



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 06:38 pm GMT

PDB ID : 3CC7  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation C2487U  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-25  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

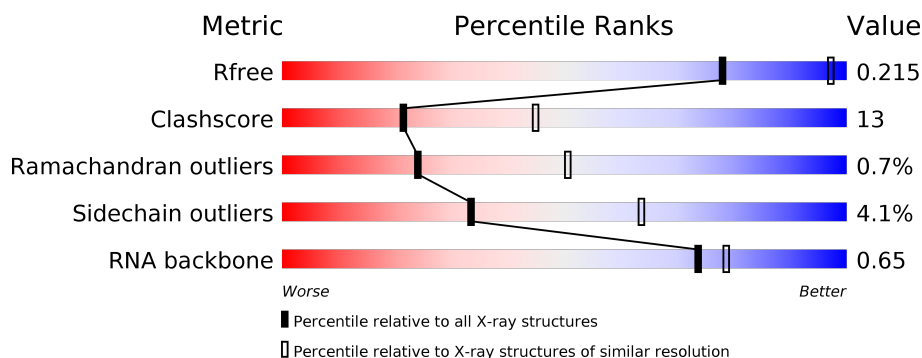
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.

















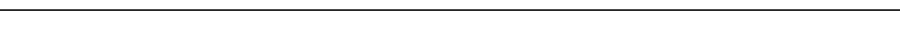




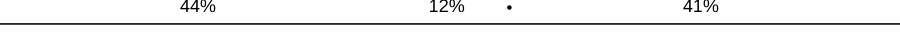
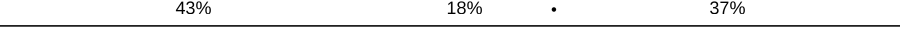




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RNA backbone	2636	1009 (3.00-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	240	70% 26% ...
2	B	338	65% 32% .
3	C	246	74% 22% .
4	D	177	49% 28% . 21%
5	E	178	79% 17% ..
6	F	120	75% 23% ..

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Mol	Chain	Length	Quality of chain
7	G	348	 6% 92%
8	H	177	 66% 23% 10%
9	I	162	 31% 12% 57%
10	J	145	 79% 16%
11	K	132	 72% 27%
12	L	165	 74% 13% 12%
13	M	196	 73% 23%
14	N	187	 72% 27%
15	O	116	 80% 18%
16	P	149	 74% 19%
17	Q	96	 83% 16%
18	R	155	 75% 19%
19	S	85	 76% 18% 5%
20	T	120	 76% 20%
21	U	67	 49% 28% 21%
22	V	71	 63% 27% 8%
23	W	154	 67% 31%
24	X	92	 57% 30% 11%
25	Y	241	 44% 12% 41%
26	Z	116	 43% 18% 37%
27	1	57	 63% 35%
28	2	50	 56% 36% 8%
29	3	92	 74% 24%
30	0	2923	 54% 34% 6% 6%
31	9	122	 38% 49% 13%

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99122 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		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
			59020	26349	10872	19054	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	85	Total	Mg	0	0
			85	85		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	2	Total	Mg	0	0
			2	2		
32	A	2	Total	Mg	0	0
			2	2		
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	10	Total 10	Cl 10	0	0
33	J	3	Total 3	Cl 3	0	0
33	B	1	Total 1	Cl 1	0	0
33	A	1	Total 1	Cl 1	0	0
33	N	1	Total 1	Cl 1	0	0
33	O	1	Total 1	Cl 1	0	0
33	R	1	Total 1	Cl 1	0	0
33	Y	1	Total 1	Cl 1	0	0
33	L	1	Total 1	Cl 1	0	0
33	3	1	Total 1	Cl 1	0	0
33	M	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	93	Total 93	Sr 93	0	0
34	J	1	Total 1	Sr 1	0	0
34	1	2	Total 2	Sr 2	0	0
34	B	2	Total 2	Sr 2	0	0
34	3	2	Total 2	Sr 2	0	0
34	A	3	Total 3	Sr 3	0	0
34	R	1	Total 1	Sr 1	0	0
34	9	2	Total 2	Sr 2	0	0
34	S	1	Total 1	Sr 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	66	Total	Na	0	0
			66	66		
35	J	1	Total	Na	0	0
			1	1		
35	Q	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	0	0
			2	2		

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	111	Total O 111 111	0	0
38	B	153	Total O 153 153	0	0
38	C	165	Total O 165 165	0	0
38	D	46	Total O 46 46	0	0
38	E	44	Total O 44 44	0	0
38	F	23	Total O 23 23	0	0
38	G	19	Total O 19 19	0	0
38	H	71	Total O 71 71	0	0
38	I	10	Total O 10 10	0	0
38	J	54	Total O 54 54	0	0
38	K	56	Total O 56 56	0	0
38	L	80	Total O 80 80	0	0
38	M	130	Total O 130 130	0	0
38	N	59	Total O 59 59	0	0
38	O	41	Total O 41 41	0	0
38	P	61	Total O 61 61	0	0
38	Q	51	Total O 51 51	0	0
38	R	78	Total O 78 78	0	0
38	S	33	Total O 33 33	0	0
38	T	37	Total O 37 37	0	0
38	U	25	Total O 25 25	0	0

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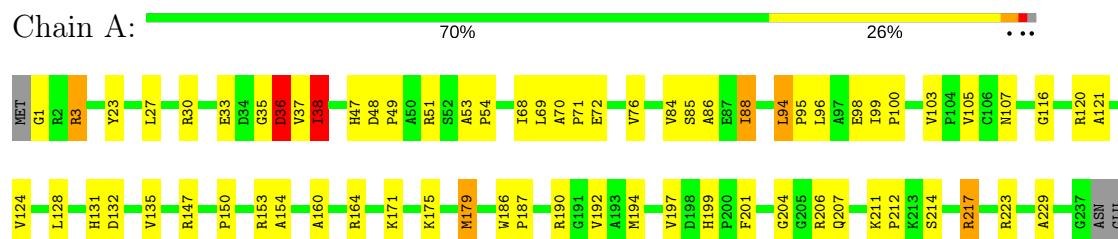
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	V	11	Total 11	O 11	0	0
38	W	63	Total 63	O 63	0	0
38	X	28	Total 28	O 28	0	0
38	Y	91	Total 91	O 91	0	0
38	Z	28	Total 28	O 28	0	0
38	1	52	Total 52	O 52	0	0
38	2	37	Total 37	O 37	0	0
38	3	68	Total 68	O 68	0	0
38	0	5951	Total 5951	O 5951	0	0
38	9	147	Total 147	O 147	0	0

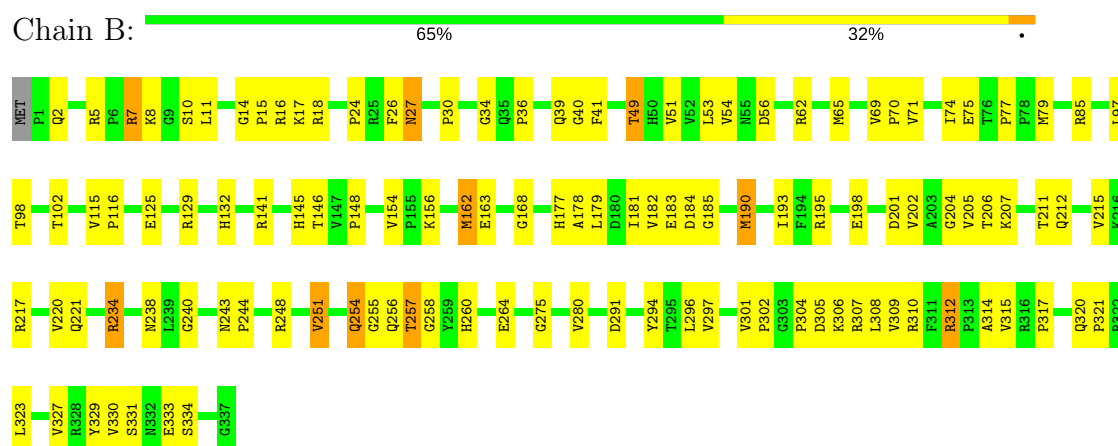
### 3 Residue-property plots [i](#)

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. 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. 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.

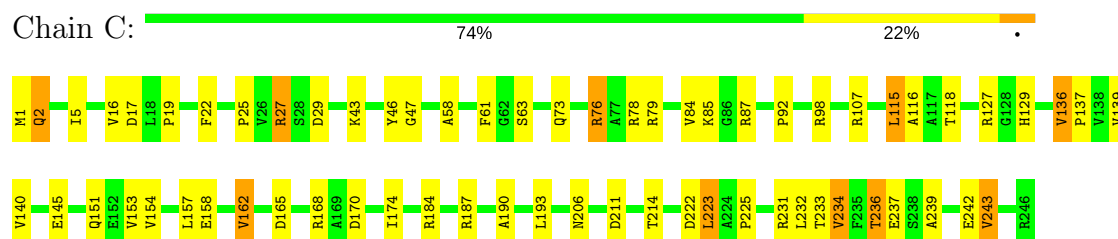
#### • Molecule 1: 50S ribosomal protein L2P



#### • Molecule 2: 50S ribosomal protein L3P

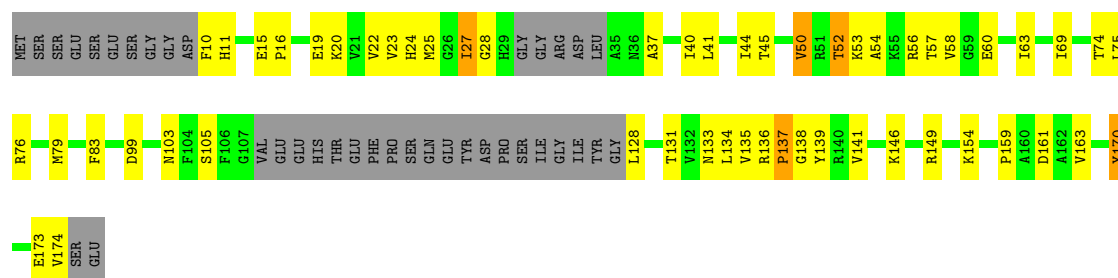


#### • Molecule 3: 50S ribosomal protein L4P




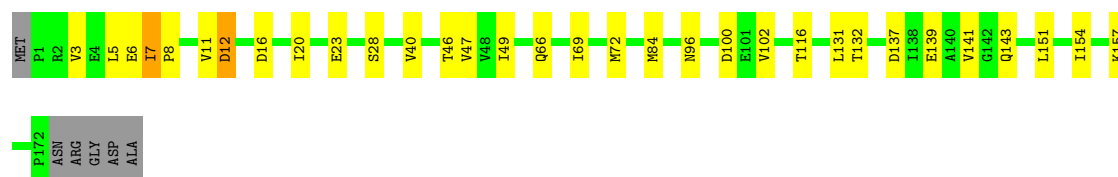
#### • Molecule 4: 50S ribosomal protein L5P





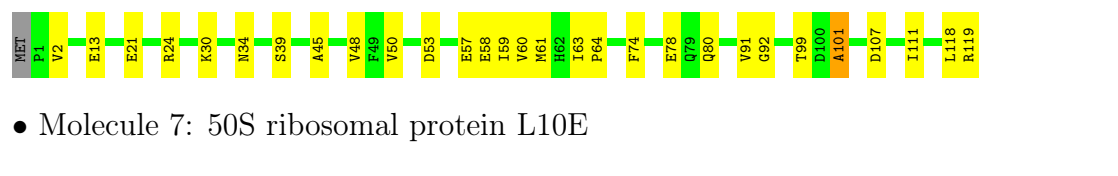
- Molecule 5: 50S ribosomal protein L6P

Chain E:  79% 17% . .

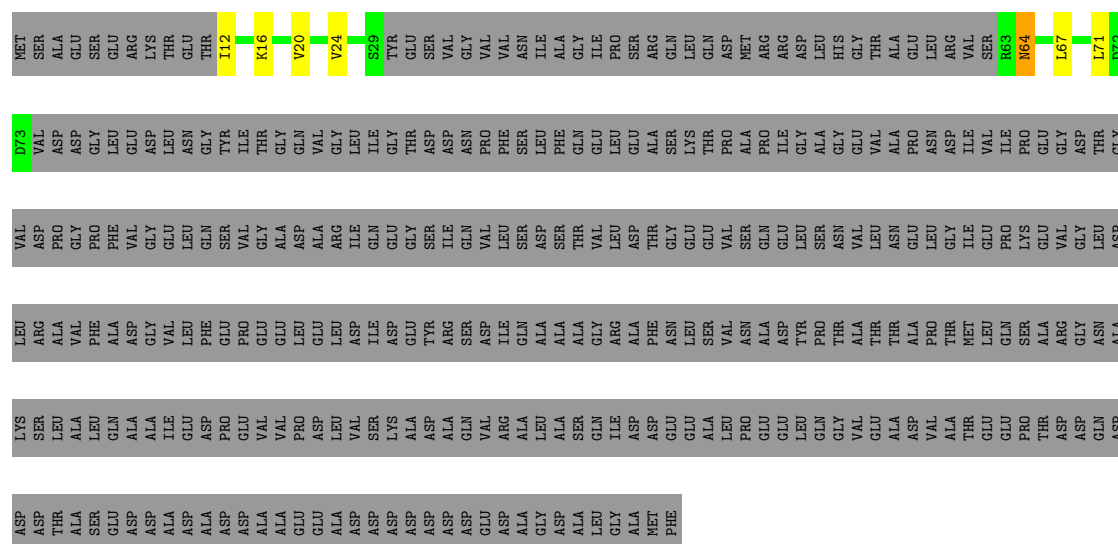


- Molecule 6: 50S ribosomal protein L7Ae

Chain F:  75% 23% .

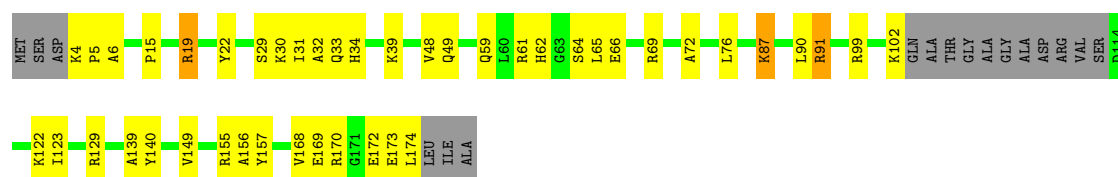


Chain G:  6% 92%



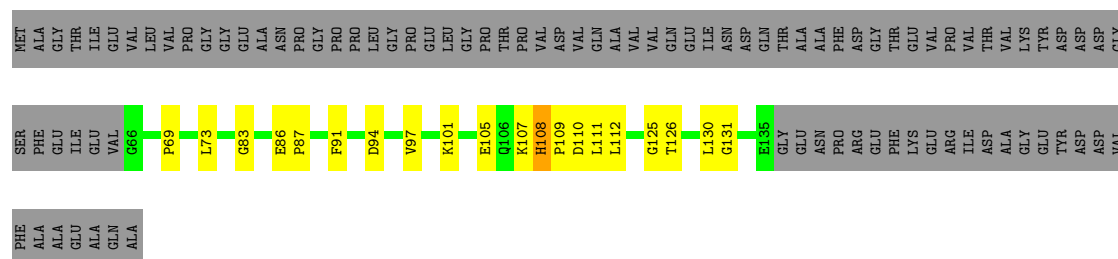
- Molecule 8: 50S ribosomal protein L10e

Chain H:  66% 23% • 10%



• Molecule 9: 50S ribosomal protein L11P

Chain I: 31% 12% 57%



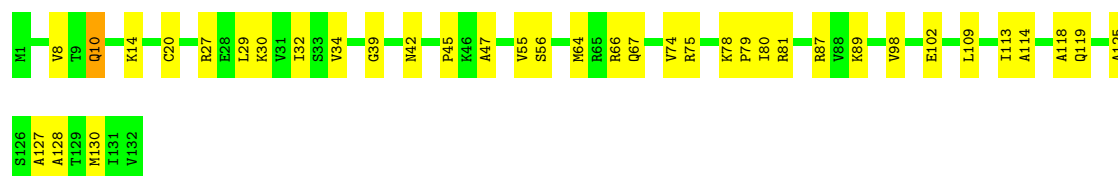
• Molecule 10: 50S ribosomal protein L13P

Chain J: 79% 16%



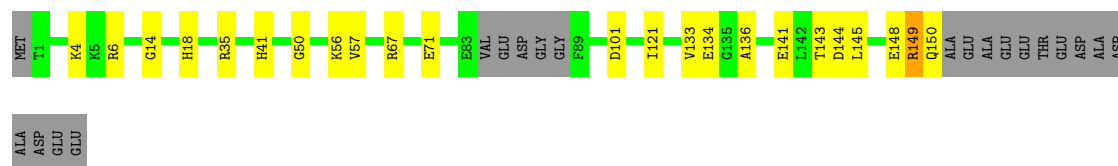
• Molecule 11: 50S ribosomal protein L14P

Chain K: 72% 27%



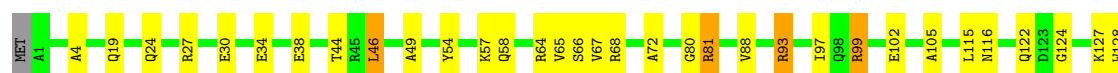
• Molecule 12: 50S ribosomal protein L15P

Chain L: 74% 13% 12%



• Molecule 13: 50S ribosomal protein L15e

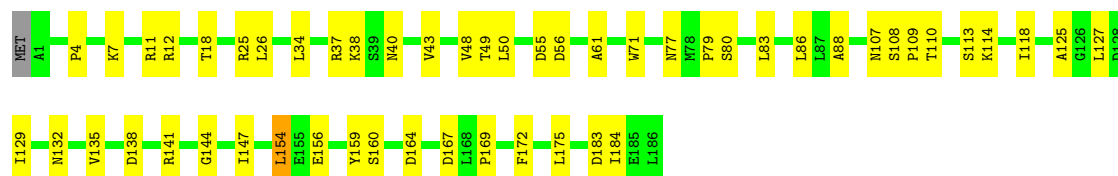
Chain M: 73% 23%





- Molecule 14: 50S ribosomal protein L18P

Chain N: 72% 27% ..



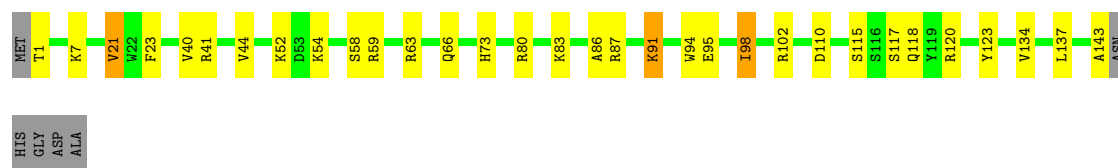
- Molecule 15: 50S ribosomal protein L18e

Chain O: 80% 18% ..



- Molecule 16: 50S ribosomal protein L19e

Chain P: 74% 19% • •



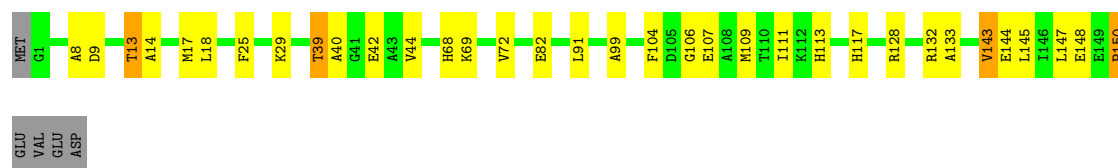
- Molecule 17: 50S ribosomal protein L21e

Chain Q: 83% 16% •



- Molecule 18: 50S ribosomal protein L22P

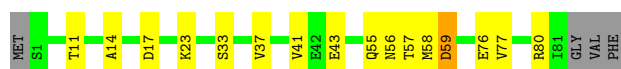
Chain R: 75% 19% • •



- Molecule 19: 50S ribosomal protein L23P

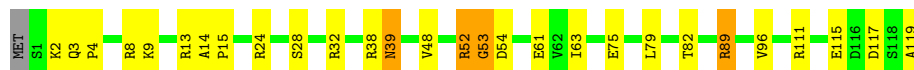
Chain S: 76% 18% 5%





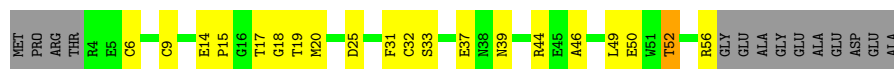
- Molecule 20: 50S ribosomal protein L24P

Chain T: 76% 20%



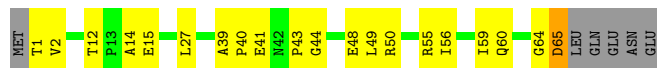
- Molecule 21: 50S ribosomal protein L24e

Chain U: 49% 28% 21%



- Molecule 22: 50S ribosomal protein L29P

Chain V: 63% 27% 8%



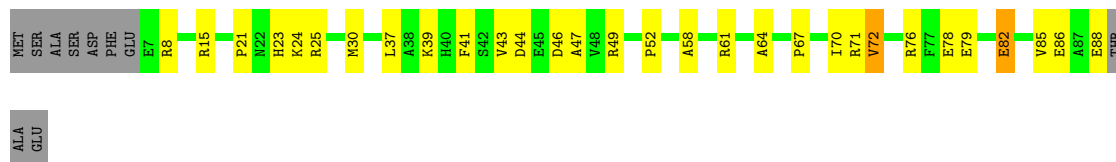
- Molecule 23: 50S ribosomal protein L30P

Chain W: 67% 31%



- Molecule 24: 50S ribosomal protein L31e

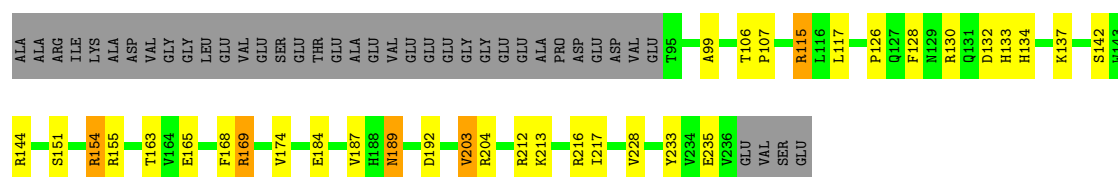
Chain X: 57% 30% 11%



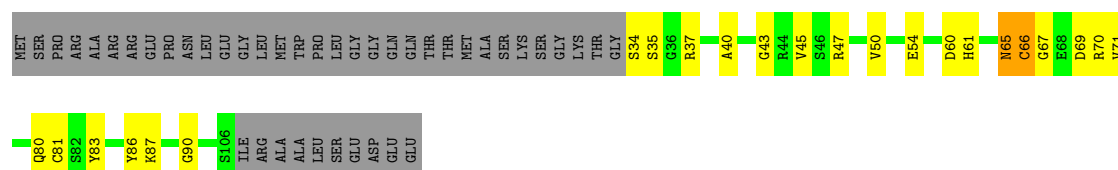
- Molecule 25: 50S ribosomal protein L32e

