Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:00 AM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

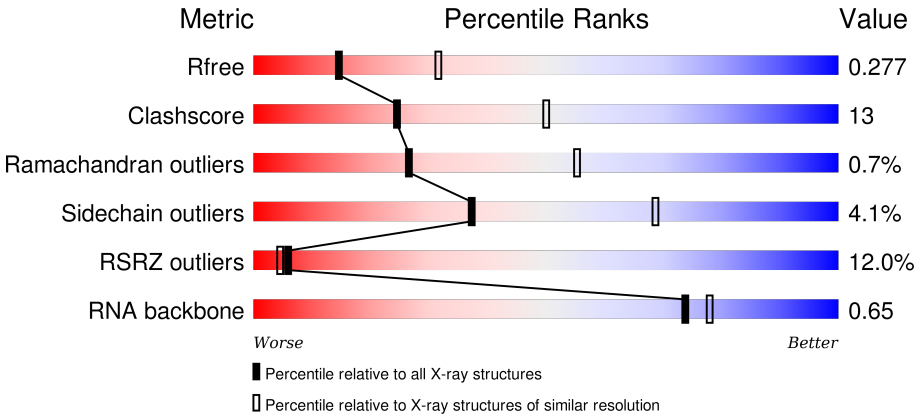
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 Å.

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



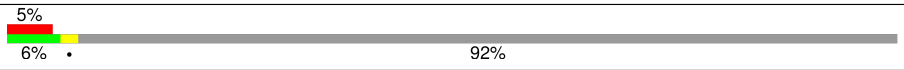
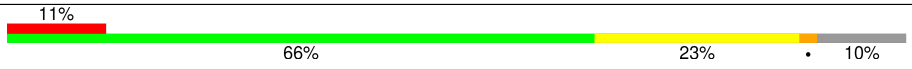
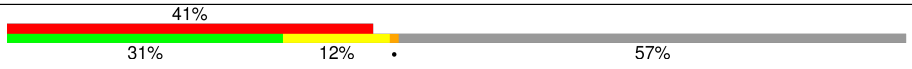
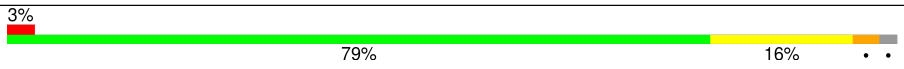
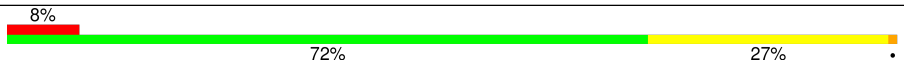
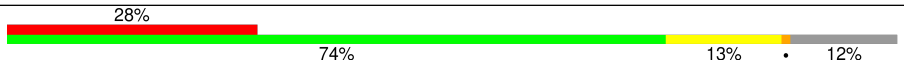
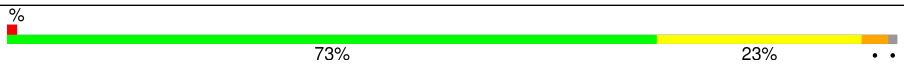
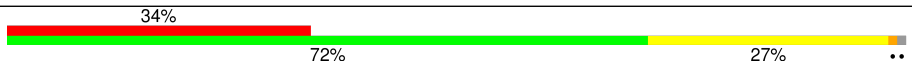
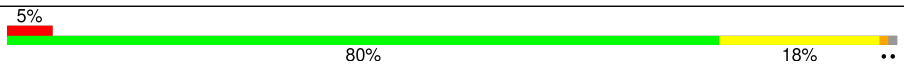
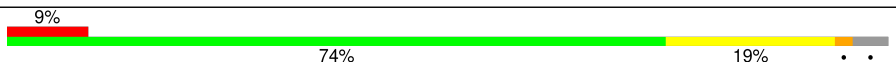
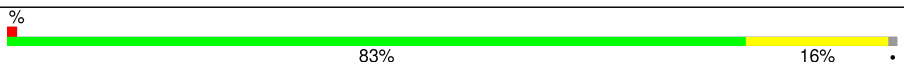
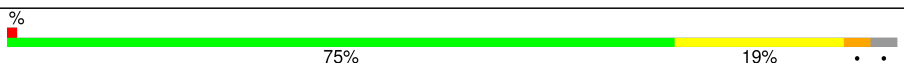
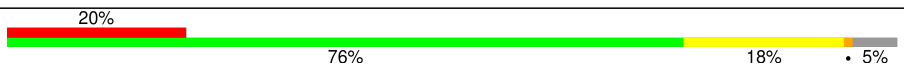
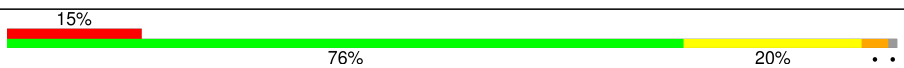
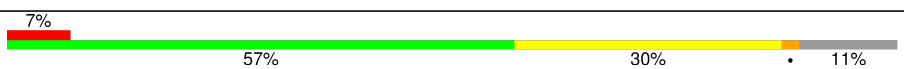
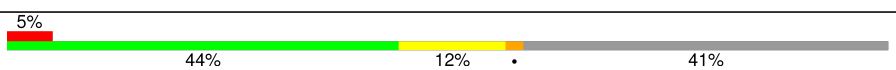
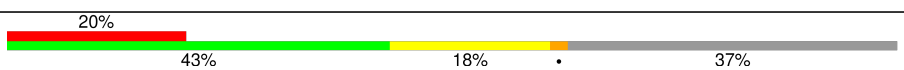
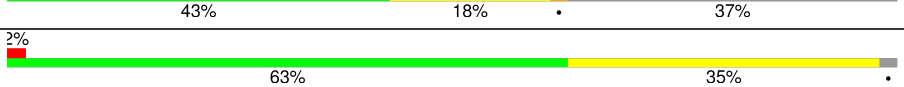
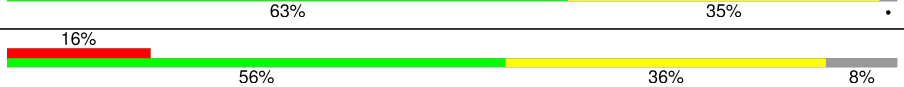
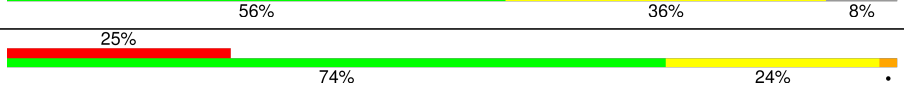
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	15% 70% 26%
2	B	338	6% 65% 32%
3	C	246	8% 74% 22%
4	D	177	56% 49% 28% 21%

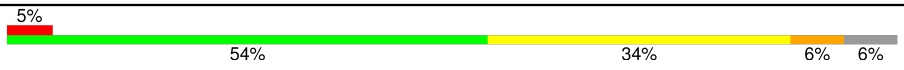
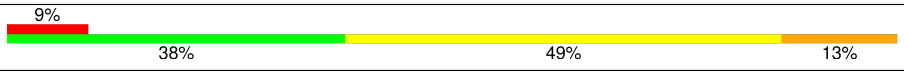
Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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
32	MG	0	8004	-	-	-	X
32	MG	0	8011	-	-	-	X
32	MG	0	8041	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	A	8051	-	-	-	X
33	K	0	8401	-	-	-	X
33	K	0	8402	-	-	-	X
34	NA	0	8502	-	-	-	X
34	NA	0	8504	-	-	-	X
34	NA	0	8508	-	-	-	X
34	NA	0	8512	-	-	-	X
34	NA	0	8517	-	-	-	X
34	NA	0	8519	-	-	-	X
34	NA	0	8523	-	-	-	X
34	NA	0	8527	-	-	-	X
34	NA	0	8530	-	-	-	X
34	NA	0	8534	-	-	-	X
34	NA	0	8535	-	-	-	X
34	NA	0	8542	-	-	-	X
34	NA	0	8546	-	-	-	X
34	NA	0	8547	-	-	-	X
34	NA	0	8550	-	-	-	X
34	NA	0	8552	-	-	-	X
34	NA	0	8553	-	-	-	X
34	NA	0	8555	-	-	-	X
34	NA	0	8559	-	-	-	X
34	NA	0	8560	-	-	-	X
34	NA	0	8562	-	-	-	X
34	NA	0	8563	-	-	-	X
34	NA	0	8565	-	-	-	X
34	NA	0	8567	-	-	-	X
34	NA	0	8568	-	-	-	X
34	NA	0	8569	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	9	8572	-	-	-	X
34	NA	R	8575	-	-	-	X
35	CL	0	8815	-	-	-	X
36	SR	B	8987	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10872	19054	2745			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	85	Total	Mg	0	0
			85	85		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	2	Total	Mg	0	0
			2	2		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	2	Total K 2 2	0	0

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

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

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	93	Total Sr 93 93	0	0
36	J	1	Total Sr 1 1	0	0
36	1	2	Total Sr 2 2	0	0
36	B	2	Total Sr 2 2	0	0
36	3	2	Total Sr 2 2	0	0
36	A	3	Total Sr 3 3	0	0
36	R	1	Total Sr 1 1	0	0
36	9	2	Total Sr 2 2	0	0
36	S	1	Total Sr 1 1	0	0
36	F	1	Total Sr 1 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5951	Total O 5951 5951	0	0
38	A	111	Total O 111 111	0	0
38	B	153	Total O 153 153	0	0
38	C	165	Total O 165 165	0	0
38	D	46	Total O 46 46	0	0
38	E	44	Total O 44 44	0	0
38	F	23	Total O 23 23	0	0
38	G	19	Total O 19 19	0	0
38	H	71	Total O 71 71	0	0
38	I	10	Total O 10 10	0	0
38	J	54	Total O 54 54	0	0
38	K	56	Total O 56 56	0	0
38	L	80	Total O 80 80	0	0
38	M	130	Total O 130 130	0	0
38	N	59	Total O 59 59	0	0
38	O	41	Total O 41 41	0	0
38	P	61	Total O 61 61	0	0
38	Q	51	Total O 51 51	0	0
38	R	78	Total O 78 78	0	0
38	S	33	Total O 33 33	0	0
38	T	37	Total O 37 37	0	0

Continued on next page...

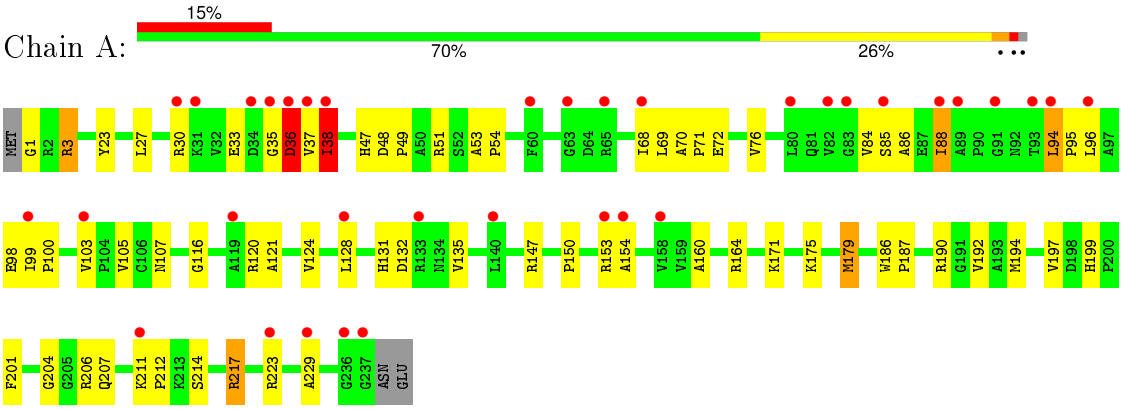
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	U	25	Total O 25 25	0	0
38	V	11	Total O 11 11	0	0
38	W	63	Total O 63 63	0	0
38	X	28	Total O 28 28	0	0
38	Y	91	Total O 91 91	0	0
38	Z	28	Total O 28 28	0	0
38	1	52	Total O 52 52	0	0
38	2	37	Total O 37 37	0	0
38	3	68	Total O 68 68	0	0
38	9	147	Total O 147 147	0	0

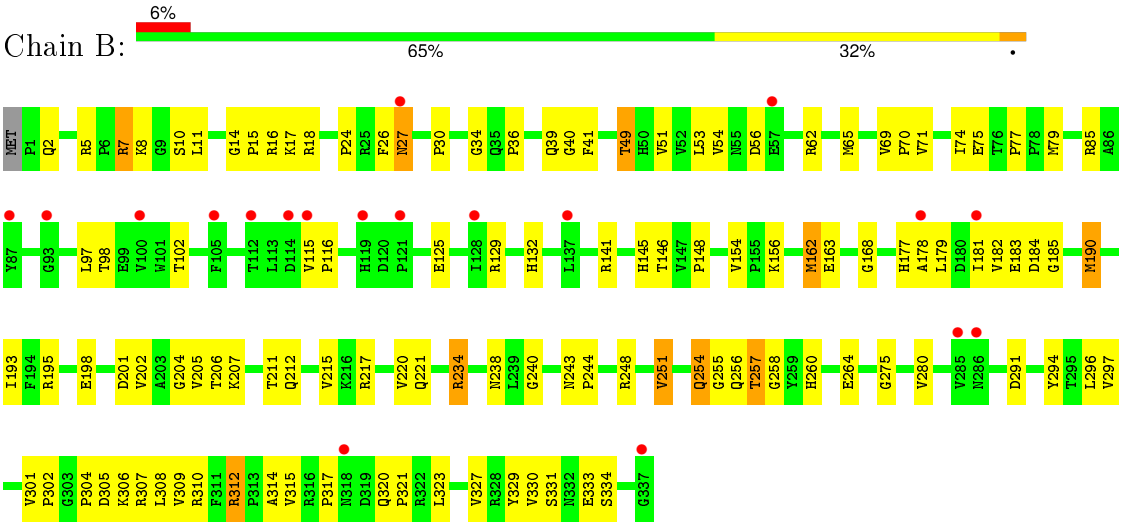
3 Residue-property plots (i)

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

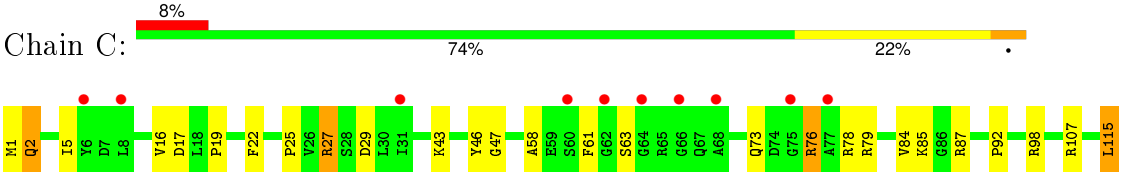
- Molecule 1: 50S ribosomal protein L2P

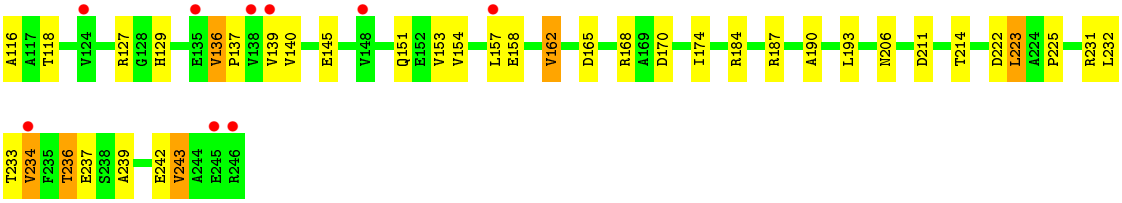


- Molecule 2: 50S ribosomal protein L3P



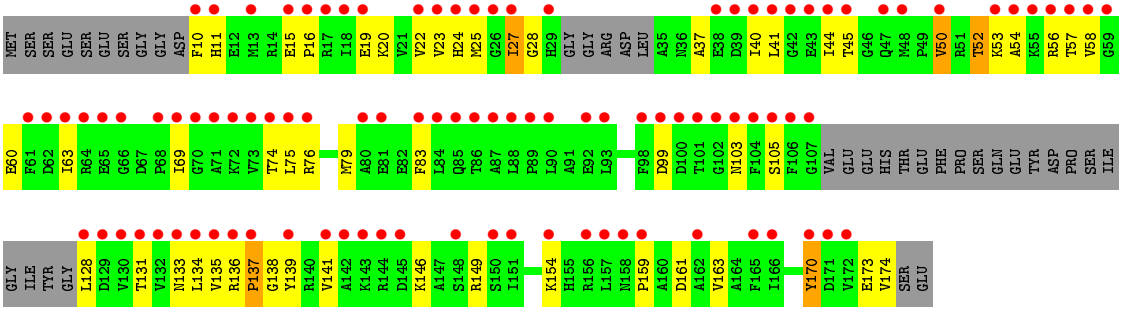
- Molecule 3: 50S ribosomal protein L4P





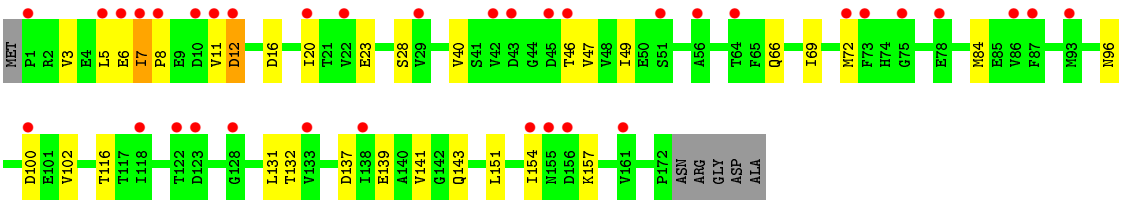
• Molecule 4: 50S ribosomal protein L5P

Chain D:



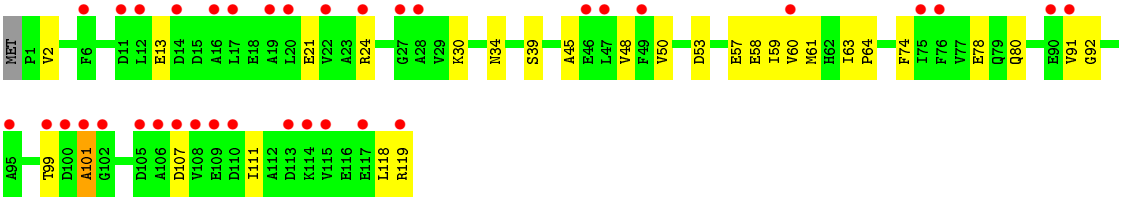
• Molecule 5: 50S ribosomal protein L6P

Chain E:



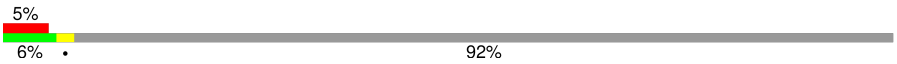
• Molecule 6: 50S ribosomal protein L7Ae

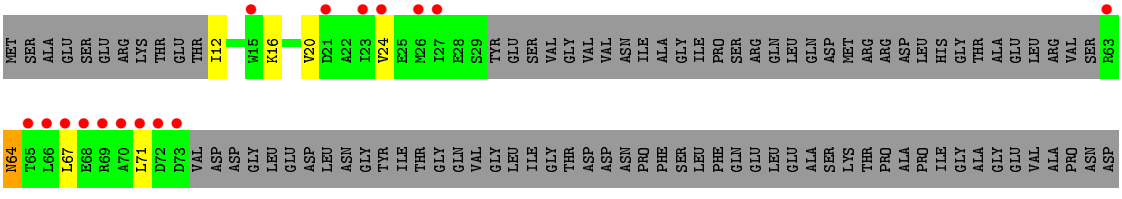
Chain F:

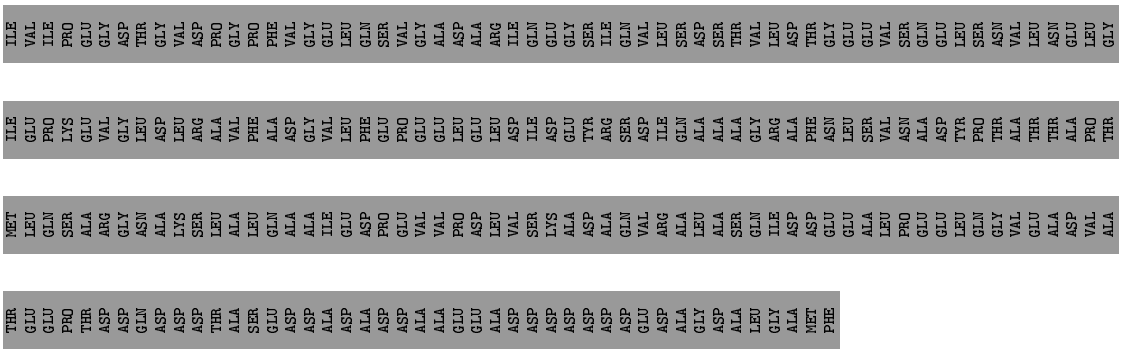


• Molecule 7: 50S ribosomal protein L10E

Chain G:

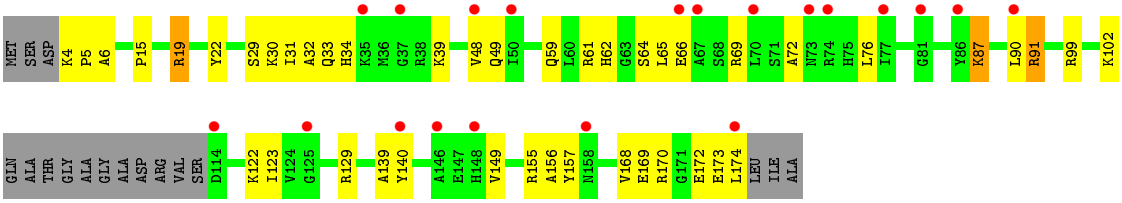






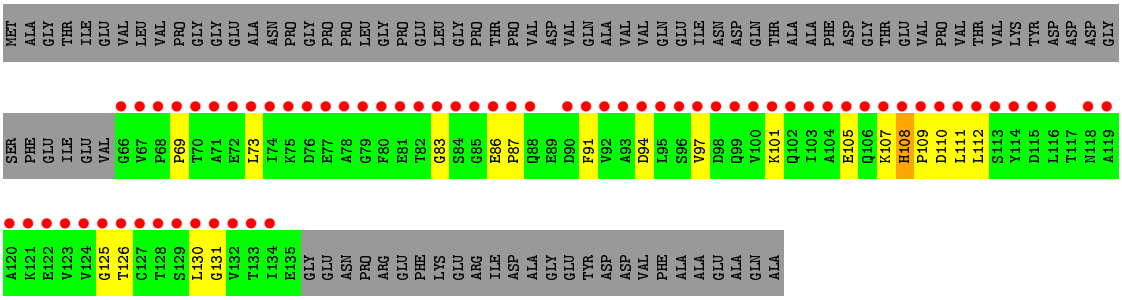
• Molecule 8: 50S ribosomal protein L10e

Chain H:



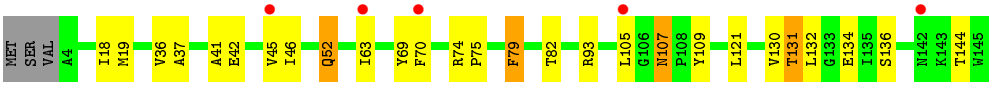
• Molecule 9: 50S ribosomal protein L11P

Chain I:



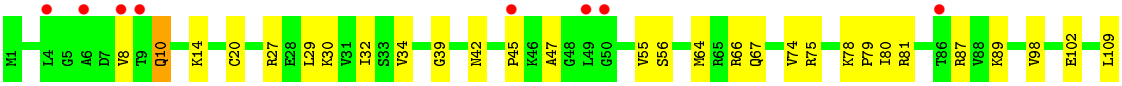
• Molecule 10: 50S ribosomal protein L13P

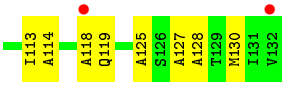
Chain J:



• Molecule 11: 50S ribosomal protein L14P

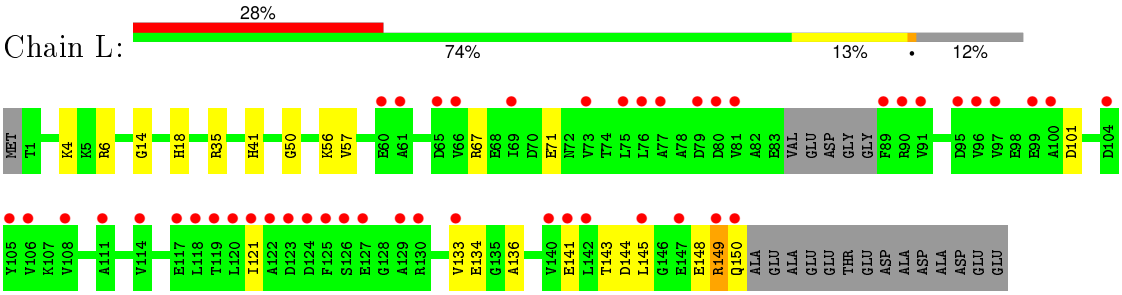
Chain K:





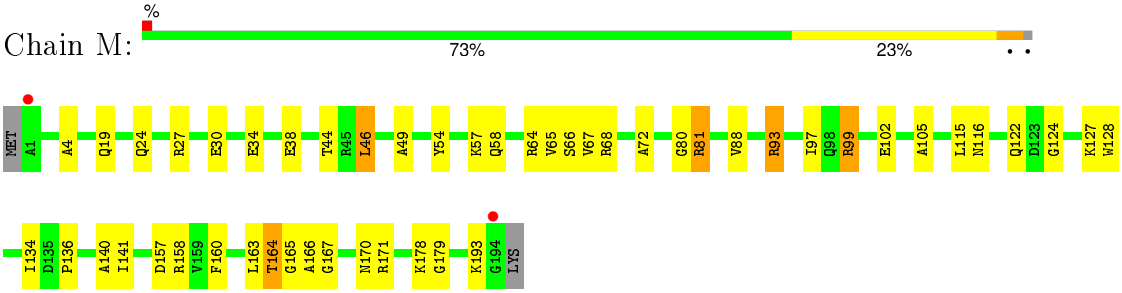
• Molecule 12: 50S ribosomal protein L15P

Chain L:



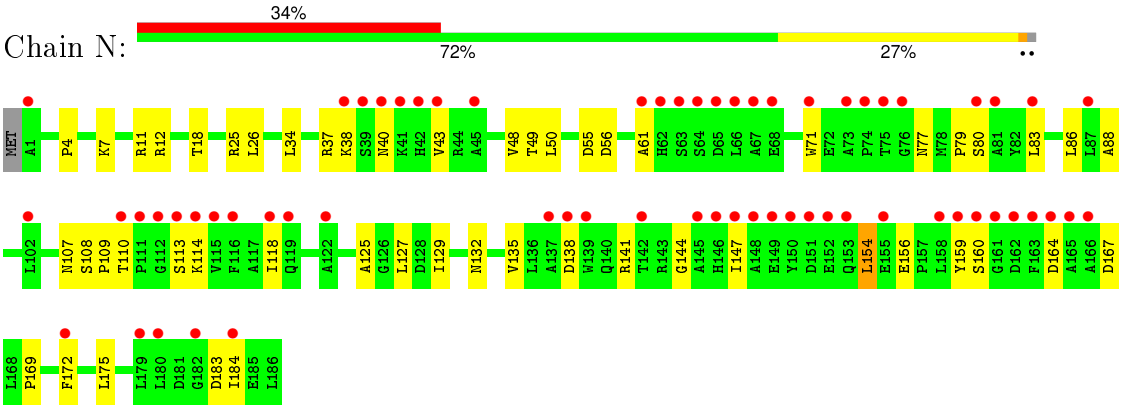
• Molecule 13: 50S ribosomal protein L15e

Chain M:



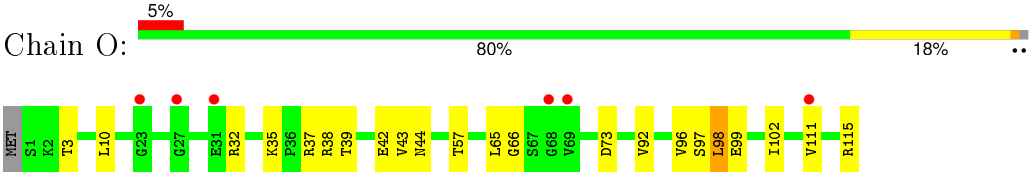
• Molecule 14: 50S ribosomal protein L18P

Chain N:



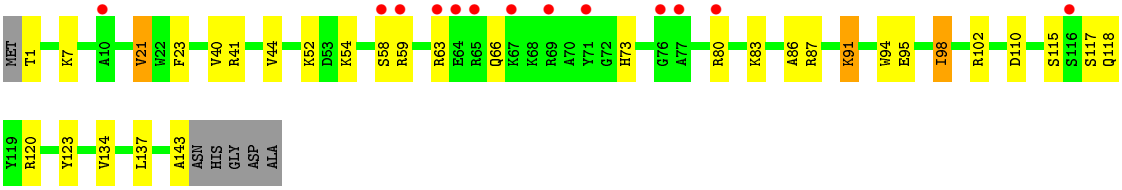
• Molecule 15: 50S ribosomal protein L18e

Chain O:

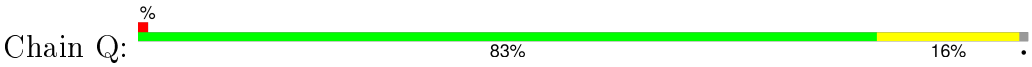


• Molecule 16: 50S ribosomal protein L19e

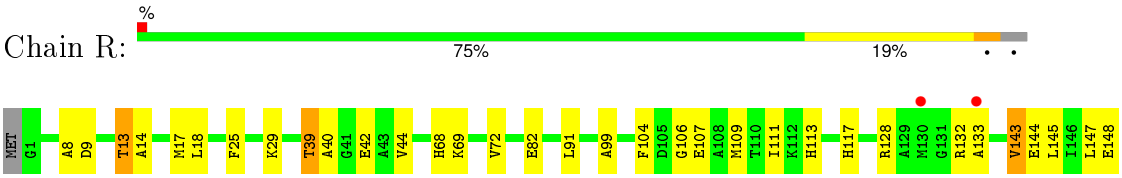
Chain P:



