Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 11:43 AM EST

PDB ID	:	3CCV
Title	:	Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2616A
Authors	:	Blaha, G.; Gurel, G.
Deposited on	:	2008-02-26
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

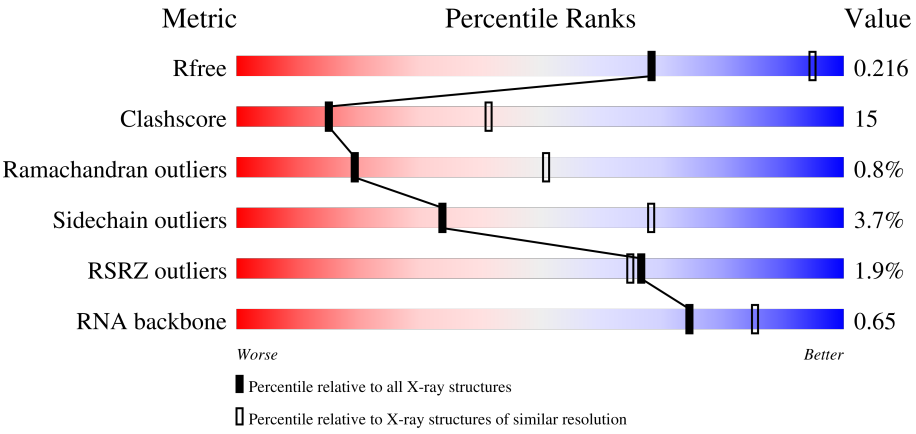
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	240	68% 28%
2	B	338	64% 32%
3	C	246	70% 28%
4	D	177	16% 50% 27% 21%

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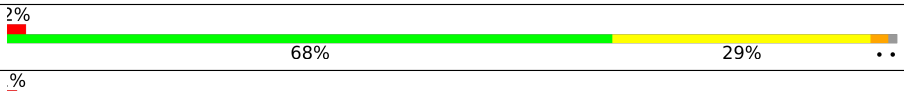
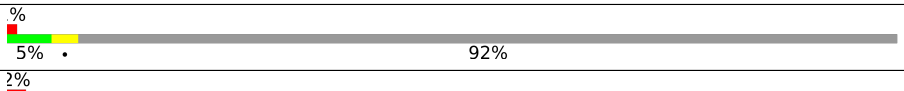
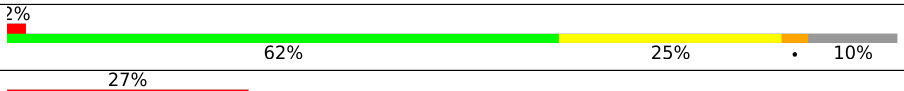
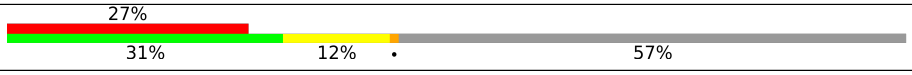
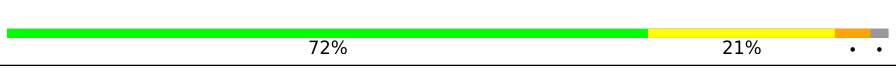
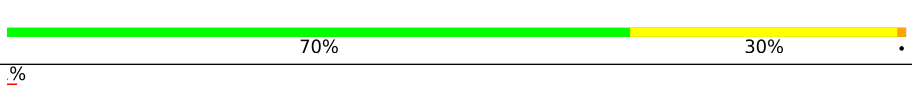
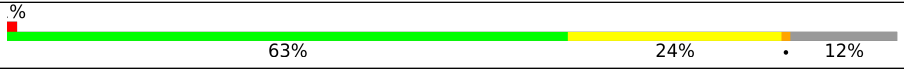
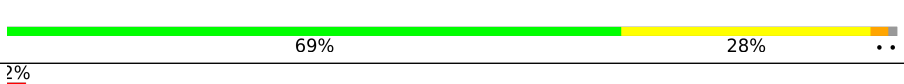
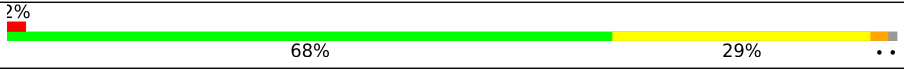
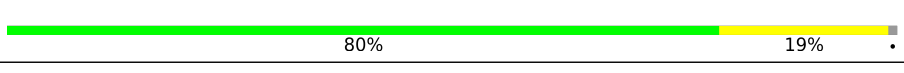
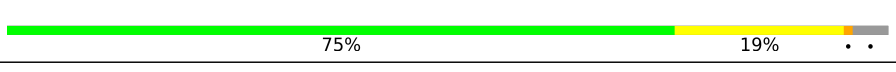
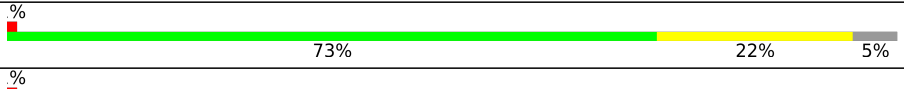
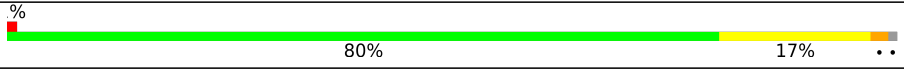
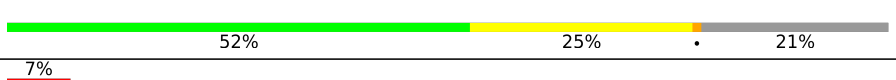
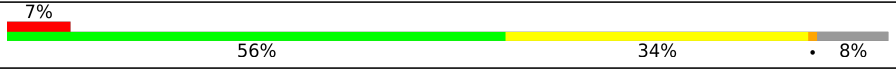
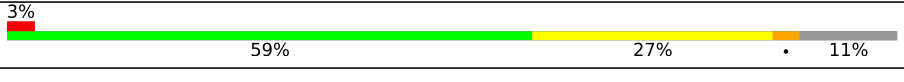
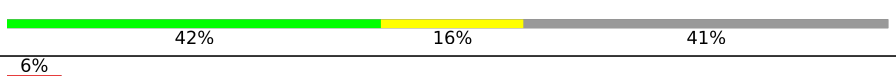
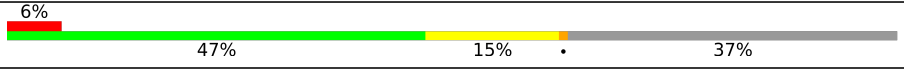
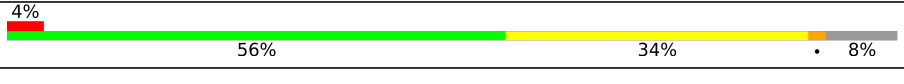
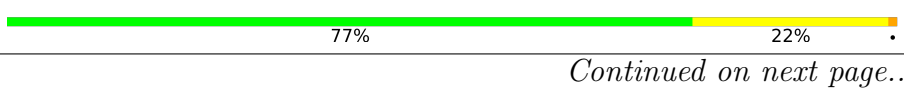
Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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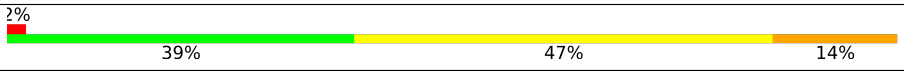
Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CL	J	8801	-	-	X	-
34	SR	0	8982	-	-	-	X
34	SR	0	9004	-	-	-	X
34	SR	0	9006	-	-	-	X
35	NA	0	8556	-	-	-	X

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 99121 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
			Total	C	N	O	S			
1	A	237	1753	1072	352	324	5	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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
			59019	26349	10873	19052	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	A	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	0	87	Total	Mg	0	0
			87	87		
32	9	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	A	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	J	3	Total Cl 3 3	0	0
33	L	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	0	10	Total Cl 10 10	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	3	Total Sr 3 3	0	0
34	B	2	Total Sr 2 2	0	0
34	F	1	Total Sr 1 1	0	0
34	R	1	Total Sr 1 1	0	0
34	S	1	Total Sr 1 1	0	0
34	Y	1	Total Sr 1 1	0	0
34	1	2	Total Sr 2 2	0	0
34	3	1	Total Sr 1 1	0	0
34	0	94	Total Sr 94 94	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	9	2	Total Sr 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	0	67	Total Na 67 67	0	0
35	9	2	Total Na 2 2	0	0

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

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

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	112	Total O 112 112	0	0
38	B	149	Total O 149 149	0	0
38	C	185	Total O 185 185	0	0
38	D	49	Total O 49 49	0	0
38	E	45	Total O 45 45	0	0
38	F	26	Total O 26 26	0	0
38	G	17	Total O 17 17	0	0
38	H	67	Total O 67 67	0	0
38	I	8	Total O 8 8	0	0
38	J	51	Total O 51 51	0	0
38	K	51	Total O 51 51	0	0
38	L	89	Total O 89 89	0	0
38	M	133	Total O 133 133	0	0
38	N	61	Total O 61 61	0	0
38	O	39	Total O 39 39	0	0
38	P	62	Total O 62 62	0	0
38	Q	45	Total O 45 45	0	0
38	R	81	Total O 81 81	0	0
38	S	32	Total O 32 32	0	0
38	T	35	Total O 35 35	0	0
38	U	29	Total O 29 29	0	0

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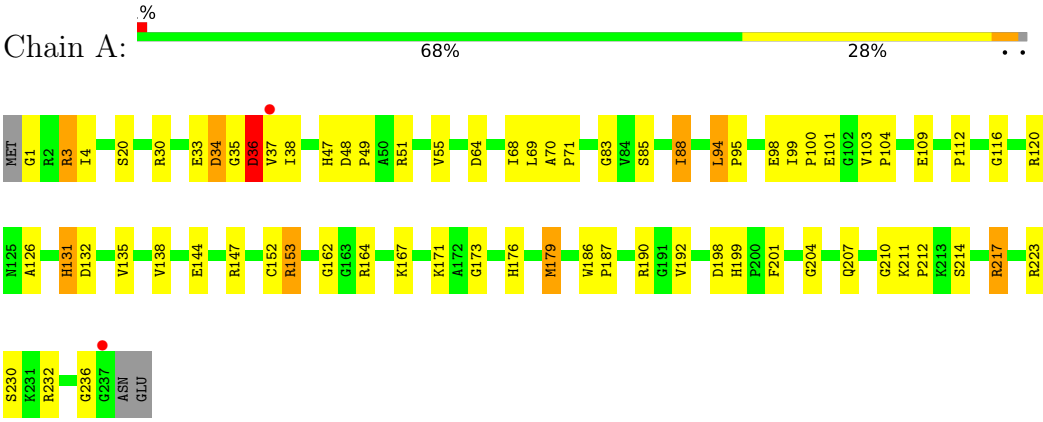
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	V	15	Total O 15 15	0	0
38	W	67	Total O 67 67	0	0
38	X	26	Total O 26 26	0	0
38	Y	98	Total O 98 98	0	0
38	Z	32	Total O 32 32	0	0
38	1	54	Total O 54 54	0	0
38	2	44	Total O 44 44	0	0
38	3	69	Total O 69 69	0	0
38	0	5910	Total O 5910 5910	0	0
38	9	142	Total O 142 142	0	0

3 Residue-property plots (i)

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

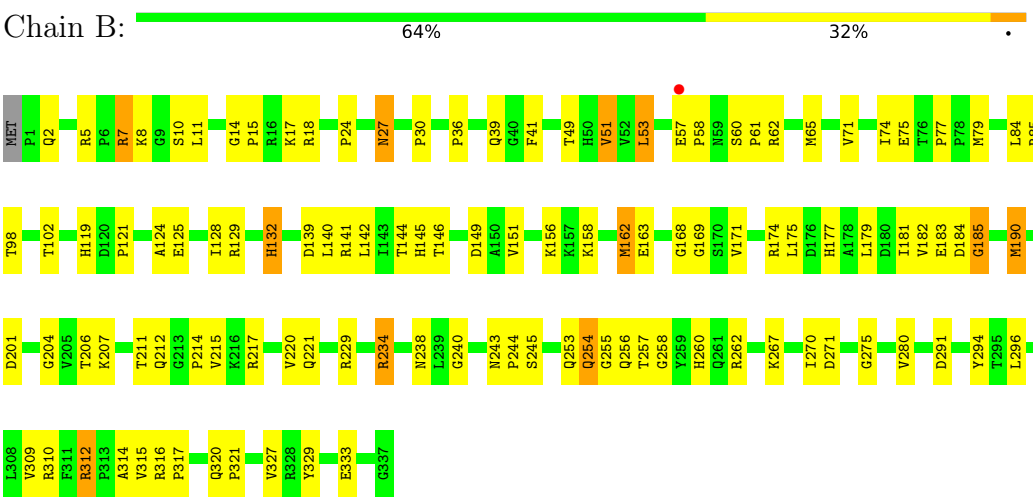
• Molecule 1: 50S ribosomal protein L2P

Chain A:



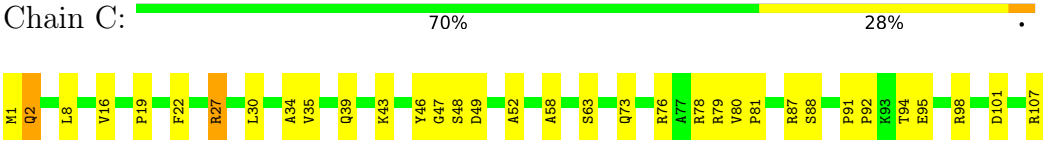
• Molecule 2: 50S ribosomal protein L3P

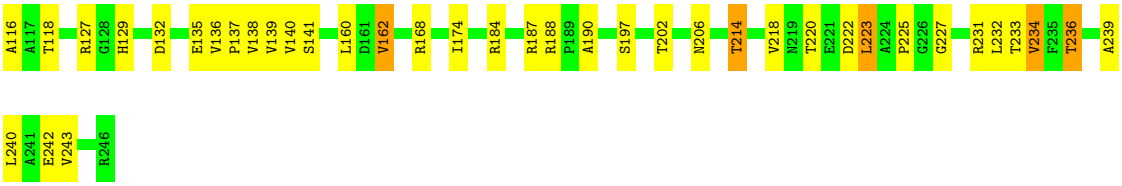
Chain B:



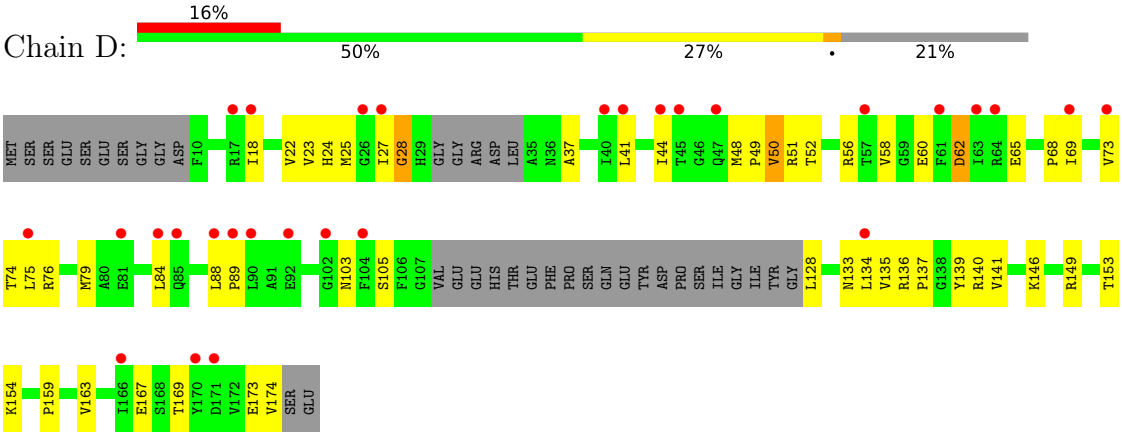
• Molecule 3: 50S ribosomal protein L4P

Chain C:

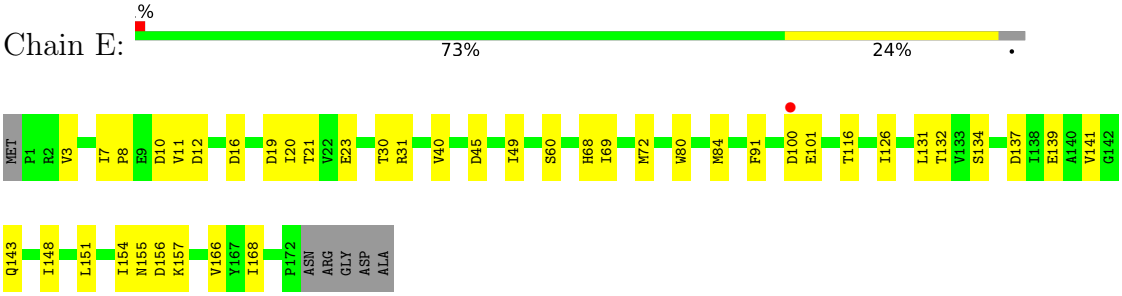




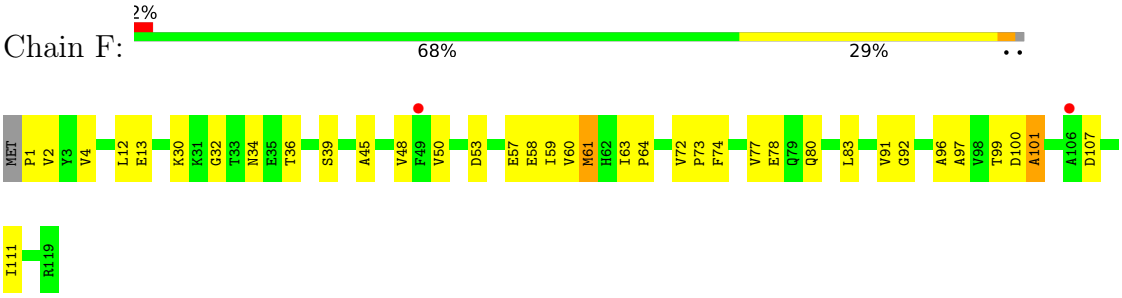
• Molecule 4: 50S ribosomal protein L5P



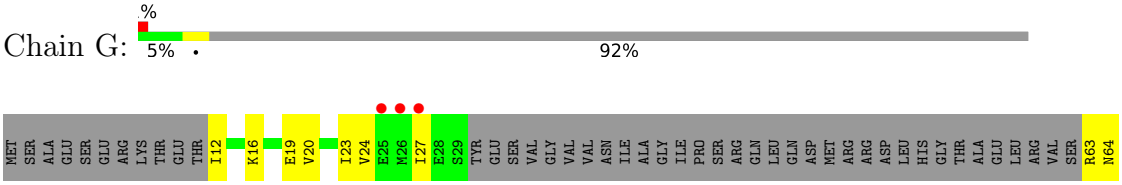
• Molecule 5: 50S ribosomal protein L6P



• Molecule 6: 50S ribosomal protein L7Ae

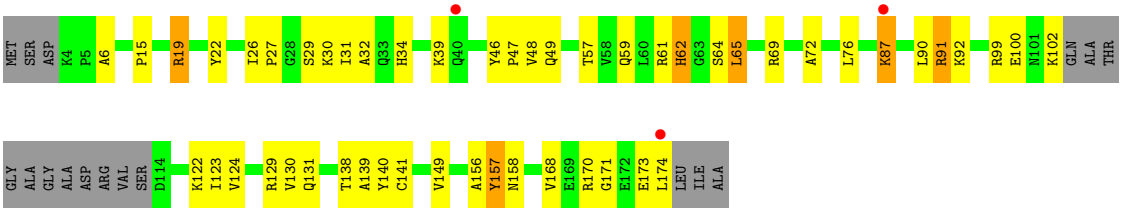


• Molecule 7: 50S ribosomal protein L10E



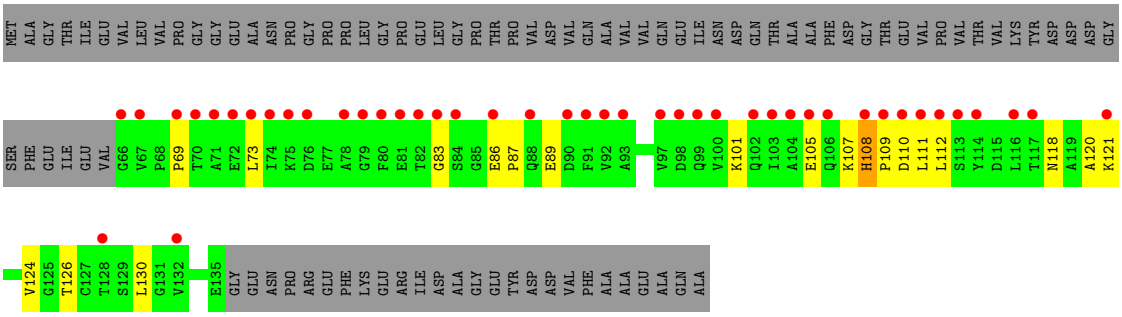
• Molecule 8: 50S ribosomal protein L10e

Chain H:



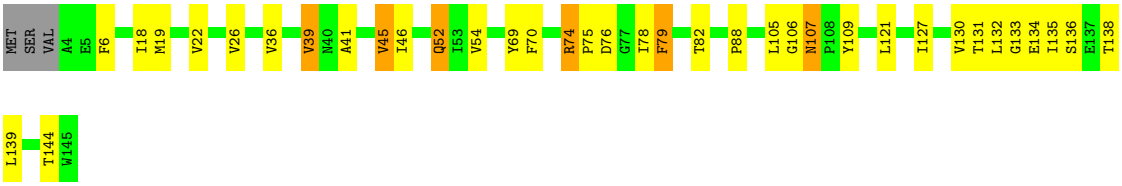
• Molecule 9: 50S ribosomal protein L11P

Chain I:



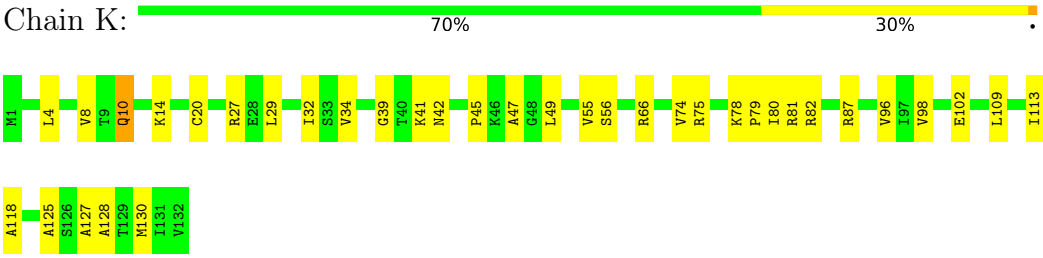
• Molecule 10: 50S ribosomal protein L13P

Chain J:



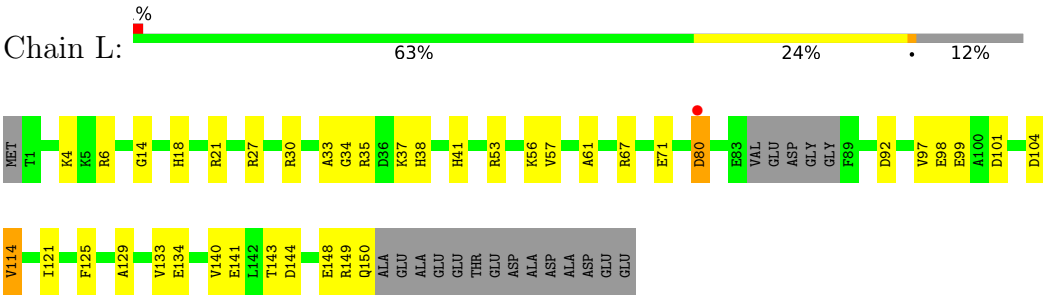
• Molecule 11: 50S ribosomal protein L14P

Chain K:



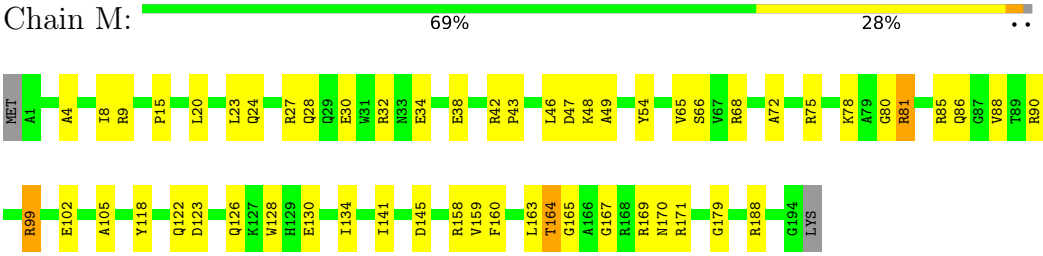
• Molecule 12: 50S ribosomal protein L15P

Chain L:



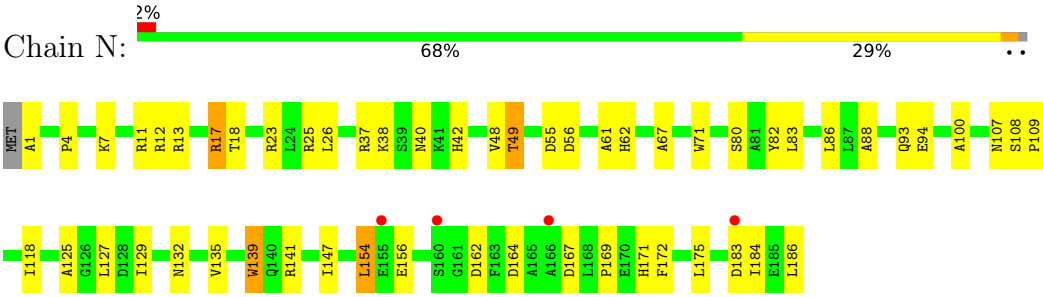
• Molecule 13: 50S ribosomal protein L15e

Chain M:



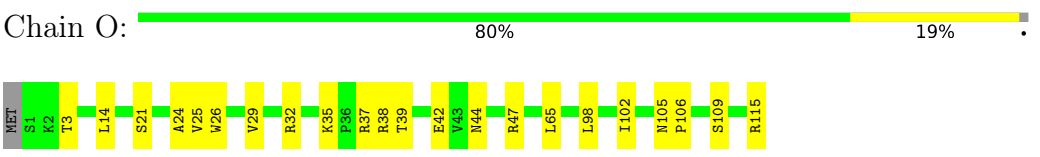
• Molecule 14: 50S ribosomal protein L18P

Chain N:



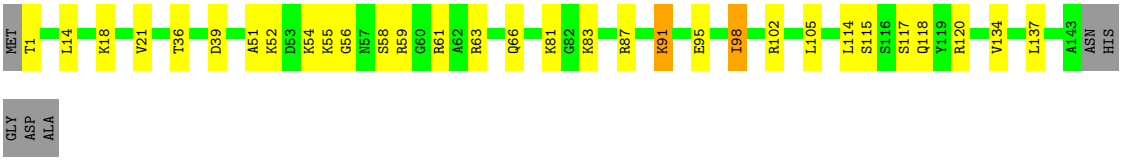
• Molecule 15: 50S ribosomal protein L18e

Chain O:

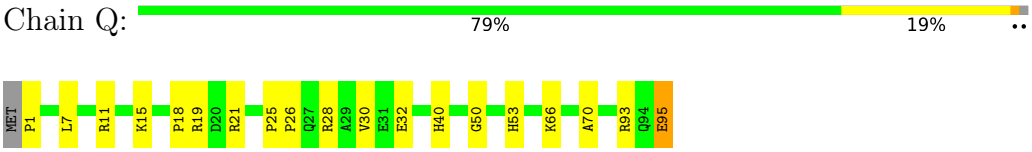


• Molecule 16: 50S ribosomal protein L19e

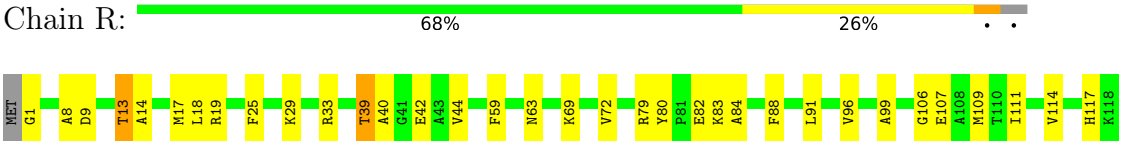
Chain P:



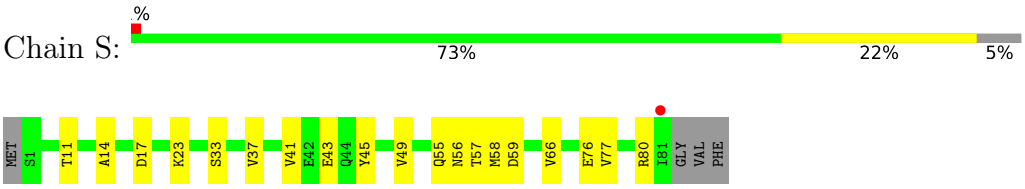
• Molecule 17: 50S ribosomal protein L21e



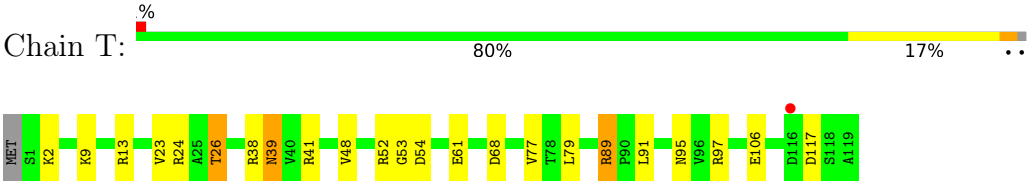
• Molecule 18: 50S ribosomal protein L22P



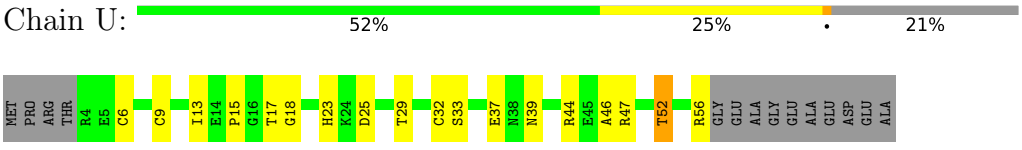
• Molecule 19: 50S ribosomal protein L23P



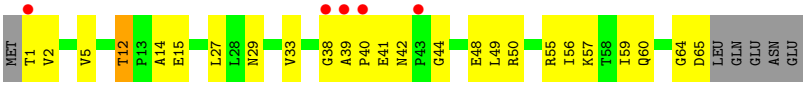
• Molecule 20: 50S ribosomal protein L24P



• Molecule 21: 50S ribosomal protein L24e

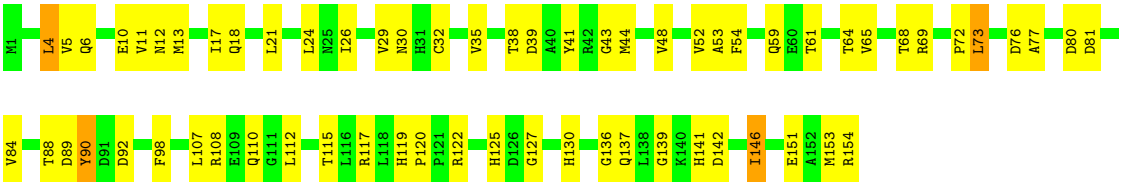


• Molecule 22: 50S ribosomal protein L29P



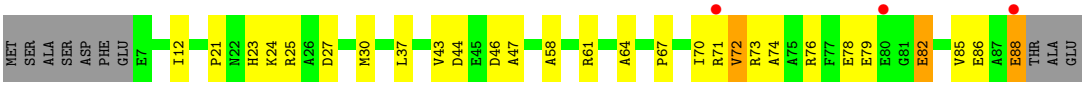
• Molecule 23: 50S ribosomal protein L30P

Chain W:



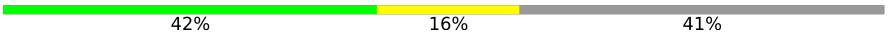
• Molecule 24: 50S ribosomal protein L31e

