74	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	47	Total	C	N	O	S	0	0	0
			393	235	92	64	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	65	Total	C	N	O	S	0	0	0
			509	320	104	80	5			

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2780	Total	C	N	O	P	0	0	0
			59673	26617	11011	19265	2780			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1510	U	UNK	conflict	GB 11612676

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

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

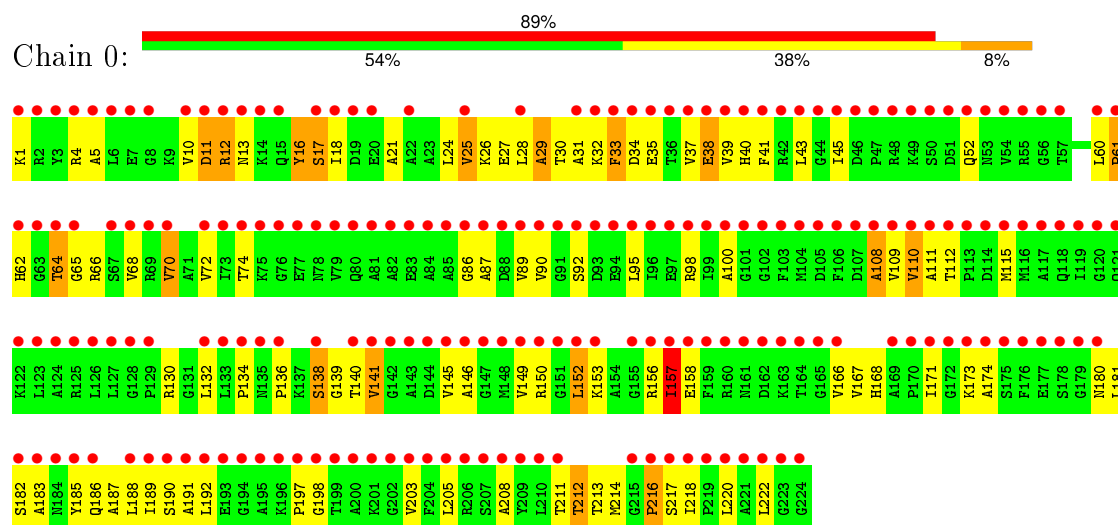
- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	X	192	Total	Mg	0	0
			192	192		
31	Y	5	Total	Mg	0	0
			5	5		
31	M	1	Total	Mg	0	0
			1	1		

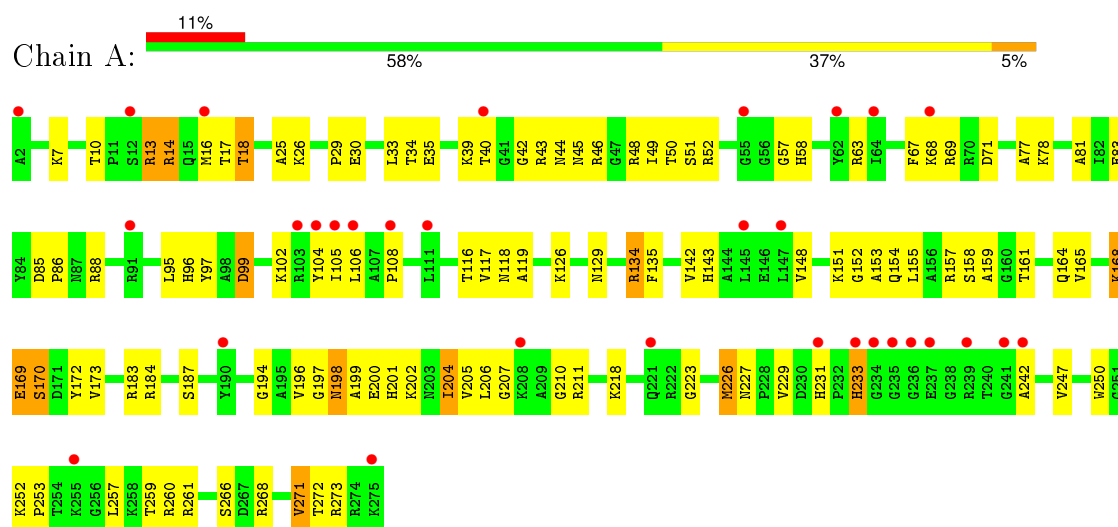
3 Residue-property plots

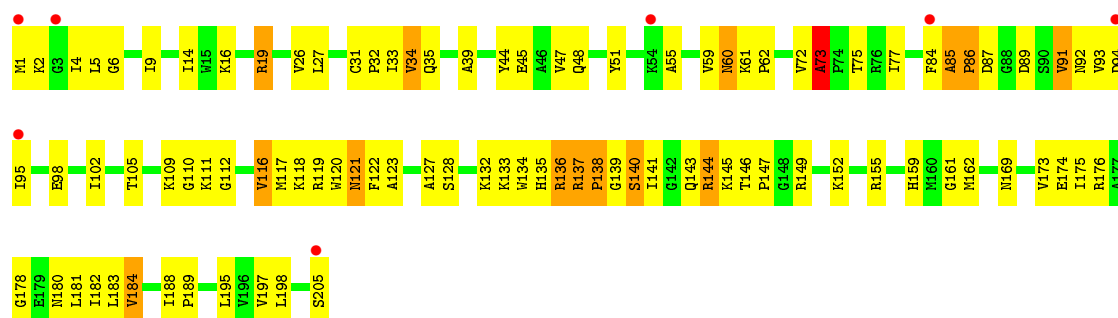
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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 L1

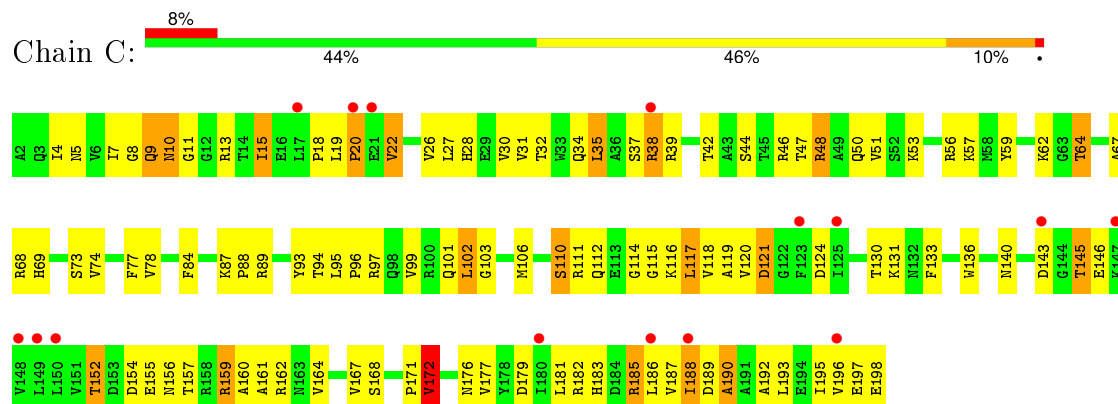


• Molecule 2: 50S ribosomal protein L2

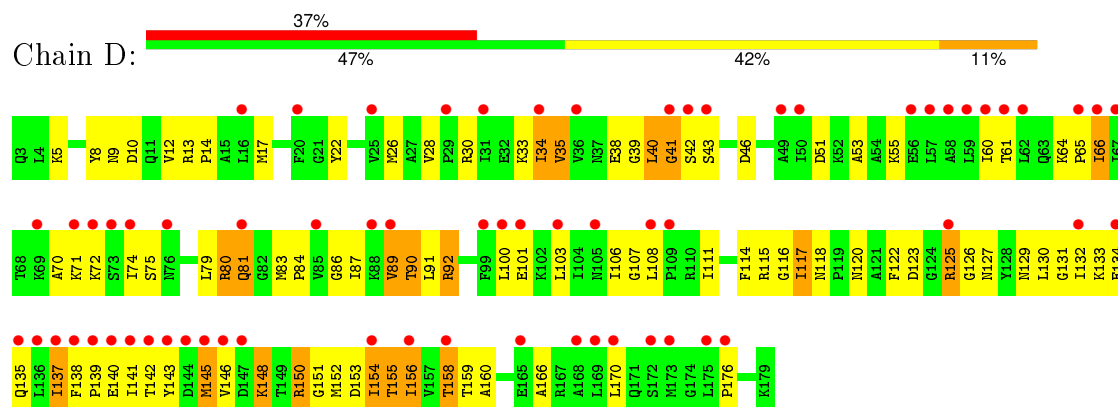




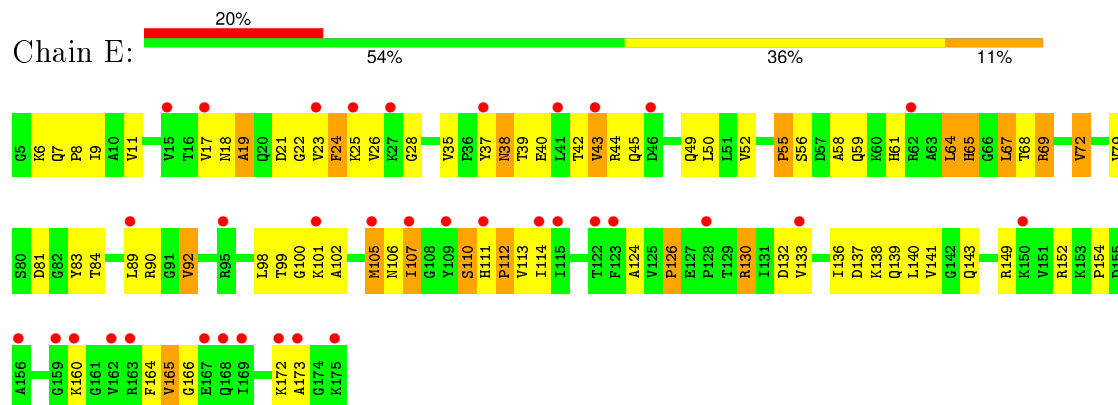
• Molecule 4: 50S ribosomal protein L4



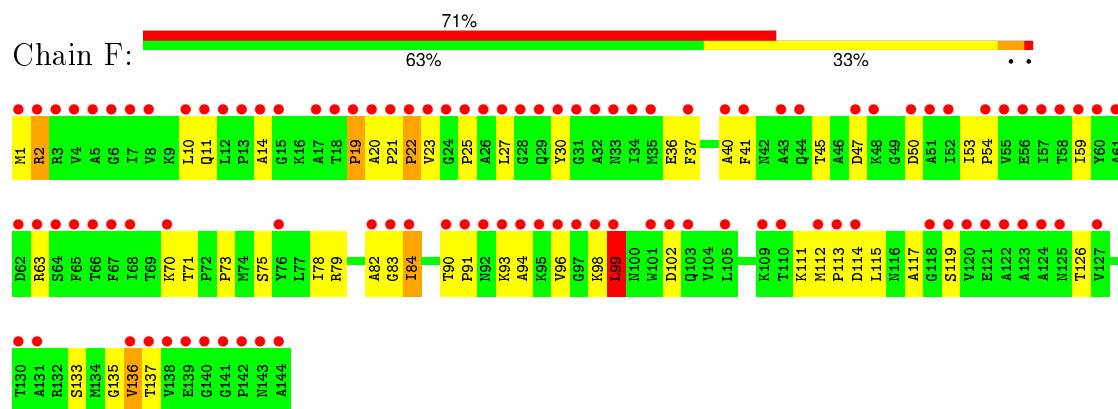
• Molecule 5: 50S ribosomal protein L5



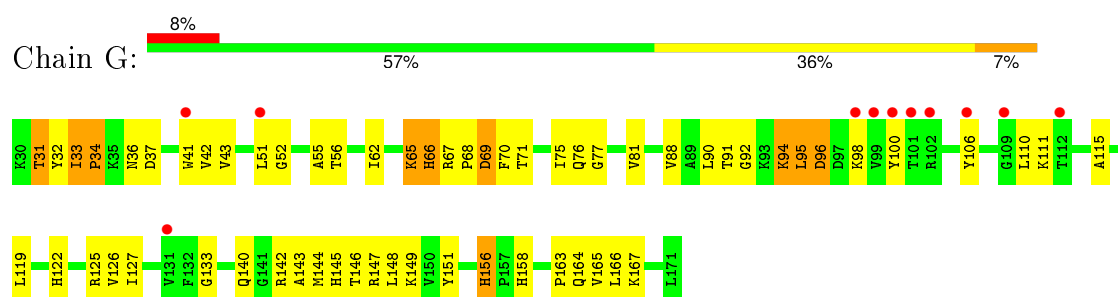
• Molecule 6: 50S ribosomal protein L6



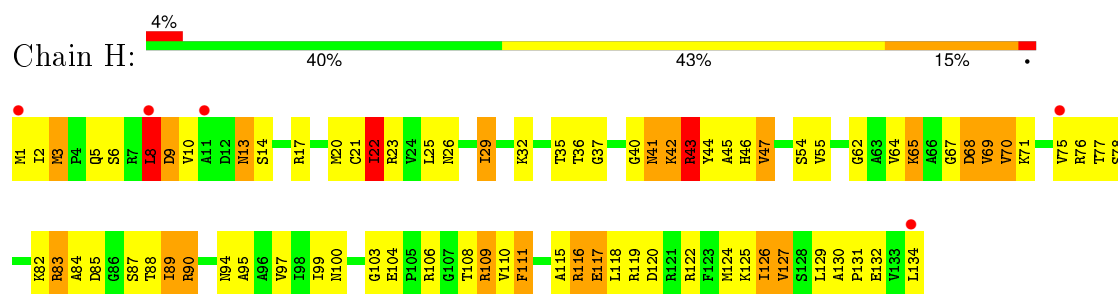
- Molecule 7: 50S ribosomal protein L11



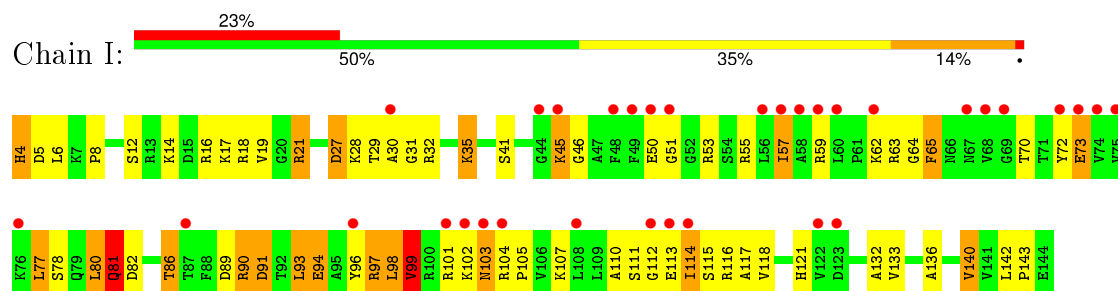
- Molecule 8: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L14

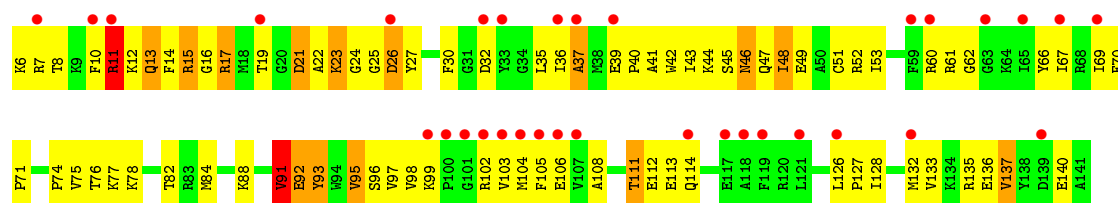


- Molecule 10: 50S ribosomal protein L15

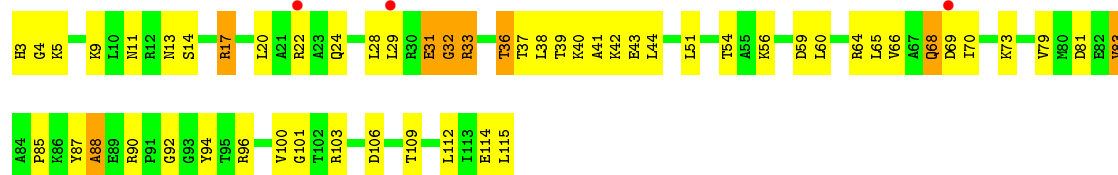


- Molecule 11: 50S ribosomal protein L16

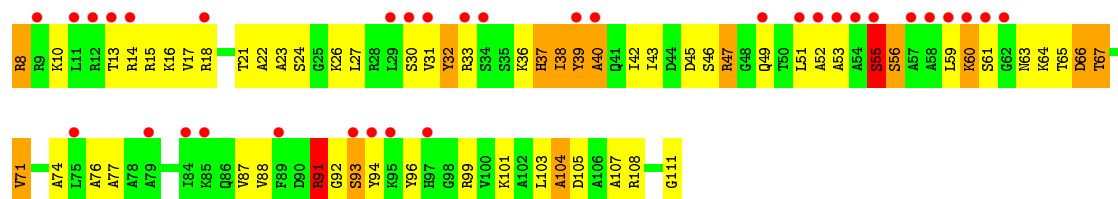




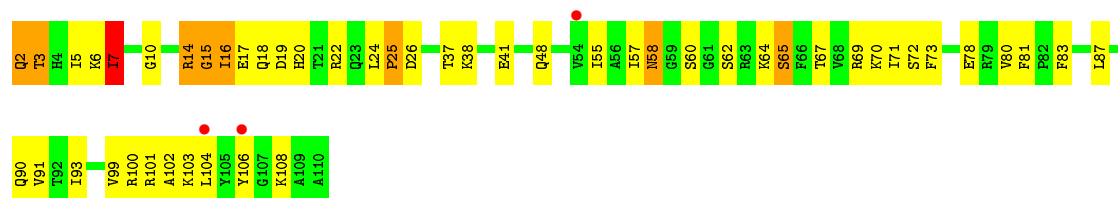
• Molecule 12: 50S ribosomal protein L17



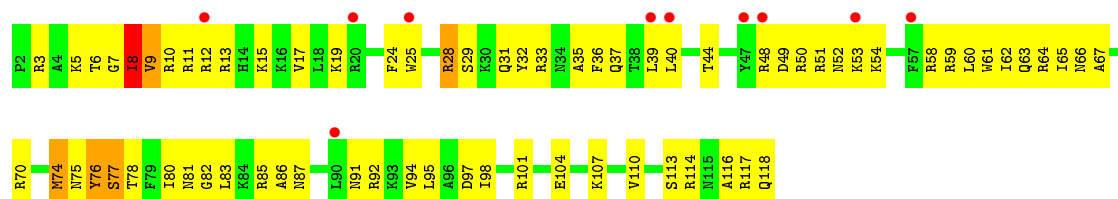
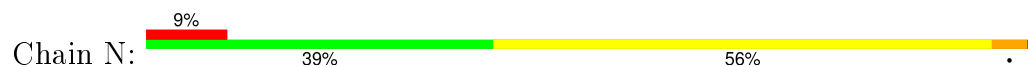
• Molecule 13: 50S ribosomal protein L18



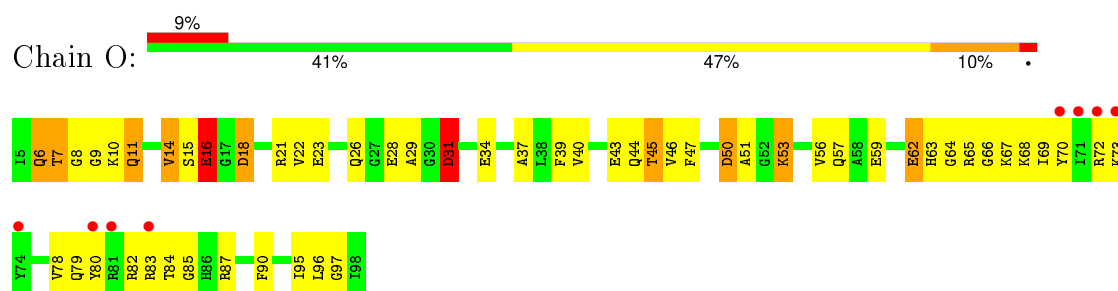
• Molecule 14: 50S ribosomal protein L19



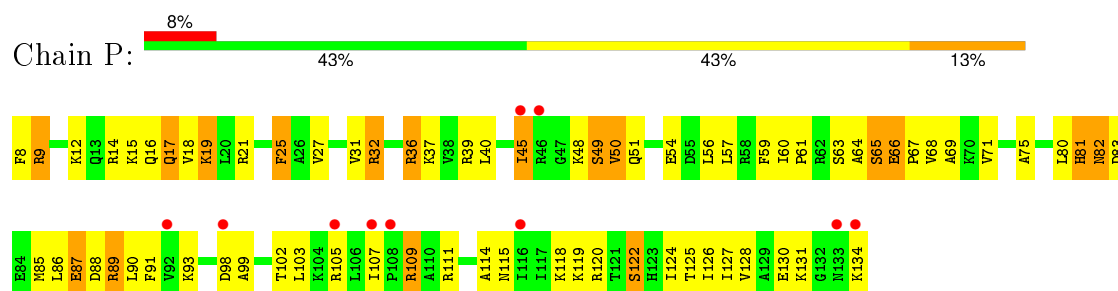
• Molecule 15: 50S ribosomal protein L20



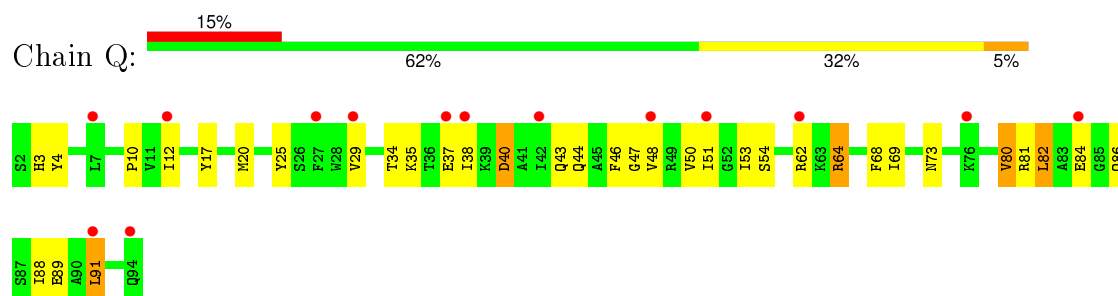
• Molecule 16: 50S ribosomal protein L21



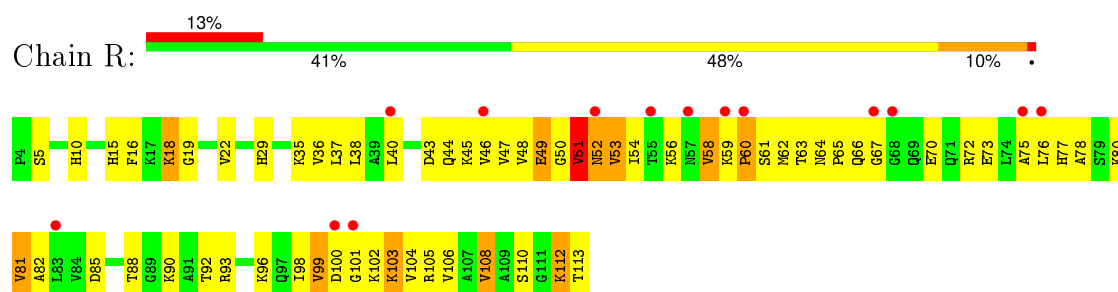
- Molecule 17: 50S ribosomal protein L22



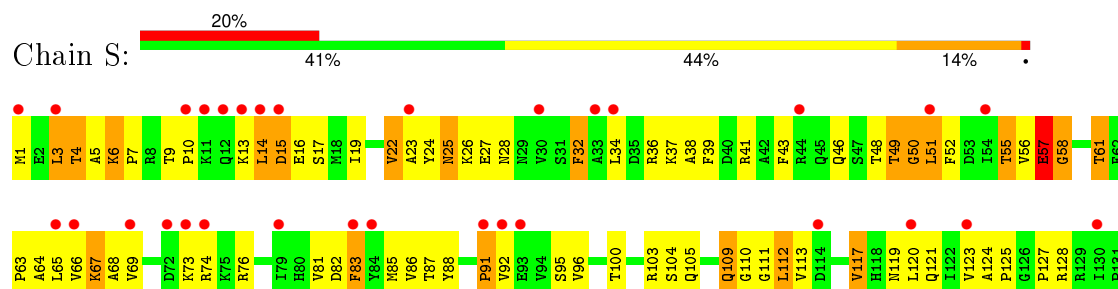
- Molecule 18: 50S ribosomal protein L23

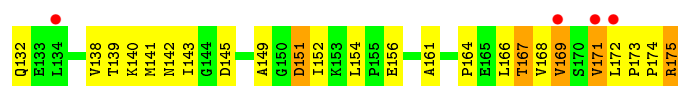


- Molecule 19: 50S ribosomal protein L24

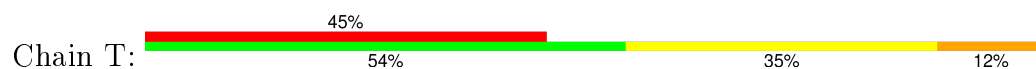


- Molecule 20: 50S ribosomal protein L25

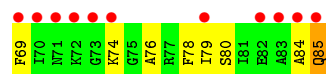
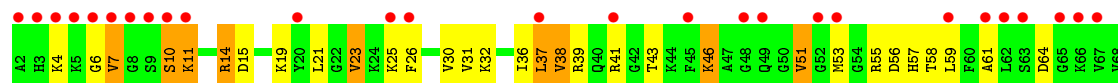




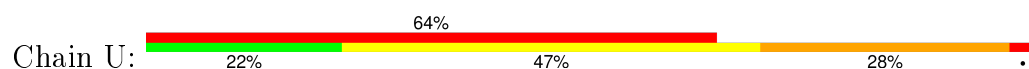
- Molecule 21: 50S ribosomal protein L27



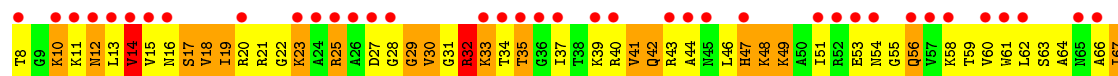
Chain T:



- Molecule 22: 50S ribosomal protein L28



Chain U:



- Molecule 23: 50S ribosomal protein L29



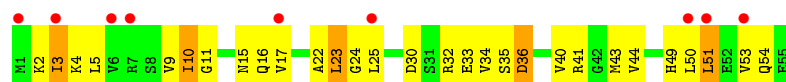
Chain V:



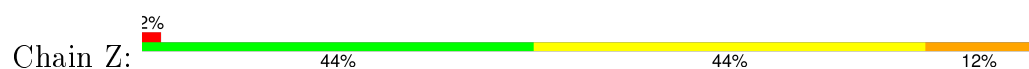
- Molecule 24: 50S ribosomal protein L30



Chain W:



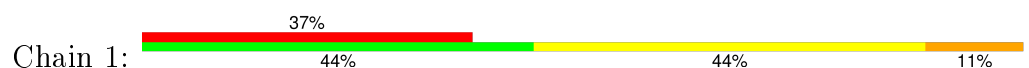
- Molecule 25: 50S ribosomal protein L32



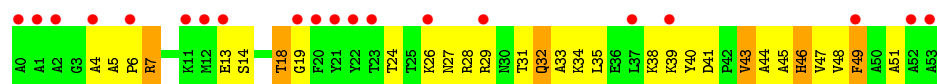
Chain Z:



- Molecule 26: 50S ribosomal protein L33



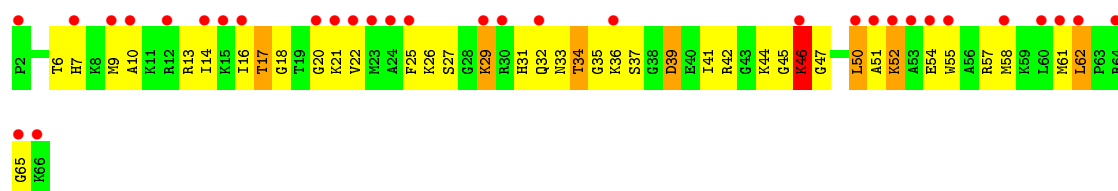
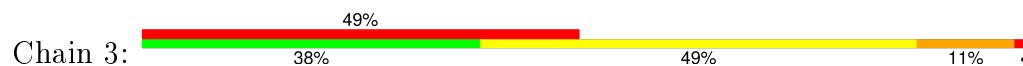
Chain 1:



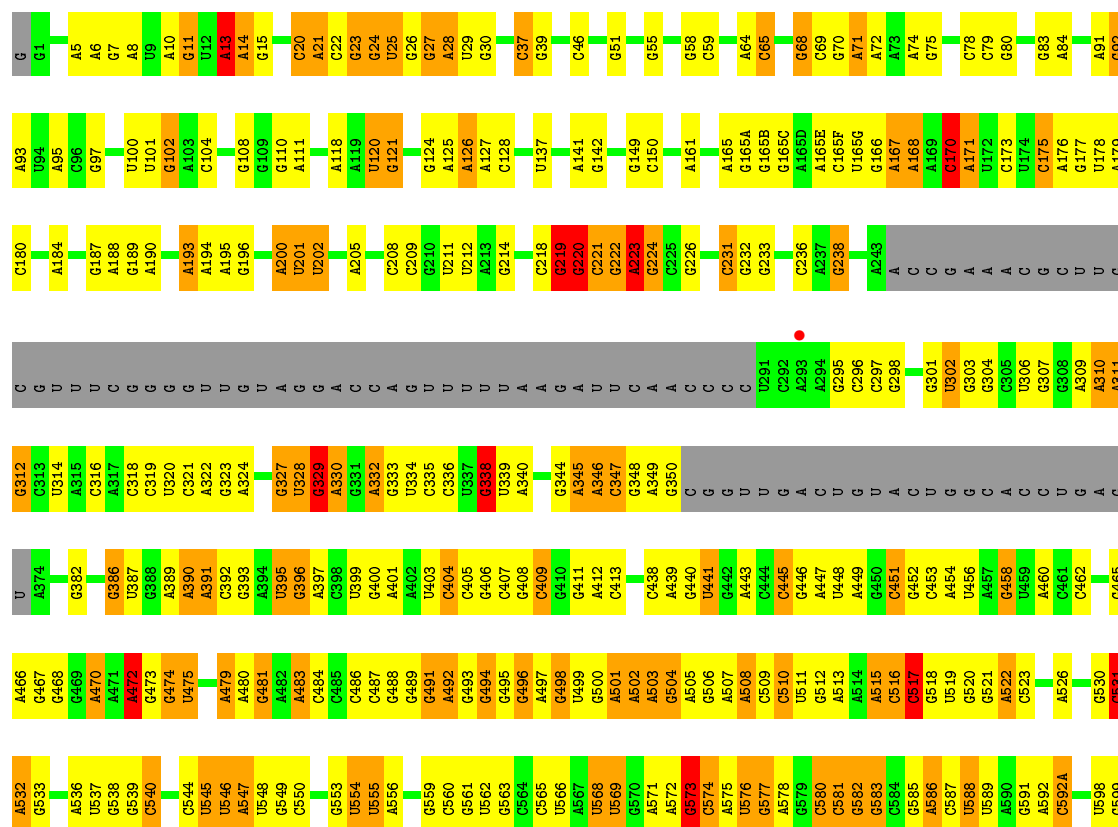
- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35

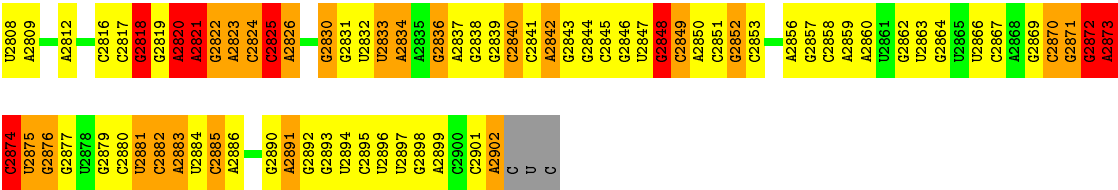


- Molecule 29: 23S ribosomal RNA

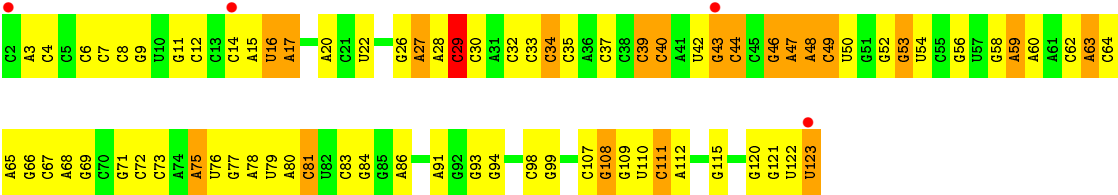








• Molecule 30: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 410.76Å 696.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.96 – 2.90 58.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (58.96-2.90) 81.6 (58.96-2.90)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.270 0.237 , 0.271	Depositor DCC
R_{free} test set	20602 reflections (4.74%)	DCC
Wilson B-factor (Å ²)	79.0	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 65.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	3 of 530819 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	89337	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical 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	0	0.30	0/1674	0.49	0/2257
2	A	0.39	0/2149	0.59	0/2890
3	B	0.69	1/1568 (0.1%)	0.86	1/2105 (0.0%)
4	C	0.51	0/1530	0.73	1/2070 (0.0%)
5	D	0.36	0/1420	0.56	0/1903
6	E	0.39	0/1309	0.55	0/1771
7	F	0.33	0/1067	0.52	1/1446 (0.1%)
8	G	0.47	0/1139	0.67	0/1539
9	H	0.76	0/1007	0.91	2/1352 (0.1%)
10	I	0.52	0/1082	0.76	1/1448 (0.1%)
11	J	0.65	0/1114	0.78	0/1486
12	K	0.83	0/887	1.04	0/1188
13	L	0.52	0/784	0.73	0/1045
14	M	0.77	0/880	0.83	0/1179
15	N	0.64	0/994	0.80	1/1323 (0.1%)
16	O	0.53	0/751	0.73	0/1000
17	P	0.69	0/1027	0.83	0/1373
18	Q	0.45	0/738	0.59	0/988
19	R	0.54	0/836	0.72	0/1121
20	S	0.41	0/1371	0.67	0/1862
21	T	0.54	0/634	0.69	0/838
22	U	0.61	0/557	0.88	1/741 (0.1%)
23	V	0.41	0/538	0.57	0/714
24	W	0.51	0/426	0.68	0/568
25	Z	0.71	0/465	0.90	0/622
26	1	0.49	0/411	0.73	0/554
27	2	0.48	0/397	0.65	0/521
28	3	0.54	0/516	0.70	0/673
29	X	0.78	37/66826 (0.1%)	1.44	971/104247 (0.9%)
30	Y	0.64	0/2907	1.20	8/4529 (0.2%)
All	All	0.72	38/97004 (0.0%)	1.29	987/145353 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	3
4	C	0	1
8	G	0	1
25	Z	0	2
All	All	0	7

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	761	A	C6-N1	8.06	1.41	1.35
29	X	1999	C	N3-C4	-7.01	1.29	1.33
29	X	1638	C	N1-C6	-6.80	1.33	1.37
29	X	1661	G	C6-N1	-6.69	1.34	1.39
29	X	1661	G	C5-C4	-6.50	1.33	1.38
29	X	2879	G	N9-C8	6.44	1.42	1.37
29	X	492	A	N3-C4	-6.41	1.31	1.34
29	X	761	A	C5-C4	6.30	1.43	1.38
29	X	2879	G	C5-C4	6.25	1.42	1.38
29	X	2509	G	C6-N1	-6.18	1.35	1.39
29	X	1660	C	N3-C4	-6.06	1.29	1.33
29	X	761	A	N3-C4	6.03	1.38	1.34
29	X	2012	G	N9-C8	-6.03	1.33	1.37
29	X	2510	C	N3-C4	-6.02	1.29	1.33
29	X	1665	A	N9-C4	5.84	1.41	1.37
29	X	761	A	N9-C8	5.77	1.42	1.37
29	X	2001	A	N9-C4	-5.77	1.34	1.37
29	X	2510	C	N1-C6	-5.74	1.33	1.37
29	X	1753	A	N3-C4	-5.73	1.31	1.34
29	X	2430	A	N9-C4	5.61	1.41	1.37
29	X	1652	A	N7-C5	-5.60	1.35	1.39
29	X	2848	G	N9-C8	-5.60	1.33	1.37
29	X	1997	A	C6-N1	5.56	1.39	1.35
29	X	2574	G	C2-N3	-5.56	1.28	1.32
29	X	2580	U	C4-C5	-5.51	1.38	1.43
29	X	2510	C	C4-C5	-5.37	1.38	1.43
29	X	1637	A	N7-C5	-5.30	1.36	1.39
29	X	2008	C	C2-O2	-5.27	1.19	1.24
29	X	1992	G	N3-C4	-5.27	1.31	1.35
29	X	1998	A	N9-C4	-5.25	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	127	ALA	CA-CB	-5.23	1.41	1.52
29	X	2009	G	C5-C4	-5.21	1.34	1.38
29	X	2015	A	N3-C4	-5.19	1.31	1.34
29	X	2879	G	C8-N7	5.18	1.34	1.30
29	X	1262	A	C5-C6	-5.16	1.36	1.41
29	X	2632	A	N3-C4	-5.05	1.31	1.34
29	X	2551	C	N1-C6	-5.04	1.34	1.37
29	X	1614	A	N9-C4	-5.01	1.34	1.37

