



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:55 AM GMT

PDB ID : 3G4S  
Title : Co-crystal structure of Tiamulin bound to the large ribosomal subunit  
Authors : Gurel, G.; Blaha, G.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2009-02-04  
Resolution : 3.20 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

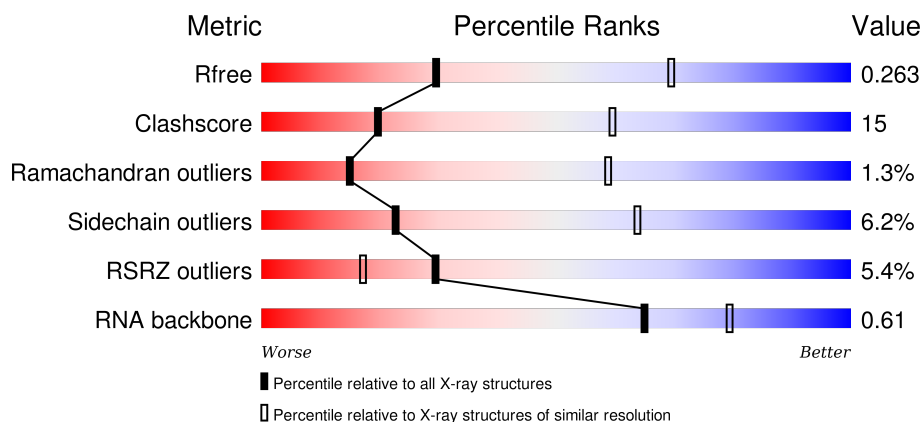
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	0	2923	<div> <div></div> <div>34% 53% 7% 6%</div> </div>
2	A	237	<div> <div>4%</div> <div>83% 16%</div> </div>
3	B	337	<div> <div></div> <div>81% 17% .</div> </div>
4	C	246	<div> <div>%</div> <div>82% 15% .</div> </div>


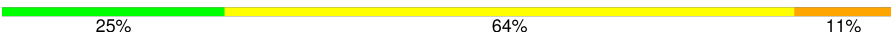
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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	172	
7	F	119	
8	G	348	
9	H	177	
10	I	70	
11	J	142	
12	K	132	
13	L	165	
14	M	194	
15	N	186	
16	O	115	
17	P	143	
18	Q	95	
19	R	150	
20	S	81	
21	T	119	
22	U	53	
23	V	65	
24	W	154	
25	X	82	
26	Y	142	
27	Z	73	
28	1	56	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	9	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
32	MG	0	8009	-	-	-	X
32	MG	0	8034	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8062	-	-	-	X
32	MG	0	8067	-	-	-	X
32	MG	0	8070	-	-	-	X
32	MG	0	8073	-	-	-	X
32	MG	0	8090	-	-	-	X
32	MG	C	8012	-	-	-	X
34	NA	0	8502	-	-	-	X
34	NA	0	8512	-	-	-	X
34	NA	0	8524	-	-	-	X
34	NA	0	8528	-	-	-	X
34	NA	0	8530	-	-	-	X
34	NA	0	8535	-	-	-	X
34	NA	0	8542	-	-	-	X
34	NA	0	8546	-	-	-	X
34	NA	0	8547	-	-	-	X
34	NA	0	8555	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8558	-	-	-	X
34	NA	0	8559	-	-	-	X
34	NA	0	8562	-	-	-	X
34	NA	0	8564	-	-	-	X
34	NA	0	8565	-	-	-	X
34	NA	0	8568	-	-	-	X
34	NA	0	8571	-	-	-	X
34	NA	9	8572	-	-	-	X
34	NA	R	8575	-	-	-	X
35	CL	B	8819	-	-	-	X
35	CL	O	8808	-	-	-	X
36	SR	0	8943	-	-	-	X
36	SR	B	8987	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	SR	L	8969	-	-	-	X
37	MUL	0	9101	-	-	-	X
38	CD	3	8704	-	-	-	X

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99167 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 2 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 3 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 4 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 5 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 6 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	172	Total	C	N	O	S	0	0	0
			1358	840	224	290	4			

- Molecule 7 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 8 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 9 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 10 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	70	Total	C	N	O	S	0	0	0
			520	323	81	115	1			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	145	Total	C	N	O		0	0	0
			1118	670	222	226				

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	194	Total	C	N	O	S	0	0	0
			1559	943	333	282	1			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 16 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	143	Total	C	N	O		0	0	0
			1137	683	229	225				

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 19 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	150	Total	C	N	O	S	0	0	0
			1150	713	209	224	4			

- Molecule 20 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	81	Total	C	N	O	S	0	0	0
			642	389	111	139	3			

- Molecule 21 is a protein called 50S ribosomal protein L24P.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 22 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	53	Total	C	N	O	S	0	0	0
			411	244	75	87	5			

- Molecule 23 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	S	0	0	0
			500	304	94	101	1			

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 25 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	X	82	Total	C	N	O	S	0	0	0
			655	402	129	123	1			

- Molecule 26 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Y	142	Total	C	N	O	0	0	0
			1131	686	228	217			

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0	0
			574	343	113	113	5			

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	84	Total	Mg	0	0
			84	84		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	1	Total K 1 1	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	9	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0

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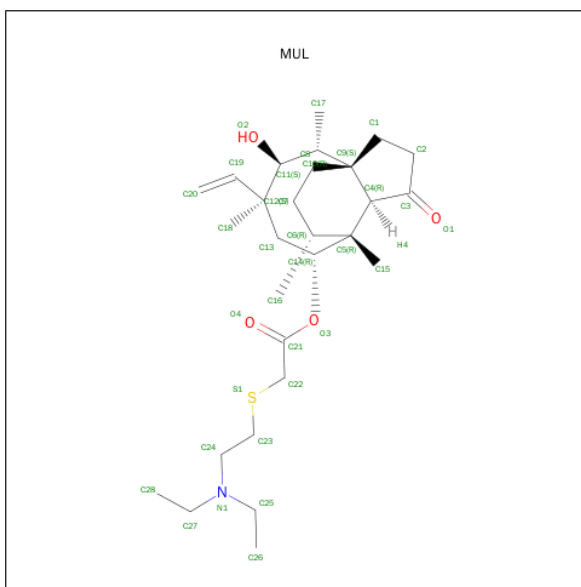
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	91	Total 91	Sr 91	0	0
36	J	1	Total 1	Sr 1	0	0
36	1	2	Total 2	Sr 2	0	0
36	H	1	Total 1	Sr 1	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	3	Total 3	Sr 3	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	2	Total 2	Sr 2	0	0
36	L	1	Total 1	Sr 1	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 1	0	0

- Molecule 37 is TIAMULIN (three-letter code: MUL) (formula: C<sub>28</sub>H<sub>47</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	0	1	Total	C	N	O	S	0	0
			34	28	1	4	1		

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total	Cd	0	0
			1	1		
38	Z	1	Total	Cd	0	0
			1	1		
38	1	1	Total	Cd	0	0
			1	1		
38	3	1	Total	Cd	0	0
			1	1		
38	U	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5940	Total	O	0	0
			5940	5940		
39	A	125	Total	O	0	0
			125	125		
39	B	140	Total	O	0	0
			140	140		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	C	158	Total 158	O 158	0	0
39	D	45	Total 45	O 45	0	0
39	E	42	Total 42	O 42	0	0
39	F	26	Total 26	O 26	0	0
39	G	18	Total 18	O 18	0	0
39	H	70	Total 70	O 70	0	0
39	I	4	Total 4	O 4	0	0
39	J	47	Total 47	O 47	0	0
39	K	58	Total 58	O 58	0	0
39	L	94	Total 94	O 94	0	0
39	M	132	Total 132	O 132	0	0
39	N	55	Total 55	O 55	0	0
39	O	43	Total 43	O 43	0	0
39	P	59	Total 59	O 59	0	0
39	Q	52	Total 52	O 52	0	0
39	R	80	Total 80	O 80	0	0
39	S	30	Total 30	O 30	0	0
39	T	30	Total 30	O 30	0	0
39	U	30	Total 30	O 30	0	0
39	V	11	Total 11	O 11	0	0
39	W	59	Total 59	O 59	0	0

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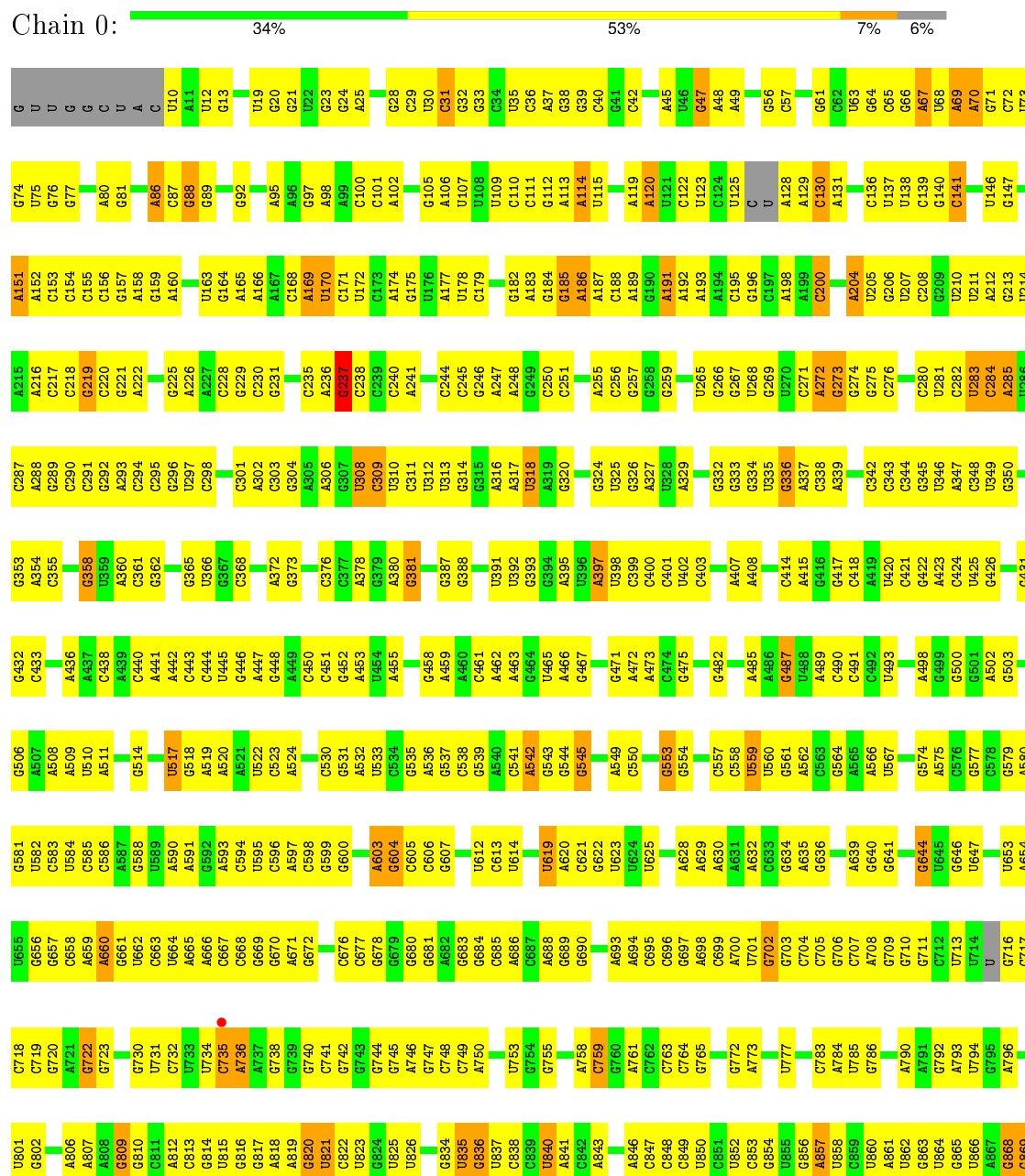
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	22	Total 22	O 22	0	0
39	Y	105	Total 105	O 105	0	0
39	Z	30	Total 30	O 30	0	0
39	1	55	Total 55	O 55	0	0
39	2	48	Total 48	O 48	0	0
39	3	62	Total 62	O 62	0	0
39	9	152	Total 152	O 152	0	0

### 3 Residue-property plots

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

#### • Molecule 1: 23S ribosomal RNA




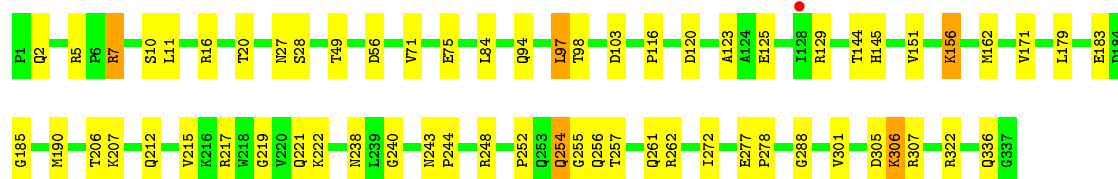


C1965	C1889	C1818	G1752	C1680	G1608	U1524	C1450	G1376	C1305		G1159	C1085	A1006	A1943	G870
U1966	U1890	G1819	C1753	G1681	C1609	G1525	C1451	C1377	U1306	C1228	G1160	A1086	A1007	G944	G871
A1969	C1892	G1820	A1754	A1682	G1610	A1526	G1452	G1378	A1307	A1230	A1161	A1088	U1008	U945	U872
G1970	C1893	A1821	G1756	A1684	G1611	A1527	G1453	A1379	A1308	A1230	G1162	U1089	C1010	C946	
G1971	C1894	A1822	G1757	A1685	C1612	A1528	G1454	U1383	U1309	U1234	U1163	U1086	G1011	U947	A875
U1972	C1824	C1824	U1758	C1686	G1614	U1531	C1456	C1384	U1310		U1164	U1097	G1012	G948	A876
A1973	U1825	G1686	A1759	C1687	A1615	U1531	C1456		G1311		G1165	A1097	A1012		A877
G1974	C1826	G1688	G1760	G1688	A1616	G1535	A1458	G1387	G1312	C1238	A1166	A1098	A1013	A951	G878
C1975	G1827	A1827	A1761	A1689	G1617	C1536	A1459	U1388	A1313	C1239	G1167	U1099	A1014	G952	G879
U1905	G1828	C1762	C1762	U1689	C1618	U1536	G1460	G1389	U1314		C1168	G1100	C1015	G953	
A1909	C1829	C1692	C1763	C1692	A1619	U1544	G1461	A1390	G1316	A1242	U1170	C1102	U1016	U954	A882
A1910	U1830	C1764	C1764		C1620	C1545	C1462	A1391		C1243	A1171	C1103		A955	U883
G1979	U1831	G1765	G1765	G1695	G1621	C1546	U1463	A1392	G1323	U1244	G1172	C1104	G1024	A957	G882
U1980	G1832	A1767	A1766	G1697	G1622	U1547	U1463		G1324	C1245	A1173	C1105	G1025	A958	G885
A1981	C1834	C1768	U1698	U1698	C1623	A1548	A1465		G1325	A1246	A1174	C1106	U1026	C959	G887
C1988	U1835	C1769	C1769		A1624	C1549		C1396	C1326		G1175	U1109	U1029	G960	U888
G1989	U1919	A1770	U1770	A1701	U1625	C1549	U1473	C1397	G1327	U1249	G1176	U1110	U1030	A961	C890
	C1920	U1772	U1772	U1702	A1626	C1554	C1474	A1399	A1328	C1251		U1111	G1031	C962	
U1992	A1921	G1773	G1773	G1703	G1627	G1555	G1475	C1400	G1331	A1252	C1179	U1112	A1032	C963	C893
C1993	A1922	G1774	G1774	G1704	A1630	G1556	U1476		C1332	C1253	A1180	G1113	G1031	G964	A894
A1994	G1923	C1775	C1775	U1558	A1631	C1557	U1477	A1407	U1333	C1254	A1181	G1114	U1041	A965	A895
G1995	A1924	G1776	G1776	U1559	A1632	U1559	U1478	U1408	U1334	C1256	C1183	U1115		G968	C896
U1996	C1844	G1707	G1707	U1561	G1633	U1561	C1483	G1409	C1335	C1257	C1184	U1116	G1044	G969	A897
	A1845			U1561	G1634		G1484			G1258	U1185	A1117	G1045	U970	G898
C1999	U1927	U1946	A1778	U1935	U1636	C1566	A1485	U1412	U1338	A1259	C1186	A1118	U1046	G	G899
G2000	C1928	A1847	A1779	C1566	G1636	G1567	A1486	G1415	G1339	A1261	A1187	U1120	U1047	U	
C2001	G1929	G1780	G1780	G1567			U1488	G1416	C1342	C1262	A1189	G1121	G1051	G	G902
C2002	A1930	C1714	C1714	C1570	U1639	C1570	A1482	U1419	C1343	C1268	A1191	A1124	G1052	C	C905
U2003	C1931	A1715	A1716	A1571	C1640	G1571	A1493	C1420	G1344	G1269	A1192	U1125	G1053	G	G906
U2004	G1932	G1785	G1785	A1572	A1641	C1572	U1493	U1347	U1347	C1273	A1193	C1126	G1055	C	A907
G2005	C1933	C1786	C1786	A1573	A1642	A1573	A1496	U1422	U1348	C1273	A1194	C1127	U1056	C	A908
C2006	A1934	G1787	G1787	C1574	C1643	A1574	G1497	C1423	G1349	A1274	G1195	U1128	A1057	U	C910
A2007	C1935	U1724	U1724	C1575	U1645	C1575	G1498	A1424	U1350	C1275	C1196	U1129	A1058	C	G911
U2008	G1855	G1725	G1725		G1646		G1498		G1351	U1276		U1130	G1059	C	A912
G2009	C1856	C1725	C1725	C1585	G1647	C1585	U1501	A1427	A1352	C1277	C1200	G1131	C1060	G	A913
A2010	A1857	G1728	G1728	G1586	G1648	G1586	A1502	C1428	C1353	A1278	C1201	A1132	C1061	A	
U2011	U1858	A1729	A1729	U1587	G1649	U1587	U1503	U1429	G1354	U1279	A1202	G1133	U1066	G	G918
U2012	C1861	C1730	C1730	G1589	A1656	G1589	A1504	G1430	A1355	G1283	G1203	G1134	A1067	A	U919
G2013	C1862	A1732	A1732	A1590	A1657	A1590	U1505	G1433	A1356	G1284	C1204	G1135	U1067	G	C920
U2016	A1866	A1733	A1733	A1591	A1657	A1591	U1506	G1434	A1357	G1284	U1205	U1136	C1068	G	G921
U2017	G1867	C1734	C1734	G1592	A1661	G1592	C1507	A1434	A1358	G1287	U1206	G1137	C1069	A	A922
A2018	C1868	C1735	C1735	C1593	C1662	C1593	C1508	U1435	A1359	A1287	A1207	G1138	A1070	G	A923
A2022		A1736	A1736	C1594	A1663	C1594	U1509	G1436	C1360	U1288	C1208	U1139	G1071	U	
C2026	U1803	G1739	G1739	G1596	G1665	U1596	U1511	G1438	G1361	C1289	C1209	C1140	A1072	C	A926
U2027	A1804	U1740	U1740	U1597	A1666	A1597	G1512	C1439	U1362	U1283	G1210	U1141	A1073	G	U927
U2028	G1805	U1741	U1741	A1598	A1667	A1598	C1513	U1440	G1364	A1294	C1212	C1142	G1074	C	
G2032	C1806	G1742	G1742	U1599	U1668	U1599	C1514	G1441	C1365	G1295	C1213	U1149	G1075	A	U932
U2033	U1807	G1743	G1743	G1600	A1673	G1600	A1514	A1442	C1366	A1296	G1214	A1150	G1076	C	C933
G2034	A1881	G1744	G1744	G1601	U1673	G1601	U1516	A1443	A1367	U1297	A1215	G1151	A1077	C	G934
C2035	C1882	G1745	G1745	C1602	C1675	A1602	C1517	G1444	U1368	G1298	G1216	A1152	C1078	A	G935
C2036	U1813	A1746	A1746	A1603	G1676	A1603	A1518	G1445	U1369	G1299	C1217	C1153	A1079	C	G938
C2037	G1814	A1747	A1747	G1604	G1676	G1604	A1518	U1446	A1372	G1300	U1218	G1156	A1081	U1001	A939
A2038	A1815	U1748	U1748	G1605	A1677	G1605	C1521	U1447			U1219	C1157	C1082	G1002	G940
U2039	C1816	U1749	U1749	A1606	A1678	A1606	A1522	A1448	A1375	C1303	C1220	G1158	C1084	G	U942
	U1817			G1523	C1679	A1607	G1523	G1449			G1221			A1005	




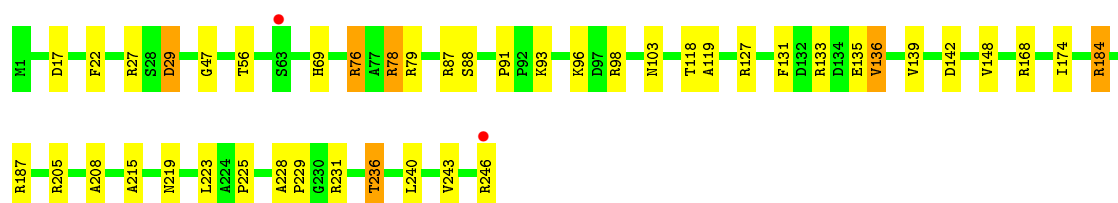
- Molecule 3: 50S ribosomal protein L3P

Chain B:  81% 17%



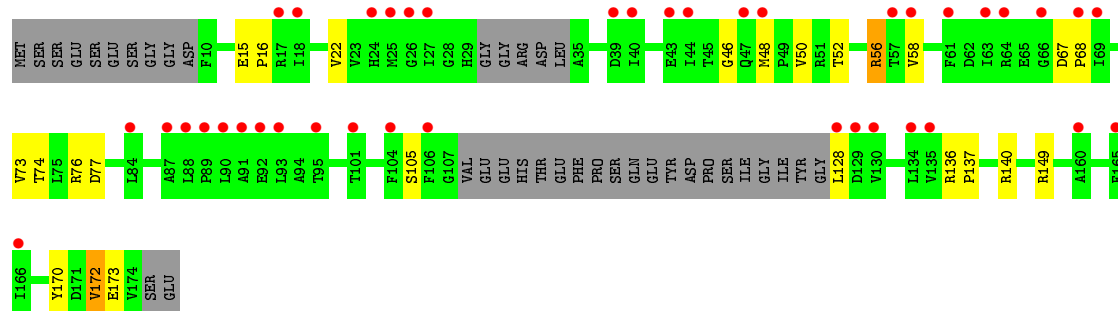
- Molecule 4: 50S ribosomal protein L4P

Chain C:  82% 15%




- Molecule 5: 50S ribosomal protein L5P

Chain D:  23% 66% 12% 21%




- Molecule 6: 50S ribosomal protein L6P

Chain E:  2% 83% 16%



- Molecule 7: 50S ribosomal protein L7Ae

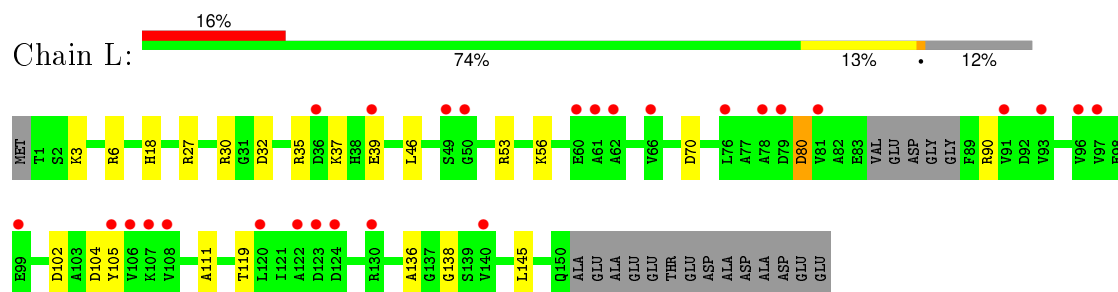
Chain F:  8% 85% 15%



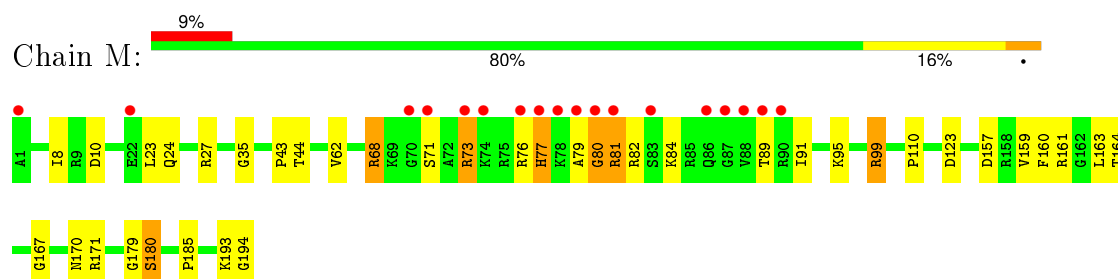
- Molecule 8: 50S ribosomal protein L10



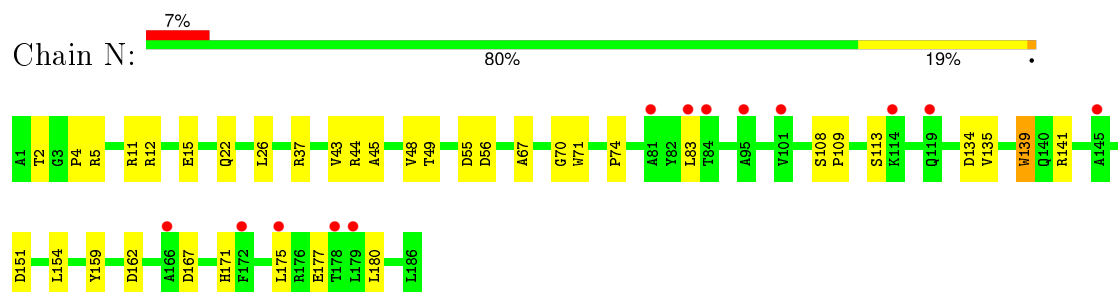
- Molecule 13: 50S ribosomal protein L15P



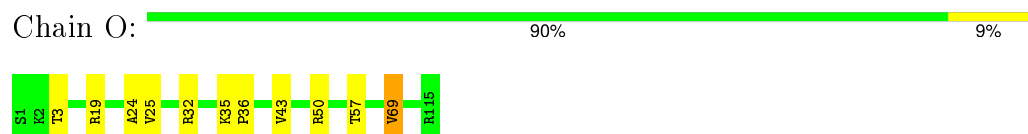
- Molecule 14: 50S ribosomal protein L15e



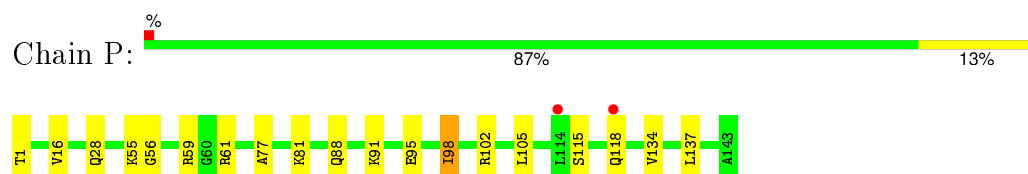
- Molecule 15: 50S ribosomal protein L18P



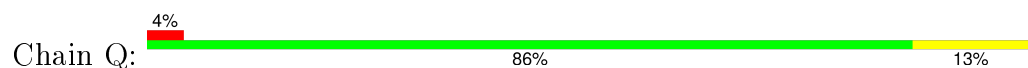
- Molecule 16: 50S ribosomal protein L18e



- Molecule 17: 50S ribosomal protein L19e

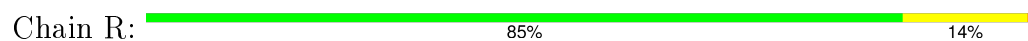


- Molecule 18: 50S ribosomal protein L21e

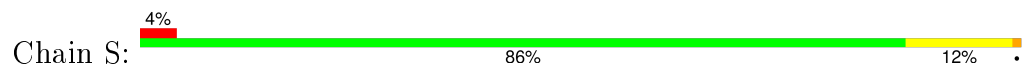




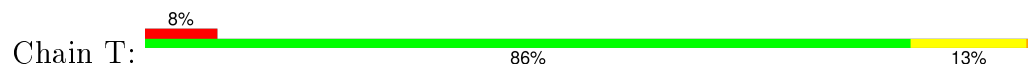
- Molecule 19: 50S ribosomal protein L22P



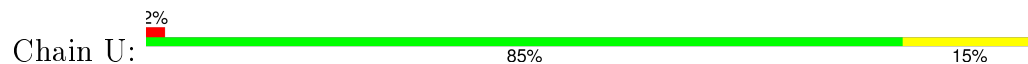
- Molecule 20: 50S ribosomal protein L23P



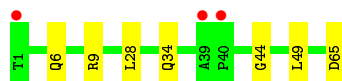
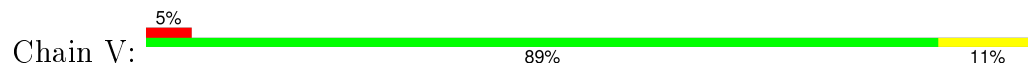
- Molecule 21: 50S ribosomal protein L24P



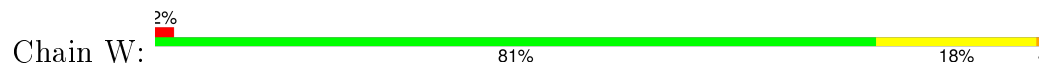
- Molecule 22: 50S ribosomal protein L24e



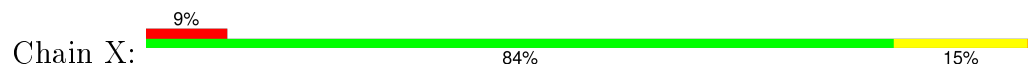
- Molecule 23: 50S ribosomal protein L29P

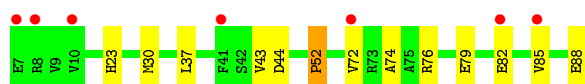


- Molecule 24: 50S ribosomal protein L30P

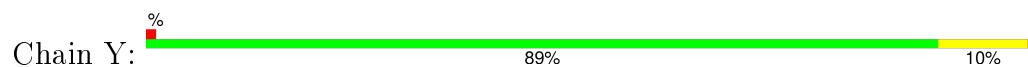


- Molecule 25: 50S ribosomal protein L31e

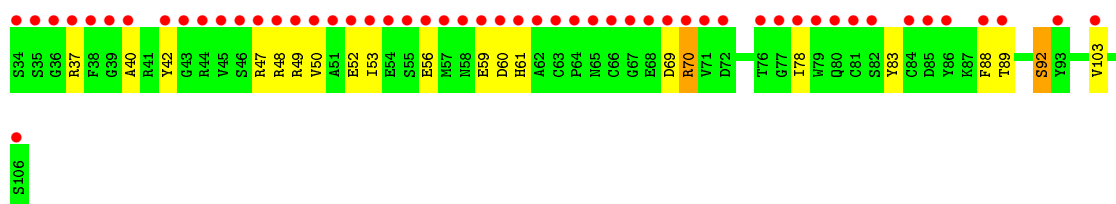




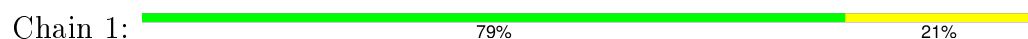
- Molecule 26: 50S ribosomal protein L32e



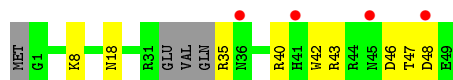
- Molecule 27: 50S ribosomal protein L37Ae



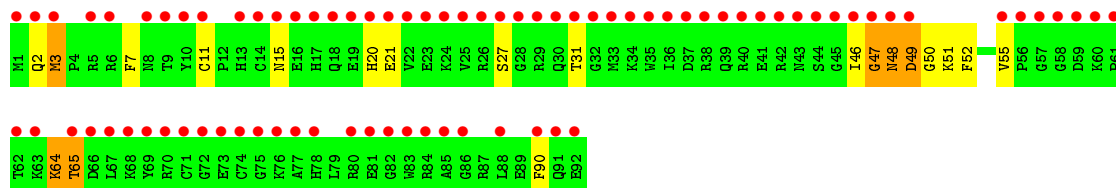
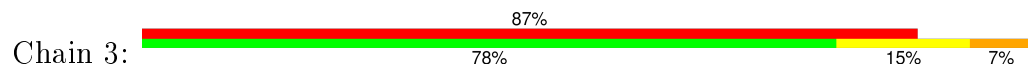
- Molecule 28: 50S ribosomal protein L37e



