



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 02:22 PM UTC

PDB ID : 3G4S / pdb_00003g4s
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

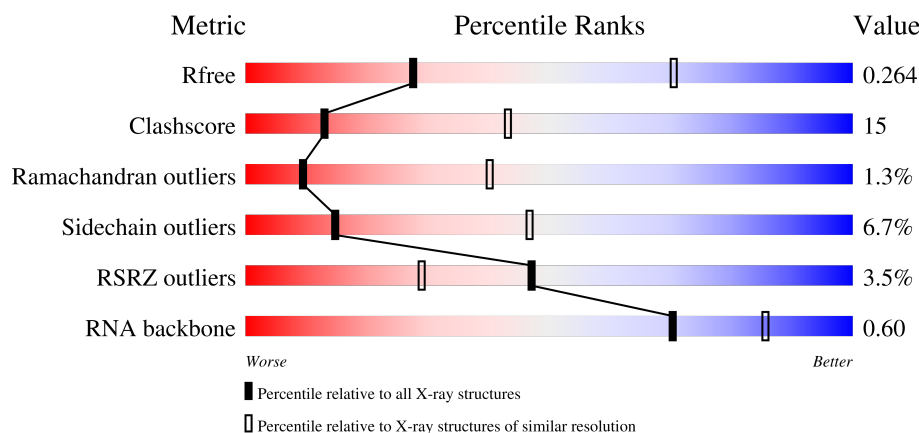
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	0	2923	
2	A	237	
3	B	337	
4	C	246	

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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	42% 74% 17% 9%
31	9	122	25% 63% 11%

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
36	SR	0	8997	-	-	-	X
36	SR	L	8969	-	-	-	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 (CCD ID: MG) (formula: Mg).

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

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	A	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	J	3	Total Cl 3 3	0	0
35	L	1	Total Cl 1 1	0	0
35	M	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

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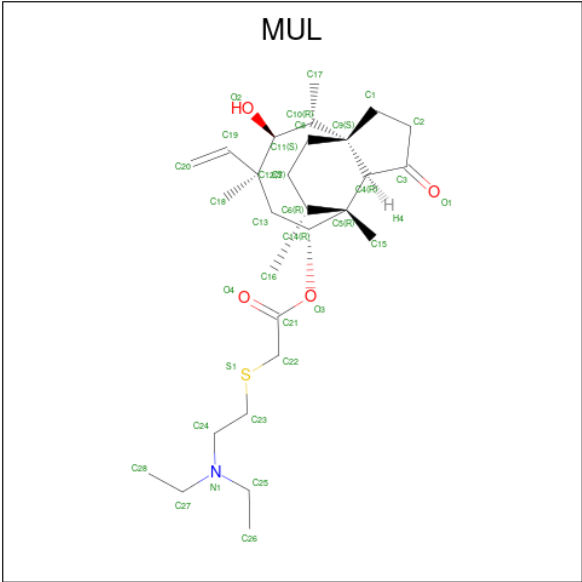
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

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

- Molecule 37 is TIAMULIN (CCD ID: MUL) (formula: C₂₈H₄₇NO₄S).



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 (CCD ID: CD) (formula: Cd).

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

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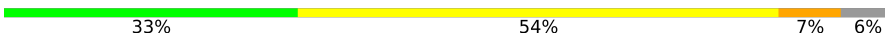
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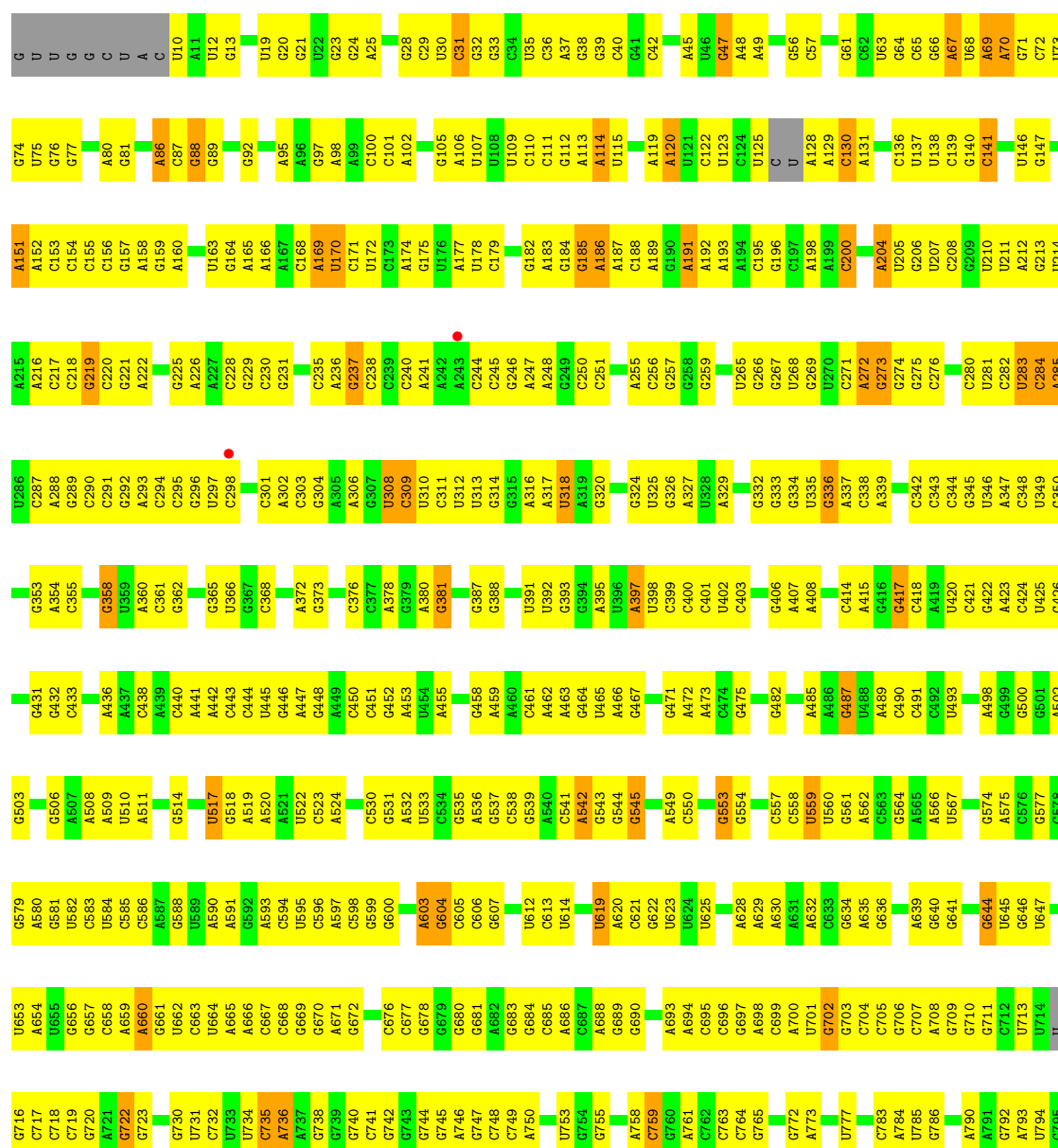
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	22	Total 22	O 22	0	0
39	Y	105	Total 105	O 105	0	0
39	Z	30	Total 30	O 30	0	0
39	1	55	Total 55	O 55	0	0
39	2	48	Total 48	O 48	0	0
39	3	62	Total 62	O 62	0	0
39	9	152	Total 152	O 152	0	0

3 Residue-property plots

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

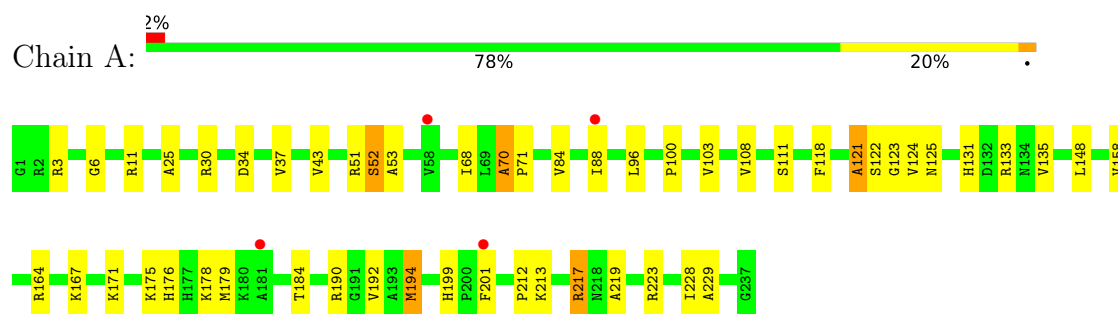
• Molecule 1: 23S ribosomal RNA

Chain 0: 

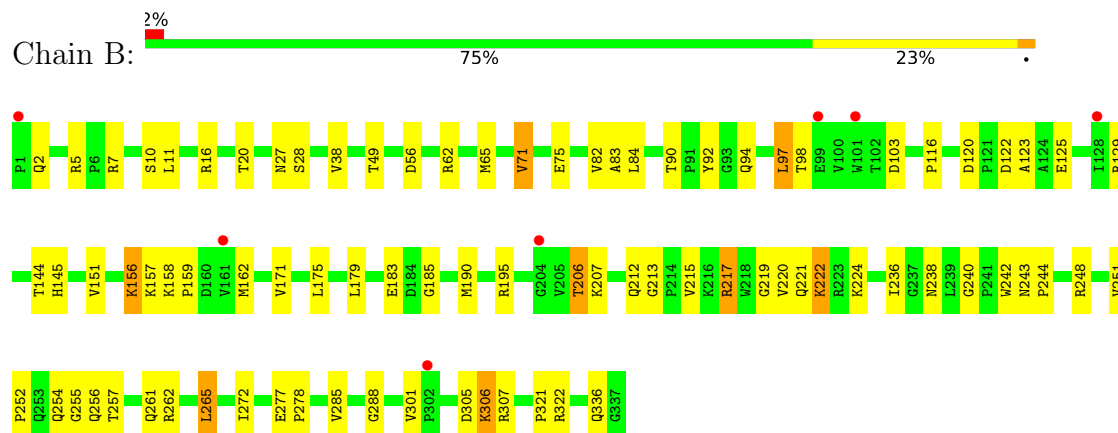


G1812	G1745	C1674	G1602	C1517	G1368	U1218	U1156	A1082	A1005	G941	G868	A796
G1813	A1746	C1675	A1603	A1518	A1369	U1219	C1157	C1083	A1006	U942	G869	U801
A1814	U1747	G1676	G1604	G1516	A1372	G1221	G1158	C1085	A1007	G943	G870	G802
C1816	U1748	U1677	G1605	C1521	G1372	G1228	G1159	C1086	U1008	G944	U872	
C1817	U1749	A1678	A1606	G1522	A1375	G1229	A1161	C1087	U1009	U945	A806	A806
C1818	G1752	C1679	G1607	G1523	G1376	C1230	G1162	A1088	C1010	U947	A807	A807
G1819	G1753	U1680	G1608	U1524	C1377	A1231	G1163	U1096	C1011	G946	A808	A808
G1820	A1754	A1682	C1450	G1525	G1378	A1232	U1164	A1097	A1012		G809	G809
A1821	A1755	G1683	G1451	A1526	A1379	A1233	G1165	A1098	A1013	A951	G878	G878
A1822	G1756	A1684	G1452	A1527	A1380	A1234	A1166	A1099	A1014	G952	C810	C810
G1823	U1757	A1685	G1453	A1528	U1309	U1234	G1167	G1099	C1015	G953	C879	C879
C1824	U1758	C1686	C1454	U1531	U1384		C1168	G1100	U1016	U954	A812	A812
U1825	A1759	C1687	C1455	U1531	U1384		C1168	G1100	U1016	U954	A812	A812
G1826	G1760	G1688	A1615	G1535	G1387	C1238	U1169	U1101	C1023	A955	U882	U882
G1827	U1761	A1689	A1616	C1536	A1388	G1239	U1170	C1102	G1024	G956	U883	U883
G1828	C1762	G1692	C1617	U1544	U1389	A1242	A1171	C1103	G1025	A957	G884	G884
A1829	C1763	C1692	G1618	C1545	G1390	C1243	A1172	A1098	C1026	G958	G886	G886
C1830	C1764	G1695	G1619	G1546	A1391	U1244	A1173	G1105	U1026	C959	G887	G887
U1831	G1765	G1696	G1620	U1547	A1392	C1245	A1174	A1106	G1027	G960	U888	U888
G1832	U1766	U1697	G1621	A1548	A1392	A1246	G1175	U1109	U1028	A961	C890	C890
C1833	A1767	G1697	G1622	U1549	C1396			G1110	U1029	C962	U821	U821
C1834	C1768	U1698	C1623	C1549	C1397	U1249	C1179	G1111	U1030	G963	U823	U823
U1835	C1769	U1698	A1624	C1549	G1326	C1250	U1180	G1112	A1032	A965	G824	G824
	U1770	A1701	U1625	C1554	G1327	C1251	A1181	G1113	U1041	G968	U825	U825
U1838	U1771	U1702	G1626	G1555	A1328	A1252	C1182	A1114	U1041	G968	U826	U826
A1839	U1772	G1703	G1627	G1556	A1328	C1252	C1183	U1115	C1044	G969	G834	G834
A1840	G1773	G1704	A1630	U1557	G1331	A1253	C1184	U1116	G1045	U970	U835	U835
C1841	G1774	C1705	A1631	G1557	C1332	C1254	U1185	A1117	G1046	G	G836	G836
	A1775	G1706	A1632	U1558	A1407	A1255	U1186	A1118	U1047	U	U837	U837
G1844	U1776	G1707	C1633	A1559	U1408	C1256	C1187	G1119	G	G	C838	C838
A1845	G1777	G1707	G1634	U1561	G1409	G1257	U1187	U1120	C	C	C839	C839
U1846	A1778	A1710	U1635	C1566	U1412	C1258	A1188	G1121	C1051	C	C905	C905
A1847	A1779	A1711	G1636	G1567	G1415	U1259	A1189	U1122	G1052	C	C906	C906
G1848	G1780	G1712	G1637	U1567	G1416	C1260	A1190	U1123	G1053	G	A907	A907
U1849	C1781	C1714	U1639	C1570	U1419	C1262	A1191	A1124	G1054	C	U840	U840
G1850	U1784	C1715	C1640	G1571	C1420	C1268	A1192	U1125	G1055	C	C841	C841
G1851	G1785	A1716	A1641	A1572	C1421	G1269	A1193	U1126	G1056	C	C842	C842
A1852	C1786	G1722	C1642	C1573	U1422		A1194	C1127	U1056	U	A843	A843
C1853	C1787	U1723	C1643	A1574	U1423		G1195	U1128	A1057	C	A846	A846
G1854	U1788	U1724	U1644	C1575	U1424		C1196	C1129	C1058	C	C847	C847
G1855	G1789	C1725	U1645	U1575	A1424		G1196	U1130	C1059	A	C848	C848
C1856	U1790	G1725	G1646	C1585				U1131	C1060	G	C849	C849
A1857	U1791	G1728	G1647	G1586				U1132	C1061	G	U850	U850
A1858	U1792	A1729	G1648	U1587	A1427		A1199	A1133	U1066	A	C851	C851
	C1792	G1730	G1649	U1588	C1428		A1200	G1134	A1067	G	U852	U852
C1861	G1793	C1731	U1503	G1589	U1429		A1202	U1135	C1068	A	C853	C853
C1862	G1794	C1732	A1504	G1590	G1430		G1203	U1136	A922	G	G854	G854
	A1797	A1732	U1505	A1590	U1430		U1205	G1137	C1069	G	U855	U855
A1866	U1798	C1733	U1506	A1591	G1433		U1206	G1138	A1070	U	G856	G856
G1867	G1799	C1734	C1507	G1592	A1434		A1207	U1139	G1071	C	A857	A857
G1868	U1800	C1735	C1508	U1593	U1436		C1208	U1140	G1072	G	U858	U858
	G1800	A1736	U1509	G1594	C1360		C1209	U1141	A1073	C	C859	C859
G1873	C1803	G1739	U1510	C1595	U1437		G1210	C1142	G1074	C	U860	U860
	A1804	U1740	U1511	U1596	A1438		G1211	U1149	G1075	A	C932	C932
G1877	G1805	U1741	G1512	A1597	C1439		C1212	U1150	G1076	C	G861	G861
G1878	U1742	A1742	C1513	U1598	U1440		G1214	A1151	A1078	A	G863	G863
U1879	G1806	G1743	C1514	A1599	G1441		G1215	G1152	C1079	C	U864	U864
C1880	U1807	G1744	A1515	G1600	A1442		A1216	A1153	C1080	U1001	G865	G865
A1881			U1673	G1601	G1443		G1217		A1081	G1002	U866	U866

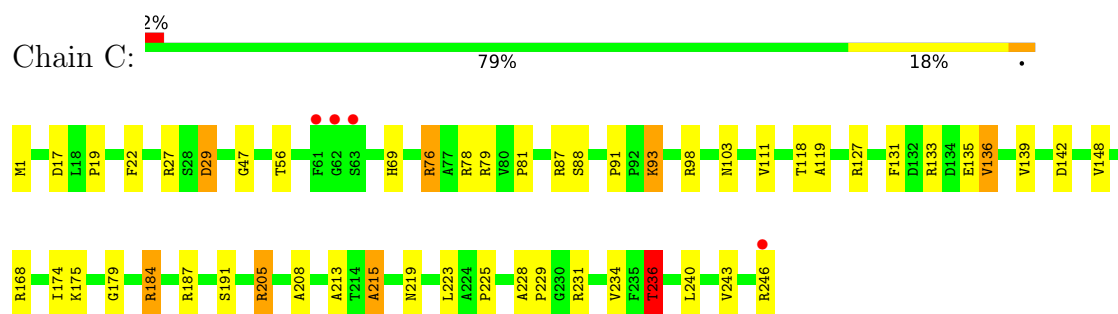
- Molecule 2: 50S ribosomal protein L2P



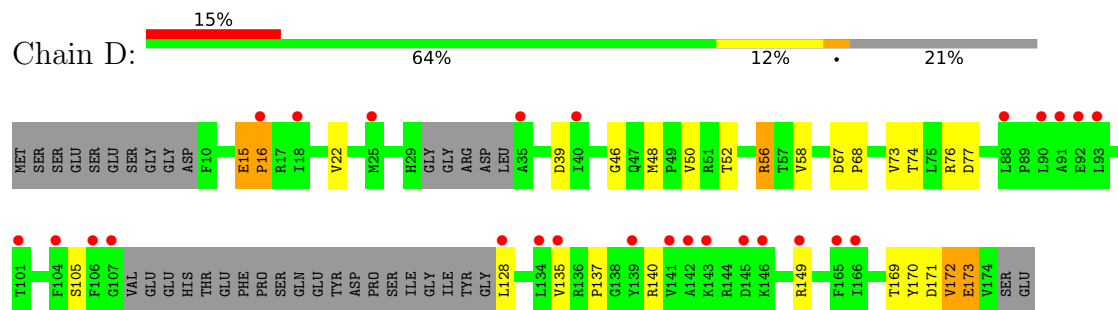
• Molecule 3: 50S ribosomal protein L3P



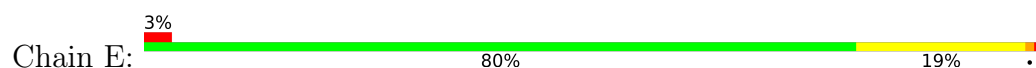
• Molecule 4: 50S ribosomal protein L4P

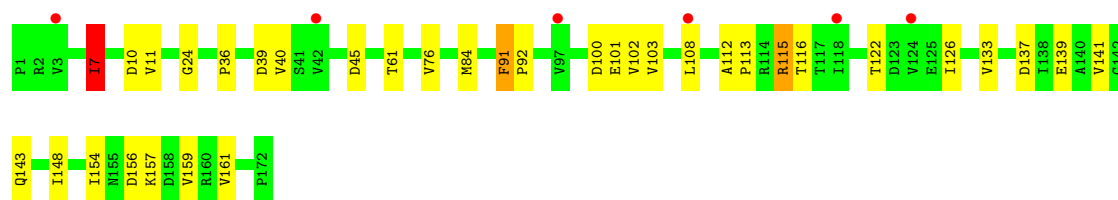


• Molecule 5: 50S ribosomal protein L5P

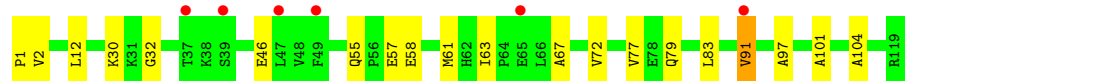
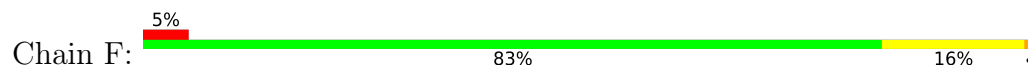


• Molecule 6: 50S ribosomal protein L6P

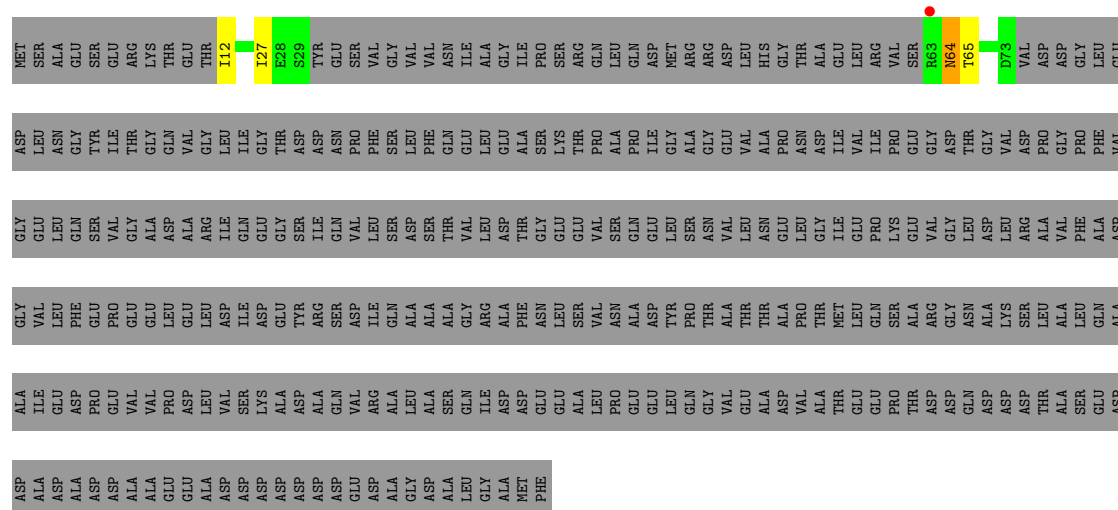




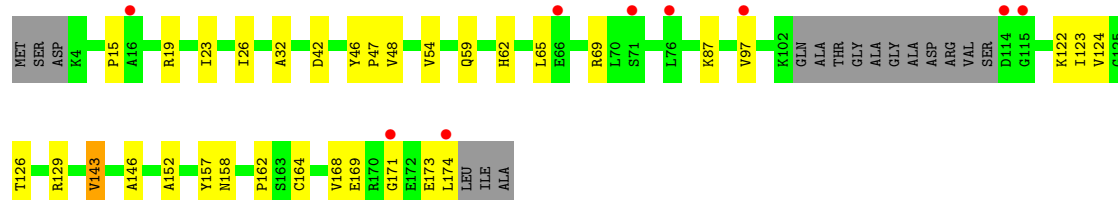
- Molecule 7: 50S ribosomal protein L7Ae



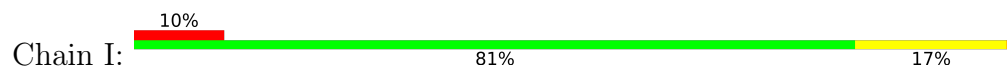
- Molecule 8: 50S ribosomal protein L10

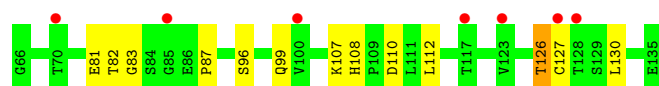


- Molecule 9: 50S ribosomal protein L10e

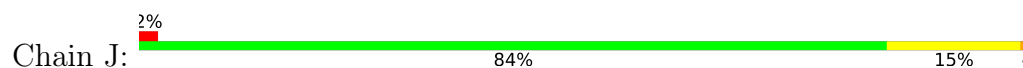


- Molecule 10: 50S ribosomal protein L11P

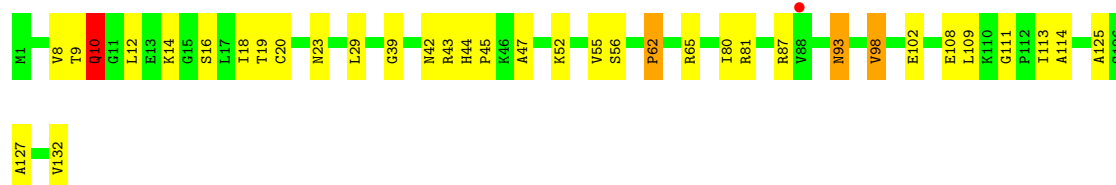




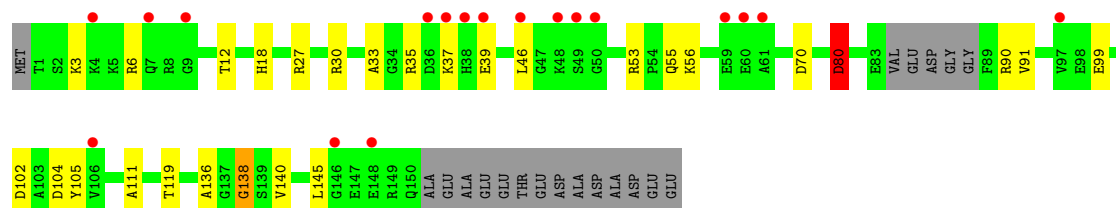
- Molecule 11: 50S ribosomal protein L13P



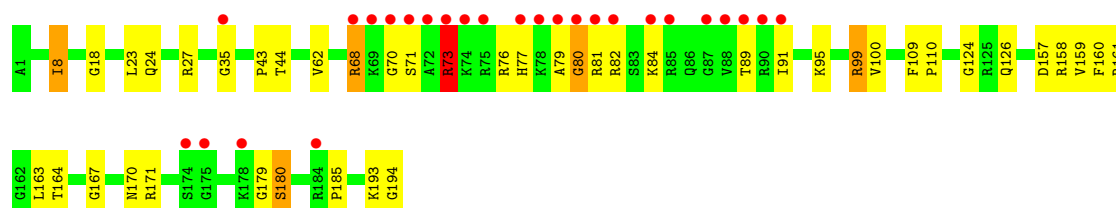
- Molecule 12: 50S ribosomal protein L14P



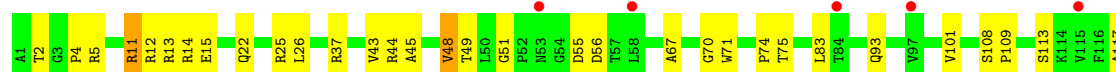
- Molecule 13: 50S ribosomal protein L15P

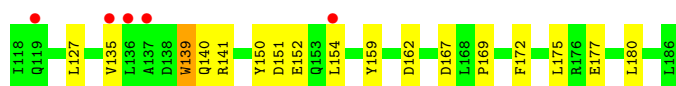


- Molecule 14: 50S ribosomal protein L15e

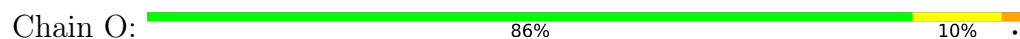


- Molecule 15: 50S ribosomal protein L18P

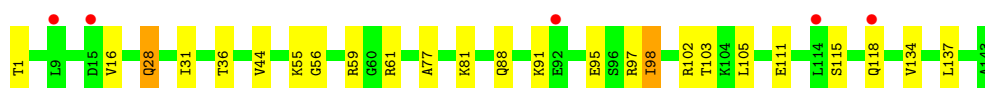
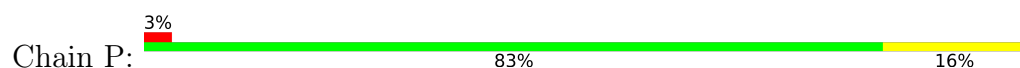




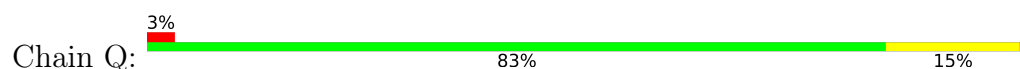
- Molecule 16: 50S ribosomal protein L18e



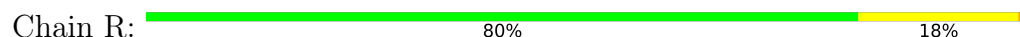
- Molecule 17: 50S ribosomal protein L19e



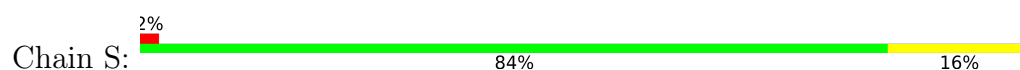
- Molecule 18: 50S ribosomal protein L21e



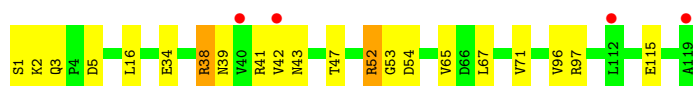
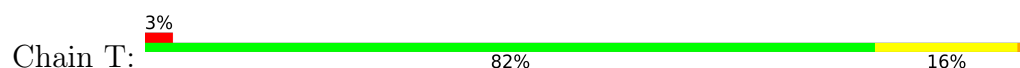
- Molecule 19: 50S ribosomal protein L22P



- Molecule 20: 50S ribosomal protein L23P

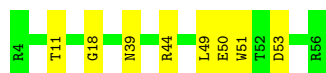


- Molecule 21: 50S ribosomal protein L24P



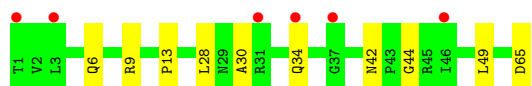
- Molecule 22: 50S ribosomal protein L24e

