



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:33 am BST

PDB ID : 3CCQ
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation A2488U
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

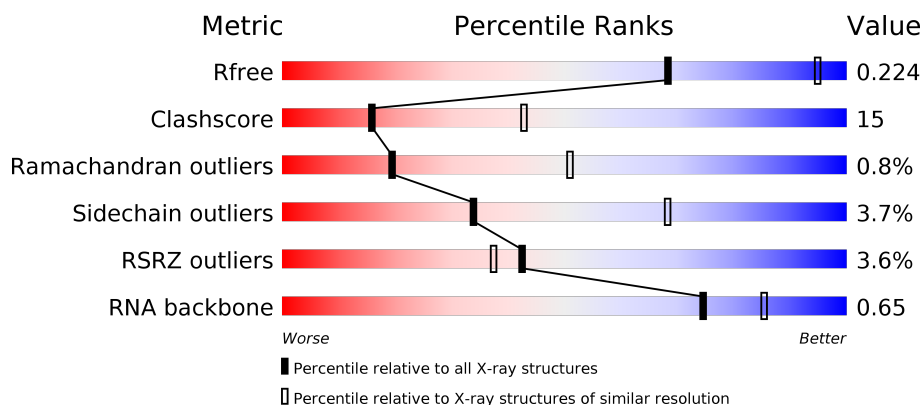
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	A	240	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>
2	B	338	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div>.</div> </div> </div>
3	C	246	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>.</div> </div> </div>
4	D	177	<div> <div>29%</div> <div> <div></div> <div>40%</div> <div>37%</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	SR	0	8947	-	-	-	X
34	SR	0	8982	-	-	-	X
34	SR	0	8986	-	-	-	X
34	SR	0	8994	-	-	-	X
34	SR	0	8996	-	-	-	X
34	SR	0	9006	-	-	-	X
35	NA	0	8509	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8562	-	-	-	X
37	K	0	8401	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99120 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

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

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

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

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

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

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O	S	0	0	0
			1130	686	228	216				

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59018	26348	10870	19055	2745			

- 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	87	Total	Mg	0	0
			87	87		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	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		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	9	Total Cl 9 9	0	0
33	J	3	Total Cl 3 3	0	0
33	Q	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	A	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	L	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	93	Total Sr 93 93	0	0
34	1	2	Total Sr 2 2	0	0
34	B	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	A	3	Total Sr 3 3	0	0
34	R	1	Total Sr 1 1	0	0
34	9	3	Total Sr 3 3	0	0
34	S	1	Total Sr 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	F	1	Total	Sr	0	0
			1	1		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	65	Total	Na	0	0
			65	65		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	B	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	R	2	Total	Na	0	0
			2	2		
35	9	2	Total	Na	0	0
			2	2		
35	S	1	Total	Na	0	0
			1	1		
35	M	1	Total	Na	0	0
			1	1		

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total	Cd	0	0
			1	1		
36	Z	1	Total	Cd	0	0
			1	1		
36	1	1	Total	Cd	0	0
			1	1		
36	3	1	Total	Cd	0	0
			1	1		
36	U	1	Total	Cd	0	0
			1	1		

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	112	Total O 112 112	0	0
38	B	142	Total O 142 142	0	0
38	C	168	Total O 168 168	0	0
38	D	45	Total O 45 45	0	0
38	E	42	Total O 42 42	0	0
38	F	26	Total O 26 26	0	0
38	G	17	Total O 17 17	0	0
38	H	65	Total O 65 65	0	0
38	I	5	Total O 5 5	0	0
38	J	56	Total O 56 56	0	0
38	K	60	Total O 60 60	0	0
38	L	82	Total O 82 82	0	0
38	M	123	Total O 123 123	0	0
38	N	59	Total O 59 59	0	0
38	O	47	Total O 47 47	0	0
38	P	59	Total O 59 59	0	0
38	Q	47	Total O 47 47	0	0
38	R	76	Total O 76 76	0	0
38	S	33	Total O 33 33	0	0

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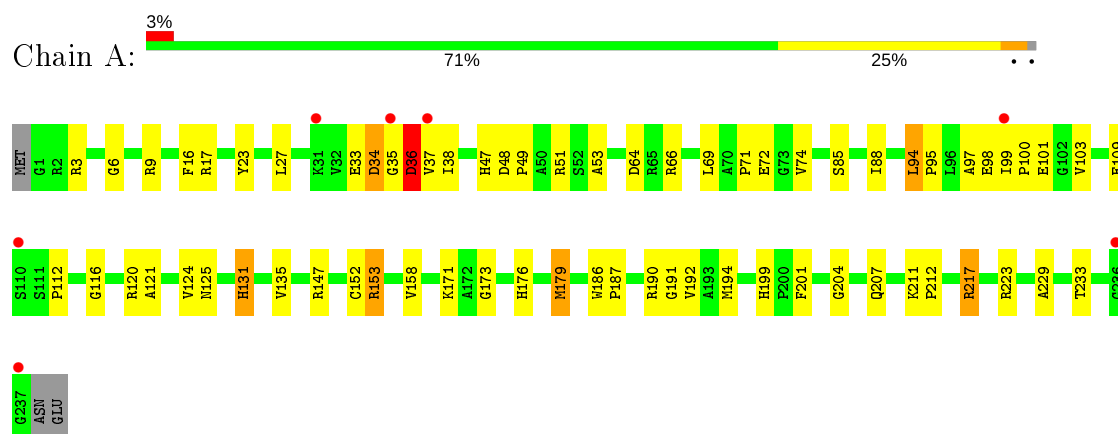
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	36	Total 36	O 36	0	0
38	U	26	Total 26	O 26	0	0
38	V	12	Total 12	O 12	0	0
38	W	66	Total 66	O 66	0	0
38	X	28	Total 28	O 28	0	0
38	Y	97	Total 97	O 97	0	0
38	Z	31	Total 31	O 31	0	0
38	1	54	Total 54	O 54	0	0
38	2	43	Total 43	O 43	0	0
38	3	68	Total 68	O 68	0	0
38	0	5950	Total 5950	O 5950	0	0
38	9	148	Total 148	O 148	0	0

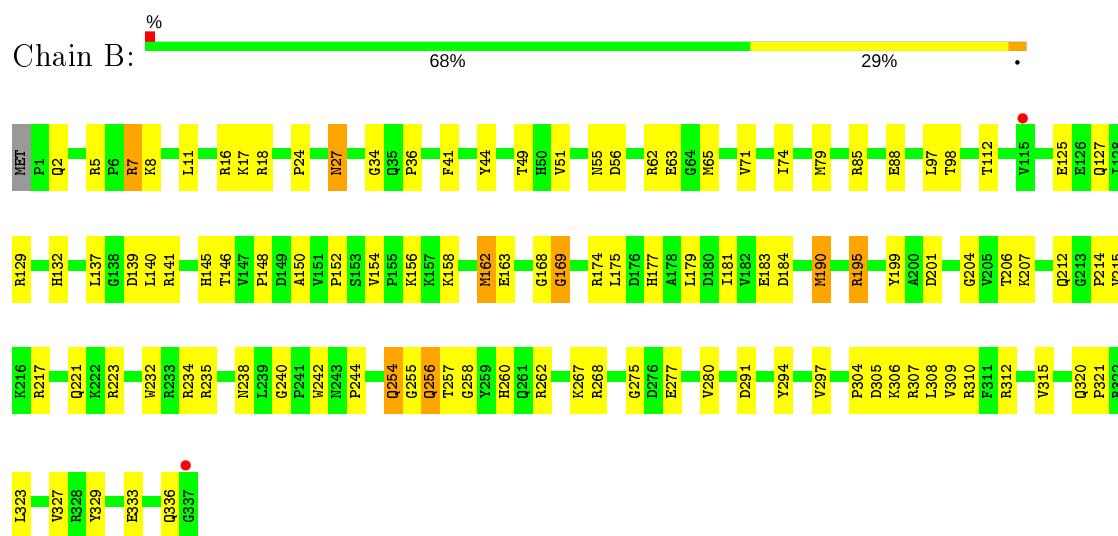
3 Residue-property plots [i](#)

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

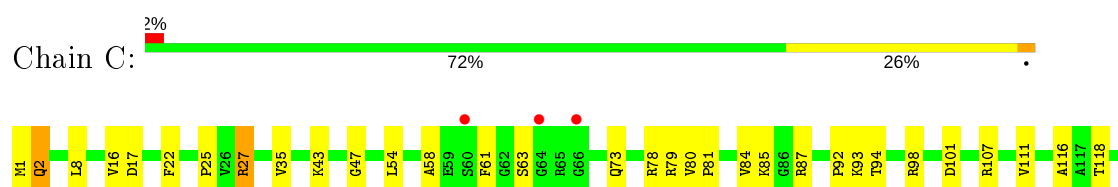
- Molecule 1: 50S ribosomal protein L2P

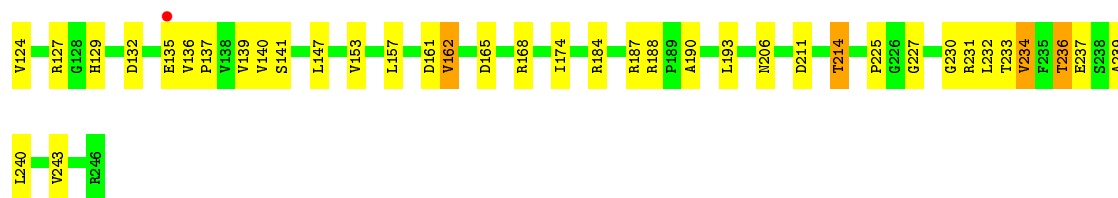


- Molecule 2: 50S ribosomal protein L3P

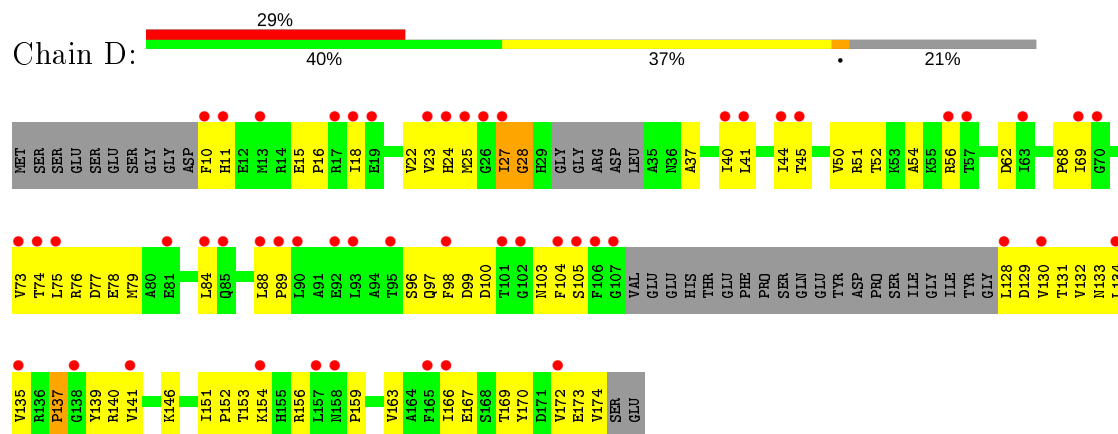


- Molecule 3: 50S ribosomal protein L4P

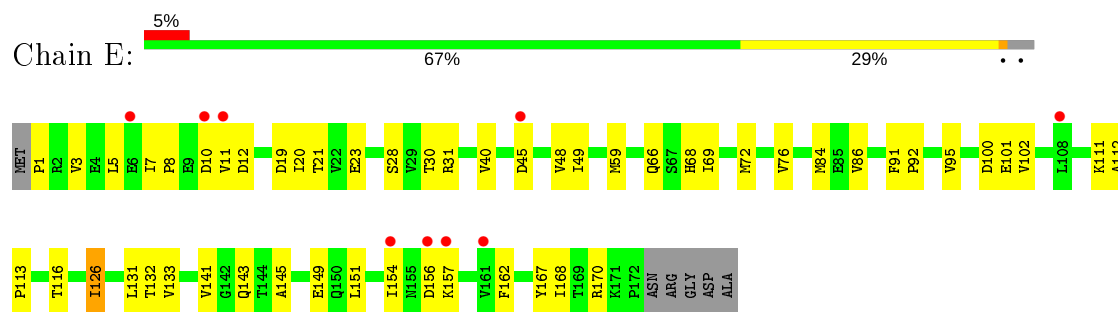




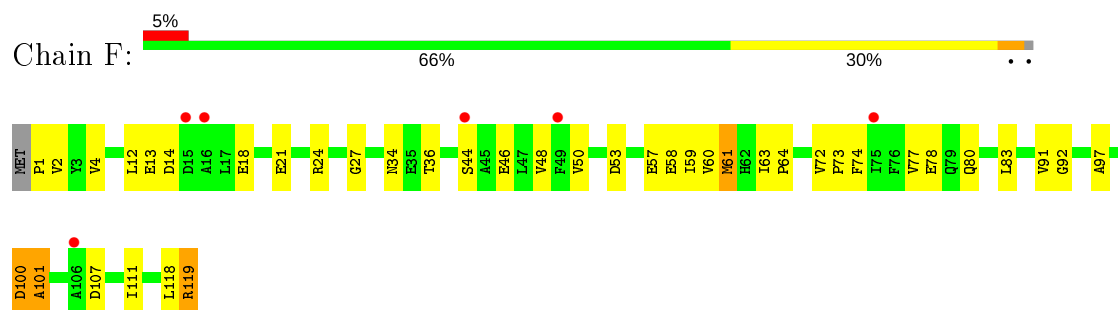
• Molecule 4: 50S ribosomal protein L5P



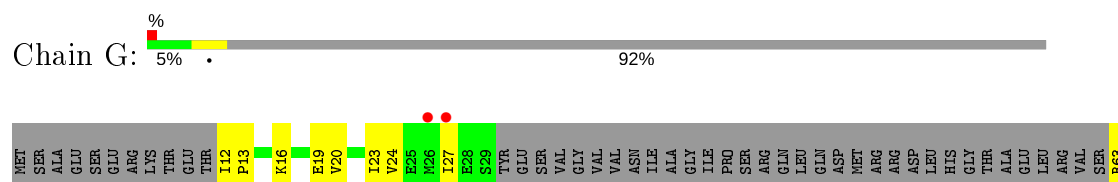
• Molecule 5: 50S ribosomal protein L6P

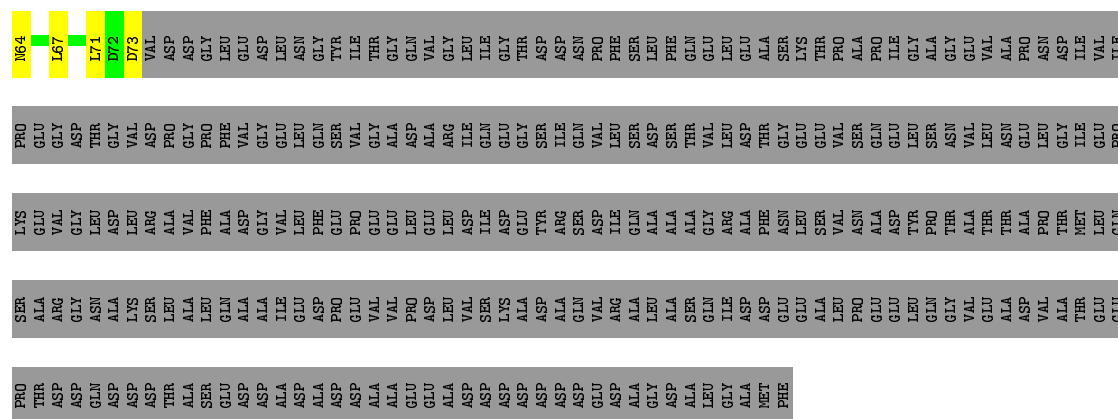


• Molecule 6: 50S ribosomal protein L7Ae

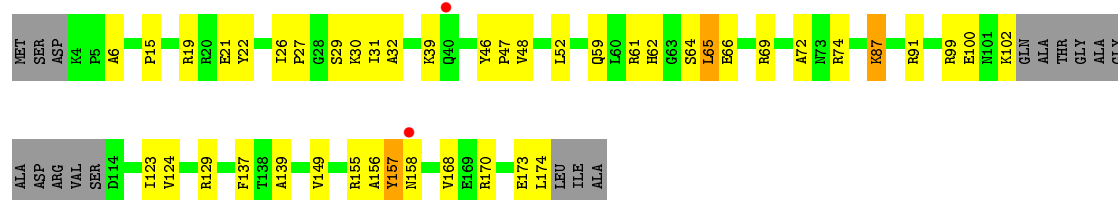


• Molecule 7: 50S ribosomal protein L10E

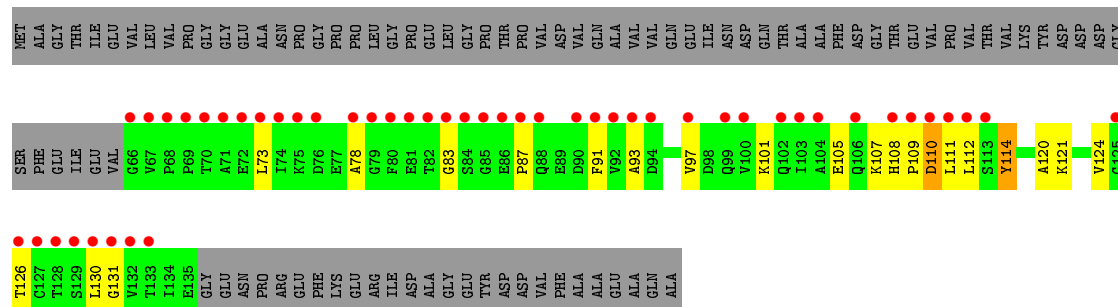




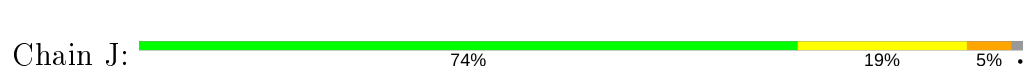
- Molecule 8: 50S ribosomal protein L10e



- Molecule 9: 50S ribosomal protein L11P

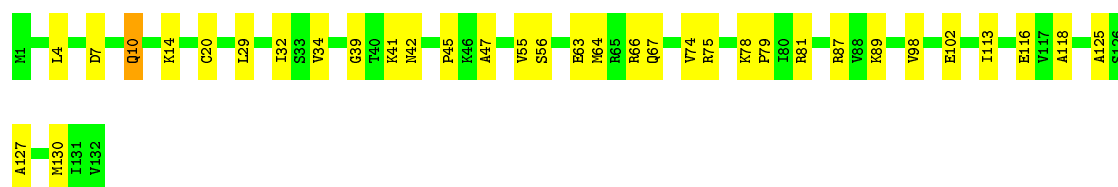


- Molecule 10: 50S ribosomal protein L13P

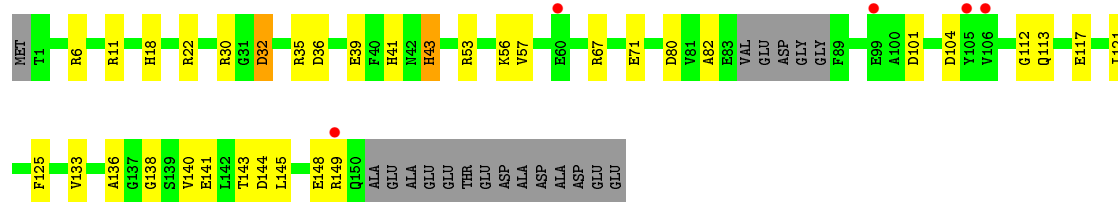


- Molecule 11: 50S ribosomal protein L14P

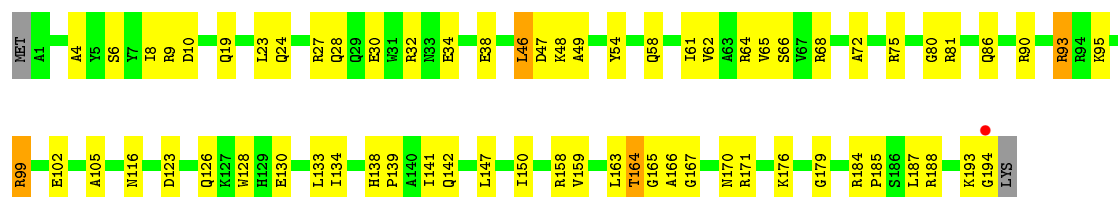




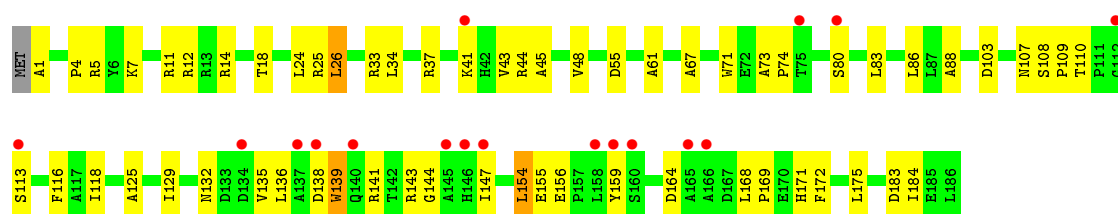
- Molecule 12: 50S ribosomal protein L15P



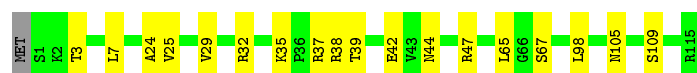
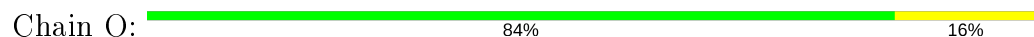
- Molecule 13: 50S ribosomal protein L15e



- Molecule 14: 50S ribosomal protein L18P

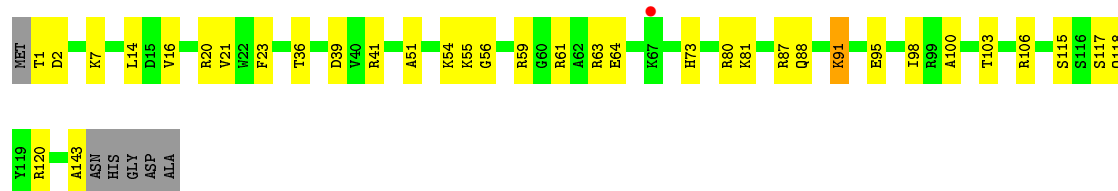


- Molecule 15: 50S ribosomal protein L18e



- Molecule 16: 50S ribosomal protein L19e





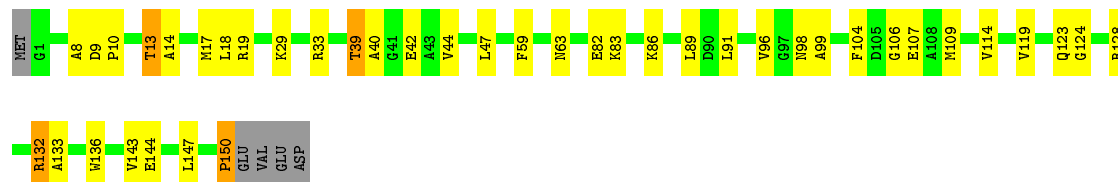
- Molecule 17: 50S ribosomal protein L21e

Chain Q: 72% 25% ..



- Molecule 18: 50S ribosomal protein L22P

Chain R: 70% 24% . .



- Molecule 19: 50S ribosomal protein L23P

Chain S: 2% 75% 20% 5%



- Molecule 20: 50S ribosomal protein L24P

Chain T: 3% 80% 18% ..



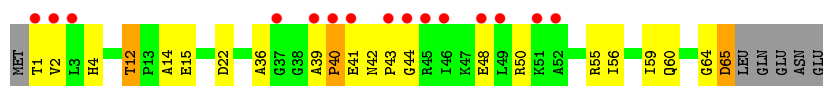
- Molecule 21: 50S ribosomal protein L24e

Chain U: 0% 51% 27% 21%



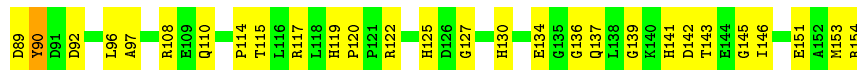
- Molecule 22: 50S ribosomal protein L29P

Chain V: 21% 61% 27% 8%



- Molecule 23: 50S ribosomal protein L30P

Chain W: 57% 42%



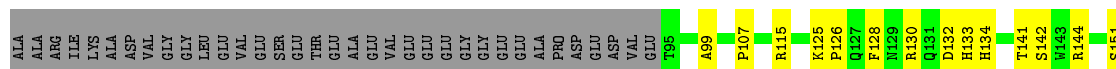
- Molecule 24: 50S ribosomal protein L31e

Chain X: 58% 32% 11%



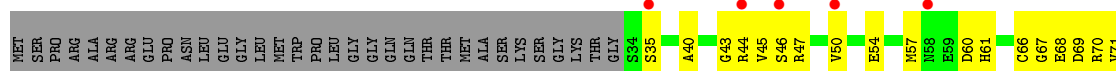
- Molecule 25: 50S ribosomal protein L32e

Chain Y: 43% 15% 41%



- Molecule 26: 50S ribosomal protein L37Ae

Chain Z: 5% 39% 24% 37%

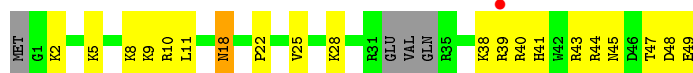


- Molecule 27: 50S ribosomal protein L37e

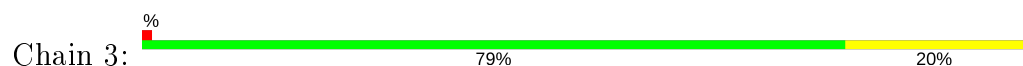
Chain 1: 68% 30%



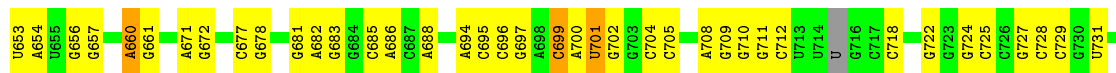
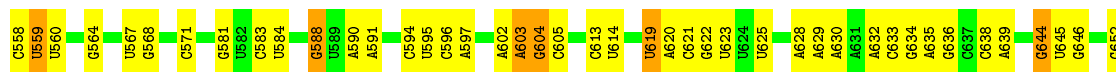
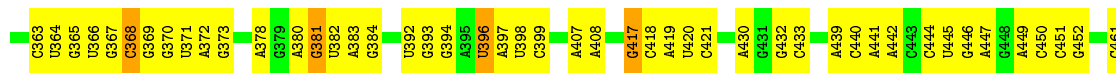
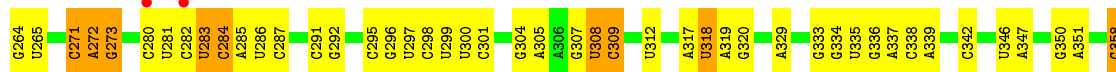
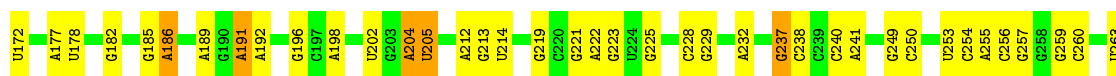
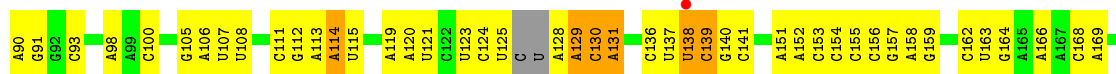
- Molecule 28: 50S ribosomal protein L39e



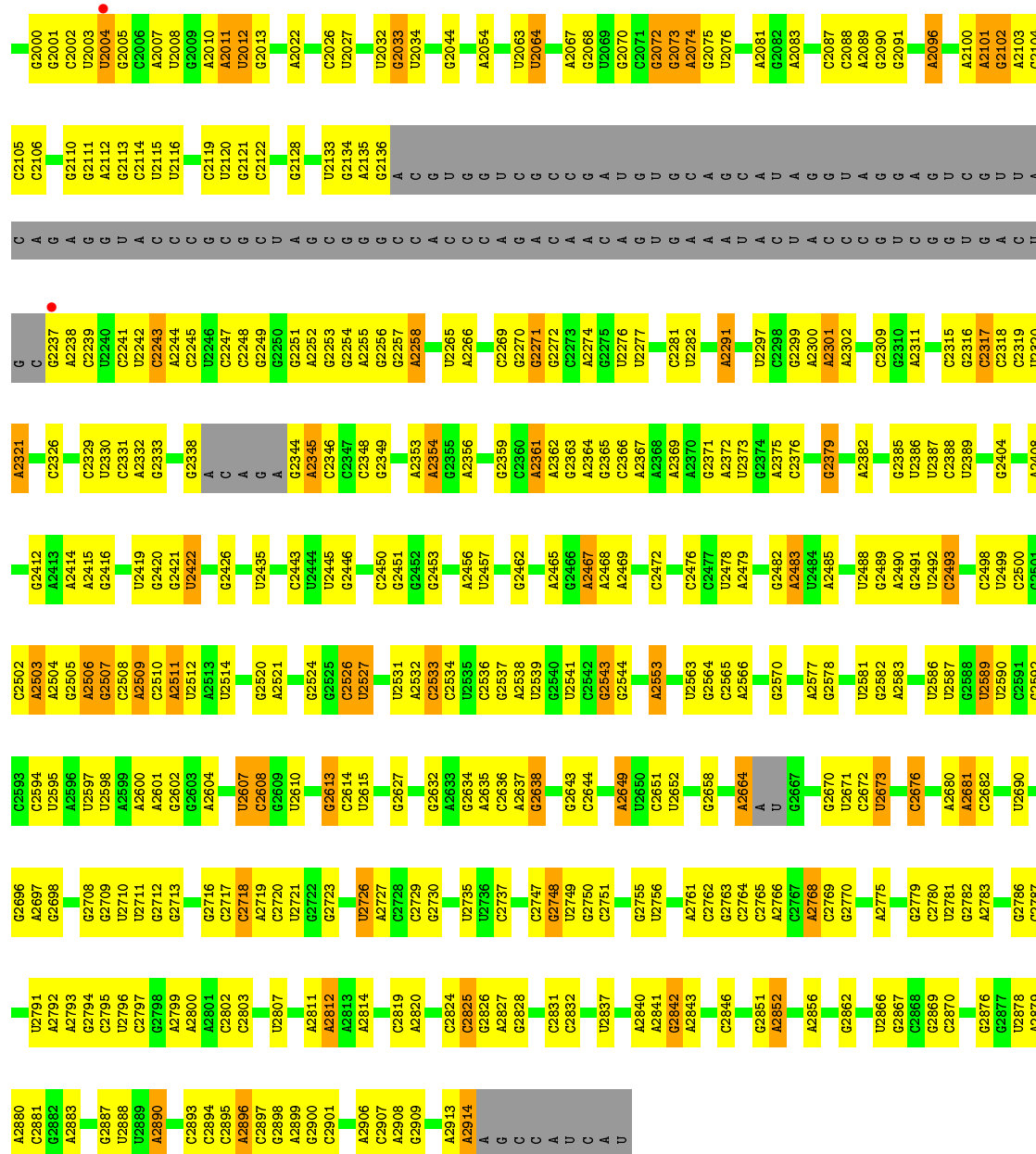
- Molecule 29: 50S ribosomal protein L44E