All (987) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	761	A	N1-C6-N6	22.08	131.85	118.60
29	X	761	A	C5-N7-C8	-17.56	95.12	103.90
29	X	2713	U	O5'-P-OP2	-17.29	89.95	110.70
29	X	761	A	C4-C5-N7	16.33	118.87	110.70
29	X	761	A	C5-C6-N6	-14.62	112.00	123.70
29	X	2879	G	C5-N7-C8	-14.56	97.02	104.30
29	X	2840	C	C6-N1-C2	14.18	125.97	120.30
29	X	2879	G	N7-C8-N9	13.73	119.97	113.10
29	X	761	A	N7-C8-N9	13.73	120.66	113.80
29	X	2879	G	C4-C5-N7	12.72	115.89	110.80
29	X	761	A	C6-C5-N7	-12.49	123.56	132.30
29	X	2616	C	O5'-P-OP1	-12.20	94.72	105.70
29	X	1779	U	C5-C6-N1	-12.03	116.69	122.70
29	X	2689	U	O5'-P-OP1	-11.60	95.26	105.70
29	X	1262	A	N1-C6-N6	11.30	125.38	118.60
29	X	568	U	O5'-P-OP2	-11.10	95.71	105.70
29	X	1660	C	O5'-P-OP2	-10.96	95.83	105.70
29	X	1999	C	C2-N3-C4	-10.94	114.43	119.90
29	X	1665	A	C8-N9-C4	-10.93	101.43	105.80
29	X	2713	U	O5'-P-OP1	10.82	123.69	110.70
29	X	2879	G	C8-N9-C4	-10.73	102.11	106.40
29	X	1999	C	C5-C6-N1	-10.56	115.72	121.00
29	X	2883	A	O5'-P-OP2	-10.45	96.30	105.70
29	X	1490	C	C6-N1-C2	-10.31	116.18	120.30
29	X	2712(A)	A	O5'-P-OP2	-10.29	96.44	105.70
29	X	1490	C	N3-C2-O2	-10.23	114.74	121.90
29	X	1286	A	O5'-P-OP2	-10.18	96.54	105.70
29	X	2060	A	O5'-P-OP2	-10.17	96.54	105.70
29	X	2874	C	O5'-P-OP2	-10.15	96.56	105.70
29	X	2879	G	C6-C5-N7	-10.14	124.32	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2840	C	C5-C6-N1	-10.13	115.93	121.00
29	X	2710	C	O5'-P-OP2	10.02	122.72	110.70
29	X	1273	U	O5'-P-OP1	-10.00	96.70	105.70
29	X	659	C	C6-N1-C2	9.99	124.30	120.30
29	X	573	G	O5'-P-OP1	-9.97	96.73	105.70
29	X	2824	C	O5'-P-OP2	-9.87	96.82	105.70
29	X	1490	C	N1-C2-O2	9.86	124.81	118.90
29	X	761	A	N9-C4-C5	-9.81	101.87	105.80
29	X	498	G	N1-C6-O6	9.81	125.79	119.90
29	X	2035	G	O5'-P-OP1	9.69	122.32	110.70
29	X	2707	C	O5'-P-OP2	-9.66	97.01	105.70
29	X	2261	C	C6-N1-C2	-9.64	116.44	120.30
29	X	1661	G	O5'-P-OP1	9.53	122.14	110.70
29	X	660	G	C8-N9-C4	9.53	110.21	106.40
29	X	2501	C	C2-N1-C1'	-9.50	108.35	118.80
29	X	2713	U	C5-C6-N1	-9.41	118.00	122.70
29	X	1668	A	C8-N9-C4	9.24	109.50	105.80
29	X	1264	G	N1-C6-O6	-9.23	114.36	119.90
29	X	2676	C	C5-C6-N1	-9.23	116.39	121.00
29	X	2892	G	N3-C4-C5	9.20	133.20	128.60
29	X	1754	A	N7-C8-N9	-9.17	109.21	113.80
29	X	2066	C	C6-N1-C2	-9.16	116.64	120.30
29	X	2571	C	C6-N1-C2	-9.12	116.65	120.30
29	X	1661	G	C5-C6-N1	9.11	116.06	111.50
29	X	2879	G	C5-C6-O6	-9.09	123.15	128.60
29	X	2508	G	N1-C6-O6	-9.08	114.45	119.90
29	X	2509	G	C5-C6-N1	9.07	116.03	111.50
29	X	2885	C	O5'-P-OP2	-9.05	97.56	105.70
29	X	2689	U	C5-C6-N1	-9.02	118.19	122.70
29	X	2519	U	O5'-P-OP1	-9.02	97.59	105.70
29	X	1264	G	O5'-P-OP2	-8.92	97.68	105.70
29	X	650	C	C2-N1-C1'	8.90	128.59	118.80
29	X	2692	C	C6-N1-C2	-8.85	116.76	120.30
29	X	1660	C	C2-N3-C4	-8.82	115.49	119.90
29	X	1659	U	OP1-P-OP2	8.80	132.79	119.60
29	X	1990	C	N1-C2-O2	8.78	124.17	118.90
29	X	2514	U	N3-C2-O2	8.71	128.30	122.20
29	X	1330	C	O5'-P-OP2	-8.71	97.86	105.70
29	X	650	C	C6-N1-C2	-8.71	116.82	120.30
29	X	2501	C	C6-N1-C1'	8.71	131.25	120.80
29	X	1261	C	C6-N1-C2	8.70	123.78	120.30
29	X	1262	A	C4-C5-N7	8.64	115.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2847	U	N3-C4-O4	8.63	125.44	119.40
29	X	2645	G	C8-N9-C4	-8.62	102.95	106.40
30	Y	32	C	C6-N1-C2	-8.61	116.85	120.30
29	X	2036	C	C6-N1-C2	-8.61	116.86	120.30
29	X	1999	C	N1-C2-N3	8.60	125.22	119.20
29	X	1754	A	C5-N7-C8	8.58	108.19	103.90
29	X	1997	A	N1-C6-N6	8.55	123.73	118.60
29	X	586	A	O5'-P-OP2	-8.54	98.02	105.70
29	X	2826	A	O5'-P-OP1	-8.53	98.02	105.70
29	X	2032	G	C5-C6-O6	-8.53	123.48	128.60
29	X	1279	A	O5'-P-OP1	8.52	120.92	110.70
29	X	2583	G	C5-C6-O6	-8.51	123.49	128.60
29	X	2032	G	N1-C6-O6	8.47	124.98	119.90
29	X	1998	A	C8-N9-C4	8.47	109.19	105.80
29	X	1656	C	O5'-P-OP2	-8.47	98.08	105.70
29	X	2001	A	O5'-P-OP2	8.38	120.76	110.70
29	X	1267	U	O5'-P-OP2	-8.35	98.19	105.70
29	X	2499	C	C6-N1-C2	-8.34	116.96	120.30
29	X	1999	C	N1-C2-O2	-8.34	113.90	118.90
29	X	2619	C	N3-C2-O2	-8.32	116.08	121.90
29	X	2580	U	C5-C4-O4	-8.31	120.91	125.90
29	X	2574	G	C8-N9-C4	-8.31	103.08	106.40
29	X	744	U	O5'-P-OP1	8.30	120.66	110.70
29	X	2676	C	C6-N1-C2	8.27	123.61	120.30
29	X	1152	C	C6-N1-C2	-8.26	117.00	120.30
29	X	27	G	O5'-P-OP1	-8.24	98.28	105.70
29	X	1490	C	C2-N1-C1'	8.21	127.83	118.80
29	X	1661	G	N7-C8-N9	-8.17	109.02	113.10
29	X	1322	A	C8-N9-C4	8.16	109.07	105.80
29	X	513	A	O5'-P-OP2	8.16	120.49	110.70
29	X	498	G	C5-C6-O6	-8.15	123.71	128.60
29	X	943	U	O5'-P-OP1	-8.14	98.37	105.70
29	X	1784	A	C8-N9-C4	8.11	109.04	105.80
29	X	1668	A	N7-C8-N9	-8.10	109.75	113.80
29	X	2619	C	N1-C2-O2	8.09	123.75	118.90
29	X	738	G	N1-C6-O6	-8.07	115.06	119.90
29	X	1668	A	O5'-P-OP2	-8.06	98.45	105.70
29	X	946	G	N1-C6-O6	-8.05	115.07	119.90
29	X	659	C	C5-C6-N1	-8.04	116.98	121.00
29	X	2501	C	N3-C4-N4	-8.02	112.38	118.00
29	X	2574	G	N3-C4-N9	-8.02	121.19	126.00
29	X	2717	G	C2-N3-C4	8.02	115.91	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1262	A	C5-C6-N6	-8.02	117.28	123.70
29	X	1673	U	C5-C4-O4	-8.02	121.09	125.90
29	X	1661	G	C6-N1-C2	-7.95	120.33	125.10
29	X	2050	C	C6-N1-C2	-7.94	117.12	120.30
29	X	962	U	O5'-P-OP1	-7.92	98.57	105.70
29	X	1277	A	O5'-P-OP2	-7.92	98.57	105.70
29	X	660	G	N7-C8-N9	-7.89	109.16	113.10
29	X	1998	A	C6-N1-C2	-7.88	113.87	118.60
29	X	1262	A	C6-C5-N7	-7.86	126.80	132.30
29	X	2659	G	N1-C6-O6	7.84	124.61	119.90
29	X	2618	G	C8-N9-C4	-7.82	103.27	106.40
29	X	2561	A	O5'-P-OP2	-7.80	98.68	105.70
29	X	1951	U	N3-C4-O4	7.79	124.86	119.40
29	X	472	A	C2-N3-C4	-7.77	106.71	110.60
29	X	645	U	N3-C2-O2	-7.77	116.76	122.20
29	X	1279	A	C8-N9-C4	7.77	108.91	105.80
29	X	2820	A	N1-C6-N6	-7.75	113.95	118.60
29	X	2600	A	O5'-P-OP1	-7.75	98.73	105.70
29	X	1777	U	N1-C2-O2	7.72	128.21	122.80
29	X	2729	C	O5'-P-OP1	-7.72	98.75	105.70
29	X	492	A	N1-C2-N3	7.72	133.16	129.30
29	X	2708	G	C8-N9-C4	7.72	109.49	106.40
29	X	1990	C	N3-C2-O2	-7.70	116.51	121.90
29	X	1646	C	N1-C2-O2	7.68	123.51	118.90
29	X	2032	G	C4-C5-N7	7.68	113.87	110.80
29	X	2546	U	N3-C2-O2	-7.68	116.82	122.20
29	X	650	C	C5-C6-N1	7.68	124.84	121.00
29	X	25	U	OP1-P-O3'	7.67	122.08	105.20
29	X	2825	C	N3-C4-N4	7.67	123.36	118.00
29	X	2551	C	N1-C2-O2	-7.66	114.31	118.90
29	X	676	A	N7-C8-N9	7.65	117.63	113.80
29	X	2443	C	N3-C2-O2	-7.64	116.55	121.90
29	X	1991	U	O5'-P-OP2	-7.63	98.83	105.70
29	X	1951	U	N3-C4-C5	-7.63	110.02	114.60
29	X	1660	C	OP1-P-OP2	7.63	131.04	119.60
29	X	1663	U	C5-C6-N1	7.62	126.51	122.70
29	X	2575	C	C6-N1-C2	-7.62	117.25	120.30
29	X	2581	G	C8-N9-C4	-7.62	103.35	106.40
29	X	2499	C	C5-C6-N1	7.62	124.81	121.00
29	X	472	A	O4'-C1'-N9	7.61	114.29	108.20
29	X	2712	C	O5'-P-OP2	-7.59	98.87	105.70
29	X	1749	A	C8-N9-C4	-7.58	102.77	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2063	C	N1-C2-O2	-7.58	114.35	118.90
29	X	2549	G	O5'-P-OP1	-7.57	98.89	105.70
29	X	2869	G	OP2-P-O3'	7.57	121.85	105.20
29	X	2695	C	N3-C2-O2	7.56	127.19	121.90
29	X	445	C	O5'-P-OP2	-7.56	98.89	105.70
29	X	1647	G	O5'-P-OP1	-7.54	98.91	105.70
29	X	782	A	N1-C6-N6	7.53	123.12	118.60
29	X	2843	G	C8-N9-C4	-7.52	103.39	106.40
29	X	30	G	C8-N9-C4	-7.52	103.39	106.40
29	X	1673	U	N3-C4-C5	7.52	119.11	114.60
29	X	531	C	C5-C6-N1	-7.50	117.25	121.00
30	Y	32	C	C5-C6-N1	7.49	124.74	121.00
29	X	1665	A	N9-C4-C5	7.48	108.79	105.80
29	X	2569	G	C5-C6-N1	-7.47	107.77	111.50
29	X	1999	C	C4-C5-C6	7.46	121.13	117.40
29	X	1630	U	N3-C4-C5	-7.44	110.13	114.60
29	X	1997	A	O5'-P-OP1	-7.44	99.00	105.70
29	X	2500	U	C5-C6-N1	7.44	126.42	122.70
29	X	676	A	C5-N7-C8	-7.42	100.19	103.90
29	X	1461	G	O5'-P-OP2	7.41	119.59	110.70
29	X	866	A	N9-C4-C5	-7.39	102.84	105.80
29	X	1616	A	C8-N9-C4	-7.39	102.84	105.80
29	X	2001	A	C2-N3-C4	-7.38	106.91	110.60
29	X	2712(A)	A	N1-C6-N6	7.36	123.02	118.60
29	X	2712(A)	A	OP2-P-O3'	7.36	121.39	105.20
29	X	2032	G	C5-N7-C8	-7.36	100.62	104.30
29	X	1652	A	N1-C6-N6	7.35	123.01	118.60
29	X	1990	C	C6-N1-C2	-7.35	117.36	120.30
29	X	2060	A	OP2-P-O3'	7.34	121.34	105.20
29	X	1662	U	C2-N3-C4	-7.32	122.61	127.00
29	X	1779	U	C4-C5-C6	7.32	124.09	119.70
29	X	2613	U	O5'-P-OP1	-7.32	99.11	105.70
29	X	1950	G	C8-N9-C4	-7.29	103.48	106.40
29	X	1660	C	N1-C2-N3	7.29	124.30	119.20
29	X	2645	G	N7-C8-N9	7.27	116.74	113.10
29	X	1653	G	N3-C2-N2	7.27	124.99	119.90
29	X	2892	G	N3-C4-N9	-7.23	121.66	126.00
29	X	327	G	C8-N9-C4	-7.22	103.51	106.40
29	X	2765	A	O4'-C1'-N9	7.21	113.97	108.20
29	X	2515	C	N3-C2-O2	-7.18	116.87	121.90
29	X	2556	C	C6-N1-C2	7.18	123.17	120.30
29	X	2021	U	O5'-P-OP2	7.17	119.30	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1661	G	N1-C6-O6	-7.16	115.60	119.90
29	X	2870	C	C6-N1-C2	-7.13	117.45	120.30
29	X	1996	C	OP1-P-OP2	-7.12	108.91	119.60
29	X	2027	G	O5'-P-OP2	-7.10	99.31	105.70
29	X	2613	U	O5'-P-OP2	7.07	119.19	110.70
29	X	1236	G	O5'-P-OP1	-7.07	99.34	105.70
29	X	2046	G	O5'-P-OP2	-7.07	99.34	105.70
29	X	598	U	C5-C6-N1	-7.06	119.17	122.70
29	X	1227	G	O5'-P-OP1	-7.06	99.35	105.70
29	X	841	G	N1-C6-O6	7.06	124.14	119.90
29	X	750	A	O5'-P-OP2	7.05	119.16	110.70
29	X	1998	A	N1-C6-N6	7.02	122.81	118.60
29	X	1206	G	C6-C5-N7	7.00	134.60	130.40
29	X	1328	G	C5-C6-N1	6.98	114.99	111.50
29	X	1285	G	N3-C2-N2	6.98	124.79	119.90
29	X	1278	G	C8-N9-C4	6.98	109.19	106.40
29	X	2392	A	C8-N9-C4	-6.97	103.01	105.80
29	X	1727	C	C6-N1-C2	6.96	123.09	120.30
29	X	1264	G	C5-C6-O6	6.96	132.78	128.60
29	X	2580	U	N3-C2-O2	6.95	127.07	122.20
29	X	25	U	C6-N1-C2	-6.94	116.84	121.00
29	X	2419	U	N3-C4-C5	-6.94	110.44	114.60
29	X	1266	G	N3-C2-N2	6.92	124.75	119.90
29	X	734	A	O4'-C1'-N9	6.90	113.72	108.20
29	X	649	G	N3-C4-C5	6.89	132.04	128.60
29	X	2684	U	OP1-P-O3'	6.88	120.33	105.20
29	X	1277	A	OP1-P-OP2	6.88	129.91	119.60
29	X	802	A	O5'-P-OP1	-6.87	99.51	105.70
29	X	2673	G	O5'-P-OP2	-6.86	99.52	105.70
29	X	2712	C	C2-N3-C4	-6.85	116.47	119.90
29	X	2451	A	N1-C2-N3	6.85	132.72	129.30
29	X	1262	A	C5-N7-C8	-6.84	100.48	103.90
29	X	788	A	N1-C6-N6	6.83	122.70	118.60
29	X	1695	G	C4-N9-C1'	6.83	135.37	126.50
29	X	1278	G	N7-C8-N9	-6.81	109.69	113.10
29	X	2488	A	N1-C6-N6	-6.81	114.51	118.60
29	X	1779	U	C2-N1-C1'	-6.81	109.53	117.70
29	X	1652	A	C6-C5-N7	-6.81	127.53	132.30
29	X	1208	C	C6-N1-C2	-6.80	117.58	120.30
29	X	1758	G	O5'-P-OP2	-6.79	99.59	105.70
29	X	673	C	C6-N1-C2	6.77	123.01	120.30
29	X	649	G	N3-C4-N9	-6.77	121.94	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1754	A	C8-N9-C4	6.77	108.51	105.80
29	X	2513	G	C8-N9-C4	-6.76	103.69	106.40
29	X	2496	C	C6-N1-C2	-6.76	117.60	120.30
29	X	2512	C	C6-N1-C2	-6.76	117.60	120.30
29	X	995	C	C5-C6-N1	-6.75	117.62	121.00
29	X	2699	C	C5-C6-N1	-6.75	117.63	121.00
29	X	1652	A	C2-N3-C4	-6.74	107.23	110.60
29	X	588	U	C6-N1-C2	6.73	125.04	121.00
29	X	2713	U	C4-C5-C6	6.73	123.74	119.70
29	X	746	C	N3-C4-C5	-6.73	119.21	121.90
29	X	2454	G	N9-C4-C5	6.72	108.09	105.40
29	X	2678	G	OP2-P-O3'	6.72	119.99	105.20
29	X	1461	G	O5'-P-OP1	-6.72	99.65	105.70
30	Y	29	C	C6-N1-C2	-6.72	117.61	120.30
29	X	1200	C	N1-C2-O2	-6.71	114.87	118.90
29	X	774	A	C2-N3-C4	-6.71	107.24	110.60
29	X	983	A	N1-C6-N6	-6.70	114.58	118.60
29	X	1210	G	C4-N9-C1'	6.70	135.21	126.50
29	X	2612	C	C2-N1-C1'	6.70	126.17	118.80
29	X	2430	A	C8-N9-C4	-6.69	103.12	105.80
29	X	1977	A	C8-N9-C4	6.69	108.48	105.80
29	X	995	C	C6-N1-C2	6.68	122.97	120.30
29	X	1156	A	N1-C6-N6	6.67	122.60	118.60
29	X	2715	C	C6-N1-C2	-6.66	117.64	120.30
29	X	1665	A	C6-N1-C2	-6.65	114.61	118.60
29	X	650	C	N3-C4-N4	6.64	122.65	118.00
29	X	1206	G	C4-N9-C1'	-6.64	117.86	126.50
29	X	1206	G	C8-N9-C1'	6.64	135.63	127.00
29	X	1262	A	N9-C4-C5	-6.64	103.15	105.80
29	X	676	A	C6-C5-N7	-6.63	127.66	132.30
29	X	1659	U	O5'-P-OP1	-6.63	99.73	105.70
29	X	492	A	C6-N1-C2	-6.63	114.62	118.60
29	X	2873	A	O5'-P-OP1	-6.62	99.74	105.70
29	X	1322	A	N7-C8-N9	-6.62	110.49	113.80
29	X	1641	A	C8-N9-C4	6.61	108.44	105.80
29	X	1003	G	C8-N9-C4	-6.61	103.76	106.40
29	X	1663	U	C4-C5-C6	-6.60	115.74	119.70
29	X	2446	G	N9-C4-C5	-6.60	102.76	105.40
29	X	1747	G	N3-C4-C5	-6.60	125.30	128.60
29	X	645	U	C6-N1-C2	-6.59	117.04	121.00
29	X	2025	C	C6-N1-C2	-6.58	117.67	120.30
29	X	1327	C	N1-C2-O2	-6.57	114.95	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	513	A	O5'-P-OP1	-6.57	99.79	105.70
29	X	1236	G	O5'-P-OP2	6.56	118.57	110.70
29	X	2001	A	OP1-P-OP2	-6.55	109.78	119.60
29	X	2511	U	O5'-P-OP2	-6.55	99.81	105.70
29	X	2454	G	C8-N9-C4	-6.54	103.78	106.40
15	N	28	ARG	NE-CZ-NH1	6.54	123.57	120.30
29	X	170	C	C5-C6-N1	6.54	124.27	121.00
29	X	1660	C	C5-C6-N1	-6.53	117.73	121.00
29	X	2712(A)	A	C5-C6-N6	-6.53	118.47	123.70
29	X	2036	C	C5-C6-N1	6.51	124.25	121.00
29	X	23	G	O5'-P-OP1	-6.51	99.84	105.70
29	X	1627	G	C8-N9-C4	6.51	109.00	106.40
29	X	2443	C	C6-N1-C2	-6.50	117.70	120.30
29	X	2879	G	C4-N9-C1'	6.49	134.94	126.50
29	X	571	A	N1-C6-N6	6.49	122.49	118.60
29	X	1998	A	C5-C6-N6	-6.48	118.52	123.70
29	X	1320	G	O5'-P-OP1	-6.48	99.87	105.70
29	X	531	C	C4-C5-C6	6.48	120.64	117.40
29	X	170	C	C2-N1-C1'	6.47	125.92	118.80
29	X	1673	U	N3-C2-O2	6.47	126.73	122.20
29	X	2689	U	C5-C4-O4	6.46	129.78	125.90
29	X	486	C	N3-C2-O2	6.46	126.42	121.90
29	X	1156	A	N9-C4-C5	-6.46	103.22	105.80
29	X	1654	A	OP2-P-O3'	6.46	119.41	105.20
29	X	957	C	N1-C2-O2	6.45	122.77	118.90
29	X	1255	U	OP1-P-O3'	6.45	119.39	105.20
29	X	845	G	N3-C4-C5	6.44	131.82	128.60
29	X	1786	A	O4'-C1'-N9	6.44	113.35	108.20
29	X	1392	A	C8-N9-C4	-6.43	103.23	105.80
29	X	2709	G	O5'-P-OP1	6.43	118.41	110.70
29	X	2731	G	O5'-P-OP2	-6.43	99.92	105.70
29	X	2271	G	C4-N9-C1'	6.42	134.85	126.50
29	X	20	C	N3-C4-N4	6.42	122.50	118.00
29	X	2009	G	N7-C8-N9	-6.42	109.89	113.10
29	X	1629	G	N3-C4-N9	-6.42	122.15	126.00
29	X	2508	G	C8-N9-C4	-6.42	103.83	106.40
29	X	2250	G	N3-C4-N9	-6.41	122.16	126.00
29	X	2822	G	N3-C4-N9	6.41	129.84	126.00
29	X	2347	C	O4'-C1'-N1	6.41	113.33	108.20
29	X	2060	A	C8-N9-C4	-6.40	103.24	105.80
29	X	2508	G	C5-C6-O6	6.40	132.44	128.60
29	X	940	G	C8-N9-C4	6.40	108.96	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1395	A	O4'-C1'-N9	6.40	113.32	108.20
29	X	1662	U	C5-C6-N1	-6.40	119.50	122.70
29	X	474	G	OP2-P-O3'	6.39	119.25	105.20
29	X	2883	A	OP1-P-O3'	6.38	119.25	105.20
29	X	2050	C	N1-C2-N3	6.38	123.67	119.20
29	X	673	C	C2-N1-C1'	-6.38	111.78	118.80
29	X	2714	G	C8-N9-C4	-6.38	103.85	106.40
29	X	2038	G	N1-C6-O6	6.37	123.72	119.90
29	X	2516	G	N3-C4-C5	-6.37	125.41	128.60
29	X	957	C	C2-N1-C1'	6.37	125.81	118.80
29	X	1616	A	O5'-P-OP1	-6.37	99.97	105.70
29	X	1779	U	N1-C2-N3	6.37	118.72	114.90
29	X	2824	C	O5'-P-OP1	6.37	118.35	110.70
29	X	516	C	C6-N1-C2	-6.37	117.75	120.30
29	X	1695	G	N3-C4-N9	6.37	129.82	126.00
29	X	1997	A	OP1-P-OP2	6.37	129.15	119.60
29	X	2583	G	N3-C2-N2	-6.37	115.44	119.90
29	X	1666	G	O4'-C1'-N9	6.36	113.28	108.20
29	X	734	A	O5'-P-OP1	6.35	118.32	110.70
29	X	2723	C	C4-C5-C6	6.34	120.57	117.40
29	X	650	C	N1-C2-O2	6.33	122.70	118.90
29	X	1661	G	C5-N7-C8	6.33	107.47	104.30
29	X	1695	G	C8-N9-C1'	-6.33	118.77	127.00
29	X	957	C	C6-N1-C1'	-6.32	113.21	120.80
29	X	2643	G	C8-N9-C4	6.32	108.93	106.40
29	X	1394	G	C6-C5-N7	-6.32	126.61	130.40
29	X	2020	A	N1-C6-N6	6.32	122.39	118.60
29	X	1027	U	C2-N1-C1'	-6.31	110.13	117.70
29	X	1665	A	N1-C2-N3	6.31	132.45	129.30
29	X	2720	U	O5'-P-OP1	-6.30	100.03	105.70
29	X	649	G	C2-N3-C4	-6.30	108.75	111.90
29	X	915	C	C6-N1-C2	-6.30	117.78	120.30
29	X	635	C	C6-N1-C2	-6.28	117.79	120.30
29	X	2045	C	C5-C4-N4	-6.28	115.81	120.20
29	X	1685	C	C6-N1-C2	6.27	122.81	120.30
29	X	2612	C	N1-C2-O2	6.27	122.66	118.90
29	X	2844	G	N3-C4-C5	-6.25	125.48	128.60
29	X	734	A	C5'-C4'-O4'	6.25	116.59	109.10
29	X	1777	U	N3-C2-O2	-6.25	117.83	122.20
29	X	2052	G	N3-C4-C5	-6.24	125.48	128.60
29	X	2271	G	N3-C4-N9	6.24	129.75	126.00
29	X	2052	G	C5-C6-O6	-6.24	124.86	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2509	G	N1-C6-O6	-6.24	116.16	119.90
29	X	2871	G	O5'-P-OP2	-6.24	100.08	105.70
29	X	2777	G	O5'-P-OP2	-6.24	100.09	105.70
29	X	2000	G	OP1-P-O3'	-6.24	91.48	105.20
29	X	2044	C	OP1-P-O3'	6.23	118.90	105.20
29	X	948	C	O5'-P-OP2	6.22	118.17	110.70
29	X	1761	C	C6-N1-C2	-6.21	117.81	120.30
29	X	1144	G	C8-N9-C4	6.21	108.89	106.40
29	X	1998	A	N7-C8-N9	-6.21	110.70	113.80
29	X	2871	G	OP1-P-OP2	6.21	128.91	119.60
29	X	1280	A	C2-N3-C4	-6.20	107.50	110.60
29	X	2572	A	N7-C8-N9	-6.18	110.71	113.80
29	X	1256	G	C5-C6-O6	-6.18	124.89	128.60
29	X	841	G	C5-C6-N1	-6.18	108.41	111.50
29	X	1264	G	N3-C4-C5	-6.18	125.51	128.60
29	X	2577	A	OP1-P-OP2	6.18	128.86	119.60
29	X	2712(A)	A	C5-N7-C8	-6.17	100.82	103.90
29	X	2271	G	N3-C4-C5	-6.17	125.52	128.60
29	X	1291	U	C5-C6-N1	-6.16	119.62	122.70
29	X	2533	A	C8-N9-C4	6.16	108.26	105.80
29	X	672	U	N1-C2-N3	6.16	118.59	114.90
29	X	338	G	N3-C4-C5	-6.15	125.53	128.60
29	X	2582	G	O5'-P-OP1	6.14	118.07	110.70
29	X	2718	G	N3-C4-C5	-6.14	125.53	128.60
29	X	1265	A	C4-C5-C6	6.14	120.07	117.00
29	X	2869	G	N3-C4-N9	-6.14	122.32	126.00
29	X	2010	G	O5'-P-OP2	6.13	118.06	110.70
29	X	2576	G	C5-C6-O6	-6.13	124.92	128.60
29	X	1675	C	N3-C4-C5	-6.12	119.45	121.90
29	X	2553	G	C2'-C3'-O3'	6.12	123.49	113.70
29	X	2049	G	C4-C5-N7	6.12	113.25	110.80
29	X	452	G	N3-C4-N9	6.11	129.67	126.00
29	X	1394	G	C4-N9-C1'	6.11	134.44	126.50
29	X	2732	G	N1-C2-N2	-6.11	110.70	116.20
29	X	2052	G	C6-N1-C2	-6.10	121.44	125.10
29	X	486	C	N1-C2-O2	-6.10	115.24	118.90
29	X	2821	A	O5'-P-OP2	-6.10	100.21	105.70
29	X	1629	G	N3-C4-C5	6.09	131.65	128.60
29	X	2723	C	N3-C4-C5	-6.09	119.46	121.90
29	X	1655	A	OP1-P-OP2	-6.09	110.47	119.60
29	X	2294	C	C6-N1-C2	-6.09	117.86	120.30
29	X	1006	C	N3-C2-O2	-6.08	117.64	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	964	C	N1-C2-O2	-6.08	115.25	118.90
29	X	2726	U	N1-C2-O2	-6.08	118.54	122.80
29	X	2574	G	N9-C4-C5	6.08	107.83	105.40
29	X	2688	C	OP1-P-O3'	6.07	118.55	105.20
29	X	2002	G	OP2-P-O3'	6.07	118.55	105.20
29	X	2038	G	C5-C6-O6	-6.07	124.96	128.60
29	X	2869	G	N3-C4-C5	6.06	131.63	128.60
29	X	2843	G	OP2-P-O3'	6.06	118.53	105.20
29	X	30	G	N9-C4-C5	6.06	107.82	105.40
29	X	1206	G	C4-C5-N7	-6.06	108.38	110.80
29	X	2684	U	C6-N1-C2	-6.06	117.36	121.00
29	X	851	C	O5'-P-OP1	-6.05	100.25	105.70
29	X	2612	C	N3-C4-C5	-6.05	119.48	121.90
29	X	2612	C	N3-C4-N4	6.05	122.24	118.00
29	X	1252	G	O5'-P-OP2	-6.05	100.25	105.70
29	X	2789	C	O5'-P-OP2	-6.04	100.26	105.70
29	X	582	G	OP2-P-O3'	6.04	118.48	105.20
29	X	1205	C	N1-C2-O2	6.04	122.52	118.90
29	X	2513	G	C5-C6-O6	6.03	132.22	128.60
29	X	220	G	O5'-P-OP1	-6.03	100.28	105.70
29	X	1394	G	C8-N9-C1'	-6.03	119.17	127.00
29	X	1784	A	N7-C8-N9	-6.02	110.79	113.80
29	X	991	C	C6-N1-C2	-6.02	117.89	120.30
29	X	2847	U	C4-C5-C6	6.02	123.31	119.70
29	X	944	G	C2-N3-C4	-6.01	108.89	111.90
29	X	1292	C	C6-N1-C2	6.01	122.70	120.30
29	X	1635	G	N9-C4-C5	-6.01	103.00	105.40
29	X	761	A	C8-N9-C4	-6.00	103.40	105.80
29	X	944	G	C5-N7-C8	-6.00	101.30	104.30
29	X	1239	C	O5'-P-OP2	6.00	117.91	110.70
29	X	744	U	O5'-P-OP2	-6.00	100.30	105.70
29	X	1652	A	N1-C2-N3	6.00	132.30	129.30
29	X	2269	A	C8-N9-C4	6.00	108.20	105.80
29	X	2768	C	C6-N1-C2	5.99	122.70	120.30
29	X	498	G	C6-C5-N7	-5.99	126.81	130.40
29	X	2443	C	C2-N1-C1'	5.99	125.39	118.80
29	X	2509	G	C2-N3-C4	5.99	114.89	111.90
29	X	2000	G	OP2-P-O3'	5.97	118.35	105.20
29	X	2572	A	C8-N9-C4	5.97	108.19	105.80
29	X	1951	U	C4-C5-C6	5.97	123.28	119.70
29	X	13	A	C8-N9-C4	-5.96	103.42	105.80
29	X	1455	G	N3-C4-C5	-5.96	125.62	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2712(A)	A	C4-C5-N7	5.96	113.68	110.70
29	X	676	A	O4'-C1'-N9	5.96	112.97	108.20
29	X	732	C	C5-C4-N4	5.96	124.37	120.20
29	X	487	C	OP2-P-O3'	5.95	118.29	105.20
29	X	799	G	C8-N9-C4	-5.95	104.02	106.40
29	X	957	C	C2-N3-C4	5.95	122.88	119.90
29	X	517	C	C2-N1-C1'	5.94	125.33	118.80
29	X	732	C	N1-C2-N3	5.94	123.36	119.20
29	X	1998	A	OP1-P-OP2	5.94	128.51	119.60
29	X	1665	A	N3-C4-C5	-5.94	122.64	126.80
29	X	512	G	O4'-C1'-N9	5.94	112.95	108.20
29	X	974	G	C8-N9-C4	-5.93	104.03	106.40
29	X	1753	A	N1-C2-N3	5.93	132.26	129.30
29	X	486	C	C6-N1-C2	5.92	122.67	120.30
29	X	1668	A	C5-N7-C8	5.92	106.86	103.90
29	X	2501	C	O4'-C1'-N1	5.92	112.93	108.20
29	X	2517	C	O5'-P-OP1	-5.92	100.38	105.70
29	X	2547	U	N1-C2-N3	5.91	118.45	114.90
29	X	2833	U	O4'-C1'-N1	5.91	112.93	108.20
29	X	1230	G	OP1-P-OP2	-5.91	110.74	119.60
29	X	2271	G	C8-N9-C1'	-5.91	119.32	127.00
29	X	2419	U	N3-C4-O4	5.91	123.54	119.40
29	X	2260	C	N3-C4-N4	-5.91	113.86	118.00
29	X	1999	C	O5'-P-OP1	5.90	117.78	110.70
29	X	475	U	C2-N1-C1'	5.90	124.78	117.70
29	X	1629	G	C2-N3-C4	-5.90	108.95	111.90
29	X	1751	U	C5-C4-O4	-5.89	122.37	125.90
29	X	2842	A	OP2-P-O3'	5.89	118.15	105.20
29	X	504	G	O4'-C1'-N9	-5.88	103.49	108.20
29	X	907	U	O4'-C1'-N1	5.88	112.90	108.20
29	X	1206	G	O4'-C1'-N9	5.88	112.90	108.20
29	X	1998	A	N1-C2-N3	5.88	132.24	129.30
29	X	1998	A	C8-N9-C1'	-5.88	117.13	127.70
29	X	2576	G	C8-N9-C4	5.88	108.75	106.40
29	X	942	G	OP2-P-O3'	5.87	118.12	105.20
29	X	516	C	N3-C2-O2	-5.87	117.79	121.90
29	X	1936	A	C2-N3-C4	-5.87	107.66	110.60
29	X	2007	U	OP2-P-O3'	5.87	118.11	105.20
29	X	2843	G	N7-C8-N9	5.87	116.03	113.10
29	X	2820	A	C5-C6-N6	5.87	128.39	123.70
29	X	1967	C	C6-N1-C2	-5.86	117.95	120.30
29	X	1649	G	C8-N9-C4	5.86	108.74	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2555	U	N3-C2-O2	5.86	126.30	122.20
29	X	2866	U	N3-C2-O2	-5.86	118.10	122.20
29	X	2273	A	N9-C4-C5	5.84	108.14	105.80
29	X	1700	A	O5'-P-OP2	5.84	117.71	110.70
29	X	948	C	C5-C6-N1	5.84	123.92	121.00
29	X	1320	G	C5-C6-O6	5.83	132.10	128.60
29	X	823	G	O5'-P-OP2	-5.83	100.46	105.70
29	X	1995	U	C5-C4-O4	-5.83	122.40	125.90
29	X	577	G	OP1-P-OP2	5.82	128.34	119.60
29	X	2680	C	C6-N1-C2	-5.82	117.97	120.30
29	X	168	A	C6-C5-N7	-5.82	128.22	132.30
29	X	1629	G	N1-C6-O6	5.82	123.39	119.90
29	X	554	U	C5-C6-N1	-5.82	119.79	122.70
29	X	1155	A	O4'-C1'-N9	5.82	112.86	108.20
29	X	635	C	N3-C2-O2	-5.82	117.83	121.90
29	X	2709	G	N3-C4-N9	5.82	129.49	126.00
29	X	1208	C	N3-C4-C5	-5.81	119.58	121.90
29	X	1673	U	C6-N1-C2	5.81	124.49	121.00
29	X	673	C	N3-C2-O2	5.81	125.97	121.90
29	X	957	C	N1-C2-N3	-5.80	115.14	119.20
29	X	1453	A	O4'-C1'-N9	-5.80	103.56	108.20
29	X	2715	C	N1-C2-O2	5.79	122.38	118.90
29	X	2012	G	N3-C4-N9	5.79	129.48	126.00
29	X	1995	U	OP2-P-O3'	5.79	117.94	105.20
29	X	488	G	O5'-P-OP2	-5.79	100.49	105.70
29	X	2690	C	N3-C4-C5	-5.79	119.58	121.90
29	X	1630	U	N3-C4-O4	5.79	123.45	119.40
29	X	1274	A	OP1-P-O3'	5.79	117.93	105.20
29	X	2261	C	C5-C6-N1	5.79	123.89	121.00
29	X	866	A	C8-N9-C4	5.78	108.11	105.80
29	X	2050	C	O5'-P-OP1	-5.78	100.50	105.70
29	X	2048	A	O5'-P-OP1	5.78	117.63	110.70
29	X	2618	G	N7-C8-N9	5.78	115.99	113.10
29	X	2266	A	N1-C6-N6	-5.77	115.14	118.60
29	X	2722	G	OP1-P-O3'	5.77	117.90	105.20
29	X	1771	C	O5'-P-OP2	-5.77	100.50	105.70
29	X	2348	U	C5-C6-N1	5.77	125.59	122.70
29	X	232	G	C8-N9-C4	-5.77	104.09	106.40
29	X	2584	U	O5'-P-OP1	-5.77	100.51	105.70
29	X	580	C	OP2-P-O3'	5.77	117.89	105.20
29	X	37	C	N1-C2-O2	5.77	122.36	118.90
29	X	744	U	C4-C5-C6	5.77	123.16	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2839	G	OP1-P-OP2	5.77	128.25	119.60
29	X	651(B)	C	C5-C6-N1	5.76	123.88	121.00
29	X	1995	U	N3-C4-O4	5.76	123.43	119.40
29	X	2272	U	C5-C6-N1	-5.76	119.82	122.70
29	X	2352	A	C8-N9-C4	5.76	108.10	105.80
29	X	951	C	C5-C6-N1	-5.76	118.12	121.00
29	X	2438	U	N3-C2-O2	-5.75	118.17	122.20
29	X	2567	G	N3-C4-C5	-5.75	125.72	128.60
29	X	2512	C	C5-C6-N1	5.75	123.87	121.00
29	X	2050	C	C2-N3-C4	-5.74	117.03	119.90
29	X	2424	C	C6-N1-C2	-5.74	118.00	120.30
29	X	2879	G	N1-C6-O6	5.74	123.34	119.90
29	X	472	A	C5-C6-N1	-5.73	114.83	117.70
29	X	2002	G	O5'-P-OP1	5.73	117.58	110.70
29	X	2549	G	OP1-P-O3'	5.73	117.81	105.20
29	X	1130	U	C5-C6-N1	-5.73	119.84	122.70
29	X	2294	C	O5'-P-OP1	-5.73	100.54	105.70
29	X	2695	C	C5-C6-N1	5.73	123.86	121.00
29	X	1292	C	C5-C6-N1	-5.73	118.14	121.00
29	X	974	G	N7-C8-N9	5.72	115.96	113.10
29	X	2544	G	C8-N9-C4	-5.72	104.11	106.40
29	X	1260	G	OP1-P-O3'	5.72	117.79	105.20
29	X	2571	C	C5-C4-N4	5.72	124.20	120.20
29	X	1217	C	C6-N1-C2	-5.72	118.01	120.30
29	X	1647	G	O5'-P-OP2	5.71	117.56	110.70
29	X	1674	G	OP1-P-OP2	5.71	128.16	119.60
29	X	1674	G	N1-C6-O6	-5.71	116.48	119.90
29	X	2611	U	OP2-P-O3'	5.71	117.75	105.20
29	X	515	A	N1-C6-N6	-5.70	115.18	118.60
29	X	2052	G	N3-C4-N9	5.69	129.41	126.00
29	X	1210	G	N3-C4-C5	-5.69	125.76	128.60
29	X	2488	A	N9-C4-C5	5.68	108.07	105.80
29	X	1326	U	C5-C4-O4	-5.68	122.49	125.90
29	X	2050	C	P-O3'-C3'	5.68	126.52	119.70
29	X	2611	U	C2-N1-C1'	5.68	124.52	117.70
29	X	2371	G	C5-C6-O6	5.68	132.01	128.60
29	X	1282	U	N3-C4-O4	5.67	123.37	119.40
29	X	2832	U	C6-N1-C2	5.67	124.40	121.00
29	X	777	A	O5'-P-OP1	-5.67	100.60	105.70
29	X	2514	U	O5'-P-OP1	-5.67	100.60	105.70
29	X	2514	U	N1-C2-O2	-5.67	118.83	122.80
29	X	1132	A	O5'-P-OP1	-5.67	100.60	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	748	G	O5'-P-OP2	-5.66	100.60	105.70
29	X	2049	G	OP1-P-O3'	5.66	117.65	105.20
29	X	1779	U	O4'-C1'-N1	5.66	112.72	108.20
29	X	1289	C	O5'-P-OP2	-5.65	100.61	105.70
29	X	2604	U	C5-C6-N1	-5.64	119.88	122.70
29	X	746	C	OP1-P-O3'	5.64	117.61	105.20
29	X	1292	C	N1-C2-O2	-5.64	115.52	118.90
29	X	2273	A	C8-N9-C4	-5.63	103.55	105.80
29	X	2067	G	C8-N9-C4	-5.62	104.15	106.40
29	X	2882	C	OP1-P-OP2	5.62	128.03	119.60
29	X	1240	C	N1-C2-O2	5.62	122.27	118.90
29	X	2001	A	N1-C2-N3	5.62	132.11	129.30
29	X	223	A	OP1-P-O3'	5.62	117.56	105.20
29	X	1754	A	O5'-P-OP2	-5.62	100.64	105.70
29	X	2006	C	C5-C6-N1	5.62	123.81	121.00
29	X	2777	G	C8-N9-C4	5.62	108.65	106.40
29	X	1264	G	C5-N7-C8	5.61	107.11	104.30
29	X	2822	G	OP1-P-OP2	5.61	128.01	119.60
29	X	2686	G	OP1-P-O3'	5.61	117.54	105.20
29	X	2732	G	N3-C2-N2	5.61	123.83	119.90
29	X	1978	A	OP2-P-O3'	5.61	117.53	105.20
29	X	2689	U	N3-C4-O4	-5.61	115.48	119.40
29	X	1662	U	N1-C2-O2	-5.60	118.88	122.80
29	X	1163	G	C5-C6-O6	5.60	131.96	128.60
29	X	1785	A	OP2-P-O3'	5.60	117.52	105.20
29	X	2419	U	C6-N1-C2	-5.60	117.64	121.00
29	X	945	A	N1-C6-N6	5.60	121.96	118.60
29	X	1511	G	C8-N9-C4	-5.60	104.16	106.40
29	X	2451	A	N9-C4-C5	5.59	108.04	105.80
29	X	2825	C	C5-C4-N4	-5.59	116.28	120.20
29	X	2035	G	P-O3'-C3'	5.59	126.41	119.70
29	X	2558	C	C5-C6-N1	5.59	123.80	121.00
29	X	2392	A	N7-C8-N9	5.58	116.59	113.80
29	X	479	A	O4'-C1'-N9	5.58	112.67	108.20
29	X	2036	C	N1-C2-O2	5.58	122.25	118.90
29	X	2250	G	N3-C2-N2	-5.58	115.99	119.90
29	X	1753	A	C6-N1-C2	-5.58	115.25	118.60
29	X	2005	A	C8-N9-C4	5.58	108.03	105.80
29	X	754	G	N7-C8-N9	-5.57	110.31	113.10
29	X	2565	A	C8-N9-C4	-5.57	103.57	105.80
30	Y	39	C	C2-N1-C1'	5.57	124.93	118.80
29	X	1755	U	C5-C6-N1	-5.56	119.92	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	673	C	N1-C2-O2	-5.56	115.56	118.90
29	X	1995	U	C5-C6-N1	5.56	125.48	122.70
29	X	2035	G	OP1-P-OP2	-5.56	111.26	119.60
29	X	1674	G	O5'-P-OP1	-5.56	100.70	105.70
29	X	2719	G	C8-N9-C4	5.56	108.62	106.40
29	X	2698	U	C5-C4-O4	5.56	129.23	125.90
29	X	2684	U	O5'-P-OP2	-5.55	100.70	105.70
29	X	1650	A	N7-C8-N9	-5.55	111.03	113.80
29	X	2514	U	OP1-P-O3'	5.55	117.41	105.20
29	X	2641	G	C8-N9-C4	5.55	108.62	106.40
29	X	2278	A	O5'-P-OP2	-5.54	100.71	105.70
29	X	753	A	N7-C8-N9	-5.54	111.03	113.80
29	X	809	G	N1-C6-O6	-5.54	116.58	119.90
29	X	2053	G	C2-N3-C4	-5.54	109.13	111.90
3	B	137	ARG	NE-CZ-NH1	-5.54	117.53	120.30
29	X	1653	G	N1-C2-N2	-5.54	111.22	116.20
29	X	2676	C	O5'-P-OP1	5.54	117.34	110.70
29	X	517	C	N3-C2-O2	-5.53	118.03	121.90
29	X	1684	C	O5'-P-OP1	5.53	117.34	110.70
29	X	2553	G	P-O3'-C3'	5.53	126.34	119.70
29	X	516	C	N1-C2-O2	5.53	122.22	118.90
29	X	2049	G	N3-C4-N9	5.52	129.31	126.00
29	X	319	C	C6-N1-C2	-5.52	118.09	120.30
29	X	1993	U	N3-C2-O2	-5.52	118.33	122.20
29	X	670	A	O4'-C1'-N9	-5.52	103.79	108.20
29	X	918	A	N1-C6-N6	-5.52	115.29	118.60
29	X	2877	G	C8-N9-C4	5.52	108.61	106.40
29	X	2566	A	OP1-P-O3'	5.51	117.33	105.20
29	X	2833	U	C6-N1-C1'	5.51	128.92	121.20
29	X	983	A	C4-C5-N7	-5.50	107.95	110.70
29	X	1653	G	N3-C4-N9	5.50	129.30	126.00
29	X	2042	A	C8-N9-C4	-5.50	103.60	105.80
29	X	1695	G	C6-C5-N7	-5.50	127.10	130.40
29	X	1266	G	N1-C2-N2	-5.50	111.25	116.20
29	X	2551	C	C2-N3-C4	-5.50	117.15	119.90
29	X	2058	A	C5-N7-C8	-5.50	101.15	103.90
29	X	957	C	C5-C4-N4	-5.49	116.36	120.20
29	X	2043	C	C6-N1-C2	-5.49	118.10	120.30
29	X	2049	G	N3-C2-N2	5.49	123.74	119.90
29	X	1157	G	OP2-P-O3'	5.49	117.28	105.20
29	X	2689	U	C2-N1-C1'	-5.49	111.11	117.70
29	X	2717	G	C8-N9-C4	-5.49	104.21	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	581	C	O5'-P-OP2	-5.48	100.77	105.70
29	X	1257	C	N3-C4-C5	-5.48	119.71	121.90
29	X	845	G	C2-N3-C4	-5.48	109.16	111.90
29	X	1998	A	C4-C5-C6	5.48	119.74	117.00
29	X	2032	G	C6-C5-N7	-5.48	127.11	130.40
29	X	1688	U	N1-C2-O2	-5.48	118.97	122.80
29	X	645	U	C5-C4-O4	5.47	129.18	125.90
29	X	2840	C	N3-C4-C5	5.47	124.09	121.90
29	X	2872	G	O5'-P-OP2	-5.47	100.78	105.70
29	X	748	G	O4'-C1'-N9	5.47	112.57	108.20
29	X	2711	A	C2-N3-C4	-5.47	107.87	110.60
29	X	2715	C	N3-C2-O2	-5.47	118.07	121.90
29	X	1256	G	N1-C6-O6	5.46	123.18	119.90
29	X	517	C	C6-N1-C2	-5.46	118.11	120.30
29	X	1297	C	N3-C4-C5	5.46	124.08	121.90
22	U	17	SER	C-N-CA	5.46	135.34	121.70
29	X	841	G	OP2-P-O3'	5.46	117.21	105.20
29	X	2500	U	N1-C2-O2	5.46	126.62	122.80
29	X	2836	G	C8-N9-C4	5.46	108.58	106.40
29	X	972	G	C8-N9-C4	-5.46	104.22	106.40
29	X	2692	C	N3-C4-C5	-5.46	119.72	121.90
29	X	1701	A	N1-C6-N6	5.45	121.87	118.60
29	X	1777	U	C2-N3-C4	5.45	130.27	127.00
29	X	1978	A	O5'-P-OP2	5.45	117.25	110.70
29	X	676	A	C4-C5-N7	5.45	113.43	110.70
29	X	2582	G	OP1-P-OP2	-5.45	111.42	119.60
29	X	1997	A	C5-C6-N6	-5.45	119.34	123.70
29	X	1261	C	N3-C2-O2	5.45	125.71	121.90
29	X	1656	C	C5-C4-N4	-5.45	116.39	120.20
29	X	2590	A	C8-N9-C4	5.45	107.98	105.80
29	X	1455	G	C8-N9-C4	-5.45	104.22	106.40
29	X	585	G	C4-C5-N7	-5.44	108.62	110.80
29	X	2593	U	C6-N1-C2	-5.44	117.73	121.00
29	X	24	G	OP1-P-OP2	5.44	127.76	119.60
29	X	1327	C	OP2-P-O3'	5.44	117.17	105.20
29	X	1627	G	N7-C8-N9	-5.43	110.38	113.10
29	X	2717	G	N9-C4-C5	5.43	107.57	105.40
29	X	2512	C	O5'-P-OP2	-5.43	100.81	105.70
29	X	1951	U	C6-N1-C2	-5.43	117.74	121.00
29	X	11	G	N1-C6-O6	5.43	123.16	119.90
29	X	472	A	N1-C2-N3	5.43	132.01	129.30
29	X	2332	U	N3-C2-O2	-5.43	118.40	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2618	G	N3-C2-N2	-5.43	116.10	119.90
29	X	1652	A	C4-C5-N7	5.42	113.41	110.70
29	X	1149	C	C6-N1-C2	-5.42	118.13	120.30
29	X	1204	C	C6-N1-C2	-5.42	118.13	120.30
29	X	2064	C	O5'-P-OP2	5.42	117.21	110.70
9	H	8	LEU	CA-CB-CG	5.42	127.75	115.30
29	X	2048	A	O5'-P-OP2	-5.42	100.83	105.70
29	X	1295	C	OP2-P-O3'	5.41	117.11	105.20
29	X	1656	C	C6-N1-C1'	-5.41	114.31	120.80
29	X	1314	C	C2-N1-C1'	5.41	124.75	118.80
29	X	2833	U	C5-C4-O4	5.41	129.15	125.90
29	X	1950	G	C2-N3-C4	5.41	114.60	111.90
29	X	329	G	OP2-P-O3'	5.40	117.09	105.20
29	X	2002	G	N1-C6-O6	5.40	123.14	119.90
29	X	2003	G	C6-N1-C2	-5.40	121.86	125.10
29	X	2581	G	N7-C8-N9	5.40	115.80	113.10
29	X	26	G	OP1-P-OP2	-5.40	111.50	119.60
29	X	706	A	C8-N9-C4	5.40	107.96	105.80
29	X	732	C	N3-C2-O2	-5.40	118.12	121.90
29	X	1955	U	O5'-P-OP2	-5.40	100.84	105.70
29	X	1980	G	C8-N9-C4	-5.40	104.24	106.40
30	Y	12	C	C6-N1-C2	5.40	122.46	120.30
29	X	2875	U	N3-C4-O4	5.39	123.18	119.40
29	X	2555	U	N1-C2-O2	-5.39	119.03	122.80
29	X	2852	G	OP1-P-OP2	-5.39	111.51	119.60
29	X	2853	C	O5'-P-OP1	5.39	117.17	110.70
29	X	1650	A	C5-N7-C8	5.39	106.59	103.90
29	X	2371	G	C4-C5-N7	-5.39	108.64	110.80
29	X	1005	C	C5-C6-N1	5.39	123.69	121.00
29	X	2576	G	C4-C5-N7	5.39	112.95	110.80
29	X	782	A	C6-C5-N7	-5.38	128.53	132.30
29	X	462	C	OP2-P-O3'	5.38	117.03	105.20
29	X	911	A	N1-C6-N6	5.38	121.83	118.60
29	X	2711	A	N1-C2-N3	5.38	131.99	129.30
29	X	2823	A	C2-N3-C4	-5.37	107.91	110.60
29	X	2690	C	N3-C2-O2	-5.37	118.14	121.90
29	X	2715	C	C5-C6-N1	5.37	123.68	121.00
29	X	1779	U	C2-N3-C4	-5.37	123.78	127.00
29	X	2881	U	C6-N1-C2	-5.36	117.78	121.00
29	X	1264	G	C4-C5-N7	-5.36	108.66	110.80
29	X	1256	G	O5'-P-OP1	-5.36	100.88	105.70
29	X	1272	A	OP1-P-OP2	5.36	127.64	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2529	G	N1-C6-O6	5.36	123.12	119.90
29	X	2714	G	P-O3'-C3'	5.36	126.13	119.70
29	X	803	U	N3-C2-O2	-5.35	118.45	122.20
29	X	676	A	N1-C6-N6	5.35	121.81	118.60
29	X	1755	U	C2-N1-C1'	-5.35	111.28	117.70
29	X	2359	C	C6-N1-C2	-5.35	118.16	120.30
29	X	2722	G	O5'-P-OP2	-5.35	100.89	105.70
29	X	2561	A	OP1-P-OP2	5.34	127.61	119.60
29	X	1779	U	C5-C4-O4	5.34	129.10	125.90
29	X	1216	C	C6-N1-C2	-5.33	118.17	120.30
29	X	2446	G	N3-C4-N9	5.33	129.20	126.00
29	X	822	U	N3-C2-O2	-5.33	118.47	122.20
29	X	231	C	C6-N1-C2	-5.33	118.17	120.30
29	X	2849	C	N1-C2-O2	-5.32	115.70	118.90
29	X	582	G	C8-N9-C4	5.32	108.53	106.40
29	X	651(B)	C	N1-C2-O2	5.32	122.09	118.90
29	X	2722	G	C8-N9-C4	-5.32	104.27	106.40
29	X	1608	A	C4-C5-C6	5.31	119.66	117.00
29	X	170	C	C6-N1-C2	-5.31	118.17	120.30
29	X	2676	C	C4-C5-C6	5.31	120.06	117.40
29	X	1663	U	O4'-C1'-N1	5.31	112.45	108.20
29	X	845	G	C5-N7-C8	-5.31	101.65	104.30
29	X	1653	G	C8-N9-C4	5.31	108.52	106.40
29	X	1695	G	N3-C4-C5	-5.31	125.95	128.60
29	X	2892	G	C2-N3-C4	-5.30	109.25	111.90
29	X	2571	C	C2-N3-C4	5.30	122.55	119.90
29	X	2879	G	C2-N3-C4	-5.30	109.25	111.90
29	X	782	A	C5-C6-N6	-5.30	119.46	123.70
29	X	2680	C	O5'-P-OP1	-5.30	100.93	105.70
29	X	2709	G	N3-C4-C5	-5.30	125.95	128.60
29	X	2684	U	C5-C6-N1	5.30	125.35	122.70
29	X	2382	G	N1-C6-O6	5.29	123.08	119.90
29	X	948	C	OP1-P-O3'	5.29	116.84	105.20
29	X	957	C	C5-C6-N1	5.29	123.65	121.00
29	X	2619	C	OP1-P-O3'	5.29	116.84	105.20
29	X	2847	U	C5-C4-O4	-5.29	122.73	125.90
29	X	1949	G	C4-C5-N7	-5.29	108.68	110.80
29	X	1980	G	O5'-P-OP2	-5.29	100.94	105.70
29	X	2618	G	N1-C6-O6	5.29	123.07	119.90
30	Y	81	C	C6-N1-C2	-5.29	118.18	120.30
29	X	944	G	N1-C6-O6	5.29	123.07	119.90
29	X	1629	G	C5-C6-N1	-5.29	108.86	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1985	G	C8-N9-C4	5.28	108.51	106.40
29	X	2680	C	N1-C2-N3	5.28	122.90	119.20
29	X	2646	U	C5-C6-N1	5.28	125.34	122.70
29	X	1536	C	N1-C2-O2	5.28	122.07	118.90
29	X	1137	G	C6-C5-N7	-5.28	127.23	130.40
29	X	907	U	C5-C6-N1	-5.28	120.06	122.70
29	X	1660	C	P-O3'-C3'	-5.28	113.37	119.70
29	X	1943	U	C6-N1-C2	5.28	124.17	121.00
29	X	1993	U	N1-C2-N3	5.28	118.06	114.90
29	X	2721	A	O5'-P-OP2	-5.27	100.95	105.70
29	X	649	G	N1-C6-O6	5.27	123.06	119.90
30	Y	84	G	C8-N9-C4	5.27	108.51	106.40
29	X	983	A	N9-C4-C5	5.27	107.91	105.80
29	X	2611	U	N1-C2-O2	5.27	126.49	122.80
29	X	20	C	C6-N1-C2	-5.27	118.19	120.30
29	X	791	C	C6-N1-C2	5.27	122.41	120.30
29	X	1394	G	C4-C5-N7	5.27	112.91	110.80
29	X	2025	C	C5-C6-N1	5.27	123.63	121.00
29	X	2500	U	C6-N1-C2	-5.26	117.84	121.00
29	X	2712(A)	A	C6-C5-N7	-5.26	128.62	132.30
29	X	1231	U	C5-C6-N1	5.26	125.33	122.70
29	X	808	A	C4-C5-C6	5.25	119.62	117.00
29	X	1265	A	O5'-P-OP2	-5.25	100.98	105.70
29	X	1137	G	N1-C6-O6	5.25	123.05	119.90
29	X	911	A	C5-C6-N6	-5.24	119.50	123.70
29	X	1394	G	N3-C4-N9	5.24	129.15	126.00
29	X	2461	C	O5'-P-OP2	-5.24	100.98	105.70
29	X	2446	G	C6-C5-N7	-5.24	127.26	130.40
29	X	2008	C	O5'-P-OP1	5.23	116.98	110.70
29	X	1252	G	C4-C5-N7	-5.23	108.71	110.80
29	X	949	U	O5'-P-OP2	5.23	116.97	110.70
29	X	2832	U	C5-C6-N1	-5.23	120.08	122.70
29	X	1165	U	C5-C6-N1	-5.23	120.09	122.70
29	X	2250	G	N7-C8-N9	5.23	115.71	113.10
29	X	850	C	C6-N1-C2	-5.23	118.21	120.30
29	X	2006	C	C6-N1-C2	-5.23	118.21	120.30
29	X	2335	A	C8-N9-C4	-5.22	103.71	105.80
29	X	650	C	C6-N1-C1'	-5.22	114.53	120.80
29	X	2250	G	N1-C2-N2	5.22	120.90	116.20
29	X	1163	G	C4-C5-N7	-5.22	108.71	110.80
29	X	2013	A	OP2-P-O3'	5.22	116.68	105.20
29	X	318	C	C6-N1-C2	-5.22	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2864	G	OP1-P-O3'	5.22	116.68	105.20
29	X	409	C	C6-N1-C2	-5.22	118.21	120.30
29	X	600	C	N1-C2-O2	5.22	122.03	118.90
29	X	1747	G	N3-C4-N9	5.22	129.13	126.00
29	X	2544	G	N3-C4-C5	-5.21	125.99	128.60
29	X	974	G	C5-N7-C8	-5.21	101.69	104.30
29	X	1675	C	C4-C5-C6	5.21	120.01	117.40
29	X	1660	C	N3-C2-O2	-5.21	118.25	121.90
29	X	1977	A	N7-C8-N9	-5.21	111.19	113.80
29	X	649	G	N3-C2-N2	-5.21	116.25	119.90
29	X	2818	G	C8-N9-C4	5.21	108.48	106.40
29	X	2683	C	N3-C4-C5	-5.21	119.82	121.90
29	X	1154	G	N1-C6-O6	5.21	123.02	119.90
29	X	218	C	C6-N1-C2	-5.21	118.22	120.30
29	X	747	U	N1-C2-O2	-5.21	119.16	122.80
30	Y	91	A	C8-N9-C4	5.20	107.88	105.80
29	X	2430	A	C2-N3-C4	5.20	113.20	110.60
29	X	1322	A	OP2-P-O3'	5.20	116.64	105.20
29	X	565	C	O5'-P-OP2	5.20	116.94	110.70
29	X	1653	G	O4'-C1'-N9	5.20	112.36	108.20
29	X	2562	U	N3-C2-O2	-5.20	118.56	122.20
29	X	2824	C	C6-N1-C2	-5.19	118.22	120.30
29	X	1652	A	C5-N7-C8	-5.19	101.31	103.90
29	X	676	A	C8-N9-C4	-5.19	103.72	105.80
29	X	2250	G	C5-N7-C8	-5.19	101.71	104.30
29	X	2709	G	O5'-P-OP2	-5.18	101.03	105.70
29	X	931	U	N3-C2-O2	-5.18	118.57	122.20
29	X	1154	G	C5-C6-O6	-5.18	125.49	128.60
29	X	2037	G	O5'-P-OP2	5.18	116.92	110.70
29	X	810	U	OP1-P-O3'	5.18	116.59	105.20
29	X	2695	C	N1-C2-O2	-5.18	115.79	118.90
7	F	99	LEU	CA-CB-CG	5.18	127.21	115.30
29	X	1616	A	N9-C4-C5	5.18	107.87	105.80
29	X	2045	C	N3-C4-N4	5.18	121.62	118.00
29	X	2272	U	N3-C4-O4	-5.17	115.78	119.40
29	X	168	A	N1-C6-N6	5.17	121.70	118.60
29	X	825	A	N1-C6-N6	5.17	121.70	118.60
29	X	1156	A	C5-C6-N6	-5.17	119.56	123.70
29	X	1027	U	O4'-C1'-N1	5.17	112.33	108.20
29	X	2572	A	C5-N7-C8	5.17	106.48	103.90
29	X	1263	U	OP2-P-O3'	5.17	116.56	105.20
29	X	983	A	C5-N7-C8	5.16	106.48	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2501	C	N3-C4-C5	5.16	123.97	121.90
29	X	2060	A	O5'-P-OP1	5.16	116.89	110.70
29	X	2271	G	C6-C5-N7	-5.15	127.31	130.40
29	X	1299	G	C2-N3-C4	-5.15	109.33	111.90
29	X	2708	G	O5'-P-OP2	-5.15	101.07	105.70
29	X	496	G	OP2-P-O3'	5.14	116.52	105.20
29	X	951	C	N3-C4-N4	-5.14	114.40	118.00
29	X	1451	C	C2-N1-C1'	5.14	124.45	118.80
29	X	2883	A	OP1-P-OP2	5.14	127.31	119.60
29	X	1613	G	N3-C4-N9	5.14	129.08	126.00
29	X	2273	A	N1-C6-N6	-5.14	115.52	118.60
29	X	732	C	N3-C4-N4	-5.14	114.40	118.00
29	X	2332	U	C4-C5-C6	5.13	122.78	119.70
29	X	2830	G	C5-N7-C8	5.13	106.87	104.30
29	X	2036	C	C2-N1-C1'	5.12	124.44	118.80
29	X	1673	U	C2-N3-C4	-5.12	123.93	127.00
29	X	491	G	C5-C6-O6	5.12	131.67	128.60
29	X	2254	C	N3-C4-N4	-5.12	114.42	118.00
29	X	2576	G	N9-C4-C5	-5.12	103.35	105.40
29	X	2728	U	N3-C2-O2	-5.12	118.62	122.20
29	X	447	A	C2-N3-C4	-5.11	108.04	110.60
29	X	1490	C	C5-C6-N1	5.11	123.56	121.00
29	X	2036	C	N3-C2-O2	-5.11	118.32	121.90
29	X	2703	C	C6-N1-C2	-5.11	118.25	120.30
29	X	2488	A	OP2-P-O3'	5.11	116.44	105.20
29	X	2721	A	N1-C2-N3	5.11	131.85	129.30
29	X	2722	G	N3-C2-N2	5.11	123.48	119.90
29	X	1027	U	C6-N1-C1'	5.11	128.35	121.20
29	X	1210	G	C8-N9-C4	-5.11	104.36	106.40
29	X	2571	C	C5-C6-N1	5.11	123.55	121.00
29	X	1664	A	O4'-C1'-N9	-5.11	104.12	108.20
29	X	2003	G	C5-C6-N1	5.11	114.05	111.50
29	X	2060	A	P-O3'-C3'	5.10	125.82	119.70
29	X	2822	G	N3-C4-C5	-5.10	126.05	128.60
29	X	824	U	C2-N3-C4	-5.10	123.94	127.00
29	X	1649	G	N7-C8-N9	-5.10	110.55	113.10
29	X	2627	G	N3-C2-N2	-5.10	116.33	119.90
29	X	2574	G	C8-N9-C1'	5.10	133.63	127.00
29	X	338	G	C4-N9-C1'	5.10	133.13	126.50
29	X	992	C	C6-N1-C2	-5.10	118.26	120.30
29	X	1606	G	N1-C6-O6	-5.10	116.84	119.90
29	X	1753	A	C4-C5-C6	5.10	119.55	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	576	U	N1-C2-O2	-5.10	119.23	122.80
29	X	1006	C	O5'-P-OP1	-5.10	101.11	105.70
29	X	1759	C	C6-N1-C2	5.10	122.34	120.30
29	X	1210	G	C8-N9-C1'	-5.09	120.38	127.00
29	X	1289	C	N3-C4-C5	5.09	123.94	121.90
29	X	2773	C	OP2-P-O3'	5.09	116.40	105.20
29	X	236	C	C6-N1-C2	5.09	122.33	120.30
29	X	2841	C	O5'-P-OP1	5.09	116.81	110.70
29	X	588	U	C5-C6-N1	-5.09	120.16	122.70
29	X	2025	C	N3-C4-N4	5.09	121.56	118.00
29	X	1992	G	O5'-P-OP1	-5.08	101.12	105.70
29	X	2617	C	C6-N1-C2	5.08	122.33	120.30
29	X	2259	G	OP2-P-O3'	5.08	116.38	105.20
29	X	2685	G	O5'-P-OP2	5.08	116.79	110.70
29	X	2516	G	N1-C6-O6	-5.08	116.86	119.90
29	X	1678	U	O5'-P-OP2	5.07	116.79	110.70
29	X	1749	A	N7-C8-N9	5.07	116.33	113.80
29	X	1929	G	O4'-C1'-N9	5.07	112.25	108.20
29	X	219	G	P-O3'-C3'	5.06	125.78	119.70
29	X	1165	U	C6-N1-C2	5.06	124.04	121.00
29	X	1320	G	N1-C6-O6	-5.06	116.86	119.90
10	I	21	ARG	NE-CZ-NH2	-5.06	117.77	120.30
29	X	2551	C	N1-C2-N3	5.06	122.74	119.20
29	X	1652	A	C5-C6-N6	-5.06	119.66	123.70
29	X	2488	A	C5-C6-N6	5.06	127.75	123.70
29	X	2447	G	O4'-C1'-N9	5.06	112.25	108.20
29	X	2453	A	N1-C2-N3	-5.06	126.77	129.30
9	H	43	ARG	NE-CZ-NH2	-5.05	117.77	120.30
29	X	669	G	C2-N3-C4	5.05	114.43	111.90
29	X	1240	C	C6-N1-C2	-5.05	118.28	120.30
29	X	1279	A	N7-C8-N9	-5.05	111.27	113.80
29	X	1613	G	N3-C2-N2	5.05	123.44	119.90
29	X	1661	G	O5'-P-OP2	-5.05	101.16	105.70
29	X	2848	G	C4-C5-C6	5.05	121.83	118.80
29	X	168	A	C4-C5-C6	5.05	119.52	117.00
29	X	574	C	O5'-P-OP1	-5.05	101.16	105.70
29	X	774	A	N3-C4-C5	5.05	130.33	126.80
29	X	956	G	O5'-P-OP2	-5.05	101.16	105.70
29	X	2046	G	OP1-P-O3'	5.05	116.30	105.20
29	X	565	C	C5-C6-N1	5.04	123.52	121.00
29	X	1726	U	C5-C6-N1	-5.04	120.18	122.70
29	X	1753	A	C8-N9-C4	-5.04	103.78	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	302	U	N3-C2-O2	-5.04	118.67	122.20
29	X	1660	C	C4-C5-C6	5.04	119.92	117.40
29	X	580	C	N1-C2-O2	-5.04	115.88	118.90
29	X	669	G	N1-C2-N2	5.04	120.73	116.20
29	X	2612	C	C2-N3-C4	5.04	122.42	119.90
29	X	2724	U	C6-N1-C2	-5.04	117.98	121.00
29	X	940	G	N3-C4-C5	5.03	131.12	128.60
29	X	599	G	OP2-P-OP3'	5.03	116.27	105.20
29	X	944	G	N7-C8-N9	5.03	115.61	113.10
29	X	1005	C	C6-N1-C2	-5.03	118.29	120.30
29	X	946	G	N3-C4-C5	-5.03	126.09	128.60
29	X	1253	G	OP2-P-OP3'	5.03	116.26	105.20
29	X	1319	G	C8-N9-C1'	-5.03	120.46	127.00
29	X	2881	U	N3-C4-C5	-5.03	111.58	114.60
29	X	998	C	C5-C6-N1	-5.03	118.49	121.00
29	X	540	C	C6-N1-C2	5.02	122.31	120.30
29	X	2250	G	O5'-P-OP2	-5.02	101.18	105.70
29	X	2558	C	C6-N1-C2	-5.02	118.29	120.30
29	X	21	A	C8-N9-C4	-5.02	103.79	105.80
29	X	2053	G	N1-C2-N3	5.02	126.91	123.90
29	X	2067	G	C6-C5-N7	-5.02	127.39	130.40
29	X	997	G	N9-C4-C5	-5.01	103.39	105.40
29	X	2844	G	N3-C4-N9	5.01	129.01	126.00
29	X	2722	G	C4-N9-C1'	5.01	133.02	126.50
29	X	738	G	O4'-C1'-N9	5.01	112.21	108.20
29	X	783	A	C8-N9-C4	-5.01	103.80	105.80
29	X	844	U	O5'-P-OP2	-5.01	101.19	105.70
29	X	866	A	O4'-C1'-N9	-5.01	104.19	108.20
4	C	35	LEU	CA-CB-CG	-5.00	103.79	115.30
29	X	1291	U	C6-N1-C2	5.00	124.00	121.00
29	X	486	C	C2-N1-C1'	-5.00	113.30	118.80
29	X	1606	G	N7-C8-N9	-5.00	110.60	113.10
29	X	2690	C	C4-C5-C6	5.00	119.90	117.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	178	GLY	Peptide
3	B	73	ALA	Peptide
3	B	85	ALA	Peptide
4	C	187	VAL	Peptide