Chain Y: 44% 12% 41%





• Molecule 26: 50S ribosomal protein L37Ae



• Molecule 27: 50S ribosomal protein L37e



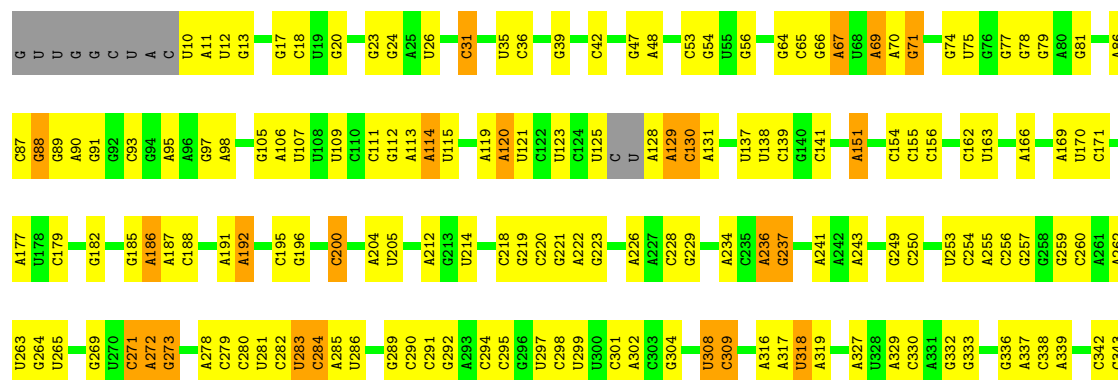
• Molecule 28: 50S ribosomal protein L39e



• Molecule 29: 50S ribosomal protein L44E



• Molecule 30: 23S ribosomal RNA



G1820	G1723	U1625	G1520	U1418	A1321	U1234	C1156	G1045	C963	U872	G775	G657	A532	C440	C344
U1724	U1725	A1626	A1521	C1420	G1322	G1235	C1157	C1051	G968	U876	U777	A660	G537	A441	G345
C1826	C1725	G1627	A1522	C1421	G1323	A1236	G1158	G1052	G969	A875	U776	G661	C538	A442	U346
A1829	G1730	A1632	U1524	C1423	G1328	C1238	A1161	G1053	U970	A876	A790	C667	G539	C444	A347
C1834	A1732	G1633	G1525	A1427	A1320	G1239	G1162	G1055	G	A878	A791	C668	U445	U445	G350
U1835	A1733	G1634	A1526	A1427	A1331	G1239	G1163	U1056	U	A879	A792	C669	C541	A446	G358
A1836	C1734	U1635	A1527	U1432	G1332	A1242	U1164	A1057	G	A882	G793	C670	A542	A447	C363
G1837	C1735	U1635	G1529	G1433	C1333	U1244	A1166	A1058	C	U883	U794	A671	G543	A448	U364
U1838	U1741	A1641	U1535	A1434	C1334	C1245	G1167	C1060	C	A886	A796	C672	G545	C450	G365
A1839	U1742	C1643	G1535	U1435	C1335	C1246	C1168	C1063	G	A892	A797	C677	G553	C451	G366
A1840	C1750	U1645	C1536	C1436	U1336	U1249	U1169	G1063	C	U890	U797	C678	A453	C452	G367
C1841	G1751	U1654	U1544	U1440	G1339	U1250	U1170	U1066	U	G898	G800	G681	C558	C453	G368
A1842	G1752	C1654	C1545	G1441	G1340	C1251	A1171	A1067	C	A899	U801	G682	U559	C454	G369
A1845	A1755	U1655	G1546	A1442	G1341	A1252	A1173	G1071	G	G902	A806	G683	U560	G458	U371
U1846	U1756	A1656	A1547	G1443	C1342	C1253	A1174	G1072	A	U903	A807	G684	G564	C461	A372
C1853	C1762	U1668	U1548	G1444	C1343	C1253	G1175	A1073	G	U904	A808	G685	U567	A462	G373
C1856	C1763	G1669	C1352	U1445	C1343	G1260	C1176	A1074	G	C906	A812	C687	U582	A466	A378
A1857	G1765	A1670	C1353	U1446	C1353	A1261	U1180	G1074	G	A907	C813	A688	C583	C467	A380
G1863	U1766	G1677	U1551	C1474	A1375	A1271	A1188	A1086	A	A912	C814	G690	U584	U468	G381
G1867	C1768	U1678	C1562	C1477	C1376	A1278	A1189	A1090	C	C920	C815	A698	G588	U470	U382
G1868	C1769	C1680	C1565	U1478	C1377	U1279	A1192	A1097	C999	C921	C816	C699	C594	C383	A384
C1873	G1773	G1681	C1566	G1481	G1378	A1280	A1193	A1098	U1001	U932	U825	C705	C604	C399	U392
U1874	A1778	A1683	C1574	G1482	C1384	U1285	A1194	G1099	A	C933	U826	G711	C605	A485	G393
C1880	A1779	G1684	C1574	G1482	C1385	A1286	A1195	A1099	U1005	C936	G834	U714	C613	A496	U396
C1882	C1787	C1692	G1593	U1488	G1387	U1288	U1198	U1109	A1006	U941	U835	U	U614	A498	C401
U1883	U1788	C1700	C1594	A1494	G1391	G1290	A1199	G1110	A1007	U942	G836	G716	G500	A499	U402
G1884	U1789	A1701	C1596	C1495	A1392	A1293	C1201	U1116	C1008	U943	U840	C717	G506	A407	A408
A1885	U1791	U1702	U1597	C1495	A1393	U1293	C1202	A1117	U1009	U944	U841	C718	A507	A508	C412
A1886	G1795	C1705	A1603	U1511	C1394	G1296	A1198	G1119	C1010	U945	C842	G724	A509	A508	G413
U1890	A1796	G1706	G1604	U1512	C1395	G1296	U1205	U1120	A1013	U947	A843	C725	U510	A509	C414
G1896	C1798	A1710	U1606	C1514	C1396	U1298	U1206	U1130	C1014	U948	U845	C729	A511	A511	U510
U1897	A1804	C1714	C1507	U1515	G1409	G1299	A1207	G1131	U1016	U949	A846	C741	A512	A512	G417
G1902	G1805	C1715	U1516	G1512	G1410	G1300	C1208	A1132	G950	C847	C848	G742	G514	A418	A419
U1903	A1904	A1717	A1615	U1516	G1411	U1304	C1209	G1135	C1023	A951	C849	G743	A635	U420	U420
U1905	G1806	A1717	A1616	A1515	G1412	C1305	G1210	U1136	C1025	G952	C853	G744	G636	U517	C421
C1906	C1818	U1722	A1617	U1517	G1417	U1306	G1211	G1137	U954	U954	C854	G745	C637	G518	C424
						A1307	C1212	G1138	A955	A955	C855	A746	A639	A521	C424
						A1308	C1213	G1139	A956	A956	C856	A747	A640	U522	C427
						G1311	C1214	U1149	G958	A957	C857	A748	G644	U523	C427
						G1312	C1215	A1150	C959	A958	C858	C759	U645	A524	C427
						A1313	C1216	G1151	G960	A959	C859	C764	G533	G533	C427
						U1314	C1217	A1152	A961	A961	C860	C765	G534	A524	C427
							C1218	G1153	C962	A962	C861	C766	G535	A524	C427
							C1219	A1154	C963	A963	C862	C767	G536	A524	C427
							C1220	G1155	C964	A964	C863	C768	G537	A524	C427
							C1221	A1156	C965	A965	C864	C769	G538	A524	C427
							C1222	G1157	C966	A966	C865	C770	G539	A524	C427
							C1223	A1158	C967	A967	C866	C771	G540	A524	C427
							C1224	G1159	C968	A968	C867	C772	G541	A524	C427
							C1225	A1160	C969	A969	C868	C773	G542	A524	C427
							C1226	G1161	C970	A970	C869	C774	G543	A524	C427
							C1227	A1162	C971	A971	C870	C775	G544	A524	C427
							C1228	G1163	C972	A972	C871	C776	G545	A524	C427
							C1229	A1164	C973	A973	C872	C777	G546	A524	C427
							C1230	G1165	C974	A974	C873	C778	G547	A524	C427
							C1231	A1166	C975	A975	C874	C779	G548	A524	C427
							C1232	G1167	C976	A976	C875	C780	G549	A524	C427
							C1233	A1168	C977	A977	C876	C781	G550	A524	C427
							C1234	G1169	C978	A978	C877	C782	G551	A524	C427
							C1235	A1170	C979	A979	C878	C783	G552	A524	C427
							C1236	G1171	C980	A980	C879	C784	G553	A524	C427
							C1237	A1172	C981	A981	C880	C785	G554	A524	C427
							C1238	G1173	C982	A982	C881	C786	G555	A524	C427
							C1239	A1174	C983	A983	C882	C787	G556	A524	C427
							C1240	G1175	C984	A984	C883	C788	G557	A524	C427
							C1241	A1176	C985	A985	C884	C789	G558	A524	C427
							C1242	G1177	C986	A986	C885	C790	G559	A524	C427
							C1243	A1178	C987	A987	C886	C791	G560	A524	C427
							C1244	G1179	C988	A988	C887	C792	G561	A524	C427
							C1245	A1180	C989	A989	C888	C793	G562	A524	C427
							C1246	G1181	C990	A990	C889	C794	G563	A524	C427
							C1247	A1182	C991	A991	C890	C795	G564	A524	C427
							C1248	G1183	C992	A992	C891	C796	G565	A524	C427
							C1249	A1184	C993	A993	C892	C797	G566	A524	C427
							C1250	G1185	C994	A994	C893	C798	G567	A524	C427
							C1251	A1186	C995	A995	C894	C799	G568	A524	C427
							C1252	G1187	C996	A996	C895	C800	G569	A524	C427
							C1253	A1188	C997	A997	C896	C801	G570	A524	C427
							C1254	G1189	C998	A998	C897	C802	G571	A524	C427
							C1255	A1190	C999	A999	C898	C803	G572	A524	C427
							C1256	G1191	C1000	A1000	C899	C804	G573	A524	C427
							C1257	A1192	C1001	A1001	C900	C805	G574	A524	C427
							C1258	G1193	C1002	A1002	C901	C806	G575	A524	C427
							C1259	A1194	C1003	A1003	C902	C807	G576	A524	C427
							C1260	G1195	C1004	A1004	C903	C808	G577	A524	C427
							C1261	A1196	C1005	A1005	C904	C809	G578	A524	C427
							C1262	G1197	C1006	A1006	C905	C810	G579	A524	C427
							C1263	A1198	C1007	A1007	C906	C811	G580	A524	C427
							C1264	G1199	C1008	A1008	C907	C812	G581	A524	C427
							C1265	A1200	C1009	A1009	C908	C813	G582	A524	C427
							C1266	G1201	C1010	A1010	C909	C814	G583	A524	C427
							C1267	A1202	C1011	A1011	C910	C815	G584	A524	C427
							C1268	G1203	C1012	A1012	C911	C816	G585	A524	C427
							C1269	A1204	C1013	A1013	C912	C817	G586	A524	C427
							C1270	G1205	C1014	A1014	C913	C818	G587	A524	C427
							C1271	A1206	C1015	A1015	C914	C819	G588	A524	C427
							C1272	G1207	C1016	A1016	C915	C820	G589	A524	C427
							C1273	A1208	C1017	A1017	C916	C821	G590	A524	C427
							C1274	G1209	C1018	A1018	C917	C822	G591	A524	C427
							C1275	A1210	C1019	A1019	C918	C823	G592	A524	C427
							C1276	G1211	C1020	A1020	C919	C824	G593	A524	C427



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.83Å 299.90Å 576.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 2.70 85.81 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.83-2.70) 90.8 (85.81-2.41)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.184 , 0.226 0.174 , 0.215	Depositor DCC
$R_{free}$ test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.32	0/1786	0.64	0/2408
2	B	0.32	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.31	0/1111	0.55	0/1498
5	E	0.32	0/1382	0.56	0/1880
6	F	0.32	0/901	0.57	0/1224
7	G	0.31	0/241	0.48	0/324
8	H	0.32	0/1302	0.63	0/1743
9	I	0.29	0/526	0.51	0/716
10	J	0.35	0/1136	0.59	0/1530
11	K	0.33	0/1004	0.65	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.34	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.61	0/1999
15	O	0.34	0/874	0.59	1/1181 (0.1%)
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.35	0/749	0.68	0/1005
18	R	1.26	7/1172 (0.6%)	1.11	6/1578 (0.4%)
19	S	0.31	0/648	0.57	0/875
20	T	0.33	0/958	0.62	1/1289 (0.1%)
21	U	0.34	0/417	0.55	0/562
22	V	0.31	0/502	0.52	0/675
23	W	0.34	0/1219	0.64	0/1655
24	X	0.34	0/664	0.58	0/895
25	Y	0.36	0/1146	0.60	0/1536
26	Z	0.35	0/584	0.60	0/781
27	1	0.37	0/438	0.61	0/578
28	2	0.34	0/401	0.55	0/529
29	3	0.36	0/771	0.57	0/1024
30	0	0.36	0/65957	0.68	17/102867 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98701 (0.0%)	0.67	26/147586 (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
30	0	0	42
31	9	0	1
All	All	1	43

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.34	2.86	1.50
18	R	150	PRO	CA-C	-18.21	1.16	1.52
18	R	150	PRO	CG-CD	13.97	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.28	1.66	1.47
18	R	150	PRO	N-CD	10.80	1.62	1.47
18	R	150	PRO	CA-CB	7.58	1.68	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.83	112.00
18	R	150	PRO	N-CA-C	-19.39	61.69	112.10
18	R	150	PRO	CA-N-CD	12.31	128.94	111.70
18	R	150	PRO	N-CA-CB	10.98	116.48	103.30
18	R	150	PRO	CA-C-O	-8.51	99.77	120.20
30	0	1878	G	N9-C1'-C2'	-6.59	104.75	112.00
18	R	150	PRO	CA-CB-CG	-6.10	92.41	104.00
30	0	1504	A	C1'-O4'-C4'	-6.07	105.04	109.90
30	0	871	G	C5'-C4'-O4'	-5.99	101.91	109.10
30	0	2291	A	N9-C1'-C2'	5.57	121.24	114.00
31	9	39	U	N1-C1'-C2'	5.48	121.12	114.00
30	0	2467	A	C1'-O4'-C4'	-5.41	105.57	109.90
30	0	1829	A	N9-C1'-C2'	-5.40	106.06	112.00
30	0	1819	G	C5'-C4'-C3'	5.26	124.42	116.00
30	0	2313	C	C5'-C4'-O4'	5.24	115.39	109.10
30	0	1504	A	N9-C1'-C2'	5.23	120.80	114.00
20	T	52	ARG	N-CA-C	5.18	124.97	111.00
30	0	2607	U	N1-C1'-C2'	5.17	120.72	114.00
30	0	2301	A	N9-C1'-C2'	5.15	120.69	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2313	C	C1'-O4'-C4'	-5.12	105.80	109.90
15	O	66	GLY	N-CA-C	5.08	125.81	113.10
30	0	699	C	C1'-O4'-C4'	-5.07	105.85	109.90
30	0	2316	G	C5'-C4'-C3'	-5.02	107.96	116.00
30	0	841	A	C1'-O4'-C4'	-5.02	105.88	109.90
30	0	777	U	O4'-C1'-N1	5.02	112.21	108.20
30	0	1120	U	C5'-C4'-C3'	-5.00	107.99	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1262	C	Sidechain
30	0	1342	C	Sidechain
30	0	1417	G	Sidechain
30	0	1432	U	Sidechain
30	0	1681	G	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1970	G	Sidechain
30	0	1979	G	Sidechain
30	0	2036	C	Sidechain
30	0	2115	U	Sidechain
30	0	221	G	Sidechain
30	0	2301	A	Sidechain
30	0	2312	G	Sidechain
30	0	2316	G	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2524	G	Sidechain
30	0	2551	C	Sidechain
30	0	2564	G	Sidechain
30	0	26	U	Sidechain
30	0	2607	U	Sidechain
30	0	2679	G	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	686	A	Sidechain
30	0	817	G	Sidechain
30	0	903	U	Sidechain
31	9	94	G	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	75	0
2	B	2625	0	2533	92	0
3	C	1860	0	1813	57	0
4	D	1094	0	1085	40	0
5	E	1357	0	1266	23	0
6	F	890	0	843	26	0
7	G	240	0	231	7	0
8	H	1282	0	1292	37	0
9	I	519	0	500	15	0
10	J	1120	0	1098	30	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	22	0
13	M	1558	0	1573	42	0
14	N	1445	0	1401	45	0
15	O	865	0	873	15	0
16	P	1136	0	1123	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	735	0	729	14	0
18	R	1149	0	1122	34	0
19	S	641	0	605	11	0
20	T	950	0	924	19	0
21	U	410	0	364	19	0
22	V	499	0	511	17	0
23	W	1196	0	1137	55	0
24	X	654	0	653	24	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	16	0
27	1	431	0	426	22	0
28	2	396	0	413	19	0
29	3	755	0	728	20	0
30	0	59020	0	29806	1142	0
31	9	2599	0	1325	101	0
32	0	85	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	10	0	0	2	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	0	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	1	0
33	O	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	2	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	J	1	0	0	0	0
34	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	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	5951	0	0	153	0
38	1	52	0	0	3	0
38	2	37	0	0	2	0
38	3	68	0	0	5	0
38	9	147	0	0	8	0
38	A	111	0	0	5	0
38	B	153	0	0	14	0
38	C	165	0	0	11	0
38	D	46	0	0	2	0
38	E	44	0	0	2	0
38	F	23	0	0	1	0
38	G	19	0	0	0	0
38	H	71	0	0	6	0
38	I	10	0	0	2	0
38	J	54	0	0	1	0
38	K	56	0	0	3	0
38	L	80	0	0	6	0
38	M	130	0	0	5	0
38	N	59	0	0	5	0
38	O	41	0	0	3	0
38	P	61	0	0	1	0
38	Q	51	0	0	2	0
38	R	78	0	0	3	0
38	S	33	0	0	2	0
38	T	37	0	0	2	0
38	U	25	0	0	3	0
38	V	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	W	63	0	0	4	0
38	X	28	0	0	1	0
38	Y	91	0	0	6	0
38	Z	28	0	0	3	0
All	All	99122	0	59907	1937	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 13.

