



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2024 – 09:47 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

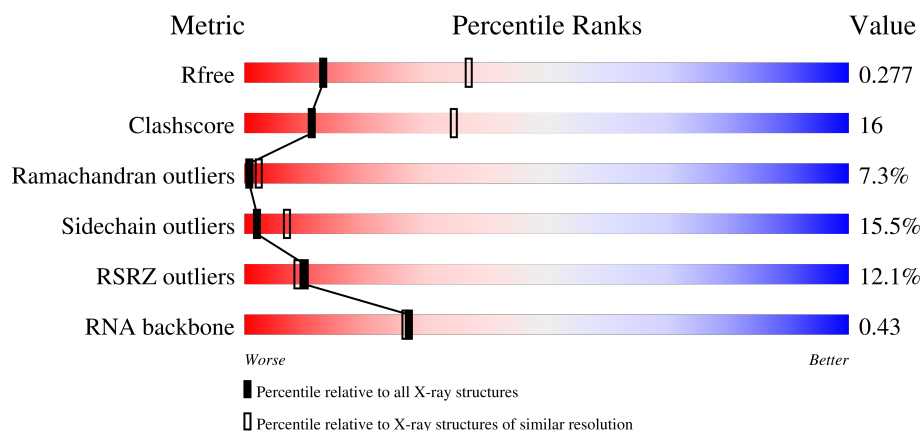
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)
RNA backbone	3690	1039 (3.10-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>26%</div> <div>54%</div> <div>38%</div> <div>8%</div> </div>
2	A	274	<div> <div>27%</div> <div>58%</div> <div>37%</div> <div>5%</div> </div>
3	B	205	<div> <div>6%</div> <div>53%</div> <div>40%</div> <div>7%</div> </div>
4	C	197	<div> <div>7%</div> <div>44%</div> <div>46%</div> <div>10%</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	6003	-	-	-	X
31	MG	X	6006	-	-	-	X
31	MG	X	6013	-	-	-	X
31	MG	X	6017	-	-	-	X
31	MG	X	6019	-	-	-	X
31	MG	X	6021	-	-	-	X
31	MG	X	6023	-	-	-	X
31	MG	X	6024	-	-	-	X
31	MG	X	6034	-	-	-	X
31	MG	X	6038	-	-	-	X
31	MG	X	6039	-	-	-	X
31	MG	X	6040	-	-	-	X
31	MG	X	6045	-	-	-	X
31	MG	X	6047	-	-	-	X
31	MG	X	6048	-	-	-	X
31	MG	X	6049	-	-	-	X
31	MG	X	6052	-	-	-	X
31	MG	X	6053	-	-	-	X
31	MG	X	6054	-	-	-	X
31	MG	X	6056	-	-	-	X
31	MG	X	6057	-	-	-	X
31	MG	X	6060	-	-	-	X
31	MG	X	6061	-	-	-	X
31	MG	X	6063	-	-	-	X
31	MG	X	6064	-	-	-	X
31	MG	X	6067	-	-	-	X
31	MG	X	6069	-	-	-	X
31	MG	X	6072	-	-	-	X
31	MG	X	6073	-	-	-	X
31	MG	X	6075	-	-	-	X
31	MG	X	6076	-	-	-	X
31	MG	X	6078	-	-	-	X
31	MG	X	6080	-	-	-	X
31	MG	X	6082	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6085	-	-	-	X
31	MG	X	6087	-	-	-	X
31	MG	X	6088	-	-	-	X
31	MG	X	6093	-	-	-	X
31	MG	X	6098	-	-	-	X
31	MG	X	6099	-	-	-	X
31	MG	X	6100	-	-	-	X
31	MG	X	6101	-	-	-	X
31	MG	X	6105	-	-	-	X
31	MG	X	6107	-	-	-	X
31	MG	X	6108	-	-	-	X
31	MG	X	6111	-	-	-	X
31	MG	X	6112	-	-	-	X
31	MG	X	6113	-	-	-	X
31	MG	X	6114	-	-	-	X
31	MG	X	6115	-	-	-	X
31	MG	X	6116	-	-	-	X
31	MG	X	6117	-	-	-	X
31	MG	X	6118	-	-	-	X
31	MG	X	6119	-	-	-	X
31	MG	X	6120	-	-	-	X
31	MG	X	6121	-	-	-	X
31	MG	X	6122	-	-	-	X
31	MG	X	6123	-	-	-	X
31	MG	X	6124	-	-	-	X
31	MG	X	6125	-	-	-	X
31	MG	X	6126	-	-	-	X
31	MG	X	6127	-	-	-	X
31	MG	X	6128	-	-	-	X
31	MG	X	6129	-	-	-	X
31	MG	X	6131	-	-	-	X
31	MG	X	6133	-	-	-	X
31	MG	X	6134	-	-	-	X
31	MG	X	6135	-	-	-	X
31	MG	X	6137	-	-	-	X
31	MG	X	6139	-	-	-	X
31	MG	X	6140	-	-	-	X
31	MG	X	6141	-	-	-	X
31	MG	X	6142	-	-	-	X
31	MG	X	6144	-	-	-	X
31	MG	X	6146	-	-	-	X
31	MG	X	6147	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6148	-	-	-	X
31	MG	X	6149	-	-	-	X
31	MG	X	6150	-	-	-	X
31	MG	X	6153	-	-	-	X
31	MG	X	6158	-	-	-	X
31	MG	X	6160	-	-	-	X
31	MG	X	6161	-	-	-	X
31	MG	X	6162	-	-	-	X
31	MG	X	6163	-	-	-	X
31	MG	X	6164	-	-	-	X
31	MG	X	6165	-	-	-	X
31	MG	X	6166	-	-	-	X
31	MG	X	6167	-	-	-	X
31	MG	X	6168	-	-	-	X
31	MG	X	6169	-	-	-	X
31	MG	X	6170	-	-	-	X
31	MG	X	6171	-	-	-	X
31	MG	X	6172	-	-	-	X
31	MG	X	6173	-	-	-	X
31	MG	X	6176	-	-	-	X
31	MG	X	6177	-	-	-	X
31	MG	X	6179	-	-	-	X
31	MG	X	6180	-	-	-	X
31	MG	X	6182	-	-	-	X
31	MG	X	6183	-	-	-	X
31	MG	X	6184	-	-	-	X
31	MG	X	6186	-	-	-	X
31	MG	X	6189	-	-	-	X
31	MG	X	6190	-	-	-	X
31	MG	X	6192	-	-	-	X
31	MG	Y	201	-	-	-	X
31	MG	Y	204	-	-	-	X
31	MG	Y	205	-	-	-	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			

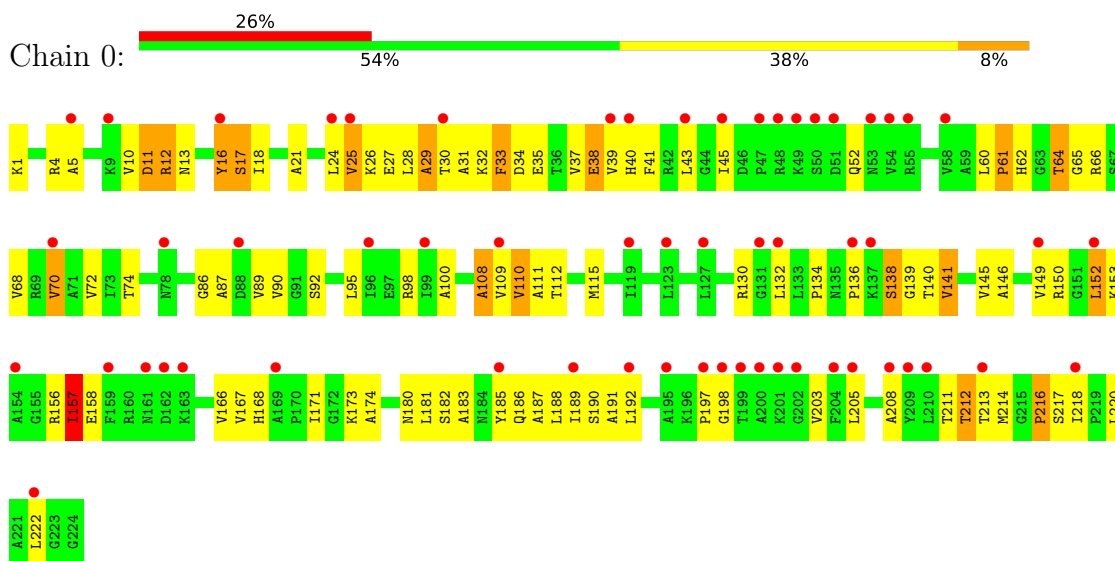
- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

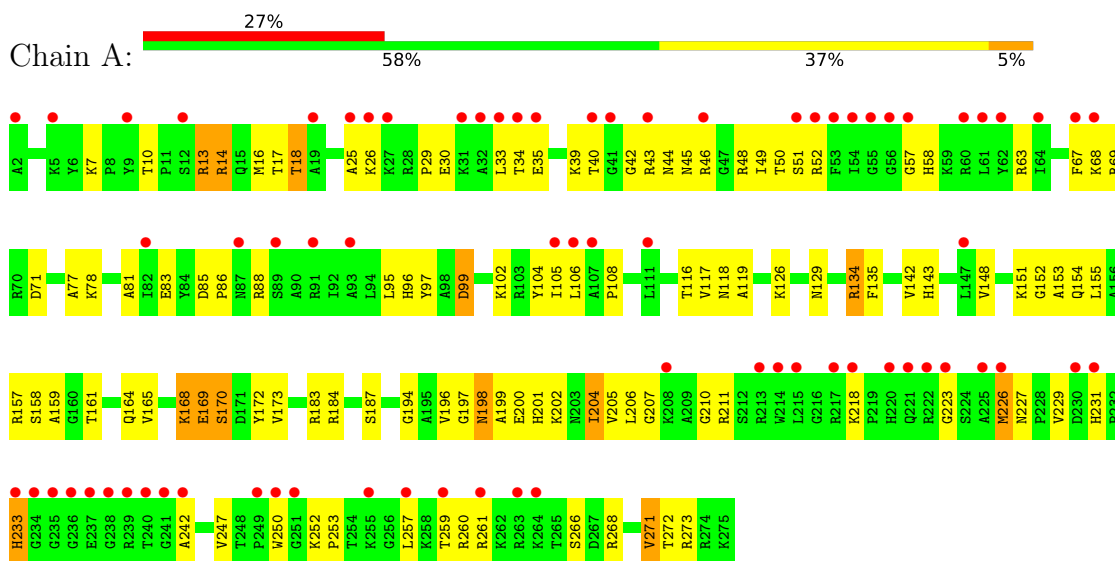
3 Residue-property plots

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

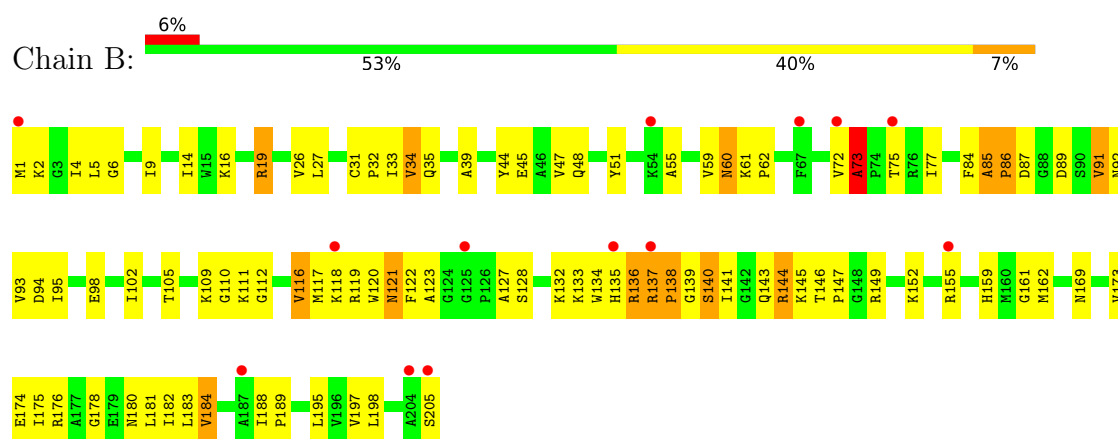
• Molecule 1: 50S ribosomal protein L1



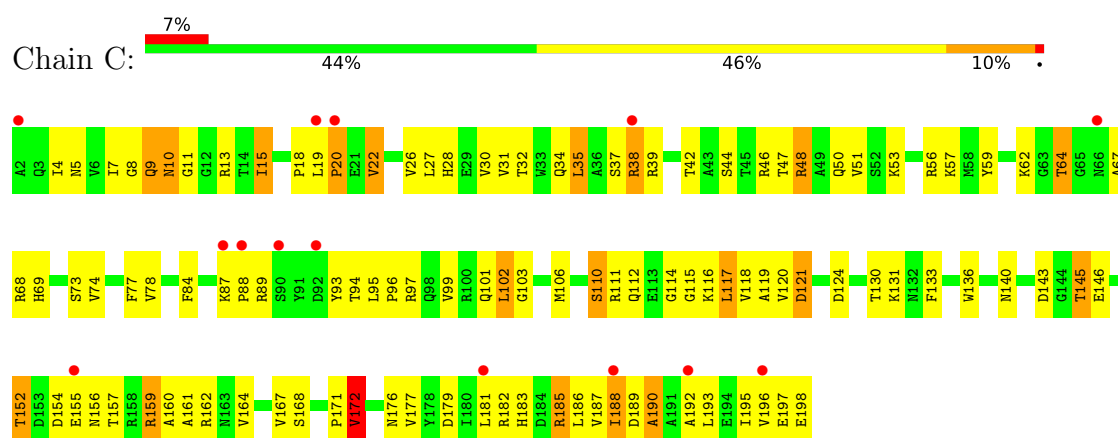
• Molecule 2: 50S ribosomal protein L2



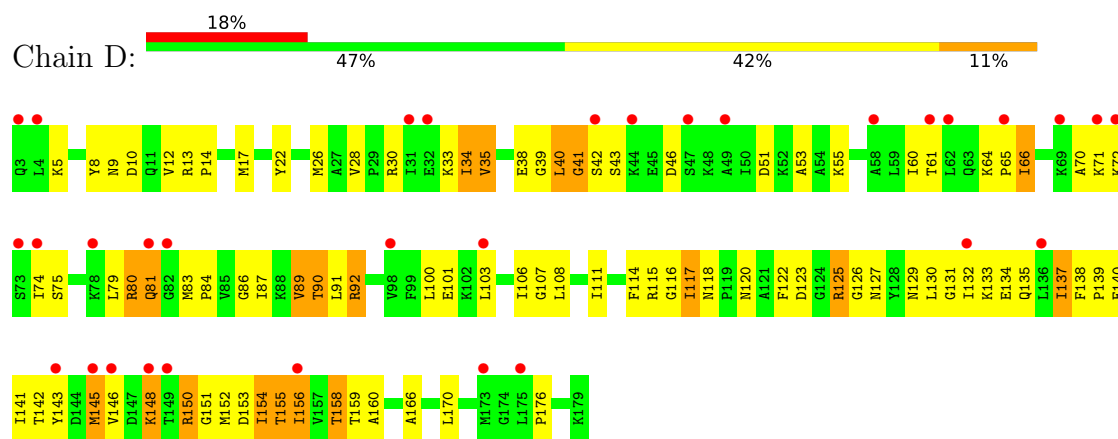
• Molecule 3: 50S ribosomal protein L3



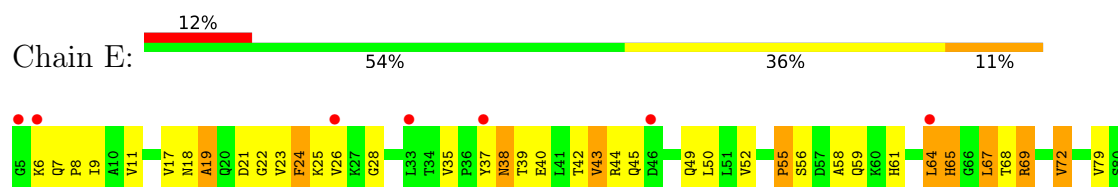
• Molecule 4: 50S ribosomal protein L4

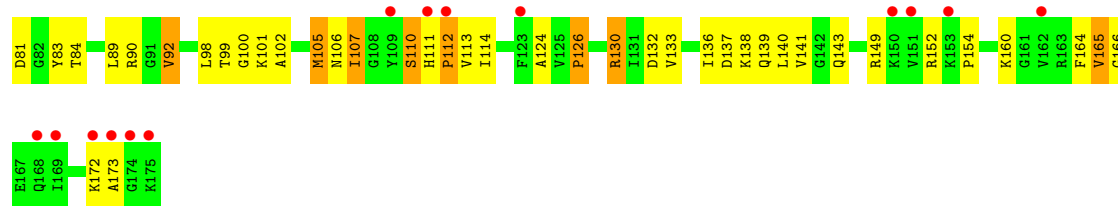


• Molecule 5: 50S ribosomal protein L5

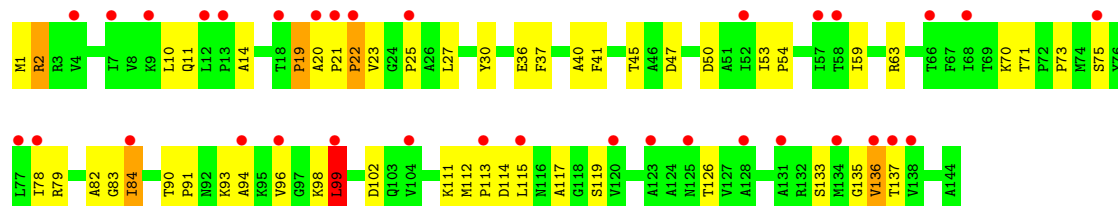


• Molecule 6: 50S ribosomal protein L6

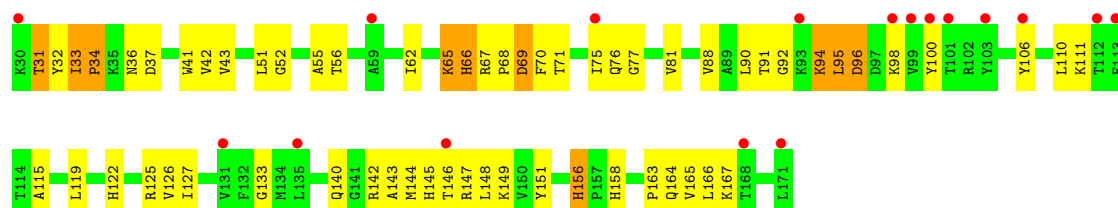




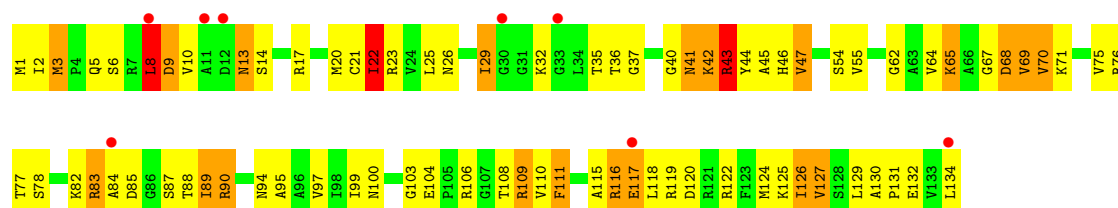
• Molecule 7: 50S ribosomal protein L11



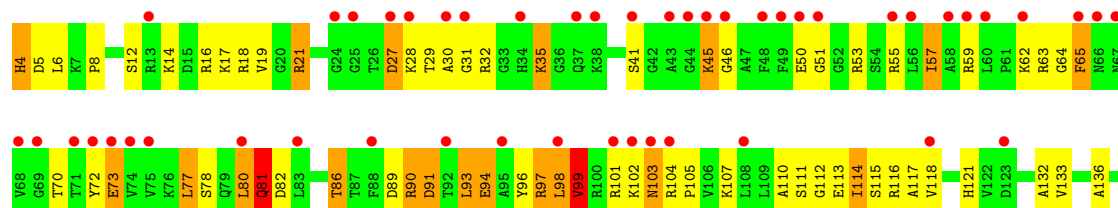
• Molecule 8: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L14

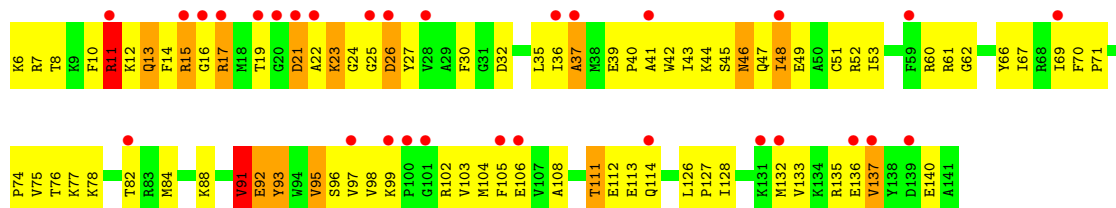


• Molecule 10: 50S ribosomal protein L15

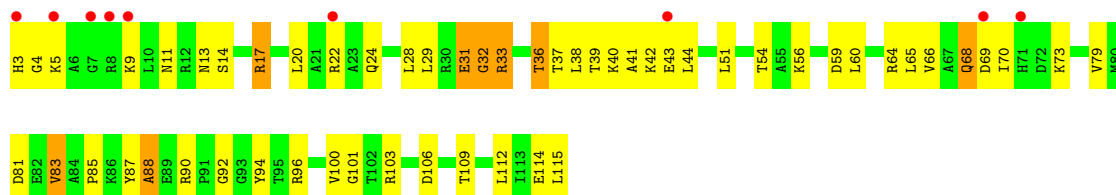




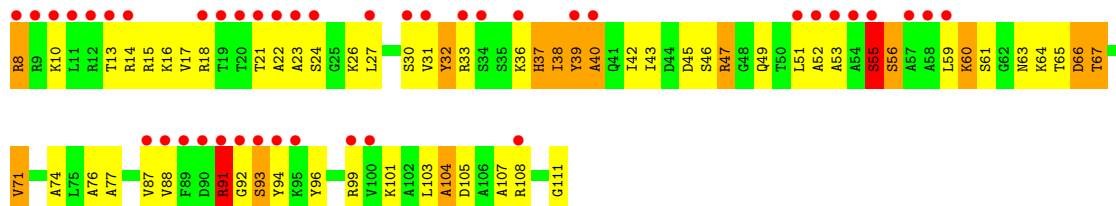
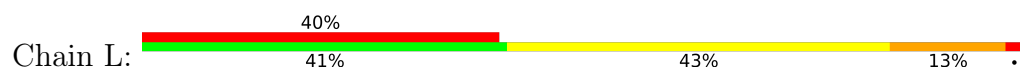
- Molecule 11: 50S ribosomal protein L16



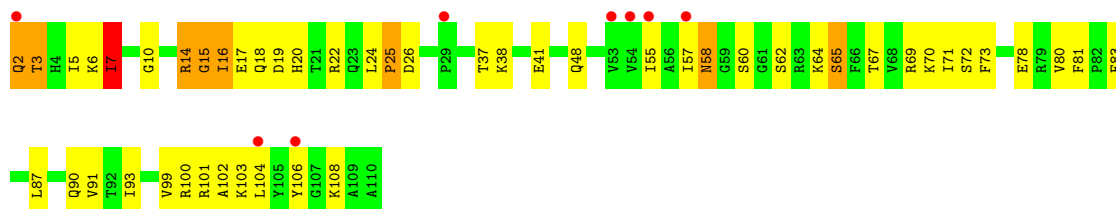
- Molecule 12: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L18

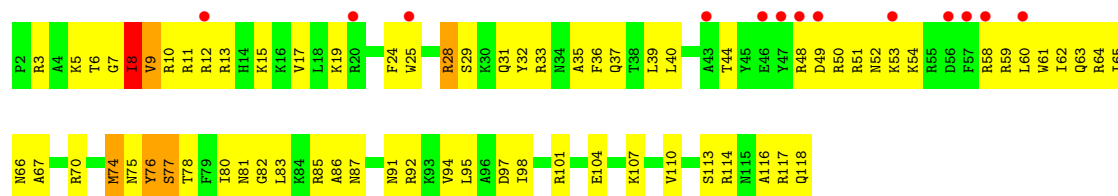


- Molecule 14: 50S ribosomal protein L19

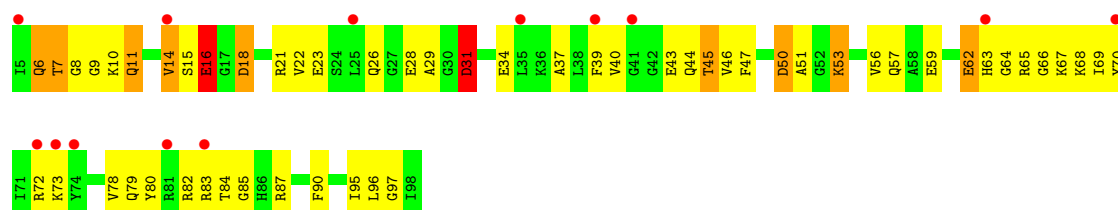
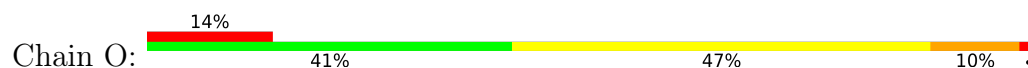


- Molecule 15: 50S ribosomal protein L20

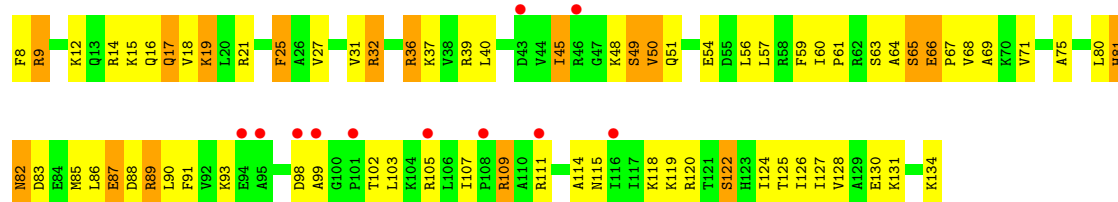
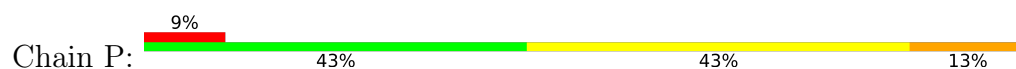




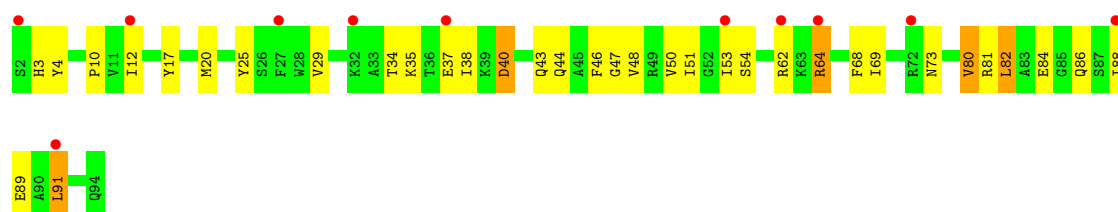
• Molecule 16: 50S ribosomal protein L21



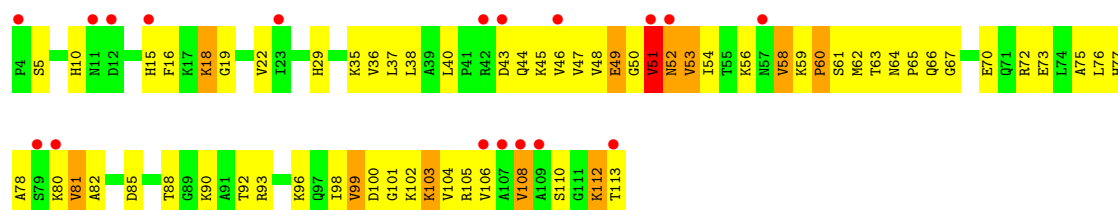
• Molecule 17: 50S ribosomal protein L22



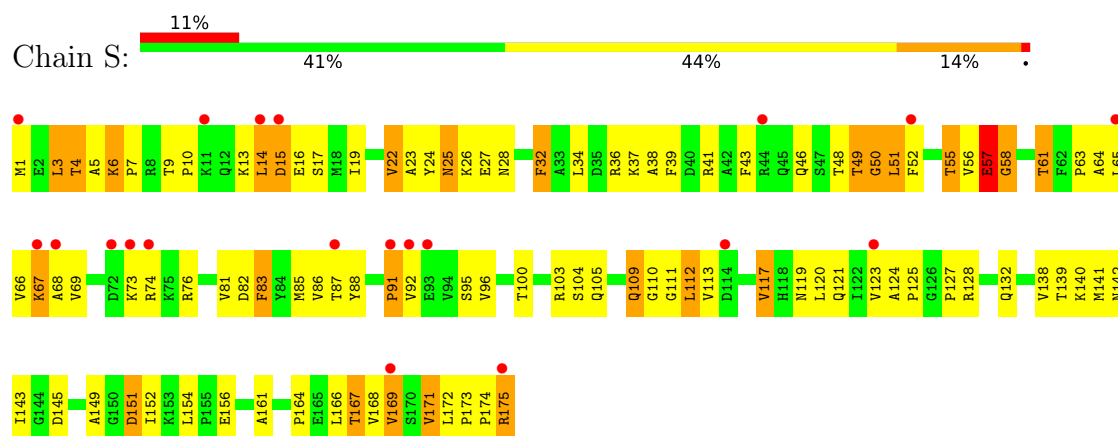
• Molecule 18: 50S ribosomal protein L23



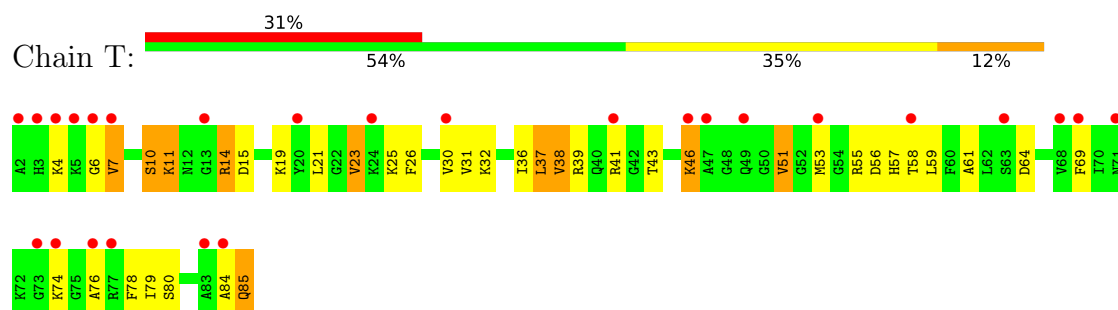
• Molecule 19: 50S ribosomal protein L24