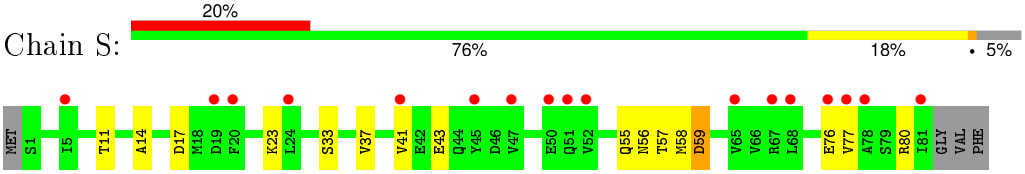
• Molecule 17: 50S ribosomal protein L21e



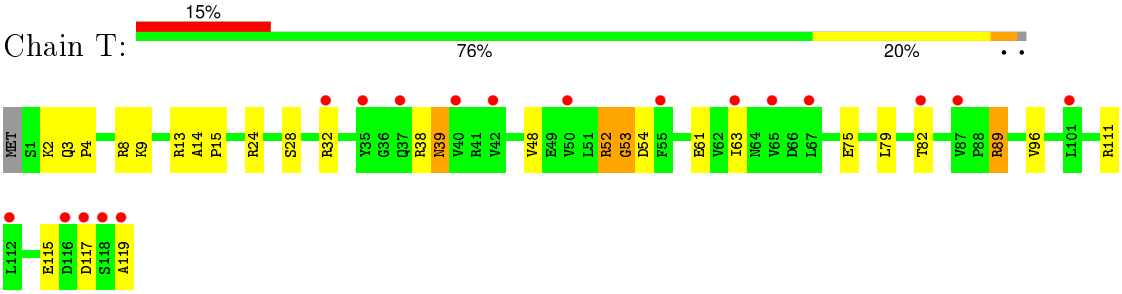
• Molecule 18: 50S ribosomal protein L22P



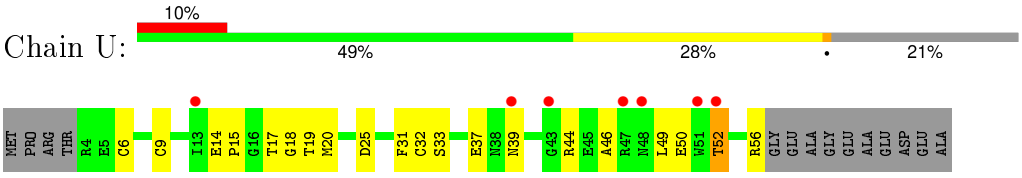
• Molecule 19: 50S ribosomal protein L23P



• Molecule 20: 50S ribosomal protein L24P

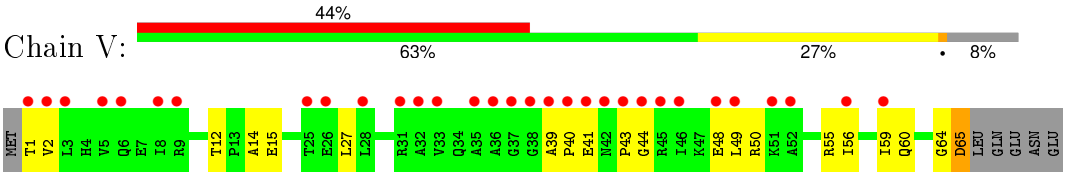


• Molecule 21: 50S ribosomal protein L24e



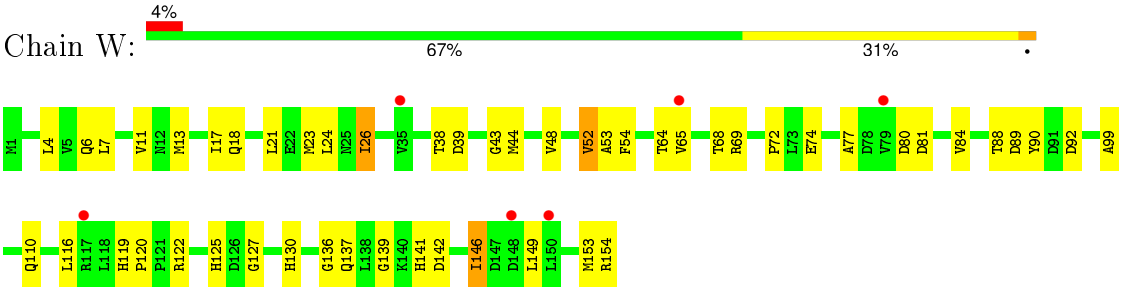
• Molecule 22: 50S ribosomal protein L29P

Chain V:



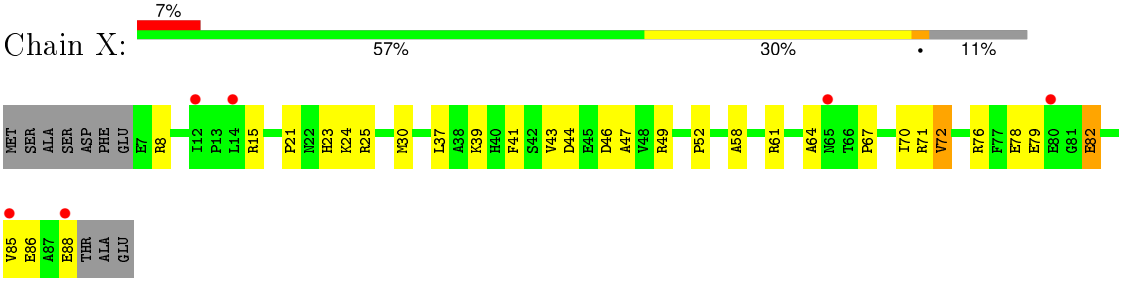
• Molecule 23: 50S ribosomal protein L30P

Chain W:



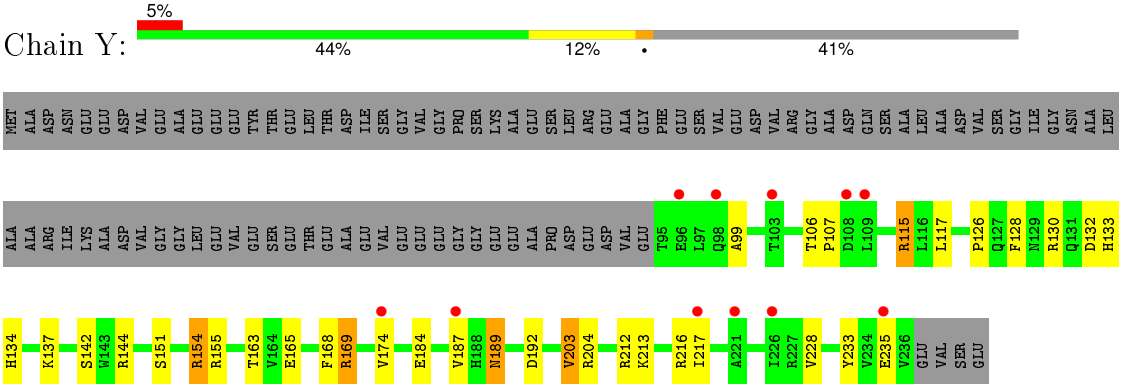
• Molecule 24: 50S ribosomal protein L31e

Chain X:



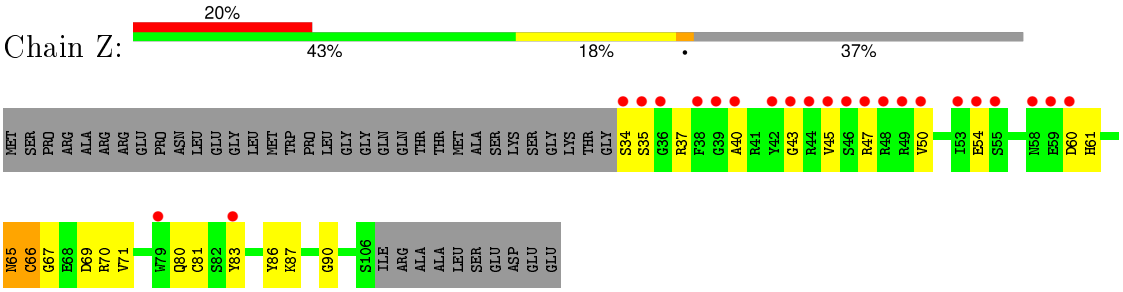
• Molecule 25: 50S ribosomal protein L32e

Chain Y:



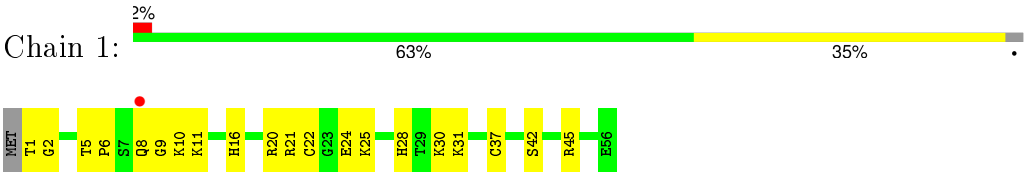
• Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



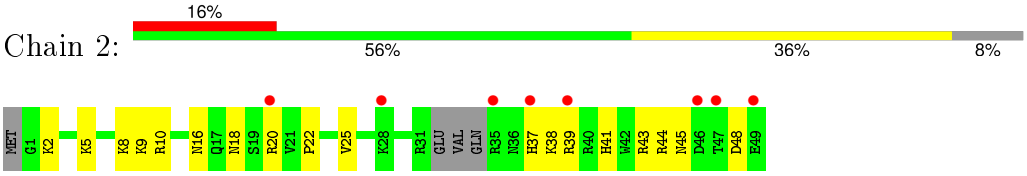
• Molecule 27: 50S ribosomal protein L37e

Chain 1:



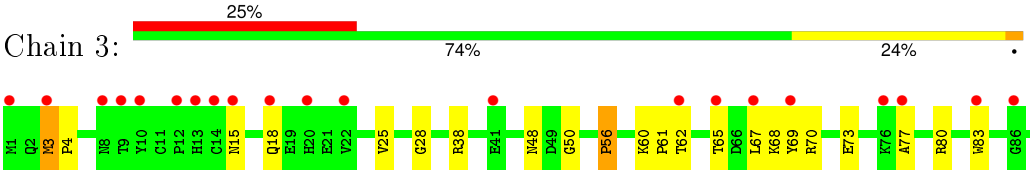
• Molecule 28: 50S ribosomal protein L39e

Chain 2:



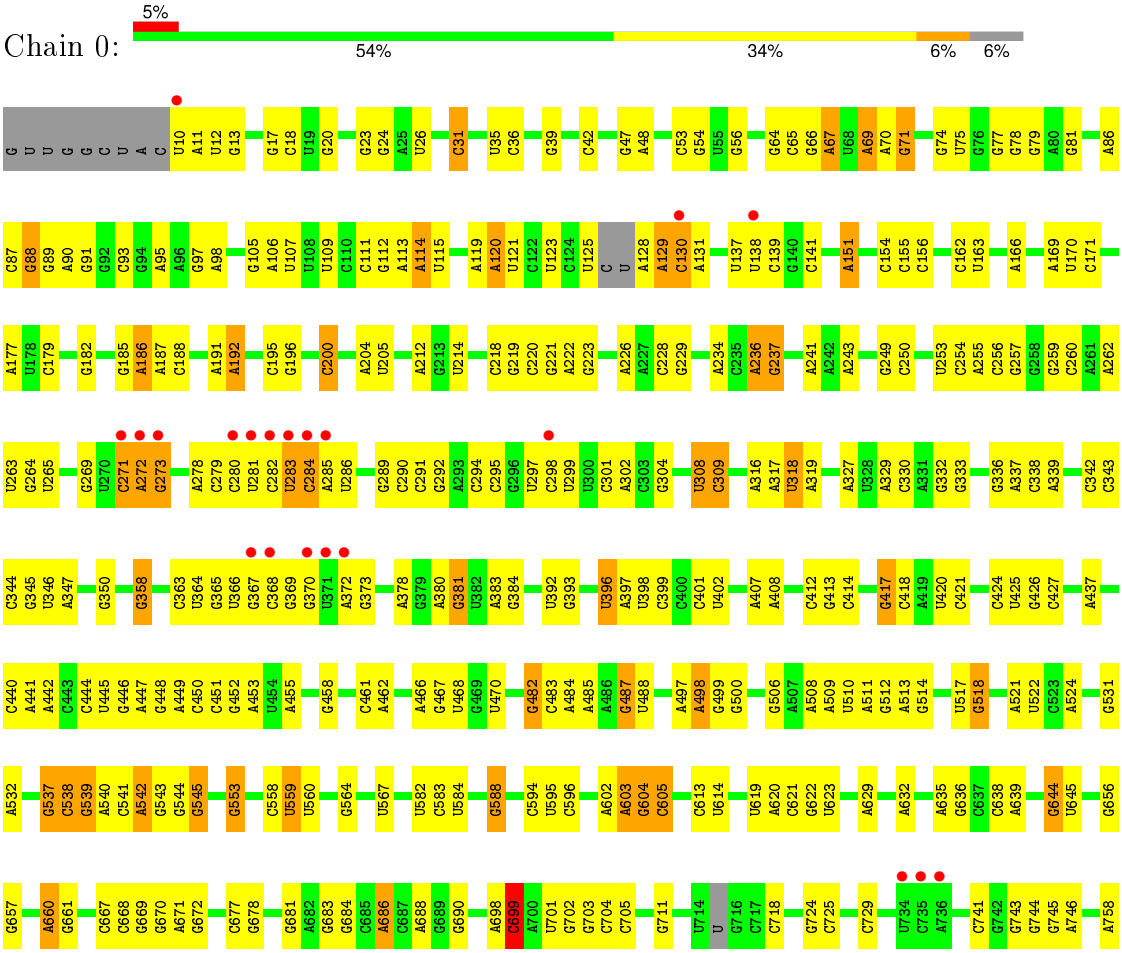
• Molecule 29: 50S ribosomal protein L44E

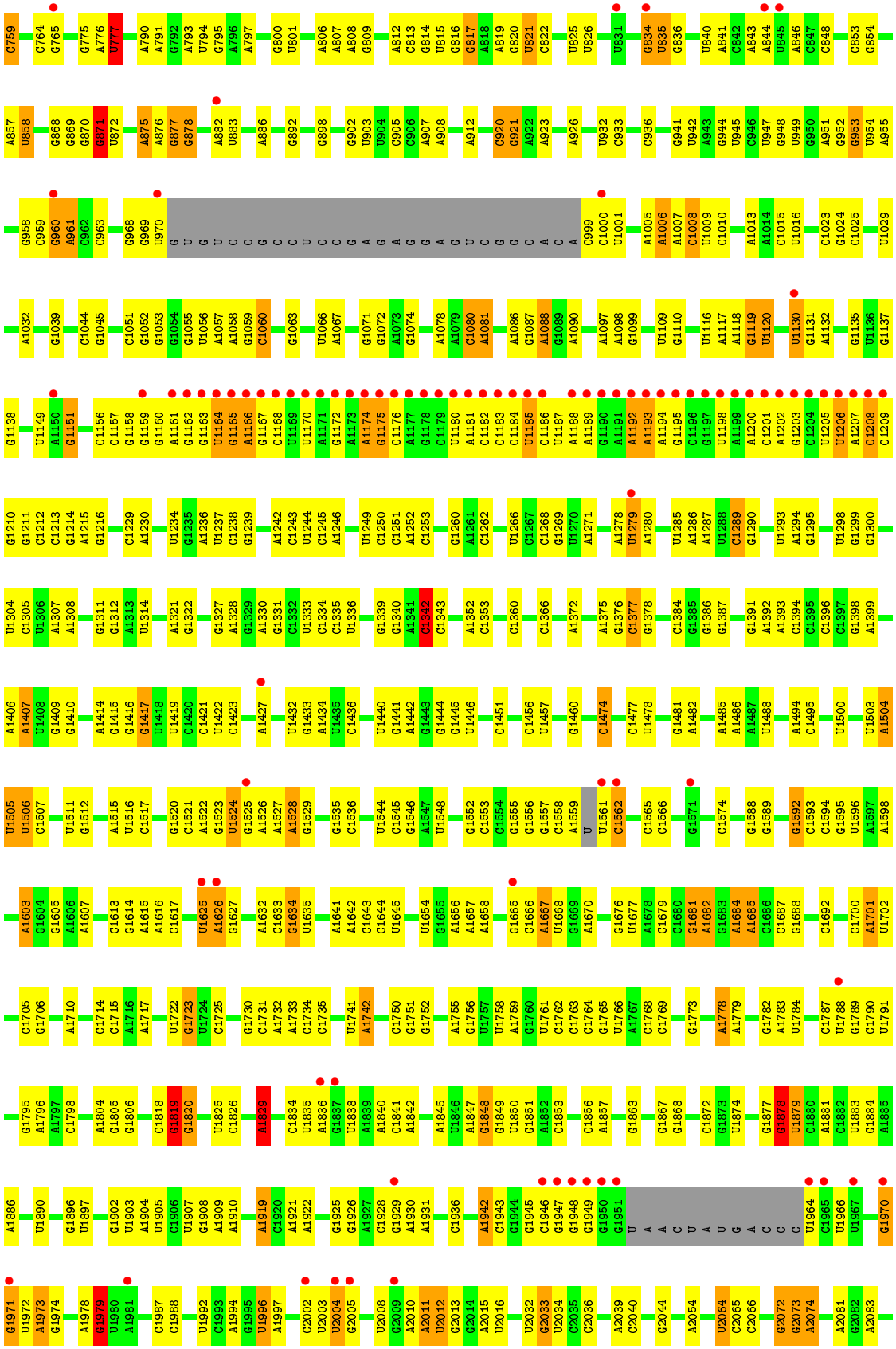
Chain 3:

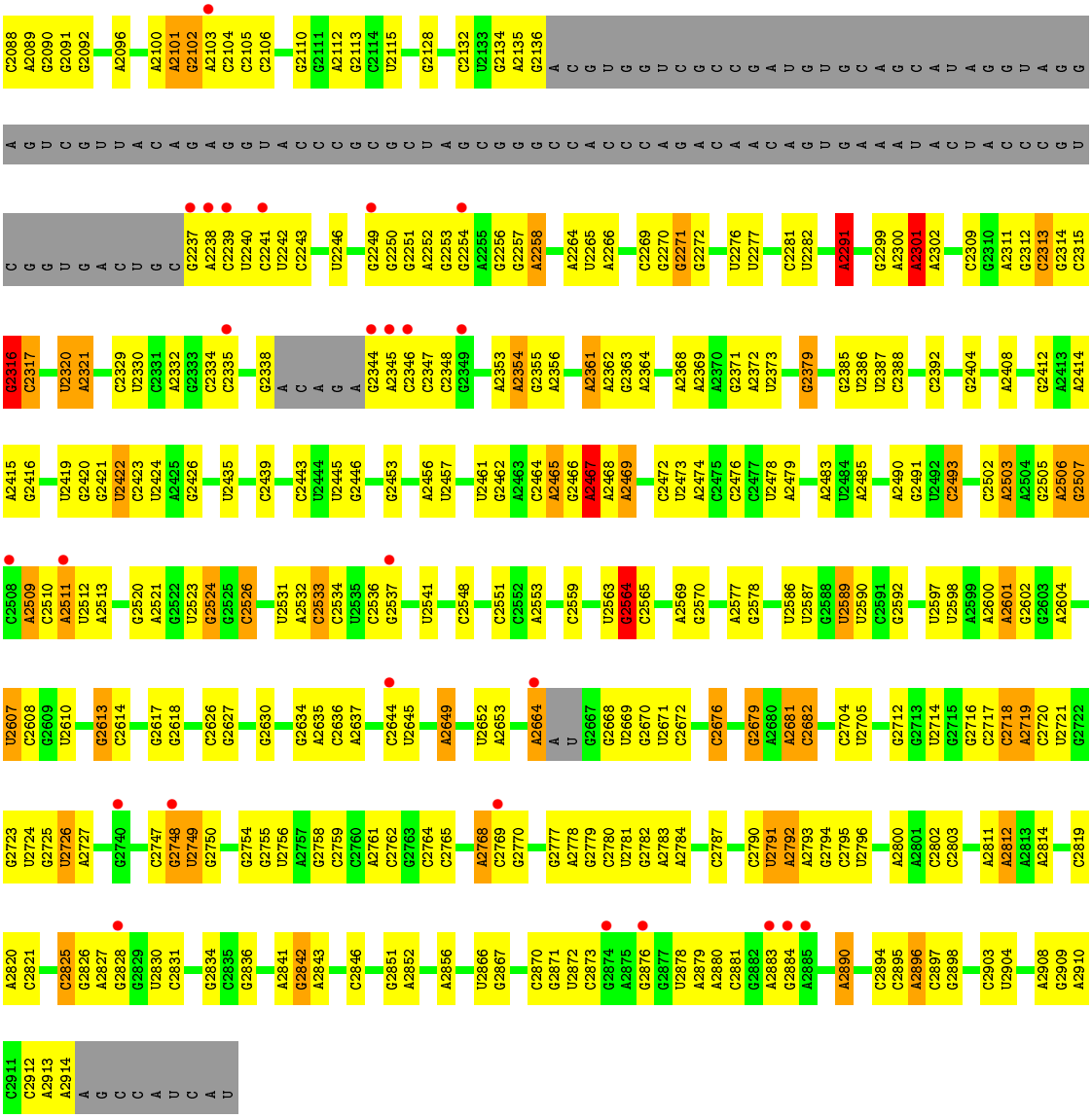


• Molecule 30: 23S ribosomal RNA

Chain 0:

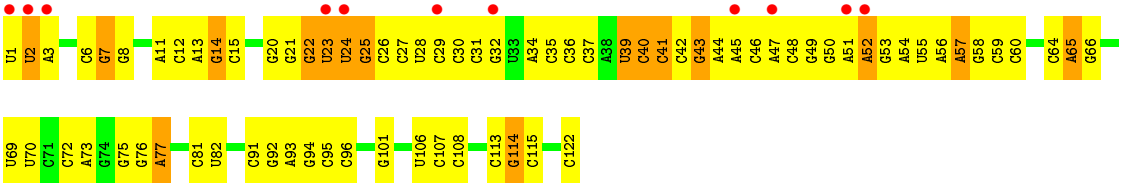



C759 C764 G765 G775 A776 U777 A790 A791 G792 A793 U794 G795 A796 A797 G800 U801 A806 A807 A808 G809 A812 C813 G814 U815 G816 G817 A818 A819 G820 U821 C822 U825 U826 U831 G834 U835 G836 U840 A841 C842 A843 A844 U845 A846 C847 C848 C853 G854
A857 U858 G868 G869 G870 G871 U872 A875 A876 G877 G878 A882 U883 A886 G892 G898 G902 U903 U904 C905 C906 A907 A908 A912 C920 G921 A922 A923 A926 U932 C933 C936 G941 U942 A943 G944 U945 C946 U947 G948 U949 G950 A951 G952 G953 U954 A955
G958 C959 G960 A961 G962 C963 G968 G969 U970 C999 C1000 U1001 A1005 A1006 A1007 C1008 U1009 C1010 A1013 A1014 C1015 U1016 C1023 G1024 C1025 U1029
A1032 G1039 C1044 G1045 C1051 G1052 G1053 G1054 G1055 U1056 A1057 A1058 G1059 C1060 G1063 U1066 A1067 G1071 G1072 A1073 G1074 A1078 A1079 C1080 A1081 A1086 G1087 A1088 G1089 A1090 A1097 A1098 G1099 U1109 G1110 U1116 A1117 A1118 G1119 U1120 U1130 G1131 A1132 G1135 U1136 G1137
G1138 U1149 A1150 G1151 C1156 C1157 G1158 G1159 G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 G1175 C1176 A1177 G1178 G1179 C1180 A1181 C1182 C1183 C1184 U1185 C1186 U1187 A1188 A1189 G1190 A1191 A1192 A1193 A1194 G1195 C1196 G1197 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208 C1209
G1210 G1211 C1212 C1213 G1214 A1215 G1216 C1229 A1230 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 U1249 C1250 C1251 A1252 C1253 G1260 A1261 C1262 U1266 C1267 C1268 G1269 U1270 A1271 A1278 U1279 A1280 U1285 A1286 A1287 U1288 C1289 G1290 U1293 A1294 G1295 U1298 G1299 G1300
U1304 C1305 U1306 A1307 A1308 G1311 G1312 A1313 U1314 A1321 G1322 G1327 A1328 G1329 A1330 G1331 C1332 U1333 C1334 C1335 U1336 G1339 G1340 A1341 C1342 C1343 A1352 C1353 C1360 C1366 A1372 A1375 G1376 C1377 G1378 C1384 G1385 G1386 G1387 G1391 A1392 A1393 C1394 C1395 C1396 C1397 G1398 A1399
A1406 A1407 U1408 G1409 G1410 A1414 G1415 G1416 G1417 U1418 U1419 C1420 C1421 U1422 C1423 A1427 U1432 G1433 A1434 U1435 C1436 U1440 C1441 A1442 G1443 G1444 G1445 U1446 C1451 C1456 U1457 G1460 C1474 C1477 U1478 G1481 A1482 A1485 A1486 A1487 U1488 A1494 C1495 U1500 U1503 A1504
U1505 U1506 C1507 U1511 G1512 A1515 U1516 C1517 G1520 C1521 A1522 G1523 U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1536 U1544 C1545 G1546 A1547 U1548 G1552 C1553 C1554 G1555 C1556 G1557 C1558 A1559 U1561 C1562 C1565 C1566 G1571 C1574 C1588 G1589 C1592 C1593 C1594 C1595 U1596 A1597 A1598
A1603 G1604 G1605 A1606 A1607 C1613 G1614 A1615 A1616 C1617 U1625 A1626 G1627 A1632 C1633 G1634 U1635 A1641 A1642 C1643 C1644 U1645 U1654 G1655 A1656 A1657 A1658 G1665 C1666 A1667 U1668 C1669 A1670 G1676 U1677 A1678 C1679 C1680 G1681 A1682 G1683 A1684 A1685 C1686 C1687 G1688 C1692 C1700 A1701 U1702
C1705 G1706 A1710 C1714 C1715 A1716 A1717 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 C1734 C1735 U1741 A1742 C1750 G1751 G1752 A1755 G1756 U1757 U1758 A1759 G1760 U1761 C1762 C1763 C1764 G1765 U1766 A1767 C1768 C1769 G1773 A1778 A1779 G1782 A1783 U1784 C1787 U1788 C1790 U1791
G1795 A1796 A1797 C1798 A1804 G1805 G1806 C1818 G1819 G1820 U1825 C1826 A1829 C1834 U1835 A1836 G1837 U1838 A1839 A1840 C1841 A1842 A1845 U1846 A1847 G1848 G1849 U1850 G1851 A1852 C1853 C1856 A1857 G1863 G1867 G1868 C1872 G1873 U1874 G1877 G1878 U1879 C1880 A1881 C1882 U1883 G1884 A1885
A1886 U1890 G1896 U1897 G1902 U1903 A1904 U1905 C1906 U1907 G1908 A1909 A1910 A1919 C1920 A1921 A1922 G1925 G1926 A1927 C1928 G1929 A1930 A1931 C1936 A1942 C1943 G1944 G1945 C1946 G1947 G1948 G1949 G1950 G1951 U1964 C1965 U1966 U1967 G1970
G1971 U1972 A1973 G1974 A1978 G1979 U1980 A1981 C1987 C1988 U1992 C1993 A1994 G1995 U1996 A1997 C2002 U2003 U2004 G2005 U2008 G2009 A2010 A2011 U2012 G2013 G2014 A2015 U2016 U2032 G2033 U2034 C2035 C2036 A2039 C2040 G2044 A2054 U2064 C2065 C2066 G2072 G2073 A2074 A2081 G2082 A2083



• 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	212.83Å 299.90Å 576.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 2.70 85.81 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.83-2.70) 90.8 (85.81-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.184 , 0.226 0.254 , 0.277	Depositor DCC
R_{free} test set	4903 reflections (1.07%)	DCC
Wilson B-factor (Å^2)	47.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 67.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 667281 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.32	0/1786	0.64	0/2408
2	B	0.32	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.31	0/1111	0.55	0/1498
5	E	0.32	0/1382	0.56	0/1880
6	F	0.32	0/901	0.57	0/1224
7	G	0.31	0/241	0.48	0/324
8	H	0.32	0/1302	0.63	0/1743
9	I	0.29	0/526	0.51	0/716
10	J	0.35	0/1136	0.59	0/1530
11	K	0.33	0/1004	0.65	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.34	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.61	0/1999
15	O	0.34	0/874	0.59	1/1181 (0.1%)
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.35	0/749	0.68	0/1005
18	R	1.26	7/1172 (0.6%)	1.11	6/1578 (0.4%)
19	S	0.31	0/648	0.57	0/875
20	T	0.33	0/958	0.62	1/1289 (0.1%)
21	U	0.34	0/417	0.55	0/562
22	V	0.31	0/502	0.52	0/675
23	W	0.34	0/1219	0.64	0/1655
24	X	0.34	0/664	0.58	0/895
25	Y	0.36	0/1146	0.60	0/1536
26	Z	0.35	0/584	0.60	0/781
27	1	0.37	0/438	0.61	0/578
28	2	0.34	0/401	0.55	0/529
29	3	0.36	0/771	0.57	0/1024
30	0	0.36	0/65957	0.68	17/102867 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98701 (0.0%)	0.67	26/147586 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
30	0	0	42
31	9	0	1
All	All	1	43

All (7) bond length outliers are listed below:

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

All (26) bond angle outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (43) planarity outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
30	0	2524	G	Sidechain
30	0	2551	C	Sidechain
30	0	2564	G	Sidechain
30	0	26	U	Sidechain
30	0	2607	U	Sidechain
30	0	2679	G	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	686	A	Sidechain
30	0	817	G	Sidechain
30	0	903	U	Sidechain
31	9	94	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	75	0
2	B	2625	0	2533	92	0
3	C	1860	0	1813	57	0
4	D	1094	0	1085	40	0
5	E	1357	0	1266	23	0
6	F	890	0	843	26	0
7	G	240	0	231	7	0
8	H	1282	0	1292	37	0
9	I	519	0	500	15	0
10	J	1120	0	1098	30	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	22	0
13	M	1558	0	1573	42	0
14	N	1445	0	1401	45	0
15	O	865	0	873	15	0
16	P	1136	0	1123	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	735	0	729	14	0
18	R	1149	0	1122	34	0
19	S	641	0	605	11	0
20	T	950	0	924	19	0
21	U	410	0	364	19	0
22	V	499	0	511	17	0
23	W	1196	0	1137	55	0
24	X	654	0	653	24	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	16	0
27	1	431	0	426	22	0
28	2	396	0	413	19	0
29	3	755	0	728	20	0
30	0	59020	0	29806	1142	0
31	9	2599	0	1325	101	0
32	0	85	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	2	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	0	93	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	2	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	J	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5951	0	0	153	0
38	1	52	0	0	3	0
38	2	37	0	0	2	0
38	3	68	0	0	5	0
38	9	147	0	0	8	0
38	A	111	0	0	5	0
38	B	153	0	0	14	0
38	C	165	0	0	11	0
38	D	46	0	0	2	0
38	E	44	0	0	2	0
38	F	23	0	0	1	0
38	G	19	0	0	0	0
38	H	71	0	0	6	0
38	I	10	0	0	2	0
38	J	54	0	0	1	0
38	K	56	0	0	3	0
38	L	80	0	0	6	0
38	M	130	0	0	5	0
38	N	59	0	0	5	0
38	O	41	0	0	3	0
38	P	61	0	0	1	0
38	Q	51	0	0	2	0
38	R	78	0	0	3	0
38	S	33	0	0	2	0
38	T	37	0	0	2	0
38	U	25	0	0	3	0
38	V	11	0	0	0	0

Continued on next page...