All (1937) 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
30:0:1160:G:C5'	30:0:1161:A:H5'	1.81	1.10
31:9:56:A:H2'	31:9:57:A:H5''	1.33	1.08
30:0:871:G:C8	30:0:871:G:H5'	1.87	1.07
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07
14:N:37:ARG:NH1	31:9:6:C:H5''	1.71	1.05
30:0:1160:G:H5'	30:0:1161:A:C5'	1.88	1.03
30:0:381:G:H5''	38:0:4345:HOH:O	1.58	1.02
30:0:1160:G:H5'	30:0:1161:A:H5'	1.02	1.02
30:0:2812:A:H2	30:0:2814:A:H62	1.03	1.02
13:M:171:ARG:HD3	30:0:156:C:H5''	1.40	1.00
10:J:82:THR:HG23	30:0:1242:A:H5'	1.44	1.00
30:0:2717:C:C2'	30:0:2718:C:H5''	1.92	0.99
11:K:10:GLN:H	11:K:10:GLN:HE21	1.06	0.99
31:9:76:G:H3'	31:9:77:A:H5''	1.42	0.99
30:0:182:G:H5'	38:0:5188:HOH:O	1.63	0.98
30:0:871:G:H8	30:0:871:G:H5'	1.23	0.98
30:0:1666:C:O2'	30:0:1667:A:H5''	1.61	0.98
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.44	0.98
30:0:1118:A:H3'	30:0:1118:A:H8	1.29	0.97
30:0:2717:C:H2'	30:0:2718:C:H5''	1.46	0.97
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.47	0.96
30:0:1474:C:H6	30:0:1474:C:H5'	1.29	0.96
15:O:3:THR:HG22	30:0:656:G:H5'	1.46	0.96
30:0:1243:C:H3'	38:0:4869:HOH:O	1.65	0.95
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.12	0.94
30:0:1187:U:HO2'	30:0:1189:A:H2	1.07	0.94
3:C:236:THR:HG22	3:C:239:ALA:H	1.31	0.94
30:0:282:C:O2'	30:0:283:U:H5'	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:115:SER:H	16:P:118:GLN:HE21	0.95	0.92
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.84	0.92
30:0:69:A:H5'	30:0:69:A:H8	1.33	0.92
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.14	0.92
30:0:871:G:H8	30:0:871:G:C5'	1.83	0.91
30:0:1205:U:H2'	30:0:1206:U:C5'	2.00	0.91
30:0:2491:G:H1'	38:0:6910:HOH:O	1.70	0.91
30:0:69:A:H5'	30:0:69:A:C8	2.06	0.91
30:0:1118:A:H3'	30:0:1118:A:C8	2.04	0.91
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.51	0.91
30:0:2533:C:H5'	30:0:2533:C:H6	1.35	0.90
8:H:49:GLN:HE21	8:H:140:TYR:HE2	1.15	0.90
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.53	0.90
4:D:154:LYS:HD2	4:D:154:LYS:H	1.37	0.89
30:0:1603:A:H5'	30:0:1605:G:O4'	1.72	0.89
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.89
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.37	0.89
30:0:1474:C:C6	30:0:1474:C:H5'	2.08	0.89
30:0:1701:A:H5'	38:0:6316:HOH:O	1.73	0.89
30:0:1183:C:H2'	38:0:6276:HOH:O	1.73	0.89
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.19	0.89
30:0:1184:C:H1'	38:0:7504:HOH:O	1.71	0.88
30:0:542:A:H5'	30:0:542:A:H8	1.38	0.88
30:0:282:C:H1'	30:0:368:C:N4	1.88	0.88
30:0:1666:C:C2'	30:0:1667:A:H5''	2.03	0.88
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.88
30:0:877:G:H5'	30:0:878:G:OP1	1.74	0.88
30:0:2251:G:H2'	30:0:2252:A:C8	2.09	0.87
30:0:558:C:C2'	30:0:559:U:H5''	2.04	0.87
2:B:238:ASN:HD22	2:B:240:GLY:H	1.20	0.87
30:0:1206:U:H6	30:0:1206:U:H5'	1.40	0.87
31:9:56:A:C2'	31:9:57:A:H5''	2.05	0.86
31:9:14:G:H5'	31:9:14:G:H8	1.39	0.86
30:0:10:U:H6	30:0:10:U:H3'	1.40	0.86
14:N:37:ARG:HH12	31:9:6:C:H5''	1.37	0.86
30:0:1372:A:H3'	38:0:7227:HOH:O	1.76	0.85
30:0:1701:A:H4'	30:0:1702:U:H5''	1.56	0.85
16:P:117:SER:HB3	30:0:1593:C:OP1	1.77	0.85
30:0:506:G:H22	30:0:509:A:C5'	1.88	0.85
30:0:871:G:C8	30:0:871:G:C5'	2.59	0.85
2:B:162:MET:HE3	2:B:308:LEU:HD21	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1205:U:H2'	30:0:1206:U:H5'	1.56	0.84
30:0:1118:A:H62	30:0:1244:U:H3	1.25	0.84
30:0:545:G:H8	30:0:545:G:H5'	1.39	0.84
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.59	0.84
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.60	0.84
30:0:1667:A:H8	30:0:1667:A:H5'	1.41	0.84
30:0:1116:U:H3	30:0:1246:A:H62	1.26	0.84
30:0:2502:C:C2'	30:0:2503:A:H5'	2.08	0.83
30:0:2506:A:HO2'	30:0:2507:G:H8	0.88	0.83
30:0:541:C:C2'	30:0:542:A:H5''	2.08	0.83
30:0:2769:C:C2'	30:0:2770:G:H5'	2.07	0.83
30:0:1300:G:H1'	38:0:4714:HOH:O	1.78	0.83
30:0:214:U:H5'	38:0:6173:HOH:O	1.77	0.83
30:0:1189:A:H1'	30:0:1209:C:O4'	1.79	0.82
30:0:506:G:H22	30:0:509:A:H5'	1.42	0.82
30:0:541:C:H2'	30:0:542:A:H5''	1.60	0.82
30:0:396:U:H1'	38:0:7666:HOH:O	1.77	0.82
28:2:41:HIS:H	28:2:45:ASN:HD22	1.25	0.82
30:0:1878:G:H1'	38:0:6153:HOH:O	1.79	0.82
30:0:2502:C:H2'	30:0:2503:A:H5'	1.60	0.82
30:0:2506:A:O2'	30:0:2507:G:H8	1.61	0.82
23:W:88:THR:HB	38:W:6679:HOH:O	1.80	0.82
30:0:1183:C:N4	30:0:1184:C:H41	1.78	0.81
30:0:236:A:H4'	30:0:237:G:H5'	1.62	0.81
30:0:1116:U:HO2'	30:0:1118:A:H2	0.82	0.81
30:0:1116:U:O2'	30:0:1118:A:H2	1.63	0.81
30:0:544:G:H2'	30:0:545:G:H5''	1.63	0.81
30:0:2783:A:H3'	38:0:5262:HOH:O	1.80	0.81
11:K:39:GLY:HA2	38:0:5251:HOH:O	1.79	0.81
30:0:559:U:H5'	30:0:559:U:H6	1.43	0.81
30:0:558:C:O2'	30:0:559:U:H5''	1.79	0.81
30:0:1632:A:H2'	30:0:1633:C:H5'	1.63	0.80
30:0:380:A:H2'	38:0:7266:HOH:O	1.81	0.80
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.28	0.80
30:0:1189:A:H3'	38:0:7718:HOH:O	1.80	0.80
30:0:2291:A:C8	30:0:2309:C:H5'	2.16	0.80
30:0:2586:U:H3	30:0:2592:G:H22	1.26	0.80
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.78	0.80
30:0:2426:G:H1'	38:0:6125:HOH:O	1.82	0.80
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.64	0.80
30:0:1603:A:H5''	30:0:1605:G:H5'	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1741:U:H5'	30:0:1742:A:OP1	1.82	0.80
16:P:115:SER:H	16:P:118:GLN:NE2	1.77	0.80
30:0:1119:G:N2	30:0:1246:A:C2	2.49	0.79
30:0:2533:C:C6	30:0:2533:C:H5'	2.15	0.79
3:C:139:VAL:HG13	38:C:8641:HOH:O	1.82	0.79
15:O:3:THR:CG2	30:0:656:G:H5'	2.11	0.79
30:0:541:C:H2'	30:0:542:A:C5'	2.12	0.79
30:0:2851:G:O2'	30:0:2852:A:H5'	1.83	0.79
20:T:9:LYS:HE3	20:T:13:ARG:NH1	1.98	0.79
30:0:2896:A:H5''	38:0:6132:HOH:O	1.81	0.78
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.65	0.78
30:0:2827:A:H2'	30:0:2828:G:O4'	1.83	0.78
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.48	0.78
33:0:8813:CL:CL	38:0:4714:HOH:O	2.39	0.78
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.13	0.78
30:0:1634:G:H3'	38:0:3915:HOH:O	1.84	0.77
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.49	0.77
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.99	0.77
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.67	0.77
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.33	0.77
30:0:2769:C:O2'	30:0:2770:G:H5'	1.85	0.77
30:0:1666:C:H2'	30:0:1667:A:C5'	2.14	0.77
13:M:164:THR:HG22	13:M:167:GLY:H	1.50	0.77
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.76
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.50	0.76
22:V:50:ARG:HH12	30:0:56:G:H5''	1.48	0.76
30:0:1209:C:H2'	30:0:1210:G:H8	1.50	0.76
5:E:143:GLN:NE2	30:0:2779:G:H21	1.82	0.76
30:0:2908:A:H2'	30:0:2909:G:O4'	1.85	0.76
30:0:282:C:H1'	30:0:368:C:H42	1.50	0.76
30:0:1080:C:H4'	30:0:1081:A:OP1	1.85	0.76
3:C:174:ILE:HD11	30:0:338:C:H4'	1.66	0.76
30:0:558:C:H2'	30:0:559:U:C5'	2.15	0.76
31:9:2:U:OP2	31:9:3:A:H5'	1.86	0.76
30:0:2768:A:O2'	30:0:2769:C:H5'	1.86	0.76
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.68	0.76
30:0:2004:U:H4'	38:0:5338:HOH:O	1.86	0.76
30:0:31:C:H4'	38:0:7463:HOH:O	1.87	0.75
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.68	0.75
30:0:2637:A:H5'	38:0:4961:HOH:O	1.85	0.75
30:0:2717:C:O2'	30:0:2718:C:H5''	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1973:A:H5'	30:0:1973:A:H8	1.52	0.74
30:0:2239:C:H2'	30:0:2240:U:H6	1.52	0.74
30:0:283:U:H5	30:0:284:C:C4	2.05	0.74
30:0:603:A:H5''	30:0:604:G:OP1	1.87	0.74
28:2:41:HIS:HD2	28:2:44:ARG:H	1.35	0.74
30:0:2748:G:H5'	38:0:7579:HOH:O	1.85	0.74
30:0:2851:G:C2'	30:0:2852:A:H5'	2.17	0.74
30:0:179:C:H5''	38:0:9320:HOH:O	1.86	0.74
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.69	0.74
30:0:1118:A:C8	30:0:1118:A:C3'	2.69	0.74
30:0:2559:C:H4'	38:0:7294:HOH:O	1.86	0.74
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.69	0.74
14:N:113:SER:HB2	38:N:8854:HOH:O	1.87	0.74
30:0:272:A:H5'	30:0:273:G:OP2	1.88	0.74
31:9:14:G:H5'	31:9:14:G:C8	2.23	0.74
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.69	0.73
30:0:1942:A:H3'	38:0:7386:HOH:O	1.88	0.73
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.69	0.73
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.71	0.73
30:0:1180:U:H2'	30:0:1181:A:O4'	1.89	0.73
16:P:115:SER:N	16:P:118:GLN:HE21	1.79	0.73
30:0:10:U:C6	30:0:10:U:H3'	2.23	0.73
30:0:1183:C:H42	30:0:1184:C:H41	1.35	0.73
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.88	0.73
30:0:2717:C:H2'	30:0:2718:C:C5'	2.19	0.73
30:0:1205:U:H2'	30:0:1206:U:H5''	1.70	0.72
30:0:338:C:H5''	38:0:3821:HOH:O	1.89	0.72
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.71	0.72
11:K:10:GLN:H	11:K:10:GLN:NE2	1.83	0.72
31:9:49:G:O2'	31:9:50:G:H5'	1.88	0.72
30:0:1279:U:O2	30:0:1279:U:H2'	1.88	0.72
30:0:2256:G:O2'	30:0:2257:G:H5'	1.88	0.72
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.87	0.72
18:R:39:THR:HG22	18:R:42:GLU:H	1.53	0.72
30:0:2420:G:O2'	30:0:2421:G:H5'	1.90	0.72
30:0:1666:C:H2'	30:0:1667:A:H5'	1.72	0.71
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.70	0.71
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.73	0.71
30:0:1666:C:C2'	30:0:1667:A:C5'	2.68	0.71
30:0:544:G:C2'	30:0:545:G:H5''	2.20	0.71
30:0:1632:A:C2'	30:0:1633:C:H5'	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:558:C:H2'	30:0:559:U:H5''	1.70	0.71
18:R:9:ASP:O	18:R:13:THR:HB	1.89	0.71
30:0:2679:G:H2'	30:0:2681:A:OP2	1.91	0.71
30:0:2010:A:H2'	38:0:5990:HOH:O	1.90	0.71
30:0:2578:G:H5'	30:0:2578:G:H8	1.54	0.71
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.37	0.71
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.72	0.71
30:0:1964:U:O2	30:0:1964:U:H2'	1.91	0.71
31:9:92:G:H2'	31:9:93:A:C8	2.26	0.71
30:0:1157:C:H2'	30:0:1158:G:H8	1.56	0.70
30:0:2635:A:O2'	30:0:2636:C:H5'	1.90	0.70
30:0:2769:C:H2'	30:0:2770:G:O4'	1.91	0.70
31:9:39:U:H1'	31:9:44:A:H61	1.55	0.70
30:0:1527:A:H1'	30:0:1528:A:C8	2.27	0.70
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.27	0.70
30:0:1174:A:C5	30:0:1201:C:H4'	2.26	0.70
3:C:174:ILE:CD1	30:0:338:C:H4'	2.21	0.70
30:0:1701:A:H4'	30:0:1702:U:C5'	2.20	0.70
30:0:31:C:H2'	38:0:7726:HOH:O	1.89	0.70
22:V:1:THR:HG23	22:V:2:VAL:H	1.56	0.70
30:0:2852:A:H5''	38:0:5264:HOH:O	1.91	0.70
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.05	0.69
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.07	0.69
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.74	0.69
30:0:1165:G:O2'	30:0:1174:A:H1'	1.92	0.69
30:0:308:U:H5'	30:0:309:C:OP1	1.91	0.69
12:L:148:GLU:HA	38:L:8870:HOH:O	1.92	0.69
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.73	0.69
30:0:2507:G:H2'	30:0:2510:C:H42	1.57	0.69
31:9:29:C:H2'	31:9:30:C:H5'	1.73	0.69
30:0:814:G:H4'	38:0:3155:HOH:O	1.91	0.69
3:C:1:MET:HG2	3:C:2:GLN:H	1.55	0.69
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.92	0.69
30:0:1603:A:C5'	30:0:1605:G:H5'	2.22	0.69
31:9:1:U:H4'	31:9:3:A:OP1	1.92	0.69
30:0:545:G:C8	30:0:545:G:H5'	2.25	0.69
12:L:133:VAL:HA	38:L:8871:HOH:O	1.92	0.69
2:B:217:ARG:HG3	2:B:257:THR:HB	1.75	0.68
30:0:281:U:H2'	30:0:282:C:O4'	1.94	0.68
31:9:7:G:H5'	38:9:9099:HOH:O	1.93	0.68
38:Y:8852:HOH:O	33:0:8817:CL:CL	2.49	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:37:ARG:NH1	31:9:6:C:C5'	2.53	0.68
2:B:258:GLY:H	2:B:260:HIS:CE1	2.12	0.68
30:0:1120:U:H5''	30:0:1120:U:C6	2.29	0.68
30:0:1819:G:H2'	30:0:1820:G:H4'	1.74	0.68
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.07	0.68
30:0:2256:G:C2'	30:0:2257:G:H5'	2.23	0.68
30:0:870:G:C2'	30:0:871:G:H5''	2.23	0.68
2:B:244:PRO:HB3	30:0:1234:U:N3	2.09	0.67
13:M:171:ARG:CD	30:0:156:C:H5''	2.20	0.67
10:J:70:PHE:HD1	30:0:2676:C:HO2'	1.40	0.67
30:0:292:G:H2'	30:0:358:G:N2	2.08	0.67
14:N:144:GLY:O	14:N:147:ILE:HG22	1.94	0.67
18:R:150:PRO:CG	18:R:150:PRO:O	2.41	0.67
27:1:42:SER:HB2	38:1:354:HOH:O	1.93	0.67
14:N:11:ARG:HD3	31:9:114:G:O6	1.94	0.67
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.94	0.67
30:0:297:U:H2'	30:0:298:C:C6	2.28	0.67
30:0:2812:A:C2	30:0:2814:A:N6	2.58	0.67
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.76	0.67
20:T:24:ARG:HH21	20:T:39:ASN:ND2	1.93	0.67
31:9:39:U:H1'	31:9:44:A:N6	2.08	0.67
30:0:1667:A:C8	30:0:1667:A:H5'	2.27	0.67
30:0:564:G:H1'	38:0:6342:HOH:O	1.94	0.67
30:0:1060:C:H6	30:0:1060:C:H5'	1.60	0.66
30:0:1474:C:C5'	30:0:1474:C:H6	2.07	0.66
3:C:27:ARG:NH2	30:0:657:G:OP1	2.28	0.66
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.58	0.66
12:L:6:ARG:HD3	30:0:1299:G:O6	1.95	0.66
30:0:2681:A:H4'	30:0:2682:C:H5'	1.75	0.66
30:0:1116:U:O2'	30:0:1118:A:C2	2.44	0.66
30:0:1205:U:C2'	30:0:1206:U:C5'	2.72	0.66
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.26	0.66
12:L:136:ALA:HB3	38:L:8871:HOH:O	1.96	0.66
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.78	0.66
30:0:1289:C:H3'	38:0:6443:HOH:O	1.95	0.66
30:0:2239:C:H2'	30:0:2240:U:C6	2.30	0.66
22:V:50:ARG:NH1	30:0:56:G:H5''	2.10	0.66
30:0:1016:U:H1'	38:0:3678:HOH:O	1.96	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.44	0.66
30:0:960:G:H2'	30:0:960:G:N3	2.11	0.66
3:C:236:THR:HG22	3:C:239:ALA:N	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:125:U:H2'	38:0:3785:HOH:O	1.96	0.65
30:0:2769:C:H2'	30:0:2770:G:H5'	1.77	0.65
30:0:2836:G:H1'	38:0:6880:HOH:O	1.95	0.65
1:A:199:HIS:HD2	1:A:201:PHE:H	1.44	0.65
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.96	0.65
30:0:2795:C:O2'	30:0:2796:U:H5'	1.95	0.65
30:0:283:U:C5	30:0:284:C:C4	2.85	0.65
30:0:960:G:N3	30:0:960:G:C2'	2.59	0.65
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.37	0.65
30:0:1183:C:N3	30:0:1184:C:C5	2.65	0.65
30:0:1189:A:O2'	30:0:1208:C:H2'	1.96	0.65
2:B:212:GLN:HA	30:0:1733:A:H4'	1.79	0.65
16:P:59:ARG:HH22	16:P:66:GLN:NE2	1.94	0.65
30:0:1451:C:H5'	30:0:1505:U:C5	2.32	0.65
30:0:704:C:O2'	30:0:705:C:H5'	1.97	0.65
30:0:1058:A:H2'	30:0:1060:C:H5''	1.78	0.64
30:0:1925:G:O2'	30:0:1926:G:H5'	1.97	0.64
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.32	0.64
30:0:363:C:H1'	38:0:5312:HOH:O	1.97	0.64
4:D:103:ASN:ND2	4:D:134:LEU:H	1.95	0.64
30:0:2414:A:H2'	30:0:2415:A:C8	2.32	0.64
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.62	0.64
30:0:2505:G:O2'	30:0:2506:A:H5'	1.97	0.64
30:0:256:C:H2'	30:0:257:G:O4'	1.96	0.64
2:B:206:THR:HG21	30:0:2716:G:H5''	1.80	0.64
30:0:1189:A:H1'	30:0:1209:C:C1'	2.28	0.64
30:0:1441:G:O2'	30:0:1442:A:H5'	1.97	0.64
30:0:1741:U:O2'	30:0:2723:G:H4'	1.97	0.64
30:0:280:C:H2'	30:0:281:U:O4'	1.97	0.64
30:0:558:C:C2'	30:0:559:U:C5'	2.74	0.64
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.63	0.64
25:Y:204:ARG:HH22	30:0:553:G:P	2.21	0.64
3:C:184:ARG:NH2	30:0:450:C:OP1	2.30	0.64
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.78	0.64
23:W:125:HIS:HD2	23:W:127:GLY:H	1.46	0.64
30:0:297:U:H2'	30:0:298:C:H6	1.63	0.64
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.26	0.64
30:0:2769:C:H2'	30:0:2770:G:C5'	2.28	0.64
30:0:10:U:C3'	30:0:10:U:C6	2.80	0.63
30:0:1205:U:C2'	30:0:1206:U:H5''	2.28	0.63
30:0:2256:G:H2'	30:0:2257:G:C5'	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:HIS:CD2	1:A:201:PHE:H	2.15	0.63
30:0:1187:U:H2'	38:0:6939:HOH:O	1.98	0.63
29:3:65:THR:HG23	29:3:67:LEU:HG	1.79	0.63
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.81	0.63
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.79	0.63
30:0:2533:C:H6	30:0:2533:C:C5'	2.09	0.63
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.64	0.63
18:R:128:ARG:NH2	30:0:2054:A:N3	2.46	0.63
21:U:46:ALA:O	21:U:52:THR:HG21	1.98	0.63
24:X:71:ARG:HD3	38:X:2171:HOH:O	1.98	0.63
30:0:1120:U:H6	30:0:1120:U:H5''	1.63	0.63
30:0:1278:A:H4'	30:0:1279:U:C4	2.33	0.63
30:0:1878:G:O2'	30:0:1879:U:C6	2.49	0.63
31:9:75:G:H1	31:9:106:U:H3	1.47	0.63
13:M:27:ARG:NH2	13:M:44:THR:HG23	2.13	0.63
30:0:2524:G:H21	30:0:2526:C:N4	1.96	0.63
30:0:317:A:H4'	38:0:3791:HOH:O	1.98	0.63
9:I:110:ASP:O	30:0:1163:G:H5'	1.99	0.63
30:0:1835:U:C5	30:0:1840:A:N7	2.60	0.63
30:0:2509:A:H2'	30:0:2510:C:O4'	1.99	0.63
30:0:2649:A:H5'	30:0:2649:A:H8	1.64	0.63
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.81	0.63
2:B:264:GLU:HG3	2:B:302:PRO:HD3	1.79	0.63
2:B:162:MET:CE	2:B:308:LEU:HD21	2.27	0.63
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.64	0.63
30:0:2604:A:H5'	38:0:5822:HOH:O	1.99	0.62
31:9:54:A:O2'	31:9:55:U:H5'	1.98	0.62
30:0:2250:G:C2	30:0:2251:G:H1'	2.34	0.62
30:0:2256:G:H2'	30:0:2257:G:H5'	1.81	0.62
30:0:853:C:H3'	38:0:4580:HOH:O	2.00	0.62
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.96	0.62
23:W:13:MET:HE1	23:W:18:GLN:HA	1.81	0.62
15:O:73:ASP:HA	15:O:92:VAL:O	2.00	0.62
30:0:2421:G:H1'	38:0:7060:HOH:O	1.98	0.62
13:M:178:LYS:HB2	38:0:6916:HOH:O	1.99	0.62
8:H:168:VAL:HG13	38:H:211:HOH:O	1.98	0.62
30:0:1701:A:H5''	30:0:1702:U:H3'	1.82	0.62
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.81	0.62
30:0:1198:U:H1'	30:0:1201:C:H5	1.63	0.62
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.81	0.62
30:0:567:U:H5''	38:0:6435:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:16:HIS:HD2	30:0:470:U:O2'	1.83	0.62
27:1:20:ARG:HG2	30:0:111:C:O2'	2.00	0.62
31:9:2:U:P	31:9:3:A:H5'	2.40	0.62
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.82	0.62
7:G:64:ASN:N	7:G:64:ASN:HD22	1.96	0.62
30:0:1166:A:H61	30:0:1180:U:H3	1.46	0.62
30:0:2404:G:H5''	38:0:5241:HOH:O	2.00	0.62
29:3:48:ASN:HD21	30:0:2468:A:H61	1.47	0.62
30:0:2670:G:O2'	30:0:2671:U:H5'	1.99	0.62
30:0:960:G:H3'	30:0:960:G:N3	2.14	0.62
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.80	0.62
11:K:10:GLN:N	11:K:10:GLN:HE21	1.87	0.62
30:0:1170:U:H2'	30:0:1172:G:OP2	2.00	0.61
30:0:1314:U:H2'	38:0:5904:HOH:O	2.00	0.61
6:F:91:VAL:HG12	6:F:92:GLY:N	2.14	0.61
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.82	0.61
25:Y:216:ARG:HD2	38:Y:8865:HOH:O	2.00	0.61
30:0:848:C:H5'	38:0:7311:HOH:O	2.00	0.61
11:K:32:ILE:HD11	11:K:56:SER:HB2	1.82	0.61
30:0:958:G:O2'	30:0:959:C:H5'	2.00	0.61
30:0:2083:A:H3'	38:0:7616:HOH:O	1.99	0.61
30:0:2613:G:O2'	30:0:2614:C:H5'	2.00	0.61
30:0:506:G:H22	30:0:509:A:H5''	1.63	0.61
31:9:20:G:O2'	31:9:21:G:H5'	2.00	0.61
13:M:157:ASP:HB3	13:M:160:PHE:HD1	1.65	0.61
14:N:4:PRO:HG3	31:9:69:U:OP1	2.00	0.61
2:B:162:MET:HG3	2:B:310:ARG:HD3	1.83	0.61
23:W:88:THR:HG22	23:W:89:ASP:H	1.65	0.61