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Mol	Chain	Res	Type	Group
8	G	37	ASP	Peptide
25	Z	37	HIS	Peptide
25	Z	52	TYR	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	0	1651	0	1693	59	0
2	A	2107	0	2190	82	0
3	B	1540	0	1600	75	0
4	C	1507	0	1525	80	0
5	D	1401	0	1481	64	0
6	E	1287	0	1336	49	0
7	F	1048	0	1088	23	0
8	G	1115	0	1144	47	0
9	H	997	0	1046	67	0
10	I	1068	0	1103	60	0
11	J	1091	0	1125	64	0
12	K	879	0	930	43	0
13	L	778	0	820	38	0
14	M	867	0	890	43	0
15	N	978	0	1020	72	0
16	O	742	0	756	37	0
17	P	1014	0	1096	60	0
18	Q	727	0	753	25	0
19	R	826	0	881	54	0
20	S	1346	0	1372	65	0
21	T	626	0	655	33	0
22	U	553	0	604	59	0
23	V	534	0	558	16	0
24	W	424	0	470	20	0
25	Z	453	0	455	38	0
26	1	404	0	416	21	0
27	2	393	0	420	19	0
28	3	509	0	565	40	0
29	X	59673	0	30060	1282	0
30	Y	2601	0	1327	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	M	1	0	0	0	0
31	X	192	0	0	0	0
31	Y	5	0	0	0	0
All	All	89337	0	59379	2369	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 16.

