



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2021 – 10:32 AM EST

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.17.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.17.1

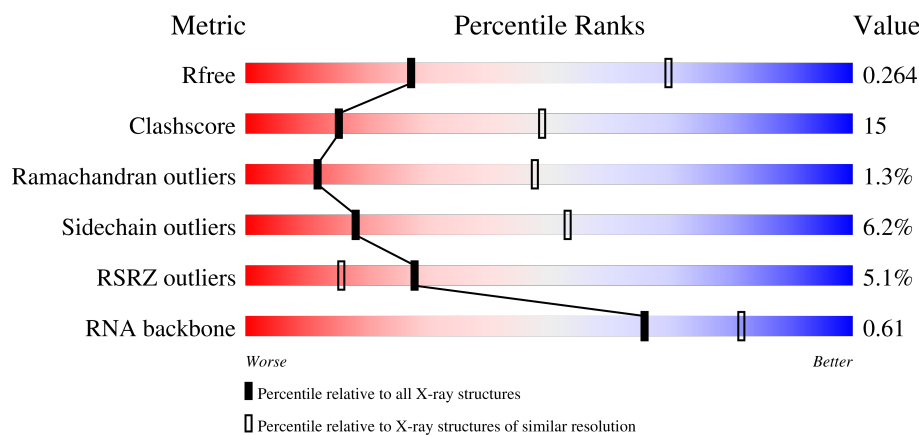
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (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  $\geq 3$ , 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	<div> <div>4%</div> <div>34%</div> <div>53%</div> <div>7%</div> <div>6%</div> </div>
2	A	237	<div> <div>4%</div> <div>83%</div> <div>16%</div> </div>
3	B	337	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
4	C	246	<div> <div>%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>

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

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Mol	Chain	Length	Quality of chain
30	3	92	<div> <div>86%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
31	9	122	<div> <div>25%</div> <div>64%</div> <div>11%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8081	-	-	-	X
32	MG	0	8090	-	-	-	X
34	NA	0	8505	-	-	-	X
34	NA	0	8506	-	-	-	X
34	NA	0	8508	-	-	-	X
34	NA	0	8509	-	-	-	X
34	NA	0	8528	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8564	-	-	-	X
34	NA	0	8566	-	-	-	X
34	NA	0	8568	-	-	-	X
36	SR	0	8922	-	-	-	X
36	SR	0	8947	-	-	-	X
36	SR	0	8994	-	-	-	X
36	SR	0	8997	-	-	-	X
36	SR	0	8998	-	-	-	X
36	SR	B	8987	-	-	-	X
36	SR	J	8986	-	-	-	X

## 2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	84	Total	Mg	0	0
			84	84		
32	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 (three-letter code: K) (formula: K).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	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 (three-letter code: 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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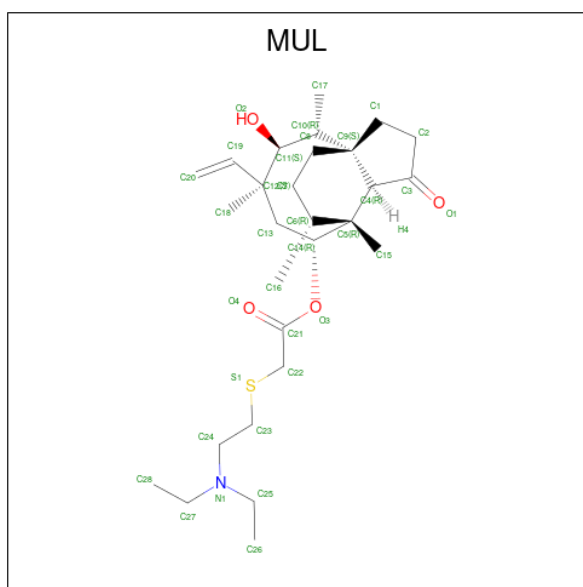
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: 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 (three-letter code: MUL) (formula: C<sub>28</sub>H<sub>47</sub>NO<sub>4</sub>S).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total	Cd	0	0
			1	1		
38	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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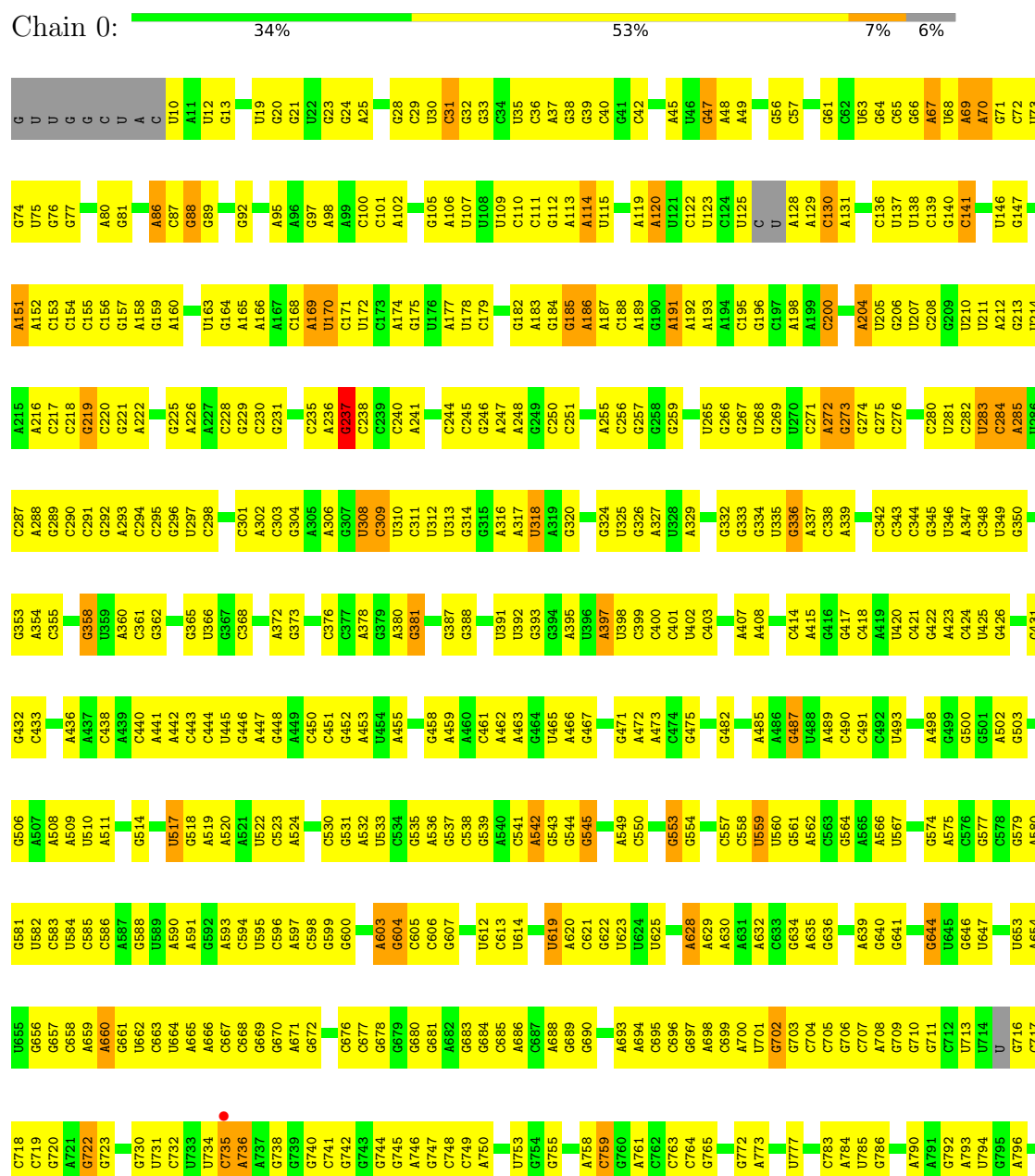
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	22	Total 22	O 22	0	0
39	Y	105	Total 105	O 105	0	0
39	Z	30	Total 30	O 30	0	0
39	1	55	Total 55	O 55	0	0
39	2	48	Total 48	O 48	0	0
39	3	62	Total 62	O 62	0	0
39	9	152	Total 152	O 152	0	0