- Molecule 29: 50S ribosomal protein L39e

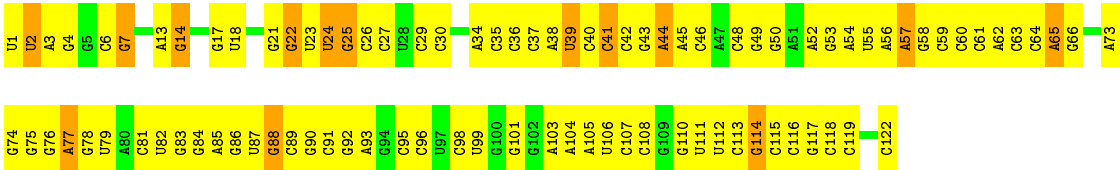


- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 5S ribosomal RNA







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.27Å 299.84Å 574.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.20 85.66 – 2.41	Depositor EDS
% Data completeness (in resolution range)	83.7 (49.84-3.20) 82.8 (85.66-2.41)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.215 , 0.290 0.200 , 0.263	Depositor DCC
$R_{free}$ test set	2920 reflections (1.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 119.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 667047 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	99167	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, MUL, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.47	0/65958	0.69	6/102869 (0.0%)
2	A	0.53	0/1787	0.77	0/2408
3	B	0.54	0/2690	0.77	1/3652 (0.0%)
4	C	0.56	0/1885	0.80	0/2552
5	D	0.70	0/1111	0.74	1/1498 (0.1%)
6	E	0.62	0/1383	0.71	0/1880
7	F	0.56	0/901	0.73	1/1224 (0.1%)
8	G	0.55	0/241	0.66	0/324
9	H	0.61	0/1302	0.78	0/1743
10	I	0.63	0/527	0.66	0/716
11	J	0.63	0/1136	0.75	0/1530
12	K	0.51	0/1004	0.78	0/1351
13	L	0.56	0/1130	0.77	0/1509
14	M	0.55	0/1583	0.79	1/2116 (0.0%)
15	N	0.60	0/1474	0.79	0/1999
16	O	0.52	0/874	0.77	0/1181
17	P	0.56	0/1148	0.69	0/1528
18	Q	0.53	0/749	0.74	0/1005
19	R	0.58	0/1173	0.74	0/1578
20	S	0.56	0/649	0.70	0/875
21	T	0.50	0/958	0.76	1/1289 (0.1%)
22	U	0.65	0/418	0.72	0/562
23	V	0.49	0/503	0.70	0/675
24	W	0.54	0/1219	0.78	0/1655
25	X	0.53	0/665	0.74	0/895
26	Y	0.55	0/1147	0.76	0/1536
27	Z	0.74	0/585	0.84	0/781
28	1	0.62	0/438	0.77	0/578
29	2	0.46	0/401	0.74	0/529
30	3	0.78	0/771	0.81	0/1024
31	9	0.38	0/2904	0.68	0/4526
All	All	0.50	0/98714	0.71	11/147588 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	25
24	W	0	1
All	All	0	26

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1504	A	N9-C1'-C2'	6.64	122.64	114.00
1	0	237	G	N9-C1'-C2'	-6.25	105.12	112.00
3	B	84	LEU	CA-CB-CG	5.84	128.74	115.30
1	0	871	G	C5'-C4'-O4'	-5.68	102.28	109.10
1	0	820	G	N9-C1'-C2'	5.65	121.34	114.00
7	F	118	LEU	CA-CB-CG	5.64	128.28	115.30
1	0	2726	U	N1-C1'-C2'	5.45	121.09	114.00
5	D	170	TYR	N-CA-C	5.31	125.34	111.00
21	T	52	ARG	N-CA-C	5.24	125.14	111.00
1	0	755	G	O4'-C4'-C3'	-5.17	98.83	104.00
14	M	80	GLY	N-CA-C	5.08	125.79	113.10

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1096	U	Sidechain
1	0	1119	G	Sidechain
1	0	1458	A	Sidechain
1	0	1635	U	Sidechain
1	0	1696	U	Sidechain
1	0	1706	G	Sidechain
1	0	1736	A	Sidechain
1	0	1817	U	Sidechain
1	0	1819	G	Sidechain
1	0	1878	G	Sidechain
1	0	1879	U	Sidechain
1	0	2492	U	Sidechain
1	0	2631	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	2726	U	Sidechain
1	0	2782	G	Sidechain
1	0	436	A	Sidechain
1	0	462	A	Sidechain
1	0	471	G	Sidechain
1	0	49	A	Sidechain
1	0	493	U	Sidechain
1	0	517	U	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	753	U	Sidechain
1	0	864	U	Sidechain
24	W	90	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	1915	0
2	A	1754	0	1766	26	0
3	B	2625	0	2533	37	0
4	C	1860	0	1813	32	0
5	D	1094	0	1085	12	0
6	E	1358	0	1266	12	0
7	F	890	0	843	7	0
8	G	240	0	231	1	0
9	H	1282	0	1292	12	0
10	I	520	0	500	6	0
11	J	1120	0	1098	16	0
12	K	994	0	1027	20	0
13	L	1118	0	1076	13	0
14	M	1559	0	1573	32	0
15	N	1445	0	1401	20	0
16	O	865	0	873	9	0
17	P	1137	0	1123	17	0
18	Q	735	0	729	9	0
19	R	1150	0	1122	15	0
20	S	642	0	605	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	T	950	0	924	13	0
22	U	411	0	368	3	0
23	V	500	0	511	3	0
24	W	1196	0	1137	25	0
25	X	655	0	653	6	0
26	Y	1131	0	1133	10	0
27	Z	574	0	535	15	0
28	1	431	0	426	8	0
29	2	396	0	413	6	0
30	3	755	0	732	16	0
31	9	2599	0	1325	113	0
32	0	84	0	0	0	0
32	2	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	1	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	2	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	91	0	0	0	0
36	1	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	3	2	0	0	0	0
36	9	2	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	L	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	34	0	47	17	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5940	0	0	278	0
39	1	55	0	0	0	0
39	2	48	0	0	1	0
39	3	62	0	0	1	0
39	9	152	0	0	12	0
39	A	125	0	0	3	0
39	B	140	0	0	2	0
39	C	158	0	0	3	0
39	D	45	0	0	1	0
39	E	42	0	0	0	0
39	F	26	0	0	2	0
39	G	18	0	0	0	0
39	H	70	0	0	1	0
39	I	4	0	0	0	0
39	J	47	0	0	1	0
39	K	58	0	0	0	0
39	L	94	0	0	4	0
39	M	132	0	0	1	0
39	N	55	0	0	1	0
39	O	43	0	0	1	0
39	P	59	0	0	0	0
39	Q	52	0	0	0	0
39	R	80	0	0	0	0
39	S	30	0	0	1	0
39	T	30	0	0	0	0
39	U	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	V	11	0	0	0	0
39	W	59	0	0	0	0
39	X	22	0	0	0	0
39	Y	105	0	0	1	0
39	Z	30	0	0	2	0
All	All	99167	0	59972	2229	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 15.