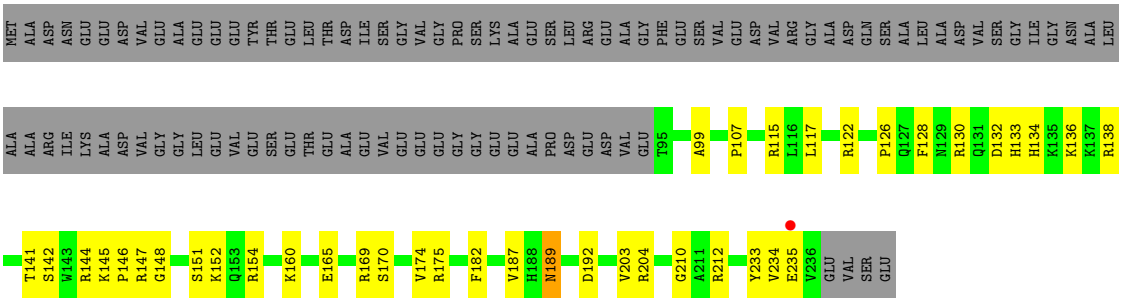
Chain X:



• Molecule 25: 50S ribosomal protein L32e

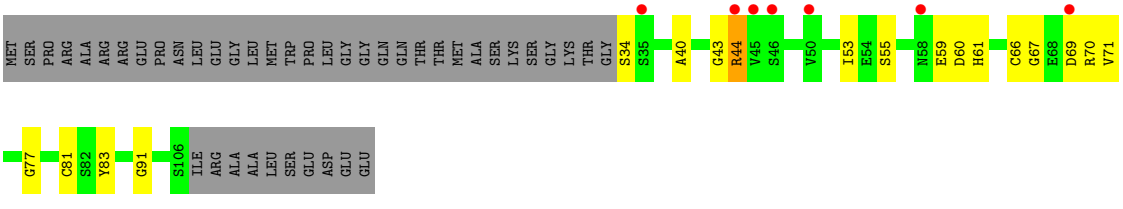
Chain Y:





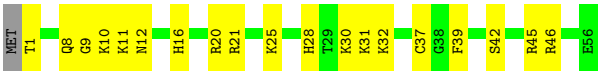
• Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



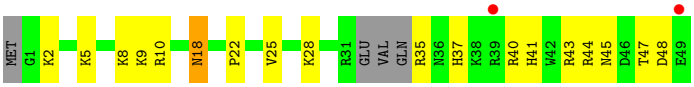
• Molecule 27: 50S ribosomal protein L37e

Chain 1:



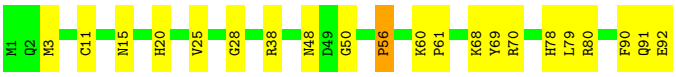
• Molecule 28: 50S ribosomal protein L39e

Chain 2:



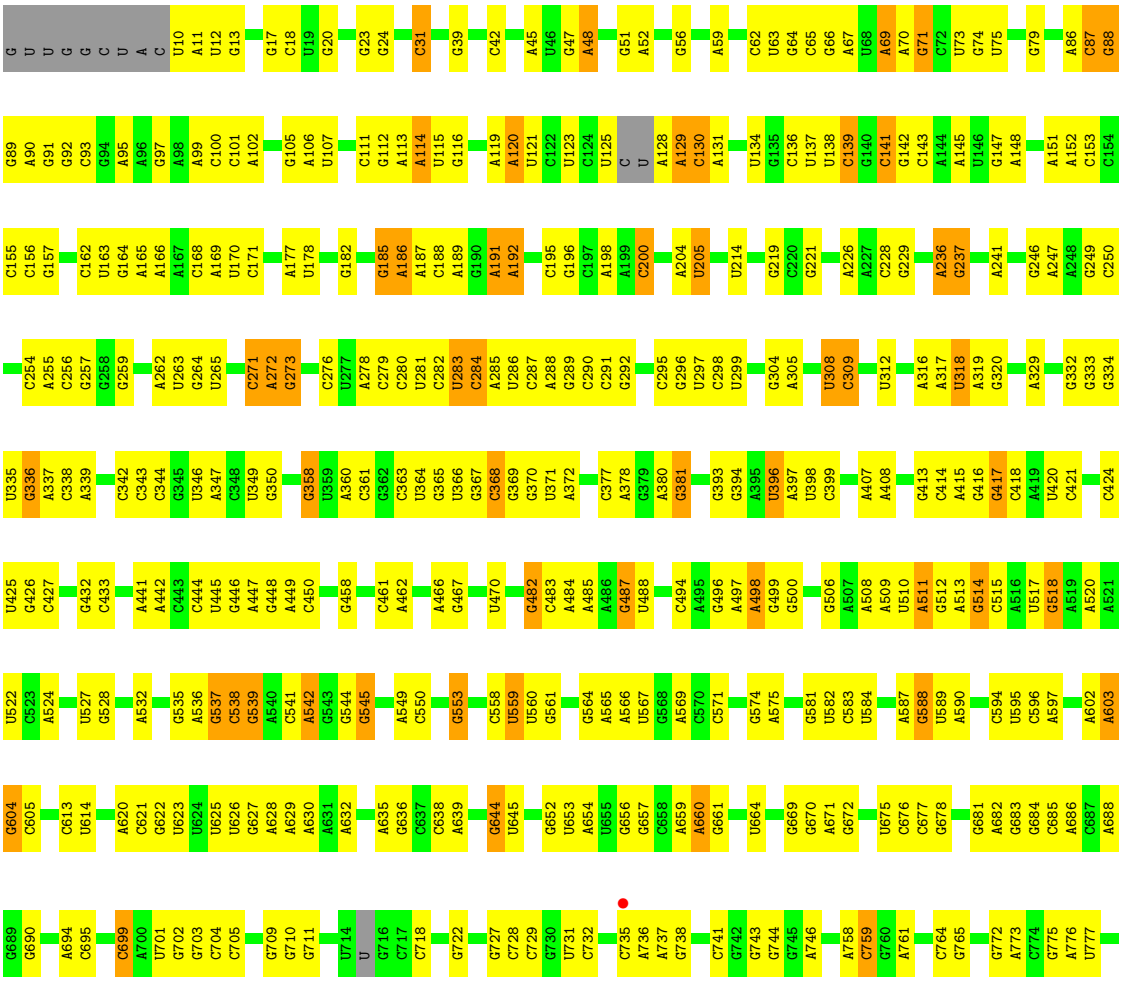
• Molecule 29: 50S ribosomal protein L44E

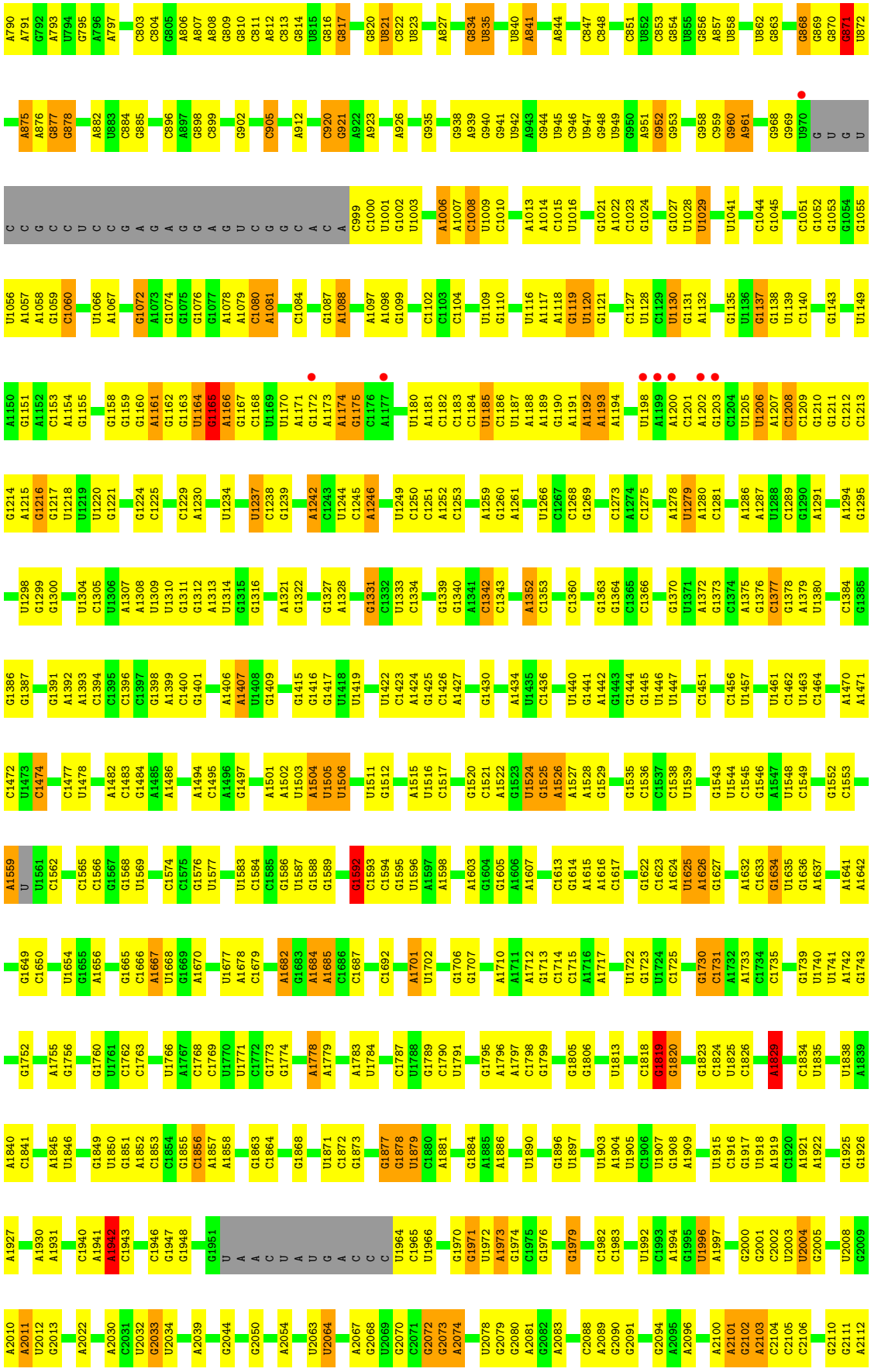
Chain 3:

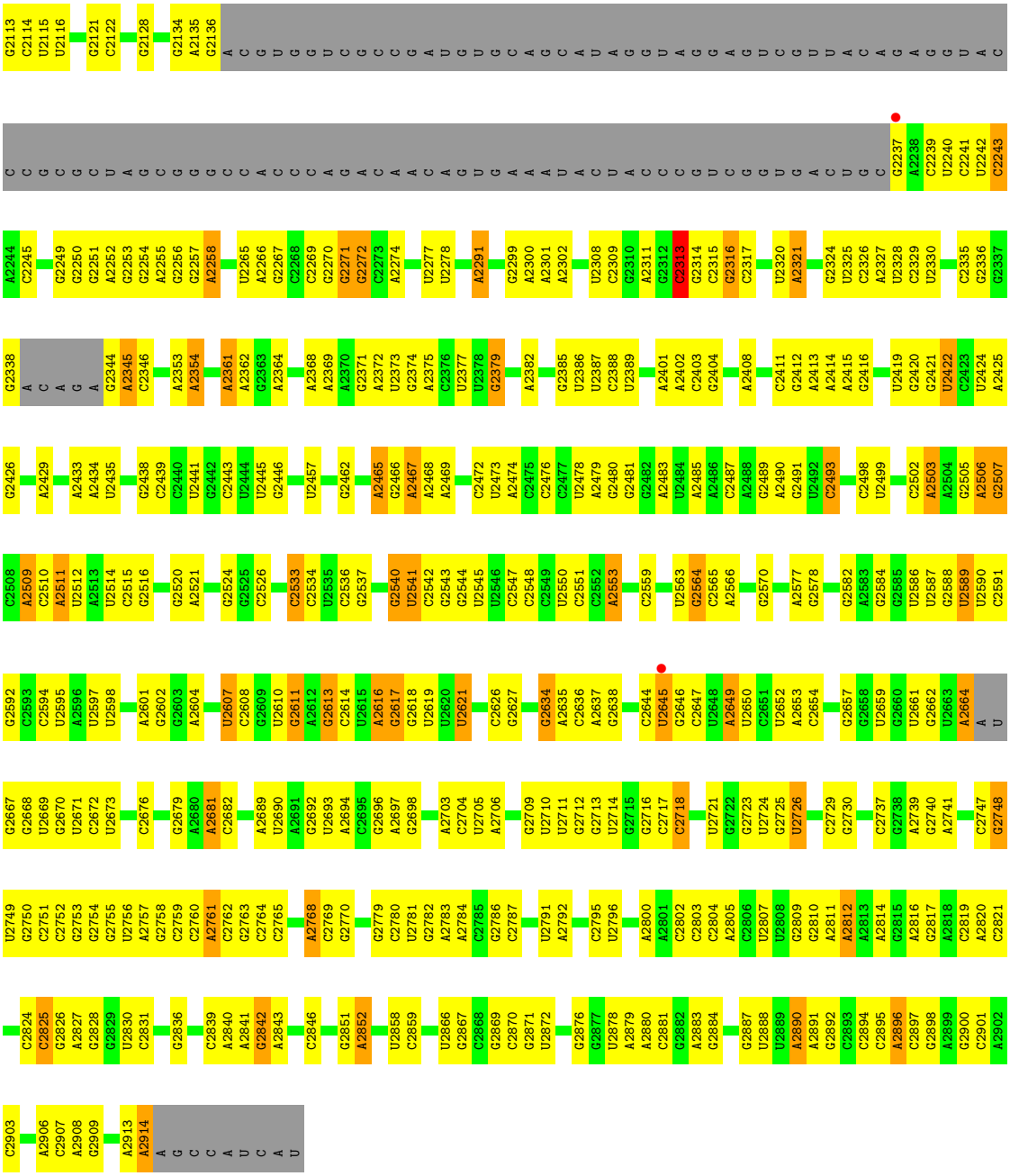


• Molecule 30: 23S RIBOSOMAL RNA

Chain 0:

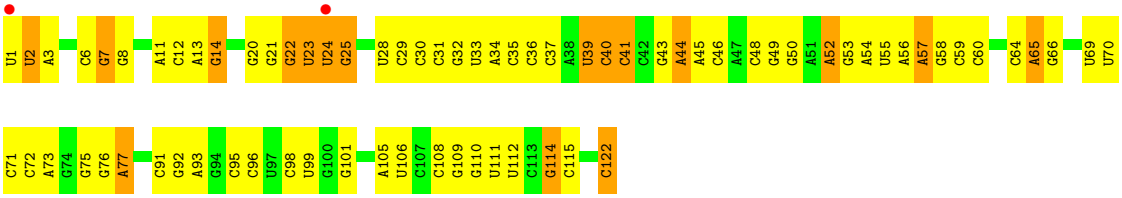



A790 A791 G792 A793 U794 G795 A796 A797 C803 C804 G805 A806 A807 A808 G809 G810 C811 A812 C813 G814 U815 G816 G817 G820 U821 C822 U823 A827 G834 U835 U840 A841 A844 C847 C848 C851 U852 C853 G854 U855 G856 A857 U858 U862 G863 G868 G869 G870 G871 U872
A875 A876 G877 G878 A882 U883 C884 G885 C896 A897 G898 C899 G902 C905 A912 C920 G921 A922 A923 A926 G935 G938 A939 G940 G941 U942 A943 G944 U945 C946 U947 G948 U949 G950 A951 G952 G953 G958 C959 G960 A961 G968 G969 U970 G U G U
C C G C C U C G G A A G G A G C A C A C999 C1000 U1001 G1002 U1003 A1006 A1007 C1008 U1009 C1010 A1013 A1014 C1015 U1016 G1021 A1022 C1023 G1024 G1027 U1028 U1029 U1041 C1044 G1045 C1051 G1052 G1053 G1054 G1055
U1056 A1057 A1058 G1059 C1060 U1066 A1067 G1072 A1073 G1074 G1075 G1076 G1077 A1078 A1079 C1080 A1081 C1084 G1087 A1088 A1097 A1098 G1099 C1102 C1103 C1104 U1109 G1110 U1116 A1117 A1118 G1119 U1120 G1121 C1127 U1128 C1129 U1130 G1131 A1132 G1135 U1136 G1137 G1138 U1139 C1140 G1143 U1149
A1150 G1151 A1152 C1153 A1154 G1155 G1158 G1159 G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 G1175 C1176 A1177 U1180 A1181 C1182 C1183 C1184 U1185 C1186 U1187 A1188 A1189 G1190 A1191 A1192 A1193 A1194 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208 C1209 G1210 G1211 C1212 C1213
G1214 A1215 G1216 G1217 U1218 U1219 U1220 G1221 G1224 C1225 C1229 A1230 U1234 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 U1249 C1250 C1251 A1252 C1253 A1259 G1260 A1261 U1266 C1267 C1268 G1269 C1273 A1274 C1275 A1278 U1279 A1280 C1281 A1286 A1287 U1288 C1289 G1290 A1291 A1294 G1295
U1298 G1299 G1300 U1304 C1305 U1306 A1307 A1308 U1309 U1310 G1311 G1312 A1313 U1314 G1315 G1316 A1321 G1322 G1327 A1328 G1331 C1332 U1333 C1334 G1339 G1340 A1341 C1342 C1343 A1352 C1353 C1360 G1363 G1364 C1365 C1366 G1370 U1371 A1372 G1373 C1374 A1375 G1376 C1377 G1378 A1379 U1380 C1384 G1385
G1386 G1387 G1391 A1392 A1393 C1394 C1395 C1396 C1397 G1398 A1399 C1400 G1401 A1406 A1407 U1408 G1409 G1415 G1416 G1417 U1418 U1419 U1422 C1423 A1424 G1425 C1426 A1427 G1430 A1434 U1435 C1436 U1440 G1441 A1442 G1443 G1444 G1445 U1446 U1447 C1451 C1456 U1457 U1461 C1462 U1463 C1464 A1470 A1471
C1472 U1473 C1474 C1477 U1478 A1482 C1483 G1484 A1485 A1486 A1494 C1495 A1496 G1497 A1501 A1502 U1503 A1504 U1505 U1506 U1511 G1512 A1515 U1516 C1517 G1520 C1521 A1522 G1523 U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1536 C1537 C1538 U1539 G1543 U1544 C1545 G1546 A1547 U1548 C1549 G1552 C1553
A1559 U U1561 C1562 C1565 C1566 G1567 G1568 U1569 C1574 C1575 G1576 U1577 U1583 C1584 C1585 G1586 U1587 G1588 G1589 G1592 C1593 C1594 G1595 U1596 A1597 A1598 A1603 G1604 G1605 A1606 A1607 C1613 G1614 A1615 A1616 C1617 G1622 C1623 A1624 U1625 A1626 G1627 A1632 C1633 G1634 A1635 G1636 A1637 A1641 A1642
G1649 C1650 U1654 G1655 A1656 G1665 C1666 A1667 U1668 G1669 A1670 U1677 A1678 C1679 A1682 G1683 A1684 A1685 C1686 C1687 C1692 A1701 U1702 G1706 G1707 A1710 A1711 A1712 G1713 C1714 C1715 A1716 A1717 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 C1734 C1735 G1739 U1740 U1741 A1742 G1743
G1752 A1755 G1756 G1760 U1761 C1762 C1763 U1766 A1767 C1768 C1769 U1770 U1771 C1772 G1773 G1774 A1778 A1779 A1783 U1784 C1787 U1788 G1789 C1790 U1791 G1795 A1796 A1797 C1798 G1799 G1805 G1806 U1813 C1818 G1819 G1820 G1823 C1824 U1825 C1826 A1829 C1834 U1835 U1838 A1839
A1840 C1841 A1845 U1846 G1849 U1850 G1851 A1852 C1853 C1854 G1855 C1856 A1857 A1858 G1863 C1864 G1868 U1871 C1872 G1873 G1877 G1878 U1879 C1880 A1881 G1884 A1885 A1886 U1890 G1896 U1897 U1903 A1904 U1905 C1906 U1907 G1908 A1909 U1915 C1916 G1917 U1918 A1919 C1920 A1921 A1922 G1925 G1926
A1927 A1930 A1931 C1940 A1941 A1942 C1943 C1946 G1947 G1948 C1951 U A A C U A U G A C C C U1964 C1965 U1966 G1970 G1971 U1972 A1973 G1974 C1975 G1976 G1979 C1982 C1983 U1992 C1993 A1994 G1995 U1996 A1997 G2000 G2001 C2002 U2003 U2004 G2005 U2008 G2009
A2010 A2011 U2012 G2013 A2022 A2030 C2031 U2032 G2033 U2034 A2039 G2044 G2050 A2054 U2063 U2064 A2067 G2068 U2069 G2070 C2071 G2072 G2073 A2074 U2078 G2079 G2080 A2081 G2082 A2083 C2088 A2089 G2090 G2091 G2094 A2095 A2096 A2100 A2101 G2102 A2103 C2104 C2105 C2106 G2110 G2111 A2112



• Molecule 31: 5S RIBOSOMAL RNA

Chain 9:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.75Å 299.01Å 574.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 2.90 85.44 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.5 (49.99-2.90) 93.6 (85.44-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.175 , 0.225 0.168 , 0.216	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	47.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 73.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	99121	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	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	0.63	0/2552
4	D	0.33	0/1111	0.56	0/1498
5	E	0.33	0/1382	0.57	0/1880
6	F	0.33	0/901	0.57	0/1224
7	G	0.32	0/241	0.49	0/324
8	H	0.34	0/1302	0.65	0/1743
9	I	0.29	0/526	0.50	0/716
10	J	0.36	0/1136	0.60	0/1530
11	K	0.36	0/1004	0.68	0/1351
12	L	0.35	0/1130	0.66	0/1509
13	M	0.34	0/1582	0.62	0/2116
14	N	0.30	0/1474	0.63	0/1999
15	O	0.34	0/874	0.59	0/1181
16	P	0.32	0/1147	0.51	0/1528
17	Q	0.34	0/749	0.67	0/1005
18	R	1.26	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.33	0/648	0.57	0/875
20	T	0.33	0/958	0.64	0/1289
21	U	0.33	0/417	0.56	0/562
22	V	0.32	0/502	0.53	0/675
23	W	0.35	0/1219	0.62	0/1655
24	X	0.34	0/664	0.59	0/895
25	Y	0.35	0/1146	0.61	0/1536
26	Z	0.36	0/584	0.61	0/781
27	1	0.39	0/438	0.60	0/578
28	2	0.33	0/401	0.56	0/529
29	3	0.34	0/771	0.56	0/1024
30	0	0.38	0/65956	0.69	13/102865 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.39	7/98700 (0.0%)	0.67	20/147584 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
23	W	0	1
30	0	0	29
All	All	1	30

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.44	2.87	1.50
18	R	150	PRO	CA-C	-18.09	1.16	1.52
18	R	150	PRO	CG-CD	13.93	1.96	1.50
18	R	150	PRO	C-O	11.89	1.47	1.23
18	R	150	PRO	N-CA	11.37	1.66	1.47
18	R	150	PRO	N-CD	10.70	1.62	1.47
18	R	150	PRO	CA-CB	7.62	1.68	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	150	PRO	CB-CA-C	-22.52	55.71	112.00
18	R	150	PRO	N-CA-C	-19.33	61.85	112.10
18	R	150	PRO	CA-N-CD	12.27	128.87	111.70
18	R	150	PRO	N-CA-CB	11.00	116.50	103.30
18	R	150	PRO	CA-C-O	-8.51	99.79	120.20
18	R	150	PRO	CA-CB-CG	-6.15	92.32	104.00
30	0	1942	A	C5'-C4'-C3'	6.08	125.73	116.00
30	0	2316	G	C5'-C4'-C3'	-5.93	106.52	116.00
31	9	39	U	N1-C1'-C2'	5.87	121.63	114.00
30	0	1504	A	N9-C1'-C2'	5.86	121.62	114.00
30	0	1504	A	C1'-O4'-C4'	-5.83	105.24	109.90
30	0	1120	U	C5'-C4'-C3'	-5.56	107.11	116.00
30	0	2726	U	N1-C1'-C2'	5.45	121.08	114.00
30	0	871	G	C5'-C4'-O4'	-5.44	102.57	109.10
30	0	2313	C	C5'-C4'-O4'	5.34	115.51	109.10
30	0	1165	G	C1'-O4'-C4'	-5.32	105.64	109.90
30	0	2467	A	C1'-O4'-C4'	-5.22	105.72	109.90
30	0	1592	G	N9-C1'-C2'	5.21	120.78	114.00
30	0	1829	A	N9-C1'-C2'	-5.19	106.29	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	841	A	C1'-O4'-C4'	-5.16	105.77	109.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain
30	0	1430	G	Sidechain
30	0	1819	G	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	205	U	Sidechain
30	0	221	G	Sidechain
30	0	2308	U	Sidechain
30	0	2313	C	Sidechain
30	0	246	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2607	U	Sidechain
30	0	2673	U	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	795	G	Sidechain
30	0	817	G	Sidechain
30	0	868	G	Sidechain
30	0	952	G	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts (i)

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	74	0
2	B	2625	0	2532	108	0
3	C	1860	0	1813	56	0
4	D	1094	0	1085	38	0
5	E	1357	0	1266	34	0
6	F	890	0	843	28	0
7	G	240	0	231	9	0
8	H	1282	0	1292	39	0
9	I	519	0	500	20	0
10	J	1120	0	1098	43	0
11	K	994	0	1027	40	0
12	L	1118	0	1076	37	0
13	M	1558	0	1573	52	0
14	N	1445	0	1401	54	0
15	O	865	0	873	23	0
16	P	1136	0	1123	25	0
17	Q	735	0	729	18	0
18	R	1149	0	1122	40	0
19	S	641	0	605	14	0
20	T	950	0	924	22	0
21	U	410	0	364	16	0
22	V	499	0	511	20	0
23	W	1196	0	1137	66	0
24	X	654	0	653	23	0
25	Y	1130	0	1133	40	0
26	Z	573	0	531	15	0
27	1	431	0	426	25	0
28	2	396	0	413	18	0
29	3	755	0	728	15	0
30	0	59019	0	29809	1374	0
31	9	2599	0	1325	96	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	10	0	0	1	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	94	0	0	0	0
34	1	2	0	0	0	0
34	3	1	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	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	67	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	1	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	5910	0	0	205	0
38	1	54	0	0	6	0
38	2	44	0	0	1	0
38	3	69	0	0	2	0
38	9	142	0	0	10	0
38	A	112	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	B	149	0	0	13	0
38	C	185	0	0	17	0
38	D	49	0	0	4	0
38	E	45	0	0	4	0
38	F	26	0	0	3	0
38	G	17	0	0	0	0
38	H	67	0	0	4	0
38	I	8	0	0	1	0
38	J	51	0	0	2	0
38	K	51	0	0	2	0
38	L	89	0	0	8	0
38	M	133	0	0	4	0
38	N	61	0	0	7	0
38	O	39	0	0	3	0
38	P	62	0	0	1	0
38	Q	45	0	0	2	0
38	R	81	0	0	3	0
38	S	32	0	0	3	0
38	T	35	0	0	3	0
38	U	29	0	0	2	0
38	V	15	0	0	2	0
38	W	67	0	0	6	0
38	X	26	0	0	4	0
38	Y	98	0	0	5	0
38	Z	32	0	0	1	0
All	All	99121	0	59909	2240	0