### 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

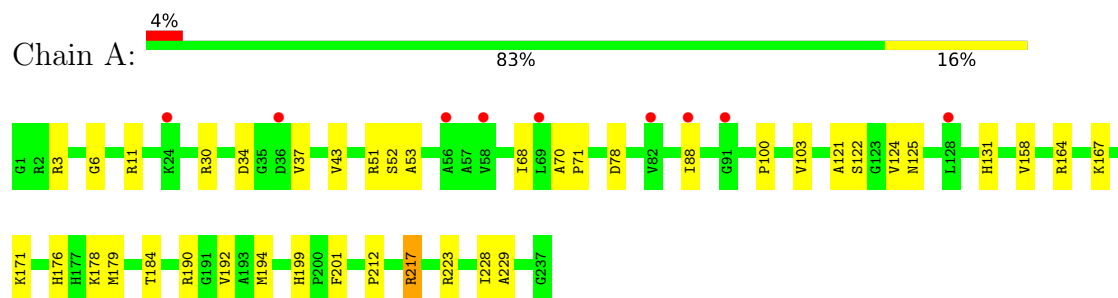


C1818	G1752	C1880	G1608	U1524	C1450	G1376	C1305	C1228	G1159	C1085	A1006	A943	G870	U801
G1819	C1783	G1681	C1609	G1525	C1451	C1377	U1306	C1228	G1160	A1086	A1007	G944	G871	G802
A1820	A1754	A1682	G1610	A1526	G1452	C1378	C1307	C1229	A1161	G1087	C1008	U945	U872	A806
A1821	A1755	G1683	G1611	A1527	G1453	A1379	A1308	A1230	G1162	A1088	U1009	C946	A875	A807
A1822	G1756	A1684	A1612	A1528	U1454	U1383	U1309	U1234	G1163	U1096	C1011	G948	A876	A808
G1823	C1613	A1685	C1613	U1531	C1455	C1384	G1311	U1234	G1164	A1097	A1012	G879	G877	G809
C1824	G1614	C1686	G1614	U1531	C1456	C1384	G1311	U1234	G1165	A1098	A1012	G948	A877	A808
U1825	A1615	A1615	A1615	U1531	C1457	C1384	G1311	U1234	G1166	A1099	A1012	G948	A878	A809
G1826	G1688	A1688	A1616	G1535	U1458	G1387	A1313	C1238	A1166	G1098	A1013	A951	G879	G810
G1827	C1617	A1689	C1617	C1536	G1459	G1388	A1314	C1239	G1167	G1099	A1014	G952	C811	C811
C1828	G1618	C1618	G1618	U1536	G1460	G1389	G1315	A1242	U1169	U1100	U1016	G953	A882	A812
A1829	G1619	U1544	G1619	U1544	U1461	A1390	G1316	C1243	U1170	C1102	G1023	A955	U883	C813
C1830	C1540	U1545	C1620	U1545	C1462	G1391	G1326	U1244	A1171	C1103	G1023	A956	U884	G814
U1831	G1621	G1546	G1621	U1546	U1463	A1392	G1324	C1245	G1172	C1104	G1024	A957	G885	G815
G1832	G1622	A1547	G1622	A1547	C1464	C1396	G1325	A1246	A1173	C1105	G1025	A958	A886	G816
U1833	C1623	U1548	C1623	U1548	A1465	G1397	C1326	U1249	A1174	C1106	U1026	G959	G887	A818
C1834	U1698	C1549	C1624	C1549	A1465	C1396	G1326	U1249	G1175	U1109	U1029	A961	U888	A819
U1835	U1625	C1554	U1625	C1554	U1473	G1398	G1327	C1250	C1176	U1110	U1030	C962	U889	G820
A1838	A1626	G1555	A1626	G1555	C1474	A1399	A1328	C1251	U1111	G1110	U1030	C962	U890	U821
U1839	G1627	G1555	G1627	G1555	G1475	C1400	A1328	A1252	U1112	G1111	U1031	C963	U891	U822
A1840	A1630	G1556	A1630	G1556	U1476	G1401	G1331	C1253	U1113	G1112	A1032	G964	U892	U823
C1841	A1631	G1557	A1631	G1557	C1477	C1401	C1332	C1254	A1181	G1113	U1041	A965	A894	G824
U1844	G1706	C1558	G1706	C1558	U1478	A1407	U1333	C1255	C1182	G1114	G1044	G968	A895	U825
A1845	U1559	A1559	U1559	A1559	C1478	U1408	C1334	C1256	C1183	U1115	G1045	G969	A896	U826
U1846	C1633	U1561	C1633	U1561	C1483	G1409	C1335	C1257	C1184	U1116	G1046	U970	A897	G834
A1847	G1634	G1484	G1634	G1484	G1484	U1412	U1338	C1258	U1185	A1117	G1047	G	G898	U835
U1848	U1635	A1485	U1635	A1485	A1485	G1415	G1339	C1259	U1186	G1118	U1047	U	G899	U836
G1849	U1636	U1486	U1636	U1486	A1486	G1416	C1342	C1260	U1187	G1119	U1047	U	G902	U837
U1850	U1639	U1487	U1639	U1487	U1488	G1416	C1343	C1261	A1189	G1120	C1051	U	G903	U838
A1851	C1640	U1488	C1640	U1488	U1488	U1419	C1344	C1262	G1190	G1121	G1052	U	G904	U839
C1852	A1641	A1492	A1641	A1492	A1493	C1420	G1347	C1268	A1191	A1124	G1053	C	U840	U840
G1853	A1642	A1493	A1642	A1493	A1493	C1421	U1348	C1269	A1192	U1125	G1054	C	A841	A841
C1854	C1643	A1496	C1643	A1496	A1496	U1422	G1349	C1273	A1193	C1126	U1056	C	C842	C842
G1855	U1645	G1497	U1645	G1497	G1497	C1423	G1350	C1274	G1195	C1127	A1057	C	U909	U909
U1856	G1646	G1498	G1646	G1498	G1498	A1424	U1351	C1275	C1196	U1128	U1057	U	C910	C910
A1857	G1647	U1501	G1647	U1501	U1501	U1427	A1352	C1276	U1130	C1129	A1058	C	G911	G911
U1858	G1648	A1502	G1648	A1502	A1502	C1428	C1353	C1277	G1131	G1131	G1059	C	A912	A846
C1859	U1649	C1507	U1649	C1507	C1507	U1429	U1354	C1278	C1201	A1132	C1060	G	A913	C847
A1860	A1656	U1508	A1656	U1508	U1508	G1430	G1355	C1279	C1202	A1133	C1061	A	G848	C848
U1861	A1657	U1509	A1657	U1509	U1509	U1431	U1356	C1280	A1203	G1134	U1066	G	U850	U850
G1862	U1658	U1511	U1658	U1511	U1511	G1432	U1357	C1281	G1204	A1135	A1067	A	C851	C851
A1863	G1665	G1512	G1665	G1512	G1512	C1433	A1358	C1282	U1205	U1136	G1068	G	G920	U852
U1864	G1666	C1513	G1666	C1513	C1513	U1440	U1359	C1283	U1206	G1137	C1069	A	G921	C853
G1865	A1667	U1514	A1667	U1514	U1514	G1441	C1360	C1284	U1207	U1138	C1070	C	A922	G854
U1866	U1668	C1515	U1668	C1515	C1515	U1442	U1361	C1285	A1208	U1139	A1071	G	U855	U855
A1867	G1673	U1516	G1673	U1516	U1516	G1443	U1362	C1286	C1209	G1140	G1072	U	G856	G856
G1868	U1674	A1517	U1674	A1517	A1517	C1439	U1363	C1287	G1210	U1141	A1073	C	A926	A857
U1869	G1675	C1518	G1675	C1518	C1518	U1440	G1364	C1288	G1211	G1074	G1074	G	U927	U858
A1870	A1676	U1519	A1676	U1519	U1519	G1441	C1365	C1289	C1212	G1075	G1075	C	C859	C859
C1871	U1677	G1521	U1677	G1521	C1521	U1442	U1366	C1290	C1213	G1076	G1076	A	U932	U860
U1872	A1678	A1522	A1678	A1522	A1522	G1443	C1367	C1291	G1214	A1150	G1077	C	C933	A861
G1873	C1679	U1523	C1679	U1523	U1523	U1444	U1368	C1292	G1215	G1151	A1078	A	G934	U862
A1874	U1679	G1524	U1679	G1524	G1524	G1445	U1369	C1293	G1216	A1152	C1080	C	G935	G863
U1875	A1680	U1525	A1680	U1525	A1525	U1446	U1370	C1294	U1217	C1153	C1081	C	G936	U864
C1876	U1681	U1526	U1681	U1526	U1526	U1447	A1372	C1295	U1218	G1154	A1082	U	A867	U865
A1877	G1682	A1527	G1682	A1527	A1527	U1448	A1373	C1296	U1219	C1155	C1083	G	G940	G866
U1878	C1683	U1528	C1683	U1528	U1528	U1449	A1374	C1297	U1220	C1156	C1084	U	U942	G867
G1879	U1684	U1529	U1684	U1529	U1529	U1450	A1375	C1298	U1221	G1157	G1084	A	G941	G868
A1880	A1685	U1530	A1685	U1530	U1530	U1451	A1376	C1299	U1222	C1158	G1085	C	U943	U869
C1881	G1686	U1531	G1686	U1531	U1531	U1452	A1377	C1300	U1223	G1159	G1086	A	U944	G890
U1882	A1686	U1532	A1686	U1532	U1532	U1453	A1378	C1301	U1224	G1160	G1087	C	U945	G891
G1883	U1687	U1533	U1687	U1533	U1533	U1454	A1379	C1302	U1225	G1161	G1088	C	U946	G892
C1884	A1687	U1534	C1687	U1534	U1534	U1455	A1380	C1303	U1226	G1162	G1089	C	U947	G893
U1885	G1688	U1535	G1688	U1535	U1535	U1456	A1381	C1304	U1227	G1163	G1090	C	U948	G894
A1886	U1689	U1536	A1689	U1536	U1536	U1457	A1382	C1305	U1228	G1164	G1091	C	U949	G895
C1887	A1689	U1537	C1689	U1537	U1537	U1458	A1383	C1306	U1229	G1165	G1092	C	U950	G896
U1888	G1690	U1538	U1690	U1538	U1538	U1459	A1384	C1307	U1230	G1166	G1093	C	U951	G897
A1889	U1691	U1539	A1691	U1539	U1539	U1460	A1385	C1308	U1231	G1167	G1094	C	U952	G898
C1890	G1692	U1540	C1692	U1540	U1540	U1461	A1386	C1309	U1232	G1168	G1095	C	U953	G899
U1891	A1693	U1541	A1693	U1541	U1541	U1462	A1387	C1310	U1233	G1169	G1096	C	U954	G900
G1892	U1694	U1542	U1694	U1542	U1542	U1463	A1388	C1311	U1234	G1170	G1097	C	U955	G901
C1893	A1695	U1543	C1695	U1543	U1543	U1464	A1389	C1312	U1235	G1171	G1098	C	U956	G902
U1894	G1696	U1544	U1696	U1544	U1544	U1465	A1390	C1313	U1236	G1172	G1099	C	U957	G903
A1895	U1697	U1545	A1697	U1545	U1545	U1466	A1391	C1314	U1237	G1173	G1100	C	U958	G904
C1896	G1698	U1546	C1698	U1546	U1546	U1467	A1392	C1315	U1238	G1174	G1101	C	U959	G905
U1897	A1699	U1547	A1699	U1547	U1547	U1468	A1393	C1316	U1239	G1175	G1102	C	U960	G906
G1898	U1699	U1548	U1699	U1548	U1548	U1469	A1394	C1317	U1240	G1176	G1103	C	U961	G907
A1899	C1699	U1549	C1699	U1549	U1549	U1470	A1395	C1318	U1241	G1177	G1104	C	U962	G908
C1900	G1700	U1550	G1700	U1550	U1550	U1471	A1396	C1319	U1242	G1178	G1105	C	U963	G909
U1901	A1701	U1551	A1701	U1551	U1551	U1472	A1397	C1320	U1243	G1179	G1106	C	U964	G910
G1902	C1702	U1552	C1702	U1552	U1552	U1473	A1398	C1321	U1244	G1180	G1107	C	U965	G911
A1903	U1703	U1553	U1703	U1553	U1553	U1474	A1399	C1322	U1245	G1181	G1108	C	U966	G912
C1904	G1704	U1554	C1704	U1554	U1554	U1475	A1400	C1323	U1246	G1182	G1109	C	U967	G913
U1905	C1705	U1555	C1705	U1555	U1555	U1476	A1401	C1324	U1247	G1183	G1110	C	U968	G914
A1906	U1706	U1556	A1706	U1556	U1556	U1477	A1402	C1325	U1248	G1184	G1111	C	U969	G915
C1907	G1707	U1557	C1707	U1557	U1557	U1478	A1403	C1326	U1249	G1185	G1112	C	U970	G916
U1908	A1708	U1558	A1708	U1558	U1558	U1479	A1404	C1327	U1250	G1186	G1113	C	U971	G917
G1909	C1709	U1559	C1709	U1559	U1559	U1480	A1405	C1328	U1251	G1187	G1114	C	U972	G918
A1910	U1710	U1560												