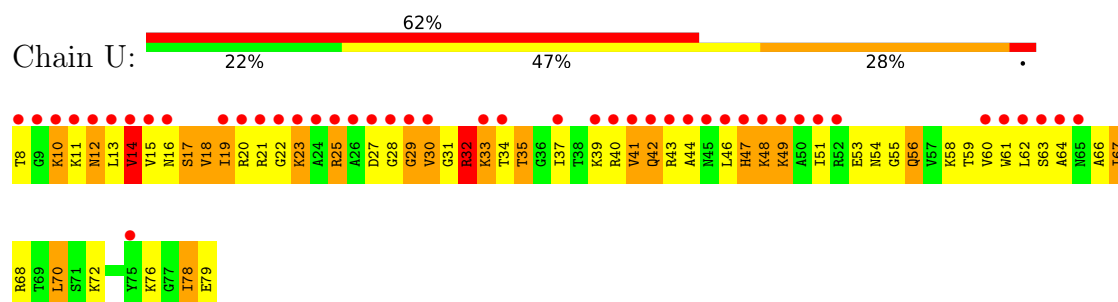
- Molecule 20: 50S ribosomal protein L25



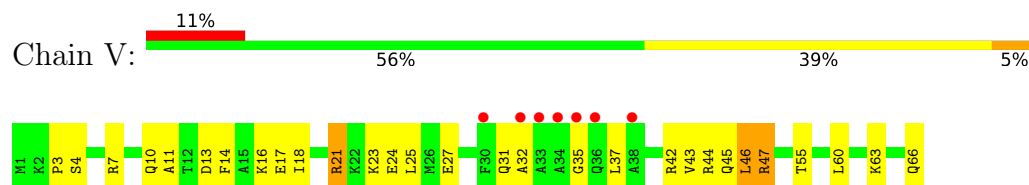
- Molecule 21: 50S ribosomal protein L27



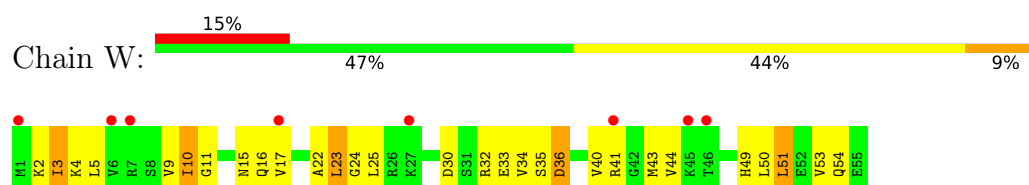
- Molecule 22: 50S ribosomal protein L28



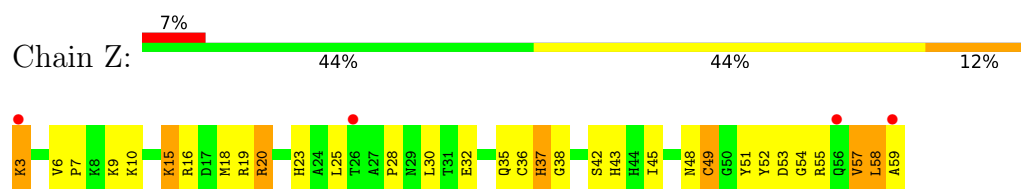
- Molecule 23: 50S ribosomal protein L29



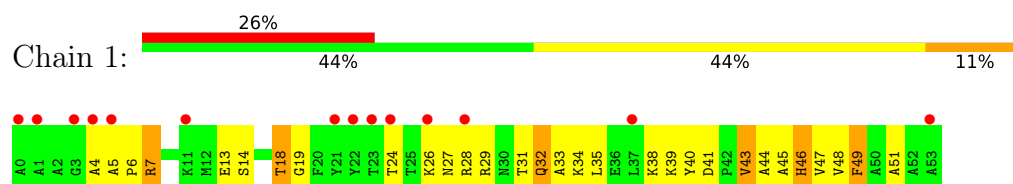
- Molecule 24: 50S ribosomal protein L30



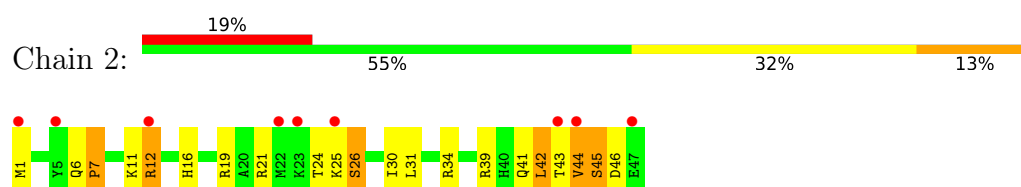
- Molecule 25: 50S ribosomal protein L32



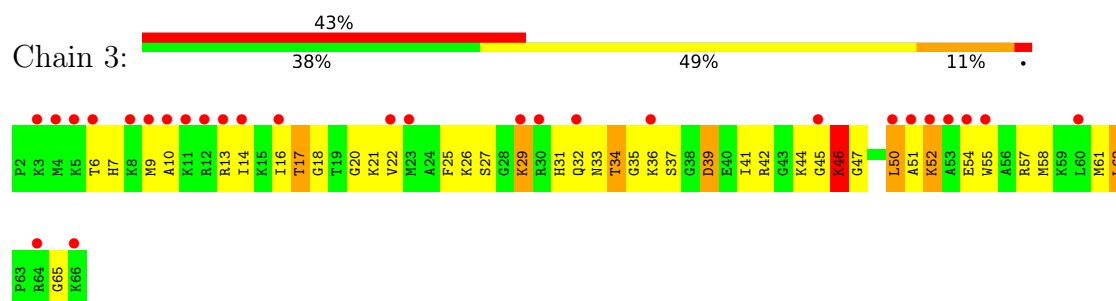
- Molecule 26: 50S ribosomal protein L33



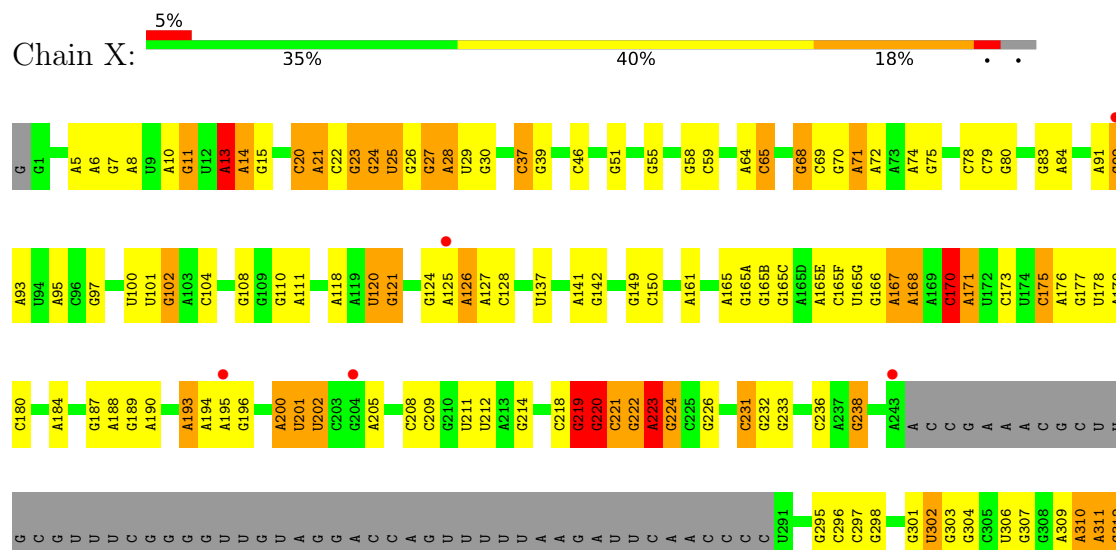
- Molecule 27: 50S ribosomal protein L34

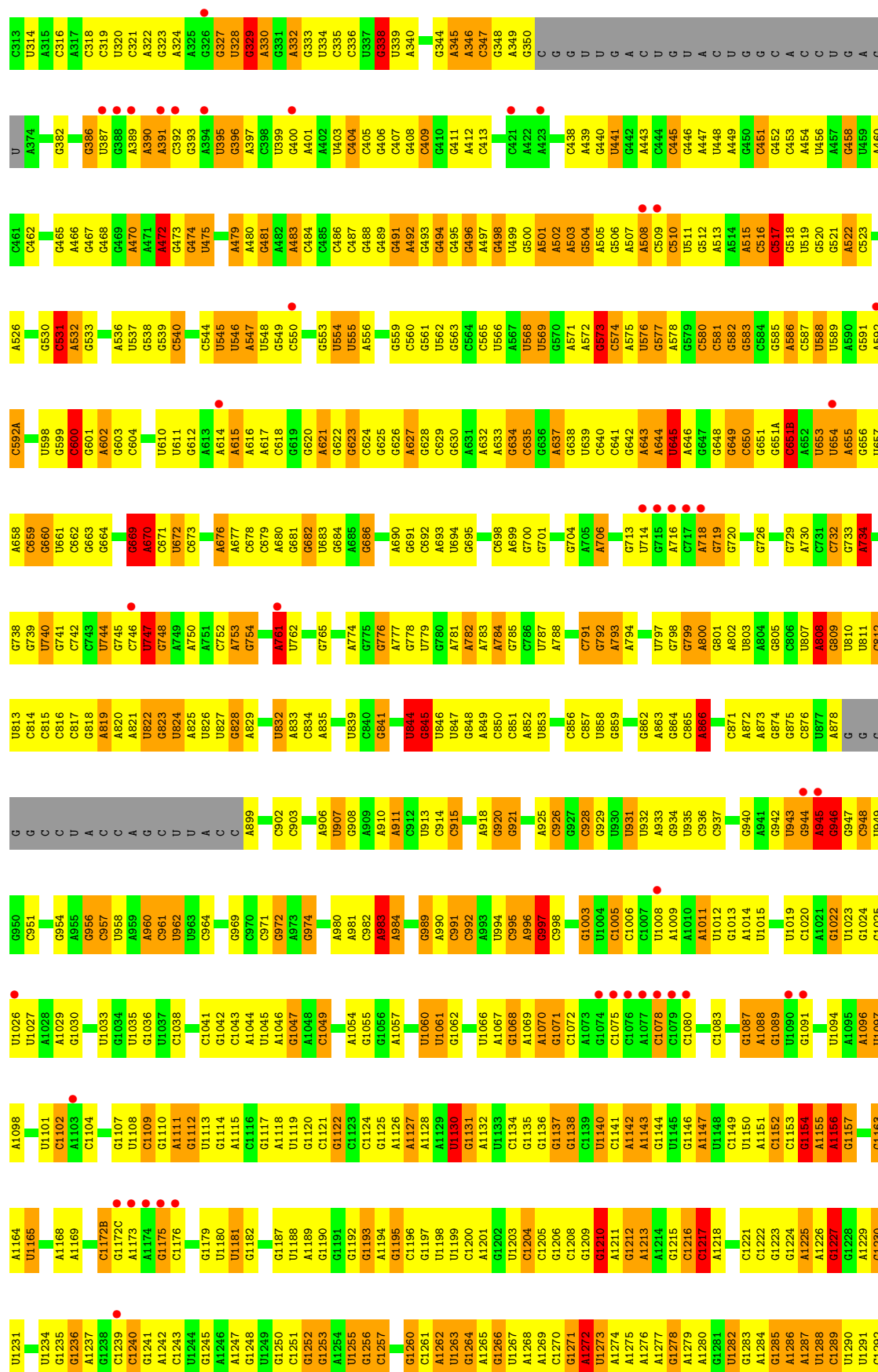


- Molecule 28: 50S ribosomal protein L35

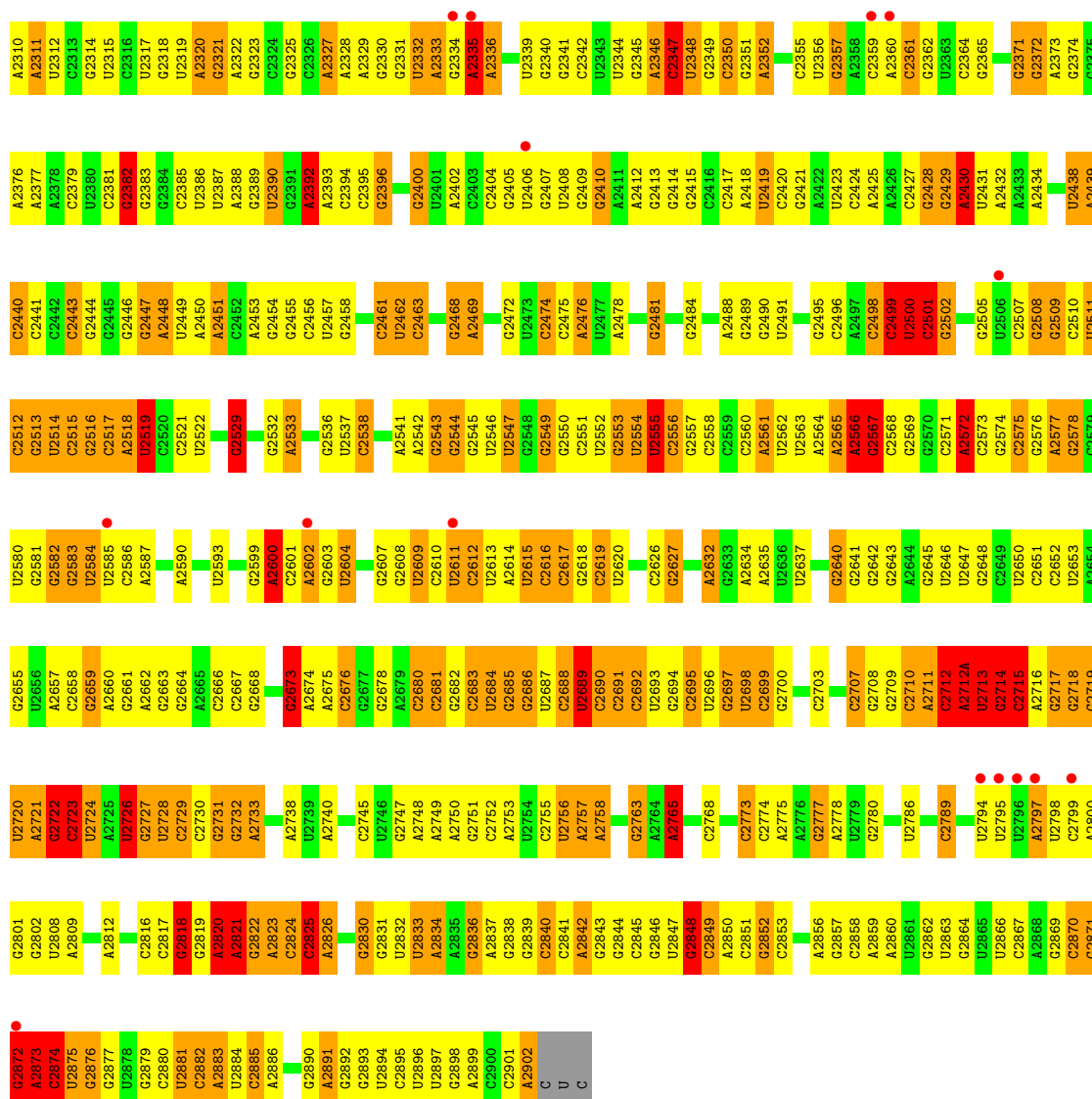


- Molecule 29: 23S ribosomal RNA



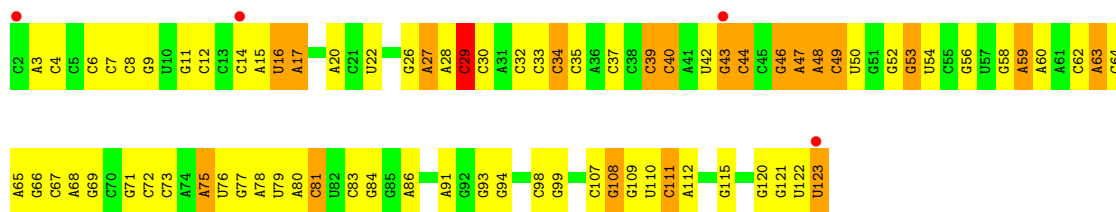


U2244	U2167	U2098	G2023	G1954	G1879	G1799	C1729	A1637	U1547	G1369	U1298
A2247	G2168	G2099	G2024	U1985	U1880	C1800	C1730	C1638	G1547	C1370	U1294
C2248	A2169	G2100	C2025	U1956	G1881	C1801	A1731	A1639	G1557	G1371	C1296
U2249	A2170	U2026	U2026	C1957	G1882	C1882	U1734	A1640	U1465	G1372	C1297
G2250	A2171	G2101	G2027	C1958	G1883	A1905	U1735	A1641	C1559	A1373	C1298
G2251	U2172	G2102	U2028	U1963	A1884	C1906	U1736	G1642	G1468	G1378	G1299
G2252	A2173	U2108	A2029	A1885	A1885	G1907	U1737	G1643	U1474	A1378	G1299
G2253	C2174	U2109	A2030	C1965	A1886	A1908	G1738	C1644	U1477	U1379	U1300
G2254	A2175	G2110	G2031	U1966	A1887	A1810	G1739	G1645	A1567	G1390	A1301
G2255	A2176	C2111	G2032	C1967	G1888	G1811	G1740	C1646	A1569	U1478	
G2256	C2177	U2112	G2035	G1968	U1892	U1812	U1741	G1647	A1570	A1384	G1309
G2257	C2178	U2113	C2036	A1969	U1893	G1813	U1742	G1648	G1480	U1390	U1312
G2258	C2179	A2114	G2037	A1970	G1814	G1745	G1746	G1649	G1481	C1391	U1313
G2259	A2182	G2115	G2038	A1900	A1915	C1746	U1747	A1650	G1482	C1392	C1314
C2260	G2116	G2116	U1971	A1901	C1816	G1747	A1652	A1651	A1483	A1393	U1315
C2261	G2117	G2117	A1902	C1902	G1817	C1748	A1653	G1652	U1484	A1394	U1316
U2262	G2118	U2118	C2043	G1903	G1818	A1749	U1749	A1654	U1584	A1395	G1317
C2263	U2119	U2119	G2044	G1904	U1818	U1750	U1750	A1655	G1486	G1318	G1318
G2264	A2186	G2120	C2045	C1905	A1819	G1751	U1751	A1656	G1487	G1405	G1319
G2265	C2187	G2121	G2046	G1906	U1820	G1752	U1752	C1657	G1488	G1406	G1320
A2266	U2188	U2122	U2047	G1907	A1921	A1753	U1753	C1658	U1489	U1412	A1321
A2267	G2189	G2123	A2047	C1908	G1822	A1754	A1754	U1659	C1490	G1413	A1322
A2268	G2190	G2124	A2048	C1909	G1823	U1755	U1755	C1660	A1491	G1414	G1323
A2269	G2191	G2125	G2049	G1910	G1824	A1756	U1756	G1661	U1592	G1415	G1324
U2270	G2192	G2126	C2050	U1911	U1825	G1757	U1757	U1662	A1493	A1416	G1325
G2271	U2194	A2126	A2051	A1912	G1826	G1758	U1758	A1663	A1494	U1417	C1327
U2272	U2195	C2128	G2052	A1913	U1827	C1759	U1759	A1664	A1495	G1418	C1328
A2273	C2196	G2129	G2053	C1914	G1828	C1760	U1760	A1665	U1496	G1422	C1329
A2274	U2197	U2130	U1991	U1915	A1829	G1761	U1761	G1666	U1497	A1423	C1330
C2275	A2198	U2131	C2055	U1916	A1832	A1762	U1762	C1667	U1499	A1424	C1331
G2276	G2203	G2132	G2056	U1917	C1833	G1763	U1763	A1668	U1500	G1332	C1332
G2277	A2204	G2133	A2057	A1918	U1834	U1770	U1770	A1669	C1501	A1427	A1336
A2278	G2205	A2135	A2058	A1919	G1835	C1771	U1771	U1673	C1502	C1428	G1337
G2279	A2210	G2136	G2060	G1921	U1836	U1772	U1772	G1674	G1503	G1429	G1337
G2280	A2211	G2137	G2061	A1997	C1838	A1773	U1773	C1675	G1504	C1430	G1338
G2281	G2211	U2138	A2062	C1999	G1839	U1774	U1774	A1676	U1505		
U2213	U2213	U2139	C2063	G2000	G1840	U1775	U1775	A1677	C1506	C1435	A1341
U2217	U2217	G2140	C2064	A2001	U1841	G1776	U1776	U1678	A1507	G1436	A1342
U2218	U2218	C2141	C2065	A1927	G1842	U1777	U1777	C1679	C1508	G1437	G1343
U2219	U2219	C2142	G2002	A1928	C1843	U1778	U1778		A1509	U1440	U1344
G2220	G2220	U2143	G2003	G1929	U1848	A1780	A1780	C1684	U1510	G1345	C1345
G2221	G2221	U2144	G2004	U1931	A1849	C1781	C1781	C1685	G1511	C1440A	G1346
G2222	G2222	U2145	C2005	U1932	G1850	C1782	U1782	C1686	U1444	A1353	A1353
G2223	G2223	U2146	G2006	A1933	U1851	A1783	U1783	G1687	G1445	G1355	G1355
G2224	A2224	G2147	A2071	A1938	C1852	U1784	U1784	U1688	U1525	G1450	G1356
A2225	U2225	G2148	G2072	U1939	A1853	A1785	A1785	G1694	G1526	C1451	U1357
U2229	U2229	U2149	U2075	U1940	A1854	A1786	U1786	G1695	G1529	U1452	U1358
G2230	G2230	U2150	U2076	C1941	G1858	U1787	U1787	G1696	U1532	C1453	A1359
U2233	U2233	C2152	A2077	C1942	U1943	C1788	U1788	G1697	C1533	U1454	G1360
G2234	G2234	G2153	A2014	U1943	G1862	U1789	U1789	A1698	C1534	G1455	G1361
G2235	U2235	G2154	U2016	G1945	U1863	C1790	U1790	G1699	U1535		
G2236	U2236	U2155	U2017	G1945	U1864	A1791	U1791	A1700	U1536		
G2237	U2237	G2156	U2018	G1945	G1874	A1794	U1794	A1701	U1537	U1458	A1365
G2238	U2238	G2157	A2090	G1949	G1875	C1795	C1795	U1726	U1538	U1459	A1366
G2239	U2239	A2158	U2091	G1950	G1876	U1796	U1796	C1727	G1539	U1460	C1367
G2240	U2240	G2159	U2092	U1951	A1877	C1797	U1797	C1728	G1546		G1368
A2309	A2309	C2164	G2094	A1953	G1878	U1798	U1798				



• Molecule 30: 5S ribosomal RNA

Chain Y: 3% 36% 47% 16%



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	0.61 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.270 0.243 , 0.277	Depositor DCC
R_{free} test set	24732 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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 2.28% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	O	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	N1-C6-O6	-5.71	116.48	119.90
29	X	1674	G	OP1-P-OP2	5.71	128.16	119.60
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-O3'	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-O3'	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	O	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
14:M:2:GLN:N	29:X:2820:A:N1	2.26	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
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
9:H:75:VAL:HG12	9:H:118:LEU:HD21	1.59	0.82
22:U:20:ARG:HB3	22:U:43:ARG:HD2	1.61	0.82
4:C:95:LEU:HD12	4:C:96:PRO:HD2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:34:THR:OG1	29:X:2420:C:OP1	1.98	0.81
13:L:37:HIS:ND1	30:Y:30:C:OP1	2.12	0.81
29:X:2689:U:O2	29:X:2713:U:H5''	1.81	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
17:P:60:ILE:HD11	25:Z:28:PRO:HD3	1.63	0.79
29:X:309:A:N3	29:X:329:G:O2'	2.15	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
16:O:7:THR:HB	16:O:22:VAL:HG11	1.66	0.77
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
29:X:679:C:H2'	29:X:680:A:H8	1.49	0.77
10:I:94:GLU:HA	10:I:97:ARG:HH11	1.50	0.77
20:S:168:VAL:HG12	20:S:169:VAL:H	1.48	0.77
11:J:15:ARG:HG3	11:J:74:PRO:HD2	1.66	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
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
22:U:23:LYS:HB3	22:U:37:ILE:HG22	1.67	0.76
30:Y:16:U:H1'	30:Y:109:G:H21	1.48	0.76
9:H:69:VAL:HG12	9:H:70:VAL:H	1.50	0.76
10:I:21:ARG:HH22	29:X:587:C:P	2.09	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
19:R:58:VAL:HG13	19:R:60:PRO:HD2	1.67	0.76
29:X:165(E):A:H2'	29:X:165(F):C:C6	2.21	0.76
5:D:150:ARG:HH21	29:X:2305:U:H3	1.30	0.76
25:Z:35:GLN:O	25:Z:37:HIS:N	2.18	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
4:C:136:TRP:O	4:C:140:ASN:ND2	2.18	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
25:Z:19:ARG:HA	29:X:2046:G:H5'	1.67	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
6:E:89:LEU:HD21	6:E:105:MET:HE1	1.69	0.75
24:W:23:LEU:HD21	24:W:43:MET:HB3	1.67	0.75
29:X:1626:A:H61	29:X:1639:U:H3	1.32	0.75
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
22:U:32:ARG:H	22:U:32:ARG:NE	1.84	0.74
23:V:63:LYS:HA	23:V:66:GLN:HG3	1.67	0.74
5:D:108:LEU:HD23	5:D:111:ILE:HD12	1.69	0.74
29:X:10:A:H2'	29:X:11:G:C8	2.22	0.74
3:B:134:TRP:CD1	3:B:137:ARG:HB2	2.22	0.74
17:P:80:LEU:HD11	17:P:87:GLU:HG3	1.69	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
10:I:17:LYS:HD2	29:X:663:G:H5''	1.68	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
1:O:182:SER:HA	1:O:185:TYR:HB3	1.69	0.73
29:X:1283:G:H22	29:X:1286:A:H5'	1.54	0.73
29:X:1418:G:O2'	29:X:1578:U:O4	2.05	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
29:X:1019:U:H3	29:X:1142:A:N6	1.86	0.73
4:C:67:ALA:HA	29:X:1255:U:C5	2.24	0.73
3:B:109:LYS:NZ	29:X:2723:C:OP1	2.19	0.73
3:B:169:ASN:ND2	29:X:2731:G:OP1	2.21	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:122:PHE:HD2	5:D:129:ASN:H	1.34	0.72
12:K:33:ARG:HB2	12:K:114:GLU:HB3	1.71	0.72
20:S:117:VAL:HG23	20:S:168:VAL:HG13	1.71	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
3:B:92:ASN:HD22	3:B:182:ILE:HG13	1.54	0.72
11:J:17:ARG:NH2	29:X:956:G:O6	2.22	0.72
25:Z:51:TYR:CE1	25:Z:55:ARG:HG3	2.25	0.72
3:B:189:PRO:HA	29:X:2680:C:H5'	1.70	0.72
4:C:193:LEU:HA	4:C:196:VAL:HG22	1.72	0.72
11:J:21:ASP:OD2	11:J:22:ALA:N	2.23	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
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
2:A:134:ARG:HB3	2:A:187:SER:HB2	1.72	0.70
3:B:62:PRO:O	29:X:2786:U:O2'	2.08	0.70
8:G:31:THR:HG21	15:N:61:TRP:NE1	2.06	0.70
29:X:303:G:H2'	29:X:304:G:C8	2.26	0.70
29:X:2291:U:O2'	29:X:2374:G:N3	2.24	0.70
9:H:1:MET:HE2	29:X:1665:A:H1'	1.74	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