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

All (2240) 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	1.43
30:0:1160:G:C5'	30:0:1161:A:H5'	1.74	1.18
30:0:871:G:C8	30:0:871:G:H5'	1.80	1.15
30:0:1160:G:H5'	30:0:1161:A:C5'	1.74	1.15
30:0:871:G:H5'	30:0:871:G:H8	1.07	1.11
14:N:37:ARG:NH1	31:9:6:C:H5"	1.63	1.09
30:0:1559:A:H1'	38:0:5862:HOH:O	1.53	1.08
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1205:U:H2'	30:0:1206:U:H5"	1.31	1.07
30:0:2717:C:C2'	30:0:2718:C:H5"	1.84	1.07
30:0:1701:A:H4'	30:0:1702:U:H5"	1.38	1.05
30:0:2717:C:H2'	30:0:2718:C:H5"	1.34	1.05
31:9:56:A:C2'	31:9:57:A:H5"	1.86	1.05
31:9:56:A:H2'	31:9:57:A:H5"	1.08	1.03
15:O:3:THR:HG22	30:0:656:G:H5'	1.37	1.02
30:0:2291:A:C8	30:0:2309:C:H5'	1.95	1.02
31:9:76:G:H3'	31:9:77:A:H5"	1.41	1.00
10:J:82:THR:HG23	30:0:1242:A:H5'	1.41	0.98
30:0:282:C:H1'	30:0:368:C:N4	1.79	0.98
30:0:1666:C:O2'	30:0:1667:A:H5"	1.64	0.98
30:0:1474:C:H6	30:0:1474:C:H5'	1.29	0.97
30:0:545:G:H5'	30:0:545:G:H8	1.24	0.97
13:M:171:ARG:HD3	30:0:156:C:H5"	1.44	0.96
30:0:1187:U:HO2'	30:0:1189:A:H2	0.98	0.96
30:0:870:G:H2'	30:0:871:G:H5"	1.48	0.95
30:0:1625:U:H4'	38:0:4666:HOH:O	1.67	0.95
30:0:871:G:H8	30:0:871:G:C5'	1.81	0.94
11:K:10:GLN:HE21	11:K:10:GLN:H	1.06	0.93
4:D:154:LYS:H	4:D:154:LYS:HD2	1.34	0.93
30:0:1205:U:H2'	30:0:1206:U:C5'	1.99	0.93
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.82	0.92
30:0:2812:A:H2	30:0:2814:A:H62	1.11	0.92
30:0:1116:U:O2'	30:0:1118:A:H2	1.51	0.92
30:0:542:A:H5'	30:0:542:A:H8	1.35	0.92
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.10	0.92
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.49	0.92
30:0:506:G:H22	30:0:509:A:C5'	1.82	0.92
3:C:236:THR:HG22	3:C:239:ALA:H	1.31	0.91
30:0:2010:A:H2'	38:0:5957:HOH:O	1.69	0.91
30:0:2533:C:H5'	30:0:2533:C:H6	1.34	0.90
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.54	0.90
30:0:69:A:H5'	30:0:69:A:C8	2.07	0.90
30:0:1184:C:H1'	38:0:7462:HOH:O	1.71	0.90
30:0:877:G:H5'	30:0:878:G:OP1	1.72	0.90
30:0:1603:A:H5'	30:0:1605:G:O4'	1.71	0.90
16:P:115:SER:H	16:P:118:GLN:HE21	1.18	0.90
15:O:3:THR:CG2	30:0:656:G:H5'	2.02	0.89
30:0:381:G:H5"	38:0:4318:HOH:O	1.72	0.89
30:0:853:C:H3'	38:0:4550:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2908:A:H2'	30:0:2909:G:O4'	1.73	0.89
30:0:1474:C:H5'	30:0:1474:C:C6	2.09	0.88
30:0:282:C:O2'	30:0:283:U:H5'	1.73	0.88
30:0:2541:U:H5'	30:0:2541:U:H6	1.37	0.88
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.18	0.88
30:0:541:C:H2'	30:0:542:A:H5"	1.55	0.88
30:0:272:A:H3'	38:0:7525:HOH:O	1.74	0.88
30:0:541:C:C2'	30:0:542:A:H5"	2.04	0.88
30:0:69:A:H5'	30:0:69:A:H8	1.39	0.87
30:0:1878:G:H1'	38:0:6119:HOH:O	1.74	0.87
30:0:2783:A:H3'	38:0:5234:HOH:O	1.75	0.87
2:B:238:ASN:HD22	2:B:240:GLY:H	1.22	0.87
30:0:1667:A:H8	30:0:1667:A:H5'	1.39	0.86
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.57	0.86
30:0:1835:U:H5	30:0:1840:A:N7	1.74	0.86
30:0:1118:A:H8	30:0:1118:A:H3'	1.39	0.86
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.58	0.85
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.58	0.85
30:0:2644:C:O2'	30:0:2645:U:H5'	1.76	0.85
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.58	0.85
30:0:1205:U:C2'	30:0:1206:U:H5"	2.06	0.85
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.59	0.85
30:0:1979:G:H2'	38:0:3289:HOH:O	1.73	0.85
28:2:18:ASN:HD21	28:2:40:ARG:H	1.24	0.84
30:0:1118:A:H3'	30:0:1118:A:C8	2.11	0.84
14:N:37:ARG:HH12	31:9:6:C:H5"	1.43	0.84
30:0:1666:C:C2'	30:0:1667:A:H5"	2.07	0.84
30:0:2506:A:O2'	30:0:2507:G:H8	1.59	0.84
30:0:1372:A:H3'	38:0:7186:HOH:O	1.78	0.84
3:C:1:MET:HG2	3:C:2:GLN:H	1.42	0.84
30:0:2769:C:C2'	30:0:2770:G:H5'	2.08	0.84
31:9:92:G:H2'	31:9:93:A:C8	2.13	0.84
30:0:1183:C:N4	30:0:1184:C:H41	1.76	0.83
30:0:182:G:H5'	38:0:5160:HOH:O	1.79	0.83
30:0:2635:A:O2'	30:0:2636:C:H5'	1.79	0.83
31:9:29:C:H2'	31:9:30:C:H5'	1.60	0.83
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.59	0.83
30:0:559:U:H6	30:0:559:U:H5'	1.43	0.83
30:0:506:G:H22	30:0:509:A:H5'	1.44	0.82
23:W:88:THR:HB	38:W:6679:HOH:O	1.78	0.82
30:0:1119:G:H22	30:0:1246:A:H2	1.25	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.25	0.82
30:0:1701:A:H5'	38:0:6284:HOH:O	1.80	0.82
30:0:545:G:H5'	30:0:545:G:C8	2.12	0.82
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.62	0.81
30:0:2586:U:H3	30:0:2592:G:H22	1.26	0.81
11:K:39:GLY:HA2	38:0:5223:HOH:O	1.79	0.81
31:9:14:G:H5'	31:9:14:G:H8	1.45	0.81
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.63	0.81
30:0:2502:C:C2'	30:0:2503:A:H5'	2.11	0.81
30:0:2502:C:H2'	30:0:2503:A:H5'	1.61	0.81
30:0:2506:A:HO2'	30:0:2507:G:H8	0.83	0.81
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.62	0.81
30:0:1119:G:N2	30:0:1246:A:C2	2.48	0.80
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.77	0.80
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.46	0.80
30:0:1175:G:H1'	30:0:1193:A:H2'	1.63	0.80
30:0:363:C:H1'	38:0:5282:HOH:O	1.82	0.80
30:0:2896:A:H5"	38:0:6099:HOH:O	1.81	0.80
30:0:283:U:H5	30:0:284:C:N3	1.79	0.80
30:0:1206:U:H5'	30:0:1206:U:H6	1.45	0.80
28:2:41:HIS:H	28:2:45:ASN:HD22	1.29	0.80
30:0:1160:G:H5'	30:0:1161:A:H5'	0.87	0.80
30:0:603:A:H5"	30:0:604:G:OP1	1.81	0.80
30:0:1973:A:H5'	30:0:1973:A:H8	1.45	0.80
30:0:1603:A:H5"	30:0:1605:G:H5'	1.63	0.79
30:0:541:C:H2'	30:0:542:A:C5'	2.12	0.79
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.64	0.79
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.17	0.78
27:1:1:THR:HA	38:0:9358:HOH:O	1.83	0.78
30:0:281:U:O2'	30:0:282:C:H5'	1.83	0.78
14:N:113:SER:HB2	38:N:8855:HOH:O	1.82	0.78
30:0:2644:C:H2'	38:0:4596:HOH:O	1.83	0.78
15:O:47:ARG:HH11	15:O:47:ARG:HG3	1.47	0.78
21:U:9:CYS:HA	21:U:52:THR:HG22	1.64	0.78
30:0:1183:C:H42	30:0:1184:C:H41	1.32	0.78
30:0:2795:C:O2'	30:0:2796:U:H5'	1.83	0.78
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.63	0.78
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.84	0.78
30:0:236:A:H4'	30:0:237:G:H5'	1.66	0.78
30:0:1189:A:H1'	30:0:1209:C:O4'	1.84	0.78
30:0:558:C:O2'	30:0:559:U:H5"	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2748:G:H5'	38:0:7537:HOH:O	1.83	0.77
30:0:1300:G:H1'	38:0:4684:HOH:O	1.83	0.77
16:P:117:SER:HB3	30:0:1593:C:OP1	1.84	0.77
30:0:1116:U:H3	30:0:1246:A:H62	1.31	0.77
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.77
12:L:133:VAL:HA	38:L:8876:HOH:O	1.84	0.77
30:0:2769:C:O2'	30:0:2770:G:H5'	1.83	0.77
30:0:871:G:C8	30:0:871:G:C5'	2.60	0.77
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.22	0.77
30:0:1183:C:H2'	38:0:6244:HOH:O	1.85	0.77
31:9:49:G:H5"	38:9:9087:HOH:O	1.84	0.77
2:B:206:THR:HG21	30:0:2716:G:H5"	1.68	0.76
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.65	0.76
30:0:2578:G:H5'	30:0:2578:G:H8	1.51	0.76
14:N:141:ARG:HH21	31:9:48:C:H4'	1.50	0.76
30:0:1209:C:H2'	30:0:1210:G:H8	1.51	0.76
30:0:192:A:H5'	38:0:7639:HOH:O	1.86	0.76
8:H:29:SER:HA	8:H:62:HIS:HD2	1.50	0.76
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.69	0.75
30:0:2533:C:H5'	30:0:2533:C:C6	2.20	0.75
30:0:2748:G:H1'	38:0:7896:HOH:O	1.85	0.75
30:0:567:U:H5"	38:0:5289:HOH:O	1.87	0.75
30:0:506:G:H22	30:0:509:A:H5"	1.51	0.75
30:0:1189:A:H1'	30:0:1209:C:C1'	2.15	0.75
30:0:847:C:H4'	38:0:3748:HOH:O	1.87	0.75
30:0:1790:C:H2'	30:0:1791:U:H6	1.52	0.75
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.15	0.74
1:A:35:GLY:O	1:A:36:ASP:HB3	1.86	0.74
30:0:1120:U:H5'	30:0:1121:G:OP2	1.86	0.74
30:0:1701:A:H4'	30:0:1702:U:C5'	2.17	0.74
30:0:558:C:C2'	30:0:559:U:H5"	2.17	0.74
30:0:1666:C:H2'	30:0:1667:A:C5'	2.16	0.74
30:0:2487:C:H5	38:0:4889:HOH:O	1.71	0.74
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.03	0.74
30:0:1080:C:H4'	30:0:1081:A:OP1	1.87	0.74
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.88	0.74
30:0:870:G:C2'	30:0:871:G:H5"	2.16	0.74
30:0:2637:A:H4'	38:0:6063:HOH:O	1.87	0.74
30:0:2717:C:H2'	30:0:2718:C:C5'	2.14	0.74
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.70	0.73
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:544:G:H2'	30:0:545:G:H5"	1.70	0.73
30:0:1441:G:O2'	30:0:1442:A:H5'	1.88	0.73
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.71	0.73
30:0:1189:A:H3'	38:0:7676:HOH:O	1.86	0.73
30:0:2541:U:H5'	30:0:2541:U:C6	2.23	0.73
30:0:2787:C:H5	38:0:4633:HOH:O	1.72	0.73
30:0:1641:A:H2'	30:0:1642:A:H5'	1.69	0.73
30:0:2717:C:O2'	30:0:2718:C:H5"	1.89	0.73
30:0:1666:C:H2'	30:0:1667:A:H5'	1.71	0.73
30:0:2524:G:H21	30:0:2526:C:N4	1.86	0.73
30:0:2679:G:H2'	30:0:2681:A:OP2	1.89	0.73
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.70	0.73
22:V:1:THR:HG23	22:V:2:VAL:H	1.54	0.73
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.70	0.73
30:0:1701:A:H5"	30:0:1702:U:H3'	1.71	0.73
30:0:271:C:H41	30:0:378:A:H2	1.33	0.73
30:0:2420:G:O2'	30:0:2421:G:H5'	1.88	0.73
30:0:396:U:H1'	38:0:7622:HOH:O	1.88	0.72
30:0:1118:A:H62	30:0:1244:U:H3	1.36	0.72
30:0:1525:G:H5'	30:0:1526:A:OP2	1.89	0.72
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.71	0.72
30:0:2102:G:H2'	38:0:7763:HOH:O	1.87	0.72
4:D:103:ASN:ND2	4:D:134:LEU:H	1.88	0.72
30:0:827:A:H1'	38:0:6214:HOH:O	1.89	0.72
30:0:2254:G:H1'	38:0:5534:HOH:O	1.89	0.72
30:0:2644:C:HO2'	30:0:2645:U:H6	1.36	0.71
30:0:1632:A:H2'	30:0:1633:C:H5'	1.72	0.71
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.25	0.71
30:0:1441:G:H1'	38:0:7761:HOH:O	1.90	0.71
3:C:139:VAL:HG13	38:C:8659:HOH:O	1.90	0.71
30:0:280:C:H2'	30:0:281:U:O4'	1.91	0.71
30:0:2769:C:H2'	30:0:2770:G:H5'	1.73	0.71
13:M:95:LYS:HE2	30:0:157:G:H4'	1.73	0.71
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.71
30:0:31:C:H4'	38:0:7421:HOH:O	1.91	0.70
30:0:2491:G:H1'	38:0:6868:HOH:O	1.90	0.70
30:0:2577:A:H8	38:0:9598:HOH:O	1.74	0.70
30:0:1730:G:H5'	30:0:1731:C:C5	2.27	0.70
30:0:2505:G:O2'	30:0:2506:A:H5'	1.92	0.70
30:0:2756:U:H3	30:0:2896:A:H2	1.35	0.70
4:D:105:SER:OG	30:0:2338:G:H1'	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.92	0.70
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.74	0.70
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.70
30:0:2073:G:OP2	30:0:2490:A:H5'	1.92	0.70
30:0:2812:A:H1'	38:0:5787:HOH:O	1.92	0.70
1:A:51:ARG:HB2	38:A:9063:HOH:O	1.91	0.70
13:M:171:ARG:CD	30:0:156:C:H5"	2.20	0.69
38:C:8676:HOH:O	30:0:2100:A:H5'	1.92	0.69
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.74	0.69
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.32	0.69
30:0:1838:U:O2'	30:0:2644:C:H5'	1.92	0.69
30:0:2135:A:O2'	30:0:2136:G:H5'	1.92	0.69
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.74	0.69
30:0:285:A:H2'	30:0:286:U:O4'	1.92	0.69
30:0:1634:G:H3'	38:0:3891:HOH:O	1.93	0.69
30:0:2004:U:H4'	38:0:5307:HOH:O	1.92	0.69
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.03	0.69
30:0:558:C:H2'	30:0:559:U:C5'	2.23	0.69
30:0:681:G:N3	30:0:681:G:H5'	2.08	0.69
30:0:2670:G:O2'	30:0:2671:U:H5'	1.92	0.69
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.57	0.69
30:0:1377:C:H5'	30:0:1377:C:H6	1.58	0.69
30:0:1451:C:H5'	30:0:1505:U:C5	2.28	0.69
30:0:1666:C:C2'	30:0:1667:A:C5'	2.70	0.69
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.88	0.69
30:0:1835:U:C5	30:0:1840:A:N7	2.59	0.69
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.73	0.68
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.08	0.68
30:0:2563:U:H2'	30:0:2565:C:O5'	1.93	0.68
24:X:78:GLU:HB3	38:X:5564:HOH:O	1.94	0.68
16:P:115:SER:H	16:P:118:GLN:NE2	1.88	0.68
30:0:960:G:N3	30:0:960:G:H2'	2.09	0.68
30:0:1667:A:H5'	30:0:1667:A:C8	2.27	0.68
30:0:2851:G:O2'	30:0:2852:A:H5'	1.94	0.68
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.08	0.68
30:0:812:A:H1'	38:0:3955:HOH:O	1.93	0.68
30:0:2005:G:H3'	30:0:2005:G:OP2	1.94	0.68
1:A:199:HIS:HD2	1:A:201:PHE:H	1.41	0.68
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.76	0.68
21:U:47:ARG:HG3	38:U:4381:HOH:O	1.94	0.68
30:0:138:U:H5"	30:0:139:C:OP2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2111:G:H1'	38:0:9049:HOH:O	1.93	0.68
20:T:2:LYS:HG2	30:0:447:A:OP1	1.93	0.68
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.75	0.68
30:0:564:G:H1'	38:0:6310:HOH:O	1.92	0.68
30:0:1528:A:H2'	30:0:1529:G:O4'	1.94	0.68
30:0:2659:U:H5"	38:0:4123:HOH:O	1.93	0.68
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.75	0.67
30:0:1730:G:H5"	30:0:1731:C:H6	1.59	0.67
30:0:2827:A:H2'	30:0:2828:G:O4'	1.94	0.67
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.74	0.67
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.76	0.67
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.60	0.67
18:R:150:PRO:CG	18:R:150:PRO:O	2.42	0.67
30:0:1562:C:O2	30:0:1562:C:H2'	1.94	0.67
30:0:1182:C:H1'	30:0:1192:A:H8	1.60	0.67
3:C:236:THR:HA	38:C:8662:HOH:O	1.95	0.67
30:0:299:U:H5'	38:0:7336:HOH:O	1.93	0.67
3:C:236:THR:HG22	3:C:239:ALA:N	2.09	0.67
14:N:37:ARG:NH1	31:9:6:C:C5'	2.52	0.67
23:W:80:ASP:O	23:W:84:VAL:HG23	1.94	0.67
29:3:48:ASN:HD21	30:0:2468:A:H61	1.43	0.67
30:0:130:C:H2'	38:0:3158:HOH:O	1.95	0.67
30:0:544:G:C2'	30:0:545:G:H5"	2.24	0.67
31:9:75:G:H1	31:9:106:U:H3	1.42	0.67
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.95	0.67
30:0:2852:A:H5"	38:0:5236:HOH:O	1.94	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.29	0.66
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.77	0.66
30:0:292:G:H2'	30:0:358:G:N2	2.10	0.66
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.76	0.66
22:V:42:ASN:HB3	38:V:7247:HOH:O	1.95	0.66
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.95	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.42	0.66
30:0:2524:G:H21	30:0:2526:C:H41	1.44	0.66
30:0:1189:A:O2'	30:0:1208:C:H2'	1.96	0.66
30:0:848:C:H5'	38:0:7271:HOH:O	1.94	0.66
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.60	0.66
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.59	0.66
33:0:8813:CL:CL	38:0:4684:HOH:O	2.51	0.66
31:9:23:U:O2'	31:9:24:U:H4'	1.96	0.66
30:0:1118:A:C8	30:0:1118:A:C3'	2.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:110:THR:HB	14:N:113:SER:OG	1.95	0.66
30:0:1834:C:H2'	30:0:1840:A:N6	2.10	0.66
26:Z:34:SER:HA	30:0:797:A:H5'	1.76	0.65
30:0:441:A:H1'	30:0:442:A:N7	2.12	0.65
31:9:92:G:H2'	31:9:93:A:H8	1.61	0.65
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.61	0.65
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.11	0.65
23:W:59:GLN:HE22	23:W:98:PHE:HB2	1.62	0.65
30:0:2812:A:C2	30:0:2814:A:N6	2.62	0.65
13:M:164:THR:HG22	13:M:167:GLY:H	1.59	0.65
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.78	0.65
30:0:482:G:H4'	30:0:508:A:N1	2.12	0.65
30:0:2755:G:H1'	38:0:4683:HOH:O	1.97	0.65
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.78	0.65
3:C:140:VAL:HB	38:C:8662:HOH:O	1.97	0.65
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.79	0.65
6:F:96:ALA:HA	38:F:3111:HOH:O	1.96	0.65
30:0:2878:U:H2'	30:0:2879:A:O4'	1.96	0.65
30:0:2748:G:H2'	38:0:7537:HOH:O	1.96	0.65
30:0:2769:C:H2'	30:0:2770:G:C5'	2.25	0.65
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.79	0.65
30:0:841:A:H5"	38:0:6907:HOH:O	1.96	0.65
31:9:14:G:H5'	31:9:14:G:C8	2.30	0.65
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.78	0.65
30:0:1477:C:H5'	30:0:1868:G:C5'	2.27	0.65
30:0:1741:U:H5'	30:0:1742:A:OP1	1.96	0.65
30:0:2559:C:H4'	38:0:7254:HOH:O	1.97	0.65
30:0:1278:A:H4'	30:0:1279:U:C4	2.32	0.65
30:0:558:C:H2'	30:0:559:U:H5'	1.79	0.64
30:0:1649:G:H1'	38:0:5533:HOH:O	1.97	0.64
30:0:2756:U:N3	30:0:2896:A:H2	1.95	0.64
3:C:184:ARG:NH2	30:0:450:C:OP1	2.30	0.64
30:0:711:G:H1'	38:0:7093:HOH:O	1.96	0.64
30:0:2768:A:H2'	30:0:2769:C:O4'	1.96	0.64
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.80	0.64
19:S:43:GLU:HB3	38:S:8989:HOH:O	1.97	0.64
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.61	0.64
10:J:41:ALA:HB3	38:J:5907:HOH:O	1.96	0.64
30:0:308:U:H5'	30:0:309:C:OP1	1.96	0.64
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.77	0.64
30:0:2256:G:O2'	30:0:2257:G:H5'	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:26:ILE:HB	38:W:5420:HOH:O	1.96	0.64
30:0:1166:A:H61	30:0:1180:U:H3	1.45	0.64
30:0:1741:U:O2'	30:0:2723:G:H4'	1.98	0.64
30:0:2894:C:O2'	30:0:2895:C:H5'	1.98	0.64
2:B:98:THR:HG22	30:0:2820:A:OP1	1.98	0.64
38:Z:8707:HOH:O	30:0:1886:A:H4'	1.97	0.64
2:B:41:PHE:HA	2:B:79:MET:HE2	1.80	0.64
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.33	0.64
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.33	0.64
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.13	0.64
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.80	0.64
12:L:114:VAL:HG11	38:L:8876:HOH:O	1.97	0.64
10:J:82:THR:CG2	30:0:1242:A:H5'	2.21	0.64
11:K:66:ARG:HH22	30:0:1994:A:P	2.21	0.64
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.80	0.64
30:0:559:U:H5'	30:0:559:U:C6	2.29	0.64
30:0:1603:A:C5'	30:0:1605:G:H5'	2.28	0.64
4:D:23:VAL:HG22	4:D:73:VAL:HB	1.80	0.63
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.33	0.63
3:C:174:ILE:HD11	30:0:338:C:H4'	1.80	0.63
30:0:1790:C:H2'	30:0:1791:U:C6	2.32	0.63
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.63	0.63
30:0:1183:C:N3	30:0:1184:C:C5	2.67	0.63
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.28	0.63
31:9:49:G:H2'	31:9:50:G:O4'	1.98	0.63
12:L:18:HIS:HD2	30:0:902:G:N7	1.97	0.63
13:M:86:GLN:NE2	30:0:2274:A:H1'	2.14	0.63
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.46	0.63
30:0:542:A:H5'	30:0:542:A:C8	2.24	0.63
2:B:254:GLN:HG2	2:B:255:GLY:N	2.14	0.63
5:E:137:ASP:O	5:E:141:VAL:HG23	1.99	0.63
38:N:8844:HOH:O	31:9:7:G:H5'	1.98	0.63
30:0:71:G:H8	38:0:3908:HOH:O	1.81	0.63
30:0:123:U:H5'	38:0:6657:HOH:O	1.97	0.63
30:0:247:A:H2'	38:0:3920:HOH:O	1.99	0.63
30:0:1187:U:H2'	38:0:6893:HOH:O	1.99	0.63
30:0:1189:A:H1'	30:0:1209:C:H1'	1.79	0.63
9:I:126:THR:O	9:I:130:LEU:HG	1.99	0.62
17:Q:25:PRO:HB2	38:Q:4350:HOH:O	1.99	0.62
30:0:2345:A:H3'	30:0:2346:C:C6	2.34	0.62
30:0:200:C:H2'	38:0:3440:HOH:O	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1973:A:H5'	30:0:1973:A:C8	2.32	0.62
30:0:2426:G:H1'	38:0:6092:HOH:O	1.98	0.62
30:0:2637:A:H5'	38:0:4930:HOH:O	1.99	0.62
3:C:174:ILE:CD1	30:0:338:C:H4'	2.30	0.62
30:0:1632:A:C2'	30:0:1633:C:H5'	2.29	0.62
30:0:2481:G:H5"	38:0:4543:HOH:O	1.98	0.62
4:D:159:PRO:O	4:D:163:VAL:HG23	2.00	0.62
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.29	0.62
30:0:371:U:H2'	30:0:372:A:H8	1.65	0.62
30:0:1249:U:H2'	30:0:1250:C:C6	2.34	0.62
30:0:2320:U:H4'	30:0:2321:A:O4'	1.99	0.62
30:0:2478:U:O2'	30:0:2479:A:H5'	1.99	0.62
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.27	0.62
28:2:35:ARG:HB2	38:2:2691:HOH:O	1.98	0.62
30:0:583:C:H2'	30:0:584:U:H6	1.64	0.62
30:0:1132:A:N6	30:0:1229:C:H2'	2.14	0.62
30:0:1730:G:C5'	30:0:1731:C:C6	2.82	0.62
15:O:25:VAL:HG12	30:0:709:G:O2'	1.99	0.62
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.81	0.62
30:0:960:G:N3	30:0:960:G:C2'	2.63	0.62
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.95	0.62
6:F:91:VAL:HG12	6:F:92:GLY:N	2.15	0.61
10:J:131:THR:HB	10:J:134:GLU:HG3	1.81	0.61
16:P:59:ARG:HH22	16:P:66:GLN:NE2	1.98	0.61
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.81	0.61
30:0:363:C:O2'	30:0:364:U:H5'	2.00	0.61
30:0:1942:A:H3'	38:0:7346:HOH:O	1.99	0.61
30:0:2541:U:H6	30:0:2541:U:C5'	2.09	0.61
30:0:2644:C:O2'	30:0:2645:U:H6	1.83	0.61
31:9:39:U:H1'	31:9:44:A:H61	1.65	0.61
31:9:58:G:C8	31:9:59:C:C5	2.88	0.61
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.63	0.61
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.82	0.61
30:0:2241:C:O2'	30:0:2242:U:H5'	2.00	0.61
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.29	0.61
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.80	0.61
8:H:19:ARG:HH12	30:0:1008:C:H5"	1.64	0.61
30:0:635:A:H2'	30:0:636:G:H5"	1.82	0.61
30:0:1172:G:H1'	38:0:4974:HOH:O	2.01	0.61
30:0:2768:A:O2'	30:0:2769:C:H5'	2.00	0.61
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1474:C:H6	30:0:1474:C:C5'	2.07	0.61
1:A:109:GLU:HG2	1:A:116:GLY:H	1.65	0.61
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.31	0.61
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.83	0.61
11:K:10:GLN:HE21	11:K:10:GLN:N	1.89	0.61
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.81	0.61
29:3:15:ASN:O	30:0:2408:A:H4'	2.01	0.61
30:0:558:C:C2'	30:0:559:U:C5'	2.79	0.61
30:0:1185:U:H5'	38:0:7462:HOH:O	1.99	0.61
30:0:2604:A:H5'	38:0:5788:HOH:O	2.01	0.61
3:C:1:MET:HG2	3:C:2:GLN:N	2.15	0.61
11:K:49:LEU:HD23	11:K:80:ILE:HD13	1.83	0.61
30:0:407:A:H5'	38:0:6024:HOH:O	2.00	0.61
1:A:36:ASP:O	1:A:38:ILE:N	2.33	0.61
12:L:6:ARG:HD3	30:0:1299:G:O6	1.99	0.61
20:T:61:GLU:HG2	38:T:3851:HOH:O	1.98	0.61
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.66	0.61
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.84	0.60
30:0:1202:A:C2'	30:0:1203:G:H5'	2.31	0.60
26:Z:34:SER:CB	30:0:797:A:H4'	2.30	0.60
30:0:514:G:H4'	38:0:5644:HOH:O	2.00	0.60
30:0:1377:C:H5'	30:0:1377:C:C6	2.36	0.60
30:0:2781:U:C2'	30:0:2782:G:H5'	2.31	0.60
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.66	0.60
27:1:8:GLN:HE22	27:1:11:LYS:NZ	1.98	0.60
30:0:969:G:H1	30:0:999:C:N4	1.98	0.60
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.84	0.60
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.36	0.60
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.83	0.60
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.84	0.60
30:0:644:G:H5'	30:0:644:G:N3	2.16	0.60
30:0:1819:G:H2'	30:0:1820:G:H4'	1.81	0.60
30:0:2414:A:H2'	30:0:2415:A:C8	2.35	0.60
1:A:199:HIS:CD2	1:A:201:PHE:H	2.18	0.60
17:Q:15:LYS:HD3	30:0:2364:A:H5"	1.83	0.60
25:Y:204:ARG:HH22	30:0:553:G:P	2.25	0.60
30:0:120:A:H2'	30:0:120:A:N3	2.16	0.60
2:B:71:VAL:HG11	2:B:296:LEU:HB3	1.81	0.60
10:J:39:VAL:HG22	10:J:106:GLY:O	2.01	0.60
30:0:625:U:H5"	30:0:1044:C:N4	2.16	0.60
30:0:920:C:H5"	30:0:921:G:O5'	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1202:A:O2'	30:0:1203:G:H5'	2.01	0.60
30:0:1342:C:C2'	30:0:1343:C:H5'	2.30	0.60
30:0:1730:G:H5"	30:0:1731:C:C6	2.36	0.60
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.02	0.60
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.01	0.60
18:R:39:THR:HG22	18:R:42:GLU:H	1.67	0.60
26:Z:40:ALA:HA	30:0:1773:G:C8	2.37	0.60
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.41	0.60
30:0:746:A:H5'	38:0:5514:HOH:O	2.02	0.60
14:N:40:ASN:ND2	31:9:28:U:H5"	2.17	0.60
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.32	0.60
30:0:1393:A:H2'	30:0:1394:C:C6	2.37	0.60
30:0:2869:G:H2'	30:0:2870:C:C6	2.36	0.60
18:R:128:ARG:NH2	30:0:2054:A:N3	2.50	0.59
27:1:16:HIS:HD2	30:0:470:U:O2'	1.83	0.59
30:0:669:G:O2'	30:0:670:G:H5'	2.02	0.59
30:0:31:C:H2'	38:0:7684:HOH:O	2.02	0.59
30:0:515:C:H5"	38:0:5644:HOH:O	2.01	0.59
30:0:2524:G:N2	30:0:2526:C:H41	2.00	0.59
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.83	0.59
30:0:283:U:C5	30:0:284:C:N3	2.67	0.59
30:0:1457:U:H5	38:0:7872:HOH:O	1.84	0.59
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.84	0.59
9:I:120:ALA:O	9:I:124:VAL:HG23	2.02	0.59
12:L:41:HIS:CD2	30:0:926:A:O2'	2.56	0.59
18:R:39:THR:HG23	18:R:107:GLU:O	2.02	0.59
20:T:9:LYS:HD3	38:0:3750:HOH:O	2.02	0.59
30:0:128:A:O2'	30:0:129:A:H5'	2.02	0.59
30:0:2498:C:O2'	30:0:2499:U:H5'	2.02	0.59
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.84	0.59
30:0:1425:G:O2'	30:0:1426:C:H5'	2.02	0.59
30:0:2403:C:H5'	38:0:6025:HOH:O	2.02	0.59
30:0:2756:U:N3	30:0:2896:A:C2	2.63	0.59
2:B:36:PRO:HG3	2:B:169:GLY:H	1.67	0.59
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.01	0.59
31:9:13:A:O2'	31:9:14:G:H5"	2.03	0.59
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.83	0.59
12:L:134:GLU:HG3	38:L:8857:HOH:O	2.03	0.59
18:R:99:ALA:HB1	18:R:109:MET:CE	2.30	0.59
30:0:1183:C:H42	30:0:1184:C:N4	2.00	0.59
30:0:1268:C:O2'	30:0:1269:G:H5'	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:O	1:A:131:HIS:HE1	1.86	0.59
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.84	0.59
30:0:1426:C:H2'	38:0:9591:HOH:O	2.03	0.59
30:0:2419:U:H5"	30:0:2420:G:H5'	1.83	0.59
30:0:2505:G:C2'	30:0:2506:A:H5'	2.33	0.59
2:B:294:TYR:HE2	38:B:9117:HOH:O	1.85	0.59
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.38	0.59
20:T:9:LYS:HB2	38:0:7421:HOH:O	2.01	0.59
27:1:28:HIS:HE1	30:0:776:A:OP1	1.86	0.58
30:0:807:A:O2'	30:0:808:A:H5'	2.03	0.58
31:9:2:U:OP2	31:9:3:A:H5'	2.03	0.58
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.18	0.58
30:0:2344:G:H2'	30:0:2344:G:N3	2.18	0.58
30:0:2637:A:C5'	38:0:4930:HOH:O	2.50	0.58
30:0:2781:U:H2'	30:0:2782:G:H5'	1.84	0.58
30:0:2900:G:H2'	30:0:2901:C:O4'	2.03	0.58
1:A:48:ASP:HB3	38:A:9063:HOH:O	2.02	0.58
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.06	0.58
11:K:8:VAL:HG13	11:K:80:ILE:HG22	1.84	0.58
18:R:29:LYS:HD3	30:0:524:A:H5"	1.85	0.58
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.84	0.58
22:V:44:GLY:HA3	30:0:92:G:H4'	1.85	0.58
23:W:52:VAL:HG22	23:W:53:ALA:H	1.68	0.58
30:0:1201:C:H5"	38:0:6233:HOH:O	2.02	0.58
31:9:1:U:H5"	31:9:3:A:OP1	2.03	0.58
14:N:11:ARG:HD3	31:9:114:G:O6	2.03	0.58
15:O:42:GLU:HB2	38:O:2176:HOH:O	2.02	0.58
30:0:1230:A:H8	30:0:1230:A:OP1	1.85	0.58
30:0:1942:A:O2'	30:0:1943:C:H5'	2.03	0.58
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.85	0.58
4:D:25:MET:HE2	4:D:41:LEU:HG	1.85	0.58
30:0:485:A:N3	30:0:487:G:H5"	2.19	0.58
30:0:2335:C:H2'	30:0:2336:G:C8	2.38	0.58
14:N:141:ARG:NH2	31:9:48:C:H4'	2.19	0.58
30:0:2533:C:H6	30:0:2533:C:C5'	2.12	0.58
2:B:162:MET:CE	2:B:310:ARG:HD3	2.33	0.58
12:L:30:ARG:HD3	30:0:164:G:H4'	1.86	0.58
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.86	0.58
20:T:41:ARG:HG2	20:T:41:ARG:HH11	1.66	0.58
30:0:1211:G:H2'	30:0:1212:C:H6	1.69	0.58
30:0:1649:G:O2'	30:0:1650:C:H5'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:179:GLY:O	30:0:399:C:H5'	2.04	0.58
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.85	0.58
30:0:1015:C:H2'	30:0:1016:U:H6	1.67	0.58
30:0:2445:U:H2'	30:0:2446:G:C8	2.39	0.58
30:0:2802:C:H2'	30:0:2803:C:H6	1.68	0.58