Chain U:  85% 15%



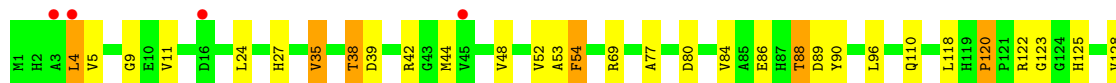
- Molecule 23: 50S ribosomal protein L29P

Chain V:  9% 85% 15%



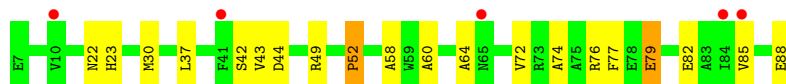
- Molecule 24: 50S ribosomal protein L30P

Chain W:  3% 75% 20% 5%



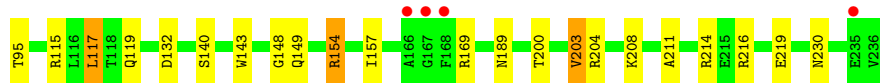
- Molecule 25: 50S ribosomal protein L31e

Chain X:  6% 76% 22%



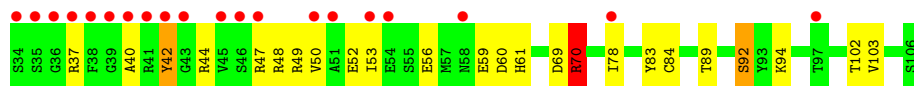
- Molecule 26: 50S ribosomal protein L32e

Chain Y:  3% 85% 13%



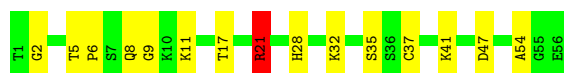
- Molecule 27: 50S ribosomal protein L37Ae

Chain Z:  27% 67% 29%

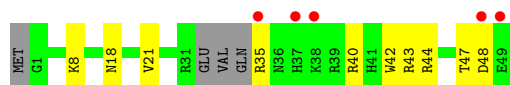


- Molecule 28: 50S ribosomal protein L37e

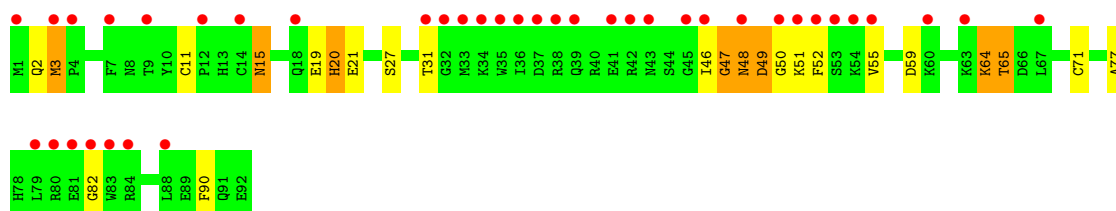
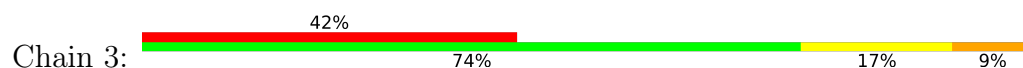
Chain 1:  73% 25%



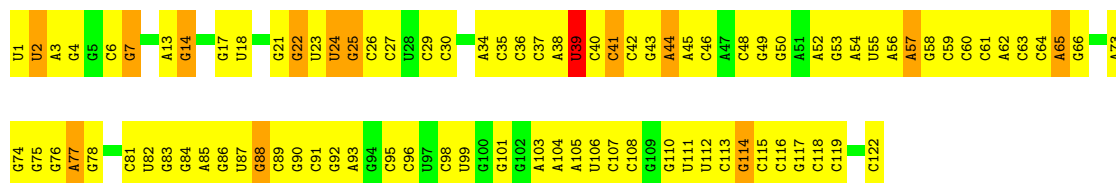
- Molecule 29: 50S ribosomal protein L39e



- 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, α , β , γ	212.27Å 299.84Å 574.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.20 49.84 – 3.20	Depositor EDS
% Data completeness (in resolution range)	83.7 (49.84-3.20) 83.7 (49.84-3.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.290 0.201 , 0.264	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 121.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	99167	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.43	0/65958	0.61	10/102869 (0.0%)
2	A	0.70	1/1787 (0.1%)	1.15	16/2408 (0.7%)
3	B	0.63	0/2690	1.14	16/3652 (0.4%)
4	C	0.65	0/1885	1.18	10/2552 (0.4%)
5	D	0.79	0/1111	1.18	9/1498 (0.6%)
6	E	0.69	1/1383 (0.1%)	1.03	4/1880 (0.2%)
7	F	0.71	1/901 (0.1%)	1.15	3/1224 (0.2%)
8	G	0.63	0/241	1.07	1/324 (0.3%)
9	H	0.65	0/1302	1.10	6/1743 (0.3%)
10	I	0.81	0/527	1.12	3/716 (0.4%)
11	J	0.64	0/1136	1.11	4/1530 (0.3%)
12	K	0.64	0/1004	1.10	5/1351 (0.4%)
13	L	0.65	0/1130	1.10	7/1509 (0.5%)
14	M	0.62	0/1583	1.12	11/2116 (0.5%)
15	N	0.68	0/1474	1.24	13/1999 (0.7%)
16	O	0.61	0/874	1.16	6/1181 (0.5%)
17	P	0.55	0/1148	1.10	7/1528 (0.5%)
18	Q	0.63	0/749	1.09	4/1005 (0.4%)
19	R	0.65	1/1173 (0.1%)	1.10	8/1578 (0.5%)
20	S	0.58	0/649	1.02	2/875 (0.2%)
21	T	0.56	0/958	1.13	7/1289 (0.5%)
22	U	0.67	0/418	1.16	2/562 (0.4%)
23	V	0.64	0/503	1.21	3/675 (0.4%)
24	W	0.68	1/1219 (0.1%)	1.20	10/1655 (0.6%)
25	X	0.69	0/665	1.22	6/895 (0.7%)
26	Y	0.62	0/1147	1.16	8/1536 (0.5%)
27	Z	0.80	0/585	1.23	6/781 (0.8%)
28	1	0.63	0/438	1.12	5/578 (0.9%)
29	2	0.55	0/401	1.03	1/529 (0.2%)
30	3	0.91	0/771	1.20	5/1024 (0.5%)
31	9	0.41	0/2904	0.57	1/4526 (0.0%)
All	All	0.51	5/98714 (0.0%)	0.79	199/147588 (0.1%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	63	ILE	CA-CB	7.77	1.58	1.54
24	W	153	MET	SD-CE	-6.01	1.64	1.79
19	R	109	MET	SD-CE	-5.77	1.65	1.79
6	E	7	ILE	CA-CB	5.21	1.60	1.54
2	A	194	MET	SD-CE	-5.07	1.66	1.79

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	170	TYR	N-CA-C	10.22	125.34	113.38
21	T	52	ARG	N-CA-C	9.15	125.14	113.88
16	O	7	LEU	N-CA-C	-8.65	101.56	112.90
16	O	43	VAL	N-CA-C	8.55	120.80	108.48
9	H	124	VAL	N-CA-C	8.54	118.81	111.90
15	N	51	GLY	CA-C-N	8.42	128.00	119.24
15	N	51	GLY	C-N-CA	8.42	128.00	119.24
24	W	35	VAL	N-CA-C	8.09	116.71	107.89
9	H	164	CYS	N-CA-C	7.91	121.78	109.52
14	M	8	ILE	N-CA-C	-7.90	105.02	111.81
2	A	70	ALA	N-CA-C	7.83	120.12	109.24
15	N	13	ARG	N-CA-C	-7.68	104.43	113.88
30	3	59	ASP	N-CA-C	7.66	118.10	108.45
22	U	18	GLY	N-CA-C	7.61	120.02	110.96
3	B	222	LYS	N-CA-C	-7.55	100.35	110.55
27	Z	84	CYS	N-CA-C	-7.50	104.09	112.57
17	P	103	THR	N-CA-C	-7.42	104.38	113.50
19	R	82	GLU	N-CA-C	7.24	120.22	111.82
1	0	1504	A	N9-C1'-C2'	7.09	122.64	112.00
13	L	33	ALA	N-CA-C	7.02	120.14	110.24
24	W	86	GLU	N-CA-C	7.02	121.84	113.28
2	A	135	VAL	N-CA-C	6.94	119.54	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	213	GLY	CA-C-N	6.93	127.22	119.32
3	B	213	GLY	C-N-CA	6.93	127.22	119.32
15	N	48	VAL	N-CA-C	6.89	117.82	108.17
18	Q	17	LYS	N-CA-C	-6.86	101.42	109.93
25	X	79	GLU	N-CA-C	6.83	118.37	111.07
1	0	834	G	C2'-C3'-O3'	-6.77	103.55	113.70
10	I	127	CYS	N-CA-C	6.75	118.43	111.14
8	G	27	ILE	N-CA-C	-6.72	106.03	111.81
13	L	55	GLN	N-CA-C	6.70	120.32	111.75
17	P	44	VAL	N-CA-C	-6.57	105.34	111.45
26	Y	117	LEU	N-CA-C	-6.52	104.97	113.12
5	D	173	GLU	N-CA-C	6.49	114.98	108.75
23	V	30	ALA	N-CA-C	-6.48	105.91	113.88
26	Y	115	ARG	N-CA-C	-6.48	105.02	113.12
15	N	117	ALA	N-CA-C	-6.48	105.51	113.41
14	M	18	GLY	N-CA-C	6.47	120.89	111.24
30	3	71	CYS	N-CA-C	6.47	119.89	109.79
3	B	217	ARG	N-CA-C	6.44	117.96	111.07
25	X	60	ALA	N-CA-C	6.42	117.97	110.97
30	3	82	GLY	N-CA-C	6.41	120.00	111.03
28	1	11	LYS	N-CA-C	6.40	118.74	109.71
26	Y	143	TRP	N-CA-C	6.38	119.24	110.24
23	V	42	ASN	CA-C-N	6.34	126.83	119.47
23	V	42	ASN	C-N-CA	6.34	126.83	119.47
6	E	11	VAL	N-CA-C	6.31	118.11	108.71
5	D	39	ASP	N-CA-C	6.31	117.95	111.14
15	N	150	TYR	N-CA-C	-6.31	106.22	114.04
6	E	161	VAL	N-CA-C	-6.24	106.20	111.56
1	0	820	G	N9-C1'-C2'	6.23	121.34	112.00
18	Q	84	ILE	N-CA-C	6.21	117.09	108.89
14	M	73	ARG	N-CA-C	-6.17	102.10	110.68
16	O	111	VAL	N-CA-C	6.17	117.00	108.12
15	N	75	THR	N-CA-C	6.16	120.95	113.38
2	A	111	SER	N-CA-C	-6.14	101.84	110.31
22	U	50	GLU	N-CA-C	6.13	118.76	111.71
25	X	77	PHE	N-CA-C	6.13	116.33	108.24
14	M	124	GLY	N-CA-C	6.08	121.78	113.99
3	B	236	ILE	N-CA-C	6.08	117.08	110.21
1	0	2726	U	N1-C1'-C2'	6.06	121.09	112.00
19	R	122	GLN	N-CA-C	-6.04	98.88	108.73
4	C	19	PRO	N-CA-C	6.03	120.70	111.11
24	W	39	ASP	N-CA-C	-6.03	105.58	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	R	13	THR	N-CA-C	6.01	118.55	109.41
5	D	77	ASP	N-CA-C	6.01	118.71	108.67
9	H	143	VAL	N-CA-C	6.00	117.47	110.62
28	1	47	ASP	N-CA-C	-5.97	100.06	109.50
4	C	215	ALA	N-CA-C	5.96	120.02	112.87
9	H	123	ILE	N-CA-C	5.94	116.68	108.84
21	T	54	ASP	N-CA-C	-5.93	104.76	112.23
4	C	213	ALA	N-CA-C	5.92	117.21	108.86
27	Z	42	TYR	N-CA-C	5.90	123.36	110.80
26	Y	203	VAL	N-CA-C	5.85	116.91	108.48
4	C	191	SER	N-CA-C	5.84	116.92	108.34
17	P	111	GLU	N-CA-C	-5.83	107.40	114.75
10	I	126	THR	N-CA-C	-5.83	107.98	114.62
19	R	106	GLY	N-CA-C	5.82	119.68	112.64
5	D	16	PRO	N-CA-C	5.81	119.64	111.33
26	Y	140	SER	N-CA-C	5.77	118.15	110.53
4	C	236	THR	N-CA-C	-5.77	100.88	110.17
16	O	51	TYR	N-CA-C	5.77	121.22	113.72
30	3	77	ALA	N-CA-C	5.76	118.35	109.07
15	N	169	PRO	N-CA-C	-5.74	108.71	114.68
19	R	137	ASN	N-CA-C	5.74	119.01	110.52
9	H	152	ALA	N-CA-C	-5.73	106.12	113.23
5	D	135	VAL	N-CA-C	5.72	115.88	107.75
13	L	12	THR	N-CA-C	5.72	120.11	113.18
11	J	69	TYR	N-CA-C	-5.72	98.62	110.80
24	W	54	PHE	N-CA-C	5.70	117.63	109.14
2	A	51	ARG	N-CA-C	5.68	119.32	111.71
20	S	20	PHE	N-CA-C	5.67	117.26	111.14
21	T	38	ARG	N-CA-C	-5.67	107.01	114.04
19	R	130	MET	N-CA-C	5.66	119.77	112.86
15	N	152	GLU	N-CA-C	-5.63	105.13	112.23
19	R	123	GLN	N-CA-C	5.63	118.44	110.50
15	N	140	GLN	N-CA-C	5.62	118.60	111.69
3	B	242	TRP	N-CA-C	-5.61	104.80	111.03
25	X	64	ALA	N-CA-C	5.61	120.26	113.41
5	D	171	ASP	N-CA-C	5.60	115.94	108.38
20	S	21	GLN	N-CA-C	5.60	120.23	113.17
4	C	93	LYS	N-CA-C	5.59	118.84	109.95
1	0	1504	A	C4'-C3'-O3'	-5.59	104.61	113.00
3	B	206	THR	N-CA-C	5.59	117.54	110.33
26	Y	119	GLN	N-CA-C	-5.58	105.26	112.68
1	0	877	G	C2'-C3'-O3'	-5.57	105.34	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	69	ARG	N-CA-C	5.57	120.96	113.72
24	W	96	LEU	N-CA-C	-5.57	104.61	111.40
4	C	175	LYS	N-CA-C	5.57	118.42	110.24
11	J	45	VAL	N-CA-C	5.56	116.37	108.42
2	A	133	ARG	N-CA-C	-5.55	106.67	113.50
12	K	9	THR	N-CA-C	-5.54	98.33	108.02
26	Y	148	GLY	N-CA-C	5.53	117.83	111.36
2	A	213	LYS	N-CA-C	5.52	118.06	111.71
18	Q	25	PRO	CA-C-N	5.52	125.14	119.56
18	Q	25	PRO	C-N-CA	5.52	125.14	119.56
3	B	159	PRO	N-CA-C	5.52	119.75	111.14
1	0	920	C	C2'-C3'-O3'	-5.52	105.42	113.70
12	K	81	ARG	N-CA-C	5.51	117.75	107.99
1	0	1080	C	C2'-C3'-O3'	-5.51	105.43	113.70
3	B	175	LEU	N-CA-C	-5.50	105.37	111.36
16	O	25	VAL	CB-CA-C	-5.49	106.03	111.30
17	P	97	ARG	N-CA-C	5.46	116.91	111.07
24	W	77	ALA	N-CA-C	5.46	122.42	110.80
28	1	21	ARG	N-CA-C	5.45	117.08	111.03
15	N	11	ARG	N-CA-C	5.44	117.64	111.11
11	J	117	ASP	N-CA-C	5.43	118.11	109.96
12	K	111	GLY	CA-C-N	5.43	125.34	119.85
12	K	111	GLY	C-N-CA	5.43	125.34	119.85
3	B	224	LYS	N-CA-C	5.43	118.67	109.76
2	A	52	SER	N-CA-C	5.42	122.34	110.80
6	E	126	ILE	N-CA-C	5.41	116.10	108.36
13	L	35	ARG	N-CA-C	5.39	118.96	112.38
2	A	25	ALA	N-CA-C	5.39	117.27	109.07
2	A	118	PHE	N-CA-C	5.38	117.81	110.55
2	A	123	GLY	N-CA-C	5.38	122.77	115.30
24	W	118	LEU	N-CA-C	5.34	118.38	110.48
15	N	14	ARG	N-CA-C	-5.33	105.39	111.14
14	M	80	GLY	N-CA-C	5.32	125.79	113.18
4	C	111	VAL	N-CA-C	-5.32	105.53	110.53
2	A	148	LEU	N-CA-C	5.30	118.36	110.52
17	P	36	THR	N-CA-C	5.30	117.37	110.53
5	D	15	GLU	CA-C-N	5.30	126.05	120.11
5	D	15	GLU	C-N-CA	5.30	126.05	120.11
27	Z	94	LYS	CA-C-N	5.29	124.74	119.24
27	Z	94	LYS	C-N-CA	5.29	124.74	119.24
3	B	265	LEU	N-CA-C	5.28	117.68	110.55
6	E	91	PHE	N-CA-C	5.28	117.28	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	123	GLY	N-CA-C	-5.28	107.25	114.64
13	L	138	GLY	N-CA-C	5.26	119.17	110.55
11	J	120	SER	N-CA-C	5.26	118.06	110.28
17	P	28	GLN	N-CA-C	5.25	117.68	111.33
30	3	20	HIS	N-CA-C	5.25	117.30	108.96
3	B	83	ALA	N-CA-C	5.23	116.23	108.60
28	1	5	THR	CA-C-N	-5.23	114.28	119.56
28	1	5	THR	C-N-CA	-5.23	114.28	119.56
2	A	121	ALA	N-CA-C	5.22	117.27	110.43
3	B	71	VAL	N-CA-C	5.21	115.78	108.17
25	X	22	ASN	N-CA-C	5.20	119.95	111.37
29	2	44	ARG	N-CA-C	5.19	117.84	111.82
3	B	158	LYS	CA-C-N	5.19	125.11	119.76
3	B	158	LYS	C-N-CA	5.19	125.11	119.76
3	B	122	ASP	N-CA-C	5.18	116.61	111.07
1	0	755	G	O4'-C4'-C3'	-5.17	98.83	104.00
15	N	172	PHE	N-CA-C	-5.17	105.56	111.14
16	O	79	VAL	N-CA-C	-5.16	105.81	110.82
4	C	205	ARG	N-CA-C	5.16	121.80	110.80
19	R	70	SER	N-CA-C	5.16	116.90	111.28
13	L	80	ASP	N-CA-C	5.15	117.70	110.23
7	F	79	GLN	N-CA-C	5.15	118.20	109.76
21	T	3	GLN	CA-C-N	5.15	125.44	119.47
21	T	3	GLN	C-N-CA	5.15	125.44	119.47
27	Z	44	ARG	N-CA-C	5.12	116.67	111.14
21	T	47	THR	N-CA-C	-5.12	101.81	109.95
21	T	34	GLU	N-CA-C	5.11	117.64	111.40
13	L	91	VAL	N-CA-C	5.11	115.63	108.17
24	W	139	GLY	N-CA-C	5.11	119.33	112.17
25	X	42	SER	N-CA-C	5.11	118.29	111.24
26	Y	211	ALA	N-CA-C	5.11	118.29	111.75
2	A	84	VAL	N-CA-C	5.10	115.77	110.82
31	9	39	U	N1-C1'-C2'	5.10	119.65	112.00
12	K	52	LYS	N-CA-C	-5.09	101.46	109.25
14	M	158	ARG	N-CA-C	5.08	118.95	112.34
10	I	107	LYS	N-CA-C	5.07	117.03	108.96
14	M	126	GLN	N-CA-C	5.07	116.54	108.79
9	H	146	ALA	N-CA-C	5.05	116.86	111.36
27	Z	70	ARG	N-CA-C	5.05	121.55	110.80
2	A	96	LEU	N-CA-C	5.04	118.20	111.75
4	C	179	GLY	N-CA-C	-5.04	106.62	113.37
17	P	31	ILE	N-CA-C	-5.04	105.65	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	100	VAL	N-CA-C	-5.04	105.63	110.72
7	F	79	GLN	CA-C-N	5.03	127.43	120.29
7	F	79	GLN	C-N-CA	5.03	127.43	120.29
2	A	219	ALA	CA-C-N	5.03	123.28	119.66
2	A	219	ALA	C-N-CA	5.03	123.28	119.66
14	M	70	GLY	N-CA-C	5.02	121.61	112.37
1	0	871	G	C5'-C4'-O4'	-5.01	102.28	109.80
14	M	109	PHE	CA-C-N	5.01	126.10	119.84
14	M	109	PHE	C-N-CA	5.01	126.10	119.84