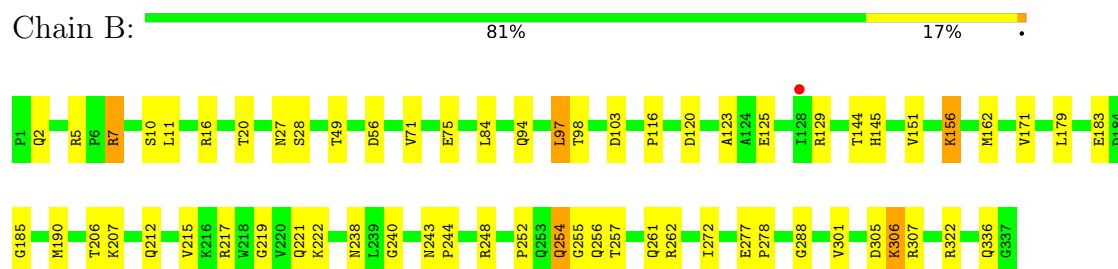




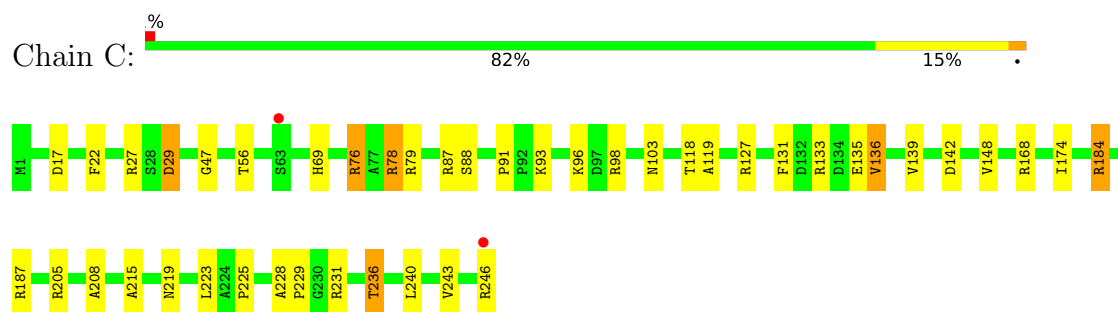
- Molecule 2: 50S ribosomal protein L2P



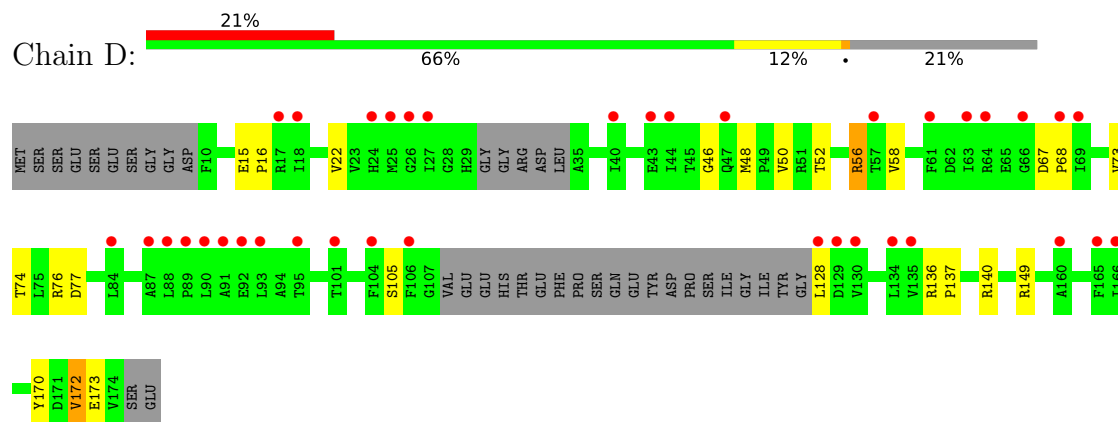
- Molecule 3: 50S ribosomal protein L3P



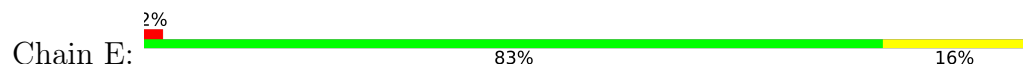
- Molecule 4: 50S ribosomal protein L4P



- Molecule 5: 50S ribosomal protein L5P

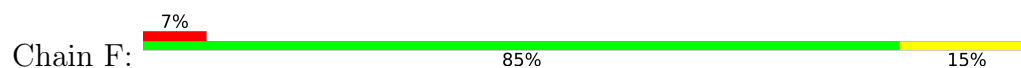


- Molecule 6: 50S ribosomal protein L6P

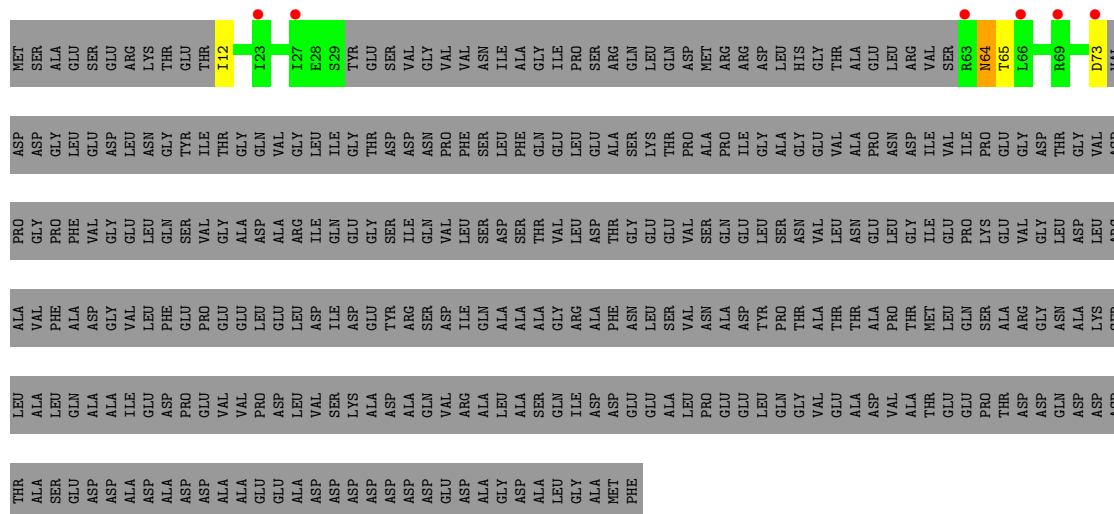




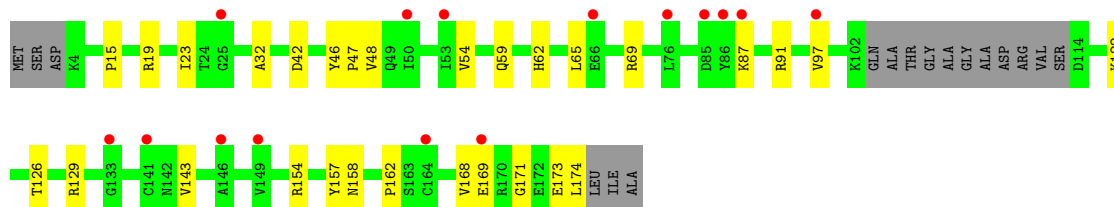
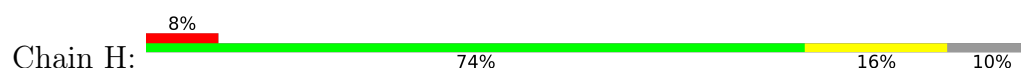
- Molecule 7: 50S ribosomal protein L7Ae



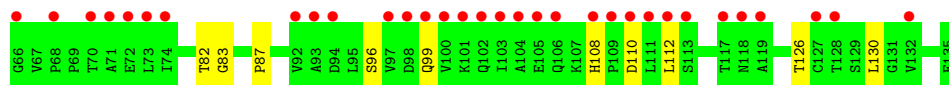
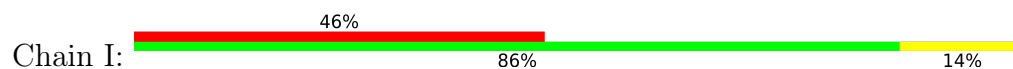
- Molecule 8: 50S ribosomal protein L10




- Molecule 9: 50S ribosomal protein L10e

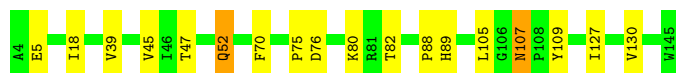


- Molecule 10: 50S ribosomal protein L11P




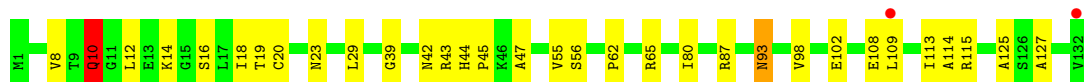
- Molecule 11: 50S ribosomal protein L13P

Chain J:  87% 11% .




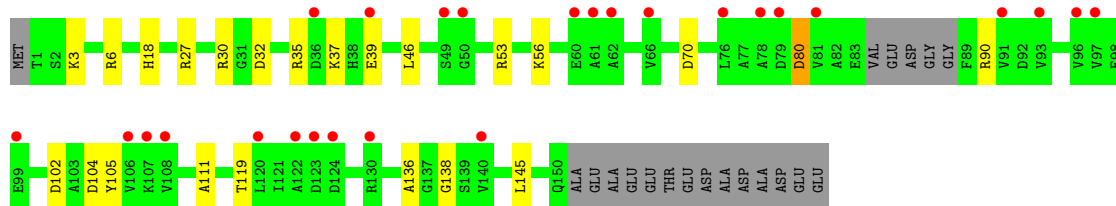
- Molecule 12: 50S ribosomal protein L14P

Chain K:  2% 76% 23% ..




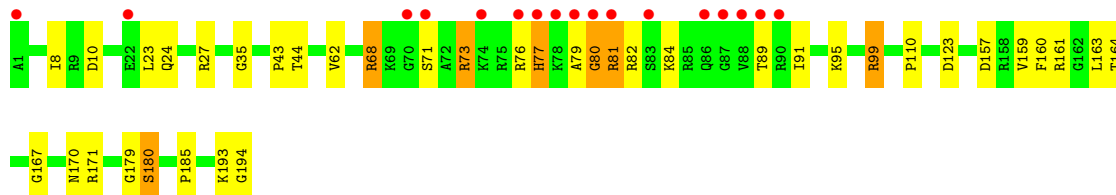
- Molecule 13: 50S ribosomal protein L15P

Chain L:  16% 74% 13% 12% .




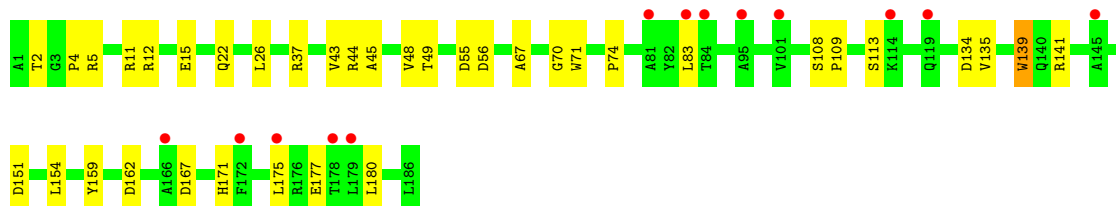
- Molecule 14: 50S ribosomal protein L15e

Chain M:  9% 80% 16% .




- Molecule 15: 50S ribosomal protein L18P

Chain N:  7% 80% 19% .



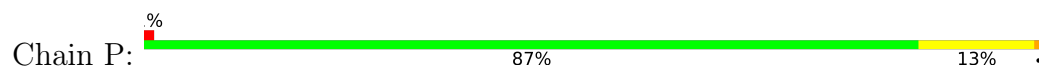
- Molecule 16: 50S ribosomal protein L18e

Chain O:  90% 9% .

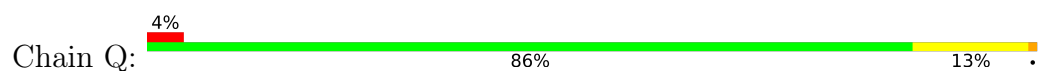




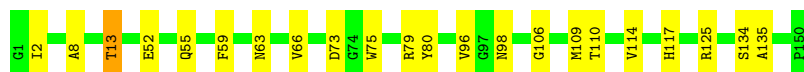
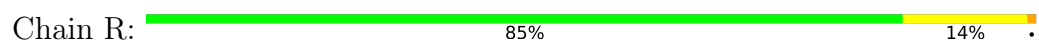
- Molecule 17: 50S ribosomal protein L19e



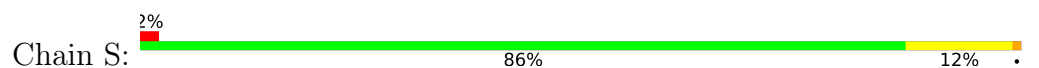
- Molecule 18: 50S ribosomal protein L21e



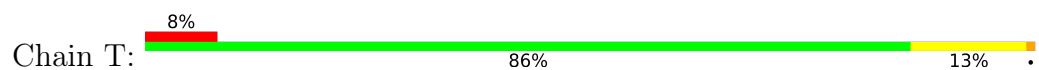
- Molecule 19: 50S ribosomal protein L22P



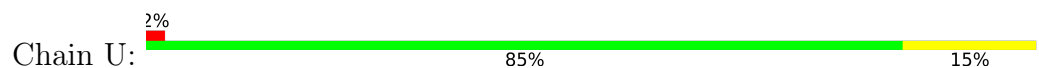
- Molecule 20: 50S ribosomal protein L23P



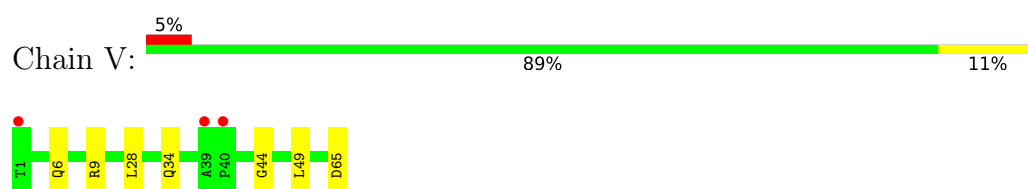
- Molecule 21: 50S ribosomal protein L24P



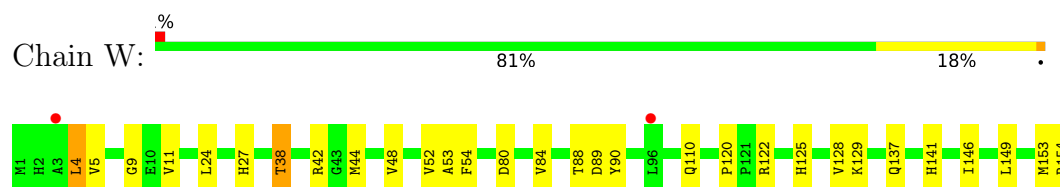
- Molecule 22: 50S ribosomal protein L24e



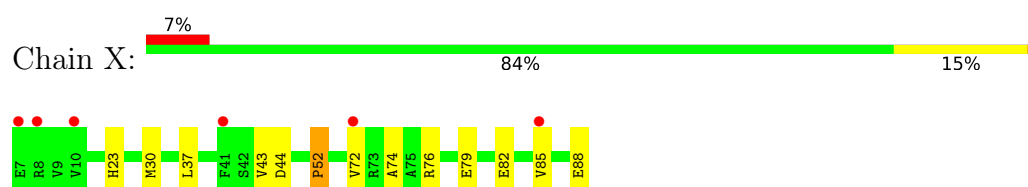
- Molecule 23: 50S ribosomal protein L29P