All (2229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:H8	1:0:871:G:H5'	1.00	1.13
1:0:1160:G:H5'	1:0:1161:A:H5'	1.28	1.13
1:0:2121:G:H4'	30:3:47:GLY:HA2	1.29	1.12
1:0:2717:C:H2'	1:0:2718:C:H5''	1.27	1.12
1:0:871:G:C8	1:0:871:G:H5'	1.88	1.08
31:9:56:A:H2'	31:9:57:A:H5''	1.33	1.07
1:0:2717:C:C2'	1:0:2718:C:H5''	1.86	1.06
1:0:541:C:H2'	1:0:542:A:H5''	1.45	0.98
31:9:76:G:H3'	31:9:77:A:H5''	1.44	0.98
1:0:506:G:H22	1:0:509:A:H5''	1.28	0.97
31:9:92:G:H2'	31:9:93:A:C8	2.00	0.96
1:0:910:C:H3'	39:0:5899:HOH:O	1.71	0.91
1:0:1205:U:H2'	1:0:1206:U:H5'	1.52	0.91
31:9:73:A:H61	31:9:108:C:H42	1.19	0.90
1:0:1166:A:H61	1:0:1180:U:H3	1.15	0.90
1:0:541:C:C2'	1:0:542:A:H5''	1.99	0.90
1:0:1778:A:H2'	1:0:1779:A:H5'	1.53	0.89
1:0:500:G:H21	19:R:98:ASN:HD21	1.20	0.89
12:K:18:ILE:HG22	12:K:93:ASN:HD22	1.38	0.88
1:0:1973:A:H2'	1:0:1974:G:O4'	1.72	0.88
1:0:821:U:H3'	39:0:8403:HOH:O	1.73	0.88
1:0:1667:A:H8	1:0:1667:A:H5'	1.37	0.87
1:0:506:G:H22	1:0:509:A:C5'	1.87	0.87
1:0:1603:A:H5'	1:0:1605:G:O4'	1.75	0.86
1:0:2415:A:H2'	1:0:2416:G:H5'	1.57	0.86
1:0:1762:C:H2'	1:0:1763:C:H6	1.41	0.85
1:0:1116:U:HO2'	1:0:1118:A:H2	0.85	0.85
1:0:1474:C:H6	1:0:1474:C:H5'	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1701:A:H4'	1:0:1702:U:H5''	1.57	0.84
1:0:1455:C:O2	1:0:1455:C:H2'	1.78	0.84
1:0:2469:A:H1'	39:0:7426:HOH:O	1.77	0.84
1:0:101:C:H2'	1:0:102:A:H8	1.43	0.84
1:0:2502:C:H2'	1:0:2503:A:H5'	1.60	0.84
1:0:2073:G:H5''	39:0:8459:HOH:O	1.75	0.84
1:0:195:C:H2'	1:0:196:G:H5'	1.59	0.84
1:0:1585:C:H2'	1:0:1586:G:H8	1.42	0.83
1:0:545:G:H8	1:0:545:G:H5'	1.41	0.83
1:0:1125:U:H2'	1:0:1126:C:H5'	1.61	0.83
1:0:1544:U:H2'	1:0:1545:C:H6	1.44	0.83
1:0:681:G:N3	1:0:681:G:H5'	1.93	0.83
1:0:1165:G:H1'	1:0:1174:A:H1'	1.60	0.82
1:0:2764:C:H2'	1:0:2765:C:H6	1.45	0.82
1:0:2716:G:H5''	3:B:206:THR:HG21	1.62	0.82
1:0:101:C:H2'	1:0:102:A:C8	2.14	0.81
14:M:24:GLN:NE2	14:M:27:ARG:HH11	1.77	0.81
1:0:213:G:H22	1:0:225:G:H2'	1.45	0.81
1:0:2472:C:O2'	1:0:2634:G:H4'	1.80	0.81
31:9:14:G:H5'	31:9:14:G:H8	1.45	0.81
15:N:141:ARG:NH2	31:9:48:C:H4'	1.96	0.81
1:0:154:C:H2'	1:0:155:C:H6	1.46	0.81
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.44	0.81
1:0:557:C:H42	1:0:600:G:H1	1.29	0.81
15:N:37:ARG:NH1	31:9:6:C:H5''	1.96	0.81
1:0:663:C:H5''	4:C:103:ASN:HD22	1.44	0.80
37:0:9101:MUL:H163	37:0:9101:MUL:C21	2.11	0.80
1:0:1800:G:H1'	17:P:88:GLN:NE2	1.97	0.80
1:0:2102:G:H2'	39:0:7719:HOH:O	1.82	0.79
1:0:2088:C:H2'	1:0:2089:A:H8	1.47	0.79
1:0:2703:A:H2'	1:0:2704:C:H6	1.45	0.79
1:0:2533:C:H5'	1:0:2533:C:H6	1.46	0.79
1:0:870:G:H2'	1:0:871:G:H5''	1.65	0.79
1:0:559:U:H5'	1:0:559:U:H6	1.48	0.79
1:0:156:C:H5''	14:M:171:ARG:HD3	1.64	0.78
1:0:2502:C:C2'	1:0:2503:A:H5'	2.13	0.78
31:9:56:A:C2'	31:9:57:A:H5''	2.11	0.78
1:0:1585:C:H2'	1:0:1586:G:C8	2.17	0.78
1:0:1447:U:H3'	1:0:1506:U:O2	1.83	0.78
1:0:1596:U:H2'	1:0:1598:A:OP2	1.83	0.78
1:0:1300:G:H1'	39:0:3448:HOH:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:110:C:H1'	39:0:6248:HOH:O	1.83	0.78
1:0:2505:G:O2'	1:0:2506:A:H5'	1.84	0.78
1:0:663:C:H5''	4:C:103:ASN:ND2	1.98	0.78
1:0:625:U:H5''	1:0:1044:C:N4	1.98	0.78
1:0:1160:G:C5'	1:0:1161:A:H5'	2.11	0.77
1:0:2816:A:H5''	1:0:2817:G:H5'	1.64	0.77
1:0:541:C:H2'	1:0:542:A:C5'	2.15	0.77
31:9:24:U:H3'	31:9:25:G:H5'	1.65	0.77
1:0:2712:G:H5'	39:0:4183:HOH:O	1.85	0.77
1:0:2264:A:H4'	39:0:4146:HOH:O	1.85	0.77
1:0:2248:C:H2'	1:0:2249:G:H8	1.47	0.77
14:M:24:GLN:HE21	14:M:27:ARG:HH11	1.29	0.77
1:0:213:G:N2	1:0:225:G:H2'	2.00	0.76
17:P:115:SER:H	17:P:118:GLN:HE21	1.32	0.76
1:0:447:A:O2'	1:0:448:G:H5'	1.85	0.76
1:0:308:U:H2'	21:T:52:ARG:NH2	1.99	0.76
1:0:2289:G:O2'	1:0:2290:U:H5'	1.86	0.76
1:0:694:A:H2'	1:0:695:C:H5'	1.67	0.76
31:9:92:G:H2'	31:9:93:A:H8	1.49	0.76
37:0:9101:MUL:H10	37:0:9101:MUL:H14	1.68	0.76
1:0:1372:A:H3'	39:0:6923:HOH:O	1.86	0.76
1:0:2270:G:H4'	2:A:223:ARG:HH12	1.49	0.75
1:0:1160:G:H5'	1:0:1161:A:C5'	2.12	0.75
1:0:1444:G:O2'	1:0:1445:G:H5'	1.86	0.75
1:0:659:A:H5''	39:O:6799:HOH:O	1.86	0.75
1:0:2466:G:H5''	39:0:8275:HOH:O	1.85	0.75
1:0:1167:G:H1	1:0:1179:C:H42	1.35	0.75
1:0:1171:A:H2'	1:0:1172:G:H5'	1.67	0.75
1:0:2371:G:H5'	39:0:3898:HOH:O	1.87	0.75
1:0:170:U:H5'	30:3:48:ASN:HD22	1.51	0.75
1:0:2780:C:H1'	6:E:143:GLN:HE21	1.51	0.75
1:0:542:A:H5'	1:0:542:A:H8	1.52	0.74
1:0:1116:U:O2'	1:0:1118:A:H2	1.67	0.74
1:0:2326:C:H2'	1:0:2327:A:H8	1.52	0.74
1:0:188:C:H5''	14:M:163:LEU:HD21	1.69	0.74
1:0:1684:A:H1'	29:2:43:ARG:HH22	1.53	0.74
1:0:2059:U:H2'	1:0:2060:A:H8	1.52	0.74
1:0:1485:A:H1'	39:0:3502:HOH:O	1.88	0.73
1:0:424:C:H2'	1:0:425:U:H6	1.53	0.73
1:0:2253:G:H2'	1:0:2254:G:H8	1.53	0.73
1:0:1692:C:H3'	39:0:8632:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1351:G:H3'	39:0:4782:HOH:O	1.87	0.73
31:9:29:C:H2'	31:9:30:C:H5'	1.70	0.73
12:K:10:GLN:H	12:K:10:GLN:NE2	1.86	0.73
1:0:1829:A:H2'	1:0:1830:C:H5'	1.71	0.73
1:0:146:U:O2'	1:0:147:G:H5'	1.89	0.73
1:0:1132:A:N6	1:0:1229:C:H2'	2.04	0.73
1:0:2326:C:H2'	1:0:2327:A:C8	2.24	0.73
1:0:2372:A:H2'	1:0:2373:U:H6	1.54	0.73
1:0:21:G:H4'	19:R:2:ILE:HG22	1.71	0.73
1:0:1701:A:H5'	39:0:5659:HOH:O	1.88	0.73
1:0:625:U:H3'	39:0:7470:HOH:O	1.87	0.72
1:0:2534:C:H1'	39:0:8122:HOH:O	1.87	0.72
1:0:2426:G:H5'	39:0:3025:HOH:O	1.89	0.72
1:0:136:C:H2'	1:0:137:U:O4'	1.89	0.72
1:0:327:A:H4'	1:0:329:A:C8	2.25	0.72
1:0:281:U:H2'	1:0:282:C:O4'	1.90	0.72
1:0:2616:G:H1'	39:0:8273:HOH:O	1.90	0.72
1:0:561:G:H2'	1:0:562:A:H8	1.55	0.72
39:D:3839:HOH:O	31:9:58:G:H1'	1.90	0.72
1:0:92:G:H4'	23:V:44:GLY:HA3	1.72	0.71
1:0:1159:G:H2'	1:0:1160:G:O4'	1.90	0.71
1:0:381:G:H5''	39:0:2945:HOH:O	1.91	0.71
1:0:905:C:H3'	39:0:4139:HOH:O	1.89	0.71
1:0:1377:C:H6	1:0:1377:C:H5'	1.55	0.71
1:0:1118:A:H3'	1:0:1118:A:C8	2.25	0.71
1:0:290:C:H1'	39:0:5406:HOH:O	1.89	0.71
1:0:2005:G:H3'	1:0:2005:G:OP2	1.91	0.71
1:0:12:U:H2'	1:0:13:G:H5'	1.70	0.71
1:0:1165:G:H21	1:0:1173:A:H5''	1.54	0.71
1:0:2637:A:H4'	39:0:3790:HOH:O	1.90	0.71
1:0:1303:C:O2	1:0:1353:C:H1'	1.90	0.71
1:0:2269:C:H2'	1:0:2270:G:O4'	1.91	0.71
1:0:282:C:H1'	1:0:368:C:N4	2.06	0.71
1:0:870:G:C2'	1:0:871:G:H5''	2.21	0.70
1:0:2059:U:H2'	1:0:2060:A:C8	2.26	0.70
1:0:1883:U:H5''	1:0:2013:G:OP2	1.90	0.70
31:9:24:U:H3'	31:9:25:G:C5'	2.20	0.70
1:0:1451:C:H5'	1:0:1505:U:C5	2.26	0.70
27:Z:60:ASP:HB3	27:Z:69:ASP:HB3	1.73	0.70
1:0:1673:U:H4'	39:S:1504:HOH:O	1.90	0.70
1:0:2271:G:H5'	39:0:3548:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1741:U:H5'	1:0:1742:A:OP1	1.91	0.70
1:0:2758:G:H2'	1:0:2759:C:C6	2.26	0.70
1:0:282:C:O2'	1:0:283:U:H5'	1.90	0.70
1:0:671:A:O2'	1:0:672:G:H2'	1.92	0.70
1:0:2710:U:H1'	39:0:7520:HOH:O	1.92	0.70
1:0:2312:G:H2'	1:0:2313:C:H5'	1.73	0.70
1:0:2461:U:O2	1:0:2466:G:H1'	1.91	0.70
1:0:1873:G:H3'	39:0:4169:HOH:O	1.91	0.70
1:0:221:G:H5''	39:0:4894:HOH:O	1.91	0.70
1:0:1130:U:H2'	1:0:1131:G:O4'	1.92	0.69
1:0:2758:G:H2'	1:0:2759:C:H6	1.56	0.69
1:0:432:G:H5''	39:0:6484:HOH:O	1.92	0.69
31:9:39:U:H3'	31:9:40:C:C5'	2.22	0.69
1:0:1347:U:H2'	1:0:1348:A:C8	2.26	0.69
1:0:2050:G:H5''	19:R:80:TYR:O	1.91	0.69
1:0:1205:U:C2'	1:0:1206:U:H5'	2.22	0.69
1:0:1682:A:O2'	1:0:1683:G:H5''	1.93	0.69
1:0:2563:U:HO2'	1:0:2564:G:H8	1.40	0.69
1:0:1186:C:H42	1:0:1190:G:H22	1.39	0.69
1:0:73:U:H2'	1:0:74:G:C8	2.28	0.69
1:0:1120:U:H5'	1:0:1121:G:OP2	1.92	0.69
1:0:1189:A:H3'	39:0:7609:HOH:O	1.92	0.69
1:0:1118:A:H3'	1:0:1118:A:H8	1.56	0.69
1:0:1856:C:H5'	1:0:1858:A:O4'	1.92	0.68
1:0:1790:C:H2'	1:0:1791:U:C6	2.28	0.68
1:0:1278:A:H4'	1:0:1279:U:C4	2.28	0.68
1:0:137:U:H2'	1:0:139:C:C5	2.29	0.68
1:0:2584:G:H4'	39:0:6824:HOH:O	1.92	0.68
1:0:2894:C:O2'	1:0:2895:C:H5'	1.94	0.68
1:0:1793:C:H2'	1:0:1793:C:O2	1.92	0.68
1:0:399:C:H5'	14:M:179:GLY:O	1.93	0.68
12:K:10:GLN:H	12:K:10:GLN:HE21	1.39	0.68
1:0:1838:U:O2'	1:0:2644:C:H5'	1.92	0.68
1:0:2812:A:H2	1:0:2814:A:H62	1.41	0.68
1:0:191:A:H2'	1:0:237:G:O6	1.93	0.68
1:0:2726:U:H5''	1:0:2749:U:H3	1.59	0.68
1:0:1120:U:H5''	1:0:1120:U:C6	2.29	0.68
1:0:2430:A:H4'	13:L:46:LEU:O	1.94	0.68
1:0:1589:G:H22	1:0:1605:G:H1'	1.58	0.68
1:0:558:C:C2'	1:0:559:U:H5''	2.24	0.68
1:0:1574:C:H2'	1:0:1575:C:H6	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1097:A:H5''	24:W:125:HIS:NE2	2.08	0.67
1:0:500:G:N2	19:R:98:ASN:HD21	1.92	0.67
1:0:2416:G:H2'	1:0:2417:C:C6	2.29	0.67
1:0:1118:A:H62	1:0:1244:U:H3	1.41	0.67
31:9:114:G:H2'	31:9:115:C:C6	2.29	0.67
1:0:2372:A:H2'	1:0:2373:U:C6	2.28	0.67
1:0:1882:C:OP1	2:A:192:VAL:HG23	1.94	0.67
1:0:1104:C:H4'	11:J:88:PRO:HD3	1.76	0.67
1:0:2332:A:H5'	5:D:56:ARG:HH22	1.58	0.67
1:0:119:A:H2'	1:0:120:A:H5''	1.77	0.67
1:0:1126:C:H6	1:0:1126:C:O5'	1.77	0.67
1:0:169:A:H1'	30:3:48:ASN:ND2	2.09	0.67
13:L:27:ARG:HH21	13:L:30:ARG:HE	1.42	0.67
1:0:2365:G:H4'	18:Q:45:PRO:O	1.95	0.67
1:0:2787:C:H5	39:0:3383:HOH:O	1.77	0.67
1:0:1829:A:H61	27:Z:42:TYR:HA	1.59	0.67
1:0:1544:U:H2'	1:0:1545:C:C6	2.28	0.66
1:0:2712:G:H1'	39:0:5039:HOH:O	1.95	0.66
1:0:2032:U:H2'	1:0:2033:G:H5''	1.76	0.66
1:0:318:U:H5'	1:0:339:A:C2	2.29	0.66
1:0:2578:G:H5'	1:0:2578:G:H8	1.59	0.66
1:0:171:C:H3'	39:0:5555:HOH:O	1.94	0.66
31:9:52:A:H2'	31:9:53:G:O4'	1.95	0.66
1:0:1667:A:C8	1:0:1667:A:H5'	2.26	0.66
1:0:1047:U:H5'	39:0:5458:HOH:O	1.94	0.66
1:0:622:G:O2'	1:0:623:U:H5'	1.95	0.66
1:0:713:U:H6	1:0:713:U:O5'	1.79	0.66
1:0:1268:C:O2'	1:0:1269:G:H5'	1.96	0.66
1:0:2498:C:O2'	1:0:2499:U:H5'	1.96	0.66
1:0:1209:C:H2'	1:0:1210:G:H8	1.59	0.66
1:0:1589:G:N2	1:0:1605:G:H1'	2.10	0.66
1:0:2506:A:O2'	1:0:2507:G:H8	1.77	0.66
1:0:848:C:H5'	39:0:7034:HOH:O	1.95	0.66
9:H:59:GLN:NE2	9:H:129:ARG:HE	1.94	0.66
1:0:2433:A:O5'	1:0:2433:A:H8	1.79	0.66
1:0:2904:U:H2'	1:0:2905:A:H8	1.61	0.66
15:N:141:ARG:HH21	31:9:48:C:H4'	1.61	0.66
1:0:877:G:H5'	1:0:878:G:OP1	1.95	0.66
1:0:183:A:H1'	14:M:161:ARG:NH1	2.11	0.66
1:0:683:G:H5''	39:0:4020:HOH:O	1.95	0.66
1:0:2296:C:H2'	1:0:2297:U:C6	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1679:C:H5'	39:0:4044:HOH:O	1.95	0.65
1:0:1743:G:H1'	39:0:3739:HOH:O	1.96	0.65
31:9:34:A:H2'	31:9:35:C:O4'	1.95	0.65
1:0:886:A:H1'	39:0:3891:HOH:O	1.95	0.65
1:0:2488:A:H1'	39:0:3221:HOH:O	1.96	0.65
1:0:1181:A:H2'	1:0:1182:C:H5'	1.76	0.65
1:0:1412:U:O4	1:0:1681:G:H2'	1.97	0.65
1:0:1165:G:O3'	1:0:1174:A:H4'	1.96	0.65
1:0:316:A:N3	1:0:336:G:O2'	2.29	0.65
1:0:2415:A:C2'	1:0:2416:G:H5'	2.25	0.65
1:0:1762:C:H2'	1:0:1763:C:C6	2.28	0.65
1:0:2088:C:H2'	1:0:2089:A:C8	2.32	0.65
1:0:1114:A:O2'	1:0:1115:U:H5'	1.96	0.65
31:9:3:A:N6	31:9:22:G:H1'	2.11	0.65
1:0:338:C:H3'	39:0:8434:HOH:O	1.96	0.65
1:0:1735:C:O2'	1:0:1736:A:H5'	1.96	0.65
1:0:431:G:H5'	39:0:7692:HOH:O	1.97	0.65
1:0:545:G:C8	1:0:545:G:H5'	2.29	0.64
1:0:2486:A:H2	37:0:9101:MUL:H221	1.63	0.64
1:0:2010:A:H2'	39:0:5197:HOH:O	1.97	0.64
1:0:1728:G:H1'	39:0:5467:HOH:O	1.96	0.64
1:0:200:C:H2'	39:0:7991:HOH:O	1.97	0.64
31:9:104:A:O2'	31:9:105:A:H5'	1.97	0.64
1:0:1626:A:H2'	1:0:1627:G:O4'	1.98	0.64
35:0:8812:CL:CL	39:0:4058:HOH:O	2.50	0.64
1:0:450:C:OP1	4:C:184:ARG:NH2	2.31	0.64
1:0:1819:G:H2'	1:0:1820:G:H4'	1.78	0.64
14:M:79:ALA:HB3	14:M:81:ARG:HH12	1.63	0.64
1:0:1015:C:H2'	1:0:1016:U:H6	1.61	0.64
1:0:932:U:O2'	1:0:1296:A:H1'	1.97	0.64
1:0:702:G:O2'	1:0:703:G:H5'	1.97	0.64
1:0:2769:C:H2'	1:0:2770:G:O4'	1.98	0.64
1:0:558:C:H2'	1:0:559:U:H5''	1.79	0.64
1:0:1307:A:H2'	1:0:1308:A:C8	2.33	0.64
1:0:2748:G:H2'	39:0:7410:HOH:O	1.98	0.64
1:0:1559:A:H1'	39:0:5067:HOH:O	1.97	0.64
1:0:1595:G:O2'	1:0:1596:U:H5'	1.98	0.64
1:0:1308:A:H4'	4:C:225:PRO:O	1.98	0.64
1:0:1483:C:O2'	1:0:1484:G:H5'	1.98	0.64
1:0:1921:A:O2'	1:0:1922:A:H5'	1.97	0.64
1:0:2898:G:H4'	3:B:288:GLY:HA2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2524:G:H21	1:0:2526:C:N4	1.96	0.64
1:0:1139:U:H2'	1:0:1140:C:C6	2.32	0.64
1:0:1184:C:H1'	39:0:7308:HOH:O	1.98	0.64
1:0:73:U:H2'	1:0:74:G:H8	1.61	0.64
1:0:1115:U:H2'	1:0:1116:U:H6	1.63	0.63
4:C:127:ARG:NH2	4:C:225:PRO:HG2	2.12	0.63
1:0:837:U:H4'	39:0:7940:HOH:O	1.98	0.63
1:0:1771:U:H1'	27:Z:47:ARG:HH21	1.62	0.63
1:0:1276:U:H3'	16:O:19:ARG:HH11	1.63	0.63
1:0:2032:U:H5''	39:0:6193:HOH:O	1.98	0.63
1:0:2526:C:O2'	1:0:2527:U:H5'	1.98	0.63
1:0:2320:U:H2'	30:3:2:GLN:O	1.98	0.63
1:0:444:C:H1'	39:0:8745:HOH:O	1.97	0.63
1:0:506:G:N2	1:0:509:A:H5''	2.08	0.63
1:0:1181:A:C2'	1:0:1182:C:H5'	2.27	0.63
1:0:958:G:H4'	31:9:105:A:H4'	1.80	0.63
1:0:1307:A:H2'	1:0:1308:A:H8	1.63	0.63
1:0:2819:C:H4'	3:B:97:LEU:O	1.98	0.63
31:9:98:C:H2'	31:9:99:U:H6	1.62	0.63
1:0:2472:C:H3'	39:0:8235:HOH:O	1.98	0.63
1:0:1061:C:H3'	39:0:4002:HOH:O	1.99	0.63
1:0:2740:G:H2'	1:0:2741:A:O4'	1.99	0.63
3:B:7:ARG:HH12	3:B:11:LEU:HD22	1.63	0.63
1:0:2332:A:H3'	1:0:2333:G:H8	1.64	0.63
1:0:1593:C:H2'	1:0:1594:C:H6	1.64	0.63
1:0:432:G:H2'	1:0:433:C:H6	1.62	0.63
1:0:1523:G:H2'	1:0:1524:U:C6	2.34	0.63
1:0:1183:C:H2'	39:0:5603:HOH:O	1.98	0.63
3:B:221:GLN:HE22	12:K:42:ASN:HD22	1.46	0.63
1:0:2256:G:H2'	1:0:2257:G:H5'	1.81	0.62
14:M:43:PRO:HG3	14:M:62:VAL:HG21	1.81	0.62
1:0:1127:C:H2'	1:0:1128:U:H5'	1.81	0.62
1:0:2714:U:H2'	1:0:2715:G:H8	1.64	0.62
1:0:1204:C:H2'	1:0:1205:U:O4'	1.99	0.62
1:0:613:C:H2'	1:0:614:U:H6	1.63	0.62
1:0:221:G:H2'	1:0:222:A:C8	2.33	0.62
1:0:2607:U:OP2	3:B:243:ASN:HB2	1.99	0.62
1:0:451:C:O2'	1:0:452:G:H5'	1.99	0.62
1:0:1220:U:H2'	1:0:1221:G:H8	1.64	0.62
1:0:219:G:H5'	1:0:220:C:H5''	1.82	0.62
37:0:9101:MUL:H263	37:0:9101:MUL:H201	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:109:U:H2'	1:0:109:U:O2	2.00	0.62
1:0:1805:G:O2'	1:0:1806:G:H5'	1.99	0.62
1:0:2314:G:O2'	1:0:2315:C:H5'	2.00	0.62
31:9:84:G:H2'	31:9:85:A:H8	1.64	0.62
1:0:1931:A:H2'	1:0:1932:G:H5'	1.81	0.62
1:0:935:G:H4'	39:0:7674:HOH:O	1.98	0.62
1:0:1139:U:H2'	1:0:1140:C:H6	1.63	0.62
1:0:1125:U:C2'	1:0:1126:C:H5'	2.29	0.62
1:0:69:A:H5'	1:0:69:A:C8	2.35	0.62
1:0:2433:A:H2	1:0:2458:U:H3	1.46	0.62
1:0:2769:C:C2'	1:0:2770:G:H5'	2.30	0.62
1:0:2887:G:H2'	1:0:2888:U:C6	2.34	0.62
1:0:1211:G:O2'	1:0:1212:C:H5'	1.99	0.62
1:0:1554:C:H1'	1:0:1632:A:H1'	1.82	0.62
1:0:1162:G:H1'	10:I:112:LEU:HD11	1.80	0.62
14:M:77:HIS:HD2	14:M:81:ARG:H	1.47	0.62
1:0:1213:C:O2'	1:0:1214:G:H5'	2.00	0.62
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.82	0.61
1:0:1008:C:H5''	9:H:19:ARG:HH12	1.63	0.61
1:0:646:G:H2'	1:0:647:U:C6	2.35	0.61
1:0:2896:A:N3	1:0:2896:A:H2'	2.15	0.61
1:0:1474:C:C6	1:0:1474:C:H5'	2.30	0.61
1:0:1391:G:H2'	1:0:1392:A:H5'	1.81	0.61
1:0:812:A:H2'	1:0:813:C:C6	2.36	0.61
1:0:2781:U:H1'	6:E:139:GLU:OE2	2.00	0.61
31:9:39:U:H3	31:9:42:C:H5''	1.64	0.61
21:T:41:ARG:HH21	21:T:67:LEU:HD21	1.64	0.61
1:0:857:A:H4'	2:A:176:HIS:CD2	2.35	0.61
1:0:1333:U:H2'	1:0:1334:C:H6	1.65	0.61
1:0:907:A:H2'	1:0:908:A:H8	1.65	0.61
1:0:1701:A:H4'	1:0:1702:U:C5'	2.27	0.61
1:0:2373:U:H1'	39:0:3565:HOH:O	2.01	0.61
1:0:178:U:H2'	1:0:179:C:H6	1.66	0.61
1:0:106:A:O2'	1:0:107:U:H5'	2.00	0.61
1:0:1527:A:H1'	1:0:1528:A:C8	2.35	0.61
14:M:27:ARG:HH22	14:M:44:THR:HG23	1.65	0.61
1:0:1347:U:H2'	1:0:1348:A:H8	1.63	0.61
1:0:183:A:C2	1:0:184:G:C4	2.88	0.61
1:0:1014:A:H5''	31:9:101:G:O2'	1.99	0.61
1:0:2627:G:H5'	39:0:3864:HOH:O	2.00	0.61
1:0:1051:C:H2'	1:0:1052:G:O4'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2295:G:N3	1:0:2361:A:H2	1.97	0.61
1:0:2426:G:H1'	39:0:5391:HOH:O	2.00	0.61
1:0:1202:A:H2'	1:0:1203:G:O4'	2.01	0.61
1:0:2486:A:C2	37:0:9101:MUL:H221	2.36	0.61
1:0:1279:U:O2	1:0:1279:U:H2'	1.98	0.61
31:9:105:A:H2'	31:9:106:U:O4'	2.01	0.61
1:0:852:U:H3'	39:0:8226:HOH:O	1.99	0.61
1:0:2041:G:O2'	1:0:2042:U:H5'	2.00	0.61
31:9:13:A:O2'	31:9:14:G:H5''	2.01	0.61
1:0:195:C:C2'	1:0:196:G:H5'	2.31	0.60
1:0:2248:C:H3'	39:0:4476:HOH:O	2.00	0.60
1:0:146:U:C2'	1:0:147:G:H5'	2.31	0.60
7:F:30:LYS:HB2	7:F:97:ALA:HB3	1.83	0.60
1:0:312:U:O2'	1:0:313:U:H5'	2.01	0.60
1:0:327:A:H4'	1:0:329:A:N7	2.15	0.60
1:0:1398:G:H2'	1:0:1399:A:H8	1.64	0.60
1:0:2548:C:H5'	3:B:252:PRO:HD2	1.83	0.60
1:0:1516:U:H2'	1:0:1517:C:O4'	2.01	0.60
1:0:287:C:H42	1:0:365:G:H1	1.49	0.60
1:0:185:G:O3'	1:0:186:A:H4'	2.00	0.60
5:D:76:ARG:NH2	31:9:44:A:H1'	2.15	0.60
1:0:1761:U:H5'	17:P:81:LYS:O	2.01	0.60
1:0:2122:C:H1'	14:M:76:ARG:HH21	1.66	0.60
37:0:9101:MUL:S1	37:0:9101:MUL:H271	2.42	0.60
1:0:2714:U:H2'	1:0:2715:G:C8	2.36	0.60
1:0:854:G:H8	39:0:8680:HOH:O	1.82	0.60
31:9:116:C:O2'	31:9:117:G:H5'	2.01	0.60
1:0:542:A:H5'	1:0:542:A:C8	2.35	0.60
1:0:1972:U:H2'	1:0:1973:A:H5'	1.83	0.60
1:0:1590:A:H1'	1:0:1606:A:C2	2.36	0.60
1:0:2385:G:H2'	1:0:2386:U:C6	2.37	0.60
1:0:1641:A:H2'	1:0:1642:A:O4'	2.01	0.60
1:0:1916:C:H2'	1:0:1917:G:H8	1.65	0.60
24:W:88:THR:HG23	24:W:110:GLN:HB3	1.83	0.60
1:0:280:C:H2'	1:0:281:U:O4'	2.02	0.60
1:0:2032:U:H2'	1:0:2033:G:C5'	2.31	0.60
1:0:2065:C:H4'	39:0:7923:HOH:O	2.01	0.60
1:0:333:G:O2'	1:0:334:G:H5'	2.02	0.60
1:0:24:G:N2	1:0:518:G:H1'	2.17	0.60
1:0:1299:G:N7	13:L:6:ARG:NH1	2.49	0.60
1:0:2769:C:O2'	1:0:2770:G:H5'	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1455:C:O2	1:0:1455:C:C2'	2.50	0.60
1:0:1398:G:H2'	1:0:1399:A:C8	2.36	0.60
1:0:630:A:H3'	39:0:5239:HOH:O	2.01	0.60
31:9:56:A:H2'	31:9:57:A:C5'	2.22	0.59
1:0:2248:C:H2'	1:0:2249:G:C8	2.34	0.59
1:0:2296:C:H2'	1:0:2297:U:H6	1.67	0.59
1:0:1255:A:H3'	39:0:6875:HOH:O	2.02	0.59
1:0:1276:U:H3'	16:O:19:ARG:NH1	2.18	0.59
1:0:105:G:O2'	1:0:106:A:H5'	2.02	0.59
1:0:1711:A:H3'	39:0:5721:HOH:O	2.02	0.59
12:K:23:ASN:ND2	12:K:108:GLU:H	2.00	0.59
1:0:1119:G:H5'	11:J:52:GLN:NE2	2.17	0.59
1:0:557:C:N4	1:0:600:G:H1	1.99	0.59
1:0:69:A:H5'	1:0:69:A:H8	1.66	0.59
1:0:1806:G:C6	1:0:1807:U:N3	2.70	0.59
1:0:1313:A:H5'	26:Y:208:LYS:O	2.01	0.59
1:0:308:U:H5'	1:0:309:C:OP1	2.03	0.59
1:0:2270:G:H4'	2:A:223:ARG:NH1	2.17	0.59
1:0:1632:A:H2'	1:0:1633:C:H5'	1.83	0.59
1:0:2324:G:H1'	39:0:5418:HOH:O	2.02	0.59
1:0:2402:A:H8	1:0:2402:A:O5'	1.86	0.59
1:0:2502:C:H2'	1:0:2503:A:C5'	2.33	0.59
1:0:595:U:H2'	1:0:596:C:H6	1.68	0.59
1:0:2828:G:O5'	1:0:2828:G:H8	1.85	0.59
1:0:820:G:H5'	1:0:821:U:H5'	1.83	0.59
1:0:2345:A:H3'	1:0:2346:C:C5	2.37	0.59
1:0:790:A:H1'	1:0:1710:A:H2'	1.85	0.59
1:0:1167:G:H2'	1:0:1168:C:C6	2.38	0.59
31:9:39:U:H1'	31:9:44:A:H61	1.68	0.59
31:9:37:C:O2'	31:9:38:A:H5'	2.03	0.59
1:0:1797:A:H4'	1:0:1798:C:C5	2.38	0.59
27:Z:59:GLU:HG2	27:Z:60:ASP:H	1.68	0.59
1:0:1015:C:H2'	1:0:1016:U:C6	2.38	0.59
1:0:2783:A:H3'	39:0:4201:HOH:O	2.02	0.59
1:0:244:C:H6	1:0:244:C:O5'	1.85	0.59
1:0:871:G:C8	1:0:871:G:C5'	2.77	0.58
1:0:558:C:H2'	1:0:559:U:C5'	2.33	0.58
1:0:1677:U:OP2	29:2:8:LYS:NZ	2.35	0.58
1:0:1790:C:H2'	1:0:1791:U:H6	1.69	0.58
1:0:2332:A:H3'	1:0:2333:G:C8	2.38	0.58
1:0:2827:A:H2'	1:0:2828:G:O4'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.85	0.58
1:0:1666:C:H2'	1:0:1667:A:C8	2.39	0.58
1:0:1921:A:H2'	1:0:1922:A:O4'	2.03	0.58
1:0:29:C:O2'	1:0:30:U:H5'	2.03	0.58
1:0:1803:C:H2'	1:0:1804:A:C8	2.37	0.58
1:0:553:G:H2'	1:0:554:G:H5'	1.86	0.58
1:0:1055:G:N2	1:0:1057:A:H3'	2.18	0.58
1:0:1931:A:C2'	1:0:1932:G:H5'	2.34	0.58
1:0:1889:C:O2'	1:0:1890:U:H5'	2.03	0.58
1:0:2433:A:H1'	39:0:7055:HOH:O	2.03	0.58
1:0:2635:A:O2'	1:0:2636:C:H5'	2.03	0.58
1:0:2748:G:H5'	39:0:7410:HOH:O	2.04	0.58
1:0:2531:U:H4'	39:0:5083:HOH:O	2.04	0.58
22:U:49:LEU:HD12	39:U:3805:HOH:O	2.02	0.58
1:0:1504:A:H4'	1:0:1506:U:C5	2.39	0.58
1:0:2768:A:H2'	1:0:2769:C:C6	2.39	0.58
1:0:164:G:H3'	39:0:8274:HOH:O	2.03	0.58
1:0:2831:C:H2'	1:0:2832:C:O4'	2.03	0.58
1:0:2410:G:H1'	39:0:7571:HOH:O	2.03	0.58
1:0:1375:A:H2'	1:0:1376:G:H5'	1.86	0.58
1:0:306:A:P	21:T:38:ARG:HH21	2.27	0.58
1:0:1163:G:OP2	1:0:1164:U:H3'	2.04	0.57
1:0:2507:G:H2'	1:0:2510:C:N4	2.19	0.57
1:0:1787:C:O2'	1:0:1788:U:H5'	2.04	0.57
1:0:1769:C:O2'	1:0:1770:U:H5'	2.02	0.57
1:0:2016:U:H2'	1:0:2017:U:O4'	2.04	0.57
1:0:822:C:O2	1:0:822:C:H2'	2.03	0.57
1:0:1057:A:H1'	1:0:2492:U:O2'	2.04	0.57
1:0:735:C:N4	30:3:15:ASN:HD21	2.03	0.57
1:0:1421:C:H2'	1:0:1422:U:H6	1.68	0.57
1:0:2312:G:C2'	1:0:2313:C:H5'	2.34	0.57
1:0:1309:U:O2'	1:0:1310:U:H5'	2.04	0.57
1:0:2613:G:O2'	1:0:2614:C:H5'	2.04	0.57
1:0:1477:C:H5'	1:0:1868:G:H5'	1.86	0.57
1:0:1446:U:H2'	20:S:55:GLN:NE2	2.20	0.57
9:H:32:ALA:H	9:H:69:ARG:HH12	1.51	0.57
1:0:2691:A:OP1	1:0:2691:A:H8	1.86	0.57
1:0:872:U:H3'	39:0:3723:HOH:O	2.05	0.57
1:0:1119:G:H2'	11:J:52:GLN:NE2	2.15	0.57
1:0:2005:G:O2'	1:0:2008:U:OP2	2.15	0.57
1:0:664:U:O2'	1:0:665:A:H5'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1201:C:H2'	1:0:1202:A:H5'	1.86	0.57
1:0:236:A:H4'	1:0:237:G:H5'	1.86	0.57
1:0:2385:G:H2'	1:0:2386:U:H6	1.68	0.57
1:0:2241:C:O2'	1:0:2242:U:H5'	2.04	0.57
24:W:52:VAL:HG22	24:W:53:ALA:H	1.69	0.57
1:0:2449:G:H2'	1:0:2450:C:C6	2.40	0.57
1:0:2676:C:H4'	11:J:70:PHE:CD1	2.40	0.57
1:0:2054:A:H4'	19:R:135:ALA:O	2.05	0.57
1:0:73:U:O2'	1:0:74:G:H5'	2.04	0.57
1:0:2378:U:H4'	39:0:3392:HOH:O	2.04	0.57
1:0:67:A:N1	1:0:109:U:H1'	2.19	0.57
1:0:2777:G:H1'	39:0:6143:HOH:O	2.04	0.57
1:0:705:C:H3'	1:0:706:G:H8	1.69	0.57
1:0:152:A:H1'	1:0:440:C:O2'	2.05	0.57
1:0:1634:G:H2'	1:0:1635:U:C6	2.39	0.57
1:0:2717:C:H2'	1:0:2718:C:C5'	2.18	0.57
1:0:1182:C:H1'	1:0:1192:A:H8	1.69	0.57
1:0:790:A:H8	39:0:5403:HOH:O	1.87	0.57
1:0:111:C:H2'	1:0:112:G:O4'	2.05	0.57
1:0:581:G:O2'	1:0:582:U:H5'	2.05	0.57
1:0:2505:G:C2'	1:0:2506:A:H5'	2.35	0.57
1:0:1829:A:C2'	1:0:1830:C:H5'	2.34	0.57
1:0:2904:U:H2'	1:0:2905:A:C8	2.40	0.57
1:0:39:G:C2	1:0:444:C:C2	2.93	0.57
1:0:343:C:H2'	1:0:344:C:H6	1.69	0.57
1:0:2336:G:H1	1:0:2348:C:H42	1.53	0.57
1:0:152:A:O2'	1:0:153:C:H5'	2.05	0.57
1:0:2673:U:C4	1:0:2674:G:C6	2.93	0.57
1:0:2735:U:H2'	1:0:2736:U:C6	2.39	0.57
1:0:2533:C:C6	1:0:2533:C:H5'	2.35	0.56
1:0:2241:C:H2'	1:0:2242:U:C6	2.40	0.56
1:0:566:A:H2'	1:0:567:U:H5'	1.86	0.56
4:C:139:VAL:HG13	39:C:6251:HOH:O	2.04	0.56
1:0:1106:A:O5'	1:0:1106:A:H8	1.87	0.56
1:0:1183:C:N4	1:0:1184:C:H41	2.03	0.56
1:0:1477:C:H5'	1:0:1868:G:C5'	2.35	0.56
1:0:2676:C:H4'	11:J:70:PHE:CE1	2.41	0.56
1:0:2689:A:H2'	1:0:2690:U:H5'	1.86	0.56
1:0:1697:G:H1'	39:0:7038:HOH:O	2.06	0.56
1:0:1383:U:H2'	1:0:1384:C:C6	2.40	0.56
1:0:1617:C:C5	1:0:1643:C:H4'	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2388:C:O2'	1:0:2389:U:H5'	2.05	0.56
1:0:1894:C:N4	1:0:1939:U:H2'	2.20	0.56
1:0:1175:G:O2'	1:0:1193:A:H2'	2.05	0.56
1:0:1165:G:H21	1:0:1173:A:C5'	2.17	0.56
1:0:2432:C:H4'	39:0:5597:HOH:O	2.05	0.56
1:0:2500:C:O2'	1:0:2501:G:H5'	2.05	0.56
1:0:2820:A:H2'	1:0:2821:C:O4'	2.05	0.56
1:0:619:U:H3'	39:0:7549:HOH:O	2.05	0.56
1:0:10:U:O4	1:0:532:A:OP2	2.22	0.56
1:0:348:C:H2'	1:0:349:U:H6	1.69	0.56
1:0:1555:G:H4'	1:0:1630:A:H2	1.70	0.56
1:0:182:G:H5'	39:0:4102:HOH:O	2.04	0.56
31:9:29:C:C2'	31:9:30:C:H5'	2.35	0.56
1:0:345:G:N2	1:0:346:U:H1'	2.21	0.56
1:0:1081:A:H5''	39:0:7126:HOH:O	2.05	0.56
3:B:179:LEU:O	3:B:183:GLU:HG2	2.06	0.56
31:9:82:U:H5''	39:9:123:HOH:O	2.05	0.56
1:0:1163:G:H5'	10:I:110:ASP:O	2.06	0.56
1:0:12:U:C2'	1:0:13:G:H5'	2.35	0.56
1:0:221:G:H2'	1:0:222:A:H8	1.71	0.56
3:B:7:ARG:NH2	3:B:11:LEU:HD13	2.21	0.56
1:0:95:A:H5''	1:0:97:G:O4'	2.06	0.56
1:0:814:G:N2	1:0:815:U:H1'	2.21	0.56
1:0:25:A:O2'	1:0:640:G:H5'	2.05	0.56
1:0:814:G:H2'	1:0:815:U:C6	2.41	0.56
1:0:1759:A:N3	1:0:1818:C:H2'	2.21	0.56
1:0:1877:G:H5''	39:0:6762:HOH:O	2.05	0.56
1:0:171:C:O2'	1:0:172:U:H5'	2.06	0.56
31:9:104:A:C2'	31:9:105:A:H5'	2.35	0.56
1:0:2439:C:H5'	39:0:4534:HOH:O	2.06	0.56
1:0:154:C:O2'	1:0:155:C:H5'	2.06	0.56
20:S:33:SER:O	20:S:37:VAL:HG23	2.06	0.56
1:0:1369:A:H5'	39:0:7798:HOH:O	2.06	0.56
1:0:636:G:H5'	1:0:2059:U:OP2	2.06	0.56
1:0:834:G:H3'	1:0:835:U:H4'	1.87	0.56
15:N:159:TYR:HE1	31:9:50:G:H5''	1.70	0.56
1:0:2751:C:H3'	39:0:7028:HOH:O	2.05	0.56
31:9:55:U:H4'	31:9:56:A:C8	2.41	0.55
1:0:1167:G:H1	1:0:1179:C:N4	2.03	0.55
1:0:1554:C:C1'	1:0:1632:A:H1'	2.36	0.55
1:0:2831:C:C2'	1:0:2832:C:H5'	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:159:VAL:HG12	35:M:8818:CL:CL	2.43	0.55
1:0:1242:A:H5'	11:J:82:THR:HG23	1.87	0.55
1:0:738:G:N2	1:0:2384:U:H4'	2.21	0.55
1:0:1099:G:H2'	1:0:1100:G:O4'	2.05	0.55
1:0:2670:G:O2'	1:0:2671:U:H5'	2.05	0.55
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.55
1:0:2256:G:C2'	1:0:2257:G:H5'	2.36	0.55
7:F:77:VAL:HG21	7:F:83:LEU:HD13	1.88	0.55
1:0:189:A:OP1	14:M:171:ARG:NH2	2.38	0.55
1:0:2781:U:O2'	1:0:2782:G:H5'	2.06	0.55
5:D:140:ARG:HB3	31:9:29:C:H5''	1.89	0.55
1:0:2768:A:H2'	1:0:2769:C:H6	1.72	0.55
1:0:68:U:O2'	1:0:69:A:H5''	2.07	0.55
1:0:226:A:H1'	1:0:393:G:N7	2.21	0.55
1:0:2906:A:H5'	1:0:2907:C:O4'	2.06	0.55
1:0:2716:G:H5'	3:B:262:ARG:HG3	1.88	0.55
1:0:1119:G:N2	1:0:1246:A:C2	2.74	0.55
1:0:612:U:H2'	1:0:613:C:C6	2.41	0.55
1:0:2782:G:O6	1:0:2790:C:H5''	2.06	0.55
1:0:290:C:O2'	1:0:291:C:H5'	2.06	0.55
1:0:338:C:H4'	4:C:174:ILE:CD1	2.36	0.55
1:0:1030:U:H5'	39:0:3468:HOH:O	2.05	0.55
1:0:1420:C:O2	1:0:1420:C:H2'	2.07	0.55
1:0:414:C:O2'	1:0:415:A:H5'	2.07	0.55
1:0:696:C:H2'	1:0:697:G:O4'	2.06	0.55
1:0:2868:C:H1'	39:0:6832:HOH:O	2.07	0.55
1:0:897:A:H2'	1:0:899:C:C5	2.42	0.55
1:0:2397:G:H2'	1:0:2398:A:H8	1.72	0.55
1:0:2465:A:H1'	39:0:3104:HOH:O	2.05	0.55
1:0:1441:G:H1'	39:0:7717:HOH:O	2.06	0.55
1:0:1784:U:O2'	1:0:1812:G:H2'	2.06	0.55
1:0:2506:A:O2'	1:0:2507:G:C8	2.56	0.55
12:K:23:ASN:HD21	12:K:108:GLU:H	1.54	0.55
1:0:2274:A:O2'	1:0:2275:G:H5'	2.07	0.55
1:0:355:C:H1'	39:0:3088:HOH:O	2.06	0.55
19:R:66:VAL:HG22	19:R:79:ARG:NH1	2.22	0.55
1:0:128:A:H3'	1:0:128:A:C8	2.41	0.55
1:0:1816:C:H6	1:0:1816:C:O5'	1.89	0.55
1:0:962:C:H2'	1:0:963:C:H5'	1.87	0.55
1:0:517:U:H2'	1:0:518:G:H5'	1.89	0.55
1:0:1850:U:H2'	1:0:1851:G:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:849:C:H2'	1:0:850:U:O4'	2.07	0.55
1:0:159:G:H1	1:0:175:G:HO2'	1.53	0.55
1:0:466:A:H2'	1:0:467:G:O4'	2.06	0.55
1:0:2764:C:H2'	1:0:2765:C:C6	2.33	0.55
1:0:1745:G:H22	1:0:2033:G:H5'	1.71	0.55
1:0:414:C:H2'	1:0:415:A:O4'	2.06	0.55
1:0:2071:C:H5'	39:0:4847:HOH:O	2.07	0.55
1:0:1159:G:H21	1:0:1189:A:H8	1.55	0.55
1:0:2431:C:H2'	1:0:2432:C:O4'	2.07	0.55
1:0:125:U:H2'	39:0:8398:HOH:O	2.07	0.55
17:P:98:ILE:HD12	17:P:102:ARG:NE	2.21	0.55
1:0:819:A:H5'	27:Z:37:ARG:HD2	1.89	0.55
1:0:1189:A:H1'	1:0:1209:C:O4'	2.07	0.55
1:0:2072:G:H3'	1:0:2073:G:C5'	2.37	0.55
14:M:27:ARG:NH2	14:M:44:THR:HG23	2.21	0.55
31:9:61:C:H2'	31:9:62:A:H8	1.72	0.55
1:0:2654:C:O2'	1:0:2655:U:H5'	2.07	0.55
39:0:4183:HOH:O	12:K:39:GLY:HA2	2.07	0.54
1:0:35:U:O2'	1:0:36:C:H5'	2.07	0.54
1:0:1167:G:H3'	39:0:7346:HOH:O	2.07	0.54
15:N:11:ARG:HD3	31:9:114:G:O6	2.08	0.54
1:0:1835:U:H5	1:0:1840:A:N7	2.06	0.54
1:0:1928:C:H2'	1:0:1929:G:O4'	2.07	0.54
6:E:137:ASP:O	6:E:141:VAL:HG23	2.06	0.54
1:0:1166:A:P	1:0:1174:A:H4'	2.46	0.54
1:0:1333:U:H2'	1:0:1334:C:C6	2.41	0.54
1:0:312:U:C2	1:0:320:G:N2	2.75	0.54
1:0:151:A:H2'	1:0:152:A:O4'	2.07	0.54
1:0:1783:A:O2'	1:0:1784:U:H5'	2.07	0.54
1:0:676:C:O2'	4:C:219:ASN:ND2	2.33	0.54
1:0:420:U:H3	1:0:2447:A:H61	1.56	0.54
1:0:250:C:H2'	1:0:251:C:H6	1.73	0.54
1:0:1010:C:H4'	15:N:4:PRO:HB2	1.89	0.54
1:0:2506:A:HO2'	1:0:2507:G:H8	1.49	0.54
1:0:1120:U:H6	1:0:1120:U:H5''	1.73	0.54
1:0:2321:A:H2	1:0:2378:U:H3	1.51	0.54
1:0:313:U:C2'	1:0:314:G:H5'	2.37	0.54
1:0:2781:U:C2'	1:0:2782:G:H5'	2.37	0.54
1:0:1016:U:H1'	39:0:8289:HOH:O	2.06	0.54
1:0:2422:U:H5'	39:0:5459:HOH:O	2.08	0.54
12:K:29:LEU:HB3	12:K:55:VAL:HG11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:590:A:H2'	1:0:591:A:O4'	2.08	0.54
31:9:76:G:C3'	31:9:77:A:H5''	2.29	0.54
1:0:1666:C:H2'	1:0:1667:A:H5'	1.90	0.54
1:0:1586:G:H1'	39:0:6211:HOH:O	2.07	0.54
1:0:2819:C:H2'	1:0:2820:A:H8	1.72	0.54
1:0:2042:U:H2'	1:0:2043:U:C6	2.42	0.54
1:0:1803:C:H2'	1:0:1804:A:H8	1.72	0.54
1:0:816:G:C6	1:0:817:G:N1	2.75	0.54
1:0:1925:G:O2'	1:0:1926:G:H5'	2.08	0.54
1:0:1730:G:C5'	1:0:1731:C:H6	2.20	0.54
1:0:1571:G:C2'	1:0:1626:A:H61	2.21	0.54
1:0:1387:G:H21	17:P:1:THR:N	2.04	0.54
1:0:1328:A:OP1	26:Y:169:ARG:HD2	2.08	0.54
1:0:2349:G:H2'	1:0:2350:G:H8	1.72	0.54
1:0:1510:G:H2'	1:0:1511:U:O4'	2.08	0.54
1:0:2908:A:H2'	1:0:2909:G:O4'	2.06	0.54
1:0:722:G:H2'	1:0:723:G:H5'	1.88	0.54
1:0:2027:U:O2'	1:0:2028:U:H5'	2.07	0.54
1:0:1747:A:C6	1:0:2035:C:O2	2.61	0.54
1:0:814:G:C2	1:0:815:U:C2	2.95	0.54
1:0:420:U:H1'	39:0:5263:HOH:O	2.07	0.54
1:0:2537:G:H5''	1:0:2538:A:H5''	1.89	0.54
1:0:491:C:N3	1:0:502:A:C2	2.75	0.54
1:0:920:C:H4'	1:0:921:G:C2	2.42	0.54
31:9:73:A:H2'	31:9:74:G:C8	2.43	0.54
1:0:2661:U:H3	1:0:2812:A:H62	1.55	0.54
1:0:2607:U:OP1	1:0:2609:G:H4'	2.07	0.54
1:0:1631:A:H2'	1:0:1632:A:C8	2.43	0.54
1:0:1099:G:P	24:W:129:LYS:HE3	2.48	0.54
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.89	0.54
1:0:2795:C:O2'	1:0:2796:U:H5'	2.07	0.54
1:0:814:G:H4'	39:0:7058:HOH:O	2.08	0.54
1:0:2439:C:H2'	1:0:2440:C:H6	1.73	0.54
1:0:2474:A:N7	1:0:2621:PSU:H4'	2.23	0.54
1:0:1461:U:H2'	1:0:1462:C:C6	2.43	0.54
1:0:847:C:H4'	39:0:8386:HOH:O	2.08	0.54
1:0:2502:C:H4'	9:H:158:ASN:ND2	2.23	0.54
1:0:2726:U:H5''	1:0:2749:U:N3	2.22	0.54
1:0:2898:G:O2'	1:0:2899:A:H5'	2.06	0.54
1:0:293:A:H2'	1:0:294:C:H6	1.73	0.54
31:9:95:C:H2'	31:9:96:C:O4'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:76:G:O5'	31:9:76:G:H8	1.91	0.53
1:0:440:C:H2'	1:0:441:A:C8	2.43	0.53
1:0:2251:G:H2'	1:0:2252:A:C8	2.43	0.53
1:0:310:U:H2'	1:0:311:C:C6	2.43	0.53
1:0:2404:G:H5''	39:0:8706:HOH:O	2.07	0.53
1:0:1187:U:O2'	1:0:1189:A:H2	1.91	0.53
1:0:1244:U:H4'	1:0:1246:A:O4'	2.08	0.53
1:0:2511:A:H2'	1:0:2512:U:O4'	2.08	0.53
1:0:1570:C:H2'	1:0:1571:G:O4'	2.08	0.53
1:0:2256:G:H2'	1:0:2257:G:C5'	2.38	0.53
1:0:907:A:H2'	1:0:908:A:C8	2.43	0.53
1:0:667:C:H2'	1:0:668:C:H6	1.72	0.53
1:0:698:A:H5''	13:L:111:ALA:HB2	1.90	0.53
17:P:105:LEU:HD21	17:P:137:LEU:HD11	1.89	0.53
1:0:2737:C:OP2	17:P:61:ARG:NH2	2.39	0.53
1:0:902:G:N7	13:L:18:HIS:HD2	2.06	0.53
1:0:272:A:H5'	1:0:273:G:OP2	2.07	0.53
1:0:1353:C:H3'	39:0:8238:HOH:O	2.08	0.53
1:0:42:C:OP2	1:0:185:G:H2'	2.08	0.53
27:Z:48:ARG:O	27:Z:52:GLU:HB2	2.09	0.53
37:0:9101:MUL:H163	37:0:9101:MUL:O3	2.09	0.53
1:0:1829:A:H5''	39:0:6825:HOH:O	2.08	0.53
18:Q:26:PRO:O	18:Q:30:VAL:HG23	2.07	0.53
1:0:1438:G:H1'	29:2:42:TRP:HZ2	1.73	0.53
1:0:31:C:O2'	1:0:32:G:H5'	2.08	0.53
1:0:1976:G:H1'	1:0:2005:G:N2	2.23	0.53
1:0:1352:A:H4'	1:0:1353:C:OP1	2.08	0.53
1:0:2508:C:H2'	39:0:6319:HOH:O	2.08	0.53
1:0:1950:G:H2'	1:0:1951:G:H8	1.74	0.53
1:0:869:G:H1'	39:0:7658:HOH:O	2.09	0.53
1:0:2809:G:H2'	1:0:2810:G:O4'	2.07	0.53
1:0:1166:A:N6	1:0:1180:U:H3	1.97	0.53
1:0:669:G:O2'	1:0:670:G:H5'	2.08	0.53
1:0:1427:A:O2'	1:0:1428:C:H5'	2.08	0.53
4:C:142:ASP:OD1	4:C:236:THR:HG23	2.09	0.53
1:0:1430:G:N2	39:0:7999:HOH:O	2.41	0.53
1:0:2486:A:H3'	39:0:3735:HOH:O	2.08	0.53
1:0:1167:G:H4'	10:I:130:LEU:HD21	1.91	0.53
1:0:1171:A:C2'	1:0:1172:G:H5'	2.39	0.53
1:0:139:C:H4'	1:0:140:G:O5'	2.09	0.53
1:0:381:G:H2'	39:0:6358:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1574:C:H2'	1:0:1575:C:C6	2.41	0.53
1:0:2433:A:H2'	1:0:2434:A:C8	2.44	0.53
1:0:2294:C:H42	1:0:2314:G:H1	1.55	0.53
1:0:1398:G:O2'	1:0:1399:A:H5'	2.09	0.53
1:0:23:G:H1'	1:0:520:A:N6	2.22	0.53
1:0:1342:C:H2'	1:0:1343:C:H5'	1.90	0.53
1:0:1423:C:O2'	1:0:1424:A:H5'	2.09	0.53
1:0:1758:U:H6	1:0:1758:U:O5'	1.92	0.53
1:0:2474:A:H4'	1:0:2475:C:O5'	2.08	0.53
1:0:1311:G:H5''	39:0:5005:HOH:O	2.06	0.53
1:0:1053:G:OP1	9:H:15:PRO:HG3	2.08	0.53
1:0:318:U:H5'	1:0:339:A:C4	2.43	0.53
1:0:1817:U:O2	17:P:81:LYS:NZ	2.32	0.53
1:0:1081:A:C6	1:0:1082:A:N1	2.76	0.53
1:0:2586:U:H3	1:0:2592:G:H22	1.55	0.53
24:W:24:LEU:HD21	24:W:44:MET:SD	2.48	0.53
1:0:2617:G:H4'	39:0:3214:HOH:O	2.08	0.53
1:0:1981:A:H3'	39:0:6149:HOH:O	2.09	0.53
1:0:710:G:OP1	16:O:24:ALA:HB3	2.09	0.53
1:0:2387:U:H2'	1:0:2388:C:C6	2.43	0.53
31:9:49:G:O2'	31:9:50:G:H5'	2.08	0.53
1:0:228:C:H2'	1:0:229:G:H5'	1.89	0.53
1:0:2742:G:H5'	39:0:5015:HOH:O	2.07	0.53
1:0:1666:C:H2'	1:0:1667:A:H8	1.72	0.53
1:0:561:G:H2'	1:0:562:A:C8	2.41	0.53
1:0:2563:U:O2'	1:0:2564:G:H8	1.92	0.53