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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
17:P:57:LEU:HD13	17:P:69:ALA:HA	1.74	0.70
29:X:1242:A:H2'	29:X:1243:C:H6	1.56	0.70
12:K:36:THR:OG1	29:X:1278:G:OP1	2.09	0.69
16:O:7:THR:O	16:O:9:GLY:N	2.25	0.69
1:0:130:ARG:HD2	29:X:2169:A:H5'	1.74	0.69
6:E:172:LYS:NZ	29:X:2529:G:OP2	2.17	0.69
3:B:60:ASN:HB3	3:B:62:PRO:HD2	1.74	0.69
12:K:11:ASN:OD1	29:X:1652:A:N6	2.25	0.69
13:L:64:LYS:HG3	30:Y:53:G:H5''	1.73	0.69
29:X:1645:G:H5''	29:X:1646:C:H5'	1.73	0.69
2:A:268:ARG:HH21	29:X:2224:G:H5''	1.56	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
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
9:H:9:ASP:N	9:H:9:ASP:OD2	2.26	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
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
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
28:3:36:LYS:HD3	28:3:41:ILE:HD12	1.75	0.69
29:X:507:A:C5'	29:X:508:A:H5'	2.23	0.69
29:X:1876:A:H2'	29:X:1877:A:H8	1.58	0.69
5:D:131:GLY:HA2	5:D:154:ILE:H	1.58	0.68
29:X:1796:U:H2'	29:X:1797:C:C6	2.27	0.68
29:X:1936:A:H2	29:X:1943:U:H3	1.41	0.68
22:U:48:LYS:HG2	22:U:49:LYS:H	1.59	0.68
1:0:40:HIS:HA	1:0:168:HIS:HB3	1.74	0.68
1:0:149:VAL:HA	1:0:152:LEU:HD12	1.75	0.68
29:X:521:G:H2'	29:X:522:A:H8	1.58	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
1:0:174:ALA:HA	1:0:181:LEU:HD21	1.76	0.68
29:X:544:C:H1'	29:X:547:A:H8	1.58	0.68
29:X:2373:A:H2'	29:X:2374:G:H8	1.57	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
7:F:96:VAL:HB	7:F:136:VAL:HG12	1.74	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
9:H:22:ILE:HD11	29:X:1952:A:N3	2.09	0.67
17:P:36:ARG:HA	17:P:39:ARG:HD2	1.77	0.67
29:X:2323:G:N1	29:X:2332:U:H5	1.92	0.67
2:A:161:THR:HG21	29:X:1819:A:H5''	1.75	0.67
15:N:13:ARG:NH1	29:X:1251:C:OP1	2.20	0.67
17:P:49:SER:O	17:P:51:GLN:N	2.28	0.67
29:X:2661:G:H2'	29:X:2662:A:C8	2.30	0.67
29:X:445:C:H2'	29:X:446:G:H5''	1.77	0.67
29:X:680:A:H2'	29:X:681:G:C8	2.30	0.67
29:X:569:U:O2'	29:X:983:A:N1	2.26	0.67
21:T:10:SER:OG	29:X:2277:G:OP2	2.13	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
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: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
29:X:650:C:H2'	29:X:651:G:H8	1.60	0.66
29:X:845:G:H8	29:X:845:G:OP2	1.78	0.66
29:X:1557:G:H3'	29:X:1558:A:H5''	1.77	0.66
9:H:124:MET:O	9:H:127:VAL:HG12	1.94	0.66
14:M:14:ARG:HH21	14:M:14:ARG:HB3	1.61	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
3:B:183:LEU:HD21	14:M:16:ILE:HD13	1.77	0.65
24:W:9:VAL:HG22	24:W:17:VAL:HG22	1.76	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)
23:V:23:LYS:O	23:V:27:GLU:HG2	1.95	0.65
29:X:2461:C:H2'	29:X:2462:U:H6	1.61	0.65
4:C:154:ASP:OD1	4:C:157:THR:OG1	2.14	0.65
29:X:699:A:H2'	29:X:700:G:O4'	1.97	0.65
29:X:2319:U:H4'	29:X:2320:A:H5'	1.77	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:34:PRO:HG3	8:G:69:ASP:OD2	1.97	0.65
8:G:88:VAL:HG21	8:G:127:ILE:HD11	1.78	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
4:C:28:HIS:CD2	10:I:8:PRO:HB3	2.32	0.64
13:L:8:ARG:HB2	13:L:8:ARG:HH11	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
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
6:E:9:ILE:HG22	6:E:11:VAL:HG13	1.80	0.64
29:X:2294:C:H2'	29:X:2295:C:H6	1.63	0.64
16:O:39:PHE:HD1	16:O:47:PHE:HB3	1.62	0.64
19:R:77:HIS:HD2	29:X:328:U:H5'	1.63	0.64
29:X:823:G:H2'	29:X:824:U:H6	1.63	0.64
29:X:1876:A:H2'	29:X:1877:A:C8	2.33	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
1:O:11:ASP:OD1	1:O:13:ASN:ND2	2.29	0.64
4:C:117:LEU:HD13	4:C:188:ILE:HD12	1.80	0.64
10:I:14:LYS:NZ	29:X:1193:G:OP1	2.27	0.64
24:W:15:ASN:OD1	24:W:16:GLN:N	2.29	0.64
29:X:616:A:H2'	29:X:617:A:C8	2.32	0.64
29:X:643:A:H2'	29:X:644:A:C8	2.33	0.64
29:X:1071:G:O2'	29:X:1089:G:OP2	2.15	0.64
1:O:16:TYR:HB3	1:O:21:ALA:HB2	1.80	0.64
16:O:21:ARG:HD3	16:O:90:PHE:CE1	2.33	0.64
29:X:1784:A:H4'	29:X:1785:A:O5'	1.98	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
6:E:28:GLY:HA3	6:E:79:VAL:HB	1.78	0.63
10:I:35:LYS:NZ	29:X:568:U:OP1	2.30	0.63
11:J:36:ILE:HG12	11:J:103:VAL:HG22	1.77	0.63
29:X:2439:A:H4'	29:X:2440:C:H5''	1.79	0.63
2:A:30:GLU:HB3	2:A:33:LEU:HB2	1.79	0.63
29:X:521:G:H2'	29:X:522:A:C8	2.33	0.63
29:X:698:C:O2'	29:X:734:A:N6	2.30	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
17:P:109:ARG:HH11	17:P:109:ARG:HG3	1.62	0.63
29:X:395:U:H2'	29:X:396:G:C8	2.34	0.63
29:X:1429:G:H2'	29:X:1430:C:C6	2.34	0.63
8:G:42:VAL:HG11	8:G:166:LEU:HB2	1.79	0.63
9:H:110:VAL:HG23	9:H:129:LEU:HB2	1.81	0.63
29:X:547:A:N3	29:X:547:A:H5''	2.14	0.63
10:I:133:VAL:HG11	10:I:140:VAL:HG23	1.79	0.63
29:X:634:G:H2'	29:X:635:C:H6	1.64	0.63
29:X:2695:C:H2'	29:X:2696:U:H6	1.64	0.63
2:A:157:ARG:NH1	29:X:1818:U:OP2	2.31	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
18:Q:35:LYS:HD2	18:Q:53:ILE:HG23	1.80	0.63
29:X:1289:C:H2'	29:X:1290:U:H6	1.64	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
2:A:259:THR:HG1	29:X:1797:C:HO2'	1.45	0.62
15:N:92:ARG:HG2	29:X:997:G:OP1	2.00	0.62
16:O:18:ASP:N	16:O:18:ASP:OD1	2.33	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
29:X:1783:A:HO2'	29:X:2607:G:HO2'	1.47	0.62
9:H:69:VAL:HG12	9:H:70:VAL:N	2.14	0.62
16:O:62:GLU:HG3	16:O:63:HIS:N	2.14	0.62
19:R:48:VAL:O	19:R:50:GLY:N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:56:VAL:O	20:S:58:GLY:N	2.33	0.62
6:E:99:THR:HB	6:E:102:ALA:HB3	1.81	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
29:X:27:G:O2'	29:X:28:A:OP2	2.16	0.62
29:X:657:U:H2'	29:X:658:A:C8	2.35	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
14:M:55:ILE:HA	14:M:104:LEU:HD12	1.82	0.61
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
29:X:2168:G:N2	29:X:2171:A:O4'	2.32	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
29:X:634:G:H2'	29:X:635:C:C6	2.35	0.61
29:X:2060:A:H1'	29:X:2502:G:C1'	2.30	0.61
29:X:2218:U:H2'	29:X:2219:U:C5	2.35	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
2:A:271:VAL:HG22	2:A:272:THR:HG23	1.82	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
19:R:76:LEU:HD22	19:R:80:LYS:HD3	1.81	0.61
20:S:39:PHE:CE1	20:S:43:PHE:HB2	2.36	0.61
29:X:807:U:H2'	29:X:808:A:H8	1.64	0.61
29:X:960:A:H5''	29:X:961:C:OP2	2.00	0.61
29:X:1450:G:H2'	29:X:1451:C:H6	1.65	0.61
29:X:2448:A:HO2'	29:X:2449:U:H5	1.45	0.61
29:X:2845:C:H2'	29:X:2846:G:C8	2.36	0.61
3:B:119:ARG:HG2	3:B:120:TRP:CD1	2.35	0.61
19:R:51:VAL:HG13	19:R:52:ASN:H	1.65	0.61
29:X:744:U:H2'	29:X:745:G:O4'	2.00	0.61
6:E:92:VAL:HG23	6:E:160:LYS:HE2	1.83	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:443:A:H2	29:X:1245:G:N3	1.97	0.61
29:X:2057:A:H2'	29:X:2058:A:C8	2.35	0.61
9:H:88:THR:HB	14:M:80:VAL:HB	1.82	0.61
12:K:28:LEU:HD21	12:K:115:LEU:HD11	1.81	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:733:G:N7	29:X:761:A:C6	2.69	0.61
29:X:1124:C:H2'	29:X:1125:G:C8	2.35	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
16:O:80:TYR:CE2	29:X:1187:G:H5''	2.36	0.60
29:X:2347:C:H2'	29:X:2348:U:C6	2.36	0.60
1:O:205:LEU:HB3	1:O:222:LEU:HD13	1.83	0.60
12:K:87:TYR:CD1	12:K:90:ARG:HD2	2.36	0.60
15:N:48:ARG:HD2	29:X:1156:A:N6	2.03	0.60
29:X:323:G:OP1	29:X:338:G:N2	2.33	0.60
29:X:1423:A:H2'	29:X:1424:G:H8	1.65	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:OD2	20:S:151:ASP:N	2.33	0.60
29:X:536:A:H2'	29:X:537:U:C6	2.36	0.60
3:B:111:LYS:NZ	29:X:2724:U:OP1	2.24	0.60
5:D:150:ARG:NH2	29:X:2305:U:H3	1.98	0.60
25:Z:15:LYS:O	25:Z:18:MET:N	2.33	0.60
5:D:166:ALA:O	5:D:170:LEU:HG	2.02	0.60
6:E:130:ARG:NH1	6:E:132:ASP:OD2	2.35	0.60
15:N:74:MET:HE2	15:N:110:VAL:HG13	1.83	0.60
1:O:72:VAL:HB	1:O:90:VAL:HG13	1.83	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
29:X:439:A:H2'	29:X:440:G:C8	2.36	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
20:S:138:VAL:HA	20:S:141:MET:HE3	1.84	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
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:2100:G:H1	29:X:2189:U:H3	1.49	0.60
29:X:2262:U:H2'	29:X:2263:C:C6	2.35	0.60
29:X:2532:G:O2'	29:X:2657:A:N1	2.34	0.60
1:O:29:ALA:HB1	1:O:35:GLU:HB3	1.82	0.59
6:E:124:ALA:HB3	6:E:132:ASP:HB2	1.83	0.59
20:S:3:LEU:HD21	20:S:56:VAL:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:171:ILE:HD12	1:0:181:LEU:HD22	1.84	0.59
2:A:13:ARG:NH2	29:X:729:G:OP2	2.25	0.59
4:C:164:VAL:HB	4:C:167:VAL:HG22	1.82	0.59
11:J:69:ILE:HG23	11:J:104:MET:HA	1.84	0.59
27:2:34:ARG:HD3	29:X:467:G:OP2	2.01	0.59
29:X:120:U:H4'	29:X:121:G:H5''	1.84	0.59
29:X:303:G:H2'	29:X:304:G:H8	1.66	0.59
29:X:650:C:H2'	29:X:651:G:C8	2.37	0.59
11:J:35:LEU:HD23	11:J:105:PHE:HD2	1.67	0.59
17:P:45:ILE:HD11	17:P:57:LEU:HG	1.83	0.59
21:T:26:PHE:HE1	29:X:857:C:H1'	1.67	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:676:A:C8	29:X:2443:C:H1'	2.37	0.59
29:X:1323:G:H2'	29:X:1324:G:H5'	1.85	0.59
2:A:260:ARG:HH22	2:A:266:SER:HB2	1.67	0.59
5:D:74:ILE:HA	5:D:79:LEU:HB2	1.83	0.59
25:Z:3:LYS:HD3	29:X:2611:U:H3'	1.83	0.59
28:3:17:THR:HG22	28:3:21:LYS:H	1.67	0.59
29:X:2307:G:H3'	29:X:2308:G:H8	1.68	0.59
30:Y:15:A:N1	30:Y:71:G:O2'	2.27	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
12:K:13:ASN:C	12:K:17:ARG:HH21	2.05	0.59
13:L:63:ASN:HB2	13:L:67:THR:HG23	1.83	0.59
17:P:86:LEU:N	17:P:130:GLU:OE2	2.34	0.59
30:Y:64:C:H2'	30:Y:65:A:H8	1.67	0.59
20:S:4:THR:HA	20:S:57:GLU:HB2	1.83	0.59
22:U:21:ARG:HH21	22:U:23:LYS:HG2	1.67	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
14:M:60:SER:HA	14:M:64:LYS:HB2	1.84	0.59
29:X:2522:U:O2'	29:X:2647:U:OP1	2.17	0.59
15:N:13:ARG:NH1	29:X:1251:C:H5''	2.17	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
1:0:68:VAL:HG21	1:0:153:LYS:HG2	1.85	0.58
11:J:23:LYS:O	20:S:73:LYS:NZ	2.36	0.58
13:L:15:ARG:NH2	29:X:2293:A:O5'	2.36	0.58
27:2:34:ARG:NH2	27:2:41:GLN:O	2.36	0.58
29:X:1450:G:H2'	29:X:1451:C:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2308:G:OP1	29:X:2310:A:N6	2.31	0.58
2:A:7:LYS:NZ	29:X:706:A:OP1	2.35	0.58
2:A:39:LYS:NZ	2:A:57:GLY:O	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
29:X:1405:C:H2'	29:X:1406:G:C8	2.38	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:1657:C:H2'	29:X:1658:C:H6	1.67	0.58
29:X:1827:U:H5'	29:X:1971:A:H5'	1.86	0.58
8:G:62:ILE:O	8:G:77:GLY:HA3	2.04	0.58
8:G:91:THR:O	8:G:94:LYS:HB2	2.03	0.58
15:N:92:ARG:HA	15:N:95:LEU:HB2	1.86	0.58
28:3:10:ALA:HB1	28:3:14:ILE:HD12	1.84	0.58
29:X:642:G:H21	29:X:645:U:H3	1.50	0.58
29:X:2438:U:O2'	29:X:2440:C:OP1	2.20	0.58
30:Y:27:A:OP2	30:Y:27:A:H8	1.86	0.58
29:X:493:G:H2'	29:X:494:G:O4'	2.04	0.58
29:X:2233:U:H2'	29:X:2234:G:C8	2.39	0.58
2:A:108:PRO:HB3	2:A:143:HIS:HE1	1.69	0.58
12:K:85:PRO:O	12:K:88:ALA:HB2	2.04	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
4:C:119:ALA:HA	4:C:189:ASP:O	2.03	0.58
10:I:19:VAL:HB	10:I:30:ALA:HB1	1.84	0.58
15:N:75:ASN:OD1	15:N:77:SER:N	2.37	0.58
25:Z:16:ARG:NH1	29:X:1263:U:OP1	2.36	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
4:C:179:ASP:OD1	4:C:182:ARG:NH2	2.37	0.58
10:I:41:SER:HB2	29:X:671:C:C6	2.39	0.58
11:J:41:ALA:HB2	11:J:128:ILE:HG21	1.85	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
22:U:51:ILE:HG12	22:U:59:THR:HB	1.86	0.58
29:X:24:G:H2'	29:X:25:U:H6	1.68	0.58
29:X:302:U:H2'	29:X:303:G:H8	1.69	0.58
29:X:740:U:H2'	29:X:741:G:C8	2.39	0.58
6:E:24:PHE:HB2	6:E:37:TYR:CD1	2.39	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
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:1283:G:N2	29:X:1286:A:H5'	2.17	0.58
6:E:37:TYR:HD2	6:E:68:THR:HG23	1.69	0.58
7:F:115:LEU:HD22	7:F:126:THR:HG21	1.86	0.58
8:G:110:LEU:HD13	29:X:1131:G:O4'	2.03	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
29:X:127:A:H5''	29:X:128:C:C6	2.39	0.58
29:X:544:C:H1'	29:X:547:A:C8	2.38	0.58
29:X:1217:C:H2'	29:X:1218:A:H8	1.69	0.58
29:X:2221:G:H2'	29:X:2222:G:C8	2.39	0.58
19:R:19:GLY:H	19:R:36:VAL:HB	1.69	0.57
4:C:22:VAL:HG11	4:C:110:SER:HB3	1.86	0.57
5:D:60:ILE:HG22	5:D:140:GLU:HB2	1.86	0.57
13:L:33:ARG:HD2	13:L:99:ARG:HB2	1.86	0.57
16:O:70:TYR:OH	29:X:1223:G:O6	2.22	0.57
21:T:39:ARG:HH21	29:X:2355:C:H1'	1.68	0.57
24:W:10:ILE:HD13	29:X:989:G:C8	2.39	0.57
29:X:14:A:C6	29:X:526:A:C2	2.92	0.57
29:X:483:A:H3'	29:X:484:C:C6	2.39	0.57
29:X:1657:C:H2'	29:X:1658:C:C6	2.39	0.57
29:X:2060:A:H1'	29:X:2502:G:O4'	2.04	0.57
29:X:2438:U:O2'	29:X:2439:A:H5''	2.04	0.57
29:X:2650:U:H2'	29:X:2651:C:H6	1.69	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
2:A:25:ALA:HB3	2:A:81:ALA:HB1	1.87	0.57
4:C:15:ILE:HG12	4:C:197:GLU:HB2	1.86	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
29:X:1353:A:H2'	29:X:1354:A:C8	2.39	0.57
29:X:1783:A:O2'	29:X:2607:G:O2'	2.21	0.57
29:X:2219:U:C3'	29:X:2220:C:H4'	2.35	0.57
29:X:2801:G:H2'	29:X:2802:G:C8	2.39	0.57
11:J:111:THR:HG23	11:J:114:GLN:HG3	1.85	0.57
29:X:165:A:H2'	29:X:165(A):G:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:465:G:C6	29:X:466:A:N6	2.73	0.57
29:X:588:U:H2'	29:X:589:U:C6	2.40	0.57
29:X:2063:C:O2	29:X:2451:A:C2	2.58	0.57
29:X:2751:G:N2	29:X:2751:G:OP1	2.32	0.57
30:Y:67:C:N4	30:Y:111:C:O2'	2.32	0.57
5:D:60:ILE:HG13	5:D:61:THR:HG23	1.85	0.57
5:D:108:LEU:HA	5:D:111:ILE:HG13	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
17:P:87:GLU:O	17:P:89:ARG:N	2.33	0.57
20:S:10:PRO:HB2	20:S:14:LEU:HD21	1.86	0.57
29:X:1936:A:H2	29:X:1943:U:N3	2.02	0.57
1:O:136:PRO:HA	1:O:141:VAL:HG11	1.86	0.57
6:E:37:TYR:CD2	6:E:68:THR:HG23	2.39	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:651(A):G:H2'	29:X:651(B):C:H4'	1.86	0.57
2:A:143:HIS:ND1	2:A:194:GLY:O	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
29:X:679:C:H2'	29:X:680:A:C8	2.35	0.57
30:Y:6:C:H2'	30:Y:7:C:C6	2.40	0.57
7:F:133:SER:HB3	29:X:1062:G:H21	1.70	0.57
8:G:31:THR:OG1	29:X:995:C:N3	2.38	0.57
10:I:90:ARG:HD2	10:I:93:LEU:HG	1.87	0.57
11:J:42:TRP:HB3	11:J:95:VAL:CG2	2.34	0.57
14:M:100:ARG:HG3	29:X:1747:G:H5''	1.87	0.57
19:R:58:VAL:HG22	19:R:59:LYS:H	1.70	0.57
22:U:27:ASP:C	22:U:32:ARG:HD3	2.24	0.57
26:1:31:THR:O	26:1:33:ALA:N	2.38	0.57
5:D:41:GLY:O	5:D:43:SER:N	2.38	0.57
17:P:50:VAL:HG21	17:P:90:LEU:HB3	1.86	0.57
22:U:14:VAL:O	22:U:16:ASN:N	2.37	0.57
29:X:474:G:C6	29:X:510:C:N4	2.73	0.57
29:X:920:G:C2	29:X:921:G:H1'	2.40	0.57
29:X:1153:C:H2'	29:X:1154:G:C8	2.39	0.57
20:S:15:ASP:O	20:S:17:SER:N	2.38	0.56
25:Z:55:ARG:NH2	25:Z:59:ALA:H	2.03	0.56
10:I:115:SER:O	10:I:136:ALA:HB1	2.04	0.56
19:R:77:HIS:CD2	29:X:328:U:H5'	2.40	0.56
22:U:48:LYS:HG2	22:U:49:LYS:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:47:THR:H	4:C:50:GLN:HG3	1.70	0.56
9:H:8:LEU:N	9:H:8:LEU:HD23	2.21	0.56
11:J:77:LYS:HG2	29:X:957:C:H5'	1.86	0.56
19:R:15:HIS:ND1	29:X:336:C:H4'	2.20	0.56
29:X:214:G:N2	29:X:226:G:H2'	2.20	0.56
29:X:536:A:H2'	29:X:537:U:H6	1.70	0.56
29:X:1224:G:O2'	29:X:1225:A:H5'	2.04	0.56
29:X:2168:G:N1	29:X:2171:A:OP2	2.37	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: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:2408:U:H2'	29:X:2409:G:H8	1.71	0.56
9:H:13:ASN:ND2	9:H:109:ARG:HG2	2.21	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
29:X:676:A:H8	29:X:2443:C:H1'	1.68	0.56
29:X:2345:G:N3	29:X:2381:C:H2'	2.21	0.56
1:O:29:ALA:O	1:O:31:ALA:N	2.38	0.56
2:A:78:LYS:NZ	29:X:1502:C:OP1	2.37	0.56
5:D:127:ASN:ND2	5:D:158:THR:O	2.39	0.56
19:R:105:ARG:HD3	19:R:112:LYS:HD3	1.87	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
3:B:120:TRP:CE3	3:B:155:ARG:HD2	2.41	0.56
6:E:67:LEU:HD11	29:X:2758:A:C5	2.41	0.56
21:T:15:ASP:OD1	29:X:2264:C:N4	2.38	0.56
27:2:12:ARG:HG3	29:X:686:G:O6	2.06	0.56
29:X:981:A:H2	29:X:2027:G:N3	2.03	0.56
30:Y:62:C:H2'	30:Y:63:A:H8	1.70	0.56
1:O:10:VAL:HG11	1:O:216:PRO:HG2	1.87	0.56
3:B:48:GLN:NE2	29:X:2635:A:O2'	2.37	0.56
16:O:83:ARG:HG2	29:X:1225:A:H4'	1.88	0.56
18:Q:84:GLU:HB2	18:Q:86:GLN:HG3	1.88	0.56
29:X:1676:A:N6	29:X:1677:A:N1	2.53	0.56
29:X:2691:C:H5''	29:X:2872:G:H5'	1.87	0.56
13:L:47:ARG:NH1	13:L:49:GLN:OE1	2.38	0.56
19:R:37:LEU:HD11	19:R:49:GLU:HG3	1.87	0.56
26:1:45: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2729:C:H2'	29:X:2730:C:H6	1.70	0.56
17:P:18:VAL:O	17:P:19:LYS:HB2	2.05	0.56
29:X:1373:A:H5''	29:X:2212:A:N6	2.21	0.56
29:X:1787:U:H2'	29:X:1788:C:H6	1.71	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
21:T:53:MET:HG3	21:T:59:LEU:HD23	1.88	0.55
2:A:168:LYS:HG3	2:A:173:VAL:HG22	1.87	0.55
3:B:105:THR:HB	3:B:197:VAL:CG1	2.36	0.55
3:B:136:ARG:HB2	29:X:1657:C:P	2.46	0.55
15:N:75:ASN:HD21	29:X:1011:A:P	2.28	0.55
29:X:515:A:H2	29:X:1260:G:N3	2.04	0.55
29:X:2229:U:H2'	29:X:2230:G:H8	1.70	0.55
6:E:143:GLN:HG3	29:X:2745:C:O2'	2.07	0.55
8:G:110:LEU:HD22	29:X:1131:G:H4'	1.88	0.55
17:P:114:ALA:O	17:P:115:ASN:ND2	2.39	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
5:D:83:MET:HG2	5:D:84:PRO:HD2	1.87	0.55
8:G:142:ARG:HA	8:G:145:HIS:CD2	2.42	0.55
8:G:151:TYR:HH	8:G:158:HIS:CD2	2.24	0.55
13:L:33:ARG:HE	13:L:38:ILE:HG21	1.70	0.55
15:N:91:ASN:ND2	29:X:996:A:H4'	2.15	0.55
26:I:19:GLY:HA3	29:X:2400:G:H4'	1.89	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
29:X:2652:C:H2'	29:X:2653:U:O4'	2.06	0.55
11:J:12:LYS:HD3	29:X:911:A:C6	2.41	0.55
11:J:49:GLU:O	11:J:53:ILE:HG13	2.07	0.55
15:N:31:GLN:NE2	29:X:580:C:H4'	2.21	0.55
15:N:37:GLN:HG3	29:X:1252:G:N1	2.21	0.55
29:X:1270:C:H5''	29:X:1271:G:O5'	2.07	0.55
29:X:2168:G:N2	29:X:2171:A:O5'	2.39	0.55
4:C:22:VAL:HG21	4:C:110:SER:HA	1.88	0.55
8:G:32:TYR:O	15:N:64:ARG:NH1	2.37	0.55
9:H:21:CYS:SG	9:H:22:ILE:N	2.80	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
29:X:864:G:H1'	29:X:914:C:N4	2.22	0.55
29:X:989:G:OP1	29:X:1157:G:O2'	2.22	0.55
29:X:1024:G:C6	29:X:1025:G:C6	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1060:U:H4'	29:X:1061:U:H5'	1.88	0.55
29:X:1678:U:O2'	29:X:1679:C:H5'	2.07	0.55
30:Y:34:C:H2'	30:Y:35:C:C6	2.42	0.55
22:U:64:ALA:O	22:U:67:ILE:HG22	2.07	0.55
28:3:33:ASN:O	28:3:36:LYS:HA	2.07	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
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:1653:G:OP2	29:X:1653:G:H8	1.90	0.55
29:X:2280:G:H1'	29:X:2327:A:H1'	1.88	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
5:D:9:ASN:O	5:D:13:ARG:HG3	2.07	0.55
6:E:37:TYR:CE2	6:E:72:VAL:HG22	2.42	0.55
17:P:59:PHE:HD1	25:Z:30:LEU:HD11	1.72	0.55
29:X:936:C:H2'	29:X:937:C:H6	1.72	0.55
29:X:2318:G:O2'	29:X:2321:G:O6	2.24	0.55
29:X:2330:G:H2'	29:X:2331:G:O4'	2.06	0.55
29:X:2619:C:O2'	29:X:2620:U:H5'	2.07	0.55
29:X:2716:A:O2'	29:X:2717:G:H5'	2.07	0.55
9:H:13:ASN:OD1	9:H:108:THR:N	2.40	0.55
12:K:87:TYR:OH	12:K:115:LEU:HB3	2.07	0.55
29:X:345:A:H2'	29:X:346:A:N7	2.22	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:2756:U:H4'	29:X:2757:A:OP1	2.07	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
29:X:2328:A:H2'	29:X:2329:A:C8	2.42	0.55
3:B:14:ILE:HD11	3:B:173:VAL:HG11	1.88	0.54
4:C:39:ARG:HG2	29:X:443:A:N7	2.21	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
14:M:104:LEU:HD23	14:M:106:TYR:HE2	1.72	0.54
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.89	0.54
20:S:91:PRO:HD3	20:S:127:PRO:HD3	1.88	0.54
21:T:51:VAL:HG11	21:T:79:ILE:O	2.06	0.54
5:D:14:PRO:HA	5:D:17:MET:HB2	1.89	0.54
8:G:92:GLY:HA2	8:G:94:LYS:H	1.71	0.54
14:M:69:ARG:HB2	14:M:78:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:20:C:H2'	29:X:21:A:H8	1.73	0.54
29:X:695:G:OP1	29:X:1380:G:O2'	2.23	0.54
29:X:1151:A:H2'	29:X:1152:C:H6	1.73	0.54
29:X:1172(B):C:H2'	29:X:1172(C):G:H2'	1.88	0.54
29:X:1429:G:H2'	29:X:1430:C:H6	1.71	0.54
4:C:56:ARG:HB2	29:X:797:U:OP2	2.07	0.54
28:3:21:LYS:HB3	28:3:55:TRP:CH2	2.42	0.54
28:3:25:PHE:HA	28:3:47:GLY:HA2	1.89	0.54
29:X:733:G:C8	29:X:761:A:N6	2.76	0.54
29:X:1203:U:H2'	29:X:1204:C:C6	2.42	0.54
30:Y:64:C:H2'	30:Y:65:A:C8	2.42	0.54
1:0:152:LEU:HD23	1:0:157:ILE:HD12	1.89	0.54
1:0:157:ILE:HD13	1:0:157:ILE:H	1.72	0.54
5:D:106:ILE:HB	5:D:139:PRO:HB3	1.89	0.54
9:H:13:ASN:HD21	9:H:109:ARG:H	1.55	0.54
28:3:29:LYS:NZ	28:3:41:ILE:HG23	2.22	0.54
29:X:936:C:H2'	29:X:937:C:C6	2.43	0.54
29:X:2314:G:H2'	29:X:2315:U:C6	2.43	0.54
29:X:2519:U:C5	29:X:2541:A:C6	2.95	0.54
2:A:151:LYS:HD3	29:X:2203:G:H4'	1.88	0.54
7:F:30:TYR:HB2	7:F:59:ILE:HD12	1.89	0.54
17:P:109:ARG:HG3	17:P:109:ARG:NH1	2.21	0.54
29:X:83:G:H1	29:X:102:G:HO2'	1.55	0.54
29:X:1127:A:C8	29:X:2518:A:H5''	2.43	0.54
29:X:2028:U:H2'	29:X:2029:A:C8	2.43	0.54
29:X:2203:G:H2'	29:X:2204:A:H8	1.71	0.54
1:0:180:ASN:HA	1:0:183:ALA:HB3	1.88	0.54
5:D:111:ILE:HG12	5:D:137:ILE:HD12	1.90	0.54
5:D:135:GLN:HG3	5:D:151:GLY:HA2	1.89	0.54
13:L:38:ILE:HD12	13:L:40:ALA:H	1.73	0.54
22:U:78:ILE:HG12	22:U:79:GLU:H	1.72	0.54
24:W:25:LEU:HD22	24:W:30:ASP:HB3	1.90	0.54
2:A:50:THR:HG22	29:X:1813:G:H21	1.72	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:44:ASN:O	2:A:46:ARG:N	2.41	0.54
3:B:144:ARG:NH1	29:X:2572:A:C4	2.75	0.54
4:C:4:ILE:HG22	4:C:13:ARG:HH12	1.73	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:126:LYS:HG3	2:A:129:ASN:OD1	2.08	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
29:X:296:C:H2'	29:X:297:C:H6	1.72	0.54
1:O:27:GLU:O	1:O:29:ALA:N	2.41	0.54
1:O:43:LEU:HD12	1:O:167:VAL:HG11	1.88	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
29:X:220:G:OP2	29:X:221:C:H5'	2.08	0.54
29:X:1787:U:H2'	29:X:1788:C:C6	2.42	0.54
29:X:2695:C:H2'	29:X:2696:U:C6	2.42	0.54
2:A:88:ARG:HD2	2:A:106:LEU:HD21	1.89	0.53
9:H:104:GLU:HG2	9:H:125:LYS:HD2	1.90	0.53
15:N:94:VAL:O	15:N:98:ILE:HG12	2.07	0.53
19:R:67:GLY:HA3	29:X:483:A:O3'	2.08	0.53
29:X:297:C:H2'	29:X:298:G:O4'	2.07	0.53
3:B:4:ILE:HG12	3:B:5:LEU:H	1.73	0.53
4:C:35:LEU:HD23	4:C:38:ARG:HD2	1.90	0.53
29:X:5:A:H2'	29:X:6:A:C8	2.43	0.53
29:X:335:C:H2'	29:X:336:C:H6	1.72	0.53
29:X:1316:U:H2'	29:X:1317:G:H8	1.73	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
22:U:17:SER:CA	22:U:18:VAL:HB	2.38	0.53
29:X:2153:G:H2'	29:X:2154:G:C8	2.44	0.53
29:X:2461:C:H2'	29:X:2462:U:C6	2.43	0.53
1:O:25:VAL:HG13	1:O:37:VAL:HG21	1.91	0.53
28:3:16:ILE:HG21	28:3:65:GLY:HA2	1.91	0.53
29:X:438:C:H2'	29:X:439:A:H8	1.74	0.53