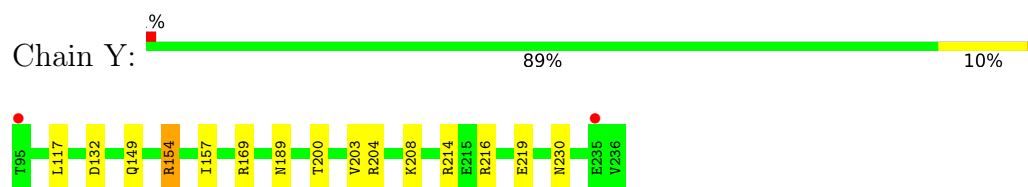
- Molecule 24: 50S ribosomal protein L30P



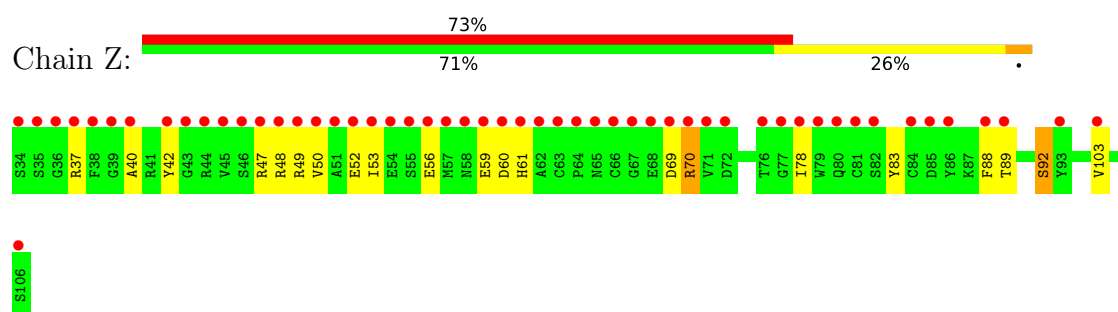
- Molecule 25: 50S ribosomal protein L31e



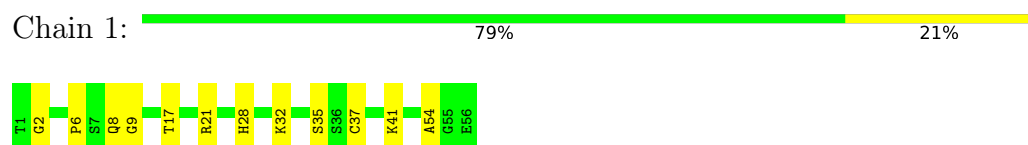
- Molecule 26: 50S ribosomal protein L32e



- Molecule 27: 50S ribosomal protein L37Ae

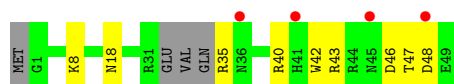


- Molecule 28: 50S ribosomal protein L37e

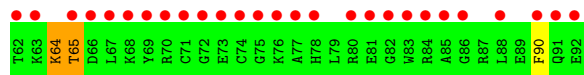
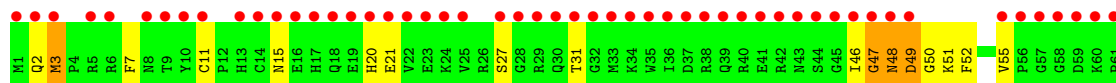
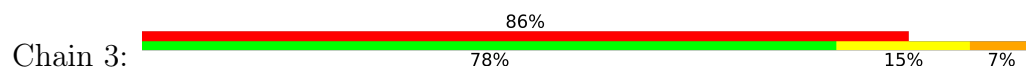


- Molecule 29: 50S ribosomal protein L39e

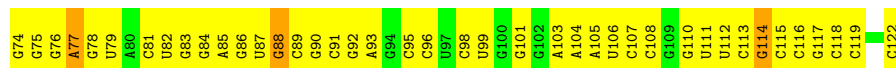




- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 5S ribosomal RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.27Å 299.84Å 574.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.20 85.66 – 2.41	Depositor EDS
% Data completeness (in resolution range)	83.7 (49.84-3.20) 82.8 (85.66-2.41)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.215 , 0.290 0.199 , 0.264	Depositor DCC
$R_{free}$ test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 119.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	87.0	wwPDB-VP

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

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: 1MA, PSU, CL, OMU, MG, K, MUL, SR, OMG, UR3, CD, NA

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

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

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

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

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

There are no chirality outliers.

All (26) planarity outliers are listed below:

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

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

## 5.2 Too-close contacts ⓘ

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:H8	1:0:871:G:H5'	1.00	1.13
1:0:1160:G:H5'	1:0:1161:A:H5'	1.28	1.13
1:0:2121:G:H4'	30:3:47:GLY:HA2	1.29	1.12
1:0:2717:C:H2'	1:0:2718:C:H5''	1.27	1.12
1:0:871:G: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1701:A:H4'	1:0:1702:U:H5''	1.57	0.84
1:0:1455:C: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:110:C:H1'	39:0:6248:HOH:O	1.83	0.78
1:0:2505:G:O2'	1:0:2506:A:H5'	1.84	0.78
1:0:625: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
1:0:1160: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
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:O: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:O: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:O: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:O:4782:HOH:O	1.87	0.73

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1741:U:H5'	1:0:1742:A:OP1	1.91	0.70
1:0:2758:G:H2'	1:0:2759:C:C6	2.26	0.70
1:0:282:C:O2'	1:0:283:U:H5'	1.90	0.70
1:0:671:A:O2'	1:0:672:G:H2'	1.92	0.70
1:0:2312: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
1:0:1205:U:C2'	1:0:1206:U:H5'	2.22	0.69
1:0:1682:A:O2'	1:0:1683:G:H5''	1.93	0.69
1:0:2563:U:HO2'	1:0:2564:G:H8	1.40	0.69
1:0:73: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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2524:G:H21	1:0:2526:C:N4	1.96	0.64
1:0:2898: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:0:2295: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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:1806:G:C6	1:0:1807:U:N3	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:1055: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:2378:U:H4'	39:0:3392:HOH:O	2.04	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
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:2256: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:849:C:H2'	1:0:850:U:O4'	2.07	0.55
1:0:962: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
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
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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:0:1817:U:O2	17:P:81:LYS:NZ	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:0:628:1MA:HM11	39:0:3514:HOH:O	2.10	0.52
1:0:809:G:H2'	1:0:810:G:C8	2.45	0.52
1:0:875: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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:574:G:O2'	1:0:575:A:H5'	2.11	0.50
1:0:2869:G:H2'	1:0:2870:C:C6	2.46	0.50
1:0:313: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:H:59:GLN:HE21	9:H:129:ARG:HE	1.59	0.49
1:0:522:U:O2'	1:0:1366:C:H5'	2.12	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
31:9:78:G:HO2'	31:9:79:U:P	2.36	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
1:0:694: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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:42:C:O5'	1:0:185:G:H5''	2.13	0.48
1:0:553:G:C2'	1:0:554:G:H5'	2.43	0.48
1:0:1174: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:444:C:H2'	1:0:445:U:C6	2.49	0.48
1:0:705: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
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
1:0:1711:A:H2	1:0:1817:U:HO2'	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:290:C:C2'	1:0:291:C:H5'	2.44	0.47
1:0:656: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
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:0:1419: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
1:0:1351:G:OP1	4:C:96:LYS:NZ	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:1278:A:H4'	1:0:1279:U:N3	2.29	0.46
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
1:0:1215: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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:0:676:C:HO2'	4:C:219:ASN:HD22	1.60	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:0:517: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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:A:178:LYS:NZ	39:A:4437:HOH:O	2.50	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
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:0:1181:A:N1	1:0:1192:A:O2'	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:0:730: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
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
1:0:944:G:H21	24:W:44:MET:HE2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:0:465: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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1965:C:H2'	1:0:1966:U:C6	2.54	0.42
1:0:2103:A:HO2'	1:0:2104:C:P	2.41	0.42
1:0:2791:U:O5'	1:0:2791:U:H6	2.02	0.42
24:W:5:VAL:HG11	24:W:153:MET:HE1	2.01	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
19:R:109:MET:HB2	19:R:109:MET:HE3	1.92	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1079:A:H4'	1:0:2078:U:H5'	2.02	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
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
1:0:1448: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
4:C:22:PHE:HD2	4:C:119:ALA:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:118:THR:O	4:C:136:VAL:HG13	2.20	0.42
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
1:0:909:U:H5	39:0:6389:HOH:O	2.03	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
1:0:913: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:472:A:N1	1:0:888:U:O2'	2.43	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
1:0:2361:A:H8	1:0:2361:A:OP2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:542: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
24:W:149:LEU:HG	24:W:153:MET:HE2	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
1:0:644:G:H1'	39:0:5820:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:0:944:G:H21	24:W:44:MET:CE	2.34	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
1:0:1400: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
1:0:2055:A:H2'	1:0:2056:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:K:125:ALA:C	12:K:127:ALA:H	2.25	0.40
15:N:113:SER:HB3	39:9:5851:HOH:O	2.21	0.40

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%)	7	37
3	B	335/337 (99%)	305 (91%)	27 (8%)	3 (1%)	17	56
4	C	244/246 (99%)	223 (91%)	18 (7%)	3 (1%)	13	49
5	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	6	35
6	E	170/172 (99%)	157 (92%)	12 (7%)	1 (1%)	25	64
7	F	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	3	24
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	145 (93%)	10 (6%)	1 (1%)	25	64
10	I	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	10	44
11	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	11	46
12	K	130/132 (98%)	116 (89%)	13 (10%)	1 (1%)	19	58
13	L	141/165 (86%)	128 (91%)	12 (8%)	1 (1%)	22	61
14	M	192/194 (99%)	180 (94%)	7 (4%)	5 (3%)	5	31
15	N	184/186 (99%)	165 (90%)	15 (8%)	4 (2%)	6	35
16	O	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
17	P	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	22	61
18	Q	93/95 (98%)	85 (91%)	6 (6%)	2 (2%)	6	35
19	R	148/150 (99%)	141 (95%)	6 (4%)	1 (1%)	22	61
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%)	12	47
26	Y	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	22	61
27	Z	71/73 (97%)	65 (92%)	4 (6%)	2 (3%)	5	29
28	1	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	8	39
29	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
30	3	90/92 (98%)	75 (83%)	11 (12%)	4 (4%)	2	19
All	All	3705/4172 (89%)	3381 (91%)	277 (8%)	47 (1%)	12	47

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%)	21	57
3	B	282/282 (100%)	263 (93%)	19 (7%)	16	50
4	C	193/193 (100%)	179 (93%)	14 (7%)	14	46
5	D	117/148 (79%)	109 (93%)	8 (7%)	16	49
6	E	152/152 (100%)	139 (91%)	13 (9%)	10	38
7	F	93/93 (100%)	91 (98%)	2 (2%)	52	79
8	G	27/282 (10%)	23 (85%)	4 (15%)	3	14
9	H	134/145 (92%)	121 (90%)	13 (10%)	8	31
10	I	58/58 (100%)	56 (97%)	2 (3%)	37	70
11	J	118/118 (100%)	112 (95%)	6 (5%)	24	60
12	K	106/106 (100%)	99 (93%)	7 (7%)	16	51
13	L	113/127 (89%)	105 (93%)	8 (7%)	14	47
14	M	158/158 (100%)	146 (92%)	12 (8%)	13	45
15	N	149/149 (100%)	135 (91%)	14 (9%)	8	33
16	O	93/93 (100%)	88 (95%)	5 (5%)	22	58
17	P	113/113 (100%)	110 (97%)	3 (3%)	44	75
18	Q	79/79 (100%)	77 (98%)	2 (2%)	47	77
19	R	117/117 (100%)	111 (95%)	6 (5%)	24	60
20	S	71/71 (100%)	68 (96%)	3 (4%)	30	65
21	T	105/105 (100%)	99 (94%)	6 (6%)	20	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	U	44/44 (100%)	40 (91%)	4 (9%)	9	34
23	V	51/51 (100%)	47 (92%)	4 (8%)	12	43
24	W	130/130 (100%)	127 (98%)	3 (2%)	50	78
25	X	66/66 (100%)	60 (91%)	6 (9%)	9	34
26	Y	120/120 (100%)	114 (95%)	6 (5%)	24	60
27	Z	60/60 (100%)	57 (95%)	3 (5%)	24	60
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	42/46 (91%)	39 (93%)	3 (7%)	14	47
30	3	79/79 (100%)	73 (92%)	6 (8%)	13	45
All	All	3095/3410 (91%)	2903 (94%)	192 (6%)	18	53