All (2369) 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)
12:K:103:ARG:HD2	29:X:1287:A:H5'	1.33	1.04
9:H:41:ASN:ND2	29:X:2674:A:O2'	1.91	1.04
15:N:48:ARG:HD2	29:X:1156:A:H61	1.20	1.03
8:G:31:THR:HG21	15:N:61:TRP:HE1	1.26	1.00
29:X:500:G:H22	29:X:503:A:H5''	1.26	0.97
3:B:75:THR:HG22	3:B:77:ILE:H	1.34	0.93
17:P:85:MET:HE3	17:P:130:GLU:HG3	1.50	0.93
28:3:29:LYS:NZ	29:X:2419:U:OP2	2.03	0.92
12:K:9:LYS:NZ	29:X:2002:G:OP2	2.04	0.91
19:R:100:ASP:HB3	19:R:101:GLY:HA3	1.52	0.91
26:1:39:LYS:HB2	26:1:49:PHE:HE2	1.35	0.89
11:J:66:TYR:HB2	11:J:106:GLU:HB2	1.56	0.87
29:X:2345:G:H4'	29:X:2346:A:H5''	1.56	0.87
22:U:20:ARG:HB3	22:U:43:ARG:HH21	1.40	0.87
15:N:91:ASN:HD21	29:X:996:A:H4'	1.40	0.87
12:K:79:VAL:HA	12:K:83:VAL:HG13	1.58	0.86
19:R:96:LYS:NZ	29:X:297:C:OP1	2.08	0.86
29:X:1212:G:H1'	29:X:1237:A:H61	1.41	0.85
29:X:1526:G:H22	29:X:1546:G:H1	1.22	0.85
10:I:21:ARG:HA	29:X:811:U:H2'	1.60	0.84
29:X:612:G:O2'	29:X:615:A:N6	2.11	0.84
29:X:2836:G:H2'	29:X:2837:A:C8	2.13	0.84
14:M:2:GLN:N	29:X:2820:A:N1	2.26	0.84
18:Q:51:ILE:HD11	18:Q:81:ARG:HE	1.44	0.83
28:3:13:ARG:NH2	29:X:222:G:OP2	2.11	0.82
22:U:27:ASP:HA	22:U:32:ARG:HH21	1.43	0.82
29:X:1360:G:H22	29:X:2213:U:H3	1.25	0.82
22:U:20:ARG:HB3	22:U:43:ARG:HD2	1.61	0.82
9:H:75:VAL:HG12	9:H:118:LEU:HD21	1.59	0.82
28:3:34:THR:OG1	29:X:2420:C:OP1	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:95:LEU:HD12	4:C:96:PRO:HD2	1.61	0.81
29:X:2689:U:O2	29:X:2713:U:H5''	1.81	0.81
13:L:37:HIS:ND1	30:Y:30:C:OP1	2.12	0.81
20:S:149:ALA:HB3	20:S:164:PRO:HA	1.62	0.81
20:S:105:GLN:O	20:S:109:GLN:NE2	2.12	0.81
30:Y:17:A:OP1	30:Y:110:U:O2'	1.98	0.80
29:X:309:A:N3	29:X:329:G:O2'	2.15	0.79
17:P:60:ILE:HD11	25:Z:28:PRO:HD3	1.63	0.79
17:P:86:LEU:HD12	17:P:89:ARG:HH21	1.45	0.79
27:2:43:THR:O	27:2:45:SER:N	2.16	0.79
5:D:75:SER:H	5:D:79:LEU:HD22	1.47	0.79
28:3:33:ASN:O	28:3:35:GLY:N	2.15	0.78
8:G:33:ILE:HG21	29:X:538:G:H5'	1.64	0.78
25:Z:19:ARG:NH2	29:X:1264:G:OP1	2.16	0.78
29:X:1019:U:H3	29:X:1142:A:H62	1.32	0.78
29:X:2601:C:H3'	29:X:2602:A:H5''	1.65	0.78
29:X:578:A:OP1	29:X:1255:U:O2'	2.01	0.78
28:3:17:THR:HG22	28:3:20:GLY:H	1.49	0.77
29:X:2693:U:H2'	29:X:2694:G:H8	1.48	0.77
16:O:7:THR:HB	16:O:22:VAL:HG11	1.66	0.77
29:X:679:C:H2'	29:X:680:A:H8	1.49	0.77
20:S:168:VAL:HG12	20:S:169:VAL:H	1.48	0.77
10:I:94:GLU:HA	10:I:97:ARG:HH11	1.50	0.77
11:J:42:TRP:HB3	11:J:95:VAL:HG21	1.66	0.77
29:X:844:U:H3'	29:X:845:G:C8	2.20	0.77
11:J:15:ARG:HG3	11:J:74:PRO:HD2	1.66	0.77
19:R:22:VAL:HG11	19:R:81:VAL:HG22	1.65	0.77
29:X:2320:A:N6	29:X:2333:A:O2'	2.17	0.76
30:Y:16:U:H1'	30:Y:109:G:H21	1.48	0.76
22:U:23:LYS:HB3	22:U:37:ILE:HG22	1.67	0.76
10:I:21:ARG:HH22	29:X:587:C:P	2.09	0.76
9:H:69:VAL:HG12	9:H:70:VAL:H	1.50	0.76
19:R:52:ASN:HA	19:R:73:GLU:HA	1.67	0.76
15:N:37:GLN:HG3	29:X:1252:G:H1	1.51	0.76
29:X:165(E):A:H2'	29:X:165(F):C:C6	2.21	0.76
19:R:58:VAL:HG13	19:R:60:PRO:HD2	1.67	0.76
25:Z:35:GLN:O	25:Z:37:HIS:N	2.18	0.76
5:D:150:ARG:HH21	29:X:2305:U:H3	1.30	0.76
29:X:500:G:N2	29:X:503:A:H5''	2.00	0.75
29:X:1042:G:N2	29:X:1113:U:O2	2.18	0.75
25:Z:19:ARG:HA	29:X:2046:G:H5'	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:12:LYS:O	11:J:13:GLN:HB2	1.87	0.75
4:C:136:TRP:O	4:C:140:ASN:ND2	2.18	0.75
29:X:2323:G:H1	29:X:2332:U:H5	1.34	0.75
13:L:65:THR:OG1	30:Y:52:G:OP1	2.04	0.75
14:M:57:ILE:O	14:M:58:ASN:ND2	2.20	0.75
29:X:2262:U:H2'	29:X:2263:C:H6	1.52	0.75
29:X:1626:A:H61	29:X:1639:U:H3	1.32	0.75
24:W:23:LEU:HD21	24:W:43:MET:HB3	1.67	0.75
6:E:89:LEU:HD21	6:E:105:MET:HE1	1.69	0.75
22:U:32:ARG:H	22:U:32:ARG:NE	1.84	0.74
1:O:150:ARG:HA	1:O:153:LYS:HB2	1.68	0.74
4:C:68:ARG:HH21	29:X:2060:A:H62	1.34	0.74
23:V:63:LYS:HA	23:V:66:GLN:HG3	1.67	0.74
29:X:10:A:H2'	29:X:11:G:C8	2.22	0.74
5:D:108:LEU:HD23	5:D:111:ILE:HD12	1.69	0.74
17:P:80:LEU:HD11	17:P:87:GLU:HG3	1.69	0.74
3:B:134:TRP:CD1	3:B:137:ARG:HB2	2.22	0.74
22:U:30:VAL:O	22:U:32:ARG:NH1	2.20	0.74
29:X:1926:U:OP2	29:X:1929:G:N1	2.17	0.74
20:S:25:ASN:HB3	20:S:28:ASN:H	1.51	0.74
29:X:1049:C:H42	29:X:2751:G:H1	1.33	0.74
15:N:54:LYS:NZ	29:X:995:C:OP2	2.20	0.73
29:X:1212:G:H1'	29:X:1237:A:N6	2.02	0.73
29:X:1905:C:H5''	29:X:1906:G:H5'	1.70	0.73
10:I:17:LYS:HD2	29:X:663:G:H5''	1.68	0.73
29:X:1283:G:H22	29:X:1286:A:H5'	1.54	0.73
1:O:182:SER:HA	1:O:185:TYR:HB3	1.69	0.73
29:X:1418:G:O2'	29:X:1578:U:O4	2.05	0.73
29:X:1019:U:H3	29:X:1142:A:N6	1.86	0.73
4:C:68:ARG:NH2	29:X:2060:A:H62	1.85	0.73
13:L:55:SER:OG	13:L:56:SER:N	2.20	0.73
4:C:67:ALA:HA	29:X:1255:U:C5	2.24	0.73
3:B:169:ASN:ND2	29:X:2731:G:OP1	2.21	0.73
3:B:109:LYS:NZ	29:X:2723:C:OP1	2.19	0.73
12:K:90:ARG:NH1	29:X:2880:C:O2'	2.22	0.73
29:X:828:G:H2'	29:X:829:A:C8	2.23	0.73
8:G:81:VAL:HG11	8:G:156:HIS:HD2	1.53	0.73
19:R:99:VAL:HG12	19:R:103:LYS:HG3	1.71	0.72
29:X:221:C:H4'	29:X:222:G:H5''	1.71	0.72
5:D:90:THR:OG1	30:Y:44:C:N3	2.20	0.72
12:K:92:GLY:HA2	12:K:94:TYR:CZ	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:117:VAL:HG23	20:S:168:VAL:HG13	1.71	0.72
12:K:33:ARG:HB2	12:K:114:GLU:HB3	1.71	0.72
5:D:122:PHE:HD2	5:D:129:ASN:H	1.34	0.72
3:B:93:VAL:O	3:B:95:ILE:N	2.20	0.72
25:Z:45:ILE:HG21	25:Z:57:VAL:HG23	1.69	0.72
29:X:2683:C:H2'	29:X:2684:U:H6	1.55	0.72
22:U:53:GLU:OE1	22:U:58:LYS:N	2.21	0.72
11:J:17:ARG:NH2	29:X:956:G:O6	2.22	0.72
3:B:92:ASN:HD22	3:B:182:ILE:HG13	1.54	0.72
25:Z:51:TYR:CE1	25:Z:55:ARG:HG3	2.25	0.72
19:R:100:ASP:HB3	19:R:101:GLY:CA	2.20	0.72
23:V:42:ARG:NH1	23:V:45:GLN:OE1	2.23	0.72
11:J:21:ASP:OD2	11:J:22:ALA:N	2.23	0.72
4:C:193:LEU:HA	4:C:196:VAL:HG22	1.72	0.72
3:B:189:PRO:HA	29:X:2680:C:H5'	1.70	0.72
10:I:111:SER:OG	10:I:112:GLY:N	2.23	0.71
13:L:33:ARG:HH22	13:L:103:LEU:HD12	1.55	0.71
15:N:37:GLN:HA	15:N:40:LEU:HD12	1.71	0.71
29:X:483:A:H3'	29:X:484:C:H6	1.54	0.71
29:X:635:C:O2'	29:X:639:U:OP1	2.03	0.71
12:K:3:HIS:O	12:K:5:LYS:N	2.22	0.71
20:S:4:THR:OG1	20:S:5:ALA:N	2.22	0.71
3:B:147:PRO:HG2	3:B:149:ARG:HG2	1.73	0.71
10:I:32:ARG:NH2	29:X:671:C:OP2	2.23	0.71
22:U:51:ILE:HG23	22:U:59:THR:HA	1.73	0.71
29:X:2373:A:H2'	29:X:2374:G:C8	2.25	0.71
29:X:678:C:H2'	29:X:679:C:H6	1.54	0.71
10:I:86:THR:OG1	10:I:116:ARG:NH1	2.24	0.71
29:X:1242:A:H2'	29:X:1243:C:C6	2.25	0.71
12:K:92:GLY:HA2	12:K:94:TYR:CE2	2.25	0.71
29:X:2304:G:H22	29:X:2312:U:H3	1.37	0.70
5:D:35:VAL:HG11	29:X:2314:G:H5'	1.72	0.70
8:G:31:THR:HG21	15:N:61:TRP:NE1	2.06	0.70
29:X:2291:U:O2'	29:X:2374:G:N3	2.24	0.70
2:A:134:ARG:HB3	2:A:187:SER:HB2	1.72	0.70
29:X:303:G:H2'	29:X:304:G:C8	2.26	0.70
3:B:62:PRO:O	29:X:2786:U:O2'	2.08	0.70
11:J:78:LYS:HD3	29:X:956:G:H5''	1.74	0.70
29:X:547:A:OP1	29:X:1221:C:H5'	1.92	0.70
29:X:1414:G:N2	29:X:1585:U:O4'	2.25	0.70
9:H:1:MET:HE2	29:X:1665:A:H1'	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2218:U:H2'	29:X:2219:U:C6	2.27	0.70
29:X:1242:A:H2'	29:X:1243:C:H6	1.56	0.70
17:P:57:LEU:HD13	17:P:69:ALA:HA	1.74	0.70
16:O:7:THR:O	16:O:9:GLY:N	2.25	0.69
12:K:36:THR:OG1	29:X:1278:G:OP1	2.09	0.69
6:E:172:LYS:NZ	29:X:2529:G:OP2	2.17	0.69
1:O:130:ARG:HD2	29:X:2169:A:H5'	1.74	0.69
12:K:11:ASN:OD1	29:X:1652:A:N6	2.25	0.69
3:B:60:ASN:HB3	3:B:62:PRO:HD2	1.74	0.69
29:X:1645:G:H5'	29:X:1646:C:H5'	1.73	0.69
13:L:64:LYS:HG3	30:Y:53:G:H5''	1.73	0.69
12:K:31:GLU:O	12:K:33:ARG:N	2.21	0.69
27:2:21:ARG:HD2	27:2:30:ILE:HD12	1.75	0.69
2:A:268:ARG:HH21	29:X:2224:G:H5''	1.56	0.69
4:C:22:VAL:HG13	4:C:106:MET:HG2	1.74	0.69
29:X:83:G:N2	29:X:102:G:H1'	2.08	0.69
20:S:3:LEU:HG	20:S:32:PHE:CD1	2.28	0.69
24:W:22:ALA:O	24:W:24:GLY:N	2.26	0.69
9:H:9:ASP:N	9:H:9:ASP:OD2	2.26	0.69
22:U:20:ARG:HB3	22:U:43:ARG:NH2	2.07	0.69
22:U:29:GLY:O	22:U:31:GLY:N	2.26	0.69
29:X:165(E):A:H2'	29:X:165(F):C:H6	1.58	0.69
29:X:1607:C:N4	29:X:1622:G:OP2	2.24	0.69
28:3:36:LYS:HD3	28:3:41:ILE:HD12	1.75	0.69
12:K:24:GLN:HB3	12:K:44:LEU:HD22	1.75	0.69
18:Q:64:ARG:HB2	18:Q:69:ILE:HD13	1.73	0.69
29:X:1876:A:H2'	29:X:1877:A:H8	1.58	0.69
29:X:507:A:C5'	29:X:508:A:H5'	2.23	0.69
5:D:131:GLY:HA2	5:D:154:ILE:H	1.58	0.68
29:X:1936:A:H2	29:X:1943:U:H3	1.41	0.68
29:X:1796:U:H2'	29:X:1797:C:C6	2.27	0.68
22:U:48:LYS:HG2	22:U:49:LYS:H	1.59	0.68
29:X:521:G:H2'	29:X:522:A:H8	1.58	0.68
1:O:149:VAL:HA	1:O:152:LEU:HD12	1.75	0.68
1:O:40:HIS:HA	1:O:168:HIS:HB3	1.74	0.68
29:X:1054:A:H2'	29:X:1055:G:C8	2.29	0.68
29:X:1163:G:H2'	29:X:1164:A:H8	1.58	0.68
29:X:2373:A:H2'	29:X:2374:G:H8	1.57	0.68
29:X:544:C:H1'	29:X:547:A:H8	1.58	0.68
1:O:174:ALA:HA	1:O:181:LEU:HD21	1.76	0.68
9:H:26:ASN:HB2	9:H:42:LYS:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:9:ILE:HD11	3:B:27:LEU:HB2	1.75	0.68
6:E:107:ILE:O	6:E:152:ARG:NH1	2.22	0.67
29:X:2357:G:N2	29:X:2360:A:OP2	2.26	0.67
26:1:39:LYS:HB2	26:1:49:PHE:CE2	2.24	0.67
29:X:507:A:H5''	29:X:508:A:H5'	1.76	0.67
7:F:96:VAL:HB	7:F:136:VAL:HG12	1.74	0.67
9:H:22:ILE:HD11	29:X:1952:A:N3	2.09	0.67
29:X:2323:G:N1	29:X:2332:U:H5	1.92	0.67
17:P:36:ARG:HA	17:P:39:ARG:HD2	1.77	0.67
17:P:49:SER:O	17:P:51:GLN:N	2.28	0.67
15:N:13:ARG:NH1	29:X:1251:C:OP1	2.20	0.67
29:X:2661:G:H2'	29:X:2662:A:C8	2.30	0.67
2:A:161:THR:HG21	29:X:1819:A:H5''	1.75	0.67
29:X:680:A:H2'	29:X:681:G:C8	2.30	0.67
29:X:445:C:H2'	29:X:446:G:H5''	1.77	0.67
29:X:569:U:O2'	29:X:983:A:N1	2.26	0.67
28:3:33:ASN:C	28:3:35:GLY:H	1.97	0.67
29:X:678:C:H2'	29:X:679:C:C6	2.29	0.67
21:T:10:SER:OG	29:X:2277:G:OP2	2.13	0.67
29:X:1526:G:N2	29:X:1546:G:H1	1.92	0.67
10:I:18:ARG:NH2	29:X:1250:G:N7	2.43	0.66
22:U:54:ASN:O	22:U:56:GLN:N	2.21	0.66
20:S:46:GLN:HB3	20:S:50:GLY:HA2	1.76	0.66
17:P:82:ASN:ND2	29:X:495:G:N3	2.41	0.66
9:H:109:ARG:HA	9:H:129:LEU:HD13	1.76	0.66
25:Z:51:TYR:CD1	25:Z:55:ARG:HG3	2.30	0.66
29:X:845:G:H8	29:X:845:G:OP2	1.78	0.66
29:X:650:C:H2'	29:X:651:G:H8	1.60	0.66
29:X:1557:G:H3'	29:X:1558:A:H5''	1.77	0.66
29:X:458:G:N2	29:X:470:A:OP2	2.26	0.66
29:X:562:U:HO2'	29:X:572:A:H8	1.44	0.66
14:M:14:ARG:HB3	14:M:14:ARG:HH21	1.61	0.66
9:H:124:MET:O	9:H:127:VAL:HG12	1.94	0.66
18:Q:10:PRO:HB3	18:Q:91:LEU:HD21	1.77	0.66
29:X:920:G:N2	29:X:2269:A:OP2	2.28	0.66
29:X:1124:C:H2'	29:X:1125:G:H8	1.60	0.66
2:A:142:VAL:HA	2:A:194:GLY:H	1.59	0.66
1:O:138:SER:OG	1:O:139:GLY:N	2.28	0.65
24:W:9:VAL:HG22	24:W:17:VAL:HG22	1.76	0.65
3:B:183:LEU:HD21	14:M:16:ILE:HD13	1.77	0.65
29:X:641:C:H42	29:X:646:A:H61	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2461:C:H2'	29:X:2462:U:H6	1.61	0.65
23:V:23:LYS:O	23:V:27:GLU:HG2	1.95	0.65
29:X:2319:U:H4'	29:X:2320:A:H5'	1.77	0.65
29:X:699:A:H2'	29:X:700:G:O4'	1.97	0.65
4:C:154:ASP:OD1	4:C:157:THR:OG1	2.14	0.65
29:X:1779:U:O2	29:X:1783:A:N6	2.30	0.65
16:O:6:GLN:HB2	16:O:11:GLN:HA	1.77	0.65
8:G:88:VAL:HG21	8:G:127:ILE:HD11	1.78	0.65
8:G:34:PRO:HG3	8:G:69:ASP:OD2	1.97	0.65
4:C:27:LEU:O	4:C:31:VAL:HG23	1.96	0.65
26:1:26:LYS:HB2	26:1:31:THR:HG21	1.79	0.65
26:1:35:LEU:HB3	26:1:51:ALA:HB2	1.77	0.65
2:A:211:ARG:NH1	29:X:1566:A:OP1	2.27	0.64
13:L:8:ARG:HH11	13:L:8:ARG:HB2	1.61	0.64
29:X:1198:U:H2'	29:X:1199:U:C6	2.32	0.64
29:X:2626:C:H2'	29:X:2627:G:H8	1.62	0.64
4:C:28:HIS:CD2	10:I:8:PRO:HB3	2.32	0.64
29:X:2035:G:OP1	29:X:2035:G:H4'	1.96	0.64
4:C:7:ILE:HB	4:C:121:ASP:O	1.97	0.64
29:X:2294:C:H2'	29:X:2295:C:H6	1.63	0.64
6:E:9:ILE:HG22	6:E:11:VAL:HG13	1.80	0.64
16:O:39:PHE:HD1	16:O:47:PHE:HB3	1.62	0.64
29:X:1876:A:H2'	29:X:1877:A:C8	2.33	0.64
29:X:823:G:H2'	29:X:824:U:H6	1.63	0.64
19:R:77:HIS:HD2	29:X:328:U:H5'	1.63	0.64
9:H:22:ILE:HD11	29:X:1952:A:C4	2.32	0.64
29:X:2101:G:H2'	29:X:2102:G:C8	2.32	0.64
29:X:616:A:H2'	29:X:617:A:C8	2.32	0.64
24:W:15:ASN:OD1	24:W:16:GLN:N	2.29	0.64
29:X:1071:G:O2'	29:X:1089:G:OP2	2.15	0.64
29:X:643:A:H2'	29:X:644:A:C8	2.33	0.64
1:O:11:ASP:OD1	1:O:13:ASN:ND2	2.29	0.64
10:I:14:LYS:NZ	29:X:1193:G:OP1	2.27	0.64
4:C:117:LEU:HD13	4:C:188:ILE:HD12	1.80	0.64
1:O:16:TYR:HB3	1:O:21:ALA:HB2	1.80	0.64
29:X:1784:A:H4'	29:X:1785:A:O5'	1.98	0.64
16:O:21:ARG:HD3	16:O:90:PHE:CE1	2.33	0.64
22:U:25:ARG:NH2	29:X:2432:A:O2'	2.31	0.64
22:U:28:GLY:O	22:U:30:VAL:N	2.30	0.63
29:X:648:G:H2'	29:X:649:G:C8	2.33	0.63
29:X:2688:C:N4	29:X:2720:U:OP2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:78:LYS:HB3	2:A:116:THR:HG22	1.79	0.63
11:J:36:ILE:HG12	11:J:103:VAL:HG22	1.77	0.63
6:E:28:GLY:HA3	6:E:79:VAL:HB	1.78	0.63
29:X:2439:A:H4'	29:X:2440:C:H5''	1.79	0.63
10:I:35:LYS:NZ	29:X:568:U:OP1	2.30	0.63
29:X:521:G:H2'	29:X:522:A:C8	2.33	0.63
29:X:823:G:H2'	29:X:824:U:C6	2.33	0.63
29:X:1664:A:C2	29:X:2726:U:C2	2.86	0.63
2:A:30:GLU:HB3	2:A:33:LEU:HB2	1.79	0.63
29:X:698:C:O2'	29:X:734:A:N6	2.30	0.63
17:P:109:ARG:HG3	17:P:109:ARG:HH11	1.62	0.63
29:X:1429:G:H2'	29:X:1430:C:C6	2.34	0.63
29:X:395:U:H2'	29:X:396:G:C8	2.34	0.63
29:X:547:A:H5''	29:X:547:A:N3	2.14	0.63
9:H:110:VAL:HG23	9:H:129:LEU:HB2	1.81	0.63
8:G:42:VAL:HG11	8:G:166:LEU:HB2	1.79	0.63
29:X:2695:C:H2'	29:X:2696:U:H6	1.64	0.63
29:X:634:G:H2'	29:X:635:C:H6	1.64	0.63
10:I:133:VAL:HG11	10:I:140:VAL:HG23	1.79	0.63
4:C:9:GLN:O	4:C:10:ASN:ND2	2.32	0.63
8:G:151:TYR:OH	8:G:158:HIS:NE2	2.32	0.63
2:A:157:ARG:NH1	29:X:1818:U:OP2	2.31	0.63
29:X:1289:C:H2'	29:X:1290:U:H6	1.64	0.63
18:Q:35:LYS:HD2	18:Q:53:ILE:HG23	1.80	0.63
15:N:58:ARG:O	15:N:62:ILE:HG13	1.98	0.62
29:X:2845:C:H2'	29:X:2846:G:H8	1.64	0.62
9:H:83:ARG:HD3	9:H:89:ILE:HD11	1.81	0.62
11:J:52:ARG:NH1	11:J:53:ILE:HG12	2.14	0.62
2:A:223:GLY:HA2	2:A:226:MET:HG3	1.81	0.62
10:I:63:ARG:NH1	29:X:2417:C:OP1	2.33	0.62
15:N:50:ARG:HA	15:N:53:LYS:HE2	1.82	0.62
17:P:15:LYS:NZ	29:X:502:A:O2'	2.17	0.62
15:N:92:ARG:HG2	29:X:997:G:OP1	2.00	0.62
2:A:259:THR:HG1	29:X:1797:C:HO2'	1.45	0.62
16:O:18:ASP:N	16:O:18:ASP:OD1	2.33	0.62
29:X:1783:A:HO2'	29:X:2607:G:HO2'	1.47	0.62
4:C:46:ARG:HB3	4:C:50:GLN:HB2	1.80	0.62
29:X:776:G:N1	29:X:2072:G:OP1	2.24	0.62
9:H:69:VAL:HG12	9:H:70:VAL:N	2.14	0.62
20:S:56:VAL:O	20:S:58:GLY:N	2.33	0.62
16:O:62:GLU:HG3	16:O:63:HIS:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:48:VAL:O	19:R:50:GLY:N	2.30	0.62
29:X:2693:U:H2'	29:X:2694:G:C8	2.34	0.62
29:X:2849:C:H4'	29:X:2850:A:H5'	1.81	0.62
6:E:99:THR:HB	6:E:102:ALA:HB3	1.81	0.62
29:X:657:U:H2'	29:X:658:A:C8	2.35	0.62
29:X:27:G:O2'	29:X:28:A:OP2	2.16	0.62
29:X:1848:A:H2'	29:X:1849:G:O4'	2.00	0.62
29:X:2219:U:H3'	29:X:2220:C:H4'	1.80	0.62
20:S:74:ARG:HH22	30:Y:94:G:H5''	1.64	0.61
29:X:1495:A:N1	29:X:1496:A:N6	2.47	0.61
14:M:55:ILE:HA	14:M:104:LEU:HD12	1.82	0.61
29:X:2168:G:N2	29:X:2171:A:O4'	2.32	0.61
29:X:2060:A:H1'	29:X:2502:G:C1'	2.30	0.61
29:X:634:G:H2'	29:X:635:C:C6	2.35	0.61
29:X:2218:U:H2'	29:X:2219:U:C5	2.35	0.61
14:M:104:LEU:HA	14:M:106:TYR:CE2	2.35	0.61
16:O:78:VAL:HG12	16:O:80:TYR:HB2	1.82	0.61
17:P:114:ALA:HB2	29:X:1614:A:N1	2.15	0.61
10:I:16:ARG:HH22	29:X:589:U:P	2.23	0.61
22:U:49:LYS:HB2	22:U:61:TRP:CE3	2.35	0.61
19:R:76:LEU:HD22	19:R:80:LYS:HD3	1.81	0.61
29:X:2845:C:H2'	29:X:2846:G:C8	2.36	0.61
29:X:807:U:H2'	29:X:808:A:H8	1.64	0.61
20:S:39:PHE:CE1	20:S:43:PHE:HB2	2.36	0.61
29:X:1450:G:H2'	29:X:1451:C:H6	1.65	0.61
5:D:103:LEU:HD12	5:D:107:GLY:HA3	1.82	0.61
9:H:99:ILE:HD12	9:H:103:GLY:HA2	1.81	0.61
2:A:271:VAL:HG22	2:A:272:THR:HG23	1.82	0.61
29:X:960:A:H5''	29:X:961:C:OP2	2.00	0.61
29:X:2448:A:HO2'	29:X:2449:U:H5	1.45	0.61
19:R:51:VAL:HG13	19:R:52:ASN:H	1.65	0.61
3:B:119:ARG:HG2	3:B:120:TRP:CD1	2.35	0.61
29:X:744:U:H2'	29:X:745:G:O4'	2.00	0.61
10:I:94:GLU:HA	10:I:97:ARG:NH1	2.15	0.61
19:R:22:VAL:HG13	19:R:82:ALA:H	1.65	0.61
29:X:2057:A:H2'	29:X:2058:A:C8	2.35	0.61
29:X:443:A:H2	29:X:1245:G:N3	1.97	0.61
6:E:92:VAL:HG23	6:E:160:LYS:HE2	1.83	0.61
12:K:28:LEU:HD21	12:K:115:LEU:HD11	1.81	0.61
9:H:88:THR:HB	14:M:80:VAL:HB	1.82	0.61
27:2:39:ARG:NH2	29:X:468:G:N7	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1188:U:H2'	29:X:1189:A:H8	1.65	0.61
29:X:1124:C:H2'	29:X:1125:G:C8	2.35	0.61
29:X:733:G:N7	29:X:761:A:C6	2.69	0.61
29:X:2874:C:H2'	29:X:2875:U:H6	1.66	0.61
1:O:112:THR:HB	1:O:115:MET:HB2	1.83	0.61
29:X:2347:C:H2'	29:X:2348:U:C6	2.36	0.60
16:O:80:TYR:CE2	29:X:1187:G:H5''	2.36	0.60
15:N:48:ARG:HD2	29:X:1156:A:N6	2.03	0.60
12:K:87:TYR:CD1	12:K:90:ARG:HD2	2.36	0.60
1:O:205:LEU:HB3	1:O:222:LEU:HD13	1.83	0.60
29:X:1423:A:H2'	29:X:1424:G:H8	1.65	0.60
29:X:323:G:OP1	29:X:338:G:N2	2.33	0.60
29:X:536:A:H2'	29:X:537:U:C6	2.36	0.60
5:D:66:ILE:HD11	30:Y:43:G:H2'	1.82	0.60
16:O:14:VAL:HG11	16:O:95:ILE:HG13	1.82	0.60
20:S:151:ASP:N	20:S:151:ASP:OD2	2.33	0.60
5:D:150:ARG:NH2	29:X:2305:U:H3	1.98	0.60
3:B:111:LYS:NZ	29:X:2724:U:OP1	2.24	0.60
25:Z:15:LYS:O	25:Z:18:MET:N	2.33	0.60
15:N:74:MET:HE2	15:N:110:VAL:HG13	1.83	0.60
6:E:130:ARG:NH1	6:E:132:ASP:OD2	2.35	0.60
5:D:166:ALA:O	5:D:170:LEU:HG	2.02	0.60
1:O:72:VAL:HB	1:O:90:VAL:HG13	1.83	0.60
29:X:439:A:H2'	29:X:440:G:C8	2.36	0.60
15:N:17:VAL:HG21	15:N:32:TYR:HE1	1.65	0.60
15:N:81:ASN:HD22	29:X:1151:A:H4'	1.66	0.60
29:X:79:C:H2'	29:X:80:G:H8	1.66	0.60
3:B:51:TYR:N	3:B:75:THR:HG21	2.16	0.60
4:C:53:LYS:HB2	4:C:73:SER:HB3	1.84	0.60
28:3:54:GLU:O	28:3:58:MET:HG2	2.01	0.60
22:U:20:ARG:CB	22:U:43:ARG:HD2	2.31	0.60
29:X:1423:A:H2'	29:X:1424:G:C8	2.37	0.60
20:S:138:VAL:HA	20:S:141:MET:HE3	1.84	0.60
29:X:2267:A:H5''	29:X:2268:A:H5'	1.83	0.60
12:K:79:VAL:HA	12:K:83:VAL:CG1	2.30	0.60
29:X:2262:U:H2'	29:X:2263:C:C6	2.35	0.60
29:X:2100:G:H1	29:X:2189:U:H3	1.49	0.60
29:X:2532:G:O2'	29:X:2657:A:N1	2.34	0.60
20:S:3:LEU:HD21	20:S:56:VAL:HG22	1.83	0.59
6:E:124:ALA:HB3	6:E:132:ASP:HB2	1.83	0.59
1:O:29:ALA:HB1	1:O:35:GLU:HB3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:650:C:H2'	29:X:651:G:C8	2.37	0.59
29:X:303:G:H2'	29:X:304:G:H8	1.66	0.59
1:0:171:ILE:HD12	1:0:181:LEU:HD22	1.84	0.59
27:2:34:ARG:HD3	29:X:467:G:OP2	2.01	0.59
11:J:69:ILE:HG23	11:J:104:MET:HA	1.84	0.59
4:C:164:VAL:HB	4:C:167:VAL:HG22	1.82	0.59
29:X:120:U:H4'	29:X:121:G:H5''	1.84	0.59
2:A:13:ARG:NH2	29:X:729:G:OP2	2.25	0.59
22:U:20:ARG:HD3	22:U:43:ARG:CZ	2.32	0.59
25:Z:16:ARG:HD2	25:Z:20:ARG:NH1	2.17	0.59
29:X:1323:G:H2'	29:X:1324:G:H5'	1.85	0.59
17:P:45:ILE:HD11	17:P:57:LEU:HG	1.83	0.59
11:J:35:LEU:HD23	11:J:105:PHE:HD2	1.67	0.59
21:T:26:PHE:HE1	29:X:857:C:H1'	1.67	0.59
29:X:676:A:C8	29:X:2443:C:H1'	2.37	0.59
5:D:74:ILE:HA	5:D:79:LEU:HB2	1.83	0.59
29:X:2307:G:H3'	29:X:2308:G:H8	1.68	0.59
28:3:17:THR:HG22	28:3:21:LYS:H	1.67	0.59
2:A:260:ARG:HH22	2:A:266:SER:HB2	1.67	0.59
30:Y:15:A:N1	30:Y:71:G:O2'	2.27	0.59
25:Z:3:LYS:HD3	29:X:2611:U:H3'	1.83	0.59
1:0:18:ILE:HG12	1:0:185:TYR:HE1	1.67	0.59
29:X:2626:C:H2'	29:X:2627:G:C8	2.38	0.59
17:P:86:LEU:N	17:P:130:GLU:OE2	2.34	0.59
13:L:63:ASN:HB2	13:L:67:THR:HG23	1.83	0.59
30:Y:64:C:H2'	30:Y:65:A:H8	1.67	0.59
12:K:13:ASN:C	12:K:17:ARG:HH21	2.05	0.59
22:U:21:ARG:HH21	22:U:23:LYS:HG2	1.67	0.59
20:S:4:THR:HA	20:S:57:GLU:HB2	1.83	0.59
15:N:44:THR:O	15:N:48:ARG:HG2	2.03	0.59
29:X:100:U:O2	29:X:102:G:N1	2.36	0.59
29:X:2522:U:O2'	29:X:2647:U:OP1	2.17	0.59
14:M:60:SER:HA	14:M:64:LYS:HB2	1.84	0.59
29:X:680:A:H2'	29:X:681:G:H8	1.67	0.59
29:X:2091:U:H5''	29:X:2092:U:H2'	1.85	0.59
15:N:13:ARG:NH1	29:X:1251:C:H5''	2.17	0.59
29:X:2308:G:OP1	29:X:2310:A:N6	2.31	0.58
1:0:68:VAL:HG21	1:0:153:LYS:HG2	1.85	0.58
29:X:1450:G:H2'	29:X:1451:C:C6	2.38	0.58
27:2:34:ARG:NH2	27:2:41:GLN:O	2.36	0.58
11:J:23:LYS:O	20:S:73:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:15:ARG:NH2	29:X:2293:A:O5'	2.36	0.58
6:E:160:LYS:NZ	29:X:2658:C:OP1	2.32	0.58
28:3:58:MET:HA	28:3:61:MET:HG3	1.86	0.58
29:X:1047:G:O2'	29:X:1109:C:N4	2.36	0.58
2:A:39:LYS:NZ	2:A:57:GLY:O	2.36	0.58
2:A:7:LYS:NZ	29:X:706:A:OP1	2.35	0.58
29:X:1405:C:H2'	29:X:1406:G:C8	2.38	0.58
29:X:1657:C:H2'	29:X:1658:C:H6	1.67	0.58
4:C:189:ASP:OD1	4:C:190:ALA:N	2.29	0.58
29:X:1412:U:H3'	29:X:1413:G:H5''	1.85	0.58
29:X:1827:U:H5'	29:X:1971:A:H5'	1.86	0.58
15:N:92:ARG:HA	15:N:95:LEU:HB2	1.86	0.58
29:X:2438:U:O2'	29:X:2440:C:OP1	2.20	0.58
28:3:10:ALA:HB1	28:3:14:ILE:HD12	1.84	0.58
8:G:91:THR:O	8:G:94:LYS:HB2	2.03	0.58
29:X:642:G:H21	29:X:645:U:H3	1.50	0.58
30:Y:27:A:H8	30:Y:27:A:OP2	1.86	0.58
8:G:62:ILE:O	8:G:77:GLY:HA3	2.04	0.58
29:X:2233:U:H2'	29:X:2234:G:C8	2.39	0.58
29:X:493:G:H2'	29:X:494:G:O4'	2.04	0.58
2:A:108:PRO:HB3	2:A:143:HIS:HE1	1.69	0.58
15:N:83:LEU:HD23	15:N:113:SER:HB2	1.84	0.58
29:X:2521:C:H2'	29:X:2522:U:C6	2.38	0.58
12:K:85:PRO:O	12:K:88:ALA:HB2	2.04	0.58
25:Z:16:ARG:NH1	29:X:1263:U:OP1	2.36	0.58
15:N:75:ASN:OD1	15:N:77:SER:N	2.37	0.58
4:C:119:ALA:HA	4:C:189:ASP:O	2.03	0.58
29:X:820:A:N3	29:X:943:U:O2'	2.31	0.58
29:X:1676:A:C2	29:X:1993:U:H5'	2.39	0.58
10:I:19:VAL:HB	10:I:30:ALA:HB1	1.84	0.58
10:I:41:SER:HB2	29:X:671:C:C6	2.39	0.58
22:U:51:ILE:HG12	22:U:59:THR:HB	1.86	0.58
29:X:302:U:H2'	29:X:303:G:H8	1.69	0.58
11:J:41:ALA:HB2	11:J:128:ILE:HG21	1.85	0.58
29:X:24:G:H2'	29:X:25:U:H6	1.68	0.58
29:X:740:U:H2'	29:X:741:G:C8	2.39	0.58
17:P:91:PHE:CD2	17:P:131:LYS:HB2	2.38	0.58
22:U:17:SER:HA	22:U:18:VAL:HB	1.86	0.58
4:C:179:ASP:OD1	4:C:182:ARG:NH2	2.37	0.58
29:X:1283:G:N2	29:X:1286:A:H5'	2.17	0.58
14:M:102:ALA:O	14:M:103:LYS:HD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:81:ASN:OD1	15:N:82:GLY:N	2.37	0.58
6:E:24:PHE:HB2	6:E:37:TYR:CD1	2.39	0.58
21:T:84:ALA:O	21:T:85:GLN:HB3	2.03	0.58
29:X:576:U:H2'	29:X:577:G:C8	2.39	0.58
29:X:544:C:H1'	29:X:547:A:C8	2.38	0.58
29:X:2221:G:H2'	29:X:2222:G:C8	2.39	0.58
6:E:37:TYR:HD2	6:E:68:THR:HG23	1.69	0.58
8:G:146:THR:O	8:G:149:LYS:NZ	2.37	0.58
11:J:32:ASP:H	11:J:108:ALA:HB2	1.68	0.58
21:T:21:LEU:HD11	21:T:41:ARG:HE	1.69	0.58
7:F:115:LEU:HD22	7:F:126:THR:HG21	1.86	0.58
29:X:1217:C:H2'	29:X:1218:A:H8	1.69	0.58
29:X:127:A:H5''	29:X:128:C:C6	2.39	0.58
8:G:110:LEU:HD13	29:X:1131:G:O4'	2.03	0.58
19:R:19:GLY:H	19:R:36:VAL:HB	1.69	0.57
29:X:483:A:H3'	29:X:484:C:C6	2.39	0.57
29:X:2060:A:H1'	29:X:2502:G:O4'	2.04	0.57
13:L:33:ARG:HD2	13:L:99:ARG:HB2	1.86	0.57
4:C:22:VAL:HG11	4:C:110:SER:HB3	1.86	0.57
24:W:10:ILE:HD13	29:X:989:G:C8	2.39	0.57
16:O:70:TYR:OH	29:X:1223:G:O6	2.22	0.57
29:X:2438:U:O2'	29:X:2439:A:H5''	2.04	0.57
29:X:1657:C:H2'	29:X:1658:C:C6	2.39	0.57
29:X:2650:U:H2'	29:X:2651:C:H6	1.69	0.57
5:D:60:ILE:HG22	5:D:140:GLU:HB2	1.86	0.57
29:X:14:A:C6	29:X:526:A:C2	2.92	0.57
21:T:39:ARG:HH21	29:X:2355:C:H1'	1.68	0.57
4:C:106:MET:O	4:C:110:SER:OG	2.18	0.57
4:C:186:LEU:HG	4:C:188:ILE:HD13	1.86	0.57
20:S:68:ALA:HB3	20:S:82:ASP:HB2	1.86	0.57
29:X:1841:U:H2'	29:X:1842:G:H8	1.69	0.57
29:X:2219:U:C3'	29:X:2220:C:H4'	2.35	0.57
29:X:1783:A:O2'	29:X:2607:G:O2'	2.21	0.57
19:R:77:HIS:HD2	29:X:328:U:H4'	1.70	0.57
29:X:1087:G:N2	29:X:1089:G:O2'	2.38	0.57
2:A:25:ALA:HB3	2:A:81:ALA:HB1	1.87	0.57
29:X:1353:A:H2'	29:X:1354:A:C8	2.39	0.57
4:C:15:ILE:HG12	4:C:197:GLU:HB2	1.86	0.57
29:X:2801:G:H2'	29:X:2802:G:C8	2.39	0.57
29:X:2751:G:N2	29:X:2751:G:OP1	2.32	0.57
29:X:588:U:H2'	29:X:589:U:C6	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:165:A:H2'	29:X:165(A):G:C8	2.40	0.57
29:X:2063:C:O2	29:X:2451:A:C2	2.58	0.57
11:J:111:THR:HG23	11:J:114:GLN:HG3	1.85	0.57
29:X:465:G:C6	29:X:466:A:N6	2.73	0.57
30:Y:67:C:N4	30:Y:111:C:O2'	2.32	0.57
17:P:87:GLU:O	17:P:89:ARG:N	2.33	0.57
5:D:108:LEU:HA	5:D:111:ILE:HG13	1.86	0.57
29:X:1936:A:H2	29:X:1943:U:N3	2.02	0.57
5:D:60:ILE:HG13	5:D:61:THR:HG23	1.85	0.57
20:S:10:PRO:HB2	20:S:14:LEU:HD21	1.86	0.57
9:H:62:GLY:O	9:H:65:LYS:HE3	2.05	0.57
9:H:119:ARG:NE	14:M:41:GLU:OE1	2.38	0.57
6:E:37:TYR:CD2	6:E:68:THR:HG23	2.39	0.57
1:O:136:PRO:HA	1:O:141:VAL:HG11	1.86	0.57
29:X:651(A):G:H2'	29:X:651(B):C:H4'	1.86	0.57
27:2:7:PRO:HB2	29:X:1309:G:H4'	1.87	0.57
29:X:322:A:H5'	29:X:340:A:H1'	1.87	0.57
29:X:679:C:H2'	29:X:680:A:C8	2.35	0.57
14:M:57:ILE:C	14:M:58:ASN:HD22	2.08	0.57
29:X:640:C:H2'	29:X:641:C:C6	2.40	0.57
2:A:143:HIS:ND1	2:A:194:GLY:O	2.35	0.57
30:Y:6:C:H2'	30:Y:7:C:C6	2.40	0.57
8:G:31:THR:OG1	29:X:995:C:N3	2.38	0.57
22:U:27:ASP:C	22:U:32:ARG:HD3	2.24	0.57
11:J:42:TRP:HB3	11:J:95:VAL:CG2	2.34	0.57
19:R:58:VAL:HG22	19:R:59:LYS:H	1.70	0.57
26:1:31:THR:O	26:1:33:ALA:N	2.38	0.57
10:I:90:ARG:HD2	10:I:93:LEU:HG	1.87	0.57
14:M:100:ARG:HG3	29:X:1747:G:H5''	1.87	0.57
7:F:133:SER:HB3	29:X:1062:G:H21	1.70	0.57
17:P:50:VAL:HG21	17:P:90:LEU:HB3	1.86	0.57
29:X:920:G:C2	29:X:921:G:H1'	2.40	0.57
5:D:41:GLY:O	5:D:43:SER:N	2.38	0.57
29:X:474:G:C6	29:X:510:C:N4	2.73	0.57
22:U:14:VAL:O	22:U:16:ASN:N	2.37	0.57
29:X:1153:C:H2'	29:X:1154:G:C8	2.39	0.57
25:Z:55:ARG:NH2	25:Z:59:ALA:H	2.03	0.56
20:S:15:ASP:O	20:S:17:SER:N	2.38	0.56
10:I:115:SER:O	10:I:136:ALA:HB1	2.04	0.56
22:U:48:LYS:HG2	22:U:49:LYS:N	2.19	0.56
19:R:77:HIS:CD2	29:X:328:U:H5'	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:536:A:H2'	29:X:537:U:H6	1.70	0.56
19:R:15:HIS:ND1	29:X:336:C:H4'	2.20	0.56
4:C:47:THR:H	4:C:50:GLN:HG3	1.70	0.56
29:X:2168:G:N1	29:X:2171:A:OP2	2.37	0.56
9:H:8:LEU:HD23	9:H:8:LEU:N	2.21	0.56
29:X:214:G:N2	29:X:226:G:H2'	2.20	0.56
11:J:77:LYS:HG2	29:X:957:C:H5'	1.86	0.56
29:X:1224:G:O2'	29:X:1225:A:H5'	2.04	0.56
3:B:91:VAL:HB	3:B:93:VAL:HG12	1.87	0.56
11:J:75:VAL:HB	11:J:93:TYR:CE2	2.41	0.56
29:X:2408:U:H2'	29:X:2409:G:H8	1.71	0.56
29:X:1939:U:OP1	29:X:2604:U:O2'	2.23	0.56
29:X:2256:G:N2	29:X:2275:C:C4	2.73	0.56
29:X:2345:G:N3	29:X:2381:C:H2'	2.21	0.56
9:H:13:ASN:ND2	9:H:109:ARG:HG2	2.21	0.56
29:X:676:A:H8	29:X:2443:C:H1'	1.68	0.56
29:X:392:C:H2'	29:X:393:G:H8	1.70	0.56
29:X:413:C:O2'	29:X:1880:U:O2'	2.17	0.56
19:R:105:ARG:HD3	19:R:112:LYS:HD3	1.87	0.56
2:A:78:LYS:NZ	29:X:1502:C:OP1	2.37	0.56
1:O:29:ALA:O	1:O:31:ALA:N	2.38	0.56
22:U:13:LEU:HD12	22:U:14:VAL:H	1.70	0.56
29:X:2182:A:H2'	29:X:2183:G:H8	1.71	0.56
5:D:127:ASN:ND2	5:D:158:THR:O	2.39	0.56
21:T:15:ASP:OD1	29:X:2264:C:N4	2.38	0.56
3:B:120:TRP:CE3	3:B:155:ARG:HD2	2.41	0.56
30:Y:62:C:H2'	30:Y:63:A:H8	1.70	0.56
27:2:12:ARG:HG3	29:X:686:G:O6	2.06	0.56
6:E:67:LEU:HD11	29:X:2758:A:C5	2.41	0.56
29:X:981:A:H2	29:X:2027:G:N3	2.03	0.56
29:X:1676:A:N6	29:X:1677:A:N1	2.53	0.56
16:O:83:ARG:HG2	29:X:1225:A:H4'	1.88	0.56
3:B:48:GLN:NE2	29:X:2635:A:O2'	2.37	0.56
29:X:2691:C:H5'	29:X:2872:G:H5'	1.87	0.56
1:O:10:VAL:HG11	1:O:216:PRO:HG2	1.87	0.56
18:Q:84:GLU:HB2	18:Q:86:GLN:HG3	1.88	0.56
26:I:45:ALA:HB1	29:X:2371:G:H4'	1.88	0.56
29:X:546:U:H5'	29:X:547:A:C2	2.41	0.56
29:X:2564:A:C6	29:X:2565:A:N1	2.74	0.56
19:R:37:LEU:HD11	19:R:49:GLU:HG3	1.87	0.56
29:X:2729:C:H2'	29:X:2730:C:H6	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:47:ARG:NH1	13:L:49:GLN:OE1	2.38	0.56
29:X:1373:A:H5''	29:X:2212:A:N6	2.21	0.56
29:X:1906:G:O2'	29:X:1907:G:H5''	2.06	0.56
29:X:2289:G:N2	29:X:2344:U:O2	2.39	0.56
17:P:18:VAL:O	17:P:19:LYS:HB2	2.05	0.56
29:X:1787:U:H2'	29:X:1788:C:H6	1.71	0.56
21:T:53:MET:HG3	21:T:59:LEU:HD23	1.88	0.55
29:X:2229:U:H2'	29:X:2230:G:H8	1.70	0.55
15:N:75:ASN:HD21	29:X:1011:A:P	2.28	0.55
3:B:136:ARG:HB2	29:X:1657:C:P	2.46	0.55
3:B:105:THR:HB	3:B:197:VAL:CG1	2.36	0.55
2:A:168:LYS:HG3	2:A:173:VAL:HG22	1.87	0.55
29:X:515:A:H2	29:X:1260:G:N3	2.04	0.55
17:P:114:ALA:O	17:P:115:ASN:ND2	2.39	0.55
8:G:110:LEU:HD22	29:X:1131:G:H4'	1.88	0.55
19:R:18:LYS:NZ	19:R:37:LEU:O	2.39	0.55
29:X:2018:G:H2'	29:X:2019:A:C8	2.41	0.55
6:E:143:GLN:HG3	29:X:2745:C:O2'	2.07	0.55
15:N:91:ASN:ND2	29:X:996:A:H4'	2.15	0.55
13:L:33:ARG:HE	13:L:38:ILE:HG21	1.70	0.55
8:G:151:TYR:HH	8:G:158:HIS:CD2	2.24	0.55
29:X:24:G:H2'	29:X:25:U:C6	2.41	0.55
29:X:2376:A:H8	29:X:2376:A:OP1	1.89	0.55
8:G:142:ARG:HA	8:G:145:HIS:CD2	2.42	0.55
29:X:2652:C:H2'	29:X:2653:U:O4'	2.06	0.55
5:D:83:MET:HG2	5:D:84:PRO:HD2	1.87	0.55
26:I:19:GLY:HA3	29:X:2400:G:H4'	1.89	0.55
11:J:12:LYS:HD3	29:X:911:A:C6	2.41	0.55
15:N:37:GLN:HG3	29:X:1252:G:N1	2.21	0.55
11:J:49:GLU:O	11:J:53:ILE:HG13	2.07	0.55
29:X:2168:G:N2	29:X:2171:A:O5'	2.39	0.55
29:X:1270:C:H5''	29:X:1271:G:O5'	2.07	0.55
15:N:31:GLN:NE2	29:X:580:C:H4'	2.21	0.55
12:K:106:ASP:HB3	29:X:1287:A:N7	2.22	0.55
15:N:33:ARG:HD2	29:X:1252:G:N3	2.22	0.55
4:C:22:VAL:HG21	4:C:110:SER:HA	1.88	0.55
9:H:21:CYS:SG	9:H:22:ILE:N	2.80	0.55
29:X:989:G:OP1	29:X:1157:G:O2'	2.22	0.55
29:X:1060:U:H4'	29:X:1061:U:H5'	1.88	0.55
30:Y:34:C:H2'	30:Y:35:C:C6	2.42	0.55
8:G:32:TYR:O	15:N:64:ARG:NH1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1024:G:C6	29:X:1025:G:C6	2.95	0.55
29:X:1678:U:O2'	29:X:1679:C:H5'	2.07	0.55
29:X:864:G:H1'	29:X:914:C:N4	2.22	0.55
28:3:33:ASN:O	28:3:36:LYS:HA	2.07	0.55
29:X:1653:G:H8	29:X:1653:G:OP2	1.90	0.55
29:X:588:U:O4	29:X:670:A:H1'	2.07	0.55
29:X:1055:G:H1	29:X:1104:C:H42	1.54	0.55
22:U:64:ALA:O	22:U:67:ILE:HG22	2.07	0.55
29:X:1268:A:H2'	29:X:1269:A:O4'	2.07	0.55
29:X:1427:A:H4'	29:X:1428:C:O5'	2.05	0.55
29:X:2280:G:H1'	29:X:2327:A:H1'	1.88	0.55
17:P:59:PHE:HD1	25:Z:30:LEU:HD11	1.72	0.55
29:X:2318:G:O2'	29:X:2321:G:O6	2.24	0.55
6:E:37:TYR:CE2	6:E:72:VAL:HG22	2.42	0.55
1:0:10:VAL:HG22	1:0:218:ILE:HD11	1.88	0.55
4:C:192:ALA:HA	4:C:195:ILE:HD11	1.88	0.55
29:X:2619:C:O2'	29:X:2620:U:H5'	2.07	0.55
29:X:936:C:H2'	29:X:937:C:H6	1.72	0.55
29:X:2716:A:O2'	29:X:2717:G:H5'	2.07	0.55
29:X:2330:G:H2'	29:X:2331:G:O4'	2.06	0.55
5:D:9:ASN:O	5:D:13:ARG:HG3	2.07	0.55
12:K:87:TYR:OH	12:K:115:LEU:HB3	2.07	0.55
9:H:13:ASN:OD1	9:H:108:THR:N	2.40	0.55
29:X:733:G:N7	29:X:761:A:N6	2.54	0.55
29:X:740:U:H2'	29:X:741:G:H8	1.72	0.55
29:X:345:A:H2'	29:X:346:A:N7	2.22	0.55
29:X:2756:U:H4'	29:X:2757:A:OP1	2.07	0.55
29:X:2328:A:H2'	29:X:2329:A:C8	2.42	0.55
13:L:22:ALA:O	13:L:24:SER:N	2.40	0.55
17:P:32:ARG:HH21	17:P:119:LYS:HG2	1.71	0.55
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.89	0.54
14:M:104:LEU:HD23	14:M:106:TYR:HE2	1.72	0.54
4:C:39:ARG:HG2	29:X:443:A:N7	2.21	0.54
21:T:51:VAL:HG11	21:T:79:ILE:O	2.06	0.54
20:S:91:PRO:HD3	20:S:127:PRO:HD3	1.88	0.54
11:J:44:LYS:HB2	11:J:47:GLN:HG3	1.88	0.54
13:L:26:LYS:HD3	13:L:87:VAL:O	2.07	0.54
3:B:14:ILE:HD11	3:B:173:VAL:HG11	1.88	0.54
29:X:1429:G:H2'	29:X:1430:C:H6	1.71	0.54
29:X:1151:A:H2'	29:X:1152:C:H6	1.73	0.54
8:G:92:GLY:HA2	8:G:94:LYS:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1172(B):C:H2'	29:X:1172(C):G:H2'	1.88	0.54
29:X:20:C:H2'	29:X:21:A:H8	1.73	0.54
14:M:69:ARG:HB2	14:M:78:GLU:HG2	1.89	0.54
29:X:695:G:OP1	29:X:1380:G:O2'	2.23	0.54
5:D:14:PRO:HA	5:D:17:MET:HB2	1.89	0.54
28:3:21:LYS:HB3	28:3:55:TRP:CH2	2.42	0.54
29:X:733:G:C8	29:X:761:A:N6	2.76	0.54
30:Y:64:C:H2'	30:Y:65:A:C8	2.42	0.54
28:3:25:PHE:HA	28:3:47:GLY:HA2	1.89	0.54
4:C:56:ARG:HB2	29:X:797:U:OP2	2.07	0.54
29:X:1203:U:H2'	29:X:1204:C:C6	2.42	0.54
28:3:29:LYS:NZ	28:3:41:ILE:HG23	2.22	0.54
29:X:2314:G:H2'	29:X:2315:U:C6	2.43	0.54
1:0:157:ILE:HD13	1:0:157:ILE:H	1.72	0.54
1:0:152:LEU:HD23	1:0:157:ILE:HD12	1.89	0.54
9:H:13:ASN:HD21	9:H:109:ARG:H	1.55	0.54
29:X:936:C:H2'	29:X:937:C:C6	2.43	0.54
29:X:2519:U:C5	29:X:2541:A:C6	2.95	0.54
5:D:106:ILE:HB	5:D:139:PRO:HB3	1.89	0.54
2:A:151:LYS:HD3	29:X:2203:G:H4'	1.88	0.54
29:X:2203:G:H2'	29:X:2204:A:H8	1.71	0.54
29:X:83:G:H1	29:X:102:G:HO2'	1.55	0.54
17:P:109:ARG:HG3	17:P:109:ARG:NH1	2.21	0.54
29:X:2028:U:H2'	29:X:2029:A:C8	2.43	0.54
7:F:30:TYR:HB2	7:F:59:ILE:HD12	1.89	0.54
29:X:1127:A:C8	29:X:2518:A:H5''	2.43	0.54
5:D:135:GLN:HG3	5:D:151:GLY:HA2	1.89	0.54
5:D:111:ILE:HG12	5:D:137:ILE:HD12	1.90	0.54
13:L:38:ILE:HD12	13:L:40:ALA:H	1.73	0.54
24:W:25:LEU:HD22	24:W:30:ASP:HB3	1.90	0.54
22:U:78:ILE:HG12	22:U:79:GLU:H	1.72	0.54
1:0:180:ASN:HA	1:0:183:ALA:HB3	1.88	0.54
5:D:116:GLY:HA2	5:D:176:PRO:HB2	1.90	0.54
8:G:43:VAL:HG23	8:G:163:PRO:HB2	1.90	0.54
2:A:50:THR:HG22	29:X:1813:G:H21	1.72	0.54
4:C:4:ILE:HG22	4:C:13:ARG:HH12	1.73	0.54
3:B:144:ARG:NH1	29:X:2572:A:C4	2.75	0.54
29:X:821:A:H5''	29:X:822:U:H6	1.73	0.54
29:X:1668:A:O4'	29:X:1669:A:C2	2.61	0.54
2:A:44:ASN:O	2:A:46:ARG:N	2.41	0.54
29:X:296:C:H2'	29:X:297:C:H6	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:141:ILE:HD11	29:X:2052:G:C8	2.42	0.54
11:J:52:ARG:HG3	11:J:67:ILE:HD11	1.90	0.54
2:A:126:LYS:HG3	2:A:129:ASN:OD1	2.08	0.54
29:X:220:G:OP2	29:X:221:C:H5'	2.08	0.54
29:X:2695:C:H2'	29:X:2696:U:C6	2.42	0.54
1:O:27:GLU:O	1:O:29:ALA:N	2.41	0.54
29:X:1787:U:H2'	29:X:1788:C:C6	2.42	0.54
1:O:65:GLY:HA3	1:O:173:LYS:HD2	1.90	0.54
7:F:78:ILE:HG12	7:F:99:LEU:HD23	1.89	0.54
1:O:43:LEU:HD12	1:O:167:VAL:HG11	1.88	0.54
29:X:297:C:H2'	29:X:298:G:O4'	2.07	0.53
19:R:67:GLY:HA3	29:X:483:A:O3'	2.08	0.53
15:N:94:VAL:O	15:N:98:ILE:HG12	2.07	0.53
9:H:104:GLU:HG2	9:H:125:LYS:HD2	1.90	0.53
2:A:88:ARG:HD2	2:A:106:LEU:HD21	1.89	0.53
29:X:335:C:H2'	29:X:336:C:H6	1.72	0.53
29:X:5:A:H2'	29:X:6:A:C8	2.43	0.53
29:X:1316:U:H2'	29:X:1317:G:H8	1.73	0.53
4:C:35:LEU:HD23	4:C:38:ARG:HD2	1.90	0.53
3:B:4:ILE:HG12	3:B:5:LEU:H	1.73	0.53
22:U:17:SER:CA	22:U:18:VAL:HB	2.38	0.53
1:O:212:THR:HG22	1:O:213:THR:H	1.74	0.53
17:P:27:VAL:HG22	17:P:125:THR:OG1	2.09	0.53
20:S:55:THR:HG22	20:S:61:THR:HB	1.89	0.53
29:X:2461:C:H2'	29:X:2462:U:C6	2.43	0.53
29:X:2153:G:H2'	29:X:2154:G:C8	2.44	0.53
29:X:2600:A:H2'	29:X:2601:C:C6	2.44	0.53
29:X:2221:G:H2'	29:X:2222:G:H8	1.72	0.53
29:X:438:C:H2'	29:X:439:A:H8	1.74	0.53
28:3:16:ILE:HG21	28:3:65:GLY:HA2	1.91	0.53
1:O:25:VAL:HG13	1:O:37:VAL:HG21	1.91	0.53
29:X:799:G:OP2	29:X:800:A:O2'	2.17	0.53
19:R:58:VAL:HA	29:X:483:A:H4'	1.91	0.53
29:X:629:C:H4'	29:X:649:G:H21	1.73	0.53
10:I:16:ARG:NH2	29:X:589:U:OP2	2.40	0.53
26:1:18:THR:HG21	26:1:43:VAL:HB	1.90	0.53
25:Z:42:SER:HB3	29:X:2885:C:H42	1.74	0.53
17:P:60:ILE:CD1	25:Z:28:PRO:HD3	2.35	0.53
29:X:1661:G:H2'	29:X:1662:U:O4'	2.08	0.53
29:X:819:A:OP2	29:X:1187:G:N2	2.31	0.53
8:G:91:THR:HG21	29:X:1140:U:H6	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2885:C:H2'	29:X:2886:A:O4'	2.07	0.53
9:H:47:VAL:HG23	9:H:77:THR:HG23	1.91	0.53
29:X:991:C:H2'	29:X:992:C:H6	1.73	0.53
29:X:2567:G:H2'	29:X:2568:C:C6	2.44	0.53
10:I:101:ARG:HE	29:X:626:G:H1	1.56	0.53
18:Q:46:PHE:O	18:Q:48:VAL:HG23	2.09	0.53
8:G:33:ILE:HD11	29:X:537:U:H4'	1.91	0.53
20:S:6:LYS:HB3	20:S:32:PHE:HA	1.91	0.53
3:B:9:ILE:HD11	3:B:27:LEU:CB	2.38	0.53
25:Z:15:LYS:HA	25:Z:18:MET:HG3	1.90	0.53
21:T:25:LYS:HB2	21:T:37:LEU:HA	1.89	0.53
16:O:43:GLU:C	16:O:45:THR:H	2.12	0.53
16:O:50:ASP:O	16:O:53:LYS:HG2	2.09	0.53
3:B:135:HIS:NE2	29:X:1658:C:OP1	2.42	0.53
29:X:2299:A:H61	29:X:2317:U:H3	1.56	0.53
29:X:1066:U:H2'	29:X:1068:G:OP2	2.08	0.53
29:X:971:C:H2'	29:X:972:G:O4'	2.09	0.53
29:X:445:C:C2'	29:X:446:G:H5''	2.38	0.53
29:X:438:C:H2'	29:X:439:A:C8	2.43	0.53
29:X:2243:U:H2'	29:X:2244:U:C6	2.44	0.53
19:R:85:ASP:HB3	19:R:88:THR:OG1	2.08	0.53
15:N:6:THR:O	15:N:9:VAL:HG23	2.09	0.53
22:U:19:ILE:HA	22:U:42:GLN:HA	1.91	0.53
29:X:2219:U:H3'	29:X:2220:C:C4'	2.38	0.52
4:C:8:GLY:H	4:C:121:ASP:HB3	1.72	0.52
18:Q:53:ILE:HG12	18:Q:54:SER:N	2.24	0.52
21:T:21:LEU:HD11	21:T:41:ARG:NE	2.24	0.52
29:X:1440:U:H2'	29:X:1440(A):C:C6	2.45	0.52
29:X:165(G):U:N3	29:X:175:C:O2	2.42	0.52
29:X:2898:G:H2'	29:X:2899:A:C8	2.44	0.52
29:X:1029:A:C8	29:X:1030:G:C8	2.97	0.52
29:X:1864:U:OP1	29:X:2410:G:O2'	2.22	0.52
29:X:2261:C:O2'	29:X:2262:U:H5'	2.09	0.52
29:X:1320:G:C2	29:X:1329:U:H5''	2.44	0.52
19:R:93:ARG:NH2	29:X:301:G:OP2	2.39	0.52
16:O:66:GLY:O	16:O:87:ARG:NH1	2.39	0.52
29:X:1222:C:H2'	29:X:1223:G:H8	1.73	0.52
29:X:1222:C:H2'	29:X:1223:G:C8	2.44	0.52
30:Y:72:C:H2'	30:Y:73:C:H6	1.74	0.52
29:X:2824:C:H2'	29:X:2825:C:O4'	2.09	0.52
12:K:38:LEU:O	12:K:41:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:44:LYS:NZ	29:X:2362:G:OP1	2.40	0.52
29:X:1858:G:H8	29:X:1884:A:N7	2.08	0.52
30:Y:80:A:H2'	30:Y:81:C:O4'	2.09	0.52
9:H:82:LYS:HB3	9:H:82:LYS:NZ	2.24	0.52
29:X:2695:C:O2'	29:X:2696:U:H5'	2.10	0.52
28:3:17:THR:HG21	28:3:21:LYS:HG3	1.90	0.52
29:X:1114:G:H2'	29:X:1115:A:H8	1.73	0.52
20:S:25:ASN:HA	20:S:85:MET:HB2	1.92	0.52
3:B:27:LEU:HD13	14:M:7:ILE:HD11	1.91	0.52
20:S:69:VAL:HG22	20:S:81:VAL:HG22	1.91	0.52
29:X:1047:G:N3	29:X:1110:G:N2	2.54	0.52
2:A:39:LYS:HZ1	2:A:58:HIS:C	2.11	0.52
21:T:43:THR:H	29:X:2331:G:H4'	1.74	0.52
15:N:6:THR:O	15:N:8:ILE:N	2.41	0.52
14:M:24:LEU:HD13	14:M:91:VAL:HG21	1.90	0.52
29:X:2272:U:H5''	29:X:2273:A:OP1	2.10	0.52
4:C:93:TYR:CE1	29:X:660:G:H5'	2.45	0.52
29:X:200:A:H2'	29:X:201:U:H5'	1.91	0.52
4:C:19:LEU:HB3	4:C:20:PRO:HA	1.90	0.52
9:H:2:ILE:HB	9:H:45:ALA:HB3	1.91	0.52
22:U:33:LYS:O	29:X:2395:C:O2'	2.19	0.52
29:X:1043:C:O2	29:X:1112:G:N2	2.30	0.52
28:3:36:LYS:HB2	28:3:37:SER:CA	2.40	0.52
20:S:109:GLN:NE2	20:S:142:ASN:OD1	2.42	0.52
29:X:2599:G:C2	29:X:2600:A:C8	2.98	0.52
29:X:1998:A:H4'	29:X:2724:U:O2'	2.10	0.52
29:X:2101:G:H2'	29:X:2102:G:H8	1.75	0.52
29:X:2430:A:H2'	29:X:2430:A:N3	2.23	0.52
10:I:72:TYR:HB3	10:I:107:LYS:HB2	1.91	0.52
7:F:21:PRO:HG2	7:F:22:PRO:HD3	1.92	0.52
24:W:4:LYS:O	24:W:51:LEU:HD12	2.10	0.52
29:X:1823:G:H2'	29:X:1824:G:H8	1.74	0.52
17:P:37:LYS:HA	17:P:40:LEU:HD12	1.92	0.52
15:N:114:ARG:O	15:N:118:GLN:HG3	2.10	0.52
8:G:96:ASP:OD1	8:G:96:ASP:N	2.41	0.52
9:H:76:ARG:O	9:H:94:ASN:HA	2.09	0.52
29:X:1479:G:H2'	29:X:1480:G:H8	1.75	0.52
29:X:559:G:H2'	29:X:560:C:O4'	2.09	0.52
15:N:3:ARG:HB3	29:X:1248:G:C5	2.42	0.52
22:U:32:ARG:HE	22:U:32:ARG:H	1.56	0.52
29:X:1266:G:O2'	29:X:2012:G:O6	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:946:G:H2'	29:X:947:G:H8	1.74	0.52
29:X:624:C:O2'	29:X:657:U:OP1	2.26	0.52
22:U:17:SER:CB	22:U:44:ALA:HA	2.39	0.52
29:X:2729:C:H2'	29:X:2730:C:C6	2.45	0.52
4:C:102:LEU:HD12	4:C:102:LEU:O	2.10	0.52
2:A:33:LEU:HD13	2:A:104:TYR:CD2	2.45	0.52
30:Y:27:A:N6	30:Y:56:G:OP2	2.39	0.52
10:I:77:LEU:O	10:I:80:LEU:N	2.43	0.52
2:A:172:TYR:CD1	2:A:184:ARG:HG2	2.44	0.52
6:E:83:TYR:CD1	6:E:138:LYS:HB2	2.45	0.52
17:P:109:ARG:NH2	29:X:2013:A:N3	2.57	0.52
29:X:1289:C:H2'	29:X:1290:U:C6	2.45	0.52
2:A:260:ARG:NH1	29:X:1799:G:OP1	2.37	0.52
29:X:1587:A:H2'	29:X:1588:A:C8	2.45	0.52
29:X:2408:U:H2'	29:X:2409:G:C8	2.45	0.52
2:A:77:ALA:HB2	2:A:97:TYR:CD1	2.44	0.52
9:H:40:GLY:HA2	29:X:2563:U:H4'	1.92	0.52
15:N:91:ASN:N	16:O:11:GLN:OE1	2.41	0.52
26:I:13:GLU:O	26:I:49:PHE:HB3	2.09	0.52
20:S:25:ASN:HB2	20:S:28:ASN:HB3	1.91	0.52
29:X:460:A:C2	29:X:470:A:C4	2.98	0.52
16:O:39:PHE:CD1	16:O:47:PHE:HB3	2.43	0.52
30:Y:7:C:O2'	30:Y:29:C:O2	2.25	0.52
13:L:39:TYR:HE1	30:Y:8:C:H1'	1.75	0.52
2:A:118:ASN:H	2:A:129:ASN:HD22	1.57	0.52
6:E:137:ASP:OD1	6:E:138:LYS:N	2.43	0.52
6:E:17:VAL:HG13	6:E:26:VAL:HG22	1.92	0.52
29:X:555:U:H2'	29:X:556:A:C8	2.44	0.52
25:Z:38:GLY:HA3	25:Z:48:ASN:ND2	2.25	0.52
30:Y:22:U:H3	30:Y:65:A:H61	1.57	0.51
29:X:2468:G:O2'	29:X:2469:A:H8	1.93	0.51
2:A:95:LEU:HD11	2:A:105:ILE:HD13	1.92	0.51
8:G:75:ILE:HG13	8:G:147:ARG:HH12	1.75	0.51
29:X:71:A:H5''	29:X:72:A:H3'	1.92	0.51
30:Y:59:A:H5'	30:Y:60:A:OP2	2.10	0.51
4:C:120:VAL:H	4:C:190:ALA:HB2	1.75	0.51
29:X:2098:U:H3	29:X:2191:G:H1	1.57	0.51
6:E:23:VAL:O	6:E:25:LYS:N	2.44	0.51
21:T:46:LYS:HZ1	21:T:76:ALA:HA	1.75	0.51
20:S:66:VAL:HG22	20:S:83:PHE:HE1	1.75	0.51
29:X:1698:A:C8	29:X:1700:A:O4'	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1360:G:N2	29:X:2213:U:H3	2.03	0.51
29:X:2356:U:H2'	29:X:2357:G:C8	2.45	0.51
29:X:630:G:N2	29:X:632:A:H3'	2.25	0.51
29:X:141:A:H2'	29:X:142:G:C8	2.44	0.51
28:3:36:LYS:HB2	28:3:37:SER:HA	1.91	0.51
27:2:45:SER:HB3	29:X:126:A:OP1	2.11	0.51
5:D:129:ASN:HB3	5:D:155:THR:HG23	1.92	0.51
10:I:86:THR:HG23	10:I:118:VAL:HG13	1.92	0.51
11:J:75:VAL:HB	11:J:93:TYR:HE2	1.75	0.51
21:T:46:LYS:NZ	21:T:76:ALA:HA	2.25	0.51
29:X:1358:G:O2'	29:X:1373:A:N6	2.42	0.51
3:B:149:ARG:O	29:X:2052:G:H1'	2.10	0.51
29:X:1779:U:C5	29:X:1784:A:N7	2.78	0.51
24:W:35:SER:O	24:W:35:SER:OG	2.29	0.51
29:X:101:U:H5''	29:X:102:G:C8	2.46	0.51
4:C:42:THR:OG1	29:X:39:G:N2	2.37	0.51
8:G:95:LEU:HA	8:G:115:ALA:HB3	1.93	0.51
29:X:2341:G:H2'	29:X:2342:C:O4'	2.11	0.51
29:X:1415:A:C6	29:X:1584:U:H4'	2.45	0.51
29:X:1991:U:H2'	29:X:1992:G:H5'	1.92	0.51
1:O:70:VAL:HG12	1:O:108:ALA:HB3	1.91	0.51
24:W:49:HIS:CD2	24:W:50:LEU:HG	2.46	0.51
18:Q:40:ASP:O	18:Q:44:GLN:HG2	2.10	0.51
29:X:1838:C:H4'	29:X:1839:G:C8	2.45	0.51
29:X:1014:A:H2'	29:X:1015:U:C6	2.46	0.51
3:B:141:ILE:HD11	29:X:2052:G:N7	2.26	0.51
19:R:77:HIS:CD2	29:X:328:U:H4'	2.46	0.51
3:B:116:VAL:HG21	3:B:138:PRO:HB3	1.93	0.51
9:H:132:GLU:HB2	14:M:73:PHE:HE1	1.75	0.51
29:X:700:G:H22	29:X:732:C:H5	1.57	0.51
29:X:2048:A:H2'	29:X:2049:G:O4'	2.10	0.51
1:O:140:THR:HG22	1:O:145:VAL:HG22	1.92	0.51
28:3:51:ALA:O	28:3:52:LYS:HB2	2.11	0.51
29:X:7:G:H2'	29:X:8:A:H8	1.76	0.51
2:A:197:GLY:O	2:A:199:ALA:N	2.44	0.51
20:S:22:VAL:HG21	30:Y:77:G:H1'	1.93	0.51
29:X:994:U:O2'	29:X:996:A:OP1	2.19	0.51
19:R:51:VAL:HG13	19:R:73:GLU:HB3	1.93	0.51
29:X:1114:G:H2'	29:X:1115:A:C8	2.46	0.51
29:X:638:G:C5	29:X:639:U:C5	2.98	0.51
29:X:983:A:C2'	29:X:984:A:H5'	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:135:HIS:CD2	29:X:1658:C:OP1	2.64	0.51
3:B:16:LYS:HD3	3:B:173:VAL:HG13	1.92	0.51
29:X:797:U:H2'	29:X:798:G:C8	2.45	0.51
29:X:2468:G:H22	29:X:2481:G:H2'	1.75	0.51
5:D:5:LYS:HB2	5:D:101:GLU:OE1	2.10	0.51
17:P:81:HIS:O	17:P:83:ASP:N	2.44	0.51
29:X:1337:G:H2'	29:X:1338:G:H8	1.76	0.51
29:X:1607:C:H4'	29:X:1608:A:O5'	2.11	0.50
29:X:1779:U:H6	29:X:1784:A:H62	1.58	0.50
29:X:2057:A:H2'	29:X:2058:A:H8	1.75	0.50
1:O:110:VAL:HG12	1:O:111:ALA:H	1.76	0.50
17:P:111:ARG:HH21	29:X:747:U:H5'	1.76	0.50
29:X:2857:G:N2	29:X:2860:A:OP2	2.24	0.50
14:M:25:PRO:HB2	14:M:93:ILE:HD11	1.93	0.50
2:A:48:ARG:NH2	29:X:778:G:H5'	2.25	0.50
15:N:86:ALA:HB2	15:N:116:ALA:HB2	1.92	0.50
28:3:17:THR:HG21	28:3:21:LYS:CG	2.41	0.50
29:X:1113:U:H2'	29:X:1114:G:H8	1.76	0.50
10:I:41:SER:HB2	29:X:671:C:C5	2.46	0.50
2:A:268:ARG:NH2	29:X:2225:A:OP1	2.45	0.50
29:X:569:U:H1'	29:X:947:G:O4'	2.12	0.50
29:X:2266:A:H4'	29:X:2267:A:N3	2.26	0.50
29:X:1810:A:H2'	29:X:1811:G:O4'	2.10	0.50
11:J:61:ARG:HD3	20:S:174:PRO:HB2	1.93	0.50
29:X:407:C:H2'	29:X:408:G:H8	1.76	0.50
29:X:1324:G:C4	29:X:1328:G:O6	2.64	0.50
29:X:1087:G:O6	29:X:1089:G:N2	2.43	0.50
29:X:1203:U:H2'	29:X:1204:C:H6	1.74	0.50
29:X:472:A:H3'	29:X:473:G:H5'	1.94	0.50
29:X:2412:A:C8	29:X:2413:G:C8	2.99	0.50
29:X:1886:A:H2'	29:X:1887:U:O4'	2.12	0.50
12:K:9:LYS:HB3	29:X:1653:G:C6	2.47	0.50
9:H:68:ASP:O	9:H:69:VAL:HB	2.11	0.50
15:N:33:ARG:HB3	29:X:1252:G:C2	2.46	0.50
29:X:2220:C:H2'	29:X:2221:G:C8	2.46	0.50
29:X:1163:G:C2	29:X:1164:A:N7	2.80	0.50
8:G:42:VAL:HA	8:G:164:GLN:H	1.76	0.50
29:X:818:G:H5'	29:X:839:U:OP1	2.10	0.50
4:C:133:PHE:CE1	4:C:161:ALA:HB2	2.45	0.50
29:X:633:A:H4'	29:X:2404:C:H5''	1.92	0.50
29:X:2031:A:C6	29:X:2498:C:H1'	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:110:GLY:HA2	3:B:161:GLY:HA3	1.93	0.50
29:X:1288:U:C2	29:X:1327:C:O2	2.65	0.50
29:X:1667:G:O2'	29:X:1991:U:O4	2.25	0.50
29:X:1416:G:O2'	29:X:1587:A:H1'	2.10	0.50
26:1:5:ALA:HB3	26:1:6:PRO:HD3	1.94	0.50
1:0:38:GLU:HB2	1:0:211:THR:HB	1.92	0.50
5:D:65:PRO:HA	5:D:89:VAL:HG13	1.93	0.50
26:1:14:SER:CA	26:1:49:PHE:HD1	2.24	0.50
28:3:44:LYS:C	28:3:46:LYS:H	2.14	0.50
18:Q:17:TYR:O	18:Q:20:MET:HG2	2.11	0.50
29:X:2817:C:C2	29:X:2830:G:N2	2.80	0.50
2:A:231:HIS:HD2	2:A:233:HIS:H	1.60	0.50
11:J:48:ILE:O	11:J:51:CYS:N	2.45	0.50
6:E:38:ASN:HB2	6:E:64:LEU:HD22	1.93	0.50
19:R:70:GLU:OE1	19:R:72:ARG:NH1	2.45	0.50
2:A:69:ARG:HD2	2:A:119:ALA:HB2	1.93	0.50
15:N:104:GLU:O	15:N:107:LYS:HB3	2.11	0.50
22:U:48:LYS:HZ1	29:X:2090:A:H2	1.60	0.50
18:Q:10:PRO:HG2	18:Q:12:ILE:HD11	1.92	0.50
29:X:807:U:H2'	29:X:808:A:C8	2.47	0.50
21:T:39:ARG:NH2	29:X:2355:C:O2	2.44	0.50
29:X:200:A:N3	29:X:202:U:H1'	2.27	0.50
29:X:2842:A:C2	29:X:2876:G:C2	2.99	0.50
29:X:753:A:O2'	29:X:754:G:H5'	2.11	0.50
29:X:1570:A:H2'	29:X:1571:A:C8	2.46	0.50
20:S:25:ASN:CB	20:S:28:ASN:HB3	2.42	0.50
29:X:1316:U:O2'	29:X:1317:G:H5'	2.11	0.50
25:Z:6:VAL:HG12	29:X:2015:A:C2	2.47	0.50
29:X:610:U:H2'	29:X:611:U:C6	2.47	0.50
15:N:28:ARG:HE	29:X:532:A:H2'	1.76	0.50
20:S:26:LYS:HG3	30:Y:108:G:P	2.52	0.50
30:Y:122:U:O5'	30:Y:122:U:H6	1.95	0.50
10:I:55:ARG:O	10:I:59:ARG:HG3	2.12	0.50
27:2:11:LYS:HE2	29:X:686:G:H5''	1.93	0.50
29:X:2728:U:H2'	29:X:2729:C:C6	2.46	0.50
24:W:3:ILE:HD11	24:W:44:VAL:HG22	1.92	0.50
20:S:19:ILE:HD11	20:S:36:ARG:HG3	1.93	0.50
29:X:390:A:H4'	29:X:391:A:H5'	1.94	0.50
29:X:1626:A:N6	29:X:1639:U:H3	2.06	0.49
15:N:10:ARG:NH1	29:X:583:G:O5'	2.45	0.49
4:C:28:HIS:O	4:C:32:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:443:A:C2	29:X:1245:G:N3	2.80	0.49
29:X:320:U:H4'	29:X:322:A:C8	2.47	0.49
20:S:55:THR:OG1	20:S:55:THR:O	2.26	0.49
9:H:23:ARG:HE	29:X:2561:A:H2	1.59	0.49
29:X:566:U:O2'	29:X:809:G:OP2	2.25	0.49
4:C:57:LYS:NZ	4:C:69:HIS:O	2.45	0.49
5:D:117:ILE:HG22	5:D:118:ASN:H	1.76	0.49
5:D:38:GLU:HB3	5:D:87:ILE:HB	1.93	0.49
4:C:89:ARG:NH2	29:X:1247:A:OP1	2.33	0.49
21:T:56:ASP:OD2	29:X:2364:C:H5'	2.11	0.49
29:X:1638:C:H4'	29:X:2710:C:O2	2.12	0.49
29:X:2712(A):A:H5'	29:X:2713:U:OP2	2.12	0.49
1:O:68:VAL:HG11	1:O:153:LYS:HG2	1.94	0.49
5:D:108:LEU:HD22	5:D:114:PHE:CE1	2.47	0.49
29:X:1285:G:N1	29:X:1329:U:OP1	2.36	0.49
3:B:141:ILE:HG23	29:X:2051:A:H4'	1.93	0.49
29:X:507:A:O5'	29:X:508:A:H5'	2.12	0.49
29:X:1779:U:C2	29:X:1783:A:N7	2.80	0.49
4:C:118:VAL:H	4:C:188:ILE:HD11	1.77	0.49
29:X:945:A:C4	29:X:2448:A:C2	3.00	0.49
29:X:2564:A:C2	29:X:2647:U:H4'	2.47	0.49
6:E:43:VAL:HB	6:E:52:VAL:HG22	1.94	0.49
18:Q:43:GLN:HG2	18:Q:48:VAL:O	2.12	0.49
10:I:64:GLY:HA2	29:X:2415:G:O3'	2.11	0.49
9:H:41:ASN:HD22	9:H:42:LYS:N	2.10	0.49
10:I:21:ARG:HG2	10:I:21:ARG:HH11	1.77	0.49
29:X:639:U:H2'	29:X:640:C:C6	2.46	0.49
29:X:1163:G:C2	29:X:1164:A:C5	3.00	0.49
11:J:25:GLY:HA3	29:X:907:U:OP1	2.12	0.49
19:R:18:LYS:HA	19:R:36:VAL:CG1	2.43	0.49
29:X:1841:U:H2'	29:X:1842:G:C8	2.46	0.49
19:R:88:THR:O	19:R:90:LYS:HE2	2.13	0.49
22:U:41:VAL:O	22:U:42:GLN:NE2	2.35	0.49
29:X:2895:C:H2'	29:X:2896:U:H6	1.77	0.49
1:O:187:ALA:HA	1:O:190:SER:HB3	1.93	0.49
9:H:55:VAL:HB	9:H:67:GLY:H	1.77	0.49
15:N:10:ARG:HH11	29:X:583:G:P	2.36	0.49
1:O:29:ALA:HB1	1:O:35:GLU:CB	2.42	0.49
29:X:214:G:O2'	29:X:226:G:O6	2.27	0.49
21:T:46:LYS:O	21:T:78:PHE:HA	2.12	0.49
29:X:1070:A:H5'	29:X:1072:C:OP2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1748:C:H2'	29:X:1749:A:C8	2.47	0.49
29:X:1240:C:C2	29:X:1241:G:C8	3.01	0.49
29:X:295:G:N2	29:X:344:G:H1'	2.27	0.49
29:X:2307:G:H3'	29:X:2308:G:C8	2.47	0.49
29:X:700:G:H1	29:X:732:C:H5	1.60	0.49
11:J:35:LEU:HD23	11:J:105:PHE:CD2	2.48	0.49
8:G:125:ARG:NH1	29:X:2640:G:OP1	2.44	0.49
10:I:114:ILE:HG21	10:I:132:ALA:O	2.11	0.49
29:X:1464:G:H2'	29:X:1465:G:H8	1.77	0.49
29:X:2836:G:H2'	29:X:2837:A:H8	1.71	0.49
13:L:33:ARG:NE	13:L:38:ILE:HG21	2.28	0.49
9:H:6:SER:OG	29:X:1666:G:H4'	2.12	0.49
2:A:148:VAL:HG11	29:X:2221:G:H21	1.77	0.49
6:E:43:VAL:HB	6:E:52:VAL:HG13	1.95	0.49
20:S:15:ASP:C	20:S:17:SER:H	2.14	0.49
29:X:1864:U:H3	29:X:1878:G:H1	1.59	0.49
2:A:97:TYR:HB3	2:A:99:ASP:HB3	1.93	0.49
5:D:26:MET:O	5:D:30:ARG:NH2	2.45	0.49
23:V:32:ALA:HB2	23:V:37:LEU:HD22	1.93	0.49
22:U:10:LYS:HD3	22:U:11:LYS:H	1.78	0.49
29:X:2070:G:C2	29:X:2071:A:C4	3.00	0.49
17:P:14:ARG:O	17:P:18:VAL:HG22	2.13	0.49
2:A:17:THR:OG1	2:A:205:VAL:N	2.37	0.49
29:X:1832:C:N4	29:X:1833:C:C4	2.81	0.49
29:X:2080:A:H2'	29:X:2081:U:C6	2.47	0.49
11:J:26:ASP:N	11:J:26:ASP:OD1	2.32	0.49
29:X:996:A:H2'	29:X:997:G:H8	1.77	0.49
11:J:43:ILE:N	11:J:95:VAL:HG22	2.28	0.49
22:U:48:LYS:HE3	29:X:2091:U:H1'	1.93	0.49
29:X:653:U:H2'	29:X:654:U:O4'	2.13	0.49
29:X:1668:A:H4'	29:X:1669:A:O5'	2.12	0.49
6:E:17:VAL:HG22	6:E:26:VAL:HG22	1.95	0.49
29:X:2205:A:H2'	29:X:2210:A:N7	2.27	0.49
29:X:1739:C:H2'	29:X:1740:G:H8	1.77	0.49
15:N:11:ARG:HH22	29:X:29:U:H4'	1.77	0.49
29:X:1756:A:H8	29:X:1756:A:O5'	1.95	0.49
19:R:43:ASP:HB3	19:R:45:LYS:HG3	1.94	0.49
29:X:2837:A:H2'	29:X:2838:G:H8	1.78	0.49
29:X:301:G:C4	29:X:302:U:C5	3.01	0.49
28:3:57:ARG:NH2	29:X:833:A:O3'	2.39	0.49
14:M:104:LEU:HA	14:M:106:TYR:HE2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1826:G:H2'	29:X:1827:U:H6	1.76	0.49
2:A:118:ASN:H	2:A:129:ASN:ND2	2.11	0.49
3:B:112:GLY:O	3:B:159:HIS:HA	2.12	0.49
7:F:14:ALA:HB1	7:F:45:THR:HB	1.95	0.49
19:R:56:LYS:HG3	29:X:481:G:OP2	2.12	0.49
2:A:102:LYS:NZ	29:X:1500:A:O2'	2.46	0.49
13:L:92:GLY:C	13:L:94:TYR:H	2.16	0.49
17:P:87:GLU:HA	17:P:90:LEU:HD13	1.95	0.49
29:X:1211:A:H4'	29:X:1212:G:OP2	2.13	0.49
19:R:80:LYS:NZ	29:X:329:G:N7	2.55	0.49
29:X:1525:G:H2'	29:X:1526:G:O4'	2.12	0.49
29:X:2203:G:H2'	29:X:2204:A:C8	2.48	0.49
9:H:9:ASP:O	9:H:95:ALA:HA	2.13	0.49
23:V:44:ARG:O	23:V:47:ARG:HB3	2.13	0.49
29:X:2584:U:H2'	29:X:2585:U:H2'	1.95	0.49
9:H:10:VAL:HG23	9:H:17:ARG:O	2.13	0.49
29:X:846:U:H4'	29:X:847:U:O5'	2.13	0.49
16:O:15:SER:O	16:O:16:GLU:HB2	2.13	0.49
15:N:54:LYS:HZ1	29:X:994:U:P	2.36	0.48
12:K:3:HIS:CD2	12:K:3:HIS:O	2.65	0.48
14:M:14:ARG:HB3	14:M:14:ARG:NH2	2.28	0.48
2:A:29:PRO:HB2	2:A:34:THR:CG2	2.43	0.48
17:P:15:LYS:HB3	29:X:502:A:H4'	1.95	0.48
29:X:79:C:H2'	29:X:80:G:C8	2.48	0.48
17:P:99:ALA:O	29:X:25:U:H5'	2.13	0.48
29:X:944:G:H3'	29:X:944:G:H8	1.78	0.48
29:X:519:U:C2	29:X:520:G:C8	3.01	0.48
29:X:2195:U:H2'	29:X:2196:C:H6	1.79	0.48
13:L:76:ALA:HB1	13:L:111:GLY:HA2	1.94	0.48
20:S:41:ARG:NH2	29:X:1041:C:OP1	2.44	0.48
20:S:121:GLN:O	20:S:161:ALA:HB3	2.13	0.48
2:A:206:LEU:HB2	29:X:1791:A:O3'	2.12	0.48
15:N:61:TRP:O	15:N:65:ILE:HG13	2.13	0.48
29:X:2323:G:C6	29:X:2332:U:H5	2.30	0.48
29:X:1323:G:O6	29:X:1324:G:C6	2.66	0.48
29:X:2055:C:H5'	29:X:2056:G:H5''	1.95	0.48
30:Y:63:A:C2	30:Y:64:C:C2	3.01	0.48
29:X:1826:G:O2'	29:X:1971:A:OP2	2.32	0.48
29:X:1309:G:H21	29:X:1611:C:H5'	1.78	0.48
29:X:1477:A:H2'	29:X:1478:G:O4'	2.13	0.48
11:J:8:THR:HG22	11:J:70:PHE:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1727:C:N3	29:X:1750:G:C6	2.81	0.48
29:X:2064:C:O2	29:X:2450:A:N6	2.46	0.48
17:P:66:GLU:HB3	17:P:67:PRO:HD3	1.95	0.48
29:X:1467:U:H1'	29:X:1468:G:C8	2.48	0.48
29:X:211:U:H2'	29:X:212:U:C6	2.47	0.48
6:E:59:GLN:NE2	29:X:1035:U:OP1	2.47	0.48
20:S:63:PRO:O	20:S:86:VAL:HG22	2.13	0.48
29:X:2346:A:H4'	29:X:2347:C:OP2	2.12	0.48
19:R:45:LYS:HA	19:R:76:LEU:O	2.14	0.48
4:C:68:ARG:NH2	29:X:2060:A:N6	2.59	0.48
29:X:545:U:H4'	29:X:546:U:OP2	2.13	0.48
29:X:2218:U:H2'	29:X:2219:U:H6	1.77	0.48
24:W:22:ALA:O	29:X:931:U:H4'	2.12	0.48
29:X:864:G:N2	29:X:913:U:C2	2.81	0.48
29:X:1753:A:H4'	29:X:2715:C:O4'	2.14	0.48
29:X:822:U:H2'	29:X:822:U:O2	2.14	0.48
29:X:672:U:C2	29:X:809:G:N2	2.81	0.48
16:O:37:ALA:HB3	16:O:51:ALA:O	2.13	0.48
17:P:25:PHE:C	17:P:25:PHE:CD2	2.87	0.48
29:X:848:G:C4	29:X:849:A:C8	3.01	0.48
29:X:2347:C:C5	29:X:2382:G:H1'	2.48	0.48
29:X:638:G:H2'	29:X:639:U:H6	1.78	0.48
29:X:2850:A:C2	29:X:2851:C:C2	3.02	0.48
14:M:55:ILE:O	14:M:103:LYS:O	2.31	0.48
12:K:14:SER:N	12:K:17:ARG:HH21	2.11	0.48
8:G:94:LYS:O	8:G:98:LYS:HB3	2.13	0.48
29:X:797:U:H2'	29:X:798:G:H8	1.77	0.48
29:X:1316:U:C2	29:X:1317:G:C8	3.01	0.48
29:X:1510:U:H2'	29:X:1511:G:C8	2.48	0.48
11:J:61:ARG:HG2	20:S:175:ARG:H	1.78	0.48
29:X:553:G:H2'	29:X:554:U:O4'	2.13	0.48
5:D:70:ALA:C	5:D:72:LYS:H	2.16	0.48
5:D:72:LYS:HG2	5:D:81:GLN:HG2	1.94	0.48
29:X:1493:A:C8	29:X:1494:A:C8	3.02	0.48
17:P:16:GLN:HG2	29:X:502:A:OP1	2.13	0.48
29:X:658:A:H2'	29:X:659:C:O4'	2.14	0.48
29:X:1850:G:H2'	29:X:1851:U:H5'	1.95	0.48
29:X:1655:A:H3'	29:X:1656:C:C6	2.49	0.48
3:B:116:VAL:HB	3:B:122:PHE:CG	2.49	0.48
25:Z:6:VAL:HG12	29:X:2015:A:N3	2.28	0.48
5:D:8:TYR:O	5:D:12:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:102:THR:HB	17:P:120:ARG:HA	1.95	0.48
29:X:2537:U:H2'	29:X:2538:C:C6	2.48	0.48
29:X:295:G:H2'	29:X:296:C:C6	2.49	0.48
6:E:105:MET:HE2	6:E:107:ILE:HD11	1.96	0.48
29:X:2219:U:C2	29:X:2220:C:H1'	2.48	0.48
20:S:3:LEU:HB3	20:S:34:LEU:HD23	1.96	0.48
29:X:1163:G:H2'	29:X:1164:A:C8	2.44	0.48
6:E:98:LEU:HD12	6:E:102:ALA:O	2.14	0.48
29:X:2874:C:H2'	29:X:2875:U:C6	2.48	0.48
15:N:82:GLY:HA3	15:N:113:SER:OG	2.13	0.48
4:C:35:LEU:HD23	4:C:35:LEU:HA	1.66	0.48
29:X:1480:G:O6	29:X:1512:C:N4	2.45	0.48
4:C:44:SER:HB2	4:C:88:PRO:HD3	1.95	0.48
29:X:2455:G:H2'	29:X:2456:C:C6	2.49	0.48
28:3:27:SER:OG	29:X:2361:C:OP1	2.21	0.48
5:D:143:TYR:HA	5:D:146:VAL:HG22	1.95	0.48
3:B:39:ALA:N	3:B:45:GLU:OE2	2.47	0.48
13:L:27:LEU:O	13:L:88:VAL:N	2.47	0.48
26:1:27:ASN:ND2	26:1:29:ARG:HB2	2.29	0.48
26:1:14:SER:HA	26:1:49:PHE:HD1	1.79	0.48
29:X:295:G:H2'	29:X:296:C:H6	1.78	0.48
