



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:32 PM UTC

PDB ID : 3CCE / pdb_00003cce
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation U2535A
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-25
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

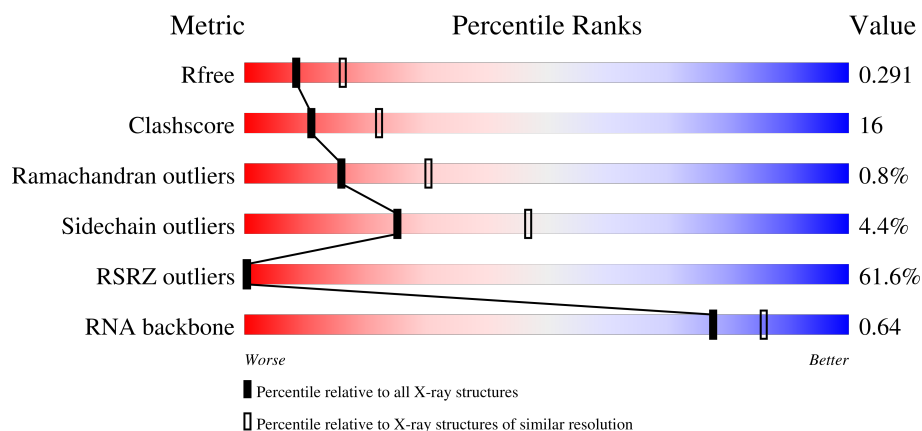
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)
RNA backbone	3983	1179 (3.00-2.52)

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

Mol	Chain	Length	Quality of chain
1	A	240	84% 63% 30% 6%
2	B	338	76% 61% 34% 5%
3	C	246	28% 64% 32%
4	D	177	67% 38% 37% 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	8037	-	-	-	X
32	MG	0	8063	-	-	-	X
33	CL	0	8814	-	-	-	X
33	CL	J	8801	-	-	X	-
33	CL	J	8802	-	-	X	-
34	SR	0	8974	-	-	-	X
35	NA	0	8518	-	-	-	X
35	NA	0	8548	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8566	-	-	-	X
35	NA	0	8569	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99124 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
			59022	26350	10876	19051	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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	2	Total	Mg	0	0
			2	2		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	0	86	Total	Mg	0	0
			86	86		
32	9	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	J	3	Total Cl 3 3	0	0
33	L	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	Q	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	0	10	Total Cl 10 10	0	0

- Molecule 34 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	3	Total Sr 3 3	0	0
34	B	2	Total Sr 2 2	0	0
34	F	1	Total Sr 1 1	0	0
34	R	1	Total Sr 1 1	0	0
34	S	1	Total Sr 1 1	0	0
34	1	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	0	92	Total Sr 92 92	0	0
34	9	4	Total Sr 4 4	0	0

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	118	Total 118	O 118	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	B	144	Total 144	O 144	0	0
38	C	179	Total 179	O 179	0	0
38	D	46	Total 46	O 46	0	0
38	E	40	Total 40	O 40	0	0
38	F	27	Total 27	O 27	0	0
38	G	19	Total 19	O 19	0	0
38	H	68	Total 68	O 68	0	0
38	I	5	Total 5	O 5	0	0
38	J	55	Total 55	O 55	0	0
38	K	52	Total 52	O 52	0	0
38	L	84	Total 84	O 84	0	0
38	M	127	Total 127	O 127	0	0
38	N	63	Total 63	O 63	0	0
38	O	40	Total 40	O 40	0	0
38	P	61	Total 61	O 61	0	0
38	Q	43	Total 43	O 43	0	0
38	R	84	Total 84	O 84	0	0
38	S	33	Total 33	O 33	0	0
38	T	33	Total 33	O 33	0	0
38	U	28	Total 28	O 28	0	0
38	V	14	Total 14	O 14	0	0

Continued on next page...

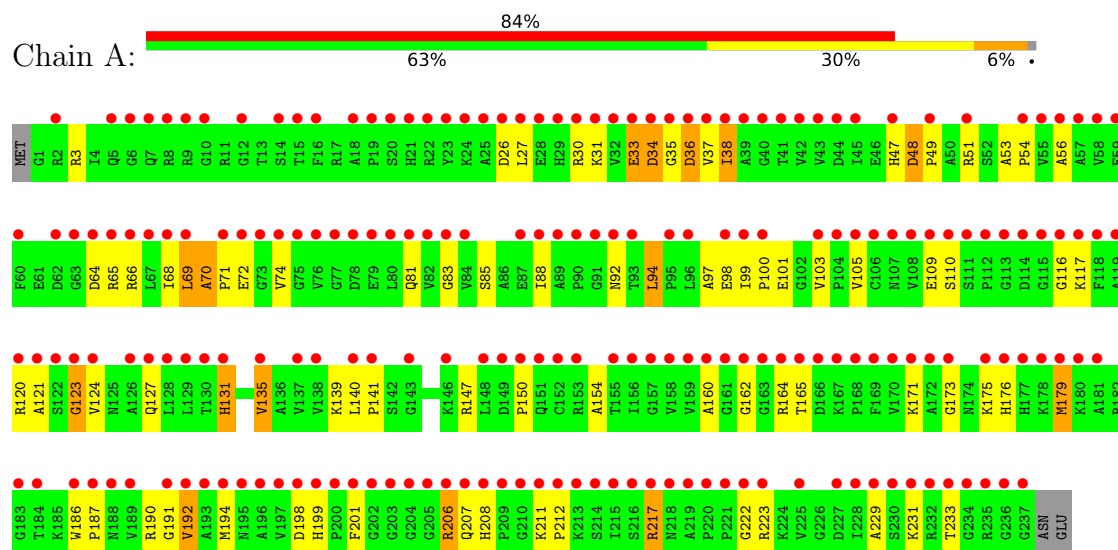
Continued from previous page...

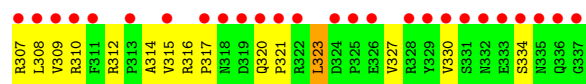
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	W	67	Total 67	O 67	0	0
38	X	30	Total 30	O 30	0	0
38	Y	100	Total 100	O 100	0	0
38	Z	32	Total 32	O 32	0	0
38	1	55	Total 55	O 55	0	0
38	2	42	Total 42	O 42	0	0
38	3	63	Total 63	O 63	0	0
38	0	5927	Total 5927	O 5927	0	0
38	9	144	Total 144	O 144	0	0

3 Residue-property plots [i](#)

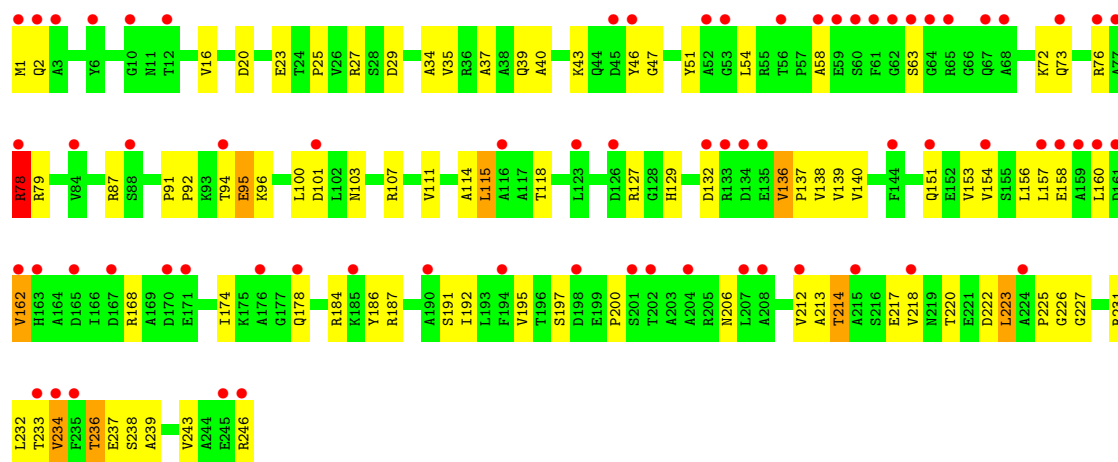
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 50S ribosomal protein L2P





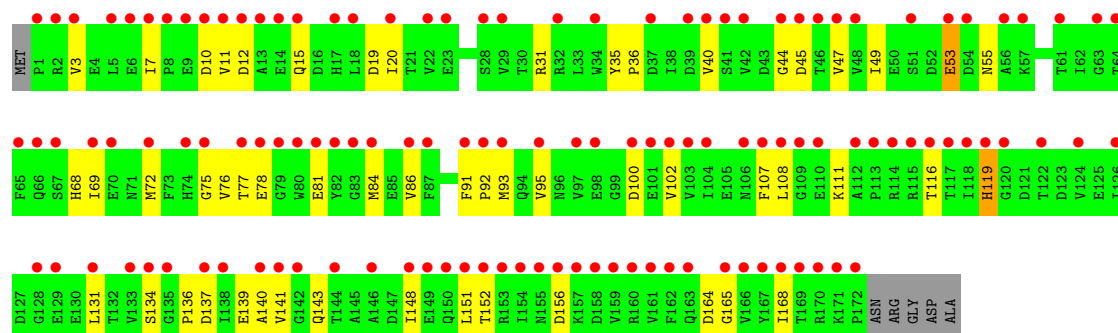
• Molecule 3: 50S ribosomal protein L4P



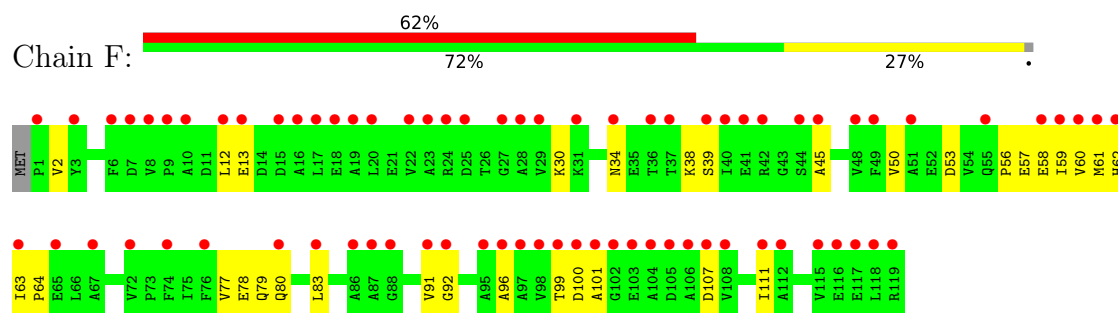
• Molecule 4: 50S ribosomal protein L5P



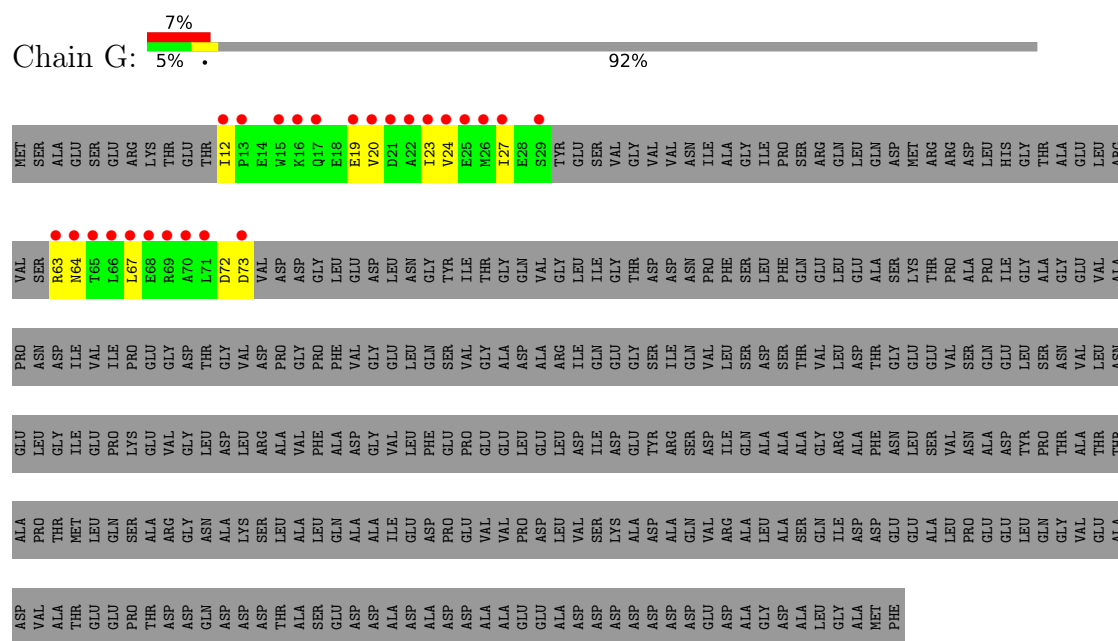
• Molecule 5: 50S ribosomal protein L6P



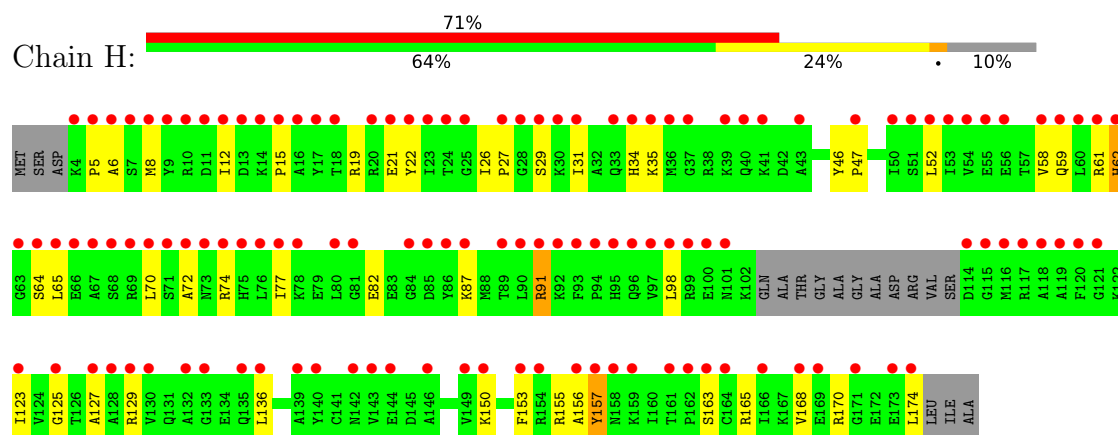
- Molecule 6: 50S ribosomal protein L7Ae



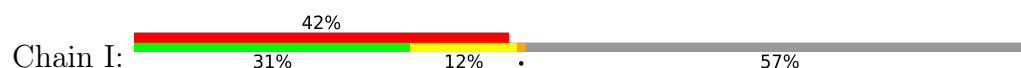
- Molecule 7: 50S ribosomal protein L10E

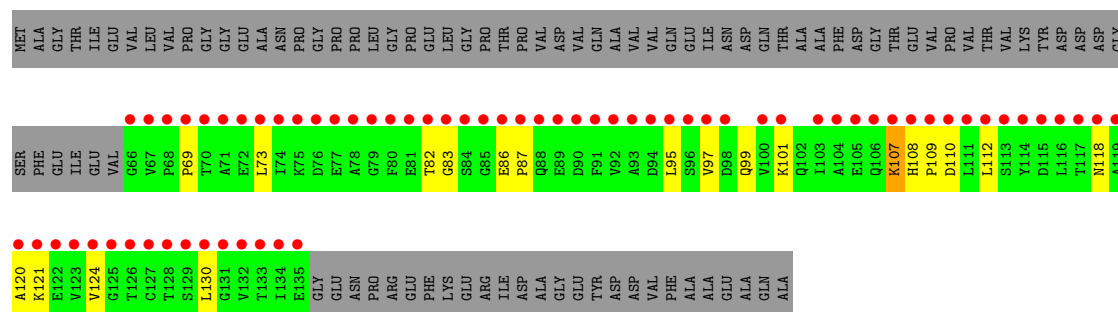


- Molecule 8: 50S ribosomal protein L10e

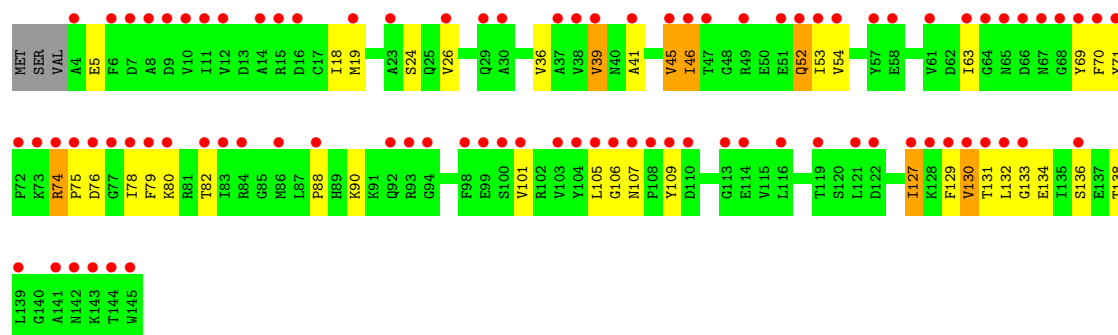


- Molecule 9: 50S ribosomal protein L11P

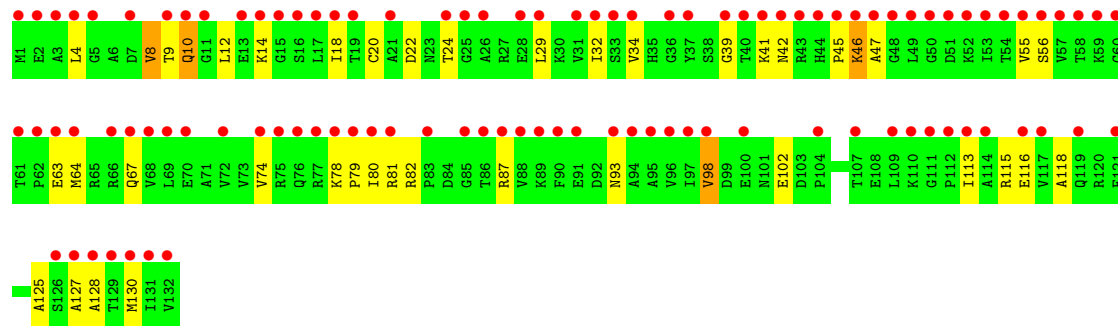
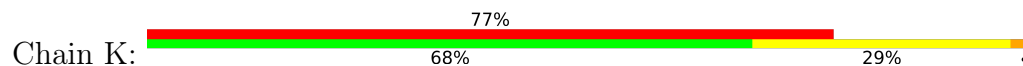




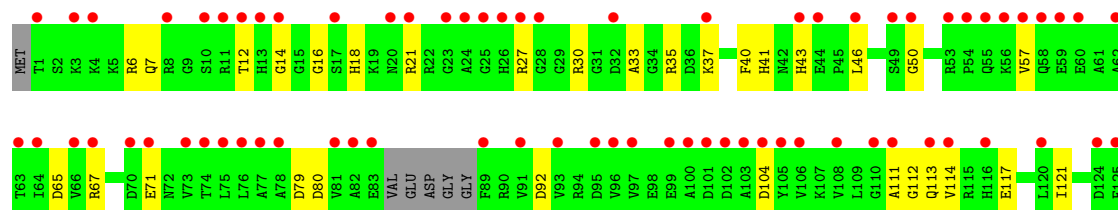
• Molecule 10: 50S ribosomal protein L13P

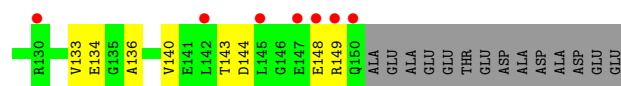


• Molecule 11: 50S ribosomal protein L14P

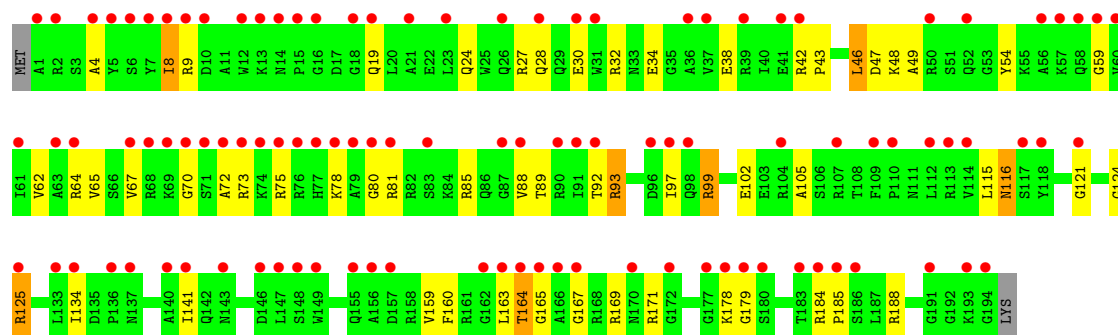


• Molecule 12: 50S ribosomal protein L15P

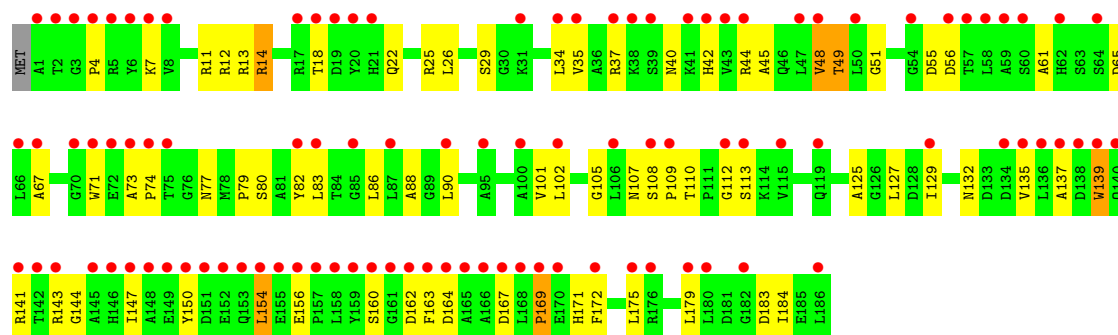




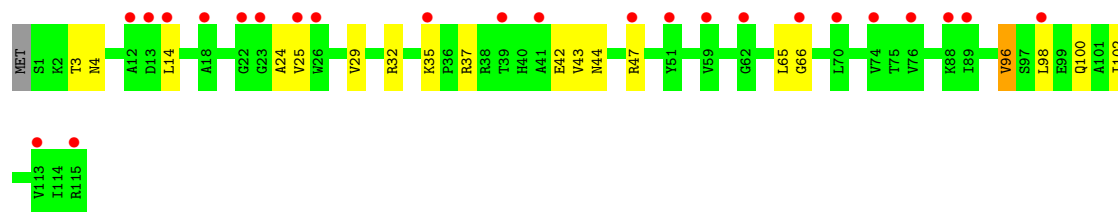
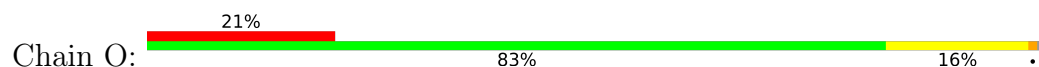
• Molecule 13: 50S ribosomal protein L15e



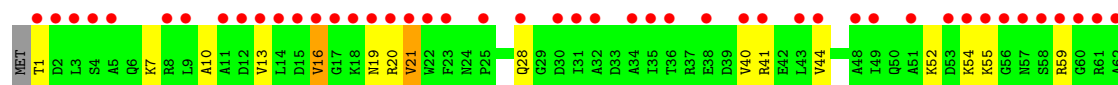
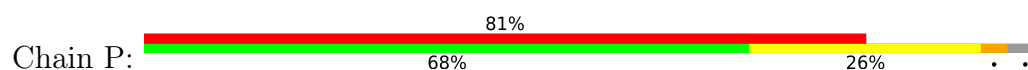
• Molecule 14: 50S ribosomal protein L18P

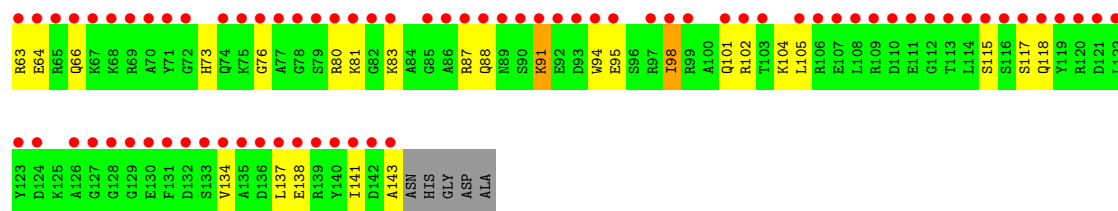


• Molecule 15: 50S ribosomal protein L18e

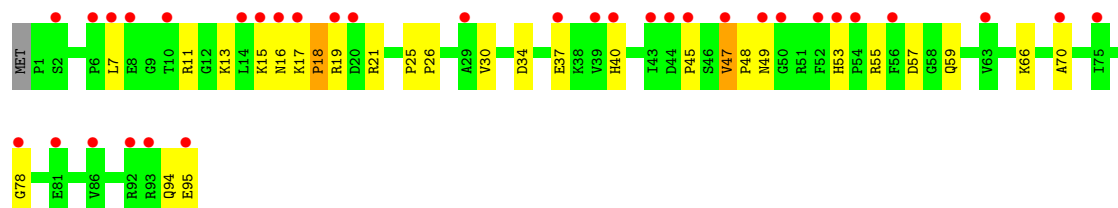


• Molecule 16: 50S ribosomal protein L19e

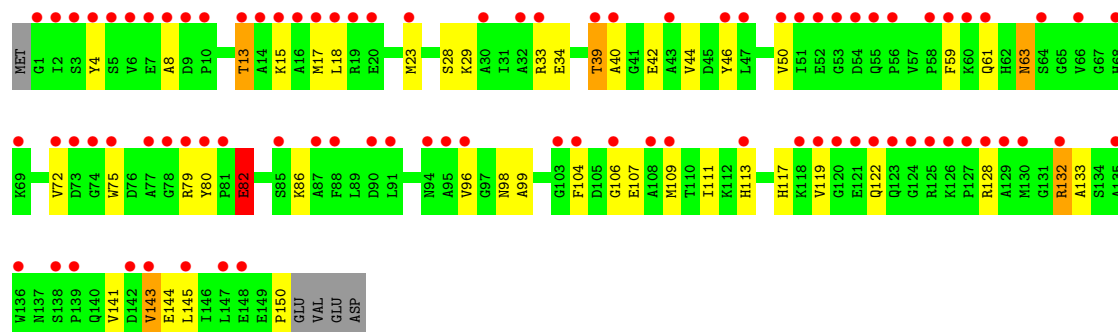




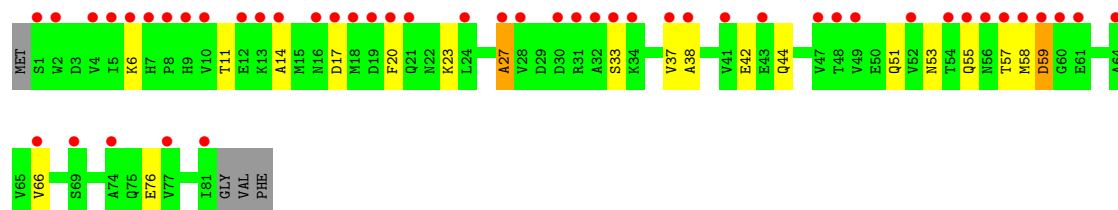
• Molecule 17: 50S ribosomal protein L21e



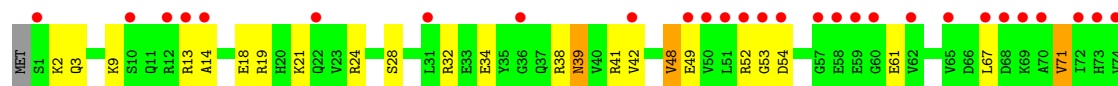
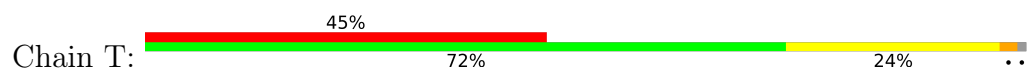
• Molecule 18: 50S ribosomal protein L22P

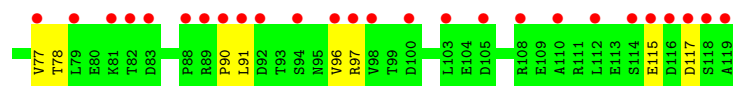


• Molecule 19: 50S ribosomal protein L23P

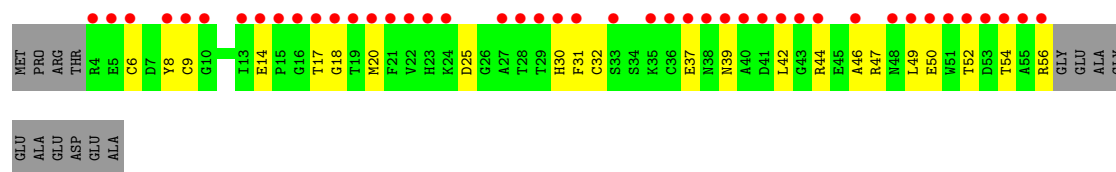


• Molecule 20: 50S ribosomal protein L24P

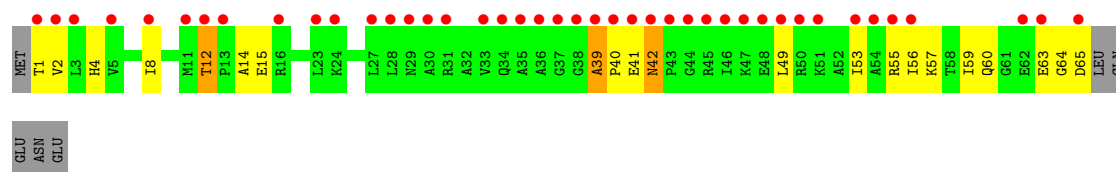




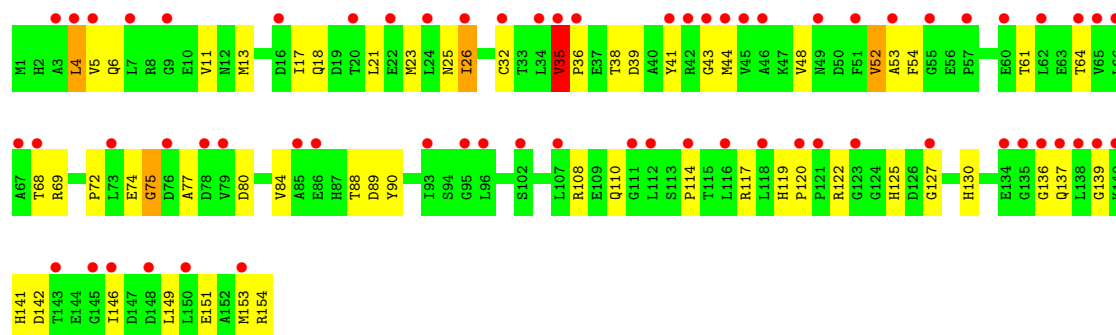
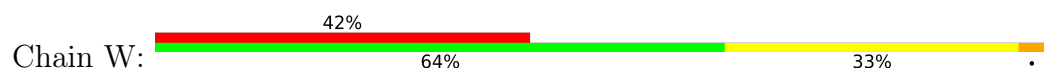
- Molecule 21: 50S ribosomal protein L24e



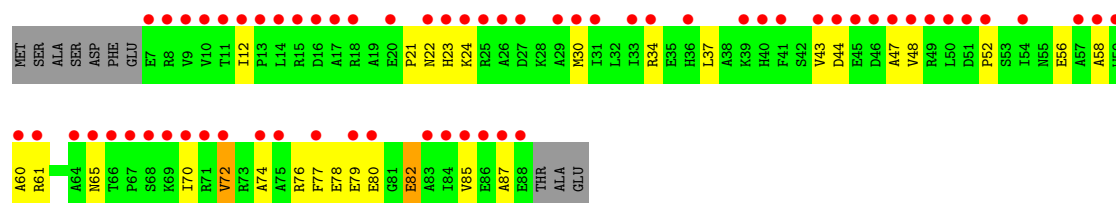
- Molecule 22: 50S ribosomal protein L29P



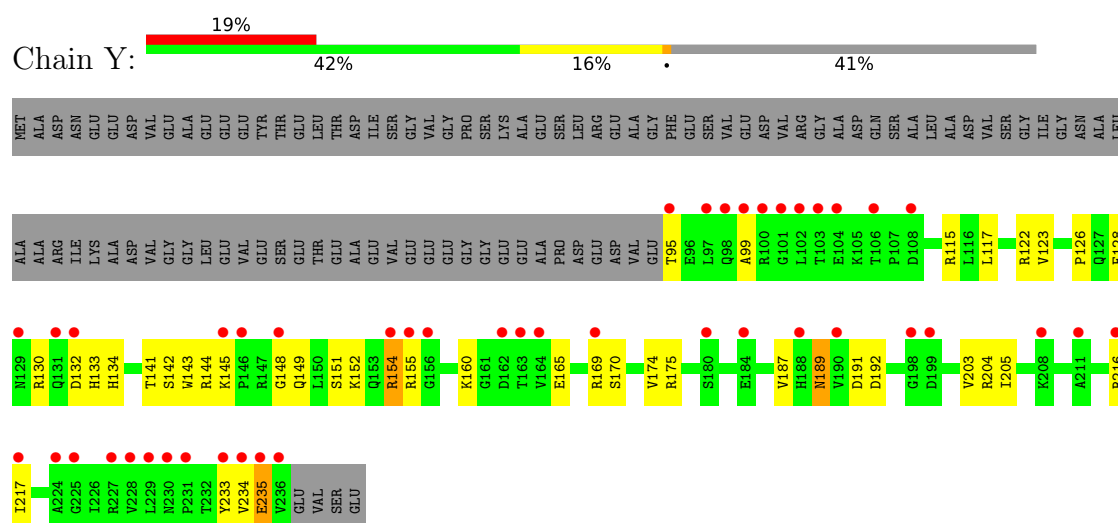
- Molecule 23: 50S ribosomal protein L30P



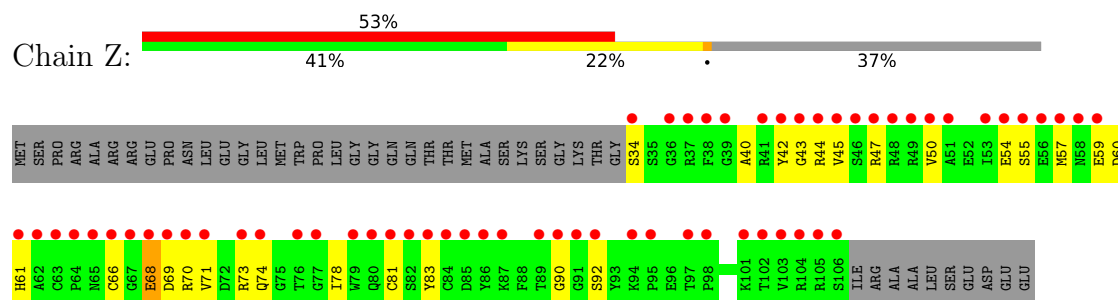
- Molecule 24: 50S ribosomal protein L31e



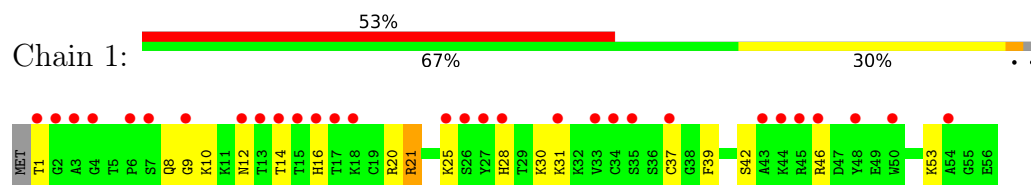
- Molecule 25: 50S ribosomal protein L32e



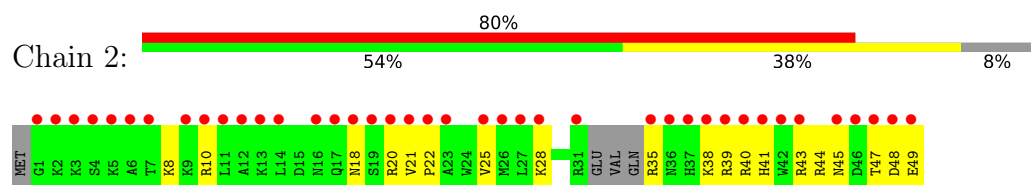
• Molecule 26: 50S ribosomal protein L37Ae



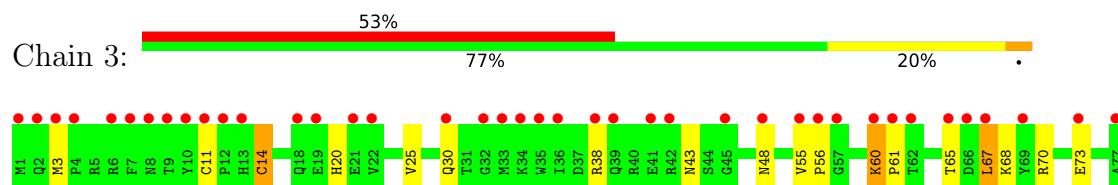
• Molecule 27: 50S ribosomal protein L37e