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
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	1926	0
2	A	1754	0	1766	27	0
3	B	2625	0	2533	40	0
4	C	1860	0	1813	31	0
5	D	1094	0	1085	12	0
6	E	1358	0	1266	13	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	17	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	16	0
20	S	642	0	605	6	0
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	24	0
25	X	655	0	653	7	0
26	Y	1131	0	1133	10	0
27	Z	574	0	535	16	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	112	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	277	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	2245	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 (2245) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:H2'	1:0:2718:C:H5''	1.27	1.12
1:0:871:G:H5'	1:0:871:G:C8	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
1:0:1166:A:H61	1:0:1180:U:H3	1.15	0.90
31:9:73:A:H61	31:9:108:C:H42	1.19	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
1:0:1701:A:H4'	1:0:1702:U:H5''	1.57	0.84
1:0:1455:C:H2'	1:0:1455:C:O2	1.78	0.84
1:0:101:C:H2'	1:0:102:A:H8	1.43	0.84
1:0:2469:A:H1'	39:0:7426:HOH:O	1.77	0.84
1:0:195:C:H2'	1:0:196:G:H5'	1.59	0.84
1:0:2073:G:H5''	39:0:8459:HOH:O	1.75	0.84
1:0:2502:C:H2'	1:0:2503:A:H5'	1.60	0.84
1:0:545:G:H5'	1:0:545:G:H8	1.41	0.83
1:0:1585:C:H2'	1:0:1586:G:H8	1.42	0.83
1:0:1125:U:H2'	1:0:1126:C:H5'	1.61	0.83
1:0:681:G:N3	1:0:681:G:H5'	1.93	0.83
1:0:1544:U:H2'	1:0:1545:C:H6	1.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:N:141:ARG:NH2	31:9:48:C:H4'	1.96	0.81
31:9:14:G:H5'	31:9:14:G:H8	1.45	0.81
1:0:154:C:H2'	1:0:155:C:H6	1.46	0.81
1:0:557:C:H42	1:0:600:G:H1	1.29	0.81
1:0:1119:G:H2'	11:J:52:GLN:HE22	1.44	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:C21	37:0:9101:MUL:H163	2.11	0.80
1:0:1800:G:H1'	17:P:88:GLN:NE2	1.97	0.80
1:0:2088:C:H2'	1:0:2089:A:H8	1.47	0.79
1:0:2102:G:H2'	39:0:7719:HOH:O	1.82	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:H6	1:0:559:U:H5'	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
1:0:1447:U:H3'	1:0:1506:U:O2	1.83	0.78
1:0:1585:C:H2'	1:0:1586:G:C8	2.17	0.78
31:9:56:A:C2'	31:9:57:A:H5''	2.11	0.78
1:0:1300:G:H1'	39:0:3448:HOH:O	1.82	0.78
1:0:1596:U:H2'	1:0:1598:A:OP2	1.83	0.78
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
1:0:625:U:H5''	1:0:1044:C:N4	1.98	0.78
1:0:663:C:H5''	4:C:103:ASN:ND2	1.98	0.78
1:0:944:G:H21	24:W:44:MET:HE2	1.49	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
1:0:447:A:O2'	1:0:448:G:H5'	1.85	0.76
17:P:115:SER:H	17:P:118:GLN:HE21	1.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:1372:A:H3'	39:0:6923:HOH:O	1.86	0.76
37:0:9101:MUL:H10	37:0:9101:MUL:H14	1.68	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
1:0:659:A:H5''	39:O:6799:HOH:O	1.86	0.75
1:0:1444:G:O2'	1:0:1445:G:H5'	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
1:0:424:C:H2'	1:0:425:U:H6	1.53	0.73
1:0:1485:A:H1'	39:0:3502:HOH:O	1.88	0.73
1:0:2253:G:H2'	1:0:2254:G:H8	1.53	0.73
1:0:1351:G:H3'	39:0:4782:HOH:O	1.87	0.73
1:0:1692:C:H3'	39:0:8632:HOH:O	1.88	0.73
12:K:10:GLN:NE2	12:K:10:GLN:H	1.86	0.73
31:9:29:C:H2'	31:9:30:C:H5'	1.70	0.73
1:0:146:U:O2'	1:0:147:G:H5'	1.89	0.73
1:0:1829:A:H2'	1:0:1830:C:H5'	1.71	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
1:0:136:C:H2'	1:0:137:U:O4'	1.89	0.72
1:0:281:U:H2'	1:0:282:C:O4'	1.90	0.72
1:0:327:A:H4'	1:0:329:A:C8	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2426:G:H5'	39:0:3025:HOH:O	1.89	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
1:0:381: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
1:0:1159:G:H2'	1:0:1160:G:O4'	1.90	0.71
1:0:1377:C:H5'	1:0:1377:C:H6	1.55	0.71
1:0:290:C:H1'	39:0:5406:HOH:O	1.89	0.71
1:0:1118:A:C8	1:0:1118:A:H3'	2.25	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
1:0:282:C:H1'	1:0:368:C:N4	2.06	0.71
1:0:2269:C:H2'	1:0:2270:G:O4'	1.91	0.71
1:0:870:G:C2'	1:0:871:G:H5''	2.21	0.70
1:0:1883:U:H5''	1:0:2013:G:OP2	1.90	0.70
1:0:2059:U:H2'	1:0:2060:A:C8	2.26	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
31:9:24:U:H3'	31:9:25:G:C5'	2.20	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
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
1:0:2312:G:H2'	1:0:2313:C:H5'	1.73	0.70
1:0:2710:U:H1'	39:0:7520:HOH:O	1.92	0.70
1:0:1873:G:H3'	39:0:4169:HOH:O	1.91	0.70
1:0:2461:U:O2	1:0:2466:G:H1'	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:73: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
1:0:1186:C:H42	1:0:1190:G:H22	1.39	0.69
1:0:1118:A:H3'	1:0:1118:A:H8	1.56	0.69
1:0:1189:A:H3'	39:0:7609:HOH:O	1.92	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
1:0:399:C:H5'	14:M:179:GLY:O	1.93	0.68
1:0:1793:C:O2	1:0:1793:C:H2'	1.92	0.68
1:0:2894:C:O2'	1:0:2895:C:H5'	1.94	0.68
1:0:1838:U:O2'	1:0:2644:C:H5'	1.92	0.68
12:K:10:GLN:H	12:K:10:GLN:HE21	1.39	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
1:0:2812:A:H2	1:0:2814:A:H62	1.41	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
1:0:558:C:C2'	1:0:559:U:H5''	2.24	0.68
1:0:1589:G:H22	1:0:1605:G:H1'	1.58	0.68
1:0:1097:A:H5''	24:W:125:HIS:NE2	2.08	0.67
1:0:1574:C:H2'	1:0:1575:C:H6	1.58	0.67
1:0:500:G:N2	19:R:98:ASN:HD21	1.92	0.67
1:0:1118:A:H62	1:0:1244:U:H3	1.41	0.67
1:0:2416:G:H2'	1:0:2417:C:C6	2.29	0.67
31:9:114:G:H2'	31:9:115:C:C6	2.29	0.67
1:0:1104:C:H4'	11:J:88:PRO:HD3	1.76	0.67
1:0:1882:C:OP1	2:A:192:VAL:HG23	1.94	0.67
1:0:2372:A:H2'	1:0:2373:U:C6	2.28	0.67
1:0:119:A:H2'	1:0:120:A:H5''	1.77	0.67
1:0:2332:A:H5'	5:D:56:ARG:HH22	1.58	0.67
1:0:169:A:H1'	30:3:48:ASN:ND2	2.09	0.67
1:0:1126:C:O5'	1:0:1126:C:H6	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:318:U:H5'	1:0:339:A:C2	2.29	0.66
1:0:1544:U:H2'	1:0:1545:C:C6	2.28	0.66
1:0:2032:U:H2'	1:0:2033:G:H5''	1.76	0.66
1:0:2578:G:H5'	1:0:2578:G:H8	1.59	0.66
1:0:2712:G:H1'	39:0:5039:HOH:O	1.95	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
1:0:622:G:O2'	1:0:623:U:H5'	1.95	0.66
1:0:713:U:O5'	1:0:713:U:H6	1.79	0.66
1:0:1047:U:H5'	39:0:5458:HOH:O	1.94	0.66
1:0:1667:A:H5'	1:0:1667:A:C8	2.26	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
1:0:848:C:H5'	39:0:7034:HOH:O	1.95	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
1:0:2433:A:H8	1:0:2433:A:O5'	1.79	0.66
1:0:2506:A:O2'	1:0:2507:G:H8	1.77	0.66
9:H:59:GLN:NE2	9:H:129:ARG:HE	1.94	0.66
1:0:2904:U:H2'	1:0:2905:A:H8	1.61	0.66
1:0:183:A:H1'	14:M:161:ARG:NH1	2.11	0.66
1:0:877:G:H5'	1:0:878:G:OP1	1.95	0.66
15:N:141:ARG:HH21	31:9:48:C:H4'	1.61	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
1:0:886:A:H1'	39:0:3891:HOH:O	1.95	0.65
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
1:0:2488: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
1:0:1762: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
1:0:2415:A:C2'	1:0:2416:G:H5'	2.25	0.65
1:0:338:C:H3'	39:0:8434:HOH:O	1.96	0.65
1:0:1114:A:O2'	1:0:1115:U:H5'	1.96	0.65
1:0:1735:C:O2'	1:0:1736:A:H5'	1.96	0.65
31:9:3:A:N6	31:9:22:G:H1'	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:431:G:H5'	39:0:7692:HOH:O	1.97	0.65
1:0:545:G:H5'	1:0:545:G:C8	2.29	0.64
1:0:1728:G:H1'	39:0:5467:HOH:O	1.96	0.64
1:0:2010:A:H2'	39:0:5197:HOH:O	1.97	0.64
1:0:2486:A:H2	37:0:9101:MUL:H221	1.63	0.64
1:0:200:C:H2'	39:0:7991:HOH:O	1.97	0.64
1:0:450:C:OP1	4:C:184:ARG:NH2	2.31	0.64
1:0:1626:A:H2'	1:0:1627:G:O4'	1.98	0.64
1:0:1819:G:H2'	1:0:1820:G:H4'	1.78	0.64
35:0:8812:CL:CL	39:0:4058:HOH:O	2.50	0.64
14:M:79:ALA:HB3	14:M:81:ARG:HH12	1.63	0.64
31:9:104:A:O2'	31:9:105:A:H5'	1.97	0.64
1:0:702:G:O2'	1:0:703:G:H5'	1.97	0.64
1:0:932:U:O2'	1:0:1296:A:H1'	1.97	0.64
1:0:1015:C:H2'	1:0:1016:U:H6	1.61	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
1:0:1308: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
1:0:1595:G:O2'	1:0:1596:U:H5'	1.98	0.64
1:0:1921:A:O2'	1:0:1922:A:H5'	1.97	0.64
1:0:1139:U:H2'	1:0:1140:C:C6	2.32	0.64
1:0:2524:G:H21	1:0:2526:C:N4	1.96	0.64
1:0:2898:G:H4'	3:B:288:GLY:HA2	1.80	0.64
1:0:73:U:H2'	1:0:74:G:H8	1.61	0.64
1:0:1184:C:H1'	39:0:7308:HOH:O	1.98	0.64
1:0:837:U:H4'	39:0:7940:HOH:O	1.98	0.63
1:0:1115:U:H2'	1:0:1116:U:H6	1.63	0.63
1:0:1276:U:H3'	16:O:19:ARG:HH11	1.63	0.63
1:0:1771:U:H1'	27:Z:47:ARG:HH21	1.62	0.63
4:C:127:ARG:NH2	4:C:225:PRO:HG2	2.12	0.63
1:0:444:C:H1'	39:0:8745:HOH:O	1.97	0.63
1:0:2032:U:H5''	39:0:6193:HOH:O	1.98	0.63
1:0:2320:U:H2'	30:3:2:GLN:O	1.98	0.63
1:0:2526:C:O2'	1:0:2527:U:H5'	1.98	0.63
1:0:506:G:N2	1:0:509:A:H5''	2.08	0.63
1:0:958:G:H4'	31:9:105:A:H4'	1.80	0.63
1:0:1181:A:C2'	1:0:1182:C:H5'	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:1061:C:H3'	39:0:4002:HOH:O	1.99	0.63
1:0:2472:C:H3'	39:0:8235:HOH:O	1.98	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
1:0:1593:C:H2'	1:0:1594:C:H6	1.64	0.63
1:0:2332:A:H3'	1:0:2333:G:H8	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
1:0:221:G:H2'	1:0:222:A:C8	2.33	0.62
1:0:451:C:O2'	1:0:452:G:H5'	1.99	0.62
1:0:613:C:H2'	1:0:614:U:H6	1.63	0.62
1:0:1204:C:H2'	1:0:1205:U:O4'	1.99	0.62
1:0:2607:U:OP2	3:B:243:ASN:HB2	1.99	0.62
1:0:219:G:H5'	1:0:220:C:H5''	1.82	0.62
1:0:1220:U:H2'	1:0:1221:G:H8	1.64	0.62
1:0:109:U:O2	1:0:109:U:H2'	2.00	0.62
1:0:935:G:H4'	39:0:7674:HOH:O	1.98	0.62
1:0:1805:G:O2'	1:0:1806:G:H5'	1.99	0.62
1:0:1931:A:H2'	1:0:1932:G:H5'	1.81	0.62
1:0:2314:G:O2'	1:0:2315:C:H5'	2.00	0.62
37:0:9101:MUL:H201	37:0:9101:MUL:H263	1.81	0.62
31:9:84:G:H2'	31:9:85:A:H8	1.64	0.62
1:0:1139:U:H2'	1:0:1140:C:H6	1.63	0.62
1:0:69:A:H5'	1:0:69:A:C8	2.35	0.62
1:0:1125:U:C2'	1:0:1126:C:H5'	2.29	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
1:0:2433: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
1:0:1162:G:H1'	10:I:112:LEU:HD11	1.80	0.62
1:0:1213:C:O2'	1:0:1214:G:H5'	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:77:HIS:HD2	14:M:81:ARG:H	1.47	0.62
25:X:37:LEU:HD13	25:X:85:VAL:HG21	1.82	0.61
1:0:646:G:H2'	1:0:647:U:C6	2.35	0.61
1:0:1008:C:H5''	9:H:19:ARG:HH12	1.63	0.61
1:0:2896:A:N3	1:0:2896:A:H2'	2.15	0.61
1:0:812:A:H2'	1:0:813:C:C6	2.36	0.61
1:0:1391:G:H2'	1:0:1392:A:H5'	1.81	0.61
1:0:1474:C:H5'	1:0:1474:C:C6	2.30	0.61
1:0:857:A:H4'	2:A:176:HIS:CD2	2.35	0.61
1:0:907:A:H2'	1:0:908:A:H8	1.65	0.61
1:0:1333:U:H2'	1:0:1334:C:H6	1.65	0.61
1:0:2781:U:H1'	6:E:139:GLU:OE2	2.00	0.61
21:T:41:ARG:HH21	21:T:67:LEU:HD21	1.64	0.61
31:9:39:U:H3	31:9:42:C:H5''	1.64	0.61
1:0:106:A:O2'	1:0:107:U:H5'	2.00	0.61
1:0:178:U:H2'	1:0:179:C:H6	1.66	0.61
1:0:1527:A:H1'	1:0:1528:A:C8	2.35	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
1:0:183: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
1:0:1051:C:H2'	1:0:1052:G:O4'	2.00	0.61
1:0:1347:U:H2'	1:0:1348:A:H8	1.63	0.61
1:0:1817:U:O2	17:P:81:LYS:NZ	2.32	0.61
1:0:2295:G:N3	1:0:2361:A:H2	1.97	0.61
1:0:2627:G:H5'	39:0:3864:HOH:O	2.00	0.61
14:M:27:ARG:HH22	14:M:44:THR:HG23	1.65	0.61
1:0:2426:G:H1'	39:0:5391:HOH:O	2.00	0.61
1:0:852:U:H3'	39:0:8226:HOH:O	1.99	0.61
1:0:1202:A:H2'	1:0:1203:G:O4'	2.01	0.61
1:0:1279:U:O2	1:0:1279:U:H2'	1.98	0.61
1:0:2041:G:O2'	1:0:2042:U:H5'	2.00	0.61
1:0:2486:A:C2	37:0:9101:MUL:H221	2.36	0.61
31:9:105:A:H2'	31:9:106:U:O4'	2.01	0.61
31:9:13:A:O2'	31:9:14:G:H5''	2.01	0.61
1:0:146:U:C2'	1:0:147:G:H5'	2.31	0.60
1:0:195:C:C2'	1:0:196:G:H5'	2.31	0.60
1:0:312:U:O2'	1:0:313:U:H5'	2.01	0.60
1:0:2248:C:H3'	39:0:4476:HOH:O	2.00	0.60
7:F:30:LYS:HB2	7:F:97:ALA:HB3	1.83	0.60
1:0:185:G:O3'	1:0:186:A:H4'	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:287:C:H42	1:0:365:G:H1	1.49	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
1:0:1516:U:H2'	1:0:1517:C:O4'	2.01	0.60
1:0:2548:C:H5'	3:B:252:PRO:HD2	1.83	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
5:D:76:ARG:NH2	31:9:44:A:H1'	2.15	0.60
37:0:9101:MUL:H271	37:0:9101:MUL:S1	2.42	0.60
1:0:854:G:H8	39:0:8680:HOH:O	1.82	0.60
1:0:2714:U:H2'	1:0:2715:G:C8	2.36	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
1:0:1590:A:H1'	1:0:1606:A:C2	2.36	0.60
1:0:1972:U:H2'	1:0:1973:A:H5'	1.83	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
1:0:24:G:N2	1:0:518:G:H1'	2.17	0.60
1:0:280:C:H2'	1:0:281:U:O4'	2.02	0.60
1:0:333:G:O2'	1:0:334:G:H5'	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
1:0:1299: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
1:0:630:A:H3'	39:0:5239:HOH:O	2.01	0.60
1:0:1398:G:H2'	1:0:1399:A:C8	2.36	0.60
1:0:1455:C:O2	1:0:1455:C:C2'	2.50	0.60
1:0:1255:A:H3'	39:0:6875:HOH:O	2.02	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
31:9:56:A:H2'	31:9:57:A:C5'	2.22	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
1:0:69:A:H5'	1:0:69:A:H8	1.66	0.59
1:0:557:C:N4	1:0:600:G:H1	1.99	0.59
1:0:1119:G:H5'	11:J:52:GLN:NE2	2.17	0.59
1:0:1313:A:H5'	26:Y:208:LYS:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1806:G:C6	1:0:1807:U:N3	2.70	0.59
24:W:5:VAL:HG11	24:W:153:MET:HE1	1.85	0.59
1:0:308:U:H5'	1:0:309:C:OP1	2.03	0.59
1:0:1632:A:H2'	1:0:1633:C:H5'	1.83	0.59
1:0:2270:G:H4'	2:A:223:ARG:NH1	2.17	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
1:0:790:A:H1'	1:0:1710:A:H2'	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
1:0:1167:G:H2'	1:0:1168:C:C6	2.38	0.59
1:0:1797:A:H4'	1:0:1798:C:C5	2.38	0.59
31:9:37:C:O2'	31:9:38:A:H5'	2.03	0.59
31:9:39:U:H1'	31:9:44:A:H61	1.68	0.59
1:0:244:C:H6	1:0:244:C:O5'	1.85	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
27:Z:59:GLU:HG2	27:Z:60:ASP:H	1.68	0.59
1:0:558:C:H2'	1:0:559:U:C5'	2.33	0.58
1:0:871:G:C8	1:0:871:G:C5'	2.77	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
1:0:2721:U:H4'	12:K:87:ARG:HG3	1.85	0.58
1:0:2827:A:H2'	1:0:2828:G:O4'	2.03	0.58
1:0:29:C:O2'	1:0:30:U:H5'	2.03	0.58
1:0:553:G:H2'	1:0:554:G:H5'	1.86	0.58
1:0:1666:C:H2'	1:0:1667:A:C8	2.39	0.58
1:0:1803:C:H2'	1:0:1804:A:C8	2.37	0.58
1:0:1921:A:H2'	1:0:1922:A:O4'	2.03	0.58
1:0:2472:C:HO2'	1:0:2634:G:H4'	1.67	0.58
1:0:1055:G:N2	1:0:1057:A:H3'	2.18	0.58
1:0:1889:C:O2'	1:0:1890:U:H5'	2.03	0.58
1:0:1931:A:C2'	1:0:1932:G:H5'	2.34	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
1:0:2531:U:H4'	39:0:5083:HOH:O	2.04	0.58
1:0:2748:G:H5'	39:0:7410:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:49:LEU:HD12	39:U:3805:HOH:O	2.02	0.58
1:0:164:G:H3'	39:0:8274:HOH:O	2.03	0.58
1:0:1375:A:H2'	1:0:1376:G:H5'	1.86	0.58
1:0:1504:A:H4'	1:0:1506:U:C5	2.39	0.58
1:0:2410:G:H1'	39:0:7571:HOH:O	2.03	0.58
1:0:2768:A:H2'	1:0:2769:C:C6	2.39	0.58
1:0:2831:C:H2'	1:0:2832:C:O4'	2.03	0.58
1:0:306:A:P	21:T:38:ARG:HH21	2.27	0.58
1:0:822:C:O2	1:0:822:C:H2'	2.03	0.57
1:0:1163:G:OP2	1:0:1164:U:H3'	2.04	0.57
1:0:1769:C:O2'	1:0:1770:U:H5'	2.02	0.57
1:0:1787:C:O2'	1:0:1788:U:H5'	2.04	0.57
1:0:2016:U:H2'	1:0:2017:U:O4'	2.04	0.57
1:0:2507:G:H2'	1:0:2510:C:N4	2.19	0.57
1:0:735:C:N4	30:3:15:ASN:HD21	2.03	0.57
1:0:1057:A:H1'	1:0:2492:U:O2'	2.04	0.57
1:0:1421:C:H2'	1:0:1422:U:H6	1.68	0.57
1:0:1309:U:O2'	1:0:1310:U:H5'	2.04	0.57
1:0:1446:U:H2'	20:S:55:GLN:NE2	2.20	0.57
1:0:1477:C:H5'	1:0:1868:G:H5'	1.86	0.57
1:0:2312:G:C2'	1:0:2313:C:H5'	2.34	0.57
1:0:2613:G:O2'	1:0:2614:C:H5'	2.04	0.57
1:0:2691:A:OP1	1:0:2691:A:H8	1.86	0.57
9:H:32:ALA:H	9:H:69:ARG:HH12	1.51	0.57
1:0:664:U:O2'	1:0:665:A:H5'	2.04	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
1:0:236:A:H4'	1:0:237:G:H5'	1.86	0.57
1:0:1201:C:H2'	1:0:1202:A:H5'	1.86	0.57
1:0:2241:C:O2'	1:0:2242:U:H5'	2.04	0.57
1:0:2385:G:H2'	1:0:2386:U:H6	1.68	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
24:W:52:VAL:HG22	24:W:53:ALA:H	1.69	0.57
1:0:67:A:N1	1:0:109:U:H1'	2.19	0.57
1:0:73:U:O2'	1:0:74:G:H5'	2.04	0.57
1:0:152:A:H1'	1:0:440:C:O2'	2.05	0.57
1:0:705:C:H3'	1:0:706:G:H8	1.69	0.57
1:0:1634:G:H2'	1:0:1635:U:C6	2.39	0.57
1:0:2054:A:H4'	19:R:135:ALA:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2378:U:H4'	39:0:3392:HOH:O	2.04	0.57
1:0:2563:U:HO2'	1:0:2564:G:H8	1.52	0.57
1:0:2777:G:H1'	39:0:6143:HOH:O	2.04	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
1:0:790:A:H8	39:0:5403:HOH:O	1.87	0.57
1:0:1182:C:H1'	1:0:1192:A:H8	1.69	0.57
1:0:2717:C:H2'	1:0:2718:C:C5'	2.18	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
1:0:1829:A:C2'	1:0:1830:C:H5'	2.34	0.57
1:0:2336:G:H1	1:0:2348:C:H42	1.53	0.57
1:0:2505:G:C2'	1:0:2506:A:H5'	2.35	0.57
1:0:2904:U:H2'	1:0:2905:A:C8	2.40	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
11:J:19:MET:HE1	11:J:78:ILE:HG22	1.86	0.57
1:0:566:A:H2'	1:0:567:U:H5'	1.86	0.56
1:0:1106:A:O5'	1:0:1106:A:H8	1.87	0.56
1:0:2241:C:H2'	1:0:2242:U:C6	2.40	0.56
1:0:2533:C:H5'	1:0:2533:C:C6	2.35	0.56
4:C:139:VAL:HG13	39:C:6251:HOH:O	2.04	0.56
1:0:1183:C:N4	1:0:1184:C:H41	2.03	0.56
1:0:1383:U:H2'	1:0:1384:C:C6	2.40	0.56
1:0:1477:C:H5'	1:0:1868:G:C5'	2.35	0.56
1:0:1617:C:C5	1:0:1643:C:H4'	2.40	0.56
1:0:1697:G:H1'	39:0:7038:HOH:O	2.06	0.56
1:0:1894:C:N4	1:0:1939:U:H2'	2.20	0.56
1:0:2388:C:O2'	1:0:2389:U:H5'	2.05	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
1:0:10: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
1:0:619:U:H3'	39:0:7549:HOH:O	2.05	0.56
1:0:1165:G:H21	1:0:1173:A:C5'	2.17	0.56
1:0:1175:G:O2'	1:0:1193:A:H2'	2.05	0.56
1:0:1555:G:H4'	1:0:1630:A:H2	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:182:G:H5'	39:0:4102:HOH:O	2.04	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
31:9:29:C:C2'	31:9:30:C:H5'	2.35	0.56
31:9:82:U:H5''	39:9:123:HOH:O	2.05	0.56
1:0:12:U:C2'	1:0:13:G:H5'	2.35	0.56
1:0:95:A:H5''	1:0:97:G:O4'	2.06	0.56
1:0:221:G:H2'	1:0:222:A:H8	1.71	0.56
1:0:814:G:N2	1:0:815:U:H1'	2.21	0.56
1:0:1163:G:H5'	10:I:110:ASP:O	2.06	0.56
3:B:7:ARG:NH2	3:B:11:LEU:HD13	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
1:0:2439:C:H5'	39:0:4534:HOH:O	2.06	0.56
31:9:104:A:C2'	31:9:105:A:H5'	2.35	0.56
1:0:154:C:O2'	1:0:155:C:H5'	2.06	0.56
1:0:1369:A:H5'	39:0:7798:HOH:O	2.06	0.56
20:S:33:SER:O	20:S:37:VAL:HG23	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
1:0:2751:C:H3'	39:0:7028:HOH:O	2.05	0.56
15:N:159:TYR:HE1	31:9:50:G:H5''	1.70	0.56
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
1:0:1167:G:H1	1:0:1179:C:N4	2.03	0.55
1:0:1242:A:H5'	11:J:82:THR:HG23	1.87	0.55
1:0:1554:C:C1'	1:0:1632:A:H1'	2.36	0.55
1:0:2670:G:O2'	1:0:2671:U:H5'	2.05	0.55
1:0:2831:C:C2'	1:0:2832:C:H5'	2.36	0.55
14:M:159:VAL:HG12	35:M:8818:CL:CL	2.43	0.55
31:9:55:U:H4'	31:9:56:A:C8	2.41	0.55
1:0:944:G:N2	24:W:44:MET:HE2	2.21	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
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.55
1:0:68:U:O2'	1:0:69:A:H5''	2.07	0.55
1:0:189:A:OP1	14:M:171:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:226:A:H1'	1:0:393:G:N7	2.21	0.55
1:0:2768:A:H2'	1:0:2769:C:H6	1.72	0.55
1:0:2781:U:O2'	1:0:2782:G:H5'	2.06	0.55
1:0:2906:A:H5'	1:0:2907:C:O4'	2.06	0.55
5:D:140:ARG:HB3	31:9:29:C:H5''	1.89	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
1:0:414:C:O2'	1:0:415:A:H5'	2.07	0.55
1:0:612:U:H2'	1:0:613:C:C6	2.41	0.55
1:0:1030:U:H5'	39:0:3468:HOH:O	2.05	0.55
1:0:1119:G:N2	1:0:1246:A:C2	2.74	0.55
1:0:1420:C:H2'	1:0:1420:C:O2	2.07	0.55
1:0:2716:G:H5'	3:B:262:ARG:HG3	1.88	0.55
1:0:2782:G:O6	1:0:2790:C:H5''	2.06	0.55
1:0:696:C:H2'	1:0:697:G:O4'	2.06	0.55
1:0:897:A:H2'	1:0:899:C:C5	2.42	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
1:0:2397: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
1:0:2868:C:H1'	39:0:6832:HOH:O	2.07	0.55
1:0:128:A:C8	1:0:128:A:H3'	2.41	0.55
1:0:355:C:H1'	39:0:3088:HOH:O	2.06	0.55
1:0:1816:C:H6	1:0:1816:C:O5'	1.89	0.55
1:0:2274:A:O2'	1:0:2275:G:H5'	2.07	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
19:R:66:VAL:HG22	19:R:79:ARG:NH1	2.22	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
1:0:517:U:H2'	1:0:518:G:H5'	1.89	0.55
1:0:522:U:HO2'	1:0:1366:C:H5'	1.72	0.55
1:0:849:C:H2'	1:0:850:U:O4'	2.07	0.55
1:0:962:C:H2'	1:0:963:C:H5'	1.87	0.55
1:0:1850:U:H2'	1:0:1851:G:H8	1.71	0.55
1:0:414:C:H2'	1:0:415:A:O4'	2.06	0.55
1:0:1745:G:H22	1:0:2033:G:H5'	1.71	0.55
1:0:2071:C:H5'	39:0:4847:HOH:O	2.07	0.55
1:0:2764:C:H2'	1:0:2765:C:C6	2.33	0.55
1:0:125:U:H2'	39:0:8398:HOH:O	2.07	0.55
1:0:819:A:H5'	27:Z:37:ARG:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:E:84:MET:HE1	6:E:148:ILE:HD13	1.89	0.55
17:P:98:ILE:HD12	17:P:102:ARG:NE	2.21	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
1:0:2654:C:O2'	1:0:2655:U:H5'	2.07	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
1:0:35: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
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
39:0:4183:HOH:O	12:K:39:GLY:HA2	2.07	0.54
6:E:137:ASP:O	6:E:141:VAL:HG23	2.06	0.54
15:N:11:ARG:HD3	31:9:114:G:O6	2.08	0.54
1:0:151:A:H2'	1:0:152:A:O4'	2.07	0.54
1:0:250:C:H2'	1:0:251:C:H6	1.73	0.54
1:0:312:U:C2	1:0:320:G:N2	2.75	0.54
1:0:420:U:H3	1:0:2447:A:H61	1.56	0.54
1:0:676:C:O2'	4:C:219:ASN:ND2	2.33	0.54
1:0:1010:C:H4'	15:N:4:PRO:HB2	1.89	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
1:0:1783:A:O2'	1:0:1784:U:H5'	2.07	0.54
1:0:313:U:C2'	1:0:314:G:H5'	2.37	0.54
1:0:1120:U:H5''	1:0:1120:U:H6	1.73	0.54
1:0:2321:A:H2	1:0:2378:U:H3	1.51	0.54
1:0:2506:A:HO2'	1:0:2507:G:H8	1.49	0.54
1:0:590:A:H2'	1:0:591:A:O4'	2.08	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
1:0:2781:U:C2'	1:0:2782:G:H5'	2.37	0.54
12:K:29:LEU:HB3	12:K:55:VAL:HG11	1.88	0.54
1:0:816:G:C6	1:0:817:G:N1	2.75	0.54
1:0:1586:G:H1'	39:0:6211:HOH:O	2.07	0.54
1:0:1666:C:H2'	1:0:1667:A:H5'	1.90	0.54
1:0:1730:G:C5'	1:0:1731:C:H6	2.20	0.54
1:0:1803:C:H2'	1:0:1804:A:H8	1.72	0.54
1:0:1925:G:O2'	1:0:1926:G:H5'	2.08	0.54
1:0:2042:U:H2'	1:0:2043:U:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2819:C:H2'	1:0:2820:A:H8	1.72	0.54
31:9:76:G:C3'	31:9:77:A:H5''	2.29	0.54
1:0:722:G:H2'	1:0:723:G:H5'	1.88	0.54
1:0:1328:A:OP1	26:Y:169:ARG:HD2	2.08	0.54
1:0:1387:G:H21	17:P:1:THR:N	2.04	0.54
1:0:1510:G:H2'	1:0:1511:U:O4'	2.08	0.54
1:0:1571:G:C2'	1:0:1626:A:H61	2.21	0.54
1:0:2027:U:O2'	1:0:2028:U:H5'	2.07	0.54
1:0:2349:G:H2'	1:0:2350:G:H8	1.72	0.54
1:0:2908:A:H2'	1:0:2909:G:O4'	2.06	0.54
1:0:420:U:H1'	39:0:5263:HOH:O	2.07	0.54
1:0:491:C:N3	1:0:502:A:C2	2.75	0.54
1:0:814:G:C2	1:0:815:U:C2	2.95	0.54
1:0:920:C:H4'	1:0:921:G:C2	2.42	0.54
1:0:1747:A:C6	1:0:2035:C:O2	2.61	0.54
1:0:2537:G:H5''	1:0:2538:A:H5''	1.89	0.54
1:0:1099:G:P	24:W:129:LYS:HE3	2.48	0.54
1:0:1631:A:H2'	1:0:1632:A:C8	2.43	0.54
1:0:2607:U:OP1	1:0:2609:G:H4'	2.07	0.54
1:0:2661:U:H3	1:0:2812:A:H62	1.55	0.54
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.89	0.54
31:9:73:A:H2'	31:9:74:G:C8	2.43	0.54
1:0:814:G:H4'	39:0:7058:HOH:O	2.08	0.54
1:0:847:C:H4'	39:0:8386:HOH:O	2.08	0.54
1:0:1461:U:H2'	1:0:1462:C:C6	2.43	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
1:0:2795:C:O2'	1:0:2796:U:H5'	2.07	0.54
1:0:293:A:H2'	1:0:294:C:H6	1.73	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
31:9:95:C:H2'	31:9:96:C:O4'	2.07	0.54
1:0:310:U:H2'	1:0:311:C:C6	2.43	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
1:0:2404:G:H5''	39:0:8706:HOH:O	2.07	0.53
31:9:76:G:O5'	31:9:76:G:H8	1.91	0.53
1:0:272:A:H5'	1:0:273:G:OP2	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:902:G:N7	13:L:18:HIS:HD2	2.06	0.53
1:0:907:A:H2'	1:0:908:A:C8	2.43	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
1:0:1570: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
1:0:2511:A:H2'	1:0:2512:U:O4'	2.08	0.53
1:0:2737:C:OP2	17:P:61:ARG:NH2	2.39	0.53
17:P:105:LEU:HD21	17:P:137:LEU:HD11	1.89	0.53
1:0:42:C:OP2	1:0:185:G:H2'	2.08	0.53
1:0:1353:C:H3'	39:0:8238:HOH:O	2.08	0.53
27:Z:48:ARG:O	27:Z:52:GLU:HB2	2.09	0.53
1:0:31:C:O2'	1:0:32:G:H5'	2.08	0.53
1:0:1438:G:H1'	29:2:42:TRP:HZ2	1.73	0.53
1:0:1829:A:H5''	39:0:6825:HOH:O	2.08	0.53
37:0:9101:MUL:H163	37:0:9101:MUL:O3	2.09	0.53
18:Q:26:PRO:O	18:Q:30:VAL:HG23	2.07	0.53
1:0:869:G:H1'	39:0:7658:HOH:O	2.09	0.53
1:0:1352:A:H4'	1:0:1353:C:OP1	2.08	0.53
1:0:1950:G:H2'	1:0:1951:G:H8	1.74	0.53
1:0:1976:G:H1'	1:0:2005:G:N2	2.23	0.53
1:0:2508:C:H2'	39:0:6319:HOH:O	2.08	0.53
1:0:2809:G:H2'	1:0:2810:G:O4'	2.07	0.53
1:0:669:G:O2'	1:0:670:G:H5'	2.08	0.53
1:0:1166:A:N6	1:0:1180:U:H3	1.97	0.53
1:0:1427:A:O2'	1:0:1428:C:H5'	2.08	0.53
1:0:1430:G:N2	39:0:7999:HOH:O	2.41	0.53
4:C:142:ASP:OD1	4:C:236:THR:HG23	2.09	0.53
1:0:23:G:H1'	1:0:520:A:N6	2.22	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
1:0:1053:G:OP1	9:H:15:PRO:HG3	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
1:0:1311:G:H5''	39:0:5005:HOH:O	2.06	0.53
1:0:1342:C:H2'	1:0:1343:C:H5'	1.90	0.53
1:0:1398:G:O2'	1:0:1399:A:H5'	2.09	0.53
1:0:1423:C:O2'	1:0:1424:A:H5'	2.09	0.53
1:0:1574:C:H2'	1:0:1575:C:C6	2.41	0.53
1:0:1758:U:H6	1:0:1758:U:O5'	1.92	0.53
1:0:2294:C:H42	1:0:2314:G:H1	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2433:A:H2'	1:0:2434:A:C8	2.44	0.53
1:0:2474:A:H4'	1:0:2475:C:O5'	2.08	0.53
1:0:2486:A:H3'	39:0:3735:HOH:O	2.08	0.53
1:0:318:U:H5'	1:0:339:A:C4	2.43	0.53
1:0:710:G:OP1	16:O:24:ALA:HB3	2.09	0.53
1:0:1081:A:C6	1:0:1082:A:N1	2.76	0.53
1:0:1981:A:H3'	39:0:6149:HOH:O	2.09	0.53
1:0:2586:U:H3	1:0:2592:G:H22	1.55	0.53
1:0:2617:G:H4'	39:0:3214:HOH:O	2.08	0.53
2:A:194:MET:HE3	2:A:199:HIS:HB2	1.91	0.53
24:W:24:LEU:HD21	24:W:44:MET:SD	2.48	0.53
1:0:228:C:H2'	1:0:229:G:H5'	1.89	0.53
1:0:2387:U:H2'	1:0:2388:C:C6	2.43	0.53
1:0:2742:G:H5'	39:0:5015:HOH:O	2.07	0.53
31:9:49:G:O2'	31:9:50:G:H5'	2.08	0.53
1:0:303:C:O2'	1:0:304:G:H5'	2.09	0.53
1:0:561:G:H2'	1:0:562:A:C8	2.41	0.53
1:0:1666:C:H2'	1:0:1667:A:H8	1.72	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
1:0:2563:U:O2'	1:0:2564:G:H8	1.92	0.53
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
1:0:2241:C:H2'	1:0:2242:U:H6	1.74	0.52
1:0:1363:G:H1'	39:0:4378:HOH:O	2.08	0.52
1:0:1741:U:C4	1:0:2033:G:C8	2.98	0.52
1:0:1972:U:H2'	1:0:1973:A:C5'	2.38	0.52
1:0:2026:C:O2'	1:0:2027:U:H5'	2.10	0.52
1:0:2089:A:O2'	1:0:2090:G:H5'	2.10	0.52
1:0:380:A:H2'	39:0:6974:HOH:O	2.09	0.52
1:0:482:G:H4'	1:0:508:A:N1	2.25	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
1:0:72:C:H5'	39:0:5110:HOH:O	2.09	0.52
1:0:640:G:O2'	1:0:641:G:H5'	2.08	0.52
1:0:656:G:H2'	1:0:657:G:H8	1.75	0.52
1:0:912:A:C4	1:0:1294:A:C2	2.97	0.52
1:0:1438:G:H1'	29:2:42:TRP:CZ2	2.45	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
1:0:2548:C:OP2	3:B:5:ARG:NH2	2.42	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
1:0:705:C:O2	1:0:705:C:H2'	2.10	0.52
1:0:960:G:N3	1:0:960:G:H2'	2.23	0.52
1:0:1363:G:H2'	1:0:1364:G:C8	2.44	0.52
1:0:1970:G:H1'	39:0:8299:HOH:O	2.08	0.52
1:0:157:G:H4'	14:M:95:LYS:HE2	1.91	0.52
1:0:809:G:H2'	1:0:810:G:C8	2.45	0.52
1:0:875:A:C2	2:A:194:MET:SD	3.03	0.52
1:0:955:A:H2'	1:0:956:G:O4'	2.10	0.52
1:0:1436:C:O2'	1:0:1437:A:H5'	2.10	0.52
1:0:2345:A:H3'	1:0:2346:C:C6	2.44	0.52
1:0:2548:C:H5''	39:0:5919:HOH:O	2.09	0.52
3:B:7:ARG:NH1	3:B:11:LEU:HD22	2.24	0.52
1:0:660:A:N6	1:0:746:A:O4'	2.42	0.52
1:0:710:G:H2'	1:0:711:G:H8	1.74	0.52
1:0:1181:A:H2'	1:0:1182:C:C5'	2.40	0.52
1:0:1359:U:C5	1:0:2101:A:C8	2.98	0.52
1:0:1461:U:H2'	1:0:1462:C:H6	1.75	0.52
1:0:2790:C:H5'	39:0:8847:HOH:O	2.08	0.52
1:0:39:G:H2'	1:0:40:C:O4'	2.09	0.52
1:0:210:U:O2'	1:0:211:U:H5'	2.10	0.52
1:0:226:A:H1'	1:0:393:G:C5	2.44	0.52
1:0:968:G:H2'	1:0:969:G:H8	1.75	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
1:0:1400: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
1:0:1688:G:C6	1:0:1692:C:C6	2.98	0.52
1:0:2121:G:H5''	39:0:9100:HOH:O	2.10	0.52
1:0:2269:C:O2'	1:0:2270:G:H5'	2.10	0.52
1:0:2718:C:H3'	39:0:6906:HOH:O	2.10	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
1:0:2703:A:H2'	1:0:2704:C:C6	2.37	0.52
31:9:29:C:H2'	31:9:30:C:C5'	2.39	0.52
31:9:119:C:H4'	39:9:2285:HOH:O	2.08	0.52
1:0:39:G:O2'	1:0:40:C:H5'	2.10	0.52
1:0:183:A:H1'	14:M:161:ARG:HH11	1.75	0.52
1:0:653:U:H2'	1:0:654:A:C8	2.45	0.52
1:0:1189:A:H1'	1:0:1209:C:C1'	2.39	0.52
1:0:1705:C:P	17:P:59:ARG:HH12	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:M:99:ARG:HE	14:M:170:ASN:HD22	1.57	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
1:0:685:C:O2	1:0:748:C:H4'	2.11	0.51
1:0:947:U:O2'	1:0:948:G:H5'	2.10	0.51
1:0:2324:G:H4'	1:0:2418:G:O2'	2.09	0.51
31:9:7:G:H5'	39:9:5071:HOH:O	2.09	0.51