- Molecule 30: 23S RIBOSOMAL RNA

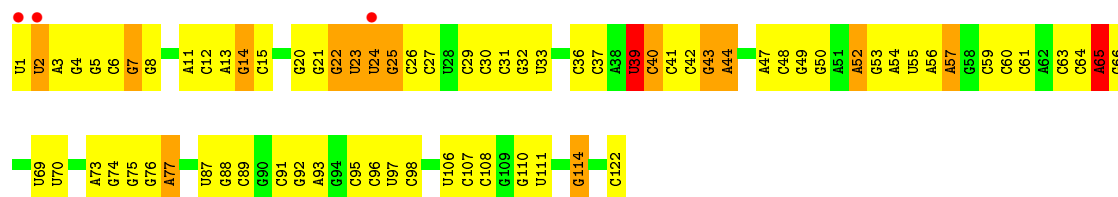


A1909	U1825	C1731	G1555	U1359	C1267	A1188	U1109	A	U932	C842	U734
U1915	C1826	A1732	A1559	C1360	C1268	A1189	U1110	C	U933	A843	C735
C1916	A1829	C1733	U	C1366	G1269	G1191	G1110	A	G935	A844	A736
A1919	C1834	C1735	U1561	A1372	C1273	A1192	U1116	C999	G936	U845	A737
C1920	U1835	A1736	C1562	G1377	A1278	A1193	U1117	C1000	C937	A846	G738
A1921	U1741	A1656	C1563	G1378	U1279	A1194	A1118	U1001	G938	C847	G743
A1922	A1742	A1657	C1564	G1379	A1279	A1195	U1119	C1002	A939	G744	G745
G1925	U1748	C1662	C1565	U1380	C1289	G1197	U1120	C1003	G940	U852	A746
C1840	A1664	A1663	C1566	G1381	U1291	U1198	G1121	A1006	U942	C854	G747
C1841	C1750	A1667	C1573	G1382	A1291	A1199	U1127	A1007	G943	U855	G748
A1842	G1751	C1574	C1575	U1383	A1294	A1200	U1128	C1008	G944	C749	G749
A1845	G1752	A1581	G1576	G1384	U1295	C1201	U1129	A1013	U945	A857	A750
G1849	A1755	C1582	U1577	C1385	G1296	A1202	U1130	A1014	C946	U858	A758
C1853	A1756	G1586	U1578	G1386	U1297	C1203	U1131	C1015	U947	U860	C759
G1854	A1670	U1587	G1588	G1387	U1298	C1204	A1132	U861	G948	U860	G759
A1931	G1675	G1589	G1589	U1388	G1299	U1205	A1133	U1016	U949	U862	A761
U1939	C1676	C1592	C1592	G1389	G1300	U1206	A1134	C1023	G950	U863	A761
C1859	G1676	C1593	C1593	U1390	U1304	A1207	U1135	G1024	A951	C764	C764
G1855	U1677	C1594	C1594	C1394	U1305	C1208	U1136	G1027	G952	G765	G765
A1857	C1679	U1500	U1500	G1395	U1306	C1209	U1137	U1028	U953	G869	G869
A1858	C1680	U1503	U1503	G1396	A1307	G1210	G1137	U1029	A954	G870	G772
C1861	G1681	C1504	C1504	G1397	A1308	C1213	G1151	C1044	G955	A872	C774
C1862	A1682	C1505	C1505	U1398	U1309	A1215	A1154	C1045	G956	G775	G775
G1863	C1683	C1506	C1506	A1399	U1310	G1216	G1155	U876	U960	A876	A776
C1864	A1684	U1507	U1507	C1407	U1314	G1217	C1156	G1052	A961	G877	U777
G1866	C1686	C1507	C1507	U1408	G1315	U1218	C1157	G1053	G877	G877	A790
C1867	U1687	U1511	U1511	G1409	G1316	U1219	G1158	G1054	G878	A791	A791
U1871	G1773	G1512	G1512	A1413	A1317	U1220	G1159	G1055	A882	U794	U794
C1872	C1692	A1515	A1515	A1414	U1318	G1226	A1161	U1056	G885	G800	G800
G1873	G1697	U1516	U1516	G1415	G1319	C1229	G1163	A1057	U801	U801	U801
G1877	A1778	G1520	G1520	G1416	C1320	A1230	U1164	A1058	C890	U806	U806
C1878	A1779	C1521	C1521	G1417	G1322	U1234	G1165	A1059	C891	A807	A807
U1878	U1702	A1522	A1522	U1418	G1325	U1237	A1166	C	A894	A808	A808
C1880	C1705	G1523	G1523	U1419	C1326	U1238	C1167	C	G	G809	G809
A1881	C1706	U1524	U1524	C1422	G1327	G1239	C1168	U1066	G898	A812	A812
C1882	G1707	A1526	A1526	C1423	A1328	U1243	U1169	A1067	C	C813	C813
G1884	C1792	U1527	U1527	A1427	G1331	A1244	A1171	G1072	G902	U814	U814
A1885	G1795	A1528	A1528	C1428	U1339	C1245	G1172	A1078	U903	U815	U815
A1886	U1710	G1529	G1529	U1428	G1340	A1246	A1173	A1079	G	G816	G816
C1889	C1714	U1535	U1535	A1434	C1342	G1247	C1175	C1080	A	G817	G817
U1890	G1715	C1536	C1536	G1441	G1343	A1247	A1177	A1081	G	A907	A907
C1894	A1716	U1538	U1538	A1442	C1344	U1248	G1178	A1086	A	A908	A908
A1895	C1717	G1543	G1543	G1443	U1350	C1250	U1179	G1087	G	G820	G820
G1896	A1717	U1544	U1544	U1444	G1351	C1251	A1180	A1088	A	U821	U821
U1897	U1722	C1545	C1545	U1446	A1352	A1252	C1182	G	G	C822	C822
C1902	G1723	G1546	G1546	U1447	C1353	C1253	C1183	A1097	G	G834	G834
U1903	U1724	C1553	C1553	C1450	A1357	G1265	U1185	A1098	U	U835	U835
A1904	C1725	A1641	A1641	C1451	A1358	U1266	C1186	G1099	G	U840	U840
U1905	G1730	C1554	C1554				U1187	C1104	C	A841	A841



- Molecule 31: 5S RIBOSOMAL RNA

Chain 9: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.33Å 299.62Å 575.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 85.65 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-2.90) 98.2 (85.65-2.41)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.186 , 0.233 0.177 , 0.224	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 82.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99120	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/1786	0.64	0/2408
2	B	0.34	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.32	0/1111	0.56	1/1498 (0.1%)
5	E	0.33	0/1382	0.57	0/1880
6	F	0.35	0/901	0.57	0/1224
7	G	0.33	0/241	0.51	0/324
8	H	0.33	0/1302	0.63	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.36	0/1136	0.61	0/1530
11	K	0.34	0/1004	0.66	0/1351
12	L	0.35	0/1130	0.64	0/1509
13	M	0.36	0/1582	0.61	0/2116
14	N	0.30	0/1474	0.61	0/1999
15	O	0.35	0/874	0.59	0/1181
16	P	0.33	0/1147	0.53	0/1528
17	Q	0.34	0/749	0.65	0/1005
18	R	1.26	7/1172 (0.6%)	1.09	6/1578 (0.4%)
19	S	0.33	0/648	0.54	0/875
20	T	0.32	0/958	0.64	0/1289
21	U	0.32	0/417	0.57	0/562
22	V	0.32	0/502	0.54	0/675
23	W	0.36	0/1219	0.63	0/1655
24	X	0.35	0/664	0.60	0/895
25	Y	0.37	0/1146	0.62	0/1536
26	Z	0.36	0/584	0.63	0/781
27	1	0.39	0/438	0.62	0/578
28	2	0.34	0/401	0.58	0/529
29	3	0.37	0/771	0.57	0/1024
30	0	0.39	0/65954	0.68	9/102862 (0.0%)
31	9	0.33	0/2904	0.68	1/4526 (0.0%)
All	All	0.40	7/98698 (0.0%)	0.67	17/147581 (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
18	R	1	0
23	W	0	1
30	0	0	32
31	9	0	3
All	All	1	36