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

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

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

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

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

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

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

such sidechains are listed below:

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

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

### 5.3.3 RNA ⓘ

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

All (280) RNA backbone outliers are listed below:

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

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

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

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

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

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

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

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

All (20) RNA pucker outliers are listed below:

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

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	OMU	0	2587	1	14,22,23	1.00	1 (7%)	14,31,34	1.17	1 (7%)
1	UR3	0	2619	1	14,22,23	0.77	0	15,32,35	0.62	0
1	OMG	0	2588	1	18,26,27	1.11	2 (11%)	20,38,41	2.59	4 (20%)
1	1MA	0	628	1,34	15,25,26	0.77	0	15,37,40	1.40	1 (6%)
1	PSU	0	2621	1	17,21,22	1.59	3 (17%)	20,30,33	5.45	4 (20%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.09	1.47	1.52
1	0	2588	OMG	C6-N1	3.65	1.39	1.33
1	0	2621	PSU	C4-N3	2.71	1.37	1.33
1	0	2587	OMU	C4-N3	2.41	1.37	1.33
1	0	2588	OMG	C8-N7	-2.22	1.30	1.34
1	0	2621	PSU	C2-N1	2.20	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.32	114.66	128.43
1	0	2621	PSU	C4-N3-C2	14.41	127.31	115.14
1	0	2588	OMG	C5-C6-N1	-8.57	111.72	123.43
1	0	2621	PSU	C5-C4-N3	-8.26	114.71	125.36
1	0	2588	OMG	C6-N1-C2	5.76	125.08	115.93
1	0	628	1MA	C2-N3-C4	-4.71	110.70	116.58
1	0	2587	OMU	C5-C4-N3	-3.95	114.61	123.31
1	0	2588	OMG	C2-N3-C4	-3.09	111.83	115.36
1	0	2621	PSU	C6-N1-C2	2.70	119.81	115.36
1	0	2588	OMG	N3-C2-N1	-2.54	123.83	127.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	1.47	5 (13%)	54,55,55	2.14	17 (31%)

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	-5.30	1.39	1.52
37	0	9101	MUL	C5-C14	-2.91	1.53	1.56
37	0	9101	MUL	C12-C11	-2.86	1.53	1.55
37	0	9101	MUL	C10-C11	-2.81	1.53	1.56
37	0	9101	MUL	C9-C10	-2.07	1.53	1.56

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	MUL	C13-C14-C5	-6.20	109.94	116.31
37	0	9101	MUL	O3-C21-C22	5.49	119.56	110.32
37	0	9101	MUL	C18-C12-C13	5.00	109.33	105.60
37	0	9101	MUL	C14-O3-C21	-3.79	110.79	117.92
37	0	9101	MUL	C8-C9-C4	3.49	111.41	106.56
37	0	9101	MUL	C1-C2-C3	-3.41	101.70	105.52
37	0	9101	MUL	C2-C1-C9	-3.32	101.13	105.61
37	0	9101	MUL	C4-C5-C6	3.30	109.76	106.61
37	0	9101	MUL	C6-C5-C14	-3.17	109.95	112.10
37	0	9101	MUL	C17-C10-C11	-3.00	109.77	112.11
37	0	9101	MUL	C9-C4-C5	-2.72	114.05	118.00
37	0	9101	MUL	C4-C9-C10	-2.69	111.91	116.04
37	0	9101	MUL	C8-C7-C6	-2.49	109.12	112.35
37	0	9101	MUL	O3-C14-C13	2.33	108.76	106.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	MUL	C23-S1-C22	-2.18	98.06	101.71
37	0	9101	MUL	C12-C19-C20	-2.13	120.96	128.86
37	0	9101	MUL	C12-C11-C10	-2.03	112.59	114.58

There are no chirality outliers.

All (3) torsion outliers are listed below:

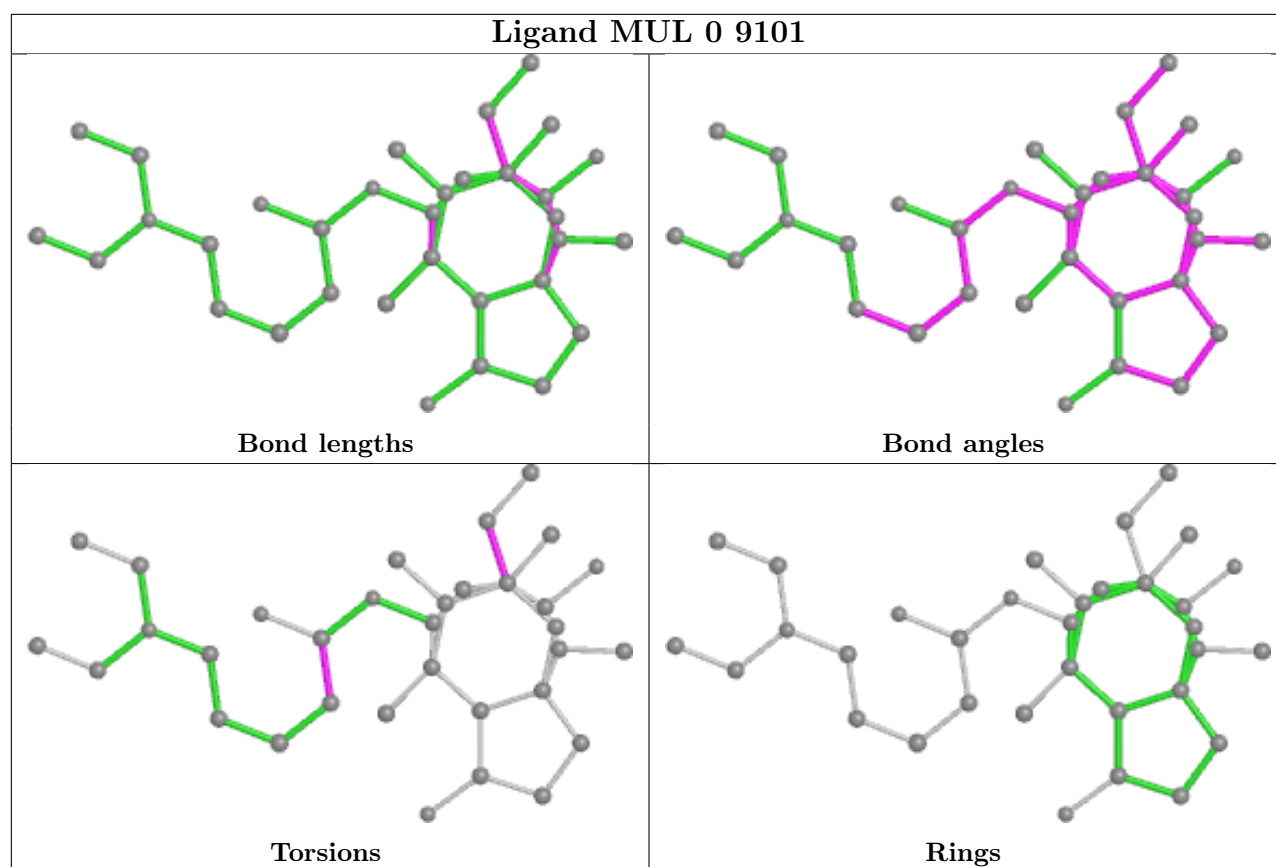
Mol	Chain	Res	Type	Atoms
37	0	9101	MUL	C13-C12-C19-C20
37	0	9101	MUL	O4-C21-C22-S1
37	0	9101	MUL	O3-C21-C22-S1

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2749/2923 (94%)	-0.66	3 (0%) 95 95	29, 74, 140, 200	0
2	A	237/237 (100%)	0.04	9 (3%) 40 26	43, 97, 143, 167	0
3	B	337/337 (100%)	-0.40	1 (0%) 94 92	40, 86, 129, 148	0
4	C	246/246 (100%)	-0.39	2 (0%) 86 78	41, 72, 103, 112	0
5	D	140/177 (79%)	1.10	37 (26%) 0 0	118, 160, 184, 191	0
6	E	172/172 (100%)	-0.13	3 (1%) 70 57	76, 104, 134, 146	0
7	F	119/119 (100%)	0.30	8 (6%) 17 10	74, 113, 153, 166	0
8	G	29/348 (8%)	1.00	6 (20%) 1 1	118, 140, 146, 150	0
9	H	160/177 (90%)	0.54	15 (9%) 8 4	77, 104, 146, 162	0
10	I	70/70 (100%)	1.85	32 (45%) 0 0	173, 199, 200, 200	0
11	J	142/142 (100%)	-0.28	0 100 100	55, 80, 104, 123	0
12	K	132/132 (100%)	-0.20	2 (1%) 73 61	54, 79, 112, 118	0
13	L	145/165 (87%)	0.66	26 (17%) 1 1	62, 121, 171, 175	0
14	M	194/194 (100%)	0.09	17 (8%) 10 5	49, 70, 145, 160	0
15	N	186/186 (100%)	0.48	13 (6%) 16 9	82, 118, 178, 187	0
16	O	115/115 (100%)	-0.44	0 100 100	66, 87, 105, 111	0
17	P	143/143 (100%)	-0.22	2 (1%) 75 63	65, 88, 117, 124	0
18	Q	95/95 (100%)	0.02	4 (4%) 36 23	67, 87, 110, 117	0
19	R	150/150 (100%)	-0.48	0 100 100	47, 72, 103, 112	0
20	S	81/81 (100%)	-0.05	2 (2%) 57 43	68, 93, 114, 130	0
21	T	119/119 (100%)	0.23	10 (8%) 11 6	69, 92, 136, 155	0
22	U	53/53 (100%)	0.09	1 (1%) 66 53	94, 114, 136, 145	0
23	V	65/65 (100%)	0.23	3 (4%) 32 20	79, 112, 164, 170	0
24	W	154/154 (100%)	-0.22	2 (1%) 77 65	56, 78, 110, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	82/82 (100%)	0.11	6 (7%) 15 9	63, 92, 125, 135	0
26	Y	142/142 (100%)	-0.33	2 (1%) 75 63	45, 73, 109, 134	0
27	Z	73/73 (100%)	5.32	53 (72%) 0 0	149, 179, 191, 194	0
28	1	56/56 (100%)	-0.31	0 100 100	42, 53, 66, 76	0
29	2	46/50 (92%)	0.26	4 (8%) 10 5	48, 95, 145, 146	0
30	3	92/92 (100%)	6.09	79 (85%) 0 0	163, 185, 199, 200	0
31	9	122/122 (100%)	-0.83	0 100 100	66, 114, 143, 191	0
All	All	6646/7217 (92%)	-0.13	342 (5%) 28 16	29, 85, 168, 200	0

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	34	SER	29.8
30	3	82	GLY	26.5
27	Z	35	SER	24.8
30	3	37	ASP	18.0
30	3	41	GLU	16.7
27	Z	46	SER	16.4
27	Z	43	GLY	15.4
30	3	34	LYS	15.1
27	Z	50	VAL	14.5
27	Z	45	VAL	14.2
30	3	32	GLY	14.1
27	Z	58	ASN	13.8
30	3	38	ARG	13.2
30	3	39	GLN	12.9
30	3	83	TRP	12.4
27	Z	44	ARG	12.4
27	Z	51	ALA	12.2
30	3	45	GLY	12.0
30	3	35	TRP	12.0
14	M	70	GLY	11.8
27	Z	59	GLU	11.4
30	3	33	MET	11.2
30	3	30	GLN	11.0
30	3	42	ARG	10.6
27	Z	54	GLU	10.5
30	3	81	GLU	10.4
27	Z	55	SER	10.4
30	3	40	ARG	10.2