29:X:2221:G:H2'	29:X:2222:G:H8	1.72	0.53
29:X:2600:A:H2'	29:X:2601:C:C6	2.44	0.53
10:I:16:ARG:NH2	29:X:589:U:OP2	2.40	0.53
19:R:58:VAL:HA	29:X:483:A:H4'	1.91	0.53
25:Z:42:SER:HB3	29:X:2885:C:H42	1.74	0.53
26:1:18:THR:HG21	26:1:43:VAL:HB	1.90	0.53
29:X:629:C:H4'	29:X:649:G:H21	1.73	0.53
29:X:799:G:OP2	29:X:800:A:O2'	2.17	0.53
8:G:91:THR:HG21	29:X:1140:U:H6	1.74	0.53
9:H:47:VAL:HG23	9:H:77:THR:HG23	1.91	0.53
10:I:101:ARG:HE	29:X:626:G:H1	1.56	0.53
17:P:60:ILE:CD1	25:Z:28:PRO:HD3	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:46:PHE:O	18:Q:48:VAL:HG23	2.09	0.53
29:X:819:A:OP2	29:X:1187:G:N2	2.31	0.53
29:X:991:C:H2'	29:X:992:C:H6	1.73	0.53
29:X:1661:G:H2'	29:X:1662:U:O4'	2.08	0.53
29:X:2567:G:H2'	29:X:2568:C:C6	2.44	0.53
29:X:2885:C:H2'	29:X:2886:A:O4'	2.07	0.53
3:B:9:ILE:HD11	3:B:27:LEU:CB	2.38	0.53
8:G:33:ILE:HD11	29:X:537:U:H4'	1.91	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
20:S:6:LYS:HB3	20:S:32:PHE:HA	1.91	0.53
21:T:25:LYS:HB2	21:T:37:LEU:HA	1.89	0.53
25:Z:15:LYS:HA	25:Z:18:MET:HG3	1.90	0.53
3:B:135:HIS:NE2	29:X:1658:C:OP1	2.42	0.53
29:X:971:C:H2'	29:X:972:G:O4'	2.09	0.53
29:X:1066:U:H2'	29:X:1068:G:OP2	2.08	0.53
29:X:2299:A:H61	29:X:2317:U:H3	1.56	0.53
15:N:6:THR:O	15:N:9:VAL:HG23	2.09	0.53
19:R:85:ASP:HB3	19:R:88:THR:OG1	2.08	0.53
22:U:19:ILE:HA	22:U:42:GLN:HA	1.91	0.53
29:X:438:C:H2'	29:X:439:A:C8	2.43	0.53
29:X:445:C:C2'	29:X:446:G:H5''	2.38	0.53
29:X:2243:U:H2'	29:X:2244:U:C6	2.44	0.53
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:165(G):U:N3	29:X:175:C:O2	2.42	0.52
29:X:1440:U:H2'	29:X:1440(A):C:C6	2.45	0.52
29:X:2219:U:H3'	29:X:2220:C:C4'	2.38	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
9:H:82:LYS:NZ	9:H:82:LYS:HB3	2.24	0.52
12:K:38:LEU:O	12:K:41:ALA:HB3	2.10	0.52
16:O:66:GLY:O	16:O:87:ARG:NH1	2.39	0.52
19:R:93:ARG:NH2	29:X:301:G:OP2	2.39	0.52
28:3:44:LYS:NZ	29:X:2362:G:OP1	2.40	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
29:X:1320:G:C2	29:X:1329:U:H5''	2.44	0.52
29:X:1858:G:H8	29:X:1884:A:N7	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2261:C:O2'	29:X:2262:U:H5'	2.09	0.52
29:X:2824:C:H2'	29:X:2825:C:O4'	2.09	0.52
30:Y:72:C:H2'	30:Y:73:C:H6	1.74	0.52
30:Y:80:A:H2'	30:Y:81:C:O4'	2.09	0.52
2:A:39:LYS:HZ1	2:A:58:HIS:C	2.11	0.52
3:B:27:LEU:HD13	14:M:7:ILE:HD11	1.91	0.52
4:C:19:LEU:HB3	4:C:20:PRO:HA	1.90	0.52
4:C:93:TYR:CE1	29:X:660:G:H5'	2.45	0.52
9:H:2:ILE:HB	9:H:45:ALA:HB3	1.91	0.52
14:M:24:LEU:HD13	14:M:91:VAL:HG21	1.90	0.52
15:N:6:THR:O	15:N:8:ILE:N	2.41	0.52
20:S:25:ASN:HA	20:S:85:MET:HB2	1.92	0.52
20:S:69:VAL:HG22	20:S:81:VAL:HG22	1.91	0.52
21:T:43:THR:H	29:X:2331:G:H4'	1.74	0.52
22:U:33:LYS:O	29:X:2395:C:O2'	2.19	0.52
28:3:17:THR:HG21	28:3:21:LYS:HG3	1.90	0.52
29:X:200:A:H2'	29:X:201:U:H5'	1.91	0.52
29:X:1043:C:O2	29:X:1112:G:N2	2.30	0.52
29:X:1047:G:N3	29:X:1110:G:N2	2.54	0.52
29:X:1114:G:H2'	29:X:1115:A:H8	1.73	0.52
29:X:2272:U:H5''	29:X:2273:A:OP1	2.10	0.52
29:X:2695:C:O2'	29:X:2696:U:H5'	2.10	0.52
7:F:21:PRO:HG2	7:F:22:PRO:HD3	1.92	0.52
8:G:96:ASP:N	8:G:96:ASP:OD1	2.41	0.52
10:I:72:TYR:HB3	10:I:107:LYS:HB2	1.91	0.52
15:N:114:ARG:O	15:N:118:GLN:HG3	2.10	0.52
17:P:37:LYS:HA	17:P:40:LEU:HD12	1.92	0.52
20:S:109:GLN:NE2	20:S:142:ASN:OD1	2.42	0.52
24:W:4:LYS:O	24:W:51:LEU:HD12	2.10	0.52
28:3:36:LYS:HB2	28:3:37:SER:CA	2.40	0.52
29:X:1823:G:H2'	29:X:1824:G:H8	1.74	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
29:X:2599:G:C2	29:X:2600:A:C8	2.98	0.52
9:H:76:ARG:O	9:H:94:ASN:HA	2.09	0.52
15:N:3:ARG:HB3	29:X:1248:G:C5	2.42	0.52
29:X:559:G:H2'	29:X:560:C:O4'	2.09	0.52
29:X:1479:G:H2'	29:X:1480:G:H8	1.75	0.52
4:C:102:LEU:HD12	4:C:102:LEU:O	2.10	0.52
22:U:17:SER:CB	22:U:44:ALA:HA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:32:ARG:H	22:U:32:ARG:HE	1.56	0.52
29:X:624:C:O2'	29:X:657:U:OP1	2.26	0.52
29:X:946:G:H2'	29:X:947:G:H8	1.74	0.52
29:X:1266:G:O2'	29:X:2012:G:O6	2.17	0.52
29:X:2729:C:H2'	29:X:2730:C:C6	2.45	0.52
2:A:33:LEU:HD13	2:A:104:TYR:CD2	2.45	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
10:I:77:LEU:O	10:I:80:LEU:N	2.43	0.52
30:Y:27:A:N6	30:Y:56:G:OP2	2.39	0.52
2:A:77:ALA:HB2	2:A:97:TYR:CD1	2.44	0.52
2:A:260:ARG:NH1	29:X:1799:G:OP1	2.37	0.52
9:H:40:GLY:HA2	29:X:2563:U:H4'	1.92	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
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:118:ASN:H	2:A:129:ASN:HD22	1.57	0.52
6:E:17:VAL:HG13	6:E:26:VAL:HG22	1.92	0.52
6:E:137:ASP:OD1	6:E:138:LYS:N	2.43	0.52
13:L:39:TYR:HE1	30:Y:8:C:H1'	1.75	0.52
15:N:91:ASN:N	16:O:11:GLN:OE1	2.41	0.52
16:O:39:PHE:CD1	16:O:47:PHE:HB3	2.43	0.52
20:S:25:ASN:HB2	20:S:28:ASN:HB3	1.91	0.52
25:Z:38:GLY:HA3	25:Z:48:ASN:ND2	2.25	0.52
26:1:13:GLU:O	26:1:49:PHE:HB3	2.09	0.52
29:X:460:A:C2	29:X:470:A:C4	2.98	0.52
29:X:555:U:H2'	29:X:556:A:C8	2.44	0.52
30:Y:7:C:O2'	30:Y:29:C:O2	2.25	0.52
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
29:X:2468:G:O2'	29:X:2469:A:H8	1.93	0.51
30:Y:22:U:H3	30:Y:65:A:H61	1.57	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
6:E:23:VAL:O	6:E:25:LYS:N	2.44	0.51
20:S:66:VAL:HG22	20:S:83:PHE:HE1	1.75	0.51
21:T:46:LYS:HZ1	21:T:76:ALA:HA	1.75	0.51
29:X:1698:A:C8	29:X:1700:A:O4'	2.63	0.51
29:X:2098:U:H3	29:X:2191:G:H1	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:141:A:H2'	29:X:142:G:C8	2.44	0.51
29:X:630:G:N2	29:X:632:A:H3'	2.25	0.51
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
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
27:2:45:SER:HB3	29:X:126:A:OP1	2.11	0.51
28:3:36:LYS:HB2	28:3:37:SER:HA	1.91	0.51
3:B:149:ARG:O	29:X:2052:G:H1'	2.10	0.51
24:W:35:SER:O	24:W:35:SER:OG	2.29	0.51
29:X:1358:G:O2'	29:X:1373:A:N6	2.42	0.51
29:X:1779:U:C5	29:X:1784:A:N7	2.78	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:101:U:H5''	29:X:102:G:C8	2.46	0.51
1:0:70:VAL:HG12	1:0:108:ALA:HB3	1.91	0.51
18:Q:40:ASP:O	18:Q:44:GLN:HG2	2.10	0.51
24:W:49:HIS:CD2	24:W:50:LEU:HG	2.46	0.51
29:X:1014:A:H2'	29:X:1015:U:C6	2.46	0.51
29:X:1415:A:C6	29:X:1584:U:H4'	2.45	0.51
29:X:1838:C:H4'	29:X:1839:G:C8	2.45	0.51
29:X:1991:U:H2'	29:X:1992:G:H5'	1.92	0.51
29:X:2341:G:H2'	29:X:2342:C:O4'	2.11	0.51
3:B:116:VAL:HG21	3:B:138:PRO:HB3	1.93	0.51
3:B:141:ILE:HD11	29:X:2052:G:N7	2.26	0.51
9:H:132:GLU:HB2	14:M:73:PHE:HE1	1.75	0.51
19:R:77:HIS:CD2	29:X:328:U:H4'	2.46	0.51
1:0:140:THR:HG22	1:0:145:VAL:HG22	1.92	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
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
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
3:B:16:LYS:HD3	3:B:173:VAL:HG13	1.92	0.51
3:B:135:HIS:CD2	29:X:1658:C:OP1	2.64	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
19:R:51:VAL:HG13	19:R:73:GLU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:638:G:C5	29:X:639:U:C5	2.98	0.51
29:X:797:U:H2'	29:X:798:G:C8	2.45	0.51
29:X:983:A:C2'	29:X:984:A:H5'	2.41	0.51
29:X:994:U:O2'	29:X:996:A:OP1	2.19	0.51
29:X:1114:G:H2'	29:X:1115:A:C8	2.46	0.51
29:X:1337:G:H2'	29:X:1338:G:H8	1.76	0.51
29:X:2468:G:H22	29:X:2481:G:H2'	1.75	0.51
1:O:110:VAL:HG12	1:O:111:ALA:H	1.76	0.50
2:A:48:ARG:NH2	29:X:778:G:H5'	2.25	0.50
14:M:25:PRO:HB2	14:M:93:ILE:HD11	1.93	0.50
15:N:86:ALA:HB2	15:N:116:ALA:HB2	1.92	0.50
17:P:111:ARG:HH21	29:X:747:U:H5'	1.76	0.50
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
29:X:2857:G:N2	29:X:2860:A:OP2	2.24	0.50
2:A:268:ARG:NH2	29:X:2225:A:OP1	2.45	0.50
10:I:41:SER:HB2	29:X:671:C:C5	2.46	0.50
11:J:61:ARG:HD3	20:S:174:PRO:HB2	1.93	0.50
28:3:17:THR:HG21	28:3:21:LYS:CG	2.41	0.50
29:X:407:C:H2'	29:X:408:G:H8	1.76	0.50
29:X:569:U:H1'	29:X:947:G:O4'	2.12	0.50
29:X:1113:U:H2'	29:X:1114:G:H8	1.76	0.50
29:X:1810:A:H2'	29:X:1811:G:O4'	2.10	0.50
29:X:2266:A:H4'	29:X:2267:A:N3	2.26	0.50
29:X:472:A:H3'	29:X:473:G:H5'	1.94	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:1324:G:C4	29:X:1328:G:O6	2.64	0.50
29:X:1886:A:H2'	29:X:1887:U:O4'	2.12	0.50
29:X:2412:A:C8	29:X:2413:G:C8	2.99	0.50
3:B:110:GLY:HA2	3:B:161:GLY:HA3	1.93	0.50
4:C:133:PHE:CE1	4:C:161:ALA:HB2	2.45	0.50
8:G:42:VAL:HA	8:G:164:GLN:H	1.76	0.50
9:H:68:ASP:O	9:H:69:VAL:HB	2.11	0.50
12:K:9:LYS:HB3	29:X:1653:G:C6	2.47	0.50
15:N:33:ARG:HB3	29:X:1252:G:C2	2.46	0.50
29:X:633:A:H4'	29:X:2404:C:H5''	1.92	0.50
29:X:818:G:H5'	29:X:839:U:OP1	2.10	0.50
29:X:1163:G:C2	29:X:1164:A:N7	2.80	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)
29:X:2220:C:H2'	29:X:2221:G:C8	2.46	0.50
1:O:38:GLU:HB2	1:O:211:THR:HB	1.92	0.50
5:D:65:PRO:HA	5:D:89:VAL:HG13	1.93	0.50
26:1:5:ALA:HB3	26:1:6:PRO:HD3	1.94	0.50
29:X:1288:U:C2	29:X:1327:C:O2	2.65	0.50
29:X:1416:G:O2'	29:X:1587:A:H1'	2.10	0.50
29:X:1667:G:O2'	29:X:1991:U:O4	2.25	0.50
2:A:69:ARG:HD2	2:A:119:ALA:HB2	1.93	0.50
2:A:231:HIS:HD2	2:A:233:HIS:H	1.60	0.50
6:E:38:ASN:HB2	6:E:64:LEU:HD22	1.93	0.50
11:J:48:ILE:O	11:J:51:CYS:N	2.45	0.50
15:N:104:GLU:O	15:N:107:LYS:HB3	2.11	0.50
18:Q:17:TYR:O	18:Q:20:MET:HG2	2.11	0.50
19:R:70:GLU:OE1	19:R:72:ARG:NH1	2.45	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
29:X:2817:C:C2	29:X:2830:G:N2	2.80	0.50
18:Q:10:PRO:HG2	18:Q:12:ILE:HD11	1.92	0.50
21:T:39:ARG:NH2	29:X:2355:C:O2	2.44	0.50
22:U:48:LYS:HZ1	29:X:2090:A:H2	1.60	0.50
29:X:200:A:N3	29:X:202:U:H1'	2.27	0.50
29:X:753:A:O2'	29:X:754:G:H5'	2.11	0.50
29:X:807:U:H2'	29:X:808:A:C8	2.47	0.50
29:X:1570:A:H2'	29:X:1571:A:C8	2.46	0.50
29:X:2842:A:C2	29:X:2876:G:C2	2.99	0.50
15:N:28:ARG:HE	29:X:532:A:H2'	1.76	0.50
20:S:25:ASN:CB	20:S:28:ASN:HB3	2.42	0.50
20:S:26:LYS:HG3	30:Y:108:G:P	2.52	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
29:X:1316:U:O2'	29:X:1317:G:H5'	2.11	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
20:S:19:ILE:HD11	20:S:36:ARG:HG3	1.93	0.50
24:W:3:ILE:HD11	24:W:44:VAL:HG22	1.92	0.50
27:2:11:LYS:HE2	29:X:686:G:H5''	1.93	0.50
29:X:390:A:H4'	29:X:391:A:H5'	1.94	0.50
29:X:2728:U:H2'	29:X:2729:C:C6	2.46	0.50
4:C:28:HIS:O	4:C:32:THR:HG23	2.12	0.49
4:C:57:LYS:NZ	4:C:69:HIS:O	2.45	0.49
4:C:89:ARG:NH2	29:X:1247:A:OP1	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:38:GLU:HB3	5:D:87:ILE:HB	1.93	0.49
5:D:117:ILE:HG22	5:D:118:ASN:H	1.76	0.49
9:H:23:ARG:HE	29:X:2561:A:H2	1.59	0.49
15:N:10:ARG:NH1	29:X:583:G:O5'	2.45	0.49
20:S:55:THR:O	20:S:55:THR:OG1	2.26	0.49
21:T:56:ASP:OD2	29:X:2364:C:H5'	2.11	0.49
29:X:320:U:H4'	29:X:322:A:C8	2.47	0.49
29:X:443:A:C2	29:X:1245:G:N3	2.80	0.49
29:X:566:U:O2'	29:X:809:G:OP2	2.25	0.49
29:X:1626:A:N6	29:X:1639:U:H3	2.06	0.49
29:X:1638:C:H4'	29:X:2710:C:O2	2.12	0.49
1:O:68:VAL:HG11	1:O:153:LYS:HG2	1.94	0.49
3:B:141:ILE:HG23	29:X:2051:A:H4'	1.93	0.49
4:C:118:VAL:H	4:C:188:ILE:HD11	1.77	0.49
5:D:108:LEU:HD22	5:D:114:PHE:CE1	2.47	0.49
6:E:43:VAL:HB	6:E:52:VAL:HG22	1.94	0.49
10:I:64:GLY:HA2	29:X:2415:G:O3'	2.11	0.49
18:Q:43:GLN:HG2	18:Q:48:VAL:O	2.12	0.49
29:X:507:A:O5'	29:X:508:A:H5'	2.12	0.49
29:X:945:A:C4	29:X:2448:A:C2	3.00	0.49
29:X:1285:G:N1	29:X:1329:U:OP1	2.36	0.49
29:X:1779:U:C2	29:X:1783:A:N7	2.80	0.49
29:X:2564:A:C2	29:X:2647:U:H4'	2.47	0.49
29:X:2712(A):A:H5'	29:X:2713:U:OP2	2.12	0.49
1:O:187:ALA:HA	1:O:190:SER:HB3	1.93	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
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
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: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
29:X:1841:U:H2'	29:X:1842:G:C8	2.46	0.49
29:X:2895:C:H2'	29:X:2896:U:H6	1.77	0.49
1:O:29:ALA:HB1	1:O:35:GLU:CB	2.42	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
21:T:46:LYS:O	21:T:78:PHE:HA	2.12	0.49
29:X:214:G:O2'	29:X:226:G:O6	2.27	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:1240:C:C2	29:X:1241:G:C8	3.01	0.49
29:X:1748:C:H2'	29:X:1749:A:C8	2.47	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
11:J:35:LEU:HD23	11:J:105:PHE:CD2	2.48	0.49
29:X:295:G:N2	29:X:344:G:H1'	2.27	0.49
29:X:700:G:H1	29:X:732:C:H5	1.60	0.49
29:X:1464:G:H2'	29:X:1465:G:H8	1.77	0.49
29:X:2307:G:H3'	29:X:2308:G:C8	2.47	0.49
2:A:97:TYR:HB3	2:A:99:ASP:HB3	1.93	0.49
2:A:148:VAL:HG11	29:X:2221:G:H21	1.77	0.49
5:D:26:MET:O	5:D:30:ARG:NH2	2.45	0.49
6:E:43:VAL:HB	6:E:52:VAL:HG13	1.95	0.49
9:H:6:SER:OG	29:X:1666:G:H4'	2.12	0.49
13:L:33:ARG:NE	13:L:38:ILE:HG21	2.28	0.49
20:S:15:ASP:C	20:S:17:SER:H	2.14	0.49
22:U:10:LYS:HD3	22:U:11:LYS:H	1.78	0.49
23:V:32:ALA:HB2	23:V:37:LEU:HD22	1.93	0.49
29:X:1864:U:H3	29:X:1878:G:H1	1.59	0.49
29:X:2836:G:H2'	29:X:2837:A:H8	1.71	0.49
2:A:17:THR:OG1	2:A:205:VAL:N	2.37	0.49
11:J:26:ASP:OD1	11:J:26:ASP:N	2.32	0.49
17:P:14:ARG:O	17:P:18:VAL:HG22	2.13	0.49
29:X:1832:C:N4	29:X:1833:C:C4	2.81	0.49
29:X:2070:G:C2	29:X:2071:A:C4	3.00	0.49
29:X:2080:A:H2'	29:X:2081:U:C6	2.47	0.49
6:E:17:VAL:HG22	6:E:26:VAL:HG22	1.95	0.49
11:J:43:ILE:N	11:J:95:VAL:HG22	2.28	0.49
15:N:11:ARG:HH22	29:X:29:U:H4'	1.77	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:996:A:H2'	29:X:997:G:H8	1.77	0.49
29:X:1668:A:H4'	29:X:1669:A:O5'	2.12	0.49
29:X:1739:C:H2'	29:X:1740:G:H8	1.77	0.49
29:X:1756:A:H8	29:X:1756:A:O5'	1.95	0.49
29:X:2205:A:H2'	29:X:2210:A:N7	2.27	0.49
2:A:102:LYS:NZ	29:X:1500:A:O2'	2.46	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
13:L:92:GLY:C	13:L:94:TYR:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:104:LEU:HA	14:M:106:TYR:HE2	1.76	0.49
19:R:43:ASP:HB3	19:R:45:LYS:HG3	1.94	0.49
19:R:56:LYS:HG3	29:X:481:G:OP2	2.12	0.49
28:3:57:ARG:NH2	29:X:833:A:O3'	2.39	0.49
29:X:301:G:C4	29:X:302:U:C5	3.01	0.49
29:X:1826:G:H2'	29:X:1827:U:H6	1.76	0.49
29:X:2837:A:H2'	29:X:2838:G:H8	1.78	0.49
9:H:9:ASP:O	9:H:95:ALA:HA	2.13	0.49
9:H:10:VAL:HG23	9:H:17:ARG:O	2.13	0.49
16:O:15:SER:O	16:O:16:GLU:HB2	2.13	0.49
17:P:87:GLU:HA	17:P:90:LEU:HD13	1.95	0.49
19:R:80:LYS:NZ	29:X:329:G:N7	2.55	0.49
23:V:44:ARG:O	23:V:47:ARG:HB3	2.13	0.49
29:X:846:U:H4'	29:X:847:U:O5'	2.13	0.49
29:X:1211:A:H4'	29:X:1212:G:OP2	2.13	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
29:X:2584:U:H2'	29:X:2585:U:H2'	1.95	0.49
2:A:29:PRO:HB2	2:A:34:THR:CG2	2.43	0.48
2:A:206:LEU:HB2	29:X:1791:A:O3'	2.12	0.48
12:K:3:HIS:O	12:K:3:HIS:CD2	2.65	0.48
13:L:76:ALA:HB1	13:L:111:GLY:HA2	1.94	0.48
14:M:14:ARG:HB3	14:M:14:ARG:NH2	2.28	0.48
15:N:54:LYS:HZ1	29:X:994:U:P	2.36	0.48
17:P:15:LYS:HB3	29:X:502:A:H4'	1.95	0.48
17:P:99:ALA:O	29:X:25:U:H5'	2.13	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
29:X:79:C:H2'	29:X:80:G:C8	2.48	0.48
29:X:519:U:C2	29:X:520:G:C8	3.01	0.48
29:X:944:G:H8	29:X:944:G:H3'	1.78	0.48
29:X:2195:U:H2'	29:X:2196:C:H6	1.79	0.48
6:E:59:GLN:NE2	29:X:1035:U:OP1	2.47	0.48
11:J:8:THR:HG22	11:J:70:PHE:HE2	1.78	0.48
15:N:61:TRP:O	15:N:65:ILE:HG13	2.13	0.48
17:P:66:GLU:HB3	17:P:67:PRO:HD3	1.95	0.48
20:S:63:PRO:O	20:S:86:VAL:HG22	2.13	0.48
29:X:211:U:H2'	29:X:212:U:C6	2.47	0.48
29:X:1309:G:H21	29:X:1611:C:H5'	1.78	0.48
29:X:1323:G:O6	29:X:1324:G:C6	2.66	0.48
29:X:1467:U:H1'	29:X:1468:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1477:A:H2'	29:X:1478:G:O4'	2.13	0.48
29:X:1727:C:N3	29:X:1750:G:C6	2.81	0.48
29:X:1826:G:O2'	29:X:1971:A:OP2	2.32	0.48
29:X:2055:C:H5'	29:X:2056:G:H5''	1.95	0.48
29:X:2064:C:O2	29:X:2450:A:N6	2.46	0.48
29:X:2323:G:C6	29:X:2332:U:H5	2.30	0.48
30:Y:63:A:C2	30:Y:64:C:C2	3.01	0.48
4:C:68:ARG:NH2	29:X:2060:A:N6	2.59	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
19:R:45:LYS:HA	19:R:76:LEU:O	2.14	0.48
24:W:22:ALA:O	29:X:931:U:H4'	2.12	0.48
29:X:545:U:H4'	29:X:546:U:OP2	2.13	0.48
29:X:672:U:C2	29:X:809:G:N2	2.81	0.48
29:X:822:U:O2	29:X:822:U:H2'	2.14	0.48
29:X:848:G:C4	29:X:849:A:C8	3.01	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:2218:U:H2'	29:X:2219:U:H6	1.77	0.48
29:X:2346:A:H4'	29:X:2347:C:OP2	2.12	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
8:G:94:LYS:O	8:G:98:LYS:HB3	2.13	0.48
11:J:61:ARG:HG2	20:S:175:ARG:H	1.78	0.48
12:K:14:SER:N	12:K:17:ARG:HH21	2.11	0.48
14:M:55:ILE:O	14:M:103:LYS:O	2.31	0.48
29:X:553:G:H2'	29:X:554:U:O4'	2.13	0.48
29:X:638:G:H2'	29:X:639:U:H6	1.78	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:1493:A:C8	29:X:1494:A:C8	3.02	0.48
29:X:1510:U:H2'	29:X:1511:G:C8	2.48	0.48
29:X:2347:C:C5	29:X:2382:G:H1'	2.48	0.48
29:X:2850:A:C2	29:X:2851:C:C2	3.02	0.48
3:B:116:VAL:HB	3:B:122:PHE:CG	2.49	0.48
5:D:8:TYR:O	5:D:12:VAL:HG23	2.14	0.48
17:P:16:GLN:HG2	29:X:502:A:OP1	2.13	0.48
17:P:102:THR:HB	17:P:120:ARG:HA	1.95	0.48
25:Z:6:VAL:HG12	29:X:2015:A:N3	2.28	0.48
29:X:658:A:H2'	29:X:659:C:O4'	2.14	0.48
29:X:1655:A:H3'	29:X:1656:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1850:G:H2'	29:X:1851:U:H5'	1.95	0.48
29:X:2537:U:H2'	29:X:2538:C:C6	2.48	0.48
3:B:39:ALA:N	3:B:45:GLU:OE2	2.47	0.48
4:C:35:LEU:HD23	4:C:35:LEU:HA	1.66	0.48
4:C:44:SER:HB2	4:C:88:PRO:HD3	1.95	0.48
5:D:143:TYR:HA	5:D:146:VAL:HG22	1.95	0.48
6:E:98:LEU:HD12	6:E:102:ALA:O	2.14	0.48
6:E:105:MET:HE2	6:E:107:ILE:HD11	1.96	0.48
13:L:27:LEU:O	13:L:88:VAL:N	2.47	0.48
15:N:82:GLY:HA3	15:N:113:SER:OG	2.13	0.48
20:S:3:LEU:HB3	20:S:34:LEU:HD23	1.96	0.48
26:1:27:ASN:ND2	26:1:29:ARG:HB2	2.29	0.48
28:3:27:SER:OG	29:X:2361:C:OP1	2.21	0.48
29:X:295:G:H2'	29:X:296:C:C6	2.49	0.48
29:X:1163:G:H2'	29:X:1164:A:C8	2.44	0.48
29:X:1480:G:O6	29:X:1512:C:N4	2.45	0.48
29:X:2219:U:C2	29:X:2220:C:H1'	2.48	0.48
29:X:2455:G:H2'	29:X:2456:C:C6	2.49	0.48
29:X:2874:C:H2'	29:X:2875:U:C6	2.48	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
17:P:21:ARG:NH2	29:X:496:G:H4'	2.28	0.48
20:S:49:THR:OG1	20:S:132:GLN:OE1	2.32	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
1:0:152:LEU:HD23	1:0:157:ILE:HG21	1.96	0.48
3:B:188:ILE:CG2	3:B:189:PRO:HD2	2.43	0.48
6:E:110:SER:OG	29:X:2667:C:N3	2.38	0.48
6:E:154:PRO:HA	6:E:160:LYS:O	2.13	0.48
28:3:44:LYS:O	28:3:46:LYS:N	2.46	0.48
29:X:165(B):G:H1	29:X:180:C:H42	1.60	0.48
29:X:492:A:H2'	29:X:493:G:O4'	2.13	0.48
29:X:1101:U:H2'	29:X:1102:C:C6	2.49	0.48
29:X:1510:U:H2'	29:X:1511:G:N9	2.29	0.48
29:X:2071:A:H2'	29:X:2072:G:H8	1.77	0.48
30:Y:3:A:H2'	30:Y:4:C:C6	2.49	0.48
3:B:44:TYR:CE1	29:X:2637:U:H5'	2.48	0.48
6:E:83:TYR:CE1	6:E:138:LYS:HB2	2.49	0.48
10:I:55:ARG:NH1	29:X:223:A:OP1	2.33	0.48
13:L:64:LYS:HG3	30:Y:53:G:C5'	2.42	0.48
20:S:123:VAL:HG23	20:S:161:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:167:THR:OG1	29:X:875:G:H4'	2.13	0.48
24:W:5:LEU:HB2	24:W:25:LEU:CD1	2.44	0.48
29:X:523:C:H5''	29:X:540:C:O2'	2.14	0.48
29:X:741:G:H2'	29:X:742:C:H6	1.78	0.48
29:X:1606:G:H5''	29:X:1607:C:OP1	2.13	0.48
29:X:1853:A:H2'	29:X:1854:A:C8	2.49	0.48
29:X:2032:G:N2	29:X:2572:A:C8	2.82	0.48
29:X:2251:G:H5''	29:X:2252:G:OP2	2.13	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
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
19:R:48:VAL:C	19:R:50:GLY:H	2.17	0.48
29:X:572:A:H5''	29:X:573:G:OP2	2.13	0.48
29:X:640:C:H2'	29:X:641:C:H6	1.79	0.48
29:X:1838:C:H4'	29:X:1839:G:H8	1.78	0.48
29:X:2684:U:C2	29:X:2685:G:C8	3.02	0.48
9:H:132:GLU:OE1	14:M:72:SER:OG	2.27	0.47
10:I:110:ALA:HB3	29:X:637:A:C5'	2.44	0.47
12:K:81:ASP:O	12:K:85:PRO:HG3	2.14	0.47
16:O:67:LYS:HG3	16:O:68:LYS:N	2.28	0.47
17:P:18:VAL:HG23	17:P:19:LYS:N	2.29	0.47
22:U:28:GLY:HA3	22:U:32:ARG:HB3	1.96	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
29:X:193:A:C8	29:X:238:G:C5	3.02	0.47
29:X:200:A:H3'	29:X:200:A:C8	2.50	0.47
29:X:1592:U:H2'	29:X:1593:G:H8	1.79	0.47
29:X:2120:G:N2	29:X:2177:C:H42	2.12	0.47
29:X:2282:G:H4'	29:X:2389:G:O2'	2.13	0.47
29:X:2304:G:N2	29:X:2312:U:H3	2.08	0.47
29:X:2443:C:O2'	29:X:2444:G:H5'	2.14	0.47
29:X:2658:C:H2'	29:X:2659:G:O4'	2.13	0.47
5:D:5:LYS:HD2	5:D:101:GLU:HB2	1.97	0.47
5:D:51:ASP:O	5:D:55:LYS:HG2	2.15	0.47
9:H:83:ARG:NH2	9:H:89:ILE:HD11	2.28	0.47
9:H:111:PHE:CD1	9:H:111:PHE:N	2.82	0.47
10:I:4:HIS:C	10:I:4:HIS:CD2	2.87	0.47
14:M:17:GLU:HG3	14:M:62:SER:HB3	1.96	0.47
19:R:112:LYS:HE3	19:R:112:LYS:HB3	1.53	0.47
20:S:43:PHE:CE2	20:S:69:VAL:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:7:ARG:HA	23:V:60:LEU:HD11	1.96	0.47
24:W:3:ILE:HD11	24:W:44:VAL:CG2	2.45	0.47
29:X:165:A:H2'	29:X:165(A):G:H8	1.77	0.47
29:X:222:G:C6	29:X:223:A:C6	3.01	0.47
29:X:407:C:H2'	29:X:408:G:C8	2.49	0.47
29:X:616:A:H2'	29:X:617:A:H8	1.76	0.47
29:X:934:G:H2'	29:X:935:U:H6	1.78	0.47
29:X:1882:C:H2'	29:X:1883:G:O4'	2.14	0.47
29:X:2564:A:OP1	29:X:2648:G:O2'	2.16	0.47
29:X:2740:A:C8	29:X:2763:G:N2	2.82	0.47
2:A:253:PRO:HD2	2:A:257:LEU:HD22	1.96	0.47
3:B:26:VAL:HG11	3:B:198:LEU:HD11	1.96	0.47
3:B:98:GLU:OE2	3:B:175:ILE:N	2.43	0.47
9:H:64:VAL:HG22	9:H:106:ARG:HH21	1.79	0.47
11:J:35:LEU:HB3	11:J:105:PHE:HB2	1.96	0.47
19:R:99:VAL:HG11	19:R:105:ARG:CZ	2.44	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
29:X:1565:C:H42	29:X:1568:G:H1	1.61	0.47
29:X:2037:G:H2'	29:X:2038:G:C8	2.49	0.47
29:X:2675:A:H2'	29:X:2676:C:O4'	2.14	0.47
4:C:28:HIS:HB2	10:I:6:LEU:HD13	1.96	0.47
7:F:75:SER:O	7:F:79:ARG:NH1	2.48	0.47
10:I:117:ALA:HB2	10:I:136:ALA:O	2.14	0.47
18:Q:43:GLN:O	18:Q:47:GLY:N	2.47	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
25:Z:55:ARG:HH21	25:Z:58:LEU:HA	1.78	0.47
26:1:38:LYS:HD2	29:X:2344:U:OP1	2.15	0.47
29:X:944:G:H3'	29:X:944:G:C8	2.49	0.47
29:X:1952:A:C6	29:X:1953:A:N1	2.82	0.47
29:X:2080:A:H2'	29:X:2081:U:H6	1.79	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
29:X:2870:C:N4	29:X:2871:G:O6	2.47	0.47
30:Y:16:U:H2'	30:Y:110:U:O2'	2.15	0.47
1:O:17:SER:OG	1:O:18:ILE:N	2.46	0.47
4:C:97:ARG:O	4:C:101:GLN:HG2	2.14	0.47
9:H:110:VAL:H	9:H:129:LEU:HB3	1.78	0.47
15:N:37:GLN:CG	29:X:1252:G:H1	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:13:ASP:O	23:V:17:GLU:HG2	2.13	0.47
29:X:200:A:H3'	29:X:200:A:H8	1.80	0.47
29:X:526:A:O2'	29:X:2043:C:O2	2.32	0.47
29:X:1216:C:O5'	29:X:1216:C:H6	1.97	0.47
29:X:1318:G:C2'	29:X:1319:G:H5'	2.44	0.47
29:X:1824:G:H2'	29:X:1825:U:H6	1.78	0.47
29:X:2681:C:C2	29:X:2724:U:O4	2.67	0.47
29:X:2712:C:O2'	29:X:2712(A):A:H5''	2.14	0.47
29:X:2801:G:H2'	29:X:2802:G:H8	1.79	0.47
2:A:16:MET:HG3	2:A:207:GLY:HA3	1.95	0.47
5:D:118:ASN:HD21	5:D:120:ASN:HB2	1.80	0.47