1:0:2240:U:O2'	1:0:2241:C:H5'	2.09	0.53
1:0:2250:G:H2'	1:0:2251:G:O4'	2.08	0.53
1:0:303:C:O2'	1:0:304:G:H5'	2.09	0.53
1:0:2241:C:H2'	1:0:2242:U:H6	1.74	0.52
1:0:523:C:O2'	1:0:524:A:H5'	2.09	0.52
1:0:734:U:H2'	1:0:736:A:OP2	2.09	0.52
1:0:1972:U:H2'	1:0:1973:A:C5'	2.38	0.52
1:0:2089:A:O2'	1:0:2090:G:H5'	2.10	0.52
1:0:1741:U:C4	1:0:2033:G:C8	2.98	0.52
1:0:2026:C:O2'	1:0:2027:U:H5'	2.10	0.52
1:0:1363:G:H1'	39:0:4378:HOH:O	2.08	0.52
1:0:482:G:H4'	1:0:508:A:N1	2.25	0.52
1:0:380:A:H2'	39:0:6974:HOH:O	2.09	0.52
1:0:1011:C:H3'	1:0:1012:A:C8	2.44	0.52
1:0:1460:G:H5'	39:0:3232:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:39:U:N3	31:9:42:C:H5''	2.24	0.52
1:0:2548:C:OP2	3:B:5:ARG:NH2	2.42	0.52
1:0:640:G:O2'	1:0:641:G:H5'	2.08	0.52
1:0:1886:A:H4'	39:Z:395:HOH:O	2.08	0.52
1:0:2018:A:H2	27:Z:40:ALA:O	1.93	0.52
1:0:1438:G:H1'	29:2:42:TRP:CZ2	2.45	0.52
1:0:72:C:H5'	39:0:5110:HOH:O	2.09	0.52
1:0:912:A:C4	1:0:1294:A:C2	2.97	0.52
1:0:656:G:H2'	1:0:657:G:H8	1.75	0.52
1:0:705:C:H2'	1:0:705:C:O2	2.10	0.52
1:0:1363:G:H2'	1:0:1364:G:C8	2.44	0.52
1:0:960:G:H2'	1:0:960:G:N3	2.23	0.52
1:0:1970:G:H1'	39:0:8299:HOH:O	2.08	0.52
3:B:7:ARG:NH1	3:B:11:LEU:HD22	2.24	0.52
1:0:2548:C:H5''	39:0:5919:HOH:O	2.09	0.52
1:0:2345:A:H3'	1:0:2346:C:C6	2.44	0.52
1:0:955:A:H2'	1:0:956:G:O4'	2.10	0.52
1:0:875:A:C2	2:A:194:MET:SD	3.03	0.52
1:0:157:G:H4'	14:M:95:LYS:HE2	1.91	0.52
1:0:1436:C:O2'	1:0:1437:A:H5'	2.10	0.52
1:0:628:1MA:HM11	39:0:3514:HOH:O	2.10	0.52
1:0:809:G:H2'	1:0:810:G:C8	2.45	0.52
1:0:1181:A:H2'	1:0:1182:C:C5'	2.40	0.52
1:0:2790:C:H5'	39:0:8847:HOH:O	2.08	0.52
1:0:1461:U:H2'	1:0:1462:C:H6	1.75	0.52
1:0:710:G:H2'	1:0:711:G:H8	1.74	0.52
1:0:660:A:N6	1:0:746:A:O4'	2.42	0.52
1:0:1359:U:C5	1:0:2101:A:C8	2.98	0.52
1:0:2121:G:H5''	39:0:9100:HOH:O	2.10	0.52
1:0:2718:C:H3'	39:0:6906:HOH:O	2.10	0.52
1:0:1130:U:H5'	39:0:7596:HOH:O	2.10	0.52
1:0:1166:A:H1'	1:0:1192:A:C2	2.45	0.52
1:0:2269:C:O2'	1:0:2270:G:H5'	2.10	0.52
1:0:1688:G:C6	1:0:1692:C:C6	2.98	0.52
1:0:39:G:H2'	1:0:40:C:O4'	2.09	0.52
1:0:1400:C:O2'	1:0:1401:G:H5'	2.08	0.52
1:0:1634:G:H2'	1:0:1635:U:H6	1.75	0.52
1:0:226:A:H1'	1:0:393:G:C5	2.44	0.52
1:0:210:U:O2'	1:0:211:U:H5'	2.10	0.52
1:0:968:G:H2'	1:0:969:G:H8	1.75	0.52
1:0:2703:A:H2'	1:0:2704:C:C6	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:29:C:H2'	31:9:30:C:C5'	2.39	0.52
1:0:640:G:C6	1:0:641:G:N7	2.78	0.52
1:0:1011:C:H3'	1:0:1012:A:H8	1.74	0.52
31:9:119:C:H4'	39:9:2285:HOH:O	2.08	0.52
1:0:1189:A:H1'	1:0:1209:C:C1'	2.39	0.52
1:0:183:A:H1'	14:M:161:ARG:HH11	1.75	0.52
1:0:39:G:O2'	1:0:40:C:H5'	2.10	0.52
1:0:1705:C:P	17:P:59:ARG:HH12	2.33	0.52
1:0:653:U:H2'	1:0:654:A:C8	2.45	0.52
14:M:99:ARG:HE	14:M:170:ASN:HD22	1.57	0.52
1:0:2392:C:H4'	18:Q:55:ARG:HH11	1.75	0.52
1:0:2851:G:O2'	1:0:2852:A:H5'	2.10	0.52
1:0:282:C:H1'	1:0:368:C:H42	1.75	0.51
1:0:284:C:H4'	1:0:285:A:H8	1.75	0.51
1:0:289:G:O2'	1:0:290:C:H5'	2.10	0.51
1:0:2324:G:H4'	1:0:2418:G:O2'	2.09	0.51
1:0:947:U:O2'	1:0:948:G:H5'	2.10	0.51
1:0:685:C:O2	1:0:748:C:H4'	2.11	0.51
31:9:7:G:H5'	39:9:5071:HOH:O	2.09	0.51
12:K:18:ILE:HG22	12:K:93:ASN:ND2	2.18	0.51
1:0:1573:A:H2'	1:0:1574:C:O4'	2.09	0.51
1:0:1736:A:H1'	39:0:7468:HOH:O	2.10	0.51
1:0:1525:G:H5'	1:0:1526:A:OP2	2.11	0.51
1:0:422:G:O2'	1:0:423:A:H5'	2.10	0.51
31:9:86:G:C2	31:9:88:G:C8	2.98	0.51
31:9:98:C:H2'	31:9:99:U:C6	2.43	0.51
1:0:301:C:O2'	1:0:302:A:H5'	2.10	0.51
1:0:1137:G:H1'	39:0:8578:HOH:O	2.10	0.51
31:9:3:A:C8	31:9:26:C:N3	2.78	0.51
1:0:2897:C:O2'	1:0:2898:G:H5'	2.11	0.51
21:T:41:ARG:NH1	21:T:42:VAL:O	2.44	0.51
1:0:968:G:H2'	1:0:969:G:C8	2.45	0.51
1:0:2880:A:H2'	1:0:2881:C:H5'	1.92	0.51
1:0:1023:C:O2'	1:0:1024:G:H5'	2.11	0.51
1:0:1218:U:H2'	1:0:1219:U:C6	2.45	0.51
1:0:593:A:H1'	39:0:8441:HOH:O	2.10	0.51
1:0:1044:C:H5''	39:0:2991:HOH:O	2.10	0.51
1:0:1445:G:N2	1:0:1678:A:H1'	2.26	0.51
1:0:45:A:H5''	1:0:47:G:H5'	1.92	0.51
1:0:120:A:H2'	1:0:120:A:N3	2.26	0.51
1:0:1375:A:C2'	1:0:1376:G:H5'	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:441:A:H1'	1:0:442:A:N7	2.25	0.51
1:0:1928:C:C4	1:0:1929:G:N7	2.78	0.51
1:0:2586:U:H3	1:0:2592:G:H1	1.58	0.51
1:0:2851:G:H2'	1:0:2902:A:H61	1.76	0.51
2:A:199:HIS:HD2	2:A:201:PHE:H	1.57	0.51
1:0:1706:G:C5	1:0:1707:G:C6	2.99	0.51
1:0:2748:G:H1'	39:0:7865:HOH:O	2.10	0.51
1:0:2065:C:O2'	1:0:2066:C:H5'	2.10	0.51
31:9:81:C:O2'	31:9:82:U:H5'	2.11	0.51
1:0:2909:G:O2'	1:0:2910:A:H5'	2.11	0.51
1:0:772:G:H2'	1:0:773:A:O4'	2.11	0.51
15:N:83:LEU:HD13	15:N:175:LEU:HD23	1.93	0.51
1:0:2481:G:H3'	39:0:3932:HOH:O	2.10	0.51
1:0:47:G:H1'	1:0:114:A:N1	2.24	0.51
1:0:2499:U:H2'	1:0:2500:C:C6	2.46	0.51
1:0:2821:C:H4'	3:B:116:PRO:HG3	1.91	0.51
31:9:84:G:H4'	39:9:4718:HOH:O	2.11	0.51
1:0:1332:C:H2'	1:0:1333:U:H6	1.75	0.51
1:0:706:G:N2	1:0:707:C:H41	2.09	0.51
1:0:1069:C:H4'	1:0:1081:A:O2'	2.10	0.51
2:A:167:LYS:HE3	27:Z:50:VAL:HG13	1.93	0.51
24:W:80:ASP:O	24:W:84:VAL:HG23	2.11	0.51
13:L:138:GLY:HA3	39:L:4360:HOH:O	2.11	0.51
1:0:870:G:H2'	1:0:871:G:C5'	2.40	0.51
37:0:9101:MUL:H11A	39:0:3722:HOH:O	2.11	0.51
1:0:1835:U:C5	1:0:1840:A:N7	2.78	0.51
1:0:1931:A:H2'	1:0:1932:G:C5'	2.40	0.51
1:0:567:U:O5'	1:0:567:U:H6	1.92	0.51
1:0:677:C:H4'	4:C:246:ARG:HH12	1.75	0.51
1:0:2061:C:H2'	1:0:2062:A:H5'	1.93	0.51
1:0:1844:C:O5'	1:0:1844:C:H6	1.93	0.51
1:0:821:U:H5''	39:0:6706:HOH:O	2.10	0.51
1:0:597:A:H2'	1:0:598:C:C6	2.46	0.51
1:0:2830:U:O2'	1:0:2831:C:H5'	2.11	0.51
24:W:48:VAL:HG12	24:W:52:VAL:HB	1.93	0.51
1:0:1363:G:P	4:C:76:ARG:HH22	2.34	0.51
1:0:2061:C:C2'	1:0:2062:A:H5'	2.41	0.51
1:0:1289:C:H3'	39:0:5826:HOH:O	2.10	0.51
1:0:694:A:C2'	1:0:695:C:H5'	2.39	0.51
1:0:74:G:H5'	23:V:9:ARG:HH22	1.76	0.51
1:0:876:A:H2'	1:0:877:G:H5'	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:10:U:C4	1:0:532:A:C8	2.99	0.51
1:0:1427:A:C2'	1:0:1428:C:H5'	2.41	0.51
1:0:1359:U:C5	1:0:2101:A:H8	2.29	0.51
6:E:7:ILE:HG23	6:E:45:ASP:O	2.11	0.51
1:0:100:C:H4'	21:T:16:LEU:HB2	1.93	0.51
1:0:1192:A:H3'	1:0:1193:A:H5'	1.93	0.50
1:0:1891:G:H1'	1:0:1972:U:O2	2.11	0.50
5:D:48:MET:O	31:9:41:C:H4'	2.10	0.50
1:0:1820:G:H2'	1:0:1821:A:H8	1.76	0.50
1:0:1878:G:H5'	39:0:3014:HOH:O	2.11	0.50
1:0:2798:G:H3'	39:0:3048:HOH:O	2.11	0.50
1:0:745:G:H4'	39:0:4576:HOH:O	2.10	0.50
1:0:1133:A:H2'	1:0:1134:G:O4'	2.11	0.50
30:3:3:MET:O	30:3:90:PHE:HA	2.11	0.50
1:0:716:G:C6	1:0:717:C:N4	2.80	0.50
1:0:1904:A:C2	1:0:1905:U:H1'	2.46	0.50
31:9:118:C:O5'	31:9:118:C:H6	1.94	0.50
1:0:1598:A:C2	1:0:1599:U:C2	2.99	0.50
1:0:1678:A:C5	1:0:1679:C:C5	2.99	0.50
31:9:59:C:H6	31:9:59:C:O5'	1.93	0.50
1:0:398:U:O3'	14:M:179:GLY:HA3	2.11	0.50
31:9:114:G:H2'	31:9:115:C:H6	1.72	0.50
1:0:301:C:H42	1:0:350:G:H1	1.58	0.50
1:0:2838:A:O2'	1:0:2839:C:H5'	2.12	0.50
1:0:1304:U:H2'	1:0:1305:C:C6	2.47	0.50
5:D:22:VAL:HG22	5:D:74:THR:HG22	1.93	0.50
1:0:447:A:OP1	21:T:2:LYS:HG2	2.10	0.50
31:9:99:U:H5'	39:9:5904:HOH:O	2.11	0.50
1:0:2295:G:N3	1:0:2361:A:C2	2.79	0.50
1:0:710:G:O2'	1:0:711:G:H5'	2.10	0.50
1:0:1942:A:H2'	1:0:1943:C:H6	1.76	0.50
1:0:1507:C:H4'	39:0:8231:HOH:O	2.10	0.50
1:0:1766:U:H4'	39:0:9080:HOH:O	2.11	0.50
1:0:1680:C:H2'	1:0:1681:G:O4'	2.11	0.50
1:0:219:G:C5'	1:0:220:C:H5''	2.40	0.50
1:0:1331:G:O2'	1:0:1332:C:H5'	2.12	0.50
1:0:2750:G:H2'	1:0:2751:C:C6	2.47	0.50
1:0:685:C:O2'	1:0:748:C:OP1	2.23	0.50
3:B:217:ARG:HG3	3:B:257:THR:HG22	1.94	0.50
1:0:894:A:OP2	39:0:3250:HOH:O	2.19	0.50
1:0:2443:C:H1'	13:L:56:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:574:G:O2'	1:0:575:A:H5'	2.11	0.50
1:0:2869:G:H2'	1:0:2870:C:C6	2.46	0.50
1:0:1496:A:H5'	1:0:1572:A:H1'	1.93	0.50
1:0:2819:C:H2'	1:0:2820:A:C8	2.46	0.50
1:0:313:U:O2'	1:0:314:G:H5'	2.10	0.50
1:0:1305:C:O2'	1:0:1306:U:H5'	2.12	0.50
1:0:690:G:H1'	1:0:731:U:O2'	2.12	0.50
1:0:2764:C:O2'	1:0:2765:C:H5'	2.12	0.50
1:0:962:C:H1'	15:N:5:ARG:NH2	2.27	0.50
4:C:56:THR:HG21	4:C:78:ARG:HB3	1.92	0.50
1:0:796:A:H5'	39:0:5974:HOH:O	2.11	0.50
31:9:2:U:H4'	39:9:5321:HOH:O	2.11	0.50
1:0:1647:G:O2'	1:0:1648:G:H5'	2.12	0.50
1:0:559:U:C5'	1:0:559:U:H6	2.23	0.50
1:0:1213:C:C2'	1:0:1214:G:H5'	2.42	0.50
1:0:1797:A:H5'	39:0:7113:HOH:O	2.12	0.50
1:0:229:G:O2'	1:0:230:C:H5'	2.12	0.50
26:Y:214:ARG:HH12	26:Y:230:ASN:ND2	2.09	0.50
1:0:1251:C:H2'	1:0:1252:A:O4'	2.12	0.50
1:0:1992:U:O2	1:0:1994:A:H8	1.95	0.50
1:0:292:G:H1'	1:0:360:A:N6	2.27	0.50
16:O:32:ARG:HH21	16:O:35:LYS:NZ	2.09	0.50
1:0:843:A:C2	1:0:846:A:C8	3.00	0.50
1:0:530:C:H4'	1:0:612:U:H4'	1.94	0.50
1:0:639:A:H2'	1:0:640:G:C8	2.47	0.50
31:9:82:U:H2'	31:9:83:G:C8	2.47	0.50
20:S:37:VAL:O	20:S:41:VAL:HG23	2.11	0.50
1:0:1511:U:H4'	39:0:6890:HOH:O	2.11	0.50
1:0:2251:G:H2'	1:0:2252:A:H8	1.76	0.50
3:B:75:GLU:OE2	3:B:151:VAL:HG13	2.12	0.50
31:9:78:G:H22	31:9:103:A:P	2.35	0.50
1:0:2484:U:H3'	39:0:3554:HOH:O	2.12	0.50
1:0:840:U:C2	1:0:2648:U:O4	2.65	0.50
26:Y:216:ARG:HD3	39:Y:4408:HOH:O	2.12	0.50
1:0:820:G:H3'	39:0:6706:HOH:O	2.12	0.49
1:0:2710:U:H6	1:0:2710:U:O5'	1.95	0.49
1:0:876:A:C2'	1:0:877:G:H5'	2.41	0.49
14:M:79:ALA:HB3	14:M:81:ARG:NH1	2.26	0.49
1:0:553:G:H5'	39:0:8126:HOH:O	2.11	0.49
1:0:1315:G:H3'	1:0:1316:G:H5'	1.93	0.49
4:C:88:SER:HB3	4:C:91:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2837:U:H2'	39:0:6433:HOH:O	2.12	0.49
1:0:1557:G:H2'	1:0:1558:C:O4'	2.11	0.49
1:0:599:G:H2'	1:0:600:G:H8	1.77	0.49
1:0:137:U:H2'	1:0:139:C:H5	1.76	0.49
1:0:2862:G:H4'	3:B:336:GLN:O	2.12	0.49
9:H:59:GLN:HE21	9:H:129:ARG:HE	1.59	0.49
1:0:2831:C:O2'	1:0:2832:C:H5'	2.12	0.49
1:0:1622:G:H2'	1:0:1623:C:H5'	1.94	0.49
1:0:2871:G:H2'	1:0:2872:U:C6	2.47	0.49
1:0:2675:A:H1'	1:0:2813:A:C2	2.47	0.49
1:0:1175:G:H2'	1:0:1176:C:C6	2.47	0.49
1:0:1447:U:H5''	1:0:1677:U:C5	2.48	0.49
1:0:635:A:H2'	1:0:636:G:H5''	1.93	0.49
1:0:1571:G:H1'	1:0:1627:G:N2	2.27	0.49
1:0:1820:G:O2'	1:0:1821:A:H5'	2.12	0.49
1:0:1342:C:C2'	1:0:1343:C:H5'	2.41	0.49
1:0:1441:G:H2'	1:0:1442:A:C8	2.46	0.49
1:0:818:A:O2'	27:Z:37:ARG:HD3	2.13	0.49
1:0:522:U:O2'	1:0:1366:C:H5'	2.12	0.49
31:9:78:G:HO2'	31:9:79:U:P	2.36	0.49
1:0:1357:A:H1'	39:0:8869:HOH:O	2.12	0.49
31:9:55:U:H4'	31:9:56:A:H8	1.77	0.49
1:0:1170:U:H1'	1:0:1172:G:N7	2.27	0.49
1:0:1400:C:C2'	1:0:1401:G:H5'	2.42	0.49
1:0:1798:C:OP2	1:0:1799:G:H5''	2.13	0.49
1:0:2611:G:H5'	1:0:2613:G:N7	2.28	0.49
1:0:1080:C:H4'	1:0:1081:A:OP1	2.13	0.49
1:0:849:C:O2'	1:0:850:U:H5'	2.12	0.49
1:0:564:G:H1'	39:0:5694:HOH:O	2.12	0.49
39:0:3007:HOH:O	2:A:212:PRO:HB2	2.12	0.49
1:0:2729:C:O2'	1:0:2730:G:H5'	2.13	0.49
1:0:2291:A:C4	1:0:2309:C:H5'	2.47	0.49
31:9:13:A:H5'	39:9:2295:HOH:O	2.13	0.49
1:0:694:A:H2'	1:0:695:C:C5'	2.41	0.49
1:0:740:G:H2'	1:0:741:C:C6	2.46	0.49
1:0:1314:U:H5''	1:0:1316:G:O4'	2.11	0.49
1:0:2885:A:H2'	1:0:2886:C:C6	2.48	0.49
1:0:2643:G:H5''	39:0:8628:HOH:O	2.13	0.49
1:0:560:U:H2'	1:0:561:G:H8	1.78	0.49
1:0:1675:C:N4	39:0:8358:HOH:O	2.44	0.49
1:0:1819:G:H2'	1:0:1820:G:C4'	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1786:C:H2'	1:0:1787:C:H6	1.78	0.49
1:0:2831:C:H2'	1:0:2832:C:C5'	2.43	0.49
1:0:1476:A:O2'	1:0:1868:G:H5'	2.13	0.49
1:0:28:G:H1'	39:0:3446:HOH:O	2.10	0.49
1:0:463:A:H5'	1:0:465:U:O4'	2.13	0.49
1:0:1183:C:H42	1:0:1184:C:H41	1.60	0.49
1:0:1119:G:H8	11:J:52:GLN:HE22	1.58	0.49
1:0:2657:G:H4'	39:0:6216:HOH:O	2.11	0.49
1:0:1447:U:C3'	1:0:1506:U:O2	2.59	0.49
1:0:2710:U:O2'	1:0:2711:U:H5'	2.13	0.49
1:0:178:U:H2'	1:0:179:C:C6	2.46	0.49
1:0:24:G:H22	1:0:518:G:H1'	1.76	0.49
31:9:81:C:C2'	31:9:82:U:H5'	2.42	0.49
3:B:305:ASP:O	3:B:306:LYS:HB2	2.12	0.49
1:0:1344:G:H1'	39:0:9105:HOH:O	2.13	0.49
1:0:1936:C:H2'	1:0:1937:U:C6	2.48	0.49
1:0:2038:A:C2	1:0:2039:A:N7	2.81	0.49
1:0:1202:A:O2'	1:0:1203:G:H5'	2.13	0.49
1:0:1453:G:H2'	1:0:1454:U:O4'	2.12	0.49
1:0:196:G:H2'	39:L:6170:HOH:O	2.11	0.49
1:0:23:G:H1'	1:0:520:A:H61	1.76	0.49
1:0:1415:G:O2'	1:0:1416:G:H5'	2.12	0.49
1:0:2266:A:H2'	1:0:2267:G:C8	2.47	0.49
1:0:1775:A:H3'	1:0:1776:A:H2'	1.95	0.49
1:0:1473:U:O2'	1:0:1474:C:H5''	2.13	0.49
1:0:1046:G:C2	1:0:1069:C:C2	3.01	0.49
1:0:677:C:H2'	1:0:678:G:H8	1.78	0.49
1:0:579:G:H2'	1:0:580:A:C8	2.47	0.49
1:0:2444:U:H2'	1:0:2445:U:O4'	2.12	0.49
25:X:43:VAL:HG13	25:X:76:ARG:HH12	1.77	0.49
1:0:245:C:C5	1:0:246:G:C5	3.01	0.49
1:0:1464:C:O2'	1:0:1465:A:H5'	2.12	0.49
1:0:820:G:N3	1:0:1831:U:H1'	2.28	0.49
1:0:1675:C:O2'	1:0:1676:G:H5'	2.13	0.49
1:0:1097:A:H5''	24:W:125:HIS:CE1	2.47	0.49
1:0:40:C:H6	1:0:40:C:O5'	1.96	0.49
1:0:1739:G:N2	1:0:2041:G:H1'	2.28	0.49
1:0:2734:G:O2'	1:0:2735:U:H5'	2.13	0.49
1:0:2617:G:H5''	39:0:8605:HOH:O	2.12	0.49
1:0:1293:U:H5'	26:Y:154:ARG:HH21	1.77	0.49
1:0:2824:C:H5''	1:0:2825:C:H5'	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2552:C:N4	39:0:8668:HOH:O	2.46	0.49
1:0:20:G:H21	19:R:117:HIS:HD2	1.60	0.49
1:0:1619:G:C5	1:0:1620:C:C4	3.01	0.49
31:9:89:C:O2'	31:9:90:G:H5'	2.12	0.49
1:0:1548:U:O2'	1:0:1549:C:H5'	2.13	0.49
1:0:1664:A:H8	1:0:1664:A:OP1	1.95	0.49
1:0:248:A:N3	1:0:248:A:H3'	2.27	0.49
1:0:2717:C:O2'	1:0:2718:C:H5''	2.09	0.48
1:0:1774:G:O2'	1:0:1775:A:H5'	2.13	0.48
1:0:1118:A:H8	1:0:1119:G:H5''	1.78	0.48
1:0:559:U:H5'	1:0:559:U:C6	2.39	0.48
1:0:2793:A:H2'	1:0:2794:G:H5'	1.94	0.48
1:0:1149:U:O5'	1:0:1151:G:H5'	2.13	0.48
1:0:1076:G:H1'	39:0:3130:HOH:O	2.13	0.48
1:0:2112:A:H2'	1:0:2113:G:C8	2.48	0.48
31:9:107:C:H2'	31:9:108:C:C6	2.48	0.48
1:0:1701:A:H5''	1:0:1702:U:H3'	1.94	0.48
1:0:169:A:H4'	39:0:5424:HOH:O	2.13	0.48
1:0:1014:A:H2'	1:0:1015:C:H5'	1.93	0.48
1:0:1806:G:C2	1:0:1807:U:O2	2.67	0.48
1:0:812:A:H2'	1:0:813:C:H6	1.76	0.48
1:0:465:U:H6	1:0:465:U:O5'	1.96	0.48
1:0:421:C:H4'	1:0:1919:A:C6	2.48	0.48
24:W:122:ARG:HH12	24:W:154:ARG:H	1.61	0.48
1:0:1841:C:OP2	1:0:2022:A:C8	2.66	0.48
1:0:1162:G:H2'	1:0:1163:G:C8	2.48	0.48
1:0:1244:U:OP1	11:J:18:ILE:HD13	2.13	0.48
15:N:12:ARG:NH2	31:9:6:C:C5	2.81	0.48
37:0:9101:MUL:H152	37:0:9101:MUL:O1	2.14	0.48
1:0:877:G:H1'	39:A:491:HOH:O	2.14	0.48
1:0:158:A:H2'	1:0:159:G:O4'	2.13	0.48
1:0:2392:C:H4'	18:Q:55:ARG:NH1	2.28	0.48
1:0:163:U:O3'	1:0:896:C:H4'	2.13	0.48
19:R:63:ASN:HD22	19:R:75:TRP:HZ2	1.60	0.48
1:0:1174:A:C5	1:0:1201:C:H4'	2.48	0.48
1:0:424:C:H2'	1:0:425:U:C6	2.43	0.48
31:9:39:U:H3'	31:9:40:C:H5''	1.96	0.48
1:0:2609:G:H22	3:B:238:ASN:HD21	1.60	0.48
1:0:19:U:H2'	1:0:20:G:O4'	2.13	0.48
1:0:1733:A:H4'	3:B:212:GLN:HA	1.96	0.48
1:0:1497:G:H2'	1:0:1498:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1449:G:H5'	39:0:7441:HOH:O	2.12	0.48
1:0:332:G:H4'	21:T:2:LYS:O	2.12	0.48
1:0:1878:G:O2'	1:0:1879:U:H6	1.96	0.48
1:0:1902:G:O2'	1:0:1903:U:H5'	2.14	0.48
1:0:579:G:H4'	39:0:6205:HOH:O	2.12	0.48
1:0:2480:G:H3'	39:0:8898:HOH:O	2.13	0.48
1:0:1824:C:O2'	1:0:1999:C:H4'	2.13	0.48
1:0:1174:A:C6	1:0:1201:C:H4'	2.48	0.48
1:0:1666:C:O2'	1:0:1667:A:H5''	2.13	0.48
1:0:1741:U:O2'	1:0:2723:G:H4'	2.14	0.48
1:0:42:C:O5'	1:0:185:G:H5''	2.13	0.48
1:0:553:G:C2'	1:0:554:G:H5'	2.43	0.48
1:0:1621:G:H2'	1:0:1622:G:O4'	2.14	0.48
1:0:2052:U:H2'	1:0:2053:G:O4'	2.14	0.48
1:0:2695:C:H2'	1:0:2696:G:C8	2.49	0.48
1:0:1163:G:H1	1:0:1184:C:H42	1.62	0.48
1:0:822:C:C2	1:0:823:U:C5	3.02	0.48
1:0:1861:C:H4'	2:A:6:GLY:O	2.13	0.48
12:K:12:LEU:HB2	12:K:47:ALA:HB3	1.95	0.48
1:0:2539:U:O2'	37:0:9101:MUL:H22	2.13	0.48
1:0:37:A:C2	1:0:446:G:C2	3.02	0.48
1:0:1635:U:H2'	1:0:1636:G:H8	1.79	0.48
1:0:1200:A:H3'	39:0:4912:HOH:O	2.12	0.48
6:E:24:GLY:HA3	6:E:76:VAL:HB	1.96	0.48
1:0:2356:A:H2'	1:0:2357:G:O4'	2.14	0.48
1:0:256:C:H2'	1:0:257:G:O4'	2.14	0.48
1:0:88:G:H2'	1:0:89:G:C8	2.48	0.48
1:0:276:C:H42	1:0:373:G:H1	1.62	0.48
1:0:1829:A:N6	27:Z:42:TYR:HA	2.28	0.48
1:0:1242:A:H5'	11:J:82:THR:CG2	2.43	0.48
1:0:1878:G:O2'	1:0:1879:U:P	2.71	0.48
12:K:55:VAL:HG12	12:K:56:SER:N	2.29	0.48
1:0:2443:C:H3'	39:0:8103:HOH:O	2.13	0.48
1:0:700:A:H4'	16:O:50:ARG:HH21	1.79	0.48
1:0:1723:G:H2'	39:0:5194:HOH:O	2.14	0.48
1:0:2743:A:H8	1:0:2743:A:H5''	1.79	0.48
1:0:2502:C:O2'	1:0:2503:A:H5'	2.14	0.48
1:0:1684:A:O2'	1:0:1685:A:H5''	2.14	0.48
1:0:2780:C:C1'	6:E:143:GLN:HE21	2.23	0.48
1:0:2768:A:O2'	1:0:2769:C:H5'	2.13	0.48
1:0:37:A:H2'	1:0:38:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:444:C:H2'	1:0:445:U:C6	2.49	0.48
1:0:314:G:N1	1:0:317:A:OP2	2.47	0.48
1:0:705:C:H3'	1:0:706:G:C8	2.48	0.48
1:0:393:G:H5''	39:0:6051:HOH:O	2.13	0.48
1:0:1850:U:H2'	1:0:1851:G:C8	2.49	0.48
1:0:247:A:C2	1:0:265:U:C2	3.02	0.48
1:0:76:G:O2'	1:0:77:G:H5'	2.13	0.48
1:0:964:G:H2'	1:0:965:A:O4'	2.14	0.48
12:K:113:ILE:HG22	12:K:114:ALA:N	2.28	0.48
1:0:951:A:C2'	1:0:952:G:H5'	2.44	0.48
1:0:447:A:C2'	1:0:448:G:H5'	2.44	0.47
1:0:1372:A:C2	1:0:2054:A:C4	3.02	0.47
1:0:2270:G:H4'	2:A:223:ARG:HH22	1.79	0.47
1:0:2781:U:H2'	1:0:2782:G:H5'	1.96	0.47
1:0:1855:G:H4'	1:0:1856:C:O5'	2.12	0.47
1:0:1391:G:N2	1:0:1434:A:H5''	2.29	0.47
1:0:2134:G:H2'	1:0:2135:A:H8	1.78	0.47
1:0:566:A:C2'	1:0:567:U:H5'	2.44	0.47
1:0:731:U:H2'	1:0:732:C:C6	2.49	0.47
1:0:1487:A:H5'	39:0:3526:HOH:O	2.14	0.47
1:0:241:A:C2	1:0:378:A:H4'	2.49	0.47
1:0:2911:C:H2'	1:0:2912:C:C6	2.48	0.47
1:0:269:G:O3'	1:0:274:G:H4'	2.14	0.47
1:0:2070:G:H2'	1:0:2072:G:OP1	2.15	0.47
14:M:24:GLN:NE2	14:M:27:ARG:NH1	2.55	0.47
37:0:9101:MUL:C10	37:0:9101:MUL:H14	2.41	0.47
1:0:2458:U:O3'	30:3:64:LYS:HB2	2.14	0.47
1:0:962:C:N4	1:0:1005:A:H61	2.12	0.47
1:0:1711:A:H2	1:0:1817:U:HO2'	1.62	0.47
1:0:2734:G:H2'	1:0:2735:U:O4'	2.13	0.47
1:0:849:C:H2'	1:0:850:U:H6	1.78	0.47
17:P:98:ILE:HD12	17:P:102:ARG:HE	1.79	0.47
1:0:1730:G:H5'	1:0:1731:C:C6	2.49	0.47
1:0:1387:G:C2	1:0:1396:C:O2	2.67	0.47
1:0:809:G:H2'	1:0:810:G:H8	1.77	0.47
1:0:1415:G:C2'	1:0:1416:G:H5'	2.44	0.47
1:0:699:C:H2'	1:0:744:G:N3	2.29	0.47
1:0:2639:G:O2'	1:0:2640:U:H5'	2.14	0.47
1:0:391:U:O2'	1:0:392:U:H5'	2.14	0.47
1:0:1448:A:O4'	1:0:1506:U:O4'	2.31	0.47
31:9:3:A:H2	31:9:21:G:N3	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:290:C:C2'	1:0:291:C:H5'	2.44	0.47
1:0:2032:U:C2'	1:0:2033:G:H5''	2.43	0.47
1:0:957:A:H2'	1:0:958:G:O4'	2.14	0.47
1:0:1515:A:H2'	1:0:1516:U:C6	2.49	0.47
1:0:128:A:C8	1:0:128:A:C3'	2.96	0.47
1:0:158:A:H5''	39:0:7993:HOH:O	2.14	0.47
1:0:656:G:H5'	16:O:3:THR:HB	1.96	0.47
1:0:2291:A:C8	1:0:2309:C:H5'	2.49	0.47
1:0:1497:G:H2'	1:0:1498:G:H8	1.78	0.47
1:0:941:G:C5	1:0:942:U:C4	3.02	0.47
1:0:2057:U:O5'	1:0:2057:U:H6	1.96	0.47
1:0:2517:A:H2'	1:0:2518:C:O4'	2.13	0.47
12:K:62:PRO:HG3	12:K:65:ARG:HH21	1.79	0.47
1:0:719:C:N3	1:0:720:G:H1'	2.29	0.47
1:0:1763:C:O2'	1:0:1764:C:H5'	2.15	0.47
1:0:2089:A:C2'	1:0:2090:G:H5'	2.45	0.47
1:0:2815:G:H4'	1:0:2816:A:OP2	2.13	0.47
1:0:137:U:OP1	1:0:259:G:O2'	2.31	0.47
1:0:221:G:H5'	39:0:6026:HOH:O	2.12	0.47
1:0:1792:C:N3	1:0:1793:C:H5	2.12	0.47
31:9:49:G:H5''	39:9:4707:HOH:O	2.13	0.47
1:0:1730:G:H2'	1:0:1730:G:N3	2.29	0.47
1:0:2038:A:H5''	3:B:222:LYS:HG3	1.96	0.47
1:0:2355:G:H5''	1:0:2356:A:OP2	2.14	0.47
1:0:325:U:O2	1:0:326:G:C8	2.67	0.47
1:0:2286:G:H1'	39:0:7013:HOH:O	2.13	0.47
1:0:2047:C:P	39:0:7641:HOH:O	2.73	0.47
1:0:825:U:H5''	1:0:826:U:OP1	2.13	0.47
1:0:2633:A:H2'	1:0:2634:G:H5'	1.97	0.47
1:0:2780:C:H2'	1:0:2781:U:C6	2.49	0.47
1:0:1377:C:H5'	1:0:1377:C:C6	2.43	0.47
1:0:683:G:O2'	1:0:684:G:H5'	2.15	0.47
1:0:37:A:H2'	1:0:38:G:H8	1.78	0.47
1:0:1324:G:H21	26:Y:204:ARG:NH2	2.13	0.47
1:0:640:G:C4	1:0:641:G:C8	3.03	0.47
1:0:1217:G:C2	1:0:1218:U:C2	3.03	0.47
1:0:894:A:H5''	39:0:7673:HOH:O	2.13	0.47
1:0:730:G:O2'	1:0:731:U:H5'	2.15	0.47
1:0:392:U:H5''	14:M:193:LYS:HG2	1.96	0.47
29:2:40:ARG:HD2	29:2:47:THR:HG22	1.96	0.47
1:0:1666:C:C2'	1:0:1667:A:H5'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2072:G:H5'	39:0:3339:HOH:O	2.13	0.47
37:0:9101:MUL:H262	37:0:9101:MUL:H242	1.71	0.47
1:0:2862:G:C6	1:0:2895:C:N4	2.83	0.47
1:0:2332:A:H5'	5:D:56:ARG:NH2	2.27	0.47
1:0:238:C:H4'	1:0:287:C:OP1	2.15	0.47
1:0:1969:A:O2'	1:0:1970:G:H5'	2.15	0.47
1:0:2642:G:C6	1:0:2643:G:C6	3.02	0.47
1:0:2554:U:H3'	39:0:6989:HOH:O	2.14	0.47
1:0:387:G:C2'	1:0:388:G:H5'	2.45	0.47
1:0:168:C:O5'	1:0:168:C:H6	1.96	0.47
1:0:1162:G:H2'	1:0:1163:G:H8	1.80	0.47
1:0:544:G:H2'	1:0:545:G:H5''	1.97	0.47
1:0:2087:C:O2'	1:0:2088:C:H5'	2.15	0.47
1:0:561:G:N3	1:0:562:A:C8	2.83	0.47
1:0:2253:G:H2'	1:0:2254:G:C8	2.40	0.47
1:0:1351:G:H1'	39:0:3441:HOH:O	2.15	0.47
1:0:2035:C:O2'	1:0:2036:C:H5'	2.15	0.47
1:0:2430:A:H2'	1:0:2431:C:C6	2.49	0.47
1:0:2499:U:H2'	1:0:2500:C:H6	1.80	0.47
31:9:35:C:H5''	39:9:4078:HOH:O	2.15	0.47
1:0:1220:U:H2'	1:0:1221:G:C8	2.47	0.47
24:W:88:THR:HG22	24:W:89:ASP:H	1.79	0.47
1:0:1851:G:H1'	39:0:3109:HOH:O	2.15	0.47
1:0:920:C:H5	1:0:2467:A:OP1	1.98	0.47
1:0:711:G:C2	1:0:718:C:C2	3.03	0.47
1:0:523:C:H2'	1:0:524:A:C8	2.49	0.47
1:0:2851:G:C2'	1:0:2852:A:H5'	2.45	0.47
1:0:57:C:H42	1:0:89:G:H1	1.63	0.47
1:0:951:A:H5''	18:Q:42:LYS:HD3	1.97	0.47
1:0:699:C:C2	1:0:744:G:C2	3.02	0.47
1:0:397:A:N3	1:0:418:C:H5'	2.30	0.47
1:0:2081:A:H2'	1:0:2082:G:O4'	2.15	0.47
1:0:1153:C:N3	1:0:2786:G:O6	2.47	0.47
1:0:208:C:C6	1:0:208:C:H3'	2.49	0.47
1:0:763:C:O2'	1:0:764:C:H5'	2.14	0.47
1:0:1656:A:H2'	1:0:1657:A:O4'	2.14	0.47
4:C:215:ALA:HB3	39:C:5535:HOH:O	2.15	0.47
1:0:2800:A:H5'	1:0:2801:A:OP2	2.15	0.47
1:0:2808:U:OP1	3:B:261:GLN:NE2	2.42	0.47
1:0:603:A:H4'	1:0:604:G:O5'	2.15	0.47
1:0:2093:G:H5''	39:0:7738:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:459:A:H4'	39:0:4567:HOH:O	2.14	0.47
6:E:91:PHE:HA	6:E:92:PRO:HD3	1.79	0.47
1:0:2119:C:O2'	1:0:2120:U:H5'	2.14	0.47
1:0:1245:C:H3'	1:0:1245:C:H6	1.79	0.47
4:C:27:ARG:HG2	4:C:27:ARG:HH11	1.79	0.47
1:0:1776:A:C8	1:0:1778:A:O4'	2.67	0.47
1:0:1119:G:C5	1:0:1243:C:C4	3.03	0.47
1:0:45:A:C5'	1:0:47:G:H5'	2.45	0.47
1:0:1575:C:H2'	1:0:1575:C:O2	2.14	0.47
1:0:639:A:C6	1:0:640:G:C6	3.02	0.47
1:0:2243:C:H5''	39:0:8382:HOH:O	2.15	0.47
1:0:292:G:O2'	1:0:360:A:N6	2.47	0.47
1:0:1826:C:O2'	1:0:1827:G:H5'	2.15	0.47
1:0:699:C:C6	1:0:744:G:N3	2.83	0.47
1:0:216:A:O2'	1:0:217:C:H5'	2.15	0.47
1:0:123:U:H1'	39:0:7179:HOH:O	2.14	0.47
1:0:1566:C:H2'	1:0:1567:G:C8	2.50	0.47
30:3:51:LYS:HB2	39:3:1812:HOH:O	2.15	0.47
1:0:621:C:H5'	26:Y:132:ASP:OD2	2.15	0.47
1:0:2651:C:H2'	1:0:2652:U:O4'	2.14	0.47
12:K:8:VAL:HG13	12:K:80:ILE:HG22	1.97	0.47
31:9:58:G:H2'	31:9:59:C:O4'	2.15	0.47
1:0:837:U:H2'	1:0:838:C:O4'	2.15	0.47
1:0:2320:U:H3'	30:3:2:GLN:HB2	1.97	0.47
1:0:2831:C:H2'	1:0:2832:C:H5'	1.97	0.47
31:9:82:U:H2'	31:9:83:G:H8	1.80	0.47
1:0:1419:U:H5'	1:0:1420:C:OP2	2.15	0.47
15:N:67:ALA:HA	15:N:71:TRP:HB3	1.96	0.47
1:0:2547:C:H1'	39:B:342:HOH:O	2.13	0.47
1:0:240:C:O2	1:0:240:C:H2'	2.14	0.47
1:0:2697:A:H2'	1:0:2698:G:O4'	2.15	0.47
1:0:1158:G:C2'	1:0:1159:G:H5'	2.45	0.47
1:0:2506:A:O2'	1:0:2507:G:O5'	2.32	0.47
1:0:1351:G:OP1	4:C:96:LYS:NZ	2.42	0.47
1:0:2893:C:O2'	1:0:2894:C:H5'	2.15	0.47
1:0:1098:A:O3'	24:W:129:LYS:HE3	2.15	0.47
1:0:849:C:C5	1:0:850:U:C5	3.03	0.47
1:0:1363:G:H2'	1:0:1364:G:H8	1.80	0.47
2:A:70:ALA:HB1	27:Z:89:THR:HG21	1.96	0.47
1:0:1978:A:H5''	39:0:7843:HOH:O	2.14	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:879:C:H3'	39:0:5621:HOH:O	2.14	0.46
1:0:2812:A:H1'	39:0:4957:HOH:O	2.15	0.46
1:0:308:U:C4	1:0:342:C:H1'	2.50	0.46
1:0:1444:G:C2'	1:0:1445:G:H5'	2.45	0.46
1:0:187:A:H5'	1:0:188:C:OP2	2.14	0.46
1:0:1278:A:H4'	1:0:1279:U:N3	2.29	0.46
1:0:1056:U:H2'	1:0:1057:A:O4'	2.15	0.46
1:0:1477:C:H2'	1:0:1478:U:O4'	2.15	0.46
1:0:738:G:H21	1:0:2384:U:H4'	1.80	0.46
1:0:174:A:H4'	1:0:175:G:OP1	2.15	0.46
1:0:661:G:C6	1:0:662:U:C4	3.03	0.46
1:0:1825:U:O2'	1:0:1826:C:H5'	2.15	0.46
1:0:1138:G:H4'	39:0:4849:HOH:O	2.15	0.46
31:9:45:A:C8	31:9:46:C:C5	3.03	0.46
1:0:1518:A:H1'	39:0:8334:HOH:O	2.15	0.46
1:0:2569:A:O5'	1:0:2569:A:H8	1.97	0.46
1:0:2070:G:H4'	39:0:2976:HOH:O	2.14	0.46
1:0:154:C:H2'	1:0:155:C:C6	2.37	0.46
1:0:2088:C:H1'	1:0:2841:A:N1	2.30	0.46
1:0:1883:U:H5'	1:0:2012:U:OP2	2.15	0.46
1:0:1920:C:H2'	1:0:1921:A:H5'	1.97	0.46
1:0:2496:C:H1'	1:0:2527:U:N3	2.30	0.46
1:0:65:C:O2'	1:0:66:G:H5'	2.14	0.46
1:0:1477:C:O2'	1:0:1478:U:H5'	2.15	0.46
1:0:1616:A:H5''	1:0:1617:C:OP1	2.15	0.46
1:0:1215:A:O3'	1:0:1216:G:C4'	2.63	0.46
1:0:1252:A:H4'	39:0:4164:HOH:O	2.14	0.46
24:W:122:ARG:HH12	24:W:154:ARG:N	2.12	0.46
1:0:1449:G:N3	1:0:1449:G:H2'	2.29	0.46
1:0:485:A:N3	1:0:487:G:H5''	2.30	0.46
1:0:2073:G:H2'	39:0:8459:HOH:O	2.16	0.46
1:0:2090:G:H2'	1:0:2091:G:C8	2.51	0.46
1:0:634:G:C2	1:0:635:A:C2	3.03	0.46
31:9:39:U:H1'	31:9:44:A:N6	2.30	0.46
1:0:1771:U:H4'	1:0:1772:C:OP2	2.15	0.46
1:0:2135:A:O4'	1:0:2243:C:N4	2.47	0.46
1:0:920:C:H4'	1:0:921:G:N3	2.29	0.46
1:0:1832:G:N2	1:0:1845:A:C4	2.83	0.46
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.56	0.46
27:Z:56:GLU:O	27:Z:61:HIS:HE1	1.98	0.46
1:0:1754:A:H2'	1:0:1755:A:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1455:C:O2	1:0:1456:C:C6	2.69	0.46
1:0:544:G:C2'	1:0:545:G:H5''	2.45	0.46
1:0:287:C:N4	1:0:365:G:H1	2.10	0.46
1:0:2134:G:O6	1:0:2258:A:H2'	2.15	0.46
1:0:722:G:C5	1:0:723:G:C8	3.03	0.46
1:0:946:C:O5'	1:0:946:C:H6	1.99	0.46
1:0:1215:A:O3'	1:0:1216:G:H4'	2.14	0.46
1:0:255:A:H2'	1:0:256:C:C6	2.50	0.46
1:0:1013:A:H5''	1:0:2302:A:N6	2.30	0.46
1:0:1977:U:OP1	1:0:1978:A:H5'	2.15	0.46
1:0:2605:G:O2'	1:0:2606:G:H5'	2.14	0.46
1:0:689:G:O2'	1:0:742:G:H1'	2.15	0.46
1:0:862:U:H4'	39:0:7515:HOH:O	2.15	0.46
10:I:96:SER:H	10:I:99:GLN:HB2	1.80	0.46
1:0:1639:U:H2'	1:0:1640:C:O5'	2.15	0.46
1:0:871:G:C6	1:0:872:U:N3	2.84	0.46
1:0:2718:C:C2	1:0:2763:G:N2	2.84	0.46
1:0:1132:A:H61	1:0:1229:C:H2'	1.79	0.46
1:0:2578:G:C8	1:0:2578:G:H5'	2.47	0.46
1:0:445:U:O2'	1:0:446:G:H5'	2.16	0.46
1:0:1523:G:C5	1:0:1524:U:C4	3.03	0.46
1:0:2714:U:O3'	3:B:10:SER:HB2	2.14	0.46
1:0:106:A:C2'	1:0:107:U:H5'	2.46	0.46
1:0:853:C:H3'	39:0:3276:HOH:O	2.14	0.46
1:0:2134:G:N2	1:0:2242:U:C2	2.83	0.46
1:0:250:C:H2'	1:0:251:C:C6	2.50	0.46
1:0:2825:C:H4'	1:0:2826:G:O4'	2.16	0.46
1:0:1253:C:O2'	1:0:1254:C:H5'	2.16	0.46
1:0:2668:G:H2'	1:0:2669:U:H6	1.79	0.46
1:0:2110:G:H4'	39:0:7642:HOH:O	2.15	0.46
1:0:2416:G:H1'	39:0:5208:HOH:O	2.14	0.46
1:0:962:C:H2'	1:0:963:C:C5'	2.46	0.46
1:0:1769:C:C2'	1:0:1770:U:H5'	2.46	0.46
1:0:353:G:H2'	1:0:354:A:C8	2.51	0.46
1:0:1556:G:O2'	1:0:1557:G:H5'	2.16	0.46
1:0:763:C:H5''	39:0:3284:HOH:O	2.16	0.46
1:0:485:A:O2'	1:0:487:G:H5'	2.16	0.46
1:0:583:C:H2'	1:0:584:U:H6	1.80	0.46
1:0:2745:C:H5''	39:0:5667:HOH:O	2.14	0.46
1:0:2096:A:C8	1:0:2539:U:C2	3.03	0.46
1:0:1684:A:H8	39:0:7816:HOH:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2796:U:H1'	6:E:143:GLN:OE1	2.16	0.46
1:0:1822:A:O2'	1:0:1823:G:H5'	2.16	0.46
1:0:677:C:H4'	4:C:246:ARG:NH1	2.30	0.46
1:0:669:G:C4	1:0:670:G:C8	3.04	0.46
1:0:522:U:O2'	1:0:523:C:H5'	2.16	0.46
1:0:1217:G:H2'	1:0:1218:U:C6	2.51	0.46
1:0:2484:U:H4'	39:0:4578:HOH:O	2.16	0.46
11:J:107:ASN:HD22	11:J:109:TYR:H	1.63	0.46
1:0:2259:C:C5	1:0:2260:A:N7	2.84	0.46
1:0:2075:G:C6	1:0:2076:U:C4	3.04	0.46
6:E:103:VAL:HG22	6:E:115:ARG:HB3	1.97	0.46
1:0:2754:G:H2'	1:0:2755:G:O4'	2.16	0.46
1:0:1463:U:H4'	39:0:6050:HOH:O	2.16	0.46
1:0:105:G:C2	1:0:106:A:C8	3.04	0.46
1:0:814:G:H2'	1:0:815:U:H6	1.81	0.46
1:0:502:A:H2'	1:0:503:G:O4'	2.15	0.46
1:0:2791:U:H4'	1:0:2792:A:OP1	2.16	0.46
1:0:2338:G:H4'	5:D:105:SER:O	2.16	0.46
1:0:295:C:C2'	1:0:296:G:H5'	2.45	0.46
1:0:2403:C:H5'	39:0:5297:HOH:O	2.14	0.46
1:0:1230:A:H8	1:0:1230:A:OP1	1.98	0.46
39:0:6068:HOH:O	31:9:83:G:H4'	2.14	0.46
2:A:125:ASN:HB3	2:A:158:VAL:HG12	1.98	0.46
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.96	0.46
1:0:160:A:C4	1:0:177:A:C2	3.04	0.46
8:G:64:ASN:HD22	8:G:64:ASN:N	2.14	0.46
15:N:37:ARG:NH1	31:9:6:C:OP1	2.46	0.46
1:0:2540:G:O2'	37:0:9101:MUL:H131	2.16	0.46
1:0:1096:U:O2'	1:0:1097:A:H5'	2.16	0.46
1:0:287:C:H2'	1:0:288:A:C8	2.51	0.46
1:0:707:C:C2	1:0:708:A:C8	3.04	0.46
1:0:230:C:H2'	1:0:231:G:H8	1.81	0.46
1:0:1880:C:H2'	1:0:1881:A:O4'	2.16	0.46
1:0:267:G:H2'	1:0:268:U:O4'	2.16	0.46
1:0:295:C:O2'	1:0:296:G:H5'	2.16	0.46
1:0:2775:A:C6	1:0:2799:A:C8	3.04	0.46
1:0:432:G:H2'	1:0:433:C:C6	2.47	0.45
1:0:878:G:H4'	1:0:1835:U:H4'	1.96	0.45
1:0:676:C:HO2'	4:C:219:ASN:HD22	1.60	0.45
1:0:893:C:H4'	1:0:894:A:OP1	2.16	0.45
1:0:2732:U:H2'	1:0:2733:U:H6	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2668:G:H2'	1:0:2669:U:C6	2.50	0.45
1:0:1794:G:OP1	17:P:134:VAL:HG23	2.16	0.45
1:0:606:C:O2'	1:0:607:G:H5'	2.16	0.45
31:9:63:C:O2'	31:9:64:C:H5'	2.16	0.45
31:9:75:G:C2	31:9:107:C:N3	2.85	0.45
1:0:1183:C:N3	1:0:1184:C:N4	2.64	0.45
1:0:820:G:H5'	1:0:821:U:C5'	2.47	0.45
1:0:2102:G:C6	37:0:9101:MUL:H173	2.51	0.45
1:0:1838:U:H3'	39:0:4588:HOH:O	2.15	0.45
1:0:2776:A:H2'	1:0:2777:G:H5'	1.98	0.45
31:9:64:C:C2'	31:9:65:A:H5'	2.46	0.45
29:2:35:ARG:N	39:2:3614:HOH:O	2.50	0.45
1:0:402:U:H2'	1:0:403:C:C6	2.51	0.45
1:0:1325:G:C2	1:0:1326:C:C6	3.04	0.45
30:3:49:ASP:HB3	30:3:52:PHE:HB2	1.98	0.45
1:0:207:U:H4'	1:0:438:C:O2	2.16	0.45
13:L:80:ASP:HB3	13:L:90:ARG:HB3	1.98	0.45
1:0:165:A:O2'	1:0:221:G:N2	2.48	0.45
1:0:1594:C:O2'	1:0:1607:A:H4'	2.16	0.45
1:0:1476:A:O2'	1:0:1477:C:H5'	2.17	0.45
1:0:2695:C:H2'	1:0:2696:G:H8	1.82	0.45
1:0:585:C:H2'	1:0:586:C:C6	2.51	0.45
1:0:2598:U:O2	1:0:2600:A:C8	2.70	0.45
7:F:67:ALA:HB1	7:F:72:VAL:O	2.17	0.45
1:0:1667:A:H2'	1:0:1668:U:C6	2.51	0.45
1:0:156:C:H5''	14:M:171:ARG:CD	2.42	0.45
1:0:1740:U:O2	1:0:2724:U:H5''	2.16	0.45
1:0:1098:A:OP1	24:W:128:VAL:HG22	2.15	0.45
1:0:2397:G:C5	1:0:2465:A:C6	3.05	0.45
1:0:1509:U:O2'	1:0:1510:G:H5'	2.16	0.45
1:0:1449:G:N3	1:0:1493:A:C2	2.84	0.45
1:0:535:G:C5	1:0:2063:U:C4	3.04	0.45
1:0:2541:U:H4'	39:0:4427:HOH:O	2.16	0.45
24:W:137:GLN:HE21	24:W:141:HIS:CE1	2.34	0.45
1:0:1368:U:H6	1:0:1368:U:O5'	2.00	0.45
1:0:1180:U:H1'	10:I:87:PRO:HD2	1.97	0.45
1:0:2297:U:O2'	1:0:2298:C:H5'	2.16	0.45
1:0:2388:C:H5''	18:Q:82:LYS:HG2	1.99	0.45
1:0:2078:U:O2'	1:0:2079:G:H5'	2.16	0.45
24:W:4:LEU:HD23	24:W:54:PHE:HB3	1.97	0.45
1:0:926:A:H4'	13:L:39:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1141:U:O2'	1:0:1142:C:H5'	2.16	0.45
1:0:883:U:C6	1:0:888:U:H5'	2.51	0.45
1:0:2106:C:H2'	1:0:2107:U:C6	2.52	0.45
1:0:1195:G:H2'	1:0:1196:C:O4'	2.16	0.45
1:0:1439:C:O5'	1:0:1439:C:H6	2.00	0.45
1:0:2717:C:OP1	3:B:207:LYS:HG3	2.16	0.45
1:0:544:G:H2'	1:0:545:G:C5'	2.47	0.45
1:0:558:C:O2'	1:0:559:U:H5''	2.17	0.45
1:0:2270:G:H2'	39:0:4485:HOH:O	2.16	0.45
1:0:876:A:N3	1:0:876:A:H2'	2.30	0.45
1:0:1220:U:H4'	9:H:174:LEU:HD21	1.98	0.45
1:0:67:A:H5''	1:0:69:A:C8	2.52	0.45
1:0:1052:G:H2'	1:0:1052:G:N3	2.32	0.45
1:0:517:U:C2'	1:0:518:G:H5'	2.47	0.45
1:0:2673:U:H4'	3:B:94:GLN:O	2.17	0.45
1:0:2689:A:C2'	1:0:2690:U:H5'	2.45	0.45
1:0:1877:G:OP1	2:A:164:ARG:NH2	2.49	0.45
15:N:159:TYR:CE1	31:9:50:G:H5''	2.49	0.45
1:0:2444:U:H2'	1:0:2445:U:H6	1.81	0.45
1:0:247:A:H2'	39:0:8624:HOH:O	2.15	0.45
1:0:421:C:H4'	1:0:1919:A:C5	2.51	0.45
1:0:255:A:C5	1:0:256:C:C4	3.04	0.45
1:0:266:G:C2	1:0:267:G:C8	3.05	0.45
1:0:860:U:H2'	1:0:861:A:C8	2.52	0.45
1:0:1909:A:H4'	39:0:8156:HOH:O	2.16	0.45
1:0:1156:C:O2'	1:0:1157:C:H5'	2.17	0.45
1:0:1447:U:OP1	1:0:1506:U:N3	2.41	0.45
1:0:329:A:H5'	1:0:347:A:C1'	2.47	0.45
31:9:53:G:O2'	31:9:54:A:H5'	2.16	0.45
1:0:443:C:H2'	1:0:444:C:C6	2.52	0.45
1:0:333:G:N1	1:0:344:C:C4	2.85	0.45
1:0:29:C:H5'	1:0:1342:C:OP1	2.16	0.45
1:0:293:A:H2'	1:0:294:C:C6	2.51	0.45
1:0:2871:G:H2'	1:0:2872:U:H6	1.82	0.45
1:0:1919:A:H4'	39:0:3679:HOH:O	2.17	0.45
22:U:39:ASN:HD22	22:U:44:ARG:HD2	1.82	0.45
19:R:96:VAL:HG13	19:R:106:GLY:HA3	1.99	0.45
1:0:1164:U:H4'	1:0:1165:G:H5''	1.99	0.45
1:0:1119:G:C8	11:J:52:GLN:NE2	2.84	0.45
1:0:1819:G:H2'	1:0:1820:G:C5'	2.47	0.45
1:0:1334:C:H1'	26:Y:204:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:178:U:O2'	1:0:179:C:H5'	2.16	0.45
1:0:2626:C:H2'	1:0:2627:G:C8	2.51	0.45
1:0:2295:G:H5'	1:0:2425:A:H4'	1.98	0.45
1:0:1917:G:H1'	1:0:1923:G:N2	2.32	0.45
1:0:193:A:H2'	1:0:414:C:O2	2.16	0.45