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Mol	Chain	Res	Type	RSRZ
30	3	48	ASN	9.8
30	3	9	THR	9.7
30	3	43	ASN	9.6
27	Z	36	GLY	9.2
30	3	36	ILE	9.0
14	M	90	ARG	8.7
27	Z	49	ARG	8.6
30	3	62	THR	8.5
27	Z	47	ARG	8.4
14	M	89	THR	8.2
30	3	31	THR	8.2
30	3	44	SER	8.1
21	T	119	ALA	7.6
30	3	71	CYS	7.5
27	Z	68	GLU	7.5
27	Z	42	TYR	7.3
30	3	56	PRO	7.2
14	M	71	SER	7.2
27	Z	63	CYS	7.2
27	Z	38	PHE	7.1
30	3	27	SER	7.1
30	3	20	HIS	7.1
30	3	58	GLY	7.0
30	3	59	ASP	6.9
30	3	14	CYS	6.7
30	3	47	GLY	6.7
30	3	49	ASP	6.4
30	3	18	GLN	6.3
30	3	5	ARG	6.3
27	Z	37	ARG	6.2
5	D	69	ILE	6.2
30	3	73	GLU	6.2
27	Z	69	ASP	6.2
30	3	57	GLY	6.2
27	Z	53	ILE	6.2
13	L	106	VAL	6.2
30	3	22	VAL	6.1
27	Z	57	MET	6.1
27	Z	82	SER	6.0
30	3	72	GLY	6.0
30	3	23	GLU	5.9
14	M	86	GLN	5.7

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Mol	Chain	Res	Type	RSRZ
27	Z	81	CYS	5.7
5	D	18	ILE	5.7
30	3	15	ASN	5.6
27	Z	48	ARG	5.6
10	I	74	ILE	5.6
30	3	10	TYR	5.5
30	3	8	ASN	5.5
5	D	134	LEU	5.5
27	Z	39	GLY	5.4
30	3	29	ARG	5.4
30	3	66	ASP	5.4
5	D	40	ILE	5.4
5	D	88	LEU	5.4
10	I	70	THR	5.4
27	Z	80	GLN	5.3
10	I	128	THR	5.2
30	3	16	GLU	5.1
30	3	78	HIS	5.1
30	3	80	ARG	5.1
30	3	19	GLU	5.1
30	3	84	ARG	5.1
30	3	21	GLU	4.9
30	3	67	LEU	4.9
7	F	106	ALA	4.9
30	3	28	GLY	4.8
15	N	84	THR	4.8
5	D	66	GLY	4.7
30	3	25	VAL	4.7
30	3	85	ALA	4.7
10	I	97	VAL	4.6
27	Z	65	ASN	4.6
10	I	106	GLN	4.6
30	3	74	CYS	4.5
14	M	77	HIS	4.5
27	Z	56	GLU	4.4
30	3	63	LYS	4.4
5	D	104	PHE	4.4
23	V	1	THR	4.4
30	3	69	TYR	4.4
10	I	117	THR	4.3
5	D	92	GLU	4.3
30	3	13	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
27	Z	67	GLY	4.2
27	Z	77	GLY	4.2
27	Z	88	PHE	4.2
30	3	11	CYS	4.2
30	3	75	GLY	4.2
30	3	55	VAL	4.2
10	I	103	ILE	4.2
15	N	119	GLN	4.1
26	Y	235	GLU	4.1
14	M	79	ALA	4.1
10	I	104	ALA	4.1
30	3	1	MET	4.1
30	3	68	LYS	4.1
30	3	60	LYS	4.0
5	D	93	LEU	4.0
10	I	100	VAL	4.0
2	A	82	VAL	3.9
8	G	73	ASP	3.9
25	X	7	GLU	3.9
30	3	17	HIS	3.9
27	Z	71	VAL	3.8
9	H	133	GLY	3.8
27	Z	52	GLU	3.8
5	D	27	ILE	3.8
30	3	76	LYS	3.8
21	T	117	ASP	3.8
30	3	46	ILE	3.8
9	H	76	LEU	3.8
10	I	94	ASP	3.8
27	Z	70	ARG	3.8
13	L	62	ALA	3.7
14	M	78	LYS	3.7
2	A	24	LYS	3.7
5	D	63	ILE	3.6
20	S	81	ILE	3.6
27	Z	103	VAL	3.6
7	F	75	ILE	3.6
30	3	61	PRO	3.6
27	Z	106	SER	3.6
14	M	80	GLY	3.6
5	D	26	GLY	3.6
30	3	91	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
8	G	66	LEU	3.5
13	L	140	VAL	3.5
14	M	76	ARG	3.5
25	X	10	VAL	3.4
13	L	61	ALA	3.4
5	D	130	VAL	3.4
27	Z	62	ALA	3.3
5	D	44	ILE	3.3
14	M	88	VAL	3.3
5	D	25	MET	3.3
10	I	73	LEU	3.3
29	2	41	HIS	3.3
13	L	76	LEU	3.3
27	Z	93	TYR	3.3
30	3	6	ARG	3.2
5	D	166	ILE	3.2
5	D	128	LEU	3.2
18	Q	95	GLU	3.2
8	G	27	ILE	3.2
13	L	107	LYS	3.2
13	L	49	SER	3.2
14	M	81	ARG	3.2
27	Z	86	TYR	3.2
30	3	65	THR	3.2
27	Z	40	ALA	3.1
30	3	77	ALA	3.1
7	F	49	PHE	3.1
10	I	111	LEU	3.1
5	D	61	PHE	3.1
15	N	172	PHE	3.1
27	Z	60	ASP	3.1
24	W	3	ALA	3.1
5	D	106	PHE	3.1
27	Z	78	ILE	3.1
15	N	179	LEU	3.1
27	Z	85	ASP	3.1
23	V	39	ALA	3.1
30	3	90	PHE	3.0
29	2	36	ASN	3.0
30	3	86	GLY	3.0
27	Z	66	CYS	3.0
21	T	99	THR	3.0