1:0:422:G:O2'	1:0:423:A:H5'	2.10	0.51
1:0:1525:G:H5'	1:0:1526:A:OP2	2.11	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
12:K:18:ILE:HG22	12:K:93:ASN:ND2	2.18	0.51
31:9:86:G:C2	31:9:88:G:C8	2.98	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
31:9:98:C:H2'	31:9:99:U:C6	2.43	0.51
1:0:593:A:H1'	39:0:8441:HOH:O	2.10	0.51
1:0:968:G:H2'	1:0:969:G:C8	2.45	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
1:0:2880:A:H2'	1:0:2881:C:H5'	1.92	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
31:9:3:A:C8	31:9:26:C:N3	2.78	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
1:0:441:A:H1'	1:0:442:A:N7	2.25	0.51
1:0:1044:C:H5''	39:0:2991:HOH:O	2.10	0.51
1:0:1375:A:C2'	1:0:1376:G:H5'	2.41	0.51
1:0:1445:G:N2	1:0:1678:A:H1'	2.26	0.51
1:0:1706:G:C5	1:0:1707:G:C6	2.99	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
1:0:772:G:H2'	1:0:773:A:O4'	2.11	0.51
1:0:2065:C:O2'	1:0:2066:C:H5'	2.10	0.51
1:0:2481:G:H3'	39:0:3932:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2748:G:H1'	39:0:7865:HOH:O	2.10	0.51
1:0:2909:G:O2'	1:0:2910:A:H5'	2.11	0.51
15:N:83:LEU:HD13	15:N:175:LEU:HD23	1.93	0.51
31:9:81:C:O2'	31:9:82:U:H5'	2.11	0.51
1:0:47:G:H1'	1:0:114:A:N1	2.24	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
1:0:1332:C:H2'	1:0:1333:U:H6	1.75	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
2:A:167:LYS:HE3	27:Z:50:VAL:HG13	1.93	0.51
13:L:138:GLY:HA3	39:L:4360:HOH:O	2.11	0.51
24:W:80:ASP:O	24:W:84:VAL:HG23	2.11	0.51
31:9:84:G:H4'	39:9:4718:HOH:O	2.11	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
1:0:870:G:H2'	1:0:871:G:C5'	2.40	0.51
1:0:1835:U:C5	1:0:1840:A:N7	2.78	0.51
1:0:1844:C:O5'	1:0:1844:C:H6	1.93	0.51
1:0:1931:A:H2'	1:0:1932:G:C5'	2.40	0.51
1:0:2061:C:H2'	1:0:2062:A:H5'	1.93	0.51
37:0:9101:MUL:H11A	39:0:3722:HOH:O	2.11	0.51
1:0:597:A:H2'	1:0:598:C:C6	2.46	0.51
1:0:821:U:H5''	39:0:6706:HOH:O	2.10	0.51
1:0:1289:C:H3'	39:0:5826:HOH:O	2.10	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
1:0:2830: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
1:0:10:U:C4	1:0:532:A:C8	2.99	0.51
1:0:74:G:H5'	23:V:9:ARG:HH22	1.76	0.51
1:0:100:C:H4'	21:T:16:LEU:HB2	1.93	0.51
1:0:694:A:C2'	1:0:695:C:H5'	2.39	0.51
1:0:876:A:H2'	1:0:877:G:H5'	1.91	0.51
1:0:1359:U:C5	1:0:2101:A:H8	2.29	0.51
1:0:1427:A:C2'	1:0:1428:C:H5'	2.41	0.51
6:E:7:ILE:HG23	6:E:45:ASP:O	2.11	0.51
1:0:716:G:C6	1:0:717:C:N4	2.80	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
1:0:1192:A:H3'	1:0:1193:A:H5'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:1891:G:H1'	1:0:1972:U:O2	2.11	0.50
1:0:1904:A:C2	1:0:1905:U:H1'	2.46	0.50
1:0:2798:G:H3'	39:0:3048:HOH:O	2.11	0.50
5:D:48:MET:O	31:9:41:C:H4'	2.10	0.50
30:3:3:MET:O	30:3:90:PHE:HA	2.11	0.50
31:9:118:C:O5'	31:9:118:C:H6	1.94	0.50
1:0:301:C:H42	1:0:350:G:H1	1.58	0.50
1:0:398:U:O3'	14:M:179:GLY:HA3	2.11	0.50
1:0:1304:U:H2'	1:0:1305:C:C6	2.47	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
1:0:2838:A:O2'	1:0:2839:C:H5'	2.12	0.50
5:D:22:VAL:HG22	5:D:74:THR:HG22	1.93	0.50
31:9:59:C:O5'	31:9:59:C:H6	1.93	0.50
31:9:114:G:H2'	31:9:115:C:H6	1.72	0.50
1:0:447:A:OP1	21:T:2:LYS:HG2	2.10	0.50
1:0:710:G:O2'	1:0:711:G:H5'	2.10	0.50
1:0:1507:C:H4'	39:0:8231:HOH:O	2.10	0.50
1:0:1942:A:H2'	1:0:1943:C:H6	1.76	0.50
1:0:2295:G:N3	1:0:2361:A:C2	2.79	0.50
31:9:99:U:H5'	39:9:5904:HOH:O	2.11	0.50
1:0:219:G:C5'	1:0:220:C:H5''	2.40	0.50
1:0:685:C:O2'	1:0:748:C:OP1	2.23	0.50
1:0:894:A:OP2	39:0:3250:HOH:O	2.19	0.50
1:0:1331:G:O2'	1:0:1332:C:H5'	2.12	0.50
1:0:1680:C:H2'	1:0:1681:G:O4'	2.11	0.50
1:0:1766:U:H4'	39:0:9080:HOH:O	2.11	0.50
1:0:2443:C:H1'	13:L:56:LYS:HE3	1.94	0.50
1:0:2750:G:H2'	1:0:2751:C:C6	2.47	0.50
3:B:217:ARG:HG3	3:B:257:THR:HG22	1.94	0.50
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
1:0:313:U:O2'	1:0:314:G:H5'	2.10	0.50
1:0:690:G:H1'	1:0:731:U:O2'	2.12	0.50
1:0:1305:C:O2'	1:0:1306:U:H5'	2.12	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
1:0:796:A:H5'	39:0:5974:HOH:O	2.11	0.50
1:0:962:C:H1'	15:N:5:ARG:NH2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1647:G:O2'	1:0:1648:G:H5'	2.12	0.50
1:0:2764:C:O2'	1:0:2765:C:H5'	2.12	0.50
4:C:56:THR:HG21	4:C:78:ARG:HB3	1.92	0.50
31:9:2:U:H4'	39:9:5321:HOH:O	2.11	0.50
1:0:229:G:O2'	1:0:230:C:H5'	2.12	0.50
1:0:292:G:H1'	1:0:360:A:N6	2.27	0.50
1:0:559:U:H6	1:0:559:U:C5'	2.23	0.50
1:0:843:A:C2	1:0:846:A:C8	3.00	0.50
1:0:1213:C:C2'	1:0:1214:G:H5'	2.42	0.50
1:0:1251:C:H2'	1:0:1252:A:O4'	2.12	0.50
1:0:1797:A:H5'	39:0:7113:HOH:O	2.12	0.50
1:0:1992:U:O2	1:0:1994:A:H8	1.95	0.50
16:O:32:ARG:HH21	16:O:35:LYS:NZ	2.09	0.50
26:Y:214:ARG:HH12	26:Y:230:ASN:ND2	2.09	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
1:0:840:U:C2	1:0:2648:U:O4	2.65	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
1:0:2484:U:H3'	39:0:3554:HOH:O	2.12	0.50
3:B:75:GLU:OE2	3:B:151:VAL:HG13	2.12	0.50
20:S:37:VAL:O	20:S:41:VAL:HG23	2.11	0.50
26:Y:216:ARG:HD3	39:Y:4408:HOH:O	2.12	0.50
31:9:78:G:H22	31:9:103:A:P	2.35	0.50
31:9:82:U:H2'	31:9:83:G:C8	2.47	0.50
1:0:553:G:H5'	39:0:8126:HOH:O	2.11	0.49
1:0:820:G:H3'	39:0:6706:HOH:O	2.12	0.49
1:0:876:A:C2'	1:0:877:G:H5'	2.41	0.49
1:0:1315:G:H3'	1:0:1316:G:H5'	1.93	0.49
1:0:1557:G:H2'	1:0:1558:C:O4'	2.11	0.49
1:0:2710:U:H6	1:0:2710:U:O5'	1.95	0.49
1:0:2837:U:H2'	39:0:6433:HOH:O	2.12	0.49
4:C:88:SER:HB3	4:C:91:PRO:HB3	1.95	0.49
14:M:79:ALA:HB3	14:M:81:ARG:NH1	2.26	0.49
1:0:137:U:H2'	1:0:139:C:H5	1.76	0.49
1:0:599:G:H2'	1:0:600:G:H8	1.77	0.49
1:0:1622:G:H2'	1:0:1623:C:H5'	1.94	0.49
1:0:2675:A:H1'	1:0:2813:A:C2	2.47	0.49
1:0:2831:C:O2'	1:0:2832:C:H5'	2.12	0.49
1:0:2862:G:H4'	3:B:336:GLN:O	2.12	0.49
1:0:2871:G:H2'	1:0:2872:U:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:59:GLN:HE21	9:H:129:ARG:HE	1.59	0.49
1:0:635:A:H2'	1:0:636:G:H5''	1.93	0.49
1:0:818:A:O2'	27:Z:37:ARG:HD3	2.13	0.49
1:0:1175:G:H2'	1:0:1176:C:C6	2.47	0.49
1:0:1342:C:C2'	1:0:1343:C:H5'	2.41	0.49
1:0:1357:A:H1'	39:0:8869:HOH:O	2.12	0.49
1:0:1441:G:H2'	1:0:1442:A:C8	2.46	0.49
1:0:1447:U:H5''	1:0:1677:U:C5	2.48	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
1:0:564:G:H1'	39:0:5694:HOH:O	2.12	0.49
1:0:849:C:O2'	1:0:850:U:H5'	2.12	0.49
1:0:1080:C:H4'	1:0:1081:A:OP1	2.13	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
1:0:2291:A:C4	1:0:2309:C:H5'	2.47	0.49
1:0:2611:G:H5'	1:0:2613:G:N7	2.28	0.49
1:0:2729:C:O2'	1:0:2730:G:H5'	2.13	0.49
39:0:3007:HOH:O	2:A:212:PRO:HB2	2.12	0.49
31:9:55:U:H4'	31:9:56:A:H8	1.77	0.49
1:0:522:U:O2'	1:0:1366:C:H5'	2.12	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
1:0:2643:G:H5''	39:0:8628:HOH:O	2.13	0.49
1:0:2885:A:H2'	1:0:2886:C:C6	2.48	0.49
31:9:13:A:H5'	39:9:2295:HOH:O	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
1:0:560:U:H2'	1:0:561:G:H8	1.78	0.49
1:0:1476:A:O2'	1:0:1868:G:H5'	2.13	0.49
1:0:1675:C:N4	39:0:8358:HOH:O	2.44	0.49
1:0:1786:C:H2'	1:0:1787:C:H6	1.78	0.49
1:0:1819:G:H2'	1:0:1820:G:C4'	2.42	0.49
1:0:2831:C:H2'	1:0:2832:C:C5'	2.43	0.49
1:0:24:G:H22	1:0:518:G:H1'	1.76	0.49
1:0:178:U:H2'	1:0:179:C:C6	2.46	0.49
1:0:1119:G:H8	11:J:52:GLN:HE22	1.58	0.49
1:0:1183:C:H42	1:0:1184:C:H41	1.60	0.49
1:0:1344:G:H1'	39:0:9105:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1447:U:C3'	1:0:1506:U:O2	2.59	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
1:0:2657:G:H4'	39:0:6216:HOH:O	2.11	0.49
1:0:2710:U:O2'	1:0:2711:U:H5'	2.13	0.49
3:B:305:ASP:O	3:B:306:LYS:HB2	2.12	0.49
31:9:81:C:C2'	31:9:82:U:H5'	2.42	0.49
1:0:23:G:H1'	1:0:520:A:H61	1.76	0.49
1:0:196:G:H2'	39:L:6170:HOH:O	2.11	0.49
1:0:1202:A:O2'	1:0:1203:G:H5'	2.13	0.49
1:0:1415:G:O2'	1:0:1416:G:H5'	2.12	0.49
1:0:1453:G:H2'	1:0:1454:U:O4'	2.12	0.49
1:0:2266:A:H2'	1:0:2267:G:C8	2.47	0.49
1:0:245:C:C5	1:0:246:G:C5	3.01	0.49
1:0:579:G:H2'	1:0:580:A:C8	2.47	0.49
1:0:677:C:H2'	1:0:678:G:H8	1.78	0.49
1:0:1046:G:C2	1:0:1069:C:C2	3.01	0.49
1:0:1464:C:O2'	1:0:1465:A:H5'	2.12	0.49
1:0:1473:U:O2'	1:0:1474:C:H5''	2.13	0.49
1:0:1775:A:H3'	1:0:1776:A:H2'	1.95	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
1:0:20:G:H21	19:R:117:HIS:HD2	1.60	0.49
1:0:40:C:O5'	1:0:40:C:H6	1.96	0.49
1:0:248:A:H3'	1:0:248:A:N3	2.27	0.49
1:0:820:G:N3	1:0:1831:U:H1'	2.28	0.49
1:0:1097:A:H5''	24:W:125:HIS:CE1	2.47	0.49
1:0:1293:U:H5'	26:Y:154:ARG:HH21	1.77	0.49
1:0:1548:U:O2'	1:0:1549:C:H5'	2.13	0.49
1:0:1619:G:C5	1:0:1620:C:C4	3.01	0.49
1:0:1664:A:H8	1:0:1664:A:OP1	1.95	0.49
1:0:1675:C:O2'	1:0:1676:G:H5'	2.13	0.49
1:0:1739:G:N2	1:0:2041:G:H1'	2.28	0.49
1:0:2552:C:N4	39:0:8668:HOH:O	2.46	0.49
1:0:2617:G:H5''	39:0:8605:HOH:O	2.12	0.49
1:0:2734:G:O2'	1:0:2735:U:H5'	2.13	0.49
1:0:2824:C:H5''	1:0:2825:C:H5'	1.95	0.49
31:9:89:C:O2'	31:9:90:G:H5'	2.12	0.49
1:0:559:U:H5'	1:0:559:U:C6	2.39	0.48
1:0:1076:G:H1'	39:0:3130:HOH:O	2.13	0.48
1:0:1118:A:H8	1:0:1119:G:H5''	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1149:U:O5'	1:0:1151:G:H5'	2.13	0.48
1:0:1774:G:O2'	1:0:1775:A:H5'	2.13	0.48
1:0:2112:A:H2'	1:0:2113:G:C8	2.48	0.48
1:0:2717:C:O2'	1:0:2718:C:H5''	2.09	0.48
1:0:2793:A:H2'	1:0:2794:G:H5'	1.94	0.48
1:0:169:A:H4'	39:0:5424:HOH:O	2.13	0.48
1:0:421:C:H4'	1:0:1919:A:C6	2.48	0.48
1:0:465:U:O5'	1:0:465:U:H6	1.96	0.48
1:0:812:A:H2'	1:0:813:C:H6	1.76	0.48
1:0:1014:A:H2'	1:0:1015:C:H5'	1.93	0.48
1:0:1701:A:H5''	1:0:1702:U:H3'	1.94	0.48
1:0:1806:G:C2	1:0:1807:U:O2	2.67	0.48
1:0:1841:C:OP2	1:0:2022:A:C8	2.66	0.48
24:W:122:ARG:HH12	24:W:154:ARG:H	1.61	0.48
31:9:107:C:H2'	31:9:108:C:C6	2.48	0.48
1:0:158:A:H2'	1:0:159:G:O4'	2.13	0.48
1:0:163:U:O3'	1:0:896:C:H4'	2.13	0.48
1:0:877:G:H1'	39:A:491:HOH:O	2.14	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
1:0:2392:C:H4'	18:Q:55:ARG:NH1	2.28	0.48
37:0:9101:MUL:H152	37:0:9101:MUL:O1	2.14	0.48
15:N:12:ARG:NH2	31:9:6:C:C5	2.81	0.48
19:R:63:ASN:HD22	19:R:75:TRP:HZ2	1.60	0.48
1:0:19:U:H2'	1:0:20:G:O4'	2.13	0.48
1:0:424:C:H2'	1:0:425:U:C6	2.43	0.48
1:0:1174:A:C5	1:0:1201:C:H4'	2.48	0.48
1:0:1449:G:H5'	39:0:7441:HOH:O	2.12	0.48
1:0:1497:G:H2'	1:0:1498:G:C8	2.48	0.48
1:0:1733:A:H4'	3:B:212:GLN:HA	1.96	0.48
1:0:2609:G:H22	3:B:238:ASN:HD21	1.60	0.48
31:9:39:U:H3'	31:9:40:C:H5''	1.96	0.48
1:0:332:G:H4'	21:T:2:LYS:O	2.12	0.48
1:0:579:G:H4'	39:0:6205:HOH:O	2.12	0.48
1:0:1824:C:O2'	1:0:1999:C:H4'	2.13	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
1:0:2480:G:H3'	39:0:8898:HOH:O	2.13	0.48
25:X:30:MET:HE1	25:X:58:ALA:HB3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1174:A:C6	1:0:1201:C:H4'	2.48	0.48
1:0:1621:G:H2'	1:0:1622:G:O4'	2.14	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
1:0:2052: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
1:0:822:C:C2	1:0:823:U:C5	3.02	0.48
1:0:1163:G:H1	1:0:1184:C:H42	1.62	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
1:0:37:A:C2	1:0:446:G:C2	3.02	0.48
1:0:88:G:H2'	1:0:89:G:C8	2.48	0.48
1:0:256:C:H2'	1:0:257:G:O4'	2.14	0.48
1:0:276:C:H42	1:0:373:G:H1	1.62	0.48
1:0:1200:A:H3'	39:0:4912:HOH:O	2.12	0.48
1:0:1635:U:H2'	1:0:1636:G:H8	1.79	0.48
1:0:2356:A:H2'	1:0:2357:G:O4'	2.14	0.48
1:0:2539:U:O2'	37:0:9101:MUL:H22	2.13	0.48
6:E:24:GLY:HA3	6:E:76:VAL:HB	1.96	0.48
1:0:700:A:H4'	16:O:50:ARG:HH21	1.79	0.48
1:0:1242:A:H5'	11:J:82:THR:CG2	2.43	0.48
1:0:1723:G:H2'	39:0:5194:HOH:O	2.14	0.48
1:0:1829:A:N6	27:Z:42:TYR:HA	2.28	0.48
1:0:1878:G:O2'	1:0:1879:U:P	2.71	0.48
1:0:2443:C:H3'	39:0:8103:HOH:O	2.13	0.48
1:0:2743:A:H5''	1:0:2743:A:H8	1.79	0.48
12:K:55:VAL:HG12	12:K:56:SER:N	2.29	0.48
1:0:37:A:H2'	1:0:38:G:C8	2.48	0.48
1:0:76:G:O2'	1:0:77:G:H5'	2.13	0.48
1:0:247:A:C2	1:0:265:U:C2	3.02	0.48
1:0:314:G:N1	1:0:317:A:OP2	2.47	0.48
1:0:393:G:H5''	39:0:6051:HOH:O	2.13	0.48
1:0:444:C:H2'	1:0:445:U:C6	2.49	0.48
1:0:705:C:H3'	1:0:706:G:C8	2.48	0.48
1:0:951:A:C2'	1:0:952:G:H5'	2.44	0.48
1:0:964:G:H2'	1:0:965:A:O4'	2.14	0.48
1:0:1684:A:O2'	1:0:1685:A:H5''	2.14	0.48
1:0:1850:U:H2'	1:0:1851:G:C8	2.49	0.48
1:0:2502:C:O2'	1:0:2503:A:H5'	2.14	0.48
1:0:2768:A:O2'	1:0:2769:C:H5'	2.13	0.48
1:0:2780:C:C1'	6:E:143:GLN:HE21	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:113:ILE:HG22	12:K:114:ALA:N	2.28	0.48
1:0:241:A:C2	1:0:378:A:H4'	2.49	0.47
1:0:269:G:O3'	1:0:274:G:H4'	2.14	0.47
1:0:447:A:C2'	1:0:448:G:H5'	2.44	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
1:0:1372:A:C2	1:0:2054:A:C4	3.02	0.47
1:0:1391:G:N2	1:0:1434:A:H5''	2.29	0.47
1:0:1487:A:H5'	39:0:3526:HOH:O	2.14	0.47
1:0:1855:G:H4'	1:0:1856:C:O5'	2.12	0.47
1:0:2134:G:H2'	1:0:2135:A:H8	1.78	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
1:0:2911:C:H2'	1:0:2912:C:C6	2.48	0.47
1:0:391:U:O2'	1:0:392:U:H5'	2.14	0.47
1:0:699:C:H2'	1:0:744:G:N3	2.29	0.47
1:0:809:G:H2'	1:0:810:G:H8	1.77	0.47
1:0:849:C:H2'	1:0:850:U:H6	1.78	0.47
1:0:962:C:N4	1:0:1005:A:H61	2.12	0.47
1:0:1387:G:C2	1:0:1396:C:O2	2.67	0.47
1:0:1415:G:C2'	1:0:1416:G:H5'	2.44	0.47
1:0:1730:G:H5'	1:0:1731:C:C6	2.49	0.47
1:0:2070:G:H2'	1:0:2072:G:OP1	2.15	0.47
1:0:2458:U:O3'	30:3:64:LYS:HB2	2.14	0.47
1:0:2639:G:O2'	1:0:2640:U:H5'	2.14	0.47
1:0:2734:G:H2'	1:0:2735:U:O4'	2.13	0.47
37:0:9101:MUL:H14	37:0:9101:MUL:C10	2.41	0.47
14:M:24:GLN:NE2	14:M:27:ARG:NH1	2.55	0.47
17:P:98:ILE:HD12	17:P:102:ARG:HE	1.79	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
1:0:290:C:C2'	1:0:291:C:H5'	2.44	0.47
1:0:656:G:H5'	16:O:3:THR:HB	1.96	0.47
1:0:719:C:N3	1:0:720:G:H1'	2.29	0.47
1:0:941:G:C5	1:0:942:U:C4	3.02	0.47
1:0:957:A:H2'	1:0:958:G:O4'	2.14	0.47
1:0:1448:A:O4'	1:0:1506:U:O4'	2.31	0.47
1:0:1497:G:H2'	1:0:1498:G:H8	1.78	0.47
1:0:1515:A:H2'	1:0:1516:U:C6	2.49	0.47
1:0:2032:U:C2'	1:0:2033:G:H5''	2.43	0.47
1:0:2057:U:O5'	1:0:2057:U:H6	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2291:A:C8	1:0:2309:C:H5'	2.49	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
31:9:3:A:H2	31:9:21:G:N3	2.12	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
1:0:325:U:O2	1:0:326:G:C8	2.67	0.47
1:0:825:U:H5''	1:0:826:U:OP1	2.13	0.47
1:0:1730:G:H2'	1:0:1730:G:N3	2.29	0.47
1:0:1763:C:O2'	1:0:1764:C:H5'	2.15	0.47
1:0:1792:C:N3	1:0:1793:C:H5	2.12	0.47
1:0:2038:A:H5''	3:B:222:LYS:HG3	1.96	0.47
1:0:2047:C:P	39:0:7641:HOH:O	2.73	0.47
1:0:2089:A:C2'	1:0:2090:G:H5'	2.45	0.47
1:0:2286:G:H1'	39:0:7013:HOH:O	2.13	0.47
1:0:2355:G:H5''	1:0:2356:A:OP2	2.14	0.47
1:0:2815:G:H4'	1:0:2816:A:OP2	2.13	0.47
31:9:49:G:H5''	39:9:4707:HOH:O	2.13	0.47
1:0:37:A:H2'	1:0:38:G:H8	1.78	0.47
1:0:392:U:H5''	14:M:193:LYS:HG2	1.96	0.47
1:0:640:G:C4	1:0:641:G:C8	3.03	0.47
1:0:683:G:O2'	1:0:684:G:H5'	2.15	0.47
1:0:730:G:O2'	1:0:731:U:H5'	2.15	0.47
1:0:894:A:H5''	39:0:7673:HOH:O	2.13	0.47
1:0:1217:G:C2	1:0:1218:U:C2	3.03	0.47
1:0:1324:G:H21	26:Y:204:ARG:NH2	2.13	0.47
1:0:1377:C:H5'	1:0:1377:C:C6	2.43	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
29:2:40:ARG:HD2	29:2:47:THR:HG22	1.96	0.47
1:0:168:C:O5'	1:0:168:C:H6	1.96	0.47
1:0:238:C:H4'	1:0:287:C:OP1	2.15	0.47
1:0:387:G:C2'	1:0:388:G:H5'	2.45	0.47
1:0:1666:C:C2'	1:0:1667:A:H5'	2.44	0.47
1:0:1969:A:O2'	1:0:1970:G:H5'	2.15	0.47
1:0:2072:G:H5'	39:0:3339:HOH:O	2.13	0.47
1:0:2332:A:H5'	5:D:56:ARG:NH2	2.27	0.47
1:0:2554:U:H3'	39:0:6989:HOH:O	2.14	0.47
1:0:2642:G:C6	1:0:2643:G:C6	3.02	0.47
1:0:2862:G:C6	1:0:2895:C:N4	2.83	0.47
37:0:9101:MUL:H262	37:0:9101:MUL:H242	1.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:57:C:H42	1:0:89:G:H1	1.63	0.47
1:0:208:C:H3'	1:0:208:C:C6	2.49	0.47
1:0:397:A:N3	1:0:418:C:H5'	2.30	0.47
1:0:459:A:H4'	39:0:4567:HOH:O	2.14	0.47
1:0:523:C:H2'	1:0:524:A:C8	2.49	0.47
1:0:544:G:H2'	1:0:545:G:H5''	1.97	0.47
1:0:561:G:N3	1:0:562:A:C8	2.83	0.47
1:0:603:A:H4'	1:0:604:G:O5'	2.15	0.47
1:0:699:C:C2	1:0:744:G:C2	3.02	0.47
1:0:711:G:C2	1:0:718:C:C2	3.03	0.47
1:0:763:C:O2'	1:0:764:C:H5'	2.14	0.47
1:0:920:C:H5	1:0:2467:A:OP1	1.98	0.47
1:0:951:A:H5''	18:Q:42:LYS:HD3	1.97	0.47
1:0:1153:C:N3	1:0:2786:G:O6	2.47	0.47
1:0:1162:G:H2'	1:0:1163:G:H8	1.80	0.47
1:0:1220:U:H2'	1:0:1221:G:C8	2.47	0.47
1:0:1245:C:H3'	1:0:1245:C:H6	1.79	0.47
1:0:1351:G:H1'	39:0:3441:HOH:O	2.15	0.47
1:0:1656:A:H2'	1:0:1657:A:O4'	2.14	0.47
1:0:1851:G:H1'	39:0:3109:HOH:O	2.15	0.47
1:0:2035:C:O2'	1:0:2036:C:H5'	2.15	0.47
1:0:2081:A:H2'	1:0:2082:G:O4'	2.15	0.47
1:0:2087:C:O2'	1:0:2088:C:H5'	2.15	0.47
1:0:2093:G:H5''	39:0:7738:HOH:O	2.15	0.47
1:0:2119:C:O2'	1:0:2120:U:H5'	2.14	0.47
1:0:2253:G:H2'	1:0:2254:G:C8	2.40	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
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
1:0:2851:G:C2'	1:0:2852:A:H5'	2.45	0.47
4:C:27:ARG:HG2	4:C:27:ARG:HH11	1.79	0.47
4:C:215:ALA:HB3	39:C:5535:HOH:O	2.15	0.47
6:E:91:PHE:HA	6:E:92:PRO:HD3	1.79	0.47
24:W:88:THR:HG22	24:W:89:ASP:H	1.79	0.47
31:9:35:C:H5''	39:9:4078:HOH:O	2.15	0.47
1:0:45:A:C5'	1:0:47:G:H5'	2.45	0.47
1:0:123:U:H1'	39:0:7179:HOH:O	2.14	0.47
1:0:216:A:O2'	1:0:217:C:H5'	2.15	0.47
1:0:292:G:O2'	1:0:360:A:N6	2.47	0.47
1:0:621:C:H5'	26:Y:132:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:639:A:C6	1:0:640:G:C6	3.02	0.47
1:0:699:C:C6	1:0:744:G:N3	2.83	0.47
1:0:1119:G:C5	1:0:1243:C:C4	3.03	0.47
1:0:1566:C:H2'	1:0:1567:G:C8	2.50	0.47
1:0:1575:C:O2	1:0:1575:C:H2'	2.14	0.47
1:0:1776:A:C8	1:0:1778:A:O4'	2.67	0.47
1:0:1826:C:O2'	1:0:1827:G:H5'	2.15	0.47
1:0:2243:C:H5''	39:0:8382:HOH:O	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
30:3:51:LYS:HB2	39:3:1812:HOH:O	2.15	0.47
1:0:240:C:O2	1:0:240:C:H2'	2.14	0.47
1:0:837:U:H2'	1:0:838:C:O4'	2.15	0.47
1:0:1233:A:N1	1:0:2604:A:O2'	2.42	0.47
1:0:1419:U:H5'	1:0:1420:C:OP2	2.15	0.47
1:0:2320:U:H3'	30:3:2:GLN:HB2	1.97	0.47
1:0:2547:C:H1'	39:B:342:HOH:O	2.13	0.47
1:0:2697:A:H2'	1:0:2698:G:O4'	2.15	0.47
1:0:2831:C:H2'	1:0:2832:C:H5'	1.97	0.47
15:N:67:ALA:HA	15:N:71:TRP:HB3	1.96	0.47
31:9:58:G:H2'	31:9:59:C:O4'	2.15	0.47
31:9:82:U:H2'	31:9:83:G:H8	1.80	0.47
1:0:849:C:C5	1:0:850:U:C5	3.03	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.49	0.47
1:0:1098:A:O3'	24:W:129:LYS:HE3	2.15	0.47
1:0:1158:G:C2'	1:0:1159:G:H5'	2.45	0.47
1:0:1363:G:H2'	1:0:1364:G:H8	1.80	0.47
1:0:1978:A:H5''	39:0:7843:HOH:O	2.14	0.47
1:0:2506:A:O2'	1:0:2507:G:O5'	2.32	0.47
1:0:2893:C:O2'	1:0:2894:C:H5'	2.15	0.47
2:A:70:ALA:HB1	27:Z:89:THR:HG21	1.96	0.47
1:0:174:A:H4'	1:0:175:G:OP1	2.15	0.46
1:0:187:A:H5'	1:0:188:C:OP2	2.14	0.46
1:0:308:U:C4	1:0:342:C:H1'	2.50	0.46
1:0:661:G:C6	1:0:662:U:C4	3.03	0.46
1:0:738:G:H21	1:0:2384:U:H4'	1.80	0.46
1:0:879:C:H3'	39:0:5621:HOH:O	2.14	0.46
1:0:1056:U:H2'	1:0:1057:A:O4'	2.15	0.46
1:0:1138:G:H4'	39:0:4849:HOH:O	2.15	0.46
1:0:1181:A:N1	1:0:1192:A:O2'	2.47	0.46
1:0:1278:A:H4'	1:0:1279:U:N3	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1444:G:C2'	1:0:1445:G:H5'	2.45	0.46
1:0:1477:C:H2'	1:0:1478:U:O4'	2.15	0.46
1:0:1518:A:H1'	39:0:8334:HOH:O	2.15	0.46
1:0:1825:U:O2'	1:0:1826:C:H5'	2.15	0.46
1:0:2569:A:H8	1:0:2569:A:O5'	1.97	0.46
1:0:2812:A:H1'	39:0:4957:HOH:O	2.15	0.46
31:9:45:A:C8	31:9:46:C:C5	3.03	0.46
1:0:65:C:O2'	1:0:66:G:H5'	2.14	0.46
1:0:154:C:H2'	1:0:155:C:C6	2.37	0.46
1:0:485:A:N3	1:0:487:G:H5''	2.30	0.46
1:0:676:C:HO2'	4:C:219:ASN:HD22	1.59	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
1:0:1449:G:N3	1:0:1449:G:H2'	2.29	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
1:0:1883: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
1:0:2070:G:H4'	39:0:2976:HOH:O	2.14	0.46
1:0:2088:C:H1'	1:0:2841:A:N1	2.30	0.46
1:0:2496:C:H1'	1:0:2527:U:N3	2.30	0.46
24:W:122:ARG:HH12	24:W:154:ARG:N	2.12	0.46
1:0:634:G:C2	1:0:635:A:C2	3.03	0.46
1:0:920:C:H4'	1:0:921:G:N3	2.29	0.46
1:0:1754:A:H2'	1:0:1755:A:O4'	2.16	0.46
1:0:1771:U:H4'	1:0:1772:C:OP2	2.15	0.46
1:0:1832:G:N2	1:0:1845:A:C4	2.83	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
1:0:2135:A:O4'	1:0:2243:C:N4	2.47	0.46
27:Z:56:GLU:O	27:Z:61:HIS:HE1	1.98	0.46
28:1:21:ARG:HD2	28:1:37:CYS:SG	2.56	0.46
31:9:39:U:H1'	31:9:44:A:N6	2.30	0.46
1:0:255:A:H2'	1:0:256:C:C6	2.50	0.46
1:0:287:C:N4	1:0:365:G:H1	2.10	0.46
1:0:544:G:C2'	1:0:545:G:H5''	2.45	0.46
1:0:689:G:O2'	1:0:742:G:H1'	2.15	0.46
1:0:722:G:C5	1:0:723:G:C8	3.03	0.46
1:0:862:U:H4'	39:0:7515:HOH:O	2.15	0.46
1:0:946:C:H6	1:0:946:C:O5'	1.99	0.46
1:0:1013:A:H5''	1:0:2302:A:N6	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1215:A:O3'	1:0:1216:G:H4'	2.14	0.46
1:0:1455:C:O2	1:0:1456:C:C6	2.69	0.46
1:0:1639:U:H2'	1:0:1640:C:O5'	2.15	0.46
1:0:1977:U:OP1	1:0:1978:A:H5'	2.15	0.46
1:0:2134:G:O6	1:0:2258:A:H2'	2.15	0.46
1:0:2605:G:O2'	1:0:2606:G:H5'	2.14	0.46
10:I:96:SER:H	10:I:99:GLN:HB2	1.80	0.46
1:0:106:A:C2'	1:0:107:U:H5'	2.46	0.46
1:0:250:C:H2'	1:0:251:C:C6	2.50	0.46
1:0:445:U:O2'	1:0:446:G:H5'	2.16	0.46
1:0:853:C:H3'	39:0:3276:HOH:O	2.14	0.46
1:0:871:G:C6	1:0:872:U:N3	2.84	0.46
1:0:1132:A:H61	1:0:1229:C:H2'	1.79	0.46
1:0:1253:C:O2'	1:0:1254:C:H5'	2.16	0.46
1:0:1523:G:C5	1:0:1524:U:C4	3.03	0.46
1:0:2110:G:H4'	39:0:7642:HOH:O	2.15	0.46
1:0:2134:G:N2	1:0:2242:U:C2	2.83	0.46
1:0:2578:G:H5'	1:0:2578:G:C8	2.47	0.46
1:0:2668:G:H2'	1:0:2669:U:H6	1.79	0.46
1:0:2714:U:O3'	3:B:10:SER:HB2	2.14	0.46
1:0:2718:C:C2	1:0:2763:G:N2	2.84	0.46
1:0:2825:C:H4'	1:0:2826:G:O4'	2.16	0.46
1:0:353:G:H2'	1:0:354:A:C8	2.51	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
1:0:763:C:H5''	39:0:3284:HOH:O	2.16	0.46
1:0:962:C:H2'	1:0:963:C:C5'	2.46	0.46
1:0:1556:G:O2'	1:0:1557:G:H5'	2.16	0.46
1:0:1769:C:C2'	1:0:1770:U:H5'	2.46	0.46
1:0:2416:G:H1'	39:0:5208:HOH:O	2.14	0.46
1:0:2745:C:H5''	39:0:5667:HOH:O	2.14	0.46
1:0:522:U:O2'	1:0:523:C:H5'	2.16	0.46
1:0:669:G:C4	1:0:670:G:C8	3.04	0.46
1:0:677:C:H4'	4:C:246:ARG:NH1	2.30	0.46
1:0:1217:G:H2'	1:0:1218:U:C6	2.51	0.46
1:0:1463:U:H4'	39:0:6050:HOH:O	2.16	0.46
1:0:1684:A:H8	39:0:7816:HOH:O	1.98	0.46
1:0:1822:A:O2'	1:0:1823:G:H5'	2.16	0.46
1:0:2075:G:C6	1:0:2076:U:C4	3.04	0.46
1:0:2096:A:C8	1:0:2539:U:C2	3.03	0.46
1:0:2259:C:C5	1:0:2260:A:N7	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2484:U:H4'	39:0:4578:HOH:O	2.16	0.46
1:0:2754:G:H2'	1:0:2755:G:O4'	2.16	0.46
1:0:2796:U:H1'	6:E:143:GLN:OE1	2.16	0.46
6:E:103:VAL:HG22	6:E:115:ARG:HB3	1.97	0.46
11:J:107:ASN:HD22	11:J:109:TYR:H	1.63	0.46
1:0:105:G:C2	1:0:106:A:C8	3.04	0.46
1:0:295:C:C2'	1:0:296:G:H5'	2.45	0.46
1:0:502:A:H2'	1:0:503:G:O4'	2.15	0.46
1:0:814:G:H2'	1:0:815:U:H6	1.81	0.46
1:0:1230:A:H8	1:0:1230:A:OP1	1.98	0.46
1:0:2338:G:H4'	5:D:105:SER:O	2.16	0.46
1:0:2403:C:H5'	39:0:5297:HOH:O	2.14	0.46
1:0:2791:U:H4'	1:0:2792:A:OP1	2.16	0.46
1:0:160:A:C4	1:0:177:A:C2	3.04	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
8:G:64:ASN:HD22	8:G:64:ASN:N	2.14	0.46
20:S:17:ASP:HB3	20:S:23:LYS:HB2	1.96	0.46
1:0:230:C:H2'	1:0:231:G:H8	1.81	0.46
1:0:267:G:H2'	1:0:268:U:O4'	2.16	0.46
1:0:287:C:H2'	1:0:288:A:C8	2.51	0.46
1:0:295:C:O2'	1:0:296:G:H5'	2.16	0.46
1:0:707:C:C2	1:0:708:A:C8	3.04	0.46
1:0:1096:U:O2'	1:0:1097:A:H5'	2.16	0.46
1:0:1880:C:H2'	1:0:1881:A:O4'	2.16	0.46
1:0:2540:G:O2'	37:0:9101:MUL:H131	2.16	0.46
1:0:2775:A:C6	1:0:2799:A:C8	3.04	0.46
15:N:37:ARG:NH1	31:9:6:C:OP1	2.46	0.46
19:R:106:GLY:HA2	19:R:109:MET:HE2	1.97	0.46
1:0:432:G:H2'	1:0:433:C:C6	2.47	0.45
1:0:606:C:O2'	1:0:607:G:H5'	2.16	0.45
1:0:878:G:H4'	1:0:1835:U:H4'	1.96	0.45
1:0:893:C:H4'	1:0:894:A:OP1	2.16	0.45
1:0:1794:G:OP1	17:P:134:VAL:HG23	2.16	0.45
1:0:2668:G:H2'	1:0:2669:U:C6	2.50	0.45
1:0:2732:U:H2'	1:0:2733:U:H6	1.80	0.45
31:9:63:C:O2'	31:9:64:C:H5'	2.16	0.45
1:0:207:U:H4'	1:0:438:C:O2	2.16	0.45
1:0:402:U:H2'	1:0:403:C:C6	2.51	0.45
1:0:820:G:H5'	1:0:821:U:C5'	2.47	0.45
1:0:1183:C:N3	1:0:1184:C:N4	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1187:U:HO2'	1:0:1188:A:H8	1.61	0.45
1:0:1325:G:C2	1:0:1326:C:C6	3.04	0.45
1:0:1838:U:H3'	39:0:4588:HOH:O	2.15	0.45
1:0:2102:G:C6	37:0:9101:MUL:H173	2.51	0.45
1:0:2776:A:H2'	1:0:2777:G:H5'	1.98	0.45
13:L:80:ASP:HB3	13:L:90:ARG:HB3	1.98	0.45
29:2:35:ARG:N	39:2:3614:HOH:O	2.50	0.45
30:3:49:ASP:HB3	30:3:52:PHE:HB2	1.98	0.45
31:9:64:C:C2'	31:9:65:A:H5'	2.46	0.45
31:9:75:G:C2	31:9:107:C:N3	2.85	0.45
1:0:165:A:O2'	1:0:221:G:N2	2.48	0.45
1:0:585:C:H2'	1:0:586:C:C6	2.51	0.45
1:0:1476:A:O2'	1:0:1477:C:H5'	2.17	0.45
1:0:1594:C:O2'	1:0:1607:A:H4'	2.16	0.45
1:0:2598:U:O2	1:0:2600:A:C8	2.70	0.45
1:0:2695:C:H2'	1:0:2696:G:H8	1.82	0.45
7:F:67:ALA:HB1	7:F:72:VAL:O	2.17	0.45
1:0:156:C:H5''	14:M:171:ARG:CD	2.42	0.45
1:0:535:G:C5	1:0:2063:U:C4	3.04	0.45
1:0:1098:A:OP1	24:W:128:VAL:HG22	2.15	0.45
1:0:1368:U:O5'	1:0:1368:U:H6	2.00	0.45
1:0:1449:G:N3	1:0:1493:A:C2	2.84	0.45
1:0:1509:U:O2'	1:0:1510:G:H5'	2.16	0.45
1:0:1667:A:H2'	1:0:1668:U:C6	2.51	0.45
1:0:1740:U:O2	1:0:2724:U:H5''	2.16	0.45
1:0:2397:G:C5	1:0:2465:A:C6	3.05	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
1:0:883:U:C6	1:0:888:U:H5'	2.51	0.45
1:0:926:A:H4'	13:L:39:GLU:HG2	1.99	0.45
1:0:1141:U:O2'	1:0:1142:C:H5'	2.16	0.45
1:0:1180:U:H1'	10:I:87:PRO:HD2	1.97	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
1:0:2078:U:O2'	1:0:2079:G:H5'	2.16	0.45
1:0:2106:C:H2'	1:0:2107:U:C6	2.52	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
24:W:4:LEU:HD23	24:W:54:PHE:HB3	1.97	0.45
1:0:67:A:H5''	1:0:69:A:C8	2.52	0.45
1:0:247:A:H2'	39:0:8624:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:421:C:H4'	1:0:1919:A:C5	2.51	0.45
1:0:472:A:N1	1:0:888:U:O2'	2.43	0.45
1:0:517:U:C2'	1:0:518:G:H5'	2.47	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
1:0:860:U:H2'	1:0:861:A:C8	2.52	0.45
1:0:876:A:H2'	1:0:876:A:N3	2.30	0.45
1:0:1052:G:H2'	1:0:1052:G:N3	2.32	0.45
1:0:1220:U:H4'	9:H:174:LEU:HD21	1.98	0.45
1:0:1877:G:OP1	2:A:164:ARG:NH2	2.49	0.45
1:0:1909:A:H4'	39:0:8156:HOH:O	2.16	0.45
1:0:2270:G:H2'	39:0:4485:HOH:O	2.16	0.45
1:0:2444:U:H2'	1:0:2445:U:H6	1.81	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
1:0:2717:C:OP1	3:B:207:LYS:HG3	2.16	0.45
15:N:159:TYR:CE1	31:9:50:G:H5''	2.49	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
1:0:329:A:H5'	1:0:347:A:C1'	2.47	0.45
1:0:333:G:N1	1:0:344:C:C4	2.85	0.45
1:0:443:C:H2'	1:0:444:C:C6	2.52	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
1:0:1919:A:H4'	39:0:3679:HOH:O	2.17	0.45
1:0:2871:G:H2'	1:0:2872:U:H6	1.82	0.45
19:R:96:VAL:HG13	19:R:106:GLY:HA3	1.99	0.45
22:U:39:ASN:HD22	22:U:44:ARG:HD2	1.82	0.45
31:9:53:G:O2'	31:9:54:A:H5'	2.16	0.45
1:0:178:U:O2'	1:0:179:C:H5'	2.16	0.45
1:0:193:A:H2'	1:0:414:C:O2	2.16	0.45
1:0:275:G:C2	1:0:376:C:C2	3.05	0.45
1:0:297:U:H2'	1:0:298:C:C6	2.52	0.45
1:0:400:C:H2'	1:0:401:C:C6	2.52	0.45
1:0:1119:G:C8	11:J:52:GLN:NE2	2.84	0.45
1:0:1164:U:H4'	1:0:1165:G:H5''	1.99	0.45
1:0:1334:C:H1'	26:Y:204:ARG:HH21	1.81	0.45
1:0:1475:G:N3	1:0:1866:A:H2	2.15	0.45
1:0:1819:G:H2'	1:0:1820:G:C5'	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1917:G:H1'	1:0:1923:G:N2	2.32	0.45
1:0:2295:G:H5'	1:0:2425:A:H4'	1.98	0.45
1:0:2493:C:O2	1:0:2493:C:H2'	2.17	0.45
1:0:2626:C:H2'	1:0:2627:G:C8	2.51	0.45
1:0:2727:A:H2'	1:0:2728:C:H5'	1.98	0.45
1:0:2823:G:O2'	1:0:2824:C:H5'	2.16	0.45
39:0:7140:HOH:O	26:Y:149:GLN:HG3	2.15	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
12:K:125:ALA:C	12:K:127:ALA:H	2.25	0.45
15:N:55:ASP:OD2	31:9:7:G:H4'	2.16	0.45
1:0:63:U:O2'	1:0:64:G: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
1:0:400:C:H2'	1:0:401:C:H6	1.82	0.45
1:0:693:A:H2'	1:0:694:A:C8	2.52	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
1:0:1398: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
1:0:1766: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
1:0:2869:G:H5'	39:0:4548:HOH:O	2.16	0.45
3:B:125:GLU:O	3:B:129:ARG:HG3	2.17	0.45
31:9:17:G:O2'	31:9:18:U:H5'	2.16	0.45
1:0:23:G:H2'	1:0:24:G:O4'	2.17	0.45
1:0:123:U:H5'	39:0:6169:HOH:O	2.17	0.45
1:0:151:A:N3	1:0:441:A:H4'	2.32	0.45
1:0:622:G:C5	1:0:623:U:C5	3.04	0.45
1:0:656:G:H2'	1:0:657:G:C8	2.52	0.45
1:0:783:C:O5'	1:0:783:C:H6	2.00	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
1:0:2269:C:C2'	1:0:2270:G:H5'	2.47	0.45
3:B:254:GLN:HG2	3:B:255:GLY:N	2.32	0.45
15:N:44:ARG:HG3	15:N:45:ALA:N	2.32	0.45
1:0:80:A:H3'	21:T:43:ASN:OD1	2.16	0.44
1:0:128:A:H3'	1:0:128:A:H8	1.81	0.44
1:0:657:G:H1'	39:0:2960:HOH:O	2.16	0.44
1:0:876:A:N7	1:0:878:G:H1'	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1258:G:H8	1:0:1258:G:O5'	2.00	0.44
1:0:1323:G:N2	1:0:1335:C:C2	2.86	0.44