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.45	2.87	1.50
18	R	150	PRO	CA-C	-18.11	1.16	1.52
18	R	150	PRO	CG-CD	13.90	1.96	1.50
18	R	150	PRO	C-O	11.92	1.47	1.23
18	R	150	PRO	N-CA	11.35	1.66	1.47
18	R	150	PRO	N-CD	10.74	1.62	1.47
18	R	150	PRO	CA-CB	7.56	1.68	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.81	112.00
18	R	150	PRO	N-CA-C	-19.38	61.71	112.10
18	R	150	PRO	CA-N-CD	12.28	128.89	111.70
18	R	150	PRO	N-CA-CB	10.98	116.47	103.30
18	R	150	PRO	CA-C-O	-8.52	99.75	120.20
31	9	39	U	N1-C1'-C2'	6.32	122.22	114.00
18	R	150	PRO	CA-CB-CG	-6.13	92.34	104.00
30	0	1592	G	N9-C1'-C2'	6.12	121.95	114.00
30	0	1504	A	C1'-O4'-C4'	-5.86	105.21	109.90
30	0	1504	A	N9-C1'-C2'	5.70	121.41	114.00
30	0	871	G	C5'-C4'-O4'	-5.36	102.67	109.10
30	0	1120	U	C5'-C4'-C3'	-5.35	107.45	116.00
30	0	841	A	C1'-O4'-C4'	-5.30	105.66	109.90
30	0	2726	U	N1-C1'-C2'	5.24	120.81	114.00
30	0	1819	G	C5'-C4'-C3'	5.05	124.07	116.00
30	0	2301	A	N9-C1'-C2'	5.01	120.52	114.00
4	D	170	TYR	N-CA-C	5.01	124.53	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	1080	C	Sidechain
30	0	1309	U	Sidechain
30	0	1327	G	Sidechain
30	0	1417	G	Sidechain
30	0	1592	G	Sidechain
30	0	1684	A	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1979	G	Sidechain
30	0	202	U	Sidechain
30	0	205	U	Sidechain
30	0	221	G	Sidechain
30	0	2492	U	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2543	G	Sidechain
30	0	2607	U	Sidechain
30	0	2632	G	Sidechain
30	0	2673	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	470	U	Sidechain
30	0	48	A	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	817	G	Sidechain
30	0	818	A	Sidechain
31	9	39	U	Sidechain
31	9	65	A	Sidechain
31	9	87	U	Sidechain
23	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	A	1753	0	1766	66	0
2	B	2625	0	2533	94	0
3	C	1860	0	1813	53	0
4	D	1094	0	1085	52	0
5	E	1357	0	1266	36	0
6	F	890	0	843	30	0
7	G	240	0	231	11	0
8	H	1282	0	1292	41	0
9	I	519	0	500	21	0
10	J	1120	0	1098	38	0
11	K	994	0	1027	39	0
12	L	1118	0	1076	33	0
13	M	1558	0	1573	59	0
14	N	1445	0	1401	54	0
15	O	865	0	873	18	0
16	P	1136	0	1123	30	0
17	Q	735	0	729	26	0
18	R	1149	0	1122	32	0
19	S	641	0	605	10	0
20	T	950	0	924	22	0
21	U	410	0	364	17	0
22	V	499	0	511	17	0
23	W	1196	0	1137	66	0
24	X	654	0	653	22	0
25	Y	1130	0	1133	33	0
26	Z	573	0	531	21	0
27	1	431	0	426	21	0
28	2	396	0	413	21	0
29	3	755	0	728	17	0
30	0	59018	0	29809	1329	0
31	9	2599	0	1325	97	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	9	0	0	3	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	1	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	93	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	65	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5950	0	0	203	0
38	1	54	0	0	3	0
38	2	43	0	0	1	0
38	3	68	0	0	6	0
38	9	148	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	A	112	0	0	5	0
38	B	142	0	0	14	0
38	C	168	0	0	13	0
38	D	45	0	0	4	0
38	E	42	0	0	4	0
38	F	26	0	0	1	0
38	G	17	0	0	1	0
38	H	65	0	0	5	0
38	I	5	0	0	0	0
38	J	56	0	0	2	0
38	K	60	0	0	5	0
38	L	82	0	0	8	0
38	M	123	0	0	2	0
38	N	59	0	0	3	0
38	O	47	0	0	4	0
38	P	59	0	0	2	0
38	Q	47	0	0	2	0
38	R	76	0	0	1	0
38	S	33	0	0	0	0
38	T	36	0	0	4	0
38	U	26	0	0	2	0
38	V	12	0	0	1	0
38	W	66	0	0	6	0
38	X	28	0	0	3	0
38	Y	97	0	0	7	0
38	Z	31	0	0	4	0
All	All	99120	0	59910	2191	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 (2191) 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.44
30:0:871:G:C8	30:0:871:G:H5'	1.75	1.21
14:N:37:ARG:NH1	31:9:6:C:H5''	1.62	1.12
31:9:56:A:H2'	31:9:57:A:H5''	1.21	1.11
30:0:1160:G:C5'	30:0:1161:A:H5'	1.79	1.11
30:0:1160:G:H5'	30:0:1161:A:C5'	1.83	1.09
30:0:871:G:H8	30:0:871:G:H5'	1.00	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:545:G:H8	30:0:545:G:H5'	1.12	1.08
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07
30:0:1474:C:H6	30:0:1474:C:H5'	1.19	1.07
30:0:1559:A:H1'	38:0:5888:HOH:O	1.54	1.07
13:M:171:ARG:HD3	30:0:156:C:H5''	1.38	1.04
30:0:69:A:H5'	30:0:69:A:C8	1.93	1.03
10:J:82:THR:HG23	30:0:1242:A:H5'	1.38	1.02
30:0:1474:C:C6	30:0:1474:C:H5'	1.96	1.01
4:D:154:LYS:HD2	4:D:154:LYS:H	1.26	1.01
30:0:1666:C:O2'	30:0:1667:A:H5''	1.62	0.99
30:0:2717:C:C2'	30:0:2718:C:H5''	1.93	0.99
31:9:76:G:H3'	31:9:77:A:H5''	1.41	0.98
30:0:69:A:H5'	30:0:69:A:H8	1.28	0.97
30:0:871:G:H8	30:0:871:G:C5'	1.78	0.96
30:0:1116:U:O2'	30:0:1118:A:H2	1.47	0.96
30:0:1205:U:H2'	30:0:1206:U:C5'	1.96	0.96
30:0:2717:C:H2'	30:0:2718:C:H5''	1.45	0.96
30:0:2812:A:H2	30:0:2814:A:H62	1.02	0.95
30:0:1603:A:H5'	30:0:1605:G:O4'	1.66	0.95
30:0:545:G:C8	30:0:545:G:H5'	2.00	0.95
30:0:1165:G:H21	30:0:1173:A:H5''	1.30	0.95
30:0:870:G:H2'	30:0:871:G:H5''	1.47	0.95
15:O:3:THR:HG22	30:0:656:G:H5'	1.45	0.95
30:0:2291:A:C8	30:0:2309:C:H5'	2.03	0.94
30:0:877:G:H5'	30:0:878:G:OP1	1.67	0.94
30:0:2316:G:H5''	38:0:6122:HOH:O	1.66	0.94
30:0:1666:C:C2'	30:0:1667:A:H5''	1.97	0.93
30:0:542:A:H5'	30:0:542:A:H8	1.30	0.93
3:C:236:THR:HG22	3:C:239:ALA:H	1.31	0.92
30:0:1206:U:H6	30:0:1206:U:H5'	1.34	0.92
30:0:2506:A:HO2'	30:0:2507:G:H8	1.10	0.92
30:0:381:G:H5''	38:0:4327:HOH:O	1.68	0.92
30:0:2502:C:C2'	30:0:2503:A:H5'	2.00	0.92
11:K:10:GLN:H	11:K:10:GLN:HE21	0.97	0.92
30:0:182:G:H5'	38:0:5177:HOH:O	1.68	0.92
16:P:115:SER:H	16:P:118:GLN:HE21	0.99	0.92
30:0:2502:C:H2'	30:0:2503:A:H5'	1.50	0.91
31:9:56:A:C2'	31:9:57:A:H5''	2.00	0.91
30:0:1160:G:H5'	30:0:1161:A:H5'	0.94	0.91
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.51	0.91
30:0:1187:U:HO2'	30:0:1189:A:H2	1.11	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2908:A:H2'	30:0:2909:G:O4'	1.69	0.90
30:0:2526:C:H5'	30:0:2526:C:H6	1.36	0.90
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.85	0.90
30:0:1835:U:H5	30:0:1840:A:N7	1.70	0.90
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.17	0.90
30:0:2004:U:H4'	38:0:5326:HOH:O	1.70	0.90
30:0:1701:A:H4'	30:0:1702:U:H5''	1.51	0.89
30:0:1184:C:H1'	38:0:7505:HOH:O	1.70	0.89
6:F:91:VAL:HG12	6:F:92:GLY:H	1.34	0.89
30:0:2526:C:H5'	30:0:2526:C:C6	2.07	0.89
31:9:29:C:H2'	31:9:30:C:H5'	1.55	0.89
30:0:282:C:H1'	30:0:368:C:N4	1.86	0.89
30:0:506:G:H22	30:0:509:A:C5'	1.86	0.89
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.55	0.88
30:0:1189:A:H1'	30:0:1209:C:O4'	1.74	0.88
38:B:9099:HOH:O	30:0:2672:C:H1'	1.72	0.88
30:0:541:C:H2'	30:0:542:A:H5''	1.56	0.88
30:0:31:C:H2'	38:0:7724:HOH:O	1.73	0.87
30:0:541:C:C2'	30:0:542:A:H5''	2.05	0.87
2:B:238:ASN:HD22	2:B:240:GLY:H	1.20	0.87
30:0:1372:A:H3'	38:0:7228:HOH:O	1.74	0.87
30:0:2769:C:C2'	30:0:2770:G:H5'	2.05	0.87
30:0:2111:G:H1'	38:0:9054:HOH:O	1.75	0.87
30:0:214:U:H5'	38:0:6171:HOH:O	1.74	0.86
30:0:1205:U:H2'	30:0:1206:U:H5''	1.57	0.86
30:0:1183:C:H2'	38:0:6275:HOH:O	1.76	0.86
30:0:1165:G:N2	30:0:1173:A:H5''	1.89	0.86
31:9:14:G:H5'	31:9:14:G:H8	1.41	0.86
2:B:162:MET:HE3	2:B:308:LEU:HD21	1.56	0.86
30:0:2586:U:H3	30:0:2592:G:H22	1.16	0.85
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.59	0.85
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.57	0.85
30:0:1165:G:H1'	30:0:1174:A:H1'	1.58	0.84
30:0:506:G:H22	30:0:509:A:H5'	1.42	0.84
30:0:2010:A:H2'	38:0:5984:HOH:O	1.77	0.84
15:O:3:THR:CG2	30:0:656:G:H5'	2.07	0.84
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.58	0.83
13:M:95:LYS:HE2	30:0:157:G:H4'	1.59	0.83
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.94	0.83
11:K:39:GLY:HA2	38:0:5241:HOH:O	1.79	0.83
30:0:1118:A:H3'	30:0:1118:A:C8	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1667:A:H8	30:0:1667:A:H5'	1.44	0.82
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.24	0.82
30:0:2073:G:H5''	38:0:3833:HOH:O	1.80	0.81
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.60	0.81
30:0:1205:U:H2'	30:0:1206:U:H5'	1.62	0.81
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.78	0.81
30:0:1118:A:H3'	30:0:1118:A:H8	1.46	0.80
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.46	0.80
30:0:559:U:H5'	30:0:559:U:H6	1.46	0.80
30:0:1666:C:H2'	30:0:1667:A:C5'	2.12	0.80
30:0:1201:C:H2'	30:0:1202:A:H5'	1.65	0.79
30:0:871:G:C8	30:0:871:G:C5'	2.57	0.79
30:0:282:C:O2'	30:0:283:U:H5'	1.81	0.79
30:0:2766:A:H5'	38:0:9567:HOH:O	1.81	0.79
30:0:2769:C:H2'	30:0:2770:G:H5'	1.62	0.79
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.63	0.79
30:0:1377:C:H6	30:0:1377:C:H5'	1.48	0.79
30:0:1300:G:H1'	38:0:4692:HOH:O	1.81	0.78
30:0:1119:G:N2	30:0:1246:A:C2	2.51	0.78
3:C:139:VAL:HG13	38:C:8646:HOH:O	1.83	0.78
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.64	0.78
30:0:2748:G:H5'	38:0:7581:HOH:O	1.83	0.78
30:0:10:U:H6	30:0:10:U:H3'	1.49	0.78
30:0:1942:A:H5'	38:0:7387:HOH:O	1.82	0.78
11:K:10:GLN:H	11:K:10:GLN:NE2	1.79	0.78
20:T:9:LYS:HE3	20:T:13:ARG:NH1	1.99	0.78
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.65	0.78
30:0:2103:A:H62	30:0:2538:A:H8	1.32	0.77
30:0:308:U:H5'	30:0:309:C:OP1	1.84	0.77
30:0:396:U:H1'	38:0:7666:HOH:O	1.83	0.77
30:0:541:C:H2'	30:0:542:A:C5'	2.14	0.77
23:W:88:THR:HB	38:W:6679:HOH:O	1.84	0.77
16:P:115:SER:H	16:P:118:GLN:NE2	1.81	0.77
30:0:2491:G:H1'	38:0:6907:HOH:O	1.86	0.76
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.68	0.76
30:0:1474:C:C5'	30:0:1474:C:H6	1.98	0.76
30:0:2533:C:H5'	30:0:2533:C:H6	1.50	0.76
30:0:870:G:C2'	30:0:871:G:H5''	2.13	0.76
30:0:2420:G:O2'	30:0:2421:G:H5'	1.86	0.76
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.48	0.76
30:0:1205:U:C2'	30:0:1206:U:H5''	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:2:U:OP2	31:9:3:A:H5'	1.85	0.76
31:9:92:G:H2'	31:9:93:A:C8	2.21	0.76
30:0:2256:G:O2'	30:0:2257:G:H5'	1.85	0.75
30:0:558:C:C2'	30:0:559:U:H5''	2.16	0.75
22:V:1:THR:HG23	22:V:2:VAL:H	1.51	0.75
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.66	0.75
30:0:1451:C:H5'	30:0:1505:U:C5	2.21	0.75
30:0:1632:A:H2'	30:0:1633:C:H5'	1.69	0.75
30:0:2256:G:C2'	30:0:2257:G:H5'	2.16	0.75
30:0:2717:C:O2'	30:0:2718:C:H5''	1.86	0.75
1:A:199:HIS:HD2	1:A:201:PHE:H	1.33	0.75
30:0:2787:C:H5	38:0:4643:HOH:O	1.69	0.75
30:0:558:C:O2'	30:0:559:U:H5''	1.87	0.75
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.69	0.75
30:0:681:G:N3	30:0:681:G:H5'	2.02	0.75
30:0:1603:A:H5''	30:0:1605:G:H5'	1.68	0.74
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.52	0.74
14:N:113:SER:HB2	38:N:8852:HOH:O	1.87	0.74
30:0:1878:G:H1'	38:0:6151:HOH:O	1.87	0.74
14:N:144:GLY:O	14:N:147:ILE:HG22	1.87	0.74
2:B:179:LEU:O	2:B:183:GLU:HG2	1.86	0.74
30:0:2135:A:O2'	30:0:2136:G:H5'	1.86	0.74
30:0:821:U:H3'	38:0:3779:HOH:O	1.87	0.74
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.69	0.74
30:0:1187:U:O2'	30:0:1189:A:H2	1.71	0.74
30:0:1116:U:H3	30:0:1246:A:H62	1.36	0.74
30:0:2103:A:HO2'	30:0:2104:C:H6	1.36	0.74
2:B:98:THR:HG22	30:0:2820:A:OP1	1.88	0.74
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.86	0.74
30:0:107:U:H2'	30:0:108:U:H5'	1.70	0.73
38:C:8660:HOH:O	30:0:2100:A:H5'	1.87	0.73
30:0:283:U:H5	30:0:284:C:N3	1.86	0.73
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.33	0.73
30:0:2426:G:H1'	38:0:6122:HOH:O	1.88	0.73
30:0:2768:A:O2'	30:0:2769:C:H5'	1.88	0.73
30:0:12:U:H2'	30:0:13:G:H5'	1.69	0.73
30:0:1183:C:N4	30:0:1184:C:H41	1.85	0.73
13:M:171:ARG:CD	30:0:156:C:H5''	2.16	0.73
30:0:1835:U:C5	30:0:1840:A:N7	2.55	0.73
2:B:336:GLN:O	30:0:2862:G:H4'	1.88	0.73
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1166:A:H61	30:0:1180:U:H3	1.37	0.72
30:0:1182:C:H1'	30:0:1192:A:H8	1.54	0.72
30:0:1666:C:C2'	30:0:1667:A:C5'	2.67	0.72
30:0:1701:A:H5'	38:0:6316:HOH:O	1.89	0.72
30:0:1741:U:H5'	30:0:1742:A:OP1	1.89	0.72
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.70	0.72
30:0:2506:A:O2'	30:0:2507:G:H8	1.72	0.72
1:A:35:GLY:O	1:A:36:ASP:HB3	1.87	0.72
30:0:1189:A:H3'	38:0:7717:HOH:O	1.89	0.72
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.72	0.72
30:0:2637:A:H5'	38:0:9282:HOH:O	1.88	0.72
22:V:1:THR:HB	30:0:93:C:H5''	1.72	0.72
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.70	0.72
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.25	0.72
30:0:2896:A:H5''	38:0:6129:HOH:O	1.90	0.72
11:K:10:GLN:N	11:K:10:GLN:HE21	1.81	0.71
31:9:14:G:H5'	31:9:14:G:C8	2.24	0.71
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.71	0.71
14:N:11:ARG:HD3	31:9:114:G:O6	1.90	0.71
24:X:71:ARG:HD3	38:X:2171:HOH:O	1.89	0.71
30:0:1973:A:H5'	30:0:1973:A:H8	1.54	0.71
30:0:2102:G:H5'	30:0:2538:A:C2	2.24	0.71
31:9:54:A:O2'	31:9:55:U:H5'	1.91	0.71
30:0:542:A:H5'	30:0:542:A:C8	2.20	0.71
30:0:564:G:H1'	38:0:6343:HOH:O	1.91	0.71
1:A:211:LYS:HB2	38:A:9077:HOH:O	1.90	0.71
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.72	0.71
30:0:10:U:C6	30:0:10:U:H3'	2.26	0.71
20:T:61:GLU:HG2	38:T:3851:HOH:O	1.90	0.71
30:0:1187:U:H2'	38:0:6936:HOH:O	1.91	0.70
5:E:143:GLN:NE2	30:0:2779:G:H21	1.89	0.70
4:D:105:SER:OG	30:0:2338:G:H1'	1.89	0.70
30:0:2578:G:H5'	30:0:2578:G:H8	1.57	0.70
38:Y:8860:HOH:O	33:0:8817:CL:CL	2.46	0.70
31:9:23:U:O2'	31:9:24:U:H4'	1.91	0.70
23:W:88:THR:HG22	23:W:89:ASP:H	1.56	0.70
30:0:2256:G:H2'	30:0:2257:G:H5'	1.73	0.70
3:C:1:MET:HG2	3:C:2:GLN:H	1.55	0.70
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.73	0.70
30:0:1205:U:C2'	30:0:1206:U:C5'	2.69	0.70
30:0:2781:U:C2'	30:0:2782:G:H5'	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2756:U:H3	30:0:2896:A:H2	1.37	0.70
31:9:64:C:H2'	31:9:65:A:H5'	1.74	0.70
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.21	0.70
6:F:91:VAL:HG12	6:F:92:GLY:N	2.07	0.70
30:0:567:U:H5''	38:0:6437:HOH:O	1.90	0.70
4:D:103:ASN:HD22	4:D:134:LEU:H	1.39	0.70
30:0:545:G:H8	30:0:545:G:C5'	2.00	0.69
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.73	0.69
30:0:1058:A:H2'	30:0:1060:C:H5''	1.74	0.69
17:Q:11:ARG:HD3	38:0:6291:HOH:O	1.92	0.69
30:0:1174:A:C5	30:0:1201:C:H4'	2.27	0.69
30:0:794:U:H3	30:0:819:A:H61	1.40	0.69
30:0:1666:C:H2'	30:0:1667:A:H5'	1.75	0.69
30:0:1377:C:H1'	38:0:9044:HOH:O	1.91	0.69
1:A:223:ARG:HH22	30:0:2271:G:P	2.16	0.69
30:0:960:G:H3'	30:0:960:G:N3	2.07	0.69
30:0:1525:G:H5'	30:0:1526:A:OP2	1.93	0.69
30:0:847:C:H4'	38:0:3762:HOH:O	1.92	0.69
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.75	0.69
14:N:37:ARG:HH12	31:9:6:C:H5''	1.51	0.69
2:B:206:THR:HG21	30:0:2716:G:H5''	1.74	0.69
13:M:164:THR:HG22	13:M:167:GLY:H	1.58	0.69
30:0:821:U:H5''	38:0:3057:HOH:O	1.93	0.68
30:0:1118:A:H62	30:0:1244:U:H3	1.39	0.68
30:0:2852:A:H5''	38:0:5254:HOH:O	1.93	0.68
30:0:271:C:H41	30:0:378:A:H2	1.40	0.68
30:0:2769:C:H2'	30:0:2770:G:C5'	2.23	0.68
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.94	0.68
22:V:50:ARG:HH12	30:0:56:G:H5''	1.59	0.68
30:0:1701:A:H4'	30:0:1702:U:C5'	2.20	0.68
30:0:2851:G:O2'	30:0:2852:A:H5'	1.92	0.68
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.74	0.68
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.75	0.68
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.93	0.68
30:0:1595:G:O2'	30:0:1596:U:H5'	1.92	0.68
30:0:2635:A:O2'	30:0:2636:C:H5'	1.94	0.68
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.75	0.68
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.11	0.68
2:B:97:LEU:HD22	2:B:127:GLN:HE21	1.57	0.68
18:R:150:PRO:O	18:R:150:PRO:CG	2.41	0.68
30:0:1132:A:N6	30:0:1229:C:H2'	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:O:8813:CL:CL	38:O:4692:HOH:O	2.48	0.68
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.09	0.68
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.76	0.68
11:K:81:ARG:HB2	11:K:87:ARG:HH11	1.59	0.67
30:O:559:U:H5'	30:O:559:U:C6	2.29	0.67
30:O:69:A:H8	30:O:69:A:C5'	2.06	0.67
30:O:506:G:H22	30:O:509:A:H5''	1.58	0.67
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.58	0.67
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.95	0.67
25:Y:212:ARG:HD2	38:Y:8904:HOH:O	1.94	0.67
30:O:2812:A:C2	30:O:2814:A:N6	2.58	0.67
8:H:155:ARG:NH1	30:O:2503:A:H5''	2.09	0.67
8:H:30:LYS:H	8:H:62:HIS:HD2	1.39	0.67
30:O:380:A:H2'	38:O:7265:HOH:O	1.93	0.67
31:9:22:G:H5'	31:9:23:U:OP1	1.95	0.67
30:O:2317:C:C6	38:O:6122:HOH:O	2.46	0.67
14:N:80:SER:HB2	38:N:8833:HOH:O	1.94	0.67
30:O:1279:U:O2	30:O:1279:U:H2'	1.95	0.67
30:O:671:A:O2'	30:O:672:G:H2'	1.94	0.67
16:P:117:SER:HB3	30:O:1593:C:OP1	1.94	0.67
30:O:1183:C:O2	30:O:1183:C:H2'	1.93	0.67
5:E:133:VAL:HG12	5:E:141:VAL:HG13	1.76	0.67
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.41	0.67
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.77	0.66
1:A:199:HIS:CD2	1:A:201:PHE:H	2.12	0.66
3:C:236:THR:HG22	3:C:239:ALA:N	2.08	0.66
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.76	0.66
30:O:1159:G:H21	30:O:1189:A:H8	1.43	0.66
30:O:2781:U:O2'	30:O:2782:G:H5'	1.96	0.66
28:2:41:HIS:HD2	28:2:44:ARG:H	1.42	0.66
2:B:5:ARG:HH11	2:B:8:LYS:HE2	1.61	0.66
12:L:39:GLU:HG2	30:O:926:A:H4'	1.76	0.66
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.94	0.66
30:O:2256:G:H2'	30:O:2257:G:C5'	2.25	0.66
31:9:64:C:C2'	31:9:65:A:H5'	2.26	0.66
10:J:82:THR:CG2	30:O:1242:A:H5'	2.21	0.66
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.76	0.66
30:O:2781:U:H2'	30:O:2782:G:H5'	1.76	0.66
28:2:18:ASN:HD21	28:2:40:ARG:H	1.41	0.66
31:9:7:G:H5'	38:9:9100:HOH:O	1.96	0.66
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:204:ARG:HH22	30:0:553:G:P	2.18	0.66
30:0:1189:A:H1'	30:0:1209:C:C1'	2.25	0.66
30:0:1377:C:H5'	30:0:1377:C:C6	2.31	0.66
30:0:2001:G:O2'	30:0:2002:C:H5'	1.96	0.66
4:D:103:ASN:ND2	4:D:134:LEU:H	1.92	0.66
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.76	0.66
30:0:2251:G:H2'	30:0:2252:A:C8	2.30	0.66
30:0:2769:C:O2'	30:0:2770:G:H5'	1.96	0.65
30:0:558:C:H2'	30:0:559:U:C5'	2.26	0.65
30:0:1118:A:C8	30:0:1118:A:C3'	2.77	0.65
30:0:1524:U:OP1	30:0:1524:U:H4'	1.96	0.65
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.78	0.65
30:0:1634:G:H3'	38:0:3903:HOH:O	1.96	0.65
30:0:2768:A:H2'	30:0:2769:C:O4'	1.96	0.65
3:C:174:ILE:HD11	30:0:338:C:H4'	1.78	0.65
30:0:603:A:H5''	30:0:604:G:OP1	1.97	0.65
30:0:1441:G:O2'	30:0:1442:A:H5'	1.97	0.65
30:0:2827:A:H2'	30:0:2828:G:O4'	1.97	0.65
30:0:1972:U:H2'	30:0:1973:A:C5'	2.26	0.65
30:0:2507:G:H2'	30:0:2510:C:H42	1.62	0.65
30:0:2613:G:O2'	30:0:2614:C:H5'	1.97	0.65
30:0:635:A:H2'	30:0:636:G:H5''	1.78	0.65
6:F:21:GLU:O	6:F:24:ARG:HG2	1.97	0.65
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.96	0.65
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.77	0.65
16:P:55:LYS:HG2	16:P:56:GLY:N	2.12	0.65
27:I:20:ARG:HG2	30:0:111:C:O2'	1.97	0.65
14:N:37:ARG:NH1	31:9:6:C:C5'	2.51	0.65
30:0:1632:A:C2'	30:0:1633:C:H5'	2.27	0.64
30:0:2005:G:H3'	30:0:2005:G:OP2	1.97	0.64
30:0:2281:C:H2'	30:0:2282:U:H5'	1.80	0.64
30:0:485:A:N3	30:0:487:G:H5''	2.12	0.64
30:0:1834:C:H2'	30:0:1840:A:N6	2.11	0.64
30:0:283:U:C5	30:0:284:C:N3	2.65	0.64
12:L:39:GLU:HG2	30:0:926:A:C4'	2.27	0.64
38:T:2217:HOH:O	30:0:317:A:H5'	1.97	0.64
30:0:1185:U:H2'	30:0:1186:C:C6	2.33	0.64
30:0:1667:A:C8	30:0:1667:A:H5'	2.29	0.64
30:0:2717:C:H2'	30:0:2718:C:C5'	2.22	0.64
30:0:283:U:H5	30:0:284:C:C2	2.15	0.64
30:0:363:C:O2'	30:0:364:U:H5'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:30:LYS:H	8:H:62:HIS:CD2	2.14	0.64
30:0:272:A:H5'	30:0:273:G:OP2	1.97	0.64
30:0:613:C:H2'	30:0:614:U:H6	1.62	0.64
14:N:12:ARG:HD3	14:N:18:THR:OG1	1.97	0.64
21:U:17:THR:HG22	21:U:18:GLY:N	2.13	0.64
30:0:2563:U:H2'	30:0:2565:C:O5'	1.98	0.64
8:H:168:VAL:HG13	38:H:213:HOH:O	1.98	0.64
30:0:2371:G:H5'	38:0:5029:HOH:O	1.98	0.64
30:0:2638:G:H5'	38:0:4946:HOH:O	1.98	0.64
3:C:184:ARG:NH2	30:0:450:C:OP1	2.31	0.64
30:0:644:G:N3	30:0:644:G:H5'	2.13	0.64
21:U:17:THR:HG22	21:U:18:GLY:H	1.62	0.64
30:0:333:G:O2'	30:0:334:G:H5'	1.97	0.63
30:0:952:G:H4'	38:0:4042:HOH:O	1.97	0.63
30:0:1596:U:H2'	30:0:1598:A:OP2	1.99	0.63
30:0:1603:A:C5'	30:0:1605:G:H5'	2.27	0.63
30:0:2404:G:H5''	38:0:5231:HOH:O	1.97	0.63
30:0:2748:G:H2'	38:0:7581:HOH:O	1.98	0.63
2:B:162:MET:HG3	2:B:310:ARG:HD3	1.80	0.63
18:R:128:ARG:NH2	30:0:2054:A:N3	2.46	0.63
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.80	0.63
30:0:2718:C:H6	30:0:2718:C:H5'	1.63	0.63
30:0:2344:G:N3	30:0:2344:G:H2'	2.14	0.63
30:0:2610:U:H4'	38:0:9484:HOH:O	1.99	0.63
30:0:420:U:H2'	30:0:421:C:C6	2.33	0.63
30:0:1166:A:P	30:0:1174:A:H4'	2.38	0.63
30:0:544:G:H2'	30:0:545:G:H5''	1.81	0.63
2:B:238:ASN:HD22	2:B:240:GLY:N	1.93	0.63
30:0:1189:A:O2'	30:0:1208:C:H2'	1.98	0.63
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.13	0.63
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.14	0.63
14:N:7:LYS:HE3	17:Q:21:ARG:O	1.99	0.63
16:P:115:SER:N	16:P:118:GLN:HE21	1.84	0.63
30:0:10:U:C3'	30:0:10:U:C6	2.82	0.63
30:0:1200:A:H3'	38:0:5774:HOH:O	1.99	0.63
30:0:1206:U:C5'	30:0:1206:U:H6	2.10	0.63
30:0:2281:C:C2'	30:0:2282:U:H5'	2.29	0.63
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.64	0.63
3:C:140:VAL:HB	38:C:8649:HOH:O	1.98	0.63
12:L:133:VAL:HA	38:L:8871:HOH:O	1.99	0.63
22:V:50:ARG:NH1	30:0:56:G:H5''	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1942:A:H3'	38:0:7387:HOH:O	1.98	0.62
27:1:16:HIS:HD2	30:0:470:U:O2'	1.81	0.62
30:0:1182:C:H1'	30:0:1192:A:C8	2.34	0.62
30:0:2781:U:H2'	30:0:2782:G:C5'	2.29	0.62
1:A:121:ALA:O	1:A:124:VAL:HG22	1.98	0.62
30:0:138:U:OP2	30:0:139:C:H5	1.82	0.62
30:0:2502:C:H2'	30:0:2503:A:C5'	2.28	0.62
30:0:2472:C:O2'	30:0:2634:G:H4'	1.99	0.62
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.36	0.62
30:0:420:U:H2'	30:0:421:C:H6	1.64	0.62
30:0:559:U:C5	30:0:560:U:C5	2.88	0.62
3:C:236:THR:HG21	38:C:8573:HOH:O	2.00	0.62
3:C:27:ARG:NH2	30:0:657:G:OP1	2.32	0.62
30:0:2241:C:O2'	30:0:2242:U:H5'	2.00	0.62
30:0:1351:G:H1'	38:0:4064:HOH:O	1.98	0.62
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.81	0.62
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.81	0.62
24:X:43:VAL:HG12	24:X:44:ASP:H	1.63	0.62
30:0:1477:C:H5'	30:0:1868:G:C5'	2.30	0.62
28:2:41:HIS:H	28:2:45:ASN:HD22	1.46	0.62
1:A:191:GLY:HA2	1:A:194:MET:CE	2.30	0.62
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.65	0.62
28:2:2:LYS:HG3	30:0:1486:A:C5	2.34	0.62
20:T:26:THR:HG23	20:T:97:ARG:HG3	1.82	0.62
30:0:107:U:C2'	30:0:108:U:H5'	2.29	0.62
30:0:2372:A:H2'	30:0:2373:U:H6	1.65	0.62
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.80	0.62
30:0:2643:G:H5''	38:0:3937:HOH:O	1.99	0.61
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.82	0.61
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.82	0.61
30:0:958:G:O2'	30:0:959:C:H5'	2.01	0.61
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.35	0.61
21:U:56:ARG:HD2	38:0:6278:HOH:O	1.98	0.61
30:0:196:G:H2'	38:0:6690:HOH:O	2.00	0.61
30:0:2802:C:H2'	30:0:2803:C:C6	2.35	0.61
30:0:1015:C:H2'	30:0:1016:U:H6	1.65	0.61
30:0:1972:U:H2'	30:0:1973:A:H5''	1.80	0.61
30:0:2509:A:OP2	30:0:2510:C:H5	1.82	0.61
30:0:407:A:H3'	38:0:4471:HOH:O	2.00	0.61
30:0:308:U:C4	30:0:342:C:H1'	2.36	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:63:GLU:HG2	38:K:6344:HOH:O	2.00	0.61
12:L:136:ALA:HB3	38:L:8871:HOH:O	2.00	0.61
23:W:80:ASP:O	23:W:84:VAL:HG23	1.99	0.61
30:0:705:C:H2'	30:0:705:C:O2	2.01	0.61
30:0:1183:C:H42	30:0:1184:C:H41	1.47	0.61
18:R:99:ALA:HB1	18:R:109:MET:CE	2.31	0.61
30:0:1174:A:C6	30:0:1201:C:H4'	2.36	0.61
27:1:1:THR:HA	38:1:435:HOH:O	2.00	0.61
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.82	0.61
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.66	0.61
12:L:30:ARG:HD3	30:0:164:G:H4'	1.82	0.61
31:9:39:U:H3'	31:9:40:C:H5''	1.83	0.61
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.15	0.61
16:P:91:LYS:O	16:P:95:GLU:HG3	2.00	0.61
30:0:1165:G:N2	30:0:1173:A:C5'	2.63	0.61
30:0:1972:U:C2'	30:0:1973:A:H5''	2.31	0.61
27:1:28:HIS:HE1	30:0:776:A:OP1	1.84	0.61
30:0:510:U:H6	38:0:7477:HOH:O	1.83	0.60
29:3:15:ASN:O	30:0:2408:A:H4'	2.01	0.60
31:9:39:U:H1'	31:9:44:A:H61	1.65	0.60
22:V:39:ALA:N	22:V:40:PRO:HD2	2.14	0.60
30:0:544:G:C2'	30:0:545:G:H5''	2.31	0.60
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.36	0.60
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.67	0.60
30:0:1379:A:H1'	38:0:9696:HOH:O	2.01	0.60
30:0:1819:G:H5'	38:0:5835:HOH:O	2.01	0.60
30:0:2768:A:H5''	38:0:4438:HOH:O	2.00	0.60
30:0:1116:U:C2'	30:0:1118:A:H2	2.14	0.60
30:0:31:C:H4'	38:0:7464:HOH:O	2.00	0.60
30:0:407:A:H5'	38:0:6054:HOH:O	2.00	0.60
30:0:69:A:C8	30:0:69:A:C5'	2.78	0.60
30:0:2787:C:C5	38:0:4643:HOH:O	2.49	0.60
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.17	0.60
30:0:2581:U:H1'	38:0:4486:HOH:O	2.01	0.60
30:0:285:A:H2'	30:0:286:U:O4'	2.01	0.60
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.66	0.60
30:0:363:C:H1'	38:0:5301:HOH:O	2.01	0.60
2:B:258:GLY:H	2:B:260:HIS:CE1	2.19	0.60
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.82	0.60
25:Y:187:VAL:HG22	25:Y:192:ASP:HB3	1.84	0.60
30:0:2893:C:O2'	30:0:2894:C:H5'	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:960:G:N3	30:0:960:G:C2'	2.65	0.60
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.32	0.60
20:T:9:LYS:HE3	20:T:13:ARG:CZ	2.32	0.60
30:0:164:G:H3'	38:0:3650:HOH:O	2.02	0.60
30:0:853:C:H3'	38:0:4563:HOH:O	2.01	0.60
30:0:2103:A:O2'	30:0:2104:C:H6	1.85	0.59
30:0:2453:G:H3'	38:0:5945:HOH:O	2.01	0.59
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.83	0.59
25:Y:216:ARG:HD2	38:Y:8873:HOH:O	2.02	0.59
30:0:2134:G:N2	30:0:2242:U:C2	2.70	0.59
13:M:86:GLN:NE2	30:0:2274:A:H1'	2.17	0.59
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.84	0.59
30:0:2637:A:H4'	38:0:4946:HOH:O	2.02	0.59
30:0:941:G:C5	30:0:942:U:C4	2.91	0.59
3:C:233:THR:HG22	3:C:234:VAL:H	1.67	0.59
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.83	0.59
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.66	0.59
30:0:2361:A:H8	30:0:2361:A:H5'	1.68	0.59
30:0:2795:C:O2'	30:0:2796:U:H5'	2.02	0.59
2:B:162:MET:CE	2:B:308:LEU:HD21	2.32	0.59
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.01	0.59
17:Q:25:PRO:HB2	38:9:9079:HOH:O	2.01	0.59
30:0:1249:U:H2'	30:0:1250:C:C6	2.36	0.59
30:0:1527:A:H1'	30:0:1528:A:C8	2.37	0.59
30:0:1819:G:H2'	30:0:1820:G:C5'	2.32	0.59
30:0:2372:A:H2'	30:0:2373:U:C6	2.37	0.59
30:0:821:U:H2'	30:0:822:C:H6	1.67	0.59
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.85	0.59
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.05	0.59
15:O:24:ALA:HB3	30:0:710:G:OP1	2.02	0.59
30:0:1625:U:H4'	38:0:4676:HOH:O	2.03	0.59
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.02	0.59
11:K:45:PRO:HB2	38:K:7169:HOH:O	2.01	0.59
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.49	0.59
30:0:1202:A:H2'	30:0:1203:G:O4'	2.03	0.59
30:0:2073:G:OP2	30:0:2490:A:H5'	2.01	0.59
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.83	0.59
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.85	0.59
30:0:1603:A:H5'	30:0:1605:G:C4'	2.33	0.59
30:0:2756:U:N3	30:0:2896:A:H2	2.01	0.59
30:0:905:C:H3'	38:0:5207:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2265:U:H2'	30:0:2266:A:C8	2.37	0.59
30:0:2846:C:H4'	38:0:5100:HOH:O	2.03	0.59
30:0:513:A:N3	38:0:3665:HOH:O	2.32	0.59
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.84	0.59
30:0:1116:U:HO2'	30:0:1118:A:H2	0.68	0.59
30:0:2756:U:N3	30:0:2896:A:C2	2.67	0.59
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.83	0.59
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.85	0.59
30:0:1120:U:H5'	30:0:1121:G:OP2	2.03	0.59
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.03	0.59
30:0:137:U:H2'	30:0:139:C:C5	2.38	0.58
30:0:2539:U:H1'	38:0:7825:HOH:O	2.02	0.58
30:0:737:A:H2'	30:0:738:G:O4'	2.02	0.58
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.84	0.58
30:0:2526:C:C6	30:0:2526:C:C5'	2.85	0.58
30:0:2607:U:H4'	38:0:9447:HOH:O	2.03	0.58
29:3:73:GLU:HB3	38:3:9052:HOH:O	2.02	0.58
14:N:37:ARG:HH11	31:9:6:C:H5"	1.61	0.58
2:B:215:VAL:HB	38:B:9087:HOH:O	2.02	0.58
30:0:1641:A:H2'	30:0:1642:A:H5'	1.85	0.58
1:A:23:TYR:HB2	30:0:1872:C:C5	2.38	0.58
2:B:145:HIS:HD2	2:B:146:THR:O	1.87	0.58
3:C:236:THR:CG2	3:C:239:ALA:H	2.10	0.58
5:E:143:GLN:HE22	30:0:2779:G:H21	1.48	0.58
10:J:76:ASP:HA	38:J:5907:HOH:O	2.03	0.58
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.43	0.58
30:0:282:C:O2'	30:0:283:U:C5'	2.52	0.58
30:0:304:G:H1'	30:0:347:A:N6	2.18	0.58
30:0:368:C:H2'	30:0:369:G:H5'	1.85	0.58
29:3:70:ARG:HB3	38:3:9064:HOH:O	2.03	0.58
8:H:48:VAL:HA	8:H:170:ARG:O	2.02	0.58
10:J:107:ASN:HD22	10:J:109:TYR:H	1.50	0.58
30:0:1919:A:H4'	38:0:4867:HOH:O	2.03	0.58
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.32	0.58
30:0:1291:A:H2	38:0:5311:HOH:O	1.86	0.58
30:0:185:G:H4'	30:0:186:A:OP1	2.02	0.58
30:0:638:C:H2'	30:0:639:A:C8	2.39	0.58
30:0:899:C:H5'	38:0:3211:HOH:O	2.03	0.58
30:0:960:G:H4'	38:0:7470:HOH:O	2.03	0.58
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.85	0.58
28:2:11:LEU:HD22	30:0:1417:G:O2'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1701:A:H5''	30:0:1702:U:H3'	1.85	0.58
20:T:52:ARG:HD2	30:0:317:A:H5''	1.85	0.58
3:C:101:ASP:HB2	30:0:750:A:O3'	2.04	0.58
28:2:2:LYS:HG3	30:0:1486:A:C4	2.39	0.58
2:B:36:PRO:HG3	2:B:169:GLY:H	1.69	0.58
3:C:2:GLN:HB3	38:C:8583:HOH:O	2.03	0.58
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.69	0.58
13:M:30:GLU:O	13:M:34:GLU:HG3	2.04	0.58
26:Z:40:ALA:HA	30:0:1773:G:C8	2.38	0.58
30:0:1206:U:C6	30:0:1206:U:H5'	2.26	0.58
30:0:1507:C:H4'	38:0:3609:HOH:O	2.03	0.58
30:0:2670:G:O2'	30:0:2671:U:H5'	2.03	0.58
9:I:107:LYS:HB3	9:I:110:ASP:HB2	1.85	0.58
14:N:141:ARG:NH2	31:9:48:C:H4'	2.19	0.58
30:0:17:G:H2'	30:0:18:C:H6	1.68	0.58
30:0:2802:C:H2'	30:0:2803:C:H6	1.66	0.58
30:0:2842:G:H2'	30:0:2843:A:H5'	1.85	0.58
30:0:877:G:C5'	30:0:878:G:OP1	2.48	0.58
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.84	0.58
2:B:112:THR:HG23	2:B:158:LYS:NZ	2.18	0.58
5:E:84:MET:HG2	5:E:168:ILE:HA	1.86	0.58
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.19	0.58
27:1:25:LYS:HD2	28:2:49:GLU:H	1.68	0.58
17:Q:19:ARG:HH21	31:9:11:A:P	2.27	0.58
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.04	0.58
12:L:6:ARG:HD3	30:0:1299:G:O6	2.03	0.57
30:0:2356:A:H5'	38:0:5655:HOH:O	2.03	0.57
30:0:2445:U:H2'	30:0:2446:G:C8	2.39	0.57
30:0:2510:C:H5'	30:0:2511:A:OP2	2.04	0.57
30:0:2755:G:H1'	38:0:4691:HOH:O	2.03	0.57
2:B:256:GLN:HG2	38:B:9121:HOH:O	2.04	0.57
7:G:16:LYS:O	7:G:20:VAL:HG23	2.03	0.57
7:G:64:ASN:N	7:G:64:ASN:HD22	2.02	0.57
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.85	0.57
30:0:2238:A:O2'	30:0:2239:C:H5'	2.03	0.57
30:0:297:U:H1'	38:0:3945:HOH:O	2.04	0.57
30:0:441:A:H1'	30:0:442:A:N7	2.20	0.57
30:0:812:A:H1'	38:0:3967:HOH:O	2.03	0.57
31:9:39:U:H1'	31:9:44:A:N6	2.18	0.57
2:B:5:ARG:NH1	2:B:8:LYS:HE2	2.19	0.57
30:0:1741:U:O2'	30:0:2723:G:H4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2004:U:H2'	30:0:2004:U:O2	2.04	0.57
29:3:48:ASN:HD21	30:0:2468:A:H61	1.50	0.57
30:0:1795:G:H2'	30:0:1796:A:O4'	2.04	0.57
23:W:44:MET:CE	30:0:944:G:H21	2.17	0.57
30:0:1278:A:H4'	30:0:1279:U:C4	2.40	0.57
30:0:232:A:H4'	38:0:6113:HOH:O	2.05	0.57
30:0:2505:G:O2'	30:0:2506:A:H5''	2.05	0.57
30:0:1167:G:H2'	30:0:1168:C:O4'	2.04	0.57
30:0:558:C:H2'	30:0:559:U:H5''	1.84	0.57
30:0:820:G:O2'	30:0:856:G:H4'	2.03	0.57
19:S:77:VAL:O	19:S:80:ARG:HG2	2.05	0.57
31:9:39:U:HO2'	31:9:42:C:H5	1.53	0.57
23:W:52:VAL:HG22	23:W:53:ALA:H	1.68	0.57
30:0:1538:C:O2'	30:0:1539:U:H5'	2.05	0.57
30:0:168:C:O5'	30:0:168:C:H6	1.88	0.57
30:0:2589:U:H2'	30:0:2590:U:C6	2.40	0.57
30:0:2597:U:H2'	30:0:2598:U:H5'	1.87	0.57
30:0:558:C:C2'	30:0:559:U:C5'	2.83	0.57
30:0:945:U:H2'	30:0:946:C:H6	1.70	0.57
12:L:41:HIS:CD2	30:0:926:A:O2'	2.58	0.57
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.68	0.57
30:0:2291:A:N9	30:0:2309:C:H5'	2.19	0.57
30:0:292:G:H2'	30:0:358:G:N2	2.20	0.57
30:0:483:C:C4	30:0:484:A:C6	2.93	0.57
1:A:51:ARG:NH1	1:A:120:ARG:O	2.38	0.57
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.86	0.57
30:0:1205:U:O2'	30:0:1206:U:H5''	2.05	0.56
38:C:8559:HOH:O	30:0:338:C:H5''	2.04	0.56
30:0:287:C:H42	30:0:365:G:H1	1.53	0.56
30:0:1214:G:H4'	38:0:4759:HOH:O	2.03	0.56
30:0:125:U:H2'	38:0:3775:HOH:O	2.04	0.56
23:W:125:HIS:HD2	23:W:127:GLY:H	1.53	0.56
30:0:119:A:H2'	30:0:120:A:H5''	1.87	0.56
30:0:1528:A:H2'	30:0:1529:G:O4'	2.05	0.56
30:0:17:G:H2'	30:0:18:C:C6	2.40	0.56
30:0:2720:C:H3'	38:0:6454:HOH:O	2.05	0.56
30:0:334:G:C5	30:0:335:U:C5	2.94	0.56
31:9:55:U:H4'	31:9:56:A:C8	2.40	0.56
14:N:147:ILE:HD12	38:9:9089:HOH:O	2.04	0.56
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.40	0.56
30:0:945:U:H2'	30:0:946:C:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.40	0.56
16:P:64:GLU:HG2	38:P:2495:HOH:O	2.05	0.56
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.06	0.56
30:0:1342:C:C2'	30:0:1343:C:H5'	2.35	0.56
23:W:139:GLY:O	23:W:141:HIS:HD2	1.87	0.56
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.71	0.56
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.08	0.56
30:0:1181:A:C2	30:0:1192:A:C8	2.94	0.56
30:0:136:C:H2'	30:0:137:U:O4'	2.05	0.56
30:0:2252:A:C5	30:0:2253:G:H1'	2.40	0.56
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.41	0.56
2:B:297:VAL:HB	38:B:9075:HOH:O	2.05	0.56
8:H:69:ARG:HD3	38:H:232:HOH:O	2.06	0.56
18:R:39:THR:HG23	18:R:107:GLU:O	2.04	0.56
30:0:1679:C:H5'	38:0:9330:HOH:O	2.05	0.56
13:M:64:ARG:HD2	38:M:8878:HOH:O	2.04	0.56
30:0:1903:U:O2'	30:0:1904:A:N7	2.39	0.56
11:K:130:MET:SD	21:U:25:ASP:O	2.64	0.56
12:L:143:THR:HG22	12:L:144:ASP:N	2.21	0.56
31:9:49:G:H2'	31:9:50:G:O4'	2.06	0.56
5:E:149:GLU:HG3	5:E:167:TYR:HA	1.86	0.56
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.87	0.56
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.88	0.56
31:9:63:C:O2'	31:9:64:C:H5'	2.06	0.56
2:B:294:TYR:HE2	38:B:9114:HOH:O	1.89	0.56
21:U:9:CYS:HA	21:U:52:THR:CG2	2.36	0.56
31:9:36:C:C5	31:9:37:C:C5	2.94	0.56
7:G:20:VAL:O	7:G:24:VAL:HG23	2.06	0.56
30:0:2253:G:O2'	30:0:2254:G:H5'	2.06	0.55
30:0:396:U:O2'	30:0:418:C:H4'	2.05	0.55
4:D:172:VAL:HG12	4:D:173:GLU:H	1.70	0.55
7:G:12:ILE:HG23	38:0:5477:HOH:O	2.07	0.55
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.87	0.55
30:0:1183:C:N3	30:0:1184:C:C5	2.74	0.55
30:0:1198:U:H1'	30:0:1201:C:H5	1.71	0.55
30:0:1664:A:H8	30:0:1664:A:OP1	1.89	0.55
30:0:1768:C:H2'	30:0:1769:C:O4'	2.06	0.55
30:0:283:U:C5	30:0:284:C:C2	2.93	0.55
30:0:960:G:C3'	30:0:960:G:N3	2.70	0.55
30:0:2419:U:H5''	30:0:2420:G:H5'	1.89	0.55
30:0:2608:C:H2'	38:0:3579:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:141:ARG:HH21	31:9:48:C:H4'	1.72	0.55
3:C:236:THR:HA	38:C:8649:HOH:O	2.05	0.55
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.87	0.55
10:J:19:MET:HE1	10:J:79:PHE:HA	1.89	0.55
9:I:111:LEU:CD2	30:0:1163:G:H4'	2.35	0.55
30:0:628:1MA:H4'	38:0:3149:HOH:O	2.06	0.55
30:0:65:C:O2'	30:0:66:G:H5'	2.06	0.55
6:F:77:VAL:HG21	6:F:83:LEU:HD13	1.88	0.55
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.41	0.55
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.88	0.55
14:N:11:ARG:HG3	14:N:14:ARG:HH12	1.71	0.55
30:0:2478:U:O2'	30:0:2479:A:H5'	2.06	0.55
30:0:2509:A:C2	30:0:2510:C:H1'	2.42	0.55
30:0:558:C:H2'	30:0:559:U:H5'	1.89	0.55