1:A:212:PRO:HB2	38:A:9024:HOH:O	2.04	0.58
2:B:145:HIS:HD2	2:B:146:THR:O	1.87	0.58
13:M:163:LEU:HD21	30:0:188:C:H5"	1.86	0.58
30:0:2032:U:H2'	30:0:2033:G:C5'	2.34	0.58
1:A:55:VAL:HG23	1:A:68:ILE:O	2.04	0.57
30:0:1165:G:O2'	30:0:1174:A:H1'	2.04	0.57
30:0:1207:A:C8	30:0:1208:C:C5	2.92	0.57
30:0:1856:C:H5'	30:0:1858:A:O4'	2.04	0.57
30:0:1596:U:H2'	30:0:1598:A:OP2	2.03	0.57
30:0:1947:G:N2	30:0:1966:U:C2	2.71	0.57
9:I:110:ASP:O	30:0:1163:G:H5'	2.04	0.57
30:0:705:C:O2	30:0:705:C:H2'	2.04	0.57
30:0:1015:C:H2'	30:0:1016:U:C6	2.39	0.57
30:0:1181:A:H2'	30:0:1182:C:H5'	1.86	0.57
30:0:1819:G:H2'	30:0:1820:G:C5'	2.34	0.57
30:0:1903:U:O2'	30:0:1904:A:N7	2.38	0.57
30:0:2472:C:O2'	30:0:2634:G:H4'	2.03	0.57
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.86	0.57
21:U:17:THR:HG22	21:U:18:GLY:N	2.18	0.57
30:0:1307:A:H2'	30:0:1308:A:C8	2.39	0.57
30:0:1463:U:H2'	30:0:1464:C:C6	2.39	0.57
30:0:1477:C:O2'	30:0:1478:U:H5'	2.04	0.57
30:0:2851:G:C2'	30:0:2852:A:H5'	2.34	0.57
22:V:1:THR:HB	30:0:93:C:H5"	1.86	0.57
22:V:38:GLY:O	22:V:41:GLU:HG3	2.05	0.57
30:0:2251:G:H2'	30:0:2252:A:C8	2.40	0.57
30:0:255:A:H2'	30:0:256:C:H6	1.68	0.57
30:0:264:G:H1'	30:0:265:U:H5	1.70	0.57
30:0:2415:A:H2'	30:0:2416:G:H5'	1.86	0.57
2:B:125:GLU:O	2:B:129:ARG:HG3	2.04	0.57
30:0:876:A:H2'	30:0:876:A:N3	2.19	0.57
30:0:1138:G:H4'	38:0:5706:HOH:O	2.03	0.57
30:0:2689:A:H2'	30:0:2690:U:H5'	1.87	0.57
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.39	0.57
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.35	0.57
30:0:941:G:C5	30:0:942:U:C4	2.93	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1588:G:C6	30:0:1589:G:N1	2.73	0.57
1:A:121:ALA:O	1:A:124:VAL:HG22	2.05	0.57
38:B:9100:HOH:O	30:0:2672:C:H1'	2.05	0.57
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.34	0.57
30:0:823:U:H3'	38:0:4446:HOH:O	2.03	0.57
30:0:1044:C:H5"	38:0:9025:HOH:O	2.05	0.57
30:0:1174:A:C5	30:0:1201:C:H4'	2.39	0.57
30:0:1603:A:H5'	30:0:1605:G:C4'	2.34	0.57
30:0:2134:G:N2	30:0:2242:U:C2	2.73	0.57
30:0:2291:A:N9	30:0:2309:C:H5'	2.19	0.57
30:0:2509:A:H2'	30:0:2510:C:O4'	2.05	0.57
2:B:140:LEU:HA	38:B:9048:HOH:O	2.05	0.57
16:P:54:LYS:HB2	30:0:1717:A:H5"	1.87	0.57
30:0:694:A:H2'	30:0:695:C:H5'	1.86	0.57
31:9:22:G:H5'	31:9:23:U:OP1	2.05	0.57
5:E:132:THR:HB	38:E:2227:HOH:O	2.05	0.56
30:0:821:U:H3'	38:0:3765:HOH:O	2.05	0.56
30:0:834:G:H3'	30:0:835:U:H4'	1.87	0.56
3:C:188:ARG:HD3	38:C:8564:HOH:O	2.05	0.56
30:0:821:U:H2'	30:0:822:C:H6	1.70	0.56
30:0:2710:U:H1'	38:0:7616:HOH:O	2.04	0.56
4:D:25:MET:CE	4:D:37:ALA:HB1	2.35	0.56
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.34	0.56
10:J:74:ARG:O	10:J:78:ILE:HG12	2.05	0.56
17:Q:19:ARG:HH21	31:9:11:A:P	2.27	0.56
30:0:671:A:O2'	30:0:672:G:H2'	2.05	0.56
30:0:952:G:N3	30:0:2302:A:H2'	2.20	0.56
30:0:1135:G:H5'	38:0:5927:HOH:O	2.05	0.56
30:0:1641:A:C2'	30:0:1642:A:H5'	2.35	0.56
31:9:29:C:C2'	31:9:30:C:H5'	2.33	0.56
17:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.04	0.56
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.69	0.56
30:0:308:U:C4	30:0:342:C:H1'	2.41	0.56
5:E:143:GLN:NE2	30:0:2779:G:H21	2.04	0.56
30:0:1160:G:O2'	30:0:1190:G:H1'	2.06	0.56
30:0:1279:U:O2	30:0:1279:U:H2'	2.05	0.56
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.87	0.56
27:1:20:ARG:HG2	30:0:111:C:O2'	2.06	0.56
30:0:316:A:N3	30:0:336:G:O2'	2.37	0.56
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.87	0.56
30:0:2256:G:H2'	30:0:2257:G:C5'	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:108:HIS:H	9:I:109:PRO:HD2	1.71	0.56
23:W:139:GLY:O	23:W:141:HIS:HD2	1.89	0.56
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.88	0.56
30:0:10:U:O4	30:0:532:A:OP2	2.23	0.56
31:9:76:G:C3'	31:9:77:A:H5"	2.28	0.56
1:A:36:ASP:HB2	1:A:85:SER:H	1.71	0.56
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.71	0.56
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.88	0.56
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.05	0.56
23:W:125:HIS:NE2	30:0:1097:A:H5"	2.21	0.56
30:0:282:C:O2'	30:0:283:U:C5'	2.50	0.56
30:0:1592:G:H2'	30:0:1593:C:C6	2.41	0.56
30:0:1768:C:H2'	30:0:1769:C:O4'	2.06	0.56
30:0:2880:A:H2'	30:0:2881:C:H5'	1.88	0.56
2:B:85:ARG:NH1	38:B:9100:HOH:O	2.39	0.56
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.33	0.56
14:N:37:ARG:NH1	31:9:6:C:OP1	2.38	0.56
14:N:169:PRO:O	14:N:172:PHE:HB3	2.06	0.56
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.88	0.56
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.37	0.56
31:9:64:C:C2'	31:9:65:A:H5'	2.36	0.56
2:B:27:ASN:HD22	2:B:27:ASN:H	1.54	0.55
19:S:76:GLU:HB3	38:S:8991:HOH:O	2.05	0.55
30:0:816:G:C6	30:0:817:G:N1	2.74	0.55
30:0:1118:A:H8	30:0:1119:G:H5"	1.71	0.55
30:0:2703:A:H2'	30:0:2704:C:H6	1.71	0.55
31:9:64:C:H2'	31:9:65:A:H5'	1.88	0.55
8:H:48:VAL:HA	8:H:170:ARG:O	2.05	0.55
30:0:1163:G:H1	30:0:1184:C:N4	2.03	0.55
30:0:1588:G:C6	30:0:1589:G:C6	2.94	0.55
30:0:1595:G:O2'	30:0:1596:U:H5'	2.06	0.55
30:0:2269:C:C2'	30:0:2270:G:H5'	2.37	0.55
30:0:2645:U:C6	30:0:2645:U:OP2	2.60	0.55
30:0:2802:C:H2'	30:0:2803:C:C6	2.41	0.55
28:2:10:ARG:NH2	30:0:121:U:OP2	2.40	0.55
30:0:1119:G:N2	30:0:1246:A:H2	1.97	0.55
30:0:1477:C:H5'	30:0:1868:G:H5"	1.88	0.55
30:0:2256:G:C2'	30:0:2257:G:H5'	2.35	0.55
5:E:84:MET:HG2	5:E:168:ILE:HA	1.88	0.55
23:W:88:THR:HG22	23:W:89:ASP:H	1.71	0.55
30:0:407:A:H3'	38:0:4460:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:735:C:H2'	30:0:736:A:H5'	1.87	0.55
30:0:1878:G:O2'	30:0:1879:U:C6	2.58	0.55
31:9:39:U:H3'	31:9:40:C:H5"	1.88	0.55
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.88	0.55
30:0:652:G:H8	38:0:3009:HOH:O	1.89	0.55
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.06	0.55
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.88	0.55
30:0:272:A:H5'	30:0:273:G:OP2	2.07	0.55
30:0:1377:C:H6	30:0:1377:C:C5'	2.18	0.55
1:A:33:GLU:H	1:A:33:GLU:CD	2.10	0.55
2:B:275:GLY:O	2:B:291:ASP:HA	2.07	0.55
30:0:810:G:H2'	30:0:811:C:C6	2.42	0.55
30:0:2626:C:H2'	30:0:2627:G:C8	2.42	0.55
4:D:154:LYS:HD2	4:D:154:LYS:N	2.15	0.55
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.71	0.55
27:1:46:ARG:HA	38:1:8971:HOH:O	2.05	0.55
28:2:18:ASN:ND2	28:2:40:ARG:H	2.01	0.55
30:0:581:G:O2'	30:0:582:U:H5'	2.06	0.55
30:0:877:G:C5'	30:0:878:G:OP1	2.52	0.55
31:9:12:C:H5'	31:9:70:U:O4'	2.06	0.55
31:9:39:U:H1'	31:9:44:A:N6	2.21	0.55
31:9:49:G:O2'	31:9:50:G:H5'	2.07	0.55
1:A:223:ARG:HD2	30:0:2272:G:OP1	2.07	0.55
38:O:7674:HOH:O	30:0:935:G:H5'	2.05	0.55
22:V:50:ARG:HH12	30:0:56:G:H5"	1.70	0.55
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.35	0.55
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.90	0.55
23:W:38:THR:HG22	23:W:39:ASP:N	2.22	0.55
30:0:2502:C:H2'	30:0:2503:A:C5'	2.36	0.55
31:9:28:U:H2'	31:9:29:C:C6	2.41	0.55
31:9:91:C:H2'	31:9:92:G:O4'	2.07	0.55
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.07	0.54
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.89	0.54
22:V:50:ARG:NH1	30:0:56:G:H5"	2.22	0.54
30:0:271:C:C2	30:0:273:G:O4'	2.60	0.54
30:0:567:U:H5"	38:0:6401:HOH:O	2.06	0.54
30:0:1174:A:C6	30:0:1201:C:H4'	2.42	0.54
30:0:1209:C:H2'	30:0:1210:G:C8	2.36	0.54
30:0:2697:A:H2'	30:0:2698:G:O4'	2.07	0.54
31:9:1:U:H4'	31:9:3:A:OP1	2.07	0.54
2:B:162:MET:HE3	2:B:310:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.19	0.54
30:0:204:A:H2'	30:0:205:U:H5'	1.88	0.54
30:0:1291:A:H2	38:0:5292:HOH:O	1.89	0.54
30:0:2616:A:H4'	30:0:2617:G:OP1	2.06	0.54
30:0:2718:C:H6	30:0:2718:C:H5'	1.73	0.54
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.89	0.54
23:W:154:ARG:NH1	30:0:588:G:O6	2.40	0.54
27:1:9:GLY:HA2	30:0:1687:C:O2	2.07	0.54
30:0:999:C:O2'	30:0:1000:C:H5'	2.07	0.54
30:0:1172:G:H5"	38:0:7257:HOH:O	2.07	0.54
21:U:9:CYS:HA	21:U:52:THR:CG2	2.35	0.54
21:U:17:THR:HG22	21:U:18:GLY:H	1.72	0.54
30:0:1484:G:H2'	38:0:9103:HOH:O	2.08	0.54
30:0:2564:G:OP2	30:0:2565:C:H5"	2.06	0.54
2:B:267:LYS:HD3	38:0:9562:HOH:O	2.06	0.54
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.22	0.54
11:K:27:ARG:HD2	38:K:3442:HOH:O	2.07	0.54
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.55	0.54
17:Q:7:LEU:HD12	30:0:2424:U:H1'	1.89	0.54
8:H:168:VAL:HG13	38:H:213:HOH:O	2.08	0.54
14:N:80:SER:HB2	38:N:8833:HOH:O	2.07	0.54
30:0:1175:G:H1'	30:0:1193:A:C2'	2.36	0.54
30:0:1559:A:OP2	30:0:1559:A:H8	1.88	0.54
30:0:1766:U:O2	30:0:1778:A:H5'	2.08	0.54
2:B:79:MET:HE1	38:B:9092:HOH:O	2.07	0.54
15:O:37:ARG:HD2	30:0:656:G:OP2	2.08	0.54
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.89	0.54
30:0:65:C:O2'	30:0:66:G:H5'	2.07	0.54
2:B:211:THR:HG23	30:0:2840:A:OP1	2.08	0.54
5:E:10:ASP:HA	38:E:6017:HOH:O	2.06	0.54
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.90	0.54
8:H:64:SER:OG	30:0:2520:G:H5'	2.07	0.54
19:S:33:SER:O	19:S:37:VAL:HG23	2.08	0.54
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.89	0.54
27:1:37:CYS:SG	27:1:39:PHE:HB2	2.48	0.54
30:0:958:G:H2'	30:0:959:C:C6	2.42	0.54
30:0:1131:G:C6	30:0:1230:A:C4	2.96	0.54
30:0:1183:C:C2	30:0:1184:C:C5	2.96	0.54
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.90	0.54
7:G:20:VAL:O	7:G:24:VAL:HG23	2.08	0.54
14:N:132:ASN:O	14:N:135:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2269:C:O2'	30:0:2270:G:H5'	2.07	0.54
30:0:420:U:H2'	30:0:421:C:C6	2.44	0.53
30:0:549:A:O2'	30:0:550:C:H5'	2.08	0.53
31:9:34:A:H2'	31:9:35:C:O4'	2.08	0.53
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.73	0.53
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.23	0.53
13:M:28:GLN:O	13:M:32:ARG:HG3	2.08	0.53
30:0:90:A:H2'	30:0:91:G:O4'	2.08	0.53
30:0:961:A:H4'	38:0:6768:HOH:O	2.07	0.53
30:0:1730:G:H5'	30:0:1731:C:H5	1.73	0.53
30:0:2070:G:H2'	30:0:2072:G:OP1	2.08	0.53
30:0:2345:A:H3'	30:0:2346:C:H6	1.71	0.53
30:0:2705:U:H2'	30:0:2706:A:C8	2.43	0.53
31:9:1:U:O3'	31:9:3:A:H5"	2.08	0.53
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.89	0.53
3:C:95:GLU:HG3	38:C:8688:HOH:O	2.07	0.53
5:E:68:HIS:O	5:E:72:MET:HG3	2.09	0.53
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.90	0.53
22:V:55:ARG:O	22:V:59:ILE:HG12	2.08	0.53
23:W:125:HIS:HB2	23:W:137:GLN:HG2	1.90	0.53
30:0:255:A:H2'	30:0:256:C:C6	2.44	0.53
30:0:1505:U:H1'	38:0:7584:HOH:O	2.07	0.53
30:0:1615:A:H5'	38:0:4180:HOH:O	2.09	0.53
30:0:1622:G:H2'	30:0:1623:C:H5'	1.90	0.53
30:0:2826:G:C6	30:0:2913:A:N6	2.75	0.53
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.91	0.53
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.89	0.53
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.89	0.53
12:L:41:HIS:HD2	30:0:926:A:O2'	1.90	0.53
13:M:188:ARG:HD3	30:0:155:C:OP2	2.08	0.53
14:N:114:LYS:O	14:N:118:ILE:HG13	2.07	0.53
30:0:297:U:H2'	30:0:298:C:C6	2.43	0.53
30:0:318:U:H5'	30:0:339:A:C2	2.44	0.53
30:0:484:A:N1	30:0:506:G:H4'	2.23	0.53
30:0:1838:U:H3'	38:0:5521:HOH:O	2.09	0.53
30:0:2597:U:H2'	30:0:2598:U:H5'	1.90	0.53
31:9:20:G:O2'	31:9:21:G:H5'	2.08	0.53
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.43	0.53
30:0:2243:C:H5"	38:0:3745:HOH:O	2.07	0.53
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.72	0.53
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:281:U:C2'	30:0:282:C:H5'	2.39	0.53
30:0:1878:G:O2'	30:0:1879:U:P	2.67	0.53
30:0:2371:G:H5'	38:0:5010:HOH:O	2.07	0.53
5:E:69:ILE:HA	5:E:72:MET:CE	2.39	0.53
13:M:164:THR:HB	38:M:8819:HOH:O	2.08	0.53
28:2:28:LYS:O	30:0:87:C:H2'	2.09	0.53
30:0:319:A:H4'	30:0:338:C:C4	2.44	0.53
30:0:1483:C:O2'	30:0:1484:G:H5'	2.09	0.53
30:0:1592:G:H2'	30:0:1593:C:H6	1.71	0.53
30:0:1921:A:O2'	30:0:1922:A:H5'	2.09	0.53
30:0:1972:U:H2'	30:0:1973:A:C5'	2.38	0.53
31:9:24:U:H3'	31:9:25:G:C5'	2.39	0.53
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.72	0.53
30:0:256:C:H2'	30:0:257:G:O4'	2.09	0.53
30:0:506:G:N2	30:0:509:A:H5"	2.22	0.53
30:0:2301:A:H5"	30:0:2302:A:H5'	1.91	0.53
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.07	0.53
28:2:41:HIS:HD2	28:2:44:ARG:H	1.56	0.53
30:0:522:U:O2'	30:0:1366:C:H5'	2.08	0.53
30:0:1202:A:H2'	30:0:1203:G:C5'	2.39	0.53
30:0:1795:G:H2'	30:0:1796:A:O4'	2.09	0.53
3:C:63:SER:OG	30:0:2101:A:H2'	2.09	0.52
22:V:39:ALA:N	22:V:40:PRO:HD2	2.24	0.52
27:1:45:ARG:NH2	38:1:8976:HOH:O	2.38	0.52
30:0:396:U:O2'	30:0:418:C:H4'	2.08	0.52
30:0:413:G:H2'	30:0:414:C:C6	2.44	0.52
30:0:1342:C:H2'	30:0:1343:C:H5'	1.91	0.52
30:0:1535:G:H2'	30:0:1536:C:C6	2.44	0.52
12:L:37:LYS:HE2	30:0:2466:G:OP2	2.09	0.52
30:0:1201:C:H2'	30:0:1202:A:H5'	1.91	0.52
30:0:1603:A:C5'	30:0:1605:G:O4'	2.53	0.52
30:0:1878:G:C1'	38:0:6119:HOH:O	2.42	0.52
30:0:2507:G:H2'	30:0:2510:C:H42	1.74	0.52
3:C:2:GLN:HB3	38:C:8534:HOH:O	2.09	0.52
3:C:218:VAL:HG12	38:C:8634:HOH:O	2.08	0.52
8:H:69:ARG:HD3	38:H:233:HOH:O	2.10	0.52
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.90	0.52
22:V:64:GLY:O	22:V:65:ASP:HB2	2.08	0.52
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.90	0.52
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.92	0.52
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1213:C:O2'	30:0:1214:G:H5'	2.10	0.52
30:0:1268:C:H2'	30:0:1269:G:H8	1.75	0.52
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.10	0.52
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.90	0.52
13:M:75:ARG:HH11	30:0:1864:C:H5	1.56	0.52
18:R:33:ARG:NH1	38:R:8946:HOH:O	2.43	0.52
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.91	0.52
30:0:613:C:H2'	30:0:614:U:H6	1.75	0.52
30:0:1855:G:H4'	30:0:1856:C:O5'	2.09	0.52
31:9:56:A:H2'	31:9:57:A:C5'	2.05	0.52
1:A:186:TRP:CG	1:A:187:PRO:HA	2.45	0.52
5:E:80:TRP:O	5:E:134:SER:HA	2.09	0.52
14:N:93:GLN:HA	14:N:93:GLN:HE21	1.74	0.52
25:Y:235:GLU:CD	25:Y:235:GLU:H	2.11	0.52
30:0:137:U:H2'	30:0:139:C:C5	2.45	0.52
30:0:1183:C:H2'	30:0:1183:C:O2	2.08	0.52
30:0:1497:G:H4'	30:0:1627:G:O2'	2.09	0.52
30:0:1679:C:H5'	38:0:9325:HOH:O	2.08	0.52
30:0:2300:A:H4'	30:0:2301:A:O5'	2.10	0.52
30:0:2433:A:H2'	30:0:2434:A:C8	2.44	0.52
30:0:2613:G:O2'	30:0:2614:C:H5'	2.09	0.52
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.89	0.52
12:L:148:GLU:HA	38:L:8875:HOH:O	2.08	0.52
13:M:30:GLU:O	13:M:34:GLU:HG3	2.10	0.52
23:W:119:HIS:HD2	23:W:120:PRO:O	1.93	0.52
25:Y:146:PRO:O	25:Y:154:ARG:HG3	2.10	0.52
30:0:2445:U:H2'	30:0:2446:G:H8	1.74	0.52
30:0:2469:A:H1'	38:0:3237:HOH:O	2.08	0.52
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.92	0.52
2:B:238:ASN:HD22	2:B:240:GLY:N	2.00	0.52
2:B:320:GLN:NE2	2:B:321:PRO:HD2	2.24	0.52
3:C:107:ARG:O	3:C:111:VAL:HG23	2.10	0.52
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.25	0.52
18:R:117:HIS:HD2	30:0:20:G:H21	1.56	0.52
20:T:38:ARG:NH1	38:T:6217:HOH:O	2.42	0.52
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.09	0.52
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.58	0.52
30:0:603:A:H1'	30:0:605:C:C2	2.44	0.52
30:0:1309:U:O2'	30:0:1310:U:H5'	2.10	0.52
30:0:1342:C:O2'	30:0:1343:C:H5'	2.09	0.52
30:0:2256:G:H2'	30:0:2257:G:H5'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2781:U:O2'	30:0:2782:G:H5'	2.08	0.52
2:B:271:ASP:HB3	2:B:296:LEU:HD12	1.91	0.52
4:D:52:THR:HG21	30:0:2346:C:O2'	2.10	0.52
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.88	0.52
16:P:58:SER:HB3	38:0:5627:HOH:O	2.10	0.52
25:Y:142:SER:OG	30:0:1331:G:OP2	2.27	0.52
30:0:645:U:O2	30:0:761:A:H2	1.92	0.52
30:0:905:C:H3'	38:0:5190:HOH:O	2.08	0.52
30:0:1202:A:H2'	30:0:1203:G:H5'	1.91	0.52
30:0:1527:A:H1'	30:0:1528:A:C8	2.45	0.52
30:0:2587:OMU:H2'	30:0:2589:U:H5"	1.92	0.52
31:9:52:A:O2'	31:9:53:G:H5'	2.10	0.52
31:9:110:G:C5	31:9:111:U:C5	2.97	0.52
1:A:171:LYS:HB2	30:0:820:G:C5	2.45	0.52
2:B:158:LYS:HD3	30:0:2846:C:OP1	2.10	0.52
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.10	0.52
6:F:57:GLU:O	6:F:61:MET:HG3	2.09	0.52
12:L:143:THR:HG21	38:L:8841:HOH:O	2.09	0.52
16:P:115:SER:N	16:P:118:GLN:HE21	1.97	0.52
21:U:9:CYS:CA	21:U:52:THR:HG22	2.39	0.52
30:0:559:U:H6	30:0:559:U:C5'	2.17	0.52
30:0:1207:A:C8	30:0:1208:C:C6	2.98	0.52
30:0:1477:C:C5'	30:0:1868:G:H5"	2.39	0.52
30:0:1825:U:O2'	30:0:1826:C:H5'	2.10	0.52
30:0:2269:C:H2'	30:0:2270:G:C5'	2.40	0.52
30:0:2836:G:H1'	38:0:6838:HOH:O	2.09	0.52
2:B:41:PHE:HB3	2:B:190:MET:CE	2.40	0.52
9:I:69:PRO:HA	30:0:1164:U:OP1	2.10	0.52
18:R:40:ALA:O	18:R:44:VAL:HG23	2.10	0.52
24:X:43:VAL:HG12	24:X:44:ASP:N	2.25	0.52
30:0:177:A:H2'	30:0:178:U:O4'	2.09	0.52
30:0:538:C:H5"	30:0:539:G:C8	2.45	0.52
30:0:1636:G:O2'	30:0:1637:A:H5'	2.09	0.52
30:0:1857:A:H5"	38:0:6701:HOH:O	2.10	0.52
30:0:2072:G:C6	30:0:2533:C:H1'	2.45	0.52
30:0:2781:U:H2'	30:0:2782:G:C5'	2.39	0.52
4:D:65:GLU:HA	38:D:6752:HOH:O	2.09	0.51
15:O:3:THR:HG22	30:0:656:G:C5'	2.26	0.51
30:0:12:U:H2'	30:0:13:G:H5'	1.92	0.51
30:0:912:A:C4	30:0:1294:A:C2	2.97	0.51
30:0:1419:U:H2'	30:0:1685:A:C2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1589:G:H4'	38:0:6857:HOH:O	2.10	0.51
30:0:2830:U:O2'	30:0:2831:C:H5'	2.09	0.51
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.26	0.51
30:0:24:G:N2	30:0:518:G:H1'	2.25	0.51
30:0:497:A:H2'	30:0:498:A:C5'	2.41	0.51
30:0:1058:A:H2'	30:0:1060:C:H5"	1.91	0.51
30:0:1165:G:H4'	30:0:1174:A:O2'	2.10	0.51
30:0:1762:C:H2'	30:0:1763:C:H6	1.76	0.51
1:A:51:ARG:NH1	1:A:120:ARG:O	2.43	0.51
1:A:210:GLY:HA3	38:A:9046:HOH:O	2.08	0.51
27:1:25:LYS:HD2	28:2:48:ASP:HA	1.92	0.51
29:3:70:ARG:HB3	38:3:8997:HOH:O	2.09	0.51
30:0:304:G:H1'	30:0:347:A:N6	2.25	0.51
30:0:558:C:H2'	30:0:559:U:H5"	1.87	0.51
30:0:661:G:C5	30:0:686:A:C2	2.99	0.51
30:0:1188:A:C6	30:0:1189:A:C6	2.98	0.51
30:0:2064:U:H5'	30:0:2652:U:H4'	1.93	0.51
30:0:2435:U:H1'	38:0:5428:HOH:O	2.11	0.51
31:9:52:A:H2'	31:9:53:G:O4'	2.09	0.51
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.91	0.51
20:T:68:ASP:HB2	38:0:5658:HOH:O	2.10	0.51
30:0:119:A:H2'	30:0:120:A:H5"	1.92	0.51
30:0:1565:C:O2'	30:0:1566:C:H5'	2.10	0.51
30:0:1976:G:H1'	30:0:2005:G:N2	2.26	0.51
30:0:2689:A:C2'	30:0:2690:U:H5'	2.39	0.51
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.76	0.51
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.39	0.51
29:3:3:MET:O	29:3:90:PHE:HA	2.10	0.51
30:0:64:G:H2'	30:0:65:C:O4'	2.11	0.51
30:0:380:A:H2'	38:0:7225:HOH:O	2.10	0.51
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.40	0.51
5:E:69:ILE:HA	5:E:72:MET:HE2	1.91	0.51
30:0:42:C:H1'	38:0:4676:HOH:O	2.10	0.51
30:0:204:A:C2'	30:0:205:U:H5'	2.40	0.51
30:0:677:C:O2'	30:0:678:G:H5'	2.10	0.51
30:0:2421:G:H3'	30:0:2422:U:C5'	2.40	0.51
30:0:2421:G:H3'	30:0:2422:U:H5"	1.92	0.51
8:H:61:ARG:HG3	38:0:4972:HOH:O	2.10	0.51
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.93	0.51
24:X:85:VAL:HG12	24:X:86:GLU:N	2.26	0.51
25:Y:133:HIS:HD2	38:Y:9065:HOH:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1730:G:C5'	30:0:1731:C:H6	2.23	0.51
2:B:212:GLN:HA	30:0:1733:A:H4'	1.91	0.51
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.92	0.51
18:R:59:PHE:O	18:R:63:ASN:HB3	2.11	0.51
20:T:97:ARG:NH2	30:0:309:C:OP1	2.44	0.51
30:0:407:A:H8	38:0:4460:HOH:O	1.94	0.51
30:0:537:G:O4'	30:0:538:C:C5	2.64	0.51
30:0:589:U:H2'	30:0:590:A:H8	1.75	0.51
30:0:1925:G:O2'	30:0:1926:G:H5'	2.11	0.51
30:0:2105:C:H2'	30:0:2106:C:C6	2.46	0.51
3:C:214:THR:HG23	38:C:8648:HOH:O	2.10	0.51
7:G:12:ILE:HG23	38:0:5457:HOH:O	2.09	0.51
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.46	0.51
30:0:1622:G:C2'	30:0:1623:C:H5'	2.41	0.51
7:G:64:ASN:HD22	7:G:64:ASN:N	2.09	0.51
12:L:92:ASP:HA	12:L:121:ILE:HB	1.91	0.51
14:N:110:THR:HB	14:N:113:SER:HG	1.74	0.51
23:W:119:HIS:HE1	38:0:9554:HOH:O	1.93	0.51
30:0:1252:A:H2'	30:0:1253:C:O4'	2.11	0.51
30:0:1482:A:O2'	30:0:1483:C:H5'	2.11	0.51
30:0:1819:G:H2'	30:0:1820:G:C4'	2.41	0.51
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.44	0.50
12:L:143:THR:HG22	12:L:144:ASP:N	2.27	0.50
16:P:83:LYS:HG2	30:0:793:A:H5"	1.93	0.50
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.92	0.50
30:0:567:U:C5'	38:0:6401:HOH:O	2.59	0.50
30:0:1205:U:C2'	30:0:1206:U:C5'	2.77	0.50
30:0:1321:A:H2'	30:0:1322:G:C8	2.47	0.50
30:0:2717:C:C2'	30:0:2718:C:C5'	2.75	0.50
2:B:132:HIS:NE2	2:B:171:VAL:HG23	2.27	0.50
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.44	0.50
25:Y:212:ARG:HD2	38:Y:9085:HOH:O	2.09	0.50
30:0:939:A:N1	30:0:1027:G:O2'	2.40	0.50
30:0:1173:A:H4'	30:0:1174:A:C8	2.45	0.50
30:0:1191:A:C2	30:0:1207:A:C2	2.99	0.50
30:0:1386:G:O2'	30:0:1387:G:H5'	2.12	0.50
30:0:1684:A:O2'	30:0:1685:A:H5"	2.12	0.50
30:0:1762:C:O2'	30:0:1763:C:H5'	2.12	0.50
30:0:1778:A:H2'	30:0:1779:A:H5'	1.92	0.50
30:0:1915:U:O2'	30:0:1916:C:H5'	2.11	0.50
30:0:2769:C:H2'	30:0:2770:G:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:PRO:HD3	1:A:152:CYS:SG	2.51	0.50
2:B:62:ARG:HA	2:B:65:MET:CE	2.41	0.50
2:B:102:THR:HG21	2:B:182:VAL:O	2.11	0.50
4:D:103:ASN:HD22	4:D:134:LEU:H	1.59	0.50
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.11	0.50
12:L:97:VAL:HG12	12:L:98:GLU:O	2.12	0.50
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.93	0.50
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.92	0.50
30:0:711:G:C2	30:0:718:C:C2	3.00	0.50
30:0:940:G:C5	30:0:1027:G:C2	3.00	0.50
30:0:1158:G:O2'	30:0:1159:G:H5'	2.11	0.50
30:0:1667:A:H2'	30:0:1668:U:C6	2.45	0.50
30:0:2385:G:H2'	30:0:2386:U:C6	2.47	0.50
38:M:8837:HOH:O	30:0:169:A:H5"	2.12	0.50
15:O:25:VAL:HG23	15:O:26:TRP:N	2.27	0.50
18:R:132:ARG:HG2	18:R:133:ALA:N	2.24	0.50
21:U:39:ASN:ND2	21:U:44:ARG:HH11	2.08	0.50
23:W:43:GLY:HA3	30:0:945:U:O2'	2.11	0.50
30:0:735:C:C2'	30:0:736:A:H5'	2.41	0.50
30:0:1130:U:H2'	30:0:1131:G:O4'	2.11	0.50
30:0:1187:U:O2'	30:0:1189:A:H2	1.79	0.50
30:0:1304:U:H2'	30:0:1305:C:C6	2.46	0.50
30:0:2089:A:O2'	30:0:2090:G:H5'	2.11	0.50
30:0:2250:G:N2	30:0:2251:G:H1'	2.27	0.50
30:0:2584:G:H4'	38:0:7115:HOH:O	2.10	0.50
30:0:2667:G:H1'	30:0:2914:A:N3	2.26	0.50
31:9:3:A:H2	31:9:21:G:N3	2.09	0.50
3:C:22:PHE:HA	3:C:116:ALA:HA	1.92	0.50
18:R:150:PRO:CG	18:R:150:PRO:CB	2.87	0.50
30:0:17:G:H2'	30:0:18:C:C6	2.47	0.50
30:0:282:C:H1'	30:0:368:C:H41	1.71	0.50
30:0:559:U:C5	30:0:560:U:C5	3.00	0.50
30:0:2724:U:H2'	30:0:2725:G:O4'	2.11	0.50
1:A:33:GLU:O	1:A:34:ASP:HB2	2.10	0.50
3:C:79:ARG:O	3:C:87:ARG:HG2	2.11	0.50
9:I:89:GLU:OE2	30:0:1181:A:H5'	2.11	0.50
10:J:19:MET:CE	10:J:132:LEU:HD11	2.41	0.50
17:Q:95:GLU:HA	30:0:949:U:H4'	1.93	0.50
25:Y:151:SER:HB3	25:Y:154:ARG:HB2	1.92	0.50
30:0:69:A:C8	30:0:69:A:C5'	2.90	0.50
30:0:332:G:O2'	30:0:333:G:H5'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1333:U:H2'	30:0:1334:C:C6	2.47	0.50
31:9:55:U:H5'	38:9:9135:HOH:O	2.11	0.50
1:A:109:GLU:HG2	1:A:116:GLY:N	2.26	0.50
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.92	0.50
10:J:107:ASN:HD22	10:J:109:TYR:H	1.58	0.50
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.93	0.50
26:Z:34:SER:HB3	30:0:797:A:H4'	1.93	0.50
30:0:1200:A:H3'	38:0:5754:HOH:O	2.11	0.50
30:0:1422:U:H2'	30:0:1423:C:C6	2.47	0.50
30:0:2372:A:H2'	30:0:2373:U:H6	1.77	0.50
30:0:2710:U:H2'	30:0:2711:U:C6	2.46	0.50
30:0:638:C:H2'	30:0:639:A:C8	2.47	0.50
30:0:920:C:H4'	30:0:921:G:C2	2.45	0.50
30:0:1170:U:H2'	30:0:1172:G:OP2	2.11	0.50
30:0:1380:U:H5'	38:0:9218:HOH:O	2.12	0.50
30:0:1762:C:H2'	30:0:1763:C:C6	2.47	0.50
30:0:2252:A:C5	30:0:2253:G:H1'	2.47	0.50
2:B:258:GLY:H	2:B:260:HIS:CE1	2.29	0.50
22:V:12:THR:HG23	22:V:14:ALA:H	1.77	0.50
30:0:876:A:N3	30:0:876:A:C2'	2.75	0.50
31:9:24:U:H3'	31:9:25:G:H5'	1.94	0.50
4:D:50:VAL:HG13	31:9:41:C:O4'	2.12	0.49
6:F:91:VAL:HG11	30:0:262:A:OP2	2.11	0.49
11:K:49:LEU:CD2	11:K:80:ILE:HD13	2.42	0.49
11:K:55:VAL:HG12	11:K:56:SER:N	2.27	0.49
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.93	0.49
30:0:136:C:H2'	30:0:137:U:O4'	2.12	0.49
30:0:2871:G:H2'	30:0:2872:U:C6	2.47	0.49
31:9:55:U:H4'	31:9:56:A:C8	2.47	0.49
8:H:34:HIS:HD2	8:H:90:LEU:O	1.95	0.49
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.46	0.49
23:W:61:THR:HG23	23:W:151:GLU:HG3	1.94	0.49
30:0:488:U:H2'	38:0:4004:HOH:O	2.12	0.49
30:0:1165:G:O2'	30:0:1174:A:C1'	2.60	0.49
30:0:1211:G:H2'	30:0:1212:C:C6	2.47	0.49
30:0:2534:C:H1'	38:0:3491:HOH:O	2.11	0.49
2:B:91:PRO:HA	10:J:144:THR:OG1	2.12	0.49
4:D:76:ARG:NE	31:9:44:A:O4'	2.44	0.49
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.13	0.49
18:R:9:ASP:O	18:R:13:THR:HB	2.11	0.49
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:R:8953:HOH:O	30:0:1370:G:H5”	2.12	0.49
25:Y:115:ARG:HH21	30:0:1266:U:H4’	1.76	0.49
30:0:559:U:H2’	30:0:560:U:O4’	2.12	0.49
30:0:790:A:H1’	30:0:1710:A:H2’	1.94	0.49
30:0:1186:C:N4	30:0:1187:U:C4	2.81	0.49
2:B:244:PRO:HB3	30:0:1234:U:N3	2.27	0.49
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.27	0.49
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.10	0.49
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.47	0.49
18:R:128:ARG:NH2	30:0:2054:A:C2	2.80	0.49
30:0:69:A:H8	30:0:69:A:C5’	2.17	0.49
30:0:947:U:O2’	30:0:948:G:H5’	2.13	0.49
30:0:1286:A:H5”	30:0:1287:A:OP1	2.13	0.49
30:0:1309:U:C2’	30:0:1310:U:H5’	2.43	0.49
30:0:1515:A:H2’	30:0:1516:U:C6	2.48	0.49
30:0:1524:U:OP1	30:0:1524:U:H4’	2.12	0.49
30:0:1972:U:C2’	30:0:1973:A:H5”	2.42	0.49
5:E:139:GLU:OE2	30:0:2781:U:H1’	2.13	0.49
14:N:1:ALA:HB2	31:9:14:G:O2’	2.13	0.49
24:X:30:MET:HG2	30:0:1384:C:H5’	1.94	0.49
30:0:483:C:C4	30:0:484:A:C6	3.01	0.49
30:0:968:G:C2	30:0:1001:U:O2	2.66	0.49
30:0:1193:A:C2	30:0:1194:A:N6	2.80	0.49
30:0:2326:C:H4’	30:0:2412:G:C4’	2.43	0.49
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.38	0.49
5:E:126:ILE:HB	5:E:131:LEU:HD23	1.94	0.49
30:0:920:C:H5’	30:0:921:G:C4	2.48	0.49
30:0:1056:U:H2’	30:0:1057:A:O4’	2.12	0.49
30:0:1119:G:N2	30:0:1246:A:N1	2.60	0.49
30:0:1245:C:O5’	30:0:1245:C:H6	1.96	0.49
30:0:1278:A:H2’	30:0:1280:A:C8	2.48	0.49
2:B:17:LYS:O	2:B:260:HIS:HD2	1.95	0.49
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.94	0.49
11:K:130:MET:SD	21:U:25:ASP:O	2.70	0.49
19:S:57:THR:HG22	19:S:58:MET:N	2.28	0.49
30:0:371:U:H2’	30:0:372:A:C8	2.47	0.49
30:0:899:C:H5’	38:0:3199:HOH:O	2.13	0.49
30:0:1706:G:H1’	30:0:1712:A:H61	1.78	0.49
30:0:1909:A:N1	30:0:2128:G:H1’	2.27	0.49
30:0:2269:C:H2’	30:0:2270:G:H5’	1.94	0.49