30:0:1679:C:H5'	38:0:9334:HOH:O	2.00	0.61
30:0:1759:A:N3	30:0:1818:C:H2'	2.16	0.61
31:9:64:C:C2'	31:9:65:A:H5'	2.30	0.61
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.82	0.61
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.83	0.61
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.81	0.61
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.83	0.61
30:0:1506:U:H6	30:0:1506:U:H5'	1.66	0.61
30:0:1641:A:H2'	30:0:1642:A:H5'	1.83	0.61
30:0:1948:G:H2'	30:0:1949:G:O4'	2.01	0.61
22:V:1:THR:HB	30:0:93:C:H5''	1.82	0.61
30:0:2787:C:H5	38:0:4664:HOH:O	1.83	0.61
27:1:10:LYS:HG3	38:1:2979:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:558:C:H2'	30:0:559:U:H5'	1.82	0.61
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.16	0.61
3:C:16:VAL:HG12	3:C:17:ASP:H	1.66	0.61
3:C:236:THR:HG21	38:C:8569:HOH:O	2.00	0.61
14:N:141:ARG:HH21	31:9:48:C:H4'	1.66	0.60
1:A:36:ASP:CB	1:A:85:SER:H	2.14	0.60
30:0:2505:G:C2'	30:0:2506:A:H5'	2.31	0.60
23:W:84:VAL:HG12	38:W:6679:HOH:O	2.01	0.60
30:0:2637:A:H4'	38:0:6094:HOH:O	2.00	0.60
30:0:936:C:H5	38:0:5991:HOH:O	1.82	0.60
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.82	0.60
14:N:40:ASN:ND2	31:9:28:U:H5''	2.16	0.60
30:0:1515:A:H2'	30:0:1516:U:C6	2.37	0.60
30:0:236:A:H4'	30:0:237:G:OP1	2.01	0.60
38:B:9109:HOH:O	30:0:2672:C:H1'	2.02	0.60
30:0:542:A:H5'	30:0:542:A:C8	2.28	0.60
30:0:836:G:H5''	38:0:9288:HOH:O	1.99	0.60
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.84	0.60
23:W:88:THR:HG22	23:W:89:ASP:N	2.17	0.60
4:D:57:THR:HG23	4:D:63:ILE:HA	1.82	0.60
11:K:27:ARG:HD2	38:K:4747:HOH:O	2.01	0.60
30:0:1080:C:O5'	30:0:1080:C:H6	1.85	0.60
30:0:2563:U:H2'	30:0:2565:C:O5'	2.01	0.60
30:0:702:G:O2'	30:0:703:G:H5'	2.02	0.60
10:J:41:ALA:HB3	38:J:5907:HOH:O	2.00	0.60
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.84	0.60
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.84	0.60
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	1.84	0.60
30:0:2089:A:O2'	30:0:2090:G:H5'	2.02	0.60
31:9:3:A:N6	31:9:22:G:H1'	2.16	0.60
30:0:2419:U:H5''	30:0:2420:G:H5'	1.83	0.59
6:F:101:ALA:HA	38:F:5413:HOH:O	2.02	0.59
8:H:102:LYS:HD3	8:H:122:LYS:HD3	1.83	0.59
30:0:368:C:H2'	30:0:369:G:H5'	1.84	0.59
9:I:87:PRO:HB3	38:I:6825:HOH:O	2.02	0.59
30:0:567:U:H5''	38:0:5320:HOH:O	2.02	0.59
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.83	0.59
13:M:80:GLY:O	13:M:81:ARG:HD3	2.01	0.59
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.32	0.59
30:0:1132:A:N6	30:0:1229:C:H2'	2.17	0.59
30:0:1790:C:H2'	30:0:1791:U:H6	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2329:C:O2'	30:0:2330:U:H5'	2.01	0.59
30:0:271:C:H41	30:0:378:A:H2	1.47	0.59
38:Z:8706:HOH:O	30:0:1886:A:H4'	2.03	0.59
30:0:2237:G:H1'	38:0:4887:HOH:O	2.02	0.59
2:B:254:GLN:HG3	38:0:9714:HOH:O	2.01	0.59
8:H:49:GLN:NE2	8:H:140:TYR:HE2	1.95	0.59
8:H:29:SER:HA	8:H:62:HIS:HD2	1.68	0.59
30:0:2718:C:H6	30:0:2718:C:H5'	1.68	0.59
30:0:119:A:H2'	30:0:120:A:H5''	1.83	0.59
30:0:1377:C:H6	30:0:1377:C:H5'	1.68	0.59
30:0:1595:G:O2'	30:0:1596:U:H5'	2.03	0.59
1:A:33:GLU:CD	1:A:33:GLU:H	2.04	0.59
3:C:236:THR:CG2	3:C:239:ALA:H	2.11	0.59
8:H:174:LEU:HA	38:H:222:HOH:O	2.02	0.59
9:I:108:HIS:H	9:I:109:PRO:HD2	1.66	0.59
18:R:39:THR:HG23	18:R:107:GLU:O	2.02	0.59
30:0:2344:G:N3	30:0:2344:G:H2'	2.17	0.59
30:0:2756:U:H3	30:0:2896:A:H2	1.43	0.59
30:0:308:U:C4	30:0:342:C:H1'	2.38	0.59
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.32	0.59
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.37	0.59
1:A:48:ASP:HB3	38:A:9060:HOH:O	2.03	0.59
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.85	0.59
7:G:16:LYS:O	7:G:20:VAL:HG23	2.03	0.59
23:W:125:HIS:CD2	23:W:127:GLY:H	2.21	0.59
31:9:64:C:H2'	31:9:65:A:H5'	1.84	0.59
7:G:12:ILE:HG23	38:0:5490:HOH:O	2.03	0.59
38:C:8655:HOH:O	30:0:2100:A:H5'	2.03	0.58
30:0:2812:A:H2	30:0:2814:A:N6	1.87	0.58
30:0:468:U:H3'	38:0:7607:HOH:O	2.03	0.58
31:9:24:U:H3'	31:9:25:G:C5'	2.32	0.58
2:B:248:ARG:O	2:B:251:VAL:HG13	2.03	0.58
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.85	0.58
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.04	0.58
30:0:2534:C:H1'	38:0:3513:HOH:O	2.01	0.58
1:A:171:LYS:HB2	30:0:820:G:C6	2.37	0.58
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.67	0.58
28:2:38:LYS:HE3	38:0:4254:HOH:O	2.01	0.58
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.85	0.58
30:0:1603:A:H5'	30:0:1605:G:C4'	2.33	0.58
30:0:1972:U:H2'	30:0:1973:A:C5'	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.03	0.58
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.19	0.58
30:0:1304:U:H2'	30:0:1305:C:C6	2.39	0.58
30:0:2252:A:C5	30:0:2253:G:H1'	2.38	0.58
30:0:2649:A:H5'	30:0:2649:A:C8	2.39	0.58
1:A:36:ASP:HB2	1:A:85:SER:H	1.68	0.58
16:P:115:SER:OG	16:P:118:GLN:HG3	2.03	0.58
28:2:10:ARG:NH2	30:0:121:U:OP2	2.32	0.58
30:0:407:A:H5'	38:0:6057:HOH:O	2.04	0.58
4:D:103:ASN:HD22	4:D:134:LEU:H	1.49	0.58
30:0:660:A:H4'	30:0:661:G:O5'	2.04	0.58
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.34	0.58
30:0:2346:C:O5'	30:0:2346:C:H6	1.86	0.58
30:0:441:A:H1'	30:0:442:A:N7	2.19	0.58
2:B:238:ASN:HD22	2:B:240:GLY:N	1.96	0.58
23:W:139:GLY:O	23:W:141:HIS:HD2	1.87	0.58
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.85	0.58
30:0:1819:G:H5'	38:0:5847:HOH:O	2.04	0.57
17:Q:11:ARG:HG3	30:0:2363:G:O2'	2.04	0.57
12:L:145:LEU:O	12:L:148:GLU:HG3	2.03	0.57
30:0:1477:C:H5'	30:0:1868:G:C5'	2.34	0.57
30:0:192:A:H5'	38:0:7682:HOH:O	2.03	0.57
30:0:567:U:C5'	38:0:6435:HOH:O	2.52	0.57
30:0:947:U:H2'	30:0:948:G:C8	2.39	0.57
30:0:228:C:H2'	30:0:229:G:H5'	1.86	0.57
30:0:644:G:N3	30:0:644:G:H5'	2.19	0.57
30:0:88:G:H2'	30:0:89:G:C8	2.39	0.57
3:C:79:ARG:O	3:C:87:ARG:HG2	2.04	0.57
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.86	0.57
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.03	0.57
22:V:39:ALA:N	22:V:40:PRO:HD2	2.19	0.57
30:0:711:G:C2	30:0:718:C:C2	2.92	0.57
31:9:1:U:O3'	31:9:3:A:H5'	2.03	0.57
30:0:2894:C:O2'	30:0:2895:C:H5'	2.05	0.57
30:0:1183:C:C2	30:0:1184:C:C5	2.93	0.57
30:0:1592:G:H2'	30:0:1593:C:H6	1.69	0.57
30:0:1714:C:O2'	30:0:1715:C:H5'	2.05	0.57
30:0:512:G:O3'	30:0:513:A:H8	1.87	0.57
1:A:51:ARG:HB2	38:A:9060:HOH:O	2.04	0.57
24:X:25:ARG:HD3	24:X:64:ALA:O	2.05	0.57
30:0:2372:A:H2'	30:0:2373:U:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:68:HIS:O	30:0:2842:G:H5'	2.05	0.57
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.86	0.57
12:L:41:HIS:HD2	30:0:926:A:O2'	1.88	0.57
30:0:1768:C:H2'	30:0:1769:C:O4'	2.05	0.57
30:0:1942:A:H5'	38:0:7386:HOH:O	2.05	0.57
30:0:396:U:O2'	30:0:418:C:H4'	2.04	0.57
30:0:541:C:H2'	30:0:542:A:H5'	1.87	0.57
30:0:1477:C:O2'	30:0:1478:U:H5'	2.05	0.56
31:9:49:G:H5''	38:9:9090:HOH:O	2.05	0.56
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.87	0.56
10:J:74:ARG:NH1	10:J:144:THR:HG21	2.20	0.56
18:R:117:HIS:HD2	30:0:20:G:H21	1.53	0.56
30:0:2269:C:H2'	30:0:2270:G:H5'	1.86	0.56
30:0:2320:U:H4'	30:0:2321:A:O4'	2.04	0.56
30:0:283:U:C5	30:0:284:C:N3	2.73	0.56
30:0:366:U:H2'	30:0:367:G:O4'	2.05	0.56
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.87	0.56
30:0:2005:G:H3'	30:0:2005:G:OP2	2.06	0.56
30:0:2668:G:H2'	30:0:2669:U:C6	2.40	0.56
30:0:485:A:N3	30:0:487:G:H5''	2.20	0.56
31:9:1:U:O3'	31:9:3:A:C5'	2.53	0.56
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.87	0.56
30:0:255:A:H2'	30:0:256:C:H6	1.71	0.56
30:0:542:A:H2'	30:0:543:G:O4'	2.05	0.56
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.86	0.56
31:9:12:C:H5'	31:9:70:U:O4'	2.04	0.56
2:B:71:VAL:HG21	2:B:296:LEU:HB3	1.87	0.56
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.70	0.56
30:0:319:A:H4'	30:0:338:C:C4	2.40	0.56
12:L:134:GLU:HG3	38:L:8854:HOH:O	2.06	0.56
23:W:44:MET:CE	30:0:944:G:H21	2.19	0.56
30:0:1206:U:C5'	30:0:1206:U:H6	2.15	0.56
3:C:63:SER:OG	30:0:2101:A:H2'	2.05	0.56
10:J:74:ARG:HH12	10:J:144:THR:HG21	1.71	0.56
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.71	0.56
30:0:2472:C:O2'	30:0:2634:G:H4'	2.05	0.56
30:0:2880:A:H2'	30:0:2881:C:H5'	1.88	0.56
30:0:363:C:H2'	30:0:364:U:H6	1.69	0.56
31:9:114:G:H2'	31:9:115:C:C6	2.41	0.56
31:9:76:G:C3'	31:9:77:A:H5''	2.28	0.56
2:B:145:HIS:HD2	2:B:146:THR:O	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:143:THR:HG22	12:L:144:ASP:H	1.71	0.56
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.79	0.56
30:0:2002:C:H2'	30:0:2003:U:H5'	1.87	0.56
29:3:70:ARG:HB3	38:3:9064:HOH:O	2.06	0.56
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.41	0.56
30:0:1213:C:O2'	30:0:1214:G:H5'	2.06	0.56
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.41	0.56
27:1:9:GLY:HA2	30:0:1687:C:O2	2.05	0.56
30:0:2064:U:H5'	30:0:2652:U:H4'	1.87	0.56
27:1:28:HIS:HE1	30:0:776:A:OP1	1.89	0.56
2:B:17:LYS:O	2:B:260:HIS:HD2	1.88	0.56
30:0:583:C:H2'	30:0:584:U:H6	1.70	0.56
7:G:20:VAL:O	7:G:24:VAL:HG23	2.06	0.56
30:0:1209:C:H2'	30:0:1210:G:C8	2.36	0.55
30:0:681:G:N3	30:0:681:G:H5'	2.21	0.55
30:0:834:G:H4'	30:0:835:U:OP2	2.05	0.55
14:N:164:ASP:CG	14:N:167:ASP:HA	2.26	0.55
30:0:1766:U:O2	30:0:1778:A:H5'	2.06	0.55
30:0:2316:G:H4'	38:0:6125:HOH:O	2.05	0.55
30:0:1904:A:H2'	30:0:1905:U:O4'	2.05	0.55
30:0:2269:C:C2'	30:0:2270:G:H5'	2.36	0.55
30:0:281:U:O2'	30:0:282:C:H5'	2.06	0.55
30:0:283:U:H5	30:0:284:C:N3	2.04	0.55
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.89	0.55
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.07	0.55
30:0:1676:G:O2'	30:0:1677:U:H5'	2.06	0.55
30:0:1834:C:H2'	30:0:1840:A:N6	2.20	0.55
30:0:236:A:C4'	30:0:237:G:H5'	2.36	0.55
30:0:65:C:O2'	30:0:66:G:H5'	2.06	0.55
30:0:1973:A:H5'	30:0:1973:A:C8	2.39	0.55
2:B:125:GLU:O	2:B:129:ARG:HG3	2.06	0.55
30:0:249:G:H2'	30:0:250:C:H6	1.71	0.55
30:0:2748:G:H1'	38:0:7936:HOH:O	2.05	0.55
30:0:2756:U:N3	30:0:2896:A:C2	2.71	0.55
31:9:22:G:H5'	31:9:23:U:OP1	2.06	0.55
12:L:18:HIS:HD2	30:0:902:G:N7	2.05	0.55
14:N:80:SER:HB2	38:N:8833:HOH:O	2.07	0.55
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	1.89	0.55
30:0:1592:G:H2'	30:0:1593:C:C6	2.42	0.55
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.89	0.55
5:E:11:VAL:HG12	5:E:12:ASP:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2748:G:H2'	38:0:7579:HOH:O	2.06	0.55
30:0:282:C:C2'	30:0:283:U:H5'	2.35	0.55
15:O:37:ARG:HD2	30:0:656:G:OP2	2.07	0.55
31:9:49:G:C2'	31:9:50:G:H5'	2.37	0.55
26:Z:40:ALA:HA	30:0:1773:G:C8	2.41	0.55
30:0:1200:A:H3'	38:0:5786:HOH:O	2.06	0.55
12:L:41:HIS:CD2	30:0:926:A:O2'	2.60	0.55
14:N:37:ARG:NH1	31:9:6:C:OP1	2.39	0.55
30:0:2768:A:H5''	38:0:4453:HOH:O	2.07	0.55
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.89	0.55
15:O:35:LYS:HD3	38:0:4645:HOH:O	2.06	0.55
13:M:163:LEU:HD21	30:0:188:C:H5''	1.89	0.54
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.37	0.54
30:0:1157:C:H2'	30:0:1158:G:C8	2.40	0.54
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.07	0.54
30:0:2064:U:H5'	30:0:2652:U:O3'	2.08	0.54
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.05	0.54
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.42	0.54
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.89	0.54
30:0:1165:G:O2'	30:0:1174:A:C1'	2.54	0.54
30:0:1681:G:H5''	30:0:1682:A:H5'	1.88	0.54
30:0:1819:G:H2'	30:0:1820:G:C4'	2.38	0.54
30:0:1878:G:O2'	30:0:1879:U:P	2.66	0.54
14:N:110:THR:HB	14:N:113:SER:OG	2.08	0.54
38:I:1549:HOH:O	30:0:1180:U:H1'	2.07	0.54
30:0:350:G:H1'	38:0:5705:HOH:O	2.06	0.54
31:9:47:A:C2	31:9:48:C:C2	2.94	0.54
2:B:177:HIS:O	2:B:181:ILE:HG13	2.07	0.54
5:E:132:THR:HB	38:E:2227:HOH:O	2.07	0.54
30:0:363:C:O2'	30:0:364:U:H5'	2.07	0.54
29:3:73:GLU:HB3	38:3:9053:HOH:O	2.08	0.54
31:9:23:U:O2'	31:9:24:U:H4'	2.07	0.54
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.89	0.54
18:R:99:ALA:HB1	18:R:109:MET:CE	2.37	0.54
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.90	0.54
30:0:1947:G:H2'	30:0:1948:G:H8	1.73	0.54
30:0:661:G:C5	30:0:686:A:C2	2.96	0.54
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.08	0.54
8:H:69:ARG:HD3	38:H:231:HOH:O	2.07	0.54
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.73	0.54
30:0:1193:A:H2	30:0:1194:A:N6	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1559:A:H4'	38:0:5895:HOH:O	2.07	0.54
30:0:1594:C:O2'	30:0:1607:A:H4'	2.08	0.54
30:0:1755:A:H2'	30:0:1756:G:O4'	2.07	0.54
30:0:1842:A:C4	30:0:1979:G:C6	2.95	0.54
30:0:2135:A:O2'	30:0:2136:G:H5'	2.06	0.54
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.89	0.54
31:9:3:A:H2	31:9:21:G:N3	2.06	0.54
9:I:126:THR:O	9:I:130:LEU:HG	2.08	0.54
23:W:130:HIS:O	23:W:136:GLY:HA3	2.08	0.54
30:0:2415:A:H2'	30:0:2416:G:H5'	1.88	0.54
30:0:2505:G:H2'	30:0:2506:A:H5'	1.89	0.54
30:0:2507:G:H2'	30:0:2510:C:N4	2.23	0.54
30:0:2781:U:C2'	30:0:2782:G:H5'	2.37	0.54
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.54
4:D:138:GLY:HA2	31:9:29:C:O3'	2.08	0.54
30:0:1878:G:O2'	30:0:1879:U:H6	1.89	0.54
30:0:877:G:C5'	30:0:878:G:OP1	2.53	0.54
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.90	0.54
16:P:58:SER:HB3	38:0:5659:HOH:O	2.08	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.08	0.54
30:0:1535:G:H2'	30:0:1536:C:C6	2.43	0.54
30:0:10:U:O4	30:0:531:G:H2'	2.08	0.54
30:0:2073:G:OP2	30:0:2490:A:H5'	2.08	0.53
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.73	0.53
14:N:160:SER:HB2	31:9:51:A:H5'	1.90	0.53
30:0:407:A:H3'	38:0:4486:HOH:O	2.08	0.53
31:9:49:G:H2'	31:9:50:G:O4'	2.09	0.53
2:B:198:GLU:HA	38:B:9133:HOH:O	2.07	0.53
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.90	0.53
30:0:1130:U:H2'	30:0:1131:G:O4'	2.08	0.53
30:0:2371:G:H5'	38:0:5041:HOH:O	2.08	0.53
30:0:2502:C:H2'	30:0:2503:A:C5'	2.37	0.53
20:T:2:LYS:HG2	30:0:447:A:OP1	2.08	0.53
30:0:24:G:N2	30:0:518:G:H1'	2.23	0.53
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.38	0.53
10:J:19:MET:CE	10:J:132:LEU:HD11	2.39	0.53
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.09	0.53
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.39	0.53
30:0:1819:G:H2'	30:0:1820:G:C5'	2.38	0.53
30:0:1850:U:H2'	30:0:1851:G:H8	1.73	0.53
30:0:2756:U:N3	30:0:2896:A:H2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:953:G:H4'	30:0:954:U:OP1	2.08	0.53
5:E:137:ASP:O	5:E:141:VAL:HG23	2.08	0.53
17:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.08	0.53
30:0:2783:A:H2'	30:0:2784:A:C8	2.44	0.53
2:B:294:TYR:HE2	38:B:9124:HOH:O	1.89	0.53
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.09	0.53
30:0:1333:U:H2'	30:0:1334:C:C6	2.44	0.53
30:0:138:U:OP2	30:0:139:C:H5	1.91	0.53
30:0:1523:G:C6	30:0:1524:U:C4	2.96	0.53
30:0:1787:C:H4'	30:0:2883:A:O4'	2.08	0.53
30:0:368:C:C2'	30:0:369:G:H5'	2.39	0.53
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.91	0.53
31:9:2:U:H4'	38:9:9103:HOH:O	2.08	0.53
21:U:17:THR:HG22	21:U:18:GLY:N	2.24	0.53
30:0:2249:G:C2	30:0:2253:G:C6	2.96	0.53
30:0:67:A:H5''	30:0:69:A:C8	2.44	0.53
30:0:947:U:H2'	30:0:948:G:H8	1.72	0.53
31:9:39:U:O2'	31:9:42:C:C5	2.61	0.53
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.90	0.53
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.90	0.53
21:U:14:GLU:O	21:U:17:THR:HB	2.08	0.53
30:0:1206:U:H2'	30:0:1207:A:O4'	2.09	0.53
30:0:123:U:H5'	38:0:6694:HOH:O	2.09	0.53
30:0:1556:G:O2'	30:0:1557:G:H5'	2.09	0.53
30:0:2597:U:H2'	30:0:2598:U:H5'	1.90	0.53
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.90	0.53
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.39	0.53
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.88	0.53
30:0:2897:C:O2'	30:0:2898:G:H5'	2.09	0.53
30:0:960:G:C3'	30:0:960:G:N3	2.72	0.53
3:C:5:ILE:HD11	3:C:16:VAL:CG2	2.39	0.53
13:M:57:LYS:HE2	13:M:140:ALA:O	2.09	0.53
30:0:1206:U:C6	30:0:1206:U:H5'	2.32	0.53
30:0:876:A:N3	30:0:876:A:H2'	2.23	0.53
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.23	0.53
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.39	0.53
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.23	0.53
30:0:1524:U:OP1	30:0:1524:U:H4'	2.09	0.52
30:0:2781:U:O2'	30:0:2782:G:H5'	2.07	0.52
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.91	0.52
23:W:80:ASP:O	23:W:84:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.91	0.52
30:0:1702:U:H1'	38:0:5805:HOH:O	2.08	0.52
30:0:2314:G:C2'	30:0:2315:C:H5'	2.39	0.52
30:0:241:A:C2	30:0:378:A:H4'	2.44	0.52
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.90	0.52
12:L:4:LYS:HE2	30:0:645:U:OP2	2.09	0.52
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.12	0.52
18:R:150:PRO:CG	18:R:150:PRO:CB	2.86	0.52
30:0:1174:A:C6	30:0:1201:C:H4'	2.45	0.52
30:0:1377:C:H5'	30:0:1377:C:C6	2.45	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.90	0.52
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.92	0.52
4:D:159:PRO:O	4:D:163:VAL:HG23	2.09	0.52
13:M:30:GLU:O	13:M:34:GLU:HG3	2.10	0.52
30:0:113:A:OP2	30:0:114:A:H2'	2.09	0.52
30:0:2478:U:O2'	30:0:2479:A:H5'	2.08	0.52
3:C:153:VAL:O	3:C:157:LEU:HG	2.09	0.52
4:D:50:VAL:HG13	31:9:41:C:O4'	2.10	0.52
17:Q:25:PRO:HB2	38:9:9082:HOH:O	2.10	0.52
19:S:43:GLU:HB3	38:S:8991:HOH:O	2.10	0.52
30:0:1135:G:H5'	38:0:5960:HOH:O	2.09	0.52
28:2:39:ARG:HG2	38:2:3143:HOH:O	2.08	0.52
12:L:143:THR:HG22	12:L:144:ASP:N	2.25	0.52
20:T:38:ARG:NH1	38:0:6725:HOH:O	2.42	0.52
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.45	0.52
30:0:2105:C:H2'	30:0:2106:C:C6	2.44	0.52
30:0:2250:G:H2'	30:0:2251:G:O4'	2.09	0.52
30:0:2664:A:OP1	30:0:2664:A:H8	1.93	0.52
30:0:2681:A:H4'	30:0:2682:C:C5'	2.39	0.52
30:0:602:A:O2'	30:0:605:C:H4'	2.09	0.52
1:A:36:ASP:HB2	1:A:84:VAL:N	2.25	0.52
4:D:138:GLY:N	38:D:7597:HOH:O	2.42	0.52
8:H:48:VAL:HA	8:H:170:ARG:O	2.10	0.52
30:0:2509:A:OP2	30:0:2510:C:H5	1.93	0.52
30:0:1444:G:O2'	30:0:1445:G:H5'	2.09	0.52
30:0:1921:A:C6	30:0:1922:A:C2	2.98	0.52
30:0:1930:A:H2'	30:0:1931:A:C8	2.45	0.52
30:0:968:G:O2'	30:0:969:G:H5'	2.10	0.52
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.91	0.52
30:0:1279:U:O2	30:0:1279:U:C2'	2.58	0.52
30:0:1289:C:O2'	30:0:1290:G:H5'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:12:U:H2'	30:0:13:G:H5'	1.91	0.52
30:0:1805:G:O2'	30:0:1806:G:H5'	2.10	0.52
30:0:2237:G:O2'	30:0:2238:A:C8	2.62	0.52
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.10	0.52
30:0:2878:U:H2'	30:0:2879:A:O4'	2.10	0.52