Continued from previous page...

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1937) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.44
30:0:1160:G:C5'	30:0:1161:A:H5'	1.81	1.10
31:9:56:A:H2'	31:9:57:A:H5"	1.33	1.08
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07
30:0:871:G:C8	30:0:871:G:H5'	1.87	1.07
14:N:37:ARG:NH1	31:9:6:C:H5"	1.71	1.05
30:0:1160:G:H5'	30:0:1161:A:C5'	1.88	1.03
30:0:1160:G:H5'	30:0:1161:A:H5'	1.02	1.02
30:0:381:G:H5"	38:0:4345:HOH:O	1.58	1.02
30:0:2812:A:H2	30:0:2814:A:H62	1.03	1.02
13:M:171:ARG:HD3	30:0:156:C:H5"	1.40	1.00
10:J:82:THR:HG23	30:0:1242:A:H5'	1.44	1.00
30:0:2717:C:C2'	30:0:2718:C:H5"	1.92	0.99
11:K:10:GLN:H	11:K:10:GLN:HE21	1.06	0.99
31:9:76:G:H3'	31:9:77:A:H5"	1.42	0.99
30:0:182:G:H5'	38:0:5188:HOH:O	1.63	0.98
30:0:871:G:H8	30:0:871:G:H5'	1.23	0.98
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.44	0.98
30:0:1666:C:O2'	30:0:1667:A:H5"	1.61	0.98
30:0:1118:A:H3'	30:0:1118:A:H8	1.29	0.97
30:0:2717:C:H2'	30:0:2718:C:H5"	1.46	0.97
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.47	0.96
30:0:1474:C:H6	30:0:1474:C:H5'	1.29	0.96
15:O:3:THR:HG22	30:0:656:G:H5'	1.46	0.96
30:0:1243:C:H3'	38:0:4869:HOH:O	1.65	0.95
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.12	0.94
30:0:1187:U:HO2'	30:0:1189:A:H2	1.07	0.94
3:C:236:THR:HG22	3:C:239:ALA:H	1.31	0.94
30:0:282:C:O2'	30:0:283:U:H5'	1.68	0.93

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:115:SER:H	16:P:118:GLN:NE2	1.77	0.80
30:0:1741:U:H5'	30:0:1742:A:OP1	1.82	0.80
30:0:1119:G:N2	30:0:1246:A:C2	2.49	0.79
30:0:2533:C:C6	30:0:2533:C:H5'	2.15	0.79
3:C:139:VAL:HG13	38:C:8641:HOH:O	1.82	0.79
15:O:3:THR:CG2	30:0:656:G:H5'	2.11	0.79
30:0:541:C:H2'	30:0:542:A:C5'	2.12	0.79
30:0:2851:G:O2'	30:0:2852:A:H5'	1.83	0.79
20:T:9:LYS:HE3	20:T:13:ARG:NH1	1.98	0.79
30:0:2896:A:H5"	38:0:6132:HOH:O	1.81	0.78
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.65	0.78
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.48	0.78
30:0:2827:A:H2'	30:0:2828:G:O4'	1.83	0.78
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.13	0.78
35:0:8813:CL:CL	38:0:4714:HOH:O	2.39	0.78
30:0:1634:G:H3'	38:0:3915:HOH:O	1.84	0.77
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.49	0.77
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.33	0.77
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.99	0.77
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.67	0.77
30:0:2769:C:O2'	30:0:2770:G:H5'	1.85	0.77
30:0:1666:C:H2'	30:0:1667:A:C5'	2.14	0.77
13:M:164:THR:HG22	13:M:167:GLY:H	1.50	0.77
22:V:50:ARG:HH12	30:0:56:G:H5"	1.48	0.76
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.50	0.76
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.76
30:0:1209:C:H2'	30:0:1210:G:H8	1.50	0.76
5:E:143:GLN:NE2	30:0:2779:G:H21	1.82	0.76
30:0:2908:A:H2'	30:0:2909:G:O4'	1.85	0.76
30:0:282:C:H1'	30:0:368:C:H42	1.50	0.76
30:0:558:C:H2'	30:0:559:U:C5'	2.15	0.76
31:9:2:U:OP2	31:9:3:A:H5'	1.86	0.76
30:0:1080:C:H4'	30:0:1081:A:OP1	1.85	0.76
3:C:174:ILE:HD11	30:0:338:C:H4'	1.66	0.76
30:0:2768:A:O2'	30:0:2769:C:H5'	1.86	0.76
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.68	0.76
30:0:2004:U:H4'	38:0:5338:HOH:O	1.86	0.76
30:0:31:C:H4'	38:0:7463:HOH:O	1.87	0.75
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.68	0.75
30:0:2637:A:H5'	38:0:4961:HOH:O	1.85	0.75
30:0:2717:C:O2'	30:0:2718:C:H5"	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:283:U:H5	30:0:284:C:C4	2.05	0.74
30:0:2239:C:H2'	30:0:2240:U:H6	1.52	0.74
30:0:1973:A:H5'	30:0:1973:A:H8	1.52	0.74
30:0:603:A:H5"	30:0:604:G:OP1	1.87	0.74
28:2:41:HIS:HD2	28:2:44:ARG:H	1.35	0.74
30:0:2851:G:C2'	30:0:2852:A:H5'	2.17	0.74
30:0:2748:G:H5'	38:0:7579:HOH:O	1.85	0.74
30:0:179:C:H5"	38:0:9320:HOH:O	1.86	0.74
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.69	0.74
30:0:1118:A:C8	30:0:1118:A:C3'	2.69	0.74
30:0:2559:C:H4'	38:0:7294:HOH:O	1.86	0.74
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.69	0.74
14:N:113:SER:HB2	38:N:8854:HOH:O	1.87	0.74
31:9:14:G:H5'	31:9:14:G:C8	2.23	0.74
30:0:272:A:H5'	30:0:273:G:OP2	1.88	0.74
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.69	0.73
30:0:1942:A:H3'	38:0:7386:HOH:O	1.88	0.73
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.69	0.73
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.71	0.73
30:0:1180:U:H2'	30:0:1181:A:O4'	1.89	0.73
16:P:115:SER:N	16:P:118:GLN:HE21	1.79	0.73
30:0:1183:C:H42	30:0:1184:C:H41	1.35	0.73
30:0:10:U:C6	30:0:10:U:H3'	2.23	0.73
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.88	0.73
30:0:2717:C:H2'	30:0:2718:C:C5'	2.19	0.73
11:K:10:GLN:H	11:K:10:GLN:NE2	1.83	0.72
30:0:1205:U:H2'	30:0:1206:U:H5"	1.70	0.72
30:0:338:C:H5"	38:0:3821:HOH:O	1.89	0.72
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.71	0.72
31:9:49:G:O2'	31:9:50:G:H5'	1.88	0.72
30:0:2256:G:O2'	30:0:2257:G:H5'	1.88	0.72
30:0:1279:U:O2	30:0:1279:U:H2'	1.88	0.72
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.87	0.72
18:R:39:THR:HG22	18:R:42:GLU:H	1.53	0.72
30:0:2420:G:O2'	30:0:2421:G:H5'	1.90	0.72
30:0:1666:C:H2'	30:0:1667:A:H5'	1.72	0.71
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.70	0.71
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.73	0.71
30:0:1666:C:C2'	30:0:1667:A:C5'	2.68	0.71
30:0:544:G:C2'	30:0:545:G:H5"	2.20	0.71
30:0:558:C:H2'	30:0:559:U:H5"	1.70	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1632:A:C2'	30:0:1633:C:H5'	2.19	0.71
18:R:9:ASP:O	18:R:13:THR:HB	1.89	0.71
30:0:2679:G:H2'	30:0:2681:A:OP2	1.91	0.71
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.72	0.71
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.37	0.71
30:0:2010:A:H2'	38:0:5990:HOH:O	1.90	0.71
30:0:2578:G:H5'	30:0:2578:G:H8	1.54	0.71
30:0:1964:U:O2	30:0:1964:U:H2'	1.91	0.71
31:9:92:G:H2'	31:9:93:A:C8	2.26	0.71
30:0:1157:C:H2'	30:0:1158:G:H8	1.56	0.70
30:0:2635:A:O2'	30:0:2636:C:H5'	1.90	0.70
30:0:2769:C:H2'	30:0:2770:G:O4'	1.91	0.70
31:9:39:U:H1'	31:9:44:A:H61	1.55	0.70
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.27	0.70
30:0:1527:A:H1'	30:0:1528:A:C8	2.27	0.70
3:C:174:ILE:CD1	30:0:338:C:H4'	2.21	0.70
30:0:1174:A:C5	30:0:1201:C:H4'	2.26	0.70
30:0:1701:A:H4'	30:0:1702:U:C5'	2.20	0.70
30:0:31:C:H2'	38:0:7726:HOH:O	1.89	0.70
22:V:1:THR:HG23	22:V:2:VAL:H	1.56	0.70
30:0:2852:A:H5"	38:0:5264:HOH:O	1.91	0.70
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.05	0.69
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.07	0.69
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.74	0.69
30:0:1165:G:O2'	30:0:1174:A:H1'	1.92	0.69
30:0:308:U:H5'	30:0:309:C:OP1	1.91	0.69
12:L:148:GLU:HA	38:L:8870:HOH:O	1.92	0.69
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.73	0.69
30:0:2507:G:H2'	30:0:2510:C:H42	1.57	0.69
31:9:29:C:H2'	31:9:30:C:H5'	1.73	0.69
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.92	0.69
3:C:1:MET:HG2	3:C:2:GLN:H	1.55	0.69
30:0:814:G:H4'	38:0:3155:HOH:O	1.91	0.69
30:0:1603:A:C5'	30:0:1605:G:H5'	2.22	0.69
31:9:1:U:H4'	31:9:3:A:OP1	1.92	0.69
30:0:545:G:C8	30:0:545:G:H5'	2.25	0.69
12:L:133:VAL:HA	38:L:8871:HOH:O	1.92	0.69
2:B:217:ARG:HG3	2:B:257:THR:HB	1.75	0.68
30:0:281:U:H2'	30:0:282:C:O4'	1.94	0.68
31:9:7:G:H5'	38:9:9099:HOH:O	1.93	0.68
38:Y:8852:HOH:O	35:0:8817:CL:CL	2.49	0.68

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:HIS:CD2	1:A:201:PHE:H	2.15	0.63
30:0:1187:U:H2'	38:0:6939:HOH:O	1.98	0.63
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.81	0.63
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.79	0.63
29:3:65:THR:HG23	29:3:67:LEU:HG	1.79	0.63
30:0:2533:C:H6	30:0:2533:C:C5'	2.09	0.63
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.64	0.63
18:R:128:ARG:NH2	30:0:2054:A:N3	2.46	0.63
24:X:71:ARG:HD3	38:X:2171:HOH:O	1.98	0.63
21:U:46:ALA:O	21:U:52:THR:HG21	1.98	0.63
30:0:1878:G:O2'	30:0:1879:U:C6	2.49	0.63
30:0:1278:A:H4'	30:0:1279:U:C4	2.33	0.63
13:M:27:ARG:NH2	13:M:44:THR:HG23	2.13	0.63
30:0:1120:U:H6	30:0:1120:U:H5"	1.63	0.63
31:9:75:G:H1	31:9:106:U:H3	1.47	0.63
30:0:2524:G:H21	30:0:2526:C:N4	1.96	0.63
9:I:110:ASP:O	30:0:1163:G:H5'	1.99	0.63
30:0:317:A:H4'	38:0:3791:HOH:O	1.98	0.63
30:0:1835:U:C5	30:0:1840:A:N7	2.60	0.63
30:0:2509:A:H2'	30:0:2510:C:O4'	1.99	0.63
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.81	0.63
30:0:2649:A:H5'	30:0:2649:A:H8	1.64	0.63
2:B:162:MET:CE	2:B:308:LEU:HD21	2.27	0.63
2:B:264:GLU:HG3	2:B:302:PRO:HD3	1.79	0.63
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.64	0.63
31:9:54:A:O2'	31:9:55:U:H5'	1.98	0.62
30:0:2604:A:H5'	38:0:5822:HOH:O	1.99	0.62
30:0:2250:G:C2	30:0:2251:G:H1'	2.34	0.62
30:0:2256:G:H2'	30:0:2257:G:H5'	1.81	0.62
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.96	0.62
30:0:853:C:H3'	38:0:4580:HOH:O	2.00	0.62
23:W:13:MET:HE1	23:W:18:GLN:HA	1.81	0.62
15:O:73:ASP:HA	15:O:92:VAL:O	2.00	0.62
30:0:2421:G:H1'	38:0:7060:HOH:O	1.98	0.62
13:M:178:LYS:HB2	38:0:6916:HOH:O	1.99	0.62
8:H:168:VAL:HG13	38:H:211:HOH:O	1.98	0.62
30:0:1701:A:H5"	30:0:1702:U:H3'	1.82	0.62
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.81	0.62
30:0:1198:U:H1'	30:0:1201:C:H5	1.63	0.62
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.81	0.62
31:9:2:U:P	31:9:3:A:H5'	2.40	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:20:ARG:HG2	30:0:111:C:O2'	2.00	0.62
30:0:567:U:H5"	38:0:6435:HOH:O	1.99	0.62
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.82	0.62
27:1:16:HIS:HD2	30:0:470:U:O2'	1.83	0.62
7:G:64:ASN:N	7:G:64:ASN:HD22	1.96	0.62
11:K:10:GLN:N	11:K:10:GLN:HE21	1.87	0.62
30:0:1166:A:H61	30:0:1180:U:H3	1.46	0.62
30:0:960:G:H3'	30:0:960:G:N3	2.14	0.62
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.80	0.62
29:3:48:ASN:HD21	30:0:2468:A:H61	1.47	0.62
30:0:2404:G:H5"	38:0:5241:HOH:O	2.00	0.62
30:0:2670:G:O2'	30:0:2671:U:H5'	1.99	0.62
6:F:91:VAL:HG12	6:F:92:GLY:N	2.14	0.61
30:0:1314:U:H2'	38:0:5904:HOH:O	2.00	0.61
30:0:1170:U:H2'	30:0:1172:G:OP2	2.00	0.61
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.82	0.61
25:Y:216:ARG:HD2	38:Y:8865:HOH:O	2.00	0.61
11:K:32:ILE:HD11	11:K:56:SER:HB2	1.82	0.61
30:0:848:C:H5'	38:0:7311:HOH:O	2.00	0.61
30:0:958:G:O2'	30:0:959:C:H5'	2.00	0.61
30:0:506:G:H22	30:0:509:A:H5"	1.63	0.61
31:9:20:G:O2'	31:9:21:G:H5'	2.00	0.61
30:0:2613:G:O2'	30:0:2614:C:H5'	2.00	0.61
13:M:157:ASP:HB3	13:M:160:PHE:HD1	1.65	0.61
30:0:2083:A:H3'	38:0:7616:HOH:O	1.99	0.61
2:B:162:MET:HG3	2:B:310:ARG:HD3	1.83	0.61
23:W:88:THR:HG22	23:W:89:ASP:H	1.65	0.61
14:N:4:PRO:HG3	31:9:69:U:OP1	2.00	0.61
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.82	0.61
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.81	0.61
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.83	0.61
30:0:1679:C:H5'	38:0:9334:HOH:O	2.00	0.61
31:9:64:C:C2'	31:9:65:A:H5'	2.30	0.61
30:0:1759:A:N3	30:0:1818:C:H2'	2.16	0.61
22:V:1:THR:HB	30:0:93:C:H5"	1.82	0.61
30:0:1948:G:H2'	30:0:1949:G:O4'	2.01	0.61
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.83	0.61
30:0:1641:A:H2'	30:0:1642:A:H5'	1.83	0.61
30:0:1506:U:H6	30:0:1506:U:H5'	1.66	0.61
30:0:2787:C:H5	38:0:4664:HOH:O	1.83	0.61
27:1:10:LYS:HG3	38:1:2979:HOH:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:558:C:H2'	30:0:559:U:H5'	1.82	0.61
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.16	0.61
3:C:236:THR:HG21	38:C:8569:HOH:O	2.00	0.61
3:C:16:VAL:HG12	3:C:17:ASP:H	1.66	0.61
14:N:141:ARG:HH21	31:9:48:C:H4'	1.66	0.60
1:A:36:ASP:CB	1:A:85:SER:H	2.14	0.60
30:0:2505:G:C2'	30:0:2506:A:H5'	2.31	0.60
23:W:84:VAL:HG12	38:W:6679:HOH:O	2.01	0.60
30:0:2637:A:H4'	38:0:6094:HOH:O	2.00	0.60
14:N:40:ASN:ND2	31:9:28:U:H5"	2.16	0.60
30:0:936:C:H5	38:0:5991:HOH:O	1.82	0.60
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.82	0.60
30:0:1515:A:H2'	30:0:1516:U:C6	2.37	0.60
30:0:542:A:H5'	30:0:542:A:C8	2.28	0.60
30:0:236:A:H4'	30:0:237:G:OP1	2.01	0.60
38:B:9109:HOH:O	30:0:2672:C:H1'	2.02	0.60
23:W:88:THR:HG22	23:W:89:ASP:N	2.17	0.60
30:0:836:G:H5"	38:0:9288:HOH:O	1.99	0.60
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.84	0.60
11:K:27:ARG:HD2	38:K:4747:HOH:O	2.01	0.60
4:D:57:THR:HG23	4:D:63:ILE:HA	1.82	0.60
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.84	0.60
30:0:1080:C:O5'	30:0:1080:C:H6	1.85	0.60
10:J:41:ALA:HB3	38:J:5907:HOH:O	2.00	0.60
30:0:702:G:O2'	30:0:703:G:H5'	2.02	0.60
30:0:2563:U:H2'	30:0:2565:C:O5'	2.01	0.60
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.84	0.60
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	1.84	0.60
31:9:3:A:N6	31:9:22:G:H1'	2.16	0.60
30:0:2089:A:O2'	30:0:2090:G:H5'	2.02	0.60
30:0:2419:U:H5"	30:0:2420:G:H5'	1.83	0.59
8:H:102:LYS:HD3	8:H:122:LYS:HD3	1.83	0.59
6:F:101:ALA:HA	38:F:5413:HOH:O	2.02	0.59
30:0:368:C:H2'	30:0:369:G:H5'	1.84	0.59
9:I:87:PRO:HB3	38:I:6825:HOH:O	2.02	0.59
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.32	0.59
30:0:567:U:H5"	38:0:5320:HOH:O	2.02	0.59
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.83	0.59
13:M:80:GLY:O	13:M:81:ARG:HD3	2.01	0.59
30:0:271:C:H41	30:0:378:A:H2	1.47	0.59
30:0:2329:C:O2'	30:0:2330:U:H5'	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1132:A:N6	30:0:1229:C:H2'	2.17	0.59
30:0:1790:C:H2'	30:0:1791:U:H6	1.67	0.59
2:B:254:GLN:HG3	38:0:9714:HOH:O	2.01	0.59
8:H:49:GLN:NE2	8:H:140:TYR:HE2	1.95	0.59
30:0:2237:G:H1'	38:0:4887:HOH:O	2.02	0.59
38:Z:8706:HOH:O	30:0:1886:A:H4'	2.03	0.59
8:H:29:SER:HA	8:H:62:HIS:HD2	1.68	0.59
30:0:2718:C:H6	30:0:2718:C:H5'	1.68	0.59
3:C:236:THR:CG2	3:C:239:ALA:H	2.11	0.59
18:R:39:THR:HG23	18:R:107:GLU:O	2.02	0.59
9:I:108:HIS:H	9:I:109:PRO:HD2	1.66	0.59
30:0:119:A:H2'	30:0:120:A:H5"	1.83	0.59
30:0:1595:G:O2'	30:0:1596:U:H5'	2.03	0.59
8:H:174:LEU:HA	38:H:222:HOH:O	2.02	0.59
30:0:1377:C:H6	30:0:1377:C:H5'	1.68	0.59
1:A:33:GLU:CD	1:A:33:GLU:H	2.04	0.59
30:0:2756:U:H3	30:0:2896:A:H2	1.43	0.59
30:0:308:U:C4	30:0:342:C:H1'	2.38	0.59
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.32	0.59
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.37	0.59
30:0:2344:G:N3	30:0:2344:G:H2'	2.17	0.59
23:W:125:HIS:CD2	23:W:127:GLY:H	2.21	0.59
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.85	0.59
7:G:16:LYS:O	7:G:20:VAL:HG23	2.03	0.59
1:A:48:ASP:HB3	38:A:9060:HOH:O	2.03	0.59
31:9:64:C:H2'	31:9:65:A:H5'	1.84	0.59
7:G:12:ILE:HG23	38:0:5490:HOH:O	2.03	0.59
30:0:2812:A:H2	30:0:2814:A:N6	1.87	0.58
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.04	0.58
31:9:24:U:H3'	31:9:25:G:C5'	2.32	0.58
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.85	0.58
2:B:248:ARG:O	2:B:251:VAL:HG13	2.03	0.58
38:C:8655:HOH:O	30:0:2100:A:H5'	2.03	0.58
30:0:468:U:H3'	38:0:7607:HOH:O	2.03	0.58
30:0:2534:C:H1'	38:0:3513:HOH:O	2.01	0.58
1:A:171:LYS:HB2	30:0:820:G:C6	2.37	0.58
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.67	0.58
28:2:38:LYS:HE3	38:0:4254:HOH:O	2.01	0.58
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.85	0.58
30:0:1603:A:H5'	30:0:1605:G:C4'	2.33	0.58
30:0:1972:U:H2'	30:0:1973:A:C5'	2.32	0.58