1:0:1387:G:H1'	17:P:28:GLN:HE22	1.80	0.44
1:0:2657:G:H5'	39:0:5938:HOH:O	2.17	0.44
9:H:168:VAL:HG13	39:H:4963:HOH:O	2.16	0.44
1:0:298:C:O5'	1:0:298:C:H6	1.99	0.44
1:0:473:A:O2'	1:0:890:C:H5'	2.17	0.44
1:0:1126:C:O5'	1:0:1126:C:C6	2.66	0.44
1:0:1454:U:H5''	1:0:1455:C:OP2	2.17	0.44
1:0:1526:A:H4'	1:0:1527:A:C5'	2.47	0.44
1:0:1592:G:O2'	1:0:1593:C:O5'	2.34	0.44
1:0:1714:C:O2'	1:0:1715:C:H5'	2.17	0.44
1:0:1845:A:OP2	2:A:190:ARG:NH1	2.50	0.44
1:0:2271:G:N3	1:0:2271:G:H2'	2.32	0.44
1:0:2407:G:C2	1:0:2408:A:C4	3.05	0.44
31:9:59:C:H2'	31:9:60:C:H6	1.82	0.44
1:0:32:G:H2'	1:0:33:G:O4'	2.18	0.44
1:0:329:A:H5'	1:0:347:A:H1'	1.99	0.44
1:0:397:A:C4	1:0:418:C:H5'	2.52	0.44
1:0:722:G:C2'	1:0:723:G:H5'	2.48	0.44
1:0:968:G:O2'	1:0:969:G:H5'	2.17	0.44
1:0:1730:G:C5'	1:0:1731:C:C6	3.00	0.44
1:0:1827:G:H2'	1:0:1828:G:C8	2.52	0.44
1:0:2087:C:C2	1:0:2658:G:C2	3.06	0.44
1:0:2428:G:H4'	39:0:4707:HOH:O	2.17	0.44
1:0:2638:G:H5'	39:0:3790:HOH:O	2.17	0.44
1:0:2842:G:H2'	1:0:2843:A:H5'	1.98	0.44
14:M:99:ARG:NE	14:M:170:ASN:HD22	2.15	0.44
18:Q:25:PRO:HA	18:Q:26:PRO:HD3	1.82	0.44
18:Q:66:LYS:HB2	18:Q:70:ALA:O	2.17	0.44
24:W:38:THR:O	24:W:42:ARG:HB2	2.17	0.44
31:9:59:C:H2'	31:9:60:C:C6	2.52	0.44
1:0:212:A:O3'	1:0:213:G:H4'	2.17	0.44
1:0:708:A:H2'	1:0:709:G:O4'	2.17	0.44
1:0:1363:G:P	4:C:76:ARG:NH2	2.90	0.44
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
1:0:1909:A:N1	1:0:2128:G:H1'	2.32	0.44
1:0:2002:C:H2'	1:0:2003:U:H5'	1.99	0.44
1:0:2451:G:H5''	39:0:6300:HOH:O	2.16	0.44
1:0:2657:G:N2	1:0:2658:G:H1'	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2814:A:O4'	1:0:2816:A:C8	2.70	0.44
1:0:2900:G:O2'	1:0:2901:C:H5'	2.17	0.44
12:K:98:VAL:HG13	12:K:102:GLU:HA	2.00	0.44
31:9:1:U:H4'	31:9:3:A:OP1	2.18	0.44
31:9:95:C:O2'	31:9:96:C:H5'	2.17	0.44
1:0:64:G:N2	1:0:70:A:C4	2.85	0.44
1:0:65:C:H2'	1:0:66:G:H8	1.82	0.44
1:0:131:A:OP2	1:0:141:C:H5	2.01	0.44
1:0:256:C:H2'	1:0:257:G:C5'	2.47	0.44
1:0:318:U:H5'	1:0:339:A:N3	2.32	0.44
1:0:962:C:C2'	1:0:963:C:H5'	2.48	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
1:0:1733:A:C2	1:0:1734:C:H1'	2.53	0.44
1:0:1886:A:H61	1:0:2016:U:H3	1.63	0.44
1:0:2103:A:O2'	1:0:2104:C:OP1	2.36	0.44
1:0:2275:G:C6	1:0:2276:U:N3	2.85	0.44
1:0:2679:G:H2'	1:0:2680:A:H3'	1.99	0.44
1:0:2726:U:O4'	1:0:2749:U:C2	2.69	0.44
1:0:2869:G:H8	1:0:2869:G:O5'	2.01	0.44
3:B:244:PRO:HG3	3:B:248:ARG:HH21	1.81	0.44
14:M:157:ASP:HB3	14:M:160:PHE:HD1	1.83	0.44
19:R:17:MET:HE1	19:R:19:ARG:NH2	2.33	0.44
28:1:28:HIS:O	28:1:32:LYS:N	2.49	0.44
31:9:54:A:H4'	39:9:7345:HOH:O	2.16	0.44
1:0:228:C:C2'	1:0:229:G:H5'	2.48	0.44
1:0:354:A:H2'	1:0:355:C:C6	2.53	0.44
1:0:1501:A:H4'	39:0:4703:HOH:O	2.17	0.44
1:0:1531:U:C2	1:0:1661:A:N1	2.85	0.44
1:0:1613:C:H2'	1:0:1614:G:O4'	2.18	0.44
1:0:1632:A:C2'	1:0:1633:C:H5'	2.46	0.44
1:0:1681:G:H5''	1:0:1682:A:H5'	1.99	0.44
1:0:1732:A:C6	1:0:2840:A:H1'	2.52	0.44
1:0:2245:C:H6	1:0:2245:C:O5'	2.01	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
1:0:2471:G:N3	1:0:2633:A:H2	2.16	0.44
1:0:2892:G:C6	1:0:2893:C:C4	3.06	0.44
5:D:15:GLU:HA	5:D:16:PRO:HD3	1.85	0.44
31:9:3:A:H2'	31:9:26:C:O2	2.18	0.44
1:0:400:C:O2'	1:0:401:C:H5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:407:A:H2'	1:0:408:A:C8	2.52	0.44
1:0:736:A:H8	39:0:6948:HOH:O	2.01	0.44
1:0:1126:C:O2'	1:0:1128:U:H6	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
1:0:1792:C:C2	1:0:1793:C:H5	2.36	0.44
1:0:2110:G:C2	1:0:2478:U:N3	2.86	0.44
1:0:2254:G:H1'	39:0:4611:HOH:O	2.18	0.44
1:0:2331:C:H1'	1:0:2356:A:C2	2.52	0.44
1:0:2554:U:C6	1:0:2577:A:N6	2.85	0.44
5:D:172:VAL:HG12	5:D:173:GLU:H	1.83	0.44
1:0:577:G:C6	1:0:581:G:O6	2.70	0.44
1:0:690:G:H4'	1:0:741:C:O2	2.18	0.44
1:0:816:G:C5	1:0:817:G:C6	3.06	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
1:0:1841:C:OP2	1:0:2022:A:H8	2.00	0.44
1:0:1923:G:H4'	30:3:31:THR:O	2.18	0.44
1:0:2001:G:O2'	1:0:2002:C:H5'	2.18	0.44
1:0:2055:A:H5'	19:R:134:SER:HB2	2.00	0.44
1:0:2066:C:H5''	39:0:4041:HOH:O	2.17	0.44
1:0:2076:U:H2'	39:0:6153: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
1:0:2832:C:H5	39:0:6957:HOH:O	2.01	0.44
3:B:272:ILE:HG22	39:B:7492:HOH:O	2.17	0.44
1:0:81:G:N3	1:0:98:A:C2	2.86	0.44
1:0:119:A:H2'	1:0:120:A:C5'	2.45	0.44
1:0:206:G:H5'	14:M:185:PRO:HD3	1.99	0.44
1:0:533:U:H2'	1:0:2814:A:C6	2.52	0.44
1:0:566:A:H2'	1:0:567:U:C5'	2.48	0.44
1:0:595:U:H2'	1:0:596:C:C6	2.51	0.44
1:0:1200:A:H5'	39:0:7124:HOH:O	2.18	0.44
1:0:1641:A:C8	1:0:1702:U:O4	2.71	0.44
1:0:2120:U:H1'	39:0:3535:HOH:O	2.17	0.44
1:0:2265:U:H2'	1:0:2266:A:C8	2.53	0.44
1:0:2587:OMU:HM23	1:0:2589:U:C6	2.53	0.44
1:0:2846:C:H4'	3:B:156:LYS:HB2	1.99	0.44
5:D:76:ARG:NH1	31:9:42:C:O2	2.50	0.44
9:H:23:ILE:HG21	9:H:97:VAL:HG11	2.00	0.44
13:L:136:ALA:HB3	39:L:6166:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:21:G:C4'	19:R:2:ILE:HG22	2.44	0.43
1:0:506:G:H22	1:0:509:A:H5'	1.76	0.43
1:0:792:G:O2'	1:0:793:A:H5'	2.18	0.43
1:0:927:U:H4'	39:0:3262:HOH:O	2.18	0.43
1:0:1185:U:H2'	1:0:1186:C:C6	2.53	0.43
1:0:1829:A:H2'	1:0:1830:C:C5'	2.46	0.43
1:0:1909:A:H2'	1:0:1910:A:C8	2.53	0.43
1:0:2321:A:H62	1:0:2380:A:H62	1.65	0.43
1:0:2420:G:O2'	1:0:2421:G:H5'	2.17	0.43
1:0:2598:U:O2	1:0:2600:A:H8	2.01	0.43
1:0:2730:G:O2'	1:0:2731:G:H5'	2.17	0.43
1:0:2853:U:C4	1:0:2906:A:N6	2.85	0.43
11:J:75:PRO:HG2	11:J:105:LEU:HD21	2.00	0.43
28:1:2:GLY:O	28:1:6:PRO:HG2	2.18	0.43
31:9:92:G:C6	31:9:93:A:N6	2.86	0.43
1:0:212:A:O4'	1:0:214:U:C6	2.71	0.43
1:0:599:G:H2'	1:0:600:G:C8	2.53	0.43
1:0:703:G:O2'	1:0:704:C:H5'	2.18	0.43
1:0:868:G:C5	1:0:887:G:C8	3.06	0.43
1:0:952:G:N3	1:0:2302:A:H2'	2.33	0.43
1:0:1448:A:H4'	39:0:6039:HOH:O	2.18	0.43
1:0:1933:G:O2'	1:0:1934:A:H5'	2.18	0.43
1:0:2507:G:O6	1:0:2511:A:H4'	2.18	0.43
1:0:2739:A:C6	1:0:2740:G:C5	3.06	0.43
19:R:63:ASN:ND2	19:R:75:TRP:HZ2	2.17	0.43
1:0:56:G:H1'	39:0:4338:HOH:O	2.18	0.43
1:0:66:G:C2	1:0:109:U:C4	3.06	0.43
1:0:235:C:O2'	1:0:236:A:H2'	2.18	0.43
1:0:530:C:H2'	1:0:531:G:O4'	2.18	0.43
1:0:596:C:H2'	1:0:597:A:C8	2.53	0.43
1:0:836:G:N3	1:0:836:G:H2'	2.34	0.43
1:0:1188:A:N7	1:0:1189:A:C2	2.87	0.43
1:0:1311:G:C2	1:0:1312:G:C8	3.06	0.43
1:0:1557:G:H2'	1:0:1558:C:H6	1.83	0.43
1:0:1689:A:H2'	1:0:1689:A:N3	2.32	0.43
1:0:1758:U:C2'	1:0:1759:A:H5'	2.48	0.43
1:0:1788:U:C2	1:0:1805:G:N2	2.87	0.43
1:0:2300:A:H4'	1:0:2301:A:O5'	2.18	0.43
1:0:2364:A:H5''	18:Q:15:LYS:HD3	2.00	0.43
1:0:2552:C:C6	1:0:2577:A:N7	2.86	0.43
5:D:149:ARG:HH12	15:N:15:GLU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:74:ALA:HB2	25:X:85:VAL:HG13	2.00	0.43
1:0:67:A:C6	1:0:109:U:H1'	2.53	0.43
1:0:281:U:O2'	1:0:282:C:H5'	2.19	0.43
1:0:549:A:C2	1:0:550:C:C2	3.06	0.43
1:0:658:C:O2'	1:0:662:U:OP1	2.30	0.43
1:0:1127:C:C2'	1:0:1128:U:H5'	2.48	0.43
1:0:1332:C:O2'	1:0:1333:U:H5'	2.19	0.43
1:0:1503:U:C2'	1:0:1504:A:H5'	2.48	0.43
1:0:1821:A:O2'	1:0:1822:A:H5'	2.17	0.43
1:0:387:G:O2'	1:0:388:G:H5'	2.18	0.43
1:0:621:C:O2'	1:0:1357:A:N1	2.45	0.43
1:0:730:G:H2'	1:0:731:U:C6	2.53	0.43
1:0:869:G:C8	1:0:869:G:OP2	2.72	0.43
1:0:938:G:N2	1:0:1031:G:H1'	2.34	0.43
1:0:1610:G:H2'	1:0:1611:G:O4'	2.18	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
1:0:1942:A:H2'	39:0:4237:HOH:O	2.18	0.43
1:0:2467:A:H5''	39:0:2924:HOH:O	2.17	0.43
1:0:2851:G:O3'	3:B:157:LYS:NZ	2.47	0.43
31:9:3:A:OP2	31:9:25:G:N2	2.51	0.43
1:0:815:U:O2'	1:0:816:G:H5'	2.19	0.43
1:0:1074:G:H4'	1:0:1260:G:C6	2.54	0.43
1:0:1076:G:C2	1:0:1084:C:N3	2.86	0.43
1:0:1086:A:N6	24:W:11:VAL:HG11	2.33	0.43
1:0:1135:G:N2	1:0:1228:C:C2	2.87	0.43
1:0:1288:U:H4'	24:W:27:HIS:CD2	2.54	0.43
1:0:1786:C:C5	1:0:1787:C:H5	2.37	0.43
1:0:1853:C:H5'	2:A:228:ILE:O	2.18	0.43
1:0:1930:A:H2'	1:0:1931:A:C8	2.52	0.43
1:0:2097:G:N2	1:0:2098:C:H1'	2.34	0.43
1:0:2103:A:H2'	1:0:2104:C:H5'	2.01	0.43
13:L:3:LYS:NZ	39:L:3752:HOH:O	2.51	0.43
27:Z:78:ILE:HD12	39:Z:3477:HOH:O	2.16	0.43
1:0:1102:C:O5'	1:0:1102:C:H6	2.02	0.43
1:0:1162:G:N2	1:0:1185:U:C2	2.87	0.43
1:0:1397:C:H1'	17:P:28:GLN:OE1	2.18	0.43
1:0:1444:G:H5''	20:S:11:THR:HG22	2.00	0.43
1:0:1742:A:H61	1:0:2037:C:H42	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1815:A:H8	1:0:1815:A:O5'	2.01	0.43
1:0:1924:A:H8	1:0:1924:A:O5'	2.01	0.43
1:0:2591:C:H2'	1:0:2592:G:H5'	2.01	0.43
1:0:2635:A:C2'	1:0:2636:C:H5'	2.48	0.43
1:0:2686:C:H2'	1:0:2687:G:C8	2.54	0.43
1:0:2781:U:H2'	1:0:2782:G:C5'	2.47	0.43
2:A:178:LYS:NZ	39:A:4437:HOH:O	2.50	0.43
31:9:59:C:H1'	39:9:2772:HOH:O	2.18	0.43
1:0:120:A:C6	28:1:17:THR:HG21	2.53	0.43
1:0:453:A:H4'	1:0:455:A:N7	2.33	0.43
1:0:661:G:C5	1:0:662:U:C4	3.07	0.43
1:0:961:A:H4'	39:0:6342:HOH:O	2.17	0.43
1:0:1118:A:C8	1:0:1118:A:C3'	2.87	0.43
1:0:1274:A:C6	1:0:1275:C:C4	3.07	0.43
1:0:1399:A:H2'	1:0:1400:C:C6	2.54	0.43
1:0:1594:C:C2	1:0:1601:G:N2	2.86	0.43
1:0:2038:A:C2	1:0:2039:A:C5	3.07	0.43
1:0:2642:G:C6	1:0:2643:G:C5	3.06	0.43
1:0:2738:G:H2'	1:0:2739:A:H8	1.84	0.43
1:0:2835:C:H42	1:0:2845:G:H1	1.65	0.43
1:0:2846:C:H2'	1:0:2847:G:H8	1.82	0.43
1:0:2882:G:H8	1:0:2882:G:O5'	2.01	0.43
39:0:3707:HOH:O	2:A:11:ARG:HD3	2.18	0.43
17:P:55:LYS:HG2	17:P:56:GLY:N	2.34	0.43
1:0:217:C:H2'	1:0:218:C:C6	2.54	0.43
1:0:464:G:HO2'	1:0:465:U:P	2.40	0.43
1:0:465:U:C5	1:0:475:G:N2	2.87	0.43
1:0:594:C:C4	1:0:595:U:N3	2.86	0.43
1:0:603:A:H5''	1:0:604:G:OP1	2.19	0.43
1:0:656:G:H1'	39:0:7042:HOH:O	2.18	0.43
1:0:865:G:O2'	1:0:866:U:H5'	2.19	0.43
1:0:1118:A:C8	1:0:1119:G:H5''	2.54	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
1:0:1730:G:H5'	1:0:1731:C:C5	2.54	0.43
1:0:2297:U:C2	1:0:2298:C:C6	3.07	0.43
1:0:2441:U:H4'	13:L:53:ARG:HD2	2.01	0.43
1:0:2699:A:H2'	1:0:2700:G:O4'	2.18	0.43
3:B:62:ARG:HA	3:B:65:MET:HE3	2.00	0.43
14:M:99:ARG:HD2	14:M:167:GLY:HA2	2.01	0.43
1:0:24:G:O2'	1:0:25:A:OP2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:287:C:H3'	1:0:287:C:C6	2.54	0.43
1:0:458:G:H2'	1:0:459:A:C8	2.54	0.43
1:0:541:C:O2'	1:0:542:A:H5''	2.17	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
1:0:1130:U:O2'	31:9:91:C:H4'	2.18	0.43
1:0:1361:C:H2'	1:0:1362:U:H6	1.83	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
1:0:2329:C:O2'	1:0:2330:U:H5'	2.19	0.43
1:0:2768:A:H5''	39:0:3093:HOH:O	2.19	0.43
39:0:3308:HOH:O	31:9:105:A:H5''	2.19	0.43
3:B:238:ASN:HD22	3:B:240:GLY:H	1.66	0.43
20:S:73:ASP:O	20:S:77:VAL:HG23	2.18	0.43
1:0:48:A:C5	1:0:113:A:C2	3.07	0.42
1:0:295:C:H2'	1:0:296:G:O4'	2.18	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
1:0:812:A:C2	1:0:813:C:C2	3.07	0.42
1:0:1185:U:H5'	39:0:7308:HOH:O	2.18	0.42
1:0:1314:U:H2'	39:0:5081:HOH:O	2.18	0.42
1:0:1849:G:H1'	1:0:2011:A:N1	2.34	0.42
1:0:1970:G:H2'	1:0:1970:G:N3	2.34	0.42
1:0:2326:C:H4'	1:0:2412:G:C4'	2.49	0.42
1:0:2383:G:C6	1:0:2384:U:C4	3.07	0.42
1:0:2577:A:H5'	39:0:7700:HOH:O	2.19	0.42
1:0:2716:G:O2'	1:0:2717:C:H5'	2.19	0.42
1:0:2795:C:H1'	39:0:8323:HOH:O	2.19	0.42
2:A:70:ALA:HA	2:A:71:PRO:HD3	1.84	0.42
6:E:112:ALA:HA	6:E:113:PRO:HD3	1.89	0.42
1:0:292:G:H2'	1:0:358:G:N2	2.34	0.42
1:0:313:U:H2'	1:0:314:G:H5'	2.00	0.42
1:0:453:A:H5''	39:0:7136:HOH:O	2.20	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
1:0:1163:G:H1	1:0:1184:C:N4	2.16	0.42
1:0:1350:U:H4'	39:0:4055:HOH:O	2.19	0.42
1:0:1585:C:N3	1:0:1611:G:C2	2.87	0.42
1:0:1698:U:H5	39:0:7522:HOH:O	2.02	0.42
1:0:1965:C:H2'	1:0:1966:U:C6	2.54	0.42
1:0:2103:A:HO2'	1:0:2104:C:P	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2791:U:O5'	1:0:2791:U:H6	2.02	0.42
1:0:256:C:H2'	1:0:257:G:H5'	2.00	0.42
1:0:324:G:C2	1:0:325:U:C6	3.07	0.42
1:0:372:A:H2'	1:0:373:G:H8	1.83	0.42
1:0:840:U:C5	1:0:2648:U:C5	3.07	0.42
1:0:889:C:H2'	1:0:890:C:C6	2.54	0.42
1:0:908:A:O2'	1:0:909:U:H5'	2.19	0.42
1:0:1014:A:C6	1:0:1015:C:H1'	2.54	0.42
1:0:1206:U:H2'	1:0:1207:A:O4'	2.20	0.42
1:0:1307:A:O5'	1:0:1307:A:H8	2.02	0.42
1:0:1379:A:H1'	39:0:5427:HOH:O	2.19	0.42
1:0:1535:G:H2'	1:0:1536:C:C6	2.54	0.42
1:0:1632:A:C3'	1:0:1633:C:H5'	2.49	0.42
1:0:1779:A:H2'	1:0:1780:G:O4'	2.19	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
37:0:9101:MUL:C10	37:0:9101:MUL:C14	2.97	0.42
14:M:68:ARG:NE	14:M:73:ARG:HH11	2.16	0.42
16:O:32:ARG:HH21	16:O:35:LYS:HZ2	1.67	0.42
31:9:36:C:C5	31:9:37:C:C4	3.07	0.42
1:0:308:U:C2'	21:T:52:ARG:NH2	2.79	0.42
1:0:801:U:O2'	1:0:802:G:H5'	2.19	0.42
1:0:946:C:H2'	1:0:947:U:C6	2.54	0.42
1:0:1338:U:O2'	1:0:1339:G:H5'	2.20	0.42
1:0:1441:G:H2'	1:0:1442:A:H8	1.82	0.42
1:0:1593:C:H2'	1:0:1594:C:C6	2.47	0.42
1:0:1676:G:C6	1:0:1677:U:N3	2.84	0.42
1:0:1755:A:H2'	1:0:1756:G:O4'	2.20	0.42
1:0:1935:C:H2'	1:0:1936:C:C6	2.54	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
1:0:64:G:H2'	1:0:65:C:O4'	2.19	0.42
1:0:217:C:OP1	1:0:395:A:O2'	2.26	0.42
1:0:338:C:H4'	4:C:174:ILE:HD11	2.01	0.42
1:0:399:C:H1'	14:M:194:GLY:OXT	2.20	0.42
1:0:784:A:H2'	1:0:785:U:O4'	2.19	0.42
1:0:1082:A:H2'	1:0:1083:C:OP1	2.20	0.42
1:0:1168:C:H5'	10:I:83:GLY:HA3	2.00	0.42
1:0:1687:C:H1'	28:1:8:GLN:O	2.20	0.42
1:0:2072:G:C6	1:0:2533:C:H1'	2.54	0.42
1:0:2414:A:H1'	39:0:3480:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:F:32:GLY:N	39:F:3111:HOH:O	2.51	0.42
1:0:314:G:C2	1:0:317:A:C8	3.07	0.42
1:0:806:A:H2'	1:0:807:A:O4'	2.20	0.42
1:0:946:C:O2'	1:0:947:U:H5'	2.20	0.42
1:0:1069:C:H2'	1:0:1070:A:O4'	2.19	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
1:0:1452:G:H1'	35:0:8803:CL:CL	2.57	0.42
1:0:1617:C:C4	1:0:1643:C:H4'	2.54	0.42
1:0:1918:U:O2	1:0:1920:C:H3'	2.19	0.42
1:0:1947:G:N2	1:0:1966:U:O2	2.52	0.42
1:0:2397:G:H2'	1:0:2398:A:C8	2.52	0.42
1:0:2485:A:H3'	39:0:5048:HOH:O	2.19	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
1:0:170:U:H5'	30:3:48:ASN:ND2	2.27	0.42
1:0:561:G:C2	1:0:562:A:N7	2.88	0.42
1:0:595:U:H3'	1:0:595:U:H6	1.85	0.42
1:0:758:A:H2'	1:0:759:C:O4'	2.20	0.42
1:0:933:C:H4'	1:0:1297:U:H4'	2.00	0.42
1:0:1456:C:H2'	1:0:1457:U:C6	2.54	0.42
1:0:1546:G:H2'	1:0:1547:A:O4'	2.20	0.42
1:0:1692:C:H2'	39:0:6064:HOH:O	2.19	0.42
1:0:1848:G:H4'	39:0:6016:HOH:O	2.20	0.42
1:0:1866:A:N7	1:0:1867:G:H1'	2.35	0.42
1:0:2319:C:H4'	1:0:2322:U:C4	2.55	0.42
1:0:2419:U:H5''	1:0:2420:G:H5'	2.02	0.42
1:0:2583:A:H4'	12:K:43:ARG:O	2.19	0.42
1:0:2715:G:OP1	3:B:16:ARG:NH2	2.53	0.42
1:0:2769:C:H2'	1:0:2770:G:H5'	2.01	0.42
39:0:6217:HOH:O	21:T:38:ARG:NH1	2.51	0.42
15:N:44:ARG:NH1	31:9:4:G:H21	2.17	0.42
1:0:122:C:H5''	39:0:8215:HOH:O	2.19	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
1:0:1079:A:H4'	1:0:2078:U:H5'	2.02	0.42
1:0:1231:A:N1	1:0:2498:C:O2'	2.50	0.42
1:0:1384:C:H5'	25:X:30:MET:HG2	2.02	0.42
1:0:1688:G:C6	1:0:1692:C:C5	3.07	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
1:0:2291:A:N9	1:0:2309:C:H5'	2.35	0.42
1:0:2300:A:H4'	1:0:2301:A:N3	2.34	0.42
1:0:2555:C:O5'	1:0:2555:C:H6	2.03	0.42
6:E:101:GLU:HB2	6:E:116:THR:O	2.20	0.42
31:9:41:C:H2'	31:9:42:C:H6	1.84	0.42
31:9:91:C:H2'	31:9:92:G:O4'	2.19	0.42
1:0:81:G:H5'	21:T:65:VAL:O	2.20	0.42
1:0:187:A:C5'	1:0:188:C:OP2	2.67	0.42
1:0:344:C:H2'	1:0:345:G:O4'	2.19	0.42
1:0:676:C:N4	1:0:677:C:N4	2.68	0.42
1:0:1025:C:H2'	1:0:1026:U:C6	2.55	0.42
1:0:1559:A:C1'	39:0:5067:HOH:O	2.63	0.42
1:0:1847:A:H2'	1:0:1848:G:O4'	2.20	0.42
1:0:2034:U:H4'	39:0:5144:HOH:O	2.20	0.42
1:0:2039:A:H2'	1:0:2040:C:C6	2.54	0.42
1:0:2289:G:C2'	1:0:2290:U:H5'	2.49	0.42
1:0:2591:C:H2'	1:0:2592:G:C5'	2.49	0.42
1:0:2750:G:H2'	1:0:2751:C:H6	1.84	0.42
2:A:100:PRO:HG2	2:A:103:VAL:HG21	2.01	0.42
9:H:32:ALA:H	9:H:69:ARG:NH1	2.17	0.42
30:3:64:LYS:HB3	30:3:65:THR:H	1.61	0.42
31:9:27:C:O5'	31:9:27:C:H6	2.03	0.42
31:9:112:U:H2'	31:9:113:C:H5'	2.01	0.42
1:0:25:A:H1'	1:0:519:A:C2	2.55	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
1:0:137:U:H3'	1:0:139:C:H41	1.85	0.42
1:0:208:C:C6	1:0:208:C:C3'	3.03	0.42
1:0:749:C:O2'	1:0:750:A:H5'	2.20	0.42
1:0:820:G:N7	2:A:171:LYS:HB2	2.35	0.42
1:0:853:C:H2'	1:0:854:G:O4'	2.20	0.42
1:0:1029:U:O2'	1:0:1273:C:OP1	2.37	0.42
1:0:1132:A:N3	1:0:2521:A:O2'	2.50	0.42
1:0:1448:A:N7	1:0:1506:U:C2	2.88	0.42
1:0:1879:U:H1'	39:0:8121:HOH:O	2.20	0.42
1:0:2044:G:H2'	1:0:2045:G:O5'	2.19	0.42
3:B:90:THR:C	3:B:92:TYR:H	2.28	0.42
4:C:22:PHE:HD2	4:C:119:ALA:HB2	1.85	0.42
4:C:118:THR:O	4:C:136:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:10:U:C4	1:0:532:A:N7	2.88	0.41
1:0:325:U:H2'	1:0:326:G:H8	1.85	0.41
1:0:640:G:C5	1:0:641:G:N7	2.88	0.41
1:0:657:G:H2'	1:0:658:C:H6	1.85	0.41
1:0:1001:U:O2'	1:0:1002:G:H5'	2.20	0.41
1:0:1388:U:H2'	1:0:1389:G:O4'	2.20	0.41
1:0:1505:U:H6	1:0:1505:U:H2'	1.76	0.41
1:0:1884:G:O6	2:A:190:ARG:HD2	2.20	0.41
1:0:1969:A:N7	1:0:1970:G:C6	2.88	0.41
1:0:2072:G:H3'	1:0:2073:G:H5''	2.01	0.41
1:0:2543:G:O3'	1:0:2590:U:H5'	2.20	0.41
1:0:397:A:O2'	1:0:417:G:N3	2.49	0.41
1:0:909:U:H5	39:0:6389:HOH:O	2.03	0.41
1:0:939:A:N1	1:0:1027:G:O2'	2.49	0.41
1:0:1262:C:H1'	24:W:120:PRO:CG	2.50	0.41
1:0:1391:G:H21	1:0:1434:A:H5''	1.85	0.41
1:0:1396:C:H1'	17:P:1:THR:O	2.19	0.41
1:0:2042:U:H1'	39:0:7090:HOH:O	2.20	0.41
1:0:2291:A:H2'	1:0:2291:A:N3	2.35	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
9:H:54:VAL:HG13	9:H:162:PRO:HG3	2.01	0.41
13:L:90:ARG:HA	13:L:119:THR:HB	2.01	0.41
1:0:24:G:C2	1:0:518:G:N3	2.88	0.41
1:0:45:A:N6	1:0:147:G:C4	2.89	0.41
1:0:109:U:O2	1:0:109:U:C2'	2.68	0.41
1:0:317:A:C5'	39:0:8405:HOH:O	2.68	0.41
1:0:422:G:C6	1:0:2446:G:C6	3.08	0.41
1:0:689:G:HO2'	1:0:742:G:H1'	1.86	0.41
1:0:913:A:H8	1:0:913:A:O5'	2.03	0.41
1:0:1528:A:H61	1:0:1663:G:H1'	1.85	0.41
1:0:1758:U:O2'	1:0:1759:A:H5'	2.20	0.41
1:0:1833:U:O2'	1:0:1834:C:H5'	2.19	0.41
1:0:1988:C:H2'	1:0:1989:G:O4'	2.20	0.41
1:0:2067:A:C4	1:0:2068:G:C8	3.08	0.41
1:0:2250:G:H2'	1:0:2251:G:C8	2.54	0.41
1:0:2278:U:H5'	39:0:4608:HOH:O	2.20	0.41
1:0:2307:A:H8	1:0:2307:A:O5'	2.03	0.41
1:0:2379:G:H4'	1:0:2380:A:H3'	2.01	0.41
1:0:2486:A:H2	37:0:9101:MUL:C22	2.32	0.41
1:0:2735:U:H2'	1:0:2736:U:H6	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:0:9101:MUL:H131	37:0:9101:MUL:H4	1.78	0.41
2:A:53:ALA:HB1	39:A:1902:HOH:O	2.20	0.41
4:C:228:ALA:HA	4:C:229:PRO:HD3	1.90	0.41
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
19:R:59:PHE:O	19:R:63:ASN:HB3	2.19	0.41
24:W:129:LYS:NZ	31:9:87:U:H2'	2.34	0.41
1:0:182:G:H2'	1:0:183:A:H8	1.86	0.41
1:0:360:A:H2'	1:0:361:C:C6	2.56	0.41
1:0:559:U:H2'	1:0:560:U:O4'	2.20	0.41
1:0:656:G:H1	1:0:749:C:H42	1.67	0.41
1:0:1061:C:H1'	1:0:2283:G:O6	2.21	0.41
1:0:1150:A:H3'	1:0:1151:G:C5'	2.51	0.41
1:0:1649:G:H5'	39:0:6234:HOH:O	2.20	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
1:0:2787:C:H2'	1:0:2788:A:O4'	2.20	0.41
11:J:127:ILE:HG22	35:J:8801:CL:CL	2.57	0.41
1:0:36:C:C2	1:0:447:A:C2	3.09	0.41
1:0:820:G:O2'	1:0:856:G:H4'	2.21	0.41
1:0:871:G:C6	1:0:872:U:C4	3.09	0.41
1:0:1041:U:H4'	1:0:1295:G:H5'	2.03	0.41
1:0:1124:A:H2'	1:0:1124:A:N3	2.34	0.41
1:0:1249:U:H2'	1:0:1250:C:C6	2.55	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
1:0:1788: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
1:0:2035:C:O5'	1:0:2035:C:H6	2.03	0.41
1:0:2059:U:C2	1:0:2060:A:C8	3.08	0.41
31:9:104:A:H2'	31:9:105:A:H5'	2.03	0.41
1:0:39:G:C2	1:0:444:C:O2	2.74	0.41
1:0:786:G:H1'	1:0:1488:U:O2	2.20	0.41
1:0:822:C:O2	1:0:822:C:C2'	2.68	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
1:0:1158:G:O2'	1:0:1159:G:H5'	2.20	0.41
1:0:1521:C:H2'	1:0:1522:A:O4'	2.21	0.41
1:0:1592:G:C5	1:0:1593:C:C4	3.08	0.41
1:0:1625:U:H5''	39:0:5289:HOH:O	2.20	0.41
1:0:2055:A:H4'	39:0:7274:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2361:A:H8	1:0:2361:A:OP2	2.04	0.41
25:X:43:VAL:HG13	25:X:76:ARG:NH1	2.35	0.41
1:0:210:U:H2'	1:0:211:U:H6	1.86	0.41
1:0:217:C:H2'	1:0:218:C:O4'	2.21	0.41
1:0:317:A:H5'	39:0:8405:HOH:O	2.21	0.41
1:0:372:A:O2'	1:0:373:G:H5'	2.20	0.41
1:0:381:G:O2'	1:0:406:G:O6	2.38	0.41
1:0:542:A:H2'	1:0:543:G:O4'	2.20	0.41
1:0:686:A:O2'	1:0:747:G:H4'	2.21	0.41
1:0:1189:A:O2'	1:0:1208:C:H2'	2.20	0.41
1:0:1566:C:H2'	1:0:1567:G:H8	1.84	0.41
1:0:1679:C:O2	1:0:1679:C:H2'	2.21	0.41
1:0:1757:U:H6	1:0:1757:U:O5'	2.04	0.41
1:0:2409:C:O2'	1:0:2410:G:H5'	2.21	0.41
2:A:217:ARG:HG2	2:A:229:ALA:HB2	2.03	0.41
31:9:73:A:H2'	31:9:74:G:O4'	2.20	0.41
1:0:313:U:H2'	1:0:314:G:C5'	2.50	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
1:0:841:A:C8	1:0:843:A:C8	3.08	0.41
1:0:960:G:H4'	39:0:7253:HOH:O	2.19	0.41
1:0:1013:A:H5''	1:0:2302:A:H61	1.86	0.41
1:0:1202:A:C2'	1:0:1203:G:H5'	2.51	0.41
1:0:1283:G:H2'	1:0:1284:G:O4'	2.20	0.41
1:0:1297:U:P	39:0:3033:HOH:O	2.78	0.41
1:0:1355:A:H2'	1:0:1355:A:N3	2.36	0.41
1:0:1359:U:O5'	1:0:1360:C:H5''	2.21	0.41
1:0:1597:A:O4'	17:P:95:GLU:HG2	2.21	0.41
1:0:1597:A:C4	1:0:1598:A:C8	3.09	0.41
1:0:1902:G:N2	1:0:1936:C:C2	2.89	0.41
1:0:2498:C:C2'	1:0:2499:U:H5'	2.50	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
12:K:20:CYS:HB2	12:K:29:LEU:HG	2.03	0.41
15:N:151:ASP:HB3	39:N:3251:HOH:O	2.20	0.41
1:0:57:C:H4'	23:V:34:GLN:HE22	1.84	0.41
1:0:61:G:N1	1:0:86:A:N6	2.69	0.41
1:0:130:C:O2'	1:0:131:A:N7	2.48	0.41
1:0:268:U:C4	1:0:269:G:C6	3.09	0.41
1:0:339:A:N6	39:0:6198:HOH:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:644:G:H1'	39:0:5820:HOH:O	2.21	0.41
1:0:861:A:H1'	1:0:1488:U:O4	2.20	0.41
1:0:871:G:C5	1:0:872:U:C4	3.09	0.41
1:0:876:A:C6	1:0:878:G:C8	3.08	0.41
1:0:918:G:C2	1:0:926:A:C2	3.09	0.41
1:0:959:C:O2	1:0:1005:A:N6	2.54	0.41
1:0:1111:U:H2'	1:0:1112:G:C8	2.55	0.41
1:0:1175:G:H1'	1:0:1193:A:C4	2.56	0.41
1:0:1257:C:O2'	1:0:1258:G:H5'	2.21	0.41
1:0:1299:G:N2	39:0:3448:HOH:O	2.54	0.41
1:0:1338:U:H2'	1:0:1339:G:O4'	2.20	0.41
1:0:1506:U:H6	1:0:1506:U:H5'	1.86	0.41
1:0:1531:U:H1'	1:0:1661:A:C2	2.56	0.41
1:0:1608:G:O2'	1:0:1609:C:H5'	2.21	0.41
1:0:1611:G:C2	1:0:1612:A:N7	2.89	0.41
1:0:1666:C:O2'	1:0:1667:A:C5'	2.69	0.41
1:0:1689:A:OP2	1:0:1689:A:H8	2.04	0.41
1:0:1851:G:O2'	1:0:1852:A:H5'	2.21	0.41
1:0:1881:A:OP1	2:A:199:HIS:HE1	2.04	0.41
1:0:1992:U:C2	1:0:1994:A:OP2	2.73	0.41
1:0:2385:G:C4	1:0:2386:U:C5	3.09	0.41
1:0:2455:A:H2'	1:0:2456:A:O4'	2.21	0.41
1:0:2590:U:H2'	1:0:2591:C:H5'	2.01	0.41
1:0:2624:A:O2'	1:0:2625:C:H5'	2.20	0.41
1:0:2629:C:O2'	1:0:2630:G:H5'	2.21	0.41
1:0:2694:A:C6	1:0:2702:A:C8	3.09	0.41
1:0:2904:U:C5	1:0:2905:A:N7	2.89	0.41
2:A:199:HIS:CD2	2:A:201:PHE:H	2.37	0.41
3:B:120:ASP:OD2	3:B:123:ALA:HB3	2.21	0.41
31:9:49:G:H2'	31:9:50:G:O4'	2.21	0.41
31:9:73:A:C6	31:9:74:G:C6	3.09	0.41
1:0:23:G:H8	1:0:23:G:O5'	2.03	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
1:0:204:A:H2'	1:0:205:U:H5'	2.02	0.41
1:0:334:G:H2'	1:0:335:U:O4'	2.21	0.41
1:0:361:C:H2'	1:0:362:G:C8	2.56	0.41
1:0:426:G:H5''	39:0:7523:HOH:O	2.20	0.41
1:0:545:G:N1	1:0:612:U:O2	2.54	0.41
1:0:629:A:H2'	1:0:630:A:H5'	2.03	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)
1:0:1156:C:H3'	1:0:1156:C:C6	2.56	0.41
1:0:1274:A:N6	1:0:1275:C:N4	2.69	0.41
1:0:1644:C:C4	1:0:1645:U:C5	3.09	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
1:0:2106:C:O5'	1:0:2106:C:H6	2.04	0.41
1:0:2594:C:O2'	1:0:2595:U:H5'	2.21	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
4:C:118:THR:HG23	4:C:231:ARG:O	2.21	0.41
14:M:180:SER:HB3	39:M:3219:HOH:O	2.21	0.41
1:0:285:A:C2	1:0:368:C:H4'	2.56	0.40
1:0:731:U:H6	1:0:731:U:O5'	2.03	0.40
1:0:958:G:H2'	1:0:959:C:C6	2.56	0.40
1:0:1044:C:H5	39:0:6095:HOH:O	2.02	0.40
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
1:0:1521:C:O2'	1:0:1522:A:H5'	2.21	0.40
1:0:1678:A:C4	1:0:1679:C:C6	3.09	0.40
1:0:1703:G:C2	1:0:1716:A:C4	3.09	0.40
1:0:2057:U:H5	39:0:4741:HOH:O	2.04	0.40
1:0:2622:A:H1'	39:0:8784:HOH:O	2.20	0.40
1:0:2765:C:H2'	1:0:2766:A:C8	2.55	0.40
39:0:6384:HOH:O	21:T:53:GLY:HA3	2.22	0.40
2:A:121:ALA:O	2:A:124:VAL:HG22	2.21	0.40
4:C:29:ASP:HB2	16:O:3:THR:HG22	2.03	0.40
5:D:67:ASP:HA	5:D:68:PRO:HD3	1.97	0.40
7:F:2:VAL:HG22	7:F:57:GLU:OE1	2.21	0.40
21:T:1:SER:OG	21:T:2:LYS:N	2.54	0.40
22:U:49:LEU:HD13	22:U:51:TRP:HE1	1.86	0.40
1:0:154:C:C2	1:0:155:C:C5	3.09	0.40
1:0:536:A:H3'	39:0:3958:HOH:O	2.21	0.40
1:0:793:A:H2'	1:0:794:U:O4'	2.20	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
1:0:1572:A:C2	1:0:1573:A:C4	3.10	0.40
1:0:2003:U:H4'	1:0:2004:U:H5	1.86	0.40
1:0:2293:G:H2'	1:0:2294:C:O5'	2.21	0.40
1:0:2321:A:H1'	1:0:2322:U:H2'	2.02	0.40
1:0:2582:G:C2	1:0:2583:A:C8	3.09	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)
1:0:2626:C:H2'	1:0:2627:G:H8	1.86	0.40
1:0:2731:G:O2'	1:0:2732:U:H5'	2.21	0.40
1:0:2757:A:C2'	1:0:2758:G:H5'	2.51	0.40
14:M:84:LYS:HA	30:3:46:ILE:O	2.21	0.40
15:N:48:VAL:CG1	15:N:55:ASP:HB3	2.51	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
1:0:12:U:H2'	1:0:13:G:C5'	2.45	0.40
1:0:35:U:H5'	4:C:47:GLY:O	2.21	0.40
1:0:210:U:H2'	1:0:211:U:C6	2.57	0.40
1:0:489:A:H2'	1:0:490:C:O4'	2.21	0.40
1:0:700:A:H2	16:O:69:VAL:HG23	1.87	0.40
1:0:863:G:N3	1:0:1459:A:H2	2.19	0.40
1:0:1059:G:C8	1:0:2491:G:H4'	2.56	0.40
1:0:1421:C:C2	1:0:1422:U:C5	3.09	0.40
1:0:1448:A:C8	1:0:1506:U:C2	3.09	0.40
1:0:1477:C:C5'	1:0:1868:G:C5'	3.00	0.40
1:0:1704:G:O3'	17:P:59:ARG:NH1	2.55	0.40
1:0:1988:C:H5	39:0:3572:HOH:O	2.04	0.40
1:0:2316:G:O2'	1:0:2462:G:O6	2.38	0.40
1:0:2319:C:C3'	1:0:2320:U:H5''	2.52	0.40
1:0:2505:G:H2'	1:0:2506:A:H5'	2.04	0.40
1:0:2722:G:C2	1:0:2761:A:N1	2.89	0.40
1:0:2768:A:H3'	1:0:2768:A:N3	2.35	0.40
1:0:2807:U:OP2	3:B:28:SER:HB2	2.21	0.40
1:0:2838:A:OP1	3:B:307:ARG:NH2	2.54	0.40
39:0:5466:HOH:O	3:B:254:GLN:HG3	2.20	0.40
3:B:215:VAL:O	3:B:219:GLY:HA2	2.22	0.40
4:C:93:LYS:O	4:C:98:ARG:NH2	2.55	0.40
27:Z:49:ARG:O	27:Z:53:ILE:HG13	2.21	0.40
31:9:110:G:C5	31:9:111:U:C5	3.09	0.40
1:0:187:A:N3	1:0:187:A:H2'	2.37	0.40
1:0:814:G:N1	1:0:815:U:C2	2.90	0.40
1:0:818:A:HO2'	27:Z:37:ARG:HD3	1.86	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
1:0:1513:C:H5'	1:0:1574:C:O2'	2.22	0.40
1:0:1587:U:H2'	1:0:1588:G:O4'	2.21	0.40
1:0:1676:G:C5	1:0:1677:U:N3	2.90	0.40
1:0:1747:A:O3'	1:0:2584:G:H5'	2.21	0.40
1:0:1910:A:C2	1:0:2128:G:N3	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2055:A:H2'	1:0:2056:C:C6	2.56	0.40
1:0:2128:G:H2'	1:0:2129:U:O4'	2.22	0.40
1:0:2294:C:N4	1:0:2314:G:H1	2.19	0.40
1:0:2428:G:C4'	39:0:4707:HOH:O	2.70	0.40
1:0:2439:C:O2'	1:0:2440:C:H5'	2.22	0.40
1:0:2537:G:H5''	1:0:2538:A:C5'	2.51	0.40
1:0:2593:C:O2'	1:0:2594:C:H5'	2.22	0.40
12:K:14:LYS:HB2	12:K:45:PRO:HG2	2.03	0.40
31:9:56:A:C3'	31:9:57:A:H5''	2.52	0.40
1:0:365:G:H2'	1:0:366:U:O4'	2.21	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
1:0:818: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
1:0:1531:U:O2	1:0:1661:A:C2	2.74	0.40
1:0:1574:C:C6	1:0:1575:C:H5	2.40	0.40
1:0:1592:G:O2'	1:0:1593:C:O4'	2.39	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
1:0:1695:G:H1'	28:1:9:GLY:HA3	2.02	0.40
1:0:1812:G:H3'	1:0:1812:G:OP1	2.21	0.40
1:0:1893:C:H2'	1:0:1894:C:H5'	2.03	0.40
1:0:2379:G:H5'	1:0:2381:C:O4'	2.21	0.40
1:0:2468:A:N6	30:3:50:GLY:HA2	2.36	0.40
1:0:2867:G:H2'	1:0:2868:C:C6	2.57	0.40
39:0:4064:HOH:O	24:W:9:GLY:HA3	2.21	0.40
6:E:154:ILE:HD11	6:E:157:LYS:HE2	2.04	0.40
15:N:113:SER:HB3	39:9:5851:HOH:O	2.21	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%)	5	31
3	B	335/337 (99%)	305 (91%)	27 (8%)	3 (1%)	14	47
4	C	244/246 (99%)	223 (91%)	18 (7%)	3 (1%)	10	42
5	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	5	29
6	E	170/172 (99%)	157 (92%)	12 (7%)	1 (1%)	21	56
7	F	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	3	20
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	145 (93%)	10 (6%)	1 (1%)	21	56
10	I	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	8	37
11	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	9	39
12	K	130/132 (98%)	116 (89%)	13 (10%)	1 (1%)	16	50
13	L	141/165 (86%)	128 (91%)	12 (8%)	1 (1%)	18	52
14	M	192/194 (99%)	180 (94%)	7 (4%)	5 (3%)	4	26
15	N	184/186 (99%)	165 (90%)	15 (8%)	4 (2%)	5	29
16	O	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
17	P	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	18	52
18	Q	93/95 (98%)	85 (91%)	6 (6%)	2 (2%)	5	29
19	R	148/150 (99%)	141 (95%)	6 (4%)	1 (1%)	18	52
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%)	9	40
26	Y	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	18	52
27	Z	71/73 (97%)	65 (92%)	4 (6%)	2 (3%)	4	25
28	1	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	6	33
29	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
30	3	90/92 (98%)	75 (83%)	11 (12%)	4 (4%)	2	15
All	All	3705/4172 (89%)	3381 (91%)	277 (8%)	47 (1%)	9	40