30:0:704:C:H2'	30:0:705:C:H6	1.75	0.52
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.10	0.52
30:0:1130:U:H5'	38:0:7710:HOH:O	2.10	0.51
30:0:1188:A:C6	30:0:1189:A:C6	2.99	0.51
30:0:185:G:H4'	30:0:186:A:OP1	2.10	0.51
30:0:200:C:H2'	38:0:3463:HOH:O	2.09	0.51
30:0:2531:U:O2'	30:0:2532:A:H5'	2.10	0.51
13:M:179:GLY:O	30:0:399:C:H5'	2.10	0.51
31:9:24:U:H3'	31:9:25:G:H5'	1.91	0.51
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.91	0.51
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.92	0.51
23:W:64:THR:O	23:W:68:THR:HG22	2.10	0.51
30:0:2250:G:N2	30:0:2251:G:H1'	2.25	0.51
30:0:2830:U:O2'	30:0:2831:C:H5'	2.09	0.51
30:0:299:U:H5'	38:0:7375:HOH:O	2.09	0.51
2:B:148:PRO:HD2	38:B:9049:HOH:O	2.10	0.51
6:F:57:GLU:O	6:F:61:MET:HG3	2.10	0.51
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.26	0.51
22:V:12:THR:HG23	22:V:14:ALA:H	1.75	0.51
23:W:119:HIS:HD2	23:W:120:PRO:O	1.92	0.51
30:0:10:U:O4	30:0:532:A:OP2	2.28	0.51
30:0:1762:C:O2'	30:0:1763:C:H5'	2.10	0.51
30:0:363:C:H2'	30:0:364:U:C6	2.46	0.51
30:0:541:C:O2'	30:0:542:A:H5''	2.11	0.51
31:9:39:U:O2'	31:9:42:C:H5	1.92	0.51
3:C:145:GLU:HG3	38:C:8569:HOH:O	2.09	0.51
23:W:24:LEU:O	23:W:26:ILE:HG22	2.10	0.51
30:0:2252:A:H2'	30:0:2253:G:H5'	1.92	0.51
30:0:228:C:C2'	30:0:229:G:H5'	2.41	0.51
30:0:2825:C:H4'	30:0:2826:G:O5'	2.10	0.51
30:0:285:A:H2'	30:0:286:U:O4'	2.10	0.51
31:9:1:U:C4'	31:9:3:A:OP1	2.59	0.51
2:B:211:THR:HG21	38:0:7492:HOH:O	2.11	0.51
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.92	0.51
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.92	0.51
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1386:G:O2'	30:0:1387:G:H5'	2.11	0.51
30:0:414:C:H5'	38:0:9667:HOH:O	2.11	0.51
30:0:958:G:H2'	30:0:959:C:C6	2.45	0.51
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.44	0.51
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.93	0.51
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.93	0.51
30:0:1205:U:O2'	30:0:1206:U:H5''	2.11	0.51
30:0:2421:G:H3'	30:0:2422:U:H5''	1.92	0.51
30:0:2781:U:H2'	30:0:2782:G:C5'	2.40	0.51
30:0:2826:G:C6	30:0:2913:A:N6	2.78	0.51
30:0:69:A:H8	30:0:69:A:C5'	2.15	0.51
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.11	0.51
25:Y:189:ASN:HD22	25:Y:189:ASN:C	2.14	0.51
30:0:1398:G:O2'	30:0:1399:A:H5'	2.11	0.51
30:0:2241:C:O2'	30:0:2242:U:H5'	2.11	0.51
30:0:541:C:C2'	30:0:542:A:C5'	2.79	0.51
30:0:790:A:H2'	30:0:791:A:O4'	2.10	0.51
31:9:91:C:H2'	31:9:92:G:O4'	2.10	0.51
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.79	0.51
24:X:23:HIS:HD2	38:0:9973:HOH:O	1.93	0.51
12:L:14:GLY:O	30:0:1295:G:H5''	2.11	0.51
30:0:2764:C:O2'	30:0:2765:C:H5'	2.10	0.51
30:0:2781:U:H2'	30:0:2782:G:H5'	1.92	0.51
30:0:282:C:O2'	30:0:283:U:C5'	2.50	0.51
30:0:346:U:H4'	38:0:6884:HOH:O	2.11	0.51
2:B:256:GLN:HG2	38:B:9132:HOH:O	2.11	0.51
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.59	0.51
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.41	0.51
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.93	0.51
19:S:33:SER:O	19:S:37:VAL:HG23	2.11	0.51
30:0:2251:G:H2'	30:0:2252:A:H8	1.72	0.51
30:0:952:G:N3	30:0:2302:A:H2'	2.26	0.51
29:3:15:ASN:O	30:0:2408:A:H4'	2.11	0.51
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.93	0.51
30:0:1419:U:H2'	30:0:1685:A:C2	2.46	0.51
2:B:41:PHE:HA	2:B:79:MET:HE2	1.92	0.51
3:C:233:THR:HG22	3:C:234:VAL:N	2.26	0.51
25:Y:184:GLU:OE2	25:Y:204:ARG:HD2	2.11	0.51
30:0:120:A:H2'	30:0:120:A:N3	2.27	0.50
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.76	0.50
30:0:1167:G:H2'	30:0:1168:C:C6	2.46	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	2.79	0.50
30:0:249:G:H2'	30:0:250:C:C6	2.46	0.50
30:0:289:G:O2'	30:0:290:C:H5'	2.12	0.50
30:0:383:A:H4'	38:0:5359:HOH:O	2.10	0.50
30:0:683:G:O2'	30:0:684:G:H5'	2.11	0.50
2:B:85:ARG:NH1	38:B:9109:HOH:O	2.44	0.50
22:V:56:ILE:O	22:V:60:GLN:HG3	2.11	0.50
30:0:1183:C:O2	30:0:1183:C:H2'	2.10	0.50
30:0:1202:A:C2'	30:0:1203:G:H5'	2.40	0.50
30:0:1494:A:H1'	30:0:1495:C:C6	2.47	0.50
30:0:1557:G:O2'	30:0:1558:C:H5'	2.11	0.50
30:0:1972:U:C2'	30:0:1973:A:H5''	2.41	0.50
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.45	0.50
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.94	0.50
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.94	0.50
30:0:1183:C:H42	30:0:1184:C:N4	2.05	0.50
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.12	0.50
30:0:559:U:C5'	30:0:559:U:H6	2.20	0.50
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.27	0.50
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.94	0.50
15:O:39:THR:O	15:O:115:ARG:NH2	2.44	0.50
22:V:44:GLY:O	22:V:48:GLU:HG2	2.12	0.50
11:K:66:ARG:HH22	30:0:1994:A:P	2.35	0.50
30:0:2610:U:H4'	38:0:9491:HOH:O	2.12	0.50
30:0:69:A:C8	30:0:69:A:C5'	2.89	0.50
30:0:858:U:H5	38:0:5459:HOH:O	1.93	0.50
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.95	0.50
30:0:95:A:H5''	30:0:97:G:O4'	2.11	0.50
1:A:135:VAL:HA	1:A:150:PRO:HD3	1.93	0.50
5:E:7:ILE:HG13	5:E:11:VAL:HB	1.93	0.50
8:H:66:GLU:HA	38:H:231:HOH:O	2.11	0.50
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.94	0.50
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.11	0.50
30:0:1588:G:C6	30:0:1589:G:N1	2.80	0.50
30:0:1795:G:H2'	30:0:1796:A:O4'	2.12	0.50
30:0:1878:G:C1'	38:0:6153:HOH:O	2.47	0.50
27:1:16:HIS:HE1	30:0:775:G:OP1	1.94	0.50
31:9:13:A:O2'	31:9:14:G:H5''	2.12	0.50
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.47	0.50
10:J:42:GLU:O	10:J:131:THR:HG23	2.12	0.50
24:X:61:ARG:NH1	24:X:67:PRO:HD3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1118:A:H8	30:0:1119:G:H5''	1.76	0.50
30:0:2421:G:H3'	30:0:2422:U:C5'	2.42	0.50
5:E:143:GLN:HE22	30:0:2779:G:H21	1.55	0.50
30:0:2793:A:N6	38:0:5912:HOH:O	2.44	0.50
30:0:2883:A:H2'	30:0:2884:G:O4'	2.12	0.50
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.47	0.50
18:R:111:ILE:HG23	18:R:145:LEU:CD1	2.41	0.50
23:W:149:LEU:HG	23:W:153:MET:CE	2.41	0.50
23:W:65:VAL:HG12	23:W:116:LEU:HD13	1.94	0.50
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.30	0.50
30:0:912:A:C4	30:0:1294:A:C2	2.99	0.50
30:0:154:C:H2'	30:0:155:C:H6	1.76	0.50
30:0:1667:A:H2'	30:0:1668:U:C6	2.47	0.50
30:0:264:G:H1'	30:0:265:U:H5	1.77	0.50
31:9:36:C:C5	31:9:37:C:C5	3.00	0.50
2:B:310:ARG:HD2	38:B:9122:HOH:O	2.12	0.50
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.93	0.50
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.93	0.50
14:N:132:ASN:O	14:N:135:VAL:HG12	2.12	0.50
23:W:139:GLY:O	23:W:141:HIS:CD2	2.64	0.50
30:0:2820:A:H2'	30:0:2821:C:C6	2.47	0.50
30:0:2896:A:N3	30:0:2896:A:H2'	2.27	0.50
30:0:79:G:H22	30:0:97:G:H1'	1.77	0.50
30:0:79:G:N2	30:0:97:G:H1'	2.27	0.50
30:0:968:G:C2	30:0:1001:U:O2	2.65	0.50
30:0:969:G:H1	30:0:999:C:N4	2.10	0.50
1:A:35:GLY:O	1:A:36:ASP:HB3	2.12	0.50
5:E:69:ILE:HA	5:E:72:MET:CE	2.41	0.50
5:E:84:MET:HB2	5:E:131:LEU:HB2	1.94	0.50
8:H:123:ILE:HD12	8:H:123:ILE:N	2.27	0.50
30:0:1149:U:H5''	30:0:1151:G:O4'	2.12	0.49
30:0:1644:C:H2'	30:0:1645:U:H6	1.77	0.49
30:0:1848:G:O2'	30:0:1849:G:H5'	2.12	0.49
30:0:2010:A:C2'	38:0:5990:HOH:O	2.56	0.49
4:D:52:THR:HG21	30:0:2347:C:H5'	1.94	0.49
30:0:2577:A:H8	38:0:9613:HOH:O	1.95	0.49
30:0:886:A:OP2	30:0:2113:G:H5'	2.11	0.49
30:0:941:G:C5	30:0:942:U:C4	3.00	0.49
31:9:95:C:O2'	31:9:96:C:H5'	2.12	0.49
19:S:76:GLU:HB3	38:S:8992:HOH:O	2.11	0.49
22:V:39:ALA:H	22:V:40:PRO:HD2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2256:G:C2'	30:0:2257:G:C5'	2.89	0.49
30:0:2793:A:H2'	30:0:2794:G:H5'	1.94	0.49
29:3:60:LYS:HG3	38:0:7595:HOH:O	2.12	0.49
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.77	0.49
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.94	0.49
2:B:254:GLN:HG2	2:B:255:GLY:N	2.27	0.49
3:C:236:THR:HA	38:C:8644:HOH:O	2.12	0.49
4:D:103:ASN:ND2	4:D:133:ASN:HD22	2.10	0.49
14:N:37:ARG:NH2	38:N:8831:HOH:O	2.45	0.49
16:P:41:ARG:HH22	30:0:1500:U:P	2.35	0.49
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.11	0.49
30:0:2092:G:H2'	30:0:2613:G:OP1	2.13	0.49
10:J:131:THR:HB	10:J:134:GLU:HG3	1.95	0.49
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.13	0.49
25:Y:154:ARG:NH1	25:Y:155:ARG:HG3	2.28	0.49
30:0:1972:U:H2'	30:0:1973:A:H5''	1.92	0.49
30:0:2724:U:H2'	30:0:2725:G:O4'	2.12	0.49
30:0:2851:G:H2'	30:0:2852:A:H5'	1.91	0.49
30:0:301:C:O2'	30:0:302:A:H5'	2.13	0.49
3:C:43:LYS:HG2	30:0:449:A:N7	2.28	0.49
1:A:51:ARG:NH1	1:A:120:ARG:O	2.46	0.49
2:B:54:VAL:HB	38:B:9087:HOH:O	2.11	0.49
30:0:1198:U:C6	30:0:1200:A:OP2	2.65	0.49
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.93	0.49
20:T:54:ASP:OD2	30:0:316:A:H5'	2.12	0.49
30:0:671:A:O2'	30:0:672:G:H2'	2.13	0.49
31:9:39:U:HO2'	31:9:42:C:H5	1.52	0.49
2:B:26:PHE:HE1	38:B:9122:HOH:O	1.96	0.49
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.93	0.49
5:E:69:ILE:HA	5:E:72:MET:HE3	1.95	0.49
13:M:193:LYS:HB3	30:0:392:U:H4'	1.94	0.49
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.95	0.49
21:U:33:SER:O	21:U:37:GLU:HG3	2.13	0.49
30:0:1666:C:HO2'	30:0:1667:A:H5''	1.70	0.49
30:0:2265:U:H2'	30:0:2266:A:C8	2.48	0.49
30:0:2356:A:H5'	38:0:5666:HOH:O	2.12	0.49
30:0:2467:A:H2'	38:0:5488:HOH:O	2.12	0.49
30:0:255:A:C4	30:0:256:C:C6	3.00	0.49
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.42	0.49
30:0:1008:C:O2'	30:0:1009:U:H5'	2.13	0.49
30:0:1552:G:H2'	30:0:1553:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.95	0.49
20:T:52:ARG:O	30:0:317:A:OP1	2.29	0.49
30:0:790:A:H1'	30:0:1710:A:H2'	1.95	0.49
30:0:2453:G:H5''	38:0:4755:HOH:O	2.13	0.49
30:0:255:A:H2'	30:0:256:C:C6	2.47	0.49
30:0:2717:C:C2'	30:0:2718:C:C5'	2.79	0.49
30:0:2769:C:C2'	30:0:2770:G:C5'	2.84	0.49
30:0:304:G:H1'	30:0:347:A:N6	2.28	0.49
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.94	0.49
8:H:30:LYS:H	8:H:62:HIS:CD2	2.30	0.49
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.93	0.49
25:Y:154:ARG:HH21	30:0:1293:U:H5'	1.78	0.49
30:0:154:C:H2'	30:0:155:C:C6	2.48	0.49
30:0:1857:A:H5''	38:0:6744:HOH:O	2.12	0.49
30:0:2002:C:C2'	30:0:2003:U:H5'	2.42	0.49
30:0:2316:G:OP1	30:0:2317:C:H1'	2.13	0.49
30:0:513:A:N3	38:0:3679:HOH:O	2.35	0.49
30:0:1158:G:O2'	30:0:1159:G:H5'	2.13	0.48
30:0:1391:G:H2'	30:0:1392:A:H5'	1.95	0.48
30:0:1562:C:O2	30:0:1562:C:H2'	2.12	0.48
30:0:282:C:O2	30:0:282:C:H2'	2.13	0.48
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.94	0.48
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.95	0.48
7:G:67:LEU:O	7:G:71:LEU:HG	2.12	0.48
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.42	0.48
21:U:37:GLU:HB3	38:U:408:HOH:O	2.11	0.48
22:V:1:THR:HG23	22:V:2:VAL:HG23	1.94	0.48
30:0:1159:G:H1	30:0:1208:C:H42	1.58	0.48
12:L:6:ARG:NH1	30:0:1299:G:N7	2.62	0.48
30:0:1825:U:O2'	30:0:1826:C:H5'	2.12	0.48
30:0:195:C:H2'	30:0:196:G:H5'	1.95	0.48
27:1:1:THR:O	30:0:1836:A:H1'	2.13	0.48
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.45	0.48
10:J:75:PRO:HB3	10:J:132:LEU:HB3	1.95	0.48
16:P:83:LYS:HG2	30:0:793:A:H5''	1.94	0.48
24:X:43:VAL:HG12	24:X:44:ASP:N	2.28	0.48
30:0:1087:G:H4'	30:0:1088:A:OP1	2.13	0.48
30:0:137:U:H2'	30:0:139:C:C5	2.47	0.48
30:0:1528:A:H2'	30:0:1529:G:O4'	2.13	0.48
30:0:1632:A:C3'	30:0:1633:C:H5'	2.43	0.48
2:B:205:VAL:O	2:B:307:ARG:NE	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:VAL:HG22	3:C:137:PRO:HA	1.95	0.48
15:O:32:ARG:HD3	15:O:32:ARG:O	2.12	0.48
19:S:37:VAL:O	19:S:41:VAL:HG23	2.13	0.48
23:W:23:MET:O	30:0:1025:C:H5'	2.12	0.48
25:Y:212:ARG:HD2	38:Y:8896:HOH:O	2.12	0.48
26:Z:80:GLN:HA	26:Z:86:TYR:O	2.12	0.48
30:0:1321:A:H2'	30:0:1322:G:C8	2.48	0.48
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.48
30:0:2300:A:H4'	30:0:2301:A:O5'	2.13	0.48
20:T:8:ARG:HD2	30:0:31:C:OP2	2.13	0.48
1:A:121:ALA:O	1:A:124:VAL:HG22	2.13	0.48
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.95	0.48
30:0:1883:U:O2'	30:0:1884:G:H5'	2.13	0.48
30:0:2301:A:H5''	30:0:2302:A:H5'	1.95	0.48
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.48
30:0:961:A:H4'	38:0:6814:HOH:O	2.12	0.48
2:B:255:GLY:O	2:B:257:THR:HG22	2.14	0.48
2:B:49:THR:HG21	2:B:331:SER:O	2.14	0.48
3:C:236:THR:H	3:C:239:ALA:HB3	1.78	0.48
6:F:48:VAL:HG23	6:F:74:PHE:CB	2.42	0.48
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.95	0.48
30:0:1165:G:H4'	30:0:1174:A:O2'	2.13	0.48
30:0:2269:C:H2'	30:0:2270:G:C5'	2.44	0.48
30:0:447:A:O2'	30:0:448:G:H5'	2.14	0.48
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.96	0.48
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.95	0.48
30:0:222:A:H2'	30:0:223:G:O4'	2.14	0.48
30:0:2564:G:OP2	30:0:2565:C:H5''	2.14	0.48
10:J:107:ASN:C	10:J:107:ASN:HD22	2.17	0.48
30:0:1130:U:H4'	38:0:6158:HOH:O	2.13	0.48
30:0:484:A:N1	30:0:506:G:H4'	2.28	0.48
30:0:920:C:H5'	30:0:921:G:C4	2.49	0.48
31:9:45:A:H2'	31:9:46:C:H6	1.79	0.48
6:F:21:GLU:O	6:F:24:ARG:HG2	2.14	0.48
18:R:104:PHE:HB3	18:R:109:MET:HE1	1.96	0.48
30:0:1051:C:H2'	30:0:1052:G:O4'	2.14	0.48
30:0:1131:G:C6	30:0:1230:A:C4	3.02	0.48
30:0:1545:C:H2'	30:0:1546:G:O4'	2.14	0.48
30:0:2912:C:H2'	30:0:2913:A:O4'	2.14	0.48
30:0:960:G:H3'	30:0:960:G:C4	2.49	0.48
29:3:48:ASN:ND2	29:3:50:GLY:H	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.94	0.48
3:C:140:VAL:HB	38:C:8644:HOH:O	2.13	0.48
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.46	0.48
15:O:57:THR:HB	15:O:111:VAL:HG23	1.95	0.48
30:0:1625:U:H5''	38:0:6053:HOH:O	2.13	0.48
30:0:1477:C:H5'	30:0:1868:G:H5''	1.96	0.48
30:0:2439:C:H5'	38:0:5518:HOH:O	2.12	0.48
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.44	0.48
2:B:275:GLY:O	2:B:291:ASP:HA	2.14	0.48
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.79	0.48
12:L:121:ILE:HG12	12:L:141:GLU:HB2	1.96	0.48
30:0:2314:G:H2'	30:0:2315:C:H5'	1.96	0.47
30:0:90:A:H2'	30:0:91:G:O4'	2.14	0.47
27:1:28:HIS:HD2	27:1:30:LYS:H	1.60	0.47
1:A:3:ARG:HD3	30:0:870:G:OP2	2.14	0.47
3:C:22:PHE:HA	3:C:116:ALA:HA	1.94	0.47
13:M:64:ARG:HD2	38:M:8881:HOH:O	2.14	0.47
14:N:114:LYS:O	14:N:118:ILE:HG13	2.14	0.47
14:N:169:PRO:O	14:N:172:PHE:HB3	2.14	0.47
14:N:43:VAL:HG13	14:N:118:ILE:HD11	1.96	0.47
23:W:65:VAL:HA	23:W:68:THR:HG22	1.95	0.47
30:0:1666:C:H2'	30:0:1667:A:H5''	1.78	0.47
30:0:1838:U:O2'	30:0:2644:C:H5'	2.14	0.47
30:0:1850:U:H2'	30:0:1851:G:C8	2.48	0.47
30:0:398:U:H2'	30:0:399:C:C6	2.49	0.47
4:D:76:ARG:NE	31:9:44:A:O4'	2.47	0.47
21:U:9:CYS:HA	21:U:52:THR:OG1	2.14	0.47
30:0:1422:U:H2'	30:0:1423:C:C6	2.50	0.47
30:0:1641:A:C2'	30:0:1642:A:H5'	2.44	0.47
30:0:1788:U:O2'	30:0:1789:G:H5'	2.14	0.47
30:0:2264:A:H2'	30:0:2265:U:C6	2.48	0.47
30:0:2506:A:H1'	38:0:3766:HOH:O	2.13	0.47
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.47
27:1:25:LYS:HD2	28:2:48:ASP:HA	1.96	0.47
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.27	0.47
8:H:61:ARG:NH1	8:H:61:ARG:HG3	2.29	0.47
30:0:1268:C:O2'	30:0:1269:G:H5'	2.14	0.47
30:0:1280:A:H3'	30:0:1280:A:OP1	2.15	0.47
30:0:2064:U:H4'	30:0:2653:A:OP1	2.13	0.47
23:W:154:ARG:NH1	30:0:588:G:O6	2.47	0.47
30:0:955:A:C2	30:0:1013:A:C4	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:NH2	1:A:38:ILE:HG13	2.28	0.47
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.79	0.47
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.50	0.47
6:F:107:ASP:O	6:F:111:ILE:HG13	2.14	0.47
16:P:143:ALA:HA	38:P:184:HOH:O	2.13	0.47
30:0:1193:A:C2	30:0:1194:A:N6	2.78	0.47
30:0:1252:A:H2'	30:0:1253:C:O4'	2.14	0.47
30:0:137:U:OP1	30:0:259:G:O2'	2.33	0.47
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.47
14:N:40:ASN:HD21	31:9:28:U:H5''	1.80	0.47
31:9:56:A:C3'	31:9:57:A:H5''	2.44	0.47
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.30	0.47
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.49	0.47
30:0:1393:A:H2'	30:0:1394:C:C6	2.49	0.47
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.48	0.47
30:0:2271:G:H5'	38:0:4783:HOH:O	2.14	0.47
30:0:2469:A:H2'	38:0:7512:HOH:O	2.15	0.47
30:0:407:A:H2'	30:0:408:A:C8	2.50	0.47
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.97	0.47
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.15	0.47
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.45	0.47
16:P:120:ARG:NH1	30:0:1594:C:C5	2.82	0.47
24:X:85:VAL:HG12	24:X:86:GLU:N	2.30	0.47
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	1.97	0.47
30:0:1118:A:C8	30:0:1119:G:H5''	2.49	0.47
30:0:1762:C:H2'	30:0:1763:C:H6	1.80	0.47
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.47	0.47
30:0:2353:A:H4'	30:0:2354:A:O5'	2.14	0.47
30:0:440:C:H2'	30:0:441:A:C8	2.50	0.47
4:D:10:PHE:CG	4:D:11:HIS:N	2.81	0.47
12:L:149:ARG:O	12:L:150:GLN:HB2	2.14	0.47
30:0:1176:C:N4	38:0:5775:HOH:O	2.48	0.47
30:0:283:U:H5	30:0:284:C:N4	2.12	0.47
17:Q:32:GLU:O	17:Q:93:ARG:NH2	2.48	0.47
30:0:2791:U:H1'	30:0:2792:A:H5''	1.97	0.47
30:0:426:G:H2'	30:0:427:C:O4'	2.15	0.47
30:0:483:C:C4	30:0:484:A:C6	3.03	0.47
27:1:22:CYS:SG	27:1:24:GLU:HB2	2.55	0.47
29:3:65:THR:HB	29:3:83:TRP:H	1.79	0.47
31:9:52:A:H2'	31:9:53:G:O4'	2.15	0.47
13:M:164:THR:HG22	13:M:166:ALA:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:11:VAL:HG11	30:0:1086:A:C6	2.49	0.47
30:0:1682:A:H2'	38:0:9820:HOH:O	2.14	0.47
30:0:2533:C:C6	30:0:2533:C:C5'	2.92	0.47
31:9:55:U:H4'	31:9:56:A:C8	2.49	0.47
6:F:91:VAL:HG12	6:F:92:GLY:H	1.78	0.47
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.44	0.47
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.45	0.47
30:0:1249:U:H2'	30:0:1250:C:C6	2.50	0.47
30:0:1477:C:C5'	30:0:1868:G:H5''	2.44	0.47
30:0:1928:C:H2'	30:0:1929:G:H5'	1.96	0.47
30:0:2281:C:H2'	30:0:2282:U:H5'	1.97	0.47
30:0:2372:A:H2'	30:0:2373:U:H6	1.78	0.47
30:0:816:G:C6	30:0:817:G:N1	2.83	0.47
2:B:297:VAL:HB	38:B:9080:HOH:O	2.15	0.47
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.97	0.47
30:0:170:U:H2'	30:0:171:C:H5'	1.95	0.46
30:0:2011:A:H4'	30:0:2012:U:O5'	2.15	0.46
30:0:2238:A:H3'	38:0:6711:HOH:O	2.15	0.46
30:0:2589:U:H2'	30:0:2590:U:C6	2.50	0.46
26:Z:34:SER:HB3	30:0:797:A:H4'	1.96	0.46
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.30	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.15	0.46
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.35	0.46
1:A:175:LYS:HG3	30:0:1847:A:OP1	2.16	0.46
27:1:11:LYS:HG2	30:0:777:U:O2'	2.15	0.46