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:68:HIS:O	30:0:2842:G:H5'	2.05	0.57
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.86	0.57
12:L:41:HIS:HD2	30:0:926:A:O2'	1.88	0.57
30:0:541:C:H2'	30:0:542:A:H5'	1.87	0.57
30:0:396:U:O2'	30:0:418:C:H4'	2.04	0.57
30:0:1942:A:H5'	38:0:7386:HOH:O	2.05	0.57
30:0:1768:C:H2'	30:0:1769:C:O4'	2.05	0.57
31:9:49:G:H5"	38:9:9090:HOH:O	2.05	0.56
30:0:1477:C:O2'	30:0:1478:U:H5'	2.05	0.56
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.87	0.56
10:J:74:ARG:NH1	10:J:144:THR:HG21	2.20	0.56
18:R:117:HIS:HD2	30:0:20:G:H21	1.53	0.56
30:0:283:U:C5	30:0:284:C:N3	2.73	0.56
30:0:2269:C:H2'	30:0:2270:G:H5'	1.86	0.56
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.87	0.56
30:0:2320:U:H4'	30:0:2321:A:O4'	2.04	0.56
30:0:366:U:H2'	30:0:367:G:O4'	2.05	0.56
31:9:1:U:O3'	31:9:3:A:C5'	2.53	0.56
30:0:2005:G:H3'	30:0:2005:G:OP2	2.06	0.56
30:0:485:A:N3	30:0:487:G:H5"	2.20	0.56
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.87	0.56
30:0:2668:G:H2'	30:0:2669:U:C6	2.40	0.56
30:0:542:A:H2'	30:0:543:G:O4'	2.05	0.56
30:0:255:A:H2'	30:0:256:C:H6	1.71	0.56
31:9:12:C:H5'	31:9:70:U:O4'	2.04	0.56
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.86	0.56
2:B:71:VAL:HG21	2:B:296:LEU:HB3	1.87	0.56
30:0:319:A:H4'	30:0:338:C:C4	2.40	0.56
8:H:19:ARG:HH12	30:0:1008:C:H5"	1.70	0.56
23:W:44:MET:CE	30:0:944:G:H21	2.19	0.56
12:L:134:GLU:HG3	38:L:8854:HOH:O	2.06	0.56
30:0:1206:U:C5'	30:0:1206:U:H6	2.15	0.56
10:J:74:ARG:HH12	10:J:144:THR:HG21	1.71	0.56
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.71	0.56
3:C:63:SER:OG	30:0:2101:A:H2'	2.05	0.56
31:9:76:G:C3'	31:9:77:A:H5"	2.28	0.56
31:9:114:G:H2'	31:9:115:C:C6	2.41	0.56
30:0:363:C:H2'	30:0:364:U:H6	1.69	0.56
30:0:2880:A:H2'	30:0:2881:C:H5'	1.88	0.56
2:B:145:HIS:HD2	2:B:146:THR:O	1.89	0.56
12:L:143:THR:HG22	12:L:144:ASP:H	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2472:C:O2'	30:0:2634:G:H4'	2.05	0.56
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.79	0.56
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.41	0.56
30:0:2002:C:H2'	30:0:2003:U:H5'	1.87	0.56
29:3:70:ARG:HB3	38:3:9064:HOH:O	2.06	0.56
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.41	0.56
2:B:17:LYS:O	2:B:260:HIS:HD2	1.88	0.56
30:0:1213:C:O2'	30:0:1214:G:H5'	2.06	0.56
27:1:9:GLY:HA2	30:0:1687:C:O2	2.05	0.56
30:0:2064:U:H5'	30:0:2652:U:H4'	1.87	0.56
27:1:28:HIS:HE1	30:0:776:A:OP1	1.89	0.56
7:G:20:VAL:O	7:G:24:VAL:HG23	2.06	0.56
30:0:583:C:H2'	30:0:584:U:H6	1.70	0.56
30:0:1209:C:H2'	30:0:1210:G:C8	2.36	0.55
30:0:834:G:H4'	30:0:835:U:OP2	2.05	0.55
14:N:164:ASP:CG	14:N:167:ASP:HA	2.26	0.55
30:0:681:G:N3	30:0:681:G:H5'	2.21	0.55
30:0:2316:G:H4'	38:0:6125:HOH:O	2.05	0.55
30:0:1766:U:O2	30:0:1778:A:H5'	2.06	0.55
30:0:281:U:O2'	30:0:282:C:H5'	2.06	0.55
30:0:283:U:H5	30:0:284:C:N3	2.04	0.55
30:0:2269:C:C2'	30:0:2270:G:H5'	2.36	0.55
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.89	0.55
30:0:1904:A:H2'	30:0:1905:U:O4'	2.05	0.55
30:0:1834:C:H2'	30:0:1840:A:N6	2.20	0.55
30:0:236:A:C4'	30:0:237:G:H5'	2.36	0.55
30:0:65:C:O2'	30:0:66:G:H5'	2.06	0.55
30:0:1676:G:O2'	30:0:1677:U:H5'	2.06	0.55
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.07	0.55
30:0:1973:A:H5'	30:0:1973:A:C8	2.39	0.55
2:B:125:GLU:O	2:B:129:ARG:HG3	2.06	0.55
30:0:2756:U:N3	30:0:2896:A:C2	2.71	0.55
31:9:22:G:H5'	31:9:23:U:OP1	2.06	0.55
30:0:2748:G:H1'	38:0:7936:HOH:O	2.05	0.55
14:N:80:SER:HB2	38:N:8833:HOH:O	2.07	0.55
30:0:249:G:H2'	30:0:250:C:H6	1.71	0.55
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	1.89	0.55
12:L:18:HIS:HD2	30:0:902:G:N7	2.05	0.55
30:0:1592:G:H2'	30:0:1593:C:C6	2.42	0.55
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.89	0.55
5:E:11:VAL:HG12	5:E:12:ASP:N	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:37:ARG:HD2	30:0:656:G:OP2	2.07	0.55
30:0:282:C:C2'	30:0:283:U:H5'	2.35	0.55
30:0:2748:G:H2'	38:0:7579:HOH:O	2.06	0.55
31:9:49:G:C2'	31:9:50:G:H5'	2.37	0.55
26:Z:40:ALA:HA	30:0:1773:G:C8	2.41	0.55
14:N:37:ARG:NH1	31:9:6:C:OP1	2.39	0.55
30:0:1200:A:H3'	38:0:5786:HOH:O	2.06	0.55
12:L:41:HIS:CD2	30:0:926:A:O2'	2.60	0.55
30:0:2768:A:H5"	38:0:4453:HOH:O	2.07	0.55
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.89	0.55
15:O:35:LYS:HD3	38:0:4645:HOH:O	2.06	0.55
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.37	0.54
13:M:163:LEU:HD21	30:0:188:C:H5"	1.89	0.54
30:0:1157:C:H2'	30:0:1158:G:C8	2.40	0.54
30:0:2064:U:H5'	30:0:2652:U:O3'	2.08	0.54
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.07	0.54
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.05	0.54
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.89	0.54
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.42	0.54
30:0:1878:G:O2'	30:0:1879:U:P	2.66	0.54
14:N:110:THR:HB	14:N:113:SER:OG	2.08	0.54
30:0:1165:G:O2'	30:0:1174:A:C1'	2.54	0.54
30:0:1819:G:H2'	30:0:1820:G:C4'	2.38	0.54
30:0:1681:G:H5"	30:0:1682:A:H5'	1.88	0.54
38:I:1549:HOH:O	30:0:1180:U:H1'	2.07	0.54
31:9:47:A:C2	31:9:48:C:C2	2.94	0.54
2:B:177:HIS:O	2:B:181:ILE:HG13	2.07	0.54
30:0:350:G:H1'	38:0:5705:HOH:O	2.06	0.54
5:E:132:THR:HB	38:E:2227:HOH:O	2.07	0.54
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.90	0.54
31:9:23:U:O2'	31:9:24:U:H4'	2.07	0.54
30:0:363:C:O2'	30:0:364:U:H5'	2.07	0.54
18:R:99:ALA:HB1	18:R:109:MET:CE	2.37	0.54
29:3:73:GLU:HB3	38:3:9053:HOH:O	2.08	0.54
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.89	0.54
8:H:69:ARG:HD3	38:H:231:HOH:O	2.07	0.54
30:0:1947:G:H2'	30:0:1948:G:H8	1.73	0.54
30:0:661:G:C5	30:0:686:A:C2	2.96	0.54
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.08	0.54
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.73	0.54
31:9:3:A:H2	31:9:21:G:N3	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1755:A:H2'	30:0:1756:G:O4'	2.07	0.54
30:0:1594:C:O2'	30:0:1607:A:H4'	2.08	0.54
30:0:1559:A:H4'	38:0:5895:HOH:O	2.07	0.54
30:0:1842:A:C4	30:0:1979:G:C6	2.95	0.54
9:I:126:THR:O	9:I:130:LEU:HG	2.08	0.54
23:W:130:HIS:O	23:W:136:GLY:HA3	2.08	0.54
30:0:1193:A:H2	30:0:1194:A:N6	2.06	0.54
30:0:2135:A:O2'	30:0:2136:G:H5'	2.06	0.54
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.89	0.54
30:0:2505:G:H2'	30:0:2506:A:H5'	1.89	0.54
30:0:2507:G:H2'	30:0:2510:C:N4	2.23	0.54
4:D:138:GLY:HA2	31:9:29:C:O3'	2.08	0.54
30:0:2415:A:H2'	30:0:2416:G:H5'	1.88	0.54
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.54
30:0:2781:U:C2'	30:0:2782:G:H5'	2.37	0.54
30:0:877:G:C5'	30:0:878:G:OP1	2.53	0.54
30:0:1878:G:O2'	30:0:1879:U:H6	1.89	0.54
16:P:58:SER:HB3	38:0:5659:HOH:O	2.08	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.08	0.54
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.90	0.54
30:0:10:U:O4	30:0:531:G:H2'	2.08	0.54
30:0:1535:G:H2'	30:0:1536:C:C6	2.43	0.54
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.73	0.53
14:N:160:SER:HB2	31:9:51:A:H5'	1.90	0.53
30:0:2073:G:OP2	30:0:2490:A:H5'	2.08	0.53
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.90	0.53
31:9:49:G:H2'	31:9:50:G:O4'	2.09	0.53
30:0:407:A:H3'	38:0:4486:HOH:O	2.08	0.53
2:B:198:GLU:HA	38:B:9133:HOH:O	2.07	0.53
30:0:2502:C:H2'	30:0:2503:A:C5'	2.37	0.53
10:J:19:MET:CE	10:J:132:LEU:HD11	2.39	0.53
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.38	0.53
30:0:1130:U:H2'	30:0:1131:G:O4'	2.08	0.53
30:0:24:G:N2	30:0:518:G:H1'	2.23	0.53
30:0:2371:G:H5'	38:0:5041:HOH:O	2.08	0.53
20:T:2:LYS:HG2	30:0:447:A:OP1	2.08	0.53
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.09	0.53
30:0:2756:U:N3	30:0:2896:A:H2	2.06	0.53
30:0:1819:G:H2'	30:0:1820:G:C5'	2.38	0.53
17:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.08	0.53
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1850:U:H2'	30:0:1851:G:H8	1.73	0.53
30:0:953:G:H4'	30:0:954:U:OP1	2.08	0.53
5:E:137:ASP:O	5:E:141:VAL:HG23	2.08	0.53
30:0:2783:A:H2'	30:0:2784:A:C8	2.44	0.53
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.09	0.53
2:B:294:TYR:HE2	38:B:9124:HOH:O	1.89	0.53
30:0:368:C:C2'	30:0:369:G:H5'	2.39	0.53
31:9:2:U:H4'	38:9:9103:HOH:O	2.08	0.53
30:0:1787:C:H4'	30:0:2883:A:O4'	2.08	0.53
30:0:138:U:OP2	30:0:139:C:H5	1.91	0.53
30:0:1333:U:H2'	30:0:1334:C:C6	2.44	0.53
30:0:1523:G:C6	30:0:1524:U:C4	2.96	0.53
21:U:17:THR:HG22	21:U:18:GLY:N	2.24	0.53
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.91	0.53
30:0:67:A:H5"	30:0:69:A:C8	2.44	0.53
30:0:2249:G:C2	30:0:2253:G:C6	2.96	0.53
31:9:39:U:O2'	31:9:42:C:C5	2.61	0.53
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.90	0.53
30:0:947:U:H2'	30:0:948:G:H8	1.72	0.53
21:U:14:GLU:O	21:U:17:THR:HB	2.08	0.53
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.90	0.53
30:0:1206:U:H2'	30:0:1207:A:O4'	2.09	0.53
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.88	0.53
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.39	0.53
30:0:2597:U:H2'	30:0:2598:U:H5'	1.90	0.53
30:0:123:U:H5'	38:0:6694:HOH:O	2.09	0.53
30:0:1556:G:O2'	30:0:1557:G:H5'	2.09	0.53
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.90	0.53
30:0:960:G:C3'	30:0:960:G:N3	2.72	0.53
3:C:5:ILE:HD11	3:C:16:VAL:CG2	2.39	0.53
13:M:57:LYS:HE2	13:M:140:ALA:O	2.09	0.53
30:0:2897:C:O2'	30:0:2898:G:H5'	2.09	0.53
30:0:1206:U:C6	30:0:1206:U:H5'	2.32	0.53
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.23	0.53
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.23	0.53
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.39	0.53
30:0:876:A:N3	30:0:876:A:H2'	2.23	0.53
23:W:80:ASP:O	23:W:84:VAL:HG23	2.09	0.52
30:0:2781:U:O2'	30:0:2782:G:H5'	2.07	0.52
30:0:1524:U:OP1	30:0:1524:U:H4'	2.09	0.52
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.91	0.52
30:0:1702:U:H1'	38:0:5805:HOH:O	2.08	0.52
30:0:241:A:C2	30:0:378:A:H4'	2.44	0.52
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.90	0.52
12:L:4:LYS:HE2	30:0:645:U:OP2	2.09	0.52
30:0:2314:G:C2'	30:0:2315:C:H5'	2.39	0.52
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.12	0.52
18:R:150:PRO:CG	18:R:150:PRO:CB	2.86	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.90	0.52
30:0:1174:A:C6	30:0:1201:C:H4'	2.45	0.52
30:0:1377:C:H5'	30:0:1377:C:C6	2.45	0.52
13:M:30:GLU:O	13:M:34:GLU:HG3	2.10	0.52
4:D:159:PRO:O	4:D:163:VAL:HG23	2.09	0.52
30:0:2587:OMU:H2'	30:0:2589:U:H5"	1.92	0.52
4:D:50:VAL:HG13	31:9:41:C:O4'	2.10	0.52
17:Q:25:PRO:HB2	38:9:9082:HOH:O	2.10	0.52
30:0:113:A:OP2	30:0:114:A:H2'	2.09	0.52
19:S:43:GLU:HB3	38:S:8991:HOH:O	2.10	0.52
3:C:153:VAL:O	3:C:157:LEU:HG	2.09	0.52
30:0:2478:U:O2'	30:0:2479:A:H5'	2.08	0.52
12:L:143:THR:HG22	12:L:144:ASP:N	2.25	0.52
28:2:39:ARG:HG2	38:2:3143:HOH:O	2.08	0.52
30:0:1135:G:H5'	38:0:5960:HOH:O	2.09	0.52
20:T:38:ARG:NH1	38:0:6725:HOH:O	2.42	0.52
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.45	0.52
30:0:2250:G:H2'	30:0:2251:G:O4'	2.09	0.52
30:0:602:A:O2'	30:0:605:C:H4'	2.09	0.52
30:0:2681:A:H4'	30:0:2682:C:C5'	2.39	0.52
4:D:138:GLY:N	38:D:7597:HOH:O	2.42	0.52
1:A:36:ASP:HB2	1:A:84:VAL:N	2.25	0.52
30:0:2105:C:H2'	30:0:2106:C:C6	2.44	0.52
8:H:48:VAL:HA	8:H:170:ARG:O	2.10	0.52
30:0:2664:A:H8	30:0:2664:A:OP1	1.93	0.52
30:0:2509:A:OP2	30:0:2510:C:H5	1.93	0.52
30:0:1921:A:C6	30:0:1922:A:C2	2.98	0.52
30:0:968:G:O2'	30:0:969:G:H5'	2.10	0.52
30:0:1444:G:O2'	30:0:1445:G:H5'	2.09	0.52
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.91	0.52
30:0:1930:A:H2'	30:0:1931:A:C8	2.45	0.52
30:0:2237:G:O2'	30:0:2238:A:C8	2.62	0.52
30:0:1279:U:C2'	30:0:1279:U:O2	2.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1289:C:O2'	30:0:1290:G:H5'	2.10	0.52
30:0:704:C:H2'	30:0:705:C:H6	1.75	0.52
30:0:1805:G:O2'	30:0:1806:G:H5'	2.10	0.52
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.10	0.52
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.10	0.52
30:0:12:U:H2'	30:0:13:G:H5'	1.91	0.52
30:0:2878:U:H2'	30:0:2879:A:O4'	2.10	0.52
30:0:1188:A:C6	30:0:1189:A:C6	2.99	0.51
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.92	0.51
31:9:24:U:H3'	31:9:25:G:H5'	1.91	0.51
23:W:64:THR:O	23:W:68:THR:HG22	2.10	0.51
30:0:1130:U:H5'	38:0:7710:HOH:O	2.10	0.51
30:0:200:C:H2'	38:0:3463:HOH:O	2.09	0.51
30:0:2531:U:O2'	30:0:2532:A:H5'	2.10	0.51
13:M:179:GLY:O	30:0:399:C:H5'	2.10	0.51
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.91	0.51
30:0:185:G:H4'	30:0:186:A:OP1	2.10	0.51
30:0:2250:G:N2	30:0:2251:G:H1'	2.25	0.51
30:0:2830:U:O2'	30:0:2831:C:H5'	2.09	0.51
22:V:12:THR:HG23	22:V:14:ALA:H	1.75	0.51
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.26	0.51
6:F:57:GLU:O	6:F:61:MET:HG3	2.10	0.51
2:B:148:PRO:HD2	38:B:9049:HOH:O	2.10	0.51
23:W:119:HIS:HD2	23:W:120:PRO:O	1.92	0.51
30:0:299:U:H5'	38:0:7375:HOH:O	2.09	0.51
23:W:24:LEU:O	23:W:26:ILE:HG22	2.10	0.51
3:C:145:GLU:HG3	38:C:8569:HOH:O	2.09	0.51
30:0:541:C:O2'	30:0:542:A:H5"	2.11	0.51
30:0:10:U:O4	30:0:532:A:OP2	2.28	0.51
31:9:39:U:O2'	31:9:42:C:H5	1.92	0.51
30:0:363:C:H2'	30:0:364:U:C6	2.46	0.51
30:0:1762:C:O2'	30:0:1763:C:H5'	2.10	0.51
30:0:285:A:H2'	30:0:286:U:O4'	2.10	0.51
30:0:2252:A:H2'	30:0:2253:G:H5'	1.92	0.51
31:9:1:U:C4'	31:9:3:A:OP1	2.59	0.51
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.92	0.51
30:0:228:C:C2'	30:0:229:G:H5'	2.41	0.51
2:B:211:THR:HG21	38:0:7492:HOH:O	2.11	0.51
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.41	0.51
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.92	0.51
30:0:2825:C:H4'	30:0:2826:G:O5'	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.93	0.51
30:0:958:G:H2'	30:0:959:C:C6	2.45	0.51
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.44	0.51
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.93	0.51
30:0:414:C:H5'	38:0:9667:HOH:O	2.11	0.51
30:0:1386:G:O2'	30:0:1387:G:H5'	2.11	0.51
30:0:69:A:H8	30:0:69:A:C5'	2.15	0.51
30:0:1205:U:O2'	30:0:1206:U:H5"	2.11	0.51
25:Y:189:ASN:HD22	25:Y:189:ASN:C	2.14	0.51
30:0:2421:G:H3'	30:0:2422:U:H5"	1.92	0.51
30:0:2781:U:H2'	30:0:2782:G:C5'	2.40	0.51
30:0:2826:G:C6	30:0:2913:A:N6	2.78	0.51
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.11	0.51
30:0:541:C:C2'	30:0:542:A:C5'	2.79	0.51
31:9:91:C:H2'	31:9:92:G:O4'	2.10	0.51
30:0:1398:G:O2'	30:0:1399:A:H5'	2.11	0.51
30:0:2241:C:O2'	30:0:2242:U:H5'	2.11	0.51
24:X:23:HIS:HD2	38:0:9973:HOH:O	1.93	0.51
30:0:790:A:H2'	30:0:791:A:O4'	2.10	0.51
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.79	0.51
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.59	0.51
30:0:282:C:O2'	30:0:283:U:C5'	2.50	0.51
2:B:256:GLN:HG2	38:B:9132:HOH:O	2.11	0.51
30:0:2781:U:H2'	30:0:2782:G:H5'	1.92	0.51
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.93	0.51
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.41	0.51
19:S:33:SER:O	19:S:37:VAL:HG23	2.11	0.51
12:L:14:GLY:O	30:0:1295:G:H5"	2.11	0.51
30:0:346:U:H4'	38:0:6884:HOH:O	2.11	0.51
30:0:2764:C:O2'	30:0:2765:C:H5'	2.10	0.51
30:0:2251:G:H2'	30:0:2252:A:H8	1.72	0.51
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.93	0.51
29:3:15:ASN:O	30:0:2408:A:H4'	2.11	0.51
30:0:952:G:N3	30:0:2302:A:H2'	2.26	0.51
25:Y:184:GLU:OE2	25:Y:204:ARG:HD2	2.11	0.51
2:B:41:PHE:HA	2:B:79:MET:HE2	1.92	0.51
30:0:1419:U:H2'	30:0:1685:A:C2	2.46	0.51
3:C:233:THR:HG22	3:C:234:VAL:N	2.26	0.51
30:0:120:A:H2'	30:0:120:A:N3	2.27	0.50
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.76	0.50
30:0:1186:C:N4	30:0:1187:U:C4	2.79	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:289:G:O2'	30:0:290:C:H5'	2.12	0.50
2:B:85:ARG:NH1	38:B:9109:HOH:O	2.44	0.50
30:0:249:G:H2'	30:0:250:C:C6	2.46	0.50
30:0:1167:G:H2'	30:0:1168:C:C6	2.46	0.50
30:0:683:G:O2'	30:0:684:G:H5'	2.11	0.50
22:V:56:ILE:O	22:V:60:GLN:HG3	2.11	0.50
30:0:383:A:H4'	38:0:5359:HOH:O	2.10	0.50
30:0:1183:C:O2	30:0:1183:C:H2'	2.10	0.50
30:0:1972:U:C2'	30:0:1973:A:H5"	2.41	0.50
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.94	0.50
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.45	0.50
30:0:1557:G:O2'	30:0:1558:C:H5'	2.11	0.50
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.94	0.50
30:0:1202:A:C2'	30:0:1203:G:H5'	2.40	0.50
30:0:1494:A:H1'	30:0:1495:C:C6	2.47	0.50
30:0:1183:C:H42	30:0:1184:C:N4	2.05	0.50
30:0:559:U:H6	30:0:559:U:C5'	2.20	0.50
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.27	0.50
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.12	0.50
22:V:44:GLY:O	22:V:48:GLU:HG2	2.12	0.50
15:O:39:THR:O	15:O:115:ARG:NH2	2.44	0.50
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.94	0.50
30:0:69:A:C8	30:0:69:A:C5'	2.89	0.50
8:H:66:GLU:HA	38:H:231:HOH:O	2.11	0.50
1:A:135:VAL:HA	1:A:150:PRO:HD3	1.93	0.50
5:E:7:ILE:HG13	5:E:11:VAL:HB	1.93	0.50
30:0:858:U:H5	38:0:5459:HOH:O	1.93	0.50
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.95	0.50
30:0:2610:U:H4'	38:0:9491:HOH:O	2.12	0.50
30:0:95:A:H5"	30:0:97:G:O4'	2.11	0.50
11:K:66:ARG:HH22	30:0:1994:A:P	2.35	0.50
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.94	0.50
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.11	0.50
30:0:1588:G:C6	30:0:1589:G:N1	2.80	0.50
31:9:13:A:O2'	31:9:14:G:H5"	2.12	0.50
30:0:1878:G:C1'	38:0:6153:HOH:O	2.47	0.50
27:1:16:HIS:HE1	30:0:775:G:OP1	1.94	0.50
24:X:61:ARG:NH1	24:X:67:PRO:HD3	2.27	0.50
30:0:1795:G:H2'	30:0:1796:A:O4'	2.12	0.50
10:J:42:GLU:O	10:J:131:THR:HG23	2.12	0.50
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.47	0.50