10:I:80:LEU:HD11	10:I:89:ASP:OD2	2.15	0.47
11:J:12:LYS:HD3	29:X:911:A:C5	2.50	0.47
12:K:43:GLU:HG3	12:K:43:GLU:O	2.15	0.47
13:L:104:ALA:O	13:L:107:ALA:N	2.47	0.47
22:U:23:LYS:HD2	22:U:35:THR:HG21	1.95	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
27:2:31:LEU:HD23	27:2:42:LEU:HD22	1.96	0.47
28:3:33:ASN:HB2	29:X:2420:C:OP2	2.15	0.47
28:3:50:LEU:HD13	28:3:50:LEU:HA	1.66	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
29:X:2458:G:C8	29:X:2490:G:C6	3.03	0.47
29:X:2549:G:C2	29:X:2550:G:N7	2.82	0.47
3:B:149:ARG:NH1	29:X:2024:G:O3'	2.48	0.47
5:D:111:ILE:HG22	5:D:114:PHE:HB2	1.96	0.47
5:D:138:PHE:HB2	5:D:141:ILE:HB	1.97	0.47
6:E:21:ASP:HB2	6:E:23:VAL:HG23	1.95	0.47
7:F:37:PHE:HA	7:F:40:ALA:HB3	1.97	0.47
10:I:81:GLN:HG2	10:I:114:ILE:HD13	1.97	0.47
13:L:74:ALA:O	13:L:77:ALA:HB3	2.15	0.47
20:S:141:MET:HG3	20:S:145:ASP:HB3	1.97	0.47
29:X:532:A:P	29:X:561:G:H21	2.37	0.47
29:X:588:U:H2'	29:X:589:U:H6	1.80	0.47
29:X:627:A:H4'	29:X:628:G:H5'	1.97	0.47
29:X:1154:G:H5''	29:X:1155:A:OP2	2.14	0.47
29:X:1656:C:H2'	29:X:1657:C:H6	1.80	0.47
29:X:2560:C:C4	29:X:2561:A:N7	2.82	0.47
29:X:2816:C:C2	29:X:2831:G:N2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:H:85:ASP:HB3	14:M:87:LEU:HD12	1.97	0.47
12:K:32:GLY:O	12:K:115:LEU:HD13	2.14	0.47
16:O:22:VAL:HG12	16:O:23:GLU:N	2.29	0.47
27:2:43:THR:O	27:2:46:ASP:N	2.42	0.47
29:X:812:C:H2'	29:X:813:U:H6	1.80	0.47
29:X:1973:G:H2'	29:X:1974:C:C6	2.50	0.47
29:X:2615:U:H2'	29:X:2616:C:C6	2.49	0.47
6:E:111:HIS:HA	6:E:112:PRO:HD2	1.63	0.47
12:K:51:LEU:HD13	12:K:70:ILE:HD11	1.95	0.47
15:N:12:ARG:HD3	15:N:12:ARG:HA	1.59	0.47
29:X:947:G:H2'	29:X:948:C:C6	2.50	0.47
29:X:2544:G:H2'	29:X:2545:G:H8	1.80	0.47
29:X:2698:U:H2'	29:X:2699:C:C6	2.50	0.47
29:X:2711:A:OP1	29:X:2712(A):A:P	2.72	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:1196:C:C2	29:X:1197:G:C8	3.03	0.47
29:X:1333:C:H6	29:X:1333:C:O5'	1.98	0.47
29:X:2119:A:O4'	29:X:2172:U:O2'	2.33	0.47
29:X:2294:C:H2'	29:X:2295:C:C6	2.47	0.47
29:X:2511:U:H2'	29:X:2512:C:H6	1.79	0.47
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
5:D:117:ILE:HG21	5:D:130:LEU:HD11	1.96	0.46
6:E:164:PHE:O	6:E:166:GLY:N	2.48	0.46
13:L:32:TYR:CE2	30:Y:9:G:H5'	2.50	0.46
17:P:12:LYS:O	17:P:16:GLN:HG3	2.15	0.46
20:S:15:ASP:OD2	20:S:15:ASP:N	2.47	0.46
22:U:46:LEU:HB2	29:X:2230:G:H4'	1.97	0.46
29:X:531:C:H5''	29:X:532:A:C4	2.50	0.46
29:X:793:A:OP2	29:X:2071:A:O2'	2.32	0.46
29:X:1136:G:H2'	29:X:1137:G:H8	1.80	0.46
29:X:1782:C:H1'	29:X:2609:U:H5'	1.97	0.46
29:X:1999:C:H5''	29:X:2723:C:O2'	2.15	0.46
29:X:2070:G:H2'	29:X:2071:A:C8	2.50	0.46
29:X:2364:C:H2'	29:X:2365:G:O4'	2.15	0.46
5:D:34:ILE:N	5:D:91:LEU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:44:LYS:HD2	11:J:47:GLN:NE2	2.30	0.46
13:L:63:ASN:HB3	13:L:66:ASP:HB2	1.97	0.46
29:X:641:C:H42	29:X:646:A:N6	2.11	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
29:X:2683:C:H2'	29:X:2684:U:C6	2.42	0.46
30:Y:34:C:H2'	30:Y:35:C:H6	1.80	0.46
5:D:39:GLY:HA2	5:D:86:GLY:HA2	1.97	0.46
6:E:8:PRO:HD2	6:E:69:ARG:HH11	1.80	0.46
8:G:67:ARG:HA	8:G:68:PRO:HD2	1.81	0.46
12:K:54:THR:HG22	12:K:66:VAL:HG23	1.97	0.46
19:R:29:HIS:CD2	19:R:51:VAL:HA	2.50	0.46
22:U:48:LYS:NZ	29:X:2229:U:O2	2.43	0.46
24:W:36:ASP:OD1	24:W:41:ARG:NH1	2.49	0.46
29:X:37:C:H4'	29:X:451:C:OP1	2.16	0.46
29:X:330:A:H2'	29:X:330:A:N3	2.30	0.46
29:X:643:A:O2'	29:X:644:A:OP1	2.30	0.46
29:X:1336:A:H2'	29:X:1337:G:C8	2.51	0.46
29:X:1525:G:C2	29:X:1526:G:H1'	2.50	0.46
29:X:1796:U:H2'	29:X:1797:C:H6	1.78	0.46
30:Y:63:A:O2'	30:Y:64:C:H5'	2.14	0.46
1:O:214:MET:HA	29:X:2175:C:O2'	2.16	0.46
2:A:33:LEU:HD13	2:A:104:TYR:HD2	1.79	0.46
4:C:30:VAL:HG11	4:C:177:VAL:HG21	1.97	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:83:G:H22	29:X:102:G:H1'	1.77	0.46
29:X:310:A:O2'	29:X:311:A:O5'	2.29	0.46
29:X:581:C:H2'	29:X:582:G:H8	1.79	0.46
29:X:2060:A:H1'	29:X:2502:G:H1'	1.97	0.46
29:X:2283:C:C6	29:X:2389:G:H2'	2.50	0.46
29:X:2396:G:C2	29:X:2421:G:C2	3.03	0.46
30:Y:71:G:C6	30:Y:72:C:C4	3.03	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
11:J:7:ARG:HE	11:J:7:ARG:HB2	1.52	0.46
14:M:67:THR:OG1	14:M:80:VAL:HG22	2.16	0.46
18:Q:29:VAL:HG11	18:Q:38:ILE:HG12	1.97	0.46
20:S:51:LEU:HA	20:S:64:ALA:O	2.15	0.46
22:U:72:LYS:HA	22:U:72:LYS:HD3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:5:A:H2'	29:X:6:A:H8	1.79	0.46
29:X:848:G:N3	29:X:933:A:H1'	2.31	0.46
29:X:1413:G:H22	29:X:1587:A:H3'	1.80	0.46
29:X:1483:A:H2'	29:X:1484:U:O4'	2.16	0.46
29:X:2210:A:N6	29:X:2211:A:N1	2.64	0.46
29:X:2242:G:H2'	29:X:2243:U:O4'	2.15	0.46
29:X:2686:G:C2	29:X:2724:U:O2	2.69	0.46
30:Y:122:U:H5''	30:Y:123:U:OP2	2.16	0.46
4:C:5:ASN:HA	4:C:119:ALA:HB3	1.98	0.46
4:C:96:PRO:HB2	4:C:99:VAL:HG23	1.97	0.46
10:I:51:GLY:HA2	29:X:832:U:O2	2.16	0.46
15:N:10:ARG:NH1	29:X:583:G:P	2.89	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
22:U:68:ARG:NH2	29:X:400:G:N7	2.57	0.46
24:W:40:VAL:HA	24:W:43:MET:HE3	1.98	0.46
29:X:20:C:H2'	29:X:21:A:C8	2.50	0.46
29:X:214:G:H22	29:X:226:G:H2'	1.80	0.46
29:X:799:G:H3'	29:X:800:A:H2'	1.97	0.46
29:X:852:A:C5	29:X:853:U:C5	3.04	0.46
29:X:1217:C:H2'	29:X:1218:A:C8	2.49	0.46
29:X:1956:U:H1'	29:X:2552:U:OP1	2.15	0.46
29:X:2212:A:H5''	29:X:2213:U:H5	1.81	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
20:S:41:ARG:HH22	29:X:1041:C:P	2.38	0.46
21:T:38:VAL:HG23	21:T:59:LEU:HB2	1.97	0.46
29:X:68:G:H2'	29:X:69:C:C6	2.51	0.46
29:X:661:U:H2'	29:X:662:C:O4'	2.16	0.46
29:X:669:G:N3	29:X:669:G:C2'	2.79	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
29:X:2256:G:N2	29:X:2275:C:N4	2.63	0.46
29:X:2276:G:C2	29:X:2277:G:C8	3.04	0.46
1:O:208:ALA:HB3	1:O:220:LEU:HB2	1.98	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
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:389:A:C8	29:X:2413:G:H4'	2.51	0.46
29:X:1194:A:C2	29:X:1195:G:H1'	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1271:G:H5''	29:X:1272:A:OP1	2.16	0.46
29:X:2266:A:H4'	29:X:2267:A:C2	2.50	0.46
29:X:2325:G:P	29:X:2325:G:H8	2.38	0.46
30:Y:6:C:H2'	30:Y:7:C:H6	1.79	0.46
4:C:42:THR:HG1	29:X:39:G:H21	1.62	0.46
8:G:81:VAL:HG11	8:G:156:HIS:CD2	2.41	0.46
21:T:43:THR:HB	29:X:2331:G:O3'	2.15	0.46
29:X:691:G:C6	29:X:692:C:C4	3.04	0.46
29:X:818:G:N7	29:X:1187:G:C6	2.84	0.46
29:X:1234:U:H2'	29:X:1235:G:O4'	2.16	0.46
29:X:1319:G:O2'	29:X:1320:G:H5'	2.16	0.46
29:X:2821:A:H2'	29:X:2822:G:C8	2.51	0.46
5:D:135:GLN:HA	5:D:138:PHE:CE1	2.50	0.46
8:G:148:LEU:HD12	8:G:149:LYS:H	1.80	0.46
15:N:85:ARG:HD3	15:N:116:ALA:O	2.16	0.46
17:P:50:VAL:O	17:P:54:GLU:HG3	2.15	0.46
17:P:109:ARG:HD2	29:X:748:G:OP2	2.15	0.46
20:S:23:ALA:N	20:S:32:PHE:HE2	2.14	0.46
22:U:17:SER:HB3	22:U:18:VAL:HB	1.98	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:1019:U:C4	29:X:1020:C:H5	2.34	0.46
29:X:1209:G:N2	29:X:1210:G:H22	2.14	0.46
29:X:2014:A:H2'	29:X:2015:A:C8	2.51	0.46
29:X:2204:A:H2	29:X:2219:U:H3	1.63	0.46
29:X:2247:A:H2'	29:X:2248:C:C6	2.51	0.46
3:B:2:LYS:HA	3:B:84:PHE:CE1	2.51	0.45
4:C:34:GLN:O	4:C:37:SER:OG	2.22	0.45
9:H:20:MET:HG2	9:H:21:CYS:O	2.16	0.45
9:H:85:ASP:OD1	9:H:87:SER:N	2.43	0.45
10:I:113:GLU:HG2	10:I:114:ILE:N	2.30	0.45
15:N:78:THR:HB	15:N:117:ARG:CZ	2.46	0.45
26:1:41:ASP:OD2	26:1:43:VAL:HG23	2.16	0.45
29:X:562:U:O2'	29:X:572:A:H8	1.97	0.45
29:X:733:G:C8	29:X:761:A:C6	3.04	0.45
29:X:862:G:H2'	29:X:863:A:O4'	2.16	0.45
29:X:1150:U:H2'	29:X:1151:A:H8	1.80	0.45
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
29:X:2330:G:N2	29:X:2386:U:O2	2.49	0.45
29:X:2339:U:H2'	29:X:2340:G:H8	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:49:ILE:HG13	29:X:779:U:OP1	2.16	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
3:B:195:LEU:HB2	14:M:3:THR:HG22	1.98	0.45
4:C:156:ASN:HA	4:C:159:ARG:HB2	1.98	0.45
6:E:24:PHE:CD1	6:E:37:TYR:HB2	2.51	0.45
9:H:13:ASN:HD21	9:H:109:ARG:HG2	1.80	0.45
15:N:74:MET:CE	15:N:110:VAL:HG13	2.44	0.45
17:P:71:VAL:HG12	17:P:126:ILE:HD12	1.97	0.45
19:R:18:LYS:HA	19:R:36:VAL:HG11	1.98	0.45
24:W:22:ALA:C	24:W:24:GLY:H	2.20	0.45
25:Z:38:GLY:HA3	25:Z:48:ASN:HD22	1.80	0.45
26:1:13:GLU:C	26:1:49:PHE:HB3	2.37	0.45
29:X:392:C:H2'	29:X:393:G:C8	2.51	0.45
29:X:399:U:H2'	29:X:400:G:O4'	2.16	0.45
29:X:2327:A:C5	29:X:2388:A:N1	2.85	0.45
29:X:2418:A:H2'	29:X:2419:U:O4'	2.16	0.45
5:D:92:ARG:HD3	30:Y:47:A:H8	1.80	0.45
9:H:13:ASN:HD21	9:H:109:ARG:N	2.13	0.45
9:H:43:ARG:HD3	9:H:44:TYR:CE2	2.51	0.45
14:M:70:LYS:HD3	14:M:72:SER:HB2	1.99	0.45
19:R:58:VAL:HA	29:X:483:A:H5'	1.97	0.45
29:X:1499:U:H2'	29:X:1500:A:C8	2.52	0.45
29:X:1840:G:C6	29:X:1841:U:C4	3.04	0.45
29:X:2060:A:C2	29:X:2502:G:C5	3.04	0.45
29:X:2307:G:C6	29:X:2308:G:H1'	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
29:X:2680:C:O2'	29:X:2681:C:H5'	2.16	0.45
2:A:250:TRP:CE2	29:X:1805:A:H5''	2.51	0.45
8:G:41:TRP:HB3	8:G:163:PRO:HB3	1.98	0.45
8:G:56:THR:HG21	29:X:1005:C:O2'	2.16	0.45
10:I:45:LYS:HE3	10:I:45:LYS:HB2	1.54	0.45
15:N:8:ILE:HD11	29:X:1215:G:O3'	2.17	0.45
17:P:109:ARG:HH11	17:P:109:ARG:CG	2.29	0.45
22:U:29:GLY:C	22:U:31:GLY:N	2.69	0.45
29:X:497:A:H2'	29:X:498:G:C8	2.52	0.45
29:X:926:C:O2'	29:X:928:C:N4	2.50	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
4:C:59:TYR:CD1	4:C:64:THR:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:130:THR:HG22	4:C:160:ALA:O	2.16	0.45
9:H:97:VAL:HG11	9:H:126:ILE:HD13	1.98	0.45
17:P:86:LEU:HD23	17:P:86:LEU:HA	1.79	0.45
18:Q:48:VAL:HG11	18:Q:82:LEU:HG	1.99	0.45
25:Z:7:PRO:HA	29:X:2615:U:N1	2.31	0.45
28:3:6:THR:HG23	28:3:62:LEU:HA	1.97	0.45
29:X:309:A:N6	29:X:1210:G:O2'	2.49	0.45
29:X:875:G:C6	29:X:876:C:C2	3.05	0.45
29:X:1196:C:O2'	29:X:1227:G:O2'	2.32	0.45
29:X:1365:A:H5'	29:X:1366:A:OP2	2.16	0.45
29:X:2056:G:C2	29:X:2057:A:C8	3.04	0.45
29:X:2195:U:H2'	29:X:2196:C:C6	2.51	0.45
29:X:2347:C:H2'	29:X:2348:U:H6	1.79	0.45
29:X:2615:U:H2'	29:X:2616:C:H6	1.82	0.45
8:G:71:THR:HB	8:G:76:GLN:NE2	2.30	0.45
17:P:75:ALA:HB1	17:P:128:VAL:HG22	1.99	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:306:U:O2'	29:X:1211:A:N7	2.50	0.45
29:X:1370:C:H2'	29:X:1371:G:O4'	2.17	0.45
29:X:1686:C:H2'	29:X:1687:G:O4'	2.17	0.45
29:X:2599:G:N3	29:X:2600:A:C8	2.85	0.45
2:A:202:LYS:HB2	29:X:1820:U:C2	2.51	0.45
4:C:103:GLY:O	4:C:106:MET:N	2.49	0.45
13:L:31:VAL:O	13:L:32:TYR:HB2	2.17	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
22:U:22:GLY:O	22:U:39:LYS:HG3	2.16	0.45
22:U:31:GLY:HA2	22:U:32:ARG:NH1	2.32	0.45
22:U:61:TRP:O	22:U:62:LEU:HD12	2.16	0.45
29:X:83:G:H21	29:X:84:A:N6	2.15	0.45
29:X:733:G:O6	29:X:761:A:C8	2.70	0.45
29:X:902:C:H2'	29:X:903:C:H6	1.81	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:2532:G:C6	29:X:2533:A:C5	3.05	0.45
29:X:2837:A:H2'	29:X:2838:G:C8	2.52	0.45
10:I:73:GLU:OE2	10:I:104:ARG:HB2	2.16	0.45
11:J:36:ILE:HD12	20:S:76:ARG:HD2	1.99	0.45
17:P:56:LEU:HD22	25:Z:28:PRO:HD2	1.99	0.45
24:W:11:GLY:HA2	29:X:969:G:O3'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:91:A:H4'	29:X:92:G:O5'	2.16	0.45
29:X:814:C:H2'	29:X:815:C:H6	1.82	0.45
29:X:2094:G:N2	29:X:2196:C:O2	2.50	0.45
29:X:2339:U:H2'	29:X:2340:G:C8	2.52	0.45
29:X:2516:G:C2'	29:X:2517:C:H5'	2.47	0.45
29:X:2727:G:H2'	29:X:2728:U:H6	1.81	0.45
29:X:2901:C:H2'	29:X:2902:A:C8	2.51	0.45
30:Y:48:A:H2'	30:Y:49:C:C6	2.52	0.45
5:D:74:ILE:HA	5:D:79:LEU:CB	2.47	0.45
16:O:85:GLY:HA3	29:X:1224:G:O3'	2.16	0.45
20:S:3:LEU:HD23	20:S:32:PHE:HB2	1.99	0.45
24:W:32:ARG:HG2	24:W:33:GLU:N	2.32	0.45
27:2:16:HIS:HB2	27:2:44:VAL:HG21	1.99	0.45
29:X:27:G:HO2'	29:X:28:A:P	2.36	0.45
29:X:440:G:C2	29:X:441:U:C2	3.04	0.45
29:X:878:A:H1'	29:X:899:A:N7	2.31	0.45
29:X:1124:C:C2	29:X:1125:G:C8	3.05	0.45
29:X:1608:A:H1'	29:X:1610:A:OP2	2.17	0.45
29:X:1849:G:H2'	29:X:1850:G:C8	2.52	0.45
29:X:1922:G:OP2	29:X:1922:G:H8	2.00	0.45
29:X:2004:G:C6	29:X:2005:A:C4	3.05	0.45
29:X:2721:A:H2'	29:X:2722:G:O4'	2.17	0.45
7:F:11:GLN:HB3	29:X:1061:U:C5	2.52	0.45
10:I:114:ILE:HD13	10:I:114:ILE:HA	1.81	0.45
11:J:27:TYR:HB2	11:J:137:VAL:HB	1.99	0.45
13:L:101:LYS:O	13:L:104:ALA:HB3	2.17	0.45
16:O:87:ARG:NH2	29:X:1222:C:OP1	2.50	0.45
20:S:111:GLY:HA3	20:S:172:LEU:O	2.17	0.45
22:U:54:ASN:C	22:U:56:GLN:H	2.14	0.45
29:X:729:G:H2'	29:X:1775:U:O2	2.17	0.45
29:X:2291:U:H2'	29:X:2292:C:C6	2.51	0.45
29:X:2404:C:C2	29:X:2405:G:C8	3.04	0.45
30:Y:54:U:H4'	30:Y:54:U:OP1	2.17	0.45
2:A:148:VAL:HB	2:A:151:LYS:HE2	1.99	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
19:R:61:SER:HA	19:R:65:PRO:HA	1.99	0.44
20:S:3:LEU:HG	20:S:32:PHE:HD1	1.80	0.44
29:X:1069:A:H4'	29:X:1070:A:H8	1.82	0.44
29:X:2101:G:N2	29:X:2189:U:O2	2.50	0.44
29:X:2307:G:C8	29:X:2308:G:C8	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:33:ILE:HA	3:B:33:ILE:HD13	1.73	0.44
4:C:120:VAL:N	4:C:190:ALA:HB2	2.33	0.44
9:H:85:ASP:OD1	9:H:87:SER:HB3	2.17	0.44
10:I:21:ARG:HG2	10:I:21:ARG:NH1	2.31	0.44
12:K:65:LEU:O	12:K:68:GLN:HG3	2.17	0.44
17:P:40:LEU:HB3	25:Z:25:LEU:HD13	1.98	0.44
23:V:31:GLN:O	23:V:35:GLY:N	2.51	0.44
29:X:382:G:N2	29:X:393:G:C4	2.86	0.44
29:X:1950:G:C8	29:X:1951:U:C5	3.05	0.44
1:O:74:THR:O	1:O:92:SER:HA	2.17	0.44
4:C:67:ALA:HA	29:X:1255:U:C6	2.51	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
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
28:3:35:GLY:N	28:3:36:LYS:HA	2.33	0.44
29:X:219:G:H4'	29:X:386:G:C5	2.52	0.44
29:X:440:G:H2'	29:X:441:U:C6	2.52	0.44
29:X:981:A:H5''	29:X:982:C:OP2	2.17	0.44
29:X:1435:C:H42	29:X:1557:G:H1	1.63	0.44
29:X:2347:C:H5	29:X:2382:G:H1'	1.83	0.44
29:X:2521:C:H2'	29:X:2522:U:O4'	2.16	0.44
1:O:1:LYS:HB2	29:X:2131:G:C8	2.53	0.44
2:A:30:GLU:O	2:A:34:THR:HG23	2.18	0.44
9:H:132:GLU:HB2	14:M:73:PHE:CE1	2.51	0.44
18:Q:54:SER:HB2	29:X:1341:A:O3'	2.17	0.44
27:2:16:HIS:CB	27:2:44:VAL:HG21	2.48	0.44
28:3:17:THR:HG23	28:3:18:GLY:N	2.31	0.44
29:X:538:G:C2	29:X:539:G:C8	3.06	0.44
29:X:651(B):C:H5''	29:X:653:U:O5'	2.17	0.44
29:X:1136:G:H2'	29:X:1137:G:C8	2.52	0.44
29:X:1729:C:H1'	29:X:2860:A:H1'	1.98	0.44
29:X:1763:G:O2'	29:X:1958:C:OP1	2.31	0.44
29:X:2696:U:H2'	29:X:2697:G:C8	2.53	0.44
30:Y:33:C:H42	30:Y:53:G:H1	1.64	0.44
2:A:108:PRO:HA	2:A:196:VAL:O	2.18	0.44
8:G:68:PRO:HA	15:N:67:ALA:HB3	1.99	0.44
11:J:36:ILE:HG22	11:J:37:ALA:O	2.18	0.44
13:L:60:LYS:O	13:L:61:SER:OG	2.23	0.44
16:O:50:ASP:HA	16:O:53:LYS:HE3	1.99	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)
18:Q:3:HIS:NE2	18:Q:44:GLN:HG3	2.32	0.44
29:X:600:C:O2	29:X:604:C:H4'	2.16	0.44
29:X:624:C:O2'	29:X:657:U:H5''	2.17	0.44
29:X:996:A:N3	29:X:997:G:C8	2.86	0.44
29:X:1118:A:H2'	29:X:1119:U:O4'	2.17	0.44
29:X:1324:G:O2'	29:X:1326:U:OP2	2.28	0.44
29:X:1593:G:H2'	29:X:1594:A:C8	2.52	0.44
29:X:1598:C:H2'	29:X:1599:C:H6	1.82	0.44
29:X:1901:A:H2'	29:X:1902:C:H6	1.82	0.44
29:X:2247:A:H2'	29:X:2248:C:H6	1.82	0.44
30:Y:3:A:C6	30:Y:4:C:N4	2.86	0.44
2:A:43:ARG:HA	2:A:48:ARG:O	2.17	0.44
3:B:60:ASN:HB3	3:B:62:PRO:CD	2.45	0.44
3:B:144:ARG:NH1	29:X:2572:A:O2'	2.50	0.44
5:D:79:LEU:HD21	29:X:2310:A:N3	2.32	0.44
5:D:80:ARG:HD3	5:D:83:MET:HB3	1.99	0.44
7:F:79:ARG:HB3	7:F:84:ILE:O	2.17	0.44
8:G:65:LYS:O	8:G:66:HIS:HB3	2.18	0.44
8:G:115:ALA:O	8:G:119:LEU:HB2	2.18	0.44
14:M:69:ARG:HD2	14:M:78:GLU:OE2	2.17	0.44
25:Z:7:PRO:HA	29:X:2615:U:C2	2.53	0.44
29:X:189:G:H2'	29:X:190:A:O4'	2.17	0.44
29:X:620:G:H4'	29:X:621:A:H5''	1.99	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
29:X:2498:C:O2'	29:X:2499:C:H5'	2.17	0.44
3:B:180:ASN:O	3:B:181:LEU:HD23	2.17	0.44
4:C:112:GLN:C	4:C:114:GLY:H	2.21	0.44
7:F:91:PRO:HA	7:F:135:GLY:HA2	2.00	0.44
8:G:106:TYR:CD2	29:X:2642:G:H5'	2.53	0.44
15:N:24:PHE:HB2	15:N:29:SER:HB3	1.99	0.44
17:P:31:VAL:O	17:P:122:SER:N	2.48	0.44
17:P:118:LYS:HD2	17:P:120:ARG:NH2	2.32	0.44
18:Q:88:ILE:HG13	18:Q:88:ILE:O	2.18	0.44
20:S:152:ILE:HG22	20:S:154:LEU:HD23	1.99	0.44
21:T:6:GLY:HA3	21:T:7:VAL:HA	1.66	0.44
21:T:21:LEU:HD21	21:T:41:ARG:HH21	1.83	0.44
22:U:22:GLY:H	22:U:39:LYS:HB2	1.81	0.44
23:V:25:LEU:HD23	23:V:25:LEU:HA	1.72	0.44
25:Z:3:LYS:HA	29:X:2577:A:O2'	2.18	0.44
27:2:26:SER:O	27:2:30:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:72:A:N1	29:X:111:A:O2'	2.46	0.44
29:X:1533:C:H2'	29:X:1534:C:O4'	2.18	0.44
29:X:1592:U:H2'	29:X:1593:G:C8	2.53	0.44
29:X:1993:U:C2	29:X:1994:C:C6	3.06	0.44
29:X:2720:U:C2	29:X:2721:A:C8	3.06	0.44
1:O:39:VAL:HG11	1:O:185:TYR:CD2	2.52	0.44
3:B:19:ARG:HA	9:H:84:ALA:O	2.16	0.44
3:B:31:CYS:HA	3:B:32:PRO:HD3	1.89	0.44
3:B:120:TRP:O	3:B:121:ASN:HB2	2.17	0.44
3:B:140:SER:HB2	29:X:2578:G:N7	2.33	0.44
5:D:72:LYS:HA	5:D:81:GLN:HA	1.99	0.44
6:E:133:VAL:HG12	6:E:141:VAL:HG13	2.00	0.44
10:I:73:GLU:HG3	10:I:105:PRO:O	2.17	0.44
11:J:70:PHE:CE2	29:X:871:C:H4'	2.53	0.44
11:J:71:PRO:HA	11:J:96:SER:HB2	2.00	0.44
15:N:11:ARG:O	15:N:15:LYS:HG3	2.18	0.44
21:T:14:ARG:HE	21:T:14:ARG:HB2	1.48	0.44
22:U:48:LYS:CG	22:U:49:LYS:H	2.19	0.44
29:X:2004:G:C4	29:X:2005:A:C8	3.06	0.44
29:X:2302:C:H42	29:X:2314:G:H1	1.64	0.44
29:X:2511:U:H2'	29:X:2512:C:C6	2.53	0.44
30:Y:65:A:H2'	30:Y:66:G:H8	1.82	0.44
1:O:60:LEU:HA	1:O:61:PRO:HD3	1.87	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
22:U:31:GLY:HA2	22:U:32:ARG:HH11	1.82	0.44
29:X:448:U:O4	29:X:583:G:H1'	2.17	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:2650:U:O2'	29:X:2651:C:H5'	2.18	0.44
29:X:2774:C:H2'	29:X:2775:A:O4'	2.18	0.44
2:A:218:LYS:HE3	2:A:218:LYS:HB3	1.86	0.43
3:B:175:ILE:HG12	3:B:182:ILE:HG12	1.99	0.43
7:F:112:MET:HG3	7:F:113:PRO:HD3	1.99	0.43
11:J:14:PHE:O	11:J:15:ARG:HG2	2.18	0.43
11:J:52:ARG:HH12	11:J:53:ILE:HG12	1.81	0.43
20:S:104:SER:HA	20:S:139:THR:HA	2.00	0.43
20:S:172:LEU:HD22	20:S:173:PRO:HD2	2.00	0.43
22:U:46:LEU:O	29:X:397:A:H5'	2.18	0.43
29:X:165(B):G:H2'	29:X:165(C):G:O4'	2.18	0.43
29:X:784:A:N7	29:X:792:G:C4	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1054:A:H2'	29:X:1055:G:H8	1.83	0.43
29:X:1091:G:N2	29:X:1101:U:H1'	2.32	0.43
29:X:1242:A:C4	29:X:1243:C:C5	3.06	0.43
29:X:1782:C:H2'	29:X:2608:G:O2'	2.17	0.43
29:X:1995:U:H3'	29:X:1996:C:H2'	2.00	0.43
29:X:2476:A:H5'	29:X:2476:A:H8	1.83	0.43
1:0:4:ARG:HG2	1:0:5:ALA:H	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
7:F:19:PRO:HB2	7:F:20:ALA:H	1.66	0.43
7:F:90:THR:OG1	7:F:93:LYS:HB2	2.18	0.43
11:J:76:THR:HA	11:J:92:GLU:H	1.84	0.43
20:S:112:LEU:HG	20:S:113:VAL:N	2.32	0.43
22:U:27:ASP:HA	22:U:32:ARG:NH2	2.21	0.43
22:U:70:LEU:HB3	22:U:79:GLU:OE2	2.18	0.43
25:Z:28:PRO:HB2	25:Z:30:LEU:HG	1.99	0.43
26:1:40:TYR:HA	26:1:46:HIS:HA	2.00	0.43
29:X:13:A:N3	29:X:15:G:O6	2.50	0.43
29:X:733:G:N7	29:X:761:A:C5	2.86	0.43
29:X:787:U:C5	29:X:791:C:N3	2.87	0.43
29:X:1036:G:C2	29:X:1120:G:C4	3.06	0.43
29:X:1422:G:H2'	29:X:1423:A:H8	1.83	0.43
29:X:1510:U:O2'	29:X:1511:G:OP1	2.32	0.43
29:X:2075:U:H3'	29:X:2238:G:H21	1.83	0.43
29:X:2320:A:H5''	29:X:2321:G:C4	2.53	0.43
29:X:2508:G:C4	29:X:2509:G:C8	3.06	0.43
29:X:2536:G:H2'	29:X:2537:U:O4'	2.17	0.43
29:X:2881:U:H2'	29:X:2882:C:C6	2.53	0.43
30:Y:7:C:H2'	30:Y:8:C:H6	1.84	0.43
30:Y:39:C:H5''	30:Y:40:C:C5	2.53	0.43
1:0:33:PHE:HB3	1:0:34:ASP:H	1.58	0.43
1:0:64:THR:HG22	1:0:65:GLY:H	1.83	0.43
2:A:40:THR:C	2:A:42:GLY:H	2.21	0.43
2:A:51:SER:OG	29:X:1814:G:H4'	2.17	0.43
3:B:72:VAL:O	3:B:73:ALA:HB3	2.18	0.43
6:E:19:ALA:HB1	6:E:24:PHE:HD2	1.83	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
16:O:73:LYS:HB2	16:O:82:ARG:HB2	1.99	0.43
19:R:38:LEU:HB3	19:R:47:VAL:CG2	2.48	0.43
19:R:100:ASP:HB2	19:R:103:LYS:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:11:ALA:HA	23:V:14:PHE:HD2	1.83	0.43
25:Z:43:HIS:N	29:X:2884:U:O4	2.48	0.43
30:Y:39:C:H5'	30:Y:40:C:OP2	2.18	0.43
9:H:3:MET:O	9:H:6:SER:HB2	2.19	0.43
9:H:5:GLN:HG2	29:X:1668:A:H5''	1.99	0.43
9:H:116:ARG:O	9:H:116:ARG:HG3	2.18	0.43
13:L:33:ARG:CZ	13:L:33:ARG:HB2	2.48	0.43
15:N:11:ARG:HH22	29:X:29:U:C4'	2.31	0.43
16:O:28:GLU:O	16:O:31:ASP:HB2	2.18	0.43
28:3:29:LYS:HE2	29:X:2418:A:P	2.59	0.43
29:X:655:A:H4'	29:X:656:G:H5'	2.00	0.43
29:X:1164:A:C2	29:X:1165:U:C2	3.06	0.43
29:X:1644:C:O2	29:X:1644:C:H2'	2.18	0.43
29:X:1676:A:N6	29:X:1677:A:C6	2.86	0.43
29:X:2212:A:C5'	29:X:2213:U:H5	2.31	0.43
29:X:2392:A:C8	29:X:2429:G:C2	3.06	0.43
29:X:2691:C:H2'	29:X:2692:C:H6	1.83	0.43
30:Y:83:C:N4	30:Y:98:C:N3	2.67	0.43
5:D:111:ILE:CG2	5:D:114:PHE:HB2	2.47	0.43
25:Z:10:LYS:HG3	29:X:1263:U:H1'	2.00	0.43
25:Z:30:LEU:HD23	25:Z:30:LEU:HA	1.82	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
29:X:1909:C:O5'	29:X:1909:C:H6	2.02	0.43
29:X:2691:C:H5''	29:X:2872:G:C5'	2.48	0.43
11:J:46:ASN:HA	11:J:49:GLU:HB2	2.00	0.43
15:N:97:ASP:O	15:N:101:ARG:HB2	2.19	0.43
20:S:50:GLY:O	20:S:51:LEU:HB3	2.18	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:516:C:C2'	29:X:517:C:H5'	2.47	0.43
29:X:980:A:H62	29:X:981:A:N6	2.15	0.43
29:X:1061:U:H3'	29:X:1062:G:H5''	2.00	0.43
29:X:1078:C:N3	29:X:1088:A:H5'	2.34	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
2:A:229:VAL:HG11	29:X:784:A:C4	2.53	0.43
4:C:145:THR:O	4:C:146:GLU:HG3	2.18	0.43
5:D:92:ARG:NH1	30:Y:46:G:H3'	2.34	0.43
6:E:99:THR:O	6:E:101:LYS:N	2.51	0.43
15:N:28:ARG:HG2	15:N:28:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:9:ARG:NH2	29:X:307:G:OP1	2.48	0.43
19:R:53:VAL:HG12	19:R:54:ILE:H	1.84	0.43
25:Z:3:LYS:HE3	25:Z:3:LYS:HB3	1.71	0.43
28:3:29:LYS:HZ3	28:3:41:ILE:HG12	1.82	0.43
29:X:643:A:C2	29:X:644:A:C4	3.07	0.43
29:X:747:U:O2	29:X:2014:A:H1'	2.18	0.43
29:X:858:U:O2	29:X:2268:A:H2'	2.19	0.43
29:X:920:G:H2'	29:X:921:G:O4'	2.19	0.43
29:X:1835:G:H1'	29:X:1931:U:C2	2.53	0.43
29:X:2311:A:H5''	29:X:2312:U:OP2	2.19	0.43
29:X:2462:U:H2'	29:X:2463:C:C6	2.54	0.43
29:X:2689:U:P	29:X:2719:G:H22	2.41	0.43
29:X:2721:A:H1'	29:X:2873:A:O2'	2.19	0.43
2:A:85:ASP:HA	2:A:86:PRO:HD3	1.79	0.43
2:A:99:ASP:OD2	29:X:1491:A:H5'	2.19	0.43
2:A:157:ARG:HH12	29:X:1817:G:H3'	1.84	0.43
4:C:78:VAL:HG13	29:X:448:U:H1'	2.00	0.43
8:G:133:GLY:HA3	29:X:1137:G:O2'	2.19	0.43
9:H:100:ASN:OD1	9:H:100:ASN:C	2.57	0.43
10:I:81:GLN:NE2	10:I:113:GLU:OE2	2.51	0.43
10:I:133:VAL:HG11	10:I:140:VAL:CG2	2.48	0.43
11:J:6:LYS:O	11:J:71:PRO:HG2	2.19	0.43