15:N:55:ASP:OD2	31:9:7:G:H4'	2.16	0.45
1:0:2823:G:O2'	1:0:2824:C:H5'	2.16	0.45
1:0:1475:G:N3	1:0:1866:A:H2	2.15	0.45
39:0:7140:HOH:O	26:Y:149:GLN:HG3	2.15	0.45
1:0:400:C:H2'	1:0:401:C:C6	2.52	0.45
3:B:56:ASP:HB2	3:B:322:ARG:HE	1.82	0.45
11:J:76:ASP:HA	39:J:5907:HOH:O	2.16	0.45
1:0:2727:A:H2'	1:0:2728:C:H5'	1.98	0.45
1:0:297:U:H2'	1:0:298:C:C6	2.52	0.45
1:0:275:G:C2	1:0:376:C:C2	3.05	0.45
1:0:2493:C:O2	1:0:2493:C:H2'	2.17	0.45
1:0:1766:U:H2'	1:0:1776:A:N6	2.31	0.45
1:0:2513:A:H2'	1:0:2514:U:O4'	2.17	0.45
1:0:693:A:H2'	1:0:694:A:C8	2.52	0.45
1:0:63:U:O2'	1:0:64:G:H5'	2.17	0.45
1:0:1398:G:H2'	1:0:1399:A:O4'	2.17	0.45
1:0:1514:C:O2'	1:0:1515:A:H5'	2.17	0.45
1:0:287:C:H3'	1:0:287:C:H6	1.81	0.45
1:0:343:C:O2'	1:0:344:C:H5'	2.17	0.45
1:0:1080:C:O5'	1:0:1080:C:H6	2.00	0.45
1:0:1328:A:C8	26:Y:169:ARG:HD3	2.51	0.45
1:0:2869:G:H5'	39:0:4548:HOH:O	2.16	0.45
1:0:400:C:H2'	1:0:401:C:H6	1.82	0.45
31:9:17:G:O2'	31:9:18:U:H5'	2.16	0.45
3:B:125:GLU:O	3:B:129:ARG:HG3	2.17	0.45
1:0:2269:C:C2'	1:0:2270:G:H5'	2.47	0.45
1:0:622:G:C5	1:0:623:U:C5	3.04	0.45
1:0:957:A:H2'	1:0:958:G:C8	2.52	0.45
1:0:1296:A:O2'	1:0:1297:U:H5'	2.16	0.45
1:0:2043:U:O3'	25:X:23:HIS:HE1	1.99	0.45
1:0:23:G:H2'	1:0:24:G:O4'	2.17	0.45
1:0:151:A:N3	1:0:441:A:H4'	2.32	0.45
1:0:656:G:H2'	1:0:657:G:C8	2.52	0.45
1:0:123:U:H5'	39:0:6169:HOH:O	2.17	0.45
15:N:44:ARG:HG3	15:N:45:ALA:N	2.32	0.45
3:B:254:GLN:HG2	3:B:255:GLY:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:783:C:O5'	1:0:783:C:H6	2.00	0.45
1:0:2657:G:H5'	39:0:5938:HOH:O	2.17	0.44
1:0:876:A:N7	1:0:878:G:H1'	2.32	0.44
1:0:128:A:H3'	1:0:128:A:H8	1.81	0.44
1:0:1387:G:H1'	17:P:28:GLN:HE22	1.80	0.44
1:0:657:G:H1'	39:0:2960:HOH:O	2.16	0.44
1:0:80:A:H3'	21:T:43:ASN:OD1	2.16	0.44
1:0:1323:G:N2	1:0:1335:C:C2	2.86	0.44
9:H:168:VAL:HG13	39:H:4963:HOH:O	2.16	0.44
1:0:1258:G:O5'	1:0:1258:G:H8	2.00	0.44
1:0:1454:U:H5''	1:0:1455:C:OP2	2.17	0.44
1:0:1126:C:O5'	1:0:1126:C:C6	2.66	0.44
31:9:59:C:H2'	31:9:60:C:H6	1.82	0.44
1:0:2271:G:N3	1:0:2271:G:H2'	2.32	0.44
1:0:1592:G:O2'	1:0:1593:C:O5'	2.34	0.44
1:0:1526:A:H4'	1:0:1527:A:C5'	2.47	0.44
1:0:1845:A:OP2	2:A:190:ARG:NH1	2.50	0.44
1:0:298:C:H6	1:0:298:C:O5'	1.99	0.44
1:0:473:A:O2'	1:0:890:C:H5'	2.17	0.44
1:0:1714:C:O2'	1:0:1715:C:H5'	2.17	0.44
1:0:2407:G:C2	1:0:2408:A:C4	3.05	0.44
1:0:2087:C:C2	1:0:2658:G:C2	3.06	0.44
1:0:329:A:H5'	1:0:347:A:H1'	1.99	0.44
31:9:59:C:H2'	31:9:60:C:C6	2.52	0.44
1:0:2638:G:H5'	39:0:3790:HOH:O	2.17	0.44
1:0:1730:G:C5'	1:0:1731:C:C6	3.00	0.44
1:0:722:G:C2'	1:0:723:G:H5'	2.48	0.44
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.82	0.44
1:0:32:G:H2'	1:0:33:G:O4'	2.18	0.44
1:0:968:G:O2'	1:0:969:G:H5'	2.17	0.44
14:M:99:ARG:NE	14:M:170:ASN:HD22	2.15	0.44
1:0:1827:G:H2'	1:0:1828:G:C8	2.52	0.44
1:0:397:A:C4	1:0:418:C:H5'	2.52	0.44
24:W:38:THR:O	24:W:42:ARG:HB2	2.17	0.44
1:0:2428:G:H4'	39:0:4707:HOH:O	2.17	0.44
18:Q:66:LYS:HB2	18:Q:70:ALA:O	2.17	0.44
1:0:2842:G:H2'	1:0:2843:A:H5'	1.98	0.44
1:0:212:A:O3'	1:0:213:G:H4'	2.17	0.44
1:0:2657:G:N2	1:0:2658:G:H1'	2.33	0.44
1:0:2814:A:O4'	1:0:2816:A:C8	2.70	0.44
31:9:1:U:H4'	31:9:3:A:OP1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1433:G:H2'	1:0:1434:A:O4'	2.17	0.44
1:0:1477:C:C5'	1:0:1868:G:H5''	2.48	0.44
1:0:708:A:H2'	1:0:709:G:O4'	2.17	0.44
31:9:95:C:O2'	31:9:96:C:H5'	2.17	0.44
1:0:1363:G:P	4:C:76:ARG:NH2	2.90	0.44
1:0:1909:A:N1	1:0:2128:G:H1'	2.32	0.44
12:K:98:VAL:HG13	12:K:102:GLU:HA	2.00	0.44
1:0:2900:G:O2'	1:0:2901:C:H5'	2.17	0.44
2:A:178:LYS:NZ	39:A:4437:HOH:O	2.50	0.44
1:0:2451:G:H5''	39:0:6300:HOH:O	2.16	0.44
1:0:2002:C:H2'	1:0:2003:U:H5'	1.99	0.44
1:0:1209:C:H2'	1:0:1210:G:C8	2.48	0.44
1:0:1544:U:O2'	1:0:1545:C:H5'	2.17	0.44
1:0:2726:U:O4'	1:0:2749:U:C2	2.69	0.44
1:0:318:U:H5'	1:0:339:A:N3	2.32	0.44
31:9:54:A:H4'	39:9:7345:HOH:O	2.16	0.44
1:0:962:C:C2'	1:0:963:C:H5'	2.48	0.44
1:0:65:C:H2'	1:0:66:G:H8	1.82	0.44
1:0:64:G:N2	1:0:70:A:C4	2.85	0.44
1:0:1886:A:H61	1:0:2016:U:H3	1.63	0.44
1:0:2275:G:C6	1:0:2276:U:N3	2.85	0.44
1:0:2869:G:O5'	1:0:2869:G:H8	2.01	0.44
1:0:1733:A:C2	1:0:1734:C:H1'	2.53	0.44
1:0:256:C:H2'	1:0:257:G:C5'	2.47	0.44
14:M:157:ASP:HB3	14:M:160:PHE:HD1	1.83	0.44
1:0:131:A:OP2	1:0:141:C:H5	2.01	0.44
3:B:244:PRO:HG3	3:B:248:ARG:HH21	1.81	0.44
1:0:2679:G:H2'	1:0:2680:A:H3'	1.99	0.44
1:0:2103:A:O2'	1:0:2104:C:OP1	2.36	0.44
28:1:28:HIS:O	28:1:32:LYS:N	2.49	0.44
1:0:2471:G:N3	1:0:2633:A:H2	2.16	0.44
31:9:3:A:H2'	31:9:26:C:O2	2.18	0.44
1:0:1681:G:H5''	1:0:1682:A:H5'	1.99	0.44
1:0:2892:G:C6	1:0:2893:C:C4	3.06	0.44
1:0:1632:A:C2'	1:0:1633:C:H5'	2.46	0.44
1:0:354:A:H2'	1:0:355:C:C6	2.53	0.44
1:0:2349:G:H2'	1:0:2350:G:C8	2.52	0.44
1:0:2467:A:H1'	39:0:3524:HOH:O	2.17	0.44
1:0:228:C:C2'	1:0:229:G:H5'	2.48	0.44
1:0:1501:A:H4'	39:0:4703:HOH:O	2.17	0.44
1:0:1613:C:H2'	1:0:1614:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1531:U:C2	1:0:1661:A:N1	2.85	0.44
1:0:1732:A:C6	1:0:2840:A:H1'	2.52	0.44
5:D:15:GLU:HA	5:D:16:PRO:HD3	1.85	0.44
1:0:2245:C:H6	1:0:2245:C:O5'	2.01	0.44
1:0:1126:C:O2'	1:0:1128:U:H6	2.01	0.44
1:0:2254:G:H1'	39:0:4611:HOH:O	2.18	0.44
1:0:1792:C:C2	1:0:1793:C:H5	2.36	0.44
1:0:736:A:H8	39:0:6948:HOH:O	2.01	0.44
1:0:1216:G:N2	1:0:1217:G:H1'	2.33	0.44
1:0:1647:G:H2'	1:0:1648:G:O4'	2.17	0.44
1:0:2554:U:C6	1:0:2577:A:N6	2.85	0.44
1:0:2331:C:H1'	1:0:2356:A:C2	2.52	0.44
1:0:2110:G:C2	1:0:2478:U:N3	2.86	0.44
1:0:400:C:O2'	1:0:401:C:H5'	2.18	0.44
5:D:172:VAL:HG12	5:D:173:GLU:H	1.83	0.44
1:0:407:A:H2'	1:0:408:A:C8	2.52	0.44
1:0:1186:C:N4	1:0:1190:G:H22	2.12	0.44
1:0:1299:G:H5'	39:0:8773:HOH:O	2.17	0.44
1:0:2461:U:C2	1:0:2466:G:H1'	2.52	0.44
1:0:2769:C:H2'	1:0:2770:G:C5'	2.48	0.44
1:0:1923:G:H4'	30:3:31:THR:O	2.18	0.44
1:0:2066:C:H5''	39:0:4041:HOH:O	2.17	0.44
1:0:2832:C:H5	39:0:6957:HOH:O	2.01	0.44
1:0:577:G:C6	1:0:581:G:O6	2.70	0.44
1:0:816:G:C5	1:0:817:G:C6	3.06	0.44
1:0:690:G:H4'	1:0:741:C:O2	2.18	0.44
1:0:1841:C:OP2	1:0:2022:A:H8	2.00	0.44
1:0:2076:U:H2'	39:0:6153:HOH:O	2.17	0.44
1:0:2001:G:O2'	1:0:2002:C:H5'	2.18	0.44
3:B:272:ILE:HG22	39:B:7492:HOH:O	2.17	0.44
1:0:2055:A:H5'	19:R:134:SER:HB2	2.00	0.44
1:0:1641:A:C8	1:0:1702:U:O4	2.71	0.44
1:0:533:U:H2'	1:0:2814:A:C6	2.52	0.44
5:D:76:ARG:NH1	31:9:42:C:O2	2.50	0.44
1:0:119:A:H2'	1:0:120:A:C5'	2.45	0.44
1:0:595:U:H2'	1:0:596:C:C6	2.51	0.44
1:0:566:A:H2'	1:0:567:U:C5'	2.48	0.44
1:0:2265:U:H2'	1:0:2266:A:C8	2.53	0.44
1:0:1200:A:H5'	39:0:7124:HOH:O	2.18	0.44
1:0:2120:U:H1'	39:0:3535:HOH:O	2.17	0.44
1:0:81:G:N3	1:0:98:A:C2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:23:ILE:HG21	9:H:97:VAL:HG11	2.00	0.44
1:O:206:G:H5'	14:M:185:PRO:HD3	1.99	0.44
1:O:2846:C:H4'	3:B:156:LYS:HB2	1.99	0.44
1:O:2587:OMU:HM23	1:O:2589:U:C6	2.53	0.44
13:L:136:ALA:HB3	39:L:6166:HOH:O	2.18	0.44
1:O:506:G:H22	1:O:509:A:H5'	1.76	0.43
31:9:92:G:C6	31:9:93:A:N6	2.86	0.43
1:O:1181:A:N1	1:O:1192:A:O2'	2.47	0.43
1:O:1185:U:H2'	1:O:1186:C:C6	2.53	0.43
1:O:1829:A:H2'	1:O:1830:C:C5'	2.46	0.43
1:O:21:G:C4'	19:R:2:ILE:HG22	2.44	0.43
1:O:2321:A:H62	1:O:2380:A:H62	1.65	0.43
1:O:2853:U:C4	1:O:2906:A:N6	2.85	0.43
1:O:2730:G:O2'	1:O:2731:G:H5'	2.17	0.43
1:O:2598:U:O2	1:O:2600:A:H8	2.01	0.43
1:O:1909:A:H2'	1:O:1910:A:C8	2.53	0.43
1:O:927:U:H4'	39:O:3262:HOH:O	2.18	0.43
28:1:2:GLY:O	28:1:6:PRO:HG2	2.18	0.43
1:O:2420:G:O2'	1:O:2421:G:H5'	2.17	0.43
11:J:75:PRO:HG2	11:J:105:LEU:HD21	2.00	0.43
1:O:792:G:O2'	1:O:793:A:H5'	2.18	0.43
1:O:212:A:O4'	1:O:214:U:C6	2.71	0.43
1:O:599:G:H2'	1:O:600:G:C8	2.53	0.43
1:O:1448:A:H4'	39:O:6039:HOH:O	2.18	0.43
1:O:2507:G:O6	1:O:2511:A:H4'	2.18	0.43
1:O:703:G:O2'	1:O:704:C:H5'	2.18	0.43
1:O:2739:A:C6	1:O:2740:G:C5	3.06	0.43
1:O:1933:G:O2'	1:O:1934:A:H5'	2.18	0.43
19:R:63:ASN:ND2	19:R:75:TRP:HZ2	2.17	0.43
1:O:952:G:N3	1:O:2302:A:H2'	2.33	0.43
1:O:868:G:C5	1:O:887:G:C8	3.06	0.43
1:O:1188:A:N7	1:O:1189:A:C2	2.87	0.43
1:O:530:C:H2'	1:O:531:G:O4'	2.18	0.43
1:O:235:C:O2'	1:O:236:A:H2'	2.18	0.43
1:O:66:G:C2	1:O:109:U:C4	3.06	0.43
1:O:1788:U:C2	1:O:1805:G:N2	2.87	0.43
25:X:74:ALA:HB2	25:X:85:VAL:HG13	2.00	0.43
1:O:596:C:H2'	1:O:597:A:C8	2.53	0.43
1:O:1758:U:C2'	1:O:1759:A:H5'	2.48	0.43
1:O:1311:G:C2	1:O:1312:G:C8	3.06	0.43
1:O:1557:G:H2'	1:O:1558:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2552:C:C6	1:0:2577:A:N7	2.86	0.43
1:0:2364:A:H5''	18:Q:15:LYS:HD3	2.00	0.43
5:D:149:ARG:HH12	15:N:15:GLU:HA	1.83	0.43
1:0:56:G:H1'	39:0:4338:HOH:O	2.18	0.43
1:0:2300:A:H4'	1:0:2301:A:O5'	2.18	0.43
1:0:836:G:N3	1:0:836:G:H2'	2.34	0.43
1:0:1689:A:N3	1:0:1689:A:H2'	2.32	0.43
1:0:1127:C:C2'	1:0:1128:U:H5'	2.48	0.43
1:0:1503:U:C2'	1:0:1504:A:H5'	2.48	0.43
1:0:281:U:O2'	1:0:282:C:H5'	2.19	0.43
1:0:1821:A:O2'	1:0:1822:A:H5'	2.17	0.43
1:0:67:A:C6	1:0:109:U:H1'	2.53	0.43
1:0:1332:C:O2'	1:0:1333:U:H5'	2.19	0.43
1:0:658:C:O2'	1:0:662:U:OP1	2.30	0.43
1:0:549:A:C2	1:0:550:C:C2	3.06	0.43
1:0:1610:G:H2'	1:0:1611:G:O4'	2.18	0.43
31:9:3:A:OP2	31:9:25:G:N2	2.51	0.43
1:0:2467:A:H5''	39:0:2924:HOH:O	2.17	0.43
1:0:869:G:C8	1:0:869:G:OP2	2.72	0.43
1:0:1942:A:H2'	39:0:4237:HOH:O	2.18	0.43
1:0:730:G:H2'	1:0:731:U:C6	2.53	0.43
1:0:1825:U:O4'	1:0:1999:C:H5''	2.19	0.43
1:0:1861:C:O2'	1:0:1862:C:H5'	2.19	0.43
1:0:387:G:O2'	1:0:388:G:H5'	2.18	0.43
1:0:938:G:N2	1:0:1031:G:H1'	2.34	0.43
1:0:1786:C:C5	1:0:1787:C:H5	2.37	0.43
1:0:1930:A:H2'	1:0:1931:A:C8	2.52	0.43
1:0:815:U:O2'	1:0:816:G:H5'	2.19	0.43
1:0:1076:G:C2	1:0:1084:C:N3	2.86	0.43
1:0:2103:A:H2'	1:0:2104:C:H5'	2.01	0.43
1:0:1853:C:H5'	2:A:228:ILE:O	2.18	0.43
1:0:1135:G:N2	1:0:1228:C:C2	2.87	0.43
1:0:2097:G:N2	1:0:2098:C:H1'	2.34	0.43
13:L:3:LYS:NZ	39:L:3752:HOH:O	2.51	0.43
1:0:1074:G:H4'	1:0:1260:G:C6	2.54	0.43
1:0:1086:A:N6	24:W:11:VAL:HG11	2.33	0.43
27:Z:78:ILE:HD12	39:Z:3477:HOH:O	2.16	0.43
1:0:1288:U:H4'	24:W:27:HIS:CD2	2.54	0.43
1:0:1162:G:N2	1:0:1185:U:C2	2.87	0.43
1:0:1444:G:H5''	20:S:11:THR:HG22	2.00	0.43
1:0:2781:U:H2'	1:0:2782:G:C5'	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:59:C:H1'	39:9:2772:HOH:O	2.18	0.43
1:0:1742:A:H61	1:0:2037:C:H42	1.66	0.43
1:0:2635:A:C2'	1:0:2636:C:H5'	2.48	0.43
1:0:1758:U:H2'	1:0:1759:A:O4'	2.19	0.43
1:0:1812:G:H4'	1:0:1814:G:O4'	2.18	0.43
1:0:1397:C:H1'	17:P:28:GLN:OE1	2.18	0.43
1:0:2591:C:H2'	1:0:2592:G:H5'	2.01	0.43
1:0:944:G:H21	24:W:44:MET:HE2	1.83	0.43
1:0:2686:C:H2'	1:0:2687:G:C8	2.54	0.43
1:0:1924:A:O5'	1:0:1924:A:H8	2.01	0.43
1:0:1102:C:H6	1:0:1102:C:O5'	2.02	0.43
1:0:1815:A:O5'	1:0:1815:A:H8	2.01	0.43
1:0:1118:A:C8	1:0:1118:A:C3'	2.87	0.43
1:0:120:A:C6	28:1:17:THR:HG21	2.53	0.43
1:0:2738:G:H2'	1:0:2739:A:H8	1.84	0.43
1:0:1594:C:C2	1:0:1601:G:N2	2.86	0.43
1:0:1399:A:H2'	1:0:1400:C:C6	2.54	0.43
1:0:661:G:C5	1:0:662:U:C4	3.07	0.43
1:0:2642:G:C6	1:0:2643:G:C5	3.06	0.43
1:0:2038:A:C2	1:0:2039:A:C5	3.07	0.43
1:0:2846:C:H2'	1:0:2847:G:H8	1.82	0.43
17:P:55:LYS:HG2	17:P:56:GLY:N	2.34	0.43
1:0:961:A:H4'	39:0:6342:HOH:O	2.17	0.43
39:0:3707:HOH:O	2:A:11:ARG:HD3	2.18	0.43
1:0:2835:C:H42	1:0:2845:G:H1	1.65	0.43
1:0:453:A:H4'	1:0:455:A:N7	2.33	0.43
1:0:1274:A:C6	1:0:1275:C:C4	3.07	0.43
1:0:2882:G:H8	1:0:2882:G:O5'	2.01	0.43
1:0:1118:A:C8	1:0:1119:G:H5''	2.54	0.43
1:0:2297:U:C2	1:0:2298:C:C6	3.07	0.43
1:0:1626:A:H2'	1:0:1627:G:C5'	2.49	0.43
1:0:1626:A:O2'	1:0:1627:G:H5'	2.19	0.43
1:0:594:C:C4	1:0:595:U:N3	2.86	0.43
1:0:1730:G:H5'	1:0:1731:C:C5	2.54	0.43
1:0:656:G:H1'	39:0:7042:HOH:O	2.18	0.43
14:M:99:ARG:HD2	14:M:167:GLY:HA2	2.01	0.43
1:0:465:U:C5	1:0:475:G:N2	2.87	0.43
1:0:217:C:H2'	1:0:218:C:C6	2.54	0.43
1:0:603:A:H5''	1:0:604:G:OP1	2.19	0.43
1:0:865:G:O2'	1:0:866:U:H5'	2.19	0.43
1:0:2441:U:H4'	13:L:53:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2699:A:H2'	1:0:2700:G:O4'	2.18	0.43
1:0:541:C:O2'	1:0:542:A:H5''	2.17	0.43
1:0:1130:U:O2'	31:9:91:C:H4'	2.18	0.43
39:0:3308:HOH:O	31:9:105:A:H5''	2.19	0.43
1:0:2768:A:H5''	39:0:3093:HOH:O	2.19	0.43
3:B:238:ASN:HD22	3:B:240:GLY:H	1.66	0.43
1:0:287:C:H3'	1:0:287:C:C6	2.54	0.43
1:0:24:G:O2'	1:0:25:A:OP2	2.31	0.43
1:0:1904:A:H2'	1:0:1905:U:H6	1.84	0.43
1:0:1933:G:C2'	1:0:1934:A:H5'	2.48	0.43
1:0:458:G:H2'	1:0:459:A:C8	2.54	0.43
1:0:759:C:C5	1:0:761:A:C8	3.07	0.43
1:0:940:G:N3	1:0:1032:A:C2	2.86	0.43
1:0:2329:C:O2'	1:0:2330:U:H5'	2.19	0.43
1:0:1361:C:H2'	1:0:1362:U:H6	1.83	0.43
20:S:73:ASP:O	20:S:77:VAL:HG23	2.18	0.43
1:0:2716:G:O2'	1:0:2717:C:H5'	2.19	0.42
1:0:1185:U:H5'	39:0:7308:HOH:O	2.18	0.42
1:0:2795:C:H1'	39:0:8323:HOH:O	2.19	0.42
1:0:2326:C:H4'	1:0:2412:G:C4'	2.49	0.42
1:0:812:A:C2	1:0:813:C:C2	3.07	0.42
1:0:343:C:H2'	1:0:344:C:C6	2.50	0.42
1:0:664:U:H5	1:0:680:G:C4	2.36	0.42
1:0:2383:G:C6	1:0:2384:U:C4	3.07	0.42
1:0:1970:G:H2'	1:0:1970:G:N3	2.34	0.42
1:0:1314:U:H2'	39:0:5081:HOH:O	2.18	0.42
1:0:2577:A:H5'	39:0:7700:HOH:O	2.19	0.42
2:A:70:ALA:HA	2:A:71:PRO:HD3	1.84	0.42
1:0:295:C:H2'	1:0:296:G:O4'	2.18	0.42
1:0:48:A:C5	1:0:113:A:C2	3.07	0.42
6:E:112:ALA:HA	6:E:113:PRO:HD3	1.89	0.42
1:0:1849:G:H1'	1:0:2011:A:N1	2.34	0.42
1:0:1163:G:H1	1:0:1184:C:N4	2.16	0.42
1:0:1585:C:N3	1:0:1611:G:C2	2.87	0.42
1:0:313:U:H2'	1:0:314:G:H5'	2.00	0.42
1:0:661:G:C5	1:0:686:A:C2	3.07	0.42
1:0:894:A:N1	4:C:87:ARG:NH2	2.67	0.42
1:0:292:G:H2'	1:0:358:G:N2	2.34	0.42
1:0:2791:U:H6	1:0:2791:U:O5'	2.02	0.42
1:0:2103:A:HO2'	1:0:2104:C:P	2.41	0.42
1:0:453:A:H5''	39:0:7136:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1965:C:H2'	1:0:1966:U:C6	2.54	0.42
24:W:5:VAL:HG11	24:W:153:MET:HE1	2.01	0.42
1:0:1698:U:H5	39:0:7522:HOH:O	2.02	0.42
1:0:1350:U:H4'	39:0:4055:HOH:O	2.19	0.42
1:0:1206:U:H2'	1:0:1207:A:O4'	2.20	0.42
1:0:1779:A:H2'	1:0:1780:G:O4'	2.19	0.42
37:0:9101:MUL:C14	37:0:9101:MUL:C10	2.97	0.42
1:0:1014:A:C6	1:0:1015:C:H1'	2.54	0.42
1:0:1307:A:O5'	1:0:1307:A:H8	2.02	0.42
1:0:1632:A:C3'	1:0:1633:C:H5'	2.49	0.42
1:0:908:A:O2'	1:0:909:U:H5'	2.19	0.42
31:9:36:C:C5	31:9:37:C:C4	3.07	0.42
16:O:32:ARG:HH21	16:O:35:LYS:HZ2	1.67	0.42
1:0:840:U:C5	1:0:2648:U:C5	3.07	0.42
1:0:256:C:H2'	1:0:257:G:H5'	2.00	0.42
1:0:372:A:H2'	1:0:373:G:H8	1.83	0.42
1:0:324:G:C2	1:0:325:U:C6	3.07	0.42
1:0:889:C:H2'	1:0:890:C:C6	2.54	0.42
1:0:2328:U:H2'	1:0:2329:C:O4'	2.19	0.42
1:0:2359:G:H3'	39:0:4829:HOH:O	2.19	0.42
1:0:1535:G:H2'	1:0:1536:C:C6	2.54	0.42
1:0:1379:A:H1'	39:0:5427:HOH:O	2.19	0.42
14:M:68:ARG:NE	14:M:73:ARG:HH11	2.16	0.42
1:0:1676:G:C6	1:0:1677:U:N3	2.84	0.42
1:0:308:U:C2'	21:T:52:ARG:NH2	2.79	0.42
1:0:2054:A:H5'	39:0:3751:HOH:O	2.18	0.42
31:9:41:C:H2'	31:9:42:C:C6	2.53	0.42
1:0:1593:C:H2'	1:0:1594:C:C6	2.47	0.42
1:0:1441:G:H2'	1:0:1442:A:H8	1.82	0.42
1:0:946:C:H2'	1:0:947:U:C6	2.54	0.42
1:0:1935:C:H2'	1:0:1936:C:C6	2.54	0.42
1:0:1755:A:H2'	1:0:1756:G:O4'	2.20	0.42
1:0:1338:U:O2'	1:0:1339:G:H5'	2.20	0.42
1:0:801:U:O2'	1:0:802:G:H5'	2.19	0.42
19:R:109:MET:HE3	19:R:109:MET:HB2	1.92	0.42
1:0:2072:G:C6	1:0:2533:C:H1'	2.54	0.42
1:0:1168:C:H5'	10:I:83:GLY:HA3	2.00	0.42
1:0:399:C:H1'	14:M:194:GLY:OXT	2.20	0.42
1:0:338:C:H4'	4:C:174:ILE:HD11	2.01	0.42
1:0:64:G:H2'	1:0:65:C:O4'	2.19	0.42
1:0:1082:A:H2'	1:0:1083:C:OP1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:217:C:OP1	1:0:395:A:O2'	2.26	0.42
1:0:2600:A:H2'	1:0:2601:A:O4'	2.20	0.42
1:0:2686:C:H2'	1:0:2687:G:H8	1.84	0.42
1:0:2414:A:H1'	39:0:3480:HOH:O	2.19	0.42
1:0:1687:C:H1'	28:1:8:GLN:O	2.20	0.42
1:0:784:A:H2'	1:0:785:U:O4'	2.19	0.42
7:F:32:GLY:N	39:F:3111:HOH:O	2.51	0.42
1:0:1157:C:O2'	1:0:1158:G:H5'	2.19	0.42
1:0:1182:C:C1'	1:0:1192:A:H8	2.31	0.42
1:0:2766:A:O2'	1:0:2767:C:H5'	2.19	0.42
1:0:2815:G:N7	11:J:80:LYS:NZ	2.68	0.42
1:0:1918:U:O2	1:0:1920:C:H3'	2.19	0.42
1:0:314:G:C2	1:0:317:A:C8	3.07	0.42
1:0:1617:C:C4	1:0:1643:C:H4'	2.54	0.42
1:0:1069:C:H2'	1:0:1070:A:O4'	2.19	0.42
1:0:2397:G:H2'	1:0:2398:A:C8	2.52	0.42
1:0:946:C:O2'	1:0:947:U:H5'	2.20	0.42
1:0:1947:G:N2	1:0:1966:U:O2	2.52	0.42
1:0:806:A:H2'	1:0:807:A:O4'	2.20	0.42
1:0:2485:A:H3'	39:0:5048:HOH:O	2.19	0.42
1:0:1452:G:H1'	35:0:8803:CL:CL	2.57	0.42
1:0:1456:C:H2'	1:0:1457:U:C6	2.54	0.42
1:0:561:G:C2	1:0:562:A:N7	2.88	0.42
1:0:170:U:H5'	30:3:48:ASN:ND2	2.27	0.42
1:0:1692:C:H2'	39:0:6064:HOH:O	2.19	0.42
1:0:933:C:H4'	1:0:1297:U:H4'	2.00	0.42
1:0:2769:C:H2'	1:0:2770:G:H5'	2.01	0.42
1:0:2319:C:H4'	1:0:2322:U:C4	2.55	0.42
1:0:2715:G:OP1	3:B:16:ARG:NH2	2.53	0.42
1:0:595:U:H6	1:0:595:U:H3'	1.85	0.42
39:0:6217:HOH:O	21:T:38:ARG:NH1	2.51	0.42
1:0:1866:A:N7	1:0:1867:G:H1'	2.35	0.42
15:N:44:ARG:NH1	31:9:4:G:H21	2.17	0.42
1:0:2419:U:H5''	1:0:2420:G:H5'	2.02	0.42
1:0:758:A:H2'	1:0:759:C:O4'	2.20	0.42
1:0:1546:G:H2'	1:0:1547:A:O4'	2.20	0.42
1:0:2583:A:H4'	12:K:43:ARG:O	2.19	0.42
1:0:1848:G:H4'	39:0:6016:HOH:O	2.20	0.42
31:9:91:C:H2'	31:9:92:G:O4'	2.19	0.42
1:0:1688:G:C6	1:0:1692:C:C5	3.07	0.42
31:9:41:C:H2'	31:9:42:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1739:G:C6	1:0:1740:U:C4	3.07	0.42
1:0:2122:C:O2	14:M:76:ARG:NH2	2.52	0.42
1:0:1384:C:H5'	25:X:30:MET:HG2	2.02	0.42
1:0:666:A:N7	1:0:667:C:C2	2.88	0.42
1:0:740:G:H2'	1:0:741:C:H6	1.84	0.42
1:0:2291:A:N9	1:0:2309:C:H5'	2.35	0.42
1:0:1079:A:H4'	1:0:2078:U:H5'	2.02	0.42
1:0:2300:A:H4'	1:0:2301:A:N3	2.34	0.42
1:0:122:C:H5''	39:0:8215:HOH:O	2.19	0.42
6:E:101:GLU:HB2	6:E:116:THR:O	2.20	0.42
1:0:2555:C:H6	1:0:2555:C:O5'	2.03	0.42
1:0:2289:G:C2'	1:0:2290:U:H5'	2.49	0.42
1:0:187:A:C5'	1:0:188:C:OP2	2.67	0.42
30:3:64:LYS:HB3	30:3:65:THR:H	1.61	0.42
1:0:1559:A:C1'	39:0:5067:HOH:O	2.63	0.42
1:0:344:C:H2'	1:0:345:G:O4'	2.19	0.42
9:H:32:ALA:H	9:H:69:ARG:NH1	2.17	0.42
1:0:2750:G:H2'	1:0:2751:C:H6	1.84	0.42
1:0:676:C:N4	1:0:677:C:N4	2.68	0.42
1:0:2591:C:H2'	1:0:2592:G:C5'	2.49	0.42
1:0:2039:A:H2'	1:0:2040:C:C6	2.54	0.42
1:0:81:G:H5'	21:T:65:VAL:O	2.20	0.42
1:0:1847:A:H2'	1:0:1848:G:O4'	2.20	0.42
1:0:1025:C:H2'	1:0:1026:U:C6	2.55	0.42
1:0:2034:U:H4'	39:0:5144:HOH:O	2.20	0.42
31:9:112:U:H2'	31:9:113:C:H5'	2.01	0.42
2:A:100:PRO:HG2	2:A:103:VAL:HG21	2.01	0.42
31:9:27:C:O5'	31:9:27:C:H6	2.03	0.42
1:0:820:G:N7	2:A:171:LYS:HB2	2.35	0.42
1:0:1448:A:N7	1:0:1506:U:C2	2.88	0.42
1:0:137:U:H3'	1:0:139:C:H41	1.85	0.42
1:0:74:G:H2'	1:0:75:U:C6	2.55	0.42
1:0:106:A:H1'	39:0:4714:HOH:O	2.19	0.42
1:0:853:C:H2'	1:0:854:G:O4'	2.20	0.42
1:0:25:A:H1'	1:0:519:A:C2	2.55	0.42
1:0:1879:U:H1'	39:0:8121:HOH:O	2.20	0.42
1:0:749:C:O2'	1:0:750:A:H5'	2.20	0.42
1:0:208:C:C6	1:0:208:C:C3'	3.03	0.42
1:0:1029:U:O2'	1:0:1273:C:OP1	2.37	0.42
4:C:118:THR:O	4:C:136:VAL:HG13	2.20	0.42
1:0:2044:G:H2'	1:0:2045:G:O5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:22:PHE:HD2	4:C:119:ALA:HB2	1.85	0.42
1:0:2072:G:H3'	1:0:2073:G:H5''	2.01	0.41
1:0:1505:U:H6	1:0:1505:U:H2'	1.76	0.41
1:0:640:G:C5	1:0:641:G:N7	2.88	0.41
1:0:10:U:C4	1:0:532:A:N7	2.88	0.41
1:0:2543:G:O3'	1:0:2590:U:H5'	2.20	0.41
1:0:657:G:H2'	1:0:658:C:H6	1.85	0.41
1:0:1969:A:N7	1:0:1970:G:C6	2.88	0.41
1:0:325:U:H2'	1:0:326:G:H8	1.85	0.41
1:0:1884:G:O6	2:A:190:ARG:HD2	2.20	0.41
1:0:1388:U:H2'	1:0:1389:G:O4'	2.20	0.41
1:0:1001:U:O2'	1:0:1002:G:H5'	2.20	0.41
1:0:1391:G:H21	1:0:1434:A:H5''	1.85	0.41
1:0:909:U:H5	39:0:6389:HOH:O	2.03	0.41
1:0:2042:U:H1'	39:0:7090:HOH:O	2.20	0.41
1:0:1396:C:H1'	17:P:1:THR:O	2.19	0.41
1:0:2291:A:H2'	1:0:2291:A:N3	2.35	0.41
13:L:90:ARG:HA	13:L:119:THR:HB	2.01	0.41
9:H:54:VAL:HG13	9:H:162:PRO:HG3	2.01	0.41
1:0:2549:C:O2'	1:0:2550:U:H5'	2.20	0.41
7:F:1:PRO:HB2	39:F:5897:HOH:O	2.20	0.41
1:0:1262:C:H1'	24:W:120:PRO:CG	2.50	0.41
1:0:2486:A:H2	37:0:9101:MUL:C22	2.32	0.41
37:0:9101:MUL:H4	37:0:9101:MUL:H131	1.78	0.41
1:0:45:A:N6	1:0:147:G:C4	2.89	0.41
1:0:2379:G:H4'	1:0:2380:A:H3'	2.01	0.41
1:0:109:U:O2	1:0:109:U:C2'	2.68	0.41
1:0:1528:A:H61	1:0:1663:G:H1'	1.85	0.41
1:0:317:A:C5'	39:0:8405:HOH:O	2.68	0.41
1:0:24:G:C2	1:0:518:G:N3	2.88	0.41
1:0:2735:U:H2'	1:0:2736:U:H6	1.83	0.41
1:0:1758:U:O2'	1:0:1759:A:H5'	2.20	0.41
24:W:129:LYS:NZ	31:9:87:U:H2'	2.34	0.41
1:0:2250:G:H2'	1:0:2251:G:C8	2.54	0.41
1:0:422:G:C6	1:0:2446:G:C6	3.08	0.41
19:R:59:PHE:O	19:R:63:ASN:HB3	2.19	0.41
1:0:2067:A:C4	1:0:2068:G:C8	3.08	0.41
4:C:228:ALA:HA	4:C:229:PRO:HD3	1.90	0.41
1:0:2278:U:H5'	39:0:4608:HOH:O	2.20	0.41
1:0:1988:C:H2'	1:0:1989:G:O4'	2.20	0.41
2:A:53:ALA:HB1	39:A:1902:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:46:TYR:HA	9:H:47:PRO:HD3	1.90	0.41
15:N:108:SER:HA	15:N:109:PRO:HD3	1.81	0.41
1:0:913:A:H8	1:0:913:A:O5'	2.03	0.41
1:0:2307:A:H8	1:0:2307:A:O5'	2.03	0.41
1:0:1833:U:O2'	1:0:1834:C:H5'	2.19	0.41
1:0:559:U:H2'	1:0:560:U:O4'	2.20	0.41
1:0:2787:C:H2'	1:0:2788:A:O4'	2.20	0.41
1:0:182:G:H2'	1:0:183:A:H8	1.86	0.41
1:0:1061:C:H1'	1:0:2283:G:O6	2.21	0.41
1:0:656:G:H1	1:0:749:C:H42	1.67	0.41
1:0:360:A:H2'	1:0:361:C:C6	2.56	0.41
1:0:1150:A:H3'	1:0:1151:G:C5'	2.51	0.41
1:0:472:A:N1	1:0:888:U:O2'	2.43	0.41
1:0:1760:G:P	1:0:1777:G:H22	2.43	0.41
1:0:2374:G:H2'	1:0:2375:A:C8	2.55	0.41
11:J:127:ILE:HG22	35:J:8801:CL:CL	2.57	0.41
1:0:1649:G:H5'	39:0:6234:HOH:O	2.20	0.41
1:0:871:G:C6	1:0:872:U:C4	3.09	0.41
1:0:820:G:O2'	1:0:856:G:H4'	2.21	0.41
1:0:36:C:C2	1:0:447:A:C2	3.09	0.41
1:0:2059:U:C2	1:0:2060:A:C8	3.08	0.41
1:0:2035:C:O5'	1:0:2035:C:H6	2.03	0.41
31:9:104:A:H2'	31:9:105:A:H5'	2.03	0.41
1:0:1788:U:O2'	1:0:1789:G:H5'	2.20	0.41
1:0:1929:G:H1'	39:0:4103:HOH:O	2.20	0.41
1:0:1486:A:N6	39:0:3379:HOH:O	2.49	0.41
1:0:1748:U:C5	1:0:1749:U:C4	3.08	0.41
1:0:1041:U:H4'	1:0:1295:G:H5'	2.03	0.41
1:0:1249:U:H2'	1:0:1250:C:C6	2.55	0.41
1:0:1124:A:N3	1:0:1124:A:H2'	2.34	0.41
1:0:1158:G:O2'	1:0:1159:G:H5'	2.20	0.41
1:0:963:C:O2	1:0:1005:A:N1	2.53	0.41
1:0:1015:C:C2	1:0:1016:U:C5	3.09	0.41
1:0:39:G:C2	1:0:444:C:O2	2.74	0.41
1:0:1592:G:C5	1:0:1593:C:C4	3.08	0.41
1:0:2361:A:H8	1:0:2361:A:OP2	2.04	0.41
1:0:822:C:C2'	1:0:822:C:O2	2.68	0.41
25:X:43:VAL:HG13	25:X:76:ARG:NH1	2.35	0.41
1:0:786:G:H1'	1:0:1488:U:O2	2.20	0.41
1:0:2055:A:H4'	39:0:7274:HOH:O	2.20	0.41
1:0:1521:C:H2'	1:0:1522:A:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1625:U:H5''	39:0:5289:HOH:O	2.20	0.41
1:0:1189:A:O2'	1:0:1208:C:H2'	2.20	0.41
1:0:542:A:H2'	1:0:543:G:O4'	2.20	0.41
31:9:73:A:H2'	31:9:74:G:O4'	2.20	0.41
1:0:1679:C:O2	1:0:1679:C:H2'	2.21	0.41
1:0:317:A:H5'	39:0:8405:HOH:O	2.21	0.41
1:0:2409:C:O2'	1:0:2410:G:H5'	2.21	0.41
1:0:686:A:O2'	1:0:747:G:H4'	2.21	0.41
1:0:210:U:H2'	1:0:211:U:H6	1.86	0.41
1:0:372:A:O2'	1:0:373:G:H5'	2.20	0.41
1:0:217:C:H2'	1:0:218:C:O4'	2.21	0.41
1:0:1566:C:H2'	1:0:1567:G:H8	1.84	0.41
24:W:149:LEU:HG	24:W:153:MET:HE2	2.03	0.41
2:A:217:ARG:HG2	2:A:229:ALA:HB2	2.03	0.41
1:0:1757:U:H6	1:0:1757:U:O5'	2.04	0.41
1:0:1202:A:C2'	1:0:1203:G:H5'	2.51	0.41
1:0:1597:A:C4	1:0:1598:A:C8	3.09	0.41
1:0:1597:A:O4'	17:P:95:GLU:HG2	2.21	0.41
1:0:2498:C:C2'	1:0:2499:U:H5'	2.50	0.41
1:0:1297:U:P	39:0:3033:HOH:O	2.78	0.41
1:0:313:U:H2'	1:0:314:G:C5'	2.50	0.41
12:K:20:CYS:HB2	12:K:29:LEU:HG	2.03	0.41
1:0:960:G:H4'	39:0:7253:HOH:O	2.19	0.41
1:0:1359:U:O5'	1:0:1360:C:H5''	2.21	0.41
1:0:841:A:C8	1:0:843:A:C8	3.08	0.41
1:0:1902:G:N2	1:0:1936:C:C2	2.89	0.41
1:0:1013:A:H5''	1:0:2302:A:H61	1.86	0.41
1:0:395:A:H3'	1:0:397:A:N7	2.36	0.41
1:0:407:A:C2	1:0:408:A:C4	3.08	0.41
1:0:765:G:H4'	4:C:69:HIS:HB2	2.02	0.41
15:N:151:ASP:HB3	39:N:3251:HOH:O	2.20	0.41
4:C:133:ARG:NH2	39:C:5086:HOH:O	2.53	0.41
7:F:58:GLU:HB3	14:M:8:ILE:HG23	2.03	0.41
1:0:1283:G:H2'	1:0:1284:G:O4'	2.20	0.41
1:0:1355:A:N3	1:0:1355:A:H2'	2.36	0.41
1:0:871:G:C5	1:0:872:U:C4	3.09	0.41
31:9:73:A:C6	31:9:74:G:C6	3.09	0.41
1:0:1175:G:H1'	1:0:1193:A:C4	2.56	0.41
1:0:1666:C:O2'	1:0:1667:A:C5'	2.69	0.41
1:0:1611:G:C2	1:0:1612:A:N7	2.89	0.41
1:0:1506:U:H6	1:0:1506:U:H5'	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1299:G:N2	39:0:3448:HOH:O	2.54	0.41
1:0:339:A:N6	39:0:6198:HOH:O	2.51	0.41
1:0:2904:U:C5	1:0:2905:A:N7	2.89	0.41
1:0:876:A:C6	1:0:878:G:C8	3.08	0.41
1:0:959:C:O2	1:0:1005:A:N6	2.54	0.41
1:0:2385:G:C4	1:0:2386:U:C5	3.09	0.41
31:9:49:G:H2'	31:9:50:G:O4'	2.21	0.41
1:0:1851:G:O2'	1:0:1852:A:H5'	2.21	0.41
1:0:2590:U:H2'	1:0:2591:C:H5'	2.01	0.41
1:0:944:G:H21	24:W:44:MET:CE	2.34	0.41
1:0:1881:A:OP1	2:A:199:HIS:HE1	2.04	0.41
2:A:199:HIS:CD2	2:A:201:PHE:H	2.37	0.41
1:0:1992:U:C2	1:0:1994:A:OP2	2.73	0.41
1:0:57:C:H4'	23:V:34:GLN:HE22	1.84	0.41
1:0:268:U:C4	1:0:269:G:C6	3.09	0.41
1:0:918:G:C2	1:0:926:A:C2	3.09	0.41
1:0:861:A:H1'	1:0:1488:U:O4	2.20	0.41
1:0:1257:C:O2'	1:0:1258:G:H5'	2.21	0.41
1:0:130:C:O2'	1:0:131:A:N7	2.48	0.41
1:0:1531:U:H1'	1:0:1661:A:C2	2.56	0.41
1:0:1689:A:OP2	1:0:1689:A:H8	2.04	0.41
1:0:1338:U:H2'	1:0:1339:G:O4'	2.20	0.41
1:0:2455:A:H2'	1:0:2456:A:O4'	2.21	0.41
1:0:2629:C:O2'	1:0:2630:G:H5'	2.21	0.41
1:0:644:G:H1'	39:0:5820:HOH:O	2.21	0.41
1:0:1111:U:H2'	1:0:1112:G:C8	2.55	0.41
3:B:120:ASP:OD2	3:B:123:ALA:HB3	2.21	0.41
1:0:61:G:N1	1:0:86:A:N6	2.69	0.41
1:0:2624:A:O2'	1:0:2625:C:H5'	2.20	0.41
1:0:1608:G:O2'	1:0:1609:C:H5'	2.21	0.41
1:0:2694:A:C6	1:0:2702:A:C8	3.09	0.41
1:0:1156:C:C6	1:0:1156:C:H3'	2.56	0.41
1:0:545:G:N1	1:0:612:U:O2	2.54	0.41
1:0:36:C:N3	1:0:447:A:C2	2.89	0.41
1:0:73:U:O5'	1:0:73:U:H6	2.03	0.41
1:0:334:G:H2'	1:0:335:U:O4'	2.21	0.41
1:0:23:G:O5'	1:0:23:G:H8	2.03	0.41
1:0:629:A:H2'	1:0:630:A:H5'	2.03	0.41
1:0:1768:C:H2'	1:0:1769:C:O4'	2.20	0.41
1:0:2017:U:H2'	1:0:2018:A:C8	2.55	0.41
1:0:822:C:O2	1:0:823:U:C5	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:361:C:H2'	1:0:362:G:C8	2.56	0.41
1:0:2732:U:H2'	1:0:2733:U:C6	2.56	0.41
1:0:2791:U:H1'	1:0:2792:A:H5''	2.02	0.41
1:0:2106:C:O5'	1:0:2106:C:H6	2.04	0.41
1:0:1274:A:N6	1:0:1275:C:N4	2.69	0.41
4:C:118:THR:HG23	4:C:231:ARG:O	2.21	0.41
1:0:204:A:H2'	1:0:205:U:H5'	2.02	0.41
1:0:2594:C:O2'	1:0:2595:U:H5'	2.21	0.41
1:0:426:G:H5''	39:0:7523:HOH:O	2.20	0.41
14:M:180:SER:HB3	39:M:3219:HOH:O	2.21	0.41
1:0:1644:C:C4	1:0:1645:U:C5	3.09	0.41
1:0:1175:G:H1'	1:0:1193:A:C8	2.56	0.40
1:0:1473:U:H1'	28:1:41:LYS:HE2	2.02	0.40
1:0:2765:C:H2'	1:0:2766:A:C8	2.55	0.40
1:0:1044:C:H5	39:0:6095:HOH:O	2.02	0.40
21:T:1:SER:OG	21:T:2:LYS:N	2.54	0.40
1:0:1678:A:C4	1:0:1679:C:C6	3.09	0.40
1:0:285:A:C2	1:0:368:C:H4'	2.56	0.40
1:0:958:G:H2'	1:0:959:C:C6	2.56	0.40
22:U:49:LEU:HD13	22:U:51:TRP:HE1	1.86	0.40
4:C:29:ASP:HB2	16:O:3:THR:HG22	2.03	0.40
1:0:731:U:O5'	1:0:731:U:H6	2.03	0.40
1:0:2057:U:H5	39:0:4741:HOH:O	2.04	0.40
1:0:1521:C:O2'	1:0:1522:A:H5'	2.21	0.40
5:D:67:ASP:HA	5:D:68:PRO:HD3	1.97	0.40
1:0:2622:A:H1'	39:0:8784:HOH:O	2.20	0.40
2:A:121:ALA:O	2:A:124:VAL:HG22	2.21	0.40
1:0:1703:G:C2	1:0:1716:A:C4	3.09	0.40
7:F:2:VAL:HG22	7:F:57:GLU:OE1	2.21	0.40
39:0:6384:HOH:O	21:T:53:GLY:HA3	2.22	0.40
1:0:154:C:C2	1:0:155:C:C5	3.09	0.40
1:0:2757:A:C2'	1:0:2758:G:H5'	2.51	0.40
1:0:1572:A:C2	1:0:1573:A:C4	3.10	0.40
1:0:2321:A:H1'	1:0:2322:U:H2'	2.02	0.40
1:0:2293:G:H2'	1:0:2294:C:O5'	2.21	0.40
1:0:2626:C:H2'	1:0:2627:G:H8	1.86	0.40
1:0:1310:U:OP2	4:C:168:ARG:NH1	2.55	0.40
1:0:1310:U:P	4:C:168:ARG:HH11	2.44	0.40
15:N:48:VAL:CG1	15:N:55:ASP:HB3	2.51	0.40
1:0:2731:G:O2'	1:0:2732:U:H5'	2.21	0.40
1:0:2597:U:H2'	1:0:2598:U:H5'	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2003:U:H4'	1:0:2004:U:H5	1.86	0.40
1:0:793:A:H2'	1:0:794:U:O4'	2.20	0.40
1:0:2582:G:C2	1:0:2583:A:C8	3.09	0.40
27:Z:70:ARG:HD3	27:Z:83:TYR:HB2	2.04	0.40
30:3:11:CYS:HB2	30:3:20:HIS:NE2	2.36	0.40
14:M:84:LYS:HA	30:3:46:ILE:O	2.21	0.40
1:0:536:A:H3'	39:0:3958:HOH:O	2.21	0.40
1:0:1448:A:C8	1:0:1506:U:C2	3.09	0.40
1:0:2505:G:H2'	1:0:2506:A:H5'	2.04	0.40
1:0:35:U:H5'	4:C:47:GLY:O	2.21	0.40
1:0:12:U:H2'	1:0:13:G:C5'	2.45	0.40
1:0:2768:A:N3	1:0:2768:A:H3'	2.35	0.40
1:0:2319:C:C3'	1:0:2320:U:H5''	2.52	0.40
1:0:1421:C:C2	1:0:1422:U:C5	3.09	0.40
1:0:1477:C:C5'	1:0:1868:G:C5'	3.00	0.40
1:0:210:U:H2'	1:0:211:U:C6	2.57	0.40
1:0:1704:G:O3'	17:P:59:ARG:NH1	2.55	0.40
1:0:2838:A:OP1	3:B:307:ARG:NH2	2.54	0.40
1:0:700:A:H2	16:O:69:VAL:HG23	1.87	0.40
39:0:5466:HOH:O	3:B:254:GLN:HG3	2.20	0.40
1:0:1988:C:H5	39:0:3572:HOH:O	2.04	0.40
1:0:489:A:H2'	1:0:490:C:O4'	2.21	0.40
3:B:215:VAL:O	3:B:219:GLY:HA2	2.22	0.40
1:0:2807:U:OP2	3:B:28:SER:HB2	2.21	0.40
1:0:1059:G:C8	1:0:2491:G:H4'	2.56	0.40
1:0:2722:G:C2	1:0:2761:A:N1	2.89	0.40
4:C:93:LYS:O	4:C:98:ARG:NH2	2.55	0.40
1:0:2316:G:O2'	1:0:2462:G:O6	2.38	0.40
31:9:110:G:C5	31:9:111:U:C5	3.09	0.40
1:0:863:G:N3	1:0:1459:A:H2	2.19	0.40
27:Z:49:ARG:O	27:Z:53:ILE:HG13	2.21	0.40
31:9:56:A:C3'	31:9:57:A:H5''	2.52	0.40
1:0:1676:G:C5	1:0:1677:U:N3	2.90	0.40
1:0:187:A:N3	1:0:187:A:H2'	2.37	0.40
1:0:1747:A:O3'	1:0:2584:G:H5'	2.21	0.40
1:0:1513:C:H5'	1:0:1574:C:O2'	2.22	0.40
1:0:2294:C:N4	1:0:2314:G:H1	2.19	0.40
1:0:1400:C:H2'	1:0:1401:G:H5'	2.03	0.40
1:0:1422:U:H2'	1:0:1423:C:C6	2.57	0.40
1:0:814:G:N1	1:0:815:U:C2	2.90	0.40
1:0:2439:C:O2'	1:0:2440:C:H5'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2537:G:H5''	1:0:2538:A:C5'	2.51	0.40
1:0:1910:A:C2	1:0:2128:G:N3	2.90	0.40
1:0:2128:G:H2'	1:0:2129:U:O4'	2.22	0.40
1:0:2428:G:C4'	39:0:4707:HOH:O	2.70	0.40
1:0:2055:A:H2'	1:0:2056:C:C6	2.56	0.40
1:0:2593:C:O2'	1:0:2594:C:H5'	2.22	0.40
1:0:1587:U:H2'	1:0:1588:G:O4'	2.21	0.40
12:K:14:LYS:HB2	12:K:45:PRO:HG2	2.03	0.40
1:0:1679:C:O2	1:0:1685:A:C2	2.75	0.40
1:0:1682:A:H1'	1:0:1685:A:OP2	2.22	0.40
1:0:1574:C:C6	1:0:1575:C:H5	2.40	0.40
1:0:2379:G:H5'	1:0:2381:C:O4'	2.21	0.40
1:0:1592:G:O2'	1:0:1593:C:O4'	2.39	0.40
1:0:365:G:H2'	1:0:366:U:O4'	2.21	0.40
1:0:1893:C:H2'	1:0:1894:C:H5'	2.03	0.40
1:0:2867:G:H2'	1:0:2868:C:C6	2.57	0.40
1:0:1812:G:OP1	1:0:1812:G:H3'	2.21	0.40
1:0:818:A:C6	1:0:819:A:N1	2.90	0.40
1:0:951:A:H2'	1:0:952:G:H5'	2.04	0.40
1:0:387:G:H2'	1:0:388:G:H5'	2.03	0.40
1:0:472:A:H5'	28:1:35:SER:OG	2.22	0.40
1:0:1531:U:O2	1:0:1661:A:C2	2.74	0.40
1:0:1695:G:H1'	28:1:9:GLY:HA3	2.02	0.40
39:0:4064:HOH:O	24:W:9:GLY:HA3	2.21	0.40
1:0:2468:A:N6	30:3:50:GLY:HA2	2.36	0.40
12:K:125:ALA:C	12:K:127:ALA:H	2.25	0.40
15:N:113:SER:HB3	39:9:5851:HOH:O	2.21	0.40
6:E:154:ILE:HD11	6:E:157:LYS:HE2	2.04	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	
2	A	235/237 (99%)	210 (89%)	20 (8%)	5 (2%)	9	46
3	B	335/337 (99%)	305 (91%)	27 (8%)	3 (1%)	21	67
4	C	244/246 (99%)	223 (91%)	18 (7%)	3 (1%)	16	60
5	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	8	45
6	E	170/172 (99%)	157 (92%)	12 (7%)	1 (1%)	30	75
7	F	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	5	31
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	145 (93%)	10 (6%)	1 (1%)	30	75
10	I	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	13	55
11	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	14	57
12	K	130/132 (98%)	116 (89%)	13 (10%)	1 (1%)	24	69
13	L	141/165 (86%)	128 (91%)	12 (8%)	1 (1%)	26	72
14	M	192/194 (99%)	180 (94%)	7 (4%)	5 (3%)	7	40
15	N	184/186 (99%)	165 (90%)	15 (8%)	4 (2%)	8	45
16	O	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
17	P	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	26	72
18	Q	93/95 (98%)	85 (91%)	6 (6%)	2 (2%)	8	45
19	R	148/150 (99%)	141 (95%)	6 (4%)	1 (1%)	26	72
20	S	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
21	T	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
22	U	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
23	V	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
24	W	152/154 (99%)	139 (91%)	13 (9%)	0	100	100
25	X	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	15	59
26	Y	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	26	72
27	Z	71/73 (97%)	65 (92%)	4 (6%)	2 (3%)	6	37
28	1	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	10	50
29	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
30	3	90/92 (98%)	75 (83%)	11 (12%)	4 (4%)	3	24
All	All	3705/4172 (89%)	3381 (91%)	277 (8%)	47 (1%)	15	59