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%)	19	52
3	B	282/282 (100%)	256 (91%)	26 (9%)	8	33
4	C	193/193 (100%)	177 (92%)	16 (8%)	10	38
5	D	117/148 (79%)	110 (94%)	7 (6%)	17	50
6	E	152/152 (100%)	139 (91%)	13 (9%)	10	36
7	F	93/93 (100%)	89 (96%)	4 (4%)	26	59
8	G	27/282 (10%)	24 (89%)	3 (11%)	6	25
9	H	134/145 (92%)	122 (91%)	12 (9%)	9	34
10	I	58/58 (100%)	55 (95%)	3 (5%)	21	54
11	J	118/118 (100%)	113 (96%)	5 (4%)	26	60
12	K	106/106 (100%)	97 (92%)	9 (8%)	10	37
13	L	113/127 (89%)	105 (93%)	8 (7%)	13	44
14	M	158/158 (100%)	150 (95%)	8 (5%)	21	54
15	N	149/149 (100%)	133 (89%)	16 (11%)	6	27
16	O	93/93 (100%)	86 (92%)	7 (8%)	12	42
17	P	113/113 (100%)	110 (97%)	3 (3%)	39	68
18	Q	79/79 (100%)	76 (96%)	3 (4%)	29	62
19	R	117/117 (100%)	111 (95%)	6 (5%)	21	54
20	S	71/71 (100%)	69 (97%)	2 (3%)	38	68
21	T	105/105 (100%)	99 (94%)	6 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	U	44/44 (100%)	42 (96%)	2 (4%)	24	58
23	V	51/51 (100%)	46 (90%)	5 (10%)	7	31
24	W	130/130 (100%)	124 (95%)	6 (5%)	24	58
25	X	66/66 (100%)	59 (89%)	7 (11%)	6	27
26	Y	120/120 (100%)	113 (94%)	7 (6%)	18	51
27	Z	60/60 (100%)	57 (95%)	3 (5%)	22	55
28	1	46/46 (100%)	45 (98%)	1 (2%)	45	71
29	2	42/46 (91%)	39 (93%)	3 (7%)	13	44
30	3	79/79 (100%)	72 (91%)	7 (9%)	9	34
All	All	3095/3410 (91%)	2887 (93%)	208 (7%)	15	47