• Molecule 28: 50S ribosomal protein L39e

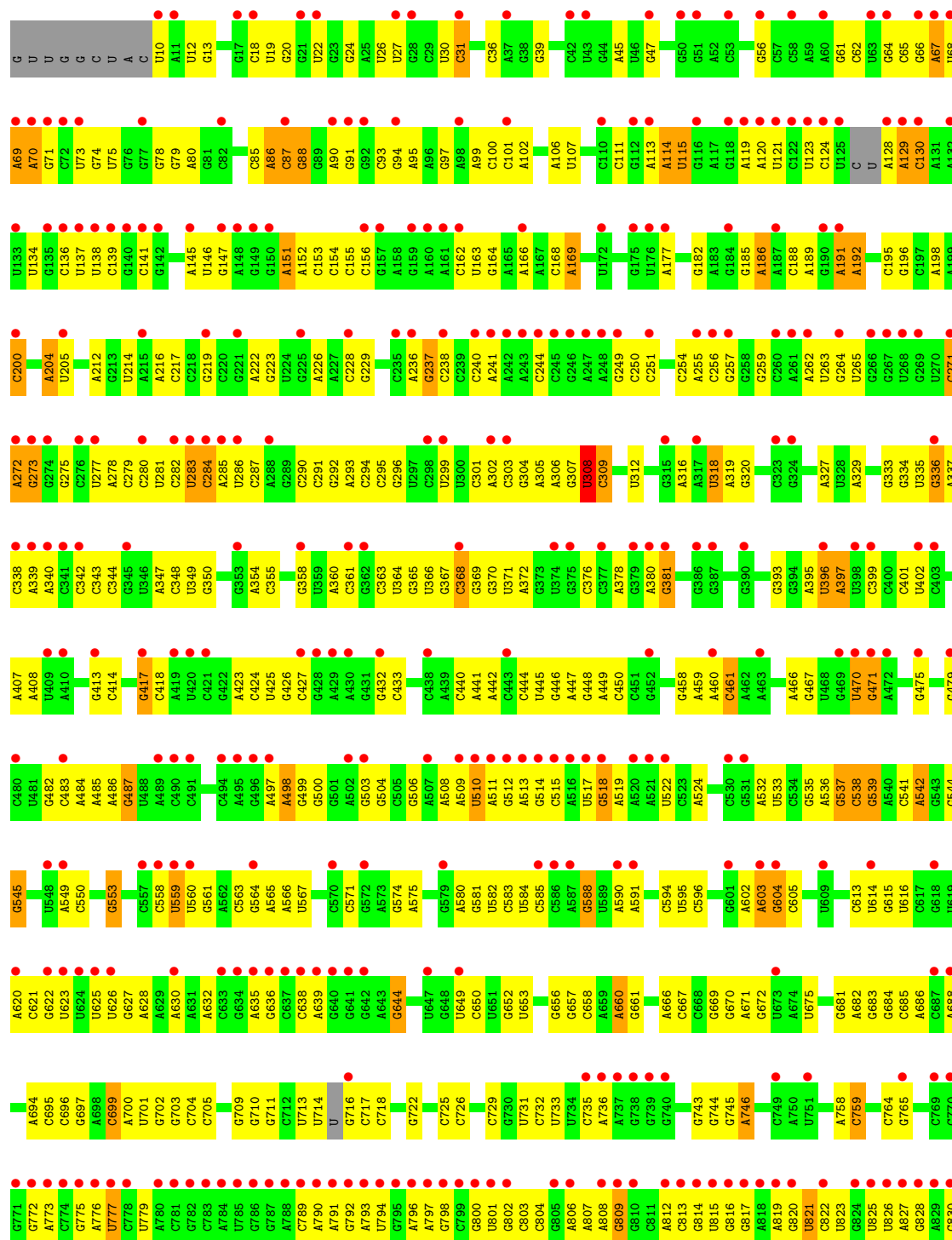


• Molecule 29: 50S ribosomal protein L44E



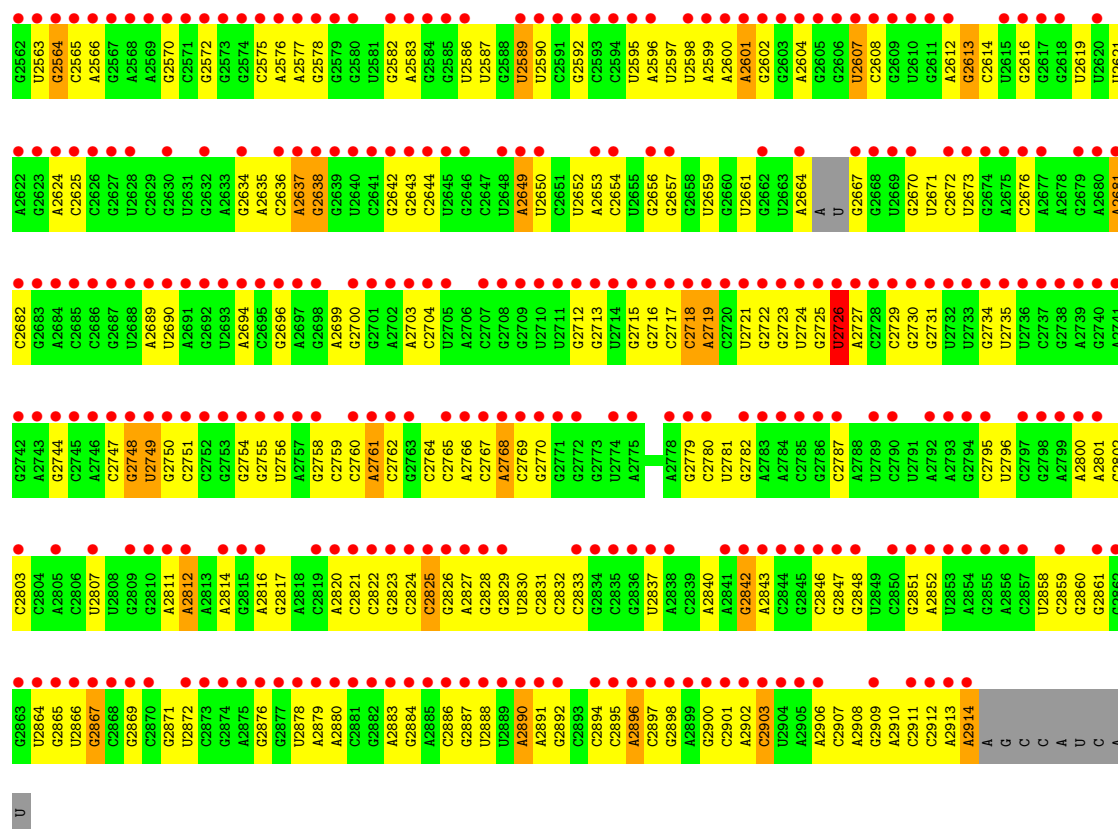


● Molecule 30: 23S RIBOSOMAL RNA

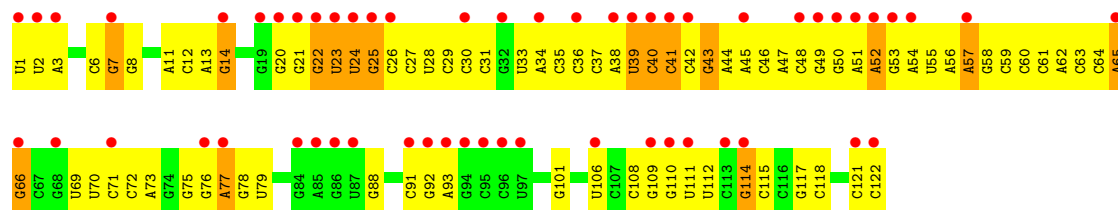


C1617	G1497	G1436	G1376	G1226	A1166	A1097	G1024	G964	U831
G1618	G1498	A1437	C1377	C1229	G1167	A1098	G1027	A965	U832
G1619	G1499	G1438	G1378	A1230	C1168	A1099	U1027	U966	G833
C1620	U1500	C1439	A1379	A1231	U1169	C1102	U1029	U967	G834
G1621	A1501	U1440	U1380	A1232	A1170	U1105	G1039	G968	U835
G1622	A1502	G1441	U1309	A1233	A1171	G1106	U1040	G969	G836
C1623	U1503	A1442	U1310	U1234	G1172	A1107	G1041	U970	U837
G1624	A1504	G1443	G1311	G1235	A1173	A1108	U1042	G	C838
U1625	U1505	G1444	G1312	A1236	A1174	A1109	U1043	U	C839
A1626	U1506	G1445	A1313	U1237	G1175	U1109	C1043	G	U840
G1627	C1507	U1446	U1314	U1238	C1176	G1110	U1044	C	A841
G1628	U1508	U1447	G1315	G1239	A1177	U1111	G1045	C	C842
U1629	U1509	A1448	G1316	C1240	G1178	U1112	G	G	A843
A1630	G1510	G1449	C1320	G1241	G1179	G1113	G1048	C	A844
C1631	U1511	C1450	A1321	A1242	U1180	U1116	U1051	C	U845
A1632	G1512	G1451	G1322	C1243	A1181	A1117	G1052	C	A846
C1633	C1513	A1452	G1323	U1244	C1182	U1118	U1053	U	C847
G1634	G1514	G1453	A1393	C1245	C1183	A1119	G1054	C	C848
U1635	U1515	U1454	G1394	A1246	C1184	U1120	U1055	C	C849
G1636	U1516	C1455	G1395	U1247	U1185	U1121	G1056	U	U850
A1637	C1517	C1456	C1396	A1248	C1186	U1122	U1057	A	C851
U1638	U1518	U1457	A1397	U1249	U1187	A1123	A1058	G	C852
C1639	A1519	G1458	G1398	C1251	A1188	U1124	G1059	G	C853
U1640	G1520	A1459	A1399	G1252	C1189	U1125	U1060	A	C854
A1641	C1521	G1460	C1400	C1253	G1190	U1126	U1061	U	U855
C1642	A1522	U1461	G1401	A1255	A1191	U1127	U1062	U	C856
C1643	G1523	C1462	G1402	U1266	A1192	C1127	U1063	C	A857
G1644	U1524	U1463	C1403	C1267	A1193	U1128	U1064	U	U858
U1645	G1525	C1464	A1404	G1268	A1194	C1129	G1065	G	C859
G1646	A1526	A1465	C1342	A1269	U1195	U1130	U1066	C	U860
U1647	U1527	C1466	C1343	G1260	C1196	U1131	U1067	C	A861
G1648	A1528	C1467	G1344	A1261	G1197	A1132	U1068	C	U862
U1649	G1529	G1468	A1345	U1266	U1198	U1133	U1069	C	C863
C1650	U1530	C1469	U1346	C1267	A1199	G1137	A1070	A	U864
G1651	G1531	A1470	G1347	G1268	A1200	G1138	G1071	G	C865
C1652	C1532	U1471	U1350	U1270	A1201	U1139	G1072	U	U866
A1653	A1533	C1472	G1351	A1271	A1202	C1140	A1073	G	C867
U1654	G1534	U1473	C1352	C1272	C1203	G1145	G1074	U	C868
G1655	C1535	C1474	A1353	C1273	U1205	C1146	G1075	U	C869
A1656	U1536	U1475	G1354	C1273	A1206	C1147	U1076	G	U871
U1657	C1537	G1476	A1355	U1278	A1207	C1148	A1077	U	C870
A1658	U1538	C1477	U1356	U1279	C1208	U1149	U1078	C	U872
G1659	G1539	U1478	A1357	A1284	C1209	A1150	C1080	U	A874
C1660	U1540	G1480	A1358	G1285	G1210	A1151	A1081	U	A875
A1661	G1541	G1481	U1359	U1286	C1211	A1152	U1082	U	A876
C1662	C1542	A1482	C1360	A1287	C1212	C1153	C1083	G	C877
U1663	U1543	G1483	G1361	U1288	C1213	A1154	C1084	U	C878
G1664	A1544	A1484	U1362	C1288	G1214	C1155	C1085	C	C879
C1665	C1545	U1485	C1363	U1289	A1215	C1156	A1086	C	C880
U1666	U1546	A1486	G1364	C1290	G1216	C1157	U1087	U	C881
A1667	A1547	C1487	C1365	A1294	C1217	U1158	A1088	C	A882
U1668	U1548	U1488	U1366	U1295	U1218	G1159	U1089	U	U883
G1669	C1549	A1489	A1367	G1296	U1219	U1160	A1090	C	C884
A1670	A1550	G1490	U1368	A1296	G1220	A1161	G1091	U	U885
U1671	U1551	C1491	A1369	U1297	A1221	G1162	G1093	C	A886
G1672	G1552	A1492	U1370	U1298	C1222	U1163	U1094	U	C887
U1673	C1553	U1493	U1371	G1299	G1223	G1164	U1095	C	U888
C1674	U1554	A1494	A1372	U1299	U1224	U1165	U1096	U	C889
G1675	C1555	G1495	C1373	G1300	G1225			C	C890
U1676	G1556	A1496	A1375						

C2500	A2433	G2350	G2286	U	A	A	A2100	A2039	C1978	U1918	A1858	A1797	C1737	U1777
G2501	A2434	C2351	C2287	A	G	G	A2101	C2040	U1980	A1919	A1859	C1798	C1738	A1678
C2502	U2435	G2352	G2288	C	U	U	G2102	G2041	A1981	C1920	U1860	G1799	G1739	C1679
A2503	G2436	C2353	C2289	C	U	G	A2103	U2042	C1982	A1921	C1861	G1800	U1740	C1680
G2504	A2437	A2354	U2290	C	A	G	C2104	G2043	C1983	G1922	G1862	A1801	U1741	C1681
U2505	G2438	G2355	U2291	C	A	G	C2105	G2044	U1985	G1923	G1863	G1802	A1742	A1682
A2506	U2439	A2356	C2292	U	C	A	C2106	G2045	U1986	A1924	C1864	C1803	G1743	G1683
G2507	G2440	G2357	C2293	C	A	A	U2107	G2046	C1987	G1925	A1865	A1804	G1744	A1684
C2508	U2441	C2360	G2294	G	G	G	A2108	C2047	G1988	G1926	A1866	G1805	G1745	A1685
A2509	U2445	U2297	U2297	U	U	U	U2109	G2048	C1989	A1927	G1867	G1806	A1746	C1686
U2510	G2446	A2362	G2298	G	C	C	G2110	C2049	U1990	C1928	G1868	U1747	C1687	C1687
A2511	A2447	A2363	C2299	G	G	G	G2111	G2050	C1991	G1929	A1869	G1808	U1748	G1688
U2512	U2448	A2364	A2300	A	U	U	A2112	G2051	A1992	U1930	C1870	U1749	U1749	A1689
A2513	C2450	G2365	A2301	C	U	U	G2113	U2052	U1993	A1931	U1871	C1750	C1750	C1690
U2514	U2451	U2366	A2302	U	A	A	C2114	G2053	C1994	G1932	C1872	G1751	G1751	A1691
C2515	G2453	A2368	A2303	G	C	C	U2115	A2054	A1995	G1933	A1873	G1752	C1752	C1692
U2516	U2454	A2369	G2304	C	A	A	U2116	A2055	U1996	A1934	A1874	C1753	C1753	A1693
A2517	A2455	A2370	A2305	G	G	G	U2117	G2056	C1997	C1935	A1875	A1754	A1754	G1694
C2518	U2457	A2371	A2306	A	A	A	A2118	G2057	A1998	C1936	C1876	A1755	A1755	G1695
U2519	U2458	A2372	U2307	G	G	G	C2119	U2058	C1999	U1939	G1877	G1756	G1756	U1696
G2520	G2459	U2373	U2308	U	U	U	U2120	A2059	G1999	U1940	C1878	U1757	U1757	G1697
A2521	U2460	G2374	C2309	C	U	U	G2121	C2061	C1940	C1941	U1879	U1758	U1758	C1698
G2522	U2461	A2375	G2310	A	A	A	C2122	A2062	G2001	A1942	C1880	A1759	A1759	C1699
U2523	G2462	C2376	A2311	C	C	C	A2123	U2063	U2002	A1943	A1881	G1760	G1760	C1700
G2524	U2463	U2377	G2312	A	A	A	G2124	U2064	C2003	C1943	C1882	U1761	U1761	A1701
U2525	A2465	U2378	C2313	C	C	C	G2125	C2065	U2004	G1944	U1883	C1762	C1762	U1702
G2526	G2466	G2379	G2314	G	G	G	U2126	C2066	G2005	G1945	A1884	C1763	C1763	G1703
A2527	U2467	A2380	C2315	C	C	C	C2127	A2067	C2006	C1946	A1885	G1764	G1764	G1704
U2528	A2468	C2381	G2316	C	C	C	G2128	G2068	A2007	G1947	A1886	G1765	G1765	C1705
G2529	A2469	U2382	C2317	C	C	C	U2129	U2069	U2008	G1948	U1887	U1766	U1766	G1706
C2530	U2470	U2383	U2320	U	U	U	C2130	G2070	G2009	G1949	C1888	A1767	A1767	G1707
U2531	G2471	U2384	A2321	A	A	A	G2131	C2071	A2010	G1950	C1889	C1768	C1768	G1708
A2532	U2472	C2385	G2322	G	G	G	C2132	U2072	A2011	U1951	U1890	C1769	C1769	G1709
G2533	U2473	U2386	U2323	C	C	C	U2133	G2073	G2012	U	G1891	U1770	U1770	A1710
A2534	A2474	G2387	G2324	C	C	C	G2134	A2074	U2013	A	C1892	U1771	U1771	A1711
U2535	C2475	U2388	U2325	G	G	G	A2135	G2075	G2014	C	C1893	G1772	G1772	A1712
G2536	G2476	G2389	C2326	C	C	C	G2136	U2076	A2015	A	C1894	G1773	G1773	G1713
C2537	U2477	U2390	U2327	C	C	C	A	C2077	U2016	U	A1895	G1774	G1774	C1714
U2538	A2478	A2401	U2328	C	C	C	C	U2078	U2017	A	G1896	A1775	A1775	C1715
G2539	U2479	A2402	C2329	A	A	A	G	G2079	A2018	U	U1897	A1776	A1776	A1716
U2540	G2480	U2411	U2330	C	C	C	U	C2080	U2019	A	G1898	G1777	G1777	A1717
U2541	A2481	G2412	U2331	C	C	C	G	A2081	C2020	G	A1899	A1778	A1778	G1718
C2542	G2482	A2413	C2332	C	C	C	G	G2082	C2021	A	C1900	G1779	G1779	G1719
G2543	A2483	A2414	G2333	C	C	C	U	A2083	A2022	C	G1901	C1720	C1720	C1720
U2544	U2484	A2415	C2334	A	A	A	C	C2084	G2023	C	G1902	G1781	G1781	C1721
C2547	A2485	G2416	C2335	G	G	G	C	A2085	A2024	U1964	U1903	G1782	G1782	U1722
U2548	G2486	U2417	G2336	C	C	C	A	C2086	G2025	C1965	A1904	A1783	A1783	G1723
C2549	A2487	U2419	G2337	C	C	C	A	C2087	U2026	U1966	U1905	U1784	U1784	U1724
U2550	G2488	G2420	G2338	A	A	A	C	A2088	U2027	U1967	C1906	G1785	G1785	C1725
C2551	U2489	U2421	A	C	C	C	U	G2089	U2028	A1968	U1907	G1786	G1786	G1726
A2553	A2490	G2422	C	A	A	A	U	G2090	C2029	A1969	G1908	C1787	C1787	G1727
U2554	G2491	U2423	A	G	G	G	C	G2091	U2030	G1970	U1909	U1788	U1788	G1728
C2557	U2492	A2424	G	U	U	U	C	G2092	C2031	G1971	A1910	G1789	G1789	A1729
G2558	A2493	U2425	U2339	G	G	G	U	G2093	U2032	U1972	C1911	C1790	C1790	G1730
U2559	C2494	G2426	A2344	A	A	A	C	A2094	G2033	A1973	A1912	U1791	U1791	G1731
A2561	U2495	U2427	U2345	A	A	A	C	A2095	U2034	G1974	C1913	G1792	G1792	A1732
G2562	G2496	G2428	C2346	A	A	A	G	A2096	C2035	G1975	C1914	C1793	C1793	A1733
U2563	A2497	U2429	U2347	U	U	U	C	G2097	C2036	G1976	U1915	G1794	G1794	G1734
C2564	U2498	A2430	C2348	A	A	A	C	C2098	U2037	U1977	C1916	C1856	C1856	C1735
U2565	U2499	U2431	G2349	C	C	C	U	A2099	A2038	A1978	G1917	A1796	A1796	A1736



• Molecule 31: 5S RIBOSOMAL RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.83Å 299.90Å 576.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 2.75 49.33 – 2.75	Depositor EDS
% Data completeness (in resolution range)	81.3 (49.33-2.75) 80.5 (49.33-2.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.183 , 0.232 (Not available) , 0.291	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	99124	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, K, CL, OMG, NA, SR, UR3, 1MA, MG, CD, 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	0.45	0/1786	0.99	8/2408 (0.3%)
2	B	0.42	0/2690	1.01	9/3652 (0.2%)
3	C	0.47	0/1885	1.01	9/2552 (0.4%)
4	D	0.41	0/1111	0.94	7/1498 (0.5%)
5	E	0.40	0/1382	0.87	1/1880 (0.1%)
6	F	0.41	0/901	0.95	2/1224 (0.2%)
7	G	0.35	0/241	0.85	0/324
8	H	0.41	0/1302	0.95	5/1743 (0.3%)
9	I	0.39	0/526	0.92	0/716
10	J	0.40	0/1136	0.94	3/1530 (0.2%)
11	K	0.42	0/1004	0.96	2/1351 (0.1%)
12	L	0.36	0/1130	0.92	1/1509 (0.1%)
13	M	0.43	0/1582	0.92	6/2116 (0.3%)
14	N	0.39	0/1474	1.05	9/1999 (0.5%)
15	O	0.43	0/874	0.94	4/1181 (0.3%)
16	P	0.39	0/1147	0.87	0/1528
17	Q	0.42	0/749	1.01	6/1005 (0.6%)
18	R	0.45	0/1172	0.98	5/1578 (0.3%)
19	S	0.41	0/648	0.92	4/875 (0.5%)
20	T	0.41	0/958	0.97	8/1289 (0.6%)
21	U	0.38	0/417	0.83	0/562
22	V	0.40	0/502	0.91	2/675 (0.3%)
23	W	0.47	0/1219	0.98	4/1655 (0.2%)
24	X	0.44	0/664	1.01	4/895 (0.4%)
25	Y	0.43	0/1146	0.94	2/1536 (0.1%)
26	Z	0.40	0/584	0.94	1/781 (0.1%)
27	1	0.43	0/438	0.92	1/578 (0.2%)
28	2	0.43	0/401	0.88	0/529
29	3	0.40	0/771	0.88	5/1024 (0.5%)
30	0	0.38	0/65960	0.60	15/102872 (0.0%)
31	9	0.38	0/2904	0.57	1/4526 (0.0%)
All	All	0.39	0/98704	0.71	124/147591 (0.1%)

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
23	W	0	1
30	0	0	26
All	All	0	27

There are no bond length outliers.

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	163	PHE	N-CA-C	-9.71	100.99	113.12
23	W	35	VAL	N-CA-C	7.45	116.48	107.61
2	B	175	LEU	N-CA-C	-7.44	103.10	111.14
4	D	136	ARG	CA-C-N	7.28	128.94	119.84
4	D	136	ARG	C-N-CA	7.28	128.94	119.84
13	M	89	THR	N-CA-C	7.14	119.06	111.28
2	B	323	LEU	N-CA-C	7.09	119.45	110.24
14	N	48	VAL	N-CA-C	6.99	117.95	108.17
17	Q	17	LYS	N-CA-C	-6.95	101.31	109.93
25	Y	143	TRP	N-CA-C	6.86	119.75	109.25
3	C	191	SER	N-CA-C	6.83	114.38	108.78
20	T	54	ASP	N-CA-C	-6.82	104.93	113.18
4	D	15	GLU	CA-C-N	6.78	128.31	119.84
4	D	15	GLU	C-N-CA	6.78	128.31	119.84
23	W	75	GLY	N-CA-C	6.75	118.90	112.08
2	B	157	LYS	N-CA-C	-6.71	106.03	114.56
18	R	141	VAL	N-CA-C	6.68	118.11	108.48
30	0	1819	G	C5'-C4'-C3'	6.53	125.79	116.00
1	A	135	VAL	N-CA-C	6.49	117.65	108.17
24	X	22	ASN	N-CA-C	6.49	119.18	111.33
14	N	51	GLY	CA-C-N	6.41	126.16	119.05
14	N	51	GLY	C-N-CA	6.41	126.16	119.05
30	0	834	G	C2'-C3'-O3'	-6.34	104.18	113.70
29	3	55	VAL	CA-C-N	6.29	127.71	119.84
29	3	55	VAL	C-N-CA	6.29	127.71	119.84
24	X	77	PHE	N-CA-C	6.24	116.84	108.23
24	X	60	ALA	N-CA-C	6.24	118.59	111.11
15	O	4	ASN	CA-C-N	6.19	125.93	119.05
15	O	4	ASN	C-N-CA	6.19	125.93	119.05
29	3	67	LEU	N-CA-C	6.16	119.06	109.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1504	A	N9-C1'-C2'	6.12	121.18	112.00
27	1	21	ARG	N-CA-C	6.08	118.81	111.40
10	J	45	VAL	N-CA-C	6.06	117.08	108.42
6	F	62	HIS	N-CA-C	6.02	117.93	111.36
19	S	59	ASP	N-CA-C	-6.01	105.24	113.30
8	H	34	HIS	N-CA-C	-5.99	106.52	113.88
4	D	170	TYR	N-CA-C	5.97	119.88	111.52
17	Q	49	ASN	N-CA-C	5.96	118.22	110.53
2	B	22	GLU	N-CA-C	-5.95	105.51	112.89
30	0	2726	U	N1-C1'-C2'	5.90	120.85	112.00
31	9	39	U	N1-C1'-C2'	5.88	120.82	112.00
3	C	192	ILE	N-CA-C	5.83	117.10	109.58
2	B	151	VAL	CA-C-N	5.80	125.17	118.85
2	B	151	VAL	C-N-CA	5.80	125.17	118.85
14	N	42	HIS	N-CA-C	5.79	118.03	109.69
29	3	60	LYS	N-CA-C	-5.79	102.31	110.29
1	A	222	GLY	N-CA-C	-5.75	107.12	114.37
29	3	43	ASN	N-CA-C	5.72	120.00	113.19
30	0	1979	G	C4'-C3'-O3'	-5.72	104.43	113.00
22	V	42	ASN	CA-C-N	5.70	126.96	119.84
22	V	42	ASN	C-N-CA	5.70	126.96	119.84
18	R	122	GLN	N-CA-C	-5.66	99.29	108.41
13	M	121	GLY	N-CA-C	5.66	118.95	111.70
12	L	7	GLN	N-CA-C	5.66	119.44	112.54
3	C	78	ARG	N-CA-C	5.65	116.54	108.74
20	T	52	ARG	N-CA-C	5.65	122.83	110.80
19	S	27	ALA	N-CA-C	-5.64	98.56	108.20
8	H	163	SER	N-CA-C	-5.62	101.32	110.20
3	C	20	ASP	N-CA-C	5.61	118.12	111.33
19	S	20	PHE	N-CA-C	5.61	118.32	111.82
1	A	48	ASP	CA-C-N	5.59	125.12	119.19
1	A	48	ASP	C-N-CA	5.59	125.12	119.19
2	B	156	LYS	N-CA-C	5.59	117.75	110.43
3	C	178	GLN	N-CA-C	5.56	119.81	113.19
14	N	150	TYR	N-CA-C	-5.56	105.62	112.90
30	0	1979	G	N9-C1'-C2'	5.55	120.33	112.00
11	K	8	VAL	N-CA-C	5.51	115.89	108.17
20	T	78	THR	N-CA-C	5.49	117.76	109.41
3	C	168	ARG	N-CA-C	-5.49	105.21	111.14
15	O	43	VAL	N-CA-C	5.43	116.12	108.36
20	T	14	ALA	CA-C-N	5.41	125.35	119.78
20	T	14	ALA	C-N-CA	5.41	125.35	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	123	VAL	N-CA-C	5.41	115.61	110.53
24	X	12	ILE	N-CA-C	5.40	113.21	107.76
30	0	920	C	C2'-C3'-O3'	-5.39	105.61	113.70
1	A	123	GLY	N-CA-C	5.37	122.67	115.59
11	K	46	LYS	N-CA-C	5.35	118.79	110.17
3	C	186	TYR	N-CA-C	5.35	118.00	110.14
13	M	125	ARG	N-CA-C	5.34	121.62	113.61
30	0	1261	A	N9-C1'-C2'	5.33	120.00	112.00
20	T	3	GLN	CA-C-N	5.33	124.79	119.24
20	T	3	GLN	C-N-CA	5.33	124.79	119.24
30	0	1120	U	C5'-C4'-C3'	-5.33	108.00	116.00
13	M	70	GLY	N-CA-C	5.31	119.60	112.17
14	N	14	ARG	N-CA-C	-5.30	105.40	111.07
13	M	73	ARG	N-CA-C	-5.30	99.35	108.56
30	0	871	G	C5'-C4'-O4'	-5.30	101.86	109.80
17	Q	13	LYS	N-CA-C	5.29	118.83	112.38
30	0	308	U	C2'-C3'-O3'	-5.29	105.77	113.70
2	B	115	VAL	CA-C-N	5.27	125.19	119.76
2	B	115	VAL	C-N-CA	5.27	125.19	119.76
13	M	8	ILE	N-CA-C	-5.25	105.41	110.72
18	R	34	GLU	N-CA-C	5.25	117.08	111.36
18	R	63	ASN	N-CA-C	5.24	119.64	112.88
30	0	921	G	N9-C1'-C2'	5.22	119.83	112.00
5	E	119	HIS	N-CA-C	5.19	117.16	108.23
3	C	236	THR	N-CA-C	-5.18	101.25	109.96
26	Z	42	TYR	N-CA-C	5.17	121.82	110.80
20	T	34	GLU	N-CA-C	5.16	116.71	111.14
1	A	70	ALA	N-CA-C	5.16	117.08	109.50
4	D	135	VAL	N-CA-C	5.14	113.98	107.70
19	S	66	VAL	N-CA-C	5.14	115.50	107.99
6	F	79	GLN	N-CA-C	5.14	117.87	109.59
8	H	125	GLY	N-CA-C	5.14	117.53	110.69
1	A	198	ASP	N-CA-C	5.13	119.59	113.23
18	R	82	GLU	N-CA-C	5.13	116.95	111.36
23	W	25	ASN	N-CA-C	5.13	119.12	112.86
8	H	58	VAL	N-CA-C	5.12	114.77	108.53
14	N	102	LEU	N-CA-C	5.11	116.50	109.15
1	A	56	ALA	N-CA-C	5.10	117.93	109.46
30	0	1592	G	N9-C1'-C2'	5.08	119.62	112.00
10	J	71	TYR	CA-C-N	5.08	125.01	119.78
10	J	71	TYR	C-N-CA	5.08	125.01	119.78
14	N	169	PRO	N-CA-C	-5.07	107.52	113.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	47	VAL	N-CA-C	5.07	112.57	107.55
4	D	137	PRO	N-CA-C	5.07	122.90	112.47
17	Q	47	VAL	CA-C-N	5.06	126.17	119.84
17	Q	47	VAL	C-N-CA	5.06	126.17	119.84
15	O	66	GLY	N-CA-C	5.05	125.16	113.18
30	0	1979	G	C2'-C3'-O3'	5.04	121.27	113.70
3	C	23	GLU	N-CA-C	-5.04	107.30	113.50
30	0	1634	G	N9-C1'-C2'	5.01	119.52	112.00
23	W	142	ASP	N-CA-C	-5.01	103.92	110.53
8	H	136	LEU	N-CA-C	-5.00	105.30	111.40

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1340	G	Sidechain
30	0	1417	G	Sidechain
30	0	1445	G	Sidechain
30	0	1653	A	Sidechain
30	0	1777	G	Sidechain
30	0	1829	A	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1972	U	Sidechain
30	0	2076	U	Sidechain
30	0	22	U	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2552	C	Sidechain
30	0	26	U	Sidechain
30	0	2607	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	470	U	Sidechain
30	0	471	G	Sidechain
30	0	518	G	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	83	0
2	B	2625	0	2533	108	0
3	C	1860	0	1813	73	0
4	D	1094	0	1085	60	0
5	E	1357	0	1266	44	0
6	F	890	0	843	23	0
7	G	240	0	231	7	0
8	H	1282	0	1292	34	0
9	I	519	0	500	24	0
10	J	1120	0	1098	39	0
11	K	994	0	1027	39	0
12	L	1118	0	1076	31	0
13	M	1558	0	1573	48	0
14	N	1445	0	1401	63	0
15	O	865	0	873	22	0
16	P	1136	0	1123	37	0
17	Q	735	0	729	20	0
18	R	1149	0	1122	36	0
19	S	641	0	605	14	0
20	T	950	0	924	21	0
21	U	410	0	364	18	0
22	V	499	0	511	16	0
23	W	1196	0	1137	61	0
24	X	654	0	653	20	0
25	Y	1130	0	1133	41	0
26	Z	573	0	531	18	0
27	1	431	0	426	25	0
28	2	396	0	413	21	0
29	3	755	0	729	15	0
30	0	59022	0	29809	1551	0
31	9	2599	0	1325	115	0
32	0	86	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	10	0	0	1	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	5	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
34	0	92	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	4	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	67	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5927	0	0	236	0
38	1	55	0	0	3	0
38	2	42	0	0	3	0
38	3	63	0	0	3	0
38	9	144	0	0	10	0
38	A	118	0	0	7	0
38	B	144	0	0	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	C	179	0	0	19	0
38	D	46	0	0	4	0
38	E	40	0	0	2	0
38	F	27	0	0	1	0
38	G	19	0	0	0	0
38	H	68	0	0	5	0
38	I	5	0	0	1	0
38	J	55	0	0	2	0
38	K	52	0	0	2	0
38	L	84	0	0	10	0
38	M	127	0	0	5	0
38	N	63	0	0	4	0
38	O	40	0	0	2	0
38	P	61	0	0	1	0
38	Q	43	0	0	1	0
38	R	84	0	0	5	0
38	S	33	0	0	2	0
38	T	33	0	0	2	0
38	U	28	0	0	2	0
38	V	14	0	0	1	0
38	W	67	0	0	5	0
38	X	30	0	0	0	0
38	Y	100	0	0	10	0
38	Z	32	0	0	0	0
All	All	99124	0	59911	2469	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 16.