30:0:2541:U:O2’	30:0:2542:C:H5’	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:56:A:C3'	31:9:57:A:H5"	2.42	0.49
1:A:179:MET:HG2	1:A:186:TRP:CB	2.43	0.49
6:F:107:ASP:O	6:F:111:ILE:HG13	2.12	0.49
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.12	0.49
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.76	0.49
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.13	0.49
14:N:17:ARG:HB3	14:N:17:ARG:HH11	1.78	0.49
30:0:1849:G:H1'	30:0:2011:A:N1	2.28	0.49
30:0:2869:G:H2'	30:0:2870:C:H6	1.78	0.49
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.43	0.49
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.45	0.49
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.94	0.49
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.28	0.49
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.42	0.49
15:O:24:ALA:HB3	30:0:710:G:OP1	2.13	0.49
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.47	0.49
30:0:2121:G:O2'	30:0:2122:C:H5'	2.13	0.49
2:B:206:THR:HG21	30:0:2716:G:C5'	2.40	0.49
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.94	0.49
13:M:78:LYS:HD3	38:0:7679:HOH:O	2.13	0.49
14:N:4:PRO:HG3	31:9:69:U:OP1	2.13	0.49
20:T:53:GLY:HA3	38:0:6800:HOH:O	2.12	0.49
30:0:226:A:H1'	30:0:393:G:C5	2.48	0.49
30:0:1066:U:H2'	30:0:1067:A:C8	2.48	0.49
30:0:1506:U:H6	30:0:1506:U:H5'	1.77	0.49
30:0:2271:G:N3	30:0:2271:G:H2'	2.28	0.49
30:0:2512:U:H4'	30:0:2514:U:O4	2.12	0.49
13:M:167:GLY:O	13:M:171:ARG:HG3	2.13	0.48
19:S:11:THR:H	19:S:14:ALA:HB3	1.77	0.48
19:S:57:THR:HG23	38:S:8979:HOH:O	2.11	0.48
30:0:191:A:C4	30:0:237:G:N7	2.81	0.48
30:0:1118:A:C8	30:0:1119:G:H5"	2.48	0.48
30:0:1545:C:H2'	30:0:1546:G:O4'	2.13	0.48
30:0:2645:U:H1'	38:0:9305:HOH:O	2.13	0.48
30:0:2664:A:H8	30:0:2664:A:OP1	1.96	0.48
30:0:2836:G:H5"	38:0:5165:HOH:O	2.12	0.48
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.78	0.48
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.48	0.48
30:0:1116:U:O2'	30:0:1118:A:C2	2.39	0.48
30:0:1447:U:H3'	30:0:1506:U:O2	2.13	0.48
30:0:1477:C:H5'	30:0:1868:G:H5'	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1972:U:H2'	30:0:1973:A:H5"	1.94	0.48
30:0:2326:C:H4'	30:0:2412:G:H4'	1.95	0.48
30:0:2329:C:O2'	30:0:2330:U:H5'	2.13	0.48
30:0:2379:G:N7	30:0:2408:A:N1	2.61	0.48
31:9:3:A:OP2	31:9:25:G:N2	2.45	0.48
3:C:43:LYS:HG2	30:0:449:A:N7	2.28	0.48
4:D:141:VAL:HG21	31:9:57:A:H8	1.78	0.48
23:W:4:LEU:O	23:W:32:CYS:HA	2.13	0.48
30:0:10:U:C4	30:0:532:A:C8	3.01	0.48
30:0:59:A:H5'	38:0:4330:HOH:O	2.12	0.48
30:0:447:A:O2'	30:0:448:G:H5'	2.13	0.48
30:0:1013:A:H1'	38:0:9158:HOH:O	2.13	0.48
30:0:2102:G:H1'	30:0:2103:A:N7	2.29	0.48
30:0:2816:A:H5"	30:0:2817:G:H5'	1.96	0.48
2:B:139:ASP:HB2	38:B:8995:HOH:O	2.12	0.48
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.77	0.48
12:L:34:GLY:HA2	38:0:5408:HOH:O	2.12	0.48
16:P:115:SER:OG	16:P:118:GLN:HG3	2.13	0.48
23:W:139:GLY:O	23:W:141:HIS:CD2	2.66	0.48
30:0:1185:U:H2'	30:0:1186:C:C6	2.48	0.48
30:0:1589:G:N2	30:0:1605:G:H1'	2.27	0.48
30:0:1667:A:C2	30:0:1668:U:C2	3.02	0.48
30:0:2420:G:H2'	30:0:2421:G:H8	1.79	0.48
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.96	0.48
2:B:119:HIS:O	2:B:121:PRO:HD3	2.13	0.48
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.94	0.48
13:M:171:ARG:NH2	30:0:189:A:OP1	2.47	0.48
23:W:88:THR:HG22	23:W:90:TYR:CD1	2.48	0.48
30:0:228:C:H2'	30:0:229:G:H5'	1.94	0.48
30:0:541:C:O2'	30:0:542:A:H5"	2.14	0.48
30:0:699:C:H6	30:0:744:G:O4'	1.96	0.48
30:0:1520:G:C6	30:0:1521:C:N4	2.82	0.48
30:0:1522:A:C2	30:0:1665:G:C6	3.02	0.48
30:0:2374:G:H2'	30:0:2375:A:C8	2.48	0.48
30:0:2493:C:O2	30:0:2493:C:H2'	2.13	0.48
16:P:1:THR:O	30:0:1396:C:H1'	2.14	0.48
20:T:106:GLU:HG3	38:T:4913:HOH:O	2.13	0.48
30:0:499:G:O2'	30:0:500:G:H5'	2.13	0.48
30:0:536:A:H3'	38:0:5049:HOH:O	2.14	0.48
30:0:1029:U:O2'	30:0:1273:C:OP1	2.27	0.48
30:0:2372:A:H2'	30:0:2373:U:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.13	0.48
5:E:101:GLU:HB2	5:E:116:THR:O	2.14	0.48
27:1:45:ARG:HB3	38:1:8967:HOH:O	2.14	0.48
30:0:346:U:H4'	38:0:6842:HOH:O	2.13	0.48
30:0:834:G:H4'	30:0:835:U:OP2	2.13	0.48
30:0:1594:C:O2'	30:0:1607:A:H4'	2.13	0.48
30:0:1739:G:O2'	30:0:1740:U:H5'	2.13	0.48
30:0:2387:U:H2'	30:0:2388:C:C6	2.48	0.48
30:0:291:C:H2'	30:0:292:G:O4'	2.14	0.48
30:0:312:U:C2	30:0:320:G:N2	2.82	0.48
30:0:1130:U:H5'	38:0:7668:HOH:O	2.13	0.48
30:0:1314:U:H5"	30:0:1316:G:O4'	2.13	0.48
31:9:1:U:C4'	31:9:3:A:OP1	2.60	0.48
31:9:45:A:C5	31:9:46:C:C5	3.02	0.48
1:A:3:ARG:HD3	30:0:870:G:OP2	2.13	0.48
1:A:126:ALA:HB1	1:A:138:VAL:CG1	2.44	0.48
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.94	0.48
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.29	0.48
30:0:289:G:O2'	30:0:290:C:H5'	2.14	0.48
30:0:304:G:H1'	30:0:347:A:H61	1.78	0.48
30:0:545:G:H8	30:0:545:G:C5'	2.12	0.48
30:0:2255:A:O2'	30:0:2256:G:H5'	2.14	0.48
10:J:107:ASN:HD22	10:J:107:ASN:C	2.16	0.48
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.96	0.48
27:1:12:ASN:O	30:0:1415:G:H5'	2.14	0.48
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.44	0.48
30:0:466:A:H2'	30:0:467:G:O4'	2.13	0.48
30:0:625:U:H3'	38:0:3250:HOH:O	2.13	0.48
30:0:820:G:H5'	30:0:821:U:H5'	1.95	0.48
30:0:1423:C:O2'	30:0:1424:A:H5'	2.14	0.48
30:0:1593:C:H1'	38:0:6105:HOH:O	2.14	0.48
30:0:2090:G:H2'	30:0:2091:G:C8	2.48	0.48
30:0:2840:A:H3'	38:0:7643:HOH:O	2.13	0.48
23:W:122:ARG:NH2	38:0:5289:HOH:O	2.46	0.47
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.14	0.47
30:0:106:A:H2'	30:0:107:U:O4'	2.14	0.47
30:0:541:C:C2'	30:0:542:A:C5'	2.79	0.47
30:0:736:A:H2'	30:0:737:A:O4'	2.14	0.47
30:0:1028:U:H1'	38:0:3639:HOH:O	2.14	0.47
31:9:110:G:C6	31:9:111:U:C5	3.02	0.47
4:D:51:ARG:NH1	4:D:68:PRO:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.29	0.47
16:P:87:ARG:HG2	38:P:185:HOH:O	2.14	0.47
30:0:185:G:O3'	30:0:186:A:H4'	2.14	0.47
30:0:559:U:C6	30:0:559:U:C3'	2.97	0.47
30:0:602:A:O2'	30:0:605:C:H4'	2.13	0.47
30:0:722:G:H22	30:0:938:G:P	2.37	0.47
30:0:1787:C:H4'	30:0:2883:A:O4'	2.14	0.47
6:F:59:ILE:CD1	30:0:263:U:C2	2.98	0.47
8:H:158:ASN:ND2	30:0:2502:C:H4'	2.30	0.47
14:N:100:ALA:O	14:N:129:ILE:HG23	2.13	0.47
22:V:12:THR:HG22	22:V:15:GLU:H	1.77	0.47
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.49	0.47
30:0:946:C:O2'	30:0:947:U:H5'	2.14	0.47
30:0:1181:A:H2'	30:0:1182:C:C5'	2.44	0.47
30:0:1181:A:C2'	30:0:1182:C:H5'	2.43	0.47
30:0:1456:C:H2'	30:0:1457:U:C6	2.49	0.47
30:0:1562:C:O2	30:0:1562:C:C2'	2.61	0.47
30:0:2032:U:O2'	30:0:2033:G:H5"	2.14	0.47
30:0:2134:G:C6	30:0:2258:A:C8	3.02	0.47
30:0:2266:A:H2'	30:0:2267:G:C8	2.49	0.47
30:0:2541:U:H3'	38:0:9060:HOH:O	2.14	0.47
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.50	0.47
30:0:968:G:O2'	30:0:969:G:H5'	2.14	0.47
30:0:1588:G:C5	30:0:1589:G:C6	3.03	0.47
30:0:1890:U:H4'	30:0:2010:A:C6	2.50	0.47
31:9:71:C:H2'	31:9:72:C:H6	1.79	0.47
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.96	0.47
8:H:31:ILE:HD11	8:H:65:LEU:HD23	1.96	0.47
23:W:64:THR:O	23:W:68:THR:HG22	2.14	0.47
25:Y:210:GLY:H	30:0:1313:A:H5"	1.78	0.47
30:0:168:C:O5'	30:0:168:C:H6	1.97	0.47
30:0:305:A:C5	30:0:329:A:C2	3.03	0.47
30:0:1137:G:H1'	38:0:3876:HOH:O	2.14	0.47
30:0:1183:C:N3	30:0:1184:C:N4	2.62	0.47
30:0:1206:U:H2'	30:0:1207:A:O4'	2.14	0.47
30:0:2000:G:O2'	30:0:2001:G:H5'	2.15	0.47
30:0:2001:G:O2'	30:0:2002:C:H5'	2.14	0.47
30:0:2712:G:O2'	30:0:2713:G:H5'	2.14	0.47
31:9:65:A:N6	31:9:112:U:C6	2.82	0.47
11:K:81:ARG:HD3	11:K:87:ARG:NH2	2.30	0.47
30:0:138:U:OP2	30:0:139:C:H5	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1153:C:N3	30:0:2786:G:O6	2.48	0.47
30:0:1406:A:H4'	30:0:1407:A:H5"	1.96	0.47
30:0:1823:G:O2'	30:0:1824:C:H5'	2.14	0.47
30:0:2335:C:H2'	30:0:2336:G:H8	1.78	0.47
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.48	0.47
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.32	0.47
11:K:41:LYS:O	11:K:42:ASN:HB2	2.15	0.47
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.95	0.47
16:P:59:ARG:O	16:P:63:ARG:HG3	2.15	0.47
19:S:77:VAL:O	19:S:80:ARG:HG2	2.15	0.47
20:T:26:THR:HA	20:T:39:ASN:HB3	1.95	0.47
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.13	0.47
23:W:13:MET:HE1	23:W:18:GLN:HA	1.95	0.47
25:Y:136:LYS:HE2	25:Y:138:ARG:NH1	2.28	0.47
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.95	0.47
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.15	0.47
30:0:283:U:C5	30:0:284:C:C4	3.03	0.47
30:0:527:U:H2'	30:0:528:G:C8	2.49	0.47
30:0:560:U:H2'	30:0:561:G:H8	1.79	0.47
30:0:814:G:H4'	38:0:3130:HOH:O	2.15	0.47
30:0:844:A:C6	30:0:882:A:C6	3.03	0.47
30:0:969:G:H1	30:0:999:C:H42	1.61	0.47
30:0:1400:C:O2'	30:0:1401:G:H5'	2.15	0.47
30:0:1548:U:O2'	30:0:1549:C:H5'	2.14	0.47
30:0:2074:A:H2'	38:0:3533:HOH:O	2.14	0.47
30:0:2239:C:O2'	30:0:2240:U:H5'	2.14	0.47
30:0:2361:A:H2'	30:0:2362:A:C8	2.49	0.47
30:0:2649:A:H5'	30:0:2649:A:C8	2.50	0.47
30:0:2871:G:H2'	30:0:2872:U:H6	1.79	0.47
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.04	0.47
18:R:122:GLN:HB3	18:R:138:SER:HB2	1.95	0.47
30:0:249:G:O2'	30:0:250:C:H5'	2.15	0.47
30:0:810:G:H2'	30:0:811:C:H6	1.79	0.47
30:0:853:C:H2'	30:0:854:G:O4'	2.14	0.47
30:0:1904:A:H2'	30:0:1905:U:O4'	2.15	0.47
30:0:2506:A:N6	30:0:2511:A:O2'	2.43	0.47
10:J:127:ILE:CG2	33:J:8801:CL:CL	2.96	0.47
14:N:147:ILE:HB	38:9:9087:HOH:O	2.15	0.47
25:Y:144:ARG:CZ	38:Y:9096:HOH:O	2.62	0.47
30:0:290:C:O2'	30:0:291:C:H5'	2.14	0.47
30:0:1014:A:H2'	30:0:1015:C:H5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1377:C:H1'	38:0:9039:HOH:O	2.15	0.47
30:0:1942:A:H2'	30:0:1943:C:H6	1.79	0.47
2:B:144:THR:HB	38:B:9092:HOH:O	2.14	0.47
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.44	0.47
10:J:6:PHE:HB3	10:J:109:TYR:OH	2.15	0.47
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.96	0.47
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.50	0.47
14:N:162:ASP:HA	38:N:8830:HOH:O	2.15	0.47
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.50	0.47
30:0:1970:G:H2'	30:0:1970:G:N3	2.30	0.47
30:0:2649:A:H5'	30:0:2649:A:H8	1.79	0.47
3:C:168:ARG:NH2	3:C:190:ALA:O	2.48	0.46
10:J:131:THR:HG22	10:J:133:GLY:N	2.30	0.46
12:L:27:ARG:HH21	12:L:30:ARG:HG2	1.80	0.46
16:P:91:LYS:O	16:P:95:GLU:HG3	2.15	0.46
16:P:114:LEU:HA	16:P:118:GLN:NE2	2.30	0.46
30:0:17:G:H2'	30:0:18:C:H6	1.79	0.46
30:0:254:C:O2	30:0:254:C:H2'	2.14	0.46
30:0:364:U:H2'	30:0:365:G:O4'	2.15	0.46
30:0:1149:U:C5	30:0:1215:A:C5	3.04	0.46
30:0:1760:G:H5'	30:0:1818:C:O2'	2.15	0.46
31:9:3:A:C2	31:9:21:G:N3	2.83	0.46
18:R:111:ILE:HG23	18:R:145:LEU:CD1	2.46	0.46
25:Y:189:ASN:ND2	25:Y:192:ASP:H	2.13	0.46
27:1:16:HIS:HE1	30:0:775:G:OP1	1.98	0.46
27:1:42:SER:HB2	38:1:8956:HOH:O	2.14	0.46
30:0:1379:A:H1'	38:0:9689:HOH:O	2.15	0.46
31:9:76:G:H3'	31:9:77:A:C5'	2.28	0.46
12:L:30:ARG:NH2	38:L:8823:HOH:O	2.44	0.46
13:M:169:ARG:NH2	38:M:8849:HOH:O	2.48	0.46
15:O:65:LEU:HD13	30:0:746:A:C6	2.51	0.46
23:W:13:MET:CE	23:W:17:ILE:HG22	2.46	0.46
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.45	0.46
30:0:162:C:H2'	30:0:163:U:H5'	1.97	0.46
30:0:1244:U:H4'	30:0:1246:A:O4'	2.16	0.46
30:0:1820:G:C6	30:0:2030:A:C2	3.04	0.46
30:0:1940:C:H4'	38:0:7346:HOH:O	2.16	0.46
30:0:2858:U:H2'	30:0:2859:C:O4'	2.15	0.46
31:9:1:U:O3'	31:9:3:A:C5'	2.63	0.46
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	1.98	0.46
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:95:A:H5”	30:0:97:G:O4’	2.14	0.46
30:0:152:A:H2’	30:0:153:C:C6	2.50	0.46
30:0:764:C:H2’	30:0:765:G:O4’	2.15	0.46
30:0:1268:C:H2’	30:0:1269:G:C8	2.50	0.46
30:0:1511:U:O2’	30:0:1512:G:H5’	2.15	0.46
30:0:1921:A:C6	30:0:1922:A:C2	3.04	0.46
30:0:2064:U:H4’	30:0:2653:A:OP1	2.14	0.46
30:0:2578:G:H5’	30:0:2578:G:C8	2.39	0.46
1:A:36:ASP:CB	1:A:85:SER:H	2.29	0.46
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.79	0.46
3:C:39:GLN:O	3:C:43:LYS:HD3	2.16	0.46
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.96	0.46
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.48	0.46
24:X:71:ARG:HD3	38:X:2171:HOH:O	2.16	0.46
27:1:1:THR:HB	38:0:7140:HOH:O	2.15	0.46
30:0:89:G:H4’	38:0:4766:HOH:O	2.16	0.46
30:0:255:A:C5	30:0:256:C:C4	3.04	0.46
30:0:1021:G:O2’	30:0:1022:A:H5’	2.16	0.46
30:0:1339:G:C6	30:0:1340:G:N1	2.84	0.46
30:0:2420:G:H2’	30:0:2421:G:C8	2.51	0.46
30:0:2783:A:H2’	30:0:2784:A:C8	2.50	0.46
30:0:2839:C:H2’	30:0:2840:A:H5”	1.96	0.46
31:9:33:U:H2’	38:9:9066:HOH:O	2.15	0.46
31:9:58:G:H3’	31:9:59:C:C6	2.49	0.46
2:B:280:VAL:HG13	2:B:333:GLU:O	2.16	0.46
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.50	0.46
3:C:132:ASP:HB3	38:C:8567:HOH:O	2.16	0.46
23:W:125:HIS:CE1	30:0:1097:A:H5”	2.51	0.46
28:2:44:ARG:HD3	38:0:6937:HOH:O	2.15	0.46
30:0:125:U:H2’	38:0:3761:HOH:O	2.15	0.46
30:0:282:C:C2’	30:0:283:U:H5’	2.45	0.46
30:0:1087:G:H4’	30:0:1088:A:OP1	2.15	0.46
30:0:1845:A:O2’	30:0:1846:U:H5’	2.15	0.46
30:0:2617:G:N3	30:0:2617:G:H2’	2.30	0.46
2:B:260:HIS:HE1	38:0:5167:HOH:O	1.97	0.46
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.98	0.46
3:C:46:TYR:CE1	30:0:450:C:H4’	2.50	0.46
4:D:52:THR:CG2	30:0:2346:C:H4’	2.45	0.46
7:G:16:LYS:O	7:G:20:VAL:HG23	2.16	0.46
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.48	0.46
30:0:407:A:H2’	30:0:408:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:704:C:H2'	30:0:705:C:H6	1.81	0.46
30:0:1044:C:H5	38:0:6604:HOH:O	1.98	0.46
30:0:1166:A:H2'	30:0:1166:A:N3	2.31	0.46
30:0:1840:A:H4'	30:0:1841:C:O5'	2.16	0.46
30:0:1878:G:O2'	30:0:1879:U:OP2	2.33	0.46
3:C:48:SER:HB3	30:0:1352:A:N1	2.31	0.46
5:E:143:GLN:HE22	30:0:2779:G:H21	1.63	0.46
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.98	0.46
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.98	0.46
13:M:81:ARG:HG3	13:M:85:ARG:HB2	1.97	0.46
13:M:159:VAL:HG13	13:M:160:PHE:N	2.31	0.46
19:S:45:TYR:O	19:S:80:ARG:NH2	2.49	0.46
23:W:10:GLU:HB2	23:W:18:GLN:NE2	2.31	0.46
24:X:85:VAL:HG12	24:X:86:GLU:H	1.80	0.46
30:0:1730:G:C5'	30:0:1731:C:C5	2.95	0.46
30:0:2032:U:H2'	30:0:2033:G:H5'	1.97	0.46
30:0:2353:A:H4'	30:0:2354:A:O5'	2.16	0.46
11:K:74:VAL:HG13	11:K:113:ILE:HG12	1.98	0.46
13:M:145:ASP:HB2	38:M:8864:HOH:O	2.15	0.46
19:S:56:ASN:O	28:2:8:LYS:NZ	2.47	0.46
30:0:772:G:H2'	30:0:773:A:O4'	2.16	0.46
30:0:862:U:H2'	30:0:863:G:H8	1.80	0.46
30:0:1052:G:H2'	30:0:1052:G:N3	2.30	0.46
30:0:1834:C:H2'	30:0:1840:A:H62	1.81	0.46
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.51	0.46
3:C:197:SER:HB3	38:C:8579:HOH:O	2.16	0.46
3:C:233:THR:HG22	3:C:234:VAL:N	2.31	0.46
14:N:94:GLU:HG3	14:N:186:LEU:HD12	1.98	0.46
30:0:424:C:H2'	30:0:425:U:C6	2.51	0.46
30:0:571:C:O5'	30:0:571:C:H6	1.99	0.46
30:0:699:C:H2'	30:0:744:G:N3	2.31	0.46
30:0:2002:C:H2'	30:0:2003:U:H5'	1.97	0.46
30:0:2250:G:H2'	30:0:2251:G:O4'	2.16	0.46
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.46
30:0:2906:A:H5'	30:0:2907:C:O4'	2.16	0.46
31:9:36:C:C5	31:9:37:C:C5	3.04	0.46
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.97	0.45
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.31	0.45
3:C:27:ARG:HG2	3:C:30:LEU:HG	1.98	0.45
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.98	0.45
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:23:ILE:O	7:G:27:ILE:HG13	2.16	0.45
8:H:91:ARG:O	30:0:1003:U:H4'	2.16	0.45
10:J:39:VAL:HG22	10:J:107:ASN:HA	1.98	0.45
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.45	0.45
12:L:18:HIS:CD2	30:0:902:G:N7	2.82	0.45
30:0:1154:A:H2'	30:0:1155:G:C8	2.51	0.45
30:0:2505:G:H2'	30:0:2506:A:H5'	1.97	0.45
31:9:58:G:H3'	31:9:59:C:C5	2.51	0.45
2:B:305:ASP:O	2:B:306:LYS:HB2	2.17	0.45
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.96	0.45
7:G:67:LEU:O	7:G:71:LEU:HG	2.15	0.45
13:M:9:ARG:HD2	30:0:380:A:OP2	2.15	0.45
23:W:24:LEU:O	23:W:26:ILE:HG22	2.16	0.45
30:0:559:U:C6	30:0:559:U:H3'	2.51	0.45
30:0:1080:C:O5'	30:0:1080:C:H6	1.99	0.45
30:0:1181:A:N1	30:0:1192:A:O2'	2.42	0.45
30:0:1626:A:H2'	30:0:1627:G:C5'	2.47	0.45
30:0:2112:A:H2'	30:0:2113:G:C8	2.51	0.45
30:0:2473:U:O3'	30:0:2474:A:H3'	2.16	0.45
30:0:2756:U:C2	30:0:2896:A:H2	2.33	0.45
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.40	0.45
8:H:31:ILE:HG23	38:H:233:HOH:O	2.16	0.45
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.98	0.45
11:K:114:ALA:HB3	11:K:117:VAL:HG23	1.99	0.45
12:L:18:HIS:HB3	38:0:9150:HOH:O	2.15	0.45
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.51	0.45
30:0:366:U:H2'	30:0:367:G:O4'	2.16	0.45
30:0:1185:U:C5'	38:0:7462:HOH:O	2.62	0.45
30:0:2506:A:O2'	30:0:2507:G:O5'	2.35	0.45
30:0:2511:A:H2'	30:0:2512:U:O4'	2.16	0.45
30:0:2825:C:H4'	30:0:2826:G:O5'	2.16	0.45
31:9:114:G:H2'	31:9:115:C:C6	2.52	0.45
2:B:27:ASN:HD21	30:0:2807:U:P	2.39	0.45
3:C:129:HIS:CE1	3:C:232:LEU:H	2.35	0.45
12:L:67:ARG:O	12:L:71:GLU:HG3	2.17	0.45
19:S:37:VAL:O	19:S:41:VAL:HG23	2.16	0.45
25:Y:148:GLY:HA3	30:0:622:G:P	2.56	0.45
30:0:214:U:H5'	38:0:6139:HOH:O	2.15	0.45
30:0:297:U:H2'	30:0:298:C:H6	1.80	0.45
30:0:816:G:H5'	30:0:1598:A:H4'	1.98	0.45
30:0:1850:U:H2'	30:0:1851:G:H8	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:55:U:H4'	31:9:56:A:H8	1.81	0.45
1:A:164:ARG:NH2	30:0:1877:G:OP1	2.49	0.45
4:D:140:ARG:HH11	4:D:140:ARG:HG3	1.80	0.45
10:J:52:GLN:HE22	30:0:1119:G:H8	1.65	0.45
15:O:21:SER:OG	15:O:106:PRO:HB2	2.15	0.45
17:Q:32:GLU:O	17:Q:93:ARG:NH2	2.50	0.45
20:T:54:ASP:OD2	30:0:316:A:H5'	2.16	0.45
25:Y:122:ARG:NH2	38:Y:9019:HOH:O	2.49	0.45
30:0:432:G:O2'	30:0:433:C:H5'	2.16	0.45
30:0:513:A:N3	38:0:3653:HOH:O	2.36	0.45
30:0:702:G:O2'	30:0:703:G:H5'	2.16	0.45
30:0:1182:C:C1'	30:0:1192:A:H8	2.28	0.45
30:0:2250:G:C2	30:0:2251:G:H1'	2.50	0.45
30:0:2740:G:H2'	30:0:2741:A:O4'	2.16	0.45
4:D:49:PRO:HA	4:D:73:VAL:HG22	1.99	0.45
10:J:19:MET:HE1	10:J:79:PHE:HA	1.98	0.45
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.51	0.45
30:0:101:C:H2'	30:0:102:A:C8	2.51	0.45
30:0:652:G:H2'	30:0:653:U:O4'	2.16	0.45
30:0:1789:G:H2'	30:0:1790:C:O5'	2.16	0.45
30:0:2439:C:H5'	38:0:5486:HOH:O	2.17	0.45
30:0:2644:C:H4'	38:0:9154:HOH:O	2.16	0.45
12:L:30:ARG:HD2	30:0:164:G:H5"	1.99	0.45
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.99	0.45
20:T:79:LEU:HG	20:T:89:ARG:HB2	1.98	0.45
24:X:25:ARG:HD2	38:X:5356:HOH:O	2.17	0.45
30:0:415:A:O2'	30:0:416:G:H5'	2.17	0.45
30:0:1198:U:C6	30:0:1200:A:OP2	2.70	0.45
30:0:2415:A:C2'	30:0:2416:G:H5'	2.46	0.45
30:0:2637:A:H5'	38:0:9275:HOH:O	2.16	0.45
2:B:256:GLN:HG2	38:B:9125:HOH:O	2.16	0.45
6:F:91:VAL:HG12	6:F:92:GLY:H	1.79	0.45
12:L:57:VAL:O	12:L:57:VAL:HG12	2.17	0.45
13:M:164:THR:CG2	13:M:165:GLY:N	2.79	0.45
23:W:122:ARG:HG3	23:W:122:ARG:HH11	1.81	0.45
30:0:113:A:OP2	30:0:114:A:H2'	2.17	0.45
30:0:1015:C:O5'	30:0:1015:C:H6	1.99	0.45
30:0:1209:C:C2	30:0:1210:G:C8	3.05	0.45
30:0:2032:U:C2'	30:0:2033:G:C5'	2.95	0.45
30:0:2324:G:N2	30:0:2377:U:H1'	2.32	0.45
30:0:2566:A:C2	30:0:2696:G:O4'	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:NH2	1:A:236:GLY:O	2.50	0.45
4:D:48:MET:HB3	31:9:41:C:H4'	1.99	0.45
12:L:150:GLN:HB3	38:L:8872:HOH:O	2.16	0.45
14:N:154:LEU:C	14:N:156:GLU:H	2.18	0.45
15:O:35:LYS:HD3	38:0:4615:HOH:O	2.17	0.45
16:P:36:THR:O	16:P:39:ASP:HB2	2.17	0.45
23:W:11:VAL:O	23:W:12:ASN:HB2	2.17	0.45
23:W:119:HIS:CG	38:0:5289:HOH:O	2.70	0.45
30:0:281:U:HO2'	30:0:282:C:H5'	1.80	0.45
30:0:587:A:H5"	38:0:7285:HOH:O	2.16	0.45
30:0:690:G:H4'	30:0:741:C:O2	2.17	0.45
30:0:1006:A:N1	30:0:2311:A:H1'	2.31	0.45
30:0:1117:A:C2	30:0:1244:U:C2	3.05	0.45
30:0:2361:A:H5'	30:0:2361:A:H8	1.82	0.45
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.99	0.45
1:A:211:LYS:HB2	38:A:9077:HOH:O	2.16	0.45
2:B:214:PRO:HD2	38:0:9075:HOH:O	2.15	0.45
2:B:215:VAL:HA	2:B:220:VAL:HG22	1.98	0.45
2:B:229:ARG:HD2	38:0:9108:HOH:O	2.17	0.45
3:C:49:ASP:HB3	3:C:52:ALA:HB2	1.99	0.45
30:0:629:A:H2'	30:0:630:A:O4'	2.17	0.45
30:0:737:A:H2'	30:0:738:G:O4'	2.17	0.45
30:0:1171:A:H2'	30:0:1172:G:H5'	1.98	0.45
30:0:1543:G:N1	30:0:1641:A:OP2	2.40	0.45
2:B:177:HIS:O	2:B:181:ILE:HG13	2.17	0.44
3:C:138:VAL:HG11	3:C:160:LEU:HD13	1.98	0.44
9:I:112:LEU:HG	30:0:1162:G:O2'	2.17	0.44
18:R:29:LYS:HD2	38:R:8943:HOH:O	2.16	0.44
24:X:25:ARG:HD3	24:X:64:ALA:O	2.16	0.44
30:0:105:G:O2'	30:0:106:A:H5'	2.17	0.44
30:0:1163:G:H2'	30:0:1164:U:C5	2.52	0.44
30:0:1188:A:N6	30:0:1189:A:N6	2.65	0.44
30:0:1224:G:H2'	30:0:1225:C:C6	2.51	0.44
30:0:2114:C:O2'	30:0:2115:U:H5'	2.17	0.44
30:0:2325:U:O2'	30:0:2411:C:H1'	2.16	0.44
31:9:35:C:H5"	38:9:9076:HOH:O	2.17	0.44
2:B:217:ARG:CG	2:B:257:THR:HG22	2.47	0.44
8:H:30:LYS:H	8:H:62:HIS:CD2	2.35	0.44
12:L:14:GLY:O	30:0:1295:G:H5"	2.17	0.44
12:L:33:ALA:HB3	38:L:8896:HOH:O	2.16	0.44
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:55:LYS:HG2	16:P:56:GLY:N	2.31	0.44
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.99	0.44
27:1:25:LYS:O	27:1:25:LYS:HG2	2.18	0.44
30:0:134:U:C2	30:0:145:A:C2	3.06	0.44
30:0:137:U:OP1	30:0:259:G:O2'	2.33	0.44
30:0:195:C:H2'	30:0:196:G:H5'	1.99	0.44
30:0:541:C:H2'	30:0:542:A:H5'	1.91	0.44
30:0:699:C:C2	30:0:743:G:N2	2.85	0.44
30:0:727:G:H3'	30:0:728:C:H6	1.82	0.44
30:0:820:G:O2'	30:0:856:G:H4'	2.18	0.44
30:0:1398:G:O2'	30:0:1399:A:H5'	2.18	0.44
30:0:1501:A:H4'	38:0:5597:HOH:O	2.17	0.44
30:0:1592:G:O2'	30:0:1593:C:O5'	2.35	0.44
30:0:1992:U:H2'	30:0:1994:A:OP2	2.17	0.44
2:B:198:GLU:HA	38:B:9126:HOH:O	2.17	0.44
2:B:243:ASN:HA	2:B:244:PRO:C	2.38	0.44
6:F:101:ALA:HA	38:F:5413:HOH:O	2.16	0.44
15:O:25:VAL:CG1	30:0:710:G:H5'	2.48	0.44
24:X:73:ARG:NH1	24:X:88:GLU:HB2	2.33	0.44
30:0:283:U:H5	30:0:284:C:C4	2.33	0.44
30:0:660:A:H4'	30:0:661:G:O5'	2.18	0.44
30:0:1206:U:C5'	30:0:1206:U:H6	2.22	0.44
30:0:1583:U:H2'	30:0:1584:C:O4'	2.18	0.44
30:0:1702:U:H1'	38:0:5772:HOH:O	2.18	0.44
30:0:2509:A:OP2	30:0:2510:C:H5	2.00	0.44
30:0:2753:G:O2'	30:0:2754:G:H5'	2.18	0.44
2:B:253:GLN:OE1	30:0:2090:G:N2	2.51	0.44
10:J:45:VAL:HG11	10:J:121:LEU:HD22	1.99	0.44
25:Y:210:GLY:N	30:0:1313:A:H5"	2.33	0.44
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.17	0.44
28:2:37:HIS:CE1	30:0:462:A:C8	3.06	0.44
30:0:295:C:H2'	30:0:296:G:O4'	2.17	0.44
30:0:535:G:C5	30:0:2063:U:C4	3.05	0.44
30:0:790:A:H2'	30:0:791:A:O4'	2.18	0.44
30:0:999:C:H2'	30:0:1000:C:O4'	2.17	0.44
30:0:1166:A:OP1	30:0:1174:A:H4'	2.16	0.44
30:0:1249:U:H2'	30:0:1250:C:H6	1.79	0.44
30:0:1714:C:O2'	30:0:1715:C:H5'	2.17	0.44
30:0:2003:U:H4'	30:0:2004:U:H5	1.83	0.44
30:0:2245:C:H6	30:0:2245:C:O5'	2.00	0.44
30:0:2401:A:H2'	30:0:2402:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLU:OE2	30:0:1855:G:H8	2.00	0.44
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.01	0.44
3:C:80:VAL:HA	3:C:81:PRO:HD3	1.84	0.44
8:H:76:LEU:HD21	8:H:149:VAL:HA	1.98	0.44
10:J:130:VAL:HG12	10:J:131:THR:N	2.33	0.44
12:L:4:LYS:HE2	30:0:645:U:OP2	2.18	0.44
17:Q:1:PRO:HA	30:0:2299:G:O6	2.17	0.44
30:0:73:U:O2'	30:0:74:G:H5'	2.18	0.44
30:0:545:G:C8	30:0:545:G:C5'	2.94	0.44
30:0:694:A:C2'	30:0:695:C:H5'	2.47	0.44
30:0:1163:G:N2	38:0:4726:HOH:O	2.49	0.44
30:0:1183:C:H41	30:0:1192:A:P	2.40	0.44
30:0:1434:A:H2'	30:0:1436:C:C5	2.52	0.44
1:A:167:LYS:HB2	26:Z:53:ILE:HD13	1.99	0.44
11:K:66:ARG:HH12	30:0:1992:U:H3'	1.82	0.44
16:P:120:ARG:NH1	30:0:1594:C:C5	2.86	0.44
26:Z:44:ARG:HB2	30:0:1886:A:O2'	2.18	0.44
30:0:758:A:H2'	30:0:759:C:O4'	2.17	0.44
30:0:1163:G:C2	30:0:1184:C:N3	2.86	0.44
30:0:1191:A:H2	30:0:1206:U:H3	1.64	0.44
30:0:1444:G:O2'	30:0:1502:A:N1	2.41	0.44
30:0:1755:A:H2'	30:0:1756:G:O4'	2.18	0.44
30:0:1805:G:O2'	30:0:1806:G:H5'	2.17	0.44
30:0:1871:U:O4'	30:0:1873:G:C8	2.71	0.44
30:0:2846:C:H4'	38:0:5080:HOH:O	2.18	0.44
31:9:31:C:H2'	31:9:32:G:O4'	2.18	0.44
2:B:51:VAL:CG1	2:B:53:LEU:HD13	2.46	0.44
2:B:75:GLU:OE2	2:B:151:VAL:HG13	2.18	0.44
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.17	0.44
11:K:41:LYS:HA	30:0:2582:G:O3'	2.18	0.44
15:O:32:ARG:O	15:O:32:ARG:HD3	2.17	0.44
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.32	0.44
25:Y:165:GLU:HB3	38:0:6704:HOH:O	2.17	0.44
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.52	0.44
30:0:241:A:N1	30:0:378:A:H4'	2.33	0.44
30:0:506:G:N2	30:0:509:A:C5'	2.66	0.44
30:0:603:A:H4'	30:0:604:G:O5'	2.17	0.44
30:0:1972:U:H2'	30:0:1973:A:H5'	1.99	0.44
30:0:2064:U:H5'	30:0:2652:U:O3'	2.18	0.44
30:0:2104:C:O2	30:0:2485:A:N1	2.51	0.44
30:0:2895:C:H2'	38:0:9570:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:1:U:C5'	31:9:3:A:OP1	2.65	0.44
1:A:95:PRO:HA	1:A:153:ARG:HA	2.00	0.44
4:D:62:ASP:HA	38:D:4233:HOH:O	2.18	0.44
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.51	0.44
8:H:57:THR:HG23	8:H:131:GLN:HA	2.00	0.44
14:N:108:SER:HA	14:N:109:PRO:HD3	1.75	0.44
30:0:512:G:O3'	30:0:513:A:H8	2.00	0.44
30:0:574:G:O2'	30:0:575:A:H5'	2.18	0.44
30:0:731:U:H2'	30:0:732:C:C6	2.53	0.44
30:0:1051:C:H2'	30:0:1052:G:O4'	2.18	0.44
30:0:1143:G:C6	30:0:1221:G:C6	3.06	0.44
30:0:1702:U:H5'	38:0:3421:HOH:O	2.16	0.44
2:B:124:ALA:O	2:B:128:ILE:HG13	2.18	0.44
3:C:16:VAL:HG21	38:C:8641:HOH:O	2.17	0.44
9:I:101:LYS:O	9:I:105:GLU:HG3	2.18	0.44
13:M:86:GLN:HE22	30:0:2274:A:H1'	1.83	0.44
20:T:23:VAL:HG23	20:T:41:ARG:HG3	1.98	0.44
25:Y:189:ASN:C	25:Y:189:ASN:HD22	2.21	0.44
30:0:494:C:H2'	30:0:496:G:OP2	2.17	0.44
30:0:596:C:H2'	30:0:597:A:C8	2.52	0.44
30:0:596:C:H2'	30:0:597:A:H8	1.83	0.44
30:0:1116:U:HO2'	30:0:1118:A:H2	0.68	0.44
30:0:1819:G:C2'	30:0:1820:G:H5'	2.47	0.44
30:0:2073:G:H5"	38:0:3823:HOH:O	2.17	0.44
30:0:2249:G:C2	30:0:2253:G:C6	3.06	0.44
30:0:2328:U:C4	30:0:2329:C:C5	3.06	0.44
30:0:2891:A:C2	30:0:2892:G:C4	3.06	0.44
30:0:2908:A:O5'	30:0:2908:A:H8	2.00	0.44
31:9:39:U:C2'	31:9:40:C:OP1	2.66	0.44
1:A:223:ARG:NH1	38:A:8985:HOH:O	2.50	0.43
2:B:315:VAL:HG23	2:B:316:ARG:HG2	2.00	0.43
9:I:87:PRO:HB3	38:I:6825:HOH:O	2.18	0.43
16:P:81:LYS:HG2	38:0:9538:HOH:O	2.18	0.43
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.99	0.43
30:0:88:G:H8	30:0:88:G:H5'	1.83	0.43
30:0:276:C:H6	30:0:276:C:O5'	2.01	0.43
30:0:1586:G:O2'	30:0:1587:U:H5'	2.18	0.43
30:0:2314:G:C2'	30:0:2315:C:H5'	2.48	0.43
30:0:2515:C:H2'	30:0:2516:G:O4'	2.18	0.43
30:0:2544:G:H2'	30:0:2545:U:O4'	2.18	0.43