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	52	SER
3	B	306	LYS
7	F	61	MET
11	J	5	GLU
14	M	80	GLY
26	Y	157	ILE
30	3	27	SER
4	C	205	ARG
7	F	91	VAL
7	F	101	ALA
15	N	167	ASP
27	Z	92	SER
30	3	47	GLY
30	3	48	ASN
2	A	34	ASP
2	A	122	SER
4	C	79	ARG
4	C	208	ALA
5	D	137	PRO
6	E	122	THR
11	J	89	HIS
14	M	82	ARG
15	N	70	GLY
15	N	139	TRP
18	Q	48	PRO
28	1	54	ALA
5	D	56	ARG
9	H	171	GLY
10	I	108	HIS
12	K	10	GLN
13	L	37	LYS
14	M	71	SER
15	N	154	LEU
17	P	77	ALA
18	Q	18	PRO
27	Z	70	ARG
30	3	64	LYS
5	D	46	GLY
2	A	37	VAL
7	F	104	ALA
2	A	88	ILE
14	M	110	PRO
19	R	114	VAL

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Mol	Chain	Res	Type
14	M	35	GLY
3	B	2	GLN
25	X	52	PRO
3	B	185	GLY

### 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	
2	A	179/179 (100%)	169 (94%)	10 (6%)	26	68
3	B	282/282 (100%)	263 (93%)	19 (7%)	20	60
4	C	193/193 (100%)	179 (93%)	14 (7%)	17	57
5	D	117/148 (79%)	109 (93%)	8 (7%)	20	59
6	E	152/152 (100%)	139 (91%)	13 (9%)	13	46
7	F	93/93 (100%)	91 (98%)	2 (2%)	60	87
8	G	27/282 (10%)	23 (85%)	4 (15%)	4	18
9	H	134/145 (92%)	121 (90%)	13 (10%)	10	39
10	I	58/58 (100%)	56 (97%)	2 (3%)	44	80
11	J	118/118 (100%)	112 (95%)	6 (5%)	29	70
12	K	106/106 (100%)	99 (93%)	7 (7%)	21	61
13	L	113/127 (89%)	105 (93%)	8 (7%)	18	57
14	M	158/158 (100%)	146 (92%)	12 (8%)	16	55
15	N	149/149 (100%)	135 (91%)	14 (9%)	11	41
16	O	93/93 (100%)	88 (95%)	5 (5%)	27	68
17	P	113/113 (100%)	110 (97%)	3 (3%)	52	85
18	Q	79/79 (100%)	77 (98%)	2 (2%)	55	86
19	R	117/117 (100%)	111 (95%)	6 (5%)	29	70
20	S	71/71 (100%)	68 (96%)	3 (4%)	36	75
21	T	105/105 (100%)	99 (94%)	6 (6%)	25	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	U	44/44 (100%)	40 (91%)	4 (9%)	12	42
23	V	51/51 (100%)	47 (92%)	4 (8%)	16	53
24	W	130/130 (100%)	127 (98%)	3 (2%)	58	87
25	X	66/66 (100%)	60 (91%)	6 (9%)	12	42
26	Y	120/120 (100%)	114 (95%)	6 (5%)	30	71
27	Z	60/60 (100%)	57 (95%)	3 (5%)	30	71
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	42/46 (91%)	39 (93%)	3 (7%)	18	57
30	3	79/79 (100%)	73 (92%)	6 (8%)	16	55
All	All	3095/3410 (91%)	2903 (94%)	192 (6%)	23	64