12:K:37:THR:HB	12:K:40:LYS:HG3	1.94	0.48
12:K:51:LEU:CD2	12:K:66:VAL:HG22	2.43	0.48
20:S:49:THR:OG1	20:S:132:GLN:OE1	2.32	0.48
17:P:21:ARG:NH2	29:X:496:G:H4'	2.28	0.48
3:B:188:ILE:CG2	3:B:189:PRO:HD2	2.43	0.48
1:0:152:LEU:HD23	1:0:157:ILE:HG21	1.96	0.48
29:X:2071:A:H2'	29:X:2072:G:H8	1.77	0.48
6:E:154:PRO:HA	6:E:160:LYS:O	2.13	0.48
29:X:492:A:H2'	29:X:493:G:O4'	2.13	0.48
28:3:44:LYS:O	28:3:46:LYS:N	2.46	0.48
29:X:1510:U:H2'	29:X:1511:G:N9	2.29	0.48
6:E:110:SER:OG	29:X:2667:C:N3	2.38	0.48
29:X:165(B):G:H1	29:X:180:C:H42	1.60	0.48
29:X:1101:U:H2'	29:X:1102:C:C6	2.49	0.48
30:Y:3:A:H2'	30:Y:4:C:C6	2.49	0.48
10:I:55:ARG:NH1	29:X:223:A:OP1	2.33	0.48
29:X:2304:G:H1	29:X:2312:U:H3	1.61	0.48
29:X:2500:U:H5''	29:X:2501:C:OP2	2.14	0.48
13:L:64:LYS:HG3	30:Y:53:G:C5'	2.42	0.48
29:X:1606:G:H5''	29:X:1607:C:OP1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:741:G:H2'	29:X:742:C:H6	1.78	0.48
24:W:5:LEU:HB2	24:W:25:LEU:CD1	2.44	0.48
29:X:2032:G:N2	29:X:2572:A:C8	2.82	0.48
6:E:83:TYR:CE1	6:E:138:LYS:HB2	2.49	0.48
20:S:123:VAL:HG23	20:S:161:ALA:HB2	1.95	0.48
29:X:523:C:H5''	29:X:540:C:O2'	2.14	0.48
29:X:1853:A:H2'	29:X:1854:A:C8	2.49	0.48
29:X:2251:G:H5''	29:X:2252:G:OP2	2.13	0.48
3:B:44:TYR:CE1	29:X:2637:U:H5'	2.48	0.48
20:S:167:THR:OG1	29:X:875:G:H4'	2.13	0.48
29:X:2684:U:C2	29:X:2685:G:C8	3.02	0.48
29:X:640:C:H2'	29:X:641:C:H6	1.79	0.48
29:X:572:A:H5''	29:X:573:G:OP2	2.13	0.48
19:R:48:VAL:C	19:R:50:GLY:H	2.17	0.48
29:X:1838:C:H4'	29:X:1839:G:H8	1.78	0.48
2:A:158:SER:OG	29:X:1820:U:O2'	2.31	0.48
7:F:111:LYS:HB3	7:F:114:ASP:HB2	1.96	0.48
22:U:28:GLY:HA3	22:U:32:ARG:HB3	1.96	0.47
29:X:2304:G:N2	29:X:2312:U:H3	2.08	0.47
10:I:110:ALA:HB3	29:X:637:A:C5'	2.44	0.47
29:X:2658:C:H2'	29:X:2659:G:O4'	2.13	0.47
29:X:2443:C:O2'	29:X:2444:G:H5'	2.14	0.47
12:K:81:ASP:O	12:K:85:PRO:HG3	2.14	0.47
27:2:12:ARG:HH11	27:2:44:VAL:HG13	1.79	0.47
27:2:12:ARG:NH1	27:2:44:VAL:HG22	2.29	0.47
17:P:18:VAL:HG23	17:P:19:LYS:N	2.29	0.47
29:X:200:A:H3'	29:X:200:A:C8	2.50	0.47
9:H:132:GLU:OE1	14:M:72:SER:OG	2.27	0.47
29:X:2282:G:H4'	29:X:2389:G:O2'	2.13	0.47
16:O:67:LYS:HG3	16:O:68:LYS:N	2.28	0.47
29:X:193:A:C8	29:X:238:G:C5	3.02	0.47
29:X:2120:G:N2	29:X:2177:C:H42	2.12	0.47
29:X:1592:U:H2'	29:X:1593:G:H8	1.79	0.47
19:R:112:LYS:HB3	19:R:112:LYS:HE3	1.53	0.47
29:X:616:A:H2'	29:X:617:A:H8	1.76	0.47
29:X:222:G:C6	29:X:223:A:C6	3.01	0.47
9:H:83:ARG:NH2	9:H:89:ILE:HD11	2.28	0.47
20:S:43:PHE:CE2	20:S:69:VAL:HG21	2.49	0.47
29:X:2564:A:OP1	29:X:2648:G:O2'	2.16	0.47
29:X:165:A:H2'	29:X:165(A):G:H8	1.77	0.47
29:X:934:G:H2'	29:X:935:U:H6	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1882:C:H2'	29:X:1883:G:O4'	2.14	0.47
5:D:5:LYS:HD2	5:D:101:GLU:HB2	1.97	0.47
29:X:407:C:H2'	29:X:408:G:C8	2.49	0.47
24:W:3:ILE:HD11	24:W:44:VAL:CG2	2.45	0.47
29:X:2740:A:C8	29:X:2763:G:N2	2.82	0.47
23:V:7:ARG:HA	23:V:60:LEU:HD11	1.96	0.47
5:D:51:ASP:O	5:D:55:LYS:HG2	2.15	0.47
14:M:17:GLU:HG3	14:M:62:SER:HB3	1.96	0.47
9:H:111:PHE:CD1	9:H:111:PHE:N	2.82	0.47
10:I:4:HIS:CD2	10:I:4:HIS:C	2.87	0.47
19:R:99:VAL:HG11	19:R:105:ARG:CZ	2.44	0.47
29:X:2675:A:H2'	29:X:2676:C:O4'	2.14	0.47
3:B:98:GLU:OE2	3:B:175:ILE:N	2.43	0.47
11:J:35:LEU:HB3	11:J:105:PHE:HB2	1.96	0.47
22:U:10:LYS:HD3	22:U:11:LYS:N	2.28	0.47
23:V:21:ARG:HG3	23:V:46:LEU:HD23	1.96	0.47
29:X:167:A:H61	29:X:170:C:H3'	1.79	0.47
2:A:253:PRO:HD2	2:A:257:LEU:HD22	1.96	0.47
29:X:2037:G:H2'	29:X:2038:G:C8	2.49	0.47
29:X:1565:C:H42	29:X:1568:G:H1	1.61	0.47
9:H:64:VAL:HG22	9:H:106:ARG:HH21	1.79	0.47
3:B:26:VAL:HG11	3:B:198:LEU:HD11	1.96	0.47
30:Y:16:U:H2'	30:Y:110:U:O2'	2.15	0.47
25:Z:55:ARG:HH21	25:Z:58:LEU:HA	1.78	0.47
10:I:117:ALA:HB2	10:I:136:ALA:O	2.14	0.47
29:X:1952:A:C6	29:X:1953:A:N1	2.82	0.47
4:C:28:HIS:HB2	10:I:6:LEU:HD13	1.96	0.47
29:X:2870:C:N4	29:X:2871:G:O6	2.47	0.47
26:1:38:LYS:HD2	29:X:2344:U:OP1	2.15	0.47
18:Q:43:GLN:O	18:Q:47:GLY:N	2.47	0.47
29:X:2080:A:H2'	29:X:2081:U:H6	1.79	0.47
29:X:944:G:C8	29:X:944:G:H3'	2.49	0.47
29:X:2393:A:H2'	29:X:2394:C:O4'	2.14	0.47
29:X:2543:G:H2'	29:X:2544:G:C8	2.50	0.47
19:R:38:LEU:HD21	19:R:40:LEU:HD13	1.96	0.47
23:V:11:ALA:HA	23:V:14:PHE:CD2	2.49	0.47
7:F:75:SER:O	7:F:79:ARG:NH1	2.48	0.47
29:X:2712:C:O2'	29:X:2712(A):A:H5''	2.14	0.47
15:N:37:GLN:CG	29:X:1252:G:H1	2.24	0.47
29:X:1318:G:C2'	29:X:1319:G:H5'	2.44	0.47
1:0:17:SER:OG	1:0:18:ILE:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2681:C:C2	29:X:2724:U:O4	2.67	0.47
9:H:110:VAL:H	9:H:129:LEU:HB3	1.78	0.47
29:X:526:A:O2'	29:X:2043:C:O2	2.32	0.47
29:X:2801:G:H2'	29:X:2802:G:H8	1.79	0.47
29:X:200:A:H3'	29:X:200:A:H8	1.80	0.47
29:X:1824:G:H2'	29:X:1825:U:H6	1.78	0.47
29:X:1216:C:H6	29:X:1216:C:O5'	1.97	0.47
4:C:97:ARG:O	4:C:101:GLN:HG2	2.14	0.47
23:V:13:ASP:O	23:V:17:GLU:HG2	2.13	0.47
28:3:33:ASN:HB2	29:X:2420:C:OP2	2.15	0.47
11:J:12:LYS:HD3	29:X:911:A:C5	2.50	0.47
22:U:23:LYS:HD2	22:U:35:THR:HG21	1.95	0.47
29:X:1113:U:H2'	29:X:1114:G:C8	2.49	0.47
29:X:1285:G:H2'	29:X:1286:A:H5''	1.95	0.47
29:X:2114:A:H61	29:X:2119:A:H62	1.63	0.47
25:Z:3:LYS:HB2	29:X:2611:U:C2	2.49	0.47
26:1:38:LYS:O	29:X:2344:U:H3'	2.15	0.47
10:I:80:LEU:HD11	10:I:89:ASP:OD2	2.15	0.47
5:D:118:ASN:HD21	5:D:120:ASN:HB2	1.80	0.47
12:K:43:GLU:HG3	12:K:43:GLU:O	2.15	0.47
28:3:50:LEU:HA	28:3:50:LEU:HD13	1.66	0.47
27:2:31:LEU:HD23	27:2:42:LEU:HD22	1.96	0.47
29:X:2458:G:C8	29:X:2490:G:C6	3.03	0.47
2:A:16:MET:HG3	2:A:207:GLY:HA3	1.95	0.47
29:X:2549:G:C2	29:X:2550:G:N7	2.82	0.47
13:L:104:ALA:O	13:L:107:ALA:N	2.47	0.47
5:D:138:PHE:HB2	5:D:141:ILE:HB	1.97	0.47
5:D:111:ILE:HG22	5:D:114:PHE:HB2	1.96	0.47
3:B:149:ARG:NH1	29:X:2024:G:O3'	2.48	0.47
29:X:588:U:H2'	29:X:589:U:H6	1.80	0.47
20:S:141:MET:HG3	20:S:145:ASP:HB3	1.97	0.47
29:X:1656:C:H2'	29:X:1657:C:H6	1.80	0.47
29:X:1154:G:H5''	29:X:1155:A:OP2	2.14	0.47
6:E:21:ASP:HB2	6:E:23:VAL:HG23	1.95	0.47
29:X:532:A:P	29:X:561:G:H21	2.37	0.47
29:X:2560:C:C4	29:X:2561:A:N7	2.82	0.47
10:I:81:GLN:HG2	10:I:114:ILE:HD13	1.97	0.47
29:X:2816:C:C2	29:X:2831:G:N2	2.83	0.47
29:X:627:A:H4'	29:X:628:G:H5'	1.97	0.47
7:F:37:PHE:HA	7:F:40:ALA:HB3	1.97	0.47
13:L:74:ALA:O	13:L:77:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:43:THR:O	27:2:46:ASP:N	2.42	0.47
16:O:22:VAL:HG12	16:O:23:GLU:N	2.29	0.47
12:K:32:GLY:O	12:K:115:LEU:HD13	2.14	0.47
9:H:85:ASP:HB3	14:M:87:LEU:HD12	1.97	0.47
2:A:231:HIS:CD2	2:A:233:HIS:H	2.32	0.47
4:C:114:GLY:N	4:C:115:GLY:HA2	2.30	0.47
29:X:812:C:H2'	29:X:813:U:H6	1.80	0.47
29:X:2615:U:H2'	29:X:2616:C:C6	2.49	0.47
29:X:1973:G:H2'	29:X:1974:C:C6	2.50	0.47
29:X:2711:A:OP1	29:X:2712(A):A:P	2.72	0.47
29:X:947:G:H2'	29:X:948:C:C6	2.50	0.47
12:K:51:LEU:HD13	12:K:70:ILE:HD11	1.95	0.47
29:X:2544:G:H2'	29:X:2545:G:H8	1.80	0.47
15:N:12:ARG:HD3	15:N:12:ARG:HA	1.59	0.47
6:E:111:HIS:HA	6:E:112:PRO:HD2	1.63	0.47
29:X:2698:U:H2'	29:X:2699:C:C6	2.50	0.47
29:X:2119:A:O4'	29:X:2172:U:O2'	2.33	0.47
29:X:1196:C:C2	29:X:1197:G:C8	3.03	0.47
29:X:2294:C:H2'	29:X:2295:C:C6	2.47	0.47
6:E:22:GLY:HA2	6:E:24:PHE:CE1	2.50	0.47
10:I:102:LYS:O	10:I:104:ARG:N	2.47	0.47
17:P:68:VAL:HG22	17:P:124:ILE:HG21	1.96	0.47
29:X:208:C:H2'	29:X:209:C:H6	1.79	0.47
29:X:2511:U:H2'	29:X:2512:C:H6	1.79	0.47
29:X:1333:C:H6	29:X:1333:C:O5'	1.98	0.47
29:X:1999:C:H5''	29:X:2723:C:O2'	2.15	0.46
22:U:46:LEU:HB2	29:X:2230:G:H4'	1.97	0.46
17:P:12:LYS:O	17:P:16:GLN:HG3	2.15	0.46
29:X:2070:G:H2'	29:X:2071:A:C8	2.50	0.46
29:X:793:A:OP2	29:X:2071:A:O2'	2.32	0.46
20:S:15:ASP:OD2	20:S:15:ASP:N	2.47	0.46
29:X:531:C:H5''	29:X:532:A:C4	2.50	0.46
5:D:117:ILE:HG21	5:D:130:LEU:HD11	1.96	0.46
29:X:2364:C:H2'	29:X:2365:G:O4'	2.15	0.46
29:X:1136:G:H2'	29:X:1137:G:H8	1.80	0.46
13:L:32:TYR:CE2	30:Y:9:G:H5'	2.50	0.46
29:X:1782:C:H1'	29:X:2609:U:H5'	1.97	0.46
3:B:47:VAL:HG12	3:B:84:PHE:HB3	1.97	0.46
4:C:111:ARG:NH1	4:C:183:HIS:O	2.47	0.46
6:E:164:PHE:O	6:E:166:GLY:N	2.48	0.46
29:X:2683:C:H2'	29:X:2684:U:C6	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:641:C:H42	29:X:646:A:N6	2.11	0.46
13:L:63:ASN:HB3	13:L:66:ASP:HB2	1.97	0.46
30:Y:34:C:H2'	30:Y:35:C:H6	1.80	0.46
11:J:44:LYS:HD2	11:J:47:GLN:NE2	2.30	0.46
29:X:1137:G:H5''	29:X:1138:G:OP2	2.15	0.46
29:X:1342:A:O2'	29:X:1344:U:OP2	2.30	0.46
5:D:34:ILE:N	5:D:91:LEU:O	2.48	0.46
29:X:1525:G:C2	29:X:1526:G:H1'	2.50	0.46
19:R:29:HIS:CD2	19:R:51:VAL:HA	2.50	0.46
29:X:1796:U:H2'	29:X:1797:C:H6	1.78	0.46
22:U:48:LYS:NZ	29:X:2229:U:O2	2.43	0.46
29:X:643:A:O2'	29:X:644:A:OP1	2.30	0.46
30:Y:63:A:O2'	30:Y:64:C:H5'	2.14	0.46
29:X:1336:A:H2'	29:X:1337:G:C8	2.51	0.46
12:K:54:THR:HG22	12:K:66:VAL:HG23	1.97	0.46
24:W:36:ASP:OD1	24:W:41:ARG:NH1	2.49	0.46
8:G:67:ARG:HA	8:G:68:PRO:HD2	1.81	0.46
29:X:37:C:H4'	29:X:451:C:OP1	2.16	0.46
6:E:8:PRO:HD2	6:E:69:ARG:HH11	1.80	0.46
5:D:39:GLY:HA2	5:D:86:GLY:HA2	1.97	0.46
29:X:330:A:N3	29:X:330:A:H2'	2.30	0.46
29:X:2060:A:H1'	29:X:2502:G:H1'	1.97	0.46
29:X:83:G:H22	29:X:102:G:H1'	1.77	0.46
29:X:581:C:H2'	29:X:582:G:H8	1.79	0.46
2:A:33:LEU:HD13	2:A:104:TYR:HD2	1.79	0.46
30:Y:71:G:C6	30:Y:72:C:C4	3.03	0.46
11:J:111:THR:HG23	11:J:114:GLN:CG	2.45	0.46
14:M:78:GLU:OE2	14:M:108:LYS:HE2	2.15	0.46
21:T:56:ASP:HB2	21:T:58:THR:OG1	2.16	0.46
29:X:2283:C:C6	29:X:2389:G:H2'	2.50	0.46
1:O:214:MET:HA	29:X:2175:C:O2'	2.16	0.46
29:X:2396:G:C2	29:X:2421:G:C2	3.03	0.46
29:X:310:A:O2'	29:X:311:A:O5'	2.29	0.46
4:C:30:VAL:HG11	4:C:177:VAL:HG21	1.97	0.46
29:X:2686:G:C2	29:X:2724:U:O2	2.69	0.46
20:S:51:LEU:HA	20:S:64:ALA:O	2.15	0.46
14:M:67:THR:OG1	14:M:80:VAL:HG22	2.16	0.46
29:X:1413:G:H22	29:X:1587:A:H3'	1.80	0.46
29:X:5:A:H2'	29:X:6:A:H8	1.79	0.46
29:X:2242:G:H2'	29:X:2243:U:O4'	2.15	0.46
30:Y:122:U:H5''	30:Y:123:U:OP2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2210:A:N6	29:X:2211:A:N1	2.64	0.46
29:X:848:G:N3	29:X:933:A:H1'	2.31	0.46
18:Q:29:VAL:HG11	18:Q:38:ILE:HG12	1.97	0.46
29:X:1483:A:H2'	29:X:1484:U:O4'	2.16	0.46
1:O:188:LEU:O	1:O:192:LEU:HB2	2.16	0.46
2:A:201:HIS:O	2:A:204:ILE:HG13	2.15	0.46
22:U:72:LYS:HA	22:U:72:LYS:HD3	1.79	0.46
11:J:7:ARG:HE	11:J:7:ARG:HB2	1.52	0.46
29:X:2212:A:H5''	29:X:2213:U:H5	1.81	0.46
4:C:96:PRO:HB2	4:C:99:VAL:HG23	1.97	0.46
29:X:799:G:H3'	29:X:800:A:H2'	1.97	0.46
24:W:40:VAL:HA	24:W:43:MET:HE3	1.98	0.46
15:N:10:ARG:NH1	29:X:583:G:P	2.89	0.46
4:C:5:ASN:HA	4:C:119:ALA:HB3	1.98	0.46
29:X:1217:C:H2'	29:X:1218:A:C8	2.49	0.46
29:X:214:G:H22	29:X:226:G:H2'	1.80	0.46
17:P:32:ARG:NH2	17:P:119:LYS:HG2	2.31	0.46
20:S:91:PRO:HB3	20:S:127:PRO:HB3	1.96	0.46
29:X:20:C:H2'	29:X:21:A:C8	2.50	0.46
29:X:2898:G:H2'	29:X:2899:A:H8	1.80	0.46
30:Y:59:A:H2'	30:Y:59:A:N3	2.31	0.46
10:I:51:GLY:HA2	29:X:832:U:O2	2.16	0.46
29:X:852:A:C5	29:X:853:U:C5	3.04	0.46
22:U:68:ARG:NH2	29:X:400:G:N7	2.57	0.46
29:X:1956:U:H1'	29:X:2552:U:OP1	2.15	0.46
29:X:2276:G:C2	29:X:2277:G:C8	3.04	0.46
29:X:2256:G:N2	29:X:2275:C:N4	2.63	0.46
21:T:38:VAL:HG23	21:T:59:LEU:HB2	1.97	0.46
29:X:1316:U:H2'	29:X:1317:G:C8	2.50	0.46
29:X:2243:U:H2'	29:X:2244:U:H6	1.78	0.46
20:S:41:ARG:HH22	29:X:1041:C:P	2.38	0.46
29:X:669:G:N3	29:X:669:G:C2'	2.79	0.46
29:X:661:U:H2'	29:X:662:C:O4'	2.16	0.46
29:X:68:G:H2'	29:X:69:C:C6	2.51	0.46
29:X:2266:A:H4'	29:X:2267:A:C2	2.50	0.46
2:A:155:LEU:HD23	29:X:1799:G:N2	2.31	0.46
4:C:119:ALA:HB1	4:C:190:ALA:HB2	1.98	0.46
30:Y:6:C:H2'	30:Y:7:C:H6	1.79	0.46
29:X:1271:G:H5''	29:X:1272:A:OP1	2.16	0.46
29:X:389:A:C8	29:X:2413:G:H4'	2.51	0.46
29:X:2325:G:H8	29:X:2325:G:P	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:208:ALA:HB3	1:O:220:LEU:HB2	1.98	0.46
29:X:1194:A:C2	29:X:1195:G:H1'	2.50	0.46
14:M:65:SER:HA	14:M:81:PHE:O	2.15	0.46
15:N:49:ASP:HA	15:N:52:ASN:HB2	1.98	0.46
29:X:1319:G:O2'	29:X:1320:G:H5'	2.16	0.46
8:G:81:VAL:HG11	8:G:156:HIS:CD2	2.41	0.46
29:X:818:G:N7	29:X:1187:G:C6	2.84	0.46
21:T:43:THR:HB	29:X:2331:G:O3'	2.15	0.46
4:C:42:THR:HG1	29:X:39:G:H21	1.62	0.46
29:X:2821:A:H2'	29:X:2822:G:C8	2.51	0.46
29:X:691:G:C6	29:X:692:C:C4	3.04	0.46
29:X:1234:U:H2'	29:X:1235:G:O4'	2.16	0.46
17:P:50:VAL:O	17:P:54:GLU:HG3	2.15	0.46
29:X:1209:G:N2	29:X:1210:G:H22	2.14	0.46
29:X:1019:U:C4	29:X:1020:C:H5	2.34	0.46
5:D:135:GLN:HA	5:D:138:PHE:CE1	2.50	0.46
29:X:2204:A:H2	29:X:2219:U:H3	1.63	0.46
20:S:23:ALA:N	20:S:32:PHE:HE2	2.14	0.46
17:P:109:ARG:HD2	29:X:748:G:OP2	2.15	0.46
22:U:17:SER:HB3	22:U:18:VAL:HB	1.98	0.46
8:G:148:LEU:HD12	8:G:149:LYS:H	1.80	0.46
29:X:2014:A:H2'	29:X:2015:A:C8	2.51	0.46
15:N:85:ARG:HD3	15:N:116:ALA:O	2.16	0.46
26:1:27:ASN:C	26:1:29:ARG:H	2.18	0.46
29:X:69:C:H2'	29:X:70:G:C8	2.51	0.46
29:X:2247:A:H2'	29:X:2248:C:C6	2.51	0.46
29:X:1210:G:H4'	29:X:1211:A:H5''	1.96	0.45
29:X:1285:G:N2	29:X:1328:G:H5'	2.30	0.45
9:H:20:MET:HG2	9:H:21:CYS:O	2.16	0.45
29:X:562:U:O2'	29:X:572:A:H8	1.97	0.45
9:H:85:ASP:OD1	9:H:87:SER:N	2.43	0.45
29:X:733:G:C8	29:X:761:A:C6	3.04	0.45
29:X:1150:U:H2'	29:X:1151:A:H8	1.80	0.45
29:X:2330:G:N2	29:X:2386:U:O2	2.49	0.45
26:1:41:ASP:OD2	26:1:43:VAL:HG23	2.16	0.45
10:I:113:GLU:HG2	10:I:114:ILE:N	2.30	0.45
3:B:2:LYS:HA	3:B:84:PHE:CE1	2.51	0.45
29:X:862:G:H2'	29:X:863:A:O4'	2.16	0.45
29:X:2339:U:H2'	29:X:2340:G:H8	1.80	0.45
15:N:78:THR:HB	15:N:117:ARG:CZ	2.46	0.45
4:C:34:GLN:O	4:C:37:SER:OG	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2418:A:H2'	29:X:2419:U:O4'	2.16	0.45
26:1:13:GLU:C	26:1:49:PHE:HB3	2.37	0.45
24:W:22:ALA:C	24:W:24:GLY:H	2.20	0.45
9:H:13:ASN:HD21	9:H:109:ARG:HG2	1.80	0.45
2:A:83:GLU:OE1	2:A:104:TYR:OH	2.28	0.45
2:A:157:ARG:HH11	29:X:1818:U:H6	1.64	0.45
15:N:74:MET:CE	15:N:110:VAL:HG13	2.44	0.45
6:E:24:PHE:CD1	6:E:37:TYR:HB2	2.51	0.45
19:R:18:LYS:HA	19:R:36:VAL:HG11	1.98	0.45
29:X:392:C:H2'	29:X:393:G:C8	2.51	0.45
29:X:2327:A:C5	29:X:2388:A:N1	2.85	0.45
3:B:195:LEU:HB2	14:M:3:THR:HG22	1.98	0.45
25:Z:38:GLY:HA3	25:Z:48:ASN:HD22	1.80	0.45
29:X:399:U:H2'	29:X:400:G:O4'	2.16	0.45
17:P:71:VAL:HG12	17:P:126:ILE:HD12	1.97	0.45
4:C:156:ASN:HA	4:C:159:ARG:HB2	1.98	0.45
2:A:49:ILE:HG13	29:X:779:U:OP1	2.16	0.45
29:X:2307:G:C6	29:X:2308:G:H1'	2.52	0.45
19:R:58:VAL:HA	29:X:483:A:H5'	1.97	0.45
29:X:2060:A:C2	29:X:2502:G:C5	3.04	0.45
29:X:2680:C:O2'	29:X:2681:C:H5'	2.16	0.45
9:H:13:ASN:HD21	9:H:109:ARG:N	2.13	0.45
29:X:1840:G:C6	29:X:1841:U:C4	3.04	0.45
14:M:70:LYS:HD3	14:M:72:SER:HB2	1.99	0.45
29:X:1499:U:H2'	29:X:1500:A:C8	2.52	0.45
29:X:2615:U:C2	29:X:2616:C:C5	3.04	0.45
29:X:2616:C:H2'	29:X:2617:C:H6	1.81	0.45
5:D:92:ARG:HD3	30:Y:47:A:H8	1.80	0.45
9:H:43:ARG:HD3	9:H:44:TYR:CE2	2.51	0.45
22:U:29:GLY:C	22:U:31:GLY:N	2.69	0.45
29:X:1330:C:O2'	29:X:1331:C:H5'	2.16	0.45
29:X:2371:G:C2	29:X:2372:G:C5	3.04	0.45
17:P:109:ARG:CG	17:P:109:ARG:HH11	2.29	0.45
8:G:41:TRP:HB3	8:G:163:PRO:HB3	1.98	0.45
15:N:8:ILE:HD11	29:X:1215:G:O3'	2.17	0.45
29:X:926:C:O2'	29:X:928:C:N4	2.50	0.45
2:A:250:TRP:CE2	29:X:1805:A:H5''	2.51	0.45
10:I:45:LYS:HB2	10:I:45:LYS:HE3	1.54	0.45
29:X:497:A:H2'	29:X:498:G:C8	2.52	0.45
8:G:56:THR:HG21	29:X:1005:C:O2'	2.16	0.45
17:P:86:LEU:HA	17:P:86:LEU:HD23	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2347:C:H2'	29:X:2348:U:H6	1.79	0.45
29:X:309:A:N6	29:X:1210:G:O2'	2.49	0.45
29:X:1196:C:O2'	29:X:1227:G:O2'	2.32	0.45
29:X:2056:G:C2	29:X:2057:A:C8	3.04	0.45
4:C:130:THR:HG22	4:C:160:ALA:O	2.16	0.45
18:Q:48:VAL:HG11	18:Q:82:LEU:HG	1.99	0.45
29:X:2195:U:H2'	29:X:2196:C:C6	2.51	0.45
29:X:875:G:C6	29:X:876:C:C2	3.05	0.45
25:Z:7:PRO:HA	29:X:2615:U:N1	2.31	0.45
29:X:2615:U:H2'	29:X:2616:C:H6	1.82	0.45
4:C:59:TYR:CD1	4:C:64:THR:HG21	2.52	0.45
9:H:97:VAL:HG11	9:H:126:ILE:HD13	1.98	0.45
29:X:1365:A:H5'	29:X:1366:A:OP2	2.16	0.45
28:3:6:THR:HG23	28:3:62:LEU:HA	1.97	0.45
29:X:306:U:O2'	29:X:1211:A:N7	2.50	0.45
29:X:2599:G:N3	29:X:2600:A:C8	2.85	0.45
23:V:27:GLU:O	23:V:31:GLN:HG3	2.16	0.45
24:W:2:LYS:HB3	24:W:54:GLN:HB3	1.98	0.45
29:X:1370:C:H2'	29:X:1371:G:O4'	2.17	0.45
17:P:75:ALA:HB1	17:P:128:VAL:HG22	1.99	0.45
29:X:1686:C:H2'	29:X:1687:G:O4'	2.17	0.45
8:G:71:THR:HB	8:G:76:GLN:NE2	2.30	0.45
29:X:2837:A:H2'	29:X:2838:G:C8	2.52	0.45
22:U:31:GLY:HA2	22:U:32:ARG:NH1	2.32	0.45
4:C:103:GLY:O	4:C:106:MET:N	2.49	0.45
29:X:83:G:H21	29:X:84:A:N6	2.15	0.45
22:U:61:TRP:O	22:U:62:LEU:HD12	2.16	0.45
29:X:1163:G:N3	29:X:1164:A:C8	2.84	0.45
29:X:1201:A:C2	29:X:1245:G:C4	3.05	0.45
29:X:733:G:O6	29:X:761:A:C8	2.70	0.45
29:X:2532:G:C6	29:X:2533:A:C5	3.05	0.45
13:L:47:ARG:C	13:L:49:GLN:H	2.20	0.45
19:R:85:ASP:CG	19:R:108:VAL:HG21	2.37	0.45
2:A:202:LYS:HB2	29:X:1820:U:C2	2.51	0.45
13:L:31:VAL:O	13:L:32:TYR:HB2	2.17	0.45
29:X:902:C:H2'	29:X:903:C:H6	1.81	0.45
22:U:22:GLY:O	22:U:39:LYS:HG3	2.16	0.45
17:P:56:LEU:HD22	25:Z:28:PRO:HD2	1.99	0.45
11:J:36:ILE:HD12	20:S:76:ARG:HD2	1.99	0.45
29:X:2727:G:H2'	29:X:2728:U:H6	1.81	0.45
29:X:2094:G:N2	29:X:2196:C:O2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:73:GLU:OE2	10:I:104:ARG:HB2	2.16	0.45
29:X:2339:U:H2'	29:X:2340:G:C8	2.52	0.45
29:X:2901:C:H2'	29:X:2902:A:C8	2.51	0.45
29:X:814:C:H2'	29:X:815:C:H6	1.82	0.45
30:Y:48:A:H2'	30:Y:49:C:C6	2.52	0.45
29:X:2516:G:C2'	29:X:2517:C:H5'	2.47	0.45
24:W:11:GLY:HA2	29:X:969:G:O3'	2.16	0.45
29:X:91:A:H4'	29:X:92:G:O5'	2.16	0.45
5:D:74:ILE:HA	5:D:79:LEU:CB	2.47	0.45
20:S:3:LEU:HD23	20:S:32:PHE:HB2	1.99	0.45
29:X:1608:A:H1'	29:X:1610:A:OP2	2.17	0.45
29:X:1124:C:C2	29:X:1125:G:C8	3.05	0.45
29:X:2721:A:H2'	29:X:2722:G:O4'	2.17	0.45
29:X:27:G:HO2'	29:X:28:A:P	2.36	0.45
29:X:1849:G:H2'	29:X:1850:G:C8	2.52	0.45
29:X:440:G:C2	29:X:441:U:C2	3.04	0.45
16:O:85:GLY:HA3	29:X:1224:G:O3'	2.16	0.45
27:2:16:HIS:HB2	27:2:44:VAL:HG21	1.99	0.45
29:X:1922:G:H8	29:X:1922:G:OP2	2.00	0.45
24:W:32:ARG:HG2	24:W:33:GLU:N	2.32	0.45
29:X:2004:G:C6	29:X:2005:A:C4	3.05	0.45
29:X:878:A:H1'	29:X:899:A:N7	2.31	0.45
29:X:2291:U:H2'	29:X:2292:C:C6	2.51	0.45
22:U:54:ASN:C	22:U:56:GLN:H	2.14	0.45
16:O:87:ARG:NH2	29:X:1222:C:OP1	2.50	0.45
29:X:729:G:H2'	29:X:1775:U:O2	2.17	0.45
7:F:11:GLN:HB3	29:X:1061:U:C5	2.52	0.45
29:X:2404:C:C2	29:X:2405:G:C8	3.04	0.45
10:I:114:ILE:HD13	10:I:114:ILE:HA	1.81	0.45
13:L:101:LYS:O	13:L:104:ALA:HB3	2.17	0.45
30:Y:54:U:H4'	30:Y:54:U:OP1	2.17	0.45
20:S:111:GLY:HA3	20:S:172:LEU:O	2.17	0.45
11:J:27:TYR:HB2	11:J:137:VAL:HB	1.99	0.45
29:X:2307:G:C8	29:X:2308:G:C8	3.05	0.44
2:A:148:VAL:HB	2:A:151:LYS:HE2	1.99	0.44
20:S:3:LEU:HG	20:S:32:PHE:HD1	1.80	0.44
3:B:176:ARG:HH21	14:M:16:ILE:HA	1.82	0.44
18:Q:4:TYR:CE2	23:V:23:LYS:HB2	2.52	0.44
29:X:2101:G:N2	29:X:2189:U:O2	2.50	0.44
29:X:1069:A:H4'	29:X:1070:A:H8	1.82	0.44
19:R:61:SER:HA	19:R:65:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:21:ARG:HG2	10:I:21:ARG:NH1	2.31	0.44
23:V:31:GLN:O	23:V:35:GLY:N	2.51	0.44
9:H:85:ASP:OD1	9:H:87:SER:HB3	2.17	0.44
4:C:120:VAL:N	4:C:190:ALA:HB2	2.33	0.44
29:X:382:G:N2	29:X:393:G:C4	2.86	0.44
17:P:40:LEU:HB3	25:Z:25:LEU:HD13	1.98	0.44
3:B:33:ILE:HA	3:B:33:ILE:HD13	1.73	0.44
12:K:65:LEU:O	12:K:68:GLN:HG3	2.17	0.44
29:X:1950:G:C8	29:X:1951:U:C5	3.05	0.44
28:3:35:GLY:N	28:3:36:LYS:HA	2.33	0.44
29:X:2347:C:H5	29:X:2382:G:H1'	1.83	0.44
4:C:67:ALA:HA	29:X:1255:U:C6	2.51	0.44
12:K:28:LEU:C	12:K:28:LEU:HD23	2.37	0.44
26:1:46:HIS:CE1	29:X:2372:G:HO2'	2.35	0.44
29:X:1435:C:H42	29:X:1557:G:H1	1.63	0.44
29:X:440:G:H2'	29:X:441:U:C6	2.52	0.44
29:X:2521:C:H2'	29:X:2522:U:O4'	2.16	0.44
29:X:981:A:H5''	29:X:982:C:OP2	2.17	0.44
4:C:168:SER:HB2	4:C:183:HIS:NE2	2.32	0.44
11:J:27:TYR:CB	11:J:137:VAL:HB	2.47	0.44
1:0:74:THR:O	1:0:92:SER:HA	2.17	0.44
29:X:219:G:H4'	29:X:386:G:C5	2.52	0.44
29:X:2696:U:H2'	29:X:2697:G:C8	2.53	0.44
29:X:538:G:C2	29:X:539:G:C8	3.06	0.44
28:3:17:THR:HG23	28:3:18:GLY:N	2.31	0.44
30:Y:33:C:H42	30:Y:53:G:H1	1.64	0.44
2:A:30:GLU:O	2:A:34:THR:HG23	2.18	0.44
18:Q:54:SER:HB2	29:X:1341:A:O3'	2.17	0.44
29:X:651(B):C:H5''	29:X:653:U:O5'	2.17	0.44
27:2:16:HIS:CB	27:2:44:VAL:HG21	2.48	0.44
9:H:132:GLU:HB2	14:M:73:PHE:CE1	2.51	0.44
29:X:1729:C:H1'	29:X:2860:A:H1'	1.98	0.44
29:X:1136:G:H2'	29:X:1137:G:C8	2.52	0.44
1:0:1:LYS:HB2	29:X:2131:G:C8	2.53	0.44
29:X:1763:G:O2'	29:X:1958:C:OP1	2.31	0.44
29:X:996:A:N3	29:X:997:G:C8	2.86	0.44
29:X:1324:G:O2'	29:X:1326:U:OP2	2.28	0.44
2:A:108:PRO:HA	2:A:196:VAL:O	2.18	0.44
11:J:36:ILE:HG22	11:J:37:ALA:O	2.18	0.44
29:X:624:C:O2'	29:X:657:U:H5''	2.17	0.44
16:O:78:VAL:O	16:O:79:GLN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:50:ASP:HA	16:O:53:LYS:HE3	1.99	0.44
18:Q:3:HIS:NE2	18:Q:44:GLN:HG3	2.32	0.44
30:Y:3:A:C6	30:Y:4:C:N4	2.86	0.44
29:X:1593:G:H2'	29:X:1594:A:C8	2.52	0.44
8:G:68:PRO:HA	15:N:67:ALA:HB3	1.99	0.44
29:X:2247:A:H2'	29:X:2248:C:H6	1.82	0.44
29:X:1901:A:H2'	29:X:1902:C:H6	1.82	0.44
29:X:600:C:O2	29:X:604:C:H4'	2.16	0.44
29:X:1118:A:H2'	29:X:1119:U:O4'	2.17	0.44
13:L:60:LYS:O	13:L:61:SER:OG	2.23	0.44
29:X:1598:C:H2'	29:X:1599:C:H6	1.82	0.44
5:D:79:LEU:HD21	29:X:2310:A:N3	2.32	0.44
3:B:60:ASN:HB3	3:B:62:PRO:CD	2.45	0.44
29:X:1664:A:H61	29:X:1996:C:H42	1.66	0.44
29:X:2018:G:C6	29:X:2019:A:C6	3.05	0.44
5:D:80:ARG:HD3	5:D:83:MET:HB3	1.99	0.44
14:M:69:ARG:HD2	14:M:78:GLU:OE2	2.17	0.44
3:B:144:ARG:NH1	29:X:2572:A:O2'	2.50	0.44
8:G:115:ALA:O	8:G:119:LEU:HB2	2.18	0.44
2:A:43:ARG:HA	2:A:48:ARG:O	2.17	0.44
29:X:2498:C:O2'	29:X:2499:C:H5'	2.17	0.44
7:F:79:ARG:HB3	7:F:84:ILE:O	2.17	0.44
25:Z:7:PRO:HA	29:X:2615:U:C2	2.53	0.44
29:X:620:G:H4'	29:X:621:A:H5''	1.99	0.44
29:X:189:G:H2'	29:X:190:A:O4'	2.17	0.44
8:G:65:LYS:O	8:G:66:HIS:HB3	2.18	0.44
27:2:26:SER:O	27:2:30:ILE:HG13	2.18	0.44
29:X:2720:U:C2	29:X:2721:A:C8	3.06	0.44
25:Z:3:LYS:HA	29:X:2577:A:O2'	2.18	0.44
29:X:1993:U:C2	29:X:1994:C:C6	3.06	0.44
21:T:21:LEU:HD21	21:T:41:ARG:HH21	1.83	0.44
29:X:72:A:N1	29:X:111:A:O2'	2.46	0.44
17:P:118:LYS:HD2	17:P:120:ARG:NH2	2.32	0.44
29:X:1592:U:H2'	29:X:1593:G:C8	2.53	0.44
4:C:112:GLN:C	4:C:114:GLY:H	2.21	0.44
22:U:22:GLY:H	22:U:39:LYS:HB2	1.81	0.44
18:Q:88:ILE:HG13	18:Q:88:ILE:O	2.18	0.44
23:V:25:LEU:HD23	23:V:25:LEU:HA	1.72	0.44
29:X:1533:C:H2'	29:X:1534:C:O4'	2.18	0.44
20:S:152:ILE:HG22	20:S:154:LEU:HD23	1.99	0.44
15:N:24:PHE:HB2	15:N:29:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:31:VAL:O	17:P:122:SER:N	2.48	0.44
3:B:180:ASN:O	3:B:181:LEU:HD23	2.17	0.44
8:G:106:TYR:CD2	29:X:2642:G:H5'	2.53	0.44
21:T:6:GLY:HA3	21:T:7:VAL:HA	1.66	0.44
7:F:91:PRO:HA	7:F:135:GLY:HA2	2.00	0.44
1:O:39:VAL:HG11	1:O:185:TYR:CD2	2.52	0.44
29:X:2302:C:H42	29:X:2314:G:H1	1.64	0.44
22:U:48:LYS:CG	22:U:49:LYS:H	2.19	0.44
3:B:120:TRP:O	3:B:121:ASN:HB2	2.17	0.44
30:Y:65:A:H2'	30:Y:66:G:H8	1.82	0.44
15:N:11:ARG:O	15:N:15:LYS:HG3	2.18	0.44
11:J:70:PHE:CE2	29:X:871:C:H4'	2.53	0.44
5:D:72:LYS:HA	5:D:81:GLN:HA	1.99	0.44
10:I:73:GLU:HG3	10:I:105:PRO:O	2.17	0.44
29:X:2511:U:H2'	29:X:2512:C:C6	2.53	0.44
29:X:2004:G:C4	29:X:2005:A:C8	3.06	0.44
21:T:14:ARG:HE	21:T:14:ARG:HB2	1.48	0.44
3:B:19:ARG:HA	9:H:84:ALA:O	2.16	0.44
3:B:140:SER:HB2	29:X:2578:G:N7	2.33	0.44
11:J:71:PRO:HA	11:J:96:SER:HB2	2.00	0.44
3:B:31:CYS:HA	3:B:32:PRO:HD3	1.89	0.44
6:E:133:VAL:HG12	6:E:141:VAL:HG13	2.00	0.44
22:U:31:GLY:HA2	22:U:32:ARG:HH11	1.82	0.44
29:X:1327:C:H2'	29:X:1328:G:C8	2.53	0.44
29:X:2372:G:C2	29:X:2373:A:N7	2.86	0.44
29:X:448:U:O4	29:X:583:G:H1'	2.17	0.44
29:X:2650:U:O2'	29:X:2651:C:H5'	2.18	0.44
1:O:60:LEU:HA	1:O:61:PRO:HD3	1.87	0.44
29:X:2774:C:H2'	29:X:2775:A:O4'	2.18	0.44
1:O:66:ARG:HH11	1:O:156:ARG:HG3	1.83	0.44
20:S:67:LYS:HE3	20:S:92:VAL:HG21	1.99	0.44
11:J:14:PHE:O	11:J:15:ARG:HG2	2.18	0.43
3:B:175:ILE:HG12	3:B:182:ILE:HG12	1.99	0.43
29:X:1242:A:C4	29:X:1243:C:C5	3.06	0.43
22:U:46:LEU:O	29:X:397:A:H5'	2.18	0.43
29:X:1054:A:H2'	29:X:1055:G:H8	1.83	0.43
29:X:1995:U:H3'	29:X:1996:C:H2'	2.00	0.43
11:J:52:ARG:HH12	11:J:53:ILE:HG12	1.81	0.43
29:X:165(B):G:H2'	29:X:165(C):G:O4'	2.18	0.43
29:X:1091:G:N2	29:X:1101:U:H1'	2.32	0.43
29:X:1782:C:H2'	29:X:2608:G:O2'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:172:LEU:HD22	20:S:173:PRO:HD2	2.00	0.43
7:F:112:MET:HG3	7:F:113:PRO:HD3	1.99	0.43
29:X:784:A:N7	29:X:792:G:C4	2.86	0.43
20:S:104:SER:HA	20:S:139:THR:HA	2.00	0.43
2:A:218:LYS:HE3	2:A:218:LYS:HB3	1.86	0.43
29:X:2476:A:H5'	29:X:2476:A:H8	1.83	0.43
22:U:27:ASP:HA	22:U:32:ARG:NH2	2.21	0.43
25:Z:28:PRO:HB2	25:Z:30:LEU:HG	1.99	0.43
29:X:2320:A:H5''	29:X:2321:G:C4	2.53	0.43
26:1:40:TYR:HA	26:1:46:HIS:HA	2.00	0.43
29:X:733:G:N7	29:X:761:A:C5	2.86	0.43
29:X:1422:G:H2'	29:X:1423:A:H8	1.83	0.43
4:C:152:THR:HG23	4:C:189:ASP:OD2	2.17	0.43
4:C:176:ASN:HD21	4:C:179:ASP:HB2	1.84	0.43
30:Y:7:C:H2'	30:Y:8:C:H6	1.84	0.43
22:U:70:LEU:HB3	22:U:79:GLU:OE2	2.18	0.43
29:X:1510:U:O2'	29:X:1511:G:OP1	2.32	0.43
29:X:2536:G:H2'	29:X:2537:U:O4'	2.17	0.43
7:F:90:THR:OG1	7:F:93:LYS:HB2	2.18	0.43
29:X:13:A:N3	29:X:15:G:O6	2.50	0.43
7:F:19:PRO:HB2	7:F:20:ALA:H	1.66	0.43
11:J:76:THR:HA	11:J:92:GLU:H	1.84	0.43
30:Y:39:C:H5''	30:Y:40:C:C5	2.53	0.43
29:X:2508:G:C4	29:X:2509:G:C8	3.06	0.43
29:X:2075:U:H3'	29:X:2238:G:H21	1.83	0.43
29:X:2881:U:H2'	29:X:2882:C:C6	2.53	0.43
1:0:4:ARG:HG2	1:0:5:ALA:H	1.83	0.43
29:X:1036:G:C2	29:X:1120:G:C4	3.06	0.43
20:S:112:LEU:HG	20:S:113:VAL:N	2.32	0.43
29:X:787:U:C5	29:X:791:C:N3	2.87	0.43
19:R:100:ASP:HB2	19:R:103:LYS:CG	2.48	0.43
12:K:24:GLN:HB3	12:K:44:LEU:CD2	2.45	0.43
13:L:8:ARG:HB2	13:L:8:ARG:NH1	2.31	0.43
6:E:19:ALA:HB1	6:E:24:PHE:HD2	1.83	0.43
2:A:40:THR:C	2:A:42:GLY:H	2.21	0.43
1:0:64:THR:HG22	1:0:65:GLY:H	1.83	0.43
25:Z:43:HIS:N	29:X:2884:U:O4	2.48	0.43
19:R:38:LEU:HB3	19:R:47:VAL:CG2	2.48	0.43
23:V:11:ALA:HA	23:V:14:PHE:HD2	1.83	0.43
30:Y:39:C:H5'	30:Y:40:C:OP2	2.18	0.43
3:B:72:VAL:O	3:B:73:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:51:SER:OG	29:X:1814:G:H4'	2.17	0.43
16:O:73:LYS:HB2	16:O:82:ARG:HB2	1.99	0.43
1:O:33:PHE:HB3	1:O:34:ASP:H	1.58	0.43
28:3:29:LYS:HE2	29:X:2418:A:P	2.59	0.43
29:X:2212:A:C5'	29:X:2213:U:H5	2.31	0.43
13:L:33:ARG:CZ	13:L:33:ARG:HB2	2.48	0.43
9:H:3:MET:O	9:H:6:SER:HB2	2.19	0.43
29:X:1164:A:C2	29:X:1165:U:C2	3.06	0.43
29:X:1676:A:N6	29:X:1677:A:C6	2.86	0.43
29:X:2691:C:H2'	29:X:2692:C:H6	1.83	0.43
9:H:5:GLN:HG2	29:X:1668:A:H5''	1.99	0.43
15:N:11:ARG:HH22	29:X:29:U:C4'	2.31	0.43
29:X:1644:C:H2'	29:X:1644:C:O2	2.18	0.43
30:Y:83:C:N4	30:Y:98:C:N3	2.67	0.43
29:X:2392:A:C8	29:X:2429:G:C2	3.06	0.43
29:X:655:A:H4'	29:X:656:G:H5'	2.00	0.43
16:O:28:GLU:O	16:O:31:ASP:HB2	2.18	0.43
9:H:116:ARG:HG3	9:H:116:ARG:O	2.18	0.43
25:Z:30:LEU:HD23	25:Z:30:LEU:HA	1.82	0.43
25:Z:10:LYS:HG3	29:X:1263:U:H1'	2.00	0.43
5:D:111:ILE:CG2	5:D:114:PHE:HB2	2.47	0.43
29:X:2691:C:H5''	29:X:2872:G:C5'	2.48	0.43
29:X:1909:C:H6	29:X:1909:C:O5'	2.02	0.43
29:X:1094:U:O2'	29:X:1096:A:N7	2.46	0.43
29:X:1641:A:N6	29:X:1642:G:C2	2.86	0.43
20:S:50:GLY:O	20:S:51:LEU:HB3	2.18	0.43
11:J:46:ASN:HA	11:J:49:GLU:HB2	2.00	0.43
25:Z:18:MET:HE2	25:Z:18:MET:HB3	1.90	0.43
29:X:24:G:N2	29:X:25:U:H1'	2.33	0.43
29:X:1061:U:H3'	29:X:1062:G:H5''	2.00	0.43
29:X:980:A:H62	29:X:981:A:N6	2.15	0.43
29:X:1511:G:C6	29:X:1512:C:C4	3.06	0.43
29:X:2856:A:H2'	29:X:2857:G:O4'	2.19	0.43
29:X:1078:C:N3	29:X:1088:A:H5'	2.34	0.43
29:X:516:C:C2'	29:X:517:C:H5'	2.47	0.43
15:N:97:ASP:O	15:N:101:ARG:HB2	2.19	0.43
28:3:29:LYS:HZ3	28:3:41:ILE:HG12	1.82	0.43
29:X:2689:U:P	29:X:2719:G:H22	2.41	0.43
29:X:2311:A:H5''	29:X:2312:U:OP2	2.19	0.43
29:X:920:G:H2'	29:X:921:G:O4'	2.19	0.43
29:X:2462:U:H2'	29:X:2463:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:643:A:C2	29:X:644:A:C4	3.07	0.43
29:X:2721:A:H1'	29:X:2873:A:O2'	2.19	0.43
6:E:99:THR:O	6:E:101:LYS:N	2.51	0.43
29:X:858:U:O2	29:X:2268:A:H2'	2.19	0.43
25:Z:3:LYS:HE3	25:Z:3:LYS:HB3	1.71	0.43
29:X:747:U:O2	29:X:2014:A:H1'	2.18	0.43
15:N:28:ARG:HH11	15:N:28:ARG:HG2	1.82	0.43
5:D:92:ARG:NH1	30:Y:46:G:H3'	2.34	0.43
2:A:229:VAL:HG11	29:X:784:A:C4	2.53	0.43
29:X:1835:G:H1'	29:X:1931:U:C2	2.53	0.43
4:C:145:THR:O	4:C:146:GLU:HG3	2.18	0.43
19:R:53:VAL:HG12	19:R:54:ILE:H	1.84	0.43
17:P:9:ARG:NH2	29:X:307:G:OP1	2.48	0.43
15:N:58:ARG:HA	15:N:61:TRP:CE3	2.54	0.43
29:X:2290:G:N2	29:X:2373:A:O2'	2.47	0.43
4:C:78:VAL:HG13	29:X:448:U:H1'	2.00	0.43
10:I:133:VAL:HG11	10:I:140:VAL:CG2	2.48	0.43
2:A:157:ARG:HH12	29:X:1817:G:H3'	1.84	0.43
29:X:2330:G:N2	29:X:2386:U:C2	2.87	0.43
2:A:99:ASP:OD2	29:X:1491:A:H5'	2.19	0.43
10:I:81:GLN:NE2	10:I:113:GLU:OE2	2.51	0.43
29:X:2543:G:C6	29:X:2544:G:C6	3.06	0.43
8:G:133:GLY:HA3	29:X:1137:G:O2'	2.19	0.43
29:X:902:C:H2'	29:X:903:C:C6	2.54	0.43
11:J:6:LYS:O	11:J:71:PRO:HG2	2.19	0.43
29:X:1619:G:H2'	29:X:1620:G:H8	1.84	0.43
11:J:39:GLU:HA	11:J:40:PRO:HD3	1.62	0.43
29:X:1179:G:N1	29:X:1180:U:C4	2.87	0.43
2:A:85:ASP:HA	2:A:86:PRO:HD3	1.79	0.43
9:H:100:ASN:C	9:H:100:ASN:OD1	2.57	0.43
13:L:67:THR:O	13:L:71:VAL:HG12	2.19	0.43
29:X:2521:C:C4	29:X:2522:U:C4	3.07	0.43
4:C:130:THR:HG21	29:X:320:U:H2'	2.00	0.43
29:X:2327:A:H3'	29:X:2328:A:C8	2.53	0.43
29:X:2716:A:C2'	29:X:2717:G:H5'	2.49	0.43
29:X:2717:G:C6	29:X:2718:G:C5	3.07	0.43
29:X:1864:U:H2'	29:X:1874:G:C8	2.54	0.43
17:P:21:ARG:HH22	29:X:496:G:H4'	1.84	0.43
15:N:24:PHE:O	15:N:29:SER:HB3	2.18	0.43
19:R:35:LYS:HB3	19:R:35:LYS:HE3	1.76	0.43
18:Q:34:THR:HB	18:Q:37:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1175:G:H2'	29:X:1176:C:C6	2.54	0.43
29:X:1745:G:O2'	29:X:1746:C:H5'	2.19	0.43
29:X:222:G:H2'	29:X:223:A:C8	2.54	0.43
29:X:335:C:H2'	29:X:336:C:C6	2.52	0.43
2:A:259:THR:OG1	29:X:1798:U:H5'	2.19	0.43
16:O:78:VAL:CG1	16:O:80:TYR:HB2	2.49	0.43
15:N:32:TYR:O	15:N:35:ALA:HB3	2.18	0.43
29:X:1151:A:H2'	29:X:1152:C:C6	2.54	0.43
29:X:1842:G:H2'	29:X:1843:C:C6	2.53	0.43
6:E:139:GLN:HB3	6:E:143:GLN:OE1	2.19	0.43
29:X:2376:A:H2'	29:X:2377:A:O4'	2.19	0.43
29:X:1885:A:H3'	29:X:1886:A:H8	1.84	0.43
21:T:55:ARG:HG2	21:T:55:ARG:H	1.68	0.43
15:N:60:LEU:HA	15:N:63:GLN:HG3	2.01	0.43
29:X:2474:C:H5'	29:X:2475:C:OP2	2.19	0.43
17:P:8:PHE:HE1	17:P:17:GLN:HB2	1.83	0.43
29:X:2655:G:O2'	29:X:2664:G:O6	2.26	0.43
1:O:109:VAL:O	1:O:134:PRO:HD3	2.18	0.43
14:M:19:ASP:O	14:M:20:HIS:ND1	2.52	0.43
29:X:591:G:C6	29:X:592(A):C:N4	2.86	0.43
8:G:90:LEU:HA	8:G:90:LEU:HD12	1.86	0.43
29:X:2349:G:O6	29:X:2382:G:N2	2.35	0.42
29:X:1637:A:H4'	29:X:2711:A:O2'	2.18	0.42
29:X:844:U:H5'	29:X:845:G:OP2	2.19	0.42
23:V:63:LYS:HG2	23:V:66:GLN:NE2	2.34	0.42
29:X:638:G:N2	29:X:650:C:H1'	2.34	0.42
29:X:638:G:N1	29:X:649:G:N1	2.67	0.42
29:X:1795:C:H2'	29:X:1796:U:O4'	2.18	0.42
9:H:83:ARG:HH21	9:H:89:ILE:HD11	1.83	0.42
14:M:104:LEU:CD2	14:M:106:TYR:HE2	2.32	0.42
1:O:72:VAL:HG13	1:O:110:VAL:HB	2.00	0.42
11:J:69:ILE:HG21	11:J:104:MET:HG2	2.00	0.42
6:E:25:LYS:HE2	6:E:25:LYS:HB3	1.81	0.42
29:X:1014:A:H2'	29:X:1015:U:H6	1.84	0.42
29:X:2507:C:C4	29:X:2583:G:C6	3.07	0.42
16:O:16:GLU:HG2	16:O:96:LEU:HD23	2.01	0.42
16:O:72:ARG:HA	16:O:82:ARG:O	2.19	0.42
29:X:2732:G:H3'	29:X:2733:A:O4'	2.19	0.42
29:X:684:G:C2	29:X:794:A:C2	3.07	0.42
29:X:1312:U:H4'	29:X:1313:U:O5'	2.19	0.42
29:X:2306:U:H5'	29:X:2307:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:155:THR:HG21	29:X:2314:G:H1'	2.01	0.42
2:A:161:THR:O	2:A:196:VAL:HG23	2.20	0.42
19:R:77:HIS:HD2	29:X:328:U:C5'	2.29	0.42
20:S:66:VAL:HG22	20:S:83:PHE:CE1	2.53	0.42
29:X:1885:A:H3'	29:X:1886:A:C8	2.54	0.42
29:X:347:C:H2'	29:X:348:G:H5'	2.01	0.42
29:X:875:G:H2'	29:X:876:C:O4'	2.19	0.42
3:B:123:ALA:HB3	29:X:2511:U:O3'	2.18	0.42
29:X:1365:A:H2'	29:X:1365:A:N3	2.34	0.42
29:X:2747:G:O6	29:X:2755:C:H5''	2.19	0.42
8:G:100:TYR:OH	8:G:126:VAL:HG13	2.19	0.42
29:X:704:G:H1'	29:X:726:G:N2	2.34	0.42
4:C:74:VAL:O	4:C:77:PHE:HB2	2.19	0.42
10:I:142:LEU:HA	10:I:143:PRO:HD3	1.91	0.42
17:P:134:LYS:HB2	29:X:2797:A:N6	2.35	0.42
20:S:1:MET:HE1	20:S:52:PHE:HB3	2.01	0.42
10:I:31:GLY:HA2	29:X:1190:G:H5''	2.01	0.42
29:X:2711:A:N6	29:X:2714:G:C5	2.88	0.42
10:I:97:ARG:HB2	10:I:97:ARG:HE	1.53	0.42
11:J:17:ARG:HB3	11:J:42:TRP:HZ2	1.84	0.42
3:B:134:TRP:HE1	3:B:139:GLY:H	1.67	0.42
3:B:174:GLU:HB3	3:B:183:LEU:HB2	2.02	0.42
3:B:5:LEU:HD22	3:B:195:LEU:HD11	2.01	0.42
21:T:37:LEU:HD11	21:T:61:ALA:N	2.34	0.42
29:X:2825:C:H5''	29:X:2826:A:OP2	2.19	0.42
11:J:61:ARG:HA	11:J:62:GLY:HA2	1.66	0.42
17:P:25:PHE:HD1	17:P:127:ILE:HD11	1.84	0.42
29:X:925:A:H2'	29:X:926:C:O4'	2.19	0.42
29:X:816:C:N3	29:X:1192:G:C2	2.87	0.42
29:X:2472:G:H2'	29:X:2475:C:H42	1.84	0.42
29:X:1821:A:O5'	29:X:1821:A:H8	2.03	0.42
20:S:143:ILE:HA	20:S:171:VAL:HG12	2.01	0.42
28:3:29:LYS:HZ1	28:3:41:ILE:HG23	1.83	0.42
24:W:22:ALA:C	24:W:24:GLY:N	2.73	0.42
13:L:15:ARG:HE	13:L:91:ARG:HH11	1.66	0.42
29:X:820:A:H1'	29:X:943:U:O2'	2.19	0.42
10:I:65:PHE:CE1	29:X:2404:C:H1'	2.54	0.42
29:X:170:C:O2'	29:X:171:A:H5'	2.20	0.42
29:X:231:C:O2	29:X:621:A:O2'	2.34	0.42
11:J:76:THR:HG22	11:J:91:VAL:HA	2.00	0.42
14:M:15:GLY:O	14:M:18:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1097:U:H2'	29:X:1098:A:O4'	2.18	0.42
1:0:95:LEU:HD13	1:0:98:ARG:HB2	2.00	0.42
29:X:2513:G:C2	29:X:2514:U:C2	3.07	0.42
8:G:52:GLY:O	8:G:55:ALA:HB3	2.19	0.42
4:C:116:LYS:HB3	4:C:185:ARG:HD3	2.02	0.42
29:X:1504:G:H2'	29:X:1505:U:O4'	2.19	0.42
4:C:48:ARG:HB3	4:C:48:ARG:HE	1.43	0.42
29:X:2697:G:C2	29:X:2711:A:C2	3.06	0.42
11:J:13:GLN:HB3	11:J:14:PHE:CD2	2.54	0.42
29:X:2332:U:H4'	29:X:2336:A:H62	1.85	0.42
29:X:2501:C:H5'	29:X:2502:G:OP1	2.18	0.42
10:I:116:ARG:HG2	10:I:117:ALA:N	2.35	0.42
26:1:34:LYS:HE3	26:1:51:ALA:O	2.19	0.42
16:O:64:GLY:HA3	16:O:90:PHE:CZ	2.55	0.42
29:X:740:U:C2	29:X:741:G:C8	3.08	0.42
29:X:980:A:N6	29:X:981:A:N6	2.67	0.42
29:X:2280:G:C2'	29:X:2281:C:H5'	2.50	0.42
10:I:12:SER:O	29:X:660:G:N2	2.52	0.42
5:D:64:LYS:HA	5:D:65:PRO:HD3	1.78	0.42
21:T:36:ILE:HD11	29:X:2364:C:O2	2.19	0.42
29:X:1745:G:C6	29:X:1746:C:N4	2.88	0.42
18:Q:68:PHE:CD1	29:X:65:C:H1'	2.55	0.42
9:H:134:LEU:HA	14:M:48:GLN:HE22	1.84	0.42
5:D:126:GLY:O	5:D:160:ALA:HB3	2.20	0.42
30:Y:78:A:H2'	30:Y:79:U:O4'	2.19	0.42
29:X:2836:G:C6	29:X:2837:A:N6	2.87	0.42
8:G:33:ILE:CD1	29:X:537:U:H4'	2.49	0.42
28:3:17:THR:CG2	28:3:21:LYS:H	2.29	0.42
19:R:15:HIS:CD2	19:R:16:PHE:HD2	2.37	0.42
17:P:36:ARG:NH1	29:X:1266:G:C8	2.87	0.42
9:H:13:ASN:ND2	9:H:108:THR:HB	2.35	0.42
29:X:1675:C:H2'	29:X:1676:A:O4'	2.20	0.42
29:X:14:A:C5	29:X:526:A:N1	2.87	0.42
29:X:1309:G:N2	29:X:1611:C:H5'	2.34	0.42
1:0:43:LEU:H	1:0:167:VAL:HG12	1.84	0.42
29:X:1235:G:C6	29:X:1236:G:N1	2.87	0.42
2:A:86:PRO:HG3	29:X:1567:A:H2'	2.02	0.42
6:E:45:GLN:HG3	6:E:49:GLN:O	2.19	0.42
28:3:39:ASP:HB3	28:3:42:ARG:NH2	2.33	0.42
12:K:100:VAL:HG12	12:K:101:GLY:N	2.33	0.42
18:Q:73:ASN:HA	29:X:58:G:OP1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:19:THR:HB	30:Y:93:G:O5'	2.20	0.42
29:X:1652:A:H3'	29:X:1653:G:C8	2.55	0.42
29:X:537:U:H2'	29:X:538:G:C8	2.55	0.42
29:X:2599:G:C4	29:X:2600:A:C8	3.08	0.42
11:J:15:ARG:HB3	11:J:16:GLY:H	1.51	0.42
15:N:33:ARG:HD3	29:X:1252:G:O4'	2.20	0.42
29:X:2263:C:H2'	29:X:2264:C:H6	1.85	0.42
25:Z:51:TYR:CD2	25:Z:54:GLY:O	2.73	0.42
29:X:1665:A:C2'	29:X:1666:G:H5'	2.50	0.42
1:O:132:LEU:HD11	29:X:2169:A:O2'	2.20	0.42
29:X:1223:G:C6	29:X:1227:G:C6	3.07	0.42
8:G:42:VAL:HG22	8:G:164:GLN:HB2	2.02	0.42
29:X:1587:A:H5'	29:X:1587:A:H8	1.85	0.42
27:2:6:GLN:HA	27:2:7:PRO:HD2	1.85	0.42
3:B:144:ARG:NH1	29:X:2572:A:N3	2.68	0.42
29:X:2884:U:C5	29:X:2885:C:C2	3.08	0.42
29:X:1111:A:O2'	29:X:1112:G:H4'	2.19	0.42
29:X:848:G:N2	29:X:932:U:H1'	2.34	0.42
22:U:22:GLY:HA3	22:U:39:LYS:CE	2.50	0.42
29:X:1142:A:O2'	29:X:1143:A:H5''	2.20	0.42
29:X:637:A:H4'	29:X:638:G:O5'	2.19	0.42
29:X:907:U:HO2'	29:X:908:G:C5'	2.32	0.42
6:E:22:GLY:HA3	6:E:39:THR:HG22	2.00	0.42
9:H:90:ARG:NH2	14:M:78:GLU:OE1	2.53	0.42
29:X:1126:A:H4'	29:X:1127:A:C5'	2.50	0.42
2:A:42:GLY:O	2:A:50:THR:N	2.49	0.42
28:3:16:ILE:HG12	28:3:65:GLY:O	2.20	0.42
29:X:472:A:C3'	29:X:473:G:H5'	2.50	0.42
10:I:81:GLN:HB3	10:I:82:ASP:H	1.50	0.42
29:X:2037:G:C6	29:X:2038:G:C6	3.08	0.42
29:X:501:A:H8	29:X:501:A:O5'	2.02	0.42
1:O:12:ARG:HG3	1:O:217:SER:O	2.20	0.42
2:A:67:PHE:HB3	2:A:153:ALA:H	1.84	0.42
29:X:1452:U:C2	29:X:1458:U:O2	2.73	0.42
2:A:159:ALA:HB1	2:A:198:ASN:HB3	2.00	0.42
29:X:1107:G:N1	29:X:1108:U:O2	2.53	0.42
15:N:39:LEU:HA	15:N:39:LEU:HD23	1.72	0.42
29:X:1770:G:C5	29:X:1771:C:C5	3.08	0.42
11:J:66:TYR:HE2	29:X:873:A:HO2'	1.62	0.42
12:K:33:ARG:HB2	12:K:114:GLU:CB	2.46	0.42
29:X:646:A:N3	29:X:2350:C:O2'	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:841:G:H1	29:X:937:C:H42	1.66	0.42
29:X:1858:G:O2'	29:X:1883:G:N2	2.45	0.42
29:X:1739:C:H2'	29:X:1740:G:C8	2.54	0.42
29:X:1297:C:C2	29:X:1298:C:C5	3.08	0.42
29:X:1344:U:H4'	29:X:1384:A:C6	2.54	0.42
8:G:65:LYS:NZ	8:G:65:LYS:HB2	2.33	0.42
16:O:57:GLN:H	16:O:97:GLY:CA	2.33	0.42
29:X:622:G:C6	29:X:623:G:N7	2.88	0.42
29:X:2140:G:H2'	29:X:2141:C:C6	2.54	0.42
29:X:2556:C:H2'	29:X:2557:G:O4'	2.20	0.42
29:X:537:U:H2'	29:X:538:G:H8	1.85	0.42
29:X:2342:C:O2'	29:X:2374:G:H5''	2.19	0.42
29:X:700:G:N2	29:X:732:C:H5	2.18	0.42
4:C:118:VAL:O	4:C:188:ILE:HG12	2.20	0.42
18:Q:53:ILE:HG13	18:Q:80:VAL:HG13	2.02	0.42
29:X:761:A:O5'	29:X:761:A:H8	2.03	0.42
21:T:23:VAL:HG22	21:T:26:PHE:CZ	2.55	0.42
30:Y:67:C:O2'	30:Y:68:A:H5'	2.20	0.42
29:X:2030:A:H4'	29:X:2031:A:C8	2.55	0.42
29:X:2667:C:H2'	29:X:2668:G:O4'	2.20	0.42
29:X:2773:C:H2'	29:X:2774:C:H6	1.84	0.42
15:N:36:PHE:O	15:N:39:LEU:HB2	2.19	0.42
5:D:148:LYS:H	5:D:148:LYS:HG3	1.55	0.42
29:X:603:G:C5	29:X:625:G:C2	3.07	0.42
6:E:61:HIS:O	6:E:65:HIS:HB2	2.19	0.42
7:F:1:MET:HB3	7:F:2:ARG:HH11	1.84	0.42
29:X:403:U:H5''	29:X:404:C:OP1	2.19	0.42
19:R:76:LEU:HA	19:R:76:LEU:HD23	1.90	0.41
29:X:1212:G:HO2'	29:X:1213:A:P	2.43	0.41
29:X:2307:G:H1'	29:X:2311:A:N6	2.35	0.41
29:X:1263:U:C4	29:X:1264:G:C6	3.08	0.41
29:X:1019:U:C4	29:X:1020:C:C5	3.08	0.41
4:C:193:LEU:HD12	4:C:193:LEU:HA	1.85	0.41
29:X:2114:A:N6	29:X:2119:A:H62	2.17	0.41
20:S:5:ALA:HB1	20:S:7:PRO:HD3	2.01	0.41
29:X:2219:U:N3	29:X:2220:C:H1'	2.34	0.41
29:X:1794:A:H2'	29:X:1795:C:H6	1.85	0.41
2:A:161:THR:H	2:A:196:VAL:HB	1.85	0.41
6:E:126:PRO:HD2	6:E:130:ARG:O	2.20	0.41
29:X:2532:G:C5	29:X:2533:A:C5	3.08	0.41
29:X:121:G:O5'	29:X:121:G:H8	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:466:A:N3	29:X:683:U:H1'	2.35	0.41
3:B:105:THR:HB	3:B:197:VAL:HG12	2.02	0.41
9:H:23:ARG:HA	9:H:23:ARG:HD2	1.88	0.41
29:X:2455:G:C6	29:X:2456:C:N4	2.88	0.41
9:H:111:PHE:N	9:H:111:PHE:HD1	2.18	0.41
3:B:2:LYS:HA	3:B:84:PHE:HE1	1.85	0.41
29:X:310:A:O3'	29:X:311:A:H8	2.03	0.41
21:T:4:LYS:HA	21:T:4:LYS:HD3	1.82	0.41
12:K:39:THR:O	12:K:42:LYS:N	2.53	0.41
29:X:1786:A:H1'	29:X:1938:A:N6	2.35	0.41
22:U:20:ARG:O	22:U:43:ARG:NH2	2.53	0.41
29:X:2260:C:H2'	29:X:2261:C:H6	1.83	0.41
29:X:2218:U:N3	29:X:2219:U:O4	2.53	0.41
4:C:26:VAL:HB	4:C:106:MET:HE1	2.02	0.41
29:X:582:G:H2'	29:X:583:G:C8	2.56	0.41
30:Y:75:A:C8	30:Y:107:C:C2	3.07	0.41
30:Y:7:C:H2'	30:Y:8:C:C6	2.56	0.41
29:X:935:U:H2'	29:X:936:C:C6	2.55	0.41
29:X:1511:G:C6	29:X:1512:C:N4	2.88	0.41
2:A:14:ARG:HB3	2:A:14:ARG:HE	1.62	0.41
9:H:115:ALA:O	9:H:117:GLU:N	2.54	0.41
1:O:41:PHE:CE2	1:O:189:ILE:HG12	2.55	0.41
29:X:612:G:C2	29:X:616:A:C6	3.09	0.41
10:I:98:LEU:O	10:I:99:VAL:HG13	2.21	0.41
29:X:648:G:C6	29:X:649:G:C6	3.08	0.41
2:A:78:LYS:HA	2:A:116:THR:HA	2.01	0.41
11:J:23:LYS:HB3	11:J:24:GLY:H	1.72	0.41
21:T:41:ARG:HH11	29:X:2387:U:H1'	1.86	0.41
29:X:2043:C:C4	29:X:2777:G:C2	3.08	0.41
17:P:40:LEU:HB3	25:Z:25:LEU:CD1	2.50	0.41
5:D:5:LYS:HE2	5:D:100:LEU:HG	2.02	0.41
15:N:25:TRP:O	15:N:28:ARG:HB2	2.20	0.41
12:K:96:ARG:NE	29:X:2882:C:OP1	2.47	0.41
10:I:57:ILE:HB	28:3:9:MET:HE2	2.02	0.41
8:G:140:GLN:O	8:G:144:MET:HG3	2.21	0.41
2:A:169:GLU:HB3	2:A:170:SER:H	1.57	0.41
11:J:135:ARG:HB3	11:J:136:GLU:H	1.68	0.41
29:X:1760:C:C2'	29:X:1761:C:H5'	2.50	0.41
29:X:2187:C:C2	29:X:2188:U:H1'	2.55	0.41
29:X:2809:A:C2	29:X:2891:A:C4	3.08	0.41
29:X:1985:G:H2'	29:X:1986:G:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:62:ILE:HG23	15:N:76:TYR:CE1	2.54	0.41
5:D:150:ARG:HB3	5:D:151:GLY:H	1.60	0.41
29:X:2335:A:O2'	29:X:2336:A:OP2	2.31	0.41
29:X:1282:U:H2'	29:X:1283:G:O4'	2.21	0.41
29:X:2684:U:N3	29:X:2685:G:C8	2.88	0.41
1:O:130:ARG:HA	1:O:130:ARG:HD3	1.98	0.41
29:X:701:G:C2	29:X:732:C:C5	3.08	0.41
4:C:28:HIS:CB	10:I:6:LEU:HD13	2.50	0.41
29:X:2720:U:H2'	29:X:2721:A:H8	1.84	0.41
29:X:2728:U:C2	29:X:2729:C:C5	3.08	0.41
4:C:192:ALA:O	4:C:195:ILE:HG13	2.19	0.41
20:S:26:LYS:N	20:S:26:LYS:HD3	2.35	0.41
29:X:2896:U:H2'	29:X:2897:U:C6	2.55	0.41
29:X:2389:G:H5''	29:X:2390:U:O5'	2.20	0.41
29:X:2833:U:O2'	29:X:2834:A:H5'	2.18	0.41
29:X:2513:G:H2'	29:X:2514:U:C6	2.55	0.41
29:X:2554:U:H2'	29:X:2555:U:C6	2.55	0.41
29:X:713:G:N2	29:X:718:A:OP2	2.53	0.41
29:X:2547:U:C5	29:X:2566:A:C5	3.09	0.41
3:B:146:THR:HG23	29:X:1130:U:C5	2.56	0.41
12:K:22:ARG:HG2	12:K:69:ASP:O	2.20	0.41
7:F:53:ILE:HA	7:F:54:PRO:HD2	1.93	0.41
16:O:40:VAL:HB	16:O:46:VAL:H	1.85	0.41
17:P:107:ILE:O	17:P:107:ILE:HG13	2.21	0.41
29:X:223:A:H2'	29:X:224:G:O4'	2.21	0.41
25:Z:10:LYS:HD2	29:X:1262:A:N3	2.35	0.41
29:X:1022:G:H22	29:X:1142:A:H2	1.68	0.41
29:X:1999:C:O2	29:X:2687:U:O2'	2.36	0.41
4:C:22:VAL:HG13	4:C:106:MET:CG	2.47	0.41
2:A:18:THR:HG23	2:A:211:ARG:NH1	2.35	0.41
18:Q:50:VAL:HG22	18:Q:82:LEU:HD12	2.02	0.41
19:R:85:ASP:HB2	19:R:92:THR:HG21	2.02	0.41
4:C:19:LEU:HB3	4:C:20:PRO:CA	2.51	0.41
29:X:1591:A:H2'	29:X:1592:U:C6	2.55	0.41
29:X:2075:U:H3'	29:X:2238:G:N2	2.34	0.41
29:X:602:A:H4'	29:X:603:G:O5'	2.19	0.41
9:H:130:ALA:HA	9:H:131:PRO:HD3	1.83	0.41
29:X:2427:C:H5''	29:X:2428:G:OP1	2.21	0.41
29:X:693:A:H2'	29:X:694:U:O4'	2.21	0.41
29:X:1360:G:N7	29:X:1361:G:C8	2.89	0.41
29:X:681:G:H2'	29:X:682:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:11:ARG:HB3	11:J:12:LYS:H	1.48	0.41
29:X:663:G:C6	29:X:664:G:C5	3.08	0.41
5:D:125:ARG:H	5:D:125:ARG:HG2	1.66	0.41
12:K:3:HIS:CG	12:K:3:HIS:O	2.72	0.41
13:L:18:ARG:HH22	29:X:2292:C:P	2.43	0.41
4:C:27:LEU:HD23	4:C:27:LEU:HA	1.83	0.41
29:X:833:A:H2'	29:X:834:C:C6	2.56	0.41
14:M:55:ILE:CG1	14:M:67:THR:HG22	2.50	0.41
11:J:24:GLY:HA2	11:J:25:GLY:HA2	1.59	0.41
29:X:23:G:C2	29:X:24:G:C8	3.08	0.41
6:E:24:PHE:CE2	6:E:43:VAL:HG13	2.55	0.41
29:X:320:U:H5''	29:X:321:C:OP1	2.21	0.41
17:P:18:VAL:HG23	17:P:19:LYS:H	1.85	0.41
29:X:2541:A:HO2'	29:X:2765:A:H2	1.64	0.41
14:M:90:GLN:OE1	14:M:91:VAL:N	2.35	0.41
29:X:600:C:N4	29:X:601:G:C5	2.89	0.41
29:X:2075:U:C4	29:X:2238:G:C6	3.09	0.41
29:X:1535:U:O2'	29:X:1537:G:N2	2.53	0.41
11:J:126:LEU:HA	11:J:127:PRO:HD3	1.85	0.41
29:X:78:C:H42	29:X:108:G:H1	1.69	0.41
29:X:1229:A:C2'	29:X:1230:G:H5'	2.50	0.41
3:B:134:TRP:CZ2	3:B:139:GLY:HA2	2.56	0.41
29:X:650:C:C2	29:X:651:G:N7	2.89	0.41
2:A:134:ARG:NH2	2:A:135:PHE:HE2	2.19	0.41
29:X:1936:A:C2	29:X:1945:G:C8	3.08	0.41
12:K:17:ARG:HE	12:K:17:ARG:HB2	1.15	0.41
29:X:651(B):C:OP2	29:X:653:U:H5'	2.21	0.41
5:D:10:ASP:HA	5:D:13:ARG:HD2	2.02	0.41
29:X:2507:C:C2	29:X:2583:G:C2	3.09	0.41
29:X:2498:C:OP2	29:X:2499:C:OP2	2.38	0.41
29:X:1464:G:H2'	29:X:1465:G:C8	2.55	0.41
23:V:24:GLU:OE1	23:V:46:LEU:HD21	2.21	0.41
3:B:1:MET:O	3:B:84:PHE:HD1	2.03	0.41
10:I:45:LYS:HB3	10:I:46:GLY:O	2.20	0.41
29:X:2547:U:C5	29:X:2566:A:C8	3.08	0.41
29:X:2457:U:O2	29:X:2495:G:C2	2.74	0.41
19:R:10:HIS:ND1	19:R:44:GLN:OE1	2.54	0.41
29:X:489:G:C2	29:X:491:G:H1'	2.56	0.41
29:X:781:A:H2	29:X:1776:G:N3	2.19	0.41
15:N:66:ASN:OD1	15:N:70:ARG:HD2	2.21	0.41
28:3:33:ASN:O	28:3:36:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:7:THR:CB	16:O:22:VAL:HG11	2.44	0.41
16:O:22:VAL:HG12	16:O:23:GLU:H	1.84	0.41
12:K:28:LEU:HD23	12:K:29:LEU:HD23	2.02	0.41
3:B:61:LYS:N	3:B:62:PRO:HD2	2.36	0.41
1:O:205:LEU:HD13	1:O:222:LEU:HD22	2.03	0.41
15:N:77:SER:HB2	29:X:1152:C:O4'	2.21	0.41
29:X:1154:G:OP2	29:X:1154:G:H8	2.03	0.41
29:X:7:G:H2'	29:X:8:A:C8	2.56	0.41
18:Q:20:MET:HB2	18:Q:25:TYR:CE1	2.55	0.41
10:I:62:LYS:HD2	29:X:2394:C:H5''	2.03	0.41
6:E:8:PRO:HD2	6:E:69:ARG:NH1	2.35	0.41
5:D:156:ILE:HG13	5:D:156:ILE:H	1.52	0.41
29:X:872:A:C6	29:X:906:A:C2	3.09	0.41
3:B:34:VAL:HG12	3:B:35:GLN:N	2.36	0.41
7:F:70:LYS:HB3	7:F:71:THR:H	1.59	0.41
29:X:2673:G:N3	29:X:2674:A:C8	2.89	0.41
16:O:11:GLN:N	16:O:11:GLN:HE21	2.19	0.41
29:X:1360:G:C8	29:X:1361:G:C8	3.09	0.41
29:X:2690:C:N4	29:X:2713:U:O3'	2.54	0.41
29:X:677:A:C4	29:X:678:C:C5	3.09	0.41
13:L:65:THR:HG1	30:Y:52:G:P	2.42	0.41
5:D:125:ARG:HG3	29:X:2315:U:O2'	2.21	0.41
25:Z:49:CYS:HB2	25:Z:51:TYR:HD1	1.86	0.41
22:U:47:HIS:HB3	29:X:397:A:OP1	2.20	0.41
15:N:13:ARG:HH12	29:X:1251:C:H3'	1.86	0.41
9:H:13:ASN:ND2	9:H:109:ARG:H	2.18	0.41
9:H:124:MET:N	9:H:124:MET:SD	2.94	0.41
29:X:1197:G:H2'	29:X:1198:U:H6	1.85	0.41
29:X:657:U:H2'	29:X:658:A:H8	1.82	0.41
11:J:41:ALA:HB2	11:J:128:ILE:CG2	2.51	0.41
29:X:864:G:H2'	29:X:865:C:C6	2.56	0.41
21:T:43:THR:O	21:T:43:THR:HG22	2.21	0.41
29:X:1127:A:N3	29:X:1127:A:H2'	2.36	0.41
7:F:41:PHE:O	7:F:45:THR:HG23	2.20	0.41
29:X:518:G:H2'	29:X:519:U:C6	2.56	0.41
29:X:208:C:H2'	29:X:209:C:C6	2.55	0.41
13:L:32:TYR:CZ	30:Y:9:G:H5'	2.56	0.41
29:X:852:A:H61	29:X:926:C:H42	1.69	0.41
29:X:2508:G:H2'	29:X:2509:G:H8	1.85	0.41
16:O:57:GLN:H	16:O:97:GLY:HA2	1.85	0.41
19:R:10:HIS:NE2	29:X:327:G:H1'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:71:LYS:HB2	5:D:71:LYS:HE3	1.90	0.41
21:T:57:HIS:N	21:T:57:HIS:CD2	2.88	0.41
29:X:2862:G:C6	29:X:2863:U:C4	3.09	0.41
27:2:19:ARG:NH1	29:X:124:G:H2'	2.36	0.41
29:X:150:C:H6	29:X:150:C:OP1	2.04	0.41
29:X:2250:G:N3	29:X:2250:G:O4'	2.52	0.41
29:X:1168:A:C2	29:X:1182:G:C2	3.09	0.41
29:X:1146:G:H2'	29:X:1147:A:O4'	2.21	0.41
17:P:51:GLN:O	17:P:54:GLU:HB2	2.21	0.41
28:3:17:THR:CG2	28:3:20:GLY:H	2.28	0.41
10:I:97:ARG:O	10:I:98:LEU:HB2	2.21	0.41
9:H:55:VAL:HB	9:H:68:ASP:H	1.85	0.41
29:X:946:G:H2'	29:X:947:G:C8	2.55	0.41
29:X:2727:G:H2'	29:X:2728:U:C6	2.55	0.41
29:X:934:G:C4	29:X:935:U:C5	3.09	0.41
29:X:600:C:N4	29:X:601:G:C6	2.89	0.41
30:Y:39:C:C5	30:Y:40:C:C4	3.09	0.41
29:X:704:G:N3	29:X:726:G:C2	2.89	0.41
21:T:69:PHE:HB2	29:X:856:C:H4'	2.03	0.41
5:D:22:TYR:CD1	5:D:28:VAL:HG22	2.56	0.41
29:X:2818:G:O2'	29:X:2819:G:H5'	2.20	0.41
29:X:2749:A:OP2	29:X:2750:A:O2'	2.31	0.41
29:X:1301:A:H2	29:X:1625(A):G:N3	2.19	0.41
7:F:10:LEU:HD13	7:F:27:LEU:HD13	2.02	0.41
29:X:177:G:O2'	29:X:178:U:OP2	2.39	0.41
29:X:2752:C:H2'	29:X:2753:A:O4'	2.20	0.41
29:X:1659:U:H2'	29:X:1660:C:O5'	2.21	0.41
22:U:32:ARG:HG2	22:U:34:THR:N	2.36	0.40
11:J:14:PHE:HD1	11:J:88:LYS:HE3	1.86	0.40
19:R:16:PHE:CE2	19:R:81:VAL:HG11	2.55	0.40
13:L:33:ARG:NH2	13:L:103:LEU:HD12	2.29	0.40
12:K:3:HIS:NE2	12:K:5:LYS:HD3	2.37	0.40
29:X:100:U:H4'	29:X:101:U:H5''	2.03	0.40
8:G:51:LEU:CD1	8:G:88:VAL:HG11	2.51	0.40
29:X:1422:G:H2'	29:X:1423:A:C8	2.55	0.40
4:C:161:ALA:HB1	4:C:167:VAL:HG21	2.03	0.40
21:T:23:VAL:HG22	21:T:26:PHE:CE2	2.56	0.40
20:S:9:THR:HA	20:S:10:PRO:HD3	1.88	0.40
29:X:1788:C:H2'	29:X:1789:A:C8	2.56	0.40
22:U:66:ALA:O	22:U:70:LEU:HB2	2.20	0.40
14:M:22:ARG:NE	14:M:24:LEU:HD21	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1499:U:H2'	29:X:1500:A:H8	1.86	0.40
7:F:73:PRO:C	7:F:75:SER:H	2.24	0.40
8:G:140:GLN:O	8:G:143:ALA:HB3	2.21	0.40
29:X:2186:A:H2'	29:X:2187:C:C6	2.56	0.40
29:X:718:A:H3'	29:X:719:G:O4'	2.21	0.40
29:X:1445:G:N3	29:X:1547:U:C2	2.89	0.40
29:X:1904:G:O2'	29:X:1928:A:N1	2.43	0.40
29:X:1324:G:N2	29:X:1331:C:C2	2.89	0.40
29:X:670:A:H4'	29:X:671:C:O5'	2.21	0.40
29:X:1414:G:HO2'	29:X:1415:A:H8	1.68	0.40
9:H:87:SER:HA	14:M:80:VAL:O	2.21	0.40
27:2:34:ARG:CZ	27:2:39:ARG:HD2	2.51	0.40
6:E:24:PHE:HB2	6:E:37:TYR:CE1	2.55	0.40
29:X:981:A:N1	29:X:2027:G:O2'	2.41	0.40
15:N:31:GLN:CD	29:X:580:C:H4'	2.41	0.40
29:X:864:G:N2	29:X:913:U:O2	2.54	0.40
29:X:2280:G:C2	29:X:2281:C:C6	3.10	0.40
29:X:2715:C:C2	29:X:2716:A:C8	3.08	0.40
29:X:1729:C:O2'	29:X:2859:A:N3	2.35	0.40
29:X:2895:C:H2'	29:X:2896:U:C6	2.55	0.40
29:X:2489:G:C6	29:X:2490:G:C6	3.09	0.40
3:B:140:SER:HB2	29:X:2575:C:O2'	2.21	0.40
14:M:18:GLN:C	14:M:20:HIS:H	2.25	0.40
29:X:1955:U:H5	29:X:2557:G:N2	2.20	0.40
29:X:866:A:H2'	29:X:866:A:N3	2.34	0.40
29:X:1634:U:H4'	29:X:1635:G:OP2	2.22	0.40
29:X:312:G:OP1	29:X:332:A:H5''	2.22	0.40
29:X:2697:G:N1	29:X:2711:A:C2	2.90	0.40
3:B:134:TRP:O	3:B:134:TRP:CG	2.74	0.40
29:X:1163:G:C2	29:X:1164:A:C8	3.09	0.40
29:X:2662:A:H8	29:X:2662:A:O5'	2.04	0.40
29:X:1783:A:C6	29:X:2587:A:C2	3.09	0.40
29:X:1150:U:H2'	29:X:1151:A:C8	2.57	0.40
29:X:2691:C:C2	29:X:2692:C:C5	3.10	0.40
2:A:44:ASN:HB2	29:X:1812:U:O2'	2.21	0.40
3:B:4:ILE:HG12	3:B:5:LEU:N	2.36	0.40
5:D:38:GLU:HG2	5:D:53:ALA:HB1	2.02	0.40
29:X:1755:U:H5''	29:X:1756:A:OP2	2.20	0.40
30:Y:46:G:C2	30:Y:50:U:O2	2.75	0.40
1:0:95:LEU:HD22	1:0:98:ARG:HD2	2.02	0.40
2:A:152:GLY:O	2:A:154:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1487:G:H2'	29:X:1488:G:H8	1.87	0.40
19:R:62:MET:HA	19:R:63:THR:HA	1.80	0.40
29:X:1121:C:H2'	29:X:1122:G:O4'	2.22	0.40
4:C:171:PRO:HB2	4:C:172:VAL:HG23	2.04	0.40
12:K:28:LEU:CD2	12:K:115:LEU:HD11	2.49	0.40
3:B:6:GLY:HA3	3:B:27:LEU:O	2.21	0.40
15:N:10:ARG:HG3	29:X:1251:C:OP1	2.21	0.40
13:L:8:ARG:C	13:L:10:LYS:H	2.25	0.40
29:X:817:C:O2'	29:X:839:U:H5''	2.21	0.40
14:M:100:ARG:O	29:X:2848:G:H3'	2.20	0.40
29:X:2519:U:C6	29:X:2541:A:N6	2.89	0.40
29:X:166:G:H2'	29:X:167:A:O4'	2.22	0.40
10:I:62:LYS:HG3	29:X:2394:C:OP1	2.21	0.40
25:Z:7:PRO:HA	29:X:2615:U:C6	2.57	0.40
13:L:32:TYR:CG	13:L:32:TYR:O	2.75	0.40
3:B:33:ILE:HG12	3:B:89:ASP:HA	2.02	0.40
11:J:76:THR:HG22	11:J:91:VAL:H	1.87	0.40
29:X:1180:U:H2'	29:X:1181:U:H6	1.87	0.40
3:B:102:ILE:HD11	3:B:184:VAL:HG21	2.02	0.40
1:O:32:LYS:HE3	29:X:2128:C:H5'	2.02	0.40
29:X:954:G:O2'	29:X:2274:A:N1	2.33	0.40
29:X:1485:C:H2'	29:X:1486:G:O4'	2.22	0.40
3:B:55:ALA:O	3:B:59:VAL:HG23	2.22	0.40
29:X:296:C:H2'	29:X:297:C:C6	2.55	0.40
29:X:617:A:H2'	29:X:618:C:C6	2.57	0.40
29:X:1319:G:C6	29:X:1320:G:O6	2.75	0.40
29:X:1196:C:N3	29:X:1197:G:N7	2.69	0.40
29:X:1197:G:C4	29:X:1198:U:C5	3.09	0.40
29:X:676:A:H8	29:X:2069:G:H21	1.65	0.40
29:X:1413:G:N2	29:X:1587:A:C8	2.90	0.40
7:F:115:LEU:C	7:F:117:ALA:H	2.25	0.40
29:X:127:A:H5''	29:X:128:C:O4'	2.21	0.40
29:X:1354:A:H2'	29:X:1355:G:O4'	2.22	0.40
29:X:1478:G:C6	29:X:1479:G:C5	3.10	0.40
29:X:2468:G:N2	29:X:2481:G:H2'	2.34	0.40
29:X:2469:A:N6	29:X:2481:G:O2'	2.55	0.40
29:X:2194:U:H2'	29:X:2195:U:O4'	2.22	0.40
29:X:179:A:H2'	29:X:180:C:O4'	2.22	0.40
2:A:227:ASN:OD1	29:X:784:A:H5''	2.22	0.40
21:T:11:LYS:HB2	21:T:11:LYS:HE2	1.81	0.40
18:Q:89:GLU:HG3	18:Q:89:GLU:H	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1731:A:H61	29:X:1741:U:H3	1.68	0.40
6:E:55:PRO:HB2	6:E:56:SER:H	1.57	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	0	222/224 (99%)	135 (61%)	65 (29%)	22 (10%)	1	2
2	A	272/274 (99%)	238 (88%)	25 (9%)	9 (3%)	5	20
3	B	203/205 (99%)	168 (83%)	24 (12%)	11 (5%)	2	7
4	C	195/197 (99%)	151 (77%)	30 (15%)	14 (7%)	1	3
5	D	175/177 (99%)	124 (71%)	39 (22%)	12 (7%)	1	4
6	E	169/171 (99%)	130 (77%)	22 (13%)	17 (10%)	1	2
7	F	142/144 (99%)	99 (70%)	34 (24%)	9 (6%)	2	5
8	G	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	3	13
9	H	132/134 (98%)	103 (78%)	19 (14%)	10 (8%)	1	3
10	I	139/141 (99%)	104 (75%)	23 (16%)	12 (9%)	1	2
11	J	134/136 (98%)	102 (76%)	20 (15%)	12 (9%)	1	2
12	K	111/113 (98%)	95 (86%)	11 (10%)	5 (4%)	3	12
13	L	102/104 (98%)	65 (64%)	21 (21%)	16 (16%)	0	0
14	M	107/109 (98%)	93 (87%)	7 (6%)	7 (6%)	1	4
15	N	115/117 (98%)	104 (90%)	8 (7%)	3 (3%)	7	26
16	O	92/94 (98%)	75 (82%)	11 (12%)	6 (6%)	1	4
17	P	125/127 (98%)	99 (79%)	16 (13%)	10 (8%)	1	3
18	Q	91/93 (98%)	87 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	R	108/110 (98%)	84 (78%)	14 (13%)	10 (9%)	1	2
20	S	173/175 (99%)	123 (71%)	32 (18%)	18 (10%)	1	1
21	T	82/84 (98%)	68 (83%)	11 (13%)	3 (4%)	4	17
22	U	70/72 (97%)	38 (54%)	16 (23%)	16 (23%)	0	0
23	V	64/66 (97%)	55 (86%)	5 (8%)	4 (6%)	2	5
24	W	53/55 (96%)	48 (91%)	3 (6%)	2 (4%)	4	16
25	Z	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	2	7
26	1	52/54 (96%)	33 (64%)	13 (25%)	6 (12%)	0	1
27	2	45/47 (96%)	40 (89%)	3 (7%)	2 (4%)	3	12
28	3	63/65 (97%)	47 (75%)	12 (19%)	4 (6%)	2	5
All	All	3431/3487 (98%)	2670 (78%)	512 (15%)	249 (7%)	1	3