31:9:28:U:H2'	31:9:29:C:C6	2.50	0.46
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.19	0.46
8:H:172:GLU:HB3	38:H:243:HOH:O	2.15	0.46
21:U:50:GLU:HB2	30:0:2866:U:C5	2.50	0.46
24:X:43:VAL:HG12	24:X:47:ALA:HB3	1.97	0.46
25:Y:165:GLU:HB3	38:0:6747:HOH:O	2.15	0.46
30:0:1907:U:O2'	30:0:1908:G:H5'	2.15	0.46
30:0:304:G:H1'	30:0:347:A:H61	1.80	0.46
30:0:559:U:C5	30:0:560:U:C5	3.03	0.46
30:0:800:G:H2'	30:0:801:U:C6	2.50	0.46
30:0:969:G:H1	30:0:999:C:H42	1.62	0.46
14:N:141:ARG:NH2	31:9:48:C:H4'	2.30	0.46
16:P:1:THR:O	30:0:1396:C:H1'	2.15	0.46
30:0:105:G:O2'	30:0:106:A:H5'	2.15	0.46
25:Y:115:ARG:NH2	30:0:1266:U:H4'	2.30	0.46
30:0:2103:A:H2'	30:0:2104:C:H5'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:699:C:C2	30:0:744:G:C2	3.03	0.46
30:0:690:G:H4'	30:0:741:C:O2	2.15	0.46
1:A:132:ASP:HB3	1:A:135:VAL:H	1.80	0.46
1:A:88:ILE:HG22	1:A:88:ILE:O	2.14	0.46
3:C:129:HIS:HD2	3:C:165:ASP:OD2	1.99	0.46
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.15	0.46
23:W:122:ARG:NH2	38:0:5320:HOH:O	2.48	0.46
30:0:1117:A:C2	30:0:1244:U:C2	3.04	0.46
10:J:82:THR:CG2	30:0:1242:A:H5'	2.30	0.46
30:0:1657:A:H2'	30:0:1658:A:C8	2.51	0.46
30:0:343:C:O2'	30:0:344:C:H5'	2.15	0.46
30:0:638:C:H2'	30:0:639:A:C8	2.51	0.46
30:0:920:C:H5''	30:0:921:G:O5'	2.15	0.46
31:9:101:G:H5''	38:9:9140:HOH:O	2.15	0.46
2:B:320:GLN:HE21	2:B:321:PRO:CD	2.24	0.46
8:H:139:ALA:HB3	8:H:149:VAL:HG21	1.97	0.46
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.31	0.46
10:J:107:ASN:HD22	10:J:109:TYR:H	1.64	0.46
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.51	0.46
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.96	0.46
30:0:11:A:H5'	30:0:12:U:OP2	2.15	0.46
30:0:1503:U:H2'	30:0:1504:A:O4'	2.15	0.46
30:0:1596:U:H2'	30:0:1598:A:OP2	2.15	0.46
30:0:2712:G:H5'	38:0:5251:HOH:O	2.15	0.46
30:0:583:C:C2	30:0:584:U:C5	3.03	0.46
1:A:51:ARG:HD2	30:0:1874:U:OP1	2.15	0.46
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.95	0.46
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.82	0.46
20:T:28:SER:O	20:T:32:ARG:HG3	2.15	0.46
30:0:1883:U:C2'	30:0:1884:G:H5'	2.46	0.46
30:0:613:C:H2'	30:0:614:U:H6	1.80	0.46
30:0:812:A:H2'	30:0:813:C:O4'	2.16	0.46
27:1:1:THR:HA	38:0:9368:HOH:O	2.16	0.46
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.54	0.46
31:9:39:U:C2'	31:9:40:C:OP1	2.63	0.46
18:R:104:PHE:CB	18:R:109:MET:HE1	2.46	0.46
24:X:30:MET:CE	24:X:58:ALA:HB3	2.45	0.46
30:0:1202:A:O2'	30:0:1203:G:H5'	2.16	0.46
30:0:1928:C:C2'	30:0:1929:G:H5'	2.46	0.46
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.98	0.46
3:C:206:ASN:HB2	30:0:329:A:OP2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:SER:HB2	38:0:4392:HOH:O	2.15	0.46
4:D:27:ILE:HB	4:D:69:ILE:O	2.15	0.46
8:H:61:ARG:HG3	38:0:5004:HOH:O	2.15	0.46
18:R:132:ARG:NH1	38:R:8984:HOH:O	2.48	0.46
10:J:63:ILE:CD1	30:0:1236:A:C8	2.99	0.46
30:0:2065:C:O2'	30:0:2066:C:H5'	2.16	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.51	0.46
30:0:2758:G:H2'	30:0:2759:C:C6	2.51	0.46
18:R:29:LYS:HD3	30:0:524:A:H5''	1.98	0.46
30:0:622:G:O2'	30:0:623:U:H5'	2.16	0.46
30:0:711:G:H1'	38:0:7133:HOH:O	2.14	0.46
30:0:71:G:H5''	38:0:3932:HOH:O	2.16	0.46
28:2:20:ARG:HD3	38:0:6163:HOH:O	2.16	0.46
31:9:29:C:C2'	31:9:30:C:H5'	2.42	0.46
6:F:91:VAL:HG11	30:0:262:A:OP2	2.16	0.46
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.97	0.46
30:0:1311:G:C2	30:0:1312:G:C8	3.04	0.46
30:0:1790:C:H2'	30:0:1791:U:C6	2.50	0.46
30:0:2241:C:H2'	30:0:2242:U:C6	2.51	0.46
30:0:2379:G:N7	30:0:2408:A:N1	2.63	0.46
1:A:206:ARG:NH2	30:0:2630:G:O6	2.49	0.46
2:B:141:ARG:N	38:B:9048:HOH:O	2.48	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.98	0.46
30:0:1511:U:O2'	30:0:1512:G:H5'	2.16	0.45
30:0:162:C:H2'	30:0:163:U:H5'	1.98	0.45
30:0:1522:A:C2	30:0:1665:G:C6	3.04	0.45
30:0:2415:A:C2'	30:0:2416:G:H5'	2.46	0.45
30:0:278:A:H2'	30:0:279:C:O4'	2.16	0.45
30:0:2831:C:H42	30:0:2909:G:H1	1.64	0.45
30:0:2872:U:H2'	30:0:2873:C:H6	1.81	0.45
30:0:2880:A:C2'	30:0:2881:C:H5'	2.46	0.45
30:0:372:A:H2'	30:0:373:G:C8	2.51	0.45
30:0:78:G:C6	30:0:79:G:C6	3.04	0.45
1:A:194:MET:HG2	30:0:875:A:C2	2.52	0.45
30:0:876:A:N3	30:0:876:A:C2'	2.80	0.45
29:3:62:THR:HB	38:3:9044:HOH:O	2.15	0.45
2:B:62:ARG:HA	2:B:65:MET:CE	2.46	0.45
30:0:1194:A:O2'	30:0:1195:G:H5'	2.16	0.45
30:0:1074:G:H4'	30:0:1260:G:C6	2.51	0.45
30:0:1339:G:C6	30:0:1340:G:N1	2.85	0.45
30:0:1778:A:H2'	30:0:1779:A:H5'	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:412:C:O2'	30:0:413:G:H5'	2.16	0.45
30:0:53:C:H2'	30:0:54:G:O4'	2.16	0.45
30:0:669:G:O2'	30:0:670:G:H5'	2.16	0.45
30:0:758:A:H2'	30:0:759:C:O4'	2.17	0.45
10:J:75:PRO:HD3	10:J:136:SER:OG	2.16	0.45
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.31	0.45
20:T:63:ILE:HD11	20:T:75:GLU:HB2	1.99	0.45
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.98	0.45
30:0:2456:A:H2'	30:0:2457:U:C6	2.51	0.45
30:0:407:A:H8	38:0:4486:HOH:O	2.00	0.45
30:0:445:U:H2'	30:0:446:G:H8	1.81	0.45
3:C:19:PRO:HG2	3:C:22:PHE:CD1	2.51	0.45
7:G:64:ASN:N	7:G:64:ASN:ND2	2.63	0.45
23:W:38:THR:HG22	23:W:39:ASP:N	2.31	0.45
30:0:1333:U:H2'	30:0:1334:C:H6	1.82	0.45
30:0:2271:G:N3	30:0:2271:G:H2'	2.31	0.45
30:0:253:U:H1'	30:0:256:C:H41	1.82	0.45
30:0:281:U:H2'	30:0:282:C:H6	1.82	0.45
30:0:506:G:N2	30:0:509:A:H5'	2.22	0.45
30:0:522:U:O2'	30:0:1366:C:H5'	2.16	0.45
31:9:3:A:OP2	31:9:25:G:N2	2.49	0.45
31:9:53:G:O2'	31:9:54:A:H5'	2.16	0.45
6:F:91:VAL:CG1	6:F:92:GLY:N	2.80	0.45
10:J:19:MET:HE1	10:J:79:PHE:HA	1.99	0.45
13:M:49:ALA:C	13:M:54:TYR:HB3	2.37	0.45
30:0:1919:A:H4'	38:0:4883:HOH:O	2.15	0.45
30:0:2493:C:O2	30:0:2493:C:H2'	2.15	0.45
31:9:40:C:H2'	31:9:41:C:OP1	2.17	0.45
31:9:57:A:N6	38:9:9066:HOH:O	2.47	0.45
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.35	0.45
11:K:113:ILE:HG22	11:K:114:ALA:N	2.32	0.45
15:O:10:LEU:HD13	15:O:99:GLU:HG3	1.99	0.45
30:0:1202:A:H2'	30:0:1203:G:H5'	1.99	0.45
30:0:1588:G:C6	30:0:1589:G:C6	3.05	0.45
30:0:1947:G:H2'	30:0:1948:G:C8	2.52	0.45
30:0:2598:U:O2	30:0:2600:A:H8	2.00	0.45
30:0:603:A:H1'	30:0:605:C:C2	2.52	0.45
4:D:20:LYS:HG2	4:D:133:ASN:HB3	1.97	0.45
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.51	0.45
11:K:125:ALA:C	11:K:127:ALA:H	2.20	0.45
18:R:132:ARG:HG2	18:R:133:ALA:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.51	0.45
24:X:78:GLU:HG2	24:X:79:GLU:H	1.81	0.45
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.99	0.45
30:0:1183:C:N3	30:0:1184:C:H5	2.15	0.45
30:0:2090:G:H2'	30:0:2091:G:C8	2.51	0.45
30:0:2281:C:C2'	30:0:2282:U:H5'	2.47	0.45
30:0:2812:A:N7	38:0:7555:HOH:O	2.36	0.45
30:0:42:C:H1'	38:0:4707:HOH:O	2.15	0.45
30:0:821:U:H3'	38:0:3789:HOH:O	2.15	0.45
1:A:164:ARG:NE	38:A:9043:HOH:O	2.49	0.45
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.99	0.45
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.99	0.45
13:M:99:ARG:HG3	38:M:8855:HOH:O	2.16	0.45
16:P:134:VAL:O	16:P:137:LEU:HB3	2.17	0.45
17:Q:1:PRO:HA	30:0:2299:G:O6	2.16	0.45
30:0:1987:C:H2'	30:0:1988:C:C6	2.51	0.45
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.52	0.45
1:A:96:LEU:HD22	1:A:128:LEU:HD13	1.99	0.45
1:A:99:ILE:O	1:A:131:HIS:HE1	2.00	0.45
1:A:186:TRP:CG	1:A:187:PRO:HA	2.52	0.45
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.99	0.45
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.98	0.45
8:H:34:HIS:HD2	8:H:90:LEU:O	2.00	0.45
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.97	0.45
23:W:149:LEU:HG	23:W:153:MET:HE2	1.99	0.45
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.32	0.45
30:0:128:A:H3'	30:0:128:A:C8	2.52	0.45
30:0:1902:G:N2	30:0:1936:C:C2	2.85	0.45
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.99	0.45
30:0:2506:A:O2'	30:0:2507:G:P	2.75	0.45
31:9:81:C:O2'	31:9:82:U:H5'	2.17	0.45
3:C:84:VAL:O	3:C:85:LYS:HB2	2.17	0.45
12:L:50:GLY:C	30:0:2453:G:H4'	2.37	0.45
18:R:113:HIS:O	18:R:145:LEU:HD12	2.17	0.45
19:S:77:VAL:O	19:S:80:ARG:HG2	2.16	0.45
23:W:119:HIS:HE1	38:0:9565:HOH:O	2.00	0.45
23:W:74:GLU:OE1	30:0:1285:U:H4'	2.17	0.45
30:0:1615:A:H5'	38:0:4210:HOH:O	2.16	0.45
30:0:1626:A:H2'	30:0:1627:G:O4'	2.17	0.45
25:Y:137:LYS:HD2	30:0:521:A:H5''	1.99	0.45
30:0:77:G:C2'	30:0:78:G:H5'	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:951:A:O2'	30:0:952:G:H5'	2.17	0.45
30:0:969:G:N2	30:0:1000:C:C2	2.84	0.45
27:1:2:GLY:O	27:1:6:PRO:HG2	2.17	0.45
31:9:1:U:O3'	31:9:3:A:OP1	2.35	0.45
3:C:168:ARG:NH2	3:C:190:ALA:O	2.50	0.45
30:0:1783:A:O2'	30:0:1784:U:H5'	2.16	0.44
30:0:1896:G:C6	30:0:1897:U:C4	3.05	0.44
30:0:1942:A:O2'	30:0:1943:C:H5'	2.17	0.44
30:0:2754:G:H2'	30:0:2755:G:O4'	2.17	0.44
30:0:542:A:O2'	30:0:543:G:H5'	2.16	0.44
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.00	0.44
2:B:62:ARG:HA	2:B:65:MET:HE2	1.99	0.44
13:M:164:THR:HB	38:M:8819:HOH:O	2.15	0.44
30:0:1406:A:H4'	30:0:1407:A:H5''	1.99	0.44
30:0:291:C:H2'	30:0:292:G:O4'	2.17	0.44
30:0:812:A:H2'	30:0:813:C:C6	2.52	0.44
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.64	0.44
29:3:65:THR:CG2	29:3:67:LEU:HG	2.46	0.44
1:A:53:ALA:HB3	38:A:9060:HOH:O	2.16	0.44
4:D:135:VAL:HG22	4:D:136:ARG:N	2.32	0.44
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.98	0.44
26:Z:37:ARG:HD2	38:Z:8719:HOH:O	2.17	0.44
30:0:1182:C:HO2'	30:0:1183:C:H5	1.64	0.44
30:0:187:A:H3'	30:0:188:C:H6	1.82	0.44
30:0:2032:U:H2'	30:0:2033:G:C5'	2.47	0.44
30:0:204:A:H2'	30:0:205:U:H5'	1.98	0.44
30:0:582:U:H2'	30:0:583:C:C6	2.53	0.44
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.38	0.44
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.76	0.44
11:K:14:LYS:HG3	11:K:32:ILE:O	2.18	0.44
14:N:108:SER:HA	14:N:109:PRO:HD3	1.81	0.44
30:0:2385:G:H2'	30:0:2386:U:C6	2.52	0.44
30:0:2464:C:H5''	30:0:2465:A:OP1	2.17	0.44
30:0:2473:U:O3'	30:0:2474:A:H3'	2.17	0.44
30:0:451:C:O2'	30:0:452:G:H5'	2.18	0.44
30:0:453:A:H4'	30:0:455:A:N7	2.32	0.44
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.44
13:M:58:GLN:HG3	38:M:8906:HOH:O	2.18	0.44
25:Y:144:ARG:NH2	38:Y:8907:HOH:O	2.51	0.44
30:0:1342:C:C2'	30:0:1343:C:H5'	2.47	0.44
30:0:185:G:H4'	30:0:186:A:H4'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1973:A:H2'	30:0:1974:G:O4'	2.18	0.44
30:0:2635:A:C2'	30:0:2636:C:H5'	2.46	0.44
30:0:558:C:HO2'	30:0:559:U:H5''	1.80	0.44
30:0:815:U:O2'	30:0:1598:A:H4'	2.17	0.44
30:0:825:U:H5''	30:0:826:U:OP1	2.18	0.44
30:0:947:U:O2'	30:0:948:G:H5'	2.16	0.44
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.47	0.44
16:P:120:ARG:NH2	16:P:123:TYR:CD2	2.85	0.44
30:0:1427:A:H61	30:0:1440:U:C1'	2.30	0.44
30:0:1592:G:C4	30:0:1593:C:C5	3.06	0.44
30:0:1592:G:O2'	30:0:1593:C:O5'	2.35	0.44
30:0:218:C:C5	30:0:220:C:C4	3.06	0.44
30:0:2276:U:H2'	30:0:2277:U:C6	2.53	0.44
30:0:2636:C:H4'	38:0:6666:HOH:O	2.18	0.44
30:0:77:G:H2'	30:0:78:G:H5'	1.99	0.44
30:0:816:G:H5'	30:0:1598:A:H4'	1.99	0.44
28:2:2:LYS:HG3	30:0:1486:A:C5	2.52	0.44
4:D:53:LYS:HE3	31:9:40:C:H42	1.82	0.44
31:9:76:G:H3'	31:9:77:A:C5'	2.31	0.44
2:B:74:ILE:HG13	38:B:9080:HOH:O	2.17	0.44
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.17	0.44
13:M:46:LEU:HG	38:M:8922:HOH:O	2.18	0.44
30:0:1603:A:C5'	30:0:1605:G:C5'	2.94	0.44
30:0:1878:G:O2'	30:0:1879:U:OP2	2.36	0.44
30:0:204:A:C2'	30:0:205:U:H5'	2.47	0.44
30:0:764:C:H2'	30:0:765:G:O4'	2.17	0.44
30:0:794:U:C2'	30:0:795:G:H5'	2.48	0.44
2:B:79:MET:HE1	38:B:9100:HOH:O	2.17	0.44
14:N:11:ARG:NH1	31:9:8:G:O6	2.50	0.44
16:P:91:LYS:O	16:P:95:GLU:HG3	2.17	0.44
30:0:1044:C:H5''	38:0:9028:HOH:O	2.18	0.44
30:0:1006:A:N1	30:0:2311:A:H1'	2.33	0.44
30:0:2461:U:O2	30:0:2466:G:H1'	2.18	0.44
30:0:2511:A:H2'	30:0:2512:U:O4'	2.17	0.44
30:0:2565:C:H4'	38:0:4868:HOH:O	2.18	0.44
30:0:441:A:H8	30:0:441:A:O5'	1.99	0.44
30:0:497:A:H2'	30:0:498:A:C5'	2.48	0.44
30:0:807:A:O2'	30:0:808:A:H5'	2.17	0.44
31:9:107:C:O2'	31:9:108:C:H5'	2.18	0.44
1:A:204:GLY:N	30:0:2634:G:OP2	2.48	0.44
2:B:280:VAL:HG13	2:B:333:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131:THR:HG21	30:0:2348:C:H1'	1.99	0.44
4:D:135:VAL:HG22	4:D:136:ARG:H	1.82	0.44
5:E:6:GLU:HG2	5:E:46:THR:HG22	1.99	0.44
6:F:60:VAL:HG13	6:F:63:ILE:HG13	1.99	0.44
8:H:30:LYS:H	8:H:62:HIS:HD2	1.65	0.44
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.83	0.44
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.53	0.44
30:0:1066:U:H2'	30:0:1067:A:C8	2.52	0.44
30:0:1189:A:H1'	30:0:1209:C:H1'	1.99	0.44
30:0:1375:A:C2'	30:0:1376:G:H5'	2.47	0.44
30:0:1588:G:C5	30:0:1589:G:C6	3.06	0.44
30:0:1903:U:O2'	30:0:1904:A:N7	2.50	0.44
30:0:2015:A:H2'	30:0:2016:U:O4'	2.18	0.44
30:0:2238:A:O2'	30:0:2239:C:H5'	2.18	0.44
30:0:2506:A:O2'	30:0:2507:G:O5'	2.36	0.44
30:0:2569:A:H2'	30:0:2570:G:O5'	2.18	0.44
30:0:383:A:H2'	30:0:384:G:O4'	2.18	0.44
30:0:629:A:C2	30:0:2074:A:C2	3.06	0.44
30:0:66:G:C2	30:0:109:U:C4	3.06	0.44
30:0:88:G:H2'	30:0:89:G:H8	1.83	0.44
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.66	0.44
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.49	0.44
11:K:89:LYS:HE2	21:U:19:THR:HG21	2.00	0.44
21:U:49:LEU:HG	38:U:3805:HOH:O	2.17	0.44
1:A:76:VAL:HG23	26:Z:87:LYS:HB3	2.00	0.44
30:0:1632:A:H2'	30:0:1633:C:C5'	2.42	0.43
30:0:177:A:O2'	30:0:892:G:H4'	2.17	0.43
16:P:73:HIS:HE1	30:0:1789:G:O6	2.01	0.43
1:A:190:ARG:HH11	30:0:1845:A:P	2.41	0.43
30:0:2842:G:H2'	30:0:2843:A:H5'	2.00	0.43
30:0:499:G:O2'	30:0:500:G:H5'	2.16	0.43
30:0:594:C:C4	30:0:595:U:C4	3.06	0.43
17:Q:19:ARG:HH21	31:9:11:A:P	2.41	0.43
31:9:55:U:H4'	31:9:56:A:H8	1.83	0.43
2:B:53:LEU:HD11	2:B:327:VAL:HG22	1.99	0.43
3:C:170:ASP:OD2	30:0:330:C:H5	2.01	0.43
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.99	0.43
10:J:70:PHE:HD1	30:0:2676:C:O2'	2.00	0.43
14:N:37:ARG:HH12	31:9:6:C:C5'	2.21	0.43
14:N:37:ARG:NE	38:N:8831:HOH:O	2.51	0.43
30:0:1119:G:N2	30:0:1246:A:H2	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:963:C:O2	30:0:1005:A:N1	2.51	0.43
29:3:91:GLN:O	29:3:92:GLU:HB2	2.18	0.43
31:9:114:G:H2'	31:9:115:C:H6	1.81	0.43
31:9:31:C:H2'	31:9:32:G:O4'	2.18	0.43
2:B:10:SER:HB2	30:0:2714:U:H4'	1.99	0.43
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.51	0.43
13:M:134:ILE:O	13:M:136:PRO:HD3	2.19	0.43
14:N:50:LEU:HA	14:N:50:LEU:HD12	1.86	0.43
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.53	0.43
30:0:1056:U:H2'	30:0:1057:A:O4'	2.18	0.43
30:0:1156:C:O5'	30:0:1156:C:H6	2.01	0.43
30:0:1565:C:H2'	30:0:1566:C:H6	1.83	0.43
30:0:1517:C:O2	30:0:1670:A:C2	2.71	0.43
30:0:271:C:C2	30:0:273:G:O4'	2.70	0.43
30:0:2870:C:O2'	30:0:2871:G:H5'	2.19	0.43
28:2:16:ASN:HB2	38:2:5203:HOH:O	2.17	0.43
31:9:3:A:C2	31:9:21:G:N3	2.85	0.43
1:A:1:GLY:HA2	1:A:197:VAL:HG23	1.99	0.43
1:A:95:PRO:O	1:A:99:ILE:HG12	2.19	0.43
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.84	0.43
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.16	0.43
18:R:40:ALA:O	18:R:44:VAL:HG23	2.18	0.43
30:0:1434:A:H2'	30:0:1436:C:C5	2.53	0.43
30:0:1456:C:H2'	30:0:1457:U:C6	2.54	0.43
30:0:1789:G:H2'	30:0:1790:C:O5'	2.18	0.43
30:0:17:G:H2'	30:0:18:C:C6	2.53	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.96	0.43
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.43
30:0:212:A:O4'	30:0:214:U:C6	2.72	0.43
30:0:294:C:H2'	30:0:295:C:O4'	2.18	0.43
30:0:559:U:H2'	30:0:560:U:O4'	2.18	0.43
30:0:677:C:O2'	30:0:678:G:H5'	2.18	0.43
30:0:960:G:C3'	30:0:960:G:C4	3.01	0.43
3:C:61:PHE:HB3	38:C:8639:HOH:O	2.18	0.43
7:G:12:ILE:HG12	38:0:5490:HOH:O	2.19	0.43
30:0:1946:C:H2'	30:0:1971:G:C8	2.53	0.43
30:0:365:G:C6	30:0:366:U:C4	3.06	0.43
30:0:424:C:H2'	30:0:425:U:C6	2.53	0.43
30:0:951:A:C2'	30:0:952:G:H5'	2.48	0.43
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.48	0.43
28:2:41:HIS:CD2	28:2:44:ARG:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ASP:O	2:B:306:LYS:HB2	2.19	0.43
3:C:242:GLU:HB2	38:C:8577:HOH:O	2.17	0.43
11:K:8:VAL:HG13	11:K:80:ILE:HG22	2.00	0.43
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.89	0.43
22:V:1:THR:HG23	22:V:2:VAL:N	2.30	0.43
30:0:35:U:H2'	30:0:36:C:C6	2.53	0.43
30:0:226:A:H1'	30:0:393:G:C5	2.54	0.43
31:9:42:C:H5'	31:9:43:G:OP2	2.19	0.43
31:9:58:G:H3'	31:9:59:C:C6	2.54	0.43
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.82	0.43
30:0:130:C:H5'	38:0:5243:HOH:O	2.19	0.43
30:0:1764:C:H2'	30:0:1765:G:O4'	2.18	0.43
30:0:1970:G:H2'	30:0:1970:G:N3	2.33	0.43
30:0:1992:U:H2'	30:0:1994:A:OP2	2.18	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.34	0.43
30:0:2523:U:O2'	30:0:2524:G:H5'	2.19	0.43
6:F:59:ILE:CD1	30:0:263:U:C2	3.01	0.43
30:0:512:G:O3'	30:0:513:A:C8	2.71	0.43
30:0:794:U:H2'	30:0:795:G:H5'	2.01	0.43
30:0:794:U:H3	30:0:819:A:H61	1.65	0.43
30:0:844:A:C6	30:0:882:A:C5	3.06	0.43
1:A:94:LEU:HG	1:A:99:ILE:HD13	2.01	0.43
8:H:64:SER:OG	30:0:2520:G:H5'	2.17	0.43
30:0:1250:C:O2'	30:0:1251:C:H5'	2.19	0.43
30:0:1589:G:N2	30:0:1605:G:H1'	2.34	0.43
30:0:2387:U:H2'	30:0:2388:C:C6	2.54	0.43
6:F:59:ILE:HD13	30:0:263:U:O4'	2.19	0.43
3:C:98:ARG:NH1	38:C:8554:HOH:O	2.51	0.43
6:F:99:THR:HG23	6:F:99:THR:O	2.19	0.43
11:K:130:MET:SD	21:U:25:ASP:O	2.77	0.43
19:S:57:THR:HG22	19:S:58:MET:N	2.33	0.43
22:V:55:ARG:O	22:V:59:ILE:HG12	2.19	0.43
25:Y:168:PHE:CE2	30:0:1090:A:H4'	2.54	0.43
30:0:1245:C:O5'	30:0:1245:C:H6	2.02	0.43
30:0:1421:C:O2'	30:0:1422:U:H5'	2.18	0.43
30:0:1616:A:H5''	30:0:1617:C:OP1	2.19	0.43
3:C:151:GLN:HG3	30:0:327:A:OP2	2.19	0.43
30:0:537:G:O4'	30:0:538:C:C5	2.71	0.43
30:0:941:G:C6	30:0:942:U:C4	3.07	0.43
31:9:59:C:H2'	31:9:60:C:C6	2.54	0.43
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:36:VAL:HG12	10:J:37:ALA:N	2.34	0.43
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.49	0.43
11:K:64:MET:HA	11:K:67:GLN:HE21	1.84	0.43
16:P:40:VAL:O	16:P:44:VAL:HG23	2.19	0.43
21:U:49:LEU:O	21:U:52:THR:HG22	2.17	0.43
25:Y:133:HIS:HD2	38:Y:8877:HOH:O	2.02	0.43
30:0:1032:A:N3	30:0:1032:A:H2'	2.33	0.43
30:0:1160:G:H5'	30:0:1161:A:C4'	2.46	0.43
30:0:1187:U:O2'	30:0:1189:A:H2	1.85	0.43
30:0:1555:G:O2'	30:0:1556:G:H5'	2.19	0.43
30:0:1644:C:C2	30:0:1645:U:C6	3.07	0.43
30:0:1996:U:O2'	30:0:1997:A:H5'	2.18	0.43
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.43
30:0:2524:G:N2	30:0:2526:C:H41	2.17	0.43
30:0:488:U:H2'	38:0:4031:HOH:O	2.18	0.43
27:1:25:LYS:O	27:1:25:LYS:HG2	2.19	0.43
31:9:52:A:O2'	31:9:53:G:H5'	2.19	0.43