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Mol	Chain	Res	Type	RSRZ
27	Z	79	TRP	3.0
14	M	87	GLY	3.0
6	E	5	LEU	3.0
10	I	92	VAL	3.0
14	M	83	SER	3.0
5	D	89	PRO	3.0
21	T	40	VAL	2.9
27	Z	76	THR	2.9
10	I	68	PRO	2.9
21	T	42	VAL	2.9
10	I	71	ALA	2.9
8	G	69	ARG	2.9
10	I	112	LEU	2.9
7	F	99	THR	2.9
30	3	88	LEU	2.9
17	P	118	GLN	2.9
8	G	23	ILE	2.9
23	V	40	PRO	2.9
15	N	83	LEU	2.9
10	I	102	GLN	2.9
30	3	2	GLN	2.9
10	I	113	SER	2.9
13	L	97	VAL	2.9
9	H	97	VAL	2.8
10	I	109	PRO	2.8
5	D	90	LEU	2.8
10	I	110	ASP	2.8
10	I	93	ALA	2.8
15	N	81	ALA	2.8
15	N	166	ALA	2.8
29	2	48	ASP	2.8
5	D	95	THR	2.8
25	X	8	ARG	2.8
9	H	87	LYS	2.8
13	L	79	ASP	2.8
30	3	3	MET	2.8
13	L	60	GLU	2.8
15	N	175	LEU	2.7
5	D	135	VAL	2.7
5	D	84	LEU	2.7
27	Z	64	PRO	2.7
10	I	98	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
18	Q	64	GLU	2.7
1	0	735	C	2.7
10	I	127	CYS	2.6
10	I	99	GLN	2.6
5	D	57	THR	2.6
1	0	970	U	2.6
15	N	114	LYS	2.6
9	H	86	TYR	2.6
21	T	118	SER	2.5
30	3	24	LYS	2.5
5	D	91	ALA	2.5
10	I	108	HIS	2.5
9	H	66	GLU	2.5
8	G	63	ARG	2.5
2	A	88	ILE	2.5
2	A	36	ASP	2.5
13	L	120	LEU	2.5
9	H	53	ILE	2.5
10	I	72	GLU	2.5
5	D	87	ALA	2.5
10	I	132	VAL	2.5
7	F	15	ASP	2.5
5	D	160	ALA	2.5
5	D	64	ARG	2.5
7	F	17	LEU	2.4
5	D	43	GLU	2.4
5	D	165	PHE	2.4
15	N	145	ALA	2.4
13	L	123	ASP	2.4
30	3	92	GLU	2.4
15	N	101	VAL	2.4
14	M	1	ALA	2.4
7	F	91	VAL	2.4
27	Z	84	CYS	2.4
21	T	101	LEU	2.4
13	L	93	VAL	2.3
5	D	101	THR	2.3
15	N	178	THR	2.3
24	W	96	LEU	2.3
25	X	72	VAL	2.3
21	T	106	GLU	2.3
10	I	101	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
21	T	74	VAL	2.3
30	3	70	ARG	2.3
3	B	128	ILE	2.3
27	Z	89	THR	2.3
9	H	149	VAL	2.3
13	L	78	ALA	2.3
2	A	128	LEU	2.3
13	L	91	VAL	2.3
20	S	28	VAL	2.3
9	H	169	GLU	2.2
13	L	36	ASP	2.2
22	U	25	ASP	2.2
1	0	1169	U	2.2
27	Z	61	HIS	2.2
2	A	58	VAL	2.2
18	Q	75	ILE	2.2
6	E	100	ASP	2.2
9	H	85	ASP	2.2
5	D	24	HIS	2.2
5	D	47	GLN	2.2
7	F	96	ALA	2.2
10	I	119	ALA	2.2
13	L	124	ASP	2.2
5	D	17	ARG	2.2
10	I	105	GLU	2.2
13	L	99	GLU	2.2
12	K	109	LEU	2.2
13	L	130	ARG	2.2
5	D	129	ASP	2.2
12	K	132	VAL	2.2
25	X	85	VAL	2.2
6	E	118	ILE	2.2
9	H	25	GLY	2.2
13	L	108	VAL	2.1
13	L	122	ALA	2.1
2	A	69	LEU	2.1
4	C	63	SER	2.1
25	X	41	PHE	2.1
9	H	141	CYS	2.1
14	M	74	LYS	2.1
2	A	56	ALA	2.1
29	2	45	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
18	Q	85	ILE	2.1
13	L	39	GLU	2.1
15	N	95	ALA	2.1
9	H	50	ILE	2.1
2	A	91	GLY	2.1
13	L	50	GLY	2.0
13	L	66	VAL	2.0
5	D	68	PRO	2.0
10	I	66	GLY	2.0
9	H	146	ALA	2.0
13	L	96	VAL	2.0
17	P	114	LEU	2.0
10	I	118	ASN	2.0
14	M	22	GLU	2.0
21	T	23	VAL	2.0
27	Z	72	ASP	2.0
4	C	246	ARG	2.0
9	H	164	CYS	2.0
26	Y	95	THR	2.0
13	L	81	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
36	SR	0	8997	1/1	-0.10	5.65	200,200,200,200	0
36	SR	0	8971	1/1	0.15	0.12	200,200,200,200	0
34	NA	0	8522	1/1	0.21	0.13	87,87,87,87	0
34	NA	S	8510	1/1	0.40	0.30	69,69,69,69	0
34	NA	0	8506	1/1	0.47	0.60	105,105,105,105	0
34	NA	0	8525	1/1	0.53	0.33	92,92,92,92	0
34	NA	0	8524	1/1	0.54	0.38	47,47,47,47	0
36	SR	B	8987	1/1	0.55	0.82	200,200,200,200	0
32	MG	0	8036	1/1	0.58	0.21	82,82,82,82	0
34	NA	0	8505	1/1	0.59	0.45	56,56,56,56	0
34	NA	0	8553	1/1	0.61	0.20	81,81,81,81	0
34	NA	0	8554	1/1	0.61	0.38	71,71,71,71	0
36	SR	0	8998	1/1	0.62	0.63	169,169,169,169	0
34	NA	9	8572	1/1	0.62	0.32	88,88,88,88	0
32	MG	0	8068	1/1	0.64	0.08	49,49,49,49	0
34	NA	0	8549	1/1	0.64	0.17	83,83,83,83	0
34	NA	0	8556	1/1	0.64	0.80	95,95,95,95	0
32	MG	0	8092	1/1	0.66	0.12	53,53,53,53	0
36	SR	J	8986	1/1	0.66	1.51	200,200,200,200	0
32	MG	0	8090	1/1	0.67	0.93	81,81,81,81	0
36	SR	A	8930	1/1	0.67	0.24	133,133,133,133	0
36	SR	0	8991	1/1	0.68	0.09	190,190,190,190	0
36	SR	0	8958	1/1	0.69	0.07	150,150,150,150	0
36	SR	0	8962	1/1	0.69	0.15	155,155,155,155	0
32	MG	0	8049	1/1	0.69	0.20	61,61,61,61	0
34	NA	0	8564	1/1	0.70	0.57	95,95,95,95	0
34	NA	0	8528	1/1	0.71	0.49	80,80,80,80	0
35	CL	3	8804	1/1	0.73	0.15	96,96,96,96	0
34	NA	0	8501	1/1	0.73	0.22	41,41,41,41	0
36	SR	0	8957	1/1	0.74	0.24	200,200,200,200	0
36	SR	0	8916	1/1	0.74	0.08	129,129,129,129	0
36	SR	0	8994	1/1	0.75	0.72	200,200,200,200	0
34	NA	Q	8540	1/1	0.75	0.29	92,92,92,92	0
32	MG	9	8074	1/1	0.76	0.13	127,127,127,127	0
34	NA	0	8527	1/1	0.76	0.24	60,60,60,60	0
36	SR	0	8922	1/1	0.77	0.47	190,190,190,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8508	1/1	0.77	0.99	70,70,70,70	0
34	NA	9	8543	1/1	0.77	0.17	57,57,57,57	0
32	MG	0	8044	1/1	0.77	0.11	49,49,49,49	0
32	MG	0	8077	1/1	0.77	0.16	47,47,47,47	0
32	MG	0	8081	1/1	0.77	0.45	104,104,104,104	0
36	SR	9	9003	1/1	0.77	0.06	200,200,200,200	0
34	NA	0	8509	1/1	0.78	0.49	66,66,66,66	0
34	NA	0	8568	1/1	0.78	0.57	51,51,51,51	0
34	NA	0	8529	1/1	0.78	0.11	49,49,49,49	0
36	SR	0	8936	1/1	0.78	0.07	109,109,109,109	0
35	CL	N	8807	1/1	0.79	0.38	134,134,134,134	0
36	SR	0	8947	1/1	0.79	0.60	200,200,200,200	0
34	NA	0	8502	1/1	0.80	0.19	51,51,51,51	0
34	NA	0	8566	1/1	0.80	0.89	51,51,51,51	0
34	NA	R	8575	1/1	0.80	0.50	96,96,96,96	0
36	SR	0	9006	1/1	0.81	0.49	200,200,200,200	0
32	MG	0	8061	1/1	0.81	0.30	42,42,42,42	0
32	MG	0	8073	1/1	0.81	0.69	110,110,110,110	0
34	NA	0	8550	1/1	0.81	0.19	98,98,98,98	0
36	SR	0	8985	1/1	0.81	0.04	173,173,173,173	0
34	NA	0	8560	1/1	0.82	0.29	64,64,64,64	0
36	SR	0	8979	1/1	0.82	0.10	200,200,200,200	0
34	NA	0	8533	1/1	0.82	0.21	68,68,68,68	0
36	SR	0	8974	1/1	0.83	0.42	191,191,191,191	0
36	SR	0	8977	1/1	0.83	0.14	197,197,197,197	0
36	SR	0	8995	1/1	0.83	0.25	128,128,128,128	0
34	NA	0	8514	1/1	0.83	0.27	61,61,61,61	0
34	NA	0	8545	1/1	0.83	0.31	40,40,40,40	0
32	MG	0	8066	1/1	0.84	0.93	70,70,70,70	0
34	NA	0	8562	1/1	0.84	1.23	85,85,85,85	0
35	CL	0	8805	1/1	0.84	0.39	97,97,97,97	0
34	NA	R	8532	1/1	0.85	0.10	57,57,57,57	0
36	SR	0	9007	1/1	0.85	0.78	180,180,180,180	0
34	NA	0	8552	1/1	0.85	0.31	68,68,68,68	0
36	SR	A	8993	1/1	0.85	0.04	177,177,177,177	0
34	NA	0	8571	1/1	0.85	0.26	89,89,89,89	0
34	NA	0	8531	1/1	0.85	0.27	42,42,42,42	0
36	SR	0	8989	1/1	0.85	0.26	196,196,196,196	0
32	MG	0	8069	1/1	0.86	0.55	68,68,68,68	0
34	NA	0	8511	1/1	0.86	0.21	64,64,64,64	0
36	SR	0	9004	1/1	0.86	0.46	200,200,200,200	0
35	CL	Y	8820	1/1	0.86	0.06	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8047	1/1	0.86	0.37	70,70,70,70	0
34	NA	0	8573	1/1	0.87	0.19	92,92,92,92	0
36	SR	0	8992	1/1	0.87	0.10	149,149,149,149	0
36	SR	0	8975	1/1	0.87	0.04	158,158,158,158	0
36	SR	0	8927	1/1	0.87	0.16	172,172,172,172	0
34	NA	0	8565	1/1	0.87	1.16	106,106,106,106	0
32	MG	0	8055	1/1	0.87	0.28	67,67,67,67	0
36	SR	0	8973	1/1	0.87	0.17	134,134,134,134	0
36	SR	0	8960	1/1	0.88	0.11	174,174,174,174	0
36	SR	0	8984	1/1	0.88	0.06	139,139,139,139	0
34	NA	0	8547	1/1	0.88	0.91	81,81,81,81	0
34	NA	M	8539	1/1	0.88	0.12	34,34,34,34	0
34	NA	0	8537	1/1	0.88	0.16	43,43,43,43	0
35	CL	0	8811	1/1	0.88	0.61	99,99,99,99	0
35	CL	0	8822	1/1	0.88	1.36	94,94,94,94	0
36	SR	H	8972	1/1	0.88	0.15	157,157,157,157	0
36	SR	0	8976	1/1	0.88	0.22	185,185,185,185	0
36	SR	9	8980	1/1	0.88	0.05	192,192,192,192	0
36	SR	0	8959	1/1	0.88	0.15	194,194,194,194	0
36	SR	0	8910	1/1	0.89	0.12	113,113,113,113	0
32	MG	0	8039	1/1	0.89	0.27	76,76,76,76	0
34	NA	0	8536	1/1	0.89	0.13	72,72,72,72	0
32	MG	0	8043	1/1	0.89	0.13	55,55,55,55	0
34	NA	0	8558	1/1	0.89	0.60	50,50,50,50	0
36	SR	0	8996	1/1	0.89	0.40	200,200,200,200	0
36	SR	0	8938	1/1	0.89	0.07	200,200,200,200	0
32	MG	0	8072	1/1	0.89	0.08	37,37,37,37	0
36	SR	0	8988	1/1	0.89	0.11	181,181,181,181	0
34	NA	0	8559	1/1	0.90	0.32	94,94,94,94	0
34	NA	0	8518	1/1	0.90	0.40	82,82,82,82	0
36	SR	0	8968	1/1	0.90	0.11	181,181,181,181	0
36	SR	0	8982	1/1	0.90	1.70	200,200,200,200	0
32	MG	0	8033	1/1	0.90	0.26	56,56,56,56	0
36	SR	F	9005	1/1	0.90	0.13	154,154,154,154	0
35	CL	0	8812	1/1	0.90	0.09	58,58,58,58	0
34	NA	0	8544	1/1	0.90	0.17	68,68,68,68	0
36	SR	0	9001	1/1	0.90	0.09	189,189,189,189	0
34	NA	0	8515	1/1	0.90	0.22	45,45,45,45	0
36	SR	0	8970	1/1	0.91	0.06	150,150,150,150	0
34	NA	J	8538	1/1	0.91	0.14	45,45,45,45	0
36	SR	L	8969	1/1	0.91	0.93	198,198,198,198	0
36	SR	0	8914	1/1	0.91	0.32	130,130,130,130	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	0.91	0.25	185,185,185,185	0
32	MG	0	8087	1/1	0.92	0.18	20,20,20,20	0
36	SR	3	8999	1/1	0.92	0.18	160,160,160,160	0
36	SR	0	8928	1/1	0.92	0.05	164,164,164,164	0
32	MG	0	8004	1/1	0.92	0.15	32,32,32,32	0
32	MG	0	8079	1/1	0.93	0.20	63,63,63,63	0
35	CL	M	8818	1/1	0.93	0.09	73,73,73,73	0
32	MG	0	8058	1/1	0.93	0.06	25,25,25,25	0
34	NA	0	8523	1/1	0.93	0.15	58,58,58,58	0
32	MG	0	8001	1/1	0.93	0.11	28,28,28,28	0
32	MG	0	8053	1/1	0.93	0.05	57,57,57,57	0
36	SR	0	8944	1/1	0.93	0.17	171,171,171,171	0
36	SR	0	8945	1/1	0.93	0.04	111,111,111,111	0
32	MG	0	8010	1/1	0.93	0.18	35,35,35,35	0
36	SR	0	8915	1/1	0.93	0.07	125,125,125,125	0
34	NA	0	8541	1/1	0.94	0.14	46,46,46,46	0
36	SR	0	8946	1/1	0.94	0.26	138,138,138,138	0
34	NA	0	8516	1/1	0.94	0.26	26,26,26,26	0
36	SR	0	8951	1/1	0.94	0.19	177,177,177,177	0
32	MG	2	8060	1/1	0.94	0.09	56,56,56,56	0
36	SR	0	8955	1/1	0.94	0.17	199,199,199,199	0
32	MG	0	8067	1/1	0.94	0.43	42,42,42,42	0
33	K	0	8402	1/1	0.94	0.21	67,67,67,67	0
32	MG	0	8032	1/1	0.94	0.08	64,64,64,64	0
34	NA	0	8574	1/1	0.94	0.80	67,67,67,67	0
36	SR	0	8901	1/1	0.94	0.12	89,89,89,89	0
36	SR	0	8963	1/1	0.94	0.15	135,135,135,135	0
36	SR	0	8967	1/1	0.94	0.07	157,157,157,157	0
34	NA	0	8551	1/1	0.94	0.16	81,81,81,81	0
32	MG	0	8031	1/1	0.94	0.34	71,71,71,71	0
32	MG	0	8082	1/1	0.94	0.41	86,86,86,86	0
32	MG	0	8085	1/1	0.94	0.13	83,83,83,83	0
32	MG	0	8071	1/1	0.94	0.12	50,50,50,50	0
36	SR	0	8924	1/1	0.94	0.17	138,138,138,138	0
32	MG	0	8089	1/1	0.94	0.29	72,72,72,72	0
32	MG	0	8040	1/1	0.94	0.32	100,100,100,100	0
36	SR	3	8932	1/1	0.94	0.29	149,149,149,149	0
32	MG	0	8035	1/1	0.94	0.12	47,47,47,47	0
35	CL	0	8803	1/1	0.94	0.08	66,66,66,66	0
32	MG	T	8057	1/1	0.94	0.03	67,67,67,67	0
37	MUL	0	9101	34/34	0.94	0.26	85,87,104,104	0
35	CL	R	8806	1/1	0.95	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	A	8929	1/1	0.95	0.17	157,157,157,157	0
32	MG	0	8088	1/1	0.95	0.05	39,39,39,39	0
32	MG	0	8038	1/1	0.95	0.12	81,81,81,81	0
36	SR	0	8954	1/1	0.95	0.12	122,122,122,122	0
32	MG	0	8021	1/1	0.95	0.10	28,28,28,28	0
36	SR	0	8908	1/1	0.95	0.06	109,109,109,109	0
35	CL	0	8815	1/1	0.95	0.24	90,90,90,90	0
36	SR	0	8940	1/1	0.95	0.03	117,117,117,117	0
36	SR	1	8913	1/1	0.95	0.17	97,97,97,97	0
34	NA	0	8526	1/1	0.95	0.27	52,52,52,52	0
32	MG	0	8015	1/1	0.95	0.10	25,25,25,25	0
36	SR	0	8981	1/1	0.95	0.10	151,151,151,151	0
32	MG	0	8037	1/1	0.95	0.29	84,84,84,84	0
36	SR	0	8966	1/1	0.95	0.10	110,110,110,110	0
34	NA	0	8542	1/1	0.96	0.52	51,51,51,51	0
32	MG	0	8005	1/1	0.96	0.27	30,30,30,30	0
34	NA	0	8561	1/1	0.96	0.36	73,73,73,73	0
32	MG	0	8003	1/1	0.96	0.16	31,31,31,31	0
32	MG	0	8029	1/1	0.96	0.12	54,54,54,54	0
34	NA	0	8548	1/1	0.96	0.25	52,52,52,52	0
32	MG	B	8042	1/1	0.96	0.08	67,67,67,67	0
34	NA	0	8567	1/1	0.96	0.21	58,58,58,58	0
36	SR	0	8964	1/1	0.96	0.09	149,149,149,149	0
34	NA	0	8530	1/1	0.96	0.31	49,49,49,49	0
35	CL	0	8813	1/1	0.96	0.15	68,68,68,68	0
36	SR	0	8934	1/1	0.96	0.09	114,114,114,114	0
35	CL	0	8814	1/1	0.96	0.41	67,67,67,67	0
34	NA	0	8521	1/1	0.96	0.11	34,34,34,34	0
32	MG	0	8065	1/1	0.96	0.14	41,41,41,41	0
36	SR	B	8950	1/1	0.96	0.28	151,151,151,151	0
36	SR	0	8941	1/1	0.96	0.31	143,143,143,143	0
36	SR	0	8942	1/1	0.96	0.08	129,129,129,129	0
36	SR	0	8943	1/1	0.96	0.17	99,99,99,99	0
35	CL	L	8810	1/1	0.96	0.24	86,86,86,86	0
34	NA	0	8535	1/1	0.96	0.54	45,45,45,45	0
34	NA	C	8503	1/1	0.96	0.32	39,39,39,39	0
36	SR	1	8952	1/1	0.96	0.19	81,81,81,81	0
32	MG	Y	8086	1/1	0.96	0.04	55,55,55,55	0
36	SR	0	8983	1/1	0.96	0.21	185,185,185,185	0
36	SR	0	8949	1/1	0.96	0.10	120,120,120,120	0
32	MG	0	8014	1/1	0.96	0.12	30,30,30,30	0
32	MG	0	8041	1/1	0.96	0.14	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
38	CD	O	8705	1/1	0.96	0.03	115,115,115,115	0
32	MG	0	8063	1/1	0.97	0.15	67,67,67,67	0
32	MG	0	8064	1/1	0.97	0.20	48,48,48,48	0
34	NA	0	8563	1/1	0.97	0.18	74,74,74,74	0
32	MG	0	8027	1/1	0.97	0.05	30,30,30,30	0
36	SR	0	8917	1/1	0.97	0.14	121,121,121,121	0
36	SR	0	8919	1/1	0.97	0.17	194,194,194,194	0
36	SR	0	8920	1/1	0.97	0.11	132,132,132,132	0
36	SR	0	9000	1/1	0.97	0.23	200,200,200,200	0
36	SR	0	8921	1/1	0.97	0.09	90,90,90,90	0
34	NA	0	8546	1/1	0.97	1.32	69,69,69,69	0
32	MG	0	8008	1/1	0.97	0.14	15,15,15,15	0
32	MG	0	8009	1/1	0.97	0.21	28,28,28,28	0
32	MG	0	8052	1/1	0.97	0.04	40,40,40,40	0
36	SR	0	8933	1/1	0.97	0.04	122,122,122,122	0
32	MG	0	8007	1/1	0.97	0.17	10,10,10,10	0
32	MG	0	8024	1/1	0.97	0.14	58,58,58,58	0
35	CL	A	8809	1/1	0.97	0.67	96,96,96,96	0
35	CL	B	8819	1/1	0.97	0.76	68,68,68,68	0
35	CL	J	8801	1/1	0.97	0.21	90,90,90,90	0
35	CL	J	8821	1/1	0.97	0.16	70,70,70,70	0
36	SR	0	8978	1/1	0.97	0.04	130,130,130,130	0
32	MG	0	8034	1/1	0.97	0.30	43,43,43,43	0
32	MG	0	8059	1/1	0.97	0.12	40,40,40,40	0
34	NA	0	8534	1/1	0.97	0.22	45,45,45,45	0
34	NA	0	8555	1/1	0.97	0.55	50,50,50,50	0
32	MG	0	8075	1/1	0.97	0.06	40,40,40,40	0
32	MG	0	8076	1/1	0.97	0.06	36,36,36,36	0
32	MG	0	8025	1/1	0.97	0.07	44,44,44,44	0
32	MG	0	8078	1/1	0.97	0.23	64,64,64,64	0
38	CD	Z	8703	1/1	0.97	0.14	155,155,155,155	0
38	CD	3	8704	1/1	0.97	0.41	176,176,176,176	0
36	SR	0	8939	1/1	0.98	0.05	145,145,145,145	0
34	NA	0	8517	1/1	0.98	0.20	30,30,30,30	0
35	CL	J	8802	1/1	0.98	0.08	100,100,100,100	0
34	NA	0	8569	1/1	0.98	0.17	72,72,72,72	0
34	NA	0	8570	1/1	0.98	0.11	65,65,65,65	0
36	SR	0	8990	1/1	0.98	0.19	111,111,111,111	0
32	MG	C	8012	1/1	0.98	0.21	19,19,19,19	0
34	NA	0	8520	1/1	0.98	0.19	57,57,57,57	0
35	CL	O	8808	1/1	0.98	0.30	98,98,98,98	0
32	MG	K	8054	1/1	0.98	0.12	32,32,32,32	0