11:J:39:GLU:HA	11:J:40:PRO:HD3	1.62	0.43
15:N:58:ARG:HA	15:N:61:TRP:CE3	2.54	0.43
29:X:902:C:H2'	29:X:903:C:C6	2.54	0.43
29:X:1179:G:N1	29:X:1180:U:C4	2.87	0.43
29:X:1619:G:H2'	29:X:1620:G:H8	1.84	0.43
29:X:2290:G:N2	29:X:2373:A:O2'	2.47	0.43
29:X:2330:G:N2	29:X:2386:U:C2	2.87	0.43
29:X:2543:G:C6	29:X:2544:G:C6	3.06	0.43
4:C:130:THR:HG21	29:X:320:U:H2'	2.00	0.43
13:L:67:THR:O	13:L:71:VAL:HG12	2.19	0.43
15:N:24:PHE:O	15:N:29:SER:HB3	2.18	0.43
17:P:21:ARG:HH22	29:X:496:G:H4'	1.84	0.43
18:Q:34:THR:HB	18:Q:37:GLU:HG3	2.00	0.43
19:R:35:LYS:HB3	19:R:35:LYS:HE3	1.76	0.43
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:1864:U:H2'	29:X:1874:G:C8	2.54	0.43
29:X:2327:A:H3'	29:X:2328:A:C8	2.53	0.43
29:X:2521:C:C4	29:X:2522:U:C4	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:109:VAL:O	1:O:134:PRO:HD3	2.18	0.43
2:A:259:THR:OG1	29:X:1798:U:H5'	2.19	0.43
6:E:139:GLN:HB3	6:E:143:GLN:OE1	2.19	0.43
8:G:90:LEU:HD12	8:G:90:LEU:HA	1.86	0.43
14:M:19:ASP:O	14:M:20:HIS:ND1	2.52	0.43
15:N:32:TYR:O	15:N:35:ALA:HB3	2.18	0.43
15:N:60:LEU:HA	15:N:63:GLN:HG3	2.01	0.43
16:O:78:VAL:CG1	16:O:80:TYR:HB2	2.49	0.43
17:P:8:PHE:HE1	17:P:17:GLN:HB2	1.83	0.43
21:T:55:ARG:H	21:T:55:ARG:HG2	1.68	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
29:X:591:G:C6	29:X:592(A):C:N4	2.86	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
29:X:1885:A:H3'	29:X:1886:A:H8	1.84	0.43
29:X:2376:A:H2'	29:X:2377:A:O4'	2.19	0.43
29:X:2474:C:H5''	29:X:2475:C:OP2	2.19	0.43
29:X:2655:G:O2'	29:X:2664:G:O6	2.26	0.43
1:O:72:VAL:HG13	1:O:110:VAL:HB	2.00	0.42
6:E:25:LYS:HE2	6:E:25:LYS:HB3	1.81	0.42
9:H:83:ARG:HH21	9:H:89:ILE:HD11	1.83	0.42
11:J:69:ILE:HG21	11:J:104:MET:HG2	2.00	0.42
14:M:104:LEU:CD2	14:M:106:TYR:HE2	2.32	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
23:V:63:LYS:HG2	23:V:66:GLN:NE2	2.34	0.42
29:X:638:G:N1	29:X:649:G:N1	2.67	0.42
29:X:638:G:N2	29:X:650:C:H1'	2.34	0.42
29:X:684:G:C2	29:X:794:A:C2	3.07	0.42
29:X:844:U:H5'	29:X:845:G:OP2	2.19	0.42
29:X:1014:A:H2'	29:X:1015:U:H6	1.84	0.42
29:X:1312:U:H4'	29:X:1313:U:O5'	2.19	0.42
29:X:1637:A:H4'	29:X:2711:A:O2'	2.18	0.42
29:X:1795:C:H2'	29:X:1796:U:O4'	2.18	0.42
29:X:2349:G:O6	29:X:2382:G:N2	2.35	0.42
29:X:2507:C:C4	29:X:2583:G:C6	3.07	0.42
29:X:2732:G:H3'	29:X:2733:A:O4'	2.19	0.42
2:A:161:THR:O	2:A:196:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:123:ALA:HB3	29:X:2511:U:O3'	2.18	0.42
4:C:74:VAL:O	4:C:77:PHE:HB2	2.19	0.42
5:D:155:THR:HG21	29:X:2314:G:H1'	2.01	0.42
8:G:100:TYR:OH	8:G:126:VAL:HG13	2.19	0.42
10:I:31:GLY:HA2	29:X:1190:G:H5''	2.01	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
19:R:77:HIS:HD2	29:X:328:U:C5'	2.29	0.42
20:S:1:MET:HE1	20:S:52:PHE:HB3	2.01	0.42
20:S:66:VAL:HG22	20:S:83:PHE:CE1	2.53	0.42
29:X:347:C:H2'	29:X:348:G:H5'	2.01	0.42
29:X:704:G:H1'	29:X:726:G:N2	2.34	0.42
29:X:875:G:H2'	29:X:876:C:O4'	2.19	0.42
29:X:1365:A:H2'	29:X:1365:A:N3	2.34	0.42
29:X:1885:A:H3'	29:X:1886:A:C8	2.54	0.42
29:X:2306:U:H5'	29:X:2307:G:C8	2.54	0.42
29:X:2747:G:O6	29:X:2755:C:H5''	2.19	0.42
3:B:5:LEU:HD22	3:B:195:LEU:HD11	2.01	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
10:I:97:ARG:HE	10:I:97:ARG:HB2	1.53	0.42
11:J:17:ARG:HB3	11:J:42:TRP:HZ2	1.84	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
20:S:143:ILE:HA	20:S:171:VAL:HG12	2.01	0.42
21:T:37:LEU:HD11	21:T:61:ALA:N	2.34	0.42
29:X:816:C:N3	29:X:1192:G:C2	2.87	0.42
29:X:925:A:H2'	29:X:926:C:O4'	2.19	0.42
29:X:1821:A:H8	29:X:1821:A:O5'	2.03	0.42
29:X:2472:G:H2'	29:X:2475:C:H42	1.84	0.42
29:X:2711:A:N6	29:X:2714:G:C5	2.88	0.42
29:X:2825:C:H5''	29:X:2826:A:OP2	2.19	0.42
1:O:95:LEU:HD13	1:O:98:ARG:HB2	2.00	0.42
4:C:48:ARG:HE	4:C:48:ARG:HB3	1.43	0.42
4:C:116:LYS:HB3	4:C:185:ARG:HD3	2.02	0.42
8:G:52:GLY:O	8:G:55:ALA:HB3	2.19	0.42
10:I:65:PHE:CE1	29:X:2404:C:H1'	2.54	0.42
11:J:76:THR:HG22	11:J:91:VAL:HA	2.00	0.42
13:L:15:ARG:HE	13:L:91:ARG:HH11	1.66	0.42
14:M:15:GLY:O	14:M:18:GLN:HG2	2.20	0.42
24:W:22:ALA:C	24:W:24:GLY:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:29:LYS:HZ1	28:3:41:ILE:HG23	1.83	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
29:X:820:A:H1'	29:X:943:U:O2'	2.19	0.42
29:X:1097:U:H2'	29:X:1098:A:O4'	2.18	0.42
29:X:1504:G:H2'	29:X:1505:U:O4'	2.19	0.42
29:X:2513:G:C2	29:X:2514:U:C2	3.07	0.42
5:D:64:LYS:HA	5:D:65:PRO:HD3	1.78	0.42
5:D:126:GLY:O	5:D:160:ALA:HB3	2.20	0.42
9:H:134:LEU:HA	14:M:48:GLN:HE22	1.84	0.42
10:I:12:SER:O	29:X:660:G:N2	2.52	0.42
10:I:116:ARG:HG2	10:I:117:ALA:N	2.35	0.42
11:J:13:GLN:HB3	11:J:14:PHE:CD2	2.54	0.42
16:O:64:GLY:HA3	16:O:90:PHE:CZ	2.55	0.42
18:Q:68:PHE:CD1	29:X:65:C:H1'	2.55	0.42
21:T:36:ILE:HD11	29:X:2364:C:O2	2.19	0.42
26:1:34:LYS:HE3	26:1:51:ALA:O	2.19	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:1745:G:C6	29:X:1746:C:N4	2.88	0.42
29:X:2280:G:C2'	29:X:2281:C:H5'	2.50	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
29:X:2697:G:C2	29:X:2711:A:C2	3.06	0.42
30:Y:78:A:H2'	30:Y:79:U:O4'	2.19	0.42
1:0:43:LEU:H	1:0:167:VAL:HG12	1.84	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
8:G:33:ILE:CD1	29:X:537:U:H4'	2.49	0.42
9:H:13:ASN:ND2	9:H:108:THR:HB	2.35	0.42
11:J:19:THR:HB	30:Y:93:G:O5'	2.20	0.42
12:K:100:VAL:HG12	12:K:101:GLY:N	2.33	0.42
17:P:36:ARG:NH1	29:X:1266:G:C8	2.87	0.42
18:Q:73:ASN:HA	29:X:58:G:OP1	2.20	0.42
19:R:15:HIS:CD2	19:R:16:PHE:HD2	2.37	0.42
28:3:17:THR:CG2	28:3:21:LYS:H	2.29	0.42
28:3:39:ASP:HB3	28:3:42:ARG:NH2	2.33	0.42
29:X:14:A:C5	29:X:526:A:N1	2.87	0.42
29:X:1235:G:C6	29:X:1236:G:N1	2.87	0.42
29:X:1309:G:N2	29:X:1611:C:H5'	2.34	0.42
29:X:1675:C:H2'	29:X:1676:A:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2836:G:C6	29:X:2837:A:N6	2.87	0.42
1:O:132:LEU:HD11	29:X:2169:A:O2'	2.20	0.42
3:B:144:ARG:NH1	29:X:2572:A:N3	2.68	0.42
8:G:42:VAL:HG22	8:G:164:GLN:HB2	2.02	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
22:U:22:GLY:HA3	22:U:39:LYS:CE	2.50	0.42
25:Z:51:TYR:CD2	25:Z:54:GLY:O	2.73	0.42
27:2:6:GLN:HA	27:2:7:PRO:HD2	1.85	0.42
29:X:537:U:H2'	29:X:538:G:C8	2.55	0.42
29:X:848:G:N2	29:X:932:U:H1'	2.34	0.42
29:X:1111:A:O2'	29:X:1112:G:H4'	2.19	0.42
29:X:1223:G:C6	29:X:1227:G:C6	3.07	0.42
29:X:1587:A:H8	29:X:1587:A:H5'	1.85	0.42
29:X:1652:A:H3'	29:X:1653:G:C8	2.55	0.42
29:X:1665:A:C2'	29:X:1666:G:H5'	2.50	0.42
29:X:2263:C:H2'	29:X:2264:C:H6	1.85	0.42
29:X:2599:G:C4	29:X:2600:A:C8	3.08	0.42
29:X:2884:U:C5	29:X:2885:C:C2	3.08	0.42
1:O:12:ARG:HG3	1:O:217:SER:O	2.20	0.42
2:A:42:GLY:O	2:A:50:THR:N	2.49	0.42
2:A:67:PHE:HB3	2:A:153:ALA:H	1.84	0.42
2:A:159:ALA:HB1	2:A:198:ASN:HB3	2.00	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
10:I:81:GLN:HB3	10:I:82:ASP:H	1.50	0.42
15:N:39:LEU:HA	15:N:39:LEU:HD23	1.72	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
29:X:501:A:O5'	29:X:501:A:H8	2.02	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
29:X:1107:G:N1	29:X:1108:U:O2	2.53	0.42
29:X:1126:A:H4'	29:X:1127:A:C5'	2.50	0.42
29:X:1142:A:O2'	29:X:1143:A:H5''	2.20	0.42
29:X:1452:U:C2	29:X:1458:U:O2	2.73	0.42
29:X:1770:G:C5	29:X:1771:C:C5	3.08	0.42
29:X:2037:G:C6	29:X:2038:G:C6	3.08	0.42
8:G:65:LYS:HB2	8:G:65:LYS:NZ	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:646:A:N3	29:X:2350:C:O2'	2.52	0.42
29:X:841:G:H1	29:X:937:C:H42	1.66	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
29:X:1739:C:H2'	29:X:1740:G:C8	2.54	0.42
29:X:1858:G:O2'	29:X:1883:G:N2	2.45	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
4:C:118:VAL:O	4:C:188:ILE:HG12	2.20	0.42
5:D:148:LYS:H	5:D:148:LYS:HG3	1.55	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
15:N:36:PHE:O	15:N:39:LEU:HB2	2.19	0.42
18:Q:53:ILE:HG13	18:Q:80:VAL:HG13	2.02	0.42
21:T:23:VAL:HG22	21:T:26:PHE:CZ	2.55	0.42
29:X:403:U:H5''	29:X:404:C:OP1	2.19	0.42
29:X:537:U:H2'	29:X:538:G:H8	1.85	0.42
29:X:603:G:C5	29:X:625:G:C2	3.07	0.42
29:X:700:G:N2	29:X:732:C:H5	2.18	0.42
29:X:761:A:H8	29:X:761:A:O5'	2.03	0.42
29:X:2030:A:H4'	29:X:2031:A:C8	2.55	0.42
29:X:2342:C:O2'	29:X:2374:G:H5''	2.19	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
30:Y:67:C:O2'	30:Y:68:A:H5'	2.20	0.42
2:A:161:THR:H	2:A:196:VAL:HB	1.85	0.41
3:B:2:LYS:HA	3:B:84:PHE:HE1	1.85	0.41
3:B:105:THR:HB	3:B:197:VAL:HG12	2.02	0.41
4:C:193:LEU:HA	4:C:193:LEU:HD12	1.85	0.41
6:E:126:PRO:HD2	6:E:130:ARG:O	2.20	0.41
9:H:23:ARG:HD2	9:H:23:ARG:HA	1.88	0.41
9:H:111:PHE:N	9:H:111:PHE:HD1	2.18	0.41
12:K:39:THR:O	12:K:42:LYS:N	2.53	0.41
19:R:76:LEU:HD23	19:R:76:LEU:HA	1.90	0.41
20:S:5:ALA:HB1	20:S:7:PRO:HD3	2.01	0.41
21:T:4:LYS:HA	21:T:4:LYS:HD3	1.82	0.41
29:X:121:G:O5'	29:X:121:G:H8	2.03	0.41
29:X:310:A:O3'	29:X:311:A:H8	2.03	0.41
29:X:466:A:N3	29:X:683:U:H1'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1019:U:C4	29:X:1020:C:C5	3.08	0.41
29:X:1212:G:HO2'	29:X:1213:A:P	2.43	0.41
29:X:1263:U:C4	29:X:1264:G:C6	3.08	0.41
29:X:1786:A:H1'	29:X:1938:A:N6	2.35	0.41
29:X:1794:A:H2'	29:X:1795:C:H6	1.85	0.41
29:X:2114:A:N6	29:X:2119:A:H62	2.17	0.41
29:X:2219:U:N3	29:X:2220:C:H1'	2.34	0.41
29:X:2307:G:H1'	29:X:2311:A:N6	2.35	0.41
29:X:2455:G:C6	29:X:2456:C:N4	2.88	0.41
29:X:2532:G:C5	29:X:2533:A:C5	3.08	0.41
1:0:41:PHE:CE2	1:0:189:ILE:HG12	2.55	0.41
2:A:14:ARG:HE	2:A:14:ARG:HB3	1.62	0.41
4:C:26:VAL:HB	4:C:106:MET:HE1	2.02	0.41
9:H:115:ALA:O	9:H:117:GLU:N	2.54	0.41
22:U:20:ARG:O	22:U:43:ARG:NH2	2.53	0.41
29:X:582:G:H2'	29:X:583:G:C8	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
29:X:2218:U:N3	29:X:2219:U:O4	2.53	0.41
29:X:2260:C:H2'	29:X:2261:C:H6	1.83	0.41
30:Y:7:C:H2'	30:Y:8:C:C6	2.56	0.41
30:Y:75:A:C8	30:Y:107:C:C2	3.07	0.41
2:A:78:LYS:HA	2:A:116:THR:HA	2.01	0.41
2:A:169:GLU:HB3	2:A:170:SER:H	1.57	0.41
5:D:5:LYS:HE2	5:D:100:LEU:HG	2.02	0.41
8:G:140:GLN:O	8:G:144:MET:HG3	2.21	0.41
10:I:57:ILE:HB	28:3:9:MET:HE2	2.02	0.41
10:I:98:LEU:O	10:I:99:VAL:HG13	2.21	0.41
11:J:23:LYS:HB3	11:J:24:GLY:H	1.72	0.41
11:J:135:ARG:HB3	11:J:136:GLU:H	1.68	0.41
12:K:96:ARG:NE	29:X:2882:C:OP1	2.47	0.41
15:N:25:TRP:O	15:N:28:ARG:HB2	2.20	0.41
17:P:40:LEU:HB3	25:Z:25:LEU:CD1	2.50	0.41
21:T:41:ARG:HH11	29:X:2387:U:H1'	1.86	0.41
29:X:612:G:C2	29:X:616:A:C6	3.09	0.41
29:X:648:G:C6	29:X:649:G:C6	3.08	0.41
29:X:1760:C:C2'	29:X:1761:C:H5'	2.50	0.41
29:X:1985:G:H2'	29:X:1986:G:H8	1.84	0.41
29:X:2043:C:C4	29:X:2777:G:C2	3.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:130:ARG:HA	1:O:130:ARG:HD3	1.98	0.41
3:B:146:THR:HG23	29:X:1130:U:C5	2.56	0.41
4:C:28:HIS:CB	10:I:6:LEU:HD13	2.50	0.41
4:C:192:ALA:O	4:C:195:ILE:HG13	2.19	0.41
5:D:150:ARG:HB3	5:D:151:GLY:H	1.60	0.41
7:F:53:ILE:HA	7:F:54:PRO:HD2	1.93	0.41
12:K:22:ARG:HG2	12:K:69:ASP:O	2.20	0.41
15:N:62:ILE:HG23	15:N:76:TYR:CE1	2.54	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
20:S:26:LYS:HD3	20:S:26:LYS:N	2.35	0.41
29:X:701:G:C2	29:X:732:C:C5	3.08	0.41
29:X:713:G:N2	29:X:718:A:OP2	2.53	0.41
29:X:1282:U:H2'	29:X:1283:G:O4'	2.21	0.41
29:X:2335:A:O2'	29:X:2336:A:OP2	2.31	0.41
29:X:2389:G:H5''	29:X:2390:U:O5'	2.20	0.41
29:X:2513:G:H2'	29:X:2514:U:C6	2.55	0.41
29:X:2547:U:C5	29:X:2566:A:C5	3.09	0.41
29:X:2554:U:H2'	29:X:2555:U:C6	2.55	0.41
29:X:2684:U:N3	29:X:2685:G:C8	2.88	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
29:X:2833:U:O2'	29:X:2834:A:H5'	2.18	0.41
29:X:2896:U:H2'	29:X:2897:U:C6	2.55	0.41
2:A:18:THR:HG23	2:A:211:ARG:NH1	2.35	0.41
4:C:19:LEU:HB3	4:C:20:PRO:CA	2.51	0.41
4:C:22:VAL:HG13	4:C:106:MET:CG	2.47	0.41
9:H:130:ALA:HA	9:H:131:PRO:HD3	1.83	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
25:Z:10:LYS:HD2	29:X:1262:A:N3	2.35	0.41
29:X:223:A:H2'	29:X:224:G:O4'	2.21	0.41
29:X:602:A:H4'	29:X:603:G:O5'	2.19	0.41
29:X:693:A:H2'	29:X:694:U:O4'	2.21	0.41
29:X:1022:G:H22	29:X:1142:A:H2	1.68	0.41
29:X:1591:A:H2'	29:X:1592:U:C6	2.55	0.41
29:X:1999:C:O2	29:X:2687:U:O2'	2.36	0.41
29:X:2075:U:H3'	29:X:2238:G:N2	2.34	0.41
29:X:2427:C:H5''	29:X:2428:G:OP1	2.21	0.41
4:C:27:LEU:HA	4:C:27:LEU:HD23	1.83	0.41
5:D:125:ARG:H	5:D:125:ARG:HG2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:24:PHE:CE2	6:E:43:VAL:HG13	2.55	0.41
11:J:11:ARG:HB3	11:J:12:LYS:H	1.48	0.41
11:J:24:GLY:HA2	11:J:25:GLY:HA2	1.59	0.41
11:J:126:LEU:HA	11:J:127:PRO:HD3	1.85	0.41
12:K:3:HIS:O	12:K:3:HIS:CG	2.72	0.41
13:L:18:ARG:HH22	29:X:2292:C:P	2.43	0.41
14:M:55:ILE:CG1	14:M:67:THR:HG22	2.50	0.41
14:M:90:GLN:OE1	14:M:91:VAL:N	2.35	0.41
17:P:18:VAL:HG23	17:P:19:LYS:H	1.85	0.41
29:X:23:G:C2	29:X:24:G:C8	3.08	0.41
29:X:78:C:H42	29:X:108:G:H1	1.69	0.41
29:X:320:U:H5''	29:X:321:C:OP1	2.21	0.41
29:X:600:C:N4	29:X:601:G:C5	2.89	0.41
29:X:663:G:C6	29:X:664:G:C5	3.08	0.41
29:X:681:G:H2'	29:X:682:G:O4'	2.20	0.41
29:X:833:A:H2'	29:X:834:C:C6	2.56	0.41
29:X:1229:A:C2'	29:X:1230:G:H5'	2.50	0.41
29:X:1360:G:N7	29:X:1361:G:C8	2.89	0.41
29:X:1535:U:O2'	29:X:1537:G:N2	2.53	0.41
29:X:2075:U:C4	29:X:2238:G:C6	3.09	0.41
29:X:2541:A:HO2'	29:X:2765:A:H2	1.64	0.41
2:A:134:ARG:NH2	2:A:135:PHE:HE2	2.19	0.41
3:B:1:MET:O	3:B:84:PHE:HD1	2.03	0.41
3:B:134:TRP:CZ2	3:B:139:GLY:HA2	2.56	0.41
5:D:10:ASP:HA	5:D:13:ARG:HD2	2.02	0.41
10:I:45:LYS:HB3	10:I:46:GLY:O	2.20	0.41
12:K:17:ARG:HE	12:K:17:ARG:HB2	1.15	0.41
19:R:10:HIS:ND1	19:R:44:GLN:OE1	2.54	0.41
23:V:24:GLU:OE1	23:V:46:LEU:HD21	2.21	0.41
29:X:489:G:C2	29:X:491:G:H1'	2.56	0.41
29:X:650:C:C2	29:X:651:G:N7	2.89	0.41
29:X:651(B):C:OP2	29:X:653:U:H5'	2.21	0.41
29:X:781:A:H2	29:X:1776:G:N3	2.19	0.41
29:X:1464:G:H2'	29:X:1465:G:C8	2.55	0.41
29:X:1936:A:C2	29:X:1945:G:C8	3.08	0.41
29:X:2457:U:O2	29:X:2495:G:C2	2.74	0.41
29:X:2498:C:OP2	29:X:2499:C:OP2	2.38	0.41
29:X:2507:C:C2	29:X:2583:G:C2	3.09	0.41
29:X:2547:U:C5	29:X:2566:A:C8	3.08	0.41
1:O:205:LEU:HD13	1:O:222:LEU:HD22	2.03	0.41
3:B:34:VAL:HG12	3:B:35:GLN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:61:LYS:N	3:B:62:PRO:HD2	2.36	0.41
5:D:156:ILE:H	5:D:156:ILE:HG13	1.52	0.41
6:E:8:PRO:HD2	6:E:69:ARG:NH1	2.35	0.41
7:F:70:LYS:HB3	7:F:71:THR:H	1.59	0.41
10:I:62:LYS:HD2	29:X:2394:C:H5'	2.03	0.41
12:K:28:LEU:HD23	12:K:29:LEU:HD23	2.02	0.41
15:N:66:ASN:OD1	15:N:70:ARG:HD2	2.21	0.41
15:N:77:SER:HB2	29:X:1152:C:O4'	2.21	0.41
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
18:Q:20:MET:HB2	18:Q:25:TYR:CE1	2.55	0.41
28:3:33:ASN:O	28:3:36:LYS:HG2	2.21	0.41
29:X:7:G:H2'	29:X:8:A:C8	2.56	0.41
29:X:872:A:C6	29:X:906:A:C2	3.09	0.41
29:X:1154:G:OP2	29:X:1154:G:H8	2.03	0.41
5:D:71:LYS:HB2	5:D:71:LYS:HE3	1.90	0.41
5:D:125:ARG:HG3	29:X:2315:U:O2'	2.21	0.41
7:F:41:PHE:O	7:F:45:THR:HG23	2.20	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
11:J:41:ALA:HB2	11:J:128:ILE:CG2	2.51	0.41
13:L:32:TYR:CZ	30:Y:9:G:H5'	2.56	0.41
13:L:65:THR:HG1	30:Y:52:G:P	2.42	0.41
15:N:13:ARG:HH12	29:X:1251:C:H3'	1.86	0.41
16:O:11:GLN:N	16:O:11:GLN:HE21	2.19	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
21:T:43:THR:HG22	21:T:43:THR:O	2.21	0.41
21:T:57:HIS:CD2	21:T:57:HIS:N	2.88	0.41
22:U:47:HIS:HB3	29:X:397:A:OP1	2.20	0.41
25:Z:49:CYS:HB2	25:Z:51:TYR:HD1	1.86	0.41
27:2:19:ARG:NH1	29:X:124:G:H2'	2.36	0.41
29:X:150:C:OP1	29:X:150:C:H6	2.04	0.41
29:X:208:C:H2'	29:X:209:C:C6	2.55	0.41
29:X:518:G:H2'	29:X:519:U:C6	2.56	0.41
29:X:657:U:H2'	29:X:658:A:H8	1.82	0.41
29:X:677:A:C4	29:X:678:C:C5	3.09	0.41
29:X:852:A:H61	29:X:926:C:H42	1.69	0.41
29:X:864:G:H2'	29:X:865:C:C6	2.56	0.41
29:X:1127:A:N3	29:X:1127:A:H2'	2.36	0.41
29:X:1146:G:H2'	29:X:1147:A:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1168:A:C2	29:X:1182:G:C2	3.09	0.41
29:X:1197:G:H2'	29:X:1198:U:H6	1.85	0.41
29:X:1360:G:C8	29:X:1361:G:C8	3.09	0.41
29:X:2250:G:O4'	29:X:2250:G:N3	2.52	0.41
29:X:2508:G:H2'	29:X:2509:G:H8	1.85	0.41
29:X:2673:G:N3	29:X:2674:A:C8	2.89	0.41
29:X:2690:C:N4	29:X:2713:U:O3'	2.54	0.41
29:X:2862:G:C6	29:X:2863:U:C4	3.09	0.41
5:D:22:TYR:CD1	5:D:28:VAL:HG22	2.56	0.41
7:F:10:LEU:HD13	7:F:27:LEU:HD13	2.02	0.41
9:H:55:VAL:HB	9:H:68:ASP:H	1.85	0.41
10:I:97:ARG:O	10:I:98:LEU:HB2	2.21	0.41
17:P:51:GLN:O	17:P:54:GLU:HB2	2.21	0.41
21:T:69:PHE:HB2	29:X:856:C:H4'	2.03	0.41
28:3:17:THR:CG2	28:3:20:GLY:H	2.28	0.41
29:X:177:G:O2'	29:X:178:U:OP2	2.39	0.41
29:X:600:C:N4	29:X:601:G:C6	2.89	0.41
29:X:704:G:N3	29:X:726:G:C2	2.89	0.41
29:X:934:G:C4	29:X:935:U:C5	3.09	0.41
29:X:946:G:H2'	29:X:947:G:C8	2.55	0.41
29:X:1301:A:H2	29:X:1625(A):G:N3	2.19	0.41
29:X:1659:U:H2'	29:X:1660:C:O5'	2.21	0.41
29:X:2727:G:H2'	29:X:2728:U:C6	2.55	0.41
29:X:2749:A:OP2	29:X:2750:A:O2'	2.31	0.41
29:X:2752:C:H2'	29:X:2753:A:O4'	2.20	0.41
29:X:2818:G:O2'	29:X:2819:G:H5'	2.20	0.41
30:Y:39:C:C5	30:Y:40:C:C4	3.09	0.41
4:C:161:ALA:HB1	4:C:167:VAL:HG21	2.03	0.40
7:F:73:PRO:C	7:F:75:SER:H	2.24	0.40
8:G:51:LEU:CD1	8:G:88:VAL:HG11	2.51	0.40
8:G:140:GLN:O	8:G:143:ALA:HB3	2.21	0.40
11:J:14:PHE:HD1	11:J:88:LYS:HE3	1.86	0.40
12:K:3:HIS:NE2	12:K:5:LYS:HD3	2.37	0.40
13:L:33:ARG:NH2	13:L:103:LEU:HD12	2.29	0.40
14:M:22:ARG:NE	14:M:24:LEU:HD21	2.35	0.40
19:R:16:PHE:CE2	19:R:81:VAL:HG11	2.55	0.40
20:S:9:THR:HA	20:S:10:PRO:HD3	1.88	0.40
21:T:23:VAL:HG22	21:T:26:PHE:CE2	2.56	0.40
22:U:32:ARG:HG2	22:U:34:THR:N	2.36	0.40
22:U:66:ALA:O	22:U:70:LEU:HB2	2.20	0.40
29:X:100:U:H4'	29:X:101:U:H5''	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:718:A:H3'	29:X:719:G:O4'	2.21	0.40
29:X:1422:G:H2'	29:X:1423:A:C8	2.55	0.40
29:X:1445:G:N3	29:X:1547:U:C2	2.89	0.40
29:X:1499:U:H2'	29:X:1500:A:H8	1.86	0.40
29:X:1788:C:H2'	29:X:1789:A:C8	2.56	0.40
29:X:1904:G:O2'	29:X:1928:A:N1	2.43	0.40
29:X:2186:A:H2'	29:X:2187:C:C6	2.56	0.40
3:B:140:SER:HB2	29:X:2575:C:O2'	2.21	0.40
6:E:24:PHE:HB2	6:E:37:TYR:CE1	2.55	0.40
9:H:87:SER:HA	14:M:80:VAL:O	2.21	0.40
14:M:18:GLN:C	14:M:20:HIS:H	2.25	0.40
15:N:31:GLN:CD	29:X:580:C:H4'	2.41	0.40
27:2:34:ARG:CZ	27:2:39:ARG:HD2	2.51	0.40
29:X:312:G:OP1	29:X:332:A:H5''	2.22	0.40
29:X:670:A:H4'	29:X:671:C:O5'	2.21	0.40
29:X:864:G:N2	29:X:913:U:O2	2.54	0.40
29:X:866:A:N3	29:X:866:A:H2'	2.34	0.40
29:X:981:A:N1	29:X:2027:G:O2'	2.41	0.40
29:X:1324:G:N2	29:X:1331:C:C2	2.89	0.40
29:X:1414:G:HO2'	29:X:1415:A:H8	1.68	0.40
29:X:1634:U:H4'	29:X:1635:G:OP2	2.22	0.40
29:X:1729:C:O2'	29:X:2859:A:N3	2.35	0.40
29:X:1955:U:H5	29:X:2557:G:N2	2.20	0.40
29:X:2280:G:C2	29:X:2281:C:C6	3.10	0.40
29:X:2489:G:C6	29:X:2490:G:C6	3.09	0.40
29:X:2715:C:C2	29:X:2716:A:C8	3.08	0.40
29:X:2895:C:H2'	29:X:2896:U:C6	2.55	0.40
1:0:95:LEU:HD22	1:0:98:ARG:HD2	2.02	0.40
2:A:44:ASN:HB2	29:X:1812:U:O2'	2.21	0.40
2:A:152:GLY:O	2:A:154:GLN:HG3	2.21	0.40
3:B:4:ILE:HG12	3:B:5:LEU:N	2.36	0.40
3:B:134:TRP:O	3:B:134:TRP:CG	2.74	0.40
4:C:171:PRO:HB2	4:C:172:VAL:HG23	2.04	0.40
5:D:38:GLU:HG2	5:D:53:ALA:HB1	2.02	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
29:X:1150:U:H2'	29:X:1151:A:C8	2.57	0.40
29:X:1163:G:C2	29:X:1164:A:C8	3.09	0.40
29:X:1487:G:H2'	29:X:1488:G:H8	1.87	0.40
29:X:1755:U:H5''	29:X:1756:A:OP2	2.20	0.40
29:X:1783:A:C6	29:X:2587:A:C2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2662:A:H8	29:X:2662:A:O5'	2.04	0.40
29:X:2691:C:C2	29:X:2692:C:C5	3.10	0.40
29:X:2697:G:N1	29:X:2711:A:C2	2.90	0.40
30:Y:46:G:C2	30:Y:50:U:O2	2.75	0.40
1:O:32:LYS:HE3	29:X:2128:C:H5'	2.02	0.40
3:B:6:GLY:HA3	3:B:27:LEU:O	2.21	0.40
3:B:33:ILE:HG12	3:B:89:ASP:HA	2.02	0.40
3:B:55:ALA:O	3:B:59:VAL:HG23	2.22	0.40
3:B:102:ILE:HD11	3:B:184:VAL:HG21	2.02	0.40
10:I:62:LYS:HG3	29:X:2394:C:OP1	2.21	0.40
11:J:76:THR:HG22	11:J:91:VAL:H	1.87	0.40
12:K:28:LEU:CD2	12:K:115:LEU:HD11	2.49	0.40
13:L:8:ARG:C	13:L:10:LYS:H	2.25	0.40
13:L:32:TYR:O	13:L:32:TYR:CG	2.75	0.40
14:M:100:ARG:O	29:X:2848:G:H3'	2.20	0.40
15:N:10:ARG:HG3	29:X:1251:C:OP1	2.21	0.40
25:Z:7:PRO:HA	29:X:2615:U:C6	2.57	0.40
29:X:166:G:H2'	29:X:167:A:O4'	2.22	0.40
29:X:817:C:O2'	29:X:839:U:H5''	2.21	0.40
29:X:954:G:O2'	29:X:2274:A:N1	2.33	0.40
29:X:1180:U:H2'	29:X:1181:U:H6	1.87	0.40
29:X:1485:C:H2'	29:X:1486:G:O4'	2.22	0.40
29:X:2519:U:C6	29:X:2541:A:N6	2.89	0.40
2:A:227:ASN:OD1	29:X:784:A:H5''	2.22	0.40
6:E:55:PRO:HB2	6:E:56:SER:H	1.57	0.40
7:F:115:LEU:C	7:F:117:ALA:H	2.25	0.40
18:Q:89:GLU:H	18:Q:89:GLU:HG3	1.65	0.40
21:T:11:LYS:HE2	21:T:11:LYS:HB2	1.81	0.40
29:X:127:A:H5''	29:X:128:C:O4'	2.21	0.40
29:X:179:A:H2'	29:X:180:C:O4'	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:676:A:H8	29:X:2069:G:H21	1.65	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:1319:G:C6	29:X:1320:G:O6	2.75	0.40
29:X:1354:A:H2'	29:X:1355:G:O4'	2.22	0.40
29:X:1413:G:N2	29:X:1587:A:C8	2.90	0.40
29:X:1478:G:C6	29:X:1479:G:C5	3.10	0.40
29:X:1731:A:H61	29:X:1741:U:H3	1.68	0.40
29:X:2194:U:H2'	29:X:2195:U:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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%)	0	1
2	A	272/274 (99%)	238 (88%)	25 (9%)	9 (3%)	3	13
3	B	203/205 (99%)	168 (83%)	24 (12%)	11 (5%)	1	5
4	C	195/197 (99%)	151 (77%)	30 (15%)	14 (7%)	1	2
5	D	175/177 (99%)	124 (71%)	39 (22%)	12 (7%)	1	2
6	E	169/171 (99%)	130 (77%)	22 (13%)	17 (10%)	0	1
7	F	142/144 (99%)	99 (70%)	34 (24%)	9 (6%)	1	3
8	G	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	2	8
9	H	132/134 (98%)	103 (78%)	19 (14%)	10 (8%)	1	2
10	I	139/141 (99%)	104 (75%)	23 (16%)	12 (9%)	0	1
11	J	134/136 (98%)	102 (76%)	20 (15%)	12 (9%)	0	1
12	K	111/113 (98%)	95 (86%)	11 (10%)	5 (4%)	2	8
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	3
15	N	115/117 (98%)	104 (90%)	8 (7%)	3 (3%)	4	17
16	O	92/94 (98%)	75 (82%)	11 (12%)	6 (6%)	1	3
17	P	125/127 (98%)	99 (79%)	16 (13%)	10 (8%)	1	2
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%)	0	1
20	S	173/175 (99%)	123 (71%)	32 (18%)	18 (10%)	0	1
21	T	82/84 (98%)	68 (83%)	11 (13%)	3 (4%)	2	11
22	U	70/72 (97%)	38 (54%)	16 (23%)	16 (23%)	0	0
23	V	64/66 (97%)	55 (86%)	5 (8%)	4 (6%)	1	3
24	W	53/55 (96%)	48 (91%)	3 (6%)	2 (4%)	2	11
25	Z	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	1	5
26	1	52/54 (96%)	33 (64%)	13 (25%)	6 (12%)	0	1
27	2	45/47 (96%)	40 (89%)	3 (7%)	2 (4%)	2	8
28	3	63/65 (97%)	47 (75%)	12 (19%)	4 (6%)	1	3
All	All	3431/3487 (98%)	2670 (78%)	512 (15%)	249 (7%)	1	2