12:L:22:ARG:HG2	38:0:3241:HOH:O	2.05	0.55
30:0:1666:C:H2'	30:0:1667:A:H5''	1.71	0.55
30:0:2353:A:H4'	30:0:2354:A:O5'	2.06	0.55
30:0:1787:C:H4'	30:0:2883:A:O4'	2.07	0.55
30:0:2908:A:O5'	30:0:2908:A:H8	1.89	0.55
38:O:1484:HOH:O	30:0:710:G:H1'	2.06	0.55
2:B:62:ARG:HA	2:B:65:MET:CE	2.36	0.55
30:0:1127:C:C5	30:0:1128:U:C4	2.95	0.55
30:0:1159:G:H1	30:0:1208:C:H42	1.54	0.55
30:0:2320:U:H4'	30:0:2321:A:O4'	2.07	0.55
30:0:2565:C:H4'	38:0:4851:HOH:O	2.06	0.55
30:0:567:U:C5'	38:0:6437:HOH:O	2.50	0.55
23:W:154:ARG:NH1	30:0:588:G:O6	2.40	0.55
30:0:960:G:H2'	30:0:960:G:N3	2.22	0.55
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.21	0.55
12:L:36:ASP:HB2	38:L:8836:HOH:O	2.07	0.55
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.07	0.55
30:0:1120:U:H5''	30:0:1120:U:C6	2.42	0.55
30:0:2896:A:N3	30:0:2896:A:H2'	2.22	0.55
30:0:89:G:H4'	38:0:4779:HOH:O	2.05	0.55
30:0:1819:G:H2'	30:0:1820:G:H4'	1.89	0.55
30:0:1838:U:H3'	38:0:5544:HOH:O	2.07	0.55
30:0:2249:G:C2	30:0:2253:G:C6	2.95	0.55
16:P:87:ARG:HG2	38:0:5970:HOH:O	2.07	0.55
30:0:1066:U:H2'	30:0:1067:A:C8	2.41	0.54
30:0:1118:A:H8	30:0:1119:G:H5''	1.73	0.54
30:0:1474:C:C5'	30:0:1474:C:C6	2.79	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:76:G:C3'	31:9:77:A:H5''	2.27	0.54
1:A:109:GLU:HG2	1:A:116:GLY:H	1.72	0.54
27:1:9:GLY:HA2	30:0:1687:C:O2	2.07	0.54
30:0:1750:C:H5''	38:0:3673:HOH:O	2.07	0.54
3:C:174:ILE:CD1	30:0:338:C:H4'	2.36	0.54
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.37	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.06	0.54
23:W:142:ASP:HB3	23:W:145:GLY:H	1.71	0.54
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.88	0.54
38:Z:8707:HOH:O	30:0:1886:A:H4'	2.06	0.54
27:1:16:HIS:HE1	30:0:775:G:OP1	1.91	0.54
30:0:876:A:N3	30:0:876:A:H2'	2.23	0.54
2:B:221:GLN:HE22	11:K:42:ASN:ND2	1.98	0.54
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.37	0.54
23:W:64:THR:O	23:W:68:THR:HG22	2.06	0.54
30:0:1016:U:H1'	38:0:3664:HOH:O	2.06	0.54
30:0:2387:U:H2'	30:0:2388:C:C6	2.42	0.54
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.42	0.54
2:B:275:GLY:O	2:B:291:ASP:HA	2.07	0.54
2:B:305:ASP:O	2:B:306:LYS:HB2	2.08	0.54
4:D:141:VAL:HG21	31:9:57:A:H8	1.72	0.54
8:H:59:GLN:HE21	8:H:129:ARG:NE	2.05	0.54
30:0:138:U:OP1	30:0:259:G:H5'	2.07	0.54
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.89	0.54
31:9:12:C:H5'	31:9:70:U:O4'	2.06	0.54
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.42	0.54
30:0:711:G:C2	30:0:718:C:C2	2.96	0.54
30:0:962:C:H2'	30:0:963:C:H5'	1.89	0.54
15:O:105:ASN:HD21	15:O:109:SER:N	2.05	0.54
20:T:68:ASP:HB2	38:0:5678:HOH:O	2.08	0.54
30:0:2271:G:N3	30:0:2271:G:H2'	2.22	0.54
31:9:1:U:O3'	31:9:3:A:H5''	2.07	0.54
13:M:159:VAL:HG12	33:M:8818:CL:CL	2.45	0.54
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.72	0.54
26:Z:75:GLY:HA3	38:Z:8717:HOH:O	2.06	0.54
30:0:2414:A:H2'	30:0:2415:A:C8	2.43	0.54
31:9:3:A:N6	31:9:22:G:H1'	2.22	0.54
8:H:87:LYS:NZ	8:H:87:LYS:HB2	2.23	0.54
23:W:13:MET:HE1	23:W:18:GLN:HA	1.88	0.54
30:0:1205:U:H5	38:0:4451:HOH:O	1.91	0.54
30:0:1342:C:O2'	30:0:1343:C:H5'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2880:A:H2'	30:0:2881:C:H5'	1.89	0.54
4:D:18:ILE:HD13	4:D:84:LEU:HD12	1.89	0.54
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.90	0.54
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.06	0.54
30:0:1450:C:H5''	38:0:9624:HOH:O	2.08	0.54
30:0:1624:A:H5'	30:0:1626:A:O4'	2.07	0.54
30:0:1926:G:H2'	30:0:1927:A:C8	2.42	0.54
30:0:567:U:H5''	38:0:5308:HOH:O	2.08	0.54
19:S:11:THR:H	19:S:14:ALA:HB3	1.73	0.54
30:0:1137:G:H1'	38:0:3888:HOH:O	2.07	0.53
2:B:254:GLN:HG2	2:B:255:GLY:N	2.23	0.53
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.90	0.53
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.90	0.53
24:X:72:VAL:HG22	24:X:85:VAL:HG12	1.90	0.53
30:0:1201:C:C2'	30:0:1202:A:H5'	2.37	0.53
30:0:1766:U:O2	30:0:1778:A:H5'	2.08	0.53
30:0:1973:A:H5'	30:0:1973:A:C8	2.41	0.53
30:0:2697:A:H2'	30:0:2698:G:O4'	2.08	0.53
1:A:17:ARG:HD2	38:A:9005:HOH:O	2.07	0.53
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.89	0.53
30:0:121:U:H2'	38:0:9854:HOH:O	2.08	0.53
30:0:1304:U:H2'	30:0:1305:C:C6	2.43	0.53
30:0:644:G:H1'	38:0:6440:HOH:O	2.08	0.53
30:0:682:A:H2'	30:0:683:G:O4'	2.08	0.53
31:9:1:U:O3'	31:9:3:A:C5'	2.57	0.53
30:0:2102:G:C5'	30:0:2538:A:C2	2.91	0.53
30:0:2311:A:H3'	38:0:7716:HOH:O	2.07	0.53
30:0:2445:U:H2'	30:0:2446:G:H8	1.72	0.53
30:0:280:C:H2'	30:0:281:U:O4'	2.07	0.53
30:0:700:A:H5''	30:0:701:U:H5'	1.91	0.53
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.89	0.53
4:D:141:VAL:HG21	31:9:57:A:C8	2.43	0.53
19:S:37:VAL:O	19:S:41:VAL:HG23	2.08	0.53
30:0:2354:A:C2	30:0:2367:A:C8	2.97	0.53
30:0:2002:C:H2'	30:0:2003:U:H5'	1.90	0.53
30:0:482:G:H4'	30:0:508:A:N1	2.24	0.53
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.90	0.53
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.44	0.53
23:W:5:VAL:HG11	23:W:153:MET:CE	2.39	0.53
30:0:1562:C:N4	38:0:5888:HOH:O	2.41	0.53
30:0:1714:C:O2'	30:0:1715:C:H5'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:407:A:H2'	30:0:408:A:C8	2.44	0.53
27:1:42:SER:HB2	38:1:354:HOH:O	2.08	0.53
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.09	0.53
30:0:559:U:C5'	30:0:559:U:H6	2.20	0.53
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.73	0.53
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.90	0.53
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.09	0.53
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.82	0.53
30:0:1495:C:H1'	30:0:1573:A:H1'	1.91	0.53
13:M:188:ARG:NH1	30:0:154:C:H3'	2.23	0.53
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.42	0.53
30:0:2256:G:C2'	30:0:2257:G:C5'	2.86	0.53
30:0:2764:C:O2'	30:0:2765:C:H5'	2.08	0.53
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.53
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.39	0.53
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.91	0.53
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.91	0.53
25:Y:141:THR:HG23	38:Y:8892:HOH:O	2.08	0.53
30:0:1060:C:H6	30:0:1060:C:H5'	1.72	0.53
10:J:107:ASN:C	10:J:107:ASN:HD22	2.13	0.53
30:0:603:A:H1'	30:0:605:C:C2	2.43	0.52
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.39	0.52
16:P:115:SER:OG	16:P:118:GLN:HG3	2.09	0.52
30:0:1183:C:C2	30:0:1184:C:C5	2.97	0.52
30:0:138:U:C5	30:0:140:G:O6	2.62	0.52
30:0:704:C:H2'	30:0:705:C:H6	1.74	0.52
31:9:13:A:O2'	31:9:14:G:H5''	2.10	0.52
1:A:99:ILE:O	1:A:131:HIS:HE1	1.92	0.52
1:A:36:ASP:O	1:A:38:ILE:N	2.41	0.52
30:0:1014:A:H2'	30:0:1015:C:H5'	1.92	0.52
30:0:2359:G:H3'	38:0:5709:HOH:O	2.09	0.52
30:0:2509:A:H2'	30:0:2510:C:O4'	2.09	0.52
30:0:282:C:O2'	30:0:283:U:H4'	2.09	0.52
30:0:304:G:H1'	30:0:347:A:H61	1.73	0.52
4:D:134:LEU:HD11	4:D:166:ILE:HD11	1.91	0.52
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.92	0.52
18:R:114:VAL:HA	18:R:144:GLU:O	2.09	0.52
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.40	0.52
30:0:2265:U:H2'	30:0:2266:A:H8	1.75	0.52
31:9:42:C:H5'	31:9:43:G:OP2	2.09	0.52
3:C:25:PRO:HG2	38:C:8521:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.91	0.52
7:G:19:GLU:O	7:G:23:ILE:HG13	2.09	0.52
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.74	0.52
20:T:28:SER:O	20:T:32:ARG:HG3	2.08	0.52
23:W:88:THR:HG22	23:W:89:ASP:N	2.23	0.52
30:0:1180:U:O2'	30:0:1181:A:H5'	2.10	0.52
30:0:1289:C:O2'	30:0:1290:G:H5'	2.09	0.52
30:0:138:U:OP2	30:0:139:C:C5	2.62	0.52
30:0:1724:U:H5''	38:0:3739:HOH:O	2.09	0.52
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.09	0.52
14:N:33:ARG:NH2	31:9:6:C:O2'	2.43	0.52
18:R:150:PRO:CG	18:R:150:PRO:CB	2.87	0.52
30:0:1185:U:H5'	38:0:7505:HOH:O	2.08	0.52
30:0:1249:U:H2'	30:0:1250:C:H6	1.75	0.52
2:B:267:LYS:HD3	38:0:9567:HOH:O	2.09	0.52
4:D:154:LYS:HD2	4:D:154:LYS:N	2.10	0.52
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.92	0.52
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.91	0.52
30:0:1175:G:O2'	30:0:1193:A:H2'	2.09	0.52
30:0:1477:C:H5'	30:0:1868:G:H5'	1.91	0.52
30:0:204:A:H2'	30:0:205:U:H5'	1.92	0.52
30:0:2072:G:C6	30:0:2533:C:H1'	2.45	0.52
30:0:2840:A:H3'	38:0:7686:HOH:O	2.09	0.52
30:0:298:C:H1'	38:0:3853:HOH:O	2.09	0.52
30:0:661:G:C5	30:0:686:A:C2	2.98	0.52
4:D:25:MET:CE	4:D:37:ALA:HB1	2.39	0.52
30:0:1878:G:O2'	30:0:1879:U:C6	2.59	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.91	0.52
30:0:2498:C:O2'	30:0:2499:U:H5'	2.09	0.52
30:0:2604:A:H4'	38:0:7644:HOH:O	2.09	0.52
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.91	0.52
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.09	0.52
12:L:121:ILE:HG12	12:L:141:GLU:HB2	1.92	0.52
13:M:188:ARG:HD3	30:0:155:C:OP2	2.09	0.52
30:0:2526:C:O2'	30:0:2527:U:H5'	2.10	0.52
3:C:16:VAL:HG12	3:C:17:ASP:H	1.73	0.52
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.92	0.52
7:G:23:ILE:O	7:G:27:ILE:HG13	2.09	0.52
18:R:18:LEU:HB2	18:R:143:VAL:HG12	1.92	0.52
30:0:545:G:C8	30:0:545:G:C5'	2.83	0.52
30:0:734:U:O2'	30:0:736:A:N7	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:821:U:H2'	30:0:822:C:C6	2.45	0.52
17:Q:95:GLU:HA	30:0:949:U:H4'	1.92	0.52
30:0:999:C:O2'	30:0:1000:C:H5'	2.10	0.52
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.08	0.52
30:0:1675:C:H3'	38:0:7847:HOH:O	2.10	0.51
30:0:1419:U:H2'	30:0:1685:A:C2	2.45	0.51
1:A:33:GLU:O	1:A:34:ASP:HB2	2.09	0.51
2:B:212:GLN:HA	30:0:1733:A:H4'	1.92	0.51
30:0:2083:A:H3'	38:0:7617:HOH:O	2.10	0.51
30:0:137:U:OP1	30:0:259:G:O2'	2.28	0.51
30:0:334:G:C6	30:0:335:U:C4	2.98	0.51
15:O:37:ARG:HD2	30:0:656:G:OP2	2.09	0.51
15:O:7:LEU:HD22	38:O:5650:HOH:O	2.10	0.51
30:0:1393:A:H2'	30:0:1394:C:C6	2.46	0.51
30:0:2637:A:OP1	30:0:2637:A:H3'	2.10	0.51
30:0:432:G:O2'	30:0:433:C:H5'	2.10	0.51
30:0:652:G:H8	38:0:3020:HOH:O	1.93	0.51
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.51
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.93	0.51
30:0:1307:A:H2'	30:0:1308:A:C8	2.46	0.51
30:0:2493:C:O2	30:0:2493:C:H2'	2.10	0.51
30:0:346:U:H4'	38:0:6881:HOH:O	2.10	0.51
27:1:16:HIS:CD2	30:0:470:U:O2'	2.63	0.51
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.91	0.51
26:Z:57:MET:SD	26:Z:73:ARG:HD2	2.51	0.51
26:Z:76:THR:HG21	30:0:1652:C:H4'	1.91	0.51
30:0:1181:A:H2'	30:0:1182:C:H5'	1.93	0.51
30:0:1422:U:H2'	30:0:1423:C:C6	2.46	0.51
30:0:466:A:H2'	30:0:467:G:O4'	2.10	0.51
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.07	0.51
31:9:95:C:O2'	31:9:96:C:H5'	2.11	0.51
4:D:62:ASP:HA	38:D:4233:HOH:O	2.10	0.51
2:B:221:GLN:NE2	11:K:42:ASN:HD22	1.96	0.51
24:X:85:VAL:HG12	24:X:86:GLU:N	2.26	0.51
30:0:120:A:H2'	30:0:120:A:N3	2.26	0.51
30:0:1477:C:O2'	30:0:1478:U:H5'	2.10	0.51
30:0:2105:C:H2'	30:0:2106:C:C6	2.45	0.51
30:0:2329:C:O2'	30:0:2330:U:H5'	2.10	0.51
30:0:553:G:H5'	38:0:3506:HOH:O	2.11	0.51
31:9:3:A:OP2	31:9:25:G:N2	2.43	0.51
5:E:21:THR:HG23	5:E:30:THR:OG1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:7:LYS:HG2	16:P:23:PHE:CE2	2.46	0.51
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.59	0.51
30:0:1056:U:H2'	30:0:1057:A:O4'	2.11	0.51
28:2:10:ARG:NH2	30:0:121:U:OP2	2.42	0.51
30:0:2826:G:C6	30:0:2913:A:N6	2.78	0.51
30:0:282:C:H2'	30:0:283:U:O4'	2.10	0.51
30:0:281:U:H2'	30:0:282:C:O4'	2.10	0.51
28:2:38:LYS:HE3	38:0:4239:HOH:O	2.10	0.51
10:J:42:GLU:O	10:J:131:THR:HG23	2.11	0.51
18:R:40:ALA:O	18:R:44:VAL:HG23	2.11	0.51
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.11	0.51
30:0:1166:A:C6	30:0:1181:A:C2	2.99	0.51
30:0:1181:A:C2'	30:0:1182:C:H5'	2.40	0.51
30:0:694:A:H2'	30:0:695:C:H5'	1.91	0.51
30:0:764:C:H2'	30:0:765:G:O4'	2.11	0.51
2:B:223:ARG:HG3	2:B:232:TRP:O	2.10	0.51
23:W:13:MET:CE	23:W:17:ILE:HG22	2.41	0.51
30:0:1183:C:O2	30:0:1183:C:C2'	2.59	0.51
30:0:1209:C:H2'	30:0:1210:G:H8	1.76	0.51
30:0:2786:G:H5''	38:0:4643:HOH:O	2.10	0.51
30:0:2894:C:O2'	30:0:2895:C:H5'	2.11	0.51
30:0:951:A:C2'	30:0:952:G:H5'	2.40	0.51
18:R:39:THR:HG22	18:R:42:GLU:H	1.75	0.51
23:W:80:ASP:HB2	38:W:3312:HOH:O	2.11	0.51
30:0:1131:G:C6	30:0:1230:A:C4	2.99	0.51
30:0:172:U:H5'	38:0:4171:HOH:O	2.11	0.51
30:0:255:A:C5	30:0:256:C:C5	2.98	0.51
30:0:255:A:H2'	30:0:256:C:H6	1.76	0.51
30:0:90:A:H2'	30:0:91:G:O4'	2.11	0.51
28:2:41:HIS:CD2	28:2:44:ARG:H	2.26	0.51
31:9:55:U:H4'	31:9:56:A:H8	1.76	0.51
3:C:63:SER:OG	30:0:2101:A:H2'	2.11	0.51
38:C:8567:HOH:O	20:T:2:LYS:HE2	2.10	0.51
25:Y:174:VAL:HG23	25:Y:177:LYS:HD2	1.93	0.51
30:0:2553:A:H2'	30:0:2553:A:N3	2.25	0.50
30:0:305:A:C5	30:0:329:A:C2	2.99	0.50
27:1:10:LYS:HG3	38:1:2979:HOH:O	2.10	0.50
1:A:173:GLY:O	1:A:176:HIS:HB3	2.10	0.50
9:I:114:TYR:N	9:I:114:TYR:CD1	2.80	0.50
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.92	0.50
30:0:1657:A:H2'	30:0:1658:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2269:C:C2'	30:0:2270:G:H5'	2.40	0.50
30:0:282:C:O2'	30:0:283:U:C4'	2.59	0.50
30:0:512:G:O3'	30:0:513:A:H8	1.93	0.50
31:9:29:C:H2'	31:9:30:C:C5'	2.36	0.50
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.93	0.50
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.11	0.50
30:0:1594:C:O2'	30:0:1607:A:H4'	2.11	0.50
30:0:398:U:H2'	30:0:399:C:C6	2.47	0.50
1:A:33:GLU:CD	1:A:33:GLU:H	2.14	0.50
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.46	0.50
30:0:1515:A:H2'	30:0:1516:U:C6	2.46	0.50
30:0:23:G:H1'	30:0:520:A:N6	2.26	0.50
31:9:75:G:H1	31:9:106:U:H3	1.59	0.50
6:F:91:VAL:CG1	6:F:92:GLY:H	2.16	0.50
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.92	0.50
14:N:37:ARG:NH1	31:9:6:C:OP1	2.44	0.50
21:U:6:CYS:HA	21:U:13:ILE:HD11	1.94	0.50
30:0:1903:U:O2'	30:0:1904:A:C8	2.63	0.50
30:0:2589:U:H2'	30:0:2590:U:H6	1.76	0.50
13:M:9:ARG:HD2	30:0:380:A:OP2	2.11	0.50
31:9:54:A:C2	31:9:55:U:N3	2.80	0.50
31:9:59:C:H6	31:9:59:C:O5'	1.94	0.50
4:D:159:PRO:O	4:D:163:VAL:HG23	2.12	0.50
5:E:7:ILE:HG22	5:E:45:ASP:O	2.10	0.50
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.76	0.50
30:0:1015:C:H2'	30:0:1016:U:C6	2.47	0.50
30:0:10:U:O4	30:0:532:A:OP2	2.30	0.50
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.45	0.50
30:0:602:A:O2'	30:0:605:C:H4'	2.11	0.50
30:0:814:G:H4'	38:0:3140:HOH:O	2.11	0.50
26:Z:50:VAL:O	26:Z:54:GLU:HG3	2.11	0.50
30:0:11:A:N3	30:0:11:A:H2'	2.26	0.50
30:0:1883:U:C2'	30:0:1884:G:H5'	2.42	0.50
30:0:2878:U:H2'	30:0:2879:A:O4'	2.12	0.50
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.94	0.50
16:P:14:LEU:HD13	16:P:51:ALA:HB2	1.93	0.50
20:T:38:ARG:NH1	38:0:6719:HOH:O	2.45	0.50
30:0:1588:G:C6	30:0:1589:G:N1	2.80	0.50
30:0:2842:G:C2'	30:0:2843:A:H5'	2.41	0.50
31:9:1:U:H4'	31:9:3:A:OP1	2.12	0.50
30:0:1170:U:H2'	30:0:1172:G:OP2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1186:C:N4	30:0:1187:U:C4	2.80	0.50
30:0:1520:G:H2'	30:0:1521:C:C6	2.46	0.50
30:0:1759:A:N3	30:0:1818:C:H2'	2.27	0.50
30:0:1840:A:H4'	30:0:1841:C:O5'	2.12	0.50
30:0:1947:G:N2	30:0:1966:U:C2	2.80	0.50
30:0:2898:G:O2'	30:0:2899:A:H5'	2.11	0.50
30:0:319:A:H4'	30:0:338:C:C4	2.47	0.50
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.93	0.50
30:0:1377:C:C5'	30:0:1377:C:H6	2.19	0.49
30:0:1896:G:C6	30:0:1897:U:C4	3.00	0.49
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.26	0.49
10:J:74:ARG:HH11	10:J:74:ARG:HB3	1.76	0.49
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.93	0.49
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.47	0.49
30:0:1350:U:H5''	38:0:5143:HOH:O	2.11	0.49
30:0:711:G:O2'	30:0:712:C:H5'	2.12	0.49
30:0:923:A:H2'	38:0:5697:HOH:O	2.12	0.49
12:L:143:THR:HG22	12:L:144:ASP:H	1.78	0.49
14:N:5:ARG:HG3	14:N:5:ARG:HH11	1.77	0.49
24:X:43:VAL:HG12	24:X:44:ASP:N	2.26	0.49
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.46	0.49
30:0:1947:G:H2'	30:0:1948:G:H8	1.77	0.49
30:0:2415:A:H2'	30:0:2416:G:H5'	1.94	0.49
31:9:107:C:O2'	31:9:108:C:H5'	2.11	0.49
13:M:75:ARG:HH11	30:0:1864:C:H5	1.59	0.49
23:W:119:HIS:HE1	38:0:9559:HOH:O	1.95	0.49
30:0:861:A:H4'	30:0:1697:G:H4'	1.94	0.49
30:0:735:C:C5	30:0:736:A:C4	2.99	0.49
30:0:920:C:H5''	30:0:921:G:O5'	2.13	0.49
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.77	0.49
30:0:939:A:C2	30:0:1027:G:N3	2.81	0.49
30:0:1221:G:C8	38:0:6014:HOH:O	2.55	0.49
30:0:1947:G:H2'	30:0:1948:G:C8	2.47	0.49
30:0:2134:G:C6	30:0:2258:A:C8	3.01	0.49
30:0:2276:U:H2'	30:0:2277:U:C6	2.47	0.49
30:0:2638:G:H1'	38:0:7796:HOH:O	2.11	0.49
30:0:2651:C:H2'	30:0:2652:U:O4'	2.12	0.49
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.37	0.49
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.53	0.49
1:A:51:ARG:HB2	38:A:9061:HOH:O	2.11	0.49
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1878:G:O2'	30:0:1879:U:P	2.71	0.49
30:0:2345:A:H3'	30:0:2346:C:C6	2.46	0.49
31:9:2:U:P	31:9:3:A:H5'	2.52	0.49
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.42	0.49
23:W:125:HIS:CD2	23:W:127:GLY:H	2.31	0.49
30:0:1119:G:H22	30:0:1246:A:H2	1.51	0.49
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.94	0.49
30:0:2385:G:H2'	30:0:2386:U:C6	2.47	0.49
30:0:291:C:H2'	30:0:292:G:O4'	2.12	0.49
30:0:370:G:O2'	30:0:371:U:H5'	2.12	0.49
30:0:711:G:C2'	30:0:712:C:H5'	2.42	0.49
27:1:20:ARG:HH21	30:0:120:A:H5'	1.77	0.49
14:N:159:TYR:HE1	31:9:50:G:H5''	1.78	0.49
2:B:17:LYS:O	2:B:260:HIS:HD2	1.94	0.49
3:C:233:THR:HG22	3:C:234:VAL:N	2.26	0.49
9:I:114:TYR:N	9:I:114:TYR:HD1	2.10	0.49
15:O:32:ARG:HD3	15:O:32:ARG:O	2.12	0.49
25:Y:186:ARG:HG2	25:Y:186:ARG:HH11	1.77	0.49
30:0:1298:U:H2'	30:0:1299:G:C8	2.48	0.49
30:0:185:G:H4'	30:0:186:A:H4'	1.93	0.49
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.47	0.49
30:0:256:C:H2'	30:0:257:G:O4'	2.12	0.49
30:0:699:C:C2	30:0:743:G:N2	2.81	0.49
30:0:806:A:H2'	30:0:807:A:O4'	2.13	0.49
30:0:941:G:C6	30:0:942:U:C4	3.01	0.49
30:0:958:G:H2'	30:0:959:C:C6	2.48	0.49
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.78	0.49
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.95	0.49
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.12	0.49
24:X:66:THR:HG23	24:X:67:PRO:HD2	1.95	0.49
30:0:1118:A:C8	30:0:1119:G:H5''	2.48	0.49
30:0:1268:C:H2'	30:0:1269:G:H8	1.77	0.49
30:0:1755:A:H2'	30:0:1756:G:O4'	2.12	0.49
30:0:1849:G:H1'	30:0:2011:A:N1	2.28	0.49
12:L:41:HIS:HD2	30:0:926:A:O2'	1.95	0.49
29:3:3:MET:O	29:3:90:PHE:HA	2.12	0.49
31:9:49:G:O2'	31:9:50:G:H5'	2.13	0.49
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.94	0.49
8:H:100:GLU:HB3	8:H:124:VAL:HG11	1.94	0.49
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.35	0.49
30:0:1667:A:H2'	30:0:1668:U:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:182:G:H5''	38:0:3730:HOH:O	2.13	0.49
30:0:2064:U:H5'	30:0:2652:U:H4'	1.95	0.49
30:0:2103:A:N7	30:0:2538:A:N7	2.60	0.49
30:0:522:U:O2'	30:0:1366:C:H5'	2.13	0.49
30:0:699:C:H6	30:0:744:G:O4'	1.96	0.49
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.28	0.49
30:0:1158:G:O2'	30:0:1159:G:H5'	2.13	0.48
30:0:1909:A:N1	30:0:2128:G:H1'	2.27	0.48
30:0:299:U:H5'	38:0:7377:HOH:O	2.12	0.48
30:0:876:A:N3	30:0:876:A:C2'	2.76	0.48
28:2:39:ARG:HG2	38:2:3143:HOH:O	2.13	0.48
2:B:41:PHE:HA	2:B:79:MET:HE2	1.94	0.48
9:I:101:LYS:O	9:I:105:GLU:HG3	2.12	0.48
14:N:132:ASN:O	14:N:135:VAL:HG12	2.13	0.48
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.95	0.48
31:9:91:C:H2'	31:9:92:G:O4'	2.13	0.48
1:A:94:LEU:N	1:A:94:LEU:HD23	2.28	0.48
8:H:64:SER:OG	30:0:2520:G:H5'	2.13	0.48
10:J:5:GLU:HA	38:J:1652:HOH:O	2.11	0.48
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.94	0.48
12:L:138:GLY:HA3	38:L:8853:HOH:O	2.13	0.48
12:L:18:HIS:HD2	30:0:902:G:N7	2.12	0.48
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.28	0.48
16:P:1:THR:O	30:0:1396:C:H1'	2.13	0.48
30:0:2534:C:H1'	38:0:3502:HOH:O	2.12	0.48
30:0:369:G:O2'	30:0:370:G:H5'	2.13	0.48
30:0:1634:G:H2'	30:0:1635:U:C6	2.48	0.48
30:0:1778:A:H2'	30:0:1779:A:H5'	1.94	0.48
30:0:2768:A:N3	30:0:2768:A:H3'	2.27	0.48
30:0:652:G:H5''	38:0:3020:HOH:O	2.12	0.48
30:0:958:G:H2'	30:0:959:C:H6	1.77	0.48
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.95	0.48
22:V:56:ILE:O	22:V:60:GLN:HG3	2.14	0.48
30:0:1592:G:O2'	30:0:1593:C:O5'	2.30	0.48
30:0:2032:U:H2'	30:0:2033:G:C5'	2.43	0.48
30:0:2851:G:C2'	30:0:2852:A:H5'	2.44	0.48
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.34	0.48
22:V:55:ARG:O	22:V:59:ILE:HG12	2.13	0.48
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.95	0.48
30:0:1615:A:H5'	38:0:4195:HOH:O	2.13	0.48
30:0:1625:U:H3'	30:0:1625:U:H6	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1972:U:C2'	30:0:1973:A:C5'	2.91	0.48
30:0:2315:C:O2'	30:0:2316:G:H5'	2.13	0.48
30:0:2900:G:H2'	30:0:2901:C:O4'	2.13	0.48
30:0:2899:A:O2'	30:0:2900:G:H5'	2.13	0.48
30:0:2906:A:H5'	30:0:2907:C:O4'	2.14	0.48
31:9:31:C:H2'	31:9:32:G:O4'	2.14	0.48
31:9:54:A:C2'	31:9:55:U:H5'	2.43	0.48
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.95	0.48
4:D:99:ASP:HB3	4:D:103:ASN:H	1.79	0.48
4:D:25:MET:SD	4:D:40:ILE:HD11	2.53	0.48
9:I:126:THR:O	9:I:130:LEU:HG	2.14	0.48
18:R:47:LEU:HB2	18:R:89:LEU:HD21	1.95	0.48
30:0:1183:C:H42	30:0:1184:C:N4	2.11	0.48
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.48
30:0:368:C:C2'	30:0:369:G:H5'	2.43	0.48
30:0:736:A:H2'	30:0:737:A:O4'	2.14	0.48
4:D:10:PHE:CG	4:D:11:HIS:N	2.81	0.48
30:0:2488:U:O2'	30:0:2489:G:H5'	2.14	0.48
30:0:318:U:H5'	30:0:339:A:C2	2.49	0.48
30:0:241:A:C2	30:0:378:A:H4'	2.49	0.48
3:C:132:ASP:HB2	3:C:161:ASP:HB3	1.95	0.48
8:H:30:LYS:N	8:H:62:HIS:HD2	2.10	0.48
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.46	0.48
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.10	0.48
14:N:154:LEU:C	14:N:156:GLU:H	2.16	0.48
19:S:33:SER:O	19:S:37:VAL:HG23	2.12	0.48
23:W:125:HIS:HB2	23:W:137:GLN:HG2	1.94	0.48
23:W:130:HIS:O	23:W:136:GLY:HA3	2.13	0.48
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.13	0.48
30:0:1173:A:C2	30:0:1177:A:C8	3.02	0.48
30:0:1221:G:H8	38:0:6014:HOH:O	1.94	0.48
30:0:1592:G:H2'	30:0:1593:C:H6	1.78	0.48
30:0:1692:C:H2'	38:0:9867:HOH:O	2.12	0.48
30:0:2133:U:H4'	30:0:2134:G:C5'	2.44	0.48
30:0:2505:G:C2'	30:0:2506:A:H5'	2.44	0.48
30:0:2672:C:O2'	30:0:2673:U:H5'	2.14	0.48
30:0:559:U:C3'	30:0:559:U:C6	2.97	0.48
30:0:633:C:O2'	30:0:634:G:H5'	2.14	0.48
30:0:843:A:C2	30:0:846:A:C8	3.02	0.48
2:B:44:TYR:OH	2:B:148:PRO:HG3	2.13	0.48
2:B:310:ARG:HD2	38:B:9112:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1198:U:C6	30:0:1200:A:OP2	2.67	0.48
30:0:128:A:O2'	30:0:129:A:H5'	2.14	0.48
30:0:1790:C:H2'	30:0:1791:U:H6	1.78	0.48
38:K:992:HOH:O	30:0:2583:A:H5'	2.13	0.48
30:0:2649:A:H5'	30:0:2649:A:H8	1.79	0.48
30:0:2718:C:H5'	30:0:2718:C:C6	2.46	0.48
30:0:2781:U:C2'	30:0:2782:G:C5'	2.91	0.48
30:0:281:U:O2'	30:0:282:C:H5'	2.14	0.48
30:0:334:G:C4	30:0:335:U:C6	3.02	0.48
30:0:484:A:N1	30:0:506:G:H4'	2.29	0.48
30:0:660:A:H4'	30:0:661:G:O5'	2.14	0.48
2:B:79:MET:HE1	38:B:9092:HOH:O	2.12	0.48
3:C:188:ARG:HD3	38:C:8563:HOH:O	2.13	0.48
22:V:4:HIS:HB3	38:V:6622:HOH:O	2.13	0.48
23:W:122:ARG:NH2	38:0:6437:HOH:O	2.46	0.48
30:0:1206:U:H2'	30:0:1207:A:O4'	2.14	0.47
30:0:2526:C:H6	30:0:2526:C:C5'	2.18	0.47
15:O:25:VAL:HG12	30:0:709:G:O2'	2.14	0.47
30:0:727:G:H3'	30:0:728:C:H6	1.79	0.47
30:0:861:A:C4'	30:0:1697:G:H4'	2.44	0.47
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.96	0.47
30:0:1634:G:H2'	30:0:1635:U:H6	1.79	0.47
30:0:1855:G:H4'	30:0:1856:C:O5'	2.13	0.47
30:0:559:U:H2'	30:0:560:U:O4'	2.15	0.47
30:0:571:C:H6	30:0:571:C:O5'	1.97	0.47
30:0:699:C:C2	30:0:744:G:C2	3.02	0.47
31:9:7:G:C5'	38:9:9100:HOH:O	2.58	0.47
1:A:36:ASP:HB2	1:A:85:SER:H	1.79	0.47
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.95	0.47
2:B:280:VAL:HG13	2:B:333:GLU:O	2.13	0.47
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.44	0.47
10:J:107:ASN:ND2	10:J:109:TYR:H	2.11	0.47
20:T:82:THR:HA	38:0:3998:HOH:O	2.12	0.47
30:0:1497:G:H4'	30:0:1627:G:O2'	2.14	0.47
30:0:619:U:H3'	38:0:3287:HOH:O	2.13	0.47
30:0:816:G:C6	30:0:817:G:N1	2.83	0.47
2:B:85:ARG:NH1	38:B:9099:HOH:O	2.47	0.47
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.49	0.47
15:O:39:THR:HB	38:0:4627:HOH:O	2.14	0.47
25:Y:107:PRO:HB3	25:Y:182:PHE:CD2	2.50	0.47
30:0:1154:A:H2'	30:0:1155:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1172:G:H1'	38:0:4992:HOH:O	2.14	0.47
30:0:1217:G:C2	30:0:1218:U:C2	3.03	0.47
30:0:12:U:C2'	30:0:13:G:H5'	2.40	0.47
30:0:2467:A:H8	38:0:7512:HOH:O	1.97	0.47
30:0:350:G:O2'	30:0:351:A:H5'	2.13	0.47
30:0:638:C:H2'	30:0:639:A:H8	1.78	0.47
30:0:724:G:O2'	30:0:725:C:H5'	2.14	0.47
30:0:963:C:O2	30:0:1005:A:N1	2.47	0.47
27:1:22:CYS:HB3	27:1:37:CYS:SG	2.55	0.47
31:9:76:G:H3'	31:9:77:A:C5'	2.30	0.47
2:B:27:ASN:H	2:B:27:ASN:HD22	1.63	0.47
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.95	0.47
16:P:103:THR:HA	16:P:106:ARG:NH2	2.29	0.47
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.43	0.47
30:0:1636:G:O2'	30:0:1637:A:H5'	2.13	0.47
30:0:1856:C:H5'	30:0:1858:A:O4'	2.15	0.47
30:0:1878:G:C1'	38:0:6151:HOH:O	2.51	0.47
30:0:2121:G:O2'	30:0:2122:C:H5'	2.14	0.47
30:0:255:A:H2'	30:0:256:C:O4'	2.14	0.47
30:0:2577:A:H5'	38:0:7788:HOH:O	2.14	0.47
30:0:2614:C:O2'	30:0:2615:U:H5'	2.14	0.47
30:0:297:U:H2'	30:0:298:C:C6	2.49	0.47
30:0:541:C:C2'	30:0:542:A:C5'	2.81	0.47
30:0:74:G:H2'	30:0:75:U:C6	2.49	0.47
30:0:968:G:C2	30:0:1001:U:O2	2.67	0.47
31:9:1:U:H5''	31:9:3:A:OP1	2.15	0.47
1:A:64:ASP:OD2	1:A:66:ARG:HD2	2.15	0.47
2:B:307:ARG:HB3	38:B:9117:HOH:O	2.15	0.47
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.95	0.47
30:0:1587:U:H2'	30:0:1588:G:O4'	2.14	0.47
30:0:2524:G:H21	30:0:2526:C:N4	2.12	0.47
30:0:2769:C:H2'	30:0:2770:G:O4'	2.15	0.47
30:0:2842:G:H2'	30:0:2843:A:C5'	2.44	0.47
13:M:28:GLN:O	13:M:32:ARG:HG3	2.15	0.47
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.45	0.47
16:P:59:ARG:O	16:P:63:ARG:HG3	2.15	0.47
30:0:1339:G:C6	30:0:1340:G:N1	2.83	0.47
11:K:66:ARG:HH22	30:0:1994:A:P	2.37	0.47
1:A:223:ARG:NH2	30:0:2271:G:OP1	2.45	0.47
30:0:2587:OMU:O3'	30:0:2587:OMU:HM22	2.15	0.47
30:0:27:U:H5	38:0:5910:HOH:O	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:736:A:H5''	38:0:4282:HOH:O	2.14	0.47
2:B:41:PHE:HB3	2:B:190:MET:CE	2.44	0.47
3:C:153:VAL:O	3:C:157:LEU:HG	2.15	0.47
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.97	0.47
10:J:90:LYS:HB2	33:J:8802:CL:CL	2.51	0.47
2:B:244:PRO:HB3	30:0:1234:U:N3	2.29	0.47
30:0:1268:C:O2'	30:0:1269:G:H5'	2.15	0.47
30:0:1803:C:H2'	30:0:1804:A:C8	2.50	0.47
30:0:1925:G:O2'	30:0:1926:G:H5'	2.15	0.47
30:0:2649:A:H5'	30:0:2649:A:C8	2.50	0.47
30:0:758:A:H2'	30:0:759:C:O4'	2.15	0.47
30:0:772:G:H2'	30:0:773:A:O4'	2.15	0.47
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.02	0.47
5:E:145:ALA:HB1	5:E:168:ILE:CD1	2.45	0.47
20:T:62:VAL:N	38:T:3851:HOH:O	2.47	0.47
23:W:122:ARG:NH2	38:0:5308:HOH:O	2.48	0.47
24:X:78:GLU:HB3	38:X:5564:HOH:O	2.15	0.47
30:0:1183:C:N3	30:0:1184:C:N4	2.62	0.47
30:0:2326:C:H4'	30:0:2412:G:C4'	2.45	0.47
30:0:24:G:N2	30:0:518:G:H1'	2.30	0.47
30:0:70:A:H4'	30:0:71:G:O5'	2.15	0.47
27:1:28:HIS:O	27:1:32:LYS:N	2.47	0.47
31:9:52:A:O2'	31:9:53:G:H5'	2.15	0.47
31:9:5:G:O2'	31:9:6:C:H5'	2.15	0.47
3:C:87:ARG:NH2	30:0:894:A:C2	2.83	0.47
5:E:11:VAL:HG12	5:E:12:ASP:N	2.30	0.47
30:0:625:U:H5''	30:0:1044:C:N4	2.30	0.47
30:0:1204:C:H2'	30:0:1205:U:O4'	2.15	0.47
30:0:2133:U:H4'	30:0:2134:G:H5'	1.96	0.47
18:R:29:LYS:HE2	30:0:524:A:C5'	2.45	0.47
30:0:834:G:H3'	30:0:835:U:H4'	1.97	0.47
30:0:862:U:H2'	30:0:863:G:H8	1.80	0.47
31:9:33:U:H2'	38:9:9066:HOH:O	2.15	0.47
1:A:112:PRO:HD3	1:A:152:CYS:SG	2.55	0.47
2:B:139:ASP:HB2	38:B:8997:HOH:O	2.14	0.47
6:F:46:GLU:OE1	6:F:100:ASP:HA	2.15	0.47
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.97	0.47
22:V:44:GLY:O	22:V:48:GLU:HG2	2.15	0.47
30:0:1181:A:N1	30:0:1192:A:O2'	2.42	0.47
30:0:1622:G:H2'	30:0:1623:C:H5'	1.97	0.47
30:0:1641:A:C2'	30:0:1642:A:H5'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:790:A:H1'	30:0:1710:A:H2'	1.97	0.47
30:0:383:A:H2'	30:0:384:G:O4'	2.15	0.47
30:0:595:U:H2'	30:0:596:C:H6	1.80	0.47
14:N:4:PRO:HG3	31:9:69:U:OP1	2.15	0.47
2:B:62:ARG:HA	2:B:65:MET:HE2	1.97	0.47
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.15	0.47
13:M:184:ARG:HG3	13:M:185:PRO:HA	1.97	0.47
23:W:4:LEU:O	23:W:32:CYS:HA	2.15	0.47
30:0:1116:U:C2'	30:0:1118:A:C2	2.92	0.46
30:0:1589:G:N2	30:0:1605:G:H1'	2.29	0.46
30:0:2533:C:C6	30:0:2533:C:H5'	2.39	0.46
30:0:153:C:O2	30:0:439:A:H2	1.98	0.46
30:0:737:A:O5'	30:0:737:A:H8	1.98	0.46
1:A:186:TRP:CG	1:A:187:PRO:HA	2.50	0.46
3:C:236:THR:HG22	3:C:239:ALA:CB	2.45	0.46
15:O:29:VAL:HG11	15:O:98:LEU:HD21	1.96	0.46
30:0:1196:C:C2	30:0:1197:G:C8	3.03	0.46
30:0:1819:G:H2'	30:0:1820:G:C4'	2.45	0.46
30:0:2511:A:H2'	30:0:2512:U:O4'	2.15	0.46
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.96	0.46
30:0:2791:U:H1'	30:0:2792:A:H5''	1.96	0.46
30:0:284:C:H6	30:0:284:C:OP2	1.98	0.46
30:0:541:C:O2'	30:0:542:A:H5''	2.15	0.46
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.46
31:9:110:G:C6	31:9:111:U:C5	3.03	0.46
4:D:77:ASP:HB3	4:D:78:GLU:H	1.55	0.46
10:J:130:VAL:HG12	10:J:131:THR:N	2.30	0.46
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.16	0.46
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.95	0.46
30:0:1666:C:HO2'	30:0:1667:A:H5''	1.72	0.46
30:0:1706:G:C6	30:0:1707:G:C6	3.04	0.46
30:0:2089:A:O2'	30:0:2090:G:H5'	2.15	0.46
30:0:2269:C:H2'	30:0:2270:G:H5'	1.96	0.46
30:0:2361:A:H2'	30:0:2362:A:O4'	2.15	0.46
30:0:264:G:H1'	30:0:265:U:H5	1.80	0.46
30:0:515:C:H5''	38:0:5665:HOH:O	2.13	0.46
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.15	0.46
2:B:62:ARG:HA	2:B:65:MET:HE3	1.97	0.46
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.80	0.46
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.50	0.46
30:0:105:G:O2'	30:0:106:A:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:128:A:H3'	30:0:128:A:C8	2.50	0.46
30:0:1948:G:H1	30:0:1964:U:H3	1.63	0.46
30:0:1966:U:O5'	30:0:1966:U:H6	1.99	0.46
30:0:2000:G:O2'	30:0:2001:G:H5'	2.15	0.46
30:0:204:A:C2'	30:0:205:U:H5'	2.45	0.46
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.16	0.46
30:0:254:C:O2	30:0:254:C:H2'	2.14	0.46
11:K:87:ARG:NH2	30:0:2720:C:O2	2.49	0.46
30:0:506:G:N2	30:0:509:A:H5'	2.21	0.46
30:0:890:C:O2'	30:0:891:G:H5'	2.16	0.46
2:B:125:GLU:O	2:B:129:ARG:HG3	2.15	0.46
2:B:112:THR:HG23	2:B:158:LYS:HZ2	1.80	0.46
10:J:19:MET:CE	10:J:132:LEU:HD11	2.45	0.46
30:0:1581:A:C5	30:0:1582:C:C5	3.03	0.46
16:P:88:GLN:HE22	30:0:1799:G:H21	1.63	0.46
30:0:419:A:H1'	30:0:1921:A:C2	2.51	0.46
30:0:2326:C:H4'	30:0:2412:G:H4'	1.97	0.46
30:0:2506:A:N6	30:0:2511:A:O2'	2.49	0.46
30:0:300:U:C4	30:0:301:C:C5	3.03	0.46
23:W:43:GLY:HA3	30:0:945:U:O2'	2.15	0.46
1:A:71:PRO:HD2	1:A:74:VAL:HG21	1.98	0.46
2:B:177:HIS:O	2:B:181:ILE:HG13	2.15	0.46
6:F:101:ALA:HA	38:F:5413:HOH:O	2.15	0.46
12:L:148:GLU:HA	38:L:8870:HOH:O	2.14	0.46
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.97	0.46
30:0:129:A:O2'	30:0:131:A:OP1	2.33	0.46
30:0:1543:G:N1	30:0:1641:A:OP2	2.35	0.46
30:0:2775:A:C6	30:0:2799:A:C8	3.04	0.46
30:0:441:A:H8	30:0:441:A:O5'	1.97	0.46
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.45	0.46
23:W:139:GLY:O	23:W:141:HIS:CD2	2.66	0.46
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.85	0.46
30:0:1156:C:O5'	30:0:1156:C:H6	1.99	0.46
30:0:1321:A:H2'	30:0:1322:G:C8	2.51	0.46
30:0:1393:A:N1	30:0:1725:C:O2'	2.39	0.46
30:0:1588:G:C6	30:0:1589:G:C6	3.04	0.46
30:0:2115:U:H2'	30:0:2116:U:C6	2.51	0.46
30:0:2658:G:H4'	30:0:2842:G:C8	2.51	0.46
2:B:214:PRO:HD2	38:0:9083:HOH:O	2.14	0.46
3:C:214:THR:HG23	38:C:8635:HOH:O	2.16	0.46
13:M:86:GLN:HE22	30:0:2274:A:H1'	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:35:LYS:HD3	38:O:4627:HOH:O	2.15	0.46
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.49	0.46
30:0:1115:U:O2'	30:0:1116:U:H5'	2.15	0.46
30:0:1130:U:H2'	30:0:1131:G:O4'	2.16	0.46
30:0:1586:G:O2'	30:0:1587:U:H5'	2.16	0.46
30:0:1973:A:H2'	30:0:1974:G:O4'	2.15	0.46
30:0:2252:A:C6	30:0:2253:G:H1'	2.51	0.46
30:0:2366:C:O5'	30:0:2366:C:H6	1.99	0.46
1:A:6:GLY:O	30:0:1861:C:H4'	2.15	0.46
9:I:78:ALA:HB1	9:I:93:ALA:HB1	1.96	0.46
30:0:2112:A:H2'	30:0:2113:G:C8	2.50	0.46
30:0:2301:A:H5''	30:0:2302:A:H5'	1.97	0.46
30:0:2385:G:H2'	30:0:2386:U:H6	1.81	0.46
30:0:2710:U:H2'	30:0:2711:U:C6	2.50	0.46
31:9:20:G:O2'	31:9:21:G:H5'	2.16	0.46
23:W:119:HIS:CD2	23:W:120:PRO:HD2	2.50	0.46
25:Y:133:HIS:HD2	38:Y:8884:HOH:O	1.98	0.46
30:0:1445:G:N2	30:0:1678:A:H1'	2.31	0.46
30:0:1598:A:N6	33:0:8815:CL:CL	2.86	0.46
16:P:73:HIS:HE1	30:0:1789:G:O6	1.98	0.46
30:0:1930:A:H2'	30:0:1931:A:C8	2.51	0.46
30:0:2831:C:C2'	30:0:2832:C:H5'	2.46	0.46
30:0:417:G:P	38:0:7458:HOH:O	2.73	0.46
30:0:440:C:H2'	30:0:441:A:C8	2.51	0.46
30:0:567:U:O2'	30:0:568:G:H5'	2.15	0.46
30:0:999:C:H2'	30:0:1000:C:O4'	2.16	0.46
2:B:140:LEU:HD12	2:B:174:ARG:HG3	1.97	0.46
4:D:131:THR:HG21	30:0:2348:C:H1'	1.96	0.46
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.98	0.46
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.98	0.46
14:N:110:THR:HB	14:N:113:SER:OG	2.16	0.46
18:R:82:GLU:HG3	18:R:83:LYS:N	2.30	0.46
22:V:39:ALA:C	22:V:41:GLU:H	2.20	0.46
23:W:26:ILE:HB	38:W:5420:HOH:O	2.15	0.46
9:I:112:LEU:HG	30:0:1162:G:O2'	2.15	0.45
30:0:1169:U:C5	30:0:1170:U:C4	3.03	0.45
30:0:1456:C:H2'	30:0:1457:U:C6	2.50	0.45
30:0:2299:G:C6	30:0:2300:A:C6	3.05	0.45
30:0:253:U:H1'	30:0:256:C:H41	1.80	0.45
28:2:28:LYS:O	30:0:87:C:H2'	2.16	0.45
1:A:95:PRO:HA	1:A:153:ARG:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.17	0.45
26:Z:46:SER:O	26:Z:50:VAL:HG23	2.16	0.45
30:0:123:U:O2'	30:0:124:C:H5'	2.16	0.45
30:0:1669:G:O2'	30:0:1670:A:H5'	2.16	0.45
30:0:861:A:H4'	30:0:1697:G:C4'	2.47	0.45
30:0:1896:G:C5	30:0:1897:U:C5	3.04	0.45
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.49	0.45
30:0:2604:A:H5'	38:0:5810:HOH:O	2.16	0.45
30:0:282:C:H1'	30:0:368:C:H41	1.74	0.45
30:0:2869:G:H2'	30:0:2870:C:C6	2.51	0.45
30:0:851:C:O2	30:0:2022:A:H2	1.99	0.45
16:P:36:THR:O	16:P:39:ASP:HB2	2.16	0.45
23:W:56:GLU:O	23:W:143:THR:HG23	2.16	0.45
23:W:88:THR:HG21	23:W:96:LEU:HD13	1.98	0.45
25:Y:177:LYS:HD3	25:Y:181:GLY:O	2.17	0.45
30:0:1188:A:C5	30:0:1189:A:C2	3.03	0.45
30:0:1309:U:O2'	30:0:1310:U:H5'	2.16	0.45
30:0:1314:U:H5''	30:0:1316:G:O4'	2.16	0.45
30:0:1506:U:H5'	30:0:1506:U:H6	1.82	0.45
30:0:1788:U:C2	30:0:1805:G:N2	2.84	0.45
30:0:2421:G:H4'	38:0:4797:HOH:O	2.16	0.45
30:0:2664:A:H8	30:0:2664:A:OP1	1.99	0.45
30:0:2712:G:O2'	30:0:2713:G:H5'	2.16	0.45
3:C:206:ASN:HB2	30:0:329:A:OP2	2.16	0.45
31:9:39:U:C2'	31:9:40:C:OP1	2.65	0.45
4:D:76:ARG:NE	31:9:44:A:O4'	2.49	0.45
1:A:109:GLU:HG2	1:A:116:GLY:N	2.30	0.45
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.79	0.45
3:C:93:LYS:O	3:C:98:ARG:NH2	2.49	0.45
8:H:52:LEU:HB3	8:H:137:PHE:HB2	1.99	0.45
14:N:44:ARG:HG3	14:N:45:ALA:N	2.32	0.45
14:N:37:ARG:HD3	33:N:8807:CL:CL	2.54	0.45
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.81	0.45
20:T:26:THR:HA	20:T:39:ASN:HB3	1.98	0.45
22:V:39:ALA:N	22:V:40:PRO:CD	2.80	0.45
30:0:1189:A:C3'	38:0:7717:HOH:O	2.59	0.45
30:0:1790:C:H2'	30:0:1791:U:C6	2.51	0.45