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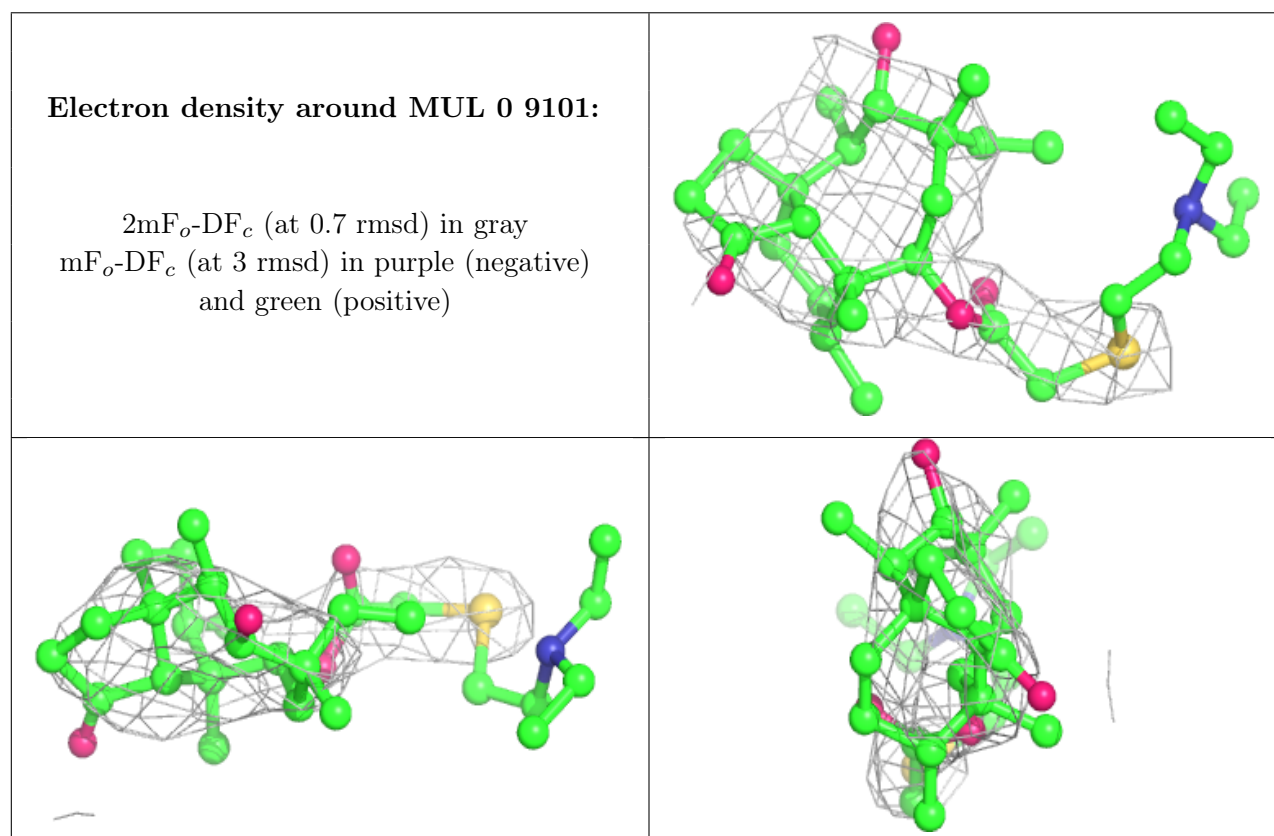
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8056	1/1	0.98	0.07	47,47,47,47	0
32	MG	0	8080	1/1	0.98	0.52	98,98,98,98	0
32	MG	0	8002	1/1	0.98	0.17	26,26,26,26	0
36	SR	0	8902	1/1	0.98	0.13	63,63,63,63	0
36	SR	0	8903	1/1	0.98	0.19	62,62,62,62	0
36	SR	0	9002	1/1	0.98	0.09	188,188,188,188	0
36	SR	0	8956	1/1	0.98	0.23	178,178,178,178	0
32	MG	0	8070	1/1	0.98	0.39	54,54,54,54	0
36	SR	0	8909	1/1	0.98	0.07	89,89,89,89	0
36	SR	0	9008	1/1	0.98	0.16	99,99,99,99	0
32	MG	0	8006	1/1	0.98	0.12	62,62,62,62	0
36	SR	0	8911	1/1	0.98	0.13	109,109,109,109	0
32	MG	0	8046	1/1	0.98	0.21	48,48,48,48	0
32	MG	0	8016	1/1	0.98	0.16	38,38,38,38	0
32	MG	0	8011	1/1	0.98	0.21	18,18,18,18	0
34	NA	0	8557	1/1	0.98	0.07	71,71,71,71	0
32	MG	0	8022	1/1	0.98	0.13	29,29,29,29	0
34	NA	0	8507	1/1	0.98	0.27	39,39,39,39	0
32	MG	0	8091	1/1	0.98	0.18	42,42,42,42	0
32	MG	0	8023	1/1	0.98	0.15	21,21,21,21	0
36	SR	0	8923	1/1	0.98	0.17	120,120,120,120	0
32	MG	0	8093	1/1	0.98	0.10	40,40,40,40	0
34	NA	0	8512	1/1	0.98	0.30	49,49,49,49	0
34	NA	0	8513	1/1	0.98	0.23	63,63,63,63	0
35	CL	0	8816	1/1	0.98	0.71	86,86,86,86	0
32	MG	A	8050	1/1	0.98	0.19	52,52,52,52	0
36	SR	0	8935	1/1	0.98	0.05	106,106,106,106	0
38	CD	U	8701	1/1	0.98	0.04	104,104,104,104	0
32	MG	A	8051	1/1	0.98	0.28	90,90,90,90	0
32	MG	0	8013	1/1	0.98	0.04	21,21,21,21	0
36	SR	0	8948	1/1	0.99	0.08	104,104,104,104	0
36	SR	0	8905	1/1	0.99	0.27	70,70,70,70	0
36	SR	0	8925	1/1	0.99	0.13	105,105,105,105	0
36	SR	0	8926	1/1	0.99	0.16	145,145,145,145	0
36	SR	0	8906	1/1	0.99	0.19	65,65,65,65	0
36	SR	0	8907	1/1	0.99	0.16	63,63,63,63	0
36	SR	0	8931	1/1	0.99	0.10	123,123,123,123	0
32	MG	0	8020	1/1	0.99	0.11	52,52,52,52	0
32	MG	0	8083	1/1	0.99	0.08	59,59,59,59	0
32	MG	0	8084	1/1	0.99	0.16	50,50,50,50	0
32	MG	0	8017	1/1	0.99	0.07	29,29,29,29	0
36	SR	0	8937	1/1	0.99	0.17	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	R	8912	1/1	0.99	0.23	106,106,106,106	0
36	SR	S	8961	1/1	0.99	0.10	127,127,127,127	0
32	MG	0	8026	1/1	0.99	0.04	32,32,32,32	0
32	MG	0	8048	1/1	0.99	0.31	38,38,38,38	0
36	SR	0	8965	1/1	0.99	0.17	135,135,135,135	0
34	NA	0	8519	1/1	0.99	0.18	44,44,44,44	0
35	CL	0	8817	1/1	0.99	0.11	63,63,63,63	0
36	SR	0	8918	1/1	0.99	0.13	84,84,84,84	0
32	MG	0	8018	1/1	0.99	0.18	42,42,42,42	0
32	MG	0	8062	1/1	0.99	0.28	47,47,47,47	0
32	MG	0	8028	1/1	0.99	0.13	14,14,14,14	0
32	MG	0	8019	1/1	0.99	0.16	10,10,10,10	0
38	CD	1	8702	1/1	0.99	0.13	68,68,68,68	0
36	SR	0	8904	1/1	0.99	0.16	64,64,64,64	0
32	MG	0	8030	1/1	1.00	0.48	60,60,60,60	0
34	NA	0	8504	1/1	1.00	0.09	22,22,22,22	0
32	MG	0	8045	1/1	1.00	0.12	44,44,44,44	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.