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

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

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

Sometimes 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 oligosaccharides 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%)	1.45	58 (25%) 2 2	238, 259, 280, 290	0
2	A	274/274 (100%)	1.30	73 (26%) 2 2	93, 135, 154, 161	0
3	B	205/205 (100%)	0.61	13 (6%) 27 23	60, 89, 107, 124	0
4	C	197/197 (100%)	0.68	14 (7%) 23 20	77, 125, 145, 159	0
5	D	177/177 (100%)	0.98	32 (18%) 4 4	155, 174, 190, 197	0
6	E	171/171 (100%)	0.76	21 (12%) 9 8	110, 148, 175, 177	0
7	F	144/144 (100%)	1.22	34 (23%) 2 2	213, 230, 235, 237	0
8	G	142/142 (100%)	0.74	17 (11%) 10 9	79, 112, 127, 144	0
9	H	134/134 (100%)	0.45	8 (5%) 29 24	62, 79, 94, 111	0
10	I	141/141 (100%)	1.66	48 (34%) 1 1	86, 138, 155, 161	0
11	J	136/136 (100%)	1.26	30 (22%) 3 2	94, 113, 135, 141	0
12	K	113/113 (100%)	0.42	9 (7%) 20 17	61, 72, 83, 88	0
13	L	104/104 (100%)	2.12	42 (40%) 1 1	121, 136, 153, 162	0
14	M	109/109 (100%)	0.33	8 (7%) 22 19	65, 80, 98, 127	0
15	N	117/117 (100%)	0.93	13 (11%) 12 10	80, 107, 126, 133	0
16	O	94/94 (100%)	1.09	13 (13%) 8 7	89, 122, 141, 152	0
17	P	127/127 (100%)	0.77	11 (8%) 17 15	71, 85, 109, 156	0
18	Q	93/93 (100%)	0.90	11 (11%) 10 9	98, 124, 140, 144	0
19	R	110/110 (100%)	1.17	18 (16%) 5 5	110, 121, 146, 157	0
20	S	175/175 (100%)	0.88	20 (11%) 11 10	124, 151, 164, 168	0
21	T	84/84 (100%)	1.61	26 (30%) 1 1	102, 117, 133, 146	0
22	U	72/72 (100%)	3.31	45 (62%) 0 0	117, 148, 161, 164	0
23	V	66/66 (100%)	0.66	7 (10%) 13 11	129, 141, 159, 163	0
24	W	55/55 (100%)	0.82	8 (14%) 7 6	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%)	0.45	4 (7%) 24 20	74, 82, 104, 112	0
26	1	54/54 (100%)	1.39	14 (25%) 2 2	125, 136, 152, 168	0
27	2	47/47 (100%)	1.33	9 (19%) 4 3	91, 108, 116, 117	0
28	3	65/65 (100%)	2.12	28 (43%) 1 1	107, 118, 127, 129	0
29	X	2780/2881 (96%)	0.17	136 (4%) 36 30	51, 111, 221, 347	0
30	Y	122/122 (100%)	0.33	4 (3%) 49 43	96, 136, 161, 172	0
All	All	6389/6490 (98%)	0.66	774 (12%) 10 9	51, 119, 242, 347	0

All (774) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	X	2137	C	20.9
29	X	2138	U	17.0
22	U	8	THR	11.5
22	U	27	ASP	11.2
29	X	2144	U	10.8
13	L	12	ARG	10.0
13	L	9	ARG	9.6
21	T	3	HIS	9.5
13	L	8	ARG	9.4
22	U	16	ASN	9.2
19	R	4	PRO	8.9
20	S	15	ASP	8.7
29	X	2602	A	8.4
29	X	1917	U	8.4
29	X	1918	A	8.2
29	X	2133	G	7.9
21	T	73	GLY	7.8
22	U	25	ARG	7.7
22	U	28	GLY	7.7
2	A	237	GLU	7.7
15	N	48	ARG	7.5
29	X	718	A	7.5
28	3	12	ARG	7.5
22	U	26	ALA	7.4
29	X	1919	A	7.3
19	R	12	ASP	7.3
16	O	72	ARG	7.2
29	X	2139	G	7.2
20	S	74	ARG	7.1

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Mol	Chain	Res	Type	RSRZ
29	X	2142	C	7.0
29	X	717	C	7.0
1	0	54	VAL	6.7
22	U	75	TYR	6.7
2	A	239	ARG	6.7
28	3	51	ALA	6.6
1	0	163	LYS	6.6
15	N	20	ARG	6.6
20	S	92	VAL	6.6
29	X	2112	G	6.6
30	Y	123	U	6.6
13	L	11	LEU	6.6
13	L	14	ARG	6.5
13	L	53	ALA	6.5
28	3	54	GLU	6.4
1	0	195	ALA	6.4
13	L	40	ALA	6.4
29	X	1173	A	6.3
29	X	1078	C	6.3
2	A	235	GLY	6.3
29	X	1075	C	6.2
29	X	1916	A	6.2
30	Y	43	G	6.0
22	U	34	THR	6.0
27	2	1	MET	6.0
29	X	2143	U	5.9
3	B	205	SER	5.9
21	T	74	LYS	5.9
29	X	2141	C	5.8
1	0	43	LEU	5.8
28	3	23	MET	5.7
20	S	73	LYS	5.7
5	D	72	LYS	5.7
29	X	614	A	5.5
22	U	12	ASN	5.5
8	G	99	VAL	5.5
22	U	14	VAL	5.4
10	I	48	PHE	5.4
12	K	69	ASP	5.4
16	O	41	GLY	5.4
29	X	2796	U	5.4
11	J	16	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
13	L	20	THR	5.4
13	L	93	SER	5.4
22	U	47	HIS	5.3
8	G	112	THR	5.3
10	I	67	ASN	5.3
29	X	1175	G	5.3
28	3	64	ARG	5.3
22	U	10	LYS	5.2
13	L	24	SER	5.2
29	X	2111	C	5.2
29	X	1026	U	5.2
22	U	13	LEU	5.2
6	E	168	GLN	5.1
10	I	43	ALA	5.1
7	F	99	LEU	5.1
29	X	2150	G	5.1
6	E	111	HIS	5.0
2	A	51	SER	5.0
22	U	63	SER	5.0
29	X	1508	C	5.0
16	O	5	ILE	4.9
15	N	53	LYS	4.9
13	L	94	TYR	4.9
22	U	30	VAL	4.9
29	X	1174	A	4.9
15	N	12	ARG	4.9
16	O	74	TYR	4.9
21	T	71	ASN	4.9
29	X	1079	C	4.9
29	X	2145	U	4.8
1	0	49	LYS	4.8
29	X	2134	A	4.8
13	L	33	ARG	4.8
1	0	162	ASP	4.8
6	E	5	GLY	4.8
29	X	1911	U	4.8
7	F	78	ILE	4.8
29	X	2125	G	4.8
26	1	0	ALA	4.8
2	A	52	ARG	4.7
14	M	104	LEU	4.7
29	X	2132	C	4.7

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Mol	Chain	Res	Type	RSRZ
14	M	106	TYR	4.7
2	A	40	THR	4.7
29	X	715	G	4.7
7	F	136	VAL	4.7
2	A	31	LYS	4.6
7	F	115	LEU	4.6
22	U	21	ARG	4.6
21	T	4	LYS	4.6
22	U	49	LYS	4.6
29	X	2334	G	4.6
2	A	231	HIS	4.6
10	I	103	ASN	4.6
10	I	62	LYS	4.6
1	O	192	LEU	4.5
22	U	29	GLY	4.5
2	A	221	GLN	4.5
29	X	2146	U	4.5
13	L	21	THR	4.5
21	T	5	LYS	4.5
12	K	3	HIS	4.4
29	X	1910	G	4.4
21	T	6	GLY	4.4
13	L	58	ALA	4.4
21	T	2	ALA	4.4
13	L	89	PHE	4.4
29	X	2126	A	4.4
29	X	2113	U	4.4
29	X	1507	A	4.4
10	I	66	ASN	4.4
29	X	1172(C)	G	4.3
8	G	93	LYS	4.3
2	A	12	SER	4.3
5	D	81	GLN	4.3
22	U	62	LEU	4.3
10	I	51	GLY	4.3
4	C	196	VAL	4.2
27	2	5	TYR	4.2
22	U	15	VAL	4.2
2	A	54	ILE	4.2
29	X	1090	U	4.2
10	I	123	ASP	4.2
29	X	1536	C	4.2

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Mol	Chain	Res	Type	RSRZ
2	A	91	ARG	4.1
13	L	23	ALA	4.1
13	L	54	ALA	4.1
9	H	117	GLU	4.1
29	X	1920	C	4.1
4	C	2	ALA	4.1
10	I	74	VAL	4.1
29	X	1509	A	4.1
2	A	236	GLY	4.0
2	A	213	ARG	4.0
22	U	40	ARG	4.0
22	U	43	ARG	4.0
17	P	98	ASP	4.0
22	U	52	ARG	4.0
10	I	46	GLY	4.0
11	J	99	LYS	4.0
22	U	39	LYS	4.0
29	X	2295	C	4.0
1	O	208	ALA	4.0
2	A	2	ALA	4.0
10	I	37	GLN	3.9
2	A	105	ILE	3.9
29	X	716	A	3.9
28	3	52	LYS	3.9
29	X	1756	A	3.9
14	M	54	VAL	3.9
22	U	44	ALA	3.9
13	L	95	LYS	3.9
20	S	11	LYS	3.9
22	U	48	LYS	3.9
2	A	238	GLY	3.9
16	O	73	LYS	3.8
18	Q	32	LYS	3.8
13	L	39	TYR	3.8
19	R	108	VAL	3.8
3	B	54	LYS	3.8
18	Q	27	PHE	3.8
23	V	34	ALA	3.8
26	1	53	ALA	3.8
22	U	22	GLY	3.8
26	1	22	TYR	3.8
19	R	11	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	0	48	ARG	3.8
2	A	27	LYS	3.8
2	A	263	ARG	3.8
13	L	10	LYS	3.8
15	N	56	ASP	3.8
20	S	72	ASP	3.8
11	J	15	ARG	3.7
28	3	3	LYS	3.7
2	A	226	MET	3.7
2	A	225	ALA	3.7
22	U	65	ASN	3.7
28	3	66	LYS	3.7
2	A	261	ARG	3.7
3	B	137	ARG	3.7
13	L	91	ARG	3.7
4	C	188	ILE	3.7
29	X	1914	C	3.7
11	J	139	ASP	3.7
11	J	11	ARG	3.7
20	S	87	THR	3.7
22	U	46	LEU	3.7
2	A	250	TRP	3.6
12	K	22	ARG	3.6
20	S	44	ARG	3.6
29	X	1080	C	3.6
15	N	43	ALA	3.6
11	J	19	THR	3.6
4	C	66	ASN	3.6
10	I	68	VAL	3.6
13	L	52	ALA	3.6
22	U	50	ALA	3.6
29	X	509	C	3.6
5	D	71	LYS	3.6
21	T	7	VAL	3.6
6	E	173	ALA	3.6
30	Y	14	C	3.6
2	A	217	ARG	3.6
5	D	73	SER	3.6
13	L	87	VAL	3.6
29	X	2110	G	3.6
22	U	23	LYS	3.6
13	L	34	SER	3.5