30:0:228:C:H2'	30:0:229:G:H5'	1.98	0.45
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.45
30:0:397:A:O2'	30:0:417:G:N3	2.39	0.45
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:110:G:C5	31:9:111:U:C5	3.04	0.45
30:0:1002:G:H2'	30:0:1003:U:O5'	2.17	0.45
30:0:1116:U:H2'	30:0:1118:A:C2	2.52	0.45
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.97	0.45
30:0:1398:G:O2'	30:0:1399:A:H5'	2.16	0.45
30:0:1563:G:H4'	38:0:4241:HOH:O	2.16	0.45
30:0:158:A:C2'	30:0:159:G:H5'	2.47	0.45
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.43	0.45
16:P:55:LYS:HD3	30:0:1716:A:H4'	1.97	0.45
30:0:2332:A:H5'	30:0:2333:G:OP2	2.17	0.45
30:0:482:G:O4'	30:0:511:A:C2	2.70	0.45
18:R:128:ARG:HH12	30:0:840:U:H2'	1.80	0.45
30:0:955:A:C2	30:0:1013:A:C4	3.05	0.45
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.78	0.45
4:D:23:VAL:HG12	4:D:130:VAL:HG22	1.98	0.45
11:K:81:ARG:HD3	11:K:87:ARG:NH1	2.31	0.45
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.45	0.45
30:0:1023:C:H2'	30:0:1024:G:O4'	2.16	0.45
30:0:1503:U:H2'	30:0:1504:A:O4'	2.16	0.45
30:0:1964:U:C2	30:0:1965:C:C5	3.05	0.45
30:0:228:C:C2'	30:0:229:G:H5'	2.46	0.45
17:Q:11:ARG:HG3	30:0:2363:G:O2'	2.16	0.45
13:M:179:GLY:O	30:0:399:C:H5'	2.17	0.45
3:C:236:THR:H	3:C:239:ALA:HB3	1.80	0.45
3:C:35:VAL:HG21	3:C:227:GLY:HA2	1.98	0.45
6:F:72:VAL:HA	6:F:73:PRO:HD3	1.87	0.45
9:I:87:PRO:HG3	38:0:7157:HOH:O	2.17	0.45
24:X:30:MET:HG2	30:0:1384:C:H5'	1.98	0.45
12:L:30:ARG:HD2	30:0:164:G:H5''	1.99	0.45
30:0:1921:A:O2'	30:0:1922:A:H5'	2.17	0.45
30:0:685:C:O2	30:0:748:C:H4'	2.17	0.45
31:9:60:C:H2'	31:9:61:C:H6	1.81	0.45
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.99	0.45
23:W:29:VAL:O	23:W:30:ASN:HB2	2.16	0.45
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.51	0.45
30:0:1573:A:N7	30:0:1574:C:C2	2.85	0.45
30:0:2251:G:H2'	30:0:2252:A:H8	1.79	0.45
38:3:9030:HOH:O	30:0:2382:A:H5'	2.16	0.45
30:0:2793:A:H2'	30:0:2794:G:H5'	1.98	0.45
30:0:559:U:H3'	30:0:559:U:C6	2.52	0.45
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:41:LYS:HD3	38:9:9060:HOH:O	2.17	0.45
19:S:6:LYS:HB2	19:S:27:ALA:O	2.17	0.45
30:0:2316:G:OP1	30:0:2317:C:H1'	2.16	0.45
30:0:2419:U:H5''	30:0:2420:G:C5'	2.46	0.45
30:0:2897:C:O2'	30:0:2898:G:H5'	2.17	0.45
30:0:962:C:C2'	30:0:963:C:H5'	2.47	0.45
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.47	0.45
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.82	0.45
3:C:127:ARG:HD3	3:C:129:HIS:CE1	2.52	0.45
5:E:10:ASP:HA	38:E:6017:HOH:O	2.17	0.45
14:N:169:PRO:O	14:N:172:PHE:HB3	2.17	0.45
17:Q:3:SER:HB3	38:Q:5998:HOH:O	2.16	0.45
23:W:69:ARG:HD2	23:W:117:ARG:O	2.16	0.45
26:Z:45:VAL:HG12	38:Z:8714:HOH:O	2.17	0.45
30:0:1120:U:H6	30:0:1120:U:H5''	1.81	0.45
30:0:1268:C:H2'	30:0:1269:G:C8	2.51	0.45
30:0:1700:C:H5''	30:0:1701:A:OP2	2.16	0.45
30:0:2002:C:C2'	30:0:2003:U:H5'	2.46	0.45
30:0:249:G:O2'	30:0:250:C:H5'	2.17	0.45
29:3:11:CYS:HB2	29:3:20:HIS:HE1	1.81	0.45
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.98	0.45
9:I:108:HIS:H	9:I:109:PRO:HD2	1.82	0.45
10:J:52:GLN:HE22	30:0:1119:G:H8	1.65	0.45
23:W:119:HIS:CG	38:0:5308:HOH:O	2.69	0.45
30:0:1209:C:O2'	30:0:1210:G:H5'	2.16	0.44
30:0:1904:A:H2'	30:0:1905:U:O4'	2.17	0.44
30:0:2831:C:H2'	30:0:2832:C:H5'	1.98	0.44
30:0:62:C:C4	30:0:63:U:C4	3.05	0.44
30:0:81:G:N3	30:0:98:A:C2	2.85	0.44
4:D:140:ARG:HG3	4:D:140:ARG:HH11	1.82	0.44
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.83	0.44
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.31	0.44
13:M:6:SER:O	13:M:10:ASP:HB2	2.17	0.44
14:N:43:VAL:HG13	14:N:118:ILE:HD11	1.98	0.44
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.99	0.44
23:W:88:THR:HG22	23:W:90:TYR:CD1	2.50	0.44
30:0:1524:U:H5''	30:0:1524:U:C6	2.52	0.44
30:0:177:A:H2'	30:0:178:U:O4'	2.16	0.44
30:0:2070:G:H2'	30:0:2072:G:OP1	2.17	0.44
30:0:2103:A:N6	30:0:2538:A:H8	2.09	0.44
30:0:812:A:H2'	30:0:813:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:920:C:H4'	30:0:921:G:N2	2.32	0.44
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.52	0.44
3:C:54:LEU:HD23	3:C:79:ARG:HG3	1.99	0.44
30:0:1626:A:H2'	30:0:1627:G:C5'	2.48	0.44
28:2:43:ARG:NH2	30:0:1684:A:H1'	2.25	0.44
30:0:2072:G:H3'	30:0:2073:G:C5'	2.47	0.44
30:0:2297:U:H1'	38:0:5197:HOH:O	2.17	0.44
30:0:2329:C:H2'	30:0:2330:U:C6	2.52	0.44
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.17	0.44
31:9:59:C:C4	31:9:60:C:N4	2.86	0.44
31:9:97:U:O2'	31:9:98:C:H5'	2.18	0.44
5:E:72:MET:O	5:E:76:VAL:HG22	2.18	0.44
11:K:89:LYS:HE2	21:U:19:THR:HG21	2.00	0.44
21:U:37:GLU:HB3	38:U:408:HOH:O	2.18	0.44
26:Z:61:HIS:O	26:Z:69:ASP:HA	2.18	0.44
30:0:1190:G:H2'	38:0:4068:HOH:O	2.15	0.44
30:0:130:C:H2'	38:0:3168:HOH:O	2.17	0.44
30:0:1712:A:H2'	30:0:1713:G:O4'	2.18	0.44
1:A:212:PRO:HA	30:0:1943:C:O4'	2.18	0.44
1:A:204:GLY:N	30:0:2634:G:OP2	2.51	0.44
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.99	0.44
3:C:168:ARG:NH2	3:C:190:ALA:O	2.51	0.44
5:E:19:ASP:HA	5:E:31:ARG:O	2.17	0.44
7:G:67:LEU:O	7:G:71:LEU:HG	2.18	0.44
24:X:47:ALA:HB1	24:X:82:GLU:HB3	2.00	0.44
30:0:1447:U:H3'	30:0:1506:U:O2	2.18	0.44
30:0:1523:G:H2'	30:0:1524:U:O4'	2.17	0.44
30:0:1592:G:H2'	30:0:1593:C:C6	2.52	0.44
30:0:1902:G:O2'	30:0:1903:U:H5'	2.17	0.44
30:0:1947:G:N2	30:0:1965:C:O2	2.50	0.44
30:0:2135:A:C2'	30:0:2136:G:H5'	2.47	0.44
30:0:2104:C:O2	30:0:2485:A:N1	2.50	0.44
30:0:506:G:N2	30:0:509:A:H5''	2.30	0.44
30:0:559:U:C4	30:0:560:U:C4	3.06	0.44
30:0:677:C:O2'	30:0:678:G:H5'	2.17	0.44
1:A:171:LYS:HB2	30:0:820:G:C5	2.53	0.44
30:0:858:U:H2'	30:0:859:C:C6	2.52	0.44
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.99	0.44
7:G:64:ASN:N	7:G:64:ASN:ND2	2.66	0.44
10:J:39:VAL:HG13	10:J:106:GLY:O	2.17	0.44
12:L:43:HIS:HD2	38:L:8827:HOH:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:167:GLY:O	13:M:171:ARG:HG3	2.17	0.44
23:W:90:TYR:N	23:W:90:TYR:CD1	2.85	0.44
26:Z:78:ILE:HD12	38:Z:8717:HOH:O	2.18	0.44
30:0:1052:G:H2'	30:0:1052:G:N3	2.31	0.44
30:0:113:A:OP2	30:0:114:A:H2'	2.17	0.44
30:0:1166:A:OP1	30:0:1174:A:H4'	2.17	0.44
30:0:1173:A:H3'	38:0:4358:HOH:O	2.16	0.44
30:0:1182:C:C1'	30:0:1192:A:C8	3.01	0.44
30:0:128:A:C8	30:0:128:A:C3'	3.01	0.44
29:3:48:ASN:ND2	30:0:169:A:H1'	2.33	0.44
30:0:1825:U:O2'	30:0:1826:C:H5'	2.18	0.44
30:0:255:A:C4	30:0:256:C:C6	3.06	0.44
30:0:295:C:H2'	30:0:296:G:O4'	2.18	0.44
30:0:39:G:N2	30:0:444:C:C2	2.86	0.44
30:0:594:C:C4	30:0:595:U:C4	3.06	0.44
30:0:645:U:O2	30:0:761:A:H2	2.00	0.44
30:0:735:C:H5	30:0:736:A:C4	2.36	0.44
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.99	0.44
5:E:170:ARG:NH2	38:E:4761:HOH:O	2.50	0.44
11:K:125:ALA:C	11:K:127:ALA:H	2.21	0.44
14:N:139:TRP:HA	14:N:139:TRP:HE3	1.81	0.44
30:0:1226:G:H5'	38:0:4543:HOH:O	2.18	0.44
30:0:1318:A:H4'	30:0:1343:C:H4'	2.00	0.44
30:0:1503:U:C2'	30:0:1504:A:H5'	2.48	0.44
30:0:2087:C:O2'	30:0:2088:C:H5'	2.18	0.44
1:A:179:MET:HG2	1:A:186:TRP:CB	2.48	0.44
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.01	0.44
1:A:94:LEU:HD12	1:A:98:GLU:HB2	2.00	0.44
13:M:80:GLY:O	13:M:81:ARG:HD2	2.17	0.44
20:T:28:SER:HA	20:T:97:ARG:HD3	2.00	0.44
24:X:25:ARG:HD2	38:X:5356:HOH:O	2.16	0.44
30:0:1135:G:H5'	38:0:5953:HOH:O	2.17	0.44
30:0:1180:U:H2'	30:0:1181:A:O4'	2.18	0.44
30:0:1553:C:O5'	30:0:1553:C:H6	2.00	0.44
30:0:1882:C:H2'	30:0:1883:U:H6	1.83	0.44
30:0:307:G:H3'	38:0:6719:HOH:O	2.18	0.44
30:0:696:C:O2'	30:0:697:G:H5'	2.17	0.44
30:0:729:C:C2	30:0:743:G:C2	3.06	0.44
30:0:734:U:H2'	30:0:736:A:OP2	2.18	0.44
8:H:39:LYS:HD2	30:0:969:G:H5'	1.98	0.44
31:9:2:U:H4'	38:9:9103:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.33	0.44
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.85	0.44
6:F:1:PRO:H3	6:F:4:VAL:HG23	1.83	0.44
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.98	0.44
12:L:113:GLN:O	30:0:700:A:N6	2.47	0.44
15:O:105:ASN:HD21	15:O:109:SER:H	1.65	0.44
18:R:104:PHE:HB3	18:R:109:MET:HE1	2.00	0.44
30:0:1279:U:C2'	30:0:1279:U:O2	2.64	0.44
30:0:2256:G:C6	30:0:2257:G:C4	3.05	0.44
4:D:52:THR:HG21	30:0:2346:C:O2'	2.17	0.44
30:0:2533:C:O2'	30:0:2534:C:H5'	2.18	0.44
6:F:59:ILE:HD13	30:0:263:U:O4'	2.17	0.44
30:0:2914:A:H5''	30:0:2914:A:H8	1.83	0.44
30:0:812:A:H2'	30:0:813:C:O4'	2.17	0.44
30:0:935:G:O2'	30:0:936:C:H5'	2.18	0.44
4:D:167:GLU:C	4:D:169:THR:H	2.21	0.44
8:H:29:SER:HA	8:H:62:HIS:HD2	1.82	0.44
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.58	0.44
30:0:553:G:O4'	30:0:1325:G:H5'	2.18	0.43
30:0:1342:C:H2'	30:0:1343:C:H5'	2.00	0.43
30:0:1386:G:O2'	30:0:1387:G:H5'	2.18	0.43
30:0:1444:G:O2'	30:0:1445:G:H5'	2.18	0.43
30:0:2796:U:H2'	30:0:2797:C:O5'	2.18	0.43
30:0:629:A:H2'	30:0:630:A:O4'	2.18	0.43
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.99	0.43
8:H:139:ALA:HB3	8:H:149:VAL:HG21	2.00	0.43
13:M:47:ASP:CG	13:M:48:LYS:N	2.71	0.43
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.52	0.43
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.82	0.43
24:X:23:HIS:CD2	24:X:24:LYS:HG3	2.53	0.43
30:0:2332:A:H3'	30:0:2333:G:H8	1.83	0.43
30:0:238:C:H4'	30:0:287:C:OP1	2.18	0.43
30:0:2717:C:C2'	30:0:2718:C:C5'	2.81	0.43
30:0:1705:C:O2	30:0:2735:U:H5''	2.18	0.43
30:0:2761:A:C4	30:0:2763:G:C8	3.06	0.43
30:0:282:C:C2'	30:0:283:U:H5'	2.47	0.43
30:0:544:G:C3'	30:0:545:G:H5''	2.46	0.43
30:0:696:C:O2'	30:0:731:U:OP1	2.35	0.43
12:L:71:GLU:HG2	30:0:700:A:C2	2.54	0.43
1:A:48:ASP:HB3	38:A:9061:HOH:O	2.18	0.43
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.18	0.43
16:P:100:ALA:HA	38:O:5526:HOH:O	2.17	0.43
17:Q:28:ARG:HG2	38:9:9079:HOH:O	2.17	0.43
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.17	0.43
30:0:1098:A:H2'	30:0:1099:G:O4'	2.18	0.43
30:0:1181:A:H2'	30:0:1182:C:C5'	2.49	0.43
30:0:312:U:C2	30:0:320:G:N2	2.87	0.43
2:B:232:TRP:CD1	2:B:235:ARG:HD2	2.52	0.43
9:I:120:ALA:O	9:I:124:VAL:HG23	2.18	0.43
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.47	0.43
20:T:52:ARG:O	30:0:317:A:OP1	2.36	0.43
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.19	0.43
24:X:34:ARG:NH1	24:X:48:VAL:O	2.51	0.43
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.53	0.43
30:0:912:A:C4	30:0:1294:A:C2	3.05	0.43
13:M:188:ARG:HH11	30:0:154:C:H3'	1.82	0.43
30:0:1622:G:C2'	30:0:1623:C:H5'	2.48	0.43
30:0:1889:C:O2'	30:0:1890:U:H5'	2.18	0.43
30:0:2491:G:H5'	38:0:9387:HOH:O	2.19	0.43
30:0:300:U:C2	30:0:301:C:C6	3.06	0.43
30:0:483:C:N4	30:0:484:A:C6	2.87	0.43
30:0:815:U:O2'	30:0:1598:A:H4'	2.19	0.43
23:W:44:MET:HE2	30:0:944:G:H21	1.83	0.43
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.19	0.43
1:A:36:ASP:CB	1:A:85:SER:H	2.31	0.43
6:F:57:GLU:O	6:F:61:MET:HG3	2.18	0.43
17:Q:45:PRO:O	30:0:2365:G:H4'	2.18	0.43
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.53	0.43
24:X:15:ARG:HH22	30:0:2856:A:P	2.41	0.43
10:J:60:ARG:NH2	30:0:1242:A:OP2	2.45	0.43
30:0:2247:C:O2'	30:0:2248:C:H5'	2.18	0.43
30:0:2421:G:H3'	30:0:2422:U:C5'	2.48	0.43
30:0:2819:C:H2'	30:0:2820:A:C8	2.53	0.43
30:0:844:A:C6	30:0:882:A:C5	3.06	0.43
30:0:962:C:H5''	38:0:4933:HOH:O	2.19	0.43
29:3:70:ARG:HD3	38:3:9064:HOH:O	2.18	0.43
2:B:162:MET:CE	2:B:310:ARG:HD3	2.48	0.43
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.33	0.43
13:M:147:LEU:O	13:M:150:ILE:HG22	2.18	0.43
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.01	0.43
14:N:7:LYS:HB3	17:Q:21:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:104:PHE:CB	18:R:109:MET:HE1	2.48	0.43
25:Y:144:ARG:NE	38:Y:8914:HOH:O	2.52	0.43
12:L:6:ARG:NH1	30:0:1299:G:N7	2.67	0.43
30:0:1482:A:H1'	38:0:9428:HOH:O	2.18	0.43
30:0:1735:C:O2'	30:0:1736:A:H5'	2.18	0.43
30:0:1842:A:C4	30:0:1979:G:C6	3.06	0.43
30:0:213:G:N2	30:0:225:G:H2'	2.34	0.43
30:0:2566:A:C2	30:0:2696:G:O4'	2.71	0.43
30:0:2727:A:N1	30:0:2756:U:C2	2.87	0.43
30:0:2869:G:H5'	38:0:5515:HOH:O	2.18	0.43
30:0:451:C:O2'	30:0:452:G:H5'	2.18	0.43
30:0:653:U:H2'	30:0:654:A:C8	2.53	0.43
27:1:25:LYS:O	27:1:25:LYS:HG2	2.19	0.43
1:A:9:ARG:HG2	1:A:16:PHE:CD2	2.54	0.43
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.79	0.43
23:W:134:GLU:OE2	31:9:97:U:H1'	2.19	0.43
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.32	0.43
30:0:1165:G:H1'	30:0:1174:A:O2'	2.19	0.43
30:0:1184:C:O2'	30:0:1185:U:OP2	2.33	0.43
30:0:1248:A:H3'	38:0:7547:HOH:O	2.17	0.43
30:0:1524:U:H5''	30:0:1524:U:H6	1.84	0.43
30:0:1684:A:O2'	30:0:1685:A:H5''	2.18	0.43
30:0:1477:C:C5'	30:0:1868:G:H5''	2.48	0.43
30:0:2075:G:C6	30:0:2076:U:C4	3.07	0.43
30:0:191:A:C4	30:0:237:G:N7	2.87	0.43
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.18	0.43
30:0:2664:A:C8	30:0:2664:A:OP1	2.72	0.43
30:0:2812:A:H2	30:0:2814:A:N6	1.86	0.43
30:0:629:A:C2	30:0:2074:A:C2	3.07	0.43
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.99	0.43
31:9:1:U:C4'	31:9:3:A:OP1	2.67	0.43
31:9:88:G:N2	31:9:89:C:C2	2.87	0.43
5:E:101:GLU:HB2	5:E:116:THR:O	2.18	0.43
11:K:74:VAL:HG13	11:K:113:ILE:HG23	2.01	0.43
13:M:193:LYS:HB3	30:0:392:U:H4'	2.00	0.43
18:R:124:GLY:HA3	18:R:136:TRP:O	2.18	0.43
30:0:111:C:H2'	30:0:112:G:O4'	2.18	0.43
30:0:1482:A:O2'	30:0:1483:C:H5'	2.18	0.43
30:0:1545:C:H2'	30:0:1546:G:O4'	2.18	0.43
30:0:1882:C:H2'	30:0:1883:U:C6	2.53	0.43
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:75:PRO:HD3	10:J:136:SER:OG	2.19	0.43
12:L:143:THR:HG21	38:L:8839:HOH:O	2.17	0.43
30:0:47:G:N3	30:0:114:A:C2	2.87	0.43
30:0:1157:C:O2'	30:0:1158:G:H5'	2.18	0.43
30:0:1176:C:N4	38:0:9957:HOH:O	2.52	0.43
30:0:1132:A:H61	30:0:1229:C:H2'	1.83	0.43
30:0:1029:U:O2'	30:0:1273:C:OP1	2.33	0.43
30:0:1819:G:H2'	30:0:1820:G:H5'	2.01	0.43
30:0:1883:U:H5'	30:0:2012:U:OP2	2.18	0.43
30:0:212:A:O3'	30:0:213:G:H4'	2.19	0.43
30:0:2255:A:O2'	30:0:2256:G:H5'	2.18	0.43
30:0:2456:A:H2'	30:0:2457:U:C6	2.54	0.43
30:0:2482:G:H4'	30:0:2483:A:C5'	2.48	0.43
30:0:2096:A:H2'	30:0:2539:U:O4'	2.19	0.43
30:0:1815:A:H4'	30:0:2751:C:O4'	2.19	0.43
30:0:722:G:H22	30:0:938:G:P	2.42	0.43
5:E:40:VAL:HA	5:E:48:VAL:O	2.19	0.43
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.48	0.43
11:K:41:LYS:HA	30:0:2582:G:O3'	2.19	0.43
13:M:24:GLN:NE2	13:M:27:ARG:NH1	2.67	0.43
25:Y:125:LYS:HB2	25:Y:126:PRO:HD2	2.00	0.43
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.19	0.43
30:0:1520:G:C6	30:0:1521:C:N4	2.87	0.43
30:0:169:A:H5''	38:0:9693:HOH:O	2.18	0.43
30:0:1787:C:O2'	30:0:1788:U:H5'	2.19	0.43
30:0:2729:C:O2'	30:0:2730:G:H5'	2.19	0.43
30:0:790:A:H2'	30:0:791:A:O4'	2.19	0.43
31:9:2:U:H4'	31:9:2:U:OP2	2.19	0.43
2:B:148:PRO:HD2	38:B:9048:HOH:O	2.19	0.43
6:F:27:GLY:HA3	6:F:101:ALA:O	2.18	0.43
6:F:57:GLU:HB2	13:M:23:LEU:HD11	1.99	0.43
8:H:65:LEU:HD12	8:H:65:LEU:HA	1.84	0.43
14:N:116:PHE:HB3	14:N:136:LEU:HD23	2.00	0.43
14:N:11:ARG:NH1	31:9:8:G:O6	2.52	0.43
14:N:164:ASP:OD2	14:N:168:LEU:HG	2.19	0.43
21:U:17:THR:CG2	21:U:18:GLY:N	2.82	0.43
30:0:1044:C:H5''	38:0:9030:HOH:O	2.18	0.42
30:0:1315:G:H4'	30:0:1316:G:OP2	2.19	0.42
30:0:1521:C:H2'	30:0:1522:A:H8	1.84	0.42
30:0:162:C:H2'	30:0:163:U:H5'	2.01	0.42
30:0:1706:G:C5	30:0:1707:G:C6	3.06	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1894:C:N4	30:0:1939:U:H2'	2.33	0.42
30:0:2026:C:O2'	30:0:2027:U:H5'	2.19	0.42
30:0:2756:U:H1'	38:0:5024:HOH:O	2.19	0.42
30:0:2866:U:H4'	30:0:2867:G:H5'	2.01	0.42
30:0:1787:C:C4'	30:0:2883:A:O4'	2.67	0.42
30:0:365:G:C6	30:0:366:U:C4	3.07	0.42
30:0:85:C:H3'	30:0:86:A:H2'	2.01	0.42
31:9:14:G:O2'	31:9:15:C:H5'	2.19	0.42
1:A:6:GLY:HA3	38:0:4633:HOH:O	2.19	0.42
18:R:82:GLU:O	18:R:86:LYS:HG3	2.19	0.42
30:0:1189:A:H1'	30:0:1209:C:H1'	2.01	0.42
30:0:1741:U:C4	30:0:2033:G:C8	3.06	0.42
30:0:1976:G:O2'	30:0:1977:U:H5'	2.19	0.42
30:0:2783:A:H5''	38:0:5252:HOH:O	2.19	0.42
30:0:366:U:H2'	30:0:367:G:O4'	2.19	0.42
30:0:907:A:H2'	30:0:908:A:C8	2.53	0.42
2:B:112:THR:HG23	2:B:158:LYS:HZ1	1.84	0.42
2:B:232:TRP:HD1	2:B:235:ARG:HD2	1.83	0.42
3:C:107:ARG:O	3:C:111:VAL:HG23	2.19	0.42
7:G:12:ILE:N	7:G:13:PRO:HD3	2.35	0.42
19:S:10:VAL:HG11	22:V:36:ALA:HA	2.00	0.42
30:0:1381:A:N3	30:0:1382:G:H1'	2.34	0.42
30:0:1603:A:C8	30:0:1605:G:C2	3.07	0.42
30:0:255:A:H2'	30:0:256:C:C6	2.54	0.42
30:0:844:A:C6	30:0:882:A:C6	3.07	0.42
29:3:71:CYS:SG	38:3:9052:HOH:O	2.61	0.42
4:D:76:ARG:NH1	31:9:42:C:O2	2.49	0.42
3:C:22:PHE:HA	3:C:116:ALA:HA	2.00	0.42
4:D:104:PHE:CE2	4:D:132:VAL:HB	2.54	0.42
5:E:68:HIS:CE1	38:0:6506:HOH:O	2.72	0.42
10:J:74:ARG:O	10:J:78:ILE:HG13	2.19	0.42
14:N:108:SER:HA	14:N:109:PRO:HD3	1.82	0.42
15:O:65:LEU:HD13	30:0:746:A:C6	2.54	0.42
26:Z:84:CYS:O	26:Z:85:ASP:HB2	2.19	0.42
30:0:1681:G:H4'	30:0:1682:A:N3	2.34	0.42
30:0:2244:A:C4	30:0:2258:A:C2	3.08	0.42
30:0:2414:A:N1	30:0:2415:A:C6	2.87	0.42
30:0:2506:A:O2'	30:0:2507:G:P	2.78	0.42
30:0:26:U:H3'	38:0:5910:HOH:O	2.18	0.42
30:0:2780:C:C4	30:0:2781:U:C4	3.08	0.42
18:R:98:ASN:HD21	30:0:500:G:H21	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:590:A:H2'	30:0:591:A:H5'	2.01	0.42
1:A:97:ALA:HA	1:A:131:HIS:NE2	2.33	0.42
2:B:51:VAL:HG23	2:B:329:TYR:O	2.20	0.42
4:D:156:ARG:NH1	38:D:5234:HOH:O	2.51	0.42
8:H:157:TYR:C	8:H:157:TYR:CD1	2.93	0.42
8:H:158:ASN:ND2	30:0:2502:C:H4'	2.35	0.42
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.67	0.42
14:N:73:ALA:HB1	14:N:74:PRO:CD	2.49	0.42
16:P:143:ALA:HA	38:P:5521:HOH:O	2.18	0.42
17:Q:94:GLN:O	17:Q:95:GLU:HB2	2.19	0.42
18:R:29:LYS:HE2	30:0:524:A:H5'	2.01	0.42
20:T:64:ASN:HB3	20:T:73:HIS:HB2	2.01	0.42
30:0:1964:U:O2	30:0:1964:U:H2'	2.18	0.42
30:0:255:A:C5	30:0:256:C:C4	3.08	0.42
30:0:2708:G:H2'	30:0:2709:G:O4'	2.19	0.42
30:0:2727:A:C5	30:0:2756:U:C4	3.07	0.42
30:0:583:C:H2'	30:0:584:U:H6	1.85	0.42
30:0:858:U:H2'	30:0:859:C:H6	1.84	0.42
31:9:1:U:O3'	31:9:3:A:OP1	2.37	0.42
31:9:74:G:C6	31:9:75:G:N7	2.87	0.42
1:A:53:ALA:HB3	38:A:9061:HOH:O	2.18	0.42
3:C:193:LEU:HA	3:C:211:ASP:O	2.20	0.42
5:E:162:PHE:CD1	5:E:162:PHE:N	2.88	0.42
11:K:14:LYS:CB	11:K:45:PRO:HG2	2.43	0.42
13:M:164:THR:CG2	13:M:165:GLY:N	2.82	0.42
14:N:37:ARG:HH11	31:9:6:C:C5'	2.28	0.42
23:W:115:THR:HG23	38:W:5420:HOH:O	2.18	0.42
30:0:1748:U:C5	30:0:1749:U:C5	3.08	0.42
30:0:1791:U:O2'	30:0:1792:C:H5'	2.20	0.42
30:0:445:U:O2'	30:0:446:G:H5'	2.19	0.42
30:0:595:U:O2'	30:0:596:C:H5'	2.20	0.42
30:0:960:G:C8	38:0:5997:HOH:O	2.57	0.42
29:3:91:GLN:O	29:3:92:GLU:HB2	2.19	0.42
31:9:106:U:O2'	31:9:107:C:H5'	2.20	0.42
17:Q:19:ARG:HH22	31:9:11:A:H3'	1.84	0.42
4:D:137:PRO:O	31:9:30:C:OP1	2.37	0.42
13:M:187:LEU:CD2	13:M:194:GLY:HA3	2.49	0.42
21:U:50:GLU:HB2	30:0:2866:U:C5	2.55	0.42
22:V:12:THR:HG23	22:V:14:ALA:H	1.85	0.42
30:0:1063:G:H8	38:0:9865:HOH:O	2.02	0.42
30:0:1185:U:C5'	38:0:7505:HOH:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1555:G:H4'	30:0:1630:A:H2	1.85	0.42
30:0:1878:G:H5'	38:0:4379:HOH:O	2.19	0.42
30:0:2450:C:C2'	30:0:2451:G:O5'	2.67	0.42
30:0:2637:A:C5'	38:0:9282:HOH:O	2.57	0.42
30:0:699:C:H2'	30:0:744:G:N3	2.34	0.42
30:0:800:G:H2'	30:0:801:U:C6	2.55	0.42
2:B:217:ARG:CD	2:B:257:THR:HG22	2.50	0.42
2:B:55:ASN:HB3	2:B:63:GLU:HA	2.00	0.42
4:D:151:ILE:HB	4:D:156:ARG:HE	1.85	0.42
4:D:23:VAL:CG2	4:D:73:VAL:HB	2.50	0.42
4:D:40:ILE:HG23	38:D:5583:HOH:O	2.20	0.42
4:D:27:ILE:HB	4:D:69:ILE:O	2.20	0.42
20:T:32:ARG:NH1	20:T:38:ARG:HH12	2.18	0.42
30:0:1119:G:N2	30:0:1246:A:H2	2.10	0.42
16:P:41:ARG:NH2	30:0:1500:U:OP2	2.51	0.42
30:0:1878:G:O2'	30:0:1879:U:OP2	2.37	0.42
13:M:171:ARG:NH2	30:0:189:A:OP1	2.52	0.42
30:0:2135:A:O4'	30:0:2243:C:N4	2.53	0.42
30:0:336:G:H5'	38:0:7404:HOH:O	2.20	0.42
30:0:907:A:H2'	30:0:908:A:H8	1.85	0.42
31:9:3:A:H2	31:9:21:G:N3	2.18	0.42
1:A:153:ARG:CB	1:A:153:ARG:HH11	2.28	0.42
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.32	0.42
6:F:107:ASP:O	6:F:111:ILE:HG13	2.19	0.42
7:G:63:ARG:N	38:G:2569:HOH:O	2.53	0.42
8:H:31:ILE:HG23	38:H:232:HOH:O	2.19	0.42
14:N:33:ARG:NH1	14:N:103:ASP:OD2	2.51	0.42
17:Q:55:ARG:HD2	38:Q:2875:HOH:O	2.19	0.42
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.02	0.42
30:0:939:A:H2	30:0:1027:G:N3	2.16	0.42
30:0:1167:G:O2'	30:0:1168:C:H5'	2.20	0.42
30:0:1178:G:C6	30:0:1179:C:N4	2.87	0.42
30:0:907:A:H4'	30:0:1328:A:C2	2.54	0.42
30:0:1343:C:H2'	30:0:1344:G:O5'	2.20	0.42
30:0:1477:C:H5'	30:0:1868:G:H5''	1.99	0.42
30:0:1515:A:H2'	30:0:1516:U:H6	1.83	0.42
30:0:1762:C:H2'	30:0:1763:C:H6	1.84	0.42
30:0:2007:A:N3	30:0:2627:G:O2'	2.48	0.42
30:0:2113:G:C6	30:0:2114:C:C4	3.08	0.42
30:0:807:A:C6	30:0:808:A:C6	3.07	0.42
30:0:947:U:O2'	30:0:948:G:H5'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.68	0.42
13:M:61:ILE:HG22	13:M:62:VAL:N	2.35	0.42
14:N:171:HIS:CE1	38:N:8858:HOH:O	2.71	0.42
21:U:33:SER:O	21:U:37:GLU:HG3	2.18	0.42
30:0:1433:G:O2'	30:0:1434:A:H5'	2.20	0.42
30:0:1992:U:H2'	30:0:1994:A:OP2	2.19	0.42
30:0:2765:C:H2'	30:0:2766:A:C8	2.54	0.42
30:0:382:U:O2'	30:0:430:A:H1'	2.19	0.42
30:0:470:U:H2'	30:0:471:G:O4'	2.20	0.42
30:0:536:A:H4'	38:0:5552:HOH:O	2.18	0.42
30:0:920:C:H5'	30:0:921:G:C4	2.55	0.42
27:1:12:ASN:O	30:0:1415:G:H5'	2.19	0.42
31:9:26:C:H2'	31:9:27:C:C6	2.55	0.42
3:C:129:HIS:HD2	3:C:165:ASP:OD2	2.03	0.42
4:D:88:LEU:N	4:D:89:PRO:CD	2.83	0.42
5:E:95:VAL:HG11	5:E:131:LEU:HD11	2.02	0.42
8:H:123:ILE:HD12	8:H:123:ILE:N	2.35	0.42
18:R:17:MET:HE3	18:R:19:ARG:NH2	2.35	0.42
30:0:152:A:H1'	30:0:440:C:O2'	2.21	0.41
30:0:1950:G:H2'	30:0:1951:G:C8	2.55	0.41
30:0:2112:A:H2'	30:0:2113:G:H8	1.85	0.41
30:0:213:G:O2'	30:0:214:U:OP2	2.38	0.41
12:L:57:VAL:HG21	30:0:2443:C:H5'	2.02	0.41
30:0:2502:C:O2'	30:0:2503:A:H5'	2.17	0.41
13:M:58:GLN:NE2	30:0:259:G:H21	2.17	0.41
2:B:27:ASN:HD21	30:0:2807:U:P	2.43	0.41
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	2.01	0.41
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.50	0.41
2:B:162:MET:HG3	2:B:310:ARG:NH1	2.35	0.41
3:C:8:LEU:HD13	3:C:147:LEU:HD21	2.01	0.41
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.84	0.41
6:F:118:LEU:O	6:F:119:ARG:HB3	2.20	0.41
6:F:14:ASP:O	6:F:18:GLU:HG3	2.20	0.41
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.53	0.41
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.41
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.18	0.41
14:N:26:LEU:HA	14:N:26:LEU:HD12	1.93	0.41
30:0:1409:G:H5'	38:0:3732:HOH:O	2.20	0.41
30:0:1414:A:H2	38:0:4921:HOH:O	2.03	0.41
30:0:1524:U:C5'	30:0:1524:U:H6	2.33	0.41
30:0:158:A:H2'	30:0:159:G:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1667:A:C2	30:0:1668:U:C2	3.07	0.41
30:0:1871:U:O4'	30:0:1873:G:C8	2.73	0.41
30:0:1883:U:H2'	30:0:1884:G:H5'	2.02	0.41
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.41
30:0:2245:C:H6	30:0:2245:C:O5'	2.02	0.41
30:0:526:U:H2'	30:0:527:U:C6	2.55	0.41
30:0:51:G:O2'	30:0:52:A:H5'	2.20	0.41
30:0:539:G:H2'	30:0:540:A:C8	2.55	0.41
30:0:969:G:H1	30:0:999:C:N4	2.18	0.41
31:9:24:U:H3'	31:9:25:G:C5'	2.51	0.41
2:B:88:GLU:HB3	2:B:97:LEU:HG	2.01	0.41
3:C:118:THR:HG22	3:C:137:PRO:HB3	2.00	0.41
3:C:61:PHE:HB3	38:C:8643:HOH:O	2.20	0.41
6:F:58:GLU:HA	6:F:61:MET:HG3	2.01	0.41
10:J:45:VAL:HG11	10:J:121:LEU:HD22	2.02	0.41
10:J:39:VAL:HG12	10:J:40:ASN:ND2	2.35	0.41
12:L:57:VAL:HG12	12:L:57:VAL:O	2.20	0.41
12:L:67:ARG:O	12:L:71:GLU:HG3	2.20	0.41
13:M:46:LEU:HG	38:M:8913:HOH:O	2.20	0.41
13:M:49:ALA:C	13:M:54:TYR:HB3	2.40	0.41
18:R:9:ASP:HA	18:R:10:PRO:HD2	1.91	0.41
23:W:11:VAL:O	23:W:12:ASN:HB2	2.19	0.41
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.54	0.41
30:0:1015:C:O5'	30:0:1015:C:H6	2.02	0.41
30:0:1119:G:C5	30:0:1243:C:C4	3.08	0.41
25:Y:212:ARG:HB2	30:0:1315:G:C4	2.55	0.41
30:0:2330:U:H4'	30:0:2331:C:OP1	2.20	0.41
30:0:2344:G:N7	38:0:4937:HOH:O	2.49	0.41
30:0:2379:G:N7	30:0:2408:A:N1	2.67	0.41
30:0:2500:C:H1'	38:0:4674:HOH:O	2.20	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.38	0.41
30:0:2508:C:H2'	38:0:6793:HOH:O	2.19	0.41
30:0:2598:U:O2	30:0:2600:A:H8	2.03	0.41
30:0:372:A:H2'	30:0:373:G:C8	2.55	0.41
30:0:708:A:H2'	30:0:709:G:O4'	2.20	0.41
5:E:95:VAL:O	5:E:126:ILE:HD12	2.20	0.41
8:H:66:GLU:HA	38:H:232:HOH:O	2.19	0.41
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.55	0.41
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.67	0.41
18:R:59:PHE:O	18:R:63:ASN:HB3	2.20	0.41
20:T:21:LYS:HA	20:T:24:ARG:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:151:SER:HB3	25:Y:154:ARG:CB	2.50	0.41
25:Y:189:ASN:HD22	25:Y:189:ASN:C	2.23	0.41
30:0:1058:A:H2'	30:0:1060:C:C5'	2.48	0.41
30:0:1213:C:O2'	30:0:1214:G:H5'	2.21	0.41
30:0:1427:A:O2'	30:0:1428:C:H5'	2.20	0.41
30:0:2011:A:H4'	30:0:2012:U:O5'	2.20	0.41
30:0:2237:G:H1'	38:0:4871:HOH:O	2.20	0.41
30:0:2269:C:H2'	30:0:2270:G:C5'	2.50	0.41
30:0:2375:A:H2'	30:0:2376:C:C6	2.56	0.41
30:0:2512:U:H4'	30:0:2514:U:O4	2.20	0.41
30:0:2791:U:H4'	30:0:2792:A:OP1	2.20	0.41
30:0:393:G:C6	30:0:394:G:C6	3.08	0.41
30:0:485:A:O2'	30:0:487:G:H5'	2.19	0.41
30:0:735:C:C5	30:0:736:A:N3	2.89	0.41
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.50	0.41
11:K:34:VAL:HB	38:K:7169:HOH:O	2.20	0.41
11:K:41:LYS:O	11:K:42:ASN:HB2	2.20	0.41
30:0:1132:A:H2'	30:0:1133:A:C8	2.56	0.41
30:0:1388:U:H2'	30:0:1389:G:O4'	2.20	0.41
30:0:1488:U:H4'	30:0:1489:G:OP1	2.21	0.41
30:0:1603:A:C5'	30:0:1605:G:O4'	2.53	0.41
30:0:1522:A:C2	30:0:1665:G:C6	3.09	0.41
30:0:1748:U:C4	30:0:1749:U:C4	3.09	0.41
30:0:1883:U:O2'	30:0:1884:G:H5'	2.20	0.41
30:0:1976:G:H1'	30:0:2005:G:N2	2.36	0.41
30:0:2067:A:H2'	30:0:2068:G:O4'	2.20	0.41
30:0:284:C:OP2	30:0:284:C:C6	2.73	0.41
30:0:491:C:O2'	30:0:492:C:H5'	2.21	0.41
30:0:699:C:C6	30:0:744:G:O4'	2.73	0.41
31:9:73:A:N1	31:9:108:C:O2	2.54	0.41
1:A:125:ASN:HB3	1:A:158:VAL:HG12	2.02	0.41
2:B:51:VAL:CG2	2:B:327:VAL:HG13	2.50	0.41
2:B:74:ILE:HG13	38:B:9075:HOH:O	2.20	0.41
4:D:96:SER:C	4:D:98:PHE:H	2.24	0.41
13:M:133:LEU:O	13:M:134:ILE:HD13	2.21	0.41
23:W:108:ARG:HE	23:W:114:PRO:HG3	1.85	0.41
25:Y:182:PHE:HD2	25:Y:200:THR:O	2.03	0.41
3:C:184:ARG:HD2	30:0:1306:U:H5''	2.01	0.41
30:0:1319:G:H1'	38:0:4701:HOH:O	2.19	0.41
30:0:1761:U:H2'	30:0:1762:C:C6	2.55	0.41
30:0:1926:G:H2'	30:0:1927:A:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:240:C:O2	30:0:240:C:H2'	2.21	0.41
30:0:2478:U:H2'	30:0:2479:A:C8	2.55	0.41
30:0:259:G:O2'	30:0:260:C:H5'	2.20	0.41
30:0:284:C:H4'	30:0:285:A:H8	1.85	0.41
30:0:300:U:N3	30:0:301:C:C5	2.88	0.41
30:0:523:C:H2'	30:0:524:A:C8	2.56	0.41
29:3:30:GLN:NE2	38:3:9046:HOH:O	2.51	0.41
31:9:2:U:C4'	38:9:9103:HOH:O	2.67	0.41
2:B:7:ARG:CG	2:B:7:ARG:HH11	2.31	0.41
3:C:140:VAL:HG12	3:C:141:SER:N	2.35	0.41
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.85	0.41
12:L:117:GLU:HG2	38:L:8860:HOH:O	2.20	0.41
13:M:139:PRO:HA	13:M:142:GLN:HB2	2.03	0.41
25:Y:216:ARG:NH1	38:Y:8834:HOH:O	2.53	0.41
30:0:1206:U:C3'	30:0:1206:U:C6	3.04	0.41
30:0:1417:G:N3	30:0:1417:G:H2'	2.35	0.41
30:0:1523:G:C6	30:0:1524:U:C4	3.09	0.41
30:0:1662:C:H2'	30:0:1663:G:O4'	2.21	0.41
30:0:2421:G:H3'	30:0:2422:U:H5''	2.02	0.41
30:0:2597:U:C2'	30:0:2598:U:H5'	2.50	0.41
5:E:111:LYS:HE3	30:0:2690:U:H4'	2.02	0.41
30:0:2878:U:OP1	30:0:2878:U:H6	2.03	0.41
30:0:64:G:H2'	30:0:65:C:O4'	2.21	0.41
30:0:853:C:H2'	30:0:854:G:O4'	2.21	0.41
31:9:5:G:C2'	31:9:6:C:H5'	2.50	0.41
2:B:137:LEU:HD21	2:B:140:LEU:HD21	2.03	0.41
4:D:154:LYS:H	4:D:154:LYS:CD	2.09	0.41
10:J:127:ILE:O	10:J:127:ILE:HG12	2.21	0.41
10:J:47:THR:O	10:J:53:ILE:HD11	2.21	0.41
24:X:78:GLU:HG2	24:X:79:GLU:H	1.86	0.41
30:0:123:U:H5'	38:0:6689:HOH:O	2.20	0.41
30:0:1265:G:H1'	38:0:5020:HOH:O	2.21	0.41
30:0:1576:G:H2'	30:0:1577:U:O4'	2.21	0.41
30:0:1762:C:H2'	30:0:1763:C:C6	2.56	0.41
30:0:2090:G:H2'	30:0:2091:G:C8	2.55	0.41
30:0:466:A:C2	30:0:476:A:C4	3.09	0.41
30:0:541:C:H2'	30:0:542:A:H5'	1.95	0.41
30:0:60:A:C2	30:0:61:G:C8	3.09	0.41
30:0:862:U:H2'	30:0:863:G:C8	2.56	0.41
1:A:212:PRO:HB2	38:0:4373:HOH:O	2.20	0.41
3:C:84:VAL:HG12	3:C:85:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.87	0.41
6:F:91:VAL:CG1	6:F:92:GLY:N	2.78	0.41
9:I:108:HIS:N	9:I:109:PRO:HD2	2.35	0.41
9:I:114:TYR:HE1	30:0:1186:C:H4'	1.85	0.41
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.21	0.41
23:W:59:GLN:NE2	23:W:97:ALA:HB3	2.36	0.41
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	2.03	0.41
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.36	0.41
30:0:1589:G:H22	30:0:1605:G:H1'	1.85	0.41
30:0:2063:U:O4	30:0:2083:A:H2	2.03	0.41
30:0:711:G:N2	30:0:718:C:C2	2.89	0.41
28:2:5:LYS:O	28:2:9:LYS:HG3	2.21	0.41
29:3:3:MET:HG3	29:3:4:PRO:HD2	2.03	0.41
2:B:195:ARG:HG2	2:B:323:LEU:HD22	2.03	0.41
5:E:132:THR:HB	38:E:2227:HOH:O	2.21	0.41
10:J:75:PRO:HB3	10:J:132:LEU:HB3	2.02	0.41
12:L:11:ARG:O	30:0:903:U:C2	2.73	0.41
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.03	0.41
22:V:12:THR:HB	22:V:15:GLU:OE2	2.20	0.41
23:W:11:VAL:HG11	30:0:1086:A:C6	2.56	0.41
30:0:1250:C:O2'	30:0:1251:C:H5'	2.20	0.41
30:0:1486:A:H4'	30:0:1487:A:OP2	2.20	0.41
30:0:1592:G:O2'	30:0:1593:C:O4'	2.32	0.41
30:0:1632:A:C3'	30:0:1633:C:H5'	2.51	0.41
30:0:1878:G:C4'	38:0:6151:HOH:O	2.69	0.41
30:0:2511:A:H4'	38:0:5487:HOH:O	2.21	0.41
30:0:2543:G:H2'	30:0:2544:G:O4'	2.21	0.41
2:B:307:ARG:HG3	30:0:2837:U:O2	2.21	0.41
20:T:2:LYS:HG2	30:0:447:A:OP1	2.21	0.41
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.49	0.41
2:B:150:ALA:O	2:B:152:PRO:HD3	2.21	0.41
10:J:132:LEU:HA	10:J:132:LEU:HD23	1.92	0.41
13:M:61:ILE:N	13:M:61:ILE:HD12	2.36	0.41
19:S:57:THR:HG22	19:S:58:MET:N	2.35	0.41
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.21	0.41
23:W:122:ARG:HH11	23:W:122:ARG:HG3	1.85	0.41
23:W:61:THR:HG23	23:W:151:GLU:HG3	2.03	0.41
30:0:1119:G:N2	30:0:1246:A:N1	2.68	0.41
30:0:1167:G:H1	30:0:1179:C:H42	1.69	0.41
30:0:1525:G:OP1	30:0:1525:G:H4'	2.21	0.41
30:0:1771:U:O2'	30:0:1773:G:N7	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2318:C:H2'	30:0:2319:C:H6	1.86	0.41
30:0:2361:A:H2'	30:0:2362:A:C8	2.55	0.41
30:0:2680:A:O2'	30:0:2681:A:C4	2.72	0.41
30:0:2712:G:H5'	38:0:5241:HOH:O	2.19	0.41
30:0:2824:C:H5''	30:0:2825:C:H5'	2.02	0.41
30:0:2088:C:H1'	30:0:2841:A:C2	2.56	0.41
30:0:2887:G:H2'	30:0:2888:U:O4'	2.20	0.41
31:9:76:G:O5'	31:9:76:G:H8	2.04	0.41
31:9:93:A:H8	31:9:93:A:O5'	2.04	0.41
1:A:233:THR:HB	30:0:1942:A:H5''	2.03	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.89	0.41
12:L:145:LEU:O	12:L:148:GLU:HG3	2.21	0.41
12:L:32:ASP:HB3	30:0:222:A:H5''	2.03	0.41
14:N:154:LEU:O	14:N:155:GLU:HB3	2.21	0.41
17:Q:34:ASP:O	17:Q:37:GLU:HB2	2.21	0.41
18:R:33:ARG:NH2	38:R:8935:HOH:O	2.54	0.41
30:0:1265:G:C5	30:0:1266:U:C5	3.09	0.40
30:0:1635:U:O2'	30:0:1636:G:H5'	2.19	0.40
30:0:2531:U:O2'	30:0:2532:A:H5'	2.21	0.40
30:0:371:U:H2'	30:0:372:A:H8	1.85	0.40
30:0:488:U:H2'	38:0:4016:HOH:O	2.21	0.40
30:0:613:C:C2	30:0:614:U:C5	3.09	0.40
30:0:932:U:O2'	30:0:1296:A:H1'	2.21	0.40
27:1:21:ARG:HD2	27:1:39:PHE:HB2	2.03	0.40
28:2:11:LEU:HA	28:2:11:LEU:HD23	1.91	0.40
3:C:80:VAL:HA	3:C:81:PRO:HD3	1.88	0.40
13:M:138:HIS:O	13:M:142:GLN:HG3	2.21	0.40
14:N:34:LEU:HD22	14:N:129:ILE:HD13	2.02	0.40
17:Q:64:GLU:HG3	17:Q:74:ASP:OD2	2.21	0.40
22:V:42:ASN:O	22:V:44:GLY:N	2.55	0.40
30:0:1252:A:H2'	30:0:1253:C:O4'	2.21	0.40
30:0:634:G:O2'	30:0:1358:A:OP1	2.36	0.40
30:0:1413:A:H2'	30:0:1414:A:O4'	2.20	0.40
30:0:1505:U:H4'	38:0:5200:HOH:O	2.22	0.40
30:0:154:C:H2'	30:0:155:C:H6	1.86	0.40
30:0:1573:A:H2'	30:0:1574:C:O4'	2.21	0.40
30:0:1632:A:H2'	30:0:1633:C:C5'	2.46	0.40
30:0:2010:A:C2'	38:0:5984:HOH:O	2.51	0.40
30:0:2119:C:O2'	30:0:2120:U:H5'	2.22	0.40
30:0:2348:C:O2'	30:0:2349:G:H5'	2.21	0.40
30:0:1838:U:O2'	30:0:2644:C:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2716:G:H1'	38:0:3037:HOH:O	2.21	0.40
30:0:625:U:H5'	38:0:3194:HOH:O	2.20	0.40
14:N:1:ALA:HB2	31:9:14:G:O2'	2.21	0.40
3:C:124:VAL:HA	3:C:230:GLY:O	2.21	0.40
8:H:100:GLU:HG2	8:H:102:LYS:HB3	2.03	0.40
13:M:164:THR:HG22	13:M:166:ALA:N	2.36	0.40
25:Y:219:GLU:HG3	25:Y:220:GLU:N	2.36	0.40
30:0:1202:A:C2'	30:0:1203:G:H5'	2.52	0.40
30:0:1511:U:O2'	30:0:1512:G:H5'	2.22	0.40
30:0:2467:A:H3'	38:0:5475:HOH:O	2.22	0.40
30:0:2765:C:H2'	30:0:2766:A:H8	1.86	0.40
3:C:43:LYS:HG2	30:0:449:A:N7	2.36	0.40
30:0:613:C:H2'	30:0:614:U:C6	2.49	0.40
30:0:622:G:O2'	30:0:623:U:H5'	2.21	0.40
27:1:25:LYS:HD2	28:2:48:ASP:HA	2.03	0.40
31:9:47:A:C2	31:9:48:C:C2	3.09	0.40
2:B:16:ARG:NH2	38:B:9021:HOH:O	2.49	0.40
5:E:1:PRO:HG2	5:E:59:MET:SD	2.61	0.40
13:M:176:LYS:HB3	13:M:176:LYS:HE2	1.95	0.40
18:R:132:ARG:HG2	18:R:133:ALA:N	2.36	0.40
21:U:20:MET:CG	21:U:28:THR:HG23	2.51	0.40
23:W:22:GLU:HG2	23:W:27:HIS:CD2	2.56	0.40
25:Y:182:PHE:CG	25:Y:202:ALA:HB2	2.57	0.40
16:P:2:ASP:OD1	30:0:1396:C:H4'	2.21	0.40
30:0:1565:C:H2'	30:0:1566:C:H6	1.86	0.40
30:0:1576:G:H2'	30:0:1577:U:C6	2.56	0.40
30:0:1588:G:C5	30:0:1589:G:C6	3.09	0.40
30:0:1603:A:C5'	30:0:1605:G:C5'	2.98	0.40
16:P:81:LYS:HB3	30:0:1707:G:O3'	2.21	0.40
30:0:1915:U:O2'	30:0:1916:C:H5'	2.22	0.40
30:0:1996:U:O2'	30:0:1997:A:H5'	2.21	0.40
30:0:222:A:H2'	30:0:223:G:O4'	2.21	0.40
30:0:2598:U:O2	30:0:2600:A:C8	2.74	0.40
30:0:37:A:H2'	30:0:38:G:C8	2.57	0.40
30:0:596:C:H2'	30:0:597:A:C8	2.56	0.40
30:0:645:U:H2'	30:0:646:G:C8	2.56	0.40
2:B:141:ARG:N	38:B:9047:HOH:O	2.54	0.40
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.95	0.40
5:E:116:THR:CG2	5:E:151:LEU:HD22	2.43	0.40
8:H:6:ALA:HB3	30:0:2521:A:P	2.61	0.40
17:Q:16:ASN:HD22	17:Q:16:ASN:HA	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:97:ARG:NH2	30:0:309:C:OP1	2.54	0.40
30:0:1188:A:C6	30:0:1189:A:C6	3.09	0.40
26:Z:70:ARG:NH2	30:0:1602:C:OP2	2.53	0.40
8:H:74:ARG:NH1	30:0:2504:A:H4'	2.36	0.40
30:0:535:G:C5	30:0:2063:U:C4	3.09	0.40
14:N:44:ARG:NH1	31:9:4:G:H21	2.20	0.40
3:C:135:GLU:HB3	38:C:8576:HOH:O	2.22	0.40
6:F:59:ILE:CD1	30:0:263:U:C2	3.04	0.40
8:H:155:ARG:NE	38:H:198:HOH:O	2.54	0.40
11:K:64:MET:HA	11:K:67:GLN:HE21	1.87	0.40
20:T:16:LEU:HB2	30:0:100:C:H4'	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	213 (91%)	18 (8%)	4 (2%)	9	31
2	B	335/338 (99%)	309 (92%)	22 (7%)	4 (1%)	13	40
3	C	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
4	D	134/177 (76%)	107 (80%)	22 (16%)	5 (4%)	3	13
5	E	170/178 (96%)	156 (92%)	14 (8%)	0	100	100
6	F	117/120 (98%)	104 (89%)	9 (8%)	4 (3%)	3	15
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	145 (93%)	11 (7%)	0	100	100
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	10	34
10	J	140/145 (97%)	132 (94%)	8 (6%)	0	100	100
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	7	26
13	M	192/196 (98%)	182 (95%)	10 (5%)	0	100	100
14	N	184/187 (98%)	169 (92%)	11 (6%)	4 (2%)	6	24
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
19	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
20	T	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	17	48
21	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
22	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	4	16
23	W	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	54
24	X	80/92 (87%)	71 (89%)	8 (10%)	1 (1%)	12	37
25	Y	140/241 (58%)	140 (100%)	0	0	100	100
26	Z	71/116 (61%)	62 (87%)	8 (11%)	1 (1%)	11	36
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	37 (88%)	5 (12%)	0	100	100
29	3	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
All	All	3705/4472 (83%)	3416 (92%)	258 (7%)	31 (1%)	19	51