All (2469) 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)
14:N:37:ARG:NH1	31:9:6:C:H5''	1.60	1.15
13:M:171:ARG:HD3	30:0:156:C:H5''	1.32	1.11
30:0:1160:G:C5'	30:0:1161:A:H5'	1.78	1.11
30:0:871:G:H5'	30:0:871:G:H8	1.12	1.11
30:0:871:G:H5'	30:0:871:G:C8	1.84	1.11
30:0:2717:C:H2'	30:0:2718:C:H5''	1.33	1.10
30:0:2291:A:C8	30:0:2309:C:H5'	1.87	1.09
30:0:1160:G:H5'	30:0:1161:A:C5'	1.82	1.08
30:0:381:G:H5''	38:0:4322:HOH:O	1.54	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:56:A:H2'	31:9:57:A:H5''	1.38	1.05
30:0:2502:C:H2'	30:0:2503:A:H5'	1.33	1.05
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.39	1.02
30:0:2502:C:C2'	30:0:2503:A:H5'	1.89	1.01
10:J:82:THR:HG23	30:0:1242:A:H5'	1.39	1.01
30:0:1209:C:H2'	30:0:1210:G:H8	1.19	1.01
31:9:76:G:H3'	31:9:77:A:H5''	1.39	1.01
30:0:282:C:H1'	30:0:368:C:N4	1.77	1.00
30:0:2717:C:C2'	30:0:2718:C:H5''	1.91	0.99
22:V:1:THR:HB	30:0:93:C:H5''	1.42	0.99
16:P:115:SER:H	16:P:118:GLN:HE21	1.08	0.99
30:0:2812:A:H2	30:0:2814:A:H62	1.07	0.98
30:0:1118:A:H8	30:0:1118:A:H3'	1.28	0.98
30:0:1372:A:H3'	38:0:7202:HOH:O	1.64	0.98
15:O:3:THR:HG22	30:0:656:G:H5'	1.45	0.97
30:0:1116:U:H3	30:0:1246:A:H62	1.11	0.96
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.12	0.95
30:0:545:G:H5'	30:0:545:G:H8	1.30	0.95
30:0:2908:A:H2'	30:0:2909:G:O4'	1.66	0.95
30:0:542:A:H5'	30:0:542:A:H8	1.32	0.95
30:0:1160:G:H5'	30:0:1161:A:H5'	0.96	0.94
30:0:1666:C:O2'	30:0:1667:A:H5''	1.67	0.94
11:K:10:GLN:HE21	11:K:10:GLN:H	1.15	0.93
30:0:2769:C:C2'	30:0:2770:G:H5'	1.98	0.93
30:0:2497:A:H1'	30:0:2526:C:N4	1.84	0.93
2:B:62:ARG:HA	2:B:65:MET:HE3	1.51	0.92
30:0:1603:A:H5'	30:0:1605:G:O4'	1.68	0.92
30:0:1118:A:H3'	30:0:1118:A:C8	2.04	0.92
30:0:1701:A:H4'	30:0:1702:U:H5''	1.49	0.92
31:9:14:G:H5'	31:9:14:G:H8	1.36	0.91
23:W:13:MET:HE2	23:W:18:GLN:HA	1.51	0.91
30:0:1205:U:H2'	30:0:1206:U:H5''	1.52	0.91
30:0:960:G:H3'	30:0:960:G:N3	1.85	0.91
30:0:2812:A:H1'	38:0:5804:HOH:O	1.71	0.91
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.34	0.91
30:0:871:G:H8	30:0:871:G:C5'	1.85	0.90
31:9:3:A:N6	31:9:22:G:H1'	1.86	0.90
30:0:282:C:O2'	30:0:283:U:H5'	1.71	0.90
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.90
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.54	0.89
30:0:1679:C:H5'	38:0:9328:HOH:O	1.72	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.55	0.89
30:0:182:G:H5'	38:0:5169:HOH:O	1.72	0.88
30:0:1474:C:H6	30:0:1474:C:H5'	1.36	0.88
30:0:2524:G:N2	30:0:2526:C:H41	1.71	0.88
30:0:1119:G:N2	30:0:1246:A:C2	2.42	0.88
30:0:1666:C:H2'	30:0:1667:A:H5'	1.55	0.87
30:0:2769:C:H2'	30:0:2770:G:H5'	1.55	0.87
30:0:2508:C:H2'	38:0:6774:HOH:O	1.72	0.87
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.71	0.87
30:0:1118:A:H62	30:0:1244:U:H3	1.23	0.87
30:0:2506:A:HO2'	30:0:2507:G:H8	0.90	0.87
31:9:56:A:C2'	31:9:57:A:H5''	2.05	0.87
30:0:1278:A:H4'	30:0:1279:U:C4	2.10	0.86
30:0:2637:A:H5'	38:0:9279:HOH:O	1.74	0.86
15:O:3:THR:CG2	30:0:656:G:H5'	2.05	0.86
30:0:1130:U:H5'	38:0:7684:HOH:O	1.75	0.86
30:0:541:C:C2'	30:0:542:A:H5''	2.05	0.86
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.57	0.86
23:W:13:MET:HE1	23:W:21:LEU:HD12	1.58	0.85
2:B:238:ASN:HD22	2:B:240:GLY:H	1.22	0.85
23:W:88:THR:HB	38:W:6679:HOH:O	1.75	0.85
30:0:558:C:C2'	30:0:559:U:H5''	2.06	0.85
31:9:49:G:H5''	38:9:9088:HOH:O	1.75	0.85
30:0:1119:G:H22	30:0:1246:A:H2	1.19	0.85
30:0:1116:U:HO2'	30:0:1118:A:H2	0.87	0.85
30:0:2884:G:H5'	38:0:4133:HOH:O	1.76	0.84
30:0:506:G:H22	30:0:509:A:C5'	1.89	0.84
31:9:54:A:O2'	31:9:55:U:H5'	1.77	0.84
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.60	0.84
30:0:1451:C:H5'	30:0:1505:U:C5	2.12	0.84
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.21	0.84
23:W:88:THR:HG22	23:W:89:ASP:H	1.41	0.83
30:0:2586:U:H3	30:0:2592:G:H22	1.23	0.83
30:0:558:C:O2'	30:0:559:U:H5''	1.79	0.83
30:0:1183:C:H2'	38:0:6259:HOH:O	1.77	0.83
30:0:877:G:H5'	30:0:878:G:OP1	1.79	0.82
30:0:282:C:H1'	30:0:368:C:H41	1.41	0.82
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.43	0.82
30:0:1209:C:H2'	30:0:1210:G:C8	2.10	0.82
31:9:92:G:H2'	31:9:93:A:C8	2.14	0.82
11:K:39:GLY:HA2	38:0:5233:HOH:O	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2524:G:H21	30:0:2526:C:H41	1.23	0.82
4:D:154:LYS:H	4:D:154:LYS:HD2	1.42	0.82
30:0:1835:U:H5	30:0:1840:A:N7	1.76	0.82
30:0:2896:A:H5''	38:0:6114:HOH:O	1.78	0.82
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.44	0.82
30:0:855:U:H5''	38:0:3639:HOH:O	1.80	0.82
30:0:559:U:H6	30:0:559:U:H5'	1.45	0.81
30:0:1741:U:H5'	30:0:1742:A:OP1	1.80	0.81
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.61	0.81
30:0:2748:G:H2'	38:0:7557:HOH:O	1.78	0.81
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.62	0.81
30:0:1527:A:H1'	30:0:1528:A:C8	2.16	0.81
30:0:2529:G:H3'	38:0:7196:HOH:O	1.80	0.81
23:W:149:LEU:HG	23:W:153:MET:HE2	1.63	0.81
30:0:506:G:H22	30:0:509:A:H5''	1.45	0.81
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.61	0.81
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.62	0.80
30:0:2497:A:H1'	30:0:2526:C:H42	1.46	0.80
30:0:541:C:H2'	30:0:542:A:C5'	2.11	0.80
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.63	0.80
22:V:1:THR:HG23	22:V:2:VAL:H	1.47	0.80
27:1:25:LYS:HD2	28:2:49:GLU:H	1.47	0.80
30:0:545:G:H5'	30:0:545:G:C8	2.15	0.80
16:P:117:SER:HB3	30:0:1593:C:OP1	1.82	0.80
30:0:2505:G:O2'	30:0:2506:A:H5'	1.82	0.80
30:0:541:C:H2'	30:0:542:A:H5''	1.64	0.79
30:0:2506:A:O2'	30:0:2507:G:H8	1.65	0.79
30:0:2570:G:H5''	38:0:4925:HOH:O	1.82	0.79
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.63	0.79
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.64	0.79
14:N:37:ARG:HH11	31:9:6:C:H5''	1.44	0.79
31:9:20:G:H3'	38:9:9054:HOH:O	1.82	0.79
30:0:1878:G:H1'	38:0:6135:HOH:O	1.81	0.79
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.65	0.79
30:0:1165:G:H21	30:0:1173:A:H5''	1.48	0.78
30:0:2604:A:H5'	38:0:5805:HOH:O	1.83	0.78
2:B:206:THR:HG21	30:0:2716:G:H5''	1.65	0.78
30:0:567:U:H5''	38:0:6420:HOH:O	1.83	0.78
30:0:1856:C:H5'	30:0:1858:A:O4'	1.83	0.78
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.66	0.78
30:0:1206:U:H5'	30:0:1206:U:H6	1.47	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2635:A:O2'	30:0:2636:C:H5'	1.83	0.78
30:0:2769:C:H2'	30:0:2770:G:C5'	2.14	0.78
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.99	0.78
14:N:37:ARG:HH12	31:9:6:C:H5''	1.49	0.78
13:M:164:THR:HG22	13:M:167:GLY:H	1.46	0.77
30:0:69:A:H5'	30:0:69:A:H8	1.49	0.77
30:0:254:C:O2	30:0:254:C:H2'	1.84	0.77
30:0:2565:C:H4'	38:0:4847:HOH:O	1.84	0.77
1:A:199:HIS:HD2	1:A:201:PHE:H	1.31	0.77
30:0:2563:U:H2'	30:0:2565:C:O5'	1.85	0.77
16:P:115:SER:H	16:P:118:GLN:NE2	1.83	0.77
30:0:711:G:H1'	38:0:7109:HOH:O	1.84	0.77
30:0:1205:U:H2'	30:0:1206:U:C5'	2.13	0.77
30:0:1300:G:H1'	38:0:4697:HOH:O	1.84	0.77
16:P:88:GLN:NE2	30:0:1800:G:H1'	1.98	0.77
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.99	0.77
30:0:1205:U:C2'	30:0:1206:U:H5''	2.15	0.76
30:0:2812:A:H2	30:0:2814:A:N6	1.83	0.76
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.67	0.76
30:0:1973:A:H5'	30:0:1973:A:H8	1.49	0.76
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.67	0.76
30:0:1184:C:H1'	38:0:7483:HOH:O	1.85	0.76
30:0:536:A:H3'	38:0:5057:HOH:O	1.86	0.76
30:0:1342:C:C2'	30:0:1343:C:H5'	2.14	0.76
30:0:2587:OMU:H5	38:0:7502:HOH:O	1.85	0.76
31:9:14:G:H5'	31:9:14:G:C8	2.18	0.76
30:0:1641:A:H2'	30:0:1642:A:H5'	1.67	0.76
30:0:1979:G:H2'	38:0:3302:HOH:O	1.85	0.76
30:0:69:A:H5'	30:0:69:A:C8	2.21	0.76
30:0:1185:U:H2'	30:0:1186:C:H6	1.50	0.76
30:0:396:U:H1'	38:0:7643:HOH:O	1.86	0.75
30:0:1474:C:H5'	30:0:1474:C:C6	2.20	0.75
30:0:1701:A:H5''	30:0:1702:U:H3'	1.68	0.75
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.69	0.75
26:Z:44:ARG:HH21	30:0:1771:U:H5'	1.52	0.75
22:V:39:ALA:H	22:V:40:PRO:HD2	1.51	0.75
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.69	0.75
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.02	0.75
30:0:1182:C:H1'	30:0:1192:A:H8	1.51	0.75
30:0:31:C:H2'	38:0:7701:HOH:O	1.86	0.75
30:0:282:C:O2	30:0:282:C:H2'	1.85	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2498:C:O2'	30:0:2499:U:H5'	1.87	0.75
30:0:1455:C:H3'	38:0:7887:HOH:O	1.86	0.74
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.34	0.74
30:0:1919:A:H4'	38:0:4863:HOH:O	1.86	0.74
30:0:2426:G:H1'	38:0:6107:HOH:O	1.87	0.74
14:N:144:GLY:O	14:N:147:ILE:HG22	1.88	0.74
30:0:1118:A:C8	30:0:1118:A:C3'	2.69	0.74
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.69	0.74
30:0:2456:A:H1'	38:0:6611:HOH:O	1.87	0.74
10:J:131:THR:HB	10:J:134:GLU:HG3	1.70	0.74
14:N:113:SER:HB2	38:N:8854:HOH:O	1.88	0.74
30:0:582:U:H2'	30:0:583:C:H6	1.53	0.74
31:9:54:A:H2	38:9:9061:HOH:O	1.70	0.74
10:J:82:THR:CG2	30:0:1242:A:H5'	2.16	0.73
30:0:564:G:H1'	38:0:6328:HOH:O	1.86	0.73
30:0:1634:G:H3'	38:0:3900:HOH:O	1.87	0.73
30:0:2073:G:H5''	38:0:3832:HOH:O	1.88	0.73
17:Q:95:GLU:HA	30:0:949:U:H4'	1.71	0.73
18:R:39:THR:HG22	18:R:42:GLU:H	1.53	0.73
23:W:80:ASP:O	23:W:84:VAL:HG23	1.88	0.73
30:0:2004:U:H4'	38:0:5318:HOH:O	1.87	0.73
30:0:2851:G:O2'	30:0:2852:A:H5'	1.89	0.73
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.53	0.73
30:0:542:A:H5'	30:0:542:A:C8	2.21	0.73
30:0:1615:A:H4'	38:0:5899:HOH:O	1.88	0.73
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.24	0.73
21:U:47:ARG:HG3	38:U:4381:HOH:O	1.89	0.73
2:B:18:ARG:HE	2:B:256:GLN:HE21	1.35	0.73
30:0:603:A:H5''	30:0:604:G:OP1	1.88	0.73
30:0:854:G:H5''	38:0:3639:HOH:O	1.88	0.73
30:0:2524:G:H21	30:0:2526:C:N4	1.85	0.73
30:0:1060:C:H6	30:0:1060:C:H5'	1.53	0.73
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.24	0.73
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.04	0.73
30:0:318:U:H5'	30:0:339:A:C2	2.24	0.73
30:0:558:C:H2'	30:0:559:U:C5'	2.19	0.73
3:C:78:ARG:HH11	3:C:78:ARG:HG3	1.54	0.73
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.89	0.73
30:0:1157:C:H2'	30:0:1158:G:H8	1.53	0.73
30:0:2420:G:O2'	30:0:2421:G:H5'	1.88	0.73
30:0:2769:C:O2'	30:0:2770:G:H5'	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:139:VAL:HG13	38:C:8654:HOH:O	1.87	0.73
30:0:1213:C:O2'	30:0:1214:G:H5'	1.89	0.73
30:0:1119:G:N2	30:0:1246:A:H2	1.84	0.73
31:9:55:U:H4'	31:9:56:A:C8	2.24	0.73
30:0:871:G:C8	30:0:871:G:C5'	2.63	0.72
30:0:214:U:H5'	38:0:6153:HOH:O	1.88	0.72
30:0:1666:C:H2'	30:0:1667:A:C5'	2.19	0.72
31:9:75:G:H1	31:9:106:U:H3	1.37	0.72
30:0:848:C:H5'	38:0:7287:HOH:O	1.89	0.72
30:0:1942:A:H3'	38:0:7363:HOH:O	1.88	0.72
30:0:1942:A:H5'	38:0:7363:HOH:O	1.88	0.72
3:C:1:MET:HG2	3:C:2:GLN:H	1.52	0.72
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.70	0.72
30:0:2010:A:H2'	38:0:5975:HOH:O	1.90	0.72
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.89	0.72
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.72	0.72
30:0:1528:A:H2'	30:0:1529:G:O4'	1.88	0.72
30:0:1595:G:O2'	30:0:1596:U:H5'	1.89	0.72
30:0:1964:U:H2'	30:0:1964:U:O2	1.88	0.72
30:0:2787:C:H5	38:0:4647:HOH:O	1.72	0.72
2:B:258:GLY:H	2:B:260:HIS:CE1	2.08	0.72
25:Y:216:ARG:HD3	38:Y:8139:HOH:O	1.90	0.72
30:0:1603:A:H5''	30:0:1605:G:H5'	1.72	0.72
30:0:1834:C:H2'	30:0:1840:A:N6	2.04	0.72
23:W:13:MET:HE2	23:W:18:GLN:CA	2.20	0.71
30:0:12:U:H2'	30:0:13:G:H5'	1.72	0.71
30:0:2481:G:H5''	38:0:4556:HOH:O	1.89	0.71
30:0:272:A:H5'	30:0:273:G:OP2	1.89	0.71
30:0:363:C:H1'	38:0:5292:HOH:O	1.90	0.71
30:0:969:G:H1	30:0:999:C:H42	1.38	0.71
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.88	0.71
30:0:603:A:H1'	30:0:605:C:C2	2.25	0.71
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.38	0.71
22:V:1:THR:CB	30:0:93:C:H5''	2.17	0.71
30:0:2748:G:H1'	38:0:7912:HOH:O	1.91	0.71
30:0:2768:A:H2'	30:0:2769:C:O4'	1.90	0.71
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.56	0.71
30:0:2533:C:H5'	30:0:2533:C:H6	1.54	0.71
14:N:141:ARG:HH12	31:9:35:C:H2'	1.56	0.71
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.73	0.71
30:0:1701:A:H5'	38:0:6302:HOH:O	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:172:VAL:HG12	4:D:173:GLU:H	1.55	0.71
30:0:870:G:C2'	30:0:871:G:H5''	2.20	0.71
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.72	0.70
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.72	0.70
31:9:7:G:H5'	38:9:9098:HOH:O	1.91	0.70
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.21	0.70
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.73	0.70
30:0:2243:C:H5''	38:0:3756:HOH:O	1.91	0.70
3:C:140:VAL:HB	38:C:8657:HOH:O	1.91	0.70
30:0:560:U:H2'	30:0:561:G:H8	1.56	0.70
30:0:960:G:N3	30:0:960:G:C3'	2.54	0.70
30:0:2502:C:H2'	30:0:2503:A:C5'	2.17	0.70
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.26	0.70
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.73	0.70
30:0:2453:G:H3'	38:0:5935:HOH:O	1.91	0.70
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.21	0.70
30:0:1116:U:O2'	30:0:1118:A:H2	1.69	0.70
30:0:1666:C:C2'	30:0:1667:A:C5'	2.70	0.70
31:9:3:A:H61	31:9:22:G:H1'	1.56	0.70
14:N:40:ASN:ND2	31:9:28:U:H5''	2.06	0.70
30:0:2005:G:H3'	30:0:2005:G:OP2	1.91	0.70
1:A:179:MET:HA	1:A:179:MET:HE3	1.72	0.69
30:0:1377:C:H5'	30:0:1377:C:H6	1.57	0.69
30:0:2578:G:H5'	30:0:2578:G:H8	1.56	0.69
30:0:2372:A:H2'	30:0:2373:U:C6	2.27	0.69
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.75	0.69
30:0:401:C:H2'	30:0:402:U:C6	2.27	0.69
30:0:441:A:H1'	30:0:442:A:N7	2.08	0.69
30:0:613:C:H2'	30:0:614:U:H6	1.57	0.69
30:0:1701:A:H4'	30:0:1702:U:C5'	2.19	0.69
30:0:2073:G:OP2	30:0:2490:A:H5'	1.93	0.69
30:0:2717:C:H2'	30:0:2718:C:C5'	2.18	0.69
31:9:13:A:O2'	31:9:14:G:H5''	1.92	0.69
9:I:110:ASP:O	30:0:1163:G:H5'	1.91	0.69
31:9:36:C:C5	31:9:37:C:C5	2.80	0.69
29:3:70:ARG:HD3	38:3:9059:HOH:O	1.90	0.69
30:0:1441:G:O2'	30:0:1442:A:H5'	1.92	0.69
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.27	0.69
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.75	0.69
30:0:625:U:H5''	30:0:1044:C:N4	2.08	0.69
30:0:1477:C:H5'	30:0:1868:G:C5'	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1667:A:H5'	30:0:1667:A:H8	1.57	0.69
28:2:41:HIS:H	28:2:45:ASN:HD22	1.39	0.69
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.74	0.69
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.74	0.69
30:0:249:G:O2'	30:0:250:C:H5'	1.93	0.69
30:0:271:C:H41	30:0:378:A:H2	1.36	0.69
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.74	0.68
30:0:544:G:H2'	30:0:545:G:H5''	1.75	0.68
30:0:2535:A:H2	38:0:4805:HOH:O	1.75	0.68
30:0:2616:G:H1'	38:0:9426:HOH:O	1.93	0.68
31:9:29:C:H2'	31:9:30:C:H5'	1.75	0.68
30:0:816:G:C6	30:0:817:G:N1	2.61	0.68
30:0:1204:C:H2'	30:0:1205:U:O4'	1.92	0.68
30:0:1730:G:H5'	30:0:1731:C:C5	2.28	0.68
10:J:19:MET:HE1	10:J:78:ILE:HG22	1.75	0.68
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.58	0.68
30:0:1819:G:H2'	30:0:1820:G:H4'	1.73	0.68
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.73	0.68
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.33	0.68
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.74	0.68
13:M:178:LYS:HB2	38:0:6895:HOH:O	1.92	0.68
30:0:2768:A:O2'	30:0:2769:C:H5'	1.94	0.68
15:O:47:ARG:HH11	15:O:47:ARG:HG3	1.58	0.68
30:0:1201:C:H2'	30:0:1202:A:H5'	1.75	0.68
30:0:1342:C:H2'	30:0:1343:C:H5'	1.76	0.68
30:0:2812:A:C2	30:0:2814:A:N6	2.58	0.68
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.76	0.67
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.24	0.67
30:0:1183:C:N4	30:0:1184:C:H41	1.92	0.67
30:0:1191:A:H2'	30:0:1193:A:H5'	1.76	0.67
30:0:2534:C:H1'	38:0:3501:HOH:O	1.95	0.67
30:0:2659:U:H5''	38:0:4130:HOH:O	1.95	0.67
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.59	0.67
30:0:1422:U:H2'	30:0:1423:C:C6	2.29	0.67
31:9:24:U:H3'	31:9:25:G:H5'	1.77	0.67
2:B:207:LYS:HG3	30:0:2717:C:OP1	1.95	0.67
1:A:199:HIS:CD2	1:A:201:PHE:H	2.12	0.67
30:0:308:U:H5'	30:0:309:C:OP1	1.93	0.67
30:0:2703:A:H2'	30:0:2704:C:H6	1.60	0.66
30:0:1165:G:H21	30:0:1173:A:C5'	2.08	0.66
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2485:A:H3'	38:0:4900:HOH:O	1.95	0.66
30:0:559:U:H5'	30:0:559:U:C6	2.29	0.66
30:0:1185:U:H2'	30:0:1186:C:C6	2.28	0.66
30:0:1603:A:C5'	30:0:1605:G:H5'	2.25	0.66
27:1:1:THR:HA	38:1:8959:HOH:O	1.94	0.66
30:0:1857:A:H5''	38:0:6720:HOH:O	1.94	0.66
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.31	0.66
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.26	0.66
30:0:1477:C:H5'	30:0:1868:G:H5'	1.77	0.66
31:9:49:G:O2'	31:9:50:G:H5'	1.96	0.66
30:0:280:C:H2'	30:0:281:U:O4'	1.96	0.66
30:0:281:U:H2'	30:0:282:C:O4'	1.94	0.66
30:0:582:U:H2'	30:0:583:C:C6	2.31	0.66
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.77	0.66
1:A:192:VAL:HG12	38:A:9055:HOH:O	1.96	0.65
30:0:506:G:H22	30:0:509:A:H5'	1.61	0.65
30:0:2509:A:H2'	30:0:2510:C:O4'	1.96	0.65
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.77	0.65
30:0:969:G:H1	30:0:999:C:N4	1.94	0.65
30:0:1855:G:H4'	30:0:1856:C:O5'	1.96	0.65
3:C:118:THR:O	3:C:136:VAL:HG13	1.96	0.65
30:0:625:U:H5'	38:0:3191:HOH:O	1.96	0.65
1:A:36:ASP:HB2	1:A:85:SER:H	1.60	0.65
30:0:1157:C:H2'	30:0:1158:G:C8	2.31	0.65
30:0:1189:A:H3'	38:0:7692:HOH:O	1.95	0.65
30:0:1211:G:H2'	30:0:1212:C:H6	1.61	0.65
30:0:1687:C:H3'	38:0:9459:HOH:O	1.94	0.65
8:H:168:VAL:HG13	38:H:212:HOH:O	1.95	0.65
18:R:117:HIS:HD2	30:0:20:G:H21	1.45	0.65
30:0:1186:C:H42	30:0:1190:G:H22	1.44	0.65
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.79	0.65
22:V:55:ARG:O	22:V:59:ILE:HG12	1.97	0.65
30:0:714:U:H4'	38:0:5753:HOH:O	1.95	0.65
30:0:2672:C:H1'	38:0:6699:HOH:O	1.96	0.65
6:F:77:VAL:HG21	6:F:83:LEU:HD13	1.77	0.65
11:K:63:GLU:HB2	38:K:6344:HOH:O	1.97	0.65
30:0:1834:C:H2'	30:0:1840:A:H62	1.61	0.65
30:0:2004:U:O5'	30:0:2004:U:H6	1.80	0.65
31:9:20:G:O2'	31:9:21:G:H5'	1.97	0.65
8:H:29:SER:HA	8:H:62:HIS:HD2	1.61	0.65
1:A:51:ARG:HB2	38:A:9068:HOH:O	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2781:U:H2'	30:0:2782:G:H5'	1.77	0.65
30:0:558:C:C2'	30:0:559:U:C5'	2.75	0.64
30:0:1632:A:H2'	30:0:1633:C:H5'	1.79	0.64
4:D:25:MET:SD	4:D:40:ILE:HD11	2.36	0.64
30:0:380:A:H2'	38:0:7242:HOH:O	1.96	0.64
30:0:558:C:H2'	30:0:559:U:H5''	1.76	0.64
30:0:1058:A:H2'	30:0:1060:C:H5''	1.79	0.64
30:0:1342:C:O2'	30:0:1343:C:H5'	1.98	0.64
30:0:1666:C:C2'	30:0:1667:A:H5''	2.27	0.64
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.80	0.64
25:Y:235:GLU:CD	25:Y:235:GLU:H	2.04	0.64
30:0:272:A:H3'	38:0:7547:HOH:O	1.96	0.64
30:0:595:U:H2'	30:0:596:C:H6	1.63	0.64
31:9:1:U:H4'	31:9:3:A:OP1	1.97	0.64
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.97	0.64
30:0:2894:C:O2'	30:0:2895:C:H5'	1.97	0.64
12:L:41:HIS:HD2	30:0:926:A:O2'	1.79	0.64
18:R:128:ARG:NH2	30:0:2054:A:N3	2.45	0.64
30:0:2361:A:H5''	38:0:9009:HOH:O	1.97	0.64
31:9:64:C:C2'	31:9:65:A:H5'	2.27	0.64
30:0:1175:G:H1'	30:0:1193:A:C8	2.32	0.64
30:0:2824:C:H5''	30:0:2825:C:H5'	1.79	0.64
1:A:194:MET:HE3	1:A:199:HIS:HB2	1.80	0.64
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.79	0.64
30:0:1116:U:H3	30:0:1246:A:N6	1.89	0.64
30:0:1398:G:O2'	30:0:1399:A:H5'	1.98	0.64
30:0:2781:U:C2'	30:0:2782:G:H5'	2.28	0.64
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.97	0.64
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.97	0.64
20:T:61:GLU:HG2	38:T:3851:HOH:O	1.97	0.63
28:2:41:HIS:HD2	28:2:44:ARG:H	1.44	0.63
30:0:541:C:C2'	30:0:542:A:C5'	2.74	0.63
30:0:544:G:C2'	30:0:545:G:H5''	2.28	0.63
30:0:1180:U:O2'	30:0:1181:A:H5'	1.98	0.63
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.80	0.63
30:0:1307:A:H2'	30:0:1308:A:C8	2.33	0.63
30:0:2510:C:H42	30:0:2564:G:H22	1.47	0.63
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.80	0.63
30:0:1165:G:H4'	30:0:1174:A:O2'	1.98	0.63
30:0:1634:G:H2'	30:0:1635:U:H6	1.63	0.63
30:0:2335:C:H2'	30:0:2336:G:H8	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.62	0.63
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.28	0.63
3:C:214:THR:HG23	38:C:8640:HOH:O	1.96	0.63
30:0:236:A:H4'	30:0:237:G:H5'	1.81	0.63
30:0:281:U:O2'	30:0:282:C:H5'	1.99	0.63
30:0:316:A:N3	30:0:336:G:O2'	2.30	0.63
31:9:56:A:C3'	31:9:57:A:H5''	2.29	0.63
27:1:25:LYS:HD2	28:2:49:GLU:N	2.13	0.63
30:0:74:G:H2'	30:0:75:U:C6	2.34	0.63
30:0:1878:G:C1'	38:0:6135:HOH:O	2.43	0.63
3:C:27:ARG:NH2	30:0:657:G:OP1	2.31	0.63
14:N:37:ARG:NH1	31:9:6:C:C5'	2.52	0.63
30:0:541:C:H2'	30:0:542:A:H5'	1.80	0.63
30:0:2717:C:O2'	30:0:2718:C:H5''	1.97	0.63
3:C:218:VAL:HG12	38:C:8628:HOH:O	1.99	0.63
6:F:91:VAL:HG12	6:F:92:GLY:N	2.13	0.63
30:0:1278:A:H4'	30:0:1279:U:N3	2.13	0.63
30:0:1377:C:H5'	30:0:1377:C:C6	2.34	0.63
31:9:33:U:H2'	38:9:9065:HOH:O	1.98	0.63
18:R:99:ALA:HB1	18:R:109:MET:CE	2.29	0.62
30:0:285:A:H2'	30:0:286:U:O4'	1.98	0.62
30:0:694:A:H2'	30:0:695:C:H5'	1.80	0.62
14:N:7:LYS:HE3	17:Q:21:ARG:O	1.99	0.62
5:E:93:MET:HE1	5:E:165:GLY:H	1.64	0.62
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.64	0.62
30:0:533:U:H3'	38:0:3754:HOH:O	1.98	0.62
30:0:2071:C:H5'	38:0:9532:HOH:O	1.99	0.62
30:0:2670:G:O2'	30:0:2671:U:H5'	1.99	0.62
31:9:64:C:H2'	31:9:65:A:H5'	1.81	0.62
3:C:236:THR:HG22	3:C:239:ALA:HB2	1.80	0.62
30:0:2320:U:H4'	30:0:2321:A:O4'	1.99	0.62
30:0:2414:A:H2'	30:0:2415:A:C8	2.34	0.62
3:C:236:THR:HG22	3:C:239:ALA:CB	2.30	0.62
30:0:200:C:H2'	38:0:3449:HOH:O	2.00	0.62
2:B:179:LEU:O	2:B:183:GLU:HG2	2.00	0.62
3:C:2:GLN:HB3	38:C:8587:HOH:O	1.98	0.62
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.82	0.62
30:0:920:C:H4'	30:0:921:G:C2	2.34	0.62
30:0:1398:G:H2'	30:0:1399:A:C8	2.34	0.62
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.82	0.62
27:1:10:LYS:HG3	38:1:8981:HOH:O	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2512:U:H4'	30:0:2514:U:O4	1.99	0.62
30:0:162:C:H2'	30:0:163:U:H5'	1.80	0.62
2:B:162:MET:HG3	2:B:310:ARG:HD3	1.82	0.61
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.82	0.61
30:0:585:C:H5''	38:0:4883:HOH:O	1.99	0.61
30:0:1132:A:N6	30:0:1229:C:H2'	2.16	0.61
30:0:1524:U:H6	30:0:1524:U:H5''	1.63	0.61
30:0:2900:G:H2'	30:0:2901:C:O4'	1.99	0.61
31:9:55:U:H4'	31:9:56:A:H8	1.62	0.61
38:C:8669:HOH:O	30:0:2100:A:H5'	1.99	0.61
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.83	0.61
30:0:137:U:H2'	30:0:139:C:C5	2.35	0.61
30:0:1654:U:H5''	38:0:7439:HOH:O	1.99	0.61
30:0:1838:U:H3'	38:0:5538:HOH:O	1.98	0.61
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.66	0.61
4:D:25:MET:HE2	4:D:41:LEU:HD11	1.80	0.61
9:I:108:HIS:H	9:I:109:PRO:HD2	1.66	0.61
30:0:1350:U:H4'	38:0:5132:HOH:O	2.00	0.61
30:0:2507:G:H2'	30:0:2510:C:N4	2.15	0.61
1:A:211:LYS:HB2	38:A:9083:HOH:O	2.00	0.61
30:0:1603:A:H5'	30:0:1605:G:C4'	2.30	0.61
30:0:1972:U:H2'	30:0:1973:A:H5''	1.83	0.61
30:0:2064:U:H5'	30:0:2652:U:H4'	1.82	0.61
12:L:18:HIS:HD2	30:0:902:G:N7	1.99	0.61
30:0:2908:A:O5'	30:0:2908:A:H8	1.83	0.61
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.82	0.61
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.28	0.61
12:L:133:VAL:HA	38:L:8873:HOH:O	2.00	0.61
29:3:48:ASN:HD21	30:0:2468:A:H61	1.48	0.61
30:0:1835:U:C5	30:0:1840:A:N7	2.65	0.61
3:C:37:ALA:HA	3:C:100:LEU:HD12	1.82	0.61
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.65	0.61
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.08	0.61
30:0:1226:G:H5'	38:0:4541:HOH:O	1.99	0.61
2:B:145:HIS:HD2	2:B:146:THR:O	1.83	0.61
12:L:6:ARG:HD3	30:0:1299:G:O6	2.00	0.61
21:U:17:THR:HG22	21:U:18:GLY:N	2.16	0.61
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.83	0.61
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.00	0.61
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.82	0.60
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:95:GLU:HG3	38:C:8682:HOH:O	2.00	0.60
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.83	0.60
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.83	0.60
30:0:401:C:H2'	30:0:402:U:H6	1.64	0.60
30:0:1181:A:C2'	30:0:1182:C:H5'	2.32	0.60
30:0:1741:U:O2'	30:0:2723:G:H4'	2.01	0.60
30:0:1819:G:H5'	38:0:4725:HOH:O	2.00	0.60
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.15	0.60
21:U:52:THR:HG22	21:U:54:THR:H	1.66	0.60
30:0:10:U:C4	30:0:532:A:N7	2.70	0.60
30:0:1819:G:H2'	30:0:1820:G:C5'	2.31	0.60
18:R:128:ARG:NH2	30:0:2054:A:C2	2.70	0.60
20:T:24:ARG:HH21	20:T:39:ASN:ND2	1.98	0.60
30:0:447:A:O2'	30:0:448:G:H5'	2.01	0.60
30:0:595:U:H2'	30:0:596:C:C6	2.37	0.60
30:0:1587:U:H2'	30:0:1588:G:O4'	2.02	0.60
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.17	0.60
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.82	0.60
29:3:73:GLU:HB3	38:3:9049:HOH:O	2.01	0.60
30:0:558:C:H2'	30:0:559:U:H5'	1.83	0.60
30:0:847:C:H4'	38:0:3759:HOH:O	1.99	0.60
30:0:2372:A:H2'	30:0:2373:U:H6	1.66	0.60
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.17	0.60
29:3:67:LEU:HD11	29:3:88:LEU:HD21	1.82	0.60
30:0:396:U:O2'	30:0:418:C:H4'	2.02	0.60
30:0:407:A:H2'	30:0:408:A:C8	2.37	0.60
30:0:541:C:O2'	30:0:542:A:H5''	2.02	0.60
30:0:1202:A:C2'	30:0:1203:G:H5'	2.32	0.60
30:0:282:C:O2'	30:0:283:U:C5'	2.49	0.60
30:0:1583:U:H1'	38:0:9989:HOH:O	2.02	0.60
30:0:2281:C:C2'	30:0:2282:U:H5'	2.32	0.60
3:C:238:SER:HB2	38:C:8577:HOH:O	2.01	0.60
13:M:163:LEU:HD21	30:0:188:C:H5''	1.84	0.60
13:M:179:GLY:O	30:0:399:C:H5'	2.02	0.60
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.83	0.60
23:W:21:LEU:HD22	23:W:26:ILE:CD1	2.32	0.60
30:0:130:C:H2'	38:0:3166:HOH:O	2.02	0.60
30:0:807:A:O2'	30:0:808:A:H5'	2.01	0.60
7:G:12:ILE:HG23	38:0:5471:HOH:O	2.02	0.59
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.83	0.59
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:164:THR:HG23	13:M:165:GLY:N	2.17	0.59
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.18	0.59
30:0:1172:G:H5''	38:0:7275:HOH:O	2.01	0.59
30:0:1676:G:O2'	30:0:1677:U:H5'	2.03	0.59
31:9:47:A:C2	31:9:48:C:C2	2.89	0.59
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.82	0.59
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.83	0.59
30:0:1206:U:H2'	30:0:1207:A:O4'	2.01	0.59
30:0:2135:A:O2'	30:0:2136:G:H5'	2.03	0.59
4:D:65:GLU:HA	38:D:6752:HOH:O	2.02	0.59
4:D:105:SER:OG	30:0:2338:G:H1'	2.03	0.59
5:E:68:HIS:O	5:E:72:MET:HG3	2.01	0.59
10:J:45:VAL:HG23	10:J:130:VAL:O	2.00	0.59
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.84	0.59
30:0:1165:G:N2	30:0:1173:A:H5''	2.15	0.59
30:0:2826:G:C6	30:0:2913:A:N6	2.70	0.59
1:A:186:TRP:CG	1:A:187:PRO:HA	2.38	0.59
13:M:164:THR:HG22	13:M:167:GLY:N	2.16	0.59
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.37	0.59
30:0:1524:U:H6	30:0:1524:U:C5'	2.16	0.59
30:0:1766:U:O2	30:0:1778:A:H5'	2.01	0.59
30:0:2505:G:C2'	30:0:2506:A:H5'	2.32	0.59
31:9:92:G:H2'	31:9:93:A:H8	1.67	0.59
3:C:16:VAL:HG21	38:C:8634:HOH:O	2.02	0.59
13:M:125:ARG:HD2	38:M:8893:HOH:O	2.02	0.59
14:N:34:LEU:HD22	14:N:129:ILE:HD13	1.83	0.59
30:0:424:C:H2'	30:0:425:U:C6	2.38	0.59
30:0:1042:U:O2'	30:0:1043:C:H5'	2.02	0.59
30:0:1165:G:N2	30:0:1173:A:C5'	2.66	0.59
30:0:2748:G:H5'	38:0:7557:HOH:O	2.02	0.59
10:J:63:ILE:HD11	30:0:1236:A:C8	2.38	0.59
30:0:482:G:H4'	30:0:508:A:N1	2.18	0.59
30:0:522:U:O2'	30:0:1366:C:H5'	2.02	0.59
30:0:853:C:H3'	38:0:4563:HOH:O	2.03	0.59
30:0:1511:U:O2'	30:0:1512:G:H5'	2.03	0.59
30:0:1641:A:C2'	30:0:1642:A:H5'	2.32	0.59
30:0:2374:G:H2'	30:0:2375:A:C8	2.37	0.59
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.85	0.59
28:2:39:ARG:HG2	38:2:3143:HOH:O	2.03	0.59
30:0:255:A:H2'	30:0:256:C:C6	2.38	0.59
30:0:1790:C:H2'	30:0:1791:U:H6	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1973:A:H5'	30:0:1973:A:C8	2.36	0.59
30:0:2324:G:N2	30:0:2377:U:H1'	2.17	0.59
1:A:36:ASP:O	1:A:38:ILE:N	2.36	0.58
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.67	0.58
27:1:9:GLY:HA2	30:0:1687:C:O2	2.02	0.58
30:0:368:C:H2'	30:0:369:G:H5'	1.84	0.58
30:0:1321:A:H2'	30:0:1322:G:C8	2.38	0.58
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.02	0.58
30:0:123:U:H5'	38:0:6671:HOH:O	2.03	0.58
30:0:1196:C:N4	30:0:1204:C:H42	2.01	0.58
30:0:1904:A:H2'	30:0:1905:U:O4'	2.03	0.58
30:0:2467:A:O2'	30:0:2468:A:H2'	2.02	0.58
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.33	0.58
3:C:79:ARG:O	3:C:87:ARG:HG2	2.03	0.58
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.67	0.58
30:0:10:U:C4	30:0:532:A:C8	2.91	0.58
30:0:2335:C:H2'	30:0:2336:G:C8	2.38	0.58
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.85	0.58
28:2:41:HIS:HB3	28:2:44:ARG:HB2	1.84	0.58
30:0:1170:U:H2'	30:0:1172:G:OP2	2.02	0.58
30:0:1182:C:C1'	30:0:1192:A:H8	2.16	0.58
30:0:1948:G:H2'	30:0:1949:G:C8	2.39	0.58
30:0:2878:U:H2'	30:0:2879:A:O4'	2.02	0.58
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.15	0.58
30:0:2281:C:H2'	30:0:2282:U:H5'	1.85	0.58
1:A:121:ALA:O	1:A:124:VAL:HG22	2.03	0.58
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.85	0.58
18:R:4:TYR:CE1	18:R:17:MET:HE2	2.38	0.58
30:0:960:G:H8	38:0:5987:HOH:O	1.85	0.58
30:0:2852:A:H5''	38:0:5246:HOH:O	2.03	0.58
3:C:76:ARG:HG2	3:C:78:ARG:HH12	1.69	0.58
3:C:237:GLU:HG3	38:C:8634:HOH:O	2.04	0.58
6:F:58:GLU:HA	6:F:61:MET:HE2	1.84	0.58
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.34	0.58
12:L:14:GLY:O	30:0:1295:G:H5''	2.03	0.58
30:0:2768:A:H5''	38:0:4434:HOH:O	2.03	0.58
22:V:64:GLY:O	22:V:65:ASP:HB2	2.04	0.58
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.86	0.58
25:Y:141:THR:HG23	38:Y:8158:HOH:O	2.03	0.58
30:0:440:C:H2'	30:0:441:A:C8	2.39	0.58
30:0:1819:G:H2'	30:0:1820:G:C4'	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:37:C:H2'	31:9:38:A:H8	1.68	0.58
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.34	0.58
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.38	0.58
30:0:681:G:N3	30:0:681:G:H5'	2.19	0.58
30:0:2643:G:H5''	38:0:3933:HOH:O	2.03	0.58
30:0:2820:A:H2'	30:0:2821:C:C6	2.38	0.58
14:N:141:ARG:NH1	31:9:35:C:H2'	2.18	0.58
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.86	0.58
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.86	0.57
19:S:76:GLU:HB3	38:S:8992:HOH:O	2.04	0.57
30:0:1947:G:H2'	30:0:1948:G:H8	1.69	0.57
30:0:2760:C:H5''	38:0:5337:HOH:O	2.03	0.57
2:B:27:ASN:HD22	2:B:27:ASN:H	1.51	0.57
3:C:174:ILE:HD11	30:0:338:C:H4'	1.85	0.57
5:E:69:ILE:HA	5:E:72:MET:HE3	1.85	0.57
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.86	0.57
27:1:16:HIS:HD2	30:0:470:U:O2'	1.86	0.57
28:2:38:LYS:HE3	38:0:4231:HOH:O	2.04	0.57
30:0:249:G:N2	30:0:250:C:C2	2.72	0.57
30:0:1730:G:C5'	30:0:1731:C:C6	2.86	0.57
2:B:238:ASN:HD22	2:B:240:GLY:N	1.97	0.57
6:F:91:VAL:HG12	6:F:92:GLY:H	1.68	0.57
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.38	0.57
30:0:185:G:H4'	30:0:186:A:OP1	2.04	0.57
30:0:360:A:H2'	30:0:361:C:O4'	2.04	0.57
30:0:395:A:H5''	38:0:3928:HOH:O	2.05	0.57
30:0:397:A:O2'	30:0:417:G:N3	2.36	0.57
30:0:1191:A:C2	30:0:1207:A:C2	2.93	0.57
30:0:1965:C:O2'	30:0:1966:U:H5'	2.04	0.57
30:0:2254:G:O2'	30:0:2255:A:H5'	2.04	0.57
30:0:2532:A:H2	38:0:7579:HOH:O	1.87	0.57
31:9:76:G:C3'	31:9:77:A:H5''	2.25	0.57
13:M:188:ARG:HD3	30:0:155:C:OP2	2.03	0.57
38:O:7674:HOH:O	30:0:653:U:H5''	2.05	0.57
31:9:3:A:C8	31:9:26:C:C2	2.93	0.57
31:9:23:U:O2'	31:9:24:U:H4'	2.05	0.57
2:B:244:PRO:HB3	30:0:1234:U:N3	2.19	0.57
21:U:14:GLU:O	21:U:17:THR:HB	2.05	0.57
28:2:35:ARG:HB2	38:2:2691:HOH:O	2.05	0.57
30:0:65:C:O2'	30:0:66:G:H5'	2.03	0.57
30:0:119:A:H2'	30:0:120:A:H5''	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:602:A:O2'	30:0:605:C:H4'	2.04	0.57
30:0:1524:U:OP1	30:0:1524:U:H4'	2.05	0.57
30:0:2314:G:C2'	30:0:2315:C:H5'	2.34	0.57
30:0:1116:U:O2'	30:0:1118:A:C2	2.50	0.57
30:0:1333:U:H2'	30:0:1334:C:C6	2.40	0.57
1:A:192:VAL:HG13	1:A:207:GLN:HB3	1.87	0.57
13:M:30:GLU:O	13:M:34:GLU:HG3	2.04	0.57
14:N:13:ARG:NH1	30:0:2368:A:C6	2.72	0.57
18:R:39:THR:HG23	18:R:107:GLU:O	2.05	0.57
30:0:1515:A:H2'	30:0:1516:U:C6	2.40	0.57
30:0:2282:U:H4'	30:0:2309:C:C5	2.39	0.57
30:0:2507:G:H2'	30:0:2510:C:H42	1.70	0.57
8:H:98:LEU:HD11	8:H:127:ALA:HB2	1.86	0.57
30:0:291:C:H2'	30:0:292:G:O4'	2.05	0.57
30:0:711:G:C2	30:0:718:C:C2	2.92	0.57
30:0:1016:U:O2'	30:0:2303:A:N7	2.38	0.57
30:0:1351:G:H1'	38:0:4693:HOH:O	2.04	0.57
3:C:174:ILE:CD1	30:0:338:C:H4'	2.35	0.56
16:P:59:ARG:O	16:P:63:ARG:HG3	2.05	0.56
30:0:538:C:H5''	30:0:539:G:C8	2.40	0.56
30:0:1189:A:O2'	30:0:1208:C:H2'	2.05	0.56
30:0:2533:C:H5'	30:0:2533:C:C6	2.38	0.56
30:0:2831:C:O2'	30:0:2832:C:H5'	2.05	0.56
30:0:2897:C:O2'	30:0:2898:G:H5'	2.05	0.56
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.87	0.56
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.85	0.56
30:0:432:G:O2'	30:0:433:C:H5'	2.05	0.56
30:0:1504:A:H4'	30:0:1506:U:C5	2.40	0.56
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.35	0.56
2:B:294:TYR:HE2	38:B:9116:HOH:O	1.88	0.56
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.88	0.56
19:S:11:THR:H	19:S:14:ALA:HB3	1.69	0.56
19:S:57:THR:HG23	38:S:8980:HOH:O	2.05	0.56
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.45	0.56
30:0:812:A:H2'	30:0:813:C:C6	2.40	0.56
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.40	0.56
30:0:851:C:O2	30:0:2022:A:H2	1.87	0.56
30:0:1634:G:H2'	30:0:1635:U:C6	2.41	0.56
30:0:2297:U:H1'	38:0:5188:HOH:O	2.04	0.56
30:0:2781:U:H2'	30:0:2782:G:C5'	2.35	0.56
18:R:104:PHE:HB3	18:R:109:MET:HE2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.05	0.56
30:0:483:C:C4	30:0:484:A:C6	2.94	0.56
30:0:484:A:N1	30:0:506:G:H4'	2.21	0.56
30:0:2282:U:H4'	30:0:2309:C:H5	1.71	0.56
30:0:2300:A:H4'	30:0:2301:A:O5'	2.05	0.56
30:0:2472:C:O2'	30:0:2634:G:H4'	2.04	0.56
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.70	0.56
4:D:56:ARG:NH2	30:0:2332:A:H5'	2.21	0.56
4:D:159:PRO:O	4:D:163:VAL:HG23	2.06	0.56
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.41	0.56
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.94	0.56
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.04	0.56
24:X:72:VAL:HG22	24:X:85:VAL:HG12	1.86	0.56
30:0:1189:A:H1'	30:0:1209:C:O4'	2.05	0.56
31:9:35:C:H5''	38:9:9075:HOH:O	2.06	0.56
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.37	0.56
30:0:559:U:C5	30:0:560:U:C5	2.94	0.56
30:0:1130:U:H2'	30:0:1131:G:O4'	2.06	0.56
30:0:2482:G:H5'	38:0:5036:HOH:O	2.05	0.56
18:R:29:LYS:HB3	38:R:8936:HOH:O	2.06	0.56
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.06	0.56
30:0:151:A:C2	30:0:152:A:C2	2.94	0.56
30:0:282:C:O2	30:0:282:C:C2'	2.54	0.56
30:0:1772:C:H5'	30:0:1773:G:C5	2.41	0.56
30:0:2831:C:C2'	30:0:2832:C:H5'	2.36	0.56
1:A:33:GLU:H	1:A:33:GLU:CD	2.14	0.56
4:D:103:ASN:ND2	4:D:134:LEU:H	2.04	0.56
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.70	0.56
2:B:156:LYS:HD3	38:0:3870:HOH:O	2.05	0.55
38:M:8868:HOH:O	30:0:2244:A:H1'	2.06	0.55
15:O:32:ARG:HH21	15:O:35:LYS:NZ	2.04	0.55
30:0:1741:U:HO2'	30:0:2723:G:H4'	1.71	0.55
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.87	0.55
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.88	0.55
30:0:553:G:O4'	30:0:1325:G:H5'	2.06	0.55
30:0:1426:C:H2'	38:0:9598:HOH:O	2.06	0.55
30:0:1545:C:H2'	30:0:1546:G:O4'	2.06	0.55
30:0:1787:C:H4'	30:0:2883:A:O4'	2.06	0.55
31:9:49:G:H2'	31:9:50:G:O4'	2.05	0.55
2:B:211:THR:HG23	30:0:2840:A:OP1	2.06	0.55
2:B:265:LEU:HD21	2:B:316:ARG:HD3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:45:PRO:HB2	38:O:7387:HOH:O	2.06	0.55
12:L:136:ALA:HB3	38:L:8873:HOH:O	2.05	0.55
14:N:37:ARG:HH11	31:9:6:C:C5'	2.15	0.55
14:N:80:SER:HB2	38:N:8833:HOH:O	2.05	0.55
30:0:1972:U:C2'	30:0:1973:A:H5''	2.36	0.55
30:0:2886:C:O2'	30:0:2887:G:H5'	2.07	0.55
21:U:39:ASN:ND2	21:U:44:ARG:HH11	2.04	0.55
29:3:3:MET:O	29:3:90:PHE:HA	2.06	0.55
30:0:960:G:N3	30:0:960:G:C2'	2.69	0.55
30:0:1191:A:C2'	30:0:1193:A:H5'	2.37	0.55
2:B:98:THR:HG22	30:0:2820:A:OP1	2.07	0.55
20:T:9:LYS:HD3	38:O:3761:HOH:O	2.06	0.55
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.42	0.55
30:0:1202:A:H2'	30:0:1203:G:C5'	2.37	0.55
30:0:2599:A:H5''	38:O:3384:HOH:O	2.05	0.55
9:I:87:PRO:HG2	30:0:1181:A:H4'	1.87	0.55
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.06	0.55
14:N:37:ARG:HD3	33:N:8807:CL:CL	2.44	0.55
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.89	0.55
30:0:669:G:O2'	30:0:670:G:H5'	2.07	0.55
30:0:1120:U:H5'	30:0:1121:G:OP2	2.07	0.55
4:D:173:GLU:HG3	4:D:174:VAL:H	1.71	0.55
15:O:25:VAL:CG1	30:0:710:G:H5'	2.36	0.55
18:R:98:ASN:HD21	30:0:500:G:H21	1.54	0.55
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.47	0.55
30:0:1790:C:H2'	30:0:1791:U:C6	2.41	0.55
2:B:86:ALA:HA	38:B:9045:HOH:O	2.05	0.55
2:B:267:LYS:HE2	38:B:8994:HOH:O	2.06	0.55
3:C:236:THR:HA	38:C:8657:HOH:O	2.07	0.55
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.42	0.55
18:R:59:PHE:O	18:R:63:ASN:HB3	2.06	0.55
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	1.88	0.55
30:0:1972:U:H2'	30:0:1973:A:C5'	2.37	0.55
4:D:103:ASN:HD22	4:D:134:LEU:H	1.54	0.55
13:M:46:LEU:HG	38:M:8921:HOH:O	2.06	0.55
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.89	0.55
15:O:96:VAL:HG13	15:O:100:GLN:HB2	1.89	0.55
23:W:154:ARG:NH1	30:0:588:G:O6	2.40	0.55
30:0:512:G:O3'	30:0:513:A:H8	1.89	0.55
30:0:794:U:H3	30:0:819:A:H61	1.54	0.55
30:0:1544:U:O2'	30:0:1545:C:H5'	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1706:G:C6	30:0:1707:G:C6	2.95	0.55
30:0:2297:U:H2'	30:0:2298:C:H6	1.71	0.55
30:0:2514:U:OP1	30:0:2572:G:H1'	2.06	0.55
31:9:24:U:H3'	31:9:25:G:C5'	2.35	0.55
6:F:96:ALA:HA	38:F:3111:HOH:O	2.06	0.54
30:0:88:G:H8	30:0:88:G:H5'	1.72	0.54
30:0:713:U:O5'	30:0:713:U:H6	1.90	0.54
30:0:1504:A:H5'	38:0:4423:HOH:O	2.06	0.54
30:0:1915:U:O2'	30:0:1916:C:H5'	2.06	0.54
30:0:2851:G:C2'	30:0:2852:A:H5'	2.37	0.54
4:D:131:THR:HG21	30:0:2348:C:H1'	1.89	0.54
30:0:515:C:H5''	38:0:5660:HOH:O	2.06	0.54
30:0:1202:A:H2'	30:0:1203:G:O4'	2.08	0.54
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.40	0.54
10:J:24:SER:HG	30:0:1102:C:HO2'	1.54	0.54
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.13	0.54
30:0:644:G:H5'	30:0:644:G:N3	2.22	0.54
30:0:1160:G:H2'	38:0:5647:HOH:O	2.07	0.54
30:0:1202:A:O2'	30:0:1203:G:H5'	2.07	0.54
30:0:1903:U:O2'	30:0:1904:A:N7	2.40	0.54
10:J:19:MET:HE2	10:J:79:PHE:HA	1.89	0.54
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.72	0.54
30:0:1730:G:H5''	30:0:1731:C:H6	1.71	0.54
2:B:119:HIS:O	2:B:121:PRO:HD3	2.07	0.54
10:J:127:ILE:CG2	33:J:8801:CL:CL	2.91	0.54
20:T:38:ARG:NH1	38:T:6217:HOH:O	2.41	0.54
14:N:4:PRO:HG3	31:9:69:U:OP1	2.07	0.54
18:R:132:ARG:HG2	18:R:133:ALA:N	2.21	0.54
21:U:9:CYS:HA	21:U:52:THR:HG23	1.90	0.54
27:1:20:ARG:HG2	30:0:111:C:O2'	2.08	0.54
30:0:1521:C:H2'	30:0:1522:A:H8	1.72	0.54
30:0:2326:C:H4'	30:0:2412:G:H4'	1.89	0.54
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.90	0.54
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.90	0.54
27:1:25:LYS:CD	28:2:49:GLU:H	2.18	0.54
30:0:553:G:H5'	38:0:3505:HOH:O	2.08	0.54
30:0:1406:A:H5'	30:0:1407:A:C8	2.42	0.54
30:0:2314:G:H2'	30:0:2315:C:H5'	1.90	0.54
12:L:46:LEU:O	30:0:2430:A:H4'	2.07	0.54
15:O:37:ARG:HD2	30:0:656:G:OP2	2.08	0.54
30:0:1041:U:H2'	30:0:1042:U:H5'	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1559:A:H4'	38:0:5879:HOH:O	2.08	0.54
4:D:64:ARG:HD3	4:D:67:ASP:HB3	1.90	0.54
9:I:118:ASN:HB3	30:0:1185:U:H5''	1.88	0.54
19:S:33:SER:O	19:S:37:VAL:HG23	2.08	0.54
23:W:13:MET:HE1	23:W:21:LEU:CD1	2.34	0.54
30:0:920:C:H5''	30:0:921:G:O5'	2.08	0.54
30:0:1573:A:H2'	30:0:1574:C:O4'	2.08	0.54
30:0:2329:C:O2'	30:0:2330:U:H5'	2.08	0.54
30:0:2421:G:H2'	38:0:4085:HOH:O	2.07	0.54
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.08	0.54
2:B:212:GLN:HA	30:0:1733:A:H4'	1.89	0.54
17:Q:25:PRO:HB2	38:9:9079:HOH:O	2.07	0.54
23:W:21:LEU:HD22	23:W:26:ILE:HD13	1.89	0.54
30:0:812:A:H1'	38:0:3964:HOH:O	2.08	0.54
30:0:1165:G:O3'	30:0:1174:A:H4'	2.08	0.54
30:0:1193:A:C2	30:0:1194:A:N6	2.76	0.54
30:0:2460:A:C2	30:0:2461:U:C2	2.95	0.54
25:Y:151:SER:HB3	25:Y:154:ARG:CB	2.38	0.53
30:0:1495:C:H1'	30:0:1573:A:H1'	1.90	0.53
30:0:1544:U:H2'	30:0:1545:C:H6	1.72	0.53
2:B:84:LEU:HD23	2:B:142:LEU:HD23	1.91	0.53
16:P:76:GLY:HA3	30:0:1785:G:OP1	2.08	0.53
30:0:822:C:H2'	30:0:823:U:H6	1.73	0.53
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.72	0.53
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.71	0.53
30:0:1803:C:H2'	30:0:1804:A:C8	2.43	0.53
30:0:2134:G:N2	30:0:2242:U:C2	2.76	0.53
4:D:27:ILE:HB	4:D:69:ILE:O	2.08	0.53
8:H:35:LYS:HE3	30:0:968:G:H1'	1.88	0.53
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.90	0.53
30:0:963:C:H2'	30:0:964:G:C8	2.43	0.53
30:0:1289:C:O2'	30:0:1290:G:H5'	2.09	0.53
30:0:2510:C:H5'	30:0:2511:A:OP2	2.08	0.53
30:0:2667:G:H1'	30:0:2914:A:N3	2.24	0.53
31:9:54:A:C2'	31:9:55:U:H5'	2.38	0.53
9:I:69:PRO:HA	30:0:1164:U:OP1	2.09	0.53
25:Y:187:VAL:HB	38:Y:8140:HOH:O	2.08	0.53
30:0:2241:C:O2'	30:0:2242:U:H5'	2.09	0.53
16:P:13:VAL:HG21	16:P:41:ARG:HG2	1.89	0.53
30:0:349:U:H2'	30:0:350:G:O4'	2.09	0.53
30:0:821:U:O2'	30:0:822:C:H5'	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1118:A:N6	30:0:1244:U:H3	1.99	0.53
30:0:2251:G:H2'	30:0:2252:A:C8	2.43	0.53
31:9:29:C:C2'	31:9:30:C:H5'	2.38	0.53
1:A:51:ARG:NH1	1:A:120:ARG:O	2.39	0.53
2:B:53:LEU:HD11	2:B:327:VAL:HG22	1.89	0.53
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.09	0.53
3:C:184:ARG:NH2	30:0:450:C:OP1	2.29	0.53
6:F:91:VAL:HG11	30:0:262:A:OP2	2.09	0.53
10:J:76:ASP:HA	38:J:8865:HOH:O	2.09	0.53
30:0:635:A:H2'	30:0:636:G:H5''	1.90	0.53
30:0:1632:A:C2'	30:0:1633:C:H5'	2.39	0.53
30:0:1909:A:N1	30:0:2128:G:H1'	2.24	0.53
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.90	0.53
5:E:107:PHE:CE1	5:E:152:THR:HB	2.43	0.53
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.89	0.53
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.90	0.53
14:N:35:VAL:HG12	14:N:37:ARG:HG2	1.91	0.53
25:Y:151:SER:HB3	25:Y:154:ARG:HB2	1.90	0.53
27:1:12:ASN:O	30:0:1415:G:H5'	2.08	0.53
30:0:222:A:H2'	30:0:223:G:O4'	2.08	0.53
30:0:574:G:O2'	30:0:575:A:H5'	2.09	0.53
30:0:1166:A:C6	30:0:1167:G:C6	2.97	0.53
10:J:107:ASN:HD22	10:J:109:TYR:H	1.57	0.53
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.09	0.53
14:N:132:ASN:O	14:N:135:VAL:HG12	2.09	0.53
30:0:128:A:O2'	30:0:129:A:H5'	2.09	0.53
30:0:559:U:H6	30:0:559:U:C5'	2.19	0.53
30:0:2065:C:O2'	30:0:2066:C:H5'	2.09	0.53
30:0:2073:G:C6	30:0:2489:G:H4'	2.44	0.53
30:0:2111:G:H1'	38:0:9051:HOH:O	2.08	0.53
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.09	0.53
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.91	0.53
14:N:139:TRP:HA	14:N:139:TRP:HE3	1.74	0.53
30:0:290:C:O2'	30:0:291:C:H5'	2.09	0.53
30:0:441:A:H8	30:0:441:A:O5'	1.92	0.53
30:0:2769:C:H2'	30:0:2770:G:O4'	2.09	0.53
30:0:24:G:N2	30:0:518:G:H1'	2.24	0.52
30:0:1181:A:H2'	30:0:1182:C:H5'	1.90	0.52
30:0:1594:C:O2'	30:0:1595:G:H5'	2.09	0.52
30:0:1625:U:H5''	38:0:6037:HOH:O	2.09	0.52
31:9:3:A:H1'	38:9:9037:HOH:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.13	0.52
30:0:615:G:H2'	30:0:616:U:C6	2.44	0.52
4:D:57:THR:HG23	4:D:63:ILE:HA	1.91	0.52
4:D:58:VAL:HB	4:D:62:ASP:HB3	1.89	0.52
14:N:48:VAL:HG11	14:N:55:ASP:HB3	1.90	0.52
30:0:90:A:H2'	30:0:91:G:O4'	2.08	0.52
30:0:204:A:H2'	30:0:205:U:H5'	1.90	0.52
30:0:1419:U:H2'	30:0:1685:A:C2	2.44	0.52
30:0:1733:A:C6	30:0:1734:C:C2	2.98	0.52
30:0:2500:C:O2'	30:0:2501:G:H5'	2.08	0.52
31:9:59:C:H2'	31:9:60:C:C6	2.43	0.52
1:A:223:ARG:HB2	30:0:2272:G:H5'	1.90	0.52
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.91	0.52
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.43	0.52
38:L:8841:HOH:O	30:0:2453:G:H5''	2.09	0.52
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.25	0.52
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.90	0.52
28:2:49:GLU:HB2	38:2:719:HOH:O	2.10	0.52
30:0:1181:A:H1'	38:0:7132:HOH:O	2.09	0.52
30:0:1216:G:O2'	30:0:1217:G:H5'	2.10	0.52
30:0:1461:U:H2'	30:0:1462:C:C6	2.44	0.52
30:0:2598:U:O2	30:0:2600:A:H8	1.92	0.52
33:0:8813:CL:CL	38:0:4697:HOH:O	2.56	0.52
1:A:206:ARG:HD3	38:0:4620:HOH:O	2.08	0.52
2:B:305:ASP:O	2:B:306:LYS:HB2	2.10	0.52
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.09	0.52
16:P:134:VAL:O	16:P:137:LEU:HB3	2.10	0.52
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.44	0.52
26:Z:74:GLN:HB2	26:Z:78:ILE:HG22	1.90	0.52
30:0:899:C:H5'	38:0:3209:HOH:O	2.09	0.52
30:0:1161:A:C6	30:0:1162:G:N7	2.77	0.52
30:0:1189:A:H1'	30:0:1209:C:C1'	2.40	0.52
30:0:1482:A:O2'	30:0:1483:C:H5'	2.10	0.52
30:0:1588:G:C6	30:0:1589:G:N1	2.77	0.52
2:B:17:LYS:O	2:B:260:HIS:HD2	1.91	0.52
17:Q:19:ARG:HH21	31:9:11:A:P	2.33	0.52
30:0:1196:C:H42	30:0:1204:C:H42	1.58	0.52
30:0:1202:A:H2'	30:0:1203:G:H5'	1.90	0.52
30:0:1309:U:O2'	30:0:1310:U:H5'	2.09	0.52
30:0:1871:U:O4'	30:0:1873:G:C8	2.63	0.52
31:9:91:C:H2'	31:9:92:G:O4'	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:SER:OG	30:0:2101:A:H2'	2.09	0.52
16:P:91:LYS:O	16:P:95:GLU:HG3	2.08	0.52
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.90	0.52
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.44	0.52
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.92	0.52
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.92	0.52
20:T:38:ARG:HH21	30:0:306:A:P	2.33	0.52
30:0:136:C:H2'	30:0:137:U:O4'	2.09	0.52
30:0:2866:U:C2	30:0:2891:A:C8	2.98	0.52
12:L:50:GLY:C	30:0:2453:G:H4'	2.35	0.52
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.10	0.52
30:0:1029:U:O2'	30:0:1273:C:OP1	2.25	0.52
30:0:2273:C:H5''	38:0:4515:HOH:O	2.10	0.52
31:9:108:C:H2'	31:9:109:G:C8	2.45	0.52
3:C:217:GLU:HG3	30:0:672:G:O6	2.10	0.52
11:K:10:GLN:H	11:K:10:GLN:NE2	1.96	0.52
11:K:18:ILE:HG22	11:K:93:ASN:HB2	1.92	0.52
18:R:33:ARG:NH1	38:R:8947:HOH:O	2.42	0.52
30:0:1964:U:O2	30:0:1964:U:C2'	2.58	0.52
30:0:2032:U:O2'	30:0:2033:G:H5''	2.09	0.52
30:0:2112:A:H2'	30:0:2113:G:C8	2.45	0.52
8:H:70:LEU:O	8:H:74:ARG:HB2	2.09	0.51
9:I:112:LEU:HD12	30:0:1162:G:H1'	1.92	0.51
22:V:56:ILE:O	22:V:60:GLN:HG3	2.09	0.51
30:0:152:A:H2'	30:0:153:C:C6	2.45	0.51
30:0:407:A:H8	38:0:4468:HOH:O	1.93	0.51
30:0:951:A:C2'	30:0:952:G:H5'	2.39	0.51
30:0:1333:U:H2'	30:0:1334:C:H6	1.75	0.51
30:0:2827:A:H2'	30:0:2828:G:O4'	2.10	0.51
31:9:59:C:O5'	31:9:59:C:H6	1.92	0.51
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.92	0.51
30:0:638:C:H2'	30:0:639:A:C8	2.46	0.51
30:0:792:G:O2'	30:0:793:A:H5'	2.11	0.51
30:0:876:A:H2'	30:0:876:A:N3	2.23	0.51
30:0:2636:C:H3'	38:0:9279:HOH:O	2.09	0.51
31:9:42:C:H5'	31:9:43:G:OP2	2.10	0.51
31:9:58:G:H1'	38:9:9067:HOH:O	2.09	0.51
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.91	0.51
30:0:154:C:H2'	30:0:155:C:H6	1.76	0.51
30:0:821:U:H2'	30:0:822:C:H6	1.75	0.51
30:0:1163:G:H2'	30:0:1164:U:C5	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2896:A:N3	30:0:2896:A:H2'	2.25	0.51
2:B:125:GLU:O	2:B:129:ARG:HG3	2.10	0.51
5:E:84:MET:HG2	5:E:168:ILE:HA	1.93	0.51
22:V:12:THR:HG23	22:V:14:ALA:H	1.74	0.51
30:0:255:A:H2'	30:0:256:C:H6	1.74	0.51
30:0:603:A:H4'	30:0:605:C:C6	2.46	0.51
30:0:1081:A:H5''	38:0:3158:HOH:O	2.10	0.51
30:0:1137:G:H1'	38:0:3884:HOH:O	2.09	0.51
30:0:1279:U:O2	30:0:1279:U:H2'	2.09	0.51
30:0:1525:G:H5'	30:0:1526:A:OP2	2.11	0.51
30:0:1755:A:H2'	30:0:1756:G:O4'	2.11	0.51
30:0:2478:U:O2'	30:0:2479:A:H5'	2.10	0.51
30:0:2566:A:C2	30:0:2696:G:O4'	2.63	0.51
30:0:2724:U:H2'	30:0:2725:G:O4'	2.10	0.51
2:B:248:ARG:O	2:B:251:VAL:HG22	2.11	0.51
23:W:43:GLY:HA3	30:0:945:U:O2'	2.11	0.51
30:0:684:G:H2'	30:0:685:C:C6	2.46	0.51
30:0:877:G:C2	30:0:885:G:O4'	2.63	0.51
30:0:1524:U:H5''	30:0:1524:U:C6	2.46	0.51
30:0:2758:G:H2'	30:0:2759:C:C6	2.46	0.51
1:A:69:LEU:HB3	38:A:9039:HOH:O	2.11	0.51
3:C:43:LYS:HG2	30:0:449:A:N7	2.26	0.51
3:C:111:VAL:HB	38:C:8519:HOH:O	2.11	0.51
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.91	0.51
23:W:88:THR:HG22	23:W:89:ASP:N	2.18	0.51
24:X:43:VAL:HG12	24:X:44:ASP:N	2.26	0.51
30:0:2823:G:H4'	30:0:2827:A:O4'	2.11	0.51
31:9:31:C:C2	31:9:50:G:C2	2.99	0.51
4:D:99:ASP:HB3	4:D:103:ASN:HB2	1.90	0.51
12:L:148:GLU:HA	38:L:8872:HOH:O	2.10	0.51
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.93	0.51
30:0:10:U:C6	30:0:10:U:H3'	2.46	0.51
30:0:821:U:H2'	30:0:822:C:C6	2.46	0.51
30:0:955:A:C2	30:0:1013:A:C4	2.99	0.51
30:0:958:G:O2'	30:0:959:C:H5'	2.10	0.51
30:0:1185:U:H5'	38:0:7483:HOH:O	2.09	0.51
30:0:2344:G:H2'	30:0:2344:G:N3	2.26	0.51
30:0:2830:U:O2'	30:0:2831:C:H5'	2.11	0.51
2:B:5:ARG:NH1	30:0:2547:C:OP2	2.44	0.51
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.45	0.51
11:K:10:GLN:HE21	11:K:10:GLN:N	1.97	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:40:VAL:O	16:P:44:VAL:HG23	2.11	0.51
30:0:1245:C:O5'	30:0:1245:C:H6	1.93	0.51
30:0:2638:G:H1'	38:0:4596:HOH:O	2.11	0.51
30:0:2768:A:H3'	30:0:2768:A:N3	2.26	0.51
1:A:179:MET:HG2	1:A:186:TRP:CB	2.41	0.51
2:B:243:ASN:HA	2:B:244:PRO:C	2.35	0.51
25:Y:204:ARG:HH22	30:0:553:G:P	2.33	0.51
30:0:407:A:H5'	38:0:6041:HOH:O	2.11	0.51
30:0:1614:G:H2'	38:0:4642:HOH:O	2.10	0.51
30:0:2102:G:H5'	30:0:2538:A:C2	2.45	0.51
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.93	0.51
26:Z:57:MET:SD	26:Z:73:ARG:HD2	2.51	0.51
30:0:18:C:H2'	30:0:19:U:C6	2.46	0.51
30:0:1118:A:C8	30:0:1119:G:H5''	2.46	0.51
30:0:1667:A:H5'	30:0:1667:A:C8	2.44	0.51
2:B:140:LEU:HD12	2:B:174:ARG:HG3	1.91	0.50
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.59	0.50
6:F:38:LYS:HE3	30:0:244:C:OP2	2.11	0.50
14:N:169:PRO:O	14:N:172:PHE:HB3	2.11	0.50
19:S:57:THR:HG22	19:S:58:MET:N	2.26	0.50
30:0:877:G:C5'	30:0:878:G:OP1	2.55	0.50
30:0:1857:A:N6	30:0:2247:C:H1'	2.26	0.50
30:0:2858:U:H2'	30:0:2859:C:C6	2.46	0.50
2:B:36:PRO:HG3	2:B:169:GLY:H	1.75	0.50
30:0:1284:G:O2'	30:0:1285:U:H5'	2.11	0.50
30:0:1829:A:C2'	30:0:1830:C:H5'	2.40	0.50
30:0:1829:A:H2'	30:0:1830:C:H5'	1.94	0.50
30:0:2347:C:H2'	30:0:2348:C:H6	1.76	0.50
30:0:2681:A:H8	38:0:5592:HOH:O	1.92	0.50
31:9:52:A:H2'	31:9:53:G:O4'	2.10	0.50
2:B:280:VAL:HG13	2:B:334:SER:HA	1.93	0.50
38:I:5331:HOH:O	30:0:1164:U:H5	1.94	0.50
30:0:694:A:C2'	30:0:695:C:H5'	2.41	0.50
30:0:1194:A:N1	30:0:1195:G:C6	2.79	0.50
30:0:2505:G:H8	38:0:5653:HOH:O	1.94	0.50
1:A:109:GLU:HG2	1:A:116:GLY:H	1.75	0.50
4:D:69:ILE:HD12	30:0:2346:C:H5'	1.93	0.50
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.75	0.50
24:X:78:GLU:HG2	24:X:79:GLU:H	1.75	0.50
30:0:1163:G:H2'	30:0:1164:U:C6	2.45	0.50
30:0:1166:A:C6	30:0:1181:A:C2	2.99	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1921:A:O2'	30:0:1922:A:H5'	2.12	0.50
30:0:2102:G:C2	30:0:2104:C:C4	3.00	0.50
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.11	0.50
22:V:39:ALA:C	22:V:41:GLU:H	2.20	0.50
30:0:255:A:O2'	30:0:256:C:H5'	2.12	0.50
30:0:920:C:H5'	30:0:921:G:C4	2.46	0.50
30:0:1118:A:H8	30:0:1119:G:H5''	1.77	0.50
30:0:1190:G:H3'	30:0:1190:G:N3	2.26	0.50
30:0:1762:C:H4'	38:0:4668:HOH:O	2.11	0.50
30:0:2256:G:C2'	30:0:2257:G:H5'	2.42	0.50
30:0:2718:C:H6	30:0:2718:C:H5'	1.77	0.50
1:A:212:PRO:HB2	38:0:4369:HOH:O	2.12	0.50
2:B:14:GLY:HA2	2:B:15:PRO:C	2.37	0.50
8:H:59:GLN:HG2	8:H:129:ARG:HG2	1.92	0.50
10:J:74:ARG:O	10:J:78:ILE:HG12	2.11	0.50
10:J:107:ASN:ND2	10:J:109:TYR:H	2.09	0.50
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.76	0.50
25:Y:235:GLU:CD	25:Y:235:GLU:N	2.70	0.50
30:0:12:U:C2'	30:0:13:G:H5'	2.41	0.50
30:0:368:C:C2'	30:0:369:G:H5'	2.42	0.50
30:0:1521:C:C2	30:0:1522:A:C8	3.00	0.50
30:0:1819:G:C2'	30:0:1820:G:H5'	2.41	0.50
30:0:2553:A:H2'	30:0:2553:A:N3	2.26	0.50
30:0:2730:G:O2'	30:0:2731:G:H5'	2.11	0.50
9:I:82:THR:CG2	30:0:1168:C:H5''	2.42	0.50
18:R:23:MET:HE3	18:R:28:SER:OG	2.12	0.50
30:0:559:U:C6	30:0:559:U:C3'	2.95	0.50
30:0:1131:G:C6	30:0:1230:A:C4	3.00	0.50
30:0:1522:A:C2	30:0:1665:G:C6	2.99	0.50
30:0:2729:C:O2'	30:0:2730:G:H5'	2.10	0.50
5:E:143:GLN:NE2	30:0:2779:G:H21	2.10	0.50
9:I:95:LEU:HD23	9:I:99:GLN:OE1	2.11	0.50
30:0:1205:U:C2'	30:0:1206:U:C5'	2.84	0.50
30:0:1406:A:H4'	30:0:1407:A:H5''	1.93	0.50
30:0:2445:U:H2'	30:0:2446:G:C8	2.47	0.50
30:0:2597:U:H2'	30:0:2598:U:H5'	1.94	0.50
4:D:88:LEU:HB2	4:D:89:PRO:HD3	1.94	0.50
9:I:87:PRO:HD3	38:0:3242:HOH:O	2.12	0.50
13:M:28:GLN:O	13:M:32:ARG:HG3	2.12	0.50
30:0:204:A:C2'	30:0:205:U:H5'	2.41	0.50
30:0:2291:A:N9	30:0:2309:C:H5'	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2756:U:H3	30:0:2896:A:H2	1.57	0.50
30:0:2909:G:H2'	30:0:2910:A:H8	1.76	0.50
1:A:199:HIS:HE1	30:0:1881:A:OP1	1.95	0.49
2:B:254:GLN:HG2	2:B:255:GLY:N	2.25	0.49
2:B:320:GLN:HE21	2:B:321:PRO:CD	2.24	0.49
13:M:171:ARG:NH2	30:0:189:A:OP1	2.45	0.49
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.12	0.49
23:W:64:THR:O	23:W:68:THR:HG22	2.11	0.49
26:Z:34:SER:HA	30:0:797:A:H5'	1.94	0.49
30:0:67:A:H5''	30:0:69:A:C8	2.47	0.49
30:0:73:U:O2'	30:0:74:G:H5'	2.12	0.49
30:0:941:G:C5	30:0:942:U:C4	3.00	0.49
30:0:1209:C:C2	30:0:1210:G:C8	3.00	0.49
30:0:1707:G:H1'	30:0:1711:A:N6	2.26	0.49
31:9:3:A:H2'	38:9:9040:HOH:O	2.11	0.49
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.38	0.49
30:0:256:C:H2'	30:0:257:G:O4'	2.12	0.49
30:0:2712:G:H5'	38:0:5233:HOH:O	2.11	0.49
1:A:33:GLU:O	1:A:34:ASP:HB2	2.12	0.49
2:B:144:THR:HG22	2:B:145:HIS:N	2.27	0.49
3:C:107:ARG:O	3:C:111:VAL:HG23	2.13	0.49
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.93	0.49
10:J:88:PRO:HA	33:J:8802:CL:CL	2.49	0.49
27:1:28:HIS:HE1	30:0:776:A:OP1	1.94	0.49
30:0:333:G:O2'	30:0:334:G:H5'	2.13	0.49
30:0:652:G:H8	38:0:3021:HOH:O	1.95	0.49
30:0:702:G:C2	30:0:703:G:C8	3.00	0.49
30:0:946:C:O2'	30:0:947:U:H5'	2.12	0.49
30:0:1878:G:O2'	30:0:1879:U:OP2	2.30	0.49
30:0:2831:C:C2	30:0:2910:A:C2	3.00	0.49
2:B:162:MET:HE1	2:B:308:LEU:HD21	1.94	0.49
4:D:50:VAL:HG13	31:9:41:C:O4'	2.12	0.49
11:K:34:VAL:HG21	11:K:46:LYS:O	2.12	0.49
16:P:81:LYS:HG2	38:0:9543:HOH:O	2.12	0.49
30:0:185:G:H4'	30:0:186:A:H4'	1.93	0.49
30:0:1909:A:H2'	30:0:1910:A:C8	2.48	0.49
2:B:214:PRO:C	2:B:220:VAL:HG22	2.37	0.49
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.76	0.49
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.41	0.49
21:U:20:MET:HE2	21:U:30:HIS:NE2	2.27	0.49
27:1:16:HIS:HE1	30:0:775:G:OP1	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:95:A:H5''	30:0:97:G:O4'	2.13	0.49
30:0:711:G:N2	30:0:718:C:C2	2.80	0.49
30:0:947:U:H2'	30:0:948:G:H8	1.77	0.49
30:0:1187:U:O2'	30:0:1189:A:H2	1.95	0.49
30:0:1377:C:H1'	38:0:9041:HOH:O	2.12	0.49
30:0:1607:A:C4	30:0:1608:G:C8	3.00	0.49
30:0:1768:C:H2'	30:0:1769:C:O4'	2.13	0.49
30:0:2004:U:H5''	30:0:2005:G:C8	2.47	0.49
30:0:2781:U:O2'	30:0:2782:G:H5'	2.12	0.49
2:B:162:MET:CE	2:B:308:LEU:HD21	2.42	0.49
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.94	0.49
11:K:130:MET:SD	21:U:25:ASP:O	2.70	0.49
15:O:25:VAL:HG12	30:0:709:G:O3'	2.13	0.49
18:R:29:LYS:HE2	30:0:524:A:C5'	2.42	0.49
20:T:18:GLU:O	20:T:21:LYS:HG2	2.11	0.49
30:0:363:C:H2'	30:0:364:U:H6	1.77	0.49
30:0:951:A:O2'	30:0:952:G:H5'	2.13	0.49
30:0:1588:G:C6	30:0:1589:G:C6	3.01	0.49
30:0:1854:C:H2'	30:0:1875:A:H61	1.78	0.49
30:0:2112:A:H2'	30:0:2113:G:H8	1.77	0.49
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.46	0.49
29:3:11:CYS:SG	29:3:14:CYS:HB2	2.52	0.49
29:3:30:GLN:NE2	38:3:9043:HOH:O	2.43	0.49
30:0:952:G:N3	30:0:2302:A:H2'	2.28	0.49
30:0:1189:A:N7	30:0:1190:G:C8	2.81	0.49
30:0:1568:G:C5	30:0:1569:U:C5	3.01	0.49
30:0:1730:G:C5'	30:0:1731:C:H6	2.25	0.49
30:0:1778:A:H2'	30:0:1779:A:H5'	1.94	0.49
1:A:53:ALA:HB3	38:A:9068:HOH:O	2.12	0.49
2:B:142:LEU:HD21	2:B:178:ALA:HB1	1.94	0.49
3:C:95:GLU:CD	3:C:95:GLU:H	2.20	0.49
25:Y:149:GLN:O	25:Y:154:ARG:NH1	2.46	0.49
30:0:1066:U:H2'	30:0:1067:A:C8	2.47	0.49
30:0:1682:A:H5''	38:0:9457:HOH:O	2.13	0.49
30:0:1730:G:H5'	30:0:1731:C:H5	1.78	0.49
30:0:2481:G:C3'	30:0:2482:G:H5''	2.42	0.49
30:0:2498:C:C2'	30:0:2499:U:H5'	2.43	0.49
31:9:31:C:C2	31:9:50:G:N2	2.81	0.49
31:9:73:A:N1	31:9:108:C:O2	2.45	0.49
1:A:81:GLN:HB2	1:A:92:ASN:ND2	2.28	0.49
8:H:150:LYS:HA	38:H:230:HOH:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:131:THR:HG22	10:J:133:GLY:H	1.78	0.49
20:T:97:ARG:NH2	30:0:309:C:OP1	2.46	0.49
23:W:23:MET:HE1	30:0:944:G:C8	2.48	0.49
25:Y:189:ASN:HD22	25:Y:192:ASP:H	1.61	0.49
26:Z:55:SER:O	26:Z:59:GLU:HG3	2.12	0.49
30:0:503:G:H2'	30:0:504:G:H8	1.77	0.49
30:0:1783:A:O2'	30:0:1784:U:H5'	2.12	0.49
30:0:2829:G:O2'	30:0:2830:U:H5'	2.13	0.49
30:0:2890:A:H5''	30:0:2890:A:H8	1.77	0.49
1:A:48:ASP:HB3	38:A:9068:HOH:O	2.13	0.49
1:A:211:LYS:HD2	38:A:9083:HOH:O	2.13	0.49
5:E:84:MET:HE1	5:E:148:ILE:CD1	2.43	0.49
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.28	0.49
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.12	0.49
30:0:1007:A:H1'	38:0:3138:HOH:O	2.12	0.49
30:0:1398:G:H2'	30:0:1399:A:H8	1.75	0.49
30:0:1816:C:H2'	30:0:1817:U:O4'	2.13	0.49
30:0:2064:U:H5'	30:0:2652:U:O3'	2.13	0.49
30:0:2578:G:H5'	30:0:2578:G:C8	2.43	0.49
30:0:2756:U:N3	30:0:2896:A:C2	2.75	0.49
30:0:2847:G:O2'	30:0:2848:G:H5'	2.12	0.49
3:C:76:ARG:HD3	38:C:8570:HOH:O	2.13	0.48
20:T:2:LYS:HG2	30:0:447:A:OP1	2.13	0.48
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.47	0.48
24:X:23:HIS:HD2	38:0:9959:HOH:O	1.96	0.48
30:0:703:G:O2'	30:0:704:C:H5'	2.13	0.48