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.94	0.49
30:0:2256:G:C2'	30:0:2257:G:C5'	2.89	0.49
29:3:60:LYS:HG3	38:0:7595:HOH:O	2.12	0.49
30:0:2793:A:H2'	30:0:2794:G:H5'	1.94	0.49
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.77	0.49
14:N:37:ARG:NH2	38:N:8831:HOH:O	2.45	0.49
3:C:236:THR:HA	38:C:8644:HOH:O	2.12	0.49
2:B:254:GLN:HG2	2:B:255:GLY:N	2.27	0.49
4:D:103:ASN:ND2	4:D:133:ASN:HD22	2.10	0.49
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.11	0.49
30:0:2092:G:H2'	30:0:2613:G:OP1	2.13	0.49
10:J:131:THR:HB	10:J:134:GLU:HG3	1.95	0.49
16:P:41:ARG:HH22	30:0:1500:U:P	2.35	0.49
25:Y:154:ARG:NH1	25:Y:155:ARG:HG3	2.28	0.49
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.13	0.49
30:0:2851:G:H2'	30:0:2852:A:H5'	1.91	0.49
30:0:1972:U:H2'	30:0:1973:A:H5"	1.92	0.49
1:A:51:ARG:NH1	1:A:120:ARG:O	2.46	0.49
30:0:301:C:O2'	30:0:302:A:H5'	2.13	0.49
30:0:2724:U:H2'	30:0:2725:G:O4'	2.12	0.49
3:C:43:LYS:HG2	30:0:449:A:N7	2.28	0.49
2:B:54:VAL:HB	38:B:9087:HOH:O	2.11	0.49
2:B:26:PHE:HE1	38:B:9122:HOH:O	1.96	0.49
31:9:39:U:HO2'	31:9:42:C:H5	1.52	0.49
30:0:1198:U:C6	30:0:1200:A:OP2	2.65	0.49
21:U:33:SER:O	21:U:37:GLU:HG3	2.13	0.49
5:E:69:ILE:HA	5:E:72:MET:HE3	1.95	0.49
13:M:193:LYS:HB3	30:0:392:U:H4'	1.94	0.49
30:0:671:A:O2'	30:0:672:G:H2'	2.13	0.49
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.93	0.49
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.95	0.49
16:P:54:LYS:HB2	30:0:1717:A:H5"	1.93	0.49
20:T:54:ASP:OD2	30:0:316:A:H5'	2.12	0.49
30:0:1666:C:HO2'	30:0:1667:A:H5"	1.70	0.49
30:0:255:A:C4	30:0:256:C:C6	3.00	0.49
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.42	0.49
30:0:2356:A:H5'	38:0:5666:HOH:O	2.12	0.49
30:0:2265:U:H2'	30:0:2266:A:C8	2.48	0.49
30:0:2467:A:H2'	38:0:5488:HOH:O	2.12	0.49
20:T:52:ARG:O	30:0:317:A:OP1	2.29	0.49
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1008:C:O2'	30:0:1009:U:H5'	2.13	0.49
30:0:1552:G:H2'	30:0:1553:C:C6	2.47	0.49
30:0:2717:C:C2'	30:0:2718:C:C5'	2.79	0.49
30:0:2769:C:C2'	30:0:2770:G:C5'	2.84	0.49
30:0:255:A:H2'	30:0:256:C:C6	2.47	0.49
8:H:30:LYS:H	8:H:62:HIS:CD2	2.30	0.49
30:0:790:A:H1'	30:0:1710:A:H2'	1.95	0.49
25:Y:154:ARG:HH21	30:0:1293:U:H5'	1.78	0.49
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.93	0.49
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.94	0.49
30:0:2453:G:H5"	38:0:4755:HOH:O	2.13	0.49
30:0:304:G:H1'	30:0:347:A:N6	2.28	0.49
30:0:2316:G:OP1	30:0:2317:C:H1'	2.13	0.49
30:0:513:A:N3	38:0:3679:HOH:O	2.35	0.49
30:0:2002:C:C2'	30:0:2003:U:H5'	2.42	0.49
30:0:154:C:H2'	30:0:155:C:C6	2.48	0.49
30:0:1857:A:H5"	38:0:6744:HOH:O	2.12	0.49
30:0:1158:G:O2'	30:0:1159:G:H5'	2.13	0.48
30:0:282:C:O2	30:0:282:C:H2'	2.13	0.48
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.42	0.48
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.94	0.48
22:V:1:THR:HG23	22:V:2:VAL:HG23	1.94	0.48
30:0:1562:C:O2	30:0:1562:C:H2'	2.12	0.48
21:U:37:GLU:HB3	38:U:408:HOH:O	2.11	0.48
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.95	0.48
30:0:1391:G:H2'	30:0:1392:A:H5'	1.95	0.48
7:G:67:LEU:O	7:G:71:LEU:HG	2.12	0.48
30:0:1159:G:H1	30:0:1208:C:H42	1.58	0.48
10:J:75:PRO:HB3	10:J:132:LEU:HB3	1.95	0.48
12:L:6:ARG:NH1	30:0:1299:G:N7	2.62	0.48
24:X:43:VAL:HG12	24:X:44:ASP:N	2.28	0.48
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.45	0.48
27:1:1:THR:O	30:0:1836:A:H1'	2.13	0.48
16:P:83:LYS:HG2	30:0:793:A:H5"	1.94	0.48
30:0:1825:U:O2'	30:0:1826:C:H5'	2.12	0.48
30:0:195:C:H2'	30:0:196:G:H5'	1.95	0.48
30:0:1632:A:C3'	30:0:1633:C:H5'	2.43	0.48
2:B:205:VAL:O	2:B:307:ARG:NE	2.47	0.48
30:0:1528:A:H2'	30:0:1529:G:O4'	2.13	0.48
30:0:137:U:H2'	30:0:139:C:C5	2.47	0.48
19:S:37:VAL:O	19:S:41:VAL:HG23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:80:GLN:HA	26:Z:86:TYR:O	2.12	0.48
23:W:23:MET:O	30:0:1025:C:H5'	2.12	0.48
3:C:136:VAL:HG22	3:C:137:PRO:HA	1.95	0.48
30:0:1087:G:H4'	30:0:1088:A:OP1	2.13	0.48
25:Y:212:ARG:HD2	38:Y:8896:HOH:O	2.12	0.48
15:O:32:ARG:HD3	15:O:32:ARG:O	2.12	0.48
20:T:8:ARG:HD2	30:0:31:C:OP2	2.13	0.48
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.48
30:0:2300:A:H4'	30:0:2301:A:O5'	2.13	0.48
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.95	0.48
30:0:1321:A:H2'	30:0:1322:G:C8	2.48	0.48
1:A:121:ALA:O	1:A:124:VAL:HG22	2.13	0.48
3:C:236:THR:H	3:C:239:ALA:HB3	1.78	0.48
2:B:255:GLY:O	2:B:257:THR:HG22	2.14	0.48
30:0:961:A:H4'	38:0:6814:HOH:O	2.12	0.48
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.48
6:F:48:VAL:HG23	6:F:74:PHE:CB	2.42	0.48
30:0:2301:A:H5"	30:0:2302:A:H5'	1.95	0.48
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.95	0.48
30:0:1883:U:O2'	30:0:1884:G:H5'	2.13	0.48
2:B:49:THR:HG21	2:B:331:SER:O	2.14	0.48
30:0:2269:C:H2'	30:0:2270:G:C5'	2.44	0.48
30:0:1165:G:H4'	30:0:1174:A:O2'	2.13	0.48
30:0:447:A:O2'	30:0:448:G:H5'	2.14	0.48
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.96	0.48
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.95	0.48
30:0:2564:G:OP2	30:0:2565:C:H5"	2.14	0.48
10:J:107:ASN:C	10:J:107:ASN:HD22	2.17	0.48
30:0:222:A:H2'	30:0:223:G:O4'	2.14	0.48
30:0:484:A:N1	30:0:506:G:H4'	2.28	0.48
18:R:104:PHE:HB3	18:R:109:MET:HE1	1.96	0.48
30:0:1130:U:H4'	38:0:6158:HOH:O	2.13	0.48
6:F:21:GLU:O	6:F:24:ARG:HG2	2.14	0.48
31:9:45:A:H2'	31:9:46:C:H6	1.79	0.48
30:0:920:C:H5'	30:0:921:G:C4	2.49	0.48
3:C:140:VAL:HB	38:C:8644:HOH:O	2.13	0.48
30:0:960:G:H3'	30:0:960:G:C4	2.49	0.48
29:3:48:ASN:ND2	29:3:50:GLY:H	2.11	0.48
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.46	0.48
30:0:1131:G:C6	30:0:1230:A:C4	3.02	0.48
30:0:2912:C:H2'	30:0:2913:A:O4'	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:57:THR:HB	15:O:111:VAL:HG23	1.95	0.48
30:0:1051:C:H2'	30:0:1052:G:O4'	2.14	0.48
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.94	0.48
30:0:1545:C:H2'	30:0:1546:G:O4'	2.14	0.48
30:0:1477:C:H5'	30:0:1868:G:H5"	1.96	0.48
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.44	0.48
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.79	0.48
30:0:2439:C:H5'	38:0:5518:HOH:O	2.12	0.48
30:0:1625:U:H5"	38:0:6053:HOH:O	2.13	0.48
2:B:275:GLY:O	2:B:291:ASP:HA	2.14	0.48
12:L:121:ILE:HG12	12:L:141:GLU:HB2	1.96	0.48
1:A:3:ARG:HD3	30:0:870:G:OP2	2.14	0.47
23:W:65:VAL:HA	23:W:68:THR:HG22	1.95	0.47
27:1:28:HIS:HD2	27:1:30:LYS:H	1.60	0.47
30:0:2314:G:H2'	30:0:2315:C:H5'	1.96	0.47
3:C:22:PHE:HA	3:C:116:ALA:HA	1.94	0.47
30:0:90:A:H2'	30:0:91:G:O4'	2.14	0.47
14:N:169:PRO:O	14:N:172:PHE:HB3	2.14	0.47
13:M:64:ARG:HD2	38:M:8881:HOH:O	2.14	0.47
14:N:114:LYS:O	14:N:118:ILE:HG13	2.14	0.47
14:N:43:VAL:HG13	14:N:118:ILE:HD11	1.96	0.47
30:0:1666:C:H2'	30:0:1667:A:H5"	1.78	0.47
4:D:76:ARG:NE	31:9:44:A:O4'	2.47	0.47
21:U:9:CYS:HA	21:U:52:THR:OG1	2.14	0.47
30:0:1850:U:H2'	30:0:1851:G:C8	2.48	0.47
30:0:398:U:H2'	30:0:399:C:C6	2.49	0.47
30:0:1838:U:O2'	30:0:2644:C:H5'	2.14	0.47
30:0:2506:A:H1'	38:0:3766:HOH:O	2.13	0.47
8:H:61:ARG:HG3	8:H:61:ARG:NH1	2.29	0.47
30:0:1641:A:C2'	30:0:1642:A:H5'	2.44	0.47
30:0:1788:U:O2'	30:0:1789:G:H5'	2.14	0.47
30:0:2264:A:H2'	30:0:2265:U:C6	2.48	0.47
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.47
27:1:25:LYS:HD2	28:2:48:ASP:HA	1.96	0.47
30:0:1422:U:H2'	30:0:1423:C:C6	2.50	0.47
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.27	0.47
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.50	0.47
1:A:30:ARG:NH2	1:A:38:ILE:HG13	2.28	0.47
30:0:2064:U:H4'	30:0:2653:A:OP1	2.13	0.47
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.79	0.47
30:0:955:A:C2	30:0:1013:A:C4	3.03	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:143:ALA:HA	38:P:184:HOH:O	2.13	0.47
30:0:1268:C:O2'	30:0:1269:G:H5'	2.14	0.47
6:F:107:ASP:O	6:F:111:ILE:HG13	2.14	0.47
23:W:154:ARG:NH1	30:0:588:G:O6	2.47	0.47
30:0:1280:A:H3'	30:0:1280:A:OP1	2.15	0.47
31:9:56:A:C3'	31:9:57:A:H5"	2.44	0.47
14:N:40:ASN:HD21	31:9:28:U:H5"	1.80	0.47
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.47
30:0:1193:A:C2	30:0:1194:A:N6	2.78	0.47
30:0:137:U:OP1	30:0:259:G:O2'	2.33	0.47
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.30	0.47
30:0:1252:A:H2'	30:0:1253:C:O4'	2.14	0.47
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.49	0.47
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.15	0.47
24:X:85:VAL:HG12	24:X:86:GLU:N	2.30	0.47
30:0:407:A:H2'	30:0:408:A:C8	2.50	0.47
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.97	0.47
16:P:120:ARG:NH1	30:0:1594:C:C5	2.82	0.47
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	1.97	0.47
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.48	0.47
30:0:1393:A:H2'	30:0:1394:C:C6	2.49	0.47
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.45	0.47
30:0:2271:G:H5'	38:0:4783:HOH:O	2.14	0.47
30:0:2469:A:H2'	38:0:7512:HOH:O	2.15	0.47
30:0:1118:A:C8	30:0:1119:G:H5"	2.49	0.47
30:0:283:U:H5	30:0:284:C:N4	2.12	0.47
30:0:2353:A:H4'	30:0:2354:A:O5'	2.14	0.47
30:0:440:C:H2'	30:0:441:A:C8	2.50	0.47
30:0:1762:C:H2'	30:0:1763:C:H6	1.80	0.47
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.47	0.47
12:L:149:ARG:O	12:L:150:GLN:HB2	2.14	0.47
4:D:10:PHE:CG	4:D:11:HIS:N	2.81	0.47
17:Q:32:GLU:O	17:Q:93:ARG:NH2	2.48	0.47
30:0:1176:C:N4	38:0:5775:HOH:O	2.48	0.47
31:9:52:A:H2'	31:9:53:G:O4'	2.15	0.47
13:M:164:THR:HG22	13:M:166:ALA:N	2.29	0.47
30:0:483:C:C4	30:0:484:A:C6	3.03	0.47
29:3:65:THR:HB	29:3:83:TRP:H	1.79	0.47
30:0:2791:U:H1'	30:0:2792:A:H5"	1.97	0.47
23:W:11:VAL:HG11	30:0:1086:A:C6	2.49	0.47
30:0:426:G:H2'	30:0:427:C:O4'	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:22:CYS:SG	27:1:24:GLU:HB2	2.55	0.47
31:9:55:U:H4'	31:9:56:A:C8	2.49	0.47
30:0:2533:C:C6	30:0:2533:C:C5'	2.92	0.47
6:F:91:VAL:HG12	6:F:92:GLY:H	1.78	0.47
30:0:1682:A:H2'	38:0:9820:HOH:O	2.14	0.47
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.45	0.47
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.44	0.47
2:B:297:VAL:HB	38:B:9080:HOH:O	2.15	0.47
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.97	0.47
30:0:816:G:C6	30:0:817:G:N1	2.83	0.47
30:0:1477:C:C5'	30:0:1868:G:H5"	2.44	0.47
30:0:2372:A:H2'	30:0:2373:U:H6	1.78	0.47
30:0:1928:C:H2'	30:0:1929:G:H5'	1.96	0.47
30:0:2281:C:H2'	30:0:2282:U:H5'	1.97	0.47
30:0:1249:U:H2'	30:0:1250:C:C6	2.50	0.47
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.35	0.46
30:0:2238:A:H3'	38:0:6711:HOH:O	2.15	0.46
30:0:2589:U:H2'	30:0:2590:U:C6	2.50	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.15	0.46
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.30	0.46
26:Z:34:SER:HB3	30:0:797:A:H4'	1.96	0.46
30:0:170:U:H2'	30:0:171:C:H5'	1.95	0.46
30:0:2011:A:H4'	30:0:2012:U:O5'	2.15	0.46
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.19	0.46
31:9:28:U:H2'	31:9:29:C:C6	2.50	0.46
24:X:43:VAL:HG12	24:X:47:ALA:HB3	1.97	0.46
27:1:11:LYS:HG2	30:0:777:U:O2'	2.15	0.46
1:A:175:LYS:HG3	30:0:1847:A:OP1	2.16	0.46
25:Y:165:GLU:HB3	38:0:6747:HOH:O	2.15	0.46
8:H:172:GLU:HB3	38:H:243:HOH:O	2.15	0.46
21:U:50:GLU:HB2	30:0:2866:U:C5	2.50	0.46
30:0:559:U:C5	30:0:560:U:C5	3.03	0.46
14:N:141:ARG:NH2	31:9:48:C:H4'	2.30	0.46
30:0:969:G:H1	30:0:999:C:H42	1.62	0.46
30:0:304:G:H1'	30:0:347:A:H61	1.80	0.46
16:P:1:THR:O	30:0:1396:C:H1'	2.15	0.46
30:0:800:G:H2'	30:0:801:U:C6	2.50	0.46
30:0:1907:U:O2'	30:0:1908:G:H5'	2.15	0.46
3:C:129:HIS:HD2	3:C:165:ASP:OD2	1.99	0.46
23:W:122:ARG:NH2	38:0:5320:HOH:O	2.48	0.46
1:A:132:ASP:HB3	1:A:135:VAL:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.15	0.46
25:Y:115:ARG:NH2	30:0:1266:U:H4'	2.30	0.46
30:0:105:G:O2'	30:0:106:A:H5'	2.15	0.46
30:0:690:G:H4'	30:0:741:C:O2	2.15	0.46
30:0:699:C:C2	30:0:744:G:C2	3.03	0.46
30:0:2103:A:H2'	30:0:2104:C:H5'	1.96	0.46
1:A:88:ILE:HG22	1:A:88:ILE:O	2.14	0.46
10:J:82:THR:CG2	30:0:1242:A:H5'	2.30	0.46
30:0:1117:A:C2	30:0:1244:U:C2	3.04	0.46
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.96	0.46
2:B:320:GLN:HE21	2:B:321:PRO:CD	2.24	0.46
23:W:125:HIS:CE1	30:0:1097:A:H5"	2.51	0.46
10:J:107:ASN:HD22	10:J:109:TYR:H	1.64	0.46
30:0:920:C:H5"	30:0:921:G:O5'	2.15	0.46
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.31	0.46
30:0:1657:A:H2'	30:0:1658:A:C8	2.51	0.46
8:H:139:ALA:HB3	8:H:149:VAL:HG21	1.97	0.46
31:9:101:G:H5"	38:9:9140:HOH:O	2.15	0.46
30:0:343:C:O2'	30:0:344:C:H5'	2.15	0.46
30:0:638:C:H2'	30:0:639:A:C8	2.51	0.46
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.95	0.46
30:0:2712:G:H5'	38:0:5251:HOH:O	2.15	0.46
30:0:1596:U:H2'	30:0:1598:A:OP2	2.15	0.46
1:A:51:ARG:HD2	30:0:1874:U:OP1	2.15	0.46
30:0:583:C:C2	30:0:584:U:C5	3.03	0.46
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.82	0.46
20:T:28:SER:O	20:T:32:ARG:HG3	2.15	0.46
30:0:11:A:H5'	30:0:12:U:OP2	2.15	0.46
30:0:1503:U:H2'	30:0:1504:A:O4'	2.15	0.46
31:9:39:U:C2'	31:9:40:C:OP1	2.63	0.46
18:R:104:PHE:CB	18:R:109:MET:HE1	2.46	0.46
24:X:30:MET:CE	24:X:58:ALA:HB3	2.45	0.46
30:0:1883:U:C2'	30:0:1884:G:H5'	2.46	0.46
27:1:1:THR:HA	38:0:9368:HOH:O	2.16	0.46
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.54	0.46
30:0:613:C:H2'	30:0:614:U:H6	1.80	0.46
30:0:812:A:H2'	30:0:813:C:O4'	2.16	0.46
1:A:214:SER:HB2	38:0:4392:HOH:O	2.15	0.46
8:H:61:ARG:HG3	38:0:5004:HOH:O	2.15	0.46
4:D:27:ILE:HB	4:D:69:ILE:O	2.15	0.46
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1202:A:O2'	30:0:1203:G:H5'	2.16	0.46
30:0:1928:C:C2'	30:0:1929:G:H5'	2.46	0.46
3:C:206:ASN:HB2	30:0:329:A:OP2	2.15	0.46
18:R:132:ARG:NH1	38:R:8984:HOH:O	2.48	0.46
18:R:29:LYS:HD3	30:0:524:A:H5"	1.98	0.46
31:9:29:C:C2'	31:9:30:C:H5'	2.42	0.46
6:F:91:VAL:HG11	30:0:262:A:OP2	2.16	0.46
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.97	0.46
30:0:711:G:H1'	38:0:7133:HOH:O	2.14	0.46
30:0:71:G:H5"	38:0:3932:HOH:O	2.16	0.46
30:0:2065:C:O2'	30:0:2066:C:H5'	2.16	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.51	0.46
10:J:63:ILE:CD1	30:0:1236:A:C8	2.99	0.46
30:0:622:G:O2'	30:0:623:U:H5'	2.16	0.46
30:0:2758:G:H2'	30:0:2759:C:C6	2.51	0.46
28:2:20:ARG:HD3	38:0:6163:HOH:O	2.16	0.46
30:0:1790:C:H2'	30:0:1791:U:C6	2.50	0.46
2:B:141:ARG:N	38:B:9048:HOH:O	2.48	0.46
30:0:2241:C:H2'	30:0:2242:U:C6	2.51	0.46
30:0:2379:G:N7	30:0:2408:A:N1	2.63	0.46
30:0:1311:G:C2	30:0:1312:G:C8	3.04	0.46
1:A:206:ARG:NH2	30:0:2630:G:O6	2.49	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.98	0.46
30:0:2831:C:H42	30:0:2909:G:H1	1.64	0.45
30:0:2415:A:C2'	30:0:2416:G:H5'	2.46	0.45
30:0:2880:A:C2'	30:0:2881:C:H5'	2.46	0.45
30:0:1522:A:C2	30:0:1665:G:C6	3.04	0.45
30:0:876:A:N3	30:0:876:A:C2'	2.80	0.45
30:0:78:G:C6	30:0:79:G:C6	3.04	0.45
1:A:194:MET:HG2	30:0:875:A:C2	2.52	0.45
30:0:1511:U:O2'	30:0:1512:G:H5'	2.16	0.45
29:3:62:THR:HB	38:3:9044:HOH:O	2.15	0.45
30:0:162:C:H2'	30:0:163:U:H5'	1.98	0.45
30:0:278:A:H2'	30:0:279:C:O4'	2.16	0.45
2:B:62:ARG:HA	2:B:65:MET:CE	2.46	0.45
30:0:372:A:H2'	30:0:373:G:C8	2.51	0.45
30:0:2872:U:H2'	30:0:2873:C:H6	1.81	0.45
10:J:75:PRO:HD3	10:J:136:SER:OG	2.16	0.45
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.98	0.45
30:0:1778:A:H2'	30:0:1779:A:H5'	1.97	0.45
30:0:1194:A:O2'	30:0:1195:G:H5'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:63:ILE:HD11	20:T:75:GLU:HB2	1.99	0.45
30:0:758:A:H2'	30:0:759:C:O4'	2.17	0.45
30:0:669:G:O2'	30:0:670:G:H5'	2.16	0.45
30:0:412:C:O2'	30:0:413:G:H5'	2.16	0.45
30:0:1339:G:C6	30:0:1340:G:N1	2.85	0.45
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.31	0.45
30:0:1074:G:H4'	30:0:1260:G:C6	2.51	0.45
30:0:53:C:H2'	30:0:54:G:O4'	2.16	0.45
7:G:64:ASN:N	7:G:64:ASN:ND2	2.63	0.45
30:0:407:A:H8	38:0:4486:HOH:O	2.00	0.45
3:C:19:PRO:HG2	3:C:22:PHE:CD1	2.51	0.45
23:W:38:THR:HG22	23:W:39:ASP:N	2.31	0.45
30:0:2456:A:H2'	30:0:2457:U:C6	2.51	0.45
30:0:445:U:H2'	30:0:446:G:H8	1.81	0.45
31:9:53:G:O2'	31:9:54:A:H5'	2.16	0.45
30:0:281:U:H2'	30:0:282:C:H6	1.82	0.45
30:0:506:G:N2	30:0:509:A:H5'	2.22	0.45
10:J:19:MET:HE1	10:J:79:PHE:HA	1.99	0.45
31:9:3:A:OP2	31:9:25:G:N2	2.49	0.45
30:0:253:U:H1'	30:0:256:C:H41	1.82	0.45
6:F:91:VAL:CG1	6:F:92:GLY:N	2.80	0.45
30:0:1333:U:H2'	30:0:1334:C:H6	1.82	0.45
30:0:2271:G:N3	30:0:2271:G:H2'	2.31	0.45
30:0:522:U:O2'	30:0:1366:C:H5'	2.16	0.45
13:M:49:ALA:C	13:M:54:TYR:HB3	2.37	0.45
31:9:57:A:N6	38:9:9066:HOH:O	2.47	0.45
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.35	0.45
31:9:40:C:H2'	31:9:41:C:OP1	2.17	0.45
11:K:113:ILE:HG22	11:K:114:ALA:N	2.32	0.45
15:O:10:LEU:HD13	15:O:99:GLU:HG3	1.99	0.45
30:0:1919:A:H4'	38:0:4883:HOH:O	2.15	0.45
30:0:2493:C:O2	30:0:2493:C:H2'	2.15	0.45
30:0:1588:G:C6	30:0:1589:G:C6	3.05	0.45
30:0:603:A:H1'	30:0:605:C:C2	2.52	0.45
4:D:20:LYS:HG2	4:D:133:ASN:HB3	1.97	0.45
30:0:1947:G:H2'	30:0:1948:G:C8	2.52	0.45
30:0:2598:U:O2	30:0:2600:A:H8	2.00	0.45
30:0:1202:A:H2'	30:0:1203:G:H5'	1.99	0.45
11:K:125:ALA:C	11:K:127:ALA:H	2.20	0.45
18:R:132:ARG:HG2	18:R:133:ALA:N	2.31	0.45
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.51	0.45
24:X:78:GLU:HG2	24:X:79:GLU:H	1.81	0.45
30:0:2812:A:N7	38:0:7555:HOH:O	2.36	0.45
13:M:99:ARG:HG3	38:M:8855:HOH:O	2.16	0.45
30:0:1183:C:N3	30:0:1184:C:H5	2.15	0.45
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.99	0.45
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.99	0.45
30:0:2090:G:H2'	30:0:2091:G:C8	2.51	0.45
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.99	0.45
30:0:2281:C:C2'	30:0:2282:U:H5'	2.47	0.45
1:A:164:ARG:NE	38:A:9043:HOH:O	2.49	0.45
16:P:134:VAL:O	16:P:137:LEU:HB3	2.17	0.45
17:Q:1:PRO:HA	30:0:2299:G:O6	2.16	0.45
30:0:821:U:H3'	38:0:3789:HOH:O	2.15	0.45
30:0:42:C:H1'	38:0:4707:HOH:O	2.15	0.45
1:A:99:ILE:O	1:A:131:HIS:HE1	2.00	0.45
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.32	0.45
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.52	0.45
23:W:149:LEU:HG	23:W:153:MET:HE2	1.99	0.45
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.99	0.45
8:H:34:HIS:HD2	8:H:90:LEU:O	2.00	0.45
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.97	0.45
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.98	0.45
30:0:1987:C:H2'	30:0:1988:C:C6	2.51	0.45
1:A:186:TRP:CG	1:A:187:PRO:HA	2.52	0.45
1:A:96:LEU:HD22	1:A:128:LEU:HD13	1.99	0.45
30:0:2506:A:O2'	30:0:2507:G:P	2.75	0.45
18:R:113:HIS:O	18:R:145:LEU:HD12	2.17	0.45
23:W:119:HIS:HE1	38:0:9565:HOH:O	2.00	0.45
12:L:50:GLY:C	30:0:2453:G:H4'	2.37	0.45
19:S:77:VAL:O	19:S:80:ARG:HG2	2.16	0.45
3:C:84:VAL:O	3:C:85:LYS:HB2	2.17	0.45
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.99	0.45
31:9:81:C:O2'	31:9:82:U:H5'	2.17	0.45
30:0:128:A:H3'	30:0:128:A:C8	2.52	0.45
30:0:1902:G:N2	30:0:1936:C:C2	2.85	0.45
31:9:1:U:O3'	31:9:3:A:OP1	2.35	0.45
30:0:969:G:N2	30:0:1000:C:C2	2.84	0.45
30:0:951:A:O2'	30:0:952:G:H5'	2.17	0.45
30:0:77:G:C2'	30:0:78:G:H5'	2.47	0.45
27:1:2:GLY:O	27:1:6:PRO:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:74:GLU:OE1	30:0:1285:U:H4'	2.17	0.45
30:0:1615:A:H5'	38:0:4210:HOH:O	2.16	0.45
30:0:1626:A:H2'	30:0:1627:G:O4'	2.17	0.45
3:C:168:ARG:NH2	3:C:190:ALA:O	2.50	0.45
25:Y:137:LYS:HD2	30:0:521:A:H5"	1.99	0.45
13:M:164:THR:HB	38:M:8819:HOH:O	2.15	0.44
30:0:542:A:O2'	30:0:543:G:H5'	2.16	0.44
30:0:1942:A:O2'	30:0:1943:C:H5'	2.17	0.44
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.00	0.44
2:B:62:ARG:HA	2:B:65:MET:HE2	1.99	0.44
30:0:1783:A:O2'	30:0:1784:U:H5'	2.16	0.44
30:0:1896:G:C6	30:0:1897:U:C4	3.05	0.44
30:0:2754:G:H2'	30:0:2755:G:O4'	2.17	0.44
30:0:291:C:H2'	30:0:292:G:O4'	2.17	0.44
29:3:65:THR:CG2	29:3:67:LEU:HG	2.46	0.44
1:A:53:ALA:HB3	38:A:9060:HOH:O	2.16	0.44
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.64	0.44
4:D:135:VAL:HG22	4:D:136:ARG:N	2.32	0.44
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.98	0.44
30:0:812:A:H2'	30:0:813:C:C6	2.52	0.44
30:0:1406:A:H4'	30:0:1407:A:H5"	1.99	0.44
26:Z:37:ARG:HD2	38:Z:8719:HOH:O	2.17	0.44
30:0:1182:C:HO2'	30:0:1183:C:H5	1.64	0.44
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.38	0.44
11:K:14:LYS:HG3	11:K:32:ILE:O	2.18	0.44
30:0:582:U:H2'	30:0:583:C:C6	2.53	0.44
30:0:187:A:H3'	30:0:188:C:H6	1.82	0.44
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.76	0.44
30:0:204:A:H2'	30:0:205:U:H5'	1.98	0.44
30:0:2032:U:H2'	30:0:2033:G:C5'	2.47	0.44
14:N:108:SER:HA	14:N:109:PRO:HD3	1.81	0.44
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.44
25:Y:144:ARG:NH2	38:Y:8907:HOH:O	2.51	0.44
30:0:2464:C:H5"	30:0:2465:A:OP1	2.17	0.44
30:0:2473:U:O3'	30:0:2474:A:H3'	2.17	0.44
30:0:2385:G:H2'	30:0:2386:U:C6	2.52	0.44
13:M:58:GLN:HG3	38:M:8906:HOH:O	2.18	0.44
30:0:451:C:O2'	30:0:452:G:H5'	2.18	0.44
30:0:453:A:H4'	30:0:455:A:N7	2.32	0.44
30:0:558:C:HO2'	30:0:559:U:H5"	1.80	0.44
30:0:1973:A:H2'	30:0:1974:G:O4'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2635:A:C2'	30:0:2636:C:H5'	2.46	0.44
30:0:815:U:O2'	30:0:1598:A:H4'	2.17	0.44
30:0:947:U:O2'	30:0:948:G:H5'	2.16	0.44
16:P:120:ARG:NH2	16:P:123:TYR:CD2	2.85	0.44
30:0:185:G:H4'	30:0:186:A:H4'	1.99	0.44
30:0:1342:C:C2'	30:0:1343:C:H5'	2.47	0.44
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.47	0.44
30:0:825:U:H5"	30:0:826:U:OP1	2.18	0.44
31:9:76:G:H3'	31:9:77:A:C5'	2.31	0.44
30:0:1592:G:C4	30:0:1593:C:C5	3.06	0.44
30:0:1592:G:O2'	30:0:1593:C:O5'	2.35	0.44
2:B:74:ILE:HG13	38:B:9080:HOH:O	2.17	0.44
30:0:2636:C:H4'	38:0:6666:HOH:O	2.18	0.44
4:D:53:LYS:HE3	31:9:40:C:H42	1.82	0.44
30:0:816:G:H5'	30:0:1598:A:H4'	1.99	0.44
30:0:77:G:H2'	30:0:78:G:H5'	1.99	0.44
30:0:218:C:C5	30:0:220:C:C4	3.06	0.44
28:2:2:LYS:HG3	30:0:1486:A:C5	2.52	0.44
30:0:2276:U:H2'	30:0:2277:U:C6	2.53	0.44
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.17	0.44
13:M:46:LEU:HG	38:M:8922:HOH:O	2.18	0.44
30:0:1427:A:H61	30:0:1440:U:C1'	2.30	0.44
30:0:1603:A:C5'	30:0:1605:G:C5'	2.94	0.44
30:0:1878:G:O2'	30:0:1879:U:OP2	2.36	0.44
14:N:11:ARG:NH1	31:9:8:G:O6	2.50	0.44
2:B:79:MET:HE1	38:B:9100:HOH:O	2.17	0.44
30:0:204:A:C2'	30:0:205:U:H5'	2.47	0.44
30:0:764:C:H2'	30:0:765:G:O4'	2.17	0.44
30:0:794:U:C2'	30:0:795:G:H5'	2.48	0.44
16:P:91:LYS:O	16:P:95:GLU:HG3	2.17	0.44
6:F:60:VAL:HG13	6:F:63:ILE:HG13	1.99	0.44
30:0:2565:C:H4'	38:0:4868:HOH:O	2.18	0.44
8:H:30:LYS:H	8:H:62:HIS:HD2	1.65	0.44
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.83	0.44
30:0:441:A:H8	30:0:441:A:O5'	1.99	0.44
1:A:204:GLY:N	30:0:2634:G:OP2	2.48	0.44
4:D:135:VAL:HG22	4:D:136:ARG:H	1.82	0.44
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.53	0.44
30:0:1006:A:N1	30:0:2311:A:H1'	2.33	0.44
30:0:497:A:H2'	30:0:498:A:C5'	2.48	0.44
30:0:2511:A:H2'	30:0:2512:U:O4'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131:THR:HG21	30:0:2348:C:H1'	1.99	0.44
30:0:1044:C:H5"	38:0:9028:HOH:O	2.18	0.44
5:E:6:GLU:HG2	5:E:46:THR:HG22	1.99	0.44
2:B:280:VAL:HG13	2:B:333:GLU:O	2.17	0.44
31:9:107:C:O2'	31:9:108:C:H5'	2.18	0.44
30:0:2461:U:O2	30:0:2466:G:H1'	2.18	0.44
30:0:807:A:O2'	30:0:808:A:H5'	2.17	0.44
30:0:1189:A:H1'	30:0:1209:C:H1'	1.99	0.44
30:0:1588:G:C5	30:0:1589:G:C6	3.06	0.44
30:0:2506:A:O2'	30:0:2507:G:O5'	2.36	0.44
30:0:2238:A:O2'	30:0:2239:C:H5'	2.18	0.44
21:U:49:LEU:HG	38:U:3805:HOH:O	2.17	0.44
30:0:88:G:H2'	30:0:89:G:H8	1.83	0.44
30:0:1903:U:O2'	30:0:1904:A:N7	2.50	0.44
30:0:66:G:C2	30:0:109:U:C4	3.06	0.44
30:0:383:A:H2'	30:0:384:G:O4'	2.18	0.44
1:A:76:VAL:HG23	26:Z:87:LYS:HB3	2.00	0.44
30:0:1066:U:H2'	30:0:1067:A:C8	2.52	0.44
11:K:89:LYS:HE2	21:U:19:THR:HG21	2.00	0.44
30:0:629:A:C2	30:0:2074:A:C2	3.06	0.44
30:0:2015:A:H2'	30:0:2016:U:O4'	2.18	0.44
30:0:2569:A:H2'	30:0:2570:G:O5'	2.18	0.44
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.49	0.44
30:0:1375:A:C2'	30:0:1376:G:H5'	2.47	0.44
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.66	0.44
31:9:55:U:H4'	31:9:56:A:H8	1.83	0.43
14:N:37:ARG:HH12	31:9:6:C:C5'	2.21	0.43
14:N:37:ARG:NE	38:N:8831:HOH:O	2.51	0.43
30:0:1632:A:H2'	30:0:1633:C:C5'	2.42	0.43
10:J:70:PHE:HD1	30:0:2676:C:O2'	2.00	0.43
2:B:53:LEU:HD11	2:B:327:VAL:HG22	1.99	0.43
16:P:73:HIS:HE1	30:0:1789:G:O6	2.01	0.43
30:0:2842:G:H2'	30:0:2843:A:H5'	2.00	0.43
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.99	0.43
1:A:190:ARG:HH11	30:0:1845:A:P	2.41	0.43
30:0:594:C:C4	30:0:595:U:C4	3.06	0.43
30:0:499:G:O2'	30:0:500:G:H5'	2.16	0.43
30:0:177:A:O2'	30:0:892:G:H4'	2.17	0.43
17:Q:19:ARG:HH21	31:9:11:A:P	2.41	0.43
3:C:170:ASP:OD2	30:0:330:C:H5	2.01	0.43
30:0:1119:G:N2	30:0:1246:A:H2	2.13	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:134:ILE:O	13:M:136:PRO:HD3	2.19	0.43
31:9:114:G:H2'	31:9:115:C:H6	1.81	0.43
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.53	0.43
31:9:31:C:H2'	31:9:32:G:O4'	2.18	0.43
30:0:963:C:O2	30:0:1005:A:N1	2.51	0.43
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.51	0.43
2:B:10:SER:HB2	30:0:2714:U:H4'	1.99	0.43
29:3:91:GLN:O	29:3:92:GLU:HB2	2.18	0.43
14:N:50:LEU:HA	14:N:50:LEU:HD12	1.86	0.43
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.84	0.43
31:9:3:A:C2	31:9:21:G:N3	2.85	0.43
30:0:271:C:C2	30:0:273:G:O4'	2.70	0.43
1:A:95:PRO:O	1:A:99:ILE:HG12	2.19	0.43
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.16	0.43
28:2:16:ASN:HB2	38:2:5203:HOH:O	2.17	0.43
30:0:1517:C:O2	30:0:1670:A:C2	2.71	0.43
30:0:1565:C:H2'	30:0:1566:C:H6	1.83	0.43
18:R:40:ALA:O	18:R:44:VAL:HG23	2.18	0.43
30:0:1056:U:H2'	30:0:1057:A:O4'	2.18	0.43
1:A:1:GLY:HA2	1:A:197:VAL:HG23	1.99	0.43
30:0:2870:C:O2'	30:0:2871:G:H5'	2.19	0.43
30:0:1156:C:O5'	30:0:1156:C:H6	2.01	0.43
30:0:559:U:H2'	30:0:560:U:O4'	2.18	0.43
30:0:212:A:O4'	30:0:214:U:C6	2.72	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.96	0.43
30:0:960:G:C3'	30:0:960:G:C4	3.01	0.43
30:0:1789:G:H2'	30:0:1790:C:O5'	2.18	0.43
7:G:12:ILE:HG12	38:0:5490:HOH:O	2.19	0.43
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.43
30:0:677:C:O2'	30:0:678:G:H5'	2.18	0.43
3:C:61:PHE:HB3	38:C:8639:HOH:O	2.18	0.43
30:0:1434:A:H2'	30:0:1436:C:C5	2.53	0.43
30:0:294:C:H2'	30:0:295:C:O4'	2.18	0.43
30:0:17:G:H2'	30:0:18:C:C6	2.53	0.43
30:0:1456:C:H2'	30:0:1457:U:C6	2.54	0.43
28:2:41:HIS:CD2	28:2:44:ARG:H	2.26	0.43
22:V:1:THR:HG23	22:V:2:VAL:N	2.30	0.43
30:0:365:G:C6	30:0:366:U:C4	3.06	0.43
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.48	0.43
30:0:951:A:C2'	30:0:952:G:H5'	2.48	0.43
30:0:1946:C:H2'	30:0:1971:G:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ASP:O	2:B:306:LYS:HB2	2.19	0.43
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.89	0.43
30:0:424:C:H2'	30:0:425:U:C6	2.53	0.43
3:C:242:GLU:HB2	38:C:8577:HOH:O	2.17	0.43
11:K:8:VAL:HG13	11:K:80:ILE:HG22	2.00	0.43
31:9:42:C:H5'	31:9:43:G:OP2	2.19	0.43
30:0:226:A:H1'	30:0:393:G:C5	2.54	0.43
31:9:58:G:H3'	31:9:59:C:C6	2.54	0.43
30:0:35:U:H2'	30:0:36:C:C6	2.53	0.43
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.82	0.43
30:0:2523:U:O2'	30:0:2524:G:H5'	2.19	0.43
1:A:94:LEU:HG	1:A:99:ILE:HD13	2.01	0.43
30:0:1970:G:H2'	30:0:1970:G:N3	2.33	0.43
30:0:512:G:O3'	30:0:513:A:C8	2.71	0.43
30:0:1992:U:H2'	30:0:1994:A:OP2	2.18	0.43
30:0:794:U:H3	30:0:819:A:H61	1.65	0.43
30:0:794:U:H2'	30:0:795:G:H5'	2.01	0.43
30:0:1764:C:H2'	30:0:1765:G:O4'	2.18	0.43
30:0:130:C:H5'	38:0:5243:HOH:O	2.19	0.43
30:0:844:A:C6	30:0:882:A:C5	3.06	0.43
6:F:59:ILE:CD1	30:0:263:U:C2	3.01	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.34	0.43
8:H:64:SER:OG	30:0:2520:G:H5'	2.17	0.43
30:0:1589:G:N2	30:0:1605:G:H1'	2.34	0.43
3:C:98:ARG:NH1	38:C:8554:HOH:O	2.51	0.43
6:F:99:THR:HG23	6:F:99:THR:O	2.19	0.43
30:0:1250:C:O2'	30:0:1251:C:H5'	2.19	0.43
6:F:59:ILE:HD13	30:0:263:U:O4'	2.19	0.43
22:V:55:ARG:O	22:V:59:ILE:HG12	2.19	0.43
30:0:2387:U:H2'	30:0:2388:C:C6	2.54	0.43
19:S:57:THR:HG22	19:S:58:MET:N	2.33	0.43
11:K:130:MET:SD	21:U:25:ASP:O	2.77	0.43
21:U:49:LEU:O	21:U:52:THR:HG22	2.17	0.43
30:0:537:G:O4'	30:0:538:C:C5	2.71	0.43
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.49	0.43
30:0:941:G:C6	30:0:942:U:C4	3.07	0.43
30:0:1421:C:O2'	30:0:1422:U:H5'	2.18	0.43
31:9:59:C:H2'	31:9:60:C:C6	2.54	0.43
10:J:36:VAL:HG12	10:J:37:ALA:N	2.34	0.43
16:P:40:VAL:O	16:P:44:VAL:HG23	2.19	0.43
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:64:MET:HA	11:K:67:GLN:HE21	1.84	0.43
30:0:1616:A:H5"	30:0:1617:C:OP1	2.19	0.43
3:C:151:GLN:HG3	30:0:327:A:OP2	2.19	0.43
25:Y:133:HIS:HD2	38:Y:8877:HOH:O	2.02	0.43
25:Y:168:PHE:CE2	30:0:1090:A:H4'	2.54	0.43
30:0:1245:C:O5'	30:0:1245:C:H6	2.02	0.43
30:0:1160:G:H5'	30:0:1161:A:C4'	2.46	0.43
31:9:52:A:O2'	31:9:53:G:H5'	2.19	0.43
30:0:1187:U:O2'	30:0:1189:A:H2	1.85	0.43
4:D:99:ASP:HB3	4:D:103:ASN:H	1.84	0.43
18:R:109:MET:HG2	18:R:148:GLU:C	2.40	0.43
30:0:2524:G:N2	30:0:2526:C:H41	2.17	0.43
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.90	0.43
30:0:1555:G:O2'	30:0:1556:G:H5'	2.19	0.43
30:0:1644:C:C2	30:0:1645:U:C6	3.07	0.43
27:1:25:LYS:O	27:1:25:LYS:HG2	2.19	0.43
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.43
30:0:488:U:H2'	38:0:4031:HOH:O	2.18	0.43
30:0:1996:U:O2'	30:0:1997:A:H5'	2.18	0.43
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.19	0.43
30:0:1032:A:N3	30:0:1032:A:H2'	2.33	0.43
14:N:38:LYS:HB2	14:N:38:LYS:HE3	1.77	0.43
30:0:2252:A:C6	30:0:2253:G:H1'	2.53	0.42
9:I:86:GLU:HG2	30:0:1180:U:H4'	2.01	0.42
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.18	0.42
30:0:1788:U:C2	30:0:1805:G:N2	2.87	0.42
30:0:2435:U:H1'	38:0:5462:HOH:O	2.19	0.42
2:B:5:ARG:NH1	2:B:8:LYS:HE2	2.34	0.42
30:0:1202:A:H2'	30:0:1203:G:C5'	2.48	0.42
31:9:45:A:H2'	31:9:46:C:C6	2.54	0.42
30:0:332:G:O2'	30:0:333:G:H5'	2.19	0.42
30:0:39:G:N2	30:0:444:C:C2	2.87	0.42
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.34	0.42
31:9:14:G:H2'	31:9:15:C:H5'	2.01	0.42
31:9:2:U:C4'	38:9:9103:HOH:O	2.67	0.42
31:9:2:U:OP2	31:9:2:U:H4'	2.19	0.42
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.20	0.42
1:A:99:ILE:O	1:A:131:HIS:CE1	2.72	0.42
18:R:113:HIS:HE1	18:R:144:GLU:CD	2.22	0.42
30:0:1761:U:H2'	30:0:1762:C:C6	2.54	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:72:C:O2'	31:9:73:A:H5'	2.19	0.42
3:C:25:PRO:HG2	38:C:8520:HOH:O	2.18	0.42
30:0:1015:C:O5'	30:0:1015:C:H6	2.02	0.42
30:0:1634:G:C6	30:0:1635:U:C4	3.07	0.42
30:0:2004:U:H2'	30:0:2005:G:OP1	2.19	0.42
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.51	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.46	0.42
8:H:31:ILE:HG23	38:H:231:HOH:O	2.18	0.42
30:0:1762:C:H2'	30:0:1763:C:C6	2.54	0.42
30:0:2819:C:H2'	30:0:2820:A:C8	2.54	0.42
1:A:179:MET:HG2	1:A:186:TRP:CG	2.55	0.42
30:0:2423:C:H2'	30:0:2424:U:C6	2.54	0.42
29:3:3:MET:HG3	29:3:4:PRO:HD2	2.01	0.42
12:L:67:ARG:O	12:L:71:GLU:HG3	2.20	0.42
38:Q:2875:HOH:O	30:0:2392:C:H4'	2.20	0.42
16:P:59:ARG:NH2	16:P:66:GLN:HE22	2.10	0.42
9:I:111:LEU:HD23	30:0:1163:G:H4'	2.01	0.42
30:0:1175:G:H1'	30:0:1193:A:H2'	2.02	0.42
30:0:2104:C:O2	30:0:2485:A:N1	2.53	0.42
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.84	0.42
1:A:179:MET:HG2	1:A:186:TRP:CB	2.49	0.42
2:B:178:ALA:O	2:B:182:VAL:HG23	2.20	0.42
24:X:15:ARG:HH22	30:0:2856:A:P	2.42	0.42
23:W:43:GLY:HA3	30:0:945:U:O2'	2.19	0.42
30:0:1416:G:C2'	30:0:1417:G:H5'	2.49	0.42
6:F:118:LEU:O	6:F:119:ARG:HB3	2.19	0.42
30:0:1561:U:H2'	30:0:1561:U:O2	2.18	0.42
30:0:254:C:O2	30:0:254:C:H2'	2.19	0.42
23:W:80:ASP:HB2	38:W:3312:HOH:O	2.18	0.42
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.42
30:0:2414:A:N1	30:0:2415:A:C6	2.88	0.42
23:W:13:MET:CE	23:W:17:ILE:HG22	2.49	0.42
20:T:32:ARG:NH1	20:T:38:ARG:HH12	2.17	0.42
30:0:2134:G:N2	30:0:2242:U:C2	2.87	0.42
30:0:344:C:H2'	30:0:345:G:O4'	2.20	0.42
30:0:2719:A:H5"	38:0:3702:HOH:O	2.19	0.42
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.83	0.42
30:0:284:C:H4'	30:0:285:A:H8	1.84	0.42
30:0:1206:U:C6	30:0:1206:U:C3'	3.02	0.42
31:9:14:G:H2'	31:9:15:C:C5'	2.50	0.42
30:0:544:G:C3'	30:0:545:G:H5"	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:603:A:H4'	30:0:604:G:O5'	2.20	0.42
30:0:2578:G:C8	30:0:2578:G:H5'	2.44	0.42
30:0:1451:C:H5'	30:0:1505:U:C4	2.54	0.42
4:D:23:VAL:HG11	4:D:83:PHE:CZ	2.55	0.42
21:U:17:THR:CG2	21:U:18:GLY:N	2.83	0.42
30:0:2134:G:C6	30:0:2258:A:C8	3.08	0.42
30:0:1987:C:H2'	30:0:1988:C:H6	1.85	0.42
30:0:2754:G:C2'	30:0:2755:G:H5'	2.49	0.42
30:0:843:A:C2	30:0:846:A:C8	3.08	0.42
14:N:34:LEU:HD22	14:N:129:ILE:HD13	2.01	0.42
30:0:1211:G:O2'	30:0:1212:C:H5'	2.19	0.42
30:0:2361:A:H2'	30:0:2362:A:O4'	2.19	0.42
30:0:243:A:H61	30:0:269:G:H1'	1.84	0.42
2:B:14:GLY:HA2	2:B:15:PRO:C	2.39	0.42
30:0:369:G:C2	30:0:370:G:C8	3.08	0.42
30:0:2505:G:H2'	30:0:2506:A:C5'	2.50	0.42
14:N:25:ARG:HB3	30:0:2415:A:C2	2.54	0.42
2:B:314:ALA:CB	2:B:317:PRO:HG3	2.50	0.42
30:0:1307:A:H2'	30:0:1308:A:C8	2.55	0.42
23:W:7:LEU:HD12	23:W:53:ALA:HB2	2.00	0.42
26:Z:45:VAL:HG12	38:Z:8713:HOH:O	2.19	0.42
30:0:466:A:H2'	30:0:467:G:O4'	2.20	0.42
30:0:1244:U:H4'	30:0:1246:A:O4'	2.20	0.42
24:X:37:LEU:O	24:X:41:PHE:HB2	2.19	0.42
30:0:2252:A:C2'	30:0:2253:G:H5'	2.49	0.42
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.30	0.42
30:0:2756:U:C2	30:0:2896:A:H2	2.38	0.42
30:0:2909:G:H2'	30:0:2910:A:H8	1.84	0.42
22:V:12:THR:HG22	22:V:15:GLU:CG	2.47	0.42
30:0:1298:U:H2'	30:0:1299:G:C8	2.54	0.42
1:A:38:ILE:HA	1:A:38:ILE:HD13	1.85	0.42
30:0:790:A:H8	38:0:6134:HOH:O	2.01	0.42
8:H:87:LYS:NZ	8:H:87:LYS:HB2	2.35	0.42
3:C:85:LYS:HA	3:C:85:LYS:HD2	1.90	0.42
30:0:1782:G:O2'	30:0:1783:A:H5'	2.19	0.42
30:0:1023:C:H2'	30:0:1024:G:O4'	2.20	0.42
15:O:96:VAL:HG12	15:O:97:SER:O	2.20	0.42
30:0:539:G:H2'	30:0:540:A:C8	2.54	0.42
18:R:69:LYS:HB2	18:R:72:VAL:HG23	2.01	0.42
8:H:4:LYS:HA	8:H:5:PRO:HD3	1.86	0.42
4:D:170:TYR:CD1	4:D:170:TYR:N	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:124:GLY:HA3	30:0:2132:C:H1'	2.02	0.42
24:X:37:LEU:HD21	24:X:72:VAL:HG11	2.02	0.42
30:0:2783:A:O2'	30:0:2784:A:H5'	2.19	0.42
14:N:159:TYR:HE1	31:9:50:G:H5"	1.85	0.42
30:0:1198:U:H1'	30:0:1201:C:C5	2.50	0.42
1:A:94:LEU:N	1:A:94:LEU:HD23	2.34	0.42
30:0:1676:G:C2'	30:0:1677:U:H5'	2.50	0.42
19:S:56:ASN:O	28:2:8:LYS:NZ	2.51	0.42
30:0:1433:G:O2'	30:0:1434:A:H5'	2.20	0.42
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.19	0.42
30:0:417:G:P	38:0:7457:HOH:O	2.77	0.42
1:A:23:TYR:HD1	30:0:1872:C:H2'	1.85	0.42
24:X:8:ARG:NH1	30:0:2904:U:H4'	2.35	0.42
2:B:27:ASN:H	2:B:27:ASN:HD22	1.67	0.42
30:0:2718:C:H5'	30:0:2718:C:C6	2.53	0.42
1:A:211:LYS:HB2	38:A:9075:HOH:O	2.19	0.42
30:0:2509:A:OP2	30:0:2510:C:C5	2.72	0.42
30:0:2712:G:P	38:0:5251:HOH:O	2.77	0.42
30:0:2908:A:C2'	30:0:2909:G:H5'	2.49	0.42
18:R:29:LYS:NZ	38:R:8944:HOH:O	2.53	0.42
2:B:243:ASN:HA	2:B:244:PRO:C	2.40	0.42
3:C:5:ILE:HD11	3:C:16:VAL:HG23	2.01	0.42
30:0:1334:C:H2'	30:0:1335:C:H6	1.85	0.42
30:0:128:A:C8	30:0:128:A:C3'	3.03	0.42
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.85	0.42
10:J:45:VAL:HG11	10:J:121:LEU:HD22	2.02	0.42
1:A:54:PRO:HG2	1:A:160:ALA:HB3	2.02	0.42
1:A:107:ASN:OD1	1:A:116:GLY:HA3	2.20	0.42
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.17	0.41
30:0:2727:A:C6	30:0:2756:U:C2	3.08	0.41
14:N:147:ILE:HB	38:9:9090:HOH:O	2.19	0.41
30:0:960:G:H2'	30:0:961:A:OP2	2.19	0.41
30:0:1789:G:C2'	30:0:1790:C:O5'	2.68	0.41
30:0:1562:C:N4	38:0:5895:HOH:O	2.53	0.41
30:0:259:G:O2'	30:0:260:C:H5'	2.20	0.41
30:0:1335:C:H2'	30:0:1336:U:C6	2.55	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.20	0.41
10:J:131:THR:HG22	10:J:134:GLU:H	1.85	0.41
25:Y:154:ARG:HH22	30:0:1071:G:H4'	1.85	0.41
30:0:821:U:H2'	30:0:822:C:H6	1.84	0.41
30:0:1406:A:H4'	30:0:1407:A:C5'	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:18:GLN:HG3	38:3:9009:HOH:O	2.20	0.41
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.20	0.41
30:0:129:A:O2'	30:0:131:A:OP1	2.36	0.41
4:D:105:SER:OG	30:0:2338:G:H1'	2.20	0.41
6:F:39:SER:HB3	6:F:45:ALA:HB2	2.02	0.41
30:0:883:U:C2'	30:0:883:U:O2	2.67	0.41
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.44	0.41
31:9:47:A:H2'	31:9:48:C:O4'	2.20	0.41
30:0:64:G:H2'	30:0:65:C:O4'	2.20	0.41
25:Y:142:SER:OG	30:0:1331:G:OP2	2.34	0.41
30:0:1052:G:C5	30:0:1063:G:C6	3.09	0.41
12:L:150:GLN:HB3	38:L:8868:HOH:O	2.20	0.41
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.51	0.41
4:D:37:ALA:O	4:D:40:ILE:HG12	2.20	0.41
19:S:11:THR:H	19:S:14:ALA:HB3	1.84	0.41
4:D:22:VAL:HG22	4:D:74:THR:HG22	2.00	0.41
30:0:420:U:H2'	30:0:421:C:C6	2.55	0.41
3:C:193:LEU:HD12	3:C:211:ASP:O	2.20	0.41
2:B:40:GLY:O	2:B:193:ILE:HD13	2.20	0.41
4:D:141:VAL:HG21	31:9:57:A:H8	1.85	0.41
14:N:37:ARG:HD3	35:N:8807:CL:CL	2.57	0.41
30:0:1185:U:H5'	38:0:7504:HOH:O	2.20	0.41
30:0:1840:A:H4'	30:0:1841:C:O5'	2.20	0.41
30:0:506:G:N2	30:0:509:A:H5"	2.32	0.41
28:2:41:HIS:CD2	28:2:43:ARG:H	2.39	0.41
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.41
9:I:69:PRO:HA	30:0:1164:U:OP1	2.21	0.41
2:B:248:ARG:NH1	38:B:9090:HOH:O	2.53	0.41
30:0:1167:G:C2	30:0:1168:C:C2	3.08	0.41
27:1:45:ARG:HB3	38:1:988:HOH:O	2.20	0.41
2:B:75:GLU:C	2:B:77:PRO:HD3	2.40	0.41
30:0:1474:C:C5'	30:0:1474:C:C6	2.89	0.41
28:2:41:HIS:N	28:2:45:ASN:HD22	2.03	0.41
30:0:151:A:C2	30:0:442:A:C8	3.09	0.41
9:I:101:LYS:O	9:I:105:GLU:HG3	2.21	0.41
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.01	0.41
31:9:45:A:C5	31:9:46:C:C5	3.08	0.41
30:0:1422:U:O2'	30:0:1423:C:H5'	2.20	0.41
30:0:729:C:C2	30:0:743:G:C2	3.08	0.41
30:0:635:A:H2'	30:0:636:G:H5"	2.02	0.41
30:0:1909:A:H2'	30:0:1910:A:C8	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1667:A:C2	30:0:1668:U:C2	3.08	0.41
30:0:2421:G:H4'	38:0:4814:HOH:O	2.20	0.41
3:C:223:LEU:HA	3:C:223:LEU:HD12	1.91	0.41
1:A:36:ASP:O	1:A:38:ILE:N	2.53	0.41
30:0:834:G:H3'	30:0:835:U:H4'	2.01	0.41
30:0:1903:U:O2'	30:0:1904:A:C8	2.68	0.41
16:P:7:LYS:HG2	16:P:23:PHE:CE2	2.55	0.41
30:0:1342:C:O2'	30:0:1343:C:H5'	2.20	0.41
28:2:37:HIS:CE1	30:0:462:A:C8	3.08	0.41
30:0:2704:C:H2'	30:0:2705:U:O4'	2.20	0.41
24:X:39:LYS:HE2	30:0:2834:G:OP1	2.20	0.41
30:0:1138:G:H4'	38:0:5739:HOH:O	2.18	0.41
10:J:52:GLN:HE22	30:0:1119:G:H8	1.69	0.41
29:3:38:ARG:HD2	30:0:396:U:OP2	2.21	0.41
16:P:59:ARG:O	16:P:63:ARG:HG3	2.21	0.41
30:0:2637:A:C5'	38:0:4961:HOH:O	2.59	0.41
30:0:2419:U:H5"	30:0:2420:G:C5'	2.50	0.41
30:0:290:C:H1'	38:0:6136:HOH:O	2.21	0.41
24:X:43:VAL:HG11	24:X:82:GLU:HA	2.01	0.41
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.20	0.41
30:0:2791:U:H4'	30:0:2792:A:OP1	2.20	0.41
30:0:2102:G:C2	30:0:2104:C:C4	3.08	0.41
19:S:57:THR:C	19:S:59:ASP:H	2.24	0.41
30:0:2361:A:H8	30:0:2361:A:H5'	1.86	0.41
30:0:243:A:H61	30:0:269:G:C1'	2.34	0.41
2:B:215:VAL:HA	2:B:220:VAL:HG22	2.02	0.41
30:0:318:U:H5'	30:0:339:A:C2	2.56	0.41
30:0:2802:C:H2'	30:0:2803:C:C6	2.55	0.41
30:0:482:G:H4'	30:0:508:A:N1	2.36	0.41
3:C:154:VAL:O	3:C:158:GLU:HG3	2.21	0.41
30:0:559:U:H5'	30:0:559:U:C6	2.35	0.41
1:A:212:PRO:HB2	38:0:4392:HOH:O	2.20	0.41
30:0:290:C:O2'	30:0:291:C:H5'	2.20	0.41
30:0:2089:A:C2'	30:0:2090:G:H5'	2.49	0.41
30:0:1377:C:C5'	30:0:1377:C:H6	2.33	0.41
1:A:217:ARG:HG2	1:A:229:ALA:HB2	2.03	0.41
16:P:94:TRP:CZ2	16:P:98:ILE:HG13	2.56	0.41
2:B:280:VAL:CG1	2:B:334:SER:HA	2.50	0.41
30:0:1481:G:H2'	30:0:1482:A:O4'	2.20	0.41
13:M:67:VAL:HB	13:M:97:ILE:HG23	2.03	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:5:THR:HG23	30:0:1688:G:O2'	2.20	0.41
29:3:69:TYR:CZ	29:3:80:ARG:HD2	2.56	0.41
30:0:1548:U:H1'	38:0:6897:HOH:O	2.19	0.41
25:Y:213:LYS:HE3	25:Y:213:LYS:HB2	1.90	0.41
13:M:167:GLY:O	13:M:171:ARG:HG3	2.21	0.41
23:W:48:VAL:HG12	23:W:48:VAL:O	2.19	0.41
31:9:13:A:OP1	31:9:113:C:H5'	2.21	0.41
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.56	0.41
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.48	0.41
11:K:30:LYS:HB3	11:K:56:SER:HB3	2.03	0.41
1:A:95:PRO:HA	1:A:153:ARG:HA	2.03	0.41
30:0:1804:A:H2'	30:0:1805:G:C8	2.56	0.41
30:0:1714:C:C2'	30:0:1715:C:H5'	2.51	0.41
14:N:160:SER:CB	31:9:51:A:H5'	2.50	0.41
16:P:83:LYS:O	16:P:86:ALA:HB3	2.21	0.41
30:0:1544:U:O2'	30:0:1545:C:H5'	2.20	0.41
30:0:2802:C:H2'	30:0:2803:C:H6	1.84	0.41
30:0:667:C:H2'	30:0:668:C:H6	1.85	0.41
18:R:17:MET:SD	38:R:8951:HOH:O	2.62	0.41
30:0:81:G:N3	30:0:98:A:C2	2.88	0.41
30:0:2617:G:C2	30:0:2618:G:C8	3.08	0.41
15:O:98:LEU:O	15:O:102:ILE:HG13	2.21	0.41
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.21	0.41
22:V:27:LEU:HA	22:V:49:LEU:HD13	2.02	0.41
13:M:164:THR:CG2	13:M:165:GLY:N	2.83	0.41
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.49	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.36	0.41
30:0:1634:G:C5	30:0:1635:U:C4	3.08	0.41
30:0:1166:A:N3	30:0:1166:A:H2'	2.35	0.41
30:0:2246:U:N3	30:0:2256:G:C2	2.89	0.41
22:V:39:ALA:C	22:V:41:GLU:H	2.23	0.41
30:0:2039:A:H2'	30:0:2040:C:C6	2.56	0.41
30:0:23:G:C6	30:0:24:G:N1	2.89	0.41
30:0:969:G:H2'	30:0:970:U:C6	2.56	0.41
15:O:115:ARG:NH1	38:O:6194:HOH:O	2.54	0.41
2:B:154:VAL:CG1	2:B:156:LYS:HG2	2.51	0.41
30:0:1945:G:O2'	30:0:1946:C:H5'	2.20	0.41
30:0:130:C:H2'	38:0:3183:HOH:O	2.20	0.41
4:D:25:MET:HE1	4:D:37:ALA:O	2.21	0.41
30:0:1909:A:N1	30:0:2128:G:H1'	2.35	0.41
31:9:34:A:H2'	31:9:35:C:O4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.51	0.41
26:Z:50:VAL:O	26:Z:54:GLU:HG3	2.20	0.41
3:C:76:ARG:NH1	3:C:76:ARG:HB3	2.36	0.41
20:T:79:LEU:HG	20:T:89:ARG:HB2	2.03	0.41
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.85	0.41
38:N:8830:HOH:O	30:0:2368:A:H8	2.04	0.41
38:K:7438:HOH:O	21:U:20:MET:HE2	2.21	0.41
30:0:1119:G:N2	30:0:1246:A:N1	2.69	0.41
30:0:2072:G:N2	38:0:6910:HOH:O	2.54	0.41
30:0:2251:G:C6	30:0:2252:A:C6	3.09	0.41
30:0:1163:G:N2	38:0:6078:HOH:O	2.54	0.41
29:3:70:ARG:HD3	38:3:9064:HOH:O	2.21	0.41
30:0:1522:A:C2'	30:0:1523:G:H5'	2.51	0.41
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.02	0.41
30:0:595:U:O2'	30:0:596:C:H5'	2.21	0.41
30:0:1613:C:H2'	30:0:1614:G:O4'	2.21	0.41
30:0:1271:A:C2	30:0:1286:A:C2	3.09	0.41
30:0:1574:C:O5'	30:0:1574:C:H6	2.04	0.41
30:0:369:G:O2'	30:0:370:G:H5'	2.21	0.40
30:0:1182:C:O2'	30:0:1183:C:H5	2.04	0.40
25:Y:189:ASN:ND2	25:Y:192:ASP:H	2.19	0.40
31:9:64:C:O2'	31:9:65:A:H5'	2.21	0.40
30:0:1758:U:H2'	30:0:1759:A:O4'	2.22	0.40
30:0:1515:A:H2'	30:0:1516:U:H6	1.82	0.40
30:0:1536:C:O5'	30:0:1536:C:H6	2.03	0.40
2:B:154:VAL:HG12	2:B:156:LYS:HG2	2.02	0.40
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.86	0.40
30:0:106:A:H2'	30:0:107:U:O4'	2.21	0.40
4:D:25:MET:HE3	4:D:37:ALA:HB1	2.04	0.40
30:0:1750:C:N4	30:0:1751:G:C6	2.89	0.40
30:0:2334:C:O2'	30:0:2335:C:H5'	2.21	0.40
30:0:745:G:H5"	30:0:746:A:OP1	2.21	0.40
30:0:401:C:H2'	30:0:402:U:C6	2.56	0.40
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.03	0.40
30:0:2332:A:C2	30:0:2355:G:C5	3.09	0.40
30:0:1520:G:C6	30:0:1521:C:C4	3.09	0.40
25:Y:106:THR:HG23	25:Y:107:PRO:HD2	2.03	0.40
30:0:1098:A:H2'	30:0:1099:G:O4'	2.21	0.40
30:0:1700:C:H5"	30:0:1701:A:OP2	2.22	0.40
30:0:2253:G:C2	30:0:2254:G:C8	3.09	0.40
30:0:2524:G:H21	30:0:2526:C:H41	1.67	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1947:G:C8	30:0:1970:G:C8	3.09	0.40
30:0:1377:C:H2'	30:0:1723:G:O6	2.21	0.40
12:L:143:THR:HG21	38:L:8837:HOH:O	2.21	0.40
2:B:234:ARG:HD3	30:0:1734:C:OP1	2.21	0.40
30:0:1192:A:H3'	30:0:1193:A:H5'	2.02	0.40
30:0:278:A:C6	30:0:279:C:C4	3.09	0.40
30:0:1617:C:C4	30:0:1643:C:H4'	2.56	0.40
30:0:74:G:H2'	30:0:75:U:C6	2.56	0.40
14:N:154:LEU:C	14:N:156:GLU:H	2.24	0.40
30:0:1327:G:N1	30:0:1330:A:OP2	2.52	0.40
30:0:1183:C:O2	30:0:1183:C:C2'	2.69	0.40
20:T:24:ARG:NH2	20:T:39:ASN:HD22	2.07	0.40
30:0:2727:A:N1	30:0:2756:U:C2	2.90	0.40
30:0:255:A:C5	30:0:256:C:C5	3.09	0.40
30:0:1163:G:C4	30:0:1164:U:C5	3.09	0.40
30:0:111:C:O2'	30:0:112:G:H5'	2.21	0.40
30:0:1947:G:N2	30:0:1966:U:C2	2.90	0.40
30:0:2782:G:O6	30:0:2790:C:H5"	2.21	0.40
30:0:200:C:H6	38:0:3463:HOH:O	2.03	0.40
8:H:76:LEU:HD21	8:H:149:VAL:HA	2.02	0.40
30:0:1896:G:H1'	38:0:4284:HOH:O	2.21	0.40
31:9:26:C:H2'	31:9:27:C:C6	2.57	0.40
30:0:1409:G:C2	30:0:1410:G:C8	3.10	0.40
30:0:2626:C:H2'	30:0:2627:G:C8	2.56	0.40
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.80	0.40
8:H:91:ARG:HG2	8:H:91:ARG:H	1.59	0.40
30:0:932:U:H2'	30:0:933:C:C6	2.57	0.40
23:W:90:TYR:CE2	23:W:99:ALA:HB2	2.56	0.40
30:0:1741:U:C5'	30:0:1742:A:OP1	2.63	0.40
31:9:39:U:H3'	31:9:40:C:H5"	2.02	0.40
30:0:853:C:H2'	30:0:854:G:O4'	2.21	0.40
1:A:86:ALA:HB3	1:A:94:LEU:HD22	2.03	0.40
30:0:2842:G:C2'	30:0:2843:A:H5'	2.51	0.40
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.21	0.40
30:0:1149:U:C5	30:0:1215:A:C5	3.09	0.40
30:0:2112:A:H2'	30:0:2113:G:C8	2.56	0.40
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.37	0.40
30:0:1503:U:H3'	30:0:1503:U:H6	1.86	0.40
30:0:445:U:H2'	30:0:446:G:C8	2.56	0.40
30:0:806:A:H2'	30:0:807:A:O4'	2.22	0.40
2:B:202:VAL:HG11	2:B:301:VAL:HG13	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1414:A:H2'	30:0:1415:G:O4'	2.21	0.40
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.95	0.40
30:0:2726:U:O2	30:0:2749:U:O5'	2.40	0.40
30:0:724:G:O2'	30:0:725:C:H5'	2.22	0.40
3:C:107:ARG:HB3	3:C:107:ARG:NH1	2.37	0.40
3:C:236:THR:HG22	3:C:239:ALA:CB	2.51	0.40
8:H:155:ARG:NH1	30:0:2503:A:H5"	2.36	0.40
30:0:1878:G:H2'	38:0:3278:HOH:O	2.21	0.40
3:C:2:GLN:HB3	38:C:8530:HOH:O	2.21	0.40
3:C:16:VAL:HG12	3:C:17:ASP:N	2.36	0.40
30:0:138:U:OP2	30:0:139:C:C5	2.73	0.40
30:0:47:G:N3	30:0:114:A:C2	2.90	0.40
23:W:149:LEU:HG	23:W:153:MET:HE1	2.03	0.40
3:C:118:THR:O	3:C:136:VAL:HG13	2.22	0.40
25:Y:144:ARG:NH1	38:Y:8871:HOH:O	2.53	0.40
30:0:2016:U:H6	30:0:2016:U:O5'	2.05	0.40
20:T:82:THR:HG21	30:0:488:U:O2'	2.21	0.40
28:2:5:LYS:O	28:2:9:LYS:HG3	2.22	0.40
30:0:234:A:H4'	30:0:437:A:O4'	2.22	0.40
30:0:517:U:H1'	38:0:7614:HOH:O	2.21	0.40
30:0:1705:C:H2'	30:0:1706:G:O4'	2.20	0.40
30:0:907:A:H2'	30:0:908:A:H8	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	235/240 (98%)	212 (90%)	18 (8%)	5 (2%)	9 23
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	21 49
3	C	244/246 (99%)	228 (93%)	16 (7%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	8 22
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100 100
6	F	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	21 49
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100 100
8	H	156/177 (88%)	149 (96%)	6 (4%)	1 (1%)	30 59
9	I	68/162 (42%)	55 (81%)	10 (15%)	3 (4%)	3 6
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100 100
11	K	130/132 (98%)	125 (96%)	5 (4%)	0	100 100
12	L	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	26 55
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	34 63
14	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	12 30
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100 100
16	P	141/149 (95%)	141 (100%)	0	0	100 100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
18	R	148/155 (96%)	140 (95%)	8 (5%)	0	100 100
19	S	79/85 (93%)	78 (99%)	1 (1%)	0	100 100
20	T	117/120 (98%)	110 (94%)	6 (5%)	1 (1%)	21 49
21	U	51/67 (76%)	47 (92%)	4 (8%)	0	100 100
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	12 30
23	W	152/154 (99%)	148 (97%)	4 (3%)	0	100 100
24	X	80/92 (87%)	73 (91%)	6 (8%)	1 (1%)	15 37
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100 100
26	Z	71/116 (61%)	61 (86%)	8 (11%)	2 (3%)	6 15
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100 100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100 100
29	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	17 42
All	All	3705/4472 (83%)	3458 (93%)	220 (6%)	27 (1%)	26 55