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.90	0.43
4:D:99:ASP:HB3	4:D:103:ASN:H	1.84	0.43
14:N:38:LYS:HB2	14:N:38:LYS:HE3	1.77	0.43
18:R:109:MET:HG2	18:R:148:GLU:C	2.40	0.43
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.19	0.43
30:0:1202:A:H2'	30:0:1203:G:C5'	2.48	0.42
30:0:1788:U:C2	30:0:1805:G:N2	2.87	0.42
30:0:2252:A:C6	30:0:2253:G:H1'	2.53	0.42
30:0:2435:U:H1'	38:0:5462:HOH:O	2.19	0.42
30:0:332:G:O2'	30:0:333:G:H5'	2.19	0.42
30:0:39:G:N2	30:0:444:C:C2	2.87	0.42
31:9:45:A:H2'	31:9:46:C:C6	2.54	0.42
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.34	0.42
2:B:5:ARG:NH1	2:B:8:LYS:HE2	2.34	0.42
9:I:86:GLU:HG2	30:0:1180:U:H4'	2.01	0.42
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.18	0.42
30:0:1015:C:O5'	30:0:1015:C:H6	2.02	0.42
30:0:1761:U:H2'	30:0:1762:C:C6	2.54	0.42
31:9:14:G:H2'	31:9:15:C:H5'	2.01	0.42
31:9:2:U:C4'	38:9:9103:HOH:O	2.67	0.42
31:9:2:U:OP2	31:9:2:U:H4'	2.19	0.42
31:9:72:C:O2'	31:9:73:A:H5'	2.19	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.18	0.42
1:A:99:ILE:O	1:A:131:HIS:CE1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:PRO:HG2	38:C:8520:HOH:O	2.18	0.42
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.20	0.42
18:R:113:HIS:HE1	18:R:144:GLU:CD	2.22	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.46	0.42
30:0:1634:G:C6	30:0:1635:U:C4	3.07	0.42
30:0:1762:C:H2'	30:0:1763:C:C6	2.54	0.42
30:0:2004:U:H2'	30:0:2005:G:OP1	2.19	0.42
38:Q:2875:HOH:O	30:0:2392:C:H4'	2.20	0.42
30:0:2423:C:H2'	30:0:2424:U:C6	2.54	0.42
30:0:2819:C:H2'	30:0:2820:A:C8	2.54	0.42
29:3:3:MET:HG3	29:3:4:PRO:HD2	2.01	0.42
1:A:179:MET:HG2	1:A:186:TRP:CG	2.55	0.42
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.51	0.42
8:H:31:ILE:HG23	38:H:231:HOH:O	2.18	0.42
12:L:67:ARG:O	12:L:71:GLU:HG3	2.20	0.42
30:0:1175:G:H1'	30:0:1193:A:H2'	2.02	0.42
30:0:1416:G:C2'	30:0:1417:G:H5'	2.49	0.42
30:0:1561:U:H2'	30:0:1561:U:O2	2.18	0.42
30:0:2104:C:O2	30:0:2485:A:N1	2.53	0.42
30:0:254:C:O2	30:0:254:C:H2'	2.19	0.42
23:W:43:GLY:HA3	30:0:945:U:O2'	2.19	0.42
1:A:179:MET:HG2	1:A:186:TRP:CB	2.49	0.42
2:B:178:ALA:O	2:B:182:VAL:HG23	2.20	0.42
6:F:118:LEU:O	6:F:119:ARG:HB3	2.19	0.42
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.84	0.42
9:I:111:LEU:HD23	30:0:1163:G:H4'	2.01	0.42
16:P:59:ARG:NH2	16:P:66:GLN:HE22	2.10	0.42
24:X:15:ARG:HH22	30:0:2856:A:P	2.42	0.42
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.42
30:0:2134:G:N2	30:0:2242:U:C2	2.87	0.42
30:0:2414:A:N1	30:0:2415:A:C6	2.88	0.42
30:0:2719:A:H5''	38:0:3702:HOH:O	2.19	0.42
30:0:344:C:H2'	30:0:345:G:O4'	2.20	0.42
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.83	0.42
20:T:32:ARG:NH1	20:T:38:ARG:HH12	2.17	0.42
23:W:13:MET:CE	23:W:17:ILE:HG22	2.49	0.42
23:W:80:ASP:HB2	38:W:3312:HOH:O	2.18	0.42
30:0:1206:U:C6	30:0:1206:U:C3'	3.02	0.42
30:0:1211:G:O2'	30:0:1212:C:H5'	2.19	0.42
30:0:1451:C:H5'	30:0:1505:U:C4	2.54	0.42
30:0:1987:C:H2'	30:0:1988:C:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2134:G:C6	30:0:2258:A:C8	3.08	0.42
30:0:2361:A:H2'	30:0:2362:A:O4'	2.19	0.42
30:0:243:A:H61	30:0:269:G:H1'	1.84	0.42
30:0:2578:G:C8	30:0:2578:G:H5'	2.44	0.42
30:0:2754:G:C2'	30:0:2755:G:H5'	2.49	0.42
30:0:284:C:H4'	30:0:285:A:H8	1.84	0.42
30:0:544:G:C3'	30:0:545:G:H5''	2.48	0.42
30:0:603:A:H4'	30:0:604:G:O5'	2.20	0.42
30:0:843:A:C2	30:0:846:A:C8	3.08	0.42
31:9:14:G:H2'	31:9:15:C:C5'	2.50	0.42
2:B:14:GLY:HA2	2:B:15:PRO:C	2.39	0.42
4:D:23:VAL:HG11	4:D:83:PHE:CZ	2.55	0.42
14:N:34:LEU:HD22	14:N:129:ILE:HD13	2.01	0.42
21:U:17:THR:CG2	21:U:18:GLY:N	2.83	0.42
30:0:1307:A:H2'	30:0:1308:A:C8	2.55	0.42
30:0:2505:G:H2'	30:0:2506:A:C5'	2.50	0.42
30:0:369:G:C2	30:0:370:G:C8	3.08	0.42
30:0:466:A:H2'	30:0:467:G:O4'	2.20	0.42
2:B:314:ALA:CB	2:B:317:PRO:HG3	2.50	0.42
14:N:25:ARG:HB3	30:0:2415:A:C2	2.54	0.42
23:W:7:LEU:HD12	23:W:53:ALA:HB2	2.00	0.42
26:Z:45:VAL:HG12	38:Z:8713:HOH:O	2.19	0.42
30:0:1023:C:H2'	30:0:1024:G:O4'	2.20	0.42
30:0:1244:U:H4'	30:0:1246:A:O4'	2.20	0.42
30:0:1298:U:H2'	30:0:1299:G:C8	2.54	0.42
30:0:1782:G:O2'	30:0:1783:A:H5'	2.19	0.42
30:0:2252:A:C2'	30:0:2253:G:H5'	2.49	0.42
30:0:2756:U:C2	30:0:2896:A:H2	2.38	0.42
30:0:2909:G:H2'	30:0:2910:A:H8	1.84	0.42
30:0:539:G:H2'	30:0:540:A:C8	2.54	0.42
30:0:790:A:H8	38:0:6134:HOH:O	2.01	0.42
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.85	0.42
3:C:85:LYS:HA	3:C:85:LYS:HD2	1.90	0.42
4:D:170:TYR:CD1	4:D:170:TYR:N	2.87	0.42
8:H:4:LYS:HA	8:H:5:PRO:HD3	1.86	0.42
8:H:87:LYS:NZ	8:H:87:LYS:HB2	2.35	0.42
13:M:124:GLY:HA3	30:0:2132:C:H1'	2.02	0.42
15:O:96:VAL:HG12	15:O:97:SER:O	2.20	0.42
18:R:69:LYS:HB2	18:R:72:VAL:HG23	2.01	0.42
22:V:12:THR:HG22	22:V:15:GLU:CG	2.47	0.42
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:37:LEU:O	24:X:41:PHE:HB2	2.19	0.42
30:0:1198:U:H1'	30:0:1201:C:C5	2.50	0.42
30:0:1433:G:O2'	30:0:1434:A:H5'	2.20	0.42
30:0:1676:G:C2'	30:0:1677:U:H5'	2.50	0.42
30:0:2783:A:O2'	30:0:2784:A:H5'	2.19	0.42
30:0:417:G:P	38:0:7457:HOH:O	2.77	0.42
14:N:159:TYR:HE1	31:9:50:G:H5''	1.85	0.42
1:A:23:TYR:HD1	30:0:1872:C:H2'	1.85	0.42
1:A:94:LEU:N	1:A:94:LEU:HD23	2.34	0.42
2:B:27:ASN:H	2:B:27:ASN:HD22	1.67	0.42
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.19	0.42
19:S:56:ASN:O	28:2:8:LYS:NZ	2.51	0.42
24:X:37:LEU:HD21	24:X:72:VAL:HG11	2.02	0.42
24:X:8:ARG:NH1	30:0:2904:U:H4'	2.35	0.42
30:0:128:A:C8	30:0:128:A:C3'	3.03	0.42
30:0:1334:C:H2'	30:0:1335:C:H6	1.85	0.42
30:0:2509:A:OP2	30:0:2510:C:C5	2.72	0.42
30:0:2712:G:P	38:0:5251:HOH:O	2.77	0.42
30:0:2718:C:H5'	30:0:2718:C:C6	2.53	0.42
30:0:2908:A:C2'	30:0:2909:G:H5'	2.49	0.42
1:A:107:ASN:OD1	1:A:116:GLY:HA3	2.20	0.42
1:A:54:PRO:HG2	1:A:160:ALA:HB3	2.02	0.42
1:A:211:LYS:HB2	38:A:9075:HOH:O	2.19	0.42
2:B:243:ASN:HA	2:B:244:PRO:C	2.40	0.42
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.85	0.42
3:C:5:ILE:HD11	3:C:16:VAL:HG23	2.01	0.42
10:J:45:VAL:HG11	10:J:121:LEU:HD22	2.02	0.42
18:R:29:LYS:NZ	38:R:8944:HOH:O	2.53	0.42
25:Y:154:ARG:HH22	30:0:1071:G:H4'	1.85	0.41
30:0:129:A:O2'	30:0:131:A:OP1	2.36	0.41
30:0:1335:C:H2'	30:0:1336:U:C6	2.55	0.41
30:0:1406:A:H4'	30:0:1407:A:C5'	2.50	0.41
30:0:1562:C:N4	38:0:5895:HOH:O	2.53	0.41
30:0:1789:G:C2'	30:0:1790:C:O5'	2.68	0.41
4:D:105:SER:OG	30:0:2338:G:H1'	2.20	0.41
30:0:259:G:O2'	30:0:260:C:H5'	2.20	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.20	0.41
30:0:2727:A:C6	30:0:2756:U:C2	3.08	0.41
30:0:821:U:H2'	30:0:822:C:H6	1.84	0.41
30:0:883:U:C2'	30:0:883:U:O2	2.67	0.41
30:0:960:G:H2'	30:0:961:A:OP2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:18:GLN:HG3	38:3:9009:HOH:O	2.20	0.41
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.20	0.41
6:F:39:SER:HB3	6:F:45:ALA:HB2	2.02	0.41
10:J:131:THR:HG22	10:J:134:GLU:H	1.85	0.41
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.17	0.41
14:N:147:ILE:HB	38:9:9090:HOH:O	2.19	0.41
30:0:1052:G:C5	30:0:1063:G:C6	3.09	0.41
25:Y:142:SER:OG	30:0:1331:G:OP2	2.34	0.41
30:0:420:U:H2'	30:0:421:C:C6	2.55	0.41
30:0:64:G:H2'	30:0:65:C:O4'	2.20	0.41
31:9:47:A:H2'	31:9:48:C:O4'	2.20	0.41
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.51	0.41
2:B:40:GLY:O	2:B:193:ILE:HD13	2.20	0.41
3:C:193:LEU:HD12	3:C:211:ASP:O	2.20	0.41
4:D:22:VAL:HG22	4:D:74:THR:HG22	2.00	0.41
4:D:37:ALA:O	4:D:40:ILE:HG12	2.20	0.41
12:L:150:GLN:HB3	38:L:8868:HOH:O	2.20	0.41
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.44	0.41
19:S:11:THR:H	19:S:14:ALA:HB3	1.84	0.41
9:I:69:PRO:HA	30:0:1164:U:OP1	2.21	0.41
30:0:1167:G:C2	30:0:1168:C:C2	3.08	0.41
30:0:1185:U:H5'	38:0:7504:HOH:O	2.20	0.41
30:0:1840:A:H4'	30:0:1841:C:O5'	2.20	0.41
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.41
30:0:506:G:N2	30:0:509:A:H5''	2.32	0.41
27:1:45:ARG:HB3	38:1:988:HOH:O	2.20	0.41
28:2:41:HIS:CD2	28:2:43:ARG:H	2.39	0.41
2:B:248:ARG:NH1	38:B:9090:HOH:O	2.53	0.41
2:B:75:GLU:C	2:B:77:PRO:HD3	2.40	0.41
4:D:141:VAL:HG21	31:9:57:A:H8	1.85	0.41
14:N:37:ARG:HD3	33:N:8807:CL:CL	2.57	0.41
30:0:1422:U:O2'	30:0:1423:C:H5'	2.20	0.41
30:0:1474:C:C5'	30:0:1474:C:C6	2.89	0.41
30:0:1909:A:H2'	30:0:1910:A:C8	2.54	0.41
30:0:151:A:C2	30:0:442:A:C8	3.09	0.41
30:0:635:A:H2'	30:0:636:G:H5''	2.02	0.41
30:0:729:C:C2	30:0:743:G:C2	3.08	0.41
28:2:41:HIS:N	28:2:45:ASN:HD22	2.03	0.41
31:9:45:A:C5	31:9:46:C:C5	3.08	0.41
9:I:101:LYS:O	9:I:105:GLU:HG3	2.21	0.41
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1138:G:H4'	38:0:5739:HOH:O	2.18	0.41
30:0:1342:C:O2'	30:0:1343:C:H5'	2.20	0.41
30:0:1667:A:C2	30:0:1668:U:C2	3.08	0.41
30:0:1903:U:O2'	30:0:1904:A:C8	2.68	0.41
30:0:2421:G:H4'	38:0:4814:HOH:O	2.20	0.41
30:0:2704:C:H2'	30:0:2705:U:O4'	2.20	0.41
28:2:37:HIS:CE1	30:0:462:A:C8	3.08	0.41
30:0:834:G:H3'	30:0:835:U:H4'	2.01	0.41
1:A:36:ASP:O	1:A:38:ILE:N	2.53	0.41
3:C:223:LEU:HA	3:C:223:LEU:HD12	1.91	0.41
16:P:7:LYS:HG2	16:P:23:PHE:CE2	2.55	0.41
24:X:39:LYS:HE2	30:0:2834:G:OP1	2.20	0.41
30:0:2102:G:C2	30:0:2104:C:C4	3.08	0.41
30:0:2361:A:H8	30:0:2361:A:H5'	1.86	0.41
30:0:2419:U:H5'	30:0:2420:G:C5'	2.50	0.41
30:0:243:A:H61	30:0:269:G:C1'	2.34	0.41
30:0:2637:A:C5'	38:0:4961:HOH:O	2.59	0.41
30:0:2791:U:H4'	30:0:2792:A:OP1	2.20	0.41
30:0:2802:C:H2'	30:0:2803:C:C6	2.55	0.41
30:0:290:C:H1'	38:0:6136:HOH:O	2.21	0.41
30:0:318:U:H5'	30:0:339:A:C2	2.56	0.41
29:3:38:ARG:HD2	30:0:396:U:OP2	2.21	0.41
30:0:482:G:H4'	30:0:508:A:N1	2.36	0.41
2:B:215:VAL:HA	2:B:220:VAL:HG22	2.02	0.41
3:C:154:VAL:O	3:C:158:GLU:HG3	2.21	0.41
10:J:52:GLN:HE22	30:0:1119:G:H8	1.69	0.41
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.20	0.41
16:P:59:ARG:O	16:P:63:ARG:HG3	2.21	0.41
19:S:57:THR:C	19:S:59:ASP:H	2.24	0.41
24:X:43:VAL:HG11	24:X:82:GLU:HA	2.01	0.41
30:0:1377:C:C5'	30:0:1377:C:H6	2.33	0.41
30:0:1481:G:H2'	30:0:1482:A:O4'	2.20	0.41
30:0:1548:U:H1'	38:0:6897:HOH:O	2.19	0.41
30:0:2089:A:C2'	30:0:2090:G:H5'	2.49	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.20	0.41
30:0:290:C:O2'	30:0:291:C:H5'	2.20	0.41
30:0:559:U:H5'	30:0:559:U:C6	2.35	0.41
27:1:5:THR:HG23	30:0:1688:G:O2'	2.20	0.41
29:3:69:TYR:CZ	29:3:80:ARG:HD2	2.56	0.41
1:A:212:PRO:HB2	38:0:4392:HOH:O	2.20	0.41
1:A:217:ARG:HG2	1:A:229:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:VAL:CG1	2:B:334:SER:HA	2.50	0.41
13:M:67:VAL:HB	13:M:97:ILE:HG23	2.03	0.41
16:P:94:TRP:CZ2	16:P:98:ILE:HG13	2.56	0.41
25:Y:213:LYS:HE3	25:Y:213:LYS:HB2	1.90	0.41
30:0:1544:U:O2'	30:0:1545:C:H5'	2.20	0.41
30:0:1714:C:C2'	30:0:1715:C:H5'	2.51	0.41
30:0:1804:A:H2'	30:0:1805:G:C8	2.56	0.41
30:0:2617:G:C2	30:0:2618:G:C8	3.08	0.41
30:0:2802:C:H2'	30:0:2803:C:H6	1.84	0.41
30:0:667:C:H2'	30:0:668:C:H6	1.85	0.41
30:0:81:G:N3	30:0:98:A:C2	2.88	0.41
31:9:13:A:OP1	31:9:113:C:H5'	2.21	0.41
1:A:95:PRO:HA	1:A:153:ARG:HA	2.03	0.41
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.48	0.41
11:K:30:LYS:HB3	11:K:56:SER:HB3	2.03	0.41
13:M:167:GLY:O	13:M:171:ARG:HG3	2.21	0.41
14:N:160:SER:CB	31:9:51:A:H5'	2.50	0.41
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.21	0.41
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.56	0.41
15:O:98:LEU:O	15:O:102:ILE:HG13	2.21	0.41
16:P:83:LYS:O	16:P:86:ALA:HB3	2.21	0.41
18:R:17:MET:SD	38:R:8951:HOH:O	2.62	0.41
22:V:27:LEU:HA	22:V:49:LEU:HD13	2.02	0.41
23:W:48:VAL:HG12	23:W:48:VAL:O	2.19	0.41
30:0:1166:A:N3	30:0:1166:A:H2'	2.35	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.36	0.41
30:0:130:C:H2'	38:0:3183:HOH:O	2.20	0.41
30:0:969:G:H2'	30:0:970:U:C6	2.56	0.41
31:9:34:A:H2'	31:9:35:C:O4'	2.21	0.41
3:C:76:ARG:NH1	3:C:76:ARG:HB3	2.36	0.41
4:D:25:MET:HE1	4:D:37:ALA:O	2.21	0.41
13:M:164:THR:CG2	13:M:165:GLY:N	2.83	0.41
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.49	0.41
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.51	0.41
15:O:115:ARG:NH1	38:O:6194:HOH:O	2.54	0.41
26:Z:50:VAL:O	26:Z:54:GLU:HG3	2.20	0.41
30:0:1634:G:C5	30:0:1635:U:C4	3.08	0.41
30:0:1909:A:N1	30:0:2128:G:H1'	2.35	0.41
30:0:1945:G:O2'	30:0:1946:C:H5'	2.20	0.41
30:0:2039:A:H2'	30:0:2040:C:C6	2.56	0.41
30:0:2246:U:N3	30:0:2256:G:C2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:N:8830:HOH:O	30:0:2368:A:H8	2.04	0.41
30:0:23:G:C6	30:0:24:G:N1	2.89	0.41
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.85	0.41
2:B:154:VAL:CG1	2:B:156:LYS:HG2	2.51	0.41
20:T:79:LEU:HG	20:T:89:ARG:HB2	2.03	0.41
38:K:7438:HOH:O	21:U:20:MET:HE2	2.21	0.41
22:V:39:ALA:C	22:V:41:GLU:H	2.23	0.41
30:0:1119:G:N2	30:0:1246:A:N1	2.69	0.41
30:0:1163:G:N2	38:0:6078:HOH:O	2.54	0.41
30:0:1271:A:C2	30:0:1286:A:C2	3.09	0.41
30:0:1522:A:C2'	30:0:1523:G:H5'	2.51	0.41
30:0:1574:C:H6	30:0:1574:C:O5'	2.04	0.41
30:0:1613:C:H2'	30:0:1614:G:O4'	2.21	0.41
30:0:2072:G:N2	38:0:6910:HOH:O	2.54	0.41
30:0:2251:G:C6	30:0:2252:A:C6	3.09	0.41
30:0:595:U:O2'	30:0:596:C:H5'	2.21	0.41
29:3:70:ARG:HD3	38:3:9064:HOH:O	2.21	0.41
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.02	0.41
30:0:106:A:H2'	30:0:107:U:O4'	2.21	0.40
30:0:1098:A:H2'	30:0:1099:G:O4'	2.21	0.40
30:0:1182:C:O2'	30:0:1183:C:H5	2.04	0.40
30:0:1515:A:H2'	30:0:1516:U:H6	1.82	0.40
30:0:1520:G:C6	30:0:1521:C:C4	3.09	0.40
30:0:1536:C:H6	30:0:1536:C:O5'	2.03	0.40
30:0:1750:C:N4	30:0:1751:G:C6	2.89	0.40
30:0:1758:U:H2'	30:0:1759:A:O4'	2.22	0.40
30:0:2332:A:C2	30:0:2355:G:C5	3.09	0.40
30:0:2334:C:O2'	30:0:2335:C:H5'	2.21	0.40
30:0:369:G:O2'	30:0:370:G:H5'	2.21	0.40
30:0:401:C:H2'	30:0:402:U:C6	2.56	0.40
30:0:745:G:H5''	30:0:746:A:OP1	2.21	0.40
31:9:64:C:O2'	31:9:65:A:H5'	2.21	0.40
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.86	0.40
2:B:154:VAL:HG12	2:B:156:LYS:HG2	2.02	0.40
4:D:25:MET:HE3	4:D:37:ALA:HB1	2.04	0.40
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.03	0.40
25:Y:106:THR:HG23	25:Y:107:PRO:HD2	2.03	0.40
25:Y:189:ASN:ND2	25:Y:192:ASP:H	2.19	0.40
30:0:1192:A:H3'	30:0:1193:A:H5'	2.02	0.40
30:0:1327:G:N1	30:0:1330:A:OP2	2.52	0.40
30:0:1617:C:C4	30:0:1643:C:H4'	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1700:C:H5''	30:0:1701:A:OP2	2.22	0.40
30:0:1377:C:H2'	30:0:1723:G:O6	2.21	0.40
30:0:1947:G:C8	30:0:1970:G:C8	3.09	0.40
30:0:2253:G:C2	30:0:2254:G:C8	3.09	0.40
30:0:2524:G:H21	30:0:2526:C:H41	1.67	0.40
30:0:278:A:C6	30:0:279:C:C4	3.09	0.40
30:0:74:G:H2'	30:0:75:U:C6	2.56	0.40
2:B:234:ARG:HD3	30:0:1734:C:OP1	2.21	0.40
12:L:143:THR:HG21	38:L:8837:HOH:O	2.21	0.40
14:N:154:LEU:C	14:N:156:GLU:H	2.24	0.40
30:0:111:C:O2'	30:0:112:G:H5'	2.21	0.40
30:0:1163:G:C4	30:0:1164:U:C5	3.09	0.40
30:0:1183:C:O2	30:0:1183:C:C2'	2.69	0.40
30:0:1409:G:C2	30:0:1410:G:C8	3.10	0.40
30:0:1896:G:H1'	38:0:4284:HOH:O	2.21	0.40
30:0:1947:G:N2	30:0:1966:U:C2	2.90	0.40
30:0:200:C:H6	38:0:3463:HOH:O	2.03	0.40
30:0:255:A:C5	30:0:256:C:C5	3.09	0.40
30:0:2626:C:H2'	30:0:2627:G:C8	2.56	0.40
30:0:2727:A:N1	30:0:2756:U:C2	2.90	0.40
30:0:2782:G:O6	30:0:2790:C:H5''	2.21	0.40
30:0:932:U:H2'	30:0:933:C:C6	2.57	0.40
31:9:26:C:H2'	31:9:27:C:C6	2.57	0.40
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.80	0.40
8:H:76:LEU:HD21	8:H:149:VAL:HA	2.02	0.40
8:H:91:ARG:HG2	8:H:91:ARG:H	1.59	0.40
20:T:24:ARG:NH2	20:T:39:ASN:HD22	2.07	0.40
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.37	0.40
30:0:1149:U:C5	30:0:1215:A:C5	3.09	0.40
30:0:1414:A:H2'	30:0:1415:G:O4'	2.21	0.40
30:0:1503:U:H3'	30:0:1503:U:H6	1.86	0.40
30:0:1741:U:C5'	30:0:1742:A:OP1	2.63	0.40
30:0:2112:A:H2'	30:0:2113:G:C8	2.56	0.40
30:0:2726:U:O2	30:0:2749:U:O5'	2.40	0.40
30:0:2842:G:C2'	30:0:2843:A:H5'	2.51	0.40
30:0:445:U:H2'	30:0:446:G:C8	2.56	0.40
30:0:724:G:O2'	30:0:725:C:H5'	2.22	0.40
30:0:806:A:H2'	30:0:807:A:O4'	2.22	0.40
30:0:853:C:H2'	30:0:854:G:O4'	2.21	0.40
31:9:39:U:H3'	31:9:40:C:H5''	2.02	0.40
1:A:86:ALA:HB3	1:A:94:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:VAL:HG11	2:B:301:VAL:HG13	2.04	0.40
3:C:107:ARG:NH1	3:C:107:ARG:HB3	2.37	0.40
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.95	0.40
23:W:90:TYR:CE2	23:W:99:ALA:HB2	2.56	0.40
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.21	0.40
30:0:47:G:N3	30:0:114:A:C2	2.90	0.40
30:0:138:U:OP2	30:0:139:C:C5	2.73	0.40
30:0:1705:C:H2'	30:0:1706:G:O4'	2.20	0.40
30:0:1878:G:H2'	38:0:3278:HOH:O	2.21	0.40
30:0:2016:U:H6	30:0:2016:U:O5'	2.05	0.40
30:0:234:A:H4'	30:0:437:A:O4'	2.22	0.40
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.36	0.40
30:0:517:U:H1'	38:0:7614:HOH:O	2.21	0.40
30:0:907:A:H2'	30:0:908:A:H8	1.85	0.40
28:2:5:LYS:O	28:2:9:LYS:HG3	2.22	0.40
3:C:118:THR:O	3:C:136:VAL:HG13	2.22	0.40
3:C:16:VAL:HG12	3:C:17:ASP:N	2.36	0.40
3:C:236:THR:HG22	3:C:239:ALA:CB	2.51	0.40
3:C:2:GLN:HB3	38:C:8530:HOH:O	2.21	0.40
20:T:82:THR:HG21	30:0:488:U:O2'	2.21	0.40
23:W:149:LEU:HG	23:W:153:MET:HE1	2.03	0.40
25:Y:144:ARG:NH1	38:Y:8871:HOH:O	2.53	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%)	212 (90%)	18 (8%)	5 (2%)	8	20
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	19	44
3	C	244/246 (99%)	228 (93%)	16 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	7	19
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
6	F	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	19	44
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	149 (96%)	6 (4%)	1 (1%)	27	54
9	I	68/162 (42%)	55 (81%)	10 (15%)	3 (4%)	3	6
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
11	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
12	L	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	24	50
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	31	58
14	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	11	27
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	141 (100%)	0	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
19	S	79/85 (93%)	78 (99%)	1 (1%)	0	100	100
20	T	117/120 (98%)	110 (94%)	6 (5%)	1 (1%)	19	44
21	U	51/67 (76%)	47 (92%)	4 (8%)	0	100	100
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	11	27
23	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
24	X	80/92 (87%)	73 (91%)	6 (8%)	1 (1%)	13	33
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
26	Z	71/116 (61%)	61 (86%)	8 (11%)	2 (3%)	5	13
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	16	38
All	All	3705/4472 (83%)	3458 (93%)	220 (6%)	27 (1%)	24	50