30:0:1180:U:H2'	30:0:1181:A:O4'	2.13	0.48
30:0:1497:G:H4'	30:0:1627:G:O2'	2.13	0.48
2:B:140:LEU:CD1	2:B:174:ARG:HG3	2.44	0.48
12:L:18:HIS:HB2	30:0:903:U:O4	2.13	0.48
15:O:32:ARG:O	15:O:32:ARG:HD3	2.13	0.48
22:V:39:ALA:N	22:V:40:PRO:HD2	2.25	0.48
30:0:69:A:H2'	30:0:70:A:OP2	2.12	0.48
30:0:499:G:O2'	30:0:500:G:H5'	2.13	0.48
30:0:613:C:H2'	30:0:614:U:C6	2.44	0.48
30:0:626:U:C4	30:0:627:G:C6	3.01	0.48
30:0:814:G:H2'	30:0:815:U:C6	2.48	0.48
30:0:1323:G:H5'	38:0:4709:HOH:O	2.13	0.48
30:0:1676:G:H1'	38:0:9434:HOH:O	2.13	0.48
31:9:61:C:H2'	31:9:62:A:H8	1.77	0.48
31:9:92:G:C6	31:9:93:A:C6	3.01	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:76:ARG:NE	31:9:44:A:O4'	2.46	0.48
16:P:88:GLN:HE21	30:0:1800:G:H1'	1.76	0.48
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.48
25:Y:154:ARG:HH22	30:0:1071:G:H4'	1.78	0.48
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.93	0.48
30:0:308:U:C4	30:0:342:C:H1'	2.48	0.48
30:0:371:U:O2'	30:0:372:A:H5'	2.13	0.48
30:0:961:A:H4'	38:0:6790:HOH:O	2.13	0.48
30:0:2353:A:H4'	30:0:2354:A:O5'	2.13	0.48
30:0:2433:A:H2'	30:0:2434:A:C8	2.48	0.48
30:0:2510:C:H42	30:0:2564:G:N2	2.11	0.48
5:E:69:ILE:HA	5:E:72:MET:CE	2.44	0.48
14:N:110:THR:HB	14:N:113:SER:OG	2.13	0.48
17:Q:7:LEU:HD12	30:0:2424:U:H1'	1.96	0.48
30:0:466:A:H2'	30:0:467:G:O4'	2.13	0.48
30:0:581:G:O2'	30:0:582:U:H5'	2.12	0.48
30:0:1087:G:H4'	30:0:1088:A:OP1	2.12	0.48
30:0:1377:C:H6	30:0:1377:C:C5'	2.25	0.48
30:0:2831:C:H6	38:0:7228:HOH:O	1.96	0.48
31:9:39:U:H1'	31:9:44:A:H61	1.78	0.48
1:A:140:LEU:HB3	1:A:141:PRO:HD2	1.94	0.48
2:B:223:ARG:HG3	2:B:232:TRP:O	2.13	0.48
11:K:12:LEU:HB2	11:K:47:ALA:HB3	1.96	0.48
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.41	0.48
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.43	0.48
24:X:61:ARG:O	30:0:2744:G:H5''	2.14	0.48
27:1:1:THR:HB	38:0:7157:HOH:O	2.13	0.48
30:0:513:A:N3	38:0:3665:HOH:O	2.35	0.48
30:0:790:A:H1'	30:0:1710:A:H2'	1.95	0.48
30:0:802:G:O2'	30:0:803:C:H5'	2.13	0.48
30:0:1190:G:H2'	38:0:4064:HOH:O	2.13	0.48
30:0:2256:G:O2'	30:0:2257:G:H5'	2.14	0.48
30:0:2754:G:C2'	30:0:2755:G:H5'	2.43	0.48
30:0:2768:A:C2'	30:0:2769:C:O4'	2.61	0.48
30:0:2908:A:O2'	30:0:2909:G:H5'	2.13	0.48
31:9:71:C:H2'	31:9:72:C:H6	1.79	0.48
4:D:23:VAL:HG12	4:D:130:VAL:HG22	1.96	0.48
5:E:93:MET:HE1	5:E:165:GLY:N	2.26	0.48
8:H:165:ARG:HB3	38:H:235:HOH:O	2.13	0.48
11:K:41:LYS:HA	30:0:2582:G:O3'	2.14	0.48
14:N:65:ASP:HB3	38:N:8821:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.95	0.48
30:0:305:A:C5	30:0:329:A:C2	3.02	0.48
30:0:1311:G:C2	30:0:1312:G:C8	3.01	0.48
30:0:1343:C:H2'	30:0:1344:G:O5'	2.14	0.48
30:0:1520:G:H2'	30:0:1521:C:C6	2.48	0.48
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.96	0.48
3:C:246:ARG:NE	38:C:8628:HOH:O	2.43	0.48
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.78	0.48
8:H:170:ARG:HD2	38:H:194:HOH:O	2.13	0.48
11:K:55:VAL:HG12	11:K:56:SER:N	2.28	0.48
12:L:117:GLU:HA	38:L:8852:HOH:O	2.13	0.48
18:R:113:HIS:HE1	18:R:144:GLU:CD	2.21	0.48
21:U:17:THR:CG2	21:U:18:GLY:N	2.77	0.48
23:W:21:LEU:HD13	23:W:26:ILE:HD11	1.95	0.48
27:1:28:HIS:HD2	27:1:30:LYS:H	1.59	0.48
30:0:661:G:C5	30:0:686:A:C2	3.02	0.48
30:0:735:C:O5'	30:0:735:C:H6	1.97	0.48
30:0:1422:U:H2'	30:0:1423:C:H6	1.76	0.48
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.39	0.48
5:E:72:MET:O	5:E:76:VAL:HG22	2.14	0.48
11:K:9:THR:HA	38:0:3293:HOH:O	2.14	0.48
12:L:143:THR:HG22	12:L:144:ASP:N	2.28	0.48
30:0:285:A:N6	30:0:367:G:H1'	2.28	0.48
30:0:1188:A:C5	30:0:1189:A:C2	3.01	0.48
30:0:1201:C:C2'	30:0:1202:A:H5'	2.42	0.48
30:0:1789:G:H2'	30:0:1790:C:O5'	2.13	0.48
30:0:1976:G:O2'	30:0:1977:U:H5'	2.14	0.48
30:0:2090:G:H2'	30:0:2091:G:C8	2.49	0.48
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.14	0.48
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.94	0.48
30:0:675:U:H6	30:0:675:U:O5'	1.97	0.48
30:0:732:C:O2'	30:0:733:U:H5'	2.13	0.48
30:0:1159:G:H1	30:0:1208:C:H42	1.61	0.48
30:0:1543:G:N1	30:0:1641:A:OP2	2.34	0.48
30:0:2419:U:H5''	30:0:2420:G:H5'	1.95	0.48
30:0:2635:A:C2'	30:0:2636:C:H5'	2.44	0.48
30:0:2656:G:C2'	30:0:2657:G:H5'	2.44	0.48
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.95	0.48
2:B:75:GLU:C	2:B:77:PRO:HD3	2.39	0.48
10:J:39:VAL:HG13	10:J:106:GLY:O	2.13	0.48
13:M:171:ARG:CD	30:0:156:C:H5''	2.23	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:77:VAL:HG11	20:T:91:LEU:HD11	1.95	0.48
23:W:41:TYR:OH	30:0:1024:G:H4'	2.14	0.48
30:0:363:C:H2'	30:0:364:U:C6	2.49	0.48
30:0:506:G:N2	30:0:509:A:H5''	2.20	0.48
30:0:1506:U:H6	30:0:1506:U:H5'	1.79	0.48
30:0:1613:C:H2'	30:0:1614:G:O4'	2.14	0.48
30:0:1902:G:N2	30:0:1936:C:C2	2.82	0.48
30:0:2837:U:H2'	38:0:6856:HOH:O	2.14	0.48
30:0:2858:U:H2'	30:0:2859:C:H6	1.78	0.48
1:A:191:GLY:HA2	1:A:194:MET:CE	2.41	0.47
38:C:8666:HOH:O	30:0:656:G:H1'	2.14	0.47
13:M:49:ALA:C	13:M:54:TYR:HB3	2.39	0.47
13:M:64:ARG:HD2	38:M:8880:HOH:O	2.14	0.47
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.94	0.47
30:0:250:C:H2'	30:0:251:C:H6	1.79	0.47
30:0:947:U:O2'	30:0:948:G:H5'	2.14	0.47
30:0:1512:G:O2'	30:0:1513:C:H5'	2.14	0.47
30:0:2074:A:H1'	38:0:9890:HOH:O	2.14	0.47
30:0:2769:C:C2'	30:0:2770:G:C5'	2.78	0.47
31:9:1:U:C4'	31:9:3:A:OP1	2.62	0.47
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.96	0.47
29:3:65:THR:HB	29:3:83:TRP:H	1.79	0.47
30:0:101:C:H2'	30:0:102:A:C8	2.49	0.47
30:0:128:A:O2'	30:0:129:A:C5'	2.62	0.47
30:0:800:G:H2'	30:0:801:U:C6	2.49	0.47
30:0:814:G:H4'	38:0:3141:HOH:O	2.14	0.47
30:0:843:A:C2	30:0:846:A:C8	3.02	0.47
30:0:1562:C:O2	30:0:1562:C:H2'	2.12	0.47
30:0:2493:C:O2	30:0:2493:C:H2'	2.14	0.47
30:0:2672:C:H2'	30:0:2673:U:H6	1.78	0.47
30:0:2869:G:H5'	38:0:5510:HOH:O	2.14	0.47
31:9:108:C:H2'	31:9:109:G:H8	1.78	0.47
1:A:65:ARG:O	1:A:66:ARG:HG3	2.15	0.47
1:A:171:LYS:HB2	30:0:820:G:C6	2.49	0.47
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.96	0.47
9:I:108:HIS:N	9:I:109:PRO:HD2	2.29	0.47
9:I:120:ALA:O	9:I:124:VAL:HG23	2.14	0.47
12:L:41:HIS:CD2	30:0:926:A:O2'	2.65	0.47
26:Z:45:VAL:HG23	30:0:1887:U:OP1	2.14	0.47
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.49	0.47
30:0:814:G:H2'	30:0:815:U:H6	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1268:C:H2'	30:0:1269:G:H8	1.79	0.47
30:0:1321:A:H2'	30:0:1322:G:H8	1.80	0.47
30:0:2134:G:H2'	30:0:2135:A:H8	1.79	0.47
30:0:2253:G:H2'	30:0:2254:G:H8	1.79	0.47
30:0:2795:C:O2'	30:0:2796:U:H5'	2.15	0.47
31:9:114:G:H2'	31:9:115:C:C6	2.49	0.47
1:A:171:LYS:HB2	30:0:820:G:C5	2.50	0.47
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.79	0.47
3:C:197:SER:HB3	38:C:8577:HOH:O	2.15	0.47
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.96	0.47
5:E:143:GLN:HE21	30:0:2780:C:C1'	2.15	0.47
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.14	0.47
30:0:660:A:H4'	30:0:661:G:O5'	2.14	0.47
30:0:671:A:O2'	30:0:672:G:H2'	2.14	0.47
30:0:834:G:H3'	30:0:835:U:H4'	1.95	0.47
30:0:1165:G:C4'	30:0:1174:A:O2'	2.60	0.47
30:0:1568:G:O2'	30:0:1569:U:H5'	2.14	0.47
30:0:1667:A:H2'	30:0:1668:U:C6	2.49	0.47
30:0:2256:G:H2'	30:0:2257:G:C5'	2.45	0.47
2:B:229:ARG:NH2	30:0:1753:C:O2	2.45	0.47
5:E:108:LEU:HD11	5:E:164:ASP:HB2	1.96	0.47
8:H:5:PRO:HD2	8:H:8:MET:SD	2.55	0.47
12:L:92:ASP:HA	12:L:121:ILE:HB	1.96	0.47
30:0:69:A:H8	30:0:69:A:C5'	2.21	0.47
30:0:1126:C:O5'	30:0:1126:C:H6	1.97	0.47
30:0:1187:U:H2'	38:0:6916:HOH:O	2.15	0.47
30:0:2105:C:O2'	30:0:2284:G:N2	2.48	0.47
30:0:2826:G:C6	30:0:2913:A:C6	3.02	0.47
1:A:186:TRP:CD1	1:A:187:PRO:HA	2.49	0.47
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.97	0.47
3:C:114:ALA:HB1	3:C:223:LEU:HB3	1.96	0.47
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.78	0.47
8:H:64:SER:OG	30:0:2520:G:H5'	2.13	0.47
12:L:35:ARG:O	12:L:40:PHE:HA	2.15	0.47
12:L:134:GLU:HG3	38:L:8856:HOH:O	2.15	0.47
14:N:61:ALA:CB	14:N:88:ALA:HB2	2.44	0.47
30:0:423:A:C5	30:0:424:C:C5	3.02	0.47
30:0:559:U:C6	30:0:559:U:H3'	2.50	0.47
30:0:1014:A:H5''	31:9:101:G:O2'	2.14	0.47
30:0:1166:A:H1'	30:0:1192:A:C2	2.50	0.47
30:0:1883:U:H5''	30:0:2013:G:OP2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2265:U:H2'	30:0:2266:A:C8	2.49	0.47
30:0:2411:C:H4'	38:0:4964:HOH:O	2.13	0.47
31:9:39:U:C2'	31:9:40:C:OP1	2.63	0.47
1:A:36:ASP:HA	1:A:83:GLY:HA3	1.97	0.47
3:C:154:VAL:O	3:C:158:GLU:HG3	2.15	0.47
4:D:37:ALA:O	4:D:40:ILE:HG12	2.14	0.47
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.96	0.47
12:L:71:GLU:HG2	30:0:700:A:C2	2.49	0.47
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.41	0.47
13:M:124:GLY:HA3	30:0:2132:C:H1'	1.96	0.47
18:R:82:GLU:O	18:R:86:LYS:HG3	2.13	0.47
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.95	0.47
25:Y:155:ARG:NH1	38:Y:8128:HOH:O	2.48	0.47
30:0:36:C:C2	30:0:447:A:C2	3.03	0.47
30:0:304:G:H1'	30:0:347:A:N6	2.29	0.47
30:0:1391:G:H2'	30:0:1392:A:H5'	1.97	0.47
30:0:1471:A:H5'	38:0:3197:HOH:O	2.15	0.47
30:0:1477:C:C5'	30:0:1868:G:H5''	2.44	0.47
30:0:1730:G:H5'	30:0:1731:C:C6	2.48	0.47
30:0:1948:G:H2'	30:0:1949:G:H8	1.79	0.47
30:0:2531:U:O2'	30:0:2532:A:H5'	2.14	0.47
30:0:2831:C:H2'	30:0:2832:C:C5'	2.45	0.47
1:A:27:LEU:HD12	1:A:69:LEU:HD22	1.95	0.47
12:L:133:VAL:HB	38:L:8856:HOH:O	2.15	0.47
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.30	0.47
14:N:154:LEU:C	14:N:156:GLU:H	2.20	0.47
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.95	0.47
30:0:151:A:H2'	30:0:152:A:O4'	2.14	0.47
30:0:1182:C:C1'	30:0:1192:A:C8	2.97	0.47
30:0:2829:G:C2	30:0:2912:C:C2	3.03	0.47
30:0:2871:G:H2'	30:0:2872:U:C6	2.50	0.47
30:0:2891:A:H2'	30:0:2891:A:N3	2.29	0.47
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.79	0.47
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.50	0.47
27:1:46:ARG:HA	38:0:3028:HOH:O	2.15	0.47
30:0:485:A:N3	30:0:487:G:H5''	2.29	0.47
30:0:560:U:H2'	30:0:561:G:C8	2.44	0.47
30:0:960:G:H3'	30:0:960:G:C4	2.47	0.47
30:0:2087:C:O2'	30:0:2088:C:H5'	2.15	0.47
30:0:1205:U:H2'	30:0:1206:U:H5'	1.96	0.47
30:0:1788:U:C2	30:0:1805:G:N2	2.83	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1789:G:C2'	30:0:1790:C:O5'	2.63	0.47
30:0:2326:C:H4'	30:0:2412:G:C4'	2.44	0.47
30:0:2831:C:H2'	30:0:2832:C:H5'	1.97	0.47
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.97	0.46
14:N:11:ARG:NH1	31:9:8:G:O6	2.48	0.46
14:N:86:LEU:O	14:N:90:LEU:HG	2.14	0.46
23:W:61:THR:HG23	23:W:151:GLU:HG3	1.97	0.46
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.29	0.46
30:0:254:C:O2	30:0:254:C:C2'	2.54	0.46
30:0:820:G:O2'	30:0:856:G:H4'	2.14	0.46
30:0:825:U:H5''	30:0:826:U:OP1	2.15	0.46
30:0:1947:G:N2	30:0:1966:U:O2	2.48	0.46
30:0:2072:G:C6	30:0:2533:C:H1'	2.50	0.46
30:0:2256:G:H2'	30:0:2257:G:H5'	1.97	0.46
30:0:2833:C:H1'	30:0:2848:G:N2	2.30	0.46
1:A:233:THR:HB	30:0:1942:A:H5''	1.98	0.46
3:C:35:VAL:HG21	3:C:227:GLY:HA2	1.96	0.46
3:C:200:PRO:HB3	3:C:212:VAL:HG23	1.97	0.46
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.98	0.46
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.97	0.46
14:N:141:ARG:HH21	31:9:48:C:H4'	1.79	0.46
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.97	0.46
28:2:28:LYS:O	30:0:87:C:H2'	2.15	0.46
30:0:10:U:C6	30:0:10:U:C3'	2.98	0.46
30:0:789:C:H5'	38:0:6228:HOH:O	2.15	0.46
30:0:920:C:H4'	30:0:921:G:N2	2.30	0.46
30:0:1174:A:C5	30:0:1201:C:H4'	2.50	0.46
30:0:1679:C:O2'	30:0:1685:A:N1	2.45	0.46
30:0:1706:G:C5	30:0:1707:G:C6	3.03	0.46
30:0:2092:G:H2'	30:0:2613:G:OP1	2.15	0.46
30:0:2106:C:H1'	30:0:2484:U:C2	2.49	0.46
30:0:2577:A:H8	38:0:9606:HOH:O	1.98	0.46
30:0:2825:C:H4'	30:0:2826:G:O5'	2.15	0.46
30:0:2911:C:O2'	30:0:2912:C:H5'	2.15	0.46
1:A:211:LYS:HD3	38:0:6884:HOH:O	2.15	0.46
13:M:47:ASP:CG	13:M:48:LYS:N	2.74	0.46
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.50	0.46
30:0:277:U:O2'	30:0:278:A:H5'	2.15	0.46
30:0:544:G:C3'	30:0:545:G:H5''	2.45	0.46
30:0:1400:C:O2'	30:0:1401:G:H5'	2.15	0.46
30:0:1557:G:O2'	30:0:1558:C:H5'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1596:U:H2'	30:0:1598:A:OP2	2.14	0.46
30:0:1634:G:C4	30:0:1635:U:C5	3.03	0.46
30:0:2598:U:O2	30:0:2600:A:C8	2.68	0.46
30:0:2871:G:H2'	30:0:2872:U:H6	1.79	0.46
31:9:3:A:H2	31:9:21:G:N3	2.14	0.46
1:A:123:GLY:HA3	1:A:162:GLY:HA2	1.96	0.46
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.50	0.46
13:M:80:GLY:O	13:M:81:ARG:HD2	2.14	0.46
15:O:25:VAL:HG12	30:0:709:G:O2'	2.16	0.46
30:0:354:A:H2'	30:0:355:C:H6	1.80	0.46
30:0:876:A:N3	30:0:876:A:C2'	2.79	0.46
30:0:1102:C:H5	38:0:3497:HOH:O	1.98	0.46
30:0:1200:A:H3'	38:0:5769:HOH:O	2.15	0.46
30:0:1878:G:C4'	38:0:6135:HOH:O	2.64	0.46
30:0:2105:C:H2'	30:0:2106:C:C6	2.50	0.46
30:0:2284:G:H1'	38:0:9576:HOH:O	2.15	0.46
30:0:2482:G:H4'	30:0:2483:A:C5'	2.45	0.46
30:0:2802:C:H2'	30:0:2803:C:C6	2.50	0.46
31:9:27:C:H2'	31:9:28:U:O4'	2.16	0.46
3:C:127:ARG:HD3	3:C:129:HIS:CE1	2.48	0.46
14:N:11:ARG:HD3	31:9:114:G:O6	2.15	0.46
16:P:101:GLN:HG3	38:0:3511:HOH:O	2.15	0.46
21:U:49:LEU:HG	38:U:3805:HOH:O	2.15	0.46
29:3:61:PRO:HG3	30:0:2462:G:O6	2.16	0.46
30:0:228:C:H2'	30:0:229:G:H5'	1.96	0.46
30:0:343:C:O2'	30:0:344:C:H5'	2.15	0.46
30:0:445:U:H2'	30:0:446:G:H8	1.81	0.46
30:0:590:A:H2'	30:0:591:A:H5'	1.97	0.46
30:0:716:G:C6	30:0:717:C:N4	2.83	0.46
30:0:1125:U:H3'	30:0:1126:C:C6	2.51	0.46
30:0:1515:A:H2'	30:0:1516:U:H6	1.80	0.46
2:B:214:PRO:HD2	38:0:9081:HOH:O	2.15	0.46
14:N:112:GLY:HA2	14:N:137:ALA:HB2	1.96	0.46
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.12	0.46
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.50	0.46
30:0:241:A:C2	30:0:378:A:H4'	2.51	0.46
30:0:1067:A:H5'	38:0:4351:HOH:O	2.15	0.46
30:0:1175:G:N7	30:0:1176:C:N3	2.63	0.46
30:0:1346:U:H2'	30:0:1347:U:C6	2.51	0.46
30:0:1420:C:H2'	30:0:1420:C:O2	2.15	0.46
30:0:1616:A:H5''	30:0:1617:C:OP1	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2613:G:O2'	30:0:2614:C:H5'	2.15	0.46
30:0:2703:A:H2'	30:0:2704:C:C6	2.46	0.46
31:9:12:C:H5'	31:9:70:U:O4'	2.15	0.46
1:A:71:PRO:HD2	1:A:74:VAL:HG21	1.98	0.46
1:A:127:GLN:HB3	1:A:139:LYS:HB3	1.98	0.46
2:B:202:VAL:HG11	2:B:301:VAL:HG13	1.98	0.46
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.30	0.46
3:C:1:MET:CG	3:C:2:GLN:H	2.26	0.46
4:D:64:ARG:HB3	4:D:67:ASP:OD2	2.15	0.46
9:I:130:LEU:HA	38:0:7420:HOH:O	2.15	0.46
14:N:175:LEU:O	14:N:179:LEU:HG	2.15	0.46
16:P:64:GLU:HG3	38:P:166:HOH:O	2.15	0.46
30:0:138:U:OP2	30:0:139:C:C5	2.69	0.46
30:0:889:C:H2'	30:0:890:C:C6	2.51	0.46
30:0:1181:A:N1	30:0:1192:A:O2'	2.49	0.46
30:0:1617:C:C4	30:0:1643:C:H4'	2.50	0.46
30:0:2061:C:C2'	30:0:2062:A:H5'	2.46	0.46
30:0:2093:G:H5''	38:0:9483:HOH:O	2.15	0.46
30:0:2346:C:H6	30:0:2346:C:O5'	1.98	0.46
30:0:2401:A:H2'	30:0:2402:A:C8	2.51	0.46
30:0:2840:A:H3'	38:0:7661:HOH:O	2.15	0.46
1:A:110:SER:HB2	1:A:117:LYS:HG3	1.98	0.46
3:C:103:ASN:HB3	38:0:9117:HOH:O	2.16	0.46
4:D:20:LYS:HA	4:D:75:LEU:O	2.15	0.46
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.97	0.46
12:L:113:GLN:C	30:0:700:A:H62	2.24	0.46
30:0:370:G:O2'	30:0:371:U:H5'	2.15	0.46
30:0:510:U:O5'	30:0:510:U:H6	1.99	0.46
30:0:729:C:C2	30:0:743:G:C2	3.04	0.46
30:0:1202:A:C8	30:0:1203:G:C8	3.04	0.46
30:0:1463:U:H2'	30:0:1464:C:C6	2.51	0.46
30:0:1741:U:C4	30:0:2033:G:C8	3.04	0.46
30:0:2908:A:C2'	30:0:2909:G:H5'	2.46	0.46
31:9:34:A:H2'	31:9:35:C:O4'	2.16	0.46
1:A:206:ARG:O	1:A:208:HIS:HD2	1.98	0.46
4:D:56:ARG:HH22	30:0:2332:A:H5'	1.79	0.46
5:E:137:ASP:O	5:E:141:VAL:HG23	2.16	0.46
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.15	0.46
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.46	0.46
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.81	0.46
30:0:39:G:N2	30:0:444:C:C2	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:162:C:C2'	30:0:163:U:H5'	2.45	0.46
30:0:417:G:P	38:0:7436:HOH:O	2.73	0.46
30:0:932:U:H2'	30:0:933:C:C6	2.51	0.46
30:0:1008:C:O2'	30:0:1009:U:H5'	2.16	0.46
30:0:1309:U:C2'	30:0:1310:U:H5'	2.46	0.46
30:0:1453:G:C2	30:0:1675:C:C2	3.04	0.46
30:0:1845:A:O2'	30:0:1846:U:H5'	2.15	0.46
30:0:1873:G:H2'	30:0:1874:U:H5'	1.98	0.46
30:0:2764:C:O2'	30:0:2765:C:H5'	2.16	0.46
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.98	0.46
3:C:156:LEU:O	3:C:160:LEU:HG	2.16	0.46
4:D:91:ALA:HB1	38:D:5198:HOH:O	2.15	0.46
10:J:107:ASN:HD22	10:J:107:ASN:C	2.24	0.46
24:X:56:GLU:HG2	30:0:1400:C:H4'	1.98	0.46
25:Y:165:GLU:HB3	38:Y:8163:HOH:O	2.16	0.46
27:1:42:SER:HB2	38:1:8957:HOH:O	2.16	0.46
30:0:238:C:H4'	30:0:287:C:OP1	2.16	0.46
30:0:560:U:C2	30:0:561:G:C8	3.04	0.46
30:0:567:U:C5'	38:0:5300:HOH:O	2.63	0.46
30:0:1156:C:O5'	30:0:1156:C:H6	1.99	0.46
30:0:1535:G:H2'	30:0:1536:C:C6	2.50	0.46
30:0:1700:C:H5''	30:0:1701:A:OP2	2.15	0.46
30:0:1838:U:C4	30:0:2644:C:N4	2.84	0.46
30:0:2103:A:N3	30:0:2103:A:H2'	2.30	0.46
31:9:3:A:OP2	31:9:25:G:N2	2.48	0.46
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.47	0.45
21:U:42:LEU:HD22	30:0:1810:C:H1'	1.98	0.45
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.46	0.45
30:0:369:G:C2	30:0:370:G:C8	3.04	0.45
30:0:630:A:H5'	38:0:9367:HOH:O	2.16	0.45
30:0:1393:A:H2'	30:0:1394:C:C6	2.51	0.45
30:0:1675:C:O2'	30:0:1676:G:H5'	2.16	0.45
30:0:1735:C:H2'	30:0:1736:A:C8	2.50	0.45
30:0:2526:C:H2'	30:0:2527:U:H5'	1.98	0.45
31:9:52:A:O2'	31:9:53:G:H5'	2.16	0.45
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.78	0.45
4:D:25:MET:HE1	4:D:37:ALA:O	2.15	0.45
11:K:34:VAL:HB	38:0:7387:HOH:O	2.15	0.45
30:0:80:A:C2	30:0:94:G:N3	2.85	0.45
30:0:137:U:OP1	30:0:259:G:O2'	2.34	0.45
30:0:340:A:C8	30:0:340:A:O5'	2.69	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:735:C:H2'	30:0:736:A:H5'	1.99	0.45
30:0:797:A:H2'	30:0:798:G:O4'	2.16	0.45
30:0:1501:A:H4'	38:0:5614:HOH:O	2.15	0.45
30:0:1636:G:O2'	30:0:1637:A:H5'	2.16	0.45
30:0:1741:U:H3'	38:0:9774:HOH:O	2.16	0.45
30:0:1973:A:H2'	30:0:1974:G:O4'	2.15	0.45
30:0:2499:U:H2'	30:0:2500:C:C6	2.51	0.45
31:9:37:C:H2'	31:9:38:A:C8	2.48	0.45
17:Q:45:PRO:O	30:0:2365:G:H4'	2.16	0.45
38:Y:8136:HOH:O	30:0:1316:G:H5''	2.15	0.45
30:0:497:A:H2'	30:0:498:A:C5'	2.46	0.45
30:0:806:A:H2'	30:0:807:A:O4'	2.17	0.45
30:0:1126:C:HO2'	30:0:1128:U:H6	1.62	0.45
30:0:2121:G:O2'	30:0:2122:C:H5'	2.16	0.45
30:0:2435:U:H1'	38:0:5442:HOH:O	2.16	0.45
30:0:2883:A:H2'	30:0:2884:G:O4'	2.17	0.45
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.45	0.45
5:E:119:HIS:O	5:E:140:ALA:HB1	2.17	0.45
10:J:46:ILE:HD11	10:J:53:ILE:HG23	1.97	0.45
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.99	0.45
20:T:41:ARG:HG2	20:T:41:ARG:HH11	1.82	0.45
30:0:364:U:H2'	30:0:365:G:C8	2.51	0.45
30:0:883:U:O2	30:0:883:U:C2'	2.64	0.45
30:0:1041:U:C2'	30:0:1042:U:H5'	2.47	0.45
30:0:1160:G:O2'	30:0:1190:G:H1'	2.17	0.45
30:0:1477:C:C5'	30:0:1868:G:C5'	2.93	0.45
30:0:1730:G:H5''	30:0:1731:C:C6	2.51	0.45
30:0:2909:G:H2'	30:0:2910:A:C8	2.51	0.45
1:A:231:LYS:HG3	30:0:1853:C:OP1	2.17	0.45
2:B:141:ARG:HG2	2:B:165:ARG:HA	1.98	0.45
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.97	0.45
4:D:104:PHE:CE2	4:D:132:VAL:HB	2.52	0.45
5:E:143:GLN:NE2	30:0:2780:C:C1'	2.79	0.45
12:L:33:ALA:HB3	38:L:8892:HOH:O	2.17	0.45
19:S:57:THR:HG22	19:S:59:ASP:H	1.80	0.45
30:0:281:U:H5	38:0:7610:HOH:O	2.00	0.45
30:0:282:C:C2'	30:0:283:U:H5'	2.46	0.45
30:0:1163:G:N2	38:0:4740:HOH:O	2.49	0.45
30:0:2064:U:H2'	30:0:2065:C:H6	1.81	0.45
30:0:2308:U:C5	30:0:2310:G:C8	3.05	0.45
30:0:2499:U:H2'	30:0:2500:C:H6	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:3:A:C8	31:9:26:C:O2	2.69	0.45
31:9:3:A:H8	31:9:26:C:O2	1.99	0.45
2:B:262:ARG:HD2	30:0:2715:G:O2'	2.17	0.45
3:C:236:THR:HG21	38:C:8577:HOH:O	2.17	0.45
12:L:12:THR:HG21	12:L:16:GLY:O	2.17	0.45
14:N:4:PRO:HD2	38:0:6790:HOH:O	2.17	0.45
30:0:134:U:C2	30:0:145:A:C2	3.05	0.45
30:0:517:U:H1'	38:0:7592:HOH:O	2.16	0.45
30:0:1098:A:H2'	30:0:1099:G:O4'	2.17	0.45
30:0:1120:U:H5''	30:0:1120:U:C6	2.52	0.45
30:0:1149:U:C5	30:0:1215:A:C5	3.04	0.45
30:0:1521:C:H2'	30:0:1522:A:C8	2.50	0.45
30:0:1815:A:H4'	30:0:2751:C:O4'	2.17	0.45
30:0:1903:U:O2'	30:0:1904:A:C8	2.69	0.45
30:0:1992:U:H2'	30:0:1994:A:OP2	2.17	0.45
30:0:2421:G:H3'	30:0:2422:U:C5'	2.47	0.45
30:0:2515:C:H2'	30:0:2516:G:O4'	2.16	0.45
30:0:2908:A:H2'	30:0:2909:G:C4'	2.45	0.45
31:9:39:U:H3'	31:9:40:C:H5''	1.99	0.45
1:A:194:MET:HE3	1:A:199:HIS:CB	2.46	0.45
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.82	0.45
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.50	0.45
3:C:54:LEU:HD23	3:C:79:ARG:HG3	1.99	0.45
4:D:10:PHE:HA	38:D:7345:HOH:O	2.15	0.45
19:S:57:THR:CG2	19:S:58:MET:N	2.79	0.45
22:V:49:LEU:O	22:V:53:ILE:HG13	2.17	0.45
24:X:79:GLU:CD	24:X:80:GLU:H	2.25	0.45
30:0:61:G:C6	30:0:62:C:C4	3.05	0.45
30:0:283:U:H5	30:0:284:C:N3	2.13	0.45
30:0:581:G:H5'	38:0:7694:HOH:O	2.16	0.45
30:0:1165:G:N2	30:0:1173:A:H5'	2.32	0.45
30:0:1175:G:C1'	30:0:1193:A:C8	2.98	0.45
30:0:1196:C:H42	30:0:1204:C:N4	2.14	0.45
30:0:1249:U:H2'	30:0:1250:C:C6	2.51	0.45
30:0:1773:G:N2	30:0:1774:G:C8	2.84	0.45
30:0:1996:U:O2'	30:0:1997:A:H5'	2.16	0.45
30:0:2004:U:H6	30:0:2004:U:P	2.40	0.45
31:9:63:C:O2'	31:9:64:C:H5'	2.17	0.45
1:A:206:ARG:HH11	1:A:206:ARG:HG3	1.82	0.45
2:B:81:ALA:HB1	2:B:142:LEU:HD13	1.99	0.45
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:171:HIS:CE1	38:N:8861:HOH:O	2.69	0.45
25:Y:144:ARG:NE	38:Y:8181:HOH:O	2.49	0.45
26:Z:34:SER:HB3	30:0:797:A:H4'	1.99	0.45
30:0:31:C:H4'	38:0:7442:HOH:O	2.17	0.45
30:0:168:C:O2'	30:0:169:A:H5'	2.16	0.45
30:0:844:A:C6	30:0:882:A:C5	3.05	0.45
30:0:2583:A:H5'	38:0:9803:HOH:O	2.17	0.45
1:A:35:GLY:O	1:A:36:ASP:HB3	2.16	0.45
1:A:54:PRO:HG2	1:A:160:ALA:HB3	1.99	0.45
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.50	0.45
2:B:211:THR:HG21	38:0:7472:HOH:O	2.17	0.45
3:C:72:LYS:HE3	38:C:8505:HOH:O	2.17	0.45
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.17	0.45
11:K:64:MET:HA	11:K:67:GLN:HE21	1.81	0.45
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.64	0.45
14:N:109:PRO:HB3	30:0:2413:A:N7	2.32	0.45
18:R:15:LYS:HE3	38:R:8982:HOH:O	2.16	0.45
23:W:52:VAL:HG22	23:W:53:ALA:H	1.82	0.45
23:W:130:HIS:O	23:W:136:GLY:HA3	2.17	0.45
30:0:240:C:O2	30:0:240:C:H2'	2.17	0.45
30:0:553:G:H3'	38:0:4084:HOH:O	2.15	0.45
30:0:559:U:H2'	30:0:560:U:O4'	2.17	0.45
30:0:968:G:H2'	30:0:969:G:H8	1.82	0.45
30:0:1577:U:O2'	30:0:1578:C:H5'	2.17	0.45
30:0:1711:A:O2'	30:0:1712:A:H5'	2.16	0.45
30:0:1825:U:O2'	30:0:1826:C:H5'	2.16	0.45
30:0:2072:G:H3'	30:0:2073:G:C5'	2.47	0.45
2:B:217:ARG:HG3	2:B:257:THR:HB	1.99	0.45
8:H:31:ILE:HG23	38:H:233:HOH:O	2.16	0.45
13:M:81:ARG:HG3	13:M:85:ARG:HB2	1.99	0.45
16:P:20:ARG:NH1	16:P:54:LYS:HD3	2.32	0.45
18:R:40:ALA:O	18:R:44:VAL:HG23	2.16	0.45
27:1:16:HIS:CD2	30:0:470:U:O2'	2.68	0.45
30:0:68:U:O2'	30:0:69:A:H5''	2.17	0.45
30:0:407:A:H3'	38:0:4468:HOH:O	2.16	0.45
30:0:884:C:H3'	38:0:9406:HOH:O	2.17	0.45
30:0:960:G:C3'	30:0:960:G:C4	3.00	0.45
30:0:1626:A:H2'	30:0:1627:G:C5'	2.47	0.45
30:0:2361:A:C5'	38:0:9009:HOH:O	2.60	0.45
30:0:2624:A:O2'	30:0:2625:C:H5'	2.17	0.45
30:0:2828:G:C6	30:0:2913:A:C2	3.05	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:GLN:O	3:C:43:LYS:HD3	2.18	0.44
3:C:46:TYR:CE1	3:C:92:PRO:HB3	2.51	0.44
4:D:12:GLU:O	4:D:15:GLU:HG2	2.17	0.44
5:E:75:GLY:HA3	5:E:136:PRO:O	2.18	0.44
14:N:37:ARG:NH1	31:9:6:C:OP1	2.50	0.44
16:P:1:THR:O	30:0:1396:C:H1'	2.17	0.44
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.16	0.44
23:W:122:ARG:HH12	23:W:154:ARG:N	2.14	0.44
30:0:45:A:H5''	30:0:47:G:O4'	2.17	0.44
30:0:1718:G:O2'	30:0:1719:G:H5'	2.17	0.44
30:0:1735:C:H2'	30:0:1736:A:H8	1.82	0.44
30:0:2269:C:H2'	30:0:2270:G:C5'	2.47	0.44
30:0:2653:A:H2'	30:0:2654:C:C6	2.52	0.44
2:B:10:SER:O	2:B:16:ARG:NH1	2.49	0.44
2:B:27:ASN:HD21	30:0:2807:U:P	2.40	0.44
3:C:1:MET:HG2	3:C:2:GLN:N	2.27	0.44
4:D:52:THR:HG21	30:0:2346:C:O2'	2.17	0.44
5:E:11:VAL:HG12	5:E:12:ASP:N	2.31	0.44
5:E:15:GLN:HG3	5:E:20:ILE:HG12	1.99	0.44
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.98	0.44
11:K:8:VAL:HG13	11:K:80:ILE:HG22	1.98	0.44
14:N:22:GLN:HA	14:N:25:ARG:CZ	2.47	0.44
18:R:29:LYS:HE2	30:0:524:A:H5'	1.99	0.44
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.48	0.44
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.98	0.44
30:0:255:A:H2'	30:0:256:C:O4'	2.17	0.44
30:0:1132:A:N3	30:0:2521:A:O2'	2.48	0.44
30:0:1676:G:C2'	30:0:1677:U:H5'	2.47	0.44
30:0:1894:C:N4	30:0:1939:U:H2'	2.31	0.44
30:0:2510:C:N4	30:0:2564:G:H22	2.12	0.44
31:9:14:G:H8	31:9:14:G:C5'	2.20	0.44
4:D:137:PRO:O	31:9:30:C:OP1	2.35	0.44
8:H:77:ILE:HG23	8:H:82:GLU:HG2	2.00	0.44
12:L:6:ARG:NH1	30:0:1299:G:N7	2.65	0.44
13:M:59:GLY:HA3	13:M:141:ILE:CD1	2.47	0.44
13:M:159:VAL:HG13	13:M:160:PHE:N	2.32	0.44
13:M:184:ARG:HG3	13:M:185:PRO:HA	2.00	0.44
16:P:137:LEU:O	16:P:141:ILE:HG13	2.17	0.44
23:W:21:LEU:HB3	23:W:26:ILE:HG12	1.99	0.44
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.52	0.44
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:74:G:H2'	30:0:75:U:H6	1.82	0.44
30:0:271:C:C2	30:0:273:G:O4'	2.70	0.44
30:0:542:A:H1'	38:0:4691:HOH:O	2.16	0.44
30:0:649:U:O2'	30:0:650:C:H5'	2.16	0.44
30:0:2505:G:H2'	30:0:2506:A:H5'	2.00	0.44
30:0:2526:C:C2'	30:0:2527:U:H5'	2.47	0.44
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.99	0.44
31:9:3:A:C8	31:9:26:C:N3	2.86	0.44
31:9:65:A:N6	31:9:112:U:C6	2.85	0.44
2:B:162:MET:CE	2:B:310:ARG:HD3	2.46	0.44
3:C:233:THR:HG22	3:C:234:VAL:N	2.32	0.44
4:D:54:ALA:HB2	4:D:69:ILE:CD1	2.48	0.44
5:E:95:VAL:HG11	5:E:131:LEU:HD21	1.98	0.44
11:K:55:VAL:CG1	11:K:56:SER:N	2.80	0.44
16:P:19:ASN:OD1	30:0:1720:C:H5	2.00	0.44
27:1:8:GLN:HG3	30:0:1688:G:H4'	1.99	0.44
30:0:195:C:H2'	30:0:196:G:H5'	1.99	0.44
30:0:796:A:C2	30:0:797:A:C4	3.05	0.44
30:0:957:A:H8	30:0:957:A:O5'	2.01	0.44
30:0:1116:U:N3	30:0:1246:A:N6	2.59	0.44
30:0:1268:C:O2'	30:0:1269:G:H5'	2.16	0.44
30:0:1503:U:H2'	30:0:1504:A:O4'	2.17	0.44
30:0:1850:U:H2'	30:0:1851:G:H8	1.82	0.44
30:0:1925:G:O2'	30:0:1926:G:H5'	2.18	0.44
30:0:2064:U:H4'	30:0:2653:A:OP1	2.17	0.44
30:0:2502:C:O2'	30:0:2503:A:H5'	2.17	0.44
31:9:45:A:C5	31:9:46:C:C5	3.05	0.44
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.77	0.44
1:A:164:ARG:HB2	26:Z:92:SER:OG	2.17	0.44
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.79	0.44
30:0:299:U:H5'	38:0:7352:HOH:O	2.16	0.44
30:0:348:C:H5	38:0:6349:HOH:O	1.99	0.44
30:0:731:U:O2'	30:0:732:C:H5'	2.18	0.44
30:0:970:U:H2'	38:0:6346:HOH:O	2.18	0.44
30:0:1268:C:H2'	30:0:1269:G:C8	2.53	0.44
30:0:1416:G:C2'	30:0:1417:G:H5'	2.47	0.44
30:0:1771:U:O2'	30:0:1773:G:N7	2.46	0.44
30:0:2734:G:O2'	30:0:2735:U:H5'	2.18	0.44
2:B:198:GLU:HA	38:B:9123:HOH:O	2.17	0.44
12:L:79:ASP:HB2	38:L:8858:HOH:O	2.17	0.44
13:M:92:THR:HB	30:0:401:C:O2'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:61:GLN:NE2	38:0:4737:HOH:O	2.50	0.44
25:Y:122:ARG:NH2	38:Y:8101:HOH:O	2.51	0.44
27:1:1:THR:O	30:0:1836:A:H1'	2.18	0.44
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.53	0.44
30:0:99:A:C8	30:0:100:C:C5	3.06	0.44
30:0:283:U:H5	30:0:284:C:C4	2.36	0.44
30:0:312:U:C2	30:0:320:G:N2	2.86	0.44
30:0:354:A:H2'	30:0:355:C:C6	2.53	0.44
30:0:535:G:C6	30:0:2064:U:C5	3.06	0.44
30:0:816:G:H5'	30:0:1598:A:H4'	2.00	0.44
30:0:1020:A:H2'	30:0:1021:G:C8	2.52	0.44
30:0:1058:A:H2'	30:0:1060:C:C5'	2.47	0.44
30:0:1421:C:H2'	30:0:1422:U:H6	1.82	0.44
30:0:2324:G:H21	30:0:2377:U:H1'	1.83	0.44
30:0:2612:A:H4'	38:0:3687:HOH:O	2.16	0.44
2:B:256:GLN:HG2	38:B:9122:HOH:O	2.17	0.44
5:E:35:TYR:CD2	5:E:36:PRO:HD2	2.53	0.44
6:F:107:ASP:O	6:F:111:ILE:HG13	2.18	0.44
7:G:19:GLU:O	7:G:23:ILE:HG13	2.18	0.44
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.48	0.44
14:N:160:SER:HB3	31:9:51:A:H5'	1.99	0.44
20:T:19:ARG:HD3	20:T:67:LEU:O	2.18	0.44
23:W:44:MET:HE2	30:0:944:G:H21	1.82	0.44
24:X:34:ARG:NH1	24:X:48:VAL:O	2.49	0.44
27:1:21:ARG:HD2	27:1:39:PHE:HB2	1.98	0.44
30:0:545:G:H8	30:0:545:G:C5'	2.14	0.44
30:0:565:A:C6	30:0:566:A:C6	3.05	0.44
30:0:1224:G:H2'	30:0:1225:C:C6	2.52	0.44
30:0:1666:C:C2'	30:0:1667:A:H5'	2.31	0.44
30:0:2672:C:H2'	30:0:2673:U:C6	2.52	0.44
31:9:56:A:H2'	31:9:57:A:C5'	2.28	0.44
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.86	0.44
3:C:40:ALA:O	3:C:43:LYS:HB2	2.18	0.44
3:C:153:VAL:O	3:C:157:LEU:HG	2.16	0.44
4:D:84:LEU:HA	4:D:87:ALA:HB3	1.99	0.44
5:E:81:GLU:HG2	5:E:134:SER:CB	2.45	0.44
13:M:169:ARG:HD2	38:M:8886:HOH:O	2.16	0.44
23:W:75:GLY:HA3	38:W:5763:HOH:O	2.17	0.44
30:0:363:C:O2'	30:0:364:U:H5'	2.18	0.44
30:0:777:U:OP2	30:0:777:U:H4'	2.17	0.44
30:0:1947:G:N2	30:0:1966:U:C2	2.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:TYR:CE2	27:1:53:LYS:HB3	2.53	0.44
30:0:537:G:O4'	30:0:538:C:C5	2.70	0.44
30:0:970:U:O5'	30:0:970:U:H6	2.01	0.44
30:0:1079:A:OP2	30:0:1080:C:N4	2.46	0.44
30:0:1186:C:N4	30:0:1187:U:C4	2.86	0.44
30:0:1206:U:H6	30:0:1206:U:C5'	2.24	0.44
30:0:1236:A:H2'	30:0:1237:U:O4'	2.17	0.44
30:0:1520:G:C2	30:0:1521:C:C2	3.06	0.44
30:0:2310:G:C2	30:0:2311:A:C5	3.05	0.44
30:0:2456:A:H5'	38:0:5708:HOH:O	2.18	0.44
3:C:195:VAL:HA	3:C:213:ALA:O	2.17	0.43
12:L:27:ARG:HH21	12:L:30:ARG:HG2	1.82	0.43
13:M:115:LEU:HD13	13:M:116:ASN:HB2	2.00	0.43
15:O:65:LEU:HD13	30:0:746:A:C6	2.53	0.43
30:0:192:A:H5'	38:0:7657:HOH:O	2.17	0.43
30:0:758:A:H2'	30:0:759:C:O4'	2.17	0.43
30:0:1593:C:O2'	30:0:1594:C:H5'	2.18	0.43
30:0:1695:G:C6	30:0:1696:U:C4	3.06	0.43
30:0:2015:A:H2'	30:0:2016:U:O4'	2.18	0.43
30:0:2387:U:H2'	30:0:2388:C:C6	2.53	0.43
30:0:2717:C:C2'	30:0:2718:C:C5'	2.81	0.43
30:0:2842:G:H2'	30:0:2843:A:H5'	2.00	0.43
5:E:53:GLU:HB3	5:E:55:ASN:ND2	2.33	0.43
5:E:84:MET:HG2	5:E:168:ILE:HD13	2.00	0.43
10:J:88:PRO:CA	33:J:8802:CL:CL	3.03	0.43
18:R:80:TYR:O	30:0:2050:G:H5''	2.18	0.43
22:V:4:HIS:O	22:V:8:ILE:HG13	2.18	0.43
30:0:327:A:H4'	30:0:329:A:C8	2.52	0.43
30:0:682:A:H2'	30:0:683:G:O4'	2.18	0.43
30:0:705:C:O2	30:0:705:C:H2'	2.17	0.43
30:0:958:G:H2'	30:0:959:C:C6	2.53	0.43
30:0:1069:C:H2'	30:0:1070:A:O4'	2.18	0.43
30:0:1164:U:H3	30:0:1192:A:H2	1.65	0.43
30:0:1626:A:C2'	30:0:1627:G:H5'	2.48	0.43
30:0:2107:U:O2'	30:0:2108:A:H5'	2.19	0.43
30:0:2269:C:H2'	30:0:2270:G:H5'	2.00	0.43
30:0:2595:U:O2'	30:0:2596:A:H5'	2.18	0.43
30:0:2642:G:H2'	30:0:2643:G:O4'	2.18	0.43
30:0:2649:A:H5'	30:0:2649:A:C8	2.53	0.43
30:0:2906:A:H5'	30:0:2907:C:O4'	2.17	0.43
4:D:146:LYS:HE2	14:N:107:ASN:ND2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:23:ILE:O	7:G:27:ILE:HG13	2.18	0.43
9:I:87:PRO:HG3	38:0:7132:HOH:O	2.18	0.43
16:P:73:HIS:HE1	30:0:1789:G:O6	2.01	0.43
27:1:9:GLY:HA3	30:0:1695:G:H1'	2.00	0.43
30:0:100:C:H2'	30:0:101:C:H6	1.84	0.43
30:0:130:C:H4'	38:0:5803:HOH:O	2.17	0.43
30:0:622:G:O2'	30:0:623:U:H5'	2.19	0.43
30:0:711:G:C2	30:0:718:C:N3	2.87	0.43
30:0:745:G:H5''	30:0:746:A:OP1	2.18	0.43
30:0:1205:U:H5	38:0:4448:HOH:O	2.00	0.43
30:0:1298:U:H2'	30:0:1299:G:C8	2.53	0.43
30:0:1631:A:C6	30:0:1632:A:N1	2.86	0.43
30:0:1889:C:O2	30:0:2010:A:H2	2.02	0.43
30:0:2349:G:O2'	30:0:2350:G:H5'	2.17	0.43
30:0:2801:A:H2'	30:0:2801:A:N3	2.33	0.43
31:9:23:U:C2'	31:9:24:U:H4'	2.48	0.43
6:F:91:VAL:CG1	6:F:92:GLY:N	2.81	0.43
8:H:12:ILE:HG23	8:H:129:ARG:CZ	2.48	0.43
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.82	0.43
10:J:80:LYS:HE3	10:J:101:VAL:O	2.19	0.43
13:M:67:VAL:HB	13:M:97:ILE:HG23	2.01	0.43
16:P:98:ILE:HD12	16:P:102:ARG:CZ	2.48	0.43
30:0:367:G:H8	30:0:367:G:OP2	2.01	0.43
30:0:483:C:N4	30:0:484:A:C6	2.86	0.43
30:0:871:G:H4'	38:0:4418:HOH:O	2.18	0.43
30:0:1074:G:H4'	30:0:1260:G:C6	2.54	0.43
30:0:1368:U:O5'	30:0:1368:U:H6	2.01	0.43
30:0:1503:U:H6	30:0:1503:U:H3'	1.82	0.43
30:0:2040:C:H5''	30:0:2759:C:O2'	2.18	0.43
30:0:2315:C:H4'	30:0:2425:A:C6	2.53	0.43
30:0:2649:A:H5'	30:0:2649:A:H8	1.83	0.43
31:9:110:G:C5	31:9:111:U:C5	3.07	0.43
1:A:64:ASP:OD1	1:A:66:ARG:HD3	2.18	0.43
5:E:84:MET:HE1	5:E:148:ILE:HD13	1.99	0.43
14:N:37:ARG:HH21	14:N:105:GLY:N	2.16	0.43
14:N:86:LEU:HD23	14:N:179:LEU:HD12	1.98	0.43
15:O:29:VAL:HG11	15:O:98:LEU:HD21	1.99	0.43
16:P:59:ARG:NH2	16:P:66:GLN:HE22	2.17	0.43
16:P:83:LYS:HG2	30:0:793:A:H5''	1.99	0.43
30:0:113:A:H2'	30:0:115:U:O4	2.19	0.43
30:0:666:A:H2'	30:0:667:C:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:725:C:H2'	30:0:726:C:O5'	2.17	0.43
30:0:1416:G:H2'	30:0:1417:G:H5'	1.99	0.43
30:0:1568:G:C6	30:0:1569:U:C4	3.06	0.43
30:0:1626:A:H2'	30:0:1627:G:H5'	1.99	0.43
30:0:2010:A:C2'	38:0:5975:HOH:O	2.59	0.43
30:0:2470:A:H5''	38:0:3249:HOH:O	2.18	0.43
30:0:2902:A:H4'	30:0:2903:C:OP1	2.19	0.43
31:9:117:G:H2'	31:9:118:C:H6	1.83	0.43
3:C:27:ARG:NH1	3:C:29:ASP:OD1	2.50	0.43
11:K:24:THR:HB	11:K:64:MET:HE2	2.00	0.43
15:O:3:THR:HG22	30:0:656:G:C5'	2.31	0.43
15:O:25:VAL:HG11	30:0:710:G:H5'	1.99	0.43
16:P:94:TRP:CH2	16:P:98:ILE:HG13	2.53	0.43
17:Q:47:VAL:HA	17:Q:48:PRO:HD3	1.81	0.43
17:Q:94:GLN:O	17:Q:95:GLU:HB2	2.18	0.43
22:V:59:ILE:O	22:V:63:GLU:HG2	2.17	0.43
23:W:139:GLY:O	23:W:141:HIS:CD2	2.71	0.43
25:Y:204:ARG:NH2	30:0:1324:G:H21	2.16	0.43
30:0:1023:C:H2'	30:0:1024:G:O4'	2.18	0.43
30:0:1163:G:H1	30:0:1184:C:N4	2.17	0.43
30:0:1314:U:H5''	30:0:1316:G:O4'	2.19	0.43
30:0:1585:C:H2'	30:0:1586:G:H8	1.84	0.43
30:0:2829:G:N2	30:0:2912:C:C2	2.86	0.43
1:A:94:LEU:HD23	1:A:94:LEU:N	2.33	0.43
1:A:94:LEU:HD12	1:A:98:GLU:HB2	2.00	0.43
2:B:51:VAL:CG2	2:B:330:VAL:HG22	2.48	0.43
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.99	0.43
4:D:12:GLU:C	4:D:14:ARG:H	2.27	0.43
5:E:7:ILE:HG22	5:E:45:ASP:O	2.19	0.43
15:O:24:ALA:HB3	30:0:710:G:OP1	2.19	0.43
30:0:790:A:H2'	30:0:791:A:O4'	2.18	0.43
30:0:912:A:C4	30:0:1294:A:C2	3.06	0.43
30:0:1181:A:O2'	30:0:1182:C:H5'	2.18	0.43
30:0:1474:C:H6	30:0:1474:C:C5'	2.18	0.43
30:0:1626:A:H2'	30:0:1627:G:O4'	2.19	0.43
30:0:1950:G:O2'	30:0:1951:G:H5'	2.19	0.43
30:0:2421:G:H3'	30:0:2422:U:H5''	2.00	0.43
30:0:2716:G:O2'	30:0:2717:C:H5'	2.19	0.43
31:9:59:C:H2'	31:9:60:C:H6	1.83	0.43
31:9:64:C:O2'	31:9:65:A:H5'	2.18	0.43
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.06	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:PRO:HG2	38:C:8520:HOH:O	2.17	0.43
12:L:67:ARG:O	12:L:71:GLU:HG3	2.19	0.43
14:N:108:SER:HA	14:N:109:PRO:HD3	1.78	0.43
30:0:512:G:O3'	30:0:513:A:C8	2.70	0.43
30:0:1132:A:H3'	38:0:4832:HOH:O	2.18	0.43
30:0:1175:G:O2'	30:0:1193:A:H2'	2.19	0.43
30:0:1453:G:N2	30:0:1675:C:C2	2.87	0.43
30:0:1705:C:H2'	30:0:1706:G:O4'	2.19	0.43
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.48	0.43
4:D:154:LYS:H	4:D:154:LYS:CD	2.20	0.43
4:D:167:GLU:C	4:D:169:THR:H	2.27	0.43
6:F:59:ILE:CD1	30:0:263:U:C2	3.02	0.43
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.19	0.43
14:N:44:ARG:HG3	14:N:45:ALA:N	2.34	0.43
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.99	0.43
23:W:119:HIS:HE1	38:0:9560:HOH:O	2.02	0.43
30:0:64:G:H2'	30:0:65:C:O4'	2.19	0.43
30:0:590:A:C2'	30:0:591:A:H5'	2.48	0.43
30:0:1138:G:H4'	38:0:5722:HOH:O	2.18	0.43
30:0:1463:U:H2'	30:0:1464:C:H6	1.83	0.43
30:0:1971:G:H5''	38:0:7084:HOH:O	2.18	0.43
30:0:2241:C:H2'	30:0:2242:U:C6	2.54	0.43
30:0:2362:A:H2'	30:0:2363:G:C8	2.54	0.43
30:0:2589:U:H2'	30:0:2590:U:C6	2.54	0.43
30:0:2761:A:H2'	38:0:5654:HOH:O	2.19	0.43
31:9:65:A:C2'	31:9:66:G:OP2	2.66	0.43
31:9:117:G:H2'	31:9:118:C:C6	2.53	0.43
1:A:173:GLY:O	1:A:176:HIS:HB3	2.19	0.43
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.32	0.43
3:C:27:ARG:HH11	3:C:27:ARG:HG3	1.83	0.43
4:D:96:SER:O	30:0:2337:G:H5''	2.19	0.43
5:E:108:LEU:CD1	5:E:164:ASP:HB2	2.49	0.43
7:G:63:ARG:O	7:G:67:LEU:HG	2.18	0.43
10:J:75:PRO:HD3	10:J:136:SER:OG	2.18	0.43
18:R:29:LYS:HE2	30:0:524:A:H5''	2.01	0.43
23:W:26:ILE:HB	38:W:5420:HOH:O	2.18	0.43
30:0:764:C:H2'	30:0:765:G:O4'	2.19	0.43
30:0:779:U:H5'	30:0:1836:A:C2	2.54	0.43
30:0:1015:C:H2'	30:0:1016:U:C6	2.54	0.43
30:0:1158:G:O2'	30:0:1159:G:H5'	2.19	0.43
30:0:1409:G:C2	30:0:1410:G:C8	3.07	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1483:C:O2'	30:0:1484:G:H5'	2.18	0.43
30:0:1528:A:H61	30:0:1663:G:H1'	1.84	0.43
30:0:1559:A:OP2	30:0:1559:A:H8	2.02	0.43
30:0:1829:A:C8	30:0:1885:A:C8	3.07	0.43
30:0:2249:G:C2	30:0:2253:G:C6	3.07	0.43
30:0:2314:G:O2'	30:0:2315:C:H5'	2.19	0.43
31:9:121:C:O5'	31:9:121:C:H6	2.02	0.43
2:B:82:VAL:O	2:B:82:VAL:HG12	2.19	0.42
14:N:29:SER:HB3	30:0:2415:A:O2'	2.19	0.42
24:X:61:ARG:HD2	24:X:65:ASN:O	2.19	0.42
28:2:20:ARG:HG2	28:2:21:VAL:N	2.33	0.42
30:0:69:A:C8	30:0:69:A:C5'	2.98	0.42
30:0:1213:C:C2'	30:0:1214:G:H5'	2.48	0.42
30:0:1413:A:H2'	30:0:1414:A:O4'	2.19	0.42
30:0:1482:A:H1'	38:0:9422:HOH:O	2.19	0.42
30:0:1555:G:H4'	30:0:1630:A:H2	1.84	0.42
30:0:2293:G:C2	30:0:2316:G:C6	3.07	0.42
30:0:2374:G:H2'	30:0:2375:A:H8	1.83	0.42
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.80	0.42
14:N:73:ALA:HB1	14:N:74:PRO:CD	2.49	0.42
17:Q:55:ARG:HD2	38:Q:2875:HOH:O	2.18	0.42
18:R:128:ARG:HH22	30:0:2054:A:H2	1.65	0.42
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.33	0.42
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.98	0.42
30:0:56:G:N3	30:0:70:A:C2	2.87	0.42
30:0:137:U:H3'	30:0:139:C:H41	1.83	0.42
30:0:216:A:O2'	30:0:217:C:H5'	2.19	0.42
30:0:319:A:H4'	30:0:338:C:C4	2.53	0.42
30:0:808:A:C5	30:0:809:G:H1'	2.54	0.42
30:0:917:U:O5'	30:0:917:U:H6	2.02	0.42
30:0:941:G:C6	30:0:942:U:C4	3.08	0.42
30:0:1116:U:C2	30:0:1246:A:N6	2.87	0.42
30:0:1406:A:H4'	30:0:1407:A:C5'	2.50	0.42
30:0:1769:C:C4	30:0:1770:U:C4	3.08	0.42
30:0:2347:C:H2'	30:0:2348:C:C6	2.54	0.42
30:0:2519:C:H2'	30:0:2520:G:O4'	2.19	0.42
30:0:2726:U:O2	30:0:2749:U:O5'	2.36	0.42
1:A:211:LYS:HG2	38:0:7044:HOH:O	2.19	0.42
2:B:70:PRO:HG3	30:0:2719:A:C2	2.54	0.42
4:D:22:VAL:HA	4:D:73:VAL:O	2.19	0.42
5:E:77:THR:OG1	5:E:78:GLU:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:107:PHE:CZ	5:E:152:THR:HB	2.55	0.42
21:U:52:THR:HG22	21:U:54:THR:N	2.32	0.42
30:0:78:G:C6	30:0:79:G:C6	3.07	0.42
30:0:699:C:C6	30:0:744:G:C4	3.07	0.42
30:0:1185:U:C5'	38:0:7483:HOH:O	2.66	0.42
30:0:2017:U:O2'	30:0:2018:A:C8	2.68	0.42
30:0:2755:G:H1'	38:0:4696:HOH:O	2.19	0.42
30:0:2822:C:O2'	30:0:2827:A:H4'	2.19	0.42
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.49	0.42
16:P:16:VAL:HG22	16:P:20:ARG:CZ	2.50	0.42
26:Z:40:ALA:HA	30:0:1773:G:C8	2.54	0.42
30:0:69:A:C2'	30:0:70:A:OP2	2.67	0.42
30:0:305:A:C6	30:0:329:A:N3	2.87	0.42
30:0:536:A:H8	38:0:5057:HOH:O	2.01	0.42
30:0:1057:A:H1'	30:0:2492:U:O2'	2.19	0.42
30:0:1163:G:N2	30:0:1184:C:N3	2.67	0.42
30:0:1167:G:H3'	38:0:7514:HOH:O	2.19	0.42
30:0:1189:A:N7	30:0:1190:G:N7	2.67	0.42
30:0:1211:G:H2'	30:0:1212:C:C6	2.48	0.42
30:0:1400:C:C2'	30:0:1401:G:H5'	2.49	0.42
30:0:1603:A:H5'	30:0:1605:G:C5'	2.48	0.42
30:0:1850:U:H2'	30:0:1851:G:C8	2.53	0.42
30:0:2003:U:O2'	30:0:2004:U:H5	2.02	0.42
30:0:2061:C:H2'	30:0:2062:A:H5'	2.00	0.42
30:0:2119:C:O2'	30:0:2120:U:H5'	2.19	0.42
30:0:2456:A:H2'	30:0:2457:U:C6	2.55	0.42
30:0:2512:U:O5'	30:0:2512:U:H6	2.02	0.42
2:B:275:GLY:O	2:B:291:ASP:HA	2.19	0.42
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.84	0.42
4:D:76:ARG:NH1	31:9:42:C:O2	2.53	0.42
9:I:82:THR:HG22	30:0:1168:C:H5''	2.00	0.42
14:N:55:ASP:OD2	31:9:7:G:H4'	2.20	0.42
30:0:138:U:OP2	30:0:139:C:H5	2.02	0.42
30:0:459:A:H4'	38:0:9454:HOH:O	2.20	0.42
30:0:470:U:H2'	30:0:471:G:O4'	2.20	0.42
30:0:807:A:H2'	30:0:808:A:O4'	2.19	0.42
30:0:939:A:C2	30:0:1027:G:N3	2.88	0.42
30:0:952:G:H4'	38:0:4039:HOH:O	2.19	0.42
30:0:1015:C:H2'	30:0:1016:U:H6	1.85	0.42
30:0:1381:A:N3	30:0:1382:G:H1'	2.35	0.42
30:0:2310:G:N1	30:0:2311:A:C5	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2661:U:H3	30:0:2812:A:H62	1.66	0.42
30:0:2879:A:H2'	30:0:2880:A:O4'	2.19	0.42
31:9:14:G:C8	31:9:14:G:C5'	2.99	0.42
31:9:39:U:H1'	31:9:44:A:N6	2.35	0.42
2:B:310:ARG:HD2	38:B:9114:HOH:O	2.19	0.42
3:C:206:ASN:HB2	30:0:329:A:OP2	2.19	0.42
4:D:101:THR:O	4:D:101:THR:HG22	2.19	0.42
9:I:118:ASN:HB3	30:0:1185:U:C5'	2.49	0.42
9:I:130:LEU:HD21	30:0:1167:G:H4'	2.02	0.42
14:N:164:ASP:CG	14:N:167:ASP:HA	2.45	0.42
18:R:72:VAL:CG1	18:R:75:TRP:HB3	2.50	0.42
28:2:10:ARG:NH2	30:0:121:U:OP2	2.39	0.42
28:2:48:ASP:O	28:2:49:GLU:HB2	2.19	0.42
30:0:191:A:C4	30:0:237:G:N7	2.88	0.42
30:0:657:G:H2'	30:0:658:C:C6	2.55	0.42
30:0:722:G:H22	30:0:938:G:P	2.42	0.42
30:0:849:C:H1'	38:0:6632:HOH:O	2.19	0.42
30:0:1211:G:O2'	30:0:1212:C:H5'	2.19	0.42
30:0:1603:A:C5'	30:0:1605:G:C5'	2.96	0.42
30:0:1966:U:H2'	30:0:1967:U:H2'	2.00	0.42
30:0:1976:G:O2'	30:0:1977:U:C5'	2.68	0.42
30:0:2388:C:O2'	30:0:2389:U:H5'	2.19	0.42
30:0:2816:A:H5''	30:0:2817:G:H5'	2.01	0.42
2:B:140:LEU:HD13	2:B:175:LEU:HA	2.01	0.42
18:R:99:ALA:O	18:R:104:PHE:HB2	2.19	0.42
38:W:7873:HOH:O	30:0:1287:A:H8	2.03	0.42
30:0:85:C:H5''	30:0:86:A:OP2	2.20	0.42
30:0:120:A:H2'	30:0:120:A:N3	2.34	0.42
30:0:137:U:O5'	30:0:137:U:H6	2.02	0.42
30:0:212:A:O4'	30:0:214:U:C6	2.72	0.42
30:0:287:C:H6	30:0:287:C:O5'	2.03	0.42
30:0:307:G:H3'	30:0:342:C:OP2	2.19	0.42
30:0:485:A:H4'	30:0:486:A:OP1	2.20	0.42
30:0:1097:A:C6	30:0:1098:A:C6	3.08	0.42
30:0:1193:A:H1'	30:0:1194:A:N7	2.35	0.42
30:0:1754:A:H2'	30:0:1755:A:O4'	2.19	0.42
30:0:2355:G:H2'	38:0:5650:HOH:O	2.18	0.42
30:0:2524:G:H5''	38:0:4744:HOH:O	2.19	0.42
2:B:254:GLN:NE2	38:B:9058:HOH:O	2.52	0.42
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.29	0.42
19:S:57:THR:C	19:S:59:ASP:H	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:41:ARG:NH1	20:T:42:VAL:O	2.53	0.42
30:0:2333:G:H2'	30:0:2334:C:H6	1.84	0.42
30:0:2575:C:H2'	30:0:2576:A:O4'	2.19	0.42
1:A:30:ARG:HG2	1:A:31:LYS:N	2.35	0.42
1:A:164:ARG:NH2	30:0:1876:C:O3'	2.53	0.42
2:B:53:LEU:HD21	2:B:270:ILE:HD12	2.01	0.42
2:B:137:LEU:HD21	2:B:140:LEU:HD21	2.02	0.42
2:B:215:VAL:HA	2:B:220:VAL:HG22	2.01	0.42
4:D:19:GLU:O	4:D:76:ARG:HG2	2.19	0.42
4:D:21:VAL:HA	4:D:131:THR:O	2.20	0.42
4:D:51:ARG:HD3	38:D:7636:HOH:O	2.20	0.42
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.42
20:T:9:LYS:HB2	38:0:7442:HOH:O	2.20	0.42
30:0:293:A:C4	30:0:360:A:C2	3.08	0.42
30:0:295:C:H2'	30:0:296:G:O4'	2.20	0.42
30:0:834:G:H4'	30:0:835:U:OP2	2.19	0.42
30:0:2324:G:C2	30:0:2377:U:O2	2.73	0.42
30:0:2497:A:C2	30:0:2524:G:C2	3.07	0.42
3:C:73:GLN:NE2	3:C:73:GLN:HA	2.35	0.42
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.20	0.42
21:U:50:GLU:HB2	30:0:2866:U:C5	2.54	0.42
23:W:48:VAL:HG12	23:W:48:VAL:O	2.20	0.42
27:1:25:LYS:HG3	28:2:49:GLU:H	1.85	0.42
30:0:130:C:H5'	38:0:5226:HOH:O	2.20	0.42
30:0:264:G:H1'	30:0:265:U:H5	1.85	0.42
30:0:844:A:C6	30:0:882:A:C6	3.08	0.42
30:0:1544:U:H2'	30:0:1545:C:C6	2.53	0.42
30:0:2134:G:C6	30:0:2258:A:C8	3.08	0.42
30:0:2727:A:C6	30:0:2756:U:C2	3.08	0.42
30:0:2911:C:H2'	30:0:2912:C:C6	2.54	0.42
2:B:84:LEU:O	2:B:99:GLU:HA	2.20	0.41
7:G:20:VAL:O	7:G:24:VAL:HG23	2.20	0.41
11:K:14:LYS:CB	11:K:45:PRO:HG2	2.50	0.41
12:L:57:VAL:HG21	30:0:2443:C:H5'	2.02	0.41
12:L:57:VAL:O	12:L:57:VAL:HG12	2.20	0.41
13:M:47:ASP:CG	13:M:48:LYS:H	2.27	0.41
17:Q:40:HIS:HE1	30:0:949:U:O2'	2.03	0.41
20:T:48:VAL:HG22	20:T:97:ARG:O	2.19	0.41
23:W:13:MET:CE	23:W:18:GLN:HA	2.35	0.41
30:0:212:A:N1	30:0:226:A:H5''	2.35	0.41
30:0:583:C:C2	30:0:584:U:C5	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:803:C:H2'	30:0:804:C:C6	2.55	0.41
30:0:1175:G:H1'	30:0:1193:A:N9	2.33	0.41
30:0:2269:C:C2'	30:0:2270:G:H5'	2.50	0.41
30:0:2297:U:H2'	30:0:2298:C:C6	2.53	0.41
30:0:2333:G:H2'	30:0:2334:C:C6	2.55	0.41
30:0:2534:C:H2'	30:0:2535:A:C8	2.55	0.41
1:A:97:ALA:HB2	1:A:150:PRO:HB2	2.02	0.41
1:A:179:MET:HG2	1:A:186:TRP:HB2	2.02	0.41
2:B:229:ARG:HD2	38:B:8989:HOH:O	2.20	0.41
5:E:10:ASP:HA	38:E:6017:HOH:O	2.20	0.41
6:F:99:THR:HG23	6:F:99:THR:O	2.20	0.41
8:H:91:ARG:H	8:H:91:ARG:HG2	1.54	0.41
11:K:41:LYS:O	11:K:42:ASN:HB2	2.20	0.41
13:M:9:ARG:HD2	30:0:380:A:OP2	2.20	0.41
18:R:79:ARG:HB3	30:0:2050:G:OP1	2.20	0.41
18:R:96:VAL:HG13	18:R:106:GLY:HA3	2.02	0.41
20:T:28:SER:O	20:T:32:ARG:HG3	2.19	0.41
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.50	0.41
26:Z:34:SER:CB	30:0:797:A:H4'	2.50	0.41
30:0:226:A:H1'	30:0:393:G:C5	2.55	0.41
30:0:636:G:H5'	30:0:2059:U:OP2	2.20	0.41
30:0:830:G:C5	30:0:831:U:C4	3.08	0.41
30:0:1355:A:H4'	38:0:5766:HOH:O	2.19	0.41
30:0:2350:G:H2'	30:0:2351:C:C6	2.56	0.41
1:A:141:PRO:HG2	30:0:1855:G:O6	2.20	0.41
2:B:124:ALA:O	2:B:128:ILE:HG13	2.21	0.41
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.54	0.41
18:R:132:ARG:NH2	38:R:8987:HOH:O	2.53	0.41
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.83	0.41
30:0:349:U:O2'	30:0:350:G:H5'	2.20	0.41
30:0:567:U:H5''	38:0:5300:HOH:O	2.19	0.41
30:0:696:C:O2'	30:0:697:G:H5'	2.19	0.41
30:0:1056:U:H2'	30:0:1057:A:O4'	2.20	0.41
30:0:1154:A:H2'	30:0:1155:G:O4'	2.20	0.41
30:0:1162:G:C6	30:0:1163:G:C6	3.09	0.41
30:0:1172:G:H1'	38:0:4984:HOH:O	2.20	0.41
30:0:1598:A:C2	30:0:1599:U:C2	3.07	0.41
30:0:1971:G:C5'	38:0:7084:HOH:O	2.67	0.41
30:0:2766:A:O2'	30:0:2767:C:H5'	2.20	0.41
31:9:3:A:C6	31:9:22:G:H1'	2.52	0.41
1:A:211:LYS:NZ	38:0:7459:HOH:O	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.20	0.41
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.88	0.41
11:K:22:ASP:HB2	38:K:5264:HOH:O	2.20	0.41
17:Q:34:ASP:O	17:Q:37:GLU:HB2	2.20	0.41
23:W:74:GLU:OE1	30:0:1285:U:H4'	2.21	0.41
30:0:30:U:O2	30:0:460:A:C2	2.74	0.41
30:0:177:A:O2'	30:0:892:G:H4'	2.20	0.41
30:0:283:U:C5	30:0:284:C:N3	2.87	0.41
30:0:445:U:H2'	30:0:446:G:C8	2.55	0.41
30:0:594:C:C4	30:0:595:U:C4	3.09	0.41
30:0:1139:U:H2'	30:0:1140:C:C6	2.55	0.41
30:0:1149:U:H5''	30:0:1151:G:O4'	2.21	0.41
30:0:1421:C:H2'	30:0:1422:U:C6	2.55	0.41
30:0:1471:A:H2'	30:0:1472:C:C6	2.55	0.41
30:0:1795:G:H2'	30:0:1796:A:O4'	2.20	0.41
30:0:1904:A:C2	30:0:1905:U:H1'	2.54	0.41
30:0:1946:C:O4'	30:0:1969:A:C2	2.73	0.41
30:0:2310:G:C2	30:0:2311:A:C8	3.08	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.20	0.41
30:0:2699:A:H2'	30:0:2700:G:O4'	2.20	0.41
2:B:248:ARG:NH2	30:0:2549:C:H1'	2.35	0.41
3:C:184:ARG:HD2	30:0:1306:U:OP1	2.21	0.41
5:E:19:ASP:HA	5:E:31:ARG:O	2.21	0.41
5:E:111:LYS:CE	30:0:2690:U:H4'	2.50	0.41
13:M:72:ALA:HB2	13:M:93:ARG:HG2	2.01	0.41
24:X:43:VAL:HG12	24:X:44:ASP:H	1.85	0.41
29:3:38:ARG:HD2	30:0:396:U:OP2	2.20	0.41
30:0:113:A:OP2	30:0:114:A:H2'	2.20	0.41
30:0:154:C:O2'	30:0:155:C:H5'	2.20	0.41
30:0:625:U:H3'	38:0:3262:HOH:O	2.20	0.41
30:0:815:U:O2'	30:0:1598:A:H4'	2.20	0.41
30:0:968:G:H2'	30:0:969:G:C8	2.54	0.41
30:0:1060:C:H6	30:0:1060:C:C5'	2.29	0.41
30:0:1933:G:O2'	30:0:1934:A:H5'	2.20	0.41
30:0:2250:G:N2	30:0:2251:G:H1'	2.36	0.41
31:9:110:G:C6	31:9:111:U:C5	3.08	0.41
8:H:91:ARG:HA	30:0:1002:G:O2'	2.20	0.41
12:L:65:ASP:CG	12:L:111:ALA:HB3	2.46	0.41
16:P:115:SER:OG	16:P:118:GLN:HG3	2.21	0.41
19:S:57:THR:HG22	19:S:59:ASP:N	2.34	0.41
30:0:168:C:O5'	30:0:168:C:H6	2.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:563:C:H2'	30:0:564:G:O4'	2.21	0.41
30:0:571:C:H6	30:0:571:C:O5'	2.03	0.41
30:0:929:A:O5'	30:0:929:A:H8	2.04	0.41
30:0:1163:G:C2	30:0:1184:C:N3	2.89	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.35	0.41
30:0:1189:A:C8	30:0:1190:G:C8	3.09	0.41
30:0:1947:G:H2'	30:0:1948:G:C8	2.52	0.41
30:0:2328:U:C4	30:0:2329:C:C5	3.08	0.41
30:0:2722:G:C2	30:0:2761:A:C2	3.09	0.41
30:0:2860:G:H2'	30:0:2861:G:O4'	2.20	0.41
30:0:2891:A:C2	30:0:2892:G:C4	3.09	0.41
31:9:28:U:O2	31:9:57:A:N6	2.53	0.41
1:A:36:ASP:CB	1:A:85:SER:H	2.29	0.41
12:L:30:ARG:NH1	38:L:8811:HOH:O	2.48	0.41
19:S:6:LYS:HB2	19:S:27:ALA:O	2.20	0.41
21:U:56:ARG:NH1	30:0:2890:A:C2	2.89	0.41
25:Y:145:LYS:HD2	38:0:9965:HOH:O	2.20	0.41
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.36	0.41
30:0:301:C:O2'	30:0:302:A:H5'	2.21	0.41
30:0:681:G:N3	30:0:681:G:H2'	2.36	0.41
30:0:940:G:C5	30:0:1027:G:C2	3.09	0.41
30:0:1051:C:H2'	30:0:1052:G:O4'	2.21	0.41
30:0:1615:A:H5'	38:0:4187:HOH:O	2.19	0.41
30:0:1733:A:H2'	30:0:1734:C:O4'	2.20	0.41
30:0:1797:A:H2'	30:0:1799:G:O5'	2.21	0.41
31:9:23:U:HO2'	31:9:24:U:H4'	1.86	0.41
31:9:78:G:O2'	31:9:79:U:OP2	2.38	0.41
2:B:140:LEU:HA	38:B:9045:HOH:O	2.20	0.41
2:B:307:ARG:HD2	38:B:9119:HOH:O	2.20	0.41
4:D:13:MET:HE2	31:9:53:G:N2	2.35	0.41
8:H:157:TYR:CD1	8:H:157:TYR:C	2.99	0.41
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.20	0.41
16:P:55:LYS:HA	38:0:5633:HOH:O	2.21	0.41
23:W:38:THR:HG22	23:W:39:ASP:N	2.35	0.41
23:W:130:HIS:NE2	31:9:88:G:OP1	2.45	0.41
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	2.03	0.41
30:0:24:G:H22	30:0:518:G:H1'	1.86	0.41
30:0:250:C:H2'	30:0:251:C:C6	2.55	0.41
30:0:506:G:N1	30:0:509:A:OP2	2.54	0.41
30:0:510:U:H5''	30:0:512:G:OP2	2.21	0.41
30:0:519:A:H4'	30:0:1320:C:O3'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1255:A:N3	38:0:7772:HOH:O	2.37	0.41
30:0:1517:C:O2	30:0:1670:A:C2	2.74	0.41
30:0:1597:A:C4	30:0:1598:A:C8	3.09	0.41
30:0:1730:G:N3	30:0:1730:G:H2'	2.36	0.41
30:0:1819:G:C2'	30:0:1820:G:C5'	2.97	0.41
30:0:2712:G:O2'	30:0:2713:G:H5'	2.21	0.41
30:0:2756:U:C2	30:0:2896:A:H2	2.39	0.41
30:0:2866:U:H4'	30:0:2867:G:H5'	2.01	0.41
31:9:23:U:H2'	31:9:24:U:H4'	2.03	0.41
1:A:105:VAL:HG11	1:A:154:ALA:HB1	2.01	0.41
2:B:80:ARG:O	2:B:82:VAL:HG23	2.21	0.41
2:B:234:ARG:HD3	30:0:1734:C:OP1	2.21	0.41
2:B:254:GLN:HG3	38:0:9708:HOH:O	2.21	0.41
4:D:18:ILE:HG12	4:D:134:LEU:HD21	2.03	0.41
4:D:49:PRO:HA	4:D:73:VAL:HG22	2.02	0.41
4:D:173:GLU:HG3	4:D:174:VAL:N	2.36	0.41
8:H:52:LEU:HD13	8:H:153:PHE:HB3	2.02	0.41
13:M:75:ARG:HH21	13:M:78:LYS:HE3	1.85	0.41
14:N:7:LYS:HB3	30:0:2353:A:O2'	2.20	0.41
16:P:28:GLN:HE22	30:0:1387:G:C1'	2.33	0.41
17:Q:30:VAL:HG12	17:Q:30:VAL:O	2.21	0.41
18:R:106:GLY:HA2	18:R:109:MET:HE3	2.03	0.41
21:U:6:CYS:C	21:U:8:TYR:H	2.27	0.41
23:W:4:LEU:HD22	23:W:52:VAL:CG2	2.49	0.41
23:W:5:VAL:HG22	23:W:32:CYS:HB2	2.02	0.41
23:W:88:THR:HG23	23:W:110:GLN:CB	2.43	0.41
23:W:120:PRO:HG2	30:0:1095:U:O2	2.20	0.41
23:W:125:HIS:HD2	23:W:127:GLY:H	1.68	0.41
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.04	0.41
29:3:60:LYS:HG3	38:0:7573:HOH:O	2.19	0.41
30:0:106:A:H2'	30:0:107:U:O4'	2.21	0.41
30:0:271:C:H4'	30:0:272:A:OP1	2.21	0.41
30:0:278:A:H2'	30:0:279:C:O4'	2.19	0.41
30:0:652:G:H2'	30:0:653:U:O4'	2.20	0.41
30:0:694:A:H2'	30:0:695:C:C5'	2.50	0.41
30:0:822:C:H2'	30:0:823:U:C6	2.54	0.41
30:0:827:A:H2'	30:0:828:G:O4'	2.21	0.41
30:0:1222:A:H2'	30:0:1223:G:O4'	2.21	0.41
30:0:1305:C:H5'	38:0:9844:HOH:O	2.20	0.41
30:0:1364:G:H1'	38:0:4812:HOH:O	2.20	0.41
30:0:1597:A:C5	30:0:1598:A:C8	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1706:G:C6	30:0:1707:G:N1	2.89	0.41
30:0:1718:G:C6	30:0:1719:G:C5	3.08	0.41
30:0:1840:A:H4'	30:0:1841:C:O5'	2.21	0.41
30:0:1873:G:C2'	30:0:1874:U:H5'	2.51	0.41
30:0:1890:U:H4'	30:0:2010:A:C6	2.56	0.41
30:0:1942:A:C1'	38:0:9044:HOH:O	2.69	0.41
30:0:2361:A:H2'	30:0:2362:A:C8	2.55	0.41
30:0:2479:A:H5''	38:0:4665:HOH:O	2.21	0.41
30:0:2689:A:H2'	30:0:2690:U:H5'	2.02	0.41
30:0:2756:U:N3	30:0:2896:A:H2	2.17	0.41
30:0:2864:U:C5	30:0:2865:G:C6	3.09	0.41
31:9:65:A:O2'	31:9:66:G:P	2.79	0.41
3:C:73:GLN:HG2	30:0:475:G:OP1	2.20	0.41
29:3:48:ASN:ND2	30:0:169:A:H1'	2.36	0.41
30:0:146:U:O2'	30:0:147:G:H5'	2.21	0.41
30:0:364:U:H2'	30:0:365:G:O4'	2.21	0.41
30:0:413:G:H2'	30:0:414:C:C6	2.55	0.41
30:0:424:C:C2	30:0:425:U:C5	3.09	0.41
30:0:426:G:H2'	30:0:427:C:O4'	2.19	0.41
30:0:580:A:O4'	30:0:1111:U:H4'	2.21	0.41
30:0:1175:G:H1'	30:0:1193:A:H2'	2.03	0.41
30:0:1819:G:H2'	30:0:1820:G:H5'	1.98	0.41
30:0:2722:G:N3	30:0:2761:A:C2	2.89	0.41
30:0:2780:C:H2'	30:0:2781:U:C6	2.56	0.41
2:B:24:PRO:HD3	38:B:8991:HOH:O	2.22	0.40
4:D:135:VAL:HG22	4:D:136:ARG:N	2.36	0.40
10:J:41:ALA:HB3	38:J:8865:HOH:O	2.19	0.40
11:K:125:ALA:C	11:K:127:ALA:H	2.29	0.40
14:N:82:TYR:CD2	14:N:82:TYR:C	2.99	0.40
19:S:38:ALA:O	19:S:42:GLU:HG3	2.21	0.40
25:Y:144:ARG:CZ	38:Y:8181:HOH:O	2.69	0.40
30:0:275:G:C2	30:0:376:C:N3	2.88	0.40
30:0:334:G:C5	30:0:335:U:C5	3.09	0.40
30:0:772:G:H2'	30:0:773:A:O4'	2.21	0.40
30:0:1217:G:C2	30:0:1218:U:C2	3.09	0.40
30:0:1250:C:O2'	30:0:1251:C:H5'	2.21	0.40
30:0:2002:C:H2'	30:0:2003:U:H5'	2.03	0.40
3:C:138:VAL:O	3:C:234:VAL:HA	2.21	0.40
3:C:236:THR:CG2	3:C:239:ALA:H	2.34	0.40
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.54	0.40
8:H:27:PRO:HD3	8:H:123:ILE:HG22	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:167:GLY:O	13:M:171:ARG:HG3	2.21	0.40
15:O:32:ARG:HH21	15:O:35:LYS:HZ2	1.70	0.40
16:P:141:ILE:C	16:P:143:ALA:H	2.29	0.40
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.56	0.40
23:W:11:VAL:HG11	30:0:1086:A:C6	2.55	0.40
25:Y:152:LYS:HB3	25:Y:160:LYS:HG3	2.03	0.40
30:0:293:A:C2	30:0:294:C:C6	3.09	0.40
30:0:371:U:H2'	30:0:372:A:H8	1.86	0.40
30:0:423:A:C4	30:0:424:C:C6	3.09	0.40
30:0:725:C:C2'	30:0:726:C:O5'	2.69	0.40
30:0:921:G:H4'	30:0:924:G:N1	2.36	0.40
30:0:921:G:H4'	30:0:924:G:C6	2.56	0.40
30:0:1295:G:H2'	30:0:1296:A:C8	2.56	0.40
30:0:1587:U:C4	30:0:1588:G:C5	3.09	0.40
30:0:1669:G:H2'	30:0:1670:A:C8	2.56	0.40
30:0:1928:C:C2'	30:0:1929:G:H5'	2.51	0.40
30:0:2385:G:H2'	30:0:2386:U:C6	2.56	0.40
30:0:2846:C:H3'	38:0:7101:HOH:O	2.20	0.40
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.90	0.40
2:B:209:LYS:HB2	2:B:257:THR:O	2.21	0.40
3:C:226:GLY:HA3	30:0:1308:A:O4'	2.21	0.40
10:J:90:LYS:HB2	33:J:8802:CL:CL	2.58	0.40
11:K:81:ARG:HD3	11:K:87:ARG:NH2	2.36	0.40
13:M:42:ARG:HA	13:M:43:PRO:HD3	1.93	0.40
16:P:87:ARG:HG2	38:0:5961:HOH:O	2.22	0.40
17:Q:59:GLN:NE2	30:0:1018:A:H4'	2.36	0.40
23:W:139:GLY:O	23:W:141:HIS:HD2	2.04	0.40
25:Y:148:GLY:HA3	30:0:622:G:P	2.61	0.40
30:0:123:U:H2'	30:0:124:C:C6	2.55	0.40
30:0:303:C:N4	30:0:304:G:C6	2.89	0.40
30:0:319:A:H2'	30:0:320:G:C8	2.56	0.40
30:0:549:A:C6	30:0:550:C:C4	3.10	0.40
30:0:1182:C:H1'	30:0:1192:A:C8	2.41	0.40
30:0:1198:U:H1'	30:0:1201:C:H5	1.86	0.40
30:0:1205:U:H2'	30:0:1205:U:O2	2.21	0.40
30:0:1375:A:C2'	30:0:1376:G:H5'	2.51	0.40
30:0:1947:G:OP1	30:0:1971:G:N7	2.54	0.40
30:0:2765:C:H2'	30:0:2766:A:C8	2.56	0.40
30:0:2831:C:H2'	30:0:2832:C:O4'	2.22	0.40
1:A:109:GLU:HG2	1:A:116:GLY:N	2.36	0.40
6:F:56:PRO:HB2	6:F:58:GLU:OE1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:30:ARG:HD3	30:0:164:G:H4'	2.04	0.40
20:T:21:LYS:HA	20:T:24:ARG:HG3	2.04	0.40
23:W:108:ARG:HG3	23:W:114:PRO:HG3	2.03	0.40
25:Y:187:VAL:HG13	25:Y:205:ILE:HA	2.02	0.40
28:2:41:HIS:CD2	28:2:44:ARG:H	2.31	0.40
30:0:27:U:H5	38:0:5902:HOH:O	2.04	0.40
30:0:272:A:N1	30:0:369:G:H5'	2.35	0.40
30:0:545:G:C8	30:0:545:G:C5'	2.95	0.40
30:0:803:C:H2'	30:0:804:C:H6	1.87	0.40
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.40
30:0:1167:G:O2'	30:0:1168:C:H5'	2.22	0.40
30:0:1386:G:O2'	30:0:1387:G:H5'	2.22	0.40
30:0:1931:A:H2'	30:0:1932:G:H5'	2.04	0.40
30:0:2118:A:C5	30:0:2470:A:C5	3.09	0.40
30:0:2437:A:H2'	30:0:2438:G:C8	2.57	0.40
30:0:2802:C:H2'	30:0:2803:C:H6	1.85	0.40
30:0:2887:G:H2'	30:0:2888:U:O4'	2.22	0.40
31:9:24:U:H3'	31:9:24:U:H6	1.87	0.40
7:G:64:ASN:N	7:G:64:ASN:HD22	2.18	0.40
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.56	0.40
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.22	0.40
16:P:104:LYS:HE2	16:P:138:GLU:OE2	2.20	0.40
18:R:46:TYR:O	18:R:50:VAL:HG23	2.22	0.40
18:R:132:ARG:CZ	38:R:8987:HOH:O	2.70	0.40
20:T:49:GLU:OE2	20:T:97:ARG:HD2	2.22	0.40
25:Y:133:HIS:HD2	38:Y:8150:HOH:O	2.04	0.40
26:Z:50:VAL:O	26:Z:54:GLU:HG3	2.21	0.40
30:0:365:G:C6	30:0:366:U:C4	3.09	0.40
30:0:461:C:N3	30:0:479:G:H5'	2.36	0.40
30:0:820:G:H5'	30:0:821:U:H5'	2.02	0.40
30:0:1102:C:H4'	38:0:9561:HOH:O	2.20	0.40
30:0:1189:A:H1'	30:0:1209:C:H1'	2.02	0.40
30:0:1191:A:H2	30:0:1206:U:H3	1.69	0.40
30:0:1207:A:H5'	30:0:1208:C:OP2	2.21	0.40
30:0:1342:C:H2'	30:0:1343:C:C5'	2.47	0.40
30:0:1589:G:H4'	38:0:6875:HOH:O	2.20	0.40
30:0:2133:U:H4'	30:0:2134:G:H5'	2.02	0.40
30:0:2304:G:C6	30:0:2305:A:C5	3.10	0.40
30:0:2346:C:O5'	30:0:2346:C:C6	2.74	0.40
30:0:2543:G:H2'	30:0:2544:G:O4'	2.21	0.40
30:0:2712:G:P	38:0:5233:HOH:O	2.79	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%)	211 (90%)	22 (9%)	2 (1%)	14	28
2	B	335/338 (99%)	309 (92%)	21 (6%)	5 (2%)	8	15
3	C	244/246 (99%)	228 (93%)	16 (7%)	0	100	100
4	D	134/177 (76%)	110 (82%)	22 (16%)	2 (2%)	8	15
5	E	170/178 (96%)	160 (94%)	9 (5%)	1 (1%)	21	38
6	F	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	7	14
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	141 (90%)	14 (9%)	1 (1%)	21	38
9	I	68/162 (42%)	53 (78%)	13 (19%)	2 (3%)	3	6
10	J	140/145 (97%)	131 (94%)	8 (6%)	1 (1%)	18	34
11	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
12	L	141/165 (86%)	125 (89%)	13 (9%)	3 (2%)	5	11
13	M	192/196 (98%)	181 (94%)	10 (5%)	1 (0%)	24	43
14	N	184/187 (98%)	164 (89%)	16 (9%)	4 (2%)	5	10
15	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
16	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11	22
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
20	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	14	28
21	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
22	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	7	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	W	152/154 (99%)	146 (96%)	6 (4%)	0	100	100
24	X	80/92 (87%)	73 (91%)	5 (6%)	2 (2%)	4	8
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	62 (87%)	9 (13%)	0	100	100
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3705/4472 (83%)	3432 (93%)	244 (7%)	29 (1%)	16	30