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	36	ASP
1	A	37	VAL
6	F	101	ALA
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
1	A	34	ASP
4	D	27	ILE
6	F	44	SER
24	X	70	ILE
4	D	97	GLN
12	L	149	ARG

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Mol	Chain	Res	Type
14	N	139	TRP
26	Z	44	ARG
2	B	2	GLN
2	B	184	ASP
4	D	56	ARG
6	F	100	ASP
12	L	80	ASP
22	V	43	PRO
6	F	61	MET
9	I	83	GLY
20	T	53	GLY
23	W	49	ASN
12	L	82	ALA
2	B	34	GLY
2	B	169	GLY
4	D	28	GLY
4	D	137	PRO
22	V	40	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	171 (96%)	8 (4%)	27	61
2	B	282/283 (100%)	268 (95%)	14 (5%)	24	57
3	C	193/193 (100%)	180 (93%)	13 (7%)	16	43
4	D	117/148 (79%)	113 (97%)	4 (3%)	37	71
5	E	152/156 (97%)	148 (97%)	4 (3%)	46	77
6	F	93/94 (99%)	91 (98%)	2 (2%)	52	81
7	G	27/282 (10%)	26 (96%)	1 (4%)	34	68
8	H	134/145 (92%)	128 (96%)	6 (4%)	27	61
9	I	58/130 (45%)	56 (97%)	2 (3%)	37	71
10	J	118/121 (98%)	110 (93%)	8 (7%)	16	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	106/106 (100%)	103 (97%)	3 (3%)	43	76
12	L	113/127 (89%)	108 (96%)	5 (4%)	28	61
13	M	158/160 (99%)	151 (96%)	7 (4%)	28	61
14	N	149/150 (99%)	147 (99%)	2 (1%)	69	90
15	O	93/94 (99%)	92 (99%)	1 (1%)	73	92
16	P	113/117 (97%)	111 (98%)	2 (2%)	59	85
17	Q	79/80 (99%)	75 (95%)	4 (5%)	24	56
18	R	117/122 (96%)	112 (96%)	5 (4%)	29	62
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	101 (96%)	4 (4%)	33	67
21	U	44/53 (83%)	42 (96%)	2 (4%)	27	61
22	V	51/57 (90%)	48 (94%)	3 (6%)	19	49
23	W	130/130 (100%)	127 (98%)	3 (2%)	50	80
24	X	66/74 (89%)	63 (96%)	3 (4%)	27	61
25	Y	120/196 (61%)	116 (97%)	4 (3%)	38	72
26	Z	60/94 (64%)	59 (98%)	1 (2%)	60	86
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	79
29	3	79/79 (100%)	78 (99%)	1 (1%)	69	90
All	All	3095/3646 (85%)	2982 (96%)	113 (4%)	34	68