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	ARG
2	A	30	ARG
2	A	43	VAL
2	A	51	ARG
2	A	68	ILE
2	A	78	ASP
2	A	131	HIS
2	A	179	MET
2	A	184	THR
2	A	217	ARG
3	B	7	ARG
3	B	20	THR
3	B	27	ASN
3	B	49	THR
3	B	71	VAL
3	B	97	LEU
3	B	98	THR
3	B	103	ASP
3	B	144	THR
3	B	145	HIS
3	B	156	LYS
3	B	162	MET
3	B	171	VAL
3	B	190	MET
3	B	254	GLN

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Mol	Chain	Res	Type
3	B	256	GLN
3	B	277	GLU
3	B	278	PRO
3	B	301	VAL
4	C	17	ASP
4	C	29	ASP
4	C	76	ARG
4	C	78	ARG
4	C	131	PHE
4	C	135	GLU
4	C	136	VAL
4	C	148	VAL
4	C	184	ARG
4	C	187	ARG
4	C	223	LEU
4	C	236	THR
4	C	240	LEU
4	C	243	VAL
5	D	50	VAL
5	D	52	THR
5	D	58	VAL
5	D	73	VAL
5	D	77	ASP
5	D	128	LEU
5	D	136	ARG
5	D	172	VAL
6	E	7	ILE
6	E	10	ASP
6	E	36	PRO
6	E	39	ASP
6	E	40	VAL
6	E	61	THR
6	E	100	ASP
6	E	102	VAL
6	E	115	ARG
6	E	133	VAL
6	E	156	ASP
6	E	159	VAL
6	E	164	ASP
7	F	12	LEU
7	F	55	GLN
8	G	12	ILE

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Mol	Chain	Res	Type
8	G	64	ASN
8	G	65	THR
8	G	73	ASP
9	H	42	ASP
9	H	48	VAL
9	H	62	HIS
9	H	65	LEU
9	H	87	LYS
9	H	91	ARG
9	H	122	LYS
9	H	126	THR
9	H	143	VAL
9	H	154	ARG
9	H	157	TYR
9	H	169	GLU
9	H	173	GLU
10	I	82	THR
10	I	126	THR
11	J	39	VAL
11	J	45	VAL
11	J	47	THR
11	J	52	GLN
11	J	107	ASN
11	J	130	VAL
12	K	10	GLN
12	K	16	SER
12	K	19	THR
12	K	44	HIS
12	K	93	ASN
12	K	109	LEU
12	K	115	ARG
13	L	32	ASP
13	L	35	ARG
13	L	70	ASP
13	L	80	ASP
13	L	102	ASP
13	L	104	ASP
13	L	105	TYR
13	L	145	LEU
14	M	10	ASP
14	M	23	LEU
14	M	68	ARG

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Mol	Chain	Res	Type
14	M	73	ARG
14	M	77	HIS
14	M	81	ARG
14	M	89	THR
14	M	91	ILE
14	M	99	ARG
14	M	123	ASP
14	M	164	THR
14	M	180	SER
15	N	2	THR
15	N	22	GLN
15	N	26	LEU
15	N	43	VAL
15	N	49	THR
15	N	56	ASP
15	N	74	PRO
15	N	134	ASP
15	N	135	VAL
15	N	139	TRP
15	N	162	ASP
15	N	171	HIS
15	N	177	GLU
15	N	180	LEU
16	O	25	VAL
16	O	36	PRO
16	O	43	VAL
16	O	57	THR
16	O	69	VAL
17	P	16	VAL
17	P	91	LYS
17	P	98	ILE
18	Q	18	PRO
18	Q	57	ASP
19	R	13	THR
19	R	52	GLU
19	R	55	GLN
19	R	73	ASP
19	R	110	THR
19	R	125	ARG
20	S	17	ASP
20	S	30	ASP
20	S	44	GLN

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Mol	Chain	Res	Type
21	T	5	ASP
21	T	39	ASN
21	T	71	VAL
21	T	96	VAL
21	T	97	ARG
21	T	115	GLU
22	U	11	THR
22	U	25	ASP
22	U	32	CYS
22	U	53	ASP
23	V	6	GLN
23	V	28	LEU
23	V	49	LEU
23	V	65	ASP
24	W	4	LEU
24	W	38	THR
24	W	146	ILE
25	X	44	ASP
25	X	52	PRO
25	X	72	VAL
25	X	79	GLU
25	X	82	GLU
25	X	88	GLU
26	Y	117	LEU
26	Y	154	ARG
26	Y	189	ASN
26	Y	200	THR
26	Y	203	VAL
26	Y	219	GLU
27	Z	88	PHE
27	Z	92	SER
27	Z	103	VAL
29	2	18	ASN
29	2	46	ASP
29	2	48	ASP
30	3	3	MET
30	3	7	PHE
30	3	21	GLU
30	3	49	ASP
30	3	55	VAL
30	3	65	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such

sidechains are listed below:

Mol	Chain	Res	Type
2	A	47	HIS
2	A	176	HIS
2	A	199	HIS
3	B	27	ASN
3	B	221	GLN
3	B	238	ASN
3	B	260	HIS
3	B	320	GLN
4	C	73	GLN
4	C	103	ASN
4	C	129	HIS
5	D	103	ASN
5	D	133	ASN
6	E	55	ASN
6	E	143	GLN
6	E	150	GLN
7	F	80	GLN
8	G	64	ASN
9	H	59	GLN
9	H	73	ASN
11	J	52	GLN
11	J	107	ASN
12	K	10	GLN
12	K	23	ASN
12	K	93	ASN
13	L	18	HIS
13	L	41	HIS
13	L	113	GLN
14	M	24	GLN
14	M	29	GLN
14	M	58	GLN
14	M	170	ASN
15	N	40	ASN
15	N	107	ASN
15	N	153	GLN
16	O	100	GLN
17	P	28	GLN
17	P	50	GLN
17	P	88	GLN
17	P	118	GLN
19	R	94	ASN
19	R	98	ASN

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Mol	Chain	Res	Type
19	R	117	HIS
20	S	9	HIS
20	S	44	GLN
20	S	53	ASN
21	T	7	GLN
22	U	39	ASN
22	U	48	ASN
23	V	34	GLN
23	V	60	GLN
24	W	59	GLN
24	W	110	GLN
24	W	141	HIS
25	X	23	HIS
26	Y	129	ASN
26	Y	131	GLN
26	Y	134	HIS
26	Y	149	GLN
26	Y	189	ASN
27	Z	61	HIS
28	1	16	HIS
28	1	28	HIS
29	2	16	ASN
29	2	18	ASN
29	2	45	ASN
30	3	15	ASN
30	3	18	GLN
30	3	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	263 (9%)	19 (0%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	280 (9%)	20 (0%)

All (280) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	47	G
1	0	67	A

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Mol	Chain	Res	Type
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	138	U
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	170	U
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	198	A
1	0	200	C
1	0	204	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	318	U
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G

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Mol	Chain	Res	Type
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	702	G
1	0	735	C
1	0	736	A
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	836	G
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	882	A
1	0	885	G
1	0	898	G
1	0	905	C

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Mol	Chain	Res	Type
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1011	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1078	A
1	0	1081	A
1	0	1083	C
1	0	1088	A
1	0	1102	C
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1121	G
1	0	1129	C
1	0	1130	U
1	0	1151	G
1	0	1164	U
1	0	1165	G
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1234	U
1	0	1238	C
1	0	1239	G
1	0	1242	A
1	0	1279	U
1	0	1287	A
1	0	1289	C
1	0	1331	G

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Mol	Chain	Res	Type
1	0	1342	C
1	0	1353	C
1	0	1354	G
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1409	G
1	0	1427	A
1	0	1460	G
1	0	1474	C
1	0	1492	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1535	G
1	0	1559	A
1	0	1592	G
1	0	1605	G
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1732	A
1	0	1742	A
1	0	1752	G
1	0	1778	A
1	0	1779	A
1	0	1798	C
1	0	1819	G

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Mol	Chain	Res	Type
1	0	1820	G
1	0	1829	A
1	0	1838	U
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2063	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2104	C
1	0	2110	G
1	0	2134	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2320	U
1	0	2321	A

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Mol	Chain	Res	Type
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2420	G
1	0	2422	U
1	0	2443	C
1	0	2462	G
1	0	2465	A
1	0	2467	A
1	0	2469	A
1	0	2474	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2607	U
1	0	2608	C
1	0	2609	G
1	0	2613	G
1	0	2637	A
1	0	2649	A
1	0	2664	A
1	0	2676	C
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2792	A

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Mol	Chain	Res	Type
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	39	U
31	9	41	C
31	9	43	G
31	9	44	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	88	G
31	9	114	G
31	9	122	C

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	129	A
1	0	603	A
1	0	604	G
1	0	644	G
1	0	857	A
1	0	871	G
1	0	1080	C
1	0	1352	A
1	0	1377	C
1	0	1667	A
1	0	1730	G
1	0	1979	G
1	0	2011	A

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Mol	Chain	Res	Type
1	0	2103	A
1	0	2467	A
1	0	2536	C
1	0	2718	C
1	0	2761	A
1	0	2791	U
31	9	65	A

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	OMU	0	2587	1	12,22,23	1.00	2 (16%)	19,31,34	3.18	2 (10%)
1	OMG	0	2588	1	17,26,27	1.07	2 (11%)	21,38,41	2.53	3 (14%)
1	UR3	0	2619	1	12,22,23	0.81	0	16,32,35	0.80	0
1	PSU	0	2621	1	13,21,22	1.62	2 (15%)	18,30,33	6.11	4 (22%)
1	1MA	0	628	1,34	14,25,26	1.02	1 (7%)	15,37,40	1.15	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,34	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.98	1.47	1.52
1	0	2587	OMU	C6-C5	-2.02	1.33	1.38
1	0	2588	OMG	C8-N7	-2.01	1.30	1.34
1	0	2587	OMU	C4-N3	2.23	1.37	1.33
1	0	2621	PSU	C4-N3	2.51	1.37	1.33
1	0	628	1MA	C6-N6	2.74	1.34	1.29
1	0	2588	OMG	C6-N1	3.39	1.39	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.43	114.66	128.33
1	0	2588	OMG	C5-C6-N1	-8.68	111.72	123.59
1	0	628	1MA	C2-N3-C4	-3.68	110.70	116.40
1	0	2587	OMU	C5-C4-N3	-3.32	114.61	123.12
1	0	2588	OMG	N3-C2-N1	-2.37	123.83	127.44
1	0	2621	PSU	O4'-C1'-C2'	2.29	107.06	104.73
1	0	2621	PSU	C6-N1-C2	2.70	119.81	115.47
1	0	2588	OMG	C6-N1-C2	6.58	125.08	115.94
1	0	2587	OMU	C4-N3-C2	13.28	127.29	114.14
1	0	2621	PSU	C4-N3-C2	13.95	127.31	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0
1	0	2621	PSU	1	0
1	0	628	1MA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 304 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	MUL	0	9101	-	31,36,36	1.05	1 (3%)	28,55,55	1.38	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	MUL	0	9101	-	-	0/16/79/79	0/1/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9101	MUL	C12-C19	-3.70	1.39	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	MUL	C14-O3-C21	-3.39	110.79	118.03
37	0	9101	MUL	C1-C2-C3	-2.89	101.70	105.51
37	0	9101	MUL	C8-C7-C6	-2.45	109.12	112.34
37	0	9101	MUL	C23-S1-C22	-2.30	98.06	101.89
37	0	9101	MUL	O3-C21-C22	3.23	119.56	111.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	0	9101	MUL	17	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2749/2923 (94%)	-0.66	3 (0%) 95 95	29, 74, 140, 200	0
2	A	237/237 (100%)	0.06	9 (3%) 44 29	43, 97, 143, 167	0
3	B	337/337 (100%)	-0.38	1 (0%) 94 93	40, 86, 129, 148	0
4	C	246/246 (100%)	-0.37	2 (0%) 87 80	41, 72, 103, 112	0
5	D	140/177 (79%)	1.15	40 (28%) 1 0	118, 160, 184, 191	0
6	E	172/172 (100%)	-0.11	3 (1%) 73 60	76, 104, 134, 146	0
7	F	119/119 (100%)	0.33	9 (7%) 17 9	74, 113, 153, 166	0
8	G	29/348 (8%)	1.05	6 (20%) 1 1	118, 140, 146, 150	0
9	H	160/177 (90%)	0.58	17 (10%) 8 4	77, 104, 146, 162	0
10	I	70/70 (100%)	1.92	34 (48%) 0 0	173, 199, 200, 200	0
11	J	142/142 (100%)	-0.27	0 100 100	55, 80, 104, 123	0
12	K	132/132 (100%)	-0.18	2 (1%) 76 63	54, 79, 112, 118	0
13	L	145/165 (87%)	0.70	27 (18%) 2 1	62, 121, 171, 175	0
14	M	194/194 (100%)	0.12	18 (9%) 11 6	49, 70, 145, 160	0
15	N	186/186 (100%)	0.52	13 (6%) 19 11	82, 118, 178, 187	0
16	O	115/115 (100%)	-0.42	0 100 100	66, 87, 105, 111	0
17	P	143/143 (100%)	-0.20	2 (1%) 78 65	65, 88, 117, 124	0
18	Q	95/95 (100%)	0.05	4 (4%) 40 26	67, 87, 110, 117	0
19	R	150/150 (100%)	-0.46	0 100 100	47, 72, 103, 112	0
20	S	81/81 (100%)	-0.03	3 (3%) 45 30	68, 93, 114, 130	0
21	T	119/119 (100%)	0.26	10 (8%) 14 7	69, 92, 136, 155	0
22	U	53/53 (100%)	0.12	1 (1%) 70 55	94, 114, 136, 145	0
23	V	65/65 (100%)	0.26	3 (4%) 36 23	79, 113, 164, 170	0
24	W	154/154 (100%)	-0.20	3 (1%) 70 55	56, 78, 110, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	82/82 (100%)	0.14	7 (8%) 13 7	63, 92, 125, 135	0
26	Y	142/142 (100%)	-0.31	2 (1%) 78 65	45, 73, 109, 134	0
27	Z	73/73 (100%)	5.47	53 (72%) 0 0	149, 179, 191, 194	0
28	1	56/56 (100%)	-0.29	0 100 100	42, 53, 66, 76	0
29	2	46/50 (92%)	0.29	4 (8%) 13 7	48, 95, 145, 146	0
30	3	92/92 (100%)	6.26	80 (86%) 0 0	163, 185, 199, 200	0
31	9	122/122 (100%)	-0.83	0 100 100	66, 114, 143, 191	0
All	All	6646/7217 (92%)	-0.11	356 (5%) 29 17	29, 85, 168, 200	0

All (356) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	34	SER	30.5
30	3	82	GLY	27.0
27	Z	35	SER	25.3
30	3	37	ASP	18.5
30	3	41	GLU	17.2
27	Z	46	SER	16.7
27	Z	43	GLY	15.7
30	3	34	LYS	15.6
27	Z	50	VAL	14.9
30	3	32	GLY	14.6
27	Z	45	VAL	14.4
27	Z	58	ASN	14.0
30	3	38	ARG	13.7
30	3	39	GLN	13.2
30	3	83	TRP	12.8
27	Z	44	ARG	12.6
27	Z	51	ALA	12.5
30	3	35	TRP	12.5
30	3	45	GLY	12.3
14	M	70	GLY	12.1
27	Z	59	GLU	11.8
30	3	33	MET	11.5
30	3	30	GLN	11.3
30	3	42	ARG	10.9
27	Z	54	GLU	10.7
27	Z	55	SER	10.7
30	3	40	ARG	10.5
30	3	81	GLU	10.5

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Mol	Chain	Res	Type	RSRZ
30	3	9	THR	9.9
30	3	48	ASN	9.9
30	3	43	ASN	9.7
27	Z	36	GLY	9.5
30	3	36	ILE	9.2
14	M	90	ARG	9.1
27	Z	49	ARG	8.9
27	Z	47	ARG	8.6
30	3	62	THR	8.6
14	M	89	THR	8.5
30	3	31	THR	8.4
30	3	44	SER	8.4
21	T	119	ALA	7.8
30	3	71	CYS	7.8
27	Z	68	GLU	7.6
27	Z	42	TYR	7.6
30	3	56	PRO	7.6
14	M	71	SER	7.4
27	Z	38	PHE	7.4
27	Z	63	CYS	7.4
30	3	58	GLY	7.4
30	3	27	SER	7.2
30	3	59	ASP	7.2
30	3	20	HIS	7.2
30	3	14	CYS	7.0
30	3	47	GLY	6.8
30	3	49	ASP	6.6
30	3	5	ARG	6.5
27	Z	37	ARG	6.5
30	3	18	GLN	6.4
27	Z	53	ILE	6.4
30	3	57	GLY	6.4
27	Z	69	ASP	6.4
13	L	106	VAL	6.3
30	3	73	GLU	6.3
27	Z	57	MET	6.3
5	D	69	ILE	6.3
30	3	22	VAL	6.2
27	Z	82	SER	6.2
30	3	72	GLY	6.2
30	3	23	GLU	6.0
27	Z	81	CYS	5.9

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Mol	Chain	Res	Type	RSRZ
30	3	10	TYR	5.8
5	D	18	ILE	5.8
14	M	86	GLN	5.8
30	3	15	ASN	5.8
27	Z	48	ARG	5.8
30	3	29	ARG	5.7
10	I	74	ILE	5.7
30	3	8	ASN	5.6
5	D	134	LEU	5.6
27	Z	39	GLY	5.6
30	3	66	ASP	5.5
5	D	88	LEU	5.5
10	I	70	THR	5.5
5	D	40	ILE	5.5
27	Z	80	GLN	5.4
10	I	128	THR	5.3
30	3	84	ARG	5.3
30	3	16	GLU	5.2
30	3	80	ARG	5.2
30	3	78	HIS	5.2
30	3	19	GLU	5.2
30	3	21	GLU	5.0
30	3	67	LEU	5.0
7	F	106	ALA	5.0
30	3	28	GLY	5.0
15	N	84	THR	4.9
5	D	66	GLY	4.8
30	3	85	ALA	4.8
30	3	25	VAL	4.8
10	I	97	VAL	4.7
10	I	106	GLN	4.7
27	Z	65	ASN	4.6
30	3	74	CYS	4.6
27	Z	56	GLU	4.6
30	3	69	TYR	4.6
14	M	77	HIS	4.5
5	D	104	PHE	4.5
30	3	63	LYS	4.5
23	V	1	THR	4.5
10	I	117	THR	4.4
5	D	92	GLU	4.4
30	3	11	CYS	4.4