All (27) Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

5.3.2 Protein sidechains (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%)	171 (96%)	8 (4%)	34 65
2	B	282/283 (100%)	265 (94%)	17 (6%)	24 50
3	C	193/193 (100%)	178 (92%)	15 (8%)	16 35
4	D	117/148 (79%)	109 (93%)	8 (7%)	20 43
5	E	152/156 (97%)	147 (97%)	5 (3%)	45 76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	93/94 (99%)	93 (100%)	0	100 100
7	G	27/282 (10%)	26 (96%)	1 (4%)	41 72
8	H	134/145 (92%)	127 (95%)	7 (5%)	29 58
9	I	58/130 (45%)	57 (98%)	1 (2%)	68 90
10	J	118/121 (98%)	112 (95%)	6 (5%)	29 59
11	K	106/106 (100%)	103 (97%)	3 (3%)	51 81
12	L	113/127 (89%)	111 (98%)	2 (2%)	66 89
13	M	158/160 (99%)	150 (95%)	8 (5%)	29 59
14	N	149/150 (99%)	144 (97%)	5 (3%)	44 75
15	O	93/94 (99%)	91 (98%)	2 (2%)	60 86
16	P	113/117 (97%)	108 (96%)	5 (4%)	35 65
17	Q	79/80 (99%)	77 (98%)	2 (2%)	55 84
18	R	117/122 (96%)	113 (97%)	4 (3%)	44 75
19	S	71/74 (96%)	70 (99%)	1 (1%)	74 92
20	T	105/106 (99%)	99 (94%)	6 (6%)	25 53
21	U	44/53 (83%)	43 (98%)	1 (2%)	58 85
22	V	51/57 (90%)	50 (98%)	1 (2%)	63 87
23	W	130/130 (100%)	126 (97%)	4 (3%)	47 78
24	X	66/74 (89%)	60 (91%)	6 (9%)	12 26
25	Y	120/196 (61%)	114 (95%)	6 (5%)	30 60
26	Z	60/94 (64%)	59 (98%)	1 (2%)	68 90
27	1	46/47 (98%)	46 (100%)	0	100 100
28	2	42/46 (91%)	41 (98%)	1 (2%)	57 85
29	3	79/79 (100%)	77 (98%)	2 (2%)	55 84
All	All	3095/3646 (85%)	2967 (96%)	128 (4%)	37 69

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	2	GLN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	85	GLN
4	D	103	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	73	ASN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	40	ASN
14	N	93	GLN
14	N	107	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN

Continued on next page...