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	69	LEU
1	A	94	LEU
1	A	131	HIS
1	A	153	ARG
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN

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Mol	Chain	Res	Type
2	B	49	THR
2	B	56	ASP
2	B	71	VAL
2	B	132	HIS
2	B	162	MET
2	B	175	LEU
2	B	190	MET
2	B	195	ARG
2	B	254	GLN
2	B	256	GLN
2	B	277	GLU
3	C	2	GLN
3	C	27	ARG
3	C	78	ARG
3	C	94	THR
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	240	LEU
3	C	243	VAL
4	D	24	HIS
4	D	50	VAL
4	D	100	ASP
4	D	153	THR
5	E	86	VAL
5	E	102	VAL
5	E	126	ILE
5	E	156	ASP
6	F	12	LEU
6	F	119	ARG
7	G	73	ASP
8	H	21	GLU
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	173	GLU
9	I	110	ASP

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Mol	Chain	Res	Type
9	I	114	TYR
10	J	45	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
10	J	127	ILE
10	J	131	THR
11	K	7	ASP
11	K	10	GLN
11	K	55	VAL
12	L	32	ASP
12	L	35	ARG
12	L	43	HIS
12	L	101	ASP
12	L	104	ASP
13	M	46	LEU
13	M	68	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	130	GLU
13	M	164	THR
14	N	26	LEU
14	N	138	ASP
15	O	67	SER
16	P	91	LYS
16	P	98	ILE
17	Q	16	ASN
17	Q	18	PRO
17	Q	20	ASP
17	Q	57	ASP
18	R	13	THR
18	R	39	THR
18	R	119	VAL
18	R	123	GLN
18	R	132	ARG
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	117	ASP

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Mol	Chain	Res	Type
21	U	52	THR
21	U	53	ASP
22	V	12	THR
22	V	22	ASP
22	V	65	ASP
23	W	35	VAL
23	W	76	ASP
23	W	146	ILE
24	X	27	ASP
24	X	46	ASP
24	X	88	GLU
25	Y	163	THR
25	Y	186	ARG
25	Y	189	ASN
25	Y	203	VAL
26	Z	106	SER
28	2	18	ASN
29	3	3	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
2	B	27	ASN
2	B	127	GLN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
3	C	2	GLN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
4	D	103	ASN
5	E	74	HIS
5	E	119	HIS
5	E	143	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS

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Mol	Chain	Res	Type
8	H	59	GLN
8	H	62	HIS
8	H	158	ASN
9	I	106	GLN
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	53	ASN
14	N	93	GLN
14	N	107	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	40	HIS
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
19	S	9	HIS
19	S	44	GLN
19	S	53	ASN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	4	HIS
22	V	34	GLN
22	V	60	GLN
23	W	2	HIS
23	W	27	HIS
23	W	110	GLN

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Mol	Chain	Res	Type
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	18	ASN
28	2	37	HIS
28	2	41	HIS
28	2	45	ASN
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	22 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	260 (9%)	23 (0%)

All (260) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	130	C
30	0	131	A
30	0	138	U
30	0	139	C
30	0	141	C

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Mol	Chain	Res	Type
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	204	A
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	337	A
30	0	358	G
30	0	368	C
30	0	381	G
30	0	417	G
30	0	461	C
30	0	487	G
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A

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Mol	Chain	Res	Type
30	0	701	U
30	0	702	G
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	882	A
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1015	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1151	G

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Mol	Chain	Res	Type
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1331	G
30	0	1342	C
30	0	1353	C
30	0	1357	A
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1492	A
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1535	G
30	0	1559	A
30	0	1592	G
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A

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Mol	Chain	Res	Type
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1752	G
30	0	1774	G
30	0	1778	A
30	0	1779	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1965	C
30	0	1971	G
30	0	1973	A
30	0	1979	G
30	0	1996	U
30	0	2004	U
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2110	G

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Mol	Chain	Res	Type
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2465	A
30	0	2467	A
30	0	2469	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2526	C
30	0	2527	U
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2638	G
30	0	2649	A
30	0	2664	A
30	0	2676	C
30	0	2681	A
30	0	2682	C
30	0	2718	C

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Mol	Chain	Res	Type
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	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	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	603	A

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Mol	Chain	Res	Type
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1377	C
30	0	1474	C
30	0	1506	U
30	0	1692	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2681	A
30	0	2718	C
31	9	65	A

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

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	$\# Z > 2$
30	1MA	0	628	30,35	15,25,26	0.80	0	15,37,40	1.44	1 (6%)
30	OMG	0	2588	30	18,26,27	1.08	2 (11%)	20,38,41	2.58	5 (25%)
30	OMU	0	2587	30	14,22,23	1.02	1 (7%)	14,31,34	1.16	1 (7%)
30	PSU	0	2621	30	17,21,22	1.57	3 (17%)	20,30,33	5.47	4 (20%)
30	UR3	0	2619	30	14,22,23	0.73	0	15,32,35	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	OMU	0	2587	30	-	0/7/27/28	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	UR3	0	2619	30	-	0/5/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.97	1.48	1.52
30	0	2588	OMG	C6-N1	3.46	1.39	1.33
30	0	2587	OMU	C4-N3	2.76	1.37	1.33
30	0	2621	PSU	C4-N3	2.72	1.37	1.33
30	0	2621	PSU	C2-N1	2.26	1.42	1.38
30	0	2588	OMG	C8-N7	-2.11	1.30	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.33	114.66	128.43
30	0	2621	PSU	C4-N3-C2	14.41	127.31	115.14
30	0	2588	OMG	C5-C6-N1	-8.61	111.66	123.43
30	0	2621	PSU	C5-C4-N3	-8.24	114.74	125.36
30	0	2588	OMG	C6-N1-C2	5.84	125.21	115.93
30	0	628	1MA	C2-N3-C4	-4.78	110.61	116.58
30	0	2587	OMU	C5-C4-N3	-3.94	114.63	123.31
30	0	2588	OMG	C2-N3-C4	-2.99	111.94	115.36
30	0	2621	PSU	C6-N1-C2	2.73	119.86	115.36
30	0	2588	OMG	N3-C2-N1	-2.55	123.81	127.22
30	0	2588	OMG	C6-C5-C4	-2.04	118.85	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	628	1MA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	-0.22	7 (2%) 50 45	34, 56, 94, 116	0
2	B	337/338 (99%)	-0.42	2 (0%) 89 89	34, 58, 89, 99	0
3	C	246/246 (100%)	-0.24	4 (1%) 72 71	32, 51, 75, 87	0
4	D	140/177 (79%)	1.64	51 (36%) 0 0	69, 106, 134, 144	0
5	E	172/178 (96%)	-0.10	9 (5%) 27 23	49, 73, 97, 102	0
6	F	119/120 (99%)	-0.01	6 (5%) 28 25	52, 76, 109, 124	0
7	G	29/348 (8%)	0.52	2 (6%) 16 13	79, 103, 110, 113	0
8	H	160/177 (90%)	-0.34	2 (1%) 77 77	53, 73, 107, 111	0
9	I	70/162 (43%)	3.80	49 (70%) 0 0	137, 155, 173, 175	0
10	J	142/145 (97%)	-0.65	0 100 100	43, 57, 77, 99	0
11	K	132/132 (100%)	-0.62	0 100 100	39, 54, 79, 83	0
12	L	145/165 (87%)	0.33	5 (3%) 45 40	32, 71, 123, 134	0
13	M	194/196 (98%)	-0.48	1 (0%) 91 91	35, 49, 64, 71	0
14	N	186/187 (99%)	0.24	17 (9%) 9 6	51, 74, 121, 131	0
15	O	115/116 (99%)	-0.49	0 100 100	44, 61, 78, 85	0
16	P	143/149 (95%)	-0.41	1 (0%) 87 87	47, 61, 74, 83	0
17	Q	95/96 (98%)	-0.49	0 100 100	44, 55, 72, 85	0
18	R	150/155 (96%)	-0.50	0 100 100	37, 51, 73, 84	0
19	S	81/85 (95%)	-0.06	2 (2%) 57 55	49, 64, 87, 97	0
20	T	119/120 (99%)	-0.17	3 (2%) 57 55	42, 62, 92, 121	0
21	U	53/67 (79%)	0.01	1 (1%) 66 65	51, 64, 83, 91	0
22	V	65/71 (91%)	1.07	15 (23%) 0 0	53, 76, 130, 134	0
23	W	154/154 (100%)	-0.69	0 100 100	41, 56, 74, 88	0
24	X	82/92 (89%)	-0.31	0 100 100	49, 66, 91, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.51	1 (0%) 87 87	34, 48, 72, 94	0
26	Z	73/116 (62%)	0.19	6 (8%) 11 9	59, 77, 92, 101	0
27	1	56/57 (98%)	-0.25	0 100 100	33, 39, 48, 56	0
28	2	46/50 (92%)	-0.14	1 (2%) 62 59	41, 69, 102, 114	0
29	3	92/92 (100%)	-0.13	1 (1%) 80 80	43, 65, 78, 91	0
30	0	2749/2923 (94%)	-0.32	51 (1%) 66 65	28, 51, 95, 171	0
31	9	122/122 (100%)	-0.24	3 (2%) 57 55	45, 72, 95, 154	0
All	All	6646/7517 (88%)	-0.20	240 (3%) 42 37	28, 57, 106, 175	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	71	ALA	15.5
9	I	74	ILE	13.2
31	9	1	U	12.1
22	V	1	THR	11.8
9	I	72	GLU	11.1
22	V	43	PRO	10.6
9	I	70	THR	9.8
9	I	80	PHE	8.8
9	I	82	THR	8.6
9	I	83	GLY	8.3
14	N	166	ALA	7.9
9	I	88	GLN	7.7
9	I	132	VAL	7.0
9	I	112	LEU	6.8
9	I	79	GLY	6.7
9	I	81	GLU	6.7
9	I	128	THR	6.3
30	0	1169	U	6.1
9	I	69	PRO	5.9
22	V	40	PRO	5.7
9	I	84	SER	5.6
4	D	18	ILE	5.6
9	I	92	VAL	5.4
22	V	39	ALA	5.4
9	I	111	LEU	5.3
4	D	10	PHE	5.3
4	D	63	ILE	5.3
30	0	1170	U	5.3