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	VAL

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Mol	Chain	Res	Type
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
2	B	34	GLY
6	F	101	ALA
12	L	149	ARG
20	T	53	GLY
26	Z	66	CYS
2	B	185	GLY
4	D	27	ILE
4	D	137	PRO
8	H	19	ARG
2	B	2	GLN
22	V	43	PRO
1	A	36	ASP
4	D	56	ARG
9	I	108	HIS
29	3	56	PRO
26	Z	65	ASN
9	I	83	GLY
24	X	70	ILE
1	A	88	ILE
9	I	125	GLY
1	A	38	ILE
13	M	88	VAL

### 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%)	30	60
2	B	282/283 (100%)	265 (94%)	17 (6%)	21	46
3	C	193/193 (100%)	178 (92%)	15 (8%)	14	32
4	D	117/148 (79%)	109 (93%)	8 (7%)	17	40
5	E	152/156 (97%)	147 (97%)	5 (3%)	41	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	93/94 (99%)	93 (100%)	0	100	100
7	G	27/282 (10%)	26 (96%)	1 (4%)	37	67
8	H	134/145 (92%)	127 (95%)	7 (5%)	25	53
9	I	58/130 (45%)	57 (98%)	1 (2%)	63	87
10	J	118/121 (98%)	112 (95%)	6 (5%)	26	54
11	K	106/106 (100%)	103 (97%)	3 (3%)	47	77
12	L	113/127 (89%)	111 (98%)	2 (2%)	62	86
13	M	158/160 (99%)	150 (95%)	8 (5%)	26	54
14	N	149/150 (99%)	144 (97%)	5 (3%)	40	71
15	O	93/94 (99%)	91 (98%)	2 (2%)	55	83
16	P	113/117 (97%)	108 (96%)	5 (4%)	31	60
17	Q	79/80 (99%)	77 (98%)	2 (2%)	50	80
18	R	117/122 (96%)	113 (97%)	4 (3%)	40	71
19	S	71/74 (96%)	70 (99%)	1 (1%)	69	89
20	T	105/106 (99%)	99 (94%)	6 (6%)	23	48
21	U	44/53 (83%)	43 (98%)	1 (2%)	53	82
22	V	51/57 (90%)	50 (98%)	1 (2%)	58	84
23	W	130/130 (100%)	126 (97%)	4 (3%)	43	73
24	X	66/74 (89%)	60 (91%)	6 (9%)	10	24
25	Y	120/196 (61%)	114 (95%)	6 (5%)	27	55
26	Z	60/94 (64%)	59 (98%)	1 (2%)	63	87
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	52	81
29	3	79/79 (100%)	77 (98%)	2 (2%)	50	80
All	All	3095/3646 (85%)	2967 (96%)	128 (4%)	33	63

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	38	ILE
1	A	68	ILE
1	A	69	LEU

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Mol	Chain	Res	Type
1	A	94	LEU
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	16	ARG
2	B	27	ASN
2	B	49	THR
2	B	56	ASP
2	B	97	LEU
2	B	98	THR
2	B	132	HIS
2	B	162	MET
2	B	184	ASP
2	B	190	MET
2	B	234	ARG
2	B	251	VAL
2	B	254	GLN
2	B	257	THR
2	B	312	ARG
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	115	LEU
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	243	VAL
4	D	19	GLU
4	D	24	HIS
4	D	50	VAL
4	D	52	THR
4	D	137	PRO
4	D	149	ARG
4	D	161	ASP

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Mol	Chain	Res	Type
4	D	170	TYR
5	E	7	ILE
5	E	12	ASP
5	E	16	ASP
5	E	96	ASN
5	E	102	VAL
7	G	64	ASN
8	H	33	GLN
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	169	GLU
8	H	173	GLU
9	I	94	ASP
10	J	46	ILE
10	J	52	GLN
10	J	79	PHE
10	J	107	ASN
10	J	130	VAL
10	J	131	THR
11	K	10	GLN
11	K	55	VAL
11	K	119	GLN
12	L	35	ARG
12	L	101	ASP
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	93	ARG
13	M	99	ARG
13	M	115	LEU
13	M	116	ASN
13	M	164	THR
14	N	26	LEU
14	N	49	THR
14	N	56	ASP
14	N	127	LEU
14	N	138	ASP
15	O	43	VAL
15	O	98	LEU
16	P	21	VAL

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Mol	Chain	Res	Type
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
16	P	110	ASP
17	Q	16	ASN
17	Q	57	ASP
18	R	13	THR
18	R	39	THR
18	R	82	GLU
18	R	143	VAL
19	S	59	ASP
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	52	THR
22	V	65	ASP
23	W	26	ILE
23	W	52	VAL
23	W	142	ASP
23	W	146	ILE
24	X	46	ASP
24	X	49	ARG
24	X	52	PRO
24	X	72	VAL
24	X	82	GLU
24	X	88	GLU
25	Y	115	ARG
25	Y	154	ARG
25	Y	163	THR
25	Y	169	ARG
25	Y	189	ASN
25	Y	203	VAL
26	Z	65	ASN
28	2	18	ASN
29	3	3	MET
29	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	2	GLN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	85	GLN
4	D	103	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	73	ASN
10	J	52	GLN
10	J	107	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	40	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

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Mol	Chain	Res	Type
16	P	118	GLN
17	Q	40	HIS
18	R	22	GLN
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
18	R	122	GLN
19	S	44	GLN
20	T	39	ASN
21	U	39	ASN
22	V	60	GLN
23	W	2	HIS
23	W	28	HIS
23	W	87	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	119	GLN
25	Y	133	HIS
25	Y	134	HIS
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	41	HIS
28	2	45	ASN
29	3	20	HIS
29	3	48	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	239 (8%)	32 (1%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	255 (8%)	33 (1%)

All (255) 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	120	A
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
30	0	236	A
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	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G

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Mol	Chain	Res	Type
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	588	G
30	0	604	G
30	0	605	C
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	698	A
30	0	701	U
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	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U

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Mol	Chain	Res	Type
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
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	1279	U
30	0	1287	A
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1460	G
30	0	1474	C
30	0	1485	A
30	0	1488	U
30	0	1505	U
30	0	1506	U
30	0	1507	C

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Mol	Chain	Res	Type
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1562	C
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
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	1732	A
30	0	1742	A
30	0	1752	G
30	0	1778	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	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1996	U
30	0	2004	U
30	0	2008	U
30	0	2011	A

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Mol	Chain	Res	Type
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
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	2320	U
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	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	2513	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A

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Mol	Chain	Res	Type
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2645	U
30	0	2649	A
30	0	2664	A
30	0	2676	C
30	0	2681	A
30	0	2682	C
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	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2867	G
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
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	40	C
31	9	41	C
31	9	43	G
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A

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Mol	Chain	Res	Type
31	9	114	G
31	9	122	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	169	A
30	0	603	A
30	0	604	G
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	869	G
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1237	U
30	0	1352	A
30	0	1377	C
30	0	1474	C
30	0	1506	U
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1856	C
30	0	1878	G
30	0	1979	G
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2761	A
30	0	2791	U
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	OMU	0	2587	30	14,22,23	1.00	1 (7%)	18,31,34	3.65	2 (11%)
30	OMG	0	2588	30	19,26,27	1.08	2 (10%)	22,38,41	2.43	4 (18%)
30	UR3	0	2619	30	13,22,23	0.70	0	15,32,35	0.69	0
30	PSU	0	2621	30	16,21,22	1.67	3 (18%)	20,30,33	5.44	4 (20%)
30	1MA	0	628	30,35	16,25,26	0.97	1 (6%)	12,37,40	1.29	1 (8%)

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	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.08	1.47	1.52
30	0	2588	OMG	C8-N7	-2.11	1.30	1.34
30	0	2587	OMU	C4-N3	2.54	1.37	1.33
30	0	2621	PSU	C2-N1	2.58	1.43	1.38
30	0	628	1MA	C6-N6	2.73	1.33	1.27
30	0	2621	PSU	C4-N3	2.73	1.37	1.33
30	0	2588	OMG	C6-N1	3.39	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.45	114.39	128.41
30	0	2588	OMG	C5-C6-N1	-8.19	111.82	123.47
30	0	2621	PSU	C5-C4-N3	-8.16	114.84	125.36
30	0	628	1MA	C2-N3-C4	-3.87	110.60	116.51
30	0	2587	OMU	C5-C4-N3	-3.62	114.77	123.17
30	0	2588	OMG	C2-N3-C4	-2.84	111.84	115.16
30	0	2588	OMG	N3-C2-N1	-2.40	123.89	127.41
30	0	2621	PSU	C6-N1-C2	2.94	120.06	115.36
30	0	2588	OMG	C6-N1-C2	6.23	125.02	116.06
30	0	2621	PSU	C4-N3-C2	14.10	127.14	115.14
30	0	2587	OMU	C4-N3-C2	14.93	126.98	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.