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
8	H	19	ARG
10	J	5	GLU
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
2	B	184	ASP
9	I	107	LYS
12	L	149	ARG
14	N	162	ASP
1	A	34	ASP
2	B	34	GLY
6	F	101	ALA
12	L	80	ASP
2	B	2	GLN
2	B	245	SER
4	D	56	ARG
12	L	21	ARG
20	T	53	GLY
24	X	87	ALA
4	D	137	PRO
6	F	100	ASP
24	X	70	ILE
22	V	39	ALA
2	B	185	GLY
17	Q	78	GLY
5	E	44	GLY
9	I	83	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	88	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	164 (92%)	15 (8%)	10	19
2	B	282/283 (100%)	262 (93%)	20 (7%)	13	25
3	C	193/193 (100%)	177 (92%)	16 (8%)	10	19
4	D	117/148 (79%)	112 (96%)	5 (4%)	26	47
5	E	152/156 (97%)	148 (97%)	4 (3%)	40	63
6	F	93/94 (99%)	92 (99%)	1 (1%)	65	79
7	G	27/282 (10%)	25 (93%)	2 (7%)	13	24
8	H	134/145 (92%)	128 (96%)	6 (4%)	24	46
9	I	58/130 (45%)	58 (100%)	0	100	100
10	J	118/121 (98%)	112 (95%)	6 (5%)	21	40
11	K	106/106 (100%)	104 (98%)	2 (2%)	50	70
12	L	113/127 (89%)	108 (96%)	5 (4%)	25	47
13	M	158/160 (99%)	153 (97%)	5 (3%)	34	58
14	N	149/150 (99%)	144 (97%)	5 (3%)	32	57
15	O	93/94 (99%)	92 (99%)	1 (1%)	65	79
16	P	113/117 (97%)	108 (96%)	5 (4%)	25	47
17	Q	79/80 (99%)	75 (95%)	4 (5%)	21	40
18	R	117/122 (96%)	110 (94%)	7 (6%)	17	32
19	S	71/74 (96%)	70 (99%)	1 (1%)	59	75
20	T	105/106 (99%)	99 (94%)	6 (6%)	18	35
21	U	44/53 (83%)	44 (100%)	0	100	100
22	V	51/57 (90%)	50 (98%)	1 (2%)	48	69
23	W	130/130 (100%)	125 (96%)	5 (4%)	29	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	X	66/74 (89%)	63 (96%)	3 (4%)	24	46
25	Y	120/196 (61%)	114 (95%)	6 (5%)	22	42
26	Z	60/94 (64%)	59 (98%)	1 (2%)	53	71
27	1	46/47 (98%)	45 (98%)	1 (2%)	45	67
28	2	42/46 (91%)	41 (98%)	1 (2%)	43	65
29	3	79/79 (100%)	77 (98%)	2 (2%)	42	64
All	All	3095/3646 (85%)	2959 (96%)	136 (4%)	25	47