30:0:2662:G:N3	30:0:2816:A:H2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2896:A:N3	30:0:2896:A:H2'	2.32	0.43
2:B:24:PRO:HG2	2:B:204:GLY:HA2	2.00	0.43
3:C:88:SER:HB3	3:C:91:PRO:HB3	2.01	0.43
10:J:131:THR:HG22	10:J:133:GLY:H	1.82	0.43
10:J:135:ILE:O	10:J:139:LEU:HG	2.18	0.43
14:N:18:THR:HG21	38:N:8844:HOH:O	2.17	0.43
30:0:482:G:O4'	30:0:511:A:C2	2.70	0.43
30:0:506:G:N2	30:0:509:A:H5'	2.23	0.43
30:0:1504:A:H5'	38:0:4414:HOH:O	2.18	0.43
30:0:1568:G:O2'	30:0:1569:U:H5'	2.18	0.43
30:0:1797:A:H2'	30:0:1799:G:O5'	2.18	0.43
30:0:1996:U:O2'	30:0:1997:A:H5'	2.18	0.43
30:0:2524:G:H5"	38:0:4731:HOH:O	2.18	0.43
30:0:2705:U:H2'	30:0:2706:A:H8	1.82	0.43
2:B:185:GLY:HA2	38:B:9099:HOH:O	2.17	0.43
2:B:215:VAL:HB	38:B:9086:HOH:O	2.18	0.43
8:H:91:ARG:NH1	8:H:138:THR:OG1	2.47	0.43
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.99	0.43
11:K:74:VAL:HG21	11:K:96:VAL:HG23	1.99	0.43
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.18	0.43
20:T:52:ARG:O	30:0:317:A:OP1	2.35	0.43
23:W:21:LEU:O	23:W:26:ILE:HG23	2.19	0.43
38:3:8961:HOH:O	30:0:2382:A:H5'	2.17	0.43
30:0:398:U:H2'	30:0:399:C:C6	2.53	0.43
30:0:629:A:C2	30:0:2074:A:C2	3.06	0.43
30:0:675:U:H2'	30:0:676:C:H5'	2.00	0.43
30:0:806:A:H2'	30:0:807:A:O4'	2.19	0.43
30:0:875:A:H5'	30:0:876:A:N7	2.33	0.43
30:0:960:G:N3	30:0:960:G:H3'	2.33	0.43
30:0:1163:G:N2	30:0:1184:C:N3	2.66	0.43
30:0:1167:G:H2'	30:0:1168:C:O4'	2.18	0.43
30:0:1538:C:O2'	30:0:1539:U:H5'	2.17	0.43
30:0:2115:U:H2'	30:0:2116:U:C6	2.53	0.43
30:0:2887:G:H2'	30:0:2888:U:C6	2.53	0.43
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.81	0.43
15:O:105:ASN:HD21	15:O:109:SER:N	2.16	0.43
19:S:49:VAL:HG13	19:S:66:VAL:HG13	2.00	0.43
23:W:115:THR:HG23	38:W:5420:HOH:O	2.19	0.43
30:0:1079:A:H4'	30:0:2078:U:H5'	2.00	0.43
30:0:2067:A:H2'	30:0:2068:G:O4'	2.18	0.43
30:0:2653:A:H2'	30:0:2654:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:126:ILE:HB	5:E:131:LEU:CD2	2.48	0.43
6:F:77:VAL:HG21	6:F:83:LEU:HD13	1.99	0.43
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.83	0.43
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.19	0.43
26:Z:55:SER:O	26:Z:59:GLU:HG3	2.17	0.43
28:2:5:LYS:O	28:2:9:LYS:HG3	2.18	0.43
30:0:255:A:C5	30:0:256:C:C5	3.06	0.43
30:0:368:C:H2'	30:0:369:G:H5'	2.00	0.43
30:0:445:U:H2'	30:0:446:G:H8	1.84	0.43
30:0:699:C:C6	30:0:744:G:O4'	2.71	0.43
30:0:1127:C:C5	30:0:1128:U:C4	3.06	0.43
30:0:1333:U:H2'	30:0:1334:C:H6	1.83	0.43
30:0:1890:U:H1'	38:0:5957:HOH:O	2.18	0.43
30:0:2265:U:H2'	30:0:2266:A:C8	2.53	0.43
30:0:2543:G:O3'	30:0:2590:U:H5'	2.19	0.43
4:D:41:LEU:HA	4:D:44:ILE:HG22	2.00	0.43
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.54	0.43
14:N:38:LYS:HD2	14:N:114:LYS:HE3	2.01	0.43
16:P:134:VAL:O	16:P:137:LEU:HB3	2.19	0.43
21:U:6:CYS:HA	21:U:13:ILE:HD11	2.01	0.43
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.19	0.43
30:0:426:G:H2'	30:0:427:C:O4'	2.18	0.43
30:0:565:A:C6	30:0:566:A:C6	3.07	0.43
30:0:821:U:H2'	30:0:822:C:C6	2.50	0.43
30:0:1425:G:C2'	30:0:1426:C:H5'	2.48	0.43
30:0:1850:U:O4'	30:0:1941:A:C2	2.71	0.43
30:0:2072:G:N2	38:0:6868:HOH:O	2.51	0.43
30:0:2403:C:H2'	30:0:2404:G:O5'	2.18	0.43
31:9:98:C:O2'	31:9:99:U:H5'	2.19	0.43
1:A:123:GLY:HA3	1:A:162:GLY:HA2	1.99	0.43
2:B:5:ARG:NH1	30:0:2547:C:OP2	2.52	0.43
6:F:91:VAL:CG1	6:F:92:GLY:N	2.81	0.43
12:L:6:ARG:NH1	30:0:1299:G:N7	2.66	0.43
23:W:130:HIS:O	23:W:136:GLY:HA3	2.18	0.43
25:Y:107:PRO:HB3	25:Y:182:PHE:CD2	2.53	0.43
30:0:170:U:H2'	30:0:171:C:H5'	1.98	0.43
30:0:807:A:H2'	30:0:808:A:O4'	2.19	0.43
30:0:1250:C:O2'	30:0:1251:C:H5'	2.18	0.43
30:0:1427:A:H61	30:0:1440:U:H1'	1.82	0.43
30:0:1773:G:N2	30:0:1774:G:C8	2.86	0.43
30:0:1819:G:O2'	30:0:1820:G:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:107:LEU:O	23:W:112:LEU:HB2	2.18	0.43
24:X:76:ARG:HG3	24:X:76:ARG:NH1	2.31	0.43
26:Z:43:GLY:HA2	30:0:1771:U:O2	2.19	0.43
30:0:163:U:O3'	30:0:896:C:H4'	2.19	0.43
30:0:684:G:H2'	30:0:685:C:C6	2.54	0.43
30:0:1474:C:C6	30:0:1474:C:C5'	2.90	0.43
30:0:1634:G:H2'	30:0:1635:U:C6	2.53	0.43
30:0:2256:G:C2'	30:0:2257:G:C5'	2.97	0.43
30:0:2543:G:H2'	30:0:2544:G:O4'	2.18	0.43
31:9:105:A:H2'	31:9:106:U:O4'	2.18	0.43
5:E:11:VAL:HG12	5:E:12:ASP:N	2.34	0.43
5:E:19:ASP:HA	5:E:31:ARG:O	2.19	0.43
8:H:49:GLN:HG3	8:H:140:TYR:CE2	2.54	0.43
22:V:29:ASN:O	22:V:33:VAL:HG23	2.18	0.43
30:0:111:C:O2'	30:0:112:G:H5'	2.19	0.43
30:0:1167:G:C2	30:0:1168:C:C2	3.07	0.43
30:0:1463:U:H2'	30:0:1464:C:H6	1.83	0.43
30:0:2661:U:H3	30:0:2812:A:H62	1.65	0.43
31:9:54:A:C2	31:9:55:U:N3	2.87	0.43
1:A:101:GLU:HG2	38:A:9034:HOH:O	2.18	0.43
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.47	0.43
12:L:33:ALA:HB2	30:0:165:A:H5"	1.99	0.43
22:V:56:ILE:O	22:V:60:GLN:HG3	2.19	0.43
24:X:71:ARG:HD2	38:X:7542:HOH:O	2.18	0.43
25:Y:189:ASN:ND2	25:Y:192:ASP:N	2.66	0.43
30:0:111:C:C2'	30:0:112:G:H5'	2.49	0.43
30:0:544:G:C3'	30:0:545:G:H5"	2.48	0.43
30:0:1023:C:O2'	30:0:1024:G:H5'	2.19	0.43
30:0:1517:C:O2	30:0:1670:A:C2	2.72	0.43
30:0:1682:A:H5"	38:0:9456:HOH:O	2.19	0.43
30:0:2079:G:H2'	30:0:2080:G:O4'	2.19	0.43
30:0:2540:G:H5"	38:0:4662:HOH:O	2.19	0.43
30:0:2757:A:H2'	30:0:2758:G:O4'	2.18	0.43
7:G:19:GLU:O	7:G:23:ILE:HG13	2.19	0.42
10:J:107:ASN:ND2	10:J:109:TYR:H	2.16	0.42
14:N:37:ARG:HH11	31:9:6:C:H5"	1.71	0.42
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.92	0.42
27:1:28:HIS:HD2	27:1:30:LYS:H	1.65	0.42
30:0:699:C:C2	30:0:744:G:C2	3.06	0.42
30:0:702:G:C2	30:0:703:G:C8	3.07	0.42
30:0:920:C:H4'	30:0:921:G:N2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1461:U:H2'	30:0:1462:C:C6	2.54	0.42
30:0:1503:U:H2'	30:0:1504:A:O4'	2.19	0.42
30:0:1576:G:H2'	30:0:1577:U:O4'	2.19	0.42
30:0:2102:G:C2'	38:0:7763:HOH:O	2.59	0.42
30:0:2610:U:H3'	38:0:7521:HOH:O	2.18	0.42
30:0:2668:G:H2'	30:0:2669:U:C6	2.54	0.42
30:0:2692:G:HO2'	30:0:2693:U:P	2.41	0.42
1:A:4:ILE:HG22	1:A:198:ASP:O	2.19	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.18	0.42
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.52	0.42
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.49	0.42
12:L:61:ALA:HB2	12:L:105:TYR:CZ	2.54	0.42
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.19	0.42
18:R:106:GLY:HA2	18:R:109:MET:HE3	2.00	0.42
23:W:4:LEU:HD13	23:W:52:VAL:HG21	2.01	0.42
29:3:48:ASN:ND2	29:3:50:GLY:H	2.17	0.42
30:0:62:C:C4	30:0:63:U:C4	3.07	0.42
30:0:142:G:O2'	30:0:143:C:H5'	2.18	0.42
30:0:343:C:O2'	30:0:344:C:H5'	2.19	0.42
30:0:512:G:H5"	30:0:515:C:H1'	2.00	0.42
30:0:682:A:H2'	30:0:683:G:O4'	2.18	0.42
30:0:705:C:O2	30:0:705:C:C2'	2.67	0.42
30:0:946:C:H2'	30:0:947:U:H6	1.83	0.42
30:0:1166:A:H1'	30:0:1192:A:C2	2.55	0.42
30:0:1181:A:C2	30:0:1192:A:C8	3.06	0.42
30:0:2054:A:H5'	38:0:4901:HOH:O	2.18	0.42
30:0:2635:A:C2'	30:0:2636:C:H5'	2.49	0.42
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.87	0.42
5:E:21:THR:HG23	5:E:30:THR:OG1	2.18	0.42
14:N:132:ASN:HD22	30:0:2413:A:H4'	1.83	0.42
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.19	0.42
23:W:65:VAL:HA	23:W:68:THR:HG22	2.00	0.42
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.01	0.42
30:0:729:C:C2	30:0:743:G:C2	3.07	0.42
30:0:2474:A:N7	30:0:2621:PSU:H4'	2.34	0.42
30:0:2646:G:C5	30:0:2647:C:C5	3.07	0.42
30:0:2657:G:O2'	30:0:2842:G:N7	2.47	0.42
30:0:2809:G:H2'	30:0:2810:G:O4'	2.20	0.42
31:9:95:C:O2'	31:9:96:C:H5'	2.20	0.42
31:9:108:C:H2'	31:9:109:G:C8	2.53	0.42
2:B:53:LEU:HD21	2:B:270:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:VAL:HG12	3:C:141:SER:N	2.34	0.42
8:H:123:ILE:HD12	8:H:123:ILE:N	2.34	0.42
8:H:141:CYS:HB2	38:H:197:HOH:O	2.20	0.42
10:J:39:VAL:CG2	10:J:107:ASN:HA	2.49	0.42
13:M:93:ARG:HD2	30:0:1470:A:OP1	2.19	0.42
14:N:42:HIS:CG	14:N:62:HIS:HE1	2.37	0.42
18:R:17:MET:HE3	18:R:19:ARG:NH2	2.34	0.42
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.31	0.42
24:X:43:VAL:HG12	24:X:44:ASP:H	1.83	0.42
25:Y:152:LYS:CB	25:Y:160:LYS:HG3	2.49	0.42
25:Y:154:ARG:NH2	30:0:1072:G:OP2	2.53	0.42
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.33	0.42
30:0:48:A:N1	30:0:148:A:O2'	2.43	0.42
30:0:51:G:O2'	30:0:52:A:H5'	2.20	0.42
30:0:349:U:O2'	30:0:350:G:H5'	2.19	0.42
30:0:622:G:O2'	30:0:623:U:H5'	2.20	0.42
30:0:1298:U:H2'	30:0:1299:G:C8	2.54	0.42
30:0:1947:G:H2'	30:0:1948:G:H8	1.84	0.42
1:A:186:TRP:CD1	1:A:187:PRO:HA	2.55	0.42
2:B:84:LEU:HD23	2:B:142:LEU:HD23	2.02	0.42
3:C:35:VAL:HG21	3:C:227:GLY:HA2	2.01	0.42
4:D:135:VAL:HG22	4:D:136:ARG:N	2.34	0.42
6:F:99:THR:HG23	6:F:99:THR:O	2.19	0.42
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.34	0.42
13:M:49:ALA:C	13:M:54:TYR:HB3	2.39	0.42
14:N:71:TRP:HB2	38:N:8836:HOH:O	2.19	0.42
18:R:18:LEU:HD12	18:R:143:VAL:HG11	2.01	0.42
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.18	0.42
30:0:39:G:N2	30:0:444:C:C2	2.88	0.42
30:0:1416:G:C2'	30:0:1417:G:H5'	2.50	0.42
30:0:1616:A:H5"	30:0:1617:C:OP1	2.19	0.42
30:0:1706:G:C6	30:0:1707:G:C6	3.08	0.42
30:0:2237:G:H1'	38:0:4856:HOH:O	2.18	0.42
30:0:2316:G:H4'	38:0:6092:HOH:O	2.19	0.42
30:0:2429:A:H4'	38:0:7729:HOH:O	2.19	0.42
30:0:2626:C:H2'	30:0:2627:G:H8	1.84	0.42
1:A:36:ASP:HA	1:A:83:GLY:HA3	2.01	0.42
2:B:60:SER:HA	2:B:61:PRO:HD3	1.87	0.42
9:I:118:ASN:HB3	30:0:1185:U:H5"	2.01	0.42
30:0:360:A:H2'	30:0:361:C:O4'	2.19	0.42
30:0:567:U:O5'	30:0:567:U:H6	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:664:U:O4	30:0:681:G:H5”	2.20	0.42
30:0:851:C:O2	30:0:2022:A:H2	2.03	0.42
30:0:1098:A:H2’	30:0:1099:G:O4’	2.19	0.42
30:0:1850:U:H2’	30:0:1851:G:C8	2.55	0.42
30:0:1973:A:H2’	30:0:1974:G:O4’	2.19	0.42
30:0:2002:C:C2’	30:0:2003:U:H5’	2.49	0.42
30:0:2004:U:H6	30:0:2004:U:P	2.43	0.42
30:0:2709:G:N2	38:0:7616:HOH:O	2.51	0.42
30:0:2751:C:H2’	30:0:2752:C:H6	1.84	0.42
30:0:2883:A:H2’	30:0:2884:G:O4’	2.19	0.42
1:A:88:ILE:O	1:A:88:ILE:HG22	2.20	0.42
2:B:18:ARG:HG3	2:B:256:GLN:HG3	2.02	0.42
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.02	0.42
2:B:258:GLY:HA2	38:0:4005:HOH:O	2.20	0.42
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.20	0.42
5:E:7:ILE:HG22	5:E:45:ASP:O	2.19	0.42
10:J:22:VAL:O	10:J:26:VAL:HG23	2.20	0.42
13:M:42:ARG:HA	13:M:43:PRO:HD3	1.87	0.42
18:R:84:ALA:O	18:R:88:PHE:HD1	2.02	0.42
28:2:2:LYS:HG3	30:0:1486:A:C5	2.54	0.42
30:0:128:A:C8	30:0:128:A:H3’	2.54	0.42
30:0:130:C:H5’	38:0:5216:HOH:O	2.19	0.42
30:0:187:A:H3’	30:0:188:C:C6	2.55	0.42
30:0:236:A:H4’	30:0:237:G:OP1	2.19	0.42
30:0:417:G:P	38:0:7414:HOH:O	2.77	0.42
30:0:1058:A:H2’	30:0:1060:C:C5’	2.50	0.42
30:0:1139:U:H2’	30:0:1140:C:C6	2.54	0.42
30:0:1917:G:C6	30:0:1918:U:C4	3.07	0.42
30:0:1942:A:H2’	30:0:1943:C:C6	2.55	0.42
30:0:2645:U:O2’	30:0:2646:G:P	2.78	0.42
30:0:2761:A:C4	30:0:2763:G:C8	3.07	0.42
3:C:236:THR:HG21	38:C:8579:HOH:O	2.20	0.42
3:C:242:GLU:HB2	38:C:8587:HOH:O	2.19	0.42
5:E:11:VAL:HG13	5:E:23:GLU:O	2.19	0.42
5:E:60:SER:OG	30:0:2784:A:H1’	2.20	0.42
15:O:29:VAL:HG11	15:O:98:LEU:HD21	2.01	0.42
20:T:24:ARG:HH21	20:T:39:ASN:ND2	2.16	0.42
23:W:44:MET:CE	30:0:944:G:H21	2.33	0.42
25:Y:138:ARG:HD3	30:0:638:C:OP2	2.20	0.42
27:1:10:LYS:HG3	38:1:8981:HOH:O	2.19	0.42
30:0:309:C:O2	30:0:309:C:H2’	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:377:C:H5	38:0:3302:HOH:O	2.01	0.42
30:0:1060:C:H6	30:0:1060:C:H5'	1.85	0.42
30:0:1191:A:N3	30:0:1207:A:C2	2.87	0.42
30:0:1214:G:H4'	38:0:4747:HOH:O	2.19	0.42
30:0:1907:U:O2'	30:0:1908:G:H5'	2.20	0.42
31:9:31:C:C2	31:9:50:G:N2	2.88	0.42
1:A:103:VAL:HA	1:A:104:PRO:HD3	1.86	0.42
3:C:95:GLU:H	3:C:95:GLU:CD	2.23	0.42
4:D:167:GLU:C	4:D:169:THR:H	2.23	0.42
8:H:139:ALA:HB3	8:H:149:VAL:HG21	2.02	0.42
13:M:15:PRO:HA	13:M:20:LEU:HD23	2.02	0.42
13:M:80:GLY:O	13:M:81:ARG:HD3	2.20	0.42
13:M:122:GLN:HB2	13:M:126:GLN:O	2.20	0.42
14:N:82:TYR:CD2	14:N:82:TYR:C	2.93	0.42
15:O:39:THR:O	15:O:115:ARG:NH2	2.53	0.42
30:0:241:A:C2	30:0:378:A:H4'	2.54	0.42
30:0:569:A:H5"	30:0:587:A:N1	2.35	0.42
30:0:999:C:C2'	30:0:1000:C:H5'	2.49	0.42
30:0:1008:C:O2'	30:0:1009:U:H5'	2.20	0.42
30:0:1159:G:H1	30:0:1208:C:H42	1.68	0.42
30:0:1520:G:C6	30:0:1521:C:C4	3.07	0.42
30:0:1789:G:C2'	30:0:1790:C:O5'	2.68	0.42
30:0:1903:U:O2'	30:0:1904:A:C8	2.68	0.42
31:9:73:A:N1	31:9:108:C:O2	2.53	0.42
3:C:206:ASN:HB2	30:0:329:A:OP2	2.20	0.42
5:E:7:ILE:HA	5:E:8:PRO:HD3	1.95	0.42
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.35	0.42
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.02	0.42
14:N:171:HIS:CE1	38:N:8861:HOH:O	2.71	0.42
18:R:69:LYS:HB2	18:R:72:VAL:HG23	2.02	0.42
22:V:1:THR:CG2	22:V:2:VAL:H	2.25	0.42
23:W:29:VAL:O	23:W:30:ASN:HB2	2.19	0.42
25:Y:141:THR:HG23	38:Y:9073:HOH:O	2.19	0.42
30:0:365:G:C6	30:0:366:U:C4	3.08	0.42
30:0:699:C:C6	30:0:744:G:C4	3.08	0.42
30:0:1130:U:H2'	30:0:1131:G:C4'	2.50	0.42
30:0:1373:G:H4'	38:0:5286:HOH:O	2.20	0.42
30:0:1494:A:C4	30:0:1495:C:C5	3.08	0.42
30:0:2553:A:H2'	30:0:2553:A:N3	2.35	0.42
30:0:2739:A:C6	30:0:2740:G:C5	3.08	0.42
2:B:14:GLY:HA2	2:B:15:PRO:C	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.49	0.41
6:F:83:LEU:HD12	6:F:83:LEU:HA	1.91	0.41
20:T:41:ARG:HG2	20:T:41:ARG:NH1	2.34	0.41
24:X:30:MET:HE1	24:X:58:ALA:HB3	2.02	0.41
30:0:45:A:N6	30:0:147:G:C4	2.88	0.41
30:0:116:G:H1'	30:0:129:A:N3	2.35	0.41
30:0:424:C:H2'	30:0:425:U:H6	1.85	0.41
30:0:939:A:C2	30:0:1027:G:N3	2.88	0.41
30:0:941:G:C6	30:0:942:U:C4	3.08	0.41
30:0:1183:C:N3	30:0:1184:C:C4	2.88	0.41
30:0:1207:A:N6	38:0:5631:HOH:O	2.53	0.41
30:0:1375:A:C2'	30:0:1376:G:H5'	2.50	0.41
30:0:1416:G:H2'	30:0:1417:G:H5'	2.01	0.41
30:0:1574:C:O5'	30:0:1574:C:H6	2.03	0.41
30:0:1771:U:O2'	30:0:1773:G:N7	2.52	0.41
30:0:1878:G:O2'	30:0:1879:U:H6	2.03	0.41
30:0:1926:G:H2'	30:0:1927:A:C8	2.55	0.41
30:0:2256:G:H2'	30:0:2257:G:O5'	2.19	0.41
30:0:2425:A:H5'	30:0:2426:G:OP2	2.20	0.41
30:0:2541:U:H5"	38:0:5398:HOH:O	2.20	0.41
30:0:2587:OMU:O5'	30:0:2587:OMU:H6	2.19	0.41
30:0:2616:A:C4'	30:0:2617:G:OP1	2.67	0.41
8:H:102:LYS:HD3	8:H:122:LYS:HD3	2.02	0.41
11:K:109:LEU:CD1	11:K:113:ILE:HD11	2.50	0.41
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.56	0.41
30:0:131:A:OP2	30:0:141:C:H5	2.03	0.41
30:0:803:C:O2'	30:0:804:C:H5'	2.21	0.41
30:0:1001:U:O2'	30:0:1002:G:H5'	2.20	0.41
30:0:1202:A:H2'	30:0:1203:G:O4'	2.20	0.41
30:0:2509:A:OP2	30:0:2510:C:C5	2.73	0.41
30:0:2591:C:H2'	30:0:2592:G:O4'	2.20	0.41
30:0:2611:G:H5'	30:0:2613:G:C8	2.55	0.41
30:0:2866:U:H4'	30:0:2867:G:H5'	2.01	0.41
31:9:2:U:C1'	38:9:9099:HOH:O	2.67	0.41
31:9:2:U:H1'	38:9:9099:HOH:O	2.19	0.41
1:A:212:PRO:HA	30:0:1943:C:O4'	2.19	0.41
2:B:62:ARG:HA	2:B:65:MET:HE3	2.02	0.41
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.50	0.41
4:D:58:VAL:HG12	4:D:60:GLU:HG2	2.01	0.41
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.20	0.41
23:W:73:LEU:HD12	23:W:73:LEU:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:125:HIS:CD2	23:W:127:GLY:H	2.38	0.41
24:X:73:ARG:HH12	24:X:88:GLU:HB2	1.85	0.41
25:Y:189:ASN:HD22	25:Y:192:ASP:H	1.67	0.41
30:0:862:U:H2'	30:0:863:G:C8	2.55	0.41
30:0:1191:A:H2'	30:0:1193:A:H5'	2.02	0.41
30:0:1391:G:H2'	30:0:1392:A:H5'	2.02	0.41
30:0:1946:C:H2'	30:0:1971:G:C8	2.55	0.41
30:0:2361:A:H2'	30:0:2362:A:O4'	2.20	0.41
30:0:2438:G:H2'	30:0:2439:C:C6	2.55	0.41
30:0:2729:C:O2'	30:0:2730:G:H5'	2.19	0.41
3:C:240:LEU:HB2	38:C:8659:HOH:O	2.20	0.41
10:J:75:PRO:HD3	10:J:136:SER:OG	2.20	0.41
14:N:4:PRO:HB2	30:0:1010:C:H4'	2.02	0.41
15:O:38:ARG:HD3	30:0:654:A:OP2	2.20	0.41
17:Q:7:LEU:HD12	30:0:2424:U:C1'	2.50	0.41
20:T:26:THR:HG23	20:T:97:ARG:HG3	2.02	0.41
21:U:23:HIS:NE2	21:U:29:THR:OG1	2.41	0.41
22:V:44:GLY:O	22:V:48:GLU:HG2	2.21	0.41
29:3:69:TYR:HB2	29:3:78:HIS:CE1	2.55	0.41
30:0:23:G:H1'	30:0:520:A:N6	2.36	0.41
30:0:1398:G:H2'	30:0:1399:A:C8	2.55	0.41
30:0:1576:G:H2'	30:0:1577:U:C6	2.55	0.41
30:0:1613:C:H2'	30:0:1614:G:O4'	2.20	0.41
30:0:1940:C:H1'	38:0:9375:HOH:O	2.20	0.41
30:0:2880:A:C2'	30:0:2881:C:H5'	2.50	0.41
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.20	0.41
1:A:214:SER:HA	1:A:227:ASP:O	2.21	0.41
6:F:72:VAL:HA	6:F:73:PRO:HD3	1.86	0.41
14:N:147:ILE:HD12	38:9:9087:HOH:O	2.20	0.41
18:R:39:THR:HB	18:R:42:GLU:HG3	2.02	0.41
23:W:38:THR:HG22	23:W:39:ASP:H	1.86	0.41
30:0:370:G:N2	30:0:371:U:C2	2.89	0.41
30:0:946:C:H2'	30:0:947:U:C6	2.54	0.41
30:0:1327:G:C6	30:0:1331:G:C6	3.09	0.41
30:0:2737:C:H2'	38:0:6141:HOH:O	2.21	0.41
31:9:2:U:OP2	31:9:2:U:H4'	2.21	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.92	0.41
4:D:88:LEU:HB2	4:D:89:PRO:HD3	2.02	0.41
6:F:32:GLY:N	38:F:3111:HOH:O	2.53	0.41
8:H:92:LYS:HG3	8:H:130:VAL:HG22	2.02	0.41
13:M:24:GLN:NE2	13:M:24:GLN:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:80:TYR:O	30:0:2050:G:H5"	2.20	0.41
19:S:57:THR:C	19:S:59:ASP:H	2.24	0.41
25:Y:145:LYS:O	25:Y:147:ARG:HG2	2.20	0.41
29:3:38:ARG:HD2	30:0:396:U:OP2	2.20	0.41
30:0:334:G:H2'	30:0:335:U:O4'	2.20	0.41
30:0:659:A:H5"	38:0:7096:HOH:O	2.19	0.41
30:0:1259:A:N1	30:0:1261:A:H1'	2.35	0.41
30:0:1311:G:C2	30:0:1312:G:C8	3.08	0.41
30:0:1471:A:H2'	30:0:1472:C:C6	2.55	0.41
30:0:2088:C:H1'	30:0:2841:A:N1	2.36	0.41
30:0:2506:A:H62	30:0:2511:A:HO2'	1.66	0.41
1:A:20:SER:HB3	30:0:1872:C:H5	1.85	0.41
2:B:174:ARG:HA	2:B:177:HIS:HB3	2.03	0.41
38:D:7597:HOH:O	31:9:56:A:H2	2.04	0.41
6:F:1:PRO:H3	6:F:4:VAL:HG23	1.86	0.41
8:H:157:TYR:CD1	8:H:157:TYR:C	2.94	0.41
10:J:52:GLN:NE2	30:0:1119:G:H8	2.18	0.41
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.41
16:P:18:LYS:O	16:P:21:VAL:HG13	2.20	0.41
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.20	0.41
18:R:114:VAL:HG13	18:R:114:VAL:O	2.21	0.41
20:T:77:VAL:HG11	20:T:91:LEU:HD11	2.03	0.41
24:X:43:VAL:HG12	24:X:47:ALA:HB3	2.01	0.41
25:Y:151:SER:HB3	25:Y:154:ARG:CB	2.50	0.41
29:3:69:TYR:CZ	29:3:80:ARG:HD2	2.55	0.41
29:3:91:GLN:O	29:3:92:GLU:HB2	2.20	0.41
30:0:99:A:C8	30:0:100:C:C5	3.08	0.41
30:0:517:U:C2'	30:0:518:G:H5'	2.50	0.41
30:0:1076:G:C2	30:0:1084:C:C2	3.08	0.41
30:0:1982:C:H2'	30:0:1983:C:O4'	2.20	0.41
30:0:2083:A:H3'	38:0:7573:HOH:O	2.20	0.41
30:0:2102:G:N2	30:0:2104:C:C6	2.89	0.41
30:0:2480:G:O2'	30:0:2481:G:H5'	2.21	0.41
30:0:2526:C:H6	30:0:2526:C:H3'	1.85	0.41
30:0:2764:C:H2'	30:0:2765:C:H6	1.84	0.41
2:B:53:LEU:HD11	2:B:327:VAL:HG22	2.02	0.41
2:B:97:LEU:O	2:B:98:THR:HG23	2.21	0.41
6:F:50:VAL:CG2	6:F:63:ILE:HG21	2.51	0.41
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.51	0.41
18:R:1:GLY:HA2	18:R:119:VAL:HG21	2.02	0.41
30:0:10:U:O4	30:0:532:A:H8	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:79:G:N2	30:0:97:G:H1'	2.36	0.41
30:0:278:A:C6	30:0:279:C:C4	3.09	0.41
30:0:626:U:C4	30:0:627:G:C6	3.08	0.41
30:0:1626:A:C2'	30:0:1627:G:H5'	2.51	0.41
30:0:1896:G:C6	30:0:1897:U:C4	3.09	0.41
30:0:2607:U:H4'	38:0:9440:HOH:O	2.21	0.41
31:9:1:U:O3'	31:9:3:A:OP1	2.39	0.41
2:B:10:SER:HB2	30:0:2714:U:H4'	2.02	0.41
4:D:88:LEU:N	4:D:89:PRO:CD	2.83	0.41
5:E:166:VAL:HG12	38:E:3134:HOH:O	2.21	0.41
14:N:38:LYS:HE3	14:N:38:LYS:HB2	1.81	0.41
15:O:14:LEU:HD23	15:O:102:ILE:HD11	2.03	0.41
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.69	0.41
23:W:80:ASP:HB2	38:W:3312:HOH:O	2.21	0.41
27:1:28:HIS:O	27:1:32:LYS:N	2.47	0.41
30:0:196:G:H1'	30:0:198:A:N7	2.35	0.41
30:0:287:C:H2'	30:0:288:A:C8	2.56	0.41
30:0:393:G:C6	30:0:394:G:C6	3.09	0.41
30:0:812:A:H2'	30:0:813:C:C6	2.55	0.41
30:0:812:A:H2'	30:0:813:C:O4'	2.21	0.41
30:0:1074:G:H4'	30:0:1260:G:C6	2.56	0.41
30:0:1275:C:N3	30:0:1281:C:N4	2.69	0.41
30:0:1406:A:H4'	30:0:1407:A:C5'	2.51	0.41
30:0:1445:G:N2	30:0:1678:A:H1'	2.36	0.41
30:0:1552:G:H2'	30:0:1553:C:C6	2.56	0.41
30:0:1632:A:C3'	30:0:1633:C:H5'	2.51	0.41
30:0:1783:A:O2'	30:0:1784:U:H5'	2.21	0.41
30:0:1964:U:O2	30:0:1964:U:H2'	2.21	0.41
1:A:204:GLY:N	30:0:2634:G:OP2	2.53	0.41
2:B:57:GLU:HA	2:B:58:PRO:HD2	1.91	0.41
2:B:85:ARG:NH1	30:0:2671:U:O2	2.54	0.41
2:B:211:THR:HG21	38:0:7451:HOH:O	2.21	0.41
5:E:49:ILE:HD11	5:E:69:ILE:HD12	2.03	0.41
8:H:100:GLU:HB3	8:H:124:VAL:HG11	2.02	0.41
10:J:105:LEU:HD23	38:J:5907:HOH:O	2.21	0.41
14:N:13:ARG:NH1	30:0:2368:A:C6	2.89	0.41
17:Q:50:GLY:HA2	38:0:6025:HOH:O	2.20	0.41
18:R:79:ARG:HB3	30:0:2050:G:OP1	2.21	0.41
21:U:33:SER:O	21:U:37:GLU:HG3	2.21	0.41
30:0:74:G:O2'	30:0:75:U:H5'	2.20	0.41
30:0:594:C:C4	30:0:595:U:C4	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1084:C:H6	30:0:1084:C:O5'	2.04	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.34	0.41
30:0:1363:G:H2'	30:0:1364:G:C8	2.56	0.41
30:0:1587:U:H2'	30:0:1588:G:O4'	2.21	0.41
30:0:1641:A:H2'	30:0:1642:A:C5'	2.45	0.41
30:0:1712:A:H2'	30:0:1713:G:O4'	2.20	0.41
30:0:1743:G:H1'	38:0:4892:HOH:O	2.20	0.41
30:0:1930:A:H2'	30:0:1931:A:C8	2.55	0.41
30:0:2277:U:O2'	30:0:2278:U:H5'	2.21	0.41
30:0:2804:C:H2'	30:0:2805:A:O4'	2.21	0.41
30:0:2842:G:H2'	30:0:2843:A:H5'	2.02	0.41
31:9:58:G:N7	31:9:59:C:C4	2.89	0.41
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.54	0.40
3:C:214:THR:HG21	38:C:8608:HOH:O	2.20	0.40
4:D:18:ILE:HD13	4:D:84:LEU:HD12	2.03	0.40
4:D:25:MET:HE2	4:D:41:LEU:CG	2.50	0.40
12:L:121:ILE:HG12	12:L:141:GLU:HB2	2.04	0.40
12:L:129:ALA:O	12:L:133:VAL:HG23	2.21	0.40
18:R:82:GLU:HG3	18:R:83:LYS:N	2.35	0.40
22:V:5:VAL:HG23	38:V:2271:HOH:O	2.20	0.40
22:V:27:LEU:HA	22:V:49:LEU:HD13	2.02	0.40
29:3:38:ARG:HH11	30:0:396:U:P	2.43	0.40
29:3:79:LEU:HD13	30:0:2457:U:H1'	2.04	0.40
30:0:11:A:H5'	30:0:12:U:OP2	2.20	0.40
30:0:228:C:C2'	30:0:229:G:H5'	2.51	0.40
30:0:1041:U:H4'	30:0:1295:G:H5'	2.03	0.40
30:0:1760:G:C2	30:0:1813:U:O4'	2.74	0.40
30:0:1917:G:C5	30:0:1918:U:C4	3.09	0.40
30:0:2072:G:O2'	30:0:2489:G:N2	2.53	0.40
30:0:2617:G:C2	30:0:2618:G:C8	3.09	0.40
1:A:173:GLY:O	1:A:176:HIS:HB3	2.21	0.40
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.36	0.40
2:B:75:GLU:C	2:B:77:PRO:HD3	2.42	0.40
2:B:310:ARG:HD2	38:B:9115:HOH:O	2.21	0.40
14:N:23:ARG:HG2	14:N:23:ARG:HH11	1.87	0.40
16:P:14:LEU:HD13	16:P:51:ALA:HB2	2.03	0.40
30:0:17:G:O2'	30:0:18:C:H5'	2.20	0.40
30:0:42:C:H3'	38:0:4165:HOH:O	2.21	0.40
30:0:79:G:H22	30:0:97:G:H1'	1.86	0.40
30:0:844:A:C6	30:0:882:A:C5	3.08	0.40
30:0:1014:A:H5"	31:9:101:G:O2'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1215:A:O3'	30:0:1216:G:C4'	2.69	0.40
30:0:1819:G:C2'	30:0:1820:G:C5'	2.99	0.40
30:0:2712:G:H5'	38:0:5223:HOH:O	2.20	0.40
30:0:2712:G:P	38:0:5223:HOH:O	2.80	0.40
30:0:2791:U:H1'	30:0:2792:A:H5"	2.03	0.40
30:0:2820:A:H2'	30:0:2821:C:C6	2.55	0.40
1:A:94:LEU:HD12	1:A:98:GLU:CB	2.43	0.40
2:B:7:ARG:HH11	2:B:7:ARG:CG	2.35	0.40
3:C:135:GLU:HB3	38:C:8582:HOH:O	2.20	0.40
13:M:118:TYR:CZ	13:M:130:GLU:HB2	2.56	0.40
14:N:93:GLN:HA	14:N:93:GLN:NE2	2.35	0.40
30:0:47:G:N3	30:0:114:A:C2	2.90	0.40
30:0:517:U:H2'	30:0:518:G:H5'	2.03	0.40
30:0:1102:C:H5	38:0:3487:HOH:O	2.04	0.40
30:0:1183:C:O2	30:0:1183:C:C2'	2.70	0.40
30:0:1624:A:H5'	30:0:1626:A:O4'	2.20	0.40
30:0:2004:U:H2'	30:0:2005:G:OP1	2.22	0.40
30:0:2039:A:H4'	30:0:2760:C:O2'	2.22	0.40
30:0:2252:A:H2'	30:0:2253:G:H5'	2.03	0.40
30:0:2550:U:O2'	30:0:2551:C:H5'	2.20	0.40
30:0:2819:C:H2'	30:0:2820:A:C8	2.55	0.40
30:0:2897:C:H2'	30:0:2898:G:H8	1.85	0.40
1:A:132:ASP:HB3	1:A:135:VAL:H	1.87	0.40
1:A:230:SER:HB2	30:0:1852:A:H4'	2.04	0.40
2:B:245:SER:HB3	30:0:2094:G:H4'	2.02	0.40
7:G:64:ASN:N	7:G:64:ASN:ND2	2.69	0.40
13:M:47:ASP:CG	13:M:48:LYS:N	2.75	0.40
20:T:52:ARG:HB2	20:T:95:ASN:HB3	2.02	0.40
23:W:88:THR:HG22	23:W:89:ASP:N	2.34	0.40
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.56	0.40
27:1:10:LYS:N	38:1:8981:HOH:O	2.50	0.40
30:0:101:C:H2'	30:0:102:A:H8	1.87	0.40
30:0:129:A:H4'	30:0:130:C:OP1	2.21	0.40
30:0:249:G:H2'	30:0:250:C:H6	1.86	0.40
30:0:445:U:H2'	30:0:446:G:C8	2.57	0.40
30:0:694:A:H4'	30:0:2441:U:OP1	2.21	0.40
30:0:1139:U:H2'	30:0:1140:C:H6	1.85	0.40
30:0:1544:U:H2'	30:0:1545:C:H6	1.87	0.40
30:0:2758:G:H2'	30:0:2759:C:C6	2.56	0.40
31:9:59:C:H2'	31:9:60:C:C6	2.56	0.40
31:9:122:C:C6	38:9:9043:HOH:O	2.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:HB2	30:0:820:G:C6	2.57	0.40
2:B:149:ASP:HB2	38:B:9049:HOH:O	2.21	0.40
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.70	0.40
5:E:84:MET:HE1	5:E:148:ILE:HD12	2.04	0.40
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.68	0.40
23:W:5:VAL:HG11	23:W:153:MET:CE	2.52	0.40
30:0:272:A:N1	30:0:369:G:H5"	2.36	0.40
30:0:517:U:H1'	38:0:7571:HOH:O	2.20	0.40
30:0:951:A:O2'	30:0:952:G:H5'	2.21	0.40
30:0:1116:U:C2'	30:0:1118:A:C2	3.05	0.40
30:0:1217:G:C2	30:0:1218:U:C2	3.09	0.40
30:0:1472:C:H6	30:0:1472:C:O5'	2.04	0.40
30:0:1589:G:H22	30:0:1605:G:H1'	1.85	0.40
30:0:2327:A:H2'	30:0:2328:U:O4'	2.21	0.40
30:0:2491:G:C1'	38:0:6868:HOH:O	2.59	0.40
30:0:2824:C:H5"	30:0:2825:C:H5'	2.03	0.40
31:9:8:G:H5'	38:9:9103:HOH:O	2.21	0.40
31:9:65:A:C6	31:9:112:U:C5	3.10	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%)	19 (8%)	4 (2%)	9 31
2	B	335/338 (99%)	308 (92%)	24 (7%)	3 (1%)	17 48
3	C	244/246 (99%)	228 (93%)	15 (6%)	1 (0%)	34 66
4	D	134/177 (76%)	112 (84%)	18 (13%)	4 (3%)	4 17
5	E	170/178 (96%)	162 (95%)	8 (5%)	0	100 100
6	F	117/120 (98%)	106 (91%)	8 (7%)	3 (3%)	5 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	12	37
9	I	68/162 (42%)	55 (81%)	11 (16%)	2 (3%)	4	18
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
11	K	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	19	51
12	L	141/165 (86%)	126 (89%)	12 (8%)	3 (2%)	7	26
13	M	192/196 (98%)	185 (96%)	6 (3%)	1 (0%)	29	61
14	N	184/187 (98%)	169 (92%)	11 (6%)	4 (2%)	6	24
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
17	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
18	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
19	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
20	T	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
21	U	51/67 (76%)	46 (90%)	5 (10%)	0	100	100
22	V	63/71 (89%)	59 (94%)	4 (6%)	0	100	100
23	W	152/154 (99%)	146 (96%)	6 (4%)	0	100	100
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	12	37
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
26	Z	71/116 (61%)	63 (89%)	7 (10%)	1 (1%)	11	36
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%)	87 (97%)	2 (2%)	1 (1%)	14	42
All	All	3705/4472 (83%)	3451 (93%)	223 (6%)	31 (1%)	19	51