All (208) 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	68	ILE
2	A	108	VAL
2	A	131	HIS
2	A	175	LYS
2	A	179	MET
2	A	184	THR
2	A	217	ARG
3	B	20	THR
3	B	27	ASN
3	B	38	VAL
3	B	49	THR
3	B	71	VAL
3	B	82	VAL
3	B	84	LEU
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

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Mol	Chain	Res	Type
3	B	190	MET
3	B	195	ARG
3	B	220	VAL
3	B	251	VAL
3	B	256	GLN
3	B	265	LEU
3	B	277	GLU
3	B	278	PRO
3	B	285	VAL
3	B	301	VAL
3	B	321	PRO
4	C	1	MET
4	C	17	ASP
4	C	29	ASP
4	C	76	ARG
4	C	81	PRO
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	234	VAL
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	128	LEU
5	D	169	THR
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

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Mol	Chain	Res	Type
6	E	108	LEU
6	E	115	ARG
6	E	133	VAL
6	E	156	ASP
6	E	159	VAL
7	F	12	LEU
7	F	46	GLU
7	F	55	GLN
7	F	91	VAL
8	G	12	ILE
8	G	64	ASN
8	G	65	THR
9	H	26	ILE
9	H	42	ASP
9	H	48	VAL
9	H	62	HIS
9	H	65	LEU
9	H	87	LYS
9	H	122	LYS
9	H	126	THR
9	H	143	VAL
9	H	157	TYR
9	H	169	GLU
9	H	173	GLU
10	I	81	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	130	VAL
12	K	10	GLN
12	K	16	SER
12	K	19	THR
12	K	44	HIS
12	K	62	PRO
12	K	93	ASN
12	K	98	VAL
12	K	109	LEU
12	K	132	VAL
13	L	70	ASP

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Mol	Chain	Res	Type
13	L	80	ASP
13	L	99	GLU
13	L	102	ASP
13	L	104	ASP
13	L	105	TYR
13	L	140	VAL
13	L	145	LEU
14	M	23	LEU
14	M	68	ARG
14	M	73	ARG
14	M	89	THR
14	M	91	ILE
14	M	99	ARG
14	M	164	THR
14	M	180	SER
15	N	2	THR
15	N	22	GLN
15	N	25	ARG
15	N	26	LEU
15	N	43	VAL
15	N	49	THR
15	N	56	ASP
15	N	74	PRO
15	N	93	GLN
15	N	101	VAL
15	N	127	LEU
15	N	135	VAL
15	N	139	TRP
15	N	162	ASP
15	N	177	GLU
15	N	180	LEU
16	O	3	THR
16	O	25	VAL
16	O	36	PRO
16	O	43	VAL
16	O	57	THR
16	O	69	VAL
16	O	87	THR
17	P	16	VAL
17	P	91	LYS
17	P	98	ILE
18	Q	18	PRO

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Mol	Chain	Res	Type
18	Q	21	ARG
18	Q	76	VAL
19	R	13	THR
19	R	52	GLU
19	R	55	GLN
19	R	110	THR
19	R	138	SER
19	R	143	VAL
20	S	44	GLN
20	S	57	THR
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	53	ASP
23	V	6	GLN
23	V	13	PRO
23	V	28	LEU
23	V	49	LEU
23	V	65	ASP
24	W	4	LEU
24	W	35	VAL
24	W	38	THR
24	W	88	THR
24	W	120	PRO
24	W	146	ILE
25	X	44	ASP
25	X	49	ARG
25	X	52	PRO
25	X	72	VAL
25	X	79	GLU
25	X	82	GLU
25	X	88	GLU
26	Y	95	THR
26	Y	117	LEU
26	Y	154	ARG
26	Y	189	ASN
26	Y	200	THR
26	Y	203	VAL

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Mol	Chain	Res	Type
26	Y	219	GLU
27	Z	92	SER
27	Z	102	THR
27	Z	103	VAL
28	1	21	ARG
29	2	18	ASN
29	2	21	VAL
29	2	48	ASP
30	3	3	MET
30	3	15	ASN
30	3	19	GLU
30	3	21	GLU
30	3	49	ASP
30	3	55	VAL
30	3	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	5	GLN
2	A	131	HIS
2	A	151	GLN
2	A	199	HIS
2	A	218	ASN
3	B	55	ASN
3	B	119	HIS
3	B	177	HIS
3	B	238	ASN
3	B	243	ASN
3	B	260	HIS
3	B	320	GLN
3	B	332	ASN
4	C	39	GLN
4	C	73	GLN
4	C	103	ASN
4	C	129	HIS
4	C	151	GLN
4	C	219	ASN
5	D	133	ASN
6	E	55	ASN
6	E	143	GLN
8	G	64	ASN

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Mol	Chain	Res	Type
9	H	40	GLN
9	H	49	GLN
9	H	59	GLN
9	H	95	HIS
9	H	101	ASN
9	H	135	GLN
9	H	142	ASN
10	I	88	GLN
10	I	99	GLN
10	I	106	GLN
11	J	52	GLN
11	J	107	ASN
12	K	10	GLN
12	K	23	ASN
12	K	42	ASN
12	K	76	GLN
12	K	93	ASN
13	L	18	HIS
13	L	41	HIS
13	L	113	GLN
14	M	24	GLN
14	M	52	GLN
14	M	58	GLN
14	M	170	ASN
15	N	107	ASN
16	O	100	GLN
17	P	74	GLN
17	P	88	GLN
17	P	118	GLN
18	Q	27	GLN
18	Q	53	HIS
19	R	27	HIS
19	R	61	GLN
19	R	94	ASN
19	R	98	ASN
19	R	117	HIS
19	R	140	GLN
20	S	9	HIS
20	S	44	GLN
20	S	53	ASN
20	S	55	GLN
21	T	7	GLN

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Mol	Chain	Res	Type
21	T	73	HIS
22	U	39	ASN
23	V	34	GLN
23	V	60	GLN
24	W	14	HIS
24	W	28	HIS
24	W	59	GLN
24	W	110	GLN
24	W	141	HIS
25	X	23	HIS
25	X	36	HIS
26	Y	119	GLN
26	Y	129	ASN
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	37	HIS
29	2	45	ASN
30	3	8	ASN
30	3	15	ASN
30	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	266 (9%)	19 (0%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	283 (9%)	20 (0%)

All (283) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	47	G
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

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Mol	Chain	Res	Type
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
1	0	498	A
1	0	510	U
1	0	511	A

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Mol	Chain	Res	Type
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	645	U
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
1	0	921	G
1	0	923	A

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Mol	Chain	Res	Type
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
1	0	1342	C
1	0	1353	C

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Mol	Chain	Res	Type
1	0	1354	G
1	0	1360	C
1	0	1377	C
1	0	1378	G
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	1668	U
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	1MA	0	628	34,1	21,25,26	0.76	1 (4%)	30,37,40	0.91	2 (6%)
1	PSU	0	2621	1	18,21,22	1.43	2 (11%)	21,30,33	1.35	3 (14%)
1	UR3	0	2619	1	19,22,23	0.52	0	26,32,35	0.69	1 (3%)
1	OMU	0	2587	1	19,22,23	0.37	0	25,31,34	0.40	0
1	OMG	0	2588	1	23,26,27	0.33	0	32,38,41	0.39	0

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	1MA	0	628	34,1	-	2/7/25/26	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/9/27/28	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.50	1.42	1.36
1	0	2621	PSU	C6-C5	2.74	1.38	1.35
1	0	628	1MA	C6-N6	2.54	1.34	1.28

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.41	120.48	118.17
1	0	2621	PSU	C6-N1-C2	-3.10	119.81	122.69
1	0	628	1MA	CM1-N1-C6	2.90	124.64	120.15
1	0	2621	PSU	O2-C2-N1	2.86	125.74	122.79
1	0	628	1MA	N1-C2-N3	2.78	129.29	126.00
1	0	2619	UR3	C4-N3-C2	2.66	126.72	124.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8
1	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	36,36,36	1.49	5 (13%)	55,55,55	2.24	18 (32%)

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	-	-	3/18/79/79	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9101	MUL	C12-C19	-5.48	1.39	1.52
37	0	9101	MUL	C5-C14	-3.04	1.53	1.56
37	0	9101	MUL	C10-C11	-2.66	1.53	1.56
37	0	9101	MUL	C12-C11	-2.51	1.53	1.55
37	0	9101	MUL	C9-C10	-2.24	1.53	1.56

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	MUL	C12-C13-C14	-6.04	112.28	120.20
37	0	9101	MUL	C13-C14-C5	-5.90	109.94	116.28
37	0	9101	MUL	O3-C21-C22	5.48	119.56	110.52
37	0	9101	MUL	C18-C12-C13	5.12	109.33	105.51
37	0	9101	MUL	C14-O3-C21	-3.97	110.79	118.03
37	0	9101	MUL	C2-C1-C9	-3.59	101.13	105.63
37	0	9101	MUL	C1-C2-C3	-3.36	101.70	105.48
37	0	9101	MUL	C6-C5-C14	-3.21	109.95	112.13
37	0	9101	MUL	C17-C10-C11	-3.02	109.77	112.20
37	0	9101	MUL	C9-C4-C5	-2.89	114.05	117.94
37	0	9101	MUL	C4-C9-C10	-2.81	111.91	116.08
37	0	9101	MUL	C8-C9-C4	2.65	111.41	106.82
37	0	9101	MUL	C4-C5-C6	2.56	109.76	106.87
37	0	9101	MUL	C8-C7-C6	-2.52	109.12	112.38
37	0	9101	MUL	C23-S1-C22	-2.22	98.06	101.72
37	0	9101	MUL	C12-C11-C10	-2.21	112.59	114.75
37	0	9101	MUL	C12-C19-C20	-2.15	120.96	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	MUL	O3-C14-C13	2.01	108.76	106.37

There are no chirality outliers.

All (3) torsion outliers are listed below:

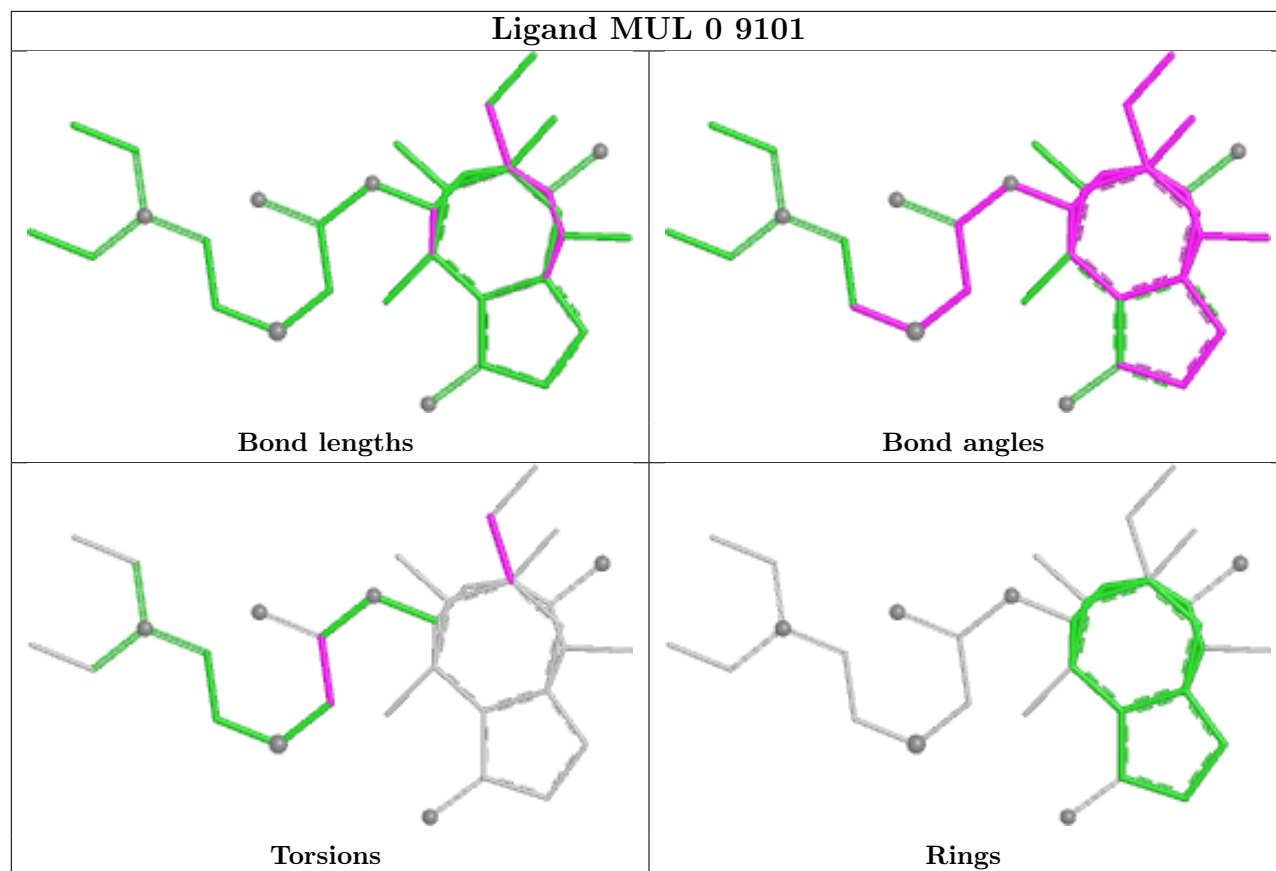
Mol	Chain	Res	Type	Atoms
37	0	9101	MUL	C13-C12-C19-C20
37	0	9101	MUL	O4-C21-C22-S1
37	0	9101	MUL	O3-C21-C22-S1