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	26	ASP
1	A	33	GLU
1	A	36	ASP
1	A	38	ILE
1	A	68	ILE
1	A	69	LEU
1	A	94	LEU
1	A	131	HIS
1	A	165	THR
1	A	175	LYS
1	A	179	MET
1	A	192	VAL
1	A	206	ARG
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	16	ARG
2	B	27	ASN
2	B	51	VAL
2	B	53	LEU
2	B	71	VAL
2	B	88	GLU
2	B	97	LEU
2	B	98	THR
2	B	140	LEU
2	B	149	ASP
2	B	162	MET
2	B	175	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	190	MET
2	B	195	ARG
2	B	254	GLN
2	B	257	THR
2	B	265	LEU
2	B	280	VAL
3	C	78	ARG
3	C	91	PRO
3	C	94	THR
3	C	95	GLU
3	C	101	ASP
3	C	115	LEU
3	C	132	ASP
3	C	136	VAL
3	C	151	GLN
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	243	VAL
4	D	24	HIS
4	D	48	MET
4	D	50	VAL
4	D	137	PRO
4	D	172	VAL
5	E	53	GLU
5	E	86	VAL
5	E	102	VAL
5	E	156	ASP
6	F	12	LEU
7	G	72	ASP
7	G	73	ASP
8	H	21	GLU
8	H	62	HIS
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
10	J	39	VAL
10	J	46	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	52	GLN
10	J	74	ARG
10	J	127	ILE
10	J	130	VAL
11	K	10	GLN
11	K	98	VAL
12	L	37	LYS
12	L	43	HIS
12	L	104	ASP
12	L	114	VAL
12	L	140	VAL
13	M	46	LEU
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	164	THR
14	N	26	LEU
14	N	49	THR
14	N	101	VAL
14	N	127	LEU
14	N	139	TRP
15	O	96	VAL
16	P	16	VAL
16	P	21	VAL
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	16	ASN
17	Q	18	PRO
17	Q	57	ASP
18	R	13	THR
18	R	39	THR
18	R	82	GLU
18	R	119	VAL
18	R	132	ARG
18	R	143	VAL
18	R	150	PRO
19	S	44	GLN
20	T	39	ASN
20	T	48	VAL
20	T	71	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
22	V	12	THR
23	W	4	LEU
23	W	26	ILE
23	W	35	VAL
23	W	52	VAL
23	W	146	ILE
24	X	52	PRO
24	X	72	VAL
24	X	82	GLU
25	Y	95	THR
25	Y	154	ARG
25	Y	189	ASN
25	Y	191	ASP
25	Y	203	VAL
25	Y	235	GLU
26	Z	68	GLU
27	1	14	THR
28	2	18	ASN
29	3	14	CYS
29	3	56	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	92	ASN
1	A	199	HIS
2	B	27	ASN
2	B	106	HIS
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	243	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
3	C	73	GLN
3	C	129	HIS
4	D	47	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	85	GLN
4	D	103	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	40	GLN
8	H	59	GLN
8	H	62	HIS
8	H	158	ASN
10	J	25	GLN
10	J	52	GLN
10	J	107	ASN
10	J	142	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
11	K	101	ASN
12	L	18	HIS
12	L	41	HIS
13	M	14	ASN
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	93	GLN
14	N	107	ASN
14	N	132	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	40	HIS
17	Q	59	GLN
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	53	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	S	55	GLN
20	T	37	GLN
20	T	39	ASN
20	T	73	HIS
21	U	39	ASN
21	U	48	ASN
22	V	60	GLN
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	133	HIS
25	Y	134	HIS
25	Y	153	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	20	HIS
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	235 (8%)	18 (0%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	251 (8%)	19 (0%)