Continued from previous page...

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

5.3.3 RNA

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

All (255) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
30	0	236	A
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	605	C
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	698	A
30	0	701	U
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1151	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1287	A
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1460	G
30	0	1474	C
30	0	1485	A
30	0	1488	U
30	0	1505	U
30	0	1506	U
30	0	1507	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1562	C
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1732	A
30	0	1742	A
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1996	U
30	0	2004	U
30	0	2008	U
30	0	2011	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2320	U
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2467	A
30	0	2469	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2513	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2645	U
30	0	2649	A
30	0	2664	A
30	0	2676	C
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2867	G
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A

Continued on next page...

Continued from previous page...

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

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	169	A
30	0	603	A
30	0	604	G
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	869	G
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1237	U
30	0	1352	A
30	0	1377	C
30	0	1474	C
30	0	1506	U
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1856	C
30	0	1878	G
30	0	1979	G
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2761	A
30	0	2791	U
31	9	65	A

5.4 Non-standard residues in protein, DNA, RNA chains (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	OMU	0	2587	30	12,22,23	1.03	1 (8%)	19,31,34	3.11	2 (10%)
30	OMG	0	2588	30	17,26,27	1.07	1 (5%)	21,38,41	2.50	3 (14%)
30	UR3	0	2619	30	12,22,23	0.71	0	16,32,35	0.75	0
30	PSU	0	2621	30	13,21,22	1.67	2 (15%)	18,30,33	6.18	3 (16%)
30	1MA	0	628	30,34	14,25,26	0.93	1 (7%)	15,37,40	1.17	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,34	-	0/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.05	1.47	1.52
30	0	2587	OMU	C4-N3	2.42	1.37	1.33
30	0	628	1MA	C6-N6	2.45	1.33	1.29
30	0	2621	PSU	C4-N3	2.61	1.37	1.33
30	0	2588	OMG	C6-N1	3.24	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	2621	PSU	N1-C2-N3	-21.86	114.39	128.33
30	0	2588	OMG	C5-C6-N1	-8.61	111.82	123.59
30	0	628	1MA	C2-N3-C4	-3.74	110.60	116.40
30	0	2587	OMU	C5-C4-N3	-3.25	114.77	123.12
30	0	2588	OMG	N3-C2-N1	-2.33	123.89	127.44
30	0	2621	PSU	C6-N1-C2	2.85	120.06	115.47
30	0	2588	OMG	C6-N1-C2	6.54	125.02	115.94
30	0	2587	OMU	C4-N3-C2	12.97	126.98	114.14
30	0	2621	PSU	C4-N3-C2	13.76	127.14	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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%)	1.01	35 (14%) 3 2	26, 50, 86, 109	0
2	B	337/338 (99%)	0.89	19 (5%) 28 26	28, 51, 79, 93	0
3	C	246/246 (100%)	0.82	19 (7%) 16 14	21, 43, 69, 77	0
4	D	140/177 (79%)	3.12	100 (71%) 0 0	56, 98, 124, 134	0
5	E	172/178 (96%)	1.33	36 (20%) 1 1	43, 66, 87, 91	0
6	F	119/120 (99%)	1.37	36 (30%) 1 0	47, 70, 99, 114	0
7	G	29/348 (8%)	2.08	16 (55%) 0 0	75, 93, 103, 106	0
8	H	160/177 (90%)	0.97	20 (12%) 5 4	34, 54, 92, 100	0
9	I	70/162 (43%)	5.97	67 (95%) 0 0	129, 145, 162, 163	0
10	J	142/145 (97%)	0.66	5 (3%) 48 48	34, 48, 70, 91	0
11	K	132/132 (100%)	0.84	10 (7%) 17 15	31, 49, 72, 78	0
12	L	145/165 (87%)	1.66	47 (32%) 1 0	24, 63, 111, 125	0
13	M	194/196 (98%)	0.44	2 (1%) 84 85	28, 40, 55, 64	0
14	N	186/187 (99%)	1.71	64 (34%) 0 0	39, 61, 111, 121	0
15	O	115/116 (99%)	0.64	6 (5%) 31 30	36, 51, 69, 79	0
16	P	143/149 (95%)	0.97	13 (9%) 11 9	37, 53, 67, 76	0
17	Q	95/96 (98%)	0.60	1 (1%) 82 83	33, 43, 59, 76	0
18	R	150/155 (96%)	0.60	2 (1%) 79 79	30, 43, 62, 77	0
19	S	81/85 (95%)	1.36	17 (20%) 1 1	38, 57, 78, 89	0
20	T	119/120 (99%)	1.23	18 (15%) 3 2	37, 54, 86, 111	0
21	U	53/67 (79%)	1.01	7 (13%) 4 4	40, 54, 72, 80	0
22	V	65/71 (91%)	2.43	31 (47%) 0 0	51, 71, 116, 122	0
23	W	154/154 (100%)	0.59	6 (3%) 43 43	32, 48, 64, 77	0
24	X	82/92 (89%)	0.95	6 (7%) 18 16	39, 58, 83, 100	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Y	142/241 (58%)	0.82	11 (7%) 16 14	23, 43, 66, 86	0
26	Z	73/116 (62%)	1.42	23 (31%) 1 0	49, 67, 83, 95	0
27	1	56/57 (98%)	0.73	1 (1%) 71 72	25, 31, 39, 47	0
28	2	46/50 (92%)	1.11	8 (17%) 2 1	31, 59, 88, 100	0
29	3	92/92 (100%)	1.40	23 (25%) 1 1	33, 55, 68, 83	0
30	0	2749/2923 (94%)	0.70	136 (4%) 33 32	19, 42, 87, 162	0
31	9	122/122 (100%)	0.76	11 (9%) 12 9	35, 61, 85, 146	0
All	All	6646/7517 (88%)	0.98	796 (11%) 6 4	19, 49, 98, 163	0