All (249) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	28	LEU
1	0	30	THR
1	0	45	ILE
1	0	157	ILE
1	0	216	PRO
2	A	170	SER
2	A	242	ALA
3	B	85	ALA
3	B	86	PRO
3	B	117	MET
3	B	121	ASN
4	C	10	ASN
4	C	64	THR
4	C	162	ARG
5	D	33	LYS
5	D	42	SER
5	D	134	GLU
6	E	55	PRO
6	E	65	HIS
6	E	92	VAL
6	E	126	PRO
6	E	165	VAL
7	F	22	PRO

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Mol	Chain	Res	Type
7	F	23	VAL
8	G	66	HIS
8	G	70	PHE
9	H	29	ILE
9	H	47	VAL
10	I	28	LYS
10	I	53	ARG
10	I	81	GLN
10	I	98	LEU
10	I	99	VAL
11	J	13	GLN
11	J	91	VAL
11	J	98	VAL
12	K	4	GLY
12	K	32	GLY
12	K	88	ALA
13	L	21	THR
13	L	23	ALA
13	L	32	TYR
13	L	40	ALA
13	L	45	ASP
13	L	104	ALA
15	N	5	LYS
15	N	7	GLY
16	O	8	GLY
16	O	31	ASP
17	P	50	VAL
17	P	65	SER
17	P	81	HIS
17	P	82	ASN
17	P	88	ASP
19	R	49	GLU
19	R	58	VAL
19	R	60	PRO
20	S	57	GLU
20	S	91	PRO
20	S	125	PRO
20	S	169	VAL
22	U	15	VAL
22	U	56	GLN
22	U	60	VAL
23	V	3	PRO