All (251) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	169	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	200	C
30	0	204	A
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	368	C
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	746	A
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	884	C
30	0	885	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1124	A
30	0	1130	U
30	0	1151	G
30	0	1165	G
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1535	G
30	0	1562	C
30	0	1592	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1605	G
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	1710	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
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	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1968	A
30	0	1971	G
30	0	1973	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2238	A
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2465	A
30	0	2467	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2637	A
30	0	2638	G
30	0	2649	A
30	0	2650	U
30	0	2664	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2681	A
30	0	2682	C
30	0	2718	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	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
31	9	114	G
31	9	122	C

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	129	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	603	A
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1237	U
30	0	1352	A
30	0	1377	C
30	0	1506	U
30	0	1685	A
30	0	1979	G
30	0	2467	A
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PSU	0	2621	30	18,21,22	1.57	2 (11%)	21,30,33	1.36	3 (14%)
30	1MA	0	628	35,30	21,25,26	0.72	1 (4%)	30,37,40	0.69	1 (3%)
30	OMG	0	2588	30	23,26,27	0.29	0	32,38,41	0.36	0
30	UR3	0	2619	30	19,22,23	0.42	0	26,32,35	0.69	1 (3%)
30	OMU	0	2587	30	19,22,23	0.30	0	25,31,34	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	35,30	-	2/7/25/26	0/3/3/3
30	OMG	0	2588	30	-	0/9/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	5.17	1.43	1.36
30	0	2621	PSU	C6-C5	2.86	1.38	1.35
30	0	628	1MA	C6-N6	2.49	1.34	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C6-C5-C4	3.53	120.56	118.17
30	0	2621	PSU	C6-N1-C2	-3.01	119.90	122.69
30	0	2621	PSU	O2-C2-N1	2.96	125.83	122.79
30	0	2619	UR3	C4-N3-C2	2.77	126.81	124.58
30	0	628	1MA	N1-C2-N3	2.73	129.24	126.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8
30	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	3.05	201 (84%) 0 0	22, 47, 83, 108	0
2	B	337/338 (99%)	2.83	258 (76%) 0 0	25, 51, 79, 90	0
3	C	246/246 (100%)	1.64	70 (28%) 1 1	19, 42, 65, 81	0
4	D	140/177 (79%)	3.47	118 (84%) 0 0	58, 101, 124, 135	0
5	E	172/178 (96%)	2.75	124 (72%) 0 0	42, 66, 89, 94	0
6	F	119/120 (99%)	2.51	75 (63%) 0 0	44, 68, 96, 114	0
7	G	29/348 (8%)	3.00	25 (86%) 0 0	71, 91, 100, 102	0
8	H	160/177 (90%)	2.90	125 (78%) 0 0	55, 73, 100, 106	0
9	I	70/162 (43%)	4.61	68 (97%) 0 0	127, 145, 163, 164	0
10	J	142/145 (97%)	2.31	89 (62%) 0 0	34, 51, 71, 94	0
11	K	132/132 (100%)	2.88	102 (77%) 0 0	29, 47, 68, 77	0
12	L	145/165 (87%)	2.30	79 (54%) 0 0	26, 62, 111, 125	0
13	M	194/196 (98%)	2.25	105 (54%) 0 0	24, 38, 55, 62	0
14	N	186/187 (99%)	2.36	101 (54%) 0 0	40, 65, 111, 120	0
15	O	115/116 (99%)	1.51	24 (20%) 2 2	34, 49, 67, 76	0
16	P	143/149 (95%)	3.23	121 (84%) 0 0	34, 51, 67, 75	0
17	Q	95/96 (98%)	1.77	34 (35%) 1 0	34, 45, 61, 74	0
18	R	150/155 (96%)	2.16	88 (58%) 0 0	28, 44, 64, 74	0
19	S	81/85 (95%)	2.36	48 (59%) 0 0	35, 53, 73, 86	0
20	T	119/120 (99%)	2.12	54 (45%) 0 0	34, 52, 80, 109	0
21	U	53/67 (79%)	3.08	44 (83%) 0 0	39, 54, 73, 82	0
22	V	65/71 (91%)	2.82	42 (64%) 0 0	42, 66, 113, 122	0
23	W	154/154 (100%)	1.90	65 (42%) 0 0	36, 49, 67, 83	0
24	X	82/92 (89%)	2.82	64 (78%) 0 0	37, 57, 82, 98	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%)	1.70	45 (31%) 1 1	23, 44, 65, 87	0
26	Z	73/116 (62%)	3.47	61 (83%) 0 0	47, 66, 82, 97	0
27	1	56/57 (98%)	2.14	30 (53%) 0 0	21, 28, 35, 45	0
28	2	46/50 (92%)	2.96	40 (86%) 0 0	28, 58, 88, 95	0
29	3	92/92 (100%)	2.17	49 (53%) 0 0	34, 54, 67, 83	0
30	0	2749/2923 (94%)	2.37	1690 (61%) 0 0	19, 43, 89, 167	0
31	9	122/122 (100%)	2.02	56 (45%) 0 0	37, 67, 86, 146	0
All	All	6646/7517 (88%)	2.45	4095 (61%) 0 0	19, 49, 99, 167	0