All (796) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	74	ILE	16.9
22	V	1	THR	13.7
9	I	112	LEU	11.7
9	I	128	THR	11.2
9	I	71	ALA	11.1
31	9	1	U	11.1
9	I	70	THR	10.5
4	D	63	ILE	10.3
9	I	132	VAL	10.0
9	I	72	GLU	9.9
14	N	166	ALA	9.9
9	I	66	GLY	9.7
20	T	119	ALA	9.6
9	I	82	THR	9.4
22	V	43	PRO	9.3
19	S	81	ILE	9.2
9	I	111	LEU	8.7
9	I	106	GLN	8.5
9	I	109	PRO	8.5
9	I	130	LEU	8.4
9	I	108	HIS	8.3
9	I	100	VAL	8.3
9	I	73	LEU	8.3
9	I	80	PHE	8.2
9	I	83	GLY	8.1
22	V	39	ALA	8.1
4	D	57	THR	7.9
30	0	1177	A	7.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	69	PRO	7.8
22	V	40	PRO	7.7
4	D	26	GLY	7.7
30	0	1173	A	7.7
30	0	1166	A	7.6
9	I	91	PHE	7.5
4	D	18	ILE	7.5
4	D	69	ILE	7.4
4	D	10	PHE	7.4
9	I	67	VAL	7.4
9	I	79	GLY	7.2
30	0	1200	A	7.2
9	I	99	GLN	7.0
4	D	134	LEU	7.0
30	0	1199	A	7.0
14	N	147	ILE	7.0
30	0	1167	G	7.0
30	0	1162	G	6.9
30	0	1163	G	6.9
30	0	1198	U	6.8
30	0	1172	G	6.8
4	D	64	ARG	6.8
4	D	128	LEU	6.7
30	0	1192	A	6.7
30	0	1190	G	6.7
9	I	102	GLN	6.7
9	I	126	THR	6.6
30	0	1174	A	6.6
4	D	17	ARG	6.5
9	I	129	SER	6.5
9	I	104	ALA	6.5
9	I	88	GLN	6.4
9	I	92	VAL	6.3
30	0	735	C	6.3
9	I	123	VAL	6.3
12	L	91	VAL	6.3
6	F	106	ALA	6.3
30	0	1202	A	6.2
20	T	116	ASP	6.1
30	0	1164	U	6.1
8	H	174	LEU	6.1
9	I	68	PRO	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	86	GLU	6.1
9	I	113	SER	6.1
12	L	99	GLU	5.9
30	0	1175	G	5.9
30	0	1171	A	5.9
9	I	81	GLU	5.9
30	0	1169	U	5.8
4	D	11	HIS	5.8
14	N	81	ALA	5.8
14	N	75	THR	5.7
30	0	1168	C	5.7
30	0	2237	G	5.7
9	I	105	GLU	5.7
30	0	1161	A	5.7
9	I	76	ASP	5.7
30	0	1176	C	5.7
4	D	61	PHE	5.6
9	I	122	GLU	5.6
4	D	70	GLY	5.6
30	0	1181	A	5.6
7	G	23	ILE	5.6
4	D	142	ALA	5.6
30	0	1951	G	5.6
4	D	106	PHE	5.6
9	I	97	VAL	5.5
4	D	23	VAL	5.5
9	I	110	ASP	5.5
1	A	236	GLY	5.5
9	I	127	CYS	5.5
4	D	141	VAL	5.3
9	I	103	ILE	5.3
9	I	87	PRO	5.3
30	0	2769	C	5.3
22	V	46	ILE	5.2
30	0	1170	U	5.2
4	D	135	VAL	5.2
4	D	65	GLU	5.1
12	L	120	LEU	5.1
30	0	1165	G	5.1
30	0	1178	G	5.1
30	0	1193	A	5.1
5	E	154	ILE	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	19	GLU	5.0
4	D	58	VAL	5.0
16	P	67	LYS	5.0
30	0	1197	G	5.0
4	D	73	VAL	5.0
9	I	75	LYS	5.0
9	I	131	GLY	4.9
30	0	1180	U	4.9
30	0	282	C	4.9
12	L	106	VAL	4.9
4	D	44	ILE	4.9
22	V	2	VAL	4.9
9	I	119	ALA	4.9
4	D	13	MET	4.8
4	D	143	LYS	4.7
12	L	73	VAL	4.7
20	T	118	SER	4.7
4	D	139	TYR	4.7
4	D	102	GLY	4.7
26	Z	44	ARG	4.7
31	9	24	U	4.7
20	T	117	ASP	4.6
12	L	89	PHE	4.6
31	9	2	U	4.6
4	D	90	LEU	4.6
12	L	60	GLU	4.6
30	0	1179	C	4.6
9	I	95	LEU	4.6
14	N	76	GLY	4.5
12	L	81	VAL	4.5
30	0	1191	A	4.5
9	I	125	GLY	4.5
29	3	1	MET	4.4
25	Y	235	GLU	4.4
4	D	107	GLY	4.4
22	V	37	GLY	4.4
4	D	56	ARG	4.3
30	0	1947	G	4.3
9	I	120	ALA	4.3
5	E	5	LEU	4.3
4	D	129	ASP	4.3
14	N	115	VAL	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	133	THR	4.2
26	Z	58	ASN	4.2
30	0	2004	U	4.2
1	A	35	GLY	4.2
12	L	80	ASP	4.2
14	N	41	LYS	4.2
9	I	84	SER	4.1
12	L	75	LEU	4.1
30	0	1203	G	4.1
14	N	42	HIS	4.1
4	D	89	PRO	4.1
22	V	45	ARG	4.1
14	N	145	ALA	4.1
1	A	237	GLY	4.1
6	F	28	ALA	4.0
6	F	49	PHE	4.0
29	3	9	THR	4.0
4	D	130	VAL	4.0
12	L	121	ILE	4.0
6	F	75	ILE	4.0
4	D	62	ASP	4.0
30	0	285	A	4.0
14	N	83	LEU	4.0
12	L	123	ASP	4.0
1	A	36	ASP	4.0
14	N	61	ALA	4.0
30	0	1195	G	4.0
4	D	100	ASP	4.0
4	D	41	LEU	4.0
4	D	165	PHE	3.9
4	D	25	MET	3.9
30	0	10	U	3.9
5	E	6	GLU	3.9
30	0	1194	A	3.9
30	0	1207	A	3.9
4	D	88	LEU	3.9
6	F	16	ALA	3.9
9	I	93	ALA	3.9
29	3	22	VAL	3.9
14	N	113	SER	3.9
8	H	37	GLY	3.9
30	0	1186	C	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	Z	42	TYR	3.9
4	D	27	ILE	3.8
5	E	45	ASP	3.8
14	N	159	TYR	3.8
4	D	66	GLY	3.8
22	V	44	GLY	3.8
4	D	55	LYS	3.8
12	L	76	LEU	3.8
30	0	1948	G	3.8
30	0	960	G	3.8
7	G	27	ILE	3.8
8	H	86	TYR	3.8
4	D	99	ASP	3.7
21	U	48	ASN	3.7
22	V	32	ALA	3.7
26	Z	60	ASP	3.7
30	0	1189	A	3.7
1	A	154	ALA	3.7
12	L	77	ALA	3.7
2	B	119	HIS	3.7
28	2	49	GLU	3.7
9	I	107	LYS	3.7
4	D	104	PHE	3.7
5	E	43	ASP	3.7
19	S	77	VAL	3.7
26	Z	49	ARG	3.7
4	D	85	GLN	3.6
4	D	84	LEU	3.6
1	A	99	ILE	3.6
22	V	41	GLU	3.6
12	L	145	LEU	3.6
4	D	75	LEU	3.6
14	N	66	LEU	3.6
30	0	2664	A	3.6
22	V	28	LEU	3.6
30	0	1970	G	3.6
22	V	48	GLU	3.6
29	3	41	GLU	3.6
30	0	1206	U	3.6
26	Z	43	GLY	3.6
30	0	1950	G	3.6
12	L	105	TYR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	133	ASN	3.6
30	0	280	C	3.6
30	0	284	C	3.6
30	0	1208	C	3.6
4	D	171	ASP	3.6
5	E	10	ASP	3.6
31	9	3	A	3.6
4	D	92	GLU	3.6
4	D	98	PHE	3.6
14	N	80	SER	3.5
4	D	157	LEU	3.5
4	D	162	ALA	3.5
30	0	2238	A	3.5
2	B	100	VAL	3.5
16	P	64	GLU	3.5
7	G	63	ARG	3.5
29	3	3	MET	3.5
25	Y	108	ASP	3.5
26	Z	83	TYR	3.5
30	0	283	U	3.5
4	D	137	PRO	3.5
9	I	121	LYS	3.5
9	I	85	GLY	3.5
5	E	7	ILE	3.5
30	0	1949	G	3.4
9	I	78	ALA	3.4
2	B	115	VAL	3.4
12	L	140	VAL	3.4
8	H	74	ARG	3.4
26	Z	34	SER	3.4
11	K	118	ALA	3.4
6	F	91	VAL	3.4
24	X	85	VAL	3.4
26	Z	45	VAL	3.4
4	D	74	THR	3.4
4	D	144	ARG	3.4
22	V	36	ALA	3.4
29	3	15	ASN	3.4
30	0	1201	C	3.4
5	E	122	THR	3.4
6	F	22	VAL	3.4
4	D	47	GLN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	N	148	ALA	3.4
4	D	72	LYS	3.4
30	0	1971	G	3.4
31	9	23	U	3.3
1	A	103	VAL	3.3
14	N	64	SER	3.3
6	F	107	ASP	3.3
9	I	101	LYS	3.3
22	V	38	GLY	3.3
5	E	11	VAL	3.3
1	A	31	LYS	3.3
30	0	272	A	3.3
14	N	137	ALA	3.3
4	D	24	HIS	3.3
14	N	63	SER	3.3
14	N	38	LYS	3.3
6	F	47	LEU	3.3
9	I	90	ASP	3.3
4	D	83	PHE	3.3
26	Z	36	GLY	3.3
4	D	170	TYR	3.3
14	N	74	PRO	3.2
2	B	178	ALA	3.2
4	D	101	THR	3.2
12	L	126	SER	3.2
14	N	67	ALA	3.2
30	0	138	U	3.2
14	N	43	VAL	3.2
22	V	49	LEU	3.2
12	L	124	ASP	3.2
31	9	29	C	3.2
14	N	62	HIS	3.2
14	N	162	ASP	3.2
4	D	105	SER	3.2
19	S	68	LEU	3.2
6	F	109	GLU	3.2
19	S	45	TYR	3.2
20	T	42	VAL	3.2
13	M	1	ALA	3.2
3	C	8	LEU	3.2
1	A	88	ILE	3.1
20	T	63	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	133	VAL	3.1
19	S	47	VAL	3.1
21	U	51	TRP	3.1
22	V	35	ALA	3.1
2	B	337	GLY	3.1
3	C	135	GLU	3.1
29	3	62	THR	3.1
4	D	166	ILE	3.1
9	I	114	TYR	3.1
14	N	163	PHE	3.1
22	V	59	ILE	3.1
26	Z	55	SER	3.1
5	E	1	PRO	3.1
30	0	1184	C	3.1
4	D	156	ARG	3.1
20	T	82	THR	3.1
14	N	179	LEU	3.1
5	E	87	PHE	3.1
8	H	35	LYS	3.1
14	N	139	TRP	3.1
19	S	76	GLU	3.1
4	D	145	ASP	3.1
30	0	736	A	3.1
14	N	150	TYR	3.0
14	N	146	HIS	3.0
30	0	1182	C	3.0
31	9	51	A	3.0
8	H	48	VAL	3.0
14	N	158	LEU	3.0
6	F	99	THR	3.0
14	N	149	GLU	3.0
29	3	77	ALA	3.0
26	Z	35	SER	3.0
22	V	8	ILE	3.0
6	F	113	ASP	3.0
14	N	152	GLU	3.0
4	D	158	ASN	3.0
16	P	77	ALA	3.0
10	J	70	PHE	3.0
1	A	37	VAL	3.0
14	N	116	PHE	3.0
4	D	151	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	N	114	LYS	3.0
19	S	52	VAL	3.0
19	S	24	LEU	3.0
12	L	100	ALA	3.0
7	G	71	LEU	2.9
4	D	148	SER	2.9
30	0	1981	A	2.9
30	0	2345	A	2.9
22	V	31	ARG	2.9
4	D	53	LYS	2.9
6	F	117	GLU	2.9
6	F	115	VAL	2.9
30	0	2349	G	2.9
4	D	80	ALA	2.9
12	L	61	ALA	2.9
30	0	1626	A	2.9
4	D	40	ILE	2.9
29	3	14	CYS	2.9
6	F	17	LEU	2.9
9	I	94	ASP	2.9
13	M	194	GLY	2.9
1	A	38	ILE	2.9
9	I	116	LEU	2.9
30	0	2511	A	2.9
6	F	119	ARG	2.9
1	A	80	LEU	2.8
5	E	156	ASP	2.8
20	T	40	VAL	2.8
22	V	33	VAL	2.8
6	F	114	LYS	2.8
3	C	246	ARG	2.8
7	G	73	ASP	2.8
9	I	77	GLU	2.8
29	3	86	GLY	2.8
30	0	1159	G	2.8
9	I	118	ASN	2.8
14	N	155	GLU	2.8
1	A	83	GLY	2.8
1	A	89	ALA	2.8
12	L	150	GLN	2.8
14	N	40	ASN	2.8
24	X	65	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2884	G	2.8
7	G	72	ASP	2.8
20	T	67	LEU	2.8
21	U	43	GLY	2.8
4	D	29	HIS	2.8
26	Z	46	SER	2.8
12	L	108	VAL	2.8
4	D	42	GLY	2.8
28	2	37	HIS	2.8
4	D	81	GLU	2.8
20	T	65	VAL	2.8
30	0	2254	G	2.8
1	A	153	ARG	2.8
4	D	76	ARG	2.8
23	W	148	ASP	2.8
22	V	5	VAL	2.8
4	D	87	ALA	2.8
6	F	101	ALA	2.8
20	T	55	PHE	2.8
1	A	133	ARG	2.7
16	P	59	ARG	2.7
14	N	184	ILE	2.7
3	C	139	VAL	2.7
2	B	318	ASN	2.7
5	E	138	ILE	2.7
4	D	50	VAL	2.7
30	0	271	C	2.7
8	H	158	ASN	2.7
4	D	16	PRO	2.7
12	L	122	ALA	2.7
14	N	122	ALA	2.7
12	L	69	ILE	2.7
12	L	141	GLU	2.7
28	2	46	ASP	2.7
12	L	118	LEU	2.7
11	K	8	VAL	2.7
15	O	111	VAL	2.7
23	W	65	VAL	2.7
12	L	104	ASP	2.7
29	3	83	TRP	2.7
26	Z	54	GLU	2.7
4	D	22	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	S	19	ASP	2.7
7	G	66	LEU	2.7
30	0	2249	G	2.7
12	L	114	VAL	2.7
26	Z	50	VAL	2.7
14	N	73	ALA	2.7
29	3	13	HIS	2.7
12	L	130	ARG	2.7
6	F	100	ASP	2.7
3	C	138	VAL	2.7
9	I	134	ILE	2.7
16	P	71	TYR	2.7
6	F	19	ALA	2.7
11	K	6	ALA	2.7
25	Y	103	THR	2.7
30	0	2885	A	2.7
1	A	94	LEU	2.6
12	L	142	LEU	2.6
30	0	1946	C	2.6
30	0	370	G	2.6
30	0	2005	G	2.6
30	0	2344	G	2.6
6	F	20	LEU	2.6
19	S	51	GLN	2.6
6	F	102	GLY	2.6
4	D	68	PRO	2.6
14	N	1	ALA	2.6
6	F	105	ASP	2.6
9	I	98	ASP	2.6
8	H	50	ILE	2.6
2	B	105	PHE	2.6
6	F	6	PHE	2.6
16	P	58	SER	2.6
8	H	146	ALA	2.6
19	S	67	ARG	2.6
30	0	1196	C	2.6
19	S	20	PHE	2.6
28	2	39	ARG	2.6
1	A	119	ALA	2.6
20	T	35	TYR	2.6
12	L	147	GLU	2.6
22	V	26	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	14	ASP	2.6
28	2	20	ARG	2.6
7	G	65	THR	2.6
29	3	8	ASN	2.6
30	0	844	A	2.6
30	0	2346	C	2.6
6	F	60	VAL	2.6
3	C	148	VAL	2.6
30	0	2241	C	2.6
14	N	138	ASP	2.5
29	3	12	PRO	2.5
6	F	12	LEU	2.5
30	0	368	C	2.5
30	0	1183	C	2.5
30	0	1279	U	2.5
12	L	96	VAL	2.5
12	L	97	VAL	2.5
26	Z	38	PHE	2.5
30	0	2876	G	2.5
31	9	32	G	2.5
20	T	101	LEU	2.5
30	0	1625	U	2.5
4	D	93	LEU	2.5
5	E	86	VAL	2.5
5	E	72	MET	2.5
7	G	26	MET	2.5
4	D	132	VAL	2.5
14	N	151	ASP	2.5
8	H	140	TYR	2.5
30	0	371	U	2.5
12	L	125	PHE	2.5
8	H	148	HIS	2.5
28	2	35	ARG	2.5
30	0	1967	U	2.5
7	G	15	TRP	2.5
11	K	49	LEU	2.5
22	V	51	LYS	2.5
30	0	2239	C	2.5
4	D	86	THR	2.5
8	H	81	GLY	2.5
20	T	37	GLN	2.5
6	F	110	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	60	PHE	2.5
30	0	281	U	2.5
28	2	28	LYS	2.4
3	C	234	VAL	2.4
5	E	133	VAL	2.4
30	0	1525	G	2.4
7	G	68	GLU	2.4
29	3	91	GLN	2.4
29	3	76	LYS	2.4
22	V	9	ARG	2.4
14	N	160	SER	2.4
14	N	164	ASP	2.4
6	F	24	ARG	2.4
12	L	149	ARG	2.4
14	N	180	LEU	2.4
14	N	118	ILE	2.4
25	Y	217	ILE	2.4
21	U	47	ARG	2.4
30	0	1571	G	2.4
2	B	285	VAL	2.4
31	9	52	A	2.4
2	B	27	ASN	2.4
26	Z	47	ARG	2.4
22	V	6	GLN	2.4
14	N	161	GLY	2.4
4	D	45	THR	2.4
6	F	46	GLU	2.4
3	C	157	LEU	2.4
26	Z	53	ILE	2.4
4	D	131	THR	2.4
16	P	80	ARG	2.4
30	0	1964	U	2.4
30	0	2740	G	2.4
2	B	128	ILE	2.4
5	E	161	VAL	2.4
18	R	133	ALA	2.4
20	T	87	VAL	2.4
30	0	2002	C	2.4
4	D	48	MET	2.3
11	K	45	PRO	2.3
30	0	273	G	2.3
30	0	1837	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	S	41	VAL	2.3
5	E	73	PHE	2.3
24	X	14	LEU	2.3
5	E	100	ASP	2.3
15	O	69	VAL	2.3
11	K	9	THR	2.3
19	S	5	ILE	2.3
30	0	882	A	2.3
30	0	1150	A	2.3
15	O	31	GLU	2.3
24	X	88	GLU	2.3
2	B	93	GLY	2.3
14	N	111	PRO	2.3
20	T	112	LEU	2.3
18	R	130	MET	2.3
30	0	845	U	2.3
14	N	71	TRP	2.3
4	D	154	LYS	2.3
25	Y	109	LEU	2.3
5	E	93	MET	2.3
5	E	123	ASP	2.3
6	F	108	VAL	2.3
23	W	79	VAL	2.3
29	3	69	TYR	2.3
15	O	68	GLY	2.3
1	A	128	LEU	2.3
25	Y	98	GLN	2.3
8	H	114	ASP	2.3
1	A	211	LYS	2.3
7	G	70	ALA	2.3
5	E	22	VAL	2.3
26	Z	79	TRP	2.3
8	H	77	ILE	2.3
1	A	63	GLY	2.3
6	F	27	GLY	2.3
30	0	1965	C	2.3
8	H	70	LEU	2.3
14	N	153	GLN	2.3
7	G	21	ASP	2.3
12	L	117	GLU	2.3
29	3	20	HIS	2.3
30	0	831	U	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1185	U	2.3
1	A	68	ILE	2.3
14	N	110	THR	2.3
30	0	2644	C	2.3
12	L	65	ASP	2.3
8	H	67	ALA	2.3
14	N	45	ALA	2.3
2	B	181	ILE	2.3
2	B	57	GLU	2.2
14	N	68	GLU	2.2
30	0	2883	A	2.2
30	0	1204	C	2.2
12	L	111	ALA	2.2
1	A	91	GLY	2.2
9	I	124	VAL	2.2
25	Y	187	VAL	2.2
1	A	93	THR	2.2
5	E	64	THR	2.2
21	U	13	ILE	2.2
29	3	65	THR	2.2
7	G	67	LEU	2.2
10	J	105	LEU	2.2
1	A	85	SER	2.2
1	A	30	ARG	2.2
21	U	39	ASN	2.2
31	9	45	A	2.2
4	D	59	GLY	2.2
14	N	112	GLY	2.2
5	E	78	GLU	2.2
22	V	25	THR	2.2
1	A	34	ASP	2.2
12	L	95	ASP	2.2
8	H	73	ASN	2.2
3	C	68	ALA	2.2
3	C	124	VAL	2.2
4	D	172	VAL	2.2
19	S	65	VAL	2.2
30	0	1562	C	2.2
24	X	12	ILE	2.2
3	C	62	GLY	2.2
8	H	66	GLU	2.2
12	L	127	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2748	G	2.2
16	P	65	ARG	2.2
2	B	87	TYR	2.2
3	C	64	GLY	2.2
4	D	103	ASN	2.2
29	3	18	GLN	2.2
29	3	92	GLU	2.2
11	K	50	GLY	2.2
30	0	970	U	2.2
25	Y	221	ALA	2.2
20	T	50	VAL	2.2
26	Z	48	ARG	2.2
11	K	86	THR	2.2
21	U	52	THR	2.2
1	A	140	LEU	2.2
2	B	137	LEU	2.2
29	3	67	LEU	2.2
14	N	172	PHE	2.2
30	0	367	G	2.2
30	0	1665	G	2.2
22	V	42	ASN	2.2
3	C	77	ALA	2.2
4	D	54	ALA	2.2
22	V	52	ALA	2.2
12	L	66	VAL	2.2
14	N	142	THR	2.2
28	2	47	THR	2.2
1	A	96	LEU	2.2
3	C	245	GLU	2.2
2	B	286	ASN	2.2
4	D	136	ARG	2.2
30	0	834	G	2.2
30	0	2508	C	2.2
30	0	1188	A	2.2
30	0	1427	A	2.2
30	0	2103	A	2.2
6	F	11	ASP	2.2
14	N	65	ASP	2.2
10	J	63	ILE	2.1
11	K	4	LEU	2.1
3	C	6	TYR	2.1
12	L	90	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	95	ALA	2.1
16	P	10	ALA	2.1
19	S	78	ALA	2.1
27	1	8	GLN	2.1
30	0	734	U	2.1
30	0	1561	U	2.1
11	K	132	VAL	2.1
30	0	2828	G	2.1
3	C	60	SER	2.1
25	Y	226	ILE	2.1
31	9	47	A	2.1
5	E	8	PRO	2.1
23	W	117	ARG	2.1
24	X	80	GLU	2.1
1	A	229	ALA	2.1
4	D	71	ALA	2.1
1	A	82	VAL	2.1
7	G	24	VAL	2.1
4	D	150	SER	2.1
14	N	102	LEU	2.1
14	N	182	GLY	2.1
26	Z	39	GLY	2.1
1	A	65	ARG	2.1
1	A	223	ARG	2.1
2	B	121	PRO	2.1
5	E	155	ASN	2.1
30	0	765	G	2.1
30	0	1929	G	2.1
5	E	12	ASP	2.1
9	I	115	ASP	2.1
3	C	75	GLY	2.1
5	E	46	THR	2.1
8	H	90	LEU	2.1
9	I	96	SER	2.1
10	J	45	VAL	2.1
14	N	87	LEU	2.1
25	Y	174	VAL	2.1
3	C	31	ILE	2.1
4	D	15	GLU	2.1
14	N	39	SER	2.1
16	P	116	SER	2.1
30	0	1788	U	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	130	C	2.1
30	0	2335	C	2.1
6	F	90	GLU	2.1
10	J	142	ASN	2.1
6	F	76	PHE	2.1
14	N	119	GLN	2.1
22	V	56	ILE	2.1
15	O	23	GLY	2.1
16	P	76	GLY	2.1
22	V	3	LEU	2.1
23	W	150	LEU	2.1
1	A	158	VAL	2.1
2	B	112	THR	2.1
5	E	29	VAL	2.1
5	E	42	VAL	2.1
12	L	119	THR	2.1
5	E	118	ILE	2.1
30	0	2009	G	2.1
4	D	39	ASP	2.1
12	L	79	ASP	2.1
30	0	1205	U	2.1
4	D	38	GLU	2.1
4	D	43	GLU	2.1
19	S	50	GLU	2.1
26	Z	59	GLU	2.1
5	E	128	GLY	2.1
15	O	27	GLY	2.1
29	3	10	TYR	2.1
12	L	129	ALA	2.1
17	Q	16	ASN	2.0
5	E	20	ILE	2.0
30	0	1130	U	2.0
30	0	2537	G	2.0
3	C	66	GLY	2.0
5	E	56	ALA	2.0
26	Z	40	ALA	2.0
4	D	159	PRO	2.0
16	P	63	ARG	2.0
16	P	69	ARG	2.0
30	0	1209	C	2.0
2	B	114	ASP	2.0
25	Y	96	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	H	125	GLY	2.0
5	E	51	SER	2.0
14	N	165	ALA	2.0
30	0	2874	G	2.0
30	0	372	A	2.0
30	0	1836	A	2.0
20	T	32	ARG	2.0
23	W	35	VAL	2.0
5	E	75	GLY	2.0
30	0	298	C	2.0
30	0	1000	C	2.0
7	G	69	ARG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
30	OMU	0	2587	21/22	0.92	0.20	-	29,32,34,36	0
30	UR3	0	2619	21/22	0.93	0.23	-	34,37,39,43	0
30	1MA	0	628	23/24	0.94	0.23	-	22,25,28,28	0
30	OMG	0	2588	24/25	0.91	0.22	-	28,32,34,36	0
30	PSU	0	2621	20/21	0.93	0.22	-	24,26,33,33	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
34	NA	0	8565	1/1	0.81	1.05	60.85	57,57,57,57	0
34	NA	0	8562	1/1	0.64	0.52	54.23	62,62,62,62	0
34	NA	0	8547	1/1	0.82	0.77	36.85	51,51,51,51	0
34	NA	0	8546	1/1	-0.16	1.24	29.61	77,77,77,77	0
33	K	0	8401	1/1	0.51	0.51	24.89	88,88,88,88	0
34	NA	0	8567	1/1	0.84	0.62	23.62	65,65,65,65	0
32	MG	0	8041	1/1	0.93	0.38	18.87	19,19,19,19	0
34	NA	0	8542	1/1	0.82	0.44	18.70	42,42,42,42	0
34	NA	0	8555	1/1	0.84	0.79	18.69	61,61,61,61	0
34	NA	0	8552	1/1	0.52	0.54	14.80	59,59,59,59	0
32	MG	A	8051	1/1	0.77	0.43	14.59	72,72,72,72	0
34	NA	0	8527	1/1	0.86	0.38	14.51	43,43,43,43	0
34	NA	0	8517	1/1	0.81	0.43	14.49	31,31,31,31	0
34	NA	0	8563	1/1	0.94	0.40	14.22	65,65,65,65	0
32	MG	0	8047	1/1	0.96	0.40	12.81	44,44,44,44	0
34	NA	9	8572	1/1	0.83	0.46	12.09	64,64,64,64	0
34	NA	0	8535	1/1	0.24	0.38	10.16	46,46,46,46	0
34	NA	R	8575	1/1	0.62	0.57	9.96	82,82,82,82	0
34	NA	0	8560	1/1	0.71	0.56	9.84	92,92,92,92	0
36	SR	B	8987	1/1	0.44	0.62	8.90	200,200,200,200	0
34	NA	0	8569	1/1	0.84	0.51	8.21	53,53,53,53	0
34	NA	0	8553	1/1	0.90	0.39	7.46	67,67,67,67	0
34	NA	0	8559	1/1	0.80	0.30	7.18	71,71,71,71	0
35	CL	0	8815	1/1	0.65	0.27	6.99	58,58,58,58	0
34	NA	0	8530	1/1	0.85	0.30	6.98	47,47,47,47	0
34	NA	0	8504	1/1	0.77	0.32	6.98	33,33,33,33	0
34	NA	0	8550	1/1	0.86	0.26	6.87	55,55,55,55	0
34	NA	0	8568	1/1	0.75	0.41	6.83	53,53,53,53	0
34	NA	0	8502	1/1	0.68	0.26	4.81	55,55,55,55	0
34	NA	0	8523	1/1	0.50	0.29	4.24	29,29,29,29	0
34	NA	0	8512	1/1	0.96	0.30	3.53	38,38,38,38	0
33	K	0	8402	1/1	0.92	0.26	3.05	62,62,62,62	0
34	NA	0	8519	1/1	0.85	0.25	2.89	36,36,36,36	0
34	NA	0	8508	1/1	0.91	0.26	2.31	39,39,39,39	0
32	MG	0	8011	1/1	0.85	0.32	2.27	24,24,24,24	0
32	MG	0	8004	1/1	0.90	0.26	2.10	21,21,21,21	0
34	NA	0	8534	1/1	0.84	0.27	2.04	25,25,25,25	0
34	NA	0	8556	1/1	0.83	0.33	1.54	41,41,41,41	0
32	MG	0	8085	1/1	0.82	0.28	1.49	73,73,73,73	0
32	MG	0	8062	1/1	0.72	0.27	1.40	47,47,47,47	0
34	NA	Q	8540	1/1	0.73	0.29	1.15	41,41,41,41	0
34	NA	0	8521	1/1	0.77	0.24	0.99	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	NA	0	8564	1/1	0.87	0.23	0.93	63,63,63,63	0
34	NA	0	8520	1/1	0.93	0.23	0.75	54,54,54,54	0
36	SR	A	8929	1/1	0.94	0.24	0.71	113,113,113,113	0
35	CL	O	8808	1/1	0.94	0.27	0.70	62,62,62,62	0
32	MG	0	8087	1/1	0.69	0.23	0.70	31,31,31,31	0
32	MG	0	8012	1/1	0.91	0.23	0.02	22,22,22,22	0
36	SR	0	8903	1/1	0.89	0.19	-0.13	45,45,45,45	0
34	NA	C	8503	1/1	0.92	0.21	-0.18	31,31,31,31	0
34	NA	0	8522	1/1	0.83	0.25	-0.34	58,58,58,58	0
35	CL	B	8819	1/1	0.80	0.24	-0.42	50,50,50,50	0
34	NA	J	8538	1/1	0.46	0.22	-0.49	57,57,57,57	0
36	SR	R	8912	1/1	0.90	0.20	-0.70	73,73,73,73	0
32	MG	0	8044	1/1	0.91	0.20	-0.71	46,46,46,46	0
32	MG	0	8009	1/1	0.82	0.20	-0.72	19,19,19,19	0
32	MG	0	8001	1/1	0.82	0.21	-0.99	29,29,29,29	0
36	SR	0	8904	1/1	0.92	0.18	-1.13	49,49,49,49	0
34	NA	0	8515	1/1	0.94	0.19	-1.18	35,35,35,35	0
32	MG	0	8028	1/1	0.94	0.17	-1.21	18,18,18,18	0
35	CL	J	8821	1/1	0.82	0.20	-1.22	59,59,59,59	0
37	CD	Z	8703	1/1	0.90	0.10	-1.24	71,71,71,71	0
36	SR	0	8972	1/1	0.91	0.15	-1.32	112,112,112,112	0
32	MG	0	8008	1/1	0.89	0.16	-1.34	23,23,23,23	0
34	NA	0	8557	1/1	0.88	0.14	-1.49	68,68,68,68	0
34	NA	0	8507	1/1	0.90	0.17	-1.64	40,40,40,40	0
35	CL	0	8805	1/1	0.85	0.13	-1.66	58,58,58,58	0
36	SR	0	8902	1/1	0.92	0.21	-1.67	58,58,58,58	0
32	MG	0	8053	1/1	0.86	0.16	-1.70	53,53,53,53	0
34	NA	R	8532	1/1	0.88	0.17	-1.89	48,48,48,48	0
32	MG	B	8043	1/1	0.72	0.10	-2.03	48,48,48,48	0
34	NA	0	8537	1/1	0.92	0.14	-2.03	32,32,32,32	0
32	MG	B	8042	1/1	0.69	0.12	-2.04	47,47,47,47	0
32	MG	T	8057	1/1	0.74	0.17	-2.06	58,58,58,58	0
36	SR	0	8935	1/1	0.96	0.13	-2.07	68,68,68,68	0
32	MG	0	8045	1/1	0.86	0.17	-2.12	39,39,39,39	0
32	MG	A	8050	1/1	0.85	0.14	-2.18	24,24,24,24	0
32	MG	0	8003	1/1	0.81	0.18	-2.18	26,26,26,26	0
32	MG	0	8088	1/1	0.78	0.13	-2.20	34,34,34,34	0
36	SR	0	8943	1/1	0.67	0.13	-2.24	104,104,104,104	0
37	CD	U	8701	1/1	0.95	0.12	-2.27	51,51,51,51	0
36	SR	0	8985	1/1	0.75	0.15	-2.33	118,118,118,118	0
35	CL	0	8812	1/1	0.81	0.14	-2.43	40,40,40,40	0
37	CD	1	8702	1/1	0.86	0.08	-2.45	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	MG	0	8034	1/1	0.93	0.13	-2.67	36,36,36,36	0
36	SR	1	8913	1/1	0.90	0.10	-2.80	78,78,78,78	0
36	SR	0	8978	1/1	0.74	0.11	-3.14	108,108,108,108	0
32	MG	0	8084	1/1	0.97	0.09	-3.19	27,27,27,27	0
36	SR	0	8992	1/1	0.88	0.18	-3.28	125,125,125,125	0
36	SR	0	8975	1/1	0.78	0.11	-3.34	120,120,120,120	0
34	NA	0	8533	1/1	0.71	0.13	-3.39	55,55,55,55	0
36	SR	0	8964	1/1	0.87	0.10	-3.50	110,110,110,110	0
37	CD	3	8704	1/1	0.95	0.07	-3.52	64,64,64,64	0
32	MG	0	8058	1/1	0.88	0.11	-3.70	25,25,25,25	0
36	SR	3	8932	1/1	0.86	0.10	-3.75	67,67,67,67	0
36	SR	0	8926	1/1	0.96	0.12	-3.76	107,107,107,107	0
34	NA	0	8528	1/1	0.95	0.13	-3.82	40,40,40,40	0
34	NA	M	8539	1/1	0.91	0.16	-3.88	33,33,33,33	0
32	MG	0	8075	1/1	0.88	0.12	-4.03	49,49,49,49	0
32	MG	Y	8086	1/1	0.94	0.13	-4.12	33,33,33,33	0
32	MG	0	8006	1/1	0.90	0.12	-4.40	23,23,23,23	0
32	MG	0	8025	1/1	0.95	0.11	-4.48	31,31,31,31	0
35	CL	M	8818	1/1	0.97	0.14	-4.76	33,33,33,33	0
35	CL	3	8804	1/1	0.97	0.08	-4.82	53,53,53,53	0
32	MG	0	8014	1/1	0.91	0.16	-4.95	19,19,19,19	0
36	SR	0	8970	1/1	0.49	0.15	-4.98	115,115,115,115	0
36	SR	0	8949	1/1	0.91	0.11	-5.38	90,90,90,90	0
32	MG	0	8052	1/1	0.86	0.12	-5.46	38,38,38,38	0
32	MG	0	8070	1/1	0.89	0.14	-5.60	40,40,40,40	0
36	SR	0	8945	1/1	0.89	0.12	-5.92	105,105,105,105	0
32	MG	0	8013	1/1	0.96	0.06	-6.12	24,24,24,24	0
32	MG	0	8065	1/1	0.80	0.14	-6.15	47,47,47,47	0
36	SR	0	8969	1/1	0.84	0.13	-6.85	134,134,134,134	0
36	SR	0	8936	1/1	0.86	0.11	-7.04	84,84,84,84	0
36	SR	0	8944	1/1	0.67	0.14	-7.83	161,161,161,161	0
36	SR	0	8918	1/1	0.91	0.15	-8.18	76,76,76,76	0
36	SR	0	8910	1/1	0.87	0.12	-10.30	84,84,84,84	0
32	MG	0	8002	1/1	0.92	0.11	-11.00	21,21,21,21	0
32	MG	0	8078	1/1	0.85	0.51	-	43,43,43,43	0
32	MG	0	8017	1/1	0.72	0.25	-	23,23,23,23	0
32	MG	0	8019	1/1	0.88	0.20	-	20,20,20,20	0
36	SR	0	8947	1/1	0.64	0.27	-	178,178,178,178	0
36	SR	0	9002	1/1	0.69	0.21	-	175,175,175,175	0
35	CL	0	8816	1/1	0.92	0.15	-	54,54,54,54	0
36	SR	0	8933	1/1	0.47	0.17	-	127,127,127,127	0
36	SR	0	8905	1/1	0.64	0.24	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	NA	0	8509	1/1	0.54	0.28	-	50,50,50,50	0
32	MG	0	8083	1/1	0.89	0.40	-	55,55,55,55	0
32	MG	0	8066	1/1	0.87	0.13	-	57,57,57,57	0
36	SR	0	8960	1/1	0.55	0.14	-	141,141,141,141	0
32	MG	0	8068	1/1	0.92	0.17	-	64,64,64,64	0
32	MG	0	8036	1/1	0.45	0.21	-	49,49,49,49	0
34	NA	0	8516	1/1	0.56	0.32	-	28,28,28,28	0
36	SR	0	8990	1/1	0.95	0.18	-	113,113,113,113	0
34	NA	0	8529	1/1	0.83	0.17	-	38,38,38,38	0
34	NA	0	8541	1/1	0.61	0.39	-	50,50,50,50	0
36	SR	0	8916	1/1	0.68	0.10	-	98,98,98,98	0
36	SR	0	8955	1/1	0.53	0.30	-	189,189,189,189	0
36	SR	0	8922	1/1	0.66	0.44	-	160,160,160,160	0
34	NA	0	8514	1/1	0.75	0.38	-	41,41,41,41	0
36	SR	0	8971	1/1	0.36	0.21	-	165,165,165,165	0
36	SR	3	8999	1/1	0.93	0.12	-	93,93,93,93	0
36	SR	0	8988	1/1	0.43	0.20	-	158,158,158,158	0
32	MG	0	8020	1/1	0.87	0.10	-	38,38,38,38	0
34	NA	0	8558	1/1	0.79	0.53	-	44,44,44,44	0
36	SR	0	9006	1/1	0.23	1.35	-	200,200,200,200	0
32	MG	0	8035	1/1	0.93	0.18	-	62,62,62,62	0
36	SR	0	8914	1/1	0.90	0.31	-	107,107,107,107	0
34	NA	0	8506	1/1	0.76	0.47	-	66,66,66,66	0
32	MG	0	8005	1/1	0.93	0.22	-	29,29,29,29	0
36	SR	0	8928	1/1	0.89	0.13	-	125,125,125,125	0
35	CL	A	8809	1/1	0.76	0.24	-	60,60,60,60	0
36	SR	0	8967	1/1	0.68	0.14	-	116,116,116,116	0
36	SR	0	8907	1/1	0.84	0.21	-	53,53,53,53	0
34	NA	0	8518	1/1	0.97	0.42	-	65,65,65,65	0
32	MG	0	8073	1/1	0.83	0.15	-	79,79,79,79	0
36	SR	B	8950	1/1	0.97	0.17	-	101,101,101,101	0
34	NA	9	8543	1/1	0.64	0.15	-	47,47,47,47	0
32	MG	0	8082	1/1	0.98	0.17	-	56,56,56,56	0
35	CL	R	8806	1/1	0.95	0.19	-	42,42,42,42	0
36	SR	0	8962	1/1	0.75	0.41	-	164,164,164,164	0
35	CL	0	8813	1/1	0.93	0.08	-	44,44,44,44	0
36	SR	0	8954	1/1	0.83	0.16	-	94,94,94,94	0
34	NA	0	8574	1/1	0.75	0.71	-	61,61,61,61	0
32	MG	0	8091	1/1	0.95	0.11	-	54,54,54,54	0
32	MG	0	8090	1/1	0.94	0.19	-	55,55,55,55	0
32	MG	0	8071	1/1	0.83	0.19	-	53,53,53,53	0
35	CL	0	8811	1/1	0.84	0.16	-	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	MG	0	8033	1/1	0.86	0.12	-	51,51,51,51	0
34	NA	0	8561	1/1	0.93	0.49	-	68,68,68,68	0
32	MG	0	8076	1/1	0.97	0.14	-	32,32,32,32	0
36	SR	0	8997	1/1	0.09	1.28	-	190,190,190,190	0
32	MG	0	8056	1/1	0.80	0.20	-	41,41,41,41	0
36	SR	0	8994	1/1	0.74	0.57	-	198,198,198,198	0
35	CL	J	8801	1/1	0.86	0.16	-	54,54,54,54	0
32	MG	0	8023	1/1	0.74	0.15	-	18,18,18,18	0
36	SR	A	8930	1/1	0.97	0.06	-	100,100,100,100	0
36	SR	0	8923	1/1	0.80	0.07	-	85,85,85,85	0
32	MG	0	8031	1/1	0.87	0.33	-	55,55,55,55	0
36	SR	0	8959	1/1	0.72	0.32	-	159,159,159,159	0
32	MG	0	8092	1/1	0.42	0.17	-	51,51,51,51	0
32	MG	0	8024	1/1	0.97	0.19	-	61,61,61,61	0
32	MG	9	8074	1/1	0.86	0.29	-	74,74,74,74	0
36	SR	S	8961	1/1	0.61	0.13	-	113,113,113,113	0
34	NA	0	8566	1/1	0.66	0.44	-	58,58,58,58	0
35	CL	Y	8820	1/1	0.95	0.13	-	38,38,38,38	0
36	SR	0	8953	1/1	0.93	0.18	-	143,143,143,143	0
36	SR	A	8977	1/1	0.07	0.20	-	158,158,158,158	0
36	SR	0	8942	1/1	0.89	0.16	-	115,115,115,115	0
32	MG	0	8016	1/1	0.89	0.34	-	43,43,43,43	0
36	SR	0	8920	1/1	0.78	0.07	-	113,113,113,113	0
32	MG	0	8022	1/1	0.73	0.15	-	32,32,32,32	0
36	SR	0	8948	1/1	0.84	0.12	-	77,77,77,77	0
32	MG	0	8081	1/1	0.50	0.41	-	64,64,64,64	0
36	SR	0	8937	1/1	0.63	0.25	-	103,103,103,103	0
36	SR	0	8958	1/1	0.84	0.16	-	86,86,86,86	0
36	SR	9	8980	1/1	0.59	0.28	-	177,177,177,177	0
32	MG	0	8038	1/1	0.94	0.14	-	68,68,68,68	0
35	CL	0	8803	1/1	0.90	0.11	-	50,50,50,50	0
36	SR	0	9007	1/1	0.54	0.69	-	200,200,200,200	0
35	CL	0	8817	1/1	0.79	0.12	-	50,50,50,50	0
36	SR	0	8991	1/1	0.85	0.20	-	188,188,188,188	0
34	NA	0	8544	1/1	0.79	0.29	-	64,64,64,64	0
34	NA	0	8571	1/1	0.28	0.29	-	73,73,73,73	0
36	SR	0	8951	1/1	0.91	0.14	-	132,132,132,132	0
32	MG	0	8048	1/1	0.88	0.25	-	27,27,27,27	0
32	MG	0	8046	1/1	0.82	0.21	-	28,28,28,28	0
36	SR	0	8983	1/1	0.67	0.17	-	177,177,177,177	0
32	MG	0	8080	1/1	0.68	0.37	-	66,66,66,66	0
36	SR	0	8941	1/1	0.59	0.17	-	113,113,113,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	NA	0	8548	1/1	0.68	0.26	-	59,59,59,59	0
34	NA	0	8573	1/1	0.76	0.19	-	69,69,69,69	0
36	SR	0	8957	1/1	0.79	0.31	-	188,188,188,188	0
32	MG	0	8089	1/1	0.27	0.33	-	40,40,40,40	0
32	MG	0	8079	1/1	0.68	0.34	-	50,50,50,50	0
36	SR	0	8919	1/1	0.65	0.25	-	173,173,173,173	0
34	NA	0	8525	1/1	0.62	0.38	-	79,79,79,79	0
32	MG	0	8039	1/1	0.90	0.39	-	64,64,64,64	0
36	SR	J	8986	1/1	0.16	1.09	-	200,200,200,200	0
32	MG	0	8049	1/1	0.81	0.48	-	65,65,65,65	0
32	MG	0	8069	1/1	0.82	0.50	-	65,65,65,65	0
36	SR	0	8984	1/1	0.94	0.10	-	105,105,105,105	0
32	MG	0	8027	1/1	0.92	0.11	-	39,39,39,39	0
36	SR	0	8979	1/1	0.72	0.22	-	199,199,199,199	0
36	SR	0	8906	1/1	0.89	0.26	-	52,52,52,52	0
32	MG	0	8055	1/1	0.85	0.19	-	30,30,30,30	0
36	SR	0	8996	1/1	0.89	0.60	-	200,200,200,200	0
32	MG	0	8059	1/1	0.66	0.13	-	35,35,35,35	0
32	MG	0	8010	1/1	0.59	0.20	-	23,23,23,23	0
32	MG	0	8029	1/1	0.85	0.14	-	52,52,52,52	0
32	MG	0	8093	1/1	0.90	0.14	-	29,29,29,29	0
36	SR	0	8901	1/1	0.82	0.15	-	73,73,73,73	0
36	SR	0	9001	1/1	0.60	0.16	-	171,171,171,171	0
36	SR	0	8998	1/1	0.60	0.40	-	171,171,171,171	0
34	NA	0	8549	1/1	0.80	0.30	-	58,58,58,58	0
36	SR	0	8965	1/1	0.39	0.13	-	117,117,117,117	0
36	SR	0	8946	1/1	0.82	0.12	-	102,102,102,102	0
32	MG	0	8007	1/1	0.80	0.21	-	27,27,27,27	0
34	NA	0	8505	1/1	0.91	0.43	-	45,45,45,45	0
36	SR	0	8911	1/1	0.96	0.06	-	74,74,74,74	0
36	SR	0	8963	1/1	0.90	0.13	-	105,105,105,105	0
34	NA	0	8501	1/1	0.98	0.18	-	24,24,24,24	0
36	SR	0	9000	1/1	0.20	0.24	-	157,157,157,157	0
36	SR	F	9005	1/1	0.91	0.07	-	122,122,122,122	0
32	MG	0	8030	1/1	0.89	0.33	-	60,60,60,60	0
36	SR	0	8982	1/1	0.83	1.09	-	189,189,189,189	0
36	SR	0	8940	1/1	0.95	0.17	-	70,70,70,70	0
34	NA	0	8513	1/1	0.86	0.25	-	45,45,45,45	0
34	NA	0	8545	1/1	0.94	0.22	-	38,38,38,38	0
32	MG	0	8018	1/1	0.86	0.23	-	36,36,36,36	0
36	SR	0	8981	1/1	0.93	0.17	-	153,153,153,153	0
36	SR	0	8909	1/1	0.78	0.14	-	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
36	SR	0	8908	1/1	0.75	0.13	-	80,80,80,80	0
36	SR	0	8939	1/1	0.62	0.26	-	146,146,146,146	0
36	SR	0	8934	1/1	0.90	0.30	-	108,108,108,108	0
36	SR	0	8917	1/1	0.96	0.11	-	95,95,95,95	0
35	CL	0	8822	1/1	0.85	0.45	-	74,74,74,74	0
36	SR	0	8976	1/1	0.65	0.48	-	194,194,194,194	0
34	NA	0	8511	1/1	0.91	0.32	-	63,63,63,63	0
35	CL	N	8807	1/1	0.89	0.29	-	68,68,68,68	0
34	NA	0	8526	1/1	0.96	0.21	-	46,46,46,46	0
36	SR	0	8995	1/1	0.88	0.09	-	117,117,117,117	0
32	MG	0	8037	1/1	0.56	0.39	-	89,89,89,89	0
36	SR	0	8974	1/1	0.22	0.47	-	166,166,166,166	0
35	CL	0	8814	1/1	0.94	0.19	-	48,48,48,48	0
36	SR	1	8952	1/1	0.97	0.11	-	74,74,74,74	0
32	MG	0	8040	1/1	0.16	0.89	-	84,84,84,84	0
34	NA	0	8536	1/1	0.93	0.15	-	44,44,44,44	0
32	MG	0	8064	1/1	0.72	0.22	-	43,43,43,43	0
34	NA	0	8570	1/1	0.77	0.25	-	44,44,44,44	0
36	SR	0	8956	1/1	0.89	0.07	-	128,128,128,128	0
32	MG	0	8067	1/1	0.62	0.30	-	26,26,26,26	0
34	NA	0	8531	1/1	0.79	0.12	-	41,41,41,41	0
32	MG	0	8021	1/1	0.96	0.06	-	31,31,31,31	0
32	MG	0	8063	1/1	0.90	0.12	-	69,69,69,69	0
36	SR	0	8968	1/1	0.41	0.15	-	146,146,146,146	0
32	MG	0	8015	1/1	0.95	0.10	-	27,27,27,27	0
32	MG	0	8032	1/1	0.93	0.08	-	36,36,36,36	0
34	NA	0	8554	1/1	0.82	0.86	-	63,63,63,63	0
32	MG	K	8054	1/1	0.74	0.16	-	37,37,37,37	0
36	SR	0	8989	1/1	0.89	0.27	-	168,168,168,168	0
32	MG	0	8061	1/1	0.90	0.24	-	29,29,29,29	0
35	CL	L	8810	1/1	0.86	0.17	-	50,50,50,50	0
37	CD	O	8705	1/1	0.94	0.09	-	83,83,83,83	0
32	MG	0	8072	1/1	0.88	0.20	-	53,53,53,53	0
32	MG	0	8026	1/1	0.92	0.11	-	27,27,27,27	0
36	SR	0	9004	1/1	0.77	0.40	-	200,200,200,200	0
36	SR	0	8915	1/1	0.85	0.09	-	115,115,115,115	0
36	SR	0	8921	1/1	0.93	0.17	-	84,84,84,84	0
36	SR	0	8966	1/1	0.92	0.06	-	100,100,100,100	0
36	SR	0	8927	1/1	0.62	0.22	-	150,150,150,150	0
35	CL	J	8802	1/1	0.84	0.16	-	56,56,56,56	0
36	SR	0	8924	1/1	0.66	0.16	-	134,134,134,134	0
36	SR	0	8973	1/1	0.78	0.16	-	121,121,121,121	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
36	SR	0	8931	1/1	0.77	0.13	-	94,94,94,94	0
34	NA	0	8524	1/1	0.82	0.24	-	41,41,41,41	0
36	SR	0	9008	1/1	0.89	0.21	-	85,85,85,85	0
36	SR	0	8938	1/1	0.85	0.09	-	139,139,139,139	0
32	MG	0	8060	1/1	0.54	0.19	-	54,54,54,54	0
34	NA	0	8551	1/1	0.89	0.19	-	47,47,47,47	0
34	NA	S	8510	1/1	0.91	0.13	-	34,34,34,34	0
36	SR	9	9003	1/1	0.69	0.17	-	169,169,169,169	0
36	SR	0	8925	1/1	0.95	0.14	-	84,84,84,84	0
36	SR	0	8993	1/1	0.70	0.20	-	165,165,165,165	0
32	MG	0	8077	1/1	0.84	0.15	-	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.