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
6	F	101	ALA
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE

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Mol	Chain	Res	Type
1	A	34	ASP
4	D	27	ILE
12	L	80	ASP
12	L	149	ARG
24	X	70	ILE
26	Z	44	ARG
1	A	36	ASP
1	A	88	ILE
2	B	2	GLN
3	C	8	LEU
6	F	100	ASP
8	H	19	ARG
11	K	127	ALA
12	L	21	ARG
14	N	139	TRP
2	B	184	ASP
4	D	56	ARG
2	B	185	GLY
6	F	61	MET
9	I	108	HIS
9	I	83	GLY
29	3	56	PRO
8	H	171	GLY
4	D	28	GLY
13	M	88	VAL

5.3.2 Protein sidechains (i)

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%)	169 (94%)	10 (6%)	21 52
2	B	282/283 (100%)	267 (95%)	15 (5%)	22 54
3	C	193/193 (100%)	177 (92%)	16 (8%)	11 32
4	D	117/148 (79%)	112 (96%)	5 (4%)	29 62
5	E	152/156 (97%)	149 (98%)	3 (2%)	55 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	93/94 (99%)	92 (99%)	1 (1%)	73 92
7	G	27/282 (10%)	26 (96%)	1 (4%)	34 68
8	H	134/145 (92%)	128 (96%)	6 (4%)	27 61
9	I	58/130 (45%)	58 (100%)	0	100 100
10	J	118/121 (98%)	111 (94%)	7 (6%)	19 49
11	K	106/106 (100%)	105 (99%)	1 (1%)	78 93
12	L	113/127 (89%)	107 (95%)	6 (5%)	22 54
13	M	158/160 (99%)	152 (96%)	6 (4%)	33 67
14	N	149/150 (99%)	145 (97%)	4 (3%)	44 77
15	O	93/94 (99%)	93 (100%)	0	100 100
16	P	113/117 (97%)	110 (97%)	3 (3%)	44 77
17	Q	79/80 (99%)	77 (98%)	2 (2%)	47 78
18	R	117/122 (96%)	112 (96%)	5 (4%)	29 62
19	S	71/74 (96%)	71 (100%)	0	100 100
20	T	105/106 (99%)	100 (95%)	5 (5%)	25 58
21	U	44/53 (83%)	43 (98%)	1 (2%)	50 80
22	V	51/57 (90%)	50 (98%)	1 (2%)	55 82
23	W	130/130 (100%)	124 (95%)	6 (5%)	27 60
24	X	66/74 (89%)	59 (89%)	7 (11%)	6 20
25	Y	120/196 (61%)	118 (98%)	2 (2%)	60 86
26	Z	60/94 (64%)	60 (100%)	0	100 100
27	1	46/47 (98%)	46 (100%)	0	100 100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49 79
29	3	79/79 (100%)	78 (99%)	1 (1%)	69 90
All	All	3095/3646 (85%)	2980 (96%)	115 (4%)	34 68

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	36	ASP
1	A	64	ASP
1	A	69	LEU

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Mol	Chain	Res	Type
1	A	94	LEU
1	A	131	HIS
1	A	153	ARG
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN
2	B	49	THR
2	B	51	VAL
2	B	53	LEU
2	B	97	LEU
2	B	132	HIS
2	B	162	MET
2	B	175	LEU
2	B	190	MET
2	B	195	ARG
2	B	234	ARG
2	B	254	GLN
2	B	312	ARG
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	94	THR
3	C	101	ASP
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	202	THR
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	243	VAL
4	D	24	HIS
4	D	50	VAL
4	D	62	ASP
4	D	149	ARG
4	D	153	THR
5	E	16	ASP

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Mol	Chain	Res	Type
5	E	155	ASN
5	E	156	ASP
6	F	12	LEU
7	G	73	ASP
8	H	62	HIS
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	173	GLU
10	J	39	VAL
10	J	45	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
11	K	10	GLN
12	L	35	ARG
12	L	80	ASP
12	L	99	GLU
12	L	101	ASP
12	L	104	ASP
12	L	114	VAL
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	93	ARG
13	M	99	ARG
13	M	164	THR
14	N	17	ARG
14	N	26	LEU
14	N	49	THR
14	N	127	LEU
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	95	GLU
18	R	13	THR
18	R	39	THR
18	R	125	ARG

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Mol	Chain	Res	Type
18	R	132	ARG
18	R	143	VAL
20	T	26	THR
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	117	ASP
21	U	52	THR
22	V	12	THR
23	W	4	LEU
23	W	73	LEU
23	W	76	ASP
23	W	108	ARG
23	W	142	ASP
23	W	146	ILE
24	X	12	ILE
24	X	27	ASP
24	X	46	ASP
24	X	72	VAL
24	X	79	GLU
24	X	82	GLU
24	X	88	GLU
25	Y	189	ASN
25	Y	203	VAL
28	2	18	ASN
29	3	56	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	2	GLN
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	73	GLN
3	C	129	HIS

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Mol	Chain	Res	Type
3	C	163	HIS
4	D	103	ASN
4	D	133	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
9	I	106	GLN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
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	21	HIS
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	89	ASN
16	P	118	GLN
17	Q	16	ASN
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
18	R	123	GLN
19	S	9	HIS
19	S	44	GLN
20	T	39	ASN

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Mol	Chain	Res	Type
21	U	39	ASN
22	V	60	GLN
23	W	28	HIS
23	W	59	GLN
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	134	HIS
25	Y	189	ASN
26	Z	61	HIS
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	238 (8%)	25 (0%)
31	9	121/122 (99%)	17 (14%)	2 (1%)
All	All	2866/3045 (94%)	255 (8%)	27 (0%)

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

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Mol	Chain	Res	Type
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	185	G
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	368	C
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
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G

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Mol	Chain	Res	Type
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
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	884	C
30	0	885	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
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G

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Mol	Chain	Res	Type
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	1161	A
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1331	G
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1559	A
30	0	1592	G
30	0	1625	U

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Mol	Chain	Res	Type
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	1731	C
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	1965	C
30	0	1971	G
30	0	1973	A
30	0	1979	G
30	0	1996	U
30	0	2004	U
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G

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Mol	Chain	Res	Type
30	0	2103	A
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	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2465	A
30	0	2467	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2540	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2611	G
30	0	2613	G
30	0	2617	G
30	0	2634	G
30	0	2638	G
30	0	2645	U
30	0	2649	A
30	0	2650	U

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Mol	Chain	Res	Type
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	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	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A