All (4095) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	113	SER	11.8
9	I	71	ALA	10.9
9	I	74	ILE	10.7
9	I	100	VAL	9.5
22	V	1	THR	9.3
9	I	104	ALA	8.3
4	D	63	ILE	8.3
4	D	19	GLU	8.3
2	B	1	PRO	8.1
4	D	134	LEU	8.0
20	T	119	ALA	7.8
26	Z	34	SER	7.8
21	U	51	TRP	7.7
16	P	79	SER	7.5
9	I	124	VAL	7.3
4	D	93	LEU	7.3
4	D	88	LEU	7.2
31	9	1	U	7.1
26	Z	42	TYR	7.1
4	D	91	ALA	7.1
21	U	52	THR	7.1
4	D	102	GLY	6.9
22	V	40	PRO	6.8
1	A	80	LEU	6.7
12	L	97	VAL	6.6
5	E	45	ASP	6.5
16	P	68	LYS	6.5
3	C	62	GLY	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	2	19	SER	6.5
30	0	2569	A	6.4
4	D	18	ILE	6.4
9	I	114	TYR	6.3
9	I	83	GLY	6.3
7	G	73	ASP	6.3
2	B	18	ARG	6.3
30	0	1161	A	6.3
22	V	43	PRO	6.3
8	H	65	LEU	6.3
14	N	137	ALA	6.3
22	V	39	ALA	6.3
2	B	119	HIS	6.2
9	I	120	ALA	6.2
16	P	143	ALA	6.2
9	I	118	ASN	6.1
9	I	119	ALA	6.1
22	V	31	ARG	6.1
16	P	55	LYS	6.1
8	H	71	SER	6.1
4	D	101	THR	6.1
14	N	75	THR	6.1
4	D	135	VAL	6.0
30	0	2865	G	6.0
26	Z	44	ARG	6.0
28	2	49	GLU	6.0
1	A	43	VAL	6.0
16	P	76	GLY	6.0
26	Z	43	GLY	6.0
4	D	174	VAL	6.0
8	H	72	ALA	5.9
26	Z	62	ALA	5.9
26	Z	106	SER	5.9
26	Z	49	ARG	5.9
30	0	1785	G	5.9
9	I	112	LEU	5.8
1	A	200	PRO	5.8
9	I	128	THR	5.8
11	K	58	THR	5.8
30	0	2755	G	5.8
4	D	75	LEU	5.8
4	D	74	THR	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	78	ALA	5.8
16	P	116	SER	5.7
26	Z	39	GLY	5.7
14	N	159	TYR	5.7
4	D	133	ASN	5.7
30	0	2736	U	5.7
30	0	1701	A	5.7
26	Z	47	ARG	5.7
9	I	73	LEU	5.7
11	K	85	GLY	5.7
1	A	74	VAL	5.7
24	X	10	VAL	5.7
30	0	2725	G	5.7
9	I	69	PRO	5.6
7	G	12	ILE	5.6
9	I	103	ILE	5.6
9	I	116	LEU	5.6
30	0	798	G	5.6
30	0	1600	G	5.6
1	A	75	GLY	5.6
1	A	91	GLY	5.6
1	A	196	ALA	5.6
4	D	66	GLY	5.6
30	0	787	G	5.5
30	0	1979	G	5.5
16	P	140	TYR	5.5
6	F	97	ALA	5.5
30	0	2867	G	5.5
1	A	68	ILE	5.5
9	I	67	VAL	5.5
26	Z	46	SER	5.5
30	0	1547	A	5.5
2	B	334	SER	5.5
30	0	1601	G	5.4
4	D	104	PHE	5.4
16	P	94	TRP	5.4
9	I	115	ASP	5.4
2	B	109	LEU	5.4
6	F	44	SER	5.4
12	L	24	ALA	5.4
2	B	118	ASP	5.4
30	0	1786	C	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2728	C	5.4
24	X	22	ASN	5.4
9	I	117	THR	5.4
24	X	58	ALA	5.4
1	A	69	LEU	5.4
6	F	20	LEU	5.4
8	H	54	VAL	5.4
4	D	139	TYR	5.4
30	0	2570	G	5.3
30	0	272	A	5.3
5	E	158	ASP	5.3
9	I	107	LYS	5.3
2	B	31	SER	5.3
8	H	133	GLY	5.3
22	V	34	GLN	5.3
1	A	31	LYS	5.3
4	D	128	LEU	5.3
4	D	10	PHE	5.2
5	E	154	ILE	5.2
8	H	90	LEU	5.2
1	A	89	ALA	5.2
6	F	100	ASP	5.2
8	H	174	LEU	5.2
30	0	786	G	5.2
30	0	1561	U	5.2
30	0	1183	C	5.2
16	P	98	ILE	5.2
9	I	77	GLU	5.2
4	D	23	VAL	5.2
30	0	1525	G	5.2
30	0	1819	G	5.2
9	I	111	LEU	5.2
5	E	168	ILE	5.2
30	0	2525	G	5.1
30	0	2863	G	5.1
1	A	40	GLY	5.1
8	H	52	LEU	5.1
24	X	87	ALA	5.1
30	0	1458	A	5.1
12	L	99	GLU	5.1
26	Z	38	PHE	5.1
30	0	788	A	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	37	ALA	5.1
8	H	127	ALA	5.1
2	B	337	GLY	5.1
18	R	106	GLY	5.1
1	A	229	ALA	5.0
14	N	145	ALA	5.0
16	P	62	ALA	5.0
16	P	86	ALA	5.0
14	N	158	LEU	5.0
30	0	2100	A	5.0
30	0	1540	G	5.0
30	0	2851	G	5.0
30	0	2685	C	5.0
2	B	92	TYR	5.0
16	P	58	SER	5.0
2	B	161	VAL	5.0
9	I	123	VAL	5.0
8	H	132	ALA	5.0
2	B	144	THR	5.0
16	P	89	ASN	5.0
31	9	24	U	5.0
11	K	117	VAL	5.0
30	0	2344	G	5.0
2	B	91	PRO	5.0
5	E	172	PRO	5.0
2	B	336	GLN	5.0
5	E	117	THR	5.0
26	Z	58	ASN	5.0
26	Z	81	CYS	5.0
30	0	1171	A	5.0
1	A	29	HIS	5.0
2	B	47	GLY	5.0
9	I	85	GLY	5.0
2	B	147	VAL	5.0
14	N	150	TYR	4.9
21	U	8	TYR	4.9
8	H	119	ALA	4.9
14	N	168	LEU	4.9
24	X	14	LEU	4.9
1	A	105	VAL	4.9
2	B	69	VAL	4.9
8	H	76	LEU	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2571	C	4.9
30	0	2737	C	4.9
30	0	1409	G	4.9
1	A	78	ASP	4.9
30	0	860	U	4.9
30	0	2756	U	4.9
2	B	117	GLU	4.9
22	V	38	GLY	4.9
4	D	106	PHE	4.9
1	A	138	VAL	4.9
8	H	61	ARG	4.9
4	D	85	GLN	4.9
2	B	4	SER	4.9
30	0	2585	G	4.9
2	B	278	PRO	4.9
16	P	2	ASP	4.8
17	Q	2	SER	4.8
30	0	1567	G	4.8
9	I	109	PRO	4.8
11	K	95	ALA	4.8
9	I	70	THR	4.8
29	3	62	THR	4.8
16	P	56	GLY	4.8
30	0	1965	C	4.8
2	B	330	VAL	4.8
24	X	85	VAL	4.8
30	0	1165	G	4.8
11	K	3	ALA	4.8
5	E	7	ILE	4.8
1	A	36	ASP	4.8
28	2	48	ASP	4.8
2	B	43	GLY	4.8
4	D	165	PHE	4.8
1	A	158	VAL	4.8
6	F	118	LEU	4.8
30	0	1537	C	4.8
14	N	165	ALA	4.8
26	Z	79	TRP	4.8
4	D	89	PRO	4.8
6	F	115	VAL	4.8
16	P	75	LYS	4.7
30	0	1702	U	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2017	U	4.7
1	A	198	ASP	4.7
28	2	47	THR	4.7
16	P	85	GLY	4.7
2	B	142	LEU	4.7
7	G	71	LEU	4.7
9	I	132	VAL	4.7
11	K	11	GLY	4.7
30	0	1551	C	4.7
8	H	98	LEU	4.7
25	Y	236	VAL	4.7
30	0	2754	G	4.7
8	H	53	ILE	4.7
11	K	94	ALA	4.7
13	M	1	ALA	4.7
1	A	161	GLY	4.7
8	H	161	THR	4.7
13	M	6	SER	4.7
30	0	1596	U	4.7
4	D	16	PRO	4.7
9	I	95	LEU	4.7
1	A	211	LYS	4.7
21	U	46	ALA	4.7
5	E	160	ARG	4.7
10	J	64	GLY	4.7
13	M	194	GLY	4.7
30	0	1709	G	4.7
1	A	110	SER	4.7
2	B	53	LEU	4.7
14	N	136	LEU	4.7
23	W	66	LEU	4.7
16	P	101	GLN	4.7
11	K	14	LYS	4.7
11	K	47	ALA	4.6
13	M	72	ALA	4.6
30	0	799	C	4.6
30	0	1651	C	4.6
30	0	1787	C	4.6
16	P	78	GLY	4.6
1	A	187	PRO	4.6
30	0	1641	A	4.6
30	0	2739	A	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	47	VAL	4.6
14	N	43	VAL	4.6
30	0	1800	G	4.6
25	Y	169	ARG	4.6
30	0	1454	U	4.6
12	L	82	ALA	4.6
2	B	204	GLY	4.6
4	D	107	GLY	4.6
8	H	81	GLY	4.6
30	0	1200	A	4.6
30	0	1598	A	4.6
30	0	1710	A	4.6
2	B	7	ARG	4.6
1	A	227	ASP	4.6
9	I	84	SER	4.6
14	N	163	PHE	4.6
6	F	72	VAL	4.6
30	0	2104	C	4.6
9	I	72	GLU	4.6
9	I	134	ILE	4.6
10	J	141	ALA	4.6
30	0	827	A	4.6
2	B	292	GLY	4.6
4	D	72	LYS	4.6
14	N	50	LEU	4.6
30	0	2734	G	4.6
2	B	70	PRO	4.6
4	D	172	VAL	4.6
2	B	5	ARG	4.5
8	H	164	CYS	4.5
30	0	2886	C	4.5
30	0	790	A	4.5
30	0	1626	A	4.5
14	N	169	PRO	4.5
5	E	107	PHE	4.5
9	I	91	PHE	4.5
14	N	160	SER	4.5
2	B	123	ALA	4.5
30	0	1467	C	4.5
8	H	116	MET	4.5
30	0	1716	A	4.5
2	B	19	SER	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	39	SER	4.5
3	C	171	GLU	4.5
5	E	104	ILE	4.5
5	E	138	ILE	4.5
11	K	110	LYS	4.5
11	K	128	ALA	4.5
30	0	1571	G	4.5
30	0	1828	G	4.5
26	Z	61	HIS	4.5
20	T	51	LEU	4.5
2	B	282	GLY	4.5
8	H	153	PHE	4.5
30	0	1517	C	4.5
11	K	81	ARG	4.5
5	E	97	VAL	4.5
5	E	70	GLU	4.5
24	X	88	GLU	4.5
30	0	128	A	4.5
2	B	287	TYR	4.5
14	N	166	ALA	4.5
15	O	41	ALA	4.5
1	A	173	GLY	4.5
1	A	202	GLY	4.5
26	Z	80	GLN	4.5
30	0	960	G	4.5
30	0	1373	G	4.5
16	P	120	ARG	4.5
1	A	42	VAL	4.5
1	A	192	VAL	4.5
10	J	130	VAL	4.5
1	A	213	LYS	4.4
30	0	789	C	4.4
30	0	1803	C	4.4
30	0	1862	C	4.4
2	B	55	ASN	4.4
12	L	75	LEU	4.4
30	0	1603	A	4.4
30	0	1729	A	4.4
16	P	127	GLY	4.4
13	M	67	VAL	4.4
22	V	2	VAL	4.4
4	D	166	ILE	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	P	49	ILE	4.4
26	Z	85	ASP	4.4
5	E	155	ASN	4.4
2	B	178	ALA	4.4
8	H	16	ALA	4.4
14	N	154	LEU	4.4
30	0	2526	C	4.4
30	0	2726	U	4.4
30	0	2727	A	4.4
21	U	35	LYS	4.4
1	A	37	VAL	4.4
1	A	82	VAL	4.4
2	B	115	VAL	4.4
30	0	1541	G	4.4
30	0	2753	G	4.4
2	B	197	GLY	4.4
24	X	52	PRO	4.4
2	B	2	GLN	4.4
9	I	127	CYS	4.4
30	0	1186	C	4.4
3	C	61	PHE	4.4
1	A	55	VAL	4.4
1	A	124	VAL	4.4
30	0	1492	A	4.4
30	0	2483	A	4.4
2	B	308	LEU	4.4
24	X	23	HIS	4.4
6	F	101	ALA	4.4
8	H	67	ALA	4.4
2	B	116	PRO	4.4
2	B	121	PRO	4.4
13	M	75	ARG	4.4
26	Z	64	PRO	4.4
27	1	4	GLY	4.4
12	L	125	PHE	4.4
22	V	41	GLU	4.4
30	0	878	G	4.4
30	0	1751	G	4.4
30	0	1827	G	4.4
30	0	1901	G	4.4
30	0	2884	G	4.4
31	9	94	G	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	57	VAL	4.4
21	U	22	VAL	4.4
9	I	110	ASP	4.3
30	0	1192	A	4.3
9	I	130	LEU	4.3
1	A	160	ALA	4.3
5	E	13	ALA	4.3
1	A	231	LYS	4.3
22	V	13	PRO	4.3
2	B	219	GLY	4.3
5	E	102	VAL	4.3
26	Z	45	VAL	4.3
30	0	817	G	4.3
14	N	186	LEU	4.3
17	Q	14	LEU	4.3
30	0	1640	C	4.3
30	0	1826	C	4.3
1	A	20	SER	4.3
8	H	29	SER	4.3
29	3	60	LYS	4.3
30	0	1591	A	4.3
30	0	2568	A	4.3
2	B	138	GLY	4.3
21	U	17	THR	4.3
24	X	12	ILE	4.3
30	0	138	U	4.3
30	0	863	G	4.3
30	0	1175	G	4.3
30	0	1491	G	4.3
30	0	1507	C	4.3
30	0	1660	G	4.3
30	0	1809	G	4.3
30	0	2237	G	4.3
30	0	2537	G	4.3
30	0	2709	G	4.3
6	F	99	THR	4.3
4	D	27	ILE	4.3
4	D	44	ILE	4.3
1	A	175	LYS	4.3
21	U	39	ASN	4.3
3	C	63	SER	4.3
13	M	30	GLU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	309	VAL	4.3
30	0	1378	G	4.3
30	0	1648	G	4.3
30	0	2018	A	4.3
10	J	16	ASP	4.2
6	F	23	ALA	4.2
20	T	118	SER	4.2
21	U	31	PHE	4.2
9	I	126	THR	4.2
5	E	159	VAL	4.2
8	H	97	VAL	4.2
30	0	1405	U	4.2
30	0	1505	U	4.2
28	2	39	ARG	4.2
30	0	1750	C	4.2
30	0	2868	C	4.2
30	0	1162	G	4.2
30	0	1177	A	4.2
30	0	1728	G	4.2
30	0	2869	G	4.2
6	F	1	PRO	4.2
18	R	1	GLY	4.2
19	S	60	GLY	4.2
1	A	99	ILE	4.2
10	J	144	THR	4.2
11	K	74	VAL	4.2
12	L	76	LEU	4.2
30	0	1724	U	4.2
30	0	2016	U	4.2
1	A	114	ASP	4.2
12	L	100	ALA	4.2
13	M	79	ALA	4.2
18	R	16	ALA	4.2
30	0	1763	C	4.2
30	0	1459	A	4.2
30	0	2741	A	4.2
2	B	40	GLY	4.2
8	H	64	SER	4.2
8	H	163	SER	4.2
12	L	148	GLU	4.2
30	0	1802	G	4.2
30	0	1944	G	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	51	VAL	4.2
12	L	73	VAL	4.2
26	Z	50	VAL	4.2
29	3	65	THR	4.2
2	B	145	HIS	4.2
11	K	109	LEU	4.2
10	J	57	TYR	4.2
30	0	10	U	4.2
30	0	1890	U	4.2
30	0	2042	U	4.2
23	W	32	CYS	4.2
9	I	80	PHE	4.2
30	0	1184	C	4.2
30	0	1853	C	4.2
30	0	1886	A	4.2
30	0	1946	C	4.2
30	0	2500	C	4.2
30	0	2538	A	4.2
1	A	30	ARG	4.2
4	D	22	VAL	4.2
11	K	68	VAL	4.2
30	0	834	G	4.2
1	A	181	ALA	4.1
16	P	34	ALA	4.1
16	P	54	LYS	4.1
24	X	39	LYS	4.1
4	D	69	ILE	4.1
13	M	180	SER	4.1
5	E	87	PHE	4.1
5	E	91	PHE	4.1
1	A	177	HIS	4.1
16	P	105	LEU	4.1
28	2	14	LEU	4.1
30	0	784	A	4.1
30	0	791	A	4.1
30	0	1514	C	4.1
30	0	1693	A	4.1
30	0	1981	A	4.1
30	0	2035	C	4.1
30	0	2686	C	4.1
30	0	1723	G	4.1
30	0	1951	G	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	179	MET	4.1
1	A	218	ASN	4.1
19	S	16	ASN	4.1
10	J	6	PHE	4.1
16	P	61	ARG	4.1
2	B	23	THR	4.1
2	B	146	THR	4.1
9	I	92	VAL	4.1
22	V	27	LEU	4.1
2	B	155	PRO	4.1
11	K	37	TYR	4.1
19	S	2	TRP	4.1
30	0	1824	C	4.1
30	0	1856	C	4.1
30	0	2702	A	4.1
30	0	2792	A	4.1
10	J	51	GLU	4.1
14	N	112	GLY	4.1
18	R	53	GLY	4.1
29	3	57	GLY	4.1
30	0	2740	G	4.1
2	B	38	VAL	4.1
5	E	169	THR	4.1
12	L	1	THR	4.1
30	0	785	U	4.1
30	0	1130	U	4.1
8	H	9	TYR	4.1
1	A	6	GLY	4.1
16	P	82	GLY	4.1
30	0	1754	A	4.1
30	0	1822	A	4.1
4	D	17	ARG	4.1
30	0	1715	C	4.1
16	P	108	LEU	4.1
2	B	300	SER	4.1
30	0	1190	G	4.0
2	B	24	PRO	4.0
14	N	74	PRO	4.0
26	Z	98	PRO	4.0
4	D	78	GLU	4.0
14	N	152	GLU	4.0
2	B	199	TYR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	105	TYR	4.0
27	1	3	ALA	4.0
26	Z	70	ARG	4.0
4	D	132	VAL	4.0
30	0	886	A	4.0
30	0	1559	A	4.0
31	9	51	A	4.0
2	B	98	THR	4.0
30	0	1562	C	4.0
4	D	20	LYS	4.0
26	Z	84	CYS	4.0
4	D	81	GLU	4.0
30	0	1195	G	4.0
30	0	1489	G	4.0
30	0	2848	G	4.0
2	B	189	ALA	4.0
20	T	14	ALA	4.0
30	0	1548	U	4.0
1	A	23	TYR	4.0
2	B	303	GLY	4.0
23	W	55	GLY	4.0
1	A	67	LEU	4.0
14	N	56	ASP	4.0
11	K	31	VAL	4.0
18	R	5	SER	4.0
1	A	104	PRO	4.0
30	0	2248	C	4.0
2	B	125	GLU	4.0
8	H	21	GLU	4.0
9	I	122	GLU	4.0
1	A	236	GLY	4.0
11	K	60	GLY	4.0
18	R	91	LEU	4.0
20	T	91	LEU	4.0
30	0	2710	U	4.0
1	A	118	PHE	4.0
30	0	816	G	4.0
30	0	869	G	4.0
30	0	1608	G	4.0
30	0	1745	G	4.0
30	0	2748	G	4.0
4	D	21	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	X	72	VAL	4.0
27	1	13	THR	4.0
2	B	62	ARG	4.0
24	X	8	ARG	4.0
30	0	1485	A	4.0
30	0	1607	A	4.0
3	C	208	ALA	4.0
8	H	6	ALA	4.0
30	0	282	C	4.0
30	0	1725	C	4.0
30	0	2625	C	4.0
30	0	2729	C	4.0
16	P	119	TYR	4.0
6	F	8	VAL	4.0
12	L	108	VAL	4.0
30	0	1639	U	4.0
30	0	1825	U	4.0
30	0	1874	U	4.0
1	A	165	THR	3.9
8	H	89	THR	3.9
30	0	828	G	3.9
30	0	1546	G	3.9
1	A	156	ILE	3.9
11	K	53	ILE	3.9
22	V	46	ILE	3.9
1	A	210	GLY	3.9
30	0	1653	A	3.9
30	0	2896	A	3.9
6	F	49	PHE	3.9
11	K	64	MET	3.9
14	N	167	ASP	3.9
28	2	18	ASN	3.9
24	X	66	THR	3.9
20	T	10	SER	3.9
31	9	2	U	3.9
8	H	56	GLU	3.9
7	G	23	ILE	3.9
13	M	56	ALA	3.9
23	W	3	ALA	3.9
30	0	772	G	3.9
30	0	1160	G	3.9
30	0	1760	G	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2254	G	3.9
30	0	2730	G	3.9
2	B	8	LYS	3.9
4	D	53	LYS	3.9
23	W	62	LEU	3.9
12	L	25	GLY	3.9
10	J	79	PHE	3.9
4	D	129	ASP	3.9
26	Z	71	VAL	3.9
28	2	16	ASN	3.9
30	0	2015	A	3.9
30	0	2517	A	3.9
30	0	2854	A	3.9
30	0	2905	A	3.9
30	0	271	C	3.9
30	0	1574	C	3.9
30	0	1943	C	3.9
14	N	119	GLN	3.9
30	0	2864	U	3.9
5	E	108	LEU	3.9
6	F	12	LEU	3.9
8	H	139	ALA	3.9
9	I	108	HIS	3.9
11	K	32	ILE	3.9
18	R	87	ALA	3.9
11	K	25	GLY	3.9
13	M	80	GLY	3.9
13	M	191	GLY	3.9
14	N	135	VAL	3.9
27	1	27	TYR	3.9
30	0	1178	G	3.9
30	0	1933	G	3.9
30	0	1950	G	3.9
30	0	1970	G	3.9
4	D	131	THR	3.9
10	J	75	PRO	3.9
27	1	14	THR	3.9
16	P	102	ARG	3.9
30	0	1659	A	3.9
30	0	1804	A	3.9
16	P	90	SER	3.9
21	U	50	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	Y	235	GLU	3.9
2	B	106	HIS	3.9
13	M	163	LEU	3.9
16	P	122	LEU	3.9
30	0	1126	C	3.9
30	0	1196	C	3.9
30	0	1534	C	3.9
30	0	1700	C	3.9
30	0	2718	C	3.9
13	M	87	GLY	3.9
26	Z	36	GLY	3.9
30	0	864	U	3.9
30	0	1972	U	3.9
30	0	2732	U	3.9
30	0	2866	U	3.9
2	B	194	PHE	3.9
14	N	172	PHE	3.9
4	D	62	ASP	3.9
16	P	15	ASP	3.9
4	D	68	PRO	3.8
2	B	67	GLU	3.8
30	0	1552	G	3.8
30	0	1646	G	3.8
30	0	1649	G	3.8
30	0	1663	G	3.8
30	0	2025	G	3.8
30	0	2051	G	3.8
30	0	2731	G	3.8
30	0	2786	G	3.8
1	A	216	SER	3.8
8	H	7	SER	3.8
16	P	117	SER	3.8
30	0	129	A	3.8
30	0	1392	A	3.8
30	0	1413	A	3.8
30	0	1842	A	3.8
30	0	2885	A	3.8
30	0	2890	A	3.8
2	B	196	ALA	3.8
10	J	41	ALA	3.8
19	S	74	ALA	3.8
21	U	55	ALA	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	X	17	ALA	3.8
28	2	1	GLY	3.8
5	E	65	PHE	3.8
30	0	1984	U	3.8
12	L	91	VAL	3.8
16	P	121	ASP	3.8
20	T	13	ARG	3.8
23	W	78	ASP	3.8
26	Z	89	THR	3.8
9	I	75	LYS	3.8
28	2	3	LYS	3.8
16	P	48	ALA	3.8
4	D	26	GLY	3.8
20	T	60	GLY	3.8
30	0	1137	G	3.8
30	0	2738	G	3.8
30	0	2876	G	3.8
6	F	6	PHE	3.8
16	P	23	PHE	3.8
29	3	22	VAL	3.8
13	M	125	ARG	3.8
16	P	142	ASP	3.8
18	R	81	PRO	3.8
26	Z	95	PRO	3.8
30	0	858	U	3.8
30	0	2560	C	3.8
30	0	2767	C	3.8
2	B	335	ASN	3.8
5	E	167	TYR	3.8
12	L	44	GLU	3.8
12	L	60	GLU	3.8
16	P	138	GLU	3.8
7	G	26	MET	3.8
11	K	113	ILE	3.8
14	N	42	HIS	3.8
29	3	1	MET	3.8
2	B	37	GLY	3.8
5	E	44	GLY	3.8
5	E	79	GLY	3.8
3	C	65	ARG	3.8
11	K	98	VAL	3.8
28	2	43	ARG	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	K	79	PRO	3.8
30	0	509	A	3.8
30	0	814	G	3.8
30	0	1199	A	3.8
30	0	1393	A	3.8
30	0	1471	A	3.8
30	0	1475	G	3.8
30	0	1484	G	3.8
30	0	1789	G	3.8
30	0	2041	G	3.8
30	0	2102	G	3.8
30	0	2810	G	3.8
4	D	171	ASP	3.8
2	B	318	ASN	3.8
5	E	80	TRP	3.8
12	L	74	THR	3.8
2	B	44	TYR	3.8
30	0	1429	U	3.8
2	B	296	LEU	3.8
10	J	132	LEU	3.8
1	A	45	ILE	3.8
8	H	23	ILE	3.8
19	S	9	HIS	3.8
30	0	770	C	3.8
30	0	1208	C	3.8
30	0	2903	C	3.8
1	A	116	GLY	3.8
21	U	18	GLY	3.8
1	A	153	ARG	3.8
11	K	55	VAL	3.8
20	T	50	VAL	3.8
23	W	65	VAL	3.8
2	B	244	PRO	3.8
7	G	13	PRO	3.8
16	P	64	GLU	3.7
16	P	74	GLN	3.7
16	P	92	GLU	3.7
18	R	122	GLN	3.7
5	E	156	ASP	3.7
1	A	130	THR	3.7
1	A	184	THR	3.7
26	Z	57	MET	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	818	A	3.7
30	0	1504	A	3.7
8	H	95	HIS	3.7
21	U	42	LEU	3.7
6	F	111	ILE	3.7
30	0	2053	G	3.7
30	0	2774	U	3.7
1	A	111	SER	3.7
5	E	112	ALA	3.7
18	R	108	ALA	3.7
26	Z	90	GLY	3.7
30	0	1129	C	3.7
31	9	122	C	3.7
2	B	280	VAL	3.7
4	D	100	ASP	3.7
5	E	144	THR	3.7
6	F	25	ASP	3.7
11	K	7	ASP	3.7
27	1	12	ASN	3.7
30	0	1150	A	3.7
30	0	1942	A	3.7
30	0	1968	A	3.7
30	0	2757	A	3.7
1	A	172	ALA	3.7
1	A	230	SER	3.7
4	D	160	ALA	3.7
5	E	75	GLY	3.7
21	U	10	GLY	3.7
5	E	114	ARG	3.7
30	0	2032	U	3.7
30	0	1131	G	3.7
30	0	1410	G	3.7
30	0	2249	G	3.7
30	0	2494	G	3.7
30	0	2687	G	3.7
2	B	71	VAL	3.7
5	E	86	VAL	3.7
9	I	68	PRO	3.7
13	M	88	VAL	3.7
25	Y	146	PRO	3.7
30	0	1566	C	3.7
30	0	2695	C	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	46	THR	3.7
5	E	151	LEU	3.7
8	H	157	TYR	3.7
8	H	156	ALA	3.7
16	P	126	ALA	3.7
30	0	861	A	3.7
30	0	1978	A	3.7
10	J	70	PHE	3.7
2	B	54	VAL	3.7
6	F	98	VAL	3.7
30	0	1698	U	3.7
30	0	2052	U	3.7
3	C	67	GLN	3.7
5	E	149	GLU	3.7
30	0	1628	G	3.7
30	0	1704	G	3.7
30	0	1812	G	3.7
30	0	1814	G	3.7
30	0	2744	G	3.7
16	P	14	LEU	3.7
30	0	774	C	3.7
30	0	1000	C	3.7
30	0	1394	C	3.7
30	0	1536	C	3.7
30	0	1854	C	3.7
30	0	2287	C	3.7
30	0	2331	C	3.7
30	0	2487	C	3.7
30	0	2760	C	3.7
2	B	128	ILE	3.7
10	J	122	ASP	3.7
11	K	97	ILE	3.7
24	X	84	ILE	3.7
11	K	41	LYS	3.7
14	N	41	LYS	3.7
9	I	129	SER	3.7
12	L	96	VAL	3.7
14	N	8	VAL	3.7
30	0	1191	A	3.6
30	0	1630	A	3.6
30	0	1815	A	3.6
30	0	2490	A	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2649	A	3.6
30	0	2703	A	3.6
30	0	1599	U	3.6
13	M	77	HIS	3.6
16	P	12	ASP	3.6
19	S	6	LYS	3.6
5	E	34	TRP	3.6
26	Z	37	ARG	3.6
30	0	854	G	3.6
30	0	856	G	3.6
30	0	1604	G	3.6
30	0	1683	G	3.6
30	0	1805	G	3.6
30	0	1947	G	3.6
30	0	1971	G	3.6
30	0	2529	G	3.6
30	0	999	C	3.6
30	0	1404	C	3.6
30	0	1565	C	3.6
1	A	163	GLY	3.6
10	J	77	GLY	3.6
11	K	114	ALA	3.6
18	R	124	GLY	3.6
23	W	135	GLY	3.6
1	A	71	PRO	3.6
4	D	83	PHE	3.6
5	E	162	PHE	3.6
11	K	1	MET	3.6
16	P	25	PRO	3.6
21	U	20	MET	3.6
21	U	21	PHE	3.6
4	D	73	VAL	3.6
6	F	108	VAL	3.6
6	F	83	LEU	3.6
7	G	66	LEU	3.6
2	B	17	LYS	3.6
9	I	121	LYS	3.6
14	N	147	ILE	3.6
8	H	11	ASP	3.6
30	0	815	U	3.6
30	0	1499	U	3.6
30	0	1797	A	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1843	A	3.6
30	0	2345	A	3.6
30	0	2746	A	3.6
16	P	57	ASN	3.6
1	A	66	ARG	3.6
11	K	21	ALA	3.6
16	P	72	GLY	3.6
25	Y	101	GLY	3.6
1	A	212	PRO	3.6
30	0	87	C	3.6
30	0	471	G	3.6
30	0	795	G	3.6
30	0	1225	C	3.6
30	0	1508	C	3.6
30	0	1563	G	3.6
30	0	1633	C	3.6
30	0	2014	G	3.6
30	0	2020	C	3.6
30	0	2050	G	3.6
30	0	2580	G	3.6
4	D	12	GLU	3.6
8	H	100	GLU	3.6
4	D	40	ILE	3.6
13	M	134	ILE	3.6
8	H	18	THR	3.6
21	U	28	THR	3.6
3	C	78	ARG	3.6
16	P	87	ARG	3.6
2	B	238	ASN	3.6
20	T	83	ASP	3.6
24	X	27	ASP	3.6
29	3	8	ASN	3.6
30	0	396	U	3.6
30	0	1408	U	3.6
30	0	1461	U	3.6
30	0	1539	U	3.6
30	0	1977	U	3.6
30	0	2330	U	3.6
30	0	2419	U	3.6
30	0	2514	U	3.6
30	0	120	A	3.6
30	0	2852	A	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	222	GLY	3.6
2	B	258	GLY	3.6
2	B	273	GLY	3.6
3	C	215	ALA	3.6
6	F	16	ALA	3.6
16	P	135	ALA	3.6
22	V	36	ALA	3.6
4	D	159	PRO	3.6
1	A	103	VAL	3.6
5	E	53	GLU	3.6
5	E	150	GLN	3.6
9	I	88	GLN	3.6
13	M	71	SER	3.6
26	Z	103	VAL	3.6
5	E	57	LYS	3.6
30	0	1060	C	3.6
30	0	1153	C	3.6
30	0	1538	C	3.6
30	0	2565	C	3.6
11	K	18	ILE	3.6
13	M	8	ILE	3.6
30	0	56	G	3.6
30	0	871	G	3.6
30	0	1441	G	3.6
30	0	1592	G	3.6
30	0	1695	G	3.6
30	0	1726	G	3.6
30	0	2815	G	3.6
7	G	65	THR	3.6
4	D	77	ASP	3.6
4	D	99	ASP	3.6
1	A	183	GLY	3.6
13	M	167	GLY	3.6
23	W	9	GLY	3.6
29	3	83	TRP	3.6
30	0	1218	U	3.6
30	0	1980	U	3.6
30	0	2012	U	3.6
30	0	2246	U	3.6
30	0	829	A	3.6
30	0	1597	A	3.6
30	0	1865	A	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1881	A	3.6
31	9	52	A	3.6
2	B	171	VAL	3.6
4	D	55	LYS	3.6
16	P	137	LEU	3.6
19	S	1	SER	3.6
24	X	11	THR	3.5
30	0	1680	C	3.5
30	0	1686	C	3.5
30	0	1993	C	3.5
30	0	2329	C	3.5
30	0	2897	C	3.5
1	A	44	ASP	3.5
2	B	286	ASN	3.5
2	B	332	ASN	3.5
12	L	95	ASP	3.5
13	M	10	ASP	3.5
16	P	19	ASN	3.5
30	0	782	G	3.5
30	0	1718	G	3.5
30	0	1730	G	3.5
30	0	2023	G	3.5
31	9	14	G	3.5
1	A	157	GLY	3.5
11	K	48	GLY	3.5
11	K	111	GLY	3.5
12	L	14	GLY	3.5
1	A	186	TRP	3.5
29	3	35	TRP	3.5
2	B	57	GLU	3.5
26	Z	54	GLU	3.5
11	K	89	LYS	3.5
11	K	90	PHE	3.5
5	E	119	HIS	3.5
18	R	64	SER	3.5
21	U	36	CYS	3.5
30	0	1615	A	3.5
30	0	1852	A	3.5
30	0	1875	A	3.5
30	0	2101	A	3.5
30	0	2743	A	3.5
2	B	307	ARG	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	39	ASP	3.5
1	A	126	ALA	3.5
2	B	169	GLY	3.5
14	N	148	ALA	3.5
11	K	112	PRO	3.5
30	0	1431	C	3.5
30	0	1483	C	3.5
30	0	1769	C	3.5
30	0	2704	C	3.5
2	B	39	GLN	3.5
2	B	284	PHE	3.5
2	B	239	LEU	3.5
3	C	160	LEU	3.5
16	P	123	TYR	3.5
30	0	1211	G	3.5
30	0	1555	G	3.5
30	0	1655	G	3.5
30	0	1877	G	3.5
30	0	1945	G	3.5
30	0	2605	G	3.5
8	H	129	ARG	3.5
10	J	74	ARG	3.5
10	J	127	ILE	3.5
13	M	141	ILE	3.5
30	0	1503	U	3.5
30	0	2586	U	3.5
30	0	797	A	3.5
30	0	1776	A	3.5
13	M	78	LYS	3.5
14	N	95	ALA	3.5
27	1	43	ALA	3.5
12	L	54	PRO	3.5
2	B	221	GLN	3.5
1	A	32	VAL	3.5
4	D	141	VAL	3.5
5	E	131	LEU	3.5
13	M	149	TRP	3.5
16	P	3	LEU	3.5
21	U	49	LEU	3.5
11	K	44	HIS	3.5
27	1	45	ARG	3.5
30	0	141	C	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1731	C	3.5
30	0	1798	C	3.5
30	0	2641	C	3.5
11	K	130	MET	3.5
30	0	1799	G	3.5
30	0	1851	G	3.5
30	0	1891	G	3.5
30	0	1995	G	3.5
30	0	2582	G	3.5
30	0	1187	U	3.5
30	0	1516	U	3.5
30	0	1966	U	3.5
1	A	188	ASN	3.5
2	B	324	ASP	3.5
4	D	103	ASN	3.5
16	P	53	ASP	3.5
1	A	56	ALA	3.5
4	D	87	ALA	3.5
6	F	104	ALA	3.5
8	H	43	ALA	3.5
24	X	64	ALA	3.5
29	3	85	ALA	3.5
30	0	285	A	3.5
30	0	288	A	3.5
30	0	497	A	3.5
30	0	773	A	3.5
30	0	1476	A	3.5
30	0	1515	A	3.5
30	0	1624	A	3.5
30	0	1656	A	3.5
30	0	1717	A	3.5
30	0	1909	A	3.5
30	0	1934	A	3.5
16	P	118	GLN	3.5
23	W	4	LEU	3.5
2	B	29	TRP	3.5
12	L	81	VAL	3.5
3	C	133	ARG	3.5
2	B	74	ILE	3.4
2	B	270	ILE	3.4
26	Z	53	ILE	3.4
18	R	3	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	781	C	3.4
30	0	1374	C	3.4
30	0	1602	C	3.4
30	0	1830	C	3.4
30	0	2002	C	3.4
30	0	2040	C	3.4
11	K	46	LYS	3.4
30	0	826	U	3.4
30	0	2492	U	3.4
8	H	121	GLY	3.4
10	J	65	ASN	3.4
20	T	117	ASP	3.4
30	0	771	G	3.4
30	0	898	G	3.4
30	0	1460	G	3.4
30	0	1468	G	3.4
30	0	1497	G	3.4
30	0	1605	G	3.4
30	0	1647	G	3.4
30	0	1823	G	3.4
30	0	2606	G	3.4
30	0	2683	G	3.4
30	0	2742	G	3.4
30	0	2874	G	3.4
3	C	73	GLN	3.4
12	L	46	LEU	3.4
2	B	105	PHE	3.4
8	H	120	PHE	3.4
5	E	124	VAL	3.4
8	H	149	VAL	3.4
12	L	93	VAL	3.4
16	P	69	ARG	3.4
27	1	46	ARG	3.4
30	0	1442	A	3.4
30	0	1801	A	3.4
30	0	1930	A	3.4
30	0	2504	A	3.4
30	0	2535	A	3.4
19	S	5	ILE	3.4
19	S	81	ILE	3.4
11	K	56	SER	3.4
1	A	90	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	115	GLY	3.4
24	X	67	PRO	3.4
25	Y	198	GLY	3.4
30	0	1652	C	3.4
30	0	1708	C	3.4
30	0	2335	C	3.4
30	0	2475	C	3.4
30	0	2534	C	3.4
5	E	100	ASP	3.4
10	J	142	ASN	3.4
16	P	32	ALA	3.4
18	R	14	ALA	3.4
10	J	92	GLN	3.4
14	N	58	LEU	3.4
22	V	3	LEU	3.4
1	A	16	PHE	3.4
30	0	831	U	3.4
30	0	1835	U	3.4
30	0	1964	U	3.4
5	E	166	VAL	3.4
9	I	97	VAL	3.4
23	W	45	VAL	3.4
28	2	21	VAL	3.4
2	B	101	TRP	3.4
30	0	802	G	3.4
30	0	865	G	3.4
30	0	1614	G	3.4
30	0	1752	G	3.4
30	0	1774	G	3.4
30	0	1820	G	3.4
30	0	2421	G	3.4
30	0	2516	G	3.4
30	0	1379	A	3.4
30	0	1411	A	3.4
30	0	1642	A	3.4
30	0	1885	A	3.4
30	0	2103	A	3.4
2	B	331	SER	3.4
9	I	101	LYS	3.4
18	R	80	TYR	3.4
28	2	38	LYS	3.4
26	Z	66	CYS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	18	ALA	3.4
4	D	41	LEU	3.4
4	D	94	ALA	3.4
6	F	67	ALA	3.4
8	H	115	GLY	3.4
12	L	62	ALA	3.4
15	O	66	GLY	3.4
1	A	107	ASN	3.4
4	D	11	HIS	3.4
5	E	10	ASP	3.4
8	H	74	ARG	3.4
14	N	62	HIS	3.4
16	P	97	ARG	3.4
2	B	285	VAL	3.4
4	D	61	PHE	3.4
8	H	168	VAL	3.4
30	0	1844	C	3.4
30	0	1872	C	3.4
30	0	2515	C	3.4
30	0	2762	C	3.4
16	P	35	ILE	3.4
30	0	1180	U	3.4
30	0	1758	U	3.4
8	H	68	SER	3.4
26	Z	83	TYR	3.4
30	0	792	G	3.4
30	0	1197	G	3.4
30	0	1376	G	3.4
30	0	2013	G	3.4
30	0	2092	G	3.4
30	0	2722	G	3.4
30	0	1661	A	3.4
30	0	2509	A	3.4
30	0	2624	A	3.4
30	0	2637	A	3.4
30	0	2684	A	3.4
30	0	2697	A	3.4
30	0	2883	A	3.4
1	A	217	ARG	3.4
2	B	42	ALA	3.4
2	B	113	LEU	3.4
11	K	50	GLY	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	254	GLN	3.4
13	M	81	ARG	3.4
26	Z	48	ARG	3.4
16	P	93	ASP	3.4
2	B	311	PHE	3.4
29	3	7	PHE	3.4
1	A	228	ILE	3.3
20	T	69	LYS	3.3
30	0	277	U	3.3
30	0	1182	C	3.3
30	0	1451	C	3.3
30	0	1456	C	3.3
30	0	1472	C	3.3
30	0	1577	U	3.3
30	0	1764	C	3.3
30	0	2733	U	3.3
30	0	2901	C	3.3
2	B	329	TYR	3.3
13	M	148	SER	3.3
2	B	240	GLY	3.3
16	P	129	GLY	3.3
22	V	16	ARG	3.3
8	H	118	ALA	3.3
9	I	106	GLN	3.3
13	M	156	ALA	3.3
30	0	11	A	3.3
30	0	587	A	3.3
30	0	875	A	3.3
30	0	1173	A	3.3
30	0	1533	A	3.3
30	0	1581	A	3.3
30	0	1912	A	3.3
30	0	1941	A	3.3
30	0	2719	A	3.3
30	0	824	G	3.3
30	0	1055	G	3.3
30	0	1449	G	3.3
30	0	1532	G	3.3
30	0	1589	G	3.3
30	0	1707	G	3.3
30	0	2001	G	3.3
30	0	2288	G	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2524	G	3.3
30	0	2877	G	3.3
16	P	30	ASP	3.3
16	P	124	ASP	3.3
1	A	197	VAL	3.3
10	J	54	VAL	3.3
11	K	132	VAL	3.3
17	Q	47	VAL	3.3
2	B	156	LYS	3.3
5	E	118	ILE	3.3
10	J	46	ILE	3.3
24	X	70	ILE	3.3
11	K	61	THR	3.3
21	U	54	THR	3.3
28	2	7	THR	3.3
30	0	2735	U	3.3
30	0	1579	C	3.3
31	9	48	C	3.3
1	A	33	GLU	3.3
2	B	3	PRO	3.3
20	T	79	LEU	3.3
2	B	131	ALA	3.3
4	D	79	MET	3.3
6	F	106	ALA	3.3
9	I	93	ALA	3.3
14	N	161	GLY	3.3
16	P	17	GLY	3.3
1	A	58	VAL	3.3
1	A	169	PHE	3.3
5	E	48	VAL	3.3
6	F	76	PHE	3.3
20	T	92	ASP	3.3
30	0	1174	A	3.3
30	0	1434	A	3.3
30	0	1685	A	3.3
30	0	1997	A	3.3
30	0	2680	A	3.3
30	0	91	G	3.3
30	0	1498	G	3.3
30	0	1529	G	3.3
30	0	1588	G	3.3
30	0	1627	G	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2131	G	3.3
30	0	2630	G	3.3
30	0	2862	G	3.3
18	R	136	TRP	3.3
1	A	214	SER	3.3
4	D	96	SER	3.3
6	F	37	THR	3.3
18	R	4	TYR	3.3
25	Y	106	THR	3.3
20	T	49	GLU	3.3
22	V	50	ARG	3.3
1	A	168	PRO	3.3
2	B	159	PRO	3.3
29	3	79	LEU	3.3
1	A	10	GLY	3.3
19	S	58	MET	3.3
3	C	116	ALA	3.3
4	D	71	ALA	3.3
4	D	142	ALA	3.3
18	R	95	ALA	3.3
30	0	777	U	3.3
30	0	1638	U	3.3
30	0	1722	U	3.3
30	0	1807	U	3.3
30	0	1831	U	3.3
30	0	2043	U	3.3
12	L	56	LYS	3.3
30	0	1395	C	3.3
30	0	1620	C	3.3
30	0	1662	C	3.3
30	0	1762	C	3.3
30	0	1818	C	3.3
30	0	1834	C	3.3
30	0	1892	C	3.3
30	0	2126	C	3.3
30	0	2443	C	3.3
30	0	2745	C	3.3
2	B	271	ASP	3.3
3	C	162	VAL	3.3
6	F	91	VAL	3.3
12	L	20	ASN	3.3
9	I	90	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	P	40	VAL	3.3
19	S	49	VAL	3.3
27	1	34	CYS	3.3
30	0	857	A	3.3
30	0	1166	A	3.3
30	0	1755	A	3.3
30	0	1775	A	3.3
30	0	1821	A	3.3
30	0	2577	A	3.3
30	0	2694	A	3.3
7	G	15	TRP	3.3
16	P	22	TRP	3.3
4	D	76	ARG	3.3
2	B	11	LEU	3.3
2	B	84	LEU	3.3
4	D	57	THR	3.3
4	D	90	LEU	3.3
13	M	41	GLU	3.3
30	0	1681	G	3.3
30	0	1697	G	3.3
30	0	1765	G	3.3
30	0	2000	G	3.3
30	0	2349	G	3.3
30	0	2692	G	3.3
30	0	2708	G	3.3
30	0	2716	G	3.3
1	A	176	HIS	3.3
2	B	260	HIS	3.3
1	A	151	GLN	3.3
1	A	207	GLN	3.3
5	E	66	GLN	3.3
12	L	55	GLN	3.3
5	E	120	GLY	3.3
14	N	182	GLY	3.3
14	N	73	ALA	3.3
1	A	92	ASN	3.3
2	B	52	VAL	3.3
17	Q	86	VAL	3.3
23	W	79	VAL	3.3
30	0	832	U	3.3
30	0	883	U	3.3
30	0	1419	U	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	305	ASP	3.3
30	0	1549	C	3.2
30	0	1810	C	3.2
30	0	1899	C	3.2
30	0	1914	C	3.2
30	0	2551	C	3.2
30	0	2752	C	3.2
4	D	64	ARG	3.2
11	K	77	ARG	3.2
15	O	47	ARG	3.2
16	P	65	ARG	3.2
20	T	12	ARG	3.2
2	B	48	MET	3.2
3	C	59	GLU	3.2
8	H	24	THR	3.2
30	0	119	A	3.2
30	0	1005	A	3.2
30	0	1057	A	3.2
30	0	1246	A	3.2
30	0	1271	A	3.2
30	0	1682	A	3.2
30	0	2019	A	3.2
1	A	39	ALA	3.2
13	M	36	ALA	3.2
16	P	77	ALA	3.2
24	X	74	ALA	3.2
30	0	387	G	3.2
30	0	836	G	3.2
30	0	1433	G	3.2
30	0	1794	G	3.2
30	0	2005	G	3.2
30	0	2072	G	3.2
30	0	2289	G	3.2
30	0	2667	G	3.2
5	E	3	VAL	3.2
5	E	42	VAL	3.2
6	F	74	PHE	3.2
10	J	11	ILE	3.2
18	R	119	VAL	3.2
19	S	20	PHE	3.2
14	N	162	ASP	3.2
25	Y	108	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1770	U	3.2
2	B	137	LEU	3.2
5	E	5	LEU	3.2
10	J	86	MET	3.2
16	P	95	GLU	3.2
19	S	13	LYS	3.2
23	W	107	LEU	3.2
30	0	18	C	3.2
30	0	859	C	3.2
30	0	1564	C	3.2
30	0	1714	C	3.2
30	0	1808	C	3.2
30	0	1882	C	3.2
30	0	2077	C	3.2
30	0	2682	C	3.2
30	0	2751	C	3.2
30	0	2846	C	3.2
21	U	19	THR	3.2
2	B	60	SER	3.2
2	B	64	GLY	3.2
24	X	68	SER	3.2
29	3	45	GLY	3.2
25	Y	99	ALA	3.2
29	3	10	TYR	3.2
30	0	1783	A	3.2
1	A	159	VAL	3.2
2	B	151	VAL	3.2
5	E	22	VAL	3.2
12	L	106	VAL	3.2
11	K	43	ARG	3.2
30	0	1217	G	3.2
30	0	1430	G	3.2
30	0	1848	G	3.2
30	0	1867	G	3.2
30	0	1929	G	3.2
30	0	1976	G	3.2
30	0	1986	G	3.2
30	0	2572	G	3.2
30	0	2845	G	3.2
30	0	2861	G	3.2
28	2	28	LYS	3.2
30	0	283	U	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	420	U	3.2
30	0	888	U	3.2
30	0	1412	U	3.2
30	0	2589	U	3.2
30	0	2889	U	3.2
2	B	163	GLU	3.2
5	E	81	GLU	3.2
6	F	17	LEU	3.2
7	G	68	GLU	3.2
24	X	7	GLU	3.2
2	B	313	PRO	3.2
4	D	155	HIS	3.2
4	D	45	THR	3.2
4	D	52	THR	3.2
4	D	95	THR	3.2
11	K	9	THR	3.2
11	K	40	THR	3.2
16	P	88	GLN	3.2
16	P	113	THR	3.2
8	H	171	GLY	3.2
11	K	36	GLY	3.2
12	L	28	GLY	3.2
12	L	110	GLY	3.2
2	B	124	ALA	3.2
18	R	43	ALA	3.2
20	T	114	SER	3.2
24	X	75	ALA	3.2
28	2	4	SER	3.2
30	0	124	C	3.2
30	0	1397	C	3.2
30	0	1792	C	3.2
30	0	1975	C	3.2
30	0	2870	C	3.2
1	A	60	PHE	3.2
3	C	212	VAL	3.2
4	D	130	VAL	3.2
19	S	47	VAL	3.2
19	S	66	VAL	3.2
24	X	43	VAL	3.2
30	0	1407	A	3.2
30	0	1494	A	3.2
30	0	1779	A	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1839	A	3.2
30	0	1858	A	3.2
16	P	136	ASP	3.2
22	V	65	ASP	3.2
7	G	16	LYS	3.2
4	D	84	LEU	3.2
14	N	175	LEU	3.2
8	H	33	GLN	3.2
13	M	98	GLN	3.2
30	0	1164	U	3.2
30	0	1703	G	3.2
30	0	1756	G	3.2
30	0	2350	G	3.2
30	0	2484	U	3.2
30	0	2501	G	3.2
30	0	2527	U	3.2
30	0	2627	G	3.2
30	0	2674	G	3.2
30	0	2770	G	3.2
1	A	123	GLY	3.2
20	T	53	GLY	3.2
3	C	60	SER	3.2
4	D	80	ALA	3.2
7	G	22	ALA	3.2
5	E	133	VAL	3.2
16	P	16	VAL	3.2
16	P	131	PHE	3.2
30	0	884	C	3.1
30	0	1229	C	3.1
30	0	1450	C	3.1
30	0	1609	C	3.1
30	0	1753	C	3.1
30	0	2029	C	3.1
30	0	2508	C	3.1
3	C	76	ARG	3.1
10	J	66	ASP	3.1
13	M	2	ARG	3.1
24	X	18	ARG	3.1
25	Y	208	LYS	3.1
1	A	129	LEU	3.1
30	0	1612	A	3.1
30	0	1857	A	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2879	A	3.1
4	D	173	GLU	3.1
6	F	41	GLU	3.1
14	N	149	GLU	3.1
26	Z	59	GLU	3.1
11	K	45	PRO	3.1
5	E	163	GLN	3.1
5	E	64	THR	3.1
21	U	6	CYS	3.1
5	E	142	GLY	3.1
9	I	66	GLY	3.1
30	0	409	U	3.1
30	0	470	U	3.1
30	0	510	U	3.1
30	0	1654	U	3.1
30	0	1784	U	3.1
30	0	2724	U	3.1
5	E	126	ILE	3.1
23	W	26	ILE	3.1
1	A	201	PHE	3.1
19	S	4	VAL	3.1
20	T	98	VAL	3.1
30	0	518	G	3.1
30	0	1172	G	3.1
30	0	1510	G	3.1
30	0	1665	G	3.1
30	0	2033	G	3.1
30	0	2333	G	3.1
21	U	24	LYS	3.1
18	R	23	MET	3.1
2	B	139	ASP	3.1
3	C	134	ASP	3.1
4	D	39	ASP	3.1
1	A	96	LEU	3.1
8	H	60	LEU	3.1
14	N	66	LEU	3.1
30	0	842	C	3.1
30	0	879	C	3.1
30	0	1466	C	3.1
30	0	1513	C	3.1
30	0	1570	C	3.1
30	0	1593	C	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1623	C	3.1
30	0	1679	C	3.1
30	0	2239	C	3.1
11	K	83	PRO	3.1
14	N	146	HIS	3.1
19	S	61	GLU	3.1
30	0	1231	A	3.1
30	0	1414	A	3.1
30	0	1606	A	3.1
30	0	1657	A	3.1
2	B	164	THR	3.1
11	K	86	THR	3.1
1	A	162	GLY	3.1
4	D	28	GLY	3.1
2	B	46	ALA	3.1
2	B	193	ILE	3.1
12	L	103	ALA	3.1
13	M	63	ALA	3.1
4	D	163	VAL	3.1
5	E	141	VAL	3.1
19	S	77	VAL	3.1
10	J	143	LYS	3.1
16	P	67	LYS	3.1
20	T	97	ARG	3.1
29	3	38	ARG	3.1
30	0	1530	U	3.1
30	0	2512	U	3.1
4	D	170	TYR	3.1
8	H	73	ASN	3.1
2	B	319	ASP	3.1
10	J	121	LEU	3.1
28	2	27	LEU	3.1
14	N	155	GLU	3.1
30	0	479	G	3.1
30	0	1490	G	3.1
30	0	1948	G	3.1
30	0	2283	G	3.1
30	0	2462	G	3.1
30	0	2520	G	3.1
30	0	2592	G	3.1
30	0	2701	G	3.1
8	H	5	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	N	157	PRO	3.1
2	B	20	THR	3.1
2	B	279	THR	3.1
16	P	1	THR	3.1
30	0	130	C	3.1
30	0	1575	C	3.1
30	0	1911	C	3.1
30	0	2268	C	3.1
4	D	59	GLY	3.1
12	L	50	GLY	3.1
4	D	54	ALA	3.1
1	A	180	LYS	3.1
30	0	1007	A	3.1
30	0	1486	A	3.1
30	0	1580	A	3.1
30	0	1737	A	3.1
30	0	2612	A	3.1
30	0	2778	A	3.1
7	G	69	ARG	3.1
16	P	109	ARG	3.1
2	B	162	MET	3.1
26	Z	82	SER	3.1
28	2	31	ARG	3.1
13	M	5	TYR	3.1
2	B	27	ASN	3.1
20	T	67	LEU	3.1
1	A	109	GLU	3.1
5	E	78	GLU	3.1
10	J	76	ASP	3.1
22	V	63	GLU	3.1
26	Z	69	ASP	3.1
6	F	9	PRO	3.1
2	B	35	GLN	3.1
5	E	135	GLY	3.1
8	H	125	GLY	3.1
10	J	94	GLY	3.1
10	J	106	GLY	3.1
16	P	103	THR	3.1
23	W	139	GLY	3.1
26	Z	67	GLY	3.1
30	0	1417	G	3.1
30	0	1542	G	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2009	G	3.1
30	0	2044	G	3.1
30	0	2355	G	3.1
30	0	2558	G	3.1
30	0	2713	G	3.1
30	0	2750	G	3.1
5	E	171	LYS	3.1
6	F	19	ALA	3.1
17	Q	75	ILE	3.1
22	V	35	ALA	3.1
28	2	9	LYS	3.1
2	B	80	ARG	3.1
8	H	20	ARG	3.1
26	Z	63	CYS	3.1
30	0	570	C	3.1
30	0	881	C	3.1
30	0	1578	C	3.1
30	0	1674	C	3.1
30	0	1880	C	3.1
30	0	2049	C	3.1
30	0	2591	C	3.1
27	1	26	SER	3.1
30	0	69	A	3.0
30	0	1767	A	3.0
30	0	2266	A	3.0
30	0	2681	A	3.0
2	B	50	HIS	3.0
7	G	25	GLU	3.0
2	B	149	ASP	3.0
8	H	59	GLN	3.0
30	0	1120	U	3.0
30	0	1850	U	3.0
30	0	1879	U	3.0
30	0	2028	U	3.0
30	0	2528	U	3.0
30	0	2620	U	3.0
1	A	15	THR	3.0
8	H	4	LYS	3.0
1	A	77	GLY	3.0
1	A	204	GLY	3.0
2	B	275	GLY	3.0
6	F	59	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	K	5	GLY	3.0
1	A	57	ALA	3.0
11	K	127	ALA	3.0
16	P	106	ARG	3.0
21	U	27	ALA	3.0
24	X	25	ARG	3.0
13	M	37	VAL	3.0
18	R	143	VAL	3.0
18	R	138	SER	3.0
30	0	830	G	3.0
30	0	1795	G	3.0
30	0	1998	G	3.0
30	0	2489	G	3.0
30	0	2828	G	3.0
30	0	2882	G	3.0
30	0	2900	G	3.0
2	B	175	LEU	3.0
11	K	29	LEU	3.0
11	K	69	LEU	3.0
1	A	59	GLU	3.0
18	R	68	HIS	3.0
30	0	1146	C	3.0
30	0	1617	C	3.0
30	0	1643	C	3.0
30	0	1650	C	3.0
30	0	1841	C	3.0
30	0	1913	C	3.0
30	0	2021	C	3.0
30	0	2510	C	3.0
30	0	2894	C	3.0
19	S	56	ASN	3.0
24	X	65	ASN	3.0
1	A	112	PRO	3.0
14	N	4	PRO	3.0
2	B	114	ASP	3.0
9	I	94	ASP	3.0
17	Q	20	ASP	3.0
30	0	410	A	3.0
30	0	1181	A	3.0
30	0	1746	A	3.0
30	0	1778	A	3.0
30	0	1811	A	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1900	A	3.0
30	0	2583	A	3.0
30	0	2768	A	3.0
2	B	306	LYS	3.0
6	F	31	LYS	3.0
19	S	34	LYS	3.0
30	0	1198	U	3.0
30	0	1544	U	3.0
31	9	23	U	3.0
2	B	25	ARG	3.0
4	D	136	ARG	3.0
11	K	131	ILE	3.0
16	P	99	ARG	3.0
16	P	141	ILE	3.0
26	Z	76	THR	3.0
14	N	1	ALA	3.0
14	N	59	ALA	3.0
16	P	5	ALA	3.0
19	S	38	ALA	3.0
1	A	135	VAL	3.0
8	H	93	PHE	3.0
1	A	148	LEU	3.0
3	C	157	LEU	3.0
12	L	10	SER	3.0
15	O	14	LEU	3.0
18	R	18	LEU	3.0
22	V	49	LEU	3.0
27	1	35	SER	3.0
14	N	21	HIS	3.0
8	H	101	ASN	3.0
11	K	10	GLN	3.0
13	M	52	GLN	3.0
8	H	14	LYS	3.0
8	H	35	LYS	3.0
13	M	178	LYS	3.0
23	W	76	ASP	3.0
30	0	1155	G	3.0
30	0	1163	G	3.0
30	0	1523	G	3.0
30	0	1576	G	3.0
30	0	1610	G	3.0
30	0	1739	G	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2564	G	3.0
30	0	2723	G	3.0
30	0	2026	C	3.0
30	0	2493	C	3.0
30	0	2502	C	3.0
1	A	88	ILE	3.0
11	K	87	ARG	3.0
12	L	149	ARG	3.0
13	M	184	ARG	3.0
24	X	15	ARG	3.0
28	2	26	MET	3.0
30	0	516	A	3.0
30	0	1118	A	3.0
30	0	1154	A	3.0
30	0	1375	A	3.0
30	0	1711	A	3.0
30	0	1732	A	3.0
30	0	1895	A	3.0
30	0	2784	A	3.0
1	A	237	GLY	3.0
5	E	116	THR	3.0
8	H	84	GLY	3.0
14	N	85	GLY	3.0
16	P	128	GLY	3.0
30	0	1170	U	3.0
30	0	1887	U	3.0
30	0	2711	U	3.0
30	0	2749	U	3.0
3	C	84	VAL	3.0
18	R	66	VAL	3.0
24	X	41	PHE	3.0
10	J	145	TRP	3.0
14	N	87	LEU	3.0
25	Y	102	LEU	3.0
1	A	199	HIS	3.0
2	B	333	GLU	3.0
5	E	129	GLU	3.0
15	O	51	TYR	3.0
2	B	141	ARG	3.0
11	K	66	ARG	3.0
14	N	141	ARG	3.0
18	R	33	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	143	GLY	3.0
4	D	153	THR	3.0
5	E	61	THR	3.0
8	H	37	GLY	3.0
10	J	47	THR	3.0
12	L	77	ALA	3.0
24	X	26	ALA	3.0
30	0	116	G	3.0
30	0	147	G	3.0
30	0	390	G	3.0
30	0	1258	G	3.0
30	0	1568	G	3.0
30	0	1694	G	3.0
30	0	1917	G	3.0
30	0	1932	G	3.0
30	0	2250	G	3.0
30	0	1061	C	3.0
30	0	1179	C	3.0
30	0	1436	C	3.0
30	0	1582	C	3.0
30	0	1983	C	3.0
30	0	2241	C	3.0
30	0	2765	C	3.0
1	A	84	VAL	3.0
10	J	12	VAL	3.0
19	S	37	VAL	3.0
23	W	35	VAL	3.0
30	0	591	A	3.0
30	0	796	A	3.0
30	0	846	A	3.0
30	0	1631	A	3.0
30	0	1689	A	3.0
30	0	2011	A	3.0
30	0	2030	A	3.0
30	0	2474	A	3.0
15	O	98	LEU	2.9
30	0	1771	U	2.9
30	0	2557	U	2.9
30	0	2688	U	2.9
18	R	113	HIS	2.9
19	S	12	GLU	2.9
4	D	143	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	K	104	PRO	2.9
26	Z	55	SER	2.9
14	N	153	GLN	2.9
28	2	17	GLN	2.9
2	B	201	ASP	2.9
8	H	117	ARG	2.9
9	I	76	ASP	2.9
13	M	9	ARG	2.9
14	N	164	ASP	2.9
23	W	93	ILE	2.9
13	M	70	GLY	2.9
15	O	62	GLY	2.9
9	I	133	THR	2.9
11	K	24	THR	2.9
11	K	54	THR	2.9
15	O	39	THR	2.9
3	C	176	ALA	2.9
6	F	28	ALA	2.9
6	F	45	ALA	2.9
11	K	26	ALA	2.9
24	X	83	ALA	2.9
1	A	189	VAL	2.9
5	E	11	VAL	2.9
13	M	109	PHE	2.9
17	Q	56	PHE	2.9
18	R	104	PHE	2.9
23	W	51	PHE	2.9
1	A	27	LEU	2.9
10	J	116	LEU	2.9
11	K	17	LEU	2.9
29	3	88	LEU	2.9
8	H	62	HIS	2.9
17	Q	95	GLU	2.9
19	S	43	GLU	2.9
22	V	51	LYS	2.9
26	Z	87	LYS	2.9
30	0	244	C	2.9
30	0	853	C	2.9
30	0	430	A	2.9
30	0	870	G	2.9
30	0	1176	C	2.9
30	0	1594	C	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1618	G	2.9
30	0	1634	G	2.9
30	0	1829	A	2.9
30	0	1866	A	2.9
30	0	1873	G	2.9
30	0	1949	G	2.9
30	0	2007	A	2.9
30	0	2055	A	2.9
30	0	2251	G	2.9
30	0	2255	A	2.9
30	0	2260	A	2.9
30	0	2316	G	2.9
30	0	2747	C	2.9
30	0	2691	A	2.9
30	0	2758	G	2.9
30	0	2766	A	2.9
30	0	2826	G	2.9
30	0	2834	G	2.9
30	0	2857	C	2.9
30	0	1189	A	2.9
30	0	1193	A	2.9
30	0	1372	A	2.9
30	0	1493	A	2.9
30	0	1526	A	2.9
31	9	110	G	2.9
29	3	61	PRO	2.9
3	C	201	SER	2.9
30	0	1056	U	2.9
30	0	1185	U	2.9
30	0	1457	U	2.9
12	L	150	GLN	2.9
18	R	55	GLN	2.9
18	R	123	GLN	2.9
6	F	61	MET	2.9
2	B	195	ARG	2.9
28	2	20	ARG	2.9
10	J	109	TYR	2.9
2	B	236	ILE	2.9
7	G	27	ILE	2.9
1	A	205	GLY	2.9
1	A	234	GLY	2.9
11	K	39	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	O	22	GLY	2.9
25	Y	156	GLY	2.9
3	C	56	THR	2.9
23	W	143	THR	2.9
1	A	108	VAL	2.9
4	D	58	VAL	2.9
8	H	143	VAL	2.9
11	K	88	VAL	2.9
19	S	28	VAL	2.9
25	Y	164	VAL	2.9
1	A	128	LEU	2.9
24	X	50	LEU	2.9
2	B	226	LYS	2.9
11	K	63	GLU	2.9
13	M	57	LYS	2.9
14	N	38	LYS	2.9
16	P	130	GLU	2.9
2	B	152	PRO	2.9
5	E	1	PRO	2.9
14	N	113	SER	2.9
13	M	68	ARG	2.9
22	V	55	ARG	2.9
23	W	42	ARG	2.9
30	0	136	C	2.9
30	0	284	C	2.9
30	0	880	C	2.9
30	0	882	A	2.9
30	0	959	C	2.9
30	0	1004	C	2.9
30	0	1550	A	2.9
30	0	1705	C	2.9
30	0	1772	C	2.9
30	0	1847	A	2.9
30	0	2024	A	2.9
30	0	2601	A	2.9
30	0	2801	A	2.9
30	0	118	G	2.9
30	0	264	G	2.9
30	0	432	G	2.9
30	0	642	G	2.9
30	0	801	U	2.9
30	0	862	U	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1054	G	2.9
30	0	1075	G	2.9
30	0	1151	G	2.9
30	0	1440	U	2.9
30	0	1569	U	2.9
30	0	1780	G	2.9
30	0	2075	G	2.9
31	9	114	G	2.9
8	H	166	ILE	2.9
13	M	96	ASP	2.9
2	B	231	GLY	2.9
2	B	263	THR	2.9
11	K	129	THR	2.9
19	S	57	THR	2.9
10	J	37	ALA	2.9
20	T	110	ALA	2.9
23	W	96	LEU	2.9
25	Y	97	LEU	2.9
25	Y	234	VAL	2.9
4	D	60	GLU	2.9
5	E	9	GLU	2.9
23	W	134	GLU	2.9
24	X	13	PRO	2.9
2	B	16	ARG	2.9
16	P	59	ARG	2.9
5	E	41	SER	2.9
19	S	69	SER	2.9
10	J	63	ILE	2.9
22	V	53	ILE	2.9
20	T	36	GLY	2.9
26	Z	91	GLY	2.9
30	0	638	C	2.9
30	0	783	C	2.9
30	0	822	C	2.9
30	0	872	U	2.9
30	0	970	U	2.9
30	0	1156	C	2.9
30	0	1506	U	2.9
30	0	1768	C	2.9
30	0	1790	C	2.9
30	0	1836	A	2.9
30	0	2048	C	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2302	A	2.9
30	0	2596	A	2.9
30	0	2608	C	2.9
30	0	2636	C	2.9
30	0	2825	C	2.9
30	0	2878	U	2.9
14	N	142	THR	2.9
12	L	78	ALA	2.9
25	Y	145	LYS	2.9
10	J	61	VAL	2.9
11	K	72	VAL	2.9
14	N	47	LEU	2.9
23	W	53	ALA	2.9
8	H	58	VAL	2.9
20	T	65	VAL	2.9
23	W	112	LEU	2.9
29	3	55	VAL	2.9
30	0	140	G	2.9
30	0	820	G	2.9
30	0	1453	G	2.9
30	0	1622	G	2.9
30	0	1777	G	2.9
30	0	2091	G	2.9
30	0	2696	G	2.9
8	H	34	HIS	2.9
16	P	38	GLU	2.8
29	3	19	GLU	2.8
2	B	6	PRO	2.8
2	B	77	PRO	2.8
2	B	148	PRO	2.8
8	H	36	MET	2.8
11	K	62	PRO	2.8
8	H	154	ARG	2.8
13	M	107	ARG	2.8
24	X	34	ARG	2.8
28	2	42	TRP	2.8
1	A	38	ILE	2.8
12	L	4	LYS	2.8
12	L	23	GLY	2.8
13	M	121	GLY	2.8
16	P	110	ASP	2.8
16	P	18	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	P	81	LYS	2.8
24	X	69	LYS	2.8
20	T	112	LEU	2.8
23	W	46	ALA	2.8
25	Y	224	ALA	2.8
12	L	114	VAL	2.8
13	M	60	VAL	2.8
16	P	21	VAL	2.8
8	H	144	GLU	2.8
22	V	62	GLU	2.8
30	0	793	A	2.8
30	0	866	U	2.8
30	0	1590	A	2.8
30	0	1625	U	2.8
30	0	1678	A	2.8
30	0	1684	A	2.8
30	0	1691	A	2.8
30	0	1791	U	2.8
30	0	2022	A	2.8
30	0	2664	A	2.8
30	0	838	C	2.8
30	0	1692	C	2.8
30	0	1870	C	2.8
30	0	2360	C	2.8
30	0	2518	C	2.8
30	0	2626	C	2.8
31	9	121	C	2.8
8	H	162	PRO	2.8
25	Y	231	PRO	2.8
1	A	2	ARG	2.8
5	E	2	ARG	2.8
8	H	91	ARG	2.8
16	P	80	ARG	2.8
28	2	35	ARG	2.8
10	J	29	GLN	2.8
11	K	67	GLN	2.8
30	0	269	G	2.8
30	0	514	G	2.8
30	0	775	G	2.8
30	0	800	G	2.8
30	0	1224	G	2.8
30	0	1316	G	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1595	G	2.8
30	0	1706	G	2.8
30	0	1727	G	2.8
30	0	1849	G	2.8
30	0	1878	G	2.8
30	0	1896	G	2.8
30	0	1989	G	2.8
30	0	2779	G	2.8
30	0	2836	G	2.8
14	N	108	SER	2.8
13	M	170	ASN	2.8
1	A	24	LYS	2.8
11	K	78	LYS	2.8
13	M	193	LYS	2.8
2	B	32	ASP	2.8
2	B	281	ASP	2.8
5	E	128	GLY	2.8
14	N	19	ASP	2.8
23	W	95	GLY	2.8
23	W	123	GLY	2.8
23	W	145	GLY	2.8
1	A	155	THR	2.8
2	B	76	THR	2.8
2	B	81	ALA	2.8
2	B	206	THR	2.8
6	F	112	ALA	2.8
8	H	86	TYR	2.8
8	H	140	TYR	2.8
10	J	131	THR	2.8
14	N	6	TYR	2.8
22	V	33	VAL	2.8
27	1	37	CYS	2.8
29	3	78	HIS	2.8
18	R	52	GLU	2.8
18	R	121	GLU	2.8
2	B	95	ARG	2.8
2	B	233	ARG	2.8
5	E	92	PRO	2.8
8	H	94	PRO	2.8
9	I	87	PRO	2.8
13	M	136	PRO	2.8
16	P	8	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	T	90	PRO	2.8
29	3	12	PRO	2.8
30	0	548	U	2.8
30	0	825	U	2.8
30	0	1511	U	2.8
30	0	1645	U	2.8
30	0	2008	U	2.8
30	0	2076	U	2.8
30	0	2628	U	2.8
30	0	2837	U	2.8
10	J	52	GLN	2.8
14	N	140	GLN	2.8
30	0	37	A	2.8
30	0	302	A	2.8
30	0	808	A	2.8
30	0	1480	A	2.8
30	0	2485	A	2.8
30	0	813	C	2.8
30	0	1201	C	2.8
30	0	1243	C	2.8
30	0	1999	C	2.8
30	0	2132	C	2.8
30	0	2822	C	2.8
1	A	215	ILE	2.8
5	E	69	ILE	2.8
2	B	107	SER	2.8
18	R	15	LYS	2.8
23	W	49	ASN	2.8
30	0	604	G	2.8
30	0	805	G	2.8
30	0	921	G	2.8
30	0	969	G	2.8
30	0	1672	G	2.8
30	0	1855	G	2.8
30	0	1868	G	2.8
30	0	1974	G	2.8
30	0	2045	G	2.8
30	0	2058	G	2.8
30	0	2562	G	2.8
30	0	2573	G	2.8
1	A	26	ASP	2.8
2	B	97	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	P	9	LEU	2.8
21	U	43	GLY	2.8
2	B	83	ALA	2.8
4	D	35	ALA	2.8
10	J	14	ALA	2.8
17	Q	10	THR	2.8
5	E	40	VAL	2.8
17	Q	40	HIS	2.8
18	R	32	ALA	2.8
21	U	5	GLU	2.8
23	W	114	PRO	2.8
1	A	81	GLN	2.8
31	9	97	U	2.8
28	2	2	LYS	2.8
30	0	132	A	2.8
30	0	161	A	2.8
30	0	339	A	2.8
30	0	2054	A	2.8
30	0	2301	A	2.8
30	0	2880	A	2.8
30	0	2891	A	2.8
30	0	735	C	2.8
30	0	1147	C	2.8
30	0	1403	C	2.8
30	0	1474	C	2.8
30	0	2047	C	2.8
30	0	2787	C	2.8
31	9	113	C	2.8
11	K	93	ASN	2.8
16	P	60	GLY	2.8
16	P	112	GLY	2.8
16	P	114	LEU	2.8
22	V	23	LEU	2.8
2	B	103	ASP	2.8
2	B	110	ASP	2.8
8	H	13	ASP	2.8
16	P	132	ASP	2.8
24	X	16	ASP	2.8
24	X	46	ASP	2.8
1	A	233	THR	2.8
2	B	134	ALA	2.8
14	N	67	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	T	96	VAL	2.8
26	Z	68	GLU	2.8
24	X	71	ARG	2.8
30	0	1145	G	2.8
30	0	1676	G	2.8
30	0	1713	G	2.8
30	0	2079	G	2.8
30	0	2352	G	2.8
30	0	2567	G	2.8
30	0	2618	G	2.8
30	0	2623	G	2.8
30	0	2829	G	2.8
8	H	27	PRO	2.7
27	1	6	PRO	2.7
2	B	45	LYS	2.7
3	C	185	LYS	2.7
8	H	30	LYS	2.7
30	0	1169	U	2.7
30	0	2495	U	2.7
30	0	2523	U	2.7
31	9	87	U	2.7
1	A	140	LEU	2.7
2	B	140	LEU	2.7
2	B	153	SER	2.7
13	M	117	SER	2.7
20	T	94	SER	2.7
21	U	33	SER	2.7
24	X	59	TRP	2.7
4	D	36	ASN	2.7
10	J	68	GLY	2.7
22	V	37	GLY	2.7
21	U	23	HIS	2.7
30	0	67	A	2.7
30	0	472	A	2.7
30	0	1202	A	2.7
30	0	1230	A	2.7
30	0	1470	A	2.7
30	0	1759	A	2.7
30	0	1919	A	2.7
30	0	2799	A	2.7
2	B	205	VAL	2.7
3	C	135	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	43	GLU	2.7
5	E	23	GLU	2.7
10	J	39	VAL	2.7
11	K	19	THR	2.7
11	K	116	GLU	2.7
12	L	70	ASP	2.7
16	P	63	ARG	2.7
16	P	134	VAL	2.7
21	U	29	THR	2.7
30	0	2031	C	2.7
30	0	2130	C	2.7
30	0	2542	C	2.7
1	A	49	PRO	2.7
4	D	137	PRO	2.7
5	E	157	LYS	2.7
8	H	39	LYS	2.7
13	M	69	LYS	2.7
30	0	92	G	2.7
30	0	375	G	2.7
30	0	564	G	2.7
30	0	1099	G	2.7
30	0	1452	G	2.7
30	0	1535	G	2.7
30	0	2046	G	2.7
30	0	2253	G	2.7
30	0	2540	G	2.7
30	0	2668	G	2.7
2	B	181	ILE	2.7
5	E	20	ILE	2.7
5	E	148	ILE	2.7
14	N	180	LEU	2.7
5	E	63	GLY	2.7
9	I	125	GLY	2.7
16	P	4	SER	2.7
21	U	30	HIS	2.7
23	W	127	GLY	2.7
26	Z	77	GLY	2.7
29	3	13	HIS	2.7
29	3	32	GLY	2.7
30	0	560	U	2.7
30	0	794	U	2.7
30	0	852	U	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1813	U	2.7
16	P	107	GLU	2.7
29	3	41	GLU	2.7
29	3	81	GLU	2.7
1	A	34	ASP	2.7
2	B	102	THR	2.7
2	B	202	VAL	2.7
3	C	190	ALA	2.7
4	D	50	VAL	2.7
5	E	146	ALA	2.7
6	F	60	VAL	2.7
6	F	105	ASP	2.7
16	P	70	ALA	2.7
17	Q	92	ARG	2.7
20	T	74	VAL	2.7
23	W	85	ALA	2.7
1	A	221	PRO	2.7
30	0	60	A	2.7
30	0	145	A	2.7
30	0	502	A	2.7
30	0	521	A	2.7
30	0	776	A	2.7
30	0	1482	A	2.7
30	0	1736	A	2.7
30	0	2062	A	2.7
30	0	2353	A	2.7
30	0	2372	A	2.7
30	0	2486	A	2.7
30	0	2653	A	2.7
30	0	2812	A	2.7
8	H	40	GLN	2.7
26	Z	94	LYS	2.7
30	0	200	C	2.7
30	0	280	C	2.7
30	0	342	C	2.7
30	0	377	C	2.7
30	0	633	C	2.7
30	0	769	C	2.7
30	0	1988	C	2.7
30	0	2006	C	2.7
30	0	2088	C	2.7
30	0	2552	C	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2859	C	2.7
21	U	9	CYS	2.7
4	D	151	ILE	2.7
6	F	63	ILE	2.7
1	A	191	GLY	2.7
30	0	358	G	2.7
30	0	887	G	2.7
30	0	956	G	2.7
30	0	1053	G	2.7
30	0	1203	G	2.7
30	0	1239	G	2.7
30	0	1340	G	2.7
30	0	1389	G	2.7
30	0	1415	G	2.7
30	0	1781	G	2.7
30	0	1782	G	2.7
30	0	1863	G	2.7
30	0	2584	G	2.7
30	0	2602	G	2.7
30	0	2616	G	2.7
30	0	2847	G	2.7
30	0	2898	G	2.7
31	9	20	G	2.7
31	9	25	G	2.7
31	9	50	G	2.7
2	B	21	SER	2.7
9	I	79	GLY	2.7
13	M	186	SER	2.7
14	N	139	TRP	2.7
15	O	23	GLY	2.7
17	Q	16	ASN	2.7
17	Q	19	ARG	2.7
17	Q	49	ASN	2.7
20	T	59	GLU	2.7
20	T	115	GLU	2.7
21	U	44	ARG	2.7
21	U	56	ARG	2.7
1	A	193	ALA	2.7
2	B	297	VAL	2.7
3	C	144	PHE	2.7
3	C	224	ALA	2.7
15	O	76	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	P	44	VAL	2.7
17	Q	63	VAL	2.7
6	F	15	ASP	2.7
20	T	105	ASP	2.7
25	Y	163	THR	2.7
10	J	88	PRO	2.7
30	0	133	U	2.7
30	0	299	U	2.7
30	0	1237	U	2.7
30	0	1788	U	2.7
30	0	922	A	2.7
30	0	1058	A	2.7
30	0	1632	A	2.7
30	0	1840	A	2.7
30	0	2280	A	2.7
30	0	2783	A	2.7
2	B	272	ILE	2.7
30	0	427	C	2.7
30	0	637	C	2.7
30	0	1699	C	2.7
30	0	2098	C	2.7
30	0	2105	C	2.7
30	0	2348	C	2.7
30	0	2785	C	2.7
31	9	36	C	2.7
31	9	71	C	2.7
23	W	44	MET	2.7
1	A	232	ARG	2.7
8	H	99	ARG	2.7
13	M	113	ARG	2.7
18	R	128	ARG	2.7
25	Y	100	ARG	2.7
2	B	28	SER	2.7
2	B	289	GLU	2.7
12	L	147	GLU	2.7
2	B	222	LYS	2.7
2	B	298	LYS	2.7
5	E	103	VAL	2.7
6	F	86	ALA	2.7
12	L	111	ALA	2.7
13	M	4	ALA	2.7
22	V	24	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	W	20	THR	2.7
24	X	77	PHE	2.7
1	A	62	ASP	2.7
1	A	64	ASP	2.7
2	B	160	ASP	2.7
3	C	101	ASP	2.7
8	H	114	ASP	2.7
17	Q	54	PRO	2.7
21	U	15	PRO	2.7
30	0	157	G	2.6
30	0	246	G	2.6
30	0	413	G	2.6
30	0	1512	G	2.6
30	0	1923	G	2.6
30	0	2336	G	2.6
30	0	2338	G	2.6
30	0	2420	G	2.6
30	0	2603	G	2.6
30	0	2662	G	2.6
8	H	17	TYR	2.6
30	0	123	U	2.6
30	0	624	U	2.6
30	0	954	U	2.6
30	0	2595	U	2.6
24	X	30	MET	2.6
30	0	639	A	2.6
30	0	736	A	2.6
30	0	1152	A	2.6
30	0	1207	A	2.6
30	0	1232	A	2.6
30	0	1248	A	2.6
30	0	1869	A	2.6
30	0	1969	A	2.6
30	0	2843	A	2.6
2	B	227	HIS	2.6
5	E	153	ARG	2.6
10	J	49	ARG	2.6
12	L	13	HIS	2.6
12	L	27	ARG	2.6
18	R	125	ARG	2.6
26	Z	73	ARG	2.6
1	A	79	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	245	GLU	2.6
4	D	65	GLU	2.6
5	E	109	GLY	2.6
13	M	179	GLY	2.6
14	N	156	GLU	2.6
16	P	111	GLU	2.6
30	0	72	C	2.6
30	0	256	C	2.6
30	0	1462	C	2.6
30	0	1477	C	2.6
30	0	1666	C	2.6
30	0	1888	C	2.6
30	0	2292	C	2.6
30	0	2561	C	2.6
30	0	2594	C	2.6
30	0	2644	C	2.6
2	B	59	ASN	2.6
20	T	81	LYS	2.6
3	C	88	SER	2.6
15	O	25	VAL	2.6
17	Q	39	VAL	2.6
18	R	135	ALA	2.6
2	B	30	PRO	2.6
3	C	202	THR	2.6
10	J	119	THR	2.6
23	W	36	PRO	2.6
1	A	5	GLN	2.6
7	G	21	ASP	2.6
14	N	138	ASP	2.6
16	P	66	GLN	2.6
18	R	90	ASP	2.6
2	B	259	TYR	2.6
11	K	80	ILE	2.6
16	P	31	ILE	2.6
23	W	146	ILE	2.6
24	X	54	ILE	2.6
29	3	3	MET	2.6
30	0	267	G	2.6
30	0	381	G	2.6
30	0	640	G	2.6
30	0	810	G	2.6
30	0	835	U	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1125	U	2.6
30	0	1220	U	2.6
30	0	1524	U	2.6
30	0	1926	G	2.6
30	0	2068	G	2.6
30	0	2578	G	2.6
30	0	2615	U	2.6
30	0	2617	G	2.6
30	0	2645	U	2.6
30	0	2657	G	2.6
30	0	2809	G	2.6
5	E	115	ARG	2.6
8	H	69	ARG	2.6
19	S	7	HIS	2.6
2	B	34	GLY	2.6
2	B	108	GLU	2.6
6	F	92	GLY	2.6
7	G