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Mol	Chain	Res	Type	RSRZ
14	N	147	ILE	5.3
9	I	75	LYS	5.2
30	0	1172	G	5.2
4	D	69	ILE	5.1
12	L	60	GLU	5.1
30	0	735	C	5.1
22	V	46	ILE	5.1
9	I	86	GLU	5.0
9	I	66	GLY	5.0
20	T	119	ALA	4.9
4	D	57	THR	4.9
26	Z	35	SER	4.8
4	D	26	GLY	4.7
30	0	1175	G	4.6
9	I	130	LEU	4.6
9	I	93	ALA	4.6
9	I	131	GLY	4.6
4	D	134	LEU	4.5
30	0	1171	A	4.5
1	A	37	VAL	4.5
26	Z	46	SER	4.4
14	N	75	THR	4.3
14	N	138	ASP	4.3
4	D	75	LEU	4.3
30	0	1168	C	4.3
30	0	1173	A	4.2
1	A	237	GLY	4.2
30	0	1166	A	4.1
30	0	1174	A	4.1
30	0	1177	A	4.1
9	I	91	PHE	4.0
9	I	126	THR	4.0
9	I	127	CYS	4.0
9	I	109	PRO	4.0
4	D	101	THR	4.0
30	0	1195	G	3.9
9	I	113	SER	3.9
30	0	1176	C	3.9
4	D	27	ILE	3.9
9	I	129	SER	3.9
30	0	1198	U	3.9
30	0	1192	A	3.9

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Mol	Chain	Res	Type	RSRZ
30	0	1181	A	3.9
4	D	104	PHE	3.8
30	0	1193	A	3.8
4	D	85	GLN	3.7
4	D	44	ILE	3.7
9	I	76	ASP	3.7
30	0	1164	U	3.7
1	A	35	GLY	3.7
1	A	236	GLY	3.7
4	D	23	VAL	3.7
4	D	102	GLY	3.6
14	N	165	ALA	3.6
26	Z	58	ASN	3.6
30	0	1199	A	3.6
4	D	90	LEU	3.6
4	D	128	LEU	3.6
4	D	25	MET	3.6
6	F	106	ALA	3.6
7	G	27	ILE	3.6
4	D	17	ARG	3.6
30	0	1207	A	3.6
4	D	135	VAL	3.6
12	L	106	VAL	3.6
4	D	107	GLY	3.6
14	N	113	SER	3.5
30	0	1202	A	3.5
9	I	97	VAL	3.4
4	D	93	LEU	3.4
22	V	51	LYS	3.4
4	D	73	VAL	3.4
30	0	1165	G	3.4
30	0	1167	G	3.4
4	D	70	GLY	3.4
4	D	154	LYS	3.3
30	0	1190	G	3.3
9	I	73	LEU	3.3
30	0	970	U	3.3
22	V	44	GLY	3.3
20	T	118	SER	3.3
9	I	106	GLN	3.3
14	N	158	LEU	3.3
30	0	1178	G	3.3

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Mol	Chain	Res	Type	RSRZ
8	H	158	ASN	3.3
9	I	67	VAL	3.2
9	I	104	ALA	3.2
30	0	1947	G	3.2
22	V	52	ALA	3.2
9	I	103	ILE	3.1
9	I	85	GLY	3.1
30	0	1163	G	3.1
5	E	157	LYS	3.1
4	D	92	GLU	3.1
30	0	2237	G	3.1
5	E	108	LEU	3.1
4	D	165	PHE	3.1
4	D	130	VAL	3.1
9	I	125	GLY	3.1
9	I	100	VAL	3.0
16	P	67	LYS	3.0
31	9	2	U	3.0
4	D	106	PHE	3.0
9	I	87	PRO	3.0
30	0	1200	A	3.0
4	D	98	PHE	3.0
9	I	108	HIS	2.9
4	D	19	GLU	2.9
22	V	2	VAL	2.9
30	0	1206	U	2.9
30	0	1951	G	2.9
28	2	39	ARG	2.9
4	D	89	PRO	2.9
5	E	10	ASP	2.9
4	D	40	ILE	2.8
4	D	56	ARG	2.8
14	N	80	SER	2.8
19	S	81	ILE	2.8
5	E	45	ASP	2.8
5	E	154	ILE	2.8
22	V	48	GLU	2.7
31	9	24	U	2.7
30	0	1191	A	2.7
30	0	282	C	2.7
20	T	82	THR	2.7
12	L	99	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
6	F	49	PHE	2.6
9	I	110	ASP	2.6
19	S	76	GLU	2.6
1	A	99	ILE	2.6
4	D	24	HIS	2.6
2	B	337	GLY	2.6
30	0	1162	G	2.6
30	0	1180	U	2.6
4	D	81	GLU	2.6
9	I	99	GLN	2.6
12	L	105	TYR	2.5
4	D	41	LEU	2.5
4	D	74	THR	2.5
9	I	133	THR	2.5
4	D	11	HIS	2.5
13	M	194	GLY	2.5
5	E	11	VAL	2.5
6	F	44	SER	2.5
30	0	1194	A	2.5
7	G	26	MET	2.5
14	N	134	ASP	2.5
14	N	159	TYR	2.5
30	0	1203	G	2.5
9	I	94	ASP	2.4
3	C	60	SER	2.4
14	N	41	LYS	2.4
4	D	157	LEU	2.4
30	0	1179	C	2.4
3	C	64	GLY	2.4
4	D	158	ASN	2.4
2	B	115	VAL	2.4
1	A	31	LYS	2.4
14	N	160	SER	2.4
30	0	1208	C	2.4
9	I	90	ASP	2.4
5	E	6	GLU	2.3
5	E	156	ASP	2.3
4	D	172	VAL	2.3
30	0	1201	C	2.3
4	D	45	THR	2.3
9	I	78	ALA	2.3
30	0	280	C	2.3

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Mol	Chain	Res	Type	RSRZ
30	0	1204	C	2.3
9	I	68	PRO	2.3
4	D	95	THR	2.2
6	F	15	ASP	2.2
22	V	41	GLU	2.2
30	0	1161	A	2.2
30	0	2004	U	2.2
9	I	102	GLN	2.2
22	V	3	LEU	2.2
26	Z	50	VAL	2.2
4	D	84	LEU	2.2
4	D	88	LEU	2.2
30	0	10	U	2.2
26	Z	44	ARG	2.2
4	D	138	GLY	2.2
22	V	37	GLY	2.2
6	F	16	ALA	2.2
1	A	110	SER	2.2
6	F	75	ILE	2.2
8	H	40	GLN	2.2
29	3	13	HIS	2.2
14	N	145	ALA	2.1
30	0	1182	C	2.1
12	L	149	ARG	2.1
25	Y	235	GLU	2.1
3	C	135	GLU	2.1
14	N	112	GLY	2.1
14	N	146	HIS	2.1
4	D	13	MET	2.1
21	U	51	TRP	2.1
30	0	1196	C	2.1
30	0	138	U	2.1
5	E	161	VAL	2.1
4	D	105	SER	2.1
14	N	140	GLN	2.1
14	N	137	ALA	2.1
30	0	1965	C	2.0
22	V	45	ARG	2.0
30	0	1948	G	2.0
26	Z	83	TYR	2.0
3	C	66	GLY	2.0
4	D	141	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	166	ILE	2.0
22	V	49	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	1MA	0	628	23/24	0.98	0.18	33,37,38,39	0
30	OMG	0	2588	24/25	0.98	0.14	36,39,42,43	0
30	PSU	0	2621	20/21	0.98	0.18	34,35,47,48	0
30	UR3	0	2619	21/22	0.98	0.15	42,44,47,47	0
30	OMU	0	2587	21/22	0.99	0.13	38,40,44,45	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	SR	0	9006	1/1	-0.21	2.27	200,200,200,200	0
35	NA	0	8560	1/1	0.19	0.88	101,101,101,101	0
35	NA	0	8525	1/1	0.30	0.25	92,92,92,92	0
34	SR	0	8924	1/1	0.32	0.09	154,154,154,154	0
37	K	0	8401	1/1	0.41	0.77	128,128,128,128	0
34	SR	0	8962	1/1	0.53	0.19	169,169,169,169	0
34	SR	0	8947	1/1	0.54	0.51	200,200,200,200	0
34	SR	0	8991	1/1	0.65	0.07	199,199,199,199	0
35	NA	0	8528	1/1	0.65	0.56	66,66,66,66	0
34	SR	0	8955	1/1	0.68	0.20	199,199,199,199	0
35	NA	0	8506	1/1	0.68	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8563	1/1	0.69	0.28	88,88,88,88	0
35	NA	0	8562	1/1	0.69	1.31	78,78,78,78	0
35	NA	0	8509	1/1	0.70	0.93	85,85,85,85	0
35	NA	0	8502	1/1	0.72	0.15	66,66,66,66	0
35	NA	0	8530	1/1	0.73	0.32	59,59,59,59	0
34	SR	0	8982	1/1	0.73	2.26	200,200,200,200	0
34	SR	0	8994	1/1	0.74	0.43	200,200,200,200	0
34	SR	0	8993	1/1	0.74	0.10	176,176,176,176	0
35	NA	0	8548	1/1	0.75	0.26	58,58,58,58	0
35	NA	0	8511	1/1	0.75	0.29	69,69,69,69	0
34	SR	0	8979	1/1	0.76	0.14	200,200,200,200	0
35	NA	9	8543	1/1	0.77	0.11	74,74,74,74	0
34	SR	0	8986	1/1	0.78	0.41	200,200,200,200	0
35	NA	Q	8540	1/1	0.78	0.11	64,64,64,64	0
34	SR	0	8944	1/1	0.79	0.14	169,169,169,169	0
35	NA	0	8568	1/1	0.79	0.20	52,52,52,52	0
34	SR	0	8996	1/1	0.79	1.20	200,200,200,200	0
34	SR	B	8987	1/1	0.80	0.56	200,200,200,200	0
32	MG	0	8072	1/1	0.81	0.19	63,63,63,63	0
35	NA	S	8510	1/1	0.81	0.48	64,64,64,64	0
35	NA	0	8527	1/1	0.81	0.27	71,71,71,71	0
34	SR	0	9001	1/1	0.81	0.08	173,173,173,173	0
35	NA	0	8571	1/1	0.82	0.17	76,76,76,76	0
35	NA	0	8557	1/1	0.82	0.06	53,53,53,53	0
34	SR	0	8998	1/1	0.82	0.19	173,173,173,173	0
32	MG	0	8067	1/1	0.83	0.16	40,40,40,40	0
35	NA	0	8546	1/1	0.83	0.38	65,65,65,65	0
35	NA	0	8535	1/1	0.83	0.53	61,61,61,61	0
35	NA	J	8538	1/1	0.83	0.18	56,56,56,56	0
34	SR	0	8960	1/1	0.83	0.10	141,141,141,141	0
34	SR	A	8977	1/1	0.83	0.06	160,160,160,160	0
34	SR	0	8997	1/1	0.84	0.84	200,200,200,200	0
32	MG	9	8074	1/1	0.84	0.09	86,86,86,86	0
35	NA	0	8518	1/1	0.85	0.58	88,88,88,88	0
35	NA	0	8544	1/1	0.86	0.17	67,67,67,67	0
35	NA	0	8550	1/1	0.86	0.95	57,57,57,57	0
35	NA	0	8501	1/1	0.87	0.08	40,40,40,40	0
35	NA	0	8565	1/1	0.87	1.24	79,79,79,79	0
34	SR	0	8974	1/1	0.87	0.24	165,165,165,165	0
35	NA	0	8504	1/1	0.88	0.18	44,44,44,44	0
35	NA	0	8545	1/1	0.88	0.26	47,47,47,47	0
32	MG	0	8049	1/1	0.88	0.29	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8567	1/1	0.88	0.36	76,76,76,76	0
34	SR	0	8976	1/1	0.88	0.28	194,194,194,194	0
34	SR	0	8922	1/1	0.88	0.47	161,161,161,161	0
35	NA	0	8573	1/1	0.88	0.34	73,73,73,73	0
35	NA	0	8574	1/1	0.89	0.26	59,59,59,59	0
34	SR	0	8992	1/1	0.89	0.15	136,136,136,136	0
32	MG	0	8092	1/1	0.89	0.18	53,53,53,53	0
35	NA	0	8570	1/1	0.90	0.09	52,52,52,52	0
35	NA	0	8547	1/1	0.90	0.70	80,80,80,80	0
34	SR	0	8951	1/1	0.90	0.04	148,148,148,148	0
35	NA	0	8554	1/1	0.90	1.00	65,65,65,65	0
32	MG	0	8038	1/1	0.90	0.15	70,70,70,70	0
34	SR	0	8985	1/1	0.90	0.14	134,134,134,134	0
32	MG	0	8081	1/1	0.90	0.22	73,73,73,73	0
34	SR	0	8927	1/1	0.90	0.09	153,153,153,153	0
35	NA	0	8522	1/1	0.90	1.12	79,79,79,79	0
34	SR	0	8972	1/1	0.90	0.13	146,146,146,146	0
32	MG	0	8062	1/1	0.91	0.15	59,59,59,59	0
32	MG	0	8031	1/1	0.91	0.11	62,62,62,62	0
34	SR	0	8936	1/1	0.91	0.11	94,94,94,94	0
34	SR	0	8975	1/1	0.91	0.14	130,130,130,130	0
35	NA	0	8549	1/1	0.91	0.52	52,52,52,52	0
33	CL	O	8808	1/1	0.91	0.08	70,70,70,70	0
33	CL	0	8815	1/1	0.91	0.12	77,77,77,77	0
34	SR	0	8959	1/1	0.91	0.38	163,163,163,163	0
32	MG	0	8083	1/1	0.91	0.10	60,60,60,60	0
33	CL	A	8809	1/1	0.91	0.11	80,80,80,80	0
35	NA	0	8521	1/1	0.91	0.40	61,61,61,61	0
34	SR	0	8946	1/1	0.91	0.22	123,123,123,123	0
35	NA	0	8536	1/1	0.91	0.23	61,61,61,61	0
35	NA	0	8529	1/1	0.92	0.15	39,39,39,39	0
32	MG	0	8045	1/1	0.92	0.09	44,44,44,44	0
32	MG	0	8039	1/1	0.92	0.27	76,76,76,76	0
35	NA	0	8559	1/1	0.92	0.29	91,91,91,91	0
32	MG	0	8044	1/1	0.92	0.16	50,50,50,50	0
34	SR	0	8915	1/1	0.92	0.08	121,121,121,121	0
32	MG	0	8087	1/1	0.92	0.12	51,51,51,51	0
34	SR	0	9002	1/1	0.92	0.29	177,177,177,177	0
32	MG	0	8066	1/1	0.92	0.18	70,70,70,70	0
34	SR	A	8929	1/1	0.92	0.23	144,144,144,144	0
34	SR	0	8989	1/1	0.92	0.16	168,168,168,168	0
32	MG	0	8011	1/1	0.92	0.23	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8051	1/1	0.93	0.66	70,70,70,70	0
32	MG	0	8056	1/1	0.93	0.10	47,47,47,47	0
32	MG	0	8089	1/1	0.93	0.17	72,72,72,72	0
34	SR	0	8988	1/1	0.93	0.05	158,158,158,158	0
33	CL	N	8807	1/1	0.93	0.17	69,69,69,69	0
35	NA	0	8564	1/1	0.93	0.39	68,68,68,68	0
35	NA	0	8505	1/1	0.93	0.87	48,48,48,48	0
33	CL	0	8813	1/1	0.93	0.09	66,66,66,66	0
33	CL	Q	8811	1/1	0.93	0.15	82,82,82,82	0
35	NA	0	8526	1/1	0.93	0.08	47,47,47,47	0
34	SR	0	8942	1/1	0.93	0.08	122,122,122,122	0
32	MG	0	8075	1/1	0.93	0.03	42,42,42,42	0
32	MG	0	8077	1/1	0.93	0.07	45,45,45,45	0
32	MG	0	8037	1/1	0.93	0.14	88,88,88,88	0
32	MG	0	8091	1/1	0.93	0.07	57,57,57,57	0
35	NA	R	8575	1/1	0.93	0.25	99,99,99,99	0
32	MG	0	8006	1/1	0.93	0.10	32,32,32,32	0
34	SR	0	8928	1/1	0.93	0.06	135,135,135,135	0
35	NA	0	8569	1/1	0.93	0.15	48,48,48,48	0
34	SR	0	8965	1/1	0.93	0.09	132,132,132,132	0
33	CL	0	8814	1/1	0.94	0.21	72,72,72,72	0
34	SR	9	8980	1/1	0.94	0.15	175,175,175,175	0
34	SR	0	8969	1/1	0.94	0.12	159,159,159,159	0
35	NA	0	8561	1/1	0.94	0.22	68,68,68,68	0
35	NA	0	8512	1/1	0.94	0.14	52,52,52,52	0
34	SR	0	8901	1/1	0.94	0.08	91,91,91,91	0
32	MG	0	8033	1/1	0.94	0.09	55,55,55,55	0
32	MG	T	8057	1/1	0.94	0.12	60,60,60,60	0
35	NA	0	8551	1/1	0.94	0.37	52,52,52,52	0
33	CL	L	8810	1/1	0.94	0.09	68,68,68,68	0
34	SR	S	8961	1/1	0.94	0.06	121,121,121,121	0
34	SR	9	9003	1/1	0.94	0.09	171,171,171,171	0
35	NA	0	8515	1/1	0.94	0.20	41,41,41,41	0
34	SR	0	9000	1/1	0.94	0.07	176,176,176,176	0
34	SR	0	8973	1/1	0.94	0.05	130,130,130,130	0
32	MG	0	8055	1/1	0.94	0.16	53,53,53,53	0
34	SR	0	8995	1/1	0.94	0.15	136,136,136,136	0
32	MG	0	8014	1/1	0.94	0.20	33,33,33,33	0
32	MG	0	8060	1/1	0.94	0.08	53,53,53,53	0
32	MG	0	8036	1/1	0.94	0.12	56,56,56,56	0
34	SR	0	8968	1/1	0.94	0.03	160,160,160,160	0
33	CL	J	8821	1/1	0.95	0.14	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8070	1/1	0.95	0.12	46,46,46,46	0
32	MG	0	8082	1/1	0.95	0.78	89,89,89,89	0
35	NA	0	8520	1/1	0.95	0.07	49,49,49,49	0
35	NA	0	8533	1/1	0.95	0.10	55,55,55,55	0
35	NA	0	8523	1/1	0.95	0.09	50,50,50,50	0
33	CL	0	8803	1/1	0.95	0.10	58,58,58,58	0
34	SR	0	9008	1/1	0.95	0.17	95,95,95,95	0
32	MG	0	8093	1/1	0.95	0.08	42,42,42,42	0
33	CL	J	8802	1/1	0.95	0.21	75,75,75,75	0
35	NA	0	8516	1/1	0.95	0.11	45,45,45,45	0
32	MG	0	8053	1/1	0.95	0.19	47,47,47,47	0
34	SR	0	8966	1/1	0.95	0.10	107,107,107,107	0
35	NA	0	8537	1/1	0.95	0.18	38,38,38,38	0
35	NA	R	8532	1/1	0.96	0.12	58,58,58,58	0
35	NA	0	8519	1/1	0.96	0.20	43,43,43,43	0
32	MG	0	8040	1/1	0.96	0.21	96,96,96,96	0
34	SR	0	8943	1/1	0.96	0.04	124,124,124,124	0
32	MG	0	8035	1/1	0.96	0.10	54,54,54,54	0
32	MG	0	8046	1/1	0.96	0.14	43,43,43,43	0
34	SR	0	8971	1/1	0.96	0.07	171,171,171,171	0
34	SR	0	9004	1/1	0.96	0.31	200,200,200,200	0
32	MG	0	8016	1/1	0.96	0.14	48,48,48,48	0
35	NA	0	8556	1/1	0.96	0.82	64,64,64,64	0
32	MG	0	8041	1/1	0.96	0.21	29,29,29,29	0
34	SR	0	8908	1/1	0.96	0.08	116,116,116,116	0
35	NA	0	8542	1/1	0.96	0.45	49,49,49,49	0
35	NA	9	8572	1/1	0.96	0.89	81,81,81,81	0
32	MG	0	8047	1/1	0.96	0.32	51,51,51,51	0
33	CL	M	8818	1/1	0.96	0.10	40,40,40,40	0
32	MG	0	8001	1/1	0.96	0.11	33,33,33,33	0
34	SR	0	8963	1/1	0.96	0.17	112,112,112,112	0
34	SR	0	8953	1/1	0.96	0.13	144,144,144,144	0
32	MG	0	8003	1/1	0.96	0.19	45,45,45,45	0
34	SR	0	8917	1/1	0.96	0.10	107,107,107,107	0
35	NA	0	8555	1/1	0.96	0.81	75,75,75,75	0
34	SR	0	8921	1/1	0.96	0.15	96,96,96,96	0
32	MG	0	8013	1/1	0.97	0.06	25,25,25,25	0
34	SR	1	8913	1/1	0.97	0.14	95,95,95,95	0
34	SR	0	8957	1/1	0.97	0.13	195,195,195,195	0
32	MG	0	8079	1/1	0.97	0.11	51,51,51,51	0
32	MG	0	8002	1/1	0.97	0.15	36,36,36,36	0
32	MG	0	8020	1/1	0.97	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8050	1/1	0.97	0.09	32,32,32,32	0
32	MG	0	8024	1/1	0.97	0.12	49,49,49,49	0
34	SR	0	8939	1/1	0.97	0.10	149,149,149,149	0
32	MG	0	8021	1/1	0.97	0.05	40,40,40,40	0
34	SR	0	8919	1/1	0.97	0.07	170,170,170,170	0
35	NA	0	8558	1/1	0.97	0.23	49,49,49,49	0
33	CL	Y	8820	1/1	0.97	0.04	48,48,48,48	0
35	NA	0	8524	1/1	0.97	0.25	58,58,58,58	0
32	MG	0	8071	1/1	0.97	0.09	72,72,72,72	0
35	NA	0	8534	1/1	0.97	0.14	44,44,44,44	0
32	MG	0	8026	1/1	0.97	0.08	35,35,35,35	0
34	SR	0	8945	1/1	0.97	0.07	106,106,106,106	0
34	SR	0	8958	1/1	0.97	0.06	122,122,122,122	0
33	CL	0	8822	1/1	0.97	0.45	81,81,81,81	0
34	SR	0	8954	1/1	0.97	0.10	109,109,109,109	0
35	NA	C	8503	1/1	0.97	0.21	36,36,36,36	0
35	NA	0	8531	1/1	0.97	0.06	40,40,40,40	0
34	SR	0	9007	1/1	0.97	0.66	200,200,200,200	0
34	SR	0	8920	1/1	0.97	0.08	135,135,135,135	0
32	MG	0	8022	1/1	0.97	0.22	44,44,44,44	0
32	MG	0	8017	1/1	0.98	0.19	52,52,52,52	0
35	NA	0	8566	1/1	0.98	0.12	64,64,64,64	0
34	SR	0	8949	1/1	0.98	0.17	122,122,122,122	0
32	MG	0	8065	1/1	0.98	0.06	57,57,57,57	0
35	NA	0	8513	1/1	0.98	0.21	54,54,54,54	0
32	MG	0	8012	1/1	0.98	0.14	18,18,18,18	0
34	SR	0	8938	1/1	0.98	0.02	147,147,147,147	0
34	SR	0	8981	1/1	0.98	0.33	178,178,178,178	0
33	CL	3	8804	1/1	0.98	0.06	63,63,63,63	0
33	CL	B	8819	1/1	0.98	0.09	58,58,58,58	0
34	SR	0	8941	1/1	0.98	0.14	108,108,108,108	0
34	SR	0	8914	1/1	0.98	0.32	120,120,120,120	0
34	SR	0	8940	1/1	0.98	0.07	97,97,97,97	0
32	MG	0	8069	1/1	0.98	0.30	73,73,73,73	0
35	NA	0	8508	1/1	0.98	0.20	35,35,35,35	0
34	SR	0	8923	1/1	0.98	0.10	101,101,101,101	0
32	MG	0	8025	1/1	0.98	0.12	37,37,37,37	0
34	SR	0	8933	1/1	0.98	0.16	139,139,139,139	0
35	NA	0	8507	1/1	0.98	0.11	37,37,37,37	0
32	MG	0	8023	1/1	0.98	0.10	37,37,37,37	0
32	MG	0	8088	1/1	0.98	0.20	52,52,52,52	0
35	NA	0	8541	1/1	0.98	0.18	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8983	1/1	0.98	0.24	170,170,170,170	0
32	MG	0	8030	1/1	0.98	0.30	68,68,68,68	0
32	MG	0	8063	1/1	0.98	0.14	80,80,80,80	0
32	MG	0	8068	1/1	0.98	0.08	51,51,51,51	0
32	MG	0	8052	1/1	0.98	0.07	56,56,56,56	0
32	MG	0	8028	1/1	0.98	0.16	26,26,26,26	0
34	SR	0	8984	1/1	0.98	0.03	121,121,121,121	0
33	CL	0	8805	1/1	0.98	0.06	67,67,67,67	0
32	MG	0	8078	1/1	0.98	0.27	69,69,69,69	0
34	SR	B	8950	1/1	0.98	0.14	116,116,116,116	0
32	MG	0	8085	1/1	0.98	0.53	97,97,97,97	0
34	SR	1	8952	1/1	0.98	0.15	89,89,89,89	0
32	MG	K	8054	1/1	0.98	0.16	46,46,46,46	0
35	NA	0	8553	1/1	0.98	0.47	65,65,65,65	0
32	MG	0	8034	1/1	0.98	0.16	46,46,46,46	0
33	CL	0	8812	1/1	0.98	0.06	58,58,58,58	0
34	SR	0	8910	1/1	0.98	0.04	100,100,100,100	0
34	SR	0	8964	1/1	0.98	0.09	131,131,131,131	0
34	SR	0	8937	1/1	0.98	0.27	112,112,112,112	0
35	NA	0	8514	1/1	0.98	0.50	56,56,56,56	0
34	SR	3	8999	1/1	0.98	0.10	110,110,110,110	0
34	SR	0	8934	1/1	0.98	0.24	134,134,134,134	0
35	NA	B	8552	1/1	0.98	0.10	83,83,83,83	0
34	SR	0	8926	1/1	0.98	0.17	108,108,108,108	0
37	K	0	8402	1/1	0.98	0.25	76,76,76,76	0
33	CL	R	8806	1/1	0.98	0.18	57,57,57,57	0
33	CL	J	8801	1/1	0.99	0.07	79,79,79,79	0
34	SR	0	8911	1/1	0.99	0.08	85,85,85,85	0
32	MG	0	8043	1/1	0.99	0.06	52,52,52,52	0
32	MG	0	8064	1/1	0.99	0.19	44,44,44,44	0
34	SR	0	8970	1/1	0.99	0.02	123,123,123,123	0
32	MG	Y	8086	1/1	0.99	0.08	44,44,44,44	0
34	SR	0	8990	1/1	0.99	0.10	139,139,139,139	0
32	MG	0	8009	1/1	0.99	0.25	36,36,36,36	0
34	SR	F	9005	1/1	0.99	0.08	133,133,133,133	0
32	MG	0	8059	1/1	0.99	0.07	57,57,57,57	0
34	SR	0	8902	1/1	0.99	0.17	66,66,66,66	0
33	CL	0	8817	1/1	0.99	0.15	67,67,67,67	0
32	MG	0	8076	1/1	0.99	0.08	40,40,40,40	0
36	CD	O	8705	1/1	0.99	0.06	118,118,118,118	0
32	MG	0	8061	1/1	0.99	0.23	37,37,37,37	0
35	NA	M	8539	1/1	0.99	0.18	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8048	1/1	0.99	0.24	33,33,33,33	0
32	MG	0	8010	1/1	0.99	0.22	45,45,45,45	0
34	SR	3	8932	1/1	0.99	0.14	76,76,76,76	0
32	MG	0	8027	1/1	0.99	0.11	51,51,51,51	0
36	CD	Z	8703	1/1	0.99	0.13	75,75,75,75	0
32	MG	0	8032	1/1	0.99	0.05	44,44,44,44	0
34	SR	0	8931	1/1	0.99	0.07	113,113,113,113	0
32	MG	0	8007	1/1	0.99	0.16	32,32,32,32	0
32	MG	0	8029	1/1	0.99	0.15	49,49,49,49	0
32	MG	0	8080	1/1	0.99	0.12	75,75,75,75	0
34	SR	0	8909	1/1	0.99	0.15	88,88,88,88	0
33	CL	0	8816	1/1	0.99	0.08	79,79,79,79	0
32	MG	0	8019	1/1	0.99	0.20	28,28,28,28	0
36	CD	1	8702	1/1	0.99	0.13	67,67,67,67	0
34	SR	R	8912	1/1	0.99	0.16	92,92,92,92	0
32	MG	0	8073	1/1	0.99	0.35	73,73,73,73	0
34	SR	9	8978	1/1	0.99	0.08	135,135,135,135	0
34	SR	0	8948	1/1	0.99	0.10	92,92,92,92	0
32	MG	0	8084	1/1	0.99	0.15	33,33,33,33	0
34	SR	0	8967	1/1	0.99	0.06	133,133,133,133	0
34	SR	0	8906	1/1	0.99	0.24	64,64,64,64	0
34	SR	0	8918	1/1	0.99	0.15	80,80,80,80	0
35	NA	0	8517	1/1	0.99	0.15	31,31,31,31	0
32	MG	0	8015	1/1	0.99	0.13	30,30,30,30	0
32	MG	0	8005	1/1	0.99	0.23	35,35,35,35	0
34	SR	0	8904	1/1	0.99	0.18	65,65,65,65	0
36	CD	U	8701	1/1	0.99	0.10	63,63,63,63	0
34	SR	0	8956	1/1	0.99	0.06	155,155,155,155	0
32	MG	B	8042	1/1	0.99	0.07	44,44,44,44	0
34	SR	0	8935	1/1	0.99	0.09	79,79,79,79	0
34	SR	A	8930	1/1	0.99	0.06	97,97,97,97	0
32	MG	0	8090	1/1	0.99	0.10	65,65,65,65	0
34	SR	0	8916	1/1	1.00	0.03	120,120,120,120	0
34	SR	0	8903	1/1	1.00	0.19	59,59,59,59	0
32	MG	0	8008	1/1	1.00	0.09	28,28,28,28	0
34	SR	0	8905	1/1	1.00	0.27	61,61,61,61	0
32	MG	0	8018	1/1	1.00	0.23	40,40,40,40	0
32	MG	0	8058	1/1	1.00	0.09	22,22,22,22	0
34	SR	0	8907	1/1	1.00	0.15	56,56,56,56	0
36	CD	3	8704	1/1	1.00	0.10	74,74,74,74	0
32	MG	0	8004	1/1	1.00	0.19	32,32,32,32	0
34	SR	0	8925	1/1	1.00	0.08	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.