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Mol	Chain	Res	Type	RSRZ
27	Z	67	GLY	4.3
30	3	13	HIS	4.3
27	Z	77	GLY	4.3
30	3	75	GLY	4.3
27	Z	88	PHE	4.3
30	3	55	VAL	4.3
26	Y	235	GLU	4.2
10	I	103	ILE	4.2
15	N	119	GLN	4.2
10	I	104	ALA	4.2
30	3	1	MET	4.2
14	M	79	ALA	4.2
30	3	68	LYS	4.1
5	D	93	LEU	4.1
10	I	100	VAL	4.1
30	3	60	LYS	4.1
25	X	7	GLU	4.0
2	A	82	VAL	4.0
8	G	73	ASP	4.0
9	H	133	GLY	4.0
9	H	76	LEU	3.9
30	3	17	HIS	3.9
27	Z	71	VAL	3.9
27	Z	52	GLU	3.9
27	Z	70	ARG	3.9
30	3	76	LYS	3.9
10	I	94	ASP	3.9
21	T	117	ASP	3.9
5	D	27	ILE	3.9
30	3	46	ILE	3.9
14	M	78	LYS	3.8
13	L	62	ALA	3.8
2	A	24	LYS	3.8
5	D	63	ILE	3.7
14	M	80	GLY	3.7
27	Z	103	VAL	3.7
30	3	61	PRO	3.7
7	F	75	ILE	3.7
20	S	81	ILE	3.7
27	Z	106	SER	3.7
5	D	26	GLY	3.7
8	G	66	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
30	3	91	GLN	3.6
13	L	140	VAL	3.6
14	M	76	ARG	3.6
25	X	10	VAL	3.6
13	L	61	ALA	3.5
5	D	25	MET	3.4
5	D	130	VAL	3.4
27	Z	62	ALA	3.4
27	Z	93	TYR	3.4
13	L	76	LEU	3.4
5	D	44	ILE	3.4
14	M	88	VAL	3.4
10	I	73	LEU	3.4
30	3	6	ARG	3.4
5	D	166	ILE	3.3
18	Q	95	GLU	3.3
29	2	41	HIS	3.3
13	L	107	LYS	3.3
13	L	49	SER	3.3
14	M	81	ARG	3.3
30	3	65	THR	3.3
5	D	128	LEU	3.3
27	Z	86	TYR	3.3
8	G	27	ILE	3.3
5	D	61	PHE	3.2
15	N	172	PHE	3.2
10	I	111	LEU	3.2
30	3	90	PHE	3.2
5	D	106	PHE	3.2
7	F	49	PHE	3.2
27	Z	85	ASP	3.2
24	W	3	ALA	3.2
30	3	77	ALA	3.2
27	Z	60	ASP	3.2
15	N	179	LEU	3.1
27	Z	78	ILE	3.1
23	V	39	ALA	3.1
27	Z	66	CYS	3.1
30	3	86	GLY	3.1
21	T	99	THR	3.1
27	Z	40	ALA	3.1
27	Z	79	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
29	2	36	ASN	3.1
6	E	5	LEU	3.1
14	M	83	SER	3.1
5	D	89	PRO	3.0
10	I	68	PRO	3.0
10	I	71	ALA	3.0
27	Z	76	THR	3.0
10	I	92	VAL	3.0
8	G	69	ARG	3.0
21	T	40	VAL	3.0
7	F	99	THR	3.0
21	T	42	VAL	3.0
14	M	87	GLY	3.0
30	3	88	LEU	3.0
8	G	23	ILE	3.0
17	P	118	GLN	3.0
10	I	112	LEU	3.0
23	V	40	PRO	3.0
15	N	83	LEU	3.0
30	3	2	GLN	3.0
10	I	113	SER	2.9
10	I	109	PRO	2.9
9	H	97	VAL	2.9
10	I	102	GLN	2.9
13	L	97	VAL	2.9
5	D	95	THR	2.9
5	D	90	LEU	2.9
10	I	93	ALA	2.9
15	N	166	ALA	2.9
29	2	48	ASP	2.9
25	X	8	ARG	2.9
10	I	110	ASP	2.9
30	3	3	MET	2.9
13	L	79	ASP	2.9
15	N	81	ALA	2.9
9	H	87	LYS	2.9
15	N	175	LEU	2.8
5	D	84	LEU	2.8
13	L	60	GLU	2.8
5	D	135	VAL	2.8
27	Z	64	PRO	2.8
1	0	735	C	2.8

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Mol	Chain	Res	Type	RSRZ
10	I	98	ASP	2.7
10	I	127	CYS	2.7
18	Q	64	GLU	2.7
9	H	86	TYR	2.7
10	I	99	GLN	2.7
1	0	970	U	2.7
5	D	57	THR	2.7
15	N	114	LYS	2.7
21	T	118	SER	2.6
30	3	24	LYS	2.6
9	H	66	GLU	2.6
10	I	108	HIS	2.6
8	G	63	ARG	2.6
5	D	91	ALA	2.6
10	I	72	GLU	2.6
2	A	88	ILE	2.6
5	D	87	ALA	2.6
10	I	132	VAL	2.6
5	D	160	ALA	2.6
2	A	36	ASP	2.5
5	D	64	ARG	2.5
9	H	53	ILE	2.5
7	F	17	LEU	2.5
13	L	120	LEU	2.5
7	F	15	ASP	2.5
5	D	165	PHE	2.5
13	L	123	ASP	2.5
5	D	43	GLU	2.5
30	3	92	GLU	2.5
15	N	145	ALA	2.5
27	Z	84	CYS	2.5
7	F	91	VAL	2.5
21	T	101	LEU	2.5
14	M	1	ALA	2.4
15	N	101	VAL	2.4
15	N	178	THR	2.4
24	W	96	LEU	2.4
5	D	101	THR	2.4
21	T	106	GLU	2.4
21	T	74	VAL	2.4
25	X	72	VAL	2.4
10	I	101	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
13	L	93	VAL	2.4
30	3	70	ARG	2.4
27	Z	89	THR	2.4
3	B	128	ILE	2.4
9	H	149	VAL	2.4
9	H	169	GLU	2.3
13	L	91	VAL	2.3
1	0	1169	U	2.3
13	L	36	ASP	2.3
22	U	25	ASP	2.3
13	L	78	ALA	2.3
18	Q	75	ILE	2.3
20	S	28	VAL	2.3
2	A	128	LEU	2.3
2	A	58	VAL	2.3
5	D	17	ARG	2.3
12	K	109	LEU	2.3
9	H	85	ASP	2.3
13	L	130	ARG	2.3
10	I	119	ALA	2.3
13	L	124	ASP	2.3
27	Z	61	HIS	2.3
9	H	25	GLY	2.3
10	I	105	GLU	2.3
13	L	99	GLU	2.3
6	E	100	ASP	2.3
5	D	24	HIS	2.2
12	K	132	VAL	2.2
5	D	47	GLN	2.2
4	C	63	SER	2.2
5	D	129	ASP	2.2
25	X	85	VAL	2.2
7	F	96	ALA	2.2
6	E	118	ILE	2.2
2	A	69	LEU	2.2
25	X	41	PHE	2.2
13	L	108	VAL	2.2
9	H	141	CYS	2.2
13	L	122	ALA	2.2
14	M	74	LYS	2.2
13	L	39	GLU	2.2
13	L	50	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
29	2	45	ASN	2.2
2	A	56	ALA	2.1
15	N	95	ALA	2.1
18	Q	85	ILE	2.1
2	A	91	GLY	2.1
13	L	96	VAL	2.1
10	I	66	GLY	2.1
13	L	66	VAL	2.1
14	M	22	GLU	2.1
9	H	50	ILE	2.1
17	P	114	LEU	2.1
4	C	246	ARG	2.1
5	D	68	PRO	2.1
9	H	146	ALA	2.1
27	Z	72	ASP	2.1
10	I	79	GLY	2.1
21	T	23	VAL	2.1
9	H	164	CYS	2.1
30	3	26	ARG	2.1
26	Y	95	THR	2.1
20	S	16	ASN	2.1
10	I	134	ILE	2.0
24	W	100	LEU	2.0
13	L	81	VAL	2.0
7	F	44	SER	2.0
10	I	118	ASN	2.0
5	D	48	MET	2.0
5	D	58	VAL	2.0
9	H	93	PHE	2.0
25	X	82	GLU	2.0
5	D	39	ASP	2.0
9	H	54	VAL	2.0
13	L	105	TYR	2.0
14	M	73	ARG	2.0

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

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

less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	1MA	0	628	23/24	0.97	0.15	-	49,56,63,64	0
1	OMU	0	2587	21/22	0.98	0.12	-	60,63,64,64	0
1	UR3	0	2619	21/22	0.98	0.15	-	61,65,71,72	0
1	PSU	0	2621	20/21	0.97	0.20	-	59,63,65,66	0
1	OMG	0	2588	24/25	0.97	0.14	-	50,54,58,60	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8565	1/1	0.87	1.17	66.60	106,106,106,106	0
34	NA	0	8562	1/1	0.84	1.23	55.58	85,85,85,85	0
34	NA	0	8535	1/1	0.96	0.55	41.17	45,45,45,45	0
34	NA	0	8564	1/1	0.70	0.57	39.91	95,95,95,95	0
34	NA	0	8547	1/1	0.88	0.90	26.34	81,81,81,81	0
34	NA	0	8555	1/1	0.97	0.55	18.70	50,50,50,50	0
34	NA	0	8546	1/1	0.97	1.30	18.14	69,69,69,69	0
34	NA	0	8556	1/1	0.65	0.81	18.02	95,95,95,95	0
34	NA	0	8558	1/1	0.89	0.60	17.10	50,50,50,50	0
34	NA	0	8559	1/1	0.90	0.32	16.87	94,94,94,94	0
34	NA	0	8542	1/1	0.96	0.52	16.84	51,51,51,51	0
34	NA	R	8575	1/1	0.80	0.50	16.63	96,96,96,96	0
34	NA	0	8528	1/1	0.71	0.48	16.39	80,80,80,80	0
34	NA	9	8572	1/1	0.62	0.32	13.62	88,88,88,88	0
32	MG	0	8070	1/1	0.98	0.39	13.15	54,54,54,54	0
34	NA	0	8524	1/1	0.54	0.38	11.61	47,47,47,47	0
32	MG	0	8073	1/1	0.80	0.68	11.10	110,110,110,110	0
35	CL	B	8819	1/1	0.97	0.77	10.93	68,68,68,68	0
32	MG	0	8090	1/1	0.68	0.93	10.61	81,81,81,81	0
32	MG	0	8034	1/1	0.96	0.30	9.67	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	L	8969	1/1	0.92	0.92	8.88	198,198,198,198	0
34	NA	0	8571	1/1	0.85	0.26	8.59	89,89,89,89	0
34	NA	0	8568	1/1	0.77	0.58	8.57	51,51,51,51	0
36	SR	B	8987	1/1	0.55	0.83	8.45	200,200,200,200	0
32	MG	0	8067	1/1	0.94	0.42	7.28	42,42,42,42	0
32	MG	0	8047	1/1	0.86	0.36	5.26	70,70,70,70	0
34	NA	0	8530	1/1	0.97	0.31	4.93	49,49,49,49	0
36	SR	0	8943	1/1	0.96	0.17	4.35	99,99,99,99	0
34	NA	0	8512	1/1	0.98	0.29	3.41	49,49,49,49	0
34	NA	0	8502	1/1	0.80	0.19	3.41	51,51,51,51	0
32	MG	0	8062	1/1	0.99	0.28	2.84	47,47,47,47	0
32	MG	C	8012	1/1	0.98	0.22	2.44	19,19,19,19	0
32	MG	0	8009	1/1	0.97	0.21	2.43	28,28,28,28	0
37	MUL	0	9101	34/34	0.94	0.26	2.16	85,87,104,104	0
35	CL	O	8808	1/1	0.98	0.30	2.10	98,98,98,98	0
34	NA	Q	8540	1/1	0.74	0.30	1.84	92,92,92,92	0
34	NA	0	8517	1/1	0.98	0.20	1.83	30,30,30,30	0
34	NA	0	8522	1/1	0.21	0.14	1.75	87,87,87,87	0
34	NA	0	8569	1/1	0.98	0.17	1.06	72,72,72,72	0
34	NA	0	8533	1/1	0.83	0.21	1.05	68,68,68,68	0
34	NA	0	8534	1/1	0.97	0.22	0.99	45,45,45,45	0
32	MG	0	8011	1/1	0.98	0.21	0.99	18,18,18,18	0
32	MG	0	8084	1/1	0.99	0.16	0.95	50,50,50,50	0
34	NA	0	8553	1/1	0.62	0.20	0.86	81,81,81,81	0
32	MG	0	8010	1/1	0.93	0.18	0.59	35,35,35,35	0
34	NA	0	8563	1/1	0.97	0.18	0.51	74,74,74,74	0
32	MG	A	8050	1/1	0.98	0.20	0.49	52,52,52,52	0
34	NA	0	8551	1/1	0.94	0.16	0.44	81,81,81,81	0
32	MG	0	8065	1/1	0.97	0.14	0.33	41,41,41,41	0
34	NA	0	8537	1/1	0.88	0.15	0.26	43,43,43,43	0
34	NA	0	8550	1/1	0.81	0.19	0.21	98,98,98,98	0
32	MG	0	8003	1/1	0.96	0.16	0.16	31,31,31,31	0
32	MG	0	8002	1/1	0.98	0.17	0.08	26,26,26,26	0
36	SR	A	8929	1/1	0.95	0.17	0.07	157,157,157,157	0
33	K	0	8402	1/1	0.95	0.21	0.00	67,67,67,67	0
32	MG	0	8007	1/1	0.97	0.17	-0.09	10,10,10,10	0
32	MG	A	8051	1/1	0.99	0.27	-0.09	90,90,90,90	0
34	NA	0	8523	1/1	0.93	0.14	-0.17	58,58,58,58	0
32	MG	0	8016	1/1	0.98	0.16	-0.20	38,38,38,38	0
34	NA	0	8560	1/1	0.82	0.28	-0.23	64,64,64,64	0
36	SR	H	8972	1/1	0.88	0.15	-0.26	157,157,157,157	0
32	MG	0	8045	1/1	1.00	0.12	-0.26	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8904	1/1	0.99	0.16	-0.27	64,64,64,64	0
36	SR	A	8930	1/1	0.69	0.24	-0.27	133,133,133,133	0
36	SR	1	8913	1/1	0.95	0.18	-0.31	97,97,97,97	0
32	MG	0	8043	1/1	0.89	0.13	-0.33	55,55,55,55	0
32	MG	0	8004	1/1	0.92	0.15	-0.45	32,32,32,32	0
32	MG	0	8044	1/1	0.77	0.11	-0.53	49,49,49,49	0
35	CL	J	8821	1/1	0.97	0.17	-0.63	70,70,70,70	0
34	NA	0	8515	1/1	0.90	0.21	-0.68	45,45,45,45	0
32	MG	0	8029	1/1	0.96	0.12	-0.77	54,54,54,54	0
32	MG	0	8021	1/1	0.95	0.10	-0.82	28,28,28,28	0
32	MG	0	8006	1/1	0.98	0.12	-0.83	62,62,62,62	0
34	NA	0	8519	1/1	0.99	0.18	-0.86	44,44,44,44	0
38	CD	1	8702	1/1	0.99	0.13	-0.94	68,68,68,68	0
32	MG	0	8014	1/1	0.96	0.12	-0.97	30,30,30,30	0
34	NA	R	8532	1/1	0.84	0.11	-0.97	57,57,57,57	0
34	NA	J	8538	1/1	0.91	0.14	-1.06	45,45,45,45	0
32	MG	0	8058	1/1	0.93	0.07	-1.06	25,25,25,25	0
36	SR	3	8932	1/1	0.94	0.29	-1.15	149,149,149,149	0
35	CL	0	8812	1/1	0.90	0.09	-1.38	58,58,58,58	0
36	SR	0	8992	1/1	0.88	0.09	-1.64	149,149,149,149	0
34	NA	0	8521	1/1	0.96	0.11	-1.91	34,34,34,34	0
34	NA	0	8557	1/1	0.98	0.07	-1.98	71,71,71,71	0
36	SR	0	8910	1/1	0.89	0.12	-2.00	113,113,113,113	0
32	MG	0	8001	1/1	0.93	0.10	-2.08	28,28,28,28	0
34	NA	M	8539	1/1	0.89	0.12	-2.09	34,34,34,34	0
38	CD	U	8701	1/1	0.98	0.04	-2.17	104,104,104,104	0
32	MG	0	8041	1/1	0.97	0.14	-2.20	27,27,27,27	0
32	MG	T	8057	1/1	0.93	0.03	-2.30	67,67,67,67	0
36	SR	0	8935	1/1	0.98	0.05	-2.47	106,106,106,106	0
38	CD	3	8704	1/1	0.97	0.41	-2.51	176,176,176,176	0
32	MG	0	8025	1/1	0.97	0.07	-2.61	44,44,44,44	0
35	CL	M	8818	1/1	0.93	0.09	-3.14	73,73,73,73	0
32	MG	0	8052	1/1	0.97	0.04	-3.17	40,40,40,40	0
38	CD	Z	8703	1/1	0.97	0.14	-3.17	155,155,155,155	0
36	SR	0	8985	1/1	0.82	0.04	-3.30	173,173,173,173	0
36	SR	0	8902	1/1	0.98	0.13	-3.34	63,63,63,63	0
36	SR	0	8936	1/1	0.78	0.06	-3.47	109,109,109,109	0
36	SR	0	8975	1/1	0.87	0.04	-3.60	158,158,158,158	0
32	MG	Y	8086	1/1	0.96	0.04	-3.63	55,55,55,55	0
34	NA	0	8504	1/1	1.00	0.09	-3.85	22,22,22,22	0
36	SR	0	8949	1/1	0.96	0.10	-4.11	120,120,120,120	0
32	MG	0	8088	1/1	0.95	0.05	-4.74	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8013	1/1	0.98	0.04	-5.62	21,21,21,21	0
36	SR	0	8984	1/1	0.88	0.06	-6.86	139,139,139,139	0
32	MG	0	8075	1/1	0.97	0.06	-8.19	40,40,40,40	0
35	CL	0	8813	1/1	0.96	0.15	-	68,68,68,68	0
36	SR	0	8964	1/1	0.96	0.10	-	149,149,149,149	0
32	MG	0	8036	1/1	0.61	0.21	-	82,82,82,82	0
36	SR	0	8942	1/1	0.96	0.07	-	129,129,129,129	0
34	NA	0	8536	1/1	0.90	0.12	-	72,72,72,72	0
36	SR	0	8918	1/1	0.99	0.13	-	84,84,84,84	0
36	SR	0	8915	1/1	0.93	0.07	-	125,125,125,125	0
32	MG	0	8040	1/1	0.94	0.32	-	100,100,100,100	0
36	SR	0	8997	1/1	-0.12	5.66	-	200,200,200,200	0
36	SR	0	8959	1/1	0.87	0.15	-	194,194,194,194	0
35	CL	0	8814	1/1	0.96	0.41	-	67,67,67,67	0
32	MG	0	8028	1/1	0.99	0.13	-	14,14,14,14	0
34	NA	0	8549	1/1	0.64	0.17	-	83,83,83,83	0
36	SR	0	8957	1/1	0.74	0.23	-	200,200,200,200	0
36	SR	0	9001	1/1	0.90	0.09	-	189,189,189,189	0
34	NA	0	8513	1/1	0.98	0.23	-	63,63,63,63	0
38	CD	O	8705	1/1	0.96	0.03	-	115,115,115,115	0
32	MG	0	8030	1/1	1.00	0.48	-	60,60,60,60	0
36	SR	S	8961	1/1	0.99	0.10	-	127,127,127,127	0
32	MG	0	8023	1/1	0.98	0.16	-	21,21,21,21	0
34	NA	9	8543	1/1	0.77	0.17	-	57,57,57,57	0
32	MG	0	8027	1/1	0.97	0.05	-	30,30,30,30	0
32	MG	0	8082	1/1	0.94	0.40	-	86,86,86,86	0
34	NA	0	8507	1/1	0.98	0.27	-	39,39,39,39	0
32	MG	0	8068	1/1	0.64	0.08	-	49,49,49,49	0
32	MG	0	8083	1/1	0.99	0.08	-	59,59,59,59	0
34	NA	0	8548	1/1	0.96	0.25	-	52,52,52,52	0
36	SR	0	8962	1/1	0.69	0.15	-	155,155,155,155	0
32	MG	B	8042	1/1	0.96	0.08	-	67,67,67,67	0
32	MG	0	8080	1/1	0.98	0.51	-	98,98,98,98	0
34	NA	0	8574	1/1	0.94	0.81	-	67,67,67,67	0
36	SR	0	8976	1/1	0.88	0.22	-	185,185,185,185	0
36	SR	0	8923	1/1	0.98	0.17	-	120,120,120,120	0
36	SR	0	8998	1/1	0.62	0.62	-	169,169,169,169	0
36	SR	0	8922	1/1	0.76	0.47	-	190,190,190,190	0
36	SR	0	9008	1/1	0.98	0.16	-	99,99,99,99	0
32	MG	0	8022	1/1	0.98	0.13	-	29,29,29,29	0
34	NA	0	8541	1/1	0.94	0.15	-	46,46,46,46	0
36	SR	0	8948	1/1	0.99	0.08	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8906	1/1	0.98	0.19	-	65,65,65,65	0
36	SR	0	8978	1/1	0.97	0.04	-	130,130,130,130	0
36	SR	0	8945	1/1	0.93	0.04	-	111,111,111,111	0
34	NA	0	8561	1/1	0.96	0.36	-	73,73,73,73	0
36	SR	0	8947	1/1	0.78	0.60	-	200,200,200,200	0
32	MG	0	8019	1/1	0.99	0.16	-	10,10,10,10	0
32	MG	0	8085	1/1	0.94	0.12	-	83,83,83,83	0
36	SR	0	8974	1/1	0.84	0.42	-	191,191,191,191	0
36	SR	0	8920	1/1	0.97	0.11	-	132,132,132,132	0
32	MG	0	8079	1/1	0.93	0.20	-	63,63,63,63	0
36	SR	0	8982	1/1	0.91	1.68	-	200,200,200,200	0
34	NA	0	8570	1/1	0.98	0.11	-	65,65,65,65	0
36	SR	F	9005	1/1	0.90	0.13	-	154,154,154,154	0
36	SR	0	8911	1/1	0.98	0.13	-	109,109,109,109	0
36	SR	0	8901	1/1	0.94	0.12	-	89,89,89,89	0
35	CL	R	8806	1/1	0.95	0.17	-	62,62,62,62	0
32	MG	0	8005	1/1	0.96	0.28	-	30,30,30,30	0
36	SR	A	8993	1/1	0.85	0.04	-	177,177,177,177	0
36	SR	0	8996	1/1	0.89	0.40	-	200,200,200,200	0
34	NA	S	8510	1/1	0.38	0.30	-	69,69,69,69	0
32	MG	0	8071	1/1	0.95	0.12	-	50,50,50,50	0
32	MG	0	8046	1/1	0.98	0.21	-	48,48,48,48	0
32	MG	0	8048	1/1	0.99	0.31	-	38,38,38,38	0
32	MG	0	8055	1/1	0.88	0.26	-	67,67,67,67	0
36	SR	0	8994	1/1	0.75	0.72	-	200,200,200,200	0
35	CL	3	8804	1/1	0.73	0.15	-	96,96,96,96	0
34	NA	0	8531	1/1	0.85	0.27	-	42,42,42,42	0
36	SR	0	8971	1/1	0.17	0.12	-	200,200,200,200	0
36	SR	0	8970	1/1	0.91	0.06	-	150,150,150,150	0
36	SR	0	8925	1/1	0.99	0.13	-	105,105,105,105	0
35	CL	Y	8820	1/1	0.86	0.06	-	59,59,59,59	0
36	SR	0	8967	1/1	0.94	0.08	-	157,157,157,157	0
34	NA	0	8518	1/1	0.90	0.39	-	82,82,82,82	0
32	MG	0	8063	1/1	0.97	0.15	-	67,67,67,67	0
36	SR	B	8950	1/1	0.96	0.28	-	151,151,151,151	0
36	SR	0	8905	1/1	0.99	0.27	-	70,70,70,70	0
36	SR	0	9007	1/1	0.85	0.78	-	180,180,180,180	0
36	SR	0	8919	1/1	0.97	0.18	-	194,194,194,194	0
32	MG	0	8026	1/1	0.99	0.04	-	32,32,32,32	0
32	MG	0	8008	1/1	0.97	0.14	-	15,15,15,15	0
36	SR	0	8951	1/1	0.94	0.19	-	177,177,177,177	0
32	MG	K	8054	1/1	0.98	0.11	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8989	1/1	0.85	0.26	-	196,196,196,196	0
36	SR	0	8946	1/1	0.94	0.27	-	138,138,138,138	0
32	MG	0	8081	1/1	0.78	0.44	-	104,104,104,104	0
32	MG	9	8074	1/1	0.77	0.12	-	127,127,127,127	0
34	NA	C	8503	1/1	0.96	0.32	-	39,39,39,39	0
32	MG	0	8091	1/1	0.97	0.18	-	42,42,42,42	0
36	SR	0	9006	1/1	0.81	0.49	-	200,200,200,200	0
36	SR	0	8960	1/1	0.88	0.10	-	174,174,174,174	0
32	MG	0	8089	1/1	0.94	0.29	-	72,72,72,72	0
36	SR	0	8968	1/1	0.90	0.12	-	181,181,181,181	0
34	NA	0	8527	1/1	0.75	0.24	-	60,60,60,60	0
36	SR	9	8980	1/1	0.89	0.05	-	192,192,192,192	0
35	CL	0	8811	1/1	0.89	0.60	-	99,99,99,99	0
34	NA	0	8526	1/1	0.95	0.27	-	52,52,52,52	0
32	MG	0	8056	1/1	0.98	0.07	-	47,47,47,47	0
36	SR	0	9004	1/1	0.86	0.46	-	200,200,200,200	0
32	MG	0	8069	1/1	0.87	0.55	-	68,68,68,68	0
34	NA	0	8520	1/1	0.99	0.19	-	57,57,57,57	0
36	SR	0	8983	1/1	0.96	0.21	-	185,185,185,185	0
35	CL	0	8805	1/1	0.83	0.39	-	97,97,97,97	0
34	NA	0	8505	1/1	0.61	0.44	-	56,56,56,56	0
35	CL	A	8809	1/1	0.98	0.67	-	96,96,96,96	0
36	SR	0	8955	1/1	0.94	0.17	-	199,199,199,199	0
34	NA	0	8511	1/1	0.86	0.22	-	64,64,64,64	0
32	MG	0	8015	1/1	0.95	0.10	-	25,25,25,25	0
36	SR	3	8999	1/1	0.92	0.18	-	160,160,160,160	0
32	MG	0	8053	1/1	0.92	0.05	-	57,57,57,57	0
35	CL	0	8817	1/1	0.99	0.11	-	63,63,63,63	0
34	NA	0	8567	1/1	0.96	0.20	-	58,58,58,58	0
32	MG	0	8020	1/1	0.99	0.11	-	52,52,52,52	0
32	MG	0	8018	1/1	0.99	0.18	-	42,42,42,42	0
34	NA	0	8573	1/1	0.86	0.19	-	92,92,92,92	0
34	NA	0	8525	1/1	0.52	0.33	-	92,92,92,92	0
36	SR	0	8941	1/1	0.96	0.31	-	143,143,143,143	0
32	MG	0	8076	1/1	0.97	0.06	-	36,36,36,36	0
36	SR	1	8952	1/1	0.96	0.19	-	81,81,81,81	0
36	SR	0	8939	1/1	0.98	0.05	-	145,145,145,145	0
35	CL	0	8816	1/1	0.98	0.71	-	86,86,86,86	0
36	SR	0	8965	1/1	0.99	0.16	-	135,135,135,135	0
36	SR	0	8907	1/1	0.99	0.16	-	63,63,63,63	0
32	MG	0	8039	1/1	0.90	0.27	-	76,76,76,76	0
35	CL	0	8803	1/1	0.94	0.08	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8017	1/1	0.99	0.07	-	29,29,29,29	0
36	SR	0	8954	1/1	0.95	0.12	-	122,122,122,122	0
36	SR	0	8909	1/1	0.98	0.07	-	89,89,89,89	0
36	SR	0	8903	1/1	0.98	0.19	-	62,62,62,62	0
36	SR	0	9002	1/1	0.98	0.09	-	188,188,188,188	0
36	SR	0	8940	1/1	0.95	0.03	-	117,117,117,117	0
34	NA	0	8554	1/1	0.61	0.38	-	71,71,71,71	0
36	SR	0	8937	1/1	0.98	0.17	-	108,108,108,108	0
35	CL	0	8815	1/1	0.95	0.24	-	90,90,90,90	0
36	SR	0	8917	1/1	0.97	0.13	-	121,121,121,121	0
35	CL	N	8807	1/1	0.79	0.38	-	134,134,134,134	0
36	SR	9	9003	1/1	0.78	0.06	-	200,200,200,200	0
35	CL	0	8822	1/1	0.88	1.37	-	94,94,94,94	0
36	SR	0	8990	1/1	0.98	0.19	-	111,111,111,111	0
34	NA	0	8516	1/1	0.94	0.26	-	26,26,26,26	0
36	SR	0	8933	1/1	0.97	0.04	-	122,122,122,122	0
32	MG	0	8066	1/1	0.84	0.92	-	70,70,70,70	0
34	NA	0	8509	1/1	0.78	0.49	-	66,66,66,66	0
32	MG	0	8077	1/1	0.77	0.16	-	47,47,47,47	0
36	SR	0	8958	1/1	0.69	0.08	-	150,150,150,150	0
34	NA	0	8529	1/1	0.77	0.11	-	49,49,49,49	0
34	NA	0	8544	1/1	0.90	0.17	-	68,68,68,68	0
36	SR	R	8912	1/1	0.99	0.23	-	106,106,106,106	0
32	MG	0	8093	1/1	0.97	0.11	-	40,40,40,40	0
34	NA	0	8514	1/1	0.83	0.26	-	61,61,61,61	0
36	SR	0	8914	1/1	0.91	0.32	-	130,130,130,130	0
32	MG	0	8033	1/1	0.89	0.26	-	56,56,56,56	0
36	SR	0	8931	1/1	0.99	0.10	-	123,123,123,123	0
36	SR	0	9000	1/1	0.96	0.23	-	200,200,200,200	0
34	NA	0	8566	1/1	0.79	0.86	-	51,51,51,51	0
35	CL	J	8802	1/1	0.98	0.08	-	100,100,100,100	0
32	MG	0	8038	1/1	0.95	0.12	-	81,81,81,81	0
32	MG	0	8061	1/1	0.82	0.30	-	42,42,42,42	0
36	SR	0	8928	1/1	0.92	0.05	-	164,164,164,164	0
36	SR	0	8988	1/1	0.88	0.11	-	181,181,181,181	0
36	SR	0	8926	1/1	0.99	0.16	-	145,145,145,145	0
36	SR	J	8986	1/1	0.66	1.53	-	200,200,200,200	0
32	MG	0	8049	1/1	0.70	0.20	-	61,61,61,61	0
36	SR	0	8916	1/1	0.74	0.08	-	129,129,129,129	0
32	MG	0	8032	1/1	0.94	0.08	-	64,64,64,64	0
34	NA	0	8506	1/1	0.47	0.60	-	105,105,105,105	0
32	MG	0	8078	1/1	0.97	0.23	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8024	1/1	0.97	0.14	-	58,58,58,58	0
34	NA	0	8552	1/1	0.85	0.31	-	68,68,68,68	0
32	MG	0	8031	1/1	0.94	0.35	-	71,71,71,71	0
36	SR	0	8995	1/1	0.84	0.25	-	128,128,128,128	0
32	MG	2	8060	1/1	0.95	0.09	-	56,56,56,56	0
32	MG	0	8035	1/1	0.94	0.12	-	47,47,47,47	0
34	NA	0	8545	1/1	0.83	0.30	-	40,40,40,40	0
35	CL	L	8810	1/1	0.96	0.24	-	86,86,86,86	0
36	SR	0	8938	1/1	0.89	0.07	-	200,200,200,200	0
34	NA	0	8508	1/1	0.77	0.98	-	70,70,70,70	0
32	MG	0	8072	1/1	0.89	0.08	-	37,37,37,37	0
36	SR	0	8991	1/1	0.68	0.10	-	190,190,190,190	0
34	NA	0	8501	1/1	0.73	0.22	-	41,41,41,41	0
32	MG	0	8092	1/1	0.65	0.12	-	53,53,53,53	0
32	MG	0	8037	1/1	0.95	0.29	-	84,84,84,84	0
32	MG	0	8064	1/1	0.97	0.20	-	48,48,48,48	0
32	MG	0	8087	1/1	0.92	0.18	-	20,20,20,20	0
36	SR	0	8924	1/1	0.94	0.17	-	138,138,138,138	0
36	SR	0	8908	1/1	0.95	0.06	-	109,109,109,109	0
35	CL	J	8801	1/1	0.97	0.20	-	90,90,90,90	0
36	SR	0	8981	1/1	0.95	0.11	-	151,151,151,151	0
36	SR	0	8934	1/1	0.96	0.09	-	114,114,114,114	0
36	SR	0	8944	1/1	0.93	0.17	-	171,171,171,171	0
36	SR	0	8966	1/1	0.95	0.10	-	110,110,110,110	0
36	SR	0	8921	1/1	0.97	0.09	-	90,90,90,90	0
36	SR	0	8963	1/1	0.94	0.15	-	135,135,135,135	0
36	SR	0	8953	1/1	0.91	0.24	-	185,185,185,185	0
32	MG	0	8059	1/1	0.97	0.12	-	40,40,40,40	0
36	SR	0	8927	1/1	0.87	0.16	-	172,172,172,172	0
36	SR	0	8973	1/1	0.87	0.16	-	134,134,134,134	0
36	SR	0	8977	1/1	0.83	0.14	-	197,197,197,197	0
36	SR	0	8956	1/1	0.98	0.23	-	178,178,178,178	0
36	SR	0	8979	1/1	0.82	0.10	-	200,200,200,200	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.