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Mol	Chain	Res	Type
30	0	129	A
30	0	603	A
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1474	C
30	0	1506	U
30	0	1692	C
30	0	1730	G
30	0	2313	C
30	0	2467	A
30	0	2536	C
30	0	2616	A
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
31	9	43	G
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	OMG	0	2588	30	18,26,27	1.07	2 (11%)	19,38,41	0.71	1 (5%)
30	PSU	0	2621	30	18,21,22	1.47	2 (11%)	22,30,33	1.34	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	OMU	0	2587	30,35	19,22,23	0.31	0	26,31,34	0.36	0
30	UR3	0	2619	30	19,22,23	0.44	0	26,32,35	0.60	1 (3%)
30	1MA	0	628	30,35	16,25,26	1.38	3 (18%)	18,37,40	1.11	2 (11%)

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	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30,35	-	0/9/27/28	0/2/2/2
30	UR3	0	2619	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	C2-N1	4.76	1.43	1.36
30	0	628	1MA	C2-N3	3.61	1.33	1.29
30	0	2588	OMG	C5-C6	-2.88	1.41	1.47
30	0	2621	PSU	C6-C5	2.58	1.38	1.35
30	0	628	1MA	C6-N6	2.56	1.34	1.27
30	0	2588	OMG	C8-N7	-2.42	1.30	1.35
30	0	628	1MA	C8-N7	-2.06	1.31	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	2621	PSU	C6-C5-C4	3.59	120.71	118.20
30	0	2621	PSU	C6-N1-C2	-2.92	119.70	122.68
30	0	2621	PSU	O2-C2-N1	2.92	126.00	122.79
30	0	628	1MA	N1-C2-N3	2.84	129.33	126.02
30	0	628	1MA	C5-C6-N1	2.54	117.68	113.90
30	0	2619	UR3	C4-N3-C2	2.39	126.82	124.56
30	0	2588	OMG	O6-C6-C5	2.13	128.52	124.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2621	PSU	1	0
30	0	2587	OMU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	237/240 (98%)	-0.52	2 (0%) 86 86	25, 49, 89, 109	0
2	B	337/338 (99%)	-0.62	1 (0%) 94 94	27, 54, 81, 92	0
3	C	246/246 (100%)	-0.68	0 100 100	22, 42, 65, 77	0
4	D	140/177 (79%)	0.88	29 (20%) 1 0	65, 101, 125, 137	0
5	E	172/178 (96%)	-0.33	1 (0%) 89 89	45, 70, 92, 97	0
6	F	119/120 (99%)	-0.00	2 (1%) 70 69	48, 69, 99, 116	0
7	G	29/348 (8%)	0.67	3 (10%) 6 5	76, 95, 103, 106	0
8	H	160/177 (90%)	-0.25	3 (1%) 66 65	41, 59, 97, 103	0
9	I	70/162 (43%)	2.97	44 (62%) 0 0	127, 146, 165, 166	0
10	J	142/145 (97%)	-0.64	0 100 100	38, 51, 72, 91	0
11	K	132/132 (100%)	-0.74	0 100 100	35, 50, 74, 84	0
12	L	145/165 (87%)	-0.17	1 (0%) 87 87	25, 64, 110, 127	0
13	M	194/196 (98%)	-0.76	0 100 100	28, 40, 57, 65	0
14	N	186/187 (99%)	-0.25	4 (2%) 62 59	41, 66, 114, 123	0
15	O	115/116 (99%)	-0.63	0 100 100	34, 53, 72, 76	0
16	P	143/149 (95%)	-0.63	0 100 100	37, 54, 69, 79	0
17	Q	95/96 (98%)	-0.64	0 100 100	36, 46, 62, 76	0
18	R	150/155 (96%)	-0.75	0 100 100	30, 44, 65, 81	0
19	S	81/85 (95%)	-0.52	1 (1%) 79 79	41, 56, 78, 89	0
20	T	119/120 (99%)	-0.50	1 (0%) 86 86	39, 54, 83, 110	0
21	U	53/67 (79%)	-0.62	0 100 100	42, 55, 75, 83	0
22	V	65/71 (91%)	0.30	5 (7%) 13 10	44, 70, 119, 125	0
23	W	154/154 (100%)	-0.58	0 100 100	36, 50, 67, 80	0
24	X	82/92 (89%)	-0.36	3 (3%) 41 37	43, 60, 86, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Y	142/241 (58%)	-0.75	1 (0%) 87 87	24, 42, 67, 88	0
26	Z	73/116 (62%)	0.42	7 (9%) 8 6	55, 77, 92, 98	0
27	1	56/57 (98%)	-0.65	0 100 100	25, 30, 37, 43	0
28	2	46/50 (92%)	-0.28	2 (4%) 35 31	31, 61, 91, 101	0
29	3	92/92 (100%)	-0.30	0 100 100	36, 63, 77, 90	0
30	0	2749/2923 (94%)	-0.66	11 (0%) 92 93	19, 44, 88, 164	0
31	9	122/122 (100%)	-0.69	2 (1%) 72 71	37, 67, 89, 147	0
All	All	6646/7517 (88%)	-0.49	123 (1%) 66 65	19, 51, 100, 166	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	74	ILE	8.6
9	I	70	THR	7.3
22	V	39	ALA	7.2
22	V	40	PRO	6.9
9	I	72	GLU	6.6
9	I	71	ALA	6.4
31	9	1	U	6.2
26	Z	46	SER	6.1
9	I	108	HIS	6.1
9	I	102	GLN	5.9
9	I	76	ASP	5.7
4	D	57	THR	5.5
4	D	63	ILE	5.5
9	I	93	ALA	5.3
9	I	104	ALA	5.3
9	I	113	SER	5.2
9	I	79	GLY	4.8
14	N	166	ALA	4.7
9	I	99	GLN	4.6
9	I	112	LEU	4.6
9	I	92	VAL	4.5
9	I	128	THR	4.5
9	I	80	PHE	4.4
4	D	90	LEU	4.4
9	I	100	VAL	4.3
9	I	66	GLY	4.2
9	I	106	GLN	4.2
9	I	97	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
9	I	109	PRO	4.1
9	I	69	PRO	4.1
4	D	85	GLN	4.0
9	I	83	GLY	3.9
9	I	111	LEU	3.9
4	D	44	ILE	3.9
9	I	91	PHE	3.8
30	0	1198	U	3.8
19	S	81	ILE	3.8
9	I	67	VAL	3.6
9	I	73	LEU	3.6
31	9	24	U	3.6
25	Y	235	GLU	3.5
9	I	132	VAL	3.5
22	V	43	PRO	3.4
22	V	1	THR	3.4
9	I	78	ALA	3.4
4	D	170	TYR	3.4
9	I	82	THR	3.4
26	Z	44	ARG	3.4
9	I	88	GLN	3.3
9	I	110	ASP	3.3
4	D	89	PRO	3.3
9	I	116	LEU	3.2
1	A	37	VAL	3.2
9	I	86	GLU	3.2
9	I	98	ASP	3.1
9	I	84	SER	3.1
26	Z	45	VAL	3.0
4	D	75	LEU	3.0
4	D	18	ILE	3.0
30	0	970	U	3.0
28	2	49	GLU	3.0
24	X	88	GLU	3.0
4	D	40	ILE	3.0
26	Z	50	VAL	3.0
26	Z	58	ASN	2.9
30	0	2645	U	2.9
30	0	1172	G	2.9
9	I	103	ILE	2.8
8	H	40	GLN	2.8
4	D	92	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	17	ARG	2.8
4	D	171	ASP	2.7
9	I	81	GLU	2.7
9	I	75	LYS	2.7
4	D	61	PHE	2.6
6	F	106	ALA	2.6
9	I	105	GLU	2.6
28	2	39	ARG	2.6
22	V	38	GLY	2.5
4	D	81	GLU	2.5
30	0	1199	A	2.5
2	B	57	GLU	2.5
1	A	237	GLY	2.5
26	Z	35	SER	2.5
8	H	174	LEU	2.4
4	D	84	LEU	2.4
30	0	1200	A	2.4
12	L	80	ASP	2.4
14	N	155	GLU	2.4
4	D	27	ILE	2.4
24	X	80	GLU	2.4
30	0	1202	A	2.4
14	N	183	ASP	2.3
4	D	166	ILE	2.3
9	I	114	TYR	2.3
5	E	100	ASP	2.3
4	D	26	GLY	2.3
20	T	116	ASP	2.3
4	D	88	LEU	2.3
4	D	134	LEU	2.3
4	D	41	LEU	2.3
4	D	104	PHE	2.2
4	D	73	VAL	2.2
8	H	87	LYS	2.2
6	F	49	PHE	2.2
4	D	69	ILE	2.2
4	D	45	THR	2.1
24	X	71	ARG	2.1
4	D	102	GLY	2.1
9	I	121	LYS	2.1
7	G	25	GLU	2.1
9	I	117	THR	2.1

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Mol	Chain	Res	Type	RSRZ
7	G	27	ILE	2.1
14	N	160	SER	2.1
26	Z	69	ASP	2.1
4	D	64	ARG	2.1
7	G	26	MET	2.1
30	0	1177	A	2.0
30	0	735	C	2.0
9	I	90	ASP	2.0
30	0	1203	G	2.0
4	D	47	GLN	2.0
30	0	2237	G	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	1MA	0	628	23/24	0.98	0.17	28,29,31,32	0
30	OMU	0	2587	21/22	0.98	0.12	32,36,38,39	0
30	UR3	0	2619	21/22	0.98	0.13	45,48,53,54	0
30	PSU	0	2621	20/21	0.98	0.14	26,30,50,51	0
30	OMG	0	2588	24/25	0.99	0.12	30,35,38,40	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SR	0	9006	1/1	0.12	2.38	200,200,200,200	0
34	SR	0	8982	1/1	0.38	0.71	197,197,197,197	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	8525	1/1	0.52	0.22	83,83,83,83	0
34	SR	0	8962	1/1	0.57	0.21	155,155,155,155	0
32	MG	0	8038	1/1	0.60	0.09	66,66,66,66	0
32	MG	0	8089	1/1	0.61	0.07	42,42,42,42	0
34	SR	0	9001	1/1	0.67	0.18	176,176,176,176	0
34	SR	0	8993	1/1	0.68	0.08	173,173,173,173	0
34	SR	0	8955	1/1	0.68	0.12	198,198,198,198	0
35	NA	0	8562	1/1	0.68	0.40	55,55,55,55	0
35	NA	0	8556	1/1	0.70	0.73	55,55,55,55	0
34	SR	0	8927	1/1	0.72	0.08	170,170,170,170	0
35	NA	0	8506	1/1	0.74	0.23	63,63,63,63	0
34	SR	0	9004	1/1	0.74	1.12	200,200,200,200	0
35	NA	0	8509	1/1	0.75	0.18	63,63,63,63	0
32	MG	0	8081	1/1	0.76	0.15	74,74,74,74	0
32	MG	0	8033	1/1	0.79	0.06	49,49,49,49	0
34	SR	0	8988	1/1	0.80	0.15	162,162,162,162	0
32	MG	0	8059	1/1	0.80	0.09	50,50,50,50	0
35	NA	0	8563	1/1	0.80	0.40	67,67,67,67	0
35	NA	0	8567	1/1	0.80	0.17	72,72,72,72	0
34	SR	0	8991	1/1	0.81	0.12	186,186,186,186	0
35	NA	0	8502	1/1	0.81	0.09	51,51,51,51	0
34	SR	0	8996	1/1	0.81	0.51	200,200,200,200	0
34	SR	0	8975	1/1	0.82	0.09	137,137,137,137	0
34	SR	0	8976	1/1	0.82	0.22	194,194,194,194	0
34	SR	0	8957	1/1	0.82	0.25	200,200,200,200	0
35	NA	0	8571	1/1	0.82	0.09	61,61,61,61	0
35	NA	Q	8540	1/1	0.83	0.11	58,58,58,58	0
34	SR	0	8944	1/1	0.83	0.12	175,175,175,175	0
35	NA	0	8555	1/1	0.83	0.48	53,53,53,53	0
34	SR	0	8971	1/1	0.83	0.05	175,175,175,175	0
34	SR	0	8928	1/1	0.84	0.08	139,139,139,139	0
35	NA	0	8553	1/1	0.84	0.28	52,52,52,52	0
35	NA	9	8572	1/1	0.84	0.23	80,80,80,80	0
35	NA	0	8508	1/1	0.85	0.20	43,43,43,43	0
34	SR	0	8979	1/1	0.85	0.19	198,198,198,198	0
34	SR	Y	9002	1/1	0.85	0.13	188,188,188,188	0
35	NA	0	8574	1/1	0.85	0.37	52,52,52,52	0
35	NA	0	8549	1/1	0.85	0.23	51,51,51,51	0
35	NA	0	8536	1/1	0.86	0.06	47,47,47,47	0
35	NA	0	8547	1/1	0.86	0.98	60,60,60,60	0
34	SR	0	8998	1/1	0.86	0.12	172,172,172,172	0
34	SR	9	9003	1/1	0.86	0.07	171,171,171,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	8545	1/1	0.87	0.17	38,38,38,38	0
32	MG	0	8036	1/1	0.87	0.06	46,46,46,46	0
32	MG	0	8063	1/1	0.87	0.18	90,90,90,90	0
34	SR	A	8977	1/1	0.88	0.05	154,154,154,154	0
34	SR	S	8961	1/1	0.88	0.06	128,128,128,128	0
35	NA	0	8564	1/1	0.88	0.18	70,70,70,70	0
35	NA	0	8528	1/1	0.88	0.25	44,44,44,44	0
35	NA	0	8554	1/1	0.88	0.70	69,69,69,69	0
34	SR	0	8985	1/1	0.88	0.07	124,124,124,124	0
32	MG	0	8078	1/1	0.88	0.31	76,76,76,76	0
35	NA	0	8546	1/1	0.89	0.81	82,82,82,82	0
35	NA	0	8516	1/1	0.89	0.13	45,45,45,45	0
35	NA	0	8548	1/1	0.89	0.11	42,42,42,42	0
34	SR	0	8951	1/1	0.89	0.03	144,144,144,144	0
35	NA	0	8550	1/1	0.89	0.21	53,53,53,53	0
34	SR	0	8919	1/1	0.89	0.11	178,178,178,178	0
32	MG	A	8051	1/1	0.89	0.27	60,60,60,60	0
35	NA	0	8514	1/1	0.89	0.38	48,48,48,48	0
35	NA	0	8565	1/1	0.90	0.35	57,57,57,57	0
35	NA	0	8566	1/1	0.90	0.35	71,71,71,71	0
34	SR	0	8949	1/1	0.90	0.07	104,104,104,104	0
35	NA	0	8570	1/1	0.90	0.07	48,48,48,48	0
34	SR	0	8924	1/1	0.90	0.17	133,133,133,133	0
34	SR	B	8987	1/1	0.90	0.53	200,200,200,200	0
34	SR	0	8956	1/1	0.90	0.08	138,138,138,138	0
34	SR	0	8920	1/1	0.91	0.05	112,112,112,112	0
33	CL	O	8808	1/1	0.91	0.10	73,73,73,73	0
34	SR	0	8968	1/1	0.91	0.04	161,161,161,161	0
32	MG	0	8067	1/1	0.91	0.27	50,50,50,50	0
32	MG	T	8057	1/1	0.92	0.08	66,66,66,66	0
32	MG	0	8056	1/1	0.92	0.14	41,41,41,41	0
35	NA	0	8560	1/1	0.92	0.59	85,85,85,85	0
35	NA	0	8561	1/1	0.92	0.78	77,77,77,77	0
35	NA	0	8518	1/1	0.92	0.35	82,82,82,82	0
35	NA	0	8513	1/1	0.92	0.21	42,42,42,42	0
35	NA	0	8526	1/1	0.92	0.04	39,39,39,39	0
34	SR	0	8934	1/1	0.93	0.12	117,117,117,117	0
35	NA	0	8524	1/1	0.93	0.19	52,52,52,52	0
32	MG	0	8083	1/1	0.93	0.09	37,37,37,37	0
34	SR	9	8980	1/1	0.93	0.09	158,158,158,158	0
34	SR	0	8947	1/1	0.93	0.13	162,162,162,162	0
35	NA	0	8533	1/1	0.93	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8075	1/1	0.93	0.04	39,39,39,39	0
32	MG	0	8037	1/1	0.93	0.14	59,59,59,59	0
33	CL	Y	8820	1/1	0.93	0.06	40,40,40,40	0
34	SR	A	8929	1/1	0.93	0.09	130,130,130,130	0
34	SR	A	8930	1/1	0.93	0.05	110,110,110,110	0
32	MG	0	8006	1/1	0.93	0.15	21,21,21,21	0
34	SR	B	8950	1/1	0.93	0.15	114,114,114,114	0
35	NA	0	8552	1/1	0.93	0.29	72,72,72,72	0
34	SR	0	8931	1/1	0.93	0.09	110,110,110,110	0
32	MG	0	8022	1/1	0.94	0.14	31,31,31,31	0
35	NA	C	8503	1/1	0.94	0.09	27,27,27,27	0
35	NA	J	8538	1/1	0.94	0.07	43,43,43,43	0
32	MG	0	8060	1/1	0.94	0.10	43,43,43,43	0
35	NA	S	8510	1/1	0.94	0.06	27,27,27,27	0
34	SR	0	8948	1/1	0.94	0.11	88,88,88,88	0
34	SR	0	8983	1/1	0.94	0.06	177,177,177,177	0
33	CL	J	8801	1/1	0.94	0.10	71,71,71,71	0
34	SR	0	8926	1/1	0.94	0.11	122,122,122,122	0
32	MG	0	8016	1/1	0.94	0.27	50,50,50,50	0
35	NA	0	8557	1/1	0.94	0.14	57,57,57,57	0
35	NA	0	8558	1/1	0.94	0.32	45,45,45,45	0
35	NA	0	8559	1/1	0.94	0.18	67,67,67,67	0
34	SR	0	8992	1/1	0.94	0.15	133,133,133,133	0
32	MG	0	8066	1/1	0.94	0.30	80,80,80,80	0
33	CL	0	8805	1/1	0.94	0.07	53,53,53,53	0
34	SR	0	8997	1/1	0.94	0.62	194,194,194,194	0
34	SR	0	8960	1/1	0.94	0.04	134,134,134,134	0
34	SR	0	9000	1/1	0.94	0.06	165,165,165,165	0
35	NA	0	8527	1/1	0.94	0.16	47,47,47,47	0
33	CL	0	8815	1/1	0.94	0.07	67,67,67,67	0
34	SR	0	8936	1/1	0.94	0.11	91,91,91,91	0
35	NA	0	8535	1/1	0.94	0.36	55,55,55,55	0
34	SR	0	8938	1/1	0.94	0.07	165,165,165,165	0
34	SR	0	8941	1/1	0.94	0.15	104,104,104,104	0
32	MG	0	8031	1/1	0.95	0.17	57,57,57,57	0
35	NA	0	8507	1/1	0.95	0.17	32,32,32,32	0
34	SR	0	8966	1/1	0.95	0.07	100,100,100,100	0
32	MG	0	8032	1/1	0.95	0.04	44,44,44,44	0
34	SR	0	8969	1/1	0.95	0.21	164,164,164,164	0
34	SR	0	8970	1/1	0.95	0.02	123,123,123,123	0
32	MG	0	8046	1/1	0.95	0.16	44,44,44,44	0
34	SR	0	8973	1/1	0.95	0.10	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	8522	1/1	0.95	0.28	67,67,67,67	0
34	SR	0	8974	1/1	0.95	0.15	158,158,158,158	0
32	MG	0	8090	1/1	0.95	0.17	55,55,55,55	0
32	MG	0	8053	1/1	0.95	0.05	38,38,38,38	0
34	SR	0	8978	1/1	0.95	0.04	119,119,119,119	0
32	MG	B	8042	1/1	0.95	0.12	44,44,44,44	0
35	NA	0	8529	1/1	0.95	0.05	39,39,39,39	0
35	NA	0	8531	1/1	0.95	0.12	41,41,41,41	0
34	SR	0	8981	1/1	0.95	0.12	171,171,171,171	0
34	SR	0	8933	1/1	0.95	0.13	141,141,141,141	0
32	MG	0	8076	1/1	0.95	0.10	39,39,39,39	0
35	NA	0	8569	1/1	0.95	0.09	44,44,44,44	0
35	NA	0	8542	1/1	0.95	0.27	48,48,48,48	0
33	CL	0	8803	1/1	0.95	0.08	52,52,52,52	0
35	NA	0	8573	1/1	0.95	0.16	61,61,61,61	0
32	MG	0	8024	1/1	0.95	0.14	52,52,52,52	0
35	NA	0	8575	1/1	0.95	0.22	83,83,83,83	0
35	NA	0	8505	1/1	0.95	0.73	34,34,34,34	0
34	SR	0	8965	1/1	0.96	0.08	121,121,121,121	0
33	CL	M	8818	1/1	0.96	0.08	44,44,44,44	0
35	NA	0	8537	1/1	0.96	0.13	38,38,38,38	0
35	NA	0	8541	1/1	0.96	0.26	61,61,61,61	0
32	MG	0	8001	1/1	0.96	0.13	30,30,30,30	0
35	NA	0	8544	1/1	0.96	0.12	60,60,60,60	0
32	MG	0	8077	1/1	0.96	0.06	35,35,35,35	0
33	CL	3	8804	1/1	0.96	0.08	58,58,58,58	0
32	MG	K	8054	1/1	0.96	0.12	37,37,37,37	0
34	SR	0	8972	1/1	0.96	0.10	127,127,127,127	0
32	MG	0	8080	1/1	0.96	0.15	66,66,66,66	0
33	CL	0	8812	1/1	0.96	0.07	45,45,45,45	0
33	CL	0	8814	1/1	0.96	0.11	50,50,50,50	0
32	MG	0	8007	1/1	0.96	0.10	43,43,43,43	0
32	MG	0	8048	1/1	0.96	0.17	22,22,22,22	0
32	MG	0	8085	1/1	0.96	0.10	80,80,80,80	0
34	SR	0	8945	1/1	0.96	0.07	107,107,107,107	0
32	MG	0	8035	1/1	0.96	0.13	43,43,43,43	0
35	NA	0	8511	1/1	0.96	0.12	56,56,56,56	0
32	MG	0	8073	1/1	0.96	0.10	74,74,74,74	0
32	MG	0	8091	1/1	0.96	0.08	51,51,51,51	0
32	MG	9	8074	1/1	0.96	0.19	75,75,75,75	0
34	SR	0	8990	1/1	0.96	0.16	173,173,173,173	0
35	NA	0	8519	1/1	0.96	0.15	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	8520	1/1	0.96	0.12	40,40,40,40	0
33	CL	B	8819	1/1	0.96	0.10	51,51,51,51	0
34	SR	0	8901	1/1	0.96	0.07	84,84,84,84	0
34	SR	0	8908	1/1	0.96	0.11	83,83,83,83	0
34	SR	0	8994	1/1	0.96	0.18	192,192,192,192	0
34	SR	0	8995	1/1	0.96	0.09	136,136,136,136	0
34	SR	0	8959	1/1	0.96	0.12	159,159,159,159	0
32	MG	0	8027	1/1	0.96	0.06	31,31,31,31	0
33	CL	L	8810	1/1	0.96	0.06	52,52,52,52	0
34	SR	0	8963	1/1	0.96	0.04	131,131,131,131	0
35	NA	0	8534	1/1	0.96	0.23	64,64,64,64	0
34	SR	0	8911	1/1	0.97	0.08	75,75,75,75	0
34	SR	0	8954	1/1	0.97	0.11	100,100,100,100	0
34	SR	0	8986	1/1	0.97	0.32	200,200,200,200	0
34	SR	0	8915	1/1	0.97	0.09	110,110,110,110	0
34	SR	0	8917	1/1	0.97	0.10	111,111,111,111	0
32	MG	0	8084	1/1	0.97	0.14	29,29,29,29	0
32	MG	0	8068	1/1	0.97	0.07	52,52,52,52	0
34	SR	0	8922	1/1	0.97	0.14	155,155,155,155	0
32	MG	0	8069	1/1	0.97	0.20	57,57,57,57	0
32	MG	0	8012	1/1	0.97	0.15	22,22,22,22	0
32	MG	0	8039	1/1	0.97	0.34	67,67,67,67	0
32	MG	0	8092	1/1	0.97	0.08	66,66,66,66	0
35	NA	0	8523	1/1	0.97	0.10	46,46,46,46	0
33	CL	0	8822	1/1	0.97	0.55	83,83,83,83	0
34	SR	0	8999	1/1	0.97	0.06	93,93,93,93	0
32	MG	0	8044	1/1	0.97	0.08	45,45,45,45	0
33	CL	A	8809	1/1	0.97	0.06	65,65,65,65	0
32	MG	0	8002	1/1	0.97	0.12	30,30,30,30	0
34	SR	0	8937	1/1	0.97	0.23	102,102,102,102	0
35	NA	0	8530	1/1	0.97	0.18	41,41,41,41	0
34	SR	0	9008	1/1	0.97	0.12	84,84,84,84	0
32	MG	0	8064	1/1	0.97	0.11	41,41,41,41	0
33	CL	J	8821	1/1	0.97	0.09	60,60,60,60	0
34	SR	0	8943	1/1	0.97	0.08	99,99,99,99	0
34	SR	R	8912	1/1	0.97	0.17	83,83,83,83	0
32	MG	0	8079	1/1	0.97	0.16	39,39,39,39	0
32	MG	0	8065	1/1	0.97	0.04	33,33,33,33	0
32	MG	0	8018	1/1	0.97	0.12	27,27,27,27	0
35	NA	9	8543	1/1	0.97	0.19	44,44,44,44	0
32	MG	0	8004	1/1	0.97	0.18	25,25,25,25	0
32	MG	0	8003	1/1	0.98	0.18	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8047	1/1	0.98	0.25	50,50,50,50	0
32	MG	0	8088	1/1	0.98	0.15	32,32,32,32	0
34	SR	0	8921	1/1	0.98	0.12	77,77,77,77	0
34	SR	0	8964	1/1	0.98	0.10	124,124,124,124	0
34	SR	0	9007	1/1	0.98	0.23	191,191,191,191	0
33	CL	0	8811	1/1	0.98	0.06	63,63,63,63	0
34	SR	0	8923	1/1	0.98	0.12	87,87,87,87	0
32	MG	0	8010	1/1	0.98	0.14	48,48,48,48	0
33	CL	0	8813	1/1	0.98	0.05	46,46,46,46	0
32	MG	0	8049	1/1	0.98	0.22	58,58,58,58	0
32	MG	0	8072	1/1	0.98	0.18	43,43,43,43	0
35	NA	R	8532	1/1	0.98	0.07	45,45,45,45	0
33	CL	0	8817	1/1	0.98	0.06	51,51,51,51	0
35	NA	0	8501	1/1	0.98	0.17	33,33,33,33	0
35	NA	0	8551	1/1	0.98	0.16	38,38,38,38	0
32	MG	0	8025	1/1	0.98	0.13	27,27,27,27	0
35	NA	0	8504	1/1	0.98	0.17	31,31,31,31	0
32	MG	0	8093	1/1	0.98	0.05	27,27,27,27	0
34	SR	0	8935	1/1	0.98	0.09	80,80,80,80	0
32	MG	0	8055	1/1	0.98	0.21	30,30,30,30	0
32	MG	0	8026	1/1	0.98	0.12	33,33,33,33	0
32	MG	0	8011	1/1	0.98	0.13	23,23,23,23	0
34	SR	0	8939	1/1	0.98	0.04	145,145,145,145	0
32	MG	0	8029	1/1	0.98	0.17	46,46,46,46	0
34	SR	0	8942	1/1	0.98	0.07	115,115,115,115	0
33	CL	J	8802	1/1	0.98	0.10	66,66,66,66	0
32	MG	0	8062	1/1	0.98	0.17	44,44,44,44	0
32	MG	0	8030	1/1	0.98	0.36	72,72,72,72	0
34	SR	0	8989	1/1	0.98	0.07	159,159,159,159	0
35	NA	0	8521	1/1	0.98	0.21	50,50,50,50	0
34	SR	1	8913	1/1	0.98	0.10	91,91,91,91	0
32	MG	0	8041	1/1	0.98	0.22	29,29,29,29	0
34	SR	0	8904	1/1	0.98	0.19	55,55,55,55	0
34	SR	0	8905	1/1	0.98	0.24	69,69,69,69	0
33	CL	N	8807	1/1	0.98	0.09	71,71,71,71	0
34	SR	0	8910	1/1	0.98	0.06	99,99,99,99	0
32	MG	0	8082	1/1	0.98	0.16	73,73,73,73	0
32	MG	0	8021	1/1	0.98	0.11	32,32,32,32	0
34	SR	0	8958	1/1	0.98	0.09	97,97,97,97	0
37	K	0	8402	1/1	0.98	0.08	67,67,67,67	0
35	NA	M	8539	1/1	0.99	0.10	26,26,26,26	0
32	MG	0	8045	1/1	0.99	0.12	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SR	0	8902	1/1	0.99	0.14	37,37,37,37	0
32	MG	0	8005	1/1	0.99	0.16	31,31,31,31	0
32	MG	0	8087	1/1	0.99	0.08	31,31,31,31	0
34	SR	0	8906	1/1	0.99	0.19	53,53,53,53	0
32	MG	0	8008	1/1	0.99	0.13	24,24,24,24	0
34	SR	0	8909	1/1	0.99	0.15	86,86,86,86	0
34	SR	0	8946	1/1	0.99	0.15	99,99,99,99	0
34	SR	0	8984	1/1	0.99	0.09	114,114,114,114	0
32	MG	0	8034	1/1	0.99	0.06	38,38,38,38	0
32	MG	0	8013	1/1	0.99	0.04	21,21,21,21	0
34	SR	0	8914	1/1	0.99	0.27	121,121,121,121	0
32	MG	0	8070	1/1	0.99	0.12	43,43,43,43	0
34	SR	0	8953	1/1	0.99	0.19	160,160,160,160	0
35	NA	0	8515	1/1	0.99	0.20	35,35,35,35	0
34	SR	0	8916	1/1	0.99	0.05	104,104,104,104	0
35	NA	0	8517	1/1	0.99	0.18	46,46,46,46	0
32	MG	0	8071	1/1	0.99	0.19	50,50,50,50	0
32	MG	0	8050	1/1	0.99	0.13	28,28,28,28	0
33	CL	0	8816	1/1	0.99	0.19	67,67,67,67	0
32	MG	0	8052	1/1	0.99	0.05	39,39,39,39	0
32	MG	0	8014	1/1	0.99	0.16	21,21,21,21	0
32	MG	0	8009	1/1	0.99	0.21	28,28,28,28	0
32	MG	0	8017	1/1	0.99	0.21	23,23,23,23	0
34	SR	0	8925	1/1	0.99	0.12	87,87,87,87	0
32	MG	0	8058	1/1	0.99	0.08	16,16,16,16	0
35	NA	0	8568	1/1	0.99	0.54	36,36,36,36	0
32	MG	Y	8086	1/1	0.99	0.07	35,35,35,35	0
32	MG	0	8040	1/1	0.99	0.17	80,80,80,80	0
34	SR	0	8967	1/1	0.99	0.02	131,131,131,131	0
34	SR	F	9005	1/1	0.99	0.07	132,132,132,132	0
32	MG	0	8019	1/1	0.99	0.15	19,19,19,19	0
32	MG	0	8043	1/1	0.99	0.09	43,43,43,43	0
32	MG	0	8020	1/1	0.99	0.12	36,36,36,36	0
33	CL	R	8806	1/1	0.99	0.10	47,47,47,47	0
36	CD	Z	8703	1/1	0.99	0.06	83,83,83,83	0
36	CD	1	8702	1/1	0.99	0.12	60,60,60,60	0
36	CD	3	8704	1/1	0.99	0.06	76,76,76,76	0
37	K	0	8401	1/1	0.99	0.15	93,93,93,93	0
34	SR	3	8932	1/1	0.99	0.14	74,74,74,74	0
34	SR	0	8940	1/1	1.00	0.12	78,78,78,78	0
32	MG	0	8015	1/1	1.00	0.14	31,31,31,31	0
34	SR	1	8952	1/1	1.00	0.12	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8061	1/1	1.00	0.20	25,25,25,25	0
34	SR	0	8907	1/1	1.00	0.12	43,43,43,43	0
36	CD	O	8705	1/1	1.00	0.09	84,84,84,84	0
36	CD	U	8701	1/1	1.00	0.09	62,62,62,62	0
35	NA	0	8512	1/1	1.00	0.31	45,45,45,45	0
32	MG	0	8023	1/1	1.00	0.14	26,26,26,26	0
34	SR	0	8918	1/1	1.00	0.12	79,79,79,79	0
32	MG	0	8028	1/1	1.00	0.18	24,24,24,24	0
34	SR	0	8903	1/1	1.00	0.16	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.