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Mol	Chain	Res	Type
24	W	23	LEU
24	W	36	ASP
25	Z	36	CYS
26	1	32	GLN
26	1	46	HIS
27	2	44	VAL
28	3	34	THR
1	0	17	SER
1	0	29	ALA
1	0	62	HIS
1	0	87	ALA
1	0	138	SER
2	A	45	ASN
2	A	198	ASN
3	B	34	VAL
3	B	118	LYS
4	C	9	GLN
4	C	11	GLY
4	C	22	VAL
4	C	124	ASP
4	C	155	GLU
4	C	172	VAL
4	C	190	ALA
5	D	35	VAL
5	D	40	LEU
5	D	132	ILE
6	E	18	ASN
6	E	58	ALA
6	E	100	GLY
6	E	110	SER
7	F	47	ASP
7	F	82	ALA
8	G	36	ASN
8	G	165	VAL
9	H	37	GLY
9	H	71	LYS
10	I	78	SER
10	I	103	ASN
11	J	11	ARG
11	J	21	ASP
11	J	46	ASN
11	J	97	VAL

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Mol	Chain	Res	Type
12	K	20	LEU
12	K	109	THR
13	L	55	SER
13	L	56	SER
16	O	16	GLU
17	P	64	ALA
19	R	110	SER
20	S	16	GLU
20	S	50	GLY
20	S	88	TYR
20	S	128	ARG
20	S	156	GLU
21	T	14	ARG
22	U	18	VAL
22	U	29	GLY
22	U	30	VAL
22	U	32	ARG
22	U	55	GLY
22	U	76	LYS
23	V	4	SER
26	1	4	ALA
26	1	48	VAL
28	3	46	LYS
28	3	52	LYS
1	0	61	PRO
1	0	86	GLY
1	0	108	ALA
1	0	146	ALA
2	A	52	ARG
2	A	169	GLU
3	B	94	ASP
3	B	133	LYS
5	D	133	LYS
6	E	7	GLN
6	E	19	ALA
6	E	42	THR
6	E	173	ALA
7	F	19	PRO
7	F	98	LYS
9	H	14	SER
9	H	69	VAL
10	I	27	ASP

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Mol	Chain	Res	Type
10	I	45	LYS
10	I	86	THR
10	I	91	ASP
11	J	23	LYS
13	L	52	ALA
13	L	53	ALA
13	L	96	TYR
17	P	89	ARG
19	R	75	ALA
19	R	78	ALA
20	S	6	LYS
20	S	14	LEU
22	U	12	ASN
22	U	14	VAL
22	U	41	VAL
22	U	48	LYS
26	1	7	ARG
26	1	44	ALA
27	2	7	PRO
28	3	45	GLY
1	0	33	PHE
2	A	26	LYS
2	A	226	MET
3	B	60	ASN
4	C	159	ARG
5	D	81	GLN
5	D	145	MET
6	E	24	PHE
6	E	112	PRO
6	E	136	ILE
8	G	95	LEU
9	H	22	ILE
9	H	32	LYS
9	H	42	LYS
9	H	70	VAL
11	J	45	SER
13	L	59	LEU
13	L	93	SER
14	M	10	GLY
14	M	16	ILE
16	O	29	ALA
16	O	44	GLN

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Mol	Chain	Res	Type
16	O	45	THR
17	P	19	LYS
17	P	87	GLU
20	S	38	ALA
22	U	10	LYS
1	0	158	GLU
1	0	191	ALA
1	0	197	PRO
1	0	203	VAL
3	B	128	SER
4	C	15	ILE
6	E	107	ILE
10	I	90	ARG
11	J	15	ARG
11	J	30	PHE
13	L	46	SER
13	L	91	ARG
14	M	7	ILE
14	M	15	GLY
14	M	25	PRO
14	M	26	ASP
14	M	83	PHE
19	R	51	VAL
19	R	64	ASN
20	S	51	LEU
21	T	74	LYS
22	U	47	HIS
25	Z	53	ASP
1	0	100	ALA
2	A	210	GLY
3	B	73	ALA
5	D	123	ASP
7	F	25	PRO
7	F	94	ALA
11	J	37	ALA
13	L	51	LEU
19	R	52	ASN
19	R	108	VAL
20	S	32	PHE
20	S	37	LYS
22	U	40	ARG
25	Z	15	LYS

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Mol	Chain	Res	Type
4	C	18	PRO
7	F	83	GLY
20	S	110	GLY
1	0	89	VAL
4	C	20	PRO
5	D	41	GLY
8	G	34	PRO
17	P	61	PRO
20	S	58	GLY
21	T	30	VAL
1	0	198	GLY
15	N	8	ILE
20	S	124	ALA
23	V	43	VAL
5	D	137	ILE
23	V	18	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	167/167 (100%)	150 (90%)	17 (10%)	9	27
2	A	214/214 (100%)	190 (89%)	24 (11%)	7	22
3	B	155/155 (100%)	139 (90%)	16 (10%)	9	26
4	C	157/157 (100%)	137 (87%)	20 (13%)	5	16
5	D	153/153 (100%)	131 (86%)	22 (14%)	4	12
6	E	136/136 (100%)	114 (84%)	22 (16%)	3	9
7	F	107/107 (100%)	97 (91%)	10 (9%)	11	32
8	G	118/118 (100%)	108 (92%)	10 (8%)	13	37
9	H	103/103 (100%)	76 (74%)	27 (26%)	0	2
10	I	108/108 (100%)	85 (79%)	23 (21%)	1	4
11	J	110/110 (100%)	89 (81%)	21 (19%)	2	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	90/90 (100%)	78 (87%)	12 (13%)	5	14
13	L	74/74 (100%)	52 (70%)	22 (30%)	0	1
14	M	92/92 (100%)	79 (86%)	13 (14%)	4	12
15	N	96/96 (100%)	86 (90%)	10 (10%)	9	26
16	O	75/75 (100%)	57 (76%)	18 (24%)	1	2
17	P	109/109 (100%)	92 (84%)	17 (16%)	3	10
18	Q	75/75 (100%)	69 (92%)	6 (8%)	15	40
19	R	91/91 (100%)	76 (84%)	15 (16%)	3	8
20	S	149/149 (100%)	117 (78%)	32 (22%)	1	4
21	T	62/62 (100%)	48 (77%)	14 (23%)	1	3
22	U	57/57 (100%)	42 (74%)	15 (26%)	0	2
23	V	54/54 (100%)	48 (89%)	6 (11%)	8	22
24	W	48/48 (100%)	43 (90%)	5 (10%)	9	26
25	Z	51/51 (100%)	43 (84%)	8 (16%)	3	9
26	1	38/38 (100%)	30 (79%)	8 (21%)	1	4
27	2	40/40 (100%)	33 (82%)	7 (18%)	2	7
28	3	51/51 (100%)	40 (78%)	11 (22%)	1	3
All	All	2780/2780 (100%)	2349 (84%)	431 (16%)	3	10

All (431) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	11	ASP
1	0	12	ARG
1	0	16	TYR
1	0	24	LEU
1	0	25	VAL
1	0	26	LYS
1	0	38	GLU
1	0	52	GLN
1	0	64	THR
1	0	70	VAL
1	0	110	VAL
1	0	141	VAL
1	0	152	LEU
1	0	157	ILE

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Mol	Chain	Res	Type
1	0	166	VAL
1	0	186	GLN
1	0	212	THR
2	A	10	THR
2	A	13	ARG
2	A	14	ARG
2	A	18	THR
2	A	35	GLU
2	A	63	ARG
2	A	68	LYS
2	A	71	ASP
2	A	96	HIS
2	A	99	ASP
2	A	117	VAL
2	A	134	ARG
2	A	164	GLN
2	A	165	VAL
2	A	168	LYS
2	A	183	ARG
2	A	200	GLU
2	A	204	ILE
2	A	233	HIS
2	A	247	VAL
2	A	252	LYS
2	A	261	ARG
2	A	271	VAL
2	A	273	ARG
3	B	19	ARG
3	B	86	PRO
3	B	87	ASP
3	B	91	VAL
3	B	116	VAL
3	B	132	LYS
3	B	136	ARG
3	B	138	PRO
3	B	140	SER
3	B	143	GLN
3	B	144	ARG
3	B	145	LYS
3	B	152	LYS
3	B	162	MET
3	B	184	VAL

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Mol	Chain	Res	Type
3	B	205	SER
4	C	38	ARG
4	C	48	ARG
4	C	51	VAL
4	C	62	LYS
4	C	84	PHE
4	C	87	LYS
4	C	94	THR
4	C	102	LEU
4	C	110	SER
4	C	117	LEU
4	C	121	ASP
4	C	131	LYS
4	C	143	ASP
4	C	145	THR
4	C	152	THR
4	C	172	VAL
4	C	181	LEU
4	C	185	ARG
4	C	188	ILE
4	C	198	GLU
5	D	34	ILE
5	D	40	LEU
5	D	46	ASP
5	D	66	ILE
5	D	80	ARG
5	D	89	VAL
5	D	90	THR
5	D	92	ARG
5	D	115	ARG
5	D	117	ILE
5	D	125	ARG
5	D	142	THR
5	D	145	MET
5	D	148	LYS
5	D	150	ARG
5	D	152	MET
5	D	153	ASP
5	D	154	ILE
5	D	155	THR
5	D	156	ILE
5	D	158	THR

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Mol	Chain	Res	Type
5	D	159	THR
6	E	6	LYS
6	E	35	VAL
6	E	38	ASN
6	E	40	GLU
6	E	43	VAL
6	E	44	ARG
6	E	50	LEU
6	E	64	LEU
6	E	67	LEU
6	E	69	ARG
6	E	72	VAL
6	E	81	ASP
6	E	84	THR
6	E	90	ARG
6	E	105	MET
6	E	106	ASN
6	E	113	VAL
6	E	114	ILE
6	E	130	ARG
6	E	140	LEU
6	E	149	ARG
6	E	165	VAL
7	F	2	ARG
7	F	36	GLU
7	F	50	ASP
7	F	63	ARG
7	F	84	ILE
7	F	99	LEU
7	F	102	ASP
7	F	119	SER
7	F	136	VAL
7	F	137	THR
8	G	31	THR
8	G	33	ILE
8	G	65	LYS
8	G	69	ASP
8	G	94	LYS
8	G	96	ASP
8	G	111	LYS
8	G	122	HIS
8	G	156	HIS

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Mol	Chain	Res	Type
8	G	167	LYS
9	H	3	MET
9	H	8	LEU
9	H	9	ASP
9	H	13	ASN
9	H	22	ILE
9	H	25	LEU
9	H	29	ILE
9	H	35	THR
9	H	36	THR
9	H	41	ASN
9	H	43	ARG
9	H	46	HIS
9	H	54	SER
9	H	65	LYS
9	H	68	ASP
9	H	78	SER
9	H	83	ARG
9	H	89	ILE
9	H	90	ARG
9	H	109	ARG
9	H	111	PHE
9	H	116	ARG
9	H	117	GLU
9	H	120	ASP
9	H	122	ARG
9	H	126	ILE
9	H	127	VAL
10	I	4	HIS
10	I	5	ASP
10	I	27	ASP
10	I	29	THR
10	I	35	LYS
10	I	50	GLU
10	I	57	ILE
10	I	65	PHE
10	I	70	THR
10	I	73	GLU
10	I	77	LEU
10	I	80	LEU
10	I	81	GLN
10	I	91	ASP

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Mol	Chain	Res	Type
10	I	93	LEU
10	I	94	GLU
10	I	96	TYR
10	I	97	ARG
10	I	99	VAL
10	I	103	ASN
10	I	114	ILE
10	I	121	HIS
10	I	140	VAL
11	J	10	PHE
11	J	11	ARG
11	J	17	ARG
11	J	26	ASP
11	J	48	ILE
11	J	60	ARG
11	J	82	THR
11	J	84	MET
11	J	91	VAL
11	J	92	GLU
11	J	93	TYR
11	J	95	VAL
11	J	99	LYS
11	J	102	ARG
11	J	111	THR
11	J	112	GLU
11	J	113	GLU
11	J	132	MET
11	J	133	VAL
11	J	137	VAL
11	J	140	GLU
12	K	17	ARG
12	K	31	GLU
12	K	33	ARG
12	K	36	THR
12	K	56	LYS
12	K	59	ASP
12	K	60	LEU
12	K	64	ARG
12	K	68	GLN
12	K	73	LYS
12	K	83	VAL
12	K	112	LEU

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Mol	Chain	Res	Type
13	L	8	ARG
13	L	13	THR
13	L	14	ARG
13	L	16	LYS
13	L	17	VAL
13	L	30	SER
13	L	36	LYS
13	L	37	HIS
13	L	38	ILE
13	L	39	TYR
13	L	42	ILE
13	L	43	ILE
13	L	47	ARG
13	L	55	SER
13	L	60	LYS
13	L	66	ASP
13	L	67	THR
13	L	71	VAL
13	L	91	ARG
13	L	93	SER
13	L	105	ASP
13	L	108	ARG
14	M	2	GLN
14	M	3	THR
14	M	5	ILE
14	M	6	LYS
14	M	7	ILE
14	M	14	ARG
14	M	37	THR
14	M	38	LYS
14	M	58	ASN
14	M	65	SER
14	M	71	ILE
14	M	99	VAL
14	M	101	ARG
15	N	8	ILE
15	N	9	VAL
15	N	19	LYS
15	N	51	ARG
15	N	59	ARG
15	N	74	MET
15	N	76	TYR

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Mol	Chain	Res	Type
15	N	77	SER
15	N	80	ILE
15	N	87	ASN
16	O	6	GLN
16	O	7	THR
16	O	10	LYS
16	O	11	GLN
16	O	14	VAL
16	O	16	GLU
16	O	18	ASP
16	O	26	GLN
16	O	31	ASP
16	O	34	GLU
16	O	50	ASP
16	O	53	LYS
16	O	56	VAL
16	O	59	GLU
16	O	62	GLU
16	O	65	ARG
16	O	69	ILE
16	O	84	THR
17	P	9	ARG
17	P	17	GLN
17	P	25	PHE
17	P	32	ARG
17	P	36	ARG
17	P	45	ILE
17	P	48	LYS
17	P	49	SER
17	P	63	SER
17	P	65	SER
17	P	66	GLU
17	P	93	LYS
17	P	98	ASP
17	P	103	LEU
17	P	105	ARG
17	P	109	ARG
17	P	122	SER
18	Q	40	ASP
18	Q	62	ARG
18	Q	64	ARG
18	Q	80	VAL

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Mol	Chain	Res	Type
18	Q	82	LEU
18	Q	91	LEU
19	R	5	SER
19	R	18	LYS
19	R	46	VAL
19	R	51	VAL
19	R	53	VAL
19	R	66	GLN
19	R	81	VAL
19	R	98	ILE
19	R	99	VAL
19	R	102	LYS
19	R	103	LYS
19	R	104	VAL
19	R	106	VAL
19	R	112	LYS
19	R	113	THR
20	S	3	LEU
20	S	4	THR
20	S	13	LYS
20	S	15	ASP
20	S	22	VAL
20	S	24	TYR
20	S	25	ASN
20	S	27	GLU
20	S	48	THR
20	S	49	THR
20	S	55	THR
20	S	57	GLU
20	S	61	THR
20	S	65	LEU
20	S	67	LYS
20	S	83	PHE
20	S	87	THR
20	S	95	SER
20	S	96	VAL
20	S	100	THR
20	S	103	ARG
20	S	109	GLN
20	S	112	LEU
20	S	117	VAL
20	S	119	ASN

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Mol	Chain	Res	Type
20	S	120	LEU
20	S	140	LYS
20	S	151	ASP
20	S	166	LEU
20	S	167	THR
20	S	171	VAL
20	S	175	ARG
21	T	7	VAL
21	T	10	SER
21	T	11	LYS
21	T	19	LYS
21	T	23	VAL
21	T	31	VAL
21	T	32	LYS
21	T	37	LEU
21	T	38	VAL
21	T	46	LYS
21	T	51	VAL
21	T	64	ASP
21	T	80	SER
21	T	85	GLN
22	U	8	THR
22	U	12	ASN
22	U	14	VAL
22	U	19	ILE
22	U	23	LYS
22	U	25	ARG
22	U	32	ARG
22	U	33	LYS
22	U	35	THR
22	U	42	GLN
22	U	49	LYS
22	U	63	SER
22	U	67	ILE
22	U	70	LEU
22	U	78	ILE
23	V	10	GLN
23	V	16	LYS
23	V	21	ARG
23	V	46	LEU
23	V	47	ARG
23	V	55	THR

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Mol	Chain	Res	Type
24	W	3	ILE
24	W	10	ILE
24	W	34	VAL
24	W	51	LEU
24	W	53	VAL
25	Z	3	LYS
25	Z	9	LYS
25	Z	20	ARG
25	Z	23	HIS
25	Z	32	GLU
25	Z	49	CYS
25	Z	57	VAL
25	Z	58	LEU
26	1	7	ARG
26	1	18	THR
26	1	24	THR
26	1	28	ARG
26	1	32	GLN
26	1	43	VAL
26	1	47	VAL
26	1	49	PHE
27	2	1	MET
27	2	12	ARG
27	2	24	THR
27	2	25	LYS
27	2	26	SER
27	2	42	LEU
27	2	45	SER
28	3	7	HIS
28	3	17	THR
28	3	22	VAL
28	3	26	LYS
28	3	29	LYS
28	3	31	HIS
28	3	32	GLN
28	3	39	ASP
28	3	46	LYS
28	3	50	LEU
28	3	62	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	129	ASN
2	A	231	HIS
4	C	10	ASN
5	D	118	ASN
5	D	120	ASN
5	D	127	ASN
8	G	161	GLN
9	H	41	ASN
14	M	58	ASN
15	N	91	ASN
18	Q	86	GLN
19	R	69	GLN
19	R	77	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2776/2881 (96%)	655 (23%)	41 (1%)
30	Y	121/122 (99%)	35 (28%)	1 (0%)
All	All	2897/3003 (96%)	690 (23%)	42 (1%)

All (690) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	13	A
29	X	14	A
29	X	22	C
29	X	28	A
29	X	46	C
29	X	51	G
29	X	55	G
29	X	59	C
29	X	64	A
29	X	65	C
29	X	68	G
29	X	71	A
29	X	74	A
29	X	75	G
29	X	92	G
29	X	93	A
29	X	95	A
29	X	97	G

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Mol	Chain	Res	Type
29	X	102	G
29	X	104	C
29	X	110	G
29	X	118	A
29	X	120	U
29	X	121	G
29	X	125	A
29	X	126	A
29	X	137	U
29	X	149	G
29	X	161	A
29	X	167	A
29	X	168	A
29	X	170	C
29	X	171	A
29	X	173	C
29	X	175	C
29	X	176	A
29	X	184	A
29	X	187	G
29	X	188	A
29	X	193	A
29	X	194	A
29	X	195	A
29	X	196	G
29	X	200	A
29	X	201	U
29	X	202	U
29	X	205	A
29	X	220	G
29	X	221	C
29	X	222	G
29	X	223	A
29	X	224	G
29	X	233	G
29	X	238	G
29	X	310	A
29	X	311	A
29	X	312	G
29	X	314	U
29	X	316	C
29	X	324	A

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Mol	Chain	Res	Type
29	X	328	U
29	X	329	G
29	X	332	A
29	X	333	G
29	X	334	U
29	X	338	G
29	X	339	U
29	X	345	A
29	X	346	A
29	X	347	C
29	X	349	A
29	X	350	G
29	X	386	G
29	X	387	U
29	X	390	A
29	X	391	A
29	X	395	U
29	X	396	G
29	X	401	A
29	X	404	C
29	X	405	C
29	X	406	G
29	X	409	C
29	X	411	G
29	X	412	A
29	X	441	U
29	X	449	A
29	X	451	C
29	X	454	A
29	X	456	U
29	X	458	G
29	X	470	A
29	X	472	A
29	X	475	U
29	X	479	A
29	X	480	A
29	X	481	G
29	X	483	A
29	X	494	G
29	X	499	U
29	X	501	A
29	X	502	A

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Mol	Chain	Res	Type
29	X	503	A
29	X	504	G
29	X	505	A
29	X	506	G
29	X	508	A
29	X	509	C
29	X	510	C
29	X	511	U
29	X	517	C
29	X	522	A
29	X	530	G
29	X	531	C
29	X	532	A
29	X	533	G
29	X	545	U
29	X	546	U
29	X	547	A
29	X	548	U
29	X	549	G
29	X	550	C
29	X	555	U
29	X	563	G
29	X	569	U
29	X	573	G
29	X	574	C
29	X	575	A
29	X	583	G
29	X	586	A
29	X	592	A
29	X	592(A)	C
29	X	600	C
29	X	602	A
29	X	614	A
29	X	615	A
29	X	621	A
29	X	623	G
29	X	627	A
29	X	634	G
29	X	637	A
29	X	643	A
29	X	644	A
29	X	645	U

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Mol	Chain	Res	Type
29	X	651(B)	C
29	X	653	U
29	X	654	U
29	X	655	A
29	X	669	G
29	X	670	A
29	X	682	G
29	X	686	G
29	X	690	A
29	X	714	U
29	X	716	A
29	X	718	A
29	X	719	G
29	X	720	G
29	X	730	A
29	X	734	A
29	X	739	G
29	X	740	U
29	X	747	U
29	X	752	C
29	X	761	A
29	X	762	U
29	X	765	G
29	X	776	G
29	X	782	A
29	X	784	A
29	X	785	G
29	X	792	G
29	X	793	A
29	X	801	G
29	X	805	G
29	X	808	A
29	X	812	C
29	X	819	A
29	X	826	U
29	X	827	U
29	X	828	G
29	X	832	U
29	X	835	A
29	X	844	U
29	X	845	G
29	X	859	G

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Mol	Chain	Res	Type
29	X	866	A
29	X	874	G
29	X	910	A
29	X	915	C
29	X	920	G
29	X	921	G
29	X	926	C
29	X	928	C
29	X	929	G
29	X	945	A
29	X	946	G
29	X	958	U
29	X	961	C
29	X	962	U
29	X	974	G
29	X	983	A
29	X	984	A
29	X	989	G
29	X	990	A
29	X	996	A
29	X	997	G
29	X	1003	G
29	X	1008	U
29	X	1009	A
29	X	1011	A
29	X	1012	U
29	X	1013	G
29	X	1022	G
29	X	1023	U
29	X	1026	U
29	X	1033	U
29	X	1038	C
29	X	1044	A
29	X	1045	U
29	X	1046	A
29	X	1047	G
29	X	1049	C
29	X	1057	A
29	X	1060	U
29	X	1061	U
29	X	1067	A
29	X	1068	G

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Mol	Chain	Res	Type
29	X	1070	A
29	X	1071	G
29	X	1075	C
29	X	1078	C
29	X	1080	C
29	X	1083	C
29	X	1087	G
29	X	1088	A
29	X	1089	G
29	X	1096	A
29	X	1097	U
29	X	1102	C
29	X	1109	C
29	X	1111	A
29	X	1112	G
29	X	1117	G
29	X	1122	G
29	X	1127	A
29	X	1128	A
29	X	1130	U
29	X	1131	G
29	X	1134	C
29	X	1135	G
29	X	1138	G
29	X	1140	U
29	X	1141	C
29	X	1142	A
29	X	1143	A
29	X	1147	A
29	X	1154	G
29	X	1156	A
29	X	1169	A
29	X	1172(B)	C
29	X	1173	A
29	X	1175	G
29	X	1181	U
29	X	1193	G
29	X	1195	G
29	X	1210	G
29	X	1213	A
29	X	1217	C
29	X	1225	A

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Mol	Chain	Res	Type
29	X	1226	A
29	X	1227	G
29	X	1253	G
29	X	1256	G
29	X	1257	C
29	X	1271	G
29	X	1272	A
29	X	1273	U
29	X	1275	A
29	X	1276	A
29	X	1284	A
29	X	1287	A
29	X	1288	U
29	X	1294	U
29	X	1298	C
29	X	1300	U
29	X	1301	A
29	X	1318	G
29	X	1319	G
29	X	1321	A
29	X	1329	U
29	X	1332	G
29	X	1338	G
29	X	1341	A
29	X	1346	G
29	X	1357	U
29	X	1360	G
29	X	1365	A
29	X	1368	G
29	X	1378	A
29	X	1379	U
29	X	1390	U
29	X	1391	C
29	X	1395	A
29	X	1413	G
29	X	1414	G
29	X	1415	A
29	X	1418	G
29	X	1428	C
29	X	1437	C
29	X	1444	U
29	X	1445	G

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Mol	Chain	Res	Type
29	X	1459	A
29	X	1460	U
29	X	1468	G
29	X	1474	U
29	X	1482	G
29	X	1489	U
29	X	1490	C
29	X	1491	A
29	X	1498	C
29	X	1507	A
29	X	1508	C
29	X	1509	A
29	X	1511	G
29	X	1525	G
29	X	1529	G
29	X	1532	U
29	X	1536	C
29	X	1537	G
29	X	1546	G
29	X	1558	A
29	X	1559	C
29	X	1566	A
29	X	1569	A
29	X	1578	U
29	X	1583	G
29	X	1585	U
29	X	1586	G
29	X	1587	A
29	X	1602	U
29	X	1608	A
29	X	1609	A
29	X	1610	A
29	X	1613	G
29	X	1615	C
29	X	1616	A
29	X	1634	U
29	X	1639	U
29	X	1644	C
29	X	1648	C
29	X	1651	G
29	X	1652	A
29	X	1653	G

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Mol	Chain	Res	Type
29	X	1660	C
29	X	1674	G
29	X	1675	C
29	X	1694	C
29	X	1697	A
29	X	1700	A
29	X	1734	C
29	X	1735	U
29	X	1736	U
29	X	1737	C
29	X	1738	G
29	X	1747	G
29	X	1750	G
29	X	1754	A
29	X	1758	G
29	X	1761	C
29	X	1763	G
29	X	1773	A
29	X	1781	C
29	X	1784	A
29	X	1791	A
29	X	1797	C
29	X	1800	C
29	X	1801	C
29	X	1808	A
29	X	1816	C
29	X	1819	A
29	X	1829	A
29	X	1833	C
29	X	1843	C
29	X	1858	G
29	X	1862	G
29	X	1876	A
29	X	1880	U
29	X	1886	A
29	X	1892	C
29	X	1900	A
29	X	1901	A
29	X	1903	G
29	X	1906	G
29	X	1907	G
29	X	1910	G

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Mol	Chain	Res	Type
29	X	1912	A
29	X	1913	A
29	X	1914	C
29	X	1915	U
29	X	1916	A
29	X	1920	C
29	X	1922	G
29	X	1926	U
29	X	1936	A
29	X	1938	A
29	X	1940	U
29	X	1941	C
29	X	1951	U
29	X	1955	U
29	X	1963	U
29	X	1966	A
29	X	1967	C
29	X	1968	G
29	X	1970	A
29	X	1971	A
29	X	1972	G
29	X	1991	U
29	X	1992	G
29	X	1993	U
29	X	1996	C
29	X	1997	A
29	X	2016	U
29	X	2023	G
29	X	2031	A
29	X	2035	G
29	X	2036	C
29	X	2043	C
29	X	2046	G
29	X	2049	G
29	X	2055	C
29	X	2056	G
29	X	2060	A
29	X	2061	G
29	X	2062	A
29	X	2066	C
29	X	2069	G
29	X	2075	U

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Mol	Chain	Res	Type
29	X	2076	U
29	X	2077	A
29	X	2092	U
29	X	2093	G
29	X	2110	G
29	X	2111	C
29	X	2112	G
29	X	2114	A
29	X	2116	G
29	X	2117	A
29	X	2118	U
29	X	2119	A
29	X	2121	G
29	X	2123	G
29	X	2124	G
29	X	2125	G
29	X	2126	A
29	X	2127	G
29	X	2128	C
29	X	2132	C
29	X	2133	G
29	X	2134	A
29	X	2136	A
29	X	2137	C
29	X	2138	U
29	X	2139	G
29	X	2140	G
29	X	2142	C
29	X	2143	U
29	X	2144	U
29	X	2145	U
29	X	2146	U
29	X	2151	U
29	X	2152	C
29	X	2157	G
29	X	2158	A
29	X	2164	C
29	X	2167	U
29	X	2168	G
29	X	2170	A
29	X	2171	A
29	X	2173	A

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Mol	Chain	Res	Type
29	X	2175	C
29	X	2179	C
29	X	2182	A
29	X	2188	U
29	X	2190	G
29	X	2197	U
29	X	2198	A
29	X	2205	A
29	X	2210	A
29	X	2211	A
29	X	2212	A
29	X	2213	U
29	X	2217	U
29	X	2220	C
29	X	2221	G
29	X	2225	A
29	X	2238	G
29	X	2239	G
29	X	2250	G
29	X	2251	G
29	X	2270	U
29	X	2273	A
29	X	2280	G
29	X	2283	C
29	X	2287	A
29	X	2288	A
29	X	2289	G
29	X	2305	U
29	X	2306	U
29	X	2307	G
29	X	2308	G
29	X	2309	A
29	X	2311	A
29	X	2320	A
29	X	2321	G
29	X	2322	A
29	X	2327	A
29	X	2333	A
29	X	2334	G
29	X	2335	A
29	X	2336	A
29	X	2346	A

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Mol	Chain	Res	Type
29	X	2350	C
29	X	2352	A
29	X	2357	G
29	X	2361	C
29	X	2372	G
29	X	2379	C
29	X	2382	G
29	X	2383	G
29	X	2385	C
29	X	2390	U
29	X	2392	A
29	X	2396	G
29	X	2400	G
29	X	2402	A
29	X	2406	U
29	X	2407	G
29	X	2410	G
29	X	2414	G
29	X	2423	U
29	X	2425	A
29	X	2428	G
29	X	2429	G
29	X	2430	A
29	X	2431	U
29	X	2434	A
29	X	2439	A
29	X	2440	C
29	X	2441	C
29	X	2447	G
29	X	2448	A
29	X	2462	U
29	X	2463	C
29	X	2469	A
29	X	2474	C
29	X	2476	A
29	X	2478	A
29	X	2481	G
29	X	2484	G
29	X	2491	U
29	X	2498	C
29	X	2499	C
29	X	2500	U

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Mol	Chain	Res	Type
29	X	2501	C
29	X	2502	G
29	X	2505	G
29	X	2515	C
29	X	2518	A
29	X	2519	U
29	X	2529	G
29	X	2538	C
29	X	2542	A
29	X	2543	G
29	X	2553	G
29	X	2554	U
29	X	2555	U
29	X	2566	A
29	X	2567	G
29	X	2572	A
29	X	2573	C
29	X	2578	G
29	X	2582	G
29	X	2586	C
29	X	2600	A
29	X	2602	A
29	X	2603	G
29	X	2609	U
29	X	2610	C
29	X	2612	C
29	X	2614	A
29	X	2615	U
29	X	2632	A
29	X	2634	A
29	X	2640	G
29	X	2660	A
29	X	2663	G
29	X	2666	C
29	X	2673	G
29	X	2681	C
29	X	2682	G
29	X	2689	U
29	X	2691	C
29	X	2697	G
29	X	2700	G
29	X	2707	C

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Mol	Chain	Res	Type
29	X	2712	C
29	X	2712(A)	A
29	X	2713	U
29	X	2714	G
29	X	2715	C
29	X	2722	G
29	X	2723	C
29	X	2726	U
29	X	2727	G
29	X	2733	A
29	X	2738	A
29	X	2748	A
29	X	2756	U
29	X	2757	A
29	X	2758	A
29	X	2763	G
29	X	2765	A
29	X	2778	A
29	X	2780	G
29	X	2789	C
29	X	2794	U
29	X	2795	U
29	X	2797	A
29	X	2798	U
29	X	2799	C
29	X	2800	A
29	X	2808	U
29	X	2812	A
29	X	2818	G
29	X	2820	A
29	X	2821	A
29	X	2823	A
29	X	2825	C
29	X	2834	A
29	X	2840	C
29	X	2848	G
29	X	2852	G
29	X	2858	C
29	X	2867	C
29	X	2872	G
29	X	2873	A
29	X	2874	C

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Mol	Chain	Res	Type
29	X	2876	G
29	X	2883	A
29	X	2890	G
29	X	2891	A
29	X	2893	G
29	X	2894	U
29	X	2902	A
30	Y	11	G
30	Y	14	C
30	Y	16	U
30	Y	17	A
30	Y	20	A
30	Y	26	G
30	Y	27	A
30	Y	28	A
30	Y	29	C
30	Y	34	C
30	Y	37	C
30	Y	40	C
30	Y	42	U
30	Y	43	G
30	Y	44	C
30	Y	46	G
30	Y	47	A
30	Y	48	A
30	Y	49	C
30	Y	53	G
30	Y	58	G
30	Y	59	A
30	Y	63	A
30	Y	69	G
30	Y	75	A
30	Y	76	U
30	Y	86	A
30	Y	99	G
30	Y	108	G
30	Y	111	C
30	Y	112	A
30	Y	115	G
30	Y	120	G
30	Y	121	G
30	Y	123	U

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	219	G
29	X	310	A
29	X	330	A
29	X	453	C
29	X	501	A
29	X	506	G
29	X	508	A
29	X	614	A
29	X	643	A
29	X	644	A
29	X	669	G
29	X	734	A
29	X	800	A
29	X	929	G
29	X	960	A
29	X	1127	A
29	X	1212	G
29	X	1275	A
29	X	1413	G
29	X	1414	G
29	X	1490	C
29	X	1510	U
29	X	1585	U
29	X	1586	G
29	X	1608	A
29	X	1610	A
29	X	1662	U
29	X	1997	A
29	X	2022	U
29	X	2035	G
29	X	2051	A
29	X	2060	A
29	X	2347	C
29	X	2351	G
29	X	2430	A
29	X	2468	G
29	X	2553	G
29	X	2714	G
29	X	2756	U
29	X	2778	A
29	X	2873	A
30	Y	16	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 198 ligands modelled in this entry, 198 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	224/224 (100%)	5.93	199 (88%) 0 0	238, 259, 280, 290	0
2	A	274/274 (100%)	0.53	31 (11%) 7 4	93, 135, 154, 161	0
3	B	205/205 (100%)	0.24	7 (3%) 49 41	60, 89, 107, 124	0
4	C	197/197 (100%)	0.37	15 (7%) 17 11	77, 125, 145, 159	0
5	D	177/177 (100%)	1.65	66 (37%) 0 0	155, 174, 190, 197	0
6	E	171/171 (100%)	0.84	35 (20%) 1 1	110, 148, 175, 177	0
7	F	144/144 (100%)	3.55	102 (70%) 0 0	213, 230, 235, 237	0
8	G	142/142 (100%)	0.27	11 (7%) 16 11	79, 112, 127, 144	0
9	H	134/134 (100%)	0.03	5 (3%) 45 38	62, 79, 94, 111	0
10	I	141/141 (100%)	0.98	33 (23%) 1 0	86, 138, 155, 161	0
11	J	136/136 (100%)	1.04	33 (24%) 1 0	94, 113, 135, 141	0
12	K	113/113 (100%)	0.14	3 (2%) 58 52	61, 72, 83, 88	0
13	L	104/104 (100%)	1.48	34 (32%) 1 0	121, 136, 153, 162	0
14	M	109/109 (100%)	-0.19	3 (2%) 56 50	65, 80, 98, 127	0
15	N	117/117 (100%)	0.40	10 (8%) 13 8	80, 107, 127, 133	0
16	O	94/94 (100%)	0.08	8 (8%) 13 8	89, 122, 141, 152	0
17	P	127/127 (100%)	0.40	10 (7%) 15 10	71, 85, 109, 156	0
18	Q	93/93 (100%)	0.94	14 (15%) 3 1	98, 124, 140, 144	0
19	R	110/110 (100%)	0.57	14 (12%) 5 3	110, 121, 146, 157	0
20	S	175/175 (100%)	0.72	35 (20%) 1 1	124, 151, 164, 168	0
21	T	84/84 (100%)	2.25	38 (45%) 0 0	102, 117, 133, 146	0
22	U	72/72 (100%)	2.89	46 (63%) 0 0	117, 148, 161, 164	0
23	V	66/66 (100%)	0.35	8 (12%) 6 3	129, 141, 159, 163	0
24	W	55/55 (100%)	0.70	9 (16%) 2 1	95, 110, 126, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/57 (100%)	-0.12	1 (1%) 71 68	74, 82, 104, 112	0
26	1	54/54 (100%)	1.46	20 (37%) 0 0	125, 136, 152, 168	0
27	2	47/47 (100%)	0.21	1 (2%) 67 62	91, 108, 116, 117	0
28	3	65/65 (100%)	2.08	32 (49%) 0 0	107, 118, 127, 129	0
29	X	2780/2881 (96%)	-0.13	108 (3%) 43 36	51, 111, 221, 347	0
30	Y	122/122 (100%)	-0.53	4 (3%) 50 42	96, 136, 161, 172	0
All	All	6389/6490 (98%)	0.57	935 (14%) 3 2	51, 119, 242, 347	0