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Mol	Chain	Res	Type	RSRZ
6	E	175	LYS	3.5
18	Q	62	ARG	3.5
24	W	6	VAL	3.5
30	Y	2	C	3.5
9	H	11	ALA	3.5
10	I	59	ARG	3.5
27	2	12	ARG	3.5
1	0	9	LYS	3.5
29	X	1076	C	3.5
2	A	56	GLY	3.5
13	L	31	VAL	3.5
28	3	45	GLY	3.5
22	U	61	TRP	3.5
29	X	2360	A	3.5
5	D	42	SER	3.5
29	X	392	C	3.5
2	A	234	GLY	3.4
8	G	131	VAL	3.4
1	0	210	LEU	3.4
11	J	26	ASP	3.4
28	3	29	LYS	3.4
10	I	98	LEU	3.4
13	L	18	ARG	3.4
29	X	1937	A	3.4
29	X	2797	A	3.4
12	K	43	GLU	3.4
29	X	2032	G	3.4
10	I	58	ALA	3.4
28	3	22	VAL	3.4
26	1	1	ALA	3.4
2	A	220	HIS	3.4
16	O	81	ARG	3.4
1	0	50	SER	3.4
10	I	50	GLU	3.4
16	O	83	ARG	3.3
29	X	1074	G	3.3
13	L	27	LEU	3.3
2	A	19	ALA	3.3
11	J	17	ARG	3.3
19	R	42	ARG	3.3
23	V	36	GLN	3.3
3	B	118	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
10	I	102	LYS	3.3
13	L	36	LYS	3.3
28	3	36	LYS	3.3
11	J	137	VAL	3.3
1	0	24	LEU	3.3
29	X	92	G	3.3
7	F	123	ALA	3.3
10	I	13	ARG	3.3
10	I	101	ARG	3.3
29	X	1938	A	3.3
29	X	2335	A	3.3
2	A	53	PHE	3.3
2	A	62	TYR	3.3
29	X	1737	C	3.3
22	U	20	ARG	3.3
22	U	11	LYS	3.3
21	T	49	GLN	3.3
22	U	42	GLN	3.3
18	Q	12	ILE	3.3
10	I	44	GLY	3.3
13	L	59	LEU	3.3
3	B	125	GLY	3.2
29	X	508	A	3.2
29	X	592	A	3.2
25	Z	56	GLN	3.2
1	0	131	GLY	3.2
19	R	107	ALA	3.2
8	G	106	TYR	3.2
29	X	2794	U	3.2
1	0	205	LEU	3.2
2	A	259	THR	3.2
5	D	32	GLU	3.2
27	2	47	GLU	3.2
28	3	11	LYS	3.2
28	3	30	ARG	3.2
2	A	242	ALA	3.2
20	S	1	MET	3.2
16	O	70	TYR	3.1
10	I	118	VAL	3.1
2	A	55	GLY	3.1
23	V	33	ALA	3.1
19	R	51	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
22	U	9	GLY	3.1
15	N	57	PHE	3.1
23	V	32	ALA	3.1
1	0	218	ILE	3.1
10	I	60	LEU	3.1
7	F	138	VAL	3.1
1	0	202	GLY	3.1
10	I	25	GLY	3.1
20	S	114	ASP	3.1
7	F	7	ILE	3.1
10	I	80	LEU	3.1
2	A	233	HIS	3.1
2	A	60	ARG	3.1
5	D	149	THR	3.1
8	G	101	THR	3.1
19	R	79	SER	3.1
29	X	195	A	3.1
29	X	2136	A	3.1
16	O	14	VAL	3.0
15	N	47	TYR	3.0
2	A	87	ASN	3.0
28	3	4	MET	3.0
21	T	76	ALA	3.0
6	E	33	LEU	3.0
7	F	12	LEU	3.0
7	F	137	THR	3.0
10	I	71	THR	3.0
21	T	63	SER	3.0
29	X	2149	G	3.0
13	L	19	THR	3.0
8	G	171	LEU	3.0
13	L	57	ALA	3.0
29	X	421	C	3.0
23	V	30	PHE	3.0
29	X	2135	A	3.0
20	S	93	GLU	3.0
4	C	90	SER	3.0
29	X	1940	U	2.9
5	D	74	ILE	2.9
7	F	13	PRO	2.9
22	U	51	ILE	2.9
29	X	1537	G	2.9

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Mol	Chain	Res	Type	RSRZ
5	D	4	LEU	2.9
6	E	172	LYS	2.9
2	A	222	ARG	2.9
6	E	46	ASP	2.9
26	1	3	GLY	2.9
5	D	31	ILE	2.9
5	D	136	LEU	2.9
1	0	201	LYS	2.9
10	I	30	ALA	2.9
10	I	92	THR	2.9
24	W	7	ARG	2.9
28	3	9	MET	2.9
6	E	123	PHE	2.9
11	J	59	PHE	2.9
29	X	1939	U	2.9
1	0	96	ILE	2.9
5	D	3	GLN	2.9
17	P	105	ARG	2.9
20	S	175	ARG	2.9
29	X	2359	C	2.9
29	X	944	G	2.9
23	V	35	GLY	2.9
1	0	99	ILE	2.9
2	A	249	PRO	2.9
5	D	148	LYS	2.9
11	J	131	LYS	2.9
19	R	43	ASP	2.9
29	X	2296	U	2.9
1	0	209	TYR	2.9
29	X	761	A	2.8
1	0	123	LEU	2.8
13	L	55	SER	2.8
27	2	23	LYS	2.8
11	J	114	GLN	2.8
8	G	103	TYR	2.8
2	A	57	GLY	2.8
10	I	31	GLY	2.8
14	M	57	ILE	2.8
29	X	550	C	2.8
28	3	32	GLN	2.8
1	0	200	ALA	2.8
29	X	1538	G	2.8

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Mol	Chain	Res	Type	RSRZ
1	0	53	ASN	2.8
20	S	91	PRO	2.8
1	0	109	VAL	2.8
19	R	106	VAL	2.8
8	G	168	THR	2.8
18	Q	37	GLU	2.8
1	0	45	ILE	2.8
1	0	119	ILE	2.8
6	E	150	LYS	2.8
10	I	45	LYS	2.8
22	U	33	LYS	2.8
28	3	50	LEU	2.8
1	0	127	LEU	2.7
29	X	1912	A	2.7
6	E	169	ILE	2.7
7	F	84	ILE	2.7
1	0	198	GLY	2.7
17	P	99	ALA	2.7
22	U	60	VAL	2.7
24	W	45	LYS	2.7
28	3	8	LYS	2.7
10	I	88	PHE	2.7
7	F	52	ILE	2.7
1	0	136	PRO	2.7
1	0	197	PRO	2.7
2	A	241	GLY	2.7
29	X	1103	A	2.7
29	X	2108	C	2.7
2	A	32	ALA	2.7
2	A	208	LYS	2.7
5	D	62	LEU	2.7
5	D	103	LEU	2.7
24	W	46	THR	2.7
11	J	101	GLY	2.7
2	A	218	LYS	2.7
4	C	87	LYS	2.7
22	U	19	ILE	2.7
4	C	38	ARG	2.6
1	0	149	VAL	2.6
2	A	107	ALA	2.6
29	X	1091	G	2.6
29	X	2114	A	2.6

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Mol	Chain	Res	Type	RSRZ
24	W	1	MET	2.6
1	0	30	THR	2.6
26	1	24	THR	2.6
27	2	25	LYS	2.6
6	E	151	VAL	2.6
6	E	162	VAL	2.6
29	X	2130	U	2.6
1	0	169	ALA	2.6
2	A	111	LEU	2.6
9	H	8	LEU	2.6
16	O	25	LEU	2.6
29	X	243	A	2.6
29	X	400	G	2.6
13	L	92	GLY	2.6
26	1	23	THR	2.6
1	0	51	ASP	2.6
2	A	230	ASP	2.6
12	K	5	LYS	2.6
13	L	90	ASP	2.6
26	1	28	ARG	2.6
5	D	146	VAL	2.6
7	F	96	VAL	2.6
3	B	187	ALA	2.6
10	I	95	ALA	2.6
28	3	53	ALA	2.6
6	E	64	LEU	2.6
29	X	1659	U	2.6
11	J	48	ILE	2.6
19	R	52	ASN	2.6
22	U	45	ASN	2.6
17	P	94	GLU	2.6
2	A	43	ARG	2.6
29	X	2872	G	2.6
29	X	1176	C	2.6
13	L	88	VAL	2.6
20	S	123	VAL	2.6
1	0	132	LEU	2.6
2	A	93	ALA	2.6
1	0	204	PHE	2.6
19	R	57	ASN	2.6
4	C	20	PRO	2.6
9	H	33	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	0	199	THR	2.6
13	L	13	THR	2.6
19	R	113	THR	2.6
19	R	46	VAL	2.6
13	L	51	LEU	2.6
2	A	64	ILE	2.5
18	Q	88	ILE	2.5
14	M	2	GLN	2.5
1	0	161	ASN	2.5
5	D	82	GLY	2.5
21	T	58	THR	2.5
25	Z	26	THR	2.5
2	A	89	SER	2.5
5	D	49	ALA	2.5
19	R	109	ALA	2.5
2	A	68	LYS	2.5
29	X	2122	U	2.5
29	X	2123	G	2.5
1	0	47	PRO	2.5
21	T	41	ARG	2.5
10	I	24	GLY	2.5
4	C	19	LEU	2.5
24	W	17	VAL	2.5
5	D	58	ALA	2.5
21	T	84	ALA	2.5
15	N	49	ASP	2.5
28	3	55	TRP	2.5
2	A	223	GLY	2.5
2	A	147	LEU	2.5
29	X	2156	G	2.5
2	A	34	THR	2.5
27	2	43	THR	2.5
26	1	4	ALA	2.5
7	F	68	ILE	2.5
12	K	8	ARG	2.5
6	E	26	VAL	2.5
10	I	75	VAL	2.5
1	0	159	PHE	2.5
28	3	5	LYS	2.4
7	F	75	SER	2.4
15	N	58	ARG	2.4
17	P	108	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
7	F	104	VAL	2.4
27	2	22	MET	2.4
29	X	1535	U	2.4
29	X	2109	U	2.4
20	S	67	LYS	2.4
29	X	2116	G	2.4
29	X	2147	G	2.4
15	N	25	TRP	2.4
12	K	7	GLY	2.4
5	D	156	ILE	2.4
29	X	387	U	2.4
7	F	20	ALA	2.4
21	T	69	PHE	2.4
1	0	213	THR	2.4
8	G	100	TYR	2.4
17	P	46	ARG	2.4
1	0	222	LEU	2.4
2	A	214	TRP	2.4
5	D	175	LEU	2.4
16	O	63	HIS	2.4
21	T	13	GLY	2.4
7	F	4	VAL	2.4
10	I	73	GLU	2.4
9	H	84	ALA	2.4
29	X	125	A	2.4
29	X	1966	A	2.4
3	B	75	THR	2.4
21	T	77	ARG	2.4
2	A	106	LEU	2.4
2	A	215	LEU	2.4
11	J	20	GLY	2.4
1	0	70	VAL	2.4
5	D	98	VAL	2.4
11	J	28	VAL	2.4
5	D	44	LYS	2.4
17	P	116	ILE	2.4
11	J	105	PHE	2.4
16	O	39	PHE	2.4
20	S	68	ALA	2.4
21	T	47	ALA	2.4
22	U	64	ALA	2.4
1	0	78	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
13	L	99	ARG	2.4
29	X	388	G	2.4
6	E	109	TYR	2.3
21	T	20	TYR	2.3
2	A	33	LEU	2.3
6	E	112	PRO	2.3
7	F	22	PRO	2.3
7	F	134	MET	2.3
5	D	47	SER	2.3
7	F	120	VAL	2.3
8	G	98	LYS	2.3
9	H	12	ASP	2.3
18	Q	2	SER	2.3
11	J	106	GLU	2.3
19	R	23	ILE	2.3
8	G	146	THR	2.3
29	X	1497	U	2.3
4	C	88	PRO	2.3
11	J	132	MET	2.3
2	A	264	LYS	2.3
18	Q	53	ILE	2.3
22	U	24	ALA	2.3
10	I	55	ARG	2.3
29	X	1533	C	2.3
7	F	18	THR	2.3
28	3	6	THR	2.3
2	A	257	LEU	2.3
7	F	77	LEU	2.3
10	I	108	LEU	2.3
28	3	60	LEU	2.3
17	P	101	PRO	2.3
2	A	82	ILE	2.3
15	N	46	GLU	2.3
4	C	92	ASP	2.3
17	P	43	ASP	2.3
29	X	2140	G	2.3
2	A	5	LYS	2.3
10	I	38	LYS	2.3
25	Z	3	LYS	2.3
26	1	26	LYS	2.3
5	D	143	TYR	2.3
29	X	654	U	2.3

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Mol	Chain	Res	Type	RSRZ
29	X	2585	U	2.3
21	T	68	VAL	2.3
2	A	25	ALA	2.3
11	J	136	GLU	2.3
29	X	394	A	2.3
18	Q	72	ARG	2.3
25	Z	59	ALA	2.3
10	I	27	ASP	2.3
29	X	326	G	2.3
1	0	137	LYS	2.3
5	D	69	LYS	2.3
8	G	75	ILE	2.2
10	I	69	GLY	2.2
19	R	15	HIS	2.2
22	U	37	ILE	2.2
29	X	1806	C	2.2
29	X	1963	U	2.2
29	X	2506	U	2.2
1	0	5	ALA	2.2
1	0	154	ALA	2.2
3	B	204	ALA	2.2
7	F	131	ALA	2.2
10	I	104	ARG	2.2
13	L	108	ARG	2.2
5	D	145	MET	2.2
18	Q	91	LEU	2.2
26	1	11	LYS	2.2
1	0	189	ILE	2.2
2	A	251	GLY	2.2
7	F	57	ILE	2.2
7	F	125	ASN	2.2
11	J	69	ILE	2.2
28	3	16	ILE	2.2
1	0	55	ARG	2.2
2	A	67	PHE	2.2
29	X	2406	U	2.2
29	X	1852	C	2.2
13	L	22	ALA	2.2
2	A	61	LEU	2.2
26	1	37	LEU	2.2
6	E	6	LYS	2.2
10	I	28	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
11	J	21	ASP	2.2
29	X	423	A	2.2
29	X	2158	A	2.2
2	A	240	THR	2.2
3	B	72	VAL	2.2
14	M	55	ILE	2.2
3	B	67	PHE	2.2
2	A	35	GLU	2.2
4	C	155	GLU	2.2
2	A	255	LYS	2.2
29	X	1239	C	2.2
11	J	82	THR	2.2
14	M	53	VAL	2.2
29	X	389	A	2.2
10	I	34	HIS	2.2
17	P	111	ARG	2.2
24	W	41	ARG	2.2
7	F	128	ALA	2.2
8	G	59	ALA	2.2
10	I	56	LEU	2.2
10	I	83	LEU	2.2
15	N	60	LEU	2.2
20	S	65	LEU	2.2
29	X	1008	U	2.2
1	O	25	VAL	2.2
1	O	58	VAL	2.2
11	J	97	VAL	2.2
11	J	25	GLY	2.1
12	K	71	HIS	2.1
3	B	155	ARG	2.1
29	X	391	A	2.1
6	E	153	LYS	2.1
7	F	94	ALA	2.1
12	K	9	LYS	2.1
17	P	95	ALA	2.1
29	X	1915	U	2.1
5	D	132	ILE	2.1
13	L	100	VAL	2.1
3	B	135	HIS	2.1
5	D	61	THR	2.1
7	F	66	THR	2.1
9	H	30	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
29	X	1922	G	2.1
21	T	53	MET	2.1
5	D	78	LYS	2.1
21	T	83	ALA	2.1
29	X	2611	U	2.1
28	3	14	ILE	2.1
1	0	39	VAL	2.1
20	S	169	VAL	2.1
21	T	30	VAL	2.1
1	0	40	HIS	2.1
5	D	173	MET	2.1
10	I	41	SER	2.1
19	R	80	LYS	2.1
21	T	46	LYS	2.1
4	C	181	LEU	2.1
20	S	14	LEU	2.1
2	A	9	TYR	2.1
6	E	37	TYR	2.1
10	I	72	TYR	2.1
26	1	21	TYR	2.1
29	X	204	G	2.1
29	X	1888	G	2.1
29	X	1654	A	2.1
11	J	100	PRO	2.1
11	J	36	ILE	2.1
22	U	41	VAL	2.1
27	2	44	VAL	2.1
2	A	41	GLY	2.1
3	B	1	MET	2.1
6	E	174	GLY	2.1
1	0	88	ASP	2.1
1	0	152	LEU	2.1
23	V	38	ALA	2.1
26	1	5	ALA	2.1
28	3	10	ALA	2.1
1	0	185	TYR	2.1
29	X	746	C	2.1
5	D	65	PRO	2.1
7	F	25	PRO	2.1
7	F	113	PRO	2.1
29	X	1077	A	2.1
2	A	46	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
29	X	714	U	2.1
8	G	30	LYS	2.1
21	T	24	LYS	2.1
10	I	49	PHE	2.1
7	F	58	THR	2.0
4	C	192	ALA	2.0
11	J	22	ALA	2.0
11	J	41	ALA	2.0
13	L	30	SER	2.0
1	O	16	TYR	2.0
8	G	113	GLU	2.0
14	M	29	PRO	2.0
29	X	2152	C	2.0
18	Q	64	ARG	2.0
29	X	945	A	2.0
29	X	2795	U	2.0
11	J	37	ALA	2.0
7	F	21	PRO	2.0
2	A	26	LYS	2.0
7	F	9	LYS	2.0
24	W	27	LYS	2.0
28	3	13	ARG	2.0
8	G	135	LEU	2.0
9	H	134	LEU	2.0
10	I	65	PHE	2.0
16	O	35	LEU	2.0
20	S	52	PHE	2.0
29	X	1816	C	2.0
29	X	1965	C	2.0
29	X	2178	C	2.0
29	X	2799	C	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	X	6163	1/1	0.08	0.41	156,156,156,156	0
31	MG	X	6146	1/1	0.14	1.21	129,129,129,129	0
31	MG	X	6093	1/1	0.18	0.59	106,106,106,106	0
31	MG	X	6192	1/1	0.23	0.49	138,138,138,138	0
31	MG	X	6110	1/1	0.35	0.39	130,130,130,130	0
31	MG	X	6054	1/1	0.35	0.44	92,92,92,92	0
31	MG	X	6170	1/1	0.36	0.59	127,127,127,127	0
31	MG	X	6020	1/1	0.36	0.37	79,79,79,79	0
31	MG	X	6177	1/1	0.38	0.49	113,113,113,113	0
31	MG	X	6076	1/1	0.38	0.49	102,102,102,102	0
31	MG	X	6052	1/1	0.39	0.67	97,97,97,97	0
31	MG	X	6127	1/1	0.40	0.59	122,122,122,122	0
31	MG	X	6108	1/1	0.40	0.66	120,120,120,120	0
31	MG	X	6019	1/1	0.40	0.55	77,77,77,77	0
31	MG	X	6186	1/1	0.42	0.58	134,134,134,134	0
31	MG	X	6018	1/1	0.42	0.38	74,74,74,74	0
31	MG	Y	202	1/1	0.42	0.35	125,125,125,125	0
31	MG	X	6105	1/1	0.43	0.86	118,118,118,118	0
31	MG	X	6141	1/1	0.43	0.51	122,122,122,122	0
31	MG	X	6012	1/1	0.43	0.39	82,82,82,82	0
31	MG	X	6157	1/1	0.43	0.31	111,111,111,111	0
31	MG	X	6048	1/1	0.43	0.57	102,102,102,102	0
31	MG	X	6070	1/1	0.45	0.37	107,107,107,107	0
31	MG	X	6123	1/1	0.45	0.48	130,130,130,130	0
31	MG	X	6109	1/1	0.45	0.27	101,101,101,101	0
31	MG	X	6148	1/1	0.47	0.42	130,130,130,130	0
31	MG	X	6153	1/1	0.47	0.57	113,113,113,113	0
31	MG	X	6037	1/1	0.47	0.34	86,86,86,86	0
31	MG	X	6084	1/1	0.48	0.28	93,93,93,93	0
31	MG	X	6089	1/1	0.48	0.37	90,90,90,90	0
31	MG	X	6072	1/1	0.49	0.55	102,102,102,102	0
31	MG	X	6090	1/1	0.49	0.35	117,117,117,117	0
31	MG	X	6058	1/1	0.50	0.39	97,97,97,97	0
31	MG	X	6024	1/1	0.50	0.54	87,87,87,87	0
31	MG	X	6023	1/1	0.50	0.51	97,97,97,97	0
31	MG	X	6046	1/1	0.50	0.30	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	6057	1/1	0.50	0.69	93,93,93,93	0
31	MG	X	6125	1/1	0.51	0.44	123,123,123,123	0
31	MG	X	6051	1/1	0.52	0.31	69,69,69,69	0
31	MG	X	6111	1/1	0.52	0.61	98,98,98,98	0
31	MG	X	6038	1/1	0.53	0.57	85,85,85,85	0
31	MG	X	6190	1/1	0.53	0.63	129,129,129,129	0
31	MG	X	6033	1/1	0.54	0.39	98,98,98,98	0
31	MG	X	6175	1/1	0.54	0.38	121,121,121,121	0
31	MG	X	6164	1/1	0.54	0.59	124,124,124,124	0
31	MG	X	6182	1/1	0.54	0.55	120,120,120,120	0
31	MG	X	6139	1/1	0.55	0.43	126,126,126,126	0
31	MG	X	6172	1/1	0.55	0.55	124,124,124,124	0
31	MG	X	6137	1/1	0.55	0.42	135,135,135,135	0
31	MG	X	6113	1/1	0.56	0.55	115,115,115,115	0
31	MG	X	6007	1/1	0.56	0.27	70,70,70,70	0
31	MG	X	6181	1/1	0.56	0.31	121,121,121,121	0
31	MG	X	6025	1/1	0.56	0.31	83,83,83,83	0
31	MG	X	6160	1/1	0.57	0.56	104,104,104,104	0
31	MG	X	6006	1/1	0.57	0.58	69,69,69,69	0
31	MG	X	6003	1/1	0.57	0.47	70,70,70,70	0
31	MG	X	6166	1/1	0.57	0.48	106,106,106,106	0
31	MG	X	6078	1/1	0.57	0.49	93,93,93,93	0
31	MG	X	6102	1/1	0.57	0.24	89,89,89,89	0
31	MG	X	6011	1/1	0.57	0.37	89,89,89,89	0
31	MG	X	6167	1/1	0.58	0.55	103,103,103,103	0
31	MG	X	6049	1/1	0.58	0.68	88,88,88,88	0
31	MG	X	6189	1/1	0.58	0.48	120,120,120,120	0
31	MG	X	6088	1/1	0.59	0.53	99,99,99,99	0
31	MG	X	6077	1/1	0.59	0.39	98,98,98,98	0
31	MG	X	6065	1/1	0.59	0.33	81,81,81,81	0
31	MG	X	6121	1/1	0.59	0.58	99,99,99,99	0
31	MG	X	6014	1/1	0.59	0.40	91,91,91,91	0
31	MG	Y	205	1/1	0.59	0.59	129,129,129,129	0
31	MG	X	6032	1/1	0.60	0.33	78,78,78,78	0
31	MG	X	6173	1/1	0.60	1.13	102,102,102,102	0
31	MG	X	6144	1/1	0.60	0.57	87,87,87,87	0
31	MG	X	6029	1/1	0.60	0.31	69,69,69,69	0
31	MG	X	6116	1/1	0.61	0.40	106,106,106,106	0
31	MG	X	6101	1/1	0.61	0.48	89,89,89,89	0
31	MG	X	6162	1/1	0.61	1.43	111,111,111,111	0
31	MG	X	6064	1/1	0.61	0.52	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	X	6115	1/1	0.61	0.47	103,103,103,103	0
31	MG	X	6015	1/1	0.62	0.38	77,77,77,77	0
31	MG	X	6069	1/1	0.62	0.46	91,91,91,91	0
31	MG	X	6059	1/1	0.62	0.37	87,87,87,87	0
31	MG	X	6179	1/1	0.62	0.65	117,117,117,117	0
31	MG	X	6026	1/1	0.62	0.27	91,91,91,91	0
31	MG	X	6094	1/1	0.62	0.39	92,92,92,92	0
31	MG	X	6001	1/1	0.63	0.58	69,69,69,69	0
31	MG	X	6145	1/1	0.63	0.26	104,104,104,104	0
31	MG	X	6155	1/1	0.63	0.37	115,115,115,115	0
31	MG	X	6107	1/1	0.63	0.67	113,113,113,113	0
31	MG	X	6034	1/1	0.64	0.58	90,90,90,90	0
31	MG	X	6056	1/1	0.64	0.75	85,85,85,85	0
31	MG	X	6129	1/1	0.64	0.55	104,104,104,104	0
31	MG	X	6075	1/1	0.64	0.69	103,103,103,103	0
31	MG	X	6149	1/1	0.64	0.45	94,94,94,94	0
31	MG	X	6047	1/1	0.64	0.42	74,74,74,74	0
31	MG	X	6044	1/1	0.64	0.34	73,73,73,73	0
31	MG	X	6140	1/1	0.65	0.80	97,97,97,97	0
31	MG	X	6112	1/1	0.65	0.61	84,84,84,84	0
31	MG	X	6079	1/1	0.66	0.25	102,102,102,102	0
31	MG	X	6039	1/1	0.66	0.57	104,104,104,104	0
31	MG	X	6119	1/1	0.66	1.22	128,128,128,128	0
31	MG	X	6017	1/1	0.66	0.40	83,83,83,83	0
31	MG	X	6103	1/1	0.66	0.34	117,117,117,117	0
31	MG	X	6040	1/1	0.67	0.57	80,80,80,80	0
31	MG	X	6073	1/1	0.67	0.57	85,85,85,85	0
31	MG	X	6063	1/1	0.67	1.21	87,87,87,87	0
31	MG	X	6050	1/1	0.67	0.35	84,84,84,84	0
31	MG	X	6022	1/1	0.68	0.26	77,77,77,77	0
31	MG	X	6117	1/1	0.68	0.46	90,90,90,90	0
31	MG	X	6183	1/1	0.68	0.45	105,105,105,105	0
31	MG	X	6098	1/1	0.68	0.57	97,97,97,97	0
31	MG	X	6085	1/1	0.68	0.41	101,101,101,101	0
31	MG	X	6004	1/1	0.68	0.33	76,76,76,76	0
31	MG	X	6060	1/1	0.68	0.58	80,80,80,80	0
31	MG	X	6009	1/1	0.68	0.37	69,69,69,69	0
31	MG	X	6013	1/1	0.68	0.55	76,76,76,76	0
31	MG	X	6082	1/1	0.69	0.72	83,83,83,83	0
31	MG	X	6168	1/1	0.69	0.42	107,107,107,107	0
31	MG	X	6180	1/1	0.69	0.91	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	6067	1/1	0.69	0.50	79,79,79,79	0
31	MG	X	6133	1/1	0.70	0.59	111,111,111,111	0
31	MG	X	6135	1/1	0.70	0.50	91,91,91,91	0
31	MG	X	6171	1/1	0.70	0.57	111,111,111,111	0
31	MG	X	6134	1/1	0.71	0.57	112,112,112,112	0
31	MG	Y	201	1/1	0.71	0.56	112,112,112,112	0
31	MG	X	6021	1/1	0.71	0.45	75,75,75,75	0
31	MG	X	6185	1/1	0.71	0.39	109,109,109,109	0
31	MG	X	6161	1/1	0.72	0.54	95,95,95,95	0
31	MG	X	6120	1/1	0.72	0.98	102,102,102,102	0
31	MG	X	6031	1/1	0.72	0.36	69,69,69,69	0
31	MG	X	6128	1/1	0.72	0.79	97,97,97,97	0
31	MG	X	6080	1/1	0.72	0.61	108,108,108,108	0
31	MG	X	6124	1/1	0.72	0.80	107,107,107,107	0
31	MG	Y	204	1/1	0.72	0.44	109,109,109,109	0
31	MG	X	6176	1/1	0.72	0.46	107,107,107,107	0
31	MG	X	6174	1/1	0.73	0.35	87,87,87,87	0
31	MG	X	6042	1/1	0.73	0.34	83,83,83,83	0
31	MG	X	6100	1/1	0.74	0.52	97,97,97,97	0
31	MG	X	6099	1/1	0.74	0.59	89,89,89,89	0
31	MG	X	6156	1/1	0.74	0.40	105,105,105,105	0
31	MG	X	6114	1/1	0.74	0.41	91,91,91,91	0
31	MG	X	6158	1/1	0.74	0.97	114,114,114,114	0
31	MG	X	6184	1/1	0.75	0.65	102,102,102,102	0
31	MG	X	6147	1/1	0.75	0.45	82,82,82,82	0
31	MG	X	6061	1/1	0.76	0.40	83,83,83,83	0
31	MG	X	6151	1/1	0.76	0.26	98,98,98,98	0
31	MG	X	6142	1/1	0.77	0.52	89,89,89,89	0
31	MG	X	6045	1/1	0.77	0.76	89,89,89,89	0
31	MG	X	6126	1/1	0.77	0.79	94,94,94,94	0
31	MG	X	6053	1/1	0.77	0.68	91,91,91,91	0
31	MG	X	6122	1/1	0.78	0.70	100,100,100,100	0
31	MG	X	6118	1/1	0.79	0.66	90,90,90,90	0
31	MG	X	6169	1/1	0.79	0.44	101,101,101,101	0
31	MG	X	6016	1/1	0.79	0.21	77,77,77,77	0
31	MG	X	6150	1/1	0.79	0.48	111,111,111,111	0
31	MG	X	6131	1/1	0.79	0.72	101,101,101,101	0
31	MG	X	6165	1/1	0.80	0.77	99,99,99,99	0
31	MG	X	6087	1/1	0.80	0.47	98,98,98,98	0
31	MG	X	6138	1/1	0.80	0.65	94,94,94,94	0
31	MG	X	6027	1/1	0.80	0.68	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	MG	X	6159	1/1	0.82	0.42	111,111,111,111	0
31	MG	X	6068	1/1	0.82	0.86	90,90,90,90	0
31	MG	X	6136	1/1	0.84	0.63	122,122,122,122	0
31	MG	X	6132	1/1	0.84	0.50	94,94,94,94	0
31	MG	X	6062	1/1	0.84	0.42	85,85,85,85	0
31	MG	X	6143	1/1	0.85	0.82	100,100,100,100	0
31	MG	X	6091	1/1	0.85	0.75	88,88,88,88	0
31	MG	X	6035	1/1	0.85	0.34	86,86,86,86	0
31	MG	X	6028	1/1	0.85	0.24	88,88,88,88	0
31	MG	X	6152	1/1	0.86	0.60	112,112,112,112	0
31	MG	X	6066	1/1	0.86	0.85	84,84,84,84	0
31	MG	X	6081	1/1	0.86	0.35	78,78,78,78	0
31	MG	Y	203	1/1	0.86	0.72	102,102,102,102	0
31	MG	X	6036	1/1	0.86	0.76	82,82,82,82	0
31	MG	X	6083	1/1	0.86	0.48	91,91,91,91	0
31	MG	X	6030	1/1	0.87	0.94	83,83,83,83	0
31	MG	X	6041	1/1	0.87	0.21	83,83,83,83	0
31	MG	X	6055	1/1	0.87	0.64	90,90,90,90	0
31	MG	X	6002	1/1	0.87	0.21	78,78,78,78	0
31	MG	X	6074	1/1	0.87	0.58	80,80,80,80	0
31	MG	X	6008	1/1	0.88	0.32	81,81,81,81	0
31	MG	X	6092	1/1	0.88	0.08	93,93,93,93	0
31	MG	X	6010	1/1	0.89	0.61	69,69,69,69	0
31	MG	X	6095	1/1	0.89	0.64	79,79,79,79	0
31	MG	X	6154	1/1	0.89	0.91	113,113,113,113	0
31	MG	X	6043	1/1	0.89	0.69	69,69,69,69	0
31	MG	X	6187	1/1	0.89	0.37	92,92,92,92	0
31	MG	X	6188	1/1	0.89	0.37	98,98,98,98	0
31	MG	X	6106	1/1	0.89	0.75	80,80,80,80	0
31	MG	X	6130	1/1	0.90	0.55	108,108,108,108	0
31	MG	X	6096	1/1	0.90	0.68	89,89,89,89	0
31	MG	X	6071	1/1	0.90	0.26	81,81,81,81	0
31	MG	X	6104	1/1	0.91	0.49	86,86,86,86	0
31	MG	M	201	1/1	0.91	0.56	69,69,69,69	0
31	MG	X	6191	1/1	0.91	0.78	101,101,101,101	0
31	MG	X	6097	1/1	0.92	0.65	93,93,93,93	0
31	MG	X	6086	1/1	0.92	0.67	87,87,87,87	0
31	MG	X	6178	1/1	0.93	0.43	103,103,103,103	0
31	MG	X	6005	1/1	0.96	0.70	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.