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2923 (94%)	-0.56	5 (0%) 91 85	29, 74, 140, 200	0
2	A	237/237 (100%)	0.20	4 (1%) 69 49	43, 97, 143, 167	0
3	B	337/337 (100%)	0.19	7 (2%) 63 43	40, 86, 129, 148	0
4	C	246/246 (100%)	0.04	4 (1%) 70 51	41, 72, 103, 112	0
5	D	140/177 (79%)	1.04	26 (18%) 3 3	118, 160, 184, 191	0
6	E	172/172 (100%)	0.30	6 (3%) 47 29	76, 104, 134, 146	0
7	F	119/119 (100%)	0.32	6 (5%) 34 22	74, 113, 153, 166	0
8	G	29/348 (8%)	0.48	1 (3%) 48 30	118, 140, 146, 150	0
9	H	160/177 (90%)	0.31	9 (5%) 30 19	77, 104, 146, 162	0
10	I	70/70 (100%)	1.11	7 (10%) 12 8	173, 199, 200, 200	0
11	J	142/142 (100%)	0.15	3 (2%) 63 43	55, 80, 104, 123	0
12	K	132/132 (100%)	0.09	1 (0%) 82 67	54, 79, 112, 118	0
13	L	145/165 (87%)	0.73	18 (12%) 8 6	62, 121, 171, 175	0
14	M	194/194 (100%)	0.55	26 (13%) 7 6	49, 70, 145, 160	0
15	N	186/186 (100%)	0.48	10 (5%) 31 20	82, 118, 178, 187	0
16	O	115/115 (100%)	0.22	0 100 100	66, 87, 105, 111	0
17	P	143/143 (100%)	0.37	5 (3%) 47 29	65, 88, 117, 124	0
18	Q	95/95 (100%)	0.25	3 (3%) 50 31	67, 87, 110, 117	0
19	R	150/150 (100%)	-0.12	0 100 100	47, 72, 103, 112	0
20	S	81/81 (100%)	0.26	2 (2%) 58 39	68, 93, 114, 130	0
21	T	119/119 (100%)	0.36	4 (3%) 48 30	69, 92, 136, 155	0
22	U	53/53 (100%)	0.16	0 100 100	94, 114, 136, 145	0
23	V	65/65 (100%)	0.49	6 (9%) 14 9	79, 112, 164, 170	0
24	W	154/154 (100%)	0.25	5 (3%) 50 31	56, 78, 110, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/82 (100%)	0.23	5 (6%) 27 17	63, 92, 125, 135	0
26	Y	142/142 (100%)	0.02	4 (2%) 55 35	45, 73, 109, 134	0
27	Z	73/73 (100%)	1.78	20 (27%) 1 1	149, 179, 191, 194	0
28	1	56/56 (100%)	-0.11	0 100 100	42, 53, 66, 76	0
29	2	46/50 (92%)	0.69	5 (10%) 10 7	48, 95, 145, 146	0
30	3	92/92 (100%)	2.23	39 (42%) 0 1	163, 185, 199, 200	0
31	9	122/122 (100%)	-0.32	0 100 100	66, 114, 143, 191	0
All	All	6646/7217 (92%)	-0.02	231 (3%) 47 29	29, 85, 168, 200	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	3	35	TRP	9.5
27	Z	35	SER	9.5
27	Z	40	ALA	9.3
14	M	80	GLY	9.2
30	3	38	ARG	8.8
14	M	70	GLY	8.7
27	Z	36	GLY	8.4
30	3	83	TRP	7.8
14	M	78	LYS	7.6
30	3	39	GLN	7.4
30	3	36	ILE	7.1
5	D	18	ILE	6.1
30	3	82	GLY	6.0
27	Z	50	VAL	5.9
30	3	79	LEU	5.8
30	3	34	LYS	5.7
30	3	84	ARG	5.7
5	D	142	ALA	5.5
30	3	46	ILE	5.4
14	M	79	ALA	5.3
30	3	51	LYS	5.2
10	I	128	THR	5.1
27	Z	46	SER	5.1
5	D	134	LEU	5.1
14	M	89	THR	4.9
14	M	85	ARG	4.9
30	3	81	GLU	4.8
27	Z	42	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
30	3	7	PHE	4.6
30	3	60	LYS	4.5
17	P	118	GLN	4.5
14	M	88	VAL	4.4
5	D	88	LEU	4.4
27	Z	34	SER	4.3
27	Z	43	GLY	4.3
15	N	119	GLN	4.3
14	M	74	LYS	4.3
13	L	7	GLN	4.2
30	3	55	VAL	4.1
21	T	40	VAL	4.1
5	D	135	VAL	4.0
13	L	50	GLY	4.0
14	M	175	GLY	4.0
14	M	71	SER	4.0
13	L	48	LYS	3.9
30	3	41	GLU	3.8
3	B	99	GLU	3.8
5	D	146	LYS	3.8
27	Z	53	ILE	3.7
17	P	114	LEU	3.7
21	T	42	VAL	3.7
27	Z	45	VAL	3.7
14	M	73	ARG	3.6
30	3	33	MET	3.6
27	Z	38	PHE	3.5
5	D	143	LYS	3.5
29	2	38	LYS	3.5
29	2	48	ASP	3.5
30	3	12	PRO	3.5
5	D	92	GLU	3.5
10	I	117	THR	3.5
30	3	42	ARG	3.5
21	T	119	ALA	3.4
30	3	37	ASP	3.4
9	H	16	ALA	3.4
13	L	9	GLY	3.3
5	D	40	ILE	3.3
14	M	82	ARG	3.3
23	V	34	GLN	3.3
15	N	53	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
27	Z	39	GLY	3.3
15	N	154	LEU	3.3
13	L	49	SER	3.2
24	W	4	LEU	3.2
13	L	4	LYS	3.2
30	3	54	LYS	3.2
30	3	32	GLY	3.2
14	M	174	SER	3.2
20	S	28	VAL	3.2
27	Z	37	ARG	3.2
10	I	127	CYS	3.2
5	D	90	LEU	3.2
5	D	104	PHE	3.1
30	3	52	PHE	3.1
14	M	91	ILE	3.1
30	3	43	ASN	3.1
23	V	31	ARG	3.1
30	3	9	THR	3.1
20	S	60	GLY	3.0
7	F	37	THR	3.0
27	Z	58	ASN	3.0
3	B	204	GLY	3.0
13	L	146	GLY	3.0
24	W	3	ALA	3.0
10	I	70	THR	3.0
30	3	31	THR	3.0
5	D	93	LEU	3.0
4	C	62	GLY	3.0
4	C	61	PHE	3.0
30	3	88	LEU	3.0
30	3	53	SER	3.0
14	M	81	ARG	2.9
27	Z	41	ARG	2.9
23	V	1	THR	2.9
30	3	50	GLY	2.9
2	A	181	ALA	2.9
21	T	112	LEU	2.9
27	Z	54	GLU	2.8
5	D	149	ARG	2.8
5	D	101	THR	2.8
10	I	85	GLY	2.8
26	Y	235	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
5	D	106	PHE	2.7
4	C	63	SER	2.7
3	B	1	PRO	2.7
14	M	75	ARG	2.7
25	X	85	VAL	2.7
11	J	83	ILE	2.7
26	Y	167	GLY	2.7
18	Q	75	ILE	2.6
1	O	298	C	2.6
9	H	171	GLY	2.6
13	L	61	ALA	2.6
9	H	71	SER	2.6
10	I	123	VAL	2.6
27	Z	51	ALA	2.6
14	M	84	LYS	2.5
30	3	63	LYS	2.5
6	E	97	VAL	2.5
10	I	100	VAL	2.5
24	W	16	ASP	2.5
25	X	65	ASN	2.5
5	D	166	ILE	2.5
13	L	38	HIS	2.5
13	L	97	VAL	2.5
3	B	101	TRP	2.5
7	F	49	PHE	2.5
9	H	97	VAL	2.5
18	Q	85	ILE	2.5
12	K	88	VAL	2.5
25	X	10	VAL	2.5
3	B	302	PRO	2.4
7	F	39	SER	2.4
9	H	66	GLU	2.4
2	A	201	PHE	2.4
15	N	136	LEU	2.4
13	L	59	GLU	2.4
14	M	90	ARG	2.4
13	L	36	ASP	2.4
30	3	80	ARG	2.4
15	N	84	THR	2.4
5	D	35	ALA	2.4
15	N	137	ALA	2.4
7	F	47	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
30	3	14	CYS	2.4
5	D	107	GLY	2.3
29	2	35	ARG	2.3
25	X	41	PHE	2.3
5	D	16	PRO	2.3
30	3	45	GLY	2.3
26	Y	168	PHE	2.3
17	P	15	ASP	2.3
14	M	178	LYS	2.3
1	0	1171	A	2.3
6	E	42	VAL	2.3
8	G	63	ARG	2.3
13	L	60	GLU	2.3
9	H	115	GLY	2.3
30	3	67	LEU	2.3
5	D	139	TYR	2.3
2	A	58	VAL	2.3
13	L	37	LYS	2.2
14	M	184	ARG	2.2
24	W	45	VAL	2.2
11	J	70	PHE	2.2
14	M	77	HIS	2.2
6	E	124	VAL	2.2
30	3	48	ASN	2.2
27	Z	78	ILE	2.2
6	E	108	LEU	2.2
14	M	87	GLY	2.2
4	C	246	ARG	2.2
5	D	141	VAL	2.2
13	L	39	GLU	2.2
13	L	148	GLU	2.2
24	W	150	LEU	2.2
18	Q	1	PRO	2.2
14	M	69	LYS	2.2
27	Z	47	ARG	2.2
13	L	106	VAL	2.2
23	V	46	ILE	2.2
23	V	37	GLY	2.2
1	0	1199	A	2.2
1	0	2637	A	2.2
6	E	118	ILE	2.1
17	P	9	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
30	3	3	MET	2.1
11	J	87	LEU	2.1
5	D	25	MET	2.1
30	3	1	MET	2.1
17	P	92	GLU	2.1
5	D	145	ASP	2.1
3	B	128	ILE	2.1
23	V	3	LEU	2.1
14	M	72	ALA	2.1
5	D	165	PHE	2.1
27	Z	97	THR	2.1
5	D	91	ALA	2.1
14	M	35	GLY	2.1
29	2	49	GLU	2.1
30	3	4	PRO	2.1
15	N	97	VAL	2.1
15	N	58	LEU	2.1
9	H	114	ASP	2.1
7	F	91	VAL	2.0
2	A	88	ILE	2.0
14	M	68	ARG	2.0
1	0	243	A	2.0
3	B	161	VAL	2.0
6	E	3	VAL	2.0
13	L	46	LEU	2.0
29	2	37	HIS	2.0
26	Y	166	ALA	2.0
30	3	18	GLN	2.0
7	F	65	GLU	2.0
15	N	115	VAL	2.0
15	N	135	VAL	2.0
5	D	128	LEU	2.0
9	H	76	LEU	2.0
9	H	174	LEU	2.0
25	X	84	ILE	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PSU	0	2621	20/21	0.94	0.08	59,63,65,66	0
1	OMU	0	2587	21/22	0.96	0.08	60,63,64,64	0
1	OMG	0	2588	24/25	0.96	0.07	50,54,58,60	0
1	UR3	0	2619	21/22	0.96	0.07	61,65,71,72	0
1	1MA	0	628	23/24	0.96	0.07	49,56,63,64	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8525	1/1	0.45	0.26	92,92,92,92	0
34	NA	0	8527	1/1	0.53	0.12	60,60,60,60	0
34	NA	0	8574	1/1	0.55	0.34	67,67,67,67	0
36	SR	0	8997	1/1	0.58	0.81	200,200,200,200	0
34	NA	0	8573	1/1	0.59	0.30	92,92,92,92	0
34	NA	0	8568	1/1	0.62	0.14	51,51,51,51	0
36	SR	9	9003	1/1	0.66	0.10	200,200,200,200	0
36	SR	J	8986	1/1	0.67	0.26	200,200,200,200	0
32	MG	0	8082	1/1	0.69	0.17	86,86,86,86	0
34	NA	0	8522	1/1	0.69	0.26	87,87,87,87	0
34	NA	0	8553	1/1	0.70	0.32	81,81,81,81	0
34	NA	0	8564	1/1	0.70	0.18	95,95,95,95	0
36	SR	0	8983	1/1	0.72	0.15	185,185,185,185	0
34	NA	0	8570	1/1	0.72	0.12	65,65,65,65	0
34	NA	0	8537	1/1	0.73	0.11	43,43,43,43	0
36	SR	0	9006	1/1	0.73	0.31	200,200,200,200	0
35	CL	J	8802	1/1	0.73	0.12	100,100,100,100	0
32	MG	B	8042	1/1	0.73	0.16	67,67,67,67	0
34	NA	0	8511	1/1	0.76	0.14	64,64,64,64	0
32	MG	0	8072	1/1	0.77	0.07	37,37,37,37	0
36	SR	0	8976	1/1	0.78	0.25	185,185,185,185	0
34	NA	9	8572	1/1	0.78	0.11	88,88,88,88	0
34	NA	0	8541	1/1	0.78	0.09	46,46,46,46	0
34	NA	0	8502	1/1	0.79	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8938	1/1	0.79	0.10	200,200,200,200	0
32	MG	0	8066	1/1	0.79	0.16	70,70,70,70	0
36	SR	L	8969	1/1	0.79	0.41	198,198,198,198	0
34	NA	0	8557	1/1	0.79	0.22	71,71,71,71	0
36	SR	0	8957	1/1	0.80	0.22	200,200,200,200	0
32	MG	0	8047	1/1	0.80	0.25	70,70,70,70	0
34	NA	0	8566	1/1	0.80	0.19	51,51,51,51	0
34	NA	R	8575	1/1	0.80	0.23	96,96,96,96	0
35	CL	0	8816	1/1	0.81	0.37	86,86,86,86	0
36	SR	0	8951	1/1	0.81	0.10	177,177,177,177	0
35	CL	0	8822	1/1	0.81	0.33	94,94,94,94	0
32	MG	0	8036	1/1	0.81	0.17	82,82,82,82	0
35	CL	N	8807	1/1	0.81	0.19	134,134,134,134	0
34	NA	0	8501	1/1	0.82	0.15	41,41,41,41	0
36	SR	B	8987	1/1	0.82	0.33	200,200,200,200	0
36	SR	0	8977	1/1	0.82	0.08	197,197,197,197	0
32	MG	9	8074	1/1	0.82	0.11	127,127,127,127	0
34	NA	0	8562	1/1	0.82	0.59	85,85,85,85	0
34	NA	0	8518	1/1	0.83	0.21	82,82,82,82	0
36	SR	0	8971	1/1	0.83	0.17	200,200,200,200	0
35	CL	3	8804	1/1	0.83	0.06	96,96,96,96	0
32	MG	0	8038	1/1	0.83	0.08	81,81,81,81	0
34	NA	0	8524	1/1	0.83	0.14	47,47,47,47	0
36	SR	0	8988	1/1	0.83	0.08	181,181,181,181	0
36	SR	0	8920	1/1	0.84	0.18	132,132,132,132	0
36	SR	0	8922	1/1	0.84	0.18	190,190,190,190	0
34	NA	0	8506	1/1	0.84	0.22	105,105,105,105	0
36	SR	0	8947	1/1	0.84	0.13	200,200,200,200	0
34	NA	0	8559	1/1	0.84	0.25	94,94,94,94	0
36	SR	0	9001	1/1	0.84	0.07	189,189,189,189	0
36	SR	0	8955	1/1	0.84	0.13	199,199,199,199	0
34	NA	0	8519	1/1	0.84	0.09	44,44,44,44	0
36	SR	0	8958	1/1	0.84	0.08	150,150,150,150	0
36	SR	0	8967	1/1	0.84	0.13	157,157,157,157	0
34	NA	0	8528	1/1	0.84	0.23	80,80,80,80	0
35	CL	A	8809	1/1	0.85	0.39	96,96,96,96	0
36	SR	0	8942	1/1	0.85	0.12	129,129,129,129	0
34	NA	0	8555	1/1	0.85	0.10	50,50,50,50	0
36	SR	9	8980	1/1	0.85	0.07	192,192,192,192	0
32	MG	0	8073	1/1	0.85	0.40	110,110,110,110	0
36	SR	0	9000	1/1	0.86	0.21	200,200,200,200	0
34	NA	R	8532	1/1	0.86	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8953	1/1	0.86	0.11	185,185,185,185	0
36	SR	A	8930	1/1	0.86	0.16	133,133,133,133	0
32	MG	0	8039	1/1	0.86	0.24	76,76,76,76	0
34	NA	9	8543	1/1	0.86	0.24	57,57,57,57	0
32	MG	0	8090	1/1	0.86	0.10	81,81,81,81	0
36	SR	0	8991	1/1	0.86	0.14	190,190,190,190	0
34	NA	Q	8540	1/1	0.86	0.12	92,92,92,92	0
34	NA	0	8571	1/1	0.87	0.14	89,89,89,89	0
36	SR	0	8916	1/1	0.87	0.11	129,129,129,129	0
36	SR	0	9007	1/1	0.87	0.34	180,180,180,180	0
36	SR	0	8959	1/1	0.87	0.11	194,194,194,194	0
32	MG	0	8037	1/1	0.87	0.33	84,84,84,84	0
36	SR	0	8994	1/1	0.87	0.42	200,200,200,200	0
36	SR	0	8995	1/1	0.87	0.11	128,128,128,128	0
36	SR	3	8999	1/1	0.87	0.18	160,160,160,160	0
35	CL	0	8805	1/1	0.87	0.24	97,97,97,97	0
34	NA	S	8510	1/1	0.87	0.12	69,69,69,69	0
34	NA	0	8523	1/1	0.88	0.12	58,58,58,58	0
34	NA	0	8569	1/1	0.88	0.23	72,72,72,72	0
36	SR	0	9004	1/1	0.88	0.14	200,200,200,200	0
34	NA	0	8544	1/1	0.88	0.12	68,68,68,68	0
32	MG	0	8040	1/1	0.88	0.22	100,100,100,100	0
35	CL	B	8819	1/1	0.88	0.27	68,68,68,68	0
32	MG	0	8085	1/1	0.89	0.24	83,83,83,83	0
34	NA	0	8509	1/1	0.89	0.16	66,66,66,66	0
34	NA	0	8545	1/1	0.89	0.11	40,40,40,40	0
36	SR	A	8993	1/1	0.89	0.06	177,177,177,177	0
35	CL	0	8815	1/1	0.89	0.10	90,90,90,90	0
34	NA	M	8539	1/1	0.89	0.10	34,34,34,34	0
34	NA	0	8530	1/1	0.89	0.20	49,49,49,49	0
34	NA	0	8533	1/1	0.89	0.26	68,68,68,68	0
34	NA	0	8556	1/1	0.89	0.17	95,95,95,95	0
32	MG	0	8063	1/1	0.89	0.18	67,67,67,67	0
34	NA	0	8520	1/1	0.90	0.24	57,57,57,57	0
32	MG	0	8031	1/1	0.90	0.09	71,71,71,71	0
32	MG	0	8029	1/1	0.90	0.17	54,54,54,54	0
36	SR	0	8924	1/1	0.90	0.12	138,138,138,138	0
36	SR	0	8962	1/1	0.90	0.11	155,155,155,155	0
36	SR	0	9002	1/1	0.90	0.09	188,188,188,188	0
36	SR	0	8964	1/1	0.90	0.08	149,149,149,149	0
36	SR	0	8927	1/1	0.90	0.10	172,172,172,172	0
36	SR	0	8933	1/1	0.90	0.10	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8975	1/1	0.90	0.07	158,158,158,158	0
32	MG	0	8044	1/1	0.90	0.08	49,49,49,49	0
32	MG	0	8068	1/1	0.90	0.07	49,49,49,49	0
36	SR	0	8978	1/1	0.90	0.07	130,130,130,130	0
35	CL	L	8810	1/1	0.90	0.11	86,86,86,86	0
36	SR	3	8932	1/1	0.90	0.19	149,149,149,149	0
35	CL	0	8811	1/1	0.90	0.19	99,99,99,99	0
36	SR	0	8989	1/1	0.90	0.17	196,196,196,196	0
32	MG	0	8089	1/1	0.90	0.10	72,72,72,72	0
34	NA	0	8561	1/1	0.91	0.25	73,73,73,73	0
32	MG	0	8092	1/1	0.91	0.06	53,53,53,53	0
36	SR	0	8919	1/1	0.91	0.18	194,194,194,194	0
32	MG	0	8064	1/1	0.91	0.12	48,48,48,48	0
36	SR	0	8979	1/1	0.91	0.07	200,200,200,200	0
34	NA	0	8548	1/1	0.91	0.21	52,52,52,52	0
34	NA	0	8531	1/1	0.91	0.23	42,42,42,42	0
36	SR	B	8950	1/1	0.91	0.13	151,151,151,151	0
32	MG	0	8077	1/1	0.91	0.16	47,47,47,47	0
36	SR	0	8960	1/1	0.91	0.07	174,174,174,174	0
34	NA	0	8535	1/1	0.91	0.20	45,45,45,45	0
34	NA	0	8526	1/1	0.91	0.05	52,52,52,52	0
32	MG	0	8055	1/1	0.91	0.10	67,67,67,67	0
36	SR	0	8998	1/1	0.91	0.35	169,169,169,169	0
36	SR	0	8944	1/1	0.91	0.09	171,171,171,171	0
38	CD	3	8704	1/1	0.91	0.39	176,176,176,176	0
32	MG	0	8080	1/1	0.92	0.08	98,98,98,98	0
32	MG	0	8034	1/1	0.92	0.11	43,43,43,43	0
34	NA	0	8547	1/1	0.92	0.27	81,81,81,81	0
36	SR	0	8974	1/1	0.92	0.15	191,191,191,191	0
32	MG	0	8043	1/1	0.92	0.08	55,55,55,55	0
34	NA	0	8550	1/1	0.92	0.24	98,98,98,98	0
34	NA	0	8551	1/1	0.92	0.20	81,81,81,81	0
34	NA	0	8505	1/1	0.92	0.27	56,56,56,56	0
34	NA	0	8554	1/1	0.92	0.24	71,71,71,71	0
32	MG	A	8051	1/1	0.92	0.11	90,90,90,90	0
32	MG	0	8087	1/1	0.92	0.19	20,20,20,20	0
35	CL	M	8818	1/1	0.92	0.10	73,73,73,73	0
32	MG	2	8060	1/1	0.92	0.05	56,56,56,56	0
34	NA	0	8558	1/1	0.92	0.21	50,50,50,50	0
34	NA	0	8514	1/1	0.92	0.39	61,61,61,61	0
34	NA	0	8560	1/1	0.92	0.12	64,64,64,64	0
34	NA	0	8542	1/1	0.92	0.26	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8563	1/1	0.93	0.30	74,74,74,74	0
34	NA	0	8529	1/1	0.93	0.11	49,49,49,49	0
36	SR	0	8954	1/1	0.93	0.06	122,122,122,122	0
35	CL	0	8814	1/1	0.93	0.42	67,67,67,67	0
36	SR	0	8928	1/1	0.93	0.08	164,164,164,164	0
36	SR	0	8982	1/1	0.93	0.14	200,200,200,200	0
34	NA	0	8508	1/1	0.93	0.18	70,70,70,70	0
36	SR	0	8936	1/1	0.93	0.07	109,109,109,109	0
34	NA	0	8521	1/1	0.93	0.05	34,34,34,34	0
36	SR	0	8939	1/1	0.93	0.11	145,145,145,145	0
36	SR	0	8941	1/1	0.93	0.09	143,143,143,143	0
34	NA	C	8503	1/1	0.93	0.08	39,39,39,39	0
36	SR	0	8996	1/1	0.93	0.11	200,200,200,200	0
36	SR	0	8968	1/1	0.93	0.07	181,181,181,181	0
32	MG	0	8059	1/1	0.93	0.08	40,40,40,40	0
35	CL	0	8803	1/1	0.93	0.08	66,66,66,66	0
36	SR	0	8915	1/1	0.94	0.06	125,125,125,125	0
34	NA	0	8536	1/1	0.94	0.11	72,72,72,72	0
36	SR	0	8917	1/1	0.94	0.09	121,121,121,121	0
32	MG	0	8071	1/1	0.94	0.30	50,50,50,50	0
36	SR	0	8973	1/1	0.94	0.06	134,134,134,134	0
36	SR	0	8945	1/1	0.94	0.08	111,111,111,111	0
36	SR	0	8946	1/1	0.94	0.08	138,138,138,138	0
32	MG	0	8081	1/1	0.94	0.18	104,104,104,104	0
36	SR	0	8949	1/1	0.94	0.07	120,120,120,120	0
32	MG	0	8033	1/1	0.94	0.12	56,56,56,56	0
32	MG	0	8032	1/1	0.94	0.06	64,64,64,64	0
36	SR	0	8926	1/1	0.94	0.07	145,145,145,145	0
34	NA	0	8517	1/1	0.94	0.08	30,30,30,30	0
36	SR	F	9005	1/1	0.94	0.09	154,154,154,154	0
36	SR	H	8972	1/1	0.94	0.12	157,157,157,157	0
36	SR	0	8984	1/1	0.94	0.05	139,139,139,139	0
32	MG	0	8049	1/1	0.94	0.06	61,61,61,61	0
36	SR	0	8931	1/1	0.94	0.06	123,123,123,123	0
34	NA	0	8567	1/1	0.94	0.09	58,58,58,58	0
36	SR	0	8992	1/1	0.94	0.11	149,149,149,149	0
35	CL	R	8806	1/1	0.94	0.06	62,62,62,62	0
38	CD	Z	8703	1/1	0.94	0.23	155,155,155,155	0
32	MG	T	8057	1/1	0.94	0.07	67,67,67,67	0
35	CL	O	8808	1/1	0.95	0.12	98,98,98,98	0
36	SR	0	8935	1/1	0.95	0.06	106,106,106,106	0
36	SR	0	8963	1/1	0.95	0.05	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8056	1/1	0.95	0.07	47,47,47,47	0
36	SR	0	8966	1/1	0.95	0.06	110,110,110,110	0
36	SR	0	8937	1/1	0.95	0.07	108,108,108,108	0
35	CL	0	8812	1/1	0.95	0.13	58,58,58,58	0
36	SR	0	8901	1/1	0.95	0.06	89,89,89,89	0
36	SR	0	8908	1/1	0.95	0.06	109,109,109,109	0
36	SR	0	8910	1/1	0.95	0.07	113,113,113,113	0
34	NA	J	8538	1/1	0.95	0.12	45,45,45,45	0
32	MG	0	8030	1/1	0.95	0.17	60,60,60,60	0
32	MG	Y	8086	1/1	0.95	0.05	55,55,55,55	0
32	MG	0	8061	1/1	0.95	0.10	42,42,42,42	0
32	MG	0	8017	1/1	0.95	0.08	29,29,29,29	0
33	K	0	8402	1/1	0.95	0.09	67,67,67,67	0
36	SR	0	8923	1/1	0.95	0.05	120,120,120,120	0
35	CL	J	8801	1/1	0.95	0.06	90,90,90,90	0
36	SR	0	8985	1/1	0.95	0.06	173,173,173,173	0
34	NA	0	8512	1/1	0.95	0.24	49,49,49,49	0
36	SR	0	8956	1/1	0.95	0.09	178,178,178,178	0
34	NA	0	8513	1/1	0.95	0.38	63,63,63,63	0
37	MUL	0	9101	34/34	0.95	0.14	85,87,104,104	0
32	MG	0	8010	1/1	0.95	0.06	35,35,35,35	0
34	NA	0	8552	1/1	0.95	0.12	68,68,68,68	0
32	MG	0	8091	1/1	0.96	0.04	42,42,42,42	0
32	MG	0	8053	1/1	0.96	0.05	57,57,57,57	0
34	NA	0	8565	1/1	0.96	0.25	106,106,106,106	0
35	CL	0	8813	1/1	0.96	0.07	68,68,68,68	0
34	NA	0	8546	1/1	0.96	0.18	69,69,69,69	0
36	SR	R	8912	1/1	0.96	0.07	106,106,106,106	0
36	SR	1	8913	1/1	0.96	0.05	97,97,97,97	0
36	SR	1	8952	1/1	0.96	0.05	81,81,81,81	0
36	SR	0	8925	1/1	0.96	0.04	105,105,105,105	0
32	MG	0	8079	1/1	0.96	0.10	63,63,63,63	0
34	NA	0	8516	1/1	0.96	0.18	26,26,26,26	0
36	SR	A	8929	1/1	0.96	0.16	157,157,157,157	0
36	SR	0	8965	1/1	0.96	0.07	135,135,135,135	0
32	MG	0	8020	1/1	0.96	0.11	52,52,52,52	0
36	SR	0	8981	1/1	0.96	0.10	151,151,151,151	0
34	NA	0	8549	1/1	0.97	0.23	83,83,83,83	0
35	CL	Y	8820	1/1	0.97	0.05	59,59,59,59	0
32	MG	0	8015	1/1	0.97	0.04	25,25,25,25	0
32	MG	0	8067	1/1	0.97	0.13	42,42,42,42	0
36	SR	0	8907	1/1	0.97	0.06	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8515	1/1	0.97	0.04	45,45,45,45	0
36	SR	0	8970	1/1	0.97	0.06	150,150,150,150	0
36	SR	0	8940	1/1	0.97	0.09	117,117,117,117	0
36	SR	0	8909	1/1	0.97	0.04	89,89,89,89	0
32	MG	0	8048	1/1	0.97	0.08	38,38,38,38	0
36	SR	0	8943	1/1	0.97	0.09	99,99,99,99	0
36	SR	0	8914	1/1	0.97	0.10	130,130,130,130	0
32	MG	0	8069	1/1	0.97	0.09	68,68,68,68	0
34	NA	0	8534	1/1	0.97	0.13	45,45,45,45	0
32	MG	0	8027	1/1	0.97	0.04	30,30,30,30	0
36	SR	0	8948	1/1	0.97	0.05	104,104,104,104	0
35	CL	0	8817	1/1	0.97	0.07	63,63,63,63	0
32	MG	0	8062	1/1	0.97	0.15	47,47,47,47	0
36	SR	S	8961	1/1	0.97	0.04	127,127,127,127	0
36	SR	0	8921	1/1	0.97	0.04	90,90,90,90	0
32	MG	0	8014	1/1	0.97	0.07	30,30,30,30	0
32	MG	0	8076	1/1	0.97	0.05	36,36,36,36	0
32	MG	0	8046	1/1	0.97	0.08	48,48,48,48	0
34	NA	0	8507	1/1	0.97	0.09	39,39,39,39	0
32	MG	0	8093	1/1	0.97	0.04	40,40,40,40	0
32	MG	0	8078	1/1	0.97	0.08	64,64,64,64	0
32	MG	0	8065	1/1	0.97	0.06	41,41,41,41	0
32	MG	K	8054	1/1	0.97	0.03	32,32,32,32	0
32	MG	0	8023	1/1	0.98	0.05	21,21,21,21	0
32	MG	0	8035	1/1	0.98	0.07	47,47,47,47	0
35	CL	J	8821	1/1	0.98	0.07	70,70,70,70	0
32	MG	0	8052	1/1	0.98	0.03	40,40,40,40	0
32	MG	0	8070	1/1	0.98	0.05	54,54,54,54	0
32	MG	0	8024	1/1	0.98	0.07	58,58,58,58	0
32	MG	0	8025	1/1	0.98	0.05	44,44,44,44	0
32	MG	0	8026	1/1	0.98	0.04	32,32,32,32	0
32	MG	A	8050	1/1	0.98	0.04	52,52,52,52	0
32	MG	0	8075	1/1	0.98	0.03	40,40,40,40	0
32	MG	0	8006	1/1	0.98	0.05	62,62,62,62	0
36	SR	0	8902	1/1	0.98	0.03	63,63,63,63	0
36	SR	0	8903	1/1	0.98	0.10	62,62,62,62	0
36	SR	0	8905	1/1	0.98	0.10	70,70,70,70	0
36	SR	0	8990	1/1	0.98	0.06	111,111,111,111	0
36	SR	0	8906	1/1	0.98	0.04	65,65,65,65	0
32	MG	0	8016	1/1	0.98	0.06	38,38,38,38	0
32	MG	0	8041	1/1	0.98	0.03	27,27,27,27	0
32	MG	0	8004	1/1	0.98	0.06	32,32,32,32	0

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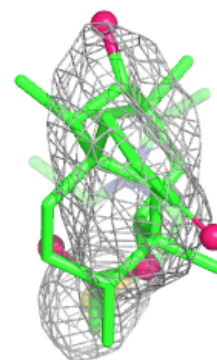
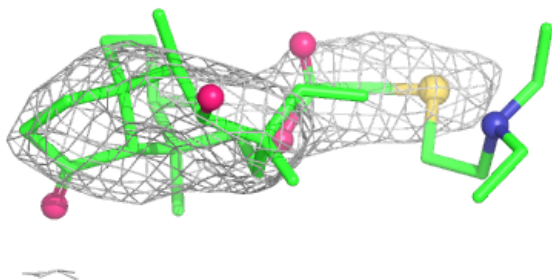
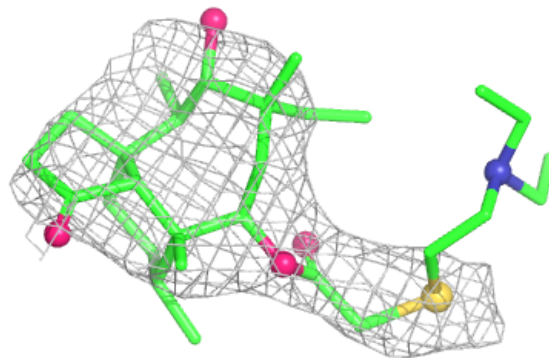
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8018	1/1	0.98	0.04	42,42,42,42	0
36	SR	0	8911	1/1	0.98	0.04	109,109,109,109	0
32	MG	0	8005	1/1	0.98	0.15	30,30,30,30	0
38	CD	O	8705	1/1	0.98	0.12	115,115,115,115	0
32	MG	0	8022	1/1	0.98	0.05	29,29,29,29	0
32	MG	0	8084	1/1	0.98	0.12	50,50,50,50	0
32	MG	C	8012	1/1	0.99	0.03	19,19,19,19	0
32	MG	0	8001	1/1	0.99	0.03	28,28,28,28	0
32	MG	0	8013	1/1	0.99	0.03	21,21,21,21	0
36	SR	0	8934	1/1	0.99	0.04	114,114,114,114	0
32	MG	0	8002	1/1	0.99	0.05	26,26,26,26	0
32	MG	0	8088	1/1	0.99	0.04	39,39,39,39	0
32	MG	0	8003	1/1	0.99	0.05	31,31,31,31	0
36	SR	0	8918	1/1	0.99	0.03	84,84,84,84	0
32	MG	0	8007	1/1	0.99	0.02	10,10,10,10	0
32	MG	0	8008	1/1	0.99	0.04	15,15,15,15	0
32	MG	0	8009	1/1	0.99	0.11	28,28,28,28	0
36	SR	0	8904	1/1	0.99	0.03	64,64,64,64	0
34	NA	0	8504	1/1	0.99	0.02	22,22,22,22	0
32	MG	0	8058	1/1	0.99	0.05	25,25,25,25	0
36	SR	0	9008	1/1	0.99	0.04	99,99,99,99	0
32	MG	0	8045	1/1	0.99	0.06	44,44,44,44	0
38	CD	U	8701	1/1	0.99	0.04	104,104,104,104	0
32	MG	0	8028	1/1	0.99	0.03	14,14,14,14	0
38	CD	1	8702	1/1	0.99	0.03	68,68,68,68	0
32	MG	0	8083	1/1	0.99	0.07	59,59,59,59	0
32	MG	0	8019	1/1	1.00	0.02	10,10,10,10	0
32	MG	0	8011	1/1	1.00	0.04	18,18,18,18	0
32	MG	0	8021	1/1	1.00	0.06	28,28,28,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MUL 0 9101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.