All (935) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	X	2137	C	31.1
29	X	1916	A	26.7
1	0	54	VAL	23.5
29	X	2112	G	20.1
1	0	86	GLY	19.9
29	X	1918	A	19.5
1	0	85	ALA	19.4
29	X	2144	U	18.6
29	X	1917	U	18.4
1	0	223	GLY	18.2
1	0	200	ALA	18.0
1	0	55	ARG	16.8
1	0	143	ALA	16.8
7	F	1	MET	16.8
1	0	14	LYS	15.5
29	X	2138	U	15.4
1	0	209	TYR	15.3
21	T	3	HIS	15.1
29	X	2113	U	14.1
29	X	1919	A	13.8
1	0	222	LEU	13.2
29	X	1914	C	13.0
7	F	25	PRO	12.8
1	0	208	ALA	12.6
1	0	164	THR	12.3
1	0	162	ASP	12.0
29	X	2145	U	12.0
1	0	69	ARG	11.8
1	0	42	ARG	11.7

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Mol	Chain	Res	Type	RSRZ
21	T	2	ALA	11.6
1	0	56	GLY	11.5
29	X	718	A	11.4
7	F	7	ILE	11.3
29	X	1507	A	11.3
1	0	102	GLY	11.3
29	X	2146	U	11.2
1	0	193	GLU	11.2
1	0	49	LYS	11.2
7	F	4	VAL	11.1
29	X	1508	C	11.0
21	T	6	GLY	11.0
29	X	2142	C	11.0
1	0	84	ALA	10.9
1	0	205	LEU	10.8
1	0	207	SER	10.8
1	0	204	PHE	10.6
1	0	203	VAL	10.5
7	F	136	VAL	10.4
29	X	2111	C	10.4
1	0	159	PHE	10.3
1	0	165	GLY	10.3
1	0	48	ARG	10.2
29	X	2143	U	10.1
29	X	2133	G	10.0
1	0	78	ASN	10.0
1	0	107	ASP	9.9
7	F	26	ALA	9.9
1	0	124	ALA	9.9
1	0	210	LEU	9.8
1	0	174	ALA	9.7
29	X	2125	G	9.5
1	0	39	VAL	9.5
29	X	1911	U	9.4
29	X	1915	U	9.3
29	X	2126	A	9.3
1	0	206	ARG	9.3
1	0	218	ILE	9.3
1	0	142	GLY	9.2
1	0	170	PRO	9.1
21	T	4	LYS	9.1
1	0	157	ILE	9.1

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Mol	Chain	Res	Type	RSRZ
1	0	90	VAL	9.1
1	0	163	LYS	9.0
29	X	1509	A	8.9
1	0	219	PRO	8.9
29	X	1173	A	8.9
1	0	194	GLY	8.9
13	L	40	ALA	8.8
7	F	12	LEU	8.8
1	0	198	GLY	8.7
1	0	87	ALA	8.6
1	0	103	PHE	8.6
29	X	2134	A	8.6
1	0	199	THR	8.5
7	F	5	ALA	8.5
1	0	82	ALA	8.4
1	0	113	PRO	8.4
1	0	189	ILE	8.4
1	0	13	ASN	8.4
1	0	19	ASP	8.3
1	0	28	LEU	8.3
1	0	88	ASP	8.3
1	0	99	ILE	8.3
29	X	717	C	8.3
1	0	67	SER	8.3
1	0	144	ASP	8.3
3	B	205	SER	8.2
22	U	28	GLY	8.2
29	X	716	A	8.2
1	0	217	SER	8.1
1	0	202	GLY	8.1
1	0	161	ASN	8.0
5	D	73	SER	8.0
1	0	136	PRO	8.0
29	X	2132	C	7.9
1	0	15	GLN	7.9
1	0	74	THR	7.9
21	T	5	LYS	7.9
29	X	2141	C	7.8
1	0	145	VAL	7.8
7	F	137	THR	7.8
7	F	96	VAL	7.7
13	L	53	ALA	7.7

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Mol	Chain	Res	Type	RSRZ
13	L	58	ALA	7.7
29	X	2796	U	7.5
1	0	196	LYS	7.5
20	S	92	VAL	7.5
1	0	50	SER	7.4
1	0	33	PHE	7.4
4	C	196	VAL	7.4
1	0	201	LYS	7.4
7	F	58	THR	7.3
1	0	216	PRO	7.3
1	0	53	ASN	7.3
7	F	18	THR	7.3
13	L	33	ARG	7.2
29	X	1912	A	7.2
22	U	16	ASN	7.2
1	0	44	GLY	7.1
1	0	89	VAL	7.1
29	X	715	G	7.0
7	F	6	GLY	7.0
7	F	2	ARG	7.0
1	0	121	GLN	7.0
1	0	6	LEU	7.0
29	X	1172(C)	G	6.9
1	0	100	ALA	6.9
1	0	140	THR	6.9
1	0	81	ALA	6.9
1	0	93	ASP	6.9
5	D	146	VAL	6.9
22	U	25	ARG	6.9
29	X	2139	G	6.9
7	F	67	PHE	6.9
1	0	146	ALA	6.8
1	0	129	PRO	6.8
7	F	29	GLN	6.8
7	F	20	ALA	6.7
29	X	2150	G	6.7
22	U	15	VAL	6.7
29	X	2110	G	6.7
5	D	31	ILE	6.7
22	U	75	TYR	6.6
7	F	23	VAL	6.6
29	X	2147	G	6.6

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Mol	Chain	Res	Type	RSRZ
13	L	59	LEU	6.6
1	0	92	SER	6.5
5	D	139	PRO	6.5
27	2	1	MET	6.5
28	3	23	MET	6.5
29	X	1536	C	6.5
1	0	40	HIS	6.4
1	0	101	GLY	6.4
7	F	66	THR	6.4
1	0	83	GLU	6.4
5	D	42	SER	6.4
1	0	80	GLN	6.4
1	0	79	VAL	6.4
20	S	15	ASP	6.4
29	X	1174	A	6.4
1	0	41	PHE	6.3
29	X	1910	G	6.3
7	F	27	LEU	6.3
29	X	1078	C	6.3
1	0	98	ARG	6.3
7	F	68	ILE	6.2
22	U	45	ASN	6.2
7	F	92	ASN	6.2
1	0	171	ILE	6.2
21	T	7	VAL	6.2
22	U	27	ASP	6.1
22	U	26	ALA	6.1
29	X	2602	A	6.1
22	U	52	ARG	6.1
7	F	95	LYS	6.1
1	0	47	PRO	6.1
7	F	119	SER	6.1
7	F	24	GLY	6.1
29	X	1920	C	6.1
1	0	122	LYS	6.0
1	0	120	GLY	6.0
1	0	135	ASN	6.0
1	0	20	GLU	6.0
1	0	134	PRO	6.0
13	L	12	ARG	6.0
1	0	95	LEU	5.9
5	D	62	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
7	F	138	VAL	5.9
29	X	2114	A	5.9
29	X	1175	G	5.9
1	0	91	GLY	5.9
17	P	134	LYS	5.9
5	D	71	LYS	5.9
1	0	180	ASN	5.9
18	Q	27	PHE	5.8
5	D	74	ILE	5.8
29	X	2797	A	5.8
22	U	12	ASN	5.8
1	0	197	PRO	5.8
7	F	94	ALA	5.7
1	0	76	GLY	5.7
7	F	32	ALA	5.7
21	T	71	ASN	5.7
13	L	54	ALA	5.7
1	0	141	VAL	5.7
30	Y	123	U	5.7
1	0	185	TYR	5.6
1	0	215	GLY	5.6
1	0	104	MET	5.6
1	0	45	ILE	5.6
5	D	72	LYS	5.5
22	U	13	LEU	5.5
29	X	2182	A	5.5
1	0	34	ASP	5.5
29	X	1913	A	5.5
7	F	101	TRP	5.5
13	L	14	ARG	5.5
1	0	147	GLY	5.5
28	3	55	TRP	5.5
1	0	57	THR	5.5
5	D	43	SER	5.4
1	0	188	LEU	5.4
30	Y	2	C	5.4
1	0	18	ILE	5.4
22	U	8	THR	5.4
7	F	113	PRO	5.4
29	X	2109	U	5.4
1	0	96	ILE	5.4
1	0	125	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
5	D	145	MET	5.3
6	E	123	PHE	5.3
7	F	120	VAL	5.3
10	I	74	VAL	5.3
20	S	74	ARG	5.3
28	3	51	ALA	5.3
21	T	69	PHE	5.3
1	0	75	LYS	5.3
28	3	22	VAL	5.3
7	F	143	ASN	5.2
1	0	123	LEU	5.2
1	0	114	ASP	5.2
1	0	106	PHE	5.2
1	0	119	ILE	5.1
22	U	57	VAL	5.1
1	0	7	GLU	5.1
1	0	4	ARG	5.1
4	C	20	PRO	5.1
5	D	61	THR	5.1
7	F	55	VAL	5.0
29	X	1075	C	5.0
7	F	37	PHE	5.0
5	D	66	ILE	5.0
10	I	67	ASN	5.0
1	0	73	ILE	5.0
7	F	30	TYR	5.0
7	F	56	GLU	5.0
7	F	62	ASP	5.0
5	D	141	ILE	5.0
13	L	51	LEU	5.0
1	0	117	ALA	4.9
29	X	2794	U	4.9
5	D	81	GLN	4.9
1	0	68	VAL	4.9
21	T	84	ALA	4.9
5	D	175	LEU	4.9
20	S	14	LEU	4.9
7	F	112	MET	4.9
7	F	3	ARG	4.8
28	3	16	ILE	4.8
1	0	32	LYS	4.8
7	F	43	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
10	I	51	GLY	4.8
1	0	151	GLY	4.8
7	F	57	ILE	4.8
7	F	142	PRO	4.8
22	U	60	VAL	4.8
21	T	82	GLU	4.8
1	0	11	ASP	4.8
7	F	14	ALA	4.8
20	S	11	LYS	4.8
1	0	97	GLU	4.7
7	F	121	GLU	4.7
13	L	39	TYR	4.7
21	T	49	GLN	4.7
29	X	1506	C	4.7
22	U	35	THR	4.7
29	X	2127	G	4.7
1	0	182	SER	4.6
4	C	150	LEU	4.6
16	O	72	ARG	4.6
26	1	21	TYR	4.6
26	1	22	TYR	4.6
29	X	2136	A	4.6
21	T	74	LYS	4.6
28	3	9	MET	4.6
1	0	126	LEU	4.6
5	D	136	LEU	4.6
1	0	17	SER	4.6
21	T	72	LYS	4.6
1	0	133	LEU	4.5
1	0	111	ALA	4.5
28	3	14	ILE	4.5
1	0	52	GLN	4.5
1	0	178	SER	4.5
5	D	99	PHE	4.5
10	I	48	PHE	4.5
5	D	65	PRO	4.5
22	U	44	ALA	4.5
29	X	2154	G	4.5
7	F	102	ASP	4.5
7	F	97	GLY	4.5
22	U	14	VAL	4.5
28	3	52	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
21	T	83	ALA	4.5
13	L	60	LYS	4.5
1	0	155	GLY	4.4
21	T	65	GLY	4.4
21	T	73	GLY	4.4
26	1	20	PHE	4.4
22	U	70	LEU	4.4
24	W	6	VAL	4.4
13	L	52	ALA	4.4
12	K	69	ASP	4.4
29	X	2181	G	4.4
29	X	2108	C	4.4
22	U	61	TRP	4.4
21	T	45	PHE	4.4
20	S	171	VAL	4.4
5	D	20	PHE	4.4
20	S	34	LEU	4.4
1	0	61	PRO	4.3
20	S	73	LYS	4.3
11	J	105	PHE	4.3
1	0	5	ALA	4.3
10	I	108	LEU	4.3
13	L	89	PHE	4.3
28	3	50	LEU	4.3
7	F	127	VAL	4.3
26	1	11	LYS	4.3
29	X	2135	A	4.3
1	0	118	GLN	4.3
28	3	10	ALA	4.3
16	O	74	TYR	4.3
29	X	2131	G	4.3
1	0	110	VAL	4.3
7	F	8	VAL	4.3
1	0	1	LYS	4.2
22	U	62	LEU	4.2
7	F	13	PRO	4.2
5	D	172	SER	4.2
6	E	133	VAL	4.2
6	E	163	ARG	4.2
29	X	1737	C	4.2
1	0	148	MET	4.2
28	3	25	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
8	G	112	THR	4.2
8	G	99	VAL	4.1
22	U	43	ARG	4.1
6	E	162	VAL	4.1
2	A	235	GLY	4.1
23	V	66	GLN	4.1
1	0	3	TYR	4.1
10	I	75	VAL	4.1
29	X	1074	G	4.1
1	0	115	MET	4.1
10	I	60	LEU	4.1
1	0	183	ALA	4.1
28	3	12	ARG	4.1
13	L	62	GLY	4.1
26	1	23	THR	4.1
7	F	34	ILE	4.1
2	A	147	LEU	4.1
24	W	50	LEU	4.1
1	0	156	ARG	4.0
1	0	116	MET	4.0
10	I	62	LYS	4.0
29	X	1537	G	4.0
1	0	172	GLY	4.0
1	0	220	LEU	4.0
5	D	125	ARG	4.0
1	0	36	THR	4.0
19	R	55	THR	4.0
5	D	36	VAL	3.9
22	U	24	ALA	3.9
29	X	2169	A	3.9
21	T	8	GLY	3.9
29	X	2178	C	3.9
22	U	10	LYS	3.9
22	U	69	THR	3.9
15	N	48	ARG	3.9
29	X	2180	U	3.9
29	X	2795	U	3.9
1	0	149	VAL	3.9
5	D	60	ILE	3.9
18	Q	94	GLN	3.9
7	F	83	GLY	3.9
7	F	51	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
13	L	93	SER	3.9
10	I	68	VAL	3.8
20	S	12	GLN	3.8
29	X	2170	A	3.8
5	D	169	LEU	3.8
26	1	1	ALA	3.8
7	F	125	ASN	3.8
28	3	54	GLU	3.8
29	X	2149	G	3.8
7	F	118	GLY	3.8
22	U	33	LYS	3.8
3	B	1	MET	3.8
11	J	119	PHE	3.8
22	U	47	HIS	3.8
1	0	10	VAL	3.8
18	Q	42	ILE	3.8
1	0	224	GLY	3.8
1	0	37	VAL	3.7
1	0	109	VAL	3.7
1	0	8	GLY	3.7
29	X	1921	G	3.7
6	E	168	GLN	3.7
7	F	22	PRO	3.7
13	L	30	SER	3.7
1	0	51	ASP	3.7
26	1	19	GLY	3.7
5	D	49	ALA	3.7
1	0	179	GLY	3.7
11	J	59	PHE	3.7
6	E	114	ILE	3.7
1	0	158	GLU	3.7
17	P	133	ASN	3.7
22	U	58	LYS	3.7
7	F	54	PRO	3.7
7	F	60	TYR	3.7
1	0	195	ALA	3.7
18	Q	84	GLU	3.7
1	0	152	LEU	3.7
20	S	65	LEU	3.7
29	X	2140	G	3.7
7	F	63	ARG	3.6
29	X	1079	C	3.6

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Mol	Chain	Res	Type	RSRZ
18	Q	12	ILE	3.6
26	1	13	GLU	3.6
2	A	111	LEU	3.6
13	L	31	VAL	3.6
10	I	69	GLY	3.6
7	F	44	GLN	3.6
7	F	140	GLY	3.6
6	E	105	MET	3.6
21	T	79	ILE	3.6
11	J	106	GLU	3.6
2	A	237	GLU	3.6
16	O	73	LYS	3.6
7	F	19	PRO	3.6
1	0	128	GLY	3.5
2	A	2	ALA	3.5
6	E	17	VAL	3.5
11	J	114	GLN	3.5
2	A	91	ARG	3.5
5	D	85	VAL	3.5
5	D	144	ASP	3.5
5	D	138	PHE	3.5
18	Q	91	LEU	3.5
1	0	62	HIS	3.5
26	1	39	LYS	3.5
1	0	60	LEU	3.5
29	X	2152	C	3.5
29	X	1510	U	3.5
8	G	100	TYR	3.5
2	A	12	SER	3.4
7	F	114	ASP	3.5
19	R	59	LYS	3.4
13	L	94	TYR	3.4
28	3	60	LEU	3.4
1	0	72	VAL	3.4
10	I	45	LYS	3.4
10	I	102	LYS	3.4
11	J	139	ASP	3.4
5	D	108	LEU	3.4
22	U	11	LYS	3.4
22	U	73	GLY	3.4
7	F	70	LYS	3.4
30	Y	43	G	3.4

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Mol	Chain	Res	Type	RSRZ
23	V	36	GLN	3.4
7	F	15	GLY	3.4
1	0	94	GLU	3.4
4	C	125	ILE	3.4
10	I	122	VAL	3.4
28	3	62	LEU	3.3
2	A	242	ALA	3.3
12	K	22	ARG	3.3
5	D	142	THR	3.3
1	0	184	ASN	3.3
21	T	20	TYR	3.3
22	U	23	LYS	3.3
20	S	114	ASP	3.3
28	3	30	ARG	3.3
29	X	2116	G	3.3
20	S	91	PRO	3.3
6	E	111	HIS	3.3
28	3	32	GLN	3.3
28	3	64	ARG	3.3
5	D	173	MET	3.3
20	S	1	MET	3.3
21	T	59	LEU	3.3
23	V	37	LEU	3.3
5	D	41	GLY	3.3
5	D	67	ILE	3.3
13	L	57	ALA	3.3
5	D	140	GLU	3.2
6	E	169	ILE	3.2
7	F	144	ALA	3.2
26	1	2	ALA	3.2
13	L	61	SER	3.2
28	3	21	LYS	3.2
5	D	76	ASN	3.2
29	X	1538	G	3.2
1	0	70	VAL	3.2
7	F	141	GLY	3.2
26	1	26	LYS	3.2
29	X	2107	U	3.2
7	F	91	PRO	3.2
13	L	34	SER	3.2
22	U	39	LYS	3.2
10	I	123	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
11	J	69	ILE	3.2
7	F	11	GLN	3.2
7	F	21	PRO	3.2
1	0	112	THR	3.2
4	C	123	PHE	3.2
22	U	51	ILE	3.2
7	F	123	ALA	3.2
20	S	83	PHE	3.2
29	X	2168	G	3.2
21	T	61	ALA	3.2
5	D	100	LEU	3.2
1	0	64	THR	3.2
11	J	36	ILE	3.1
1	0	31	ALA	3.1
21	T	66	LYS	3.1
7	F	61	ALA	3.1
15	N	47	TYR	3.1
29	X	2153	G	3.1
10	I	50	GLU	3.1
29	X	1535	U	3.1
6	E	89	LEU	3.1
1	0	190	SER	3.1
11	J	65	ILE	3.1
19	R	101	GLY	3.1
7	F	48	LYS	3.1
1	0	22	ALA	3.1
1	0	169	ALA	3.1
29	X	1176	C	3.1
5	D	29	PRO	3.1
29	X	1076	C	3.1
20	S	72	ASP	3.1
21	T	53	MET	3.1
26	1	6	PRO	3.1
1	0	127	LEU	3.1
1	0	77	GLU	3.1
7	F	84	ILE	3.1
15	N	25	TRP	3.0
6	E	173	ALA	3.0
28	3	46	LYS	3.0
11	J	26	ASP	3.0
15	N	12	ARG	3.0
24	W	7	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
29	X	2104	U	3.0
7	F	64	SER	3.0
4	C	180	ILE	3.0
5	D	168	ALA	3.0
29	X	1172(B)	C	3.0
5	D	34	ILE	3.0
7	F	35	MET	3.0
28	3	15	LYS	3.0
11	J	121	LEU	3.0
22	U	34	THR	3.0
13	L	9	ARG	3.0
20	S	66	VAL	3.0
11	J	37	ALA	3.0
18	Q	7	LEU	3.0
1	0	186	GLN	3.0
5	D	147	ASP	3.0
29	X	1540	A	2.9
13	L	29	LEU	2.9
20	S	3	LEU	2.9
10	I	73	GLU	2.9
20	S	123	VAL	2.9
24	W	1	MET	2.9
2	A	108	PRO	2.9
5	D	103	LEU	2.9
5	D	143	TYR	2.9
29	X	714	U	2.9
18	Q	48	VAL	2.9
3	B	3	GLY	2.9
7	F	99	LEU	2.9
11	J	118	ALA	2.9
20	S	51	LEU	2.9
10	I	103	ASN	2.9
28	3	66	LYS	2.9
5	D	59	LEU	2.9
9	H	134	LEU	2.9
13	L	18	ARG	2.9
20	S	33	ALA	2.9
1	0	173	LYS	2.9
2	A	275	LYS	2.9
21	T	52	GLY	2.9
28	3	58	MET	2.9
29	X	2187	C	2.9

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Mol	Chain	Res	Type	RSRZ
19	R	46	VAL	2.9
21	T	11	LYS	2.9
7	F	131	ALA	2.9
29	X	1026	U	2.9
7	F	17	ALA	2.9
28	3	61	MET	2.9
5	D	69	LYS	2.8
21	T	70	ILE	2.8
8	G	131	VAL	2.8
23	V	34	ALA	2.8
1	0	35	GLU	2.8
28	3	24	ALA	2.8
21	T	63	SER	2.8
1	0	160	ARG	2.8
1	0	191	ALA	2.8
11	J	100	PRO	2.8
13	L	84	ILE	2.8
5	D	58	ALA	2.8
5	D	176	PRO	2.8
6	E	159	GLY	2.8
15	N	20	ARG	2.8
5	D	89	VAL	2.8
6	E	37	TYR	2.8
28	3	53	ALA	2.8
5	D	109	PRO	2.7
11	J	126	LEU	2.7
7	F	110	THR	2.7
11	J	11	ARG	2.7
7	F	10	LEU	2.7
19	R	75	ALA	2.7
2	A	236	GLY	2.7
16	O	83	ARG	2.7
28	3	65	GLY	2.7
4	C	188	ILE	2.7
22	U	36	GLY	2.7
5	D	154	ILE	2.7
13	L	97	HIS	2.7
17	P	46	ARG	2.7
1	0	176	PHE	2.7
6	E	150	LYS	2.7
1	0	25	VAL	2.7
6	E	46	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
12	K	29	LEU	2.7
20	S	169	VAL	2.7
16	O	71	ILE	2.7
1	0	105	ASP	2.7
7	F	50	ASP	2.7
11	J	107	VAL	2.7
22	U	74	PRO	2.7
24	W	25	LEU	2.7
1	0	65	GLY	2.7
11	J	33	TYR	2.7
26	1	49	PHE	2.7
10	I	87	THR	2.7
2	A	106	LEU	2.7
20	S	93	GLU	2.7
9	H	11	ALA	2.7
20	S	54	ILE	2.7
6	E	175	LYS	2.7
7	F	28	GLY	2.7
29	X	2183	G	2.7
22	U	78	ILE	2.6
4	C	147	LYS	2.6
6	E	15	VAL	2.6
16	O	81	ARG	2.6
4	C	21	GLU	2.6
5	D	132	ILE	2.6
13	L	95	LYS	2.6
1	0	150	ARG	2.6
11	J	32	ASP	2.6
22	U	54	ASN	2.6
1	0	108	ALA	2.6
29	X	2129	C	2.6
5	D	135	GLN	2.6
10	I	72	TYR	2.6
10	I	104	ARG	2.6
11	J	103	VAL	2.6
19	R	68	GLY	2.6
22	U	65	ASN	2.6
9	H	1	MET	2.6
4	C	149	LEU	2.6
5	D	165	GLU	2.6
26	1	53	ALA	2.6
20	S	23	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
26	1	0	ALA	2.6
7	F	59	ILE	2.6
7	F	31	GLY	2.6
13	L	85	LYS	2.6
24	W	3	ILE	2.6
2	A	234	GLY	2.6
10	I	112	GLY	2.6
21	T	67	VAL	2.6
5	D	158	THR	2.5
29	X	1756	A	2.5
2	A	68	LYS	2.5
6	E	25	LYS	2.5
1	0	175	SER	2.5
7	F	33	ASN	2.5
1	0	63	GLY	2.5
1	0	211	THR	2.5
20	S	134	LEU	2.5
1	0	46	ASP	2.5
20	S	69	VAL	2.5
29	X	1077	A	2.5
5	D	56	GLU	2.5
4	C	17	LEU	2.5
14	M	54	VAL	2.5
11	J	117	GLU	2.5
28	3	20	GLY	2.5
14	M	104	LEU	2.5
23	V	2	LYS	2.5
11	J	7	ARG	2.5
6	E	115	ILE	2.5
2	A	190	TYR	2.5
19	R	57	ASN	2.5
10	I	76	LYS	2.5
18	Q	76	LYS	2.5
24	W	53	VAL	2.5
10	I	101	ARG	2.5
2	A	145	LEU	2.5
2	A	255	LYS	2.5
28	3	29	LYS	2.5
29	X	614	A	2.5
29	X	652	A	2.5
11	J	132	MET	2.5
28	3	2	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
10	I	113	GLU	2.5
29	X	2173	A	2.5
2	A	231	HIS	2.5
15	N	90	LEU	2.5
11	J	104	MET	2.4
29	X	2122	U	2.4
8	G	51	LEU	2.4
8	G	102	ARG	2.4
17	P	116	ILE	2.4
17	P	92	VAL	2.4
26	1	12	MET	2.4
23	V	35	GLY	2.4
13	L	11	LEU	2.4
7	F	41	PHE	2.4
7	F	82	ALA	2.4
1	0	192	LEU	2.4
6	E	27	LYS	2.4
11	J	101	GLY	2.4
6	E	156	ALA	2.4
24	W	51	LEU	2.4
6	E	43	VAL	2.4
19	R	60	PRO	2.4
9	H	8	LEU	2.4
11	J	60	ARG	2.4
3	B	54	LYS	2.4
8	G	41	TRP	2.4
11	J	99	LYS	2.4
1	0	132	LEU	2.4
7	F	109	LYS	2.4
6	E	122	THR	2.4
7	F	47	ASP	2.4
21	T	26	PHE	2.3
1	0	166	VAL	2.3
2	A	55	GLY	2.3
1	0	153	LYS	2.3
1	0	138	SER	2.3
7	F	105	LEU	2.3
6	E	167	GLU	2.3
29	X	2123	G	2.3
29	X	2334	G	2.3
1	0	2	ARG	2.3
10	I	30	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	105	ILE	2.3
17	P	107	ILE	2.3
21	T	9	SER	2.3
3	B	84	PHE	2.3
22	U	66	ALA	2.3
2	A	64	ILE	2.3
2	A	208	LYS	2.3
5	D	156	ILE	2.3
22	U	37	ILE	2.3
18	Q	62	ARG	2.3
22	U	56	GLN	2.3
24	W	17	VAL	2.3
1	0	177	GLU	2.3
17	P	108	PRO	2.3
5	D	57	LEU	2.3
16	O	70	TYR	2.3
2	A	241	GLY	2.3
7	F	52	ILE	2.3
22	U	76	LYS	2.3
3	B	94	ASP	2.3
2	A	104	TYR	2.3
16	O	80	TYR	2.3
19	R	76	LEU	2.3
21	T	41	ARG	2.3
5	D	137	ILE	2.3
18	Q	51	ILE	2.3
20	S	130	ILE	2.3
29	X	293	A	2.3
10	I	49	PHE	2.3
29	X	2148	G	2.3
6	E	160	LYS	2.3
26	1	52	ALA	2.3
10	I	96	TYR	2.3
11	J	10	PHE	2.3
23	V	30	PHE	2.3
2	A	40	THR	2.2
1	0	43	LEU	2.2
19	R	83	LEU	2.2
23	V	33	ALA	2.2
10	I	114	ILE	2.2
29	X	1092	C	2.2
22	U	20	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
11	J	19	THR	2.2
7	F	98	LYS	2.2
28	3	7	HIS	2.2
14	M	106	TYR	2.2
25	Z	56	GLN	2.2
7	F	130	THR	2.2
21	T	48	GLY	2.2
6	E	107	ILE	2.2
18	Q	37	GLU	2.2
11	J	102	ARG	2.2
28	3	36	LYS	2.2
29	X	2179	C	2.2
11	J	63	GLY	2.2
7	F	139	GLU	2.2
20	S	10	PRO	2.2
6	E	62	ARG	2.2
6	E	172	LYS	2.2
7	F	76	TYR	2.2
4	C	186	LEU	2.2
17	P	98	ASP	2.2
4	C	38	ARG	2.2
7	F	90	THR	2.2
21	T	37	LEU	2.2
10	I	56	LEU	2.2
26	1	37	LEU	2.2
21	T	10	SER	2.2
2	A	62	TYR	2.2
6	E	23	VAL	2.2
26	1	29	ARG	2.2
19	R	52	ASN	2.2
18	Q	38	ILE	2.2
9	H	75	VAL	2.2
22	U	72	LYS	2.2
15	N	40	LEU	2.2
19	R	40	LEU	2.2
20	S	172	LEU	2.2
1	0	12	ARG	2.2
2	A	239	ARG	2.2
8	G	98	LYS	2.2
5	D	25	VAL	2.2
5	D	101	GLU	2.1
22	U	53	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
4	C	143	ASP	2.1
15	N	39	LEU	2.1
2	A	221	GLN	2.1
29	X	2798	U	2.1
2	A	103	ARG	2.1
22	U	40	ARG	2.1
13	L	13	THR	2.1
15	N	57	PHE	2.1
1	O	221	ALA	2.1
17	P	105	ARG	2.1
2	A	16	MET	2.1
30	Y	14	C	2.1
4	C	148	VAL	2.1
21	T	25	LYS	2.1
20	S	120	LEU	2.1
17	P	45	ILE	2.1
5	D	105	ASN	2.1
7	F	93	LYS	2.1
7	F	124	ALA	2.1
13	L	79	ALA	2.1
5	D	134	GLU	2.1
21	T	85	GLN	2.1
6	E	128	PRO	2.1
5	D	16	LEU	2.1
13	L	75	LEU	2.1
8	G	106	TYR	2.1
15	N	53	LYS	2.1
11	J	67	ILE	2.1
29	X	2189	U	2.1
19	R	67	GLY	2.1
18	Q	29	VAL	2.1
19	R	100	ASP	2.1
7	F	122	ALA	2.1
10	I	58	ALA	2.1
20	S	84	TYR	2.1
11	J	39	GLU	2.1
20	S	30	VAL	2.1
7	F	103	GLN	2.0
6	E	95	ARG	2.0
1	O	38	GLU	2.0
20	S	13	LYS	2.0
6	E	41	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
7	F	65	PHE	2.0
2	A	233	HIS	2.0
13	L	49	GLN	2.0
6	E	101	LYS	2.0
6	E	109	TYR	2.0
8	G	109	GLY	2.0
8	G	101	THR	2.0
10	I	59	ARG	2.0
3	B	95	ILE	2.0
5	D	50	ILE	2.0
5	D	88	LYS	2.0
10	I	44	GLY	2.0
10	I	57	ILE	2.0
13	L	55	SER	2.0
20	S	79	ILE	2.0
7	F	40	ALA	2.0
26	1	4	ALA	2.0
29	X	2117	A	2.0
5	D	170	LEU	2.0
20	S	44	ARG	2.0
21	T	62	LEU	2.0
29	X	1909	C	2.0
29	X	2151	U	2.0
29	X	1539	A	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	MG	X	6158	1/1	0.86	2.46	137.84	114,114,114,114	0
31	MG	X	6036	1/1	0.94	0.84	68.71	82,82,82,82	0
31	MG	X	6169	1/1	0.94	0.57	64.22	101,101,101,101	0
31	MG	X	6011	1/1	0.86	0.45	61.47	89,89,89,89	0
31	MG	X	6147	1/1	0.87	1.00	59.12	82,82,82,82	0
31	MG	X	6112	1/1	0.94	0.68	55.61	84,84,84,84	0
31	MG	X	6142	1/1	0.86	0.77	55.05	89,89,89,89	0
31	MG	X	6014	1/1	0.78	0.42	51.05	91,91,91,91	0
31	MG	X	6118	1/1	0.93	0.72	49.43	90,90,90,90	0
31	MG	X	6063	1/1	0.96	1.29	45.95	87,87,87,87	0
31	MG	X	6180	1/1	0.77	1.58	39.84	101,101,101,101	0
31	MG	X	6056	1/1	0.92	0.88	37.40	85,85,85,85	0
31	MG	X	6057	1/1	0.87	0.99	35.04	93,93,93,93	0
31	MG	X	6091	1/1	0.94	1.11	30.96	88,88,88,88	0
31	MG	X	6013	1/1	0.83	0.57	29.03	76,76,76,76	0
31	MG	X	6121	1/1	0.79	0.80	28.44	99,99,99,99	0
31	MG	X	6001	1/1	0.92	0.56	28.42	69,69,69,69	0
31	MG	X	6072	1/1	0.85	0.55	27.26	102,102,102,102	0
31	MG	X	6040	1/1	0.94	0.78	24.98	80,80,80,80	0
31	MG	X	6019	1/1	0.91	0.80	21.60	77,77,77,77	0
31	MG	X	6066	1/1	0.86	1.07	21.45	84,84,84,84	0
31	MG	X	6125	1/1	0.97	0.46	21.03	123,123,123,123	0
31	MG	X	6023	1/1	0.87	0.52	20.86	97,97,97,97	0
31	MG	X	6093	1/1	0.51	0.69	20.29	106,106,106,106	0
31	MG	X	6185	1/1	0.95	0.59	19.04	109,109,109,109	0
31	MG	X	6060	1/1	0.97	0.68	18.05	80,80,80,80	0
31	MG	X	6004	1/1	0.92	0.35	15.58	76,76,76,76	0
31	MG	X	6135	1/1	0.86	0.75	15.29	91,91,91,91	0
31	MG	X	6058	1/1	0.76	0.52	14.49	97,97,97,97	0
31	MG	X	6024	1/1	0.93	0.61	14.32	87,87,87,87	0
31	MG	X	6070	1/1	0.96	0.58	13.52	107,107,107,107	0
31	MG	X	6017	1/1	0.91	0.48	13.23	83,83,83,83	0
31	MG	X	6008	1/1	0.88	0.42	11.77	81,81,81,81	0
31	MG	X	6151	1/1	0.86	0.34	11.47	98,98,98,98	0
31	MG	X	6062	1/1	0.94	0.41	11.36	85,85,85,85	0
31	MG	X	6006	1/1	0.81	0.48	11.02	69,69,69,69	0
31	MG	X	6016	1/1	0.84	0.35	10.88	77,77,77,77	0
31	MG	X	6041	1/1	0.70	0.35	10.81	83,83,83,83	0
31	MG	X	6059	1/1	0.90	0.45	10.29	87,87,87,87	0
31	MG	X	6018	1/1	0.82	0.46	10.26	74,74,74,74	0
31	MG	X	6020	1/1	0.77	0.34	10.10	79,79,79,79	0
31	MG	X	6007	1/1	0.93	0.46	9.93	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	MG	X	6140	1/1	0.91	1.02	8.58	97,97,97,97	0
31	MG	X	6022	1/1	0.80	0.40	7.87	77,77,77,77	0
31	MG	X	6035	1/1	0.89	0.43	7.82	86,86,86,86	0
31	MG	X	6054	1/1	0.95	0.54	7.23	92,92,92,92	0
31	MG	X	6002	1/1	0.93	0.33	6.46	78,78,78,78	0
31	MG	X	6071	1/1	0.91	0.39	6.20	81,81,81,81	0
31	MG	X	6117	1/1	0.78	0.36	5.70	90,90,90,90	0
31	MG	X	6084	1/1	0.92	0.30	3.98	93,93,93,93	0
31	MG	X	6051	1/1	0.91	0.39	3.84	69,69,69,69	0
31	MG	X	6092	1/1	0.93	0.26	3.57	93,93,93,93	0
31	MG	X	6078	1/1	0.94	0.57	1.90	93,93,93,93	0
31	MG	X	6030	1/1	0.85	1.19	-	83,83,83,83	0
31	MG	X	6190	1/1	0.84	1.32	-	129,129,129,129	0
31	MG	X	6155	1/1	0.83	0.33	-	115,115,115,115	0
31	MG	X	6065	1/1	0.96	0.61	-	81,81,81,81	0
31	MG	X	6109	1/1	0.85	0.31	-	101,101,101,101	0
31	MG	X	6165	1/1	0.88	0.98	-	99,99,99,99	0
31	MG	X	6021	1/1	0.90	0.70	-	75,75,75,75	0
31	MG	X	6153	1/1	0.96	0.62	-	113,113,113,113	0
31	MG	X	6150	1/1	0.94	0.69	-	111,111,111,111	0
31	MG	X	6085	1/1	0.77	0.36	-	101,101,101,101	0
31	MG	X	6128	1/1	0.93	0.81	-	97,97,97,97	0
31	MG	X	6113	1/1	0.77	0.53	-	115,115,115,115	0
31	MG	X	6144	1/1	0.65	0.36	-	87,87,87,87	0
31	MG	X	6163	1/1	0.93	0.37	-	156,156,156,156	0
31	MG	Y	201	1/1	0.87	0.85	-	112,112,112,112	0
31	MG	X	6034	1/1	0.88	0.81	-	90,90,90,90	0
31	MG	X	6010	1/1	0.92	0.83	-	69,69,69,69	0
31	MG	X	6111	1/1	0.77	0.70	-	98,98,98,98	0
31	MG	X	6152	1/1	0.95	0.93	-	112,112,112,112	0
31	MG	X	6106	1/1	0.94	0.54	-	80,80,80,80	0
31	MG	X	6098	1/1	0.65	1.03	-	97,97,97,97	0
31	MG	X	6183	1/1	0.58	0.71	-	105,105,105,105	0
31	MG	X	6069	1/1	0.96	0.51	-	91,91,91,91	0
31	MG	X	6045	1/1	0.92	1.02	-	89,89,89,89	0
31	MG	X	6101	1/1	0.93	0.88	-	89,89,89,89	0
31	MG	X	6176	1/1	0.88	0.50	-	107,107,107,107	0
31	MG	X	6191	1/1	0.74	1.56	-	101,101,101,101	0
31	MG	X	6175	1/1	0.64	0.41	-	121,121,121,121	0
31	MG	X	6075	1/1	0.91	0.85	-	103,103,103,103	0
31	MG	X	6131	1/1	0.94	0.86	-	101,101,101,101	0
31	MG	X	6139	1/1	0.95	0.54	-	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	6047	1/1	0.89	0.54	-	74,74,74,74	0
31	MG	Y	202	1/1	0.91	0.43	-	125,125,125,125	0
31	MG	X	6009	1/1	0.97	0.67	-	69,69,69,69	0
31	MG	X	6077	1/1	0.94	0.64	-	98,98,98,98	0
31	MG	Y	205	1/1	0.83	0.90	-	129,129,129,129	0
31	MG	X	6087	1/1	0.97	0.54	-	98,98,98,98	0
31	MG	X	6083	1/1	0.88	0.80	-	91,91,91,91	0
31	MG	X	6055	1/1	0.90	0.64	-	90,90,90,90	0
31	MG	X	6105	1/1	0.87	1.40	-	118,118,118,118	0
31	MG	X	6089	1/1	0.95	0.51	-	90,90,90,90	0
31	MG	X	6156	1/1	0.79	0.63	-	105,105,105,105	0
31	MG	X	6127	1/1	0.86	0.59	-	122,122,122,122	0
31	MG	X	6108	1/1	0.36	0.63	-	120,120,120,120	0
31	MG	X	6115	1/1	0.88	0.73	-	103,103,103,103	0
31	MG	X	6080	1/1	0.83	0.71	-	108,108,108,108	0
31	MG	X	6177	1/1	0.49	0.59	-	113,113,113,113	0
31	MG	X	6043	1/1	0.97	0.85	-	69,69,69,69	0
31	MG	X	6050	1/1	0.97	0.50	-	84,84,84,84	0
31	MG	X	6074	1/1	0.86	0.74	-	80,80,80,80	0
31	MG	X	6052	1/1	0.85	0.52	-	97,97,97,97	0
31	MG	X	6096	1/1	0.97	1.19	-	89,89,89,89	0
31	MG	X	6189	1/1	0.87	0.75	-	120,120,120,120	0
31	MG	X	6148	1/1	0.99	0.57	-	130,130,130,130	0
31	MG	X	6015	1/1	0.91	0.55	-	77,77,77,77	0
31	MG	X	6026	1/1	0.94	0.41	-	91,91,91,91	0
31	MG	X	6114	1/1	0.88	0.55	-	91,91,91,91	0
31	MG	X	6027	1/1	0.89	1.03	-	86,86,86,86	0
31	MG	X	6170	1/1	0.73	1.96	-	127,127,127,127	0
31	MG	X	6167	1/1	0.56	0.56	-	103,103,103,103	0
31	MG	X	6146	1/1	0.79	1.51	-	129,129,129,129	0
31	MG	X	6164	1/1	0.81	0.99	-	124,124,124,124	0
31	MG	X	6038	1/1	0.71	0.67	-	85,85,85,85	0
31	MG	X	6187	1/1	0.77	0.57	-	92,92,92,92	0
31	MG	X	6116	1/1	0.97	0.59	-	106,106,106,106	0
31	MG	X	6048	1/1	0.78	0.80	-	102,102,102,102	0
31	MG	X	6088	1/1	0.94	0.87	-	99,99,99,99	0
31	MG	X	6049	1/1	0.96	0.67	-	88,88,88,88	0
31	MG	X	6137	1/1	0.85	0.57	-	135,135,135,135	0
31	MG	X	6046	1/1	0.56	0.40	-	91,91,91,91	0
31	MG	X	6119	1/1	0.46	0.53	-	128,128,128,128	0
31	MG	X	6076	1/1	0.92	0.73	-	102,102,102,102	0
31	MG	X	6188	1/1	0.91	0.44	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	6138	1/1	0.75	0.77	-	94,94,94,94	0
31	MG	Y	204	1/1	0.87	0.96	-	109,109,109,109	0
31	MG	X	6095	1/1	0.92	0.85	-	79,79,79,79	0
31	MG	X	6032	1/1	0.94	0.34	-	78,78,78,78	0
31	MG	X	6166	1/1	0.96	0.73	-	106,106,106,106	0
31	MG	X	6044	1/1	0.94	0.29	-	73,73,73,73	0
31	MG	Y	203	1/1	0.97	0.96	-	102,102,102,102	0
31	MG	M	201	1/1	0.95	0.93	-	69,69,69,69	0
31	MG	X	6110	1/1	0.81	0.38	-	130,130,130,130	0
31	MG	X	6012	1/1	0.86	0.50	-	82,82,82,82	0
31	MG	X	6182	1/1	0.88	0.97	-	120,120,120,120	0
31	MG	X	6122	1/1	0.82	0.46	-	100,100,100,100	0
31	MG	X	6168	1/1	0.91	0.84	-	107,107,107,107	0
31	MG	X	6104	1/1	0.91	0.59	-	86,86,86,86	0
31	MG	X	6064	1/1	0.91	0.63	-	96,96,96,96	0
31	MG	X	6184	1/1	0.96	0.76	-	102,102,102,102	0
31	MG	X	6033	1/1	0.93	0.53	-	98,98,98,98	0
31	MG	X	6192	1/1	0.77	0.69	-	138,138,138,138	0
31	MG	X	6178	1/1	0.93	0.58	-	103,103,103,103	0
31	MG	X	6102	1/1	0.94	0.25	-	89,89,89,89	0
31	MG	X	6141	1/1	0.74	0.60	-	122,122,122,122	0
31	MG	X	6160	1/1	0.87	0.68	-	104,104,104,104	0
31	MG	X	6133	1/1	0.72	1.20	-	111,111,111,111	0
31	MG	X	6186	1/1	0.72	1.02	-	134,134,134,134	0
31	MG	X	6031	1/1	0.96	0.53	-	69,69,69,69	0
31	MG	X	6073	1/1	0.95	0.79	-	85,85,85,85	0
31	MG	X	6029	1/1	0.94	0.43	-	69,69,69,69	0
31	MG	X	6003	1/1	0.85	0.49	-	70,70,70,70	0
31	MG	X	6082	1/1	0.91	0.75	-	83,83,83,83	0
31	MG	X	6134	1/1	0.99	0.67	-	112,112,112,112	0
31	MG	X	6086	1/1	0.98	0.92	-	87,87,87,87	0
31	MG	X	6171	1/1	0.82	0.80	-	111,111,111,111	0
31	MG	X	6081	1/1	0.93	0.42	-	78,78,78,78	0
31	MG	X	6162	1/1	0.67	0.81	-	111,111,111,111	0
31	MG	X	6103	1/1	0.94	0.32	-	117,117,117,117	0
31	MG	X	6099	1/1	0.73	0.68	-	89,89,89,89	0
31	MG	X	6005	1/1	0.96	0.89	-	69,69,69,69	0
31	MG	X	6132	1/1	0.89	0.54	-	94,94,94,94	0
31	MG	X	6053	1/1	0.98	0.84	-	91,91,91,91	0
31	MG	X	6149	1/1	0.88	0.59	-	94,94,94,94	0
31	MG	X	6123	1/1	0.88	0.48	-	130,130,130,130	0
31	MG	X	6061	1/1	0.95	0.71	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	6129	1/1	0.93	0.89	-	104,104,104,104	0
31	MG	X	6068	1/1	0.94	0.66	-	90,90,90,90	0
31	MG	X	6090	1/1	0.83	0.45	-	117,117,117,117	0
31	MG	X	6174	1/1	0.85	0.71	-	87,87,87,87	0
31	MG	X	6130	1/1	0.94	0.67	-	108,108,108,108	0
31	MG	X	6100	1/1	0.83	0.58	-	97,97,97,97	0
31	MG	X	6145	1/1	0.94	0.20	-	104,104,104,104	0
31	MG	X	6124	1/1	0.87	1.13	-	107,107,107,107	0
31	MG	X	6097	1/1	0.93	1.25	-	93,93,93,93	0
31	MG	X	6161	1/1	0.93	0.68	-	95,95,95,95	0
31	MG	X	6120	1/1	0.93	1.03	-	102,102,102,102	0
31	MG	X	6028	1/1	0.84	0.33	-	88,88,88,88	0
31	MG	X	6173	1/1	0.85	1.90	-	102,102,102,102	0
31	MG	X	6143	1/1	0.86	1.04	-	100,100,100,100	0
31	MG	X	6025	1/1	0.97	0.45	-	83,83,83,83	0
31	MG	X	6179	1/1	0.61	0.54	-	117,117,117,117	0
31	MG	X	6172	1/1	0.84	0.66	-	124,124,124,124	0
31	MG	X	6037	1/1	0.89	0.41	-	86,86,86,86	0
31	MG	X	6126	1/1	0.94	1.19	-	94,94,94,94	0
31	MG	X	6181	1/1	0.97	0.32	-	121,121,121,121	0
31	MG	X	6039	1/1	0.89	1.17	-	104,104,104,104	0
31	MG	X	6136	1/1	0.83	0.81	-	122,122,122,122	0
31	MG	X	6079	1/1	0.95	0.35	-	102,102,102,102	0
31	MG	X	6107	1/1	0.79	0.75	-	113,113,113,113	0
31	MG	X	6159	1/1	0.49	0.44	-	111,111,111,111	0
31	MG	X	6154	1/1	0.83	1.09	-	113,113,113,113	0
31	MG	X	6042	1/1	0.98	0.59	-	83,83,83,83	0
31	MG	X	6094	1/1	0.94	0.45	-	92,92,92,92	0
31	MG	X	6157	1/1	0.82	0.31	-	111,111,111,111	0
31	MG	X	6067	1/1	0.91	0.49	-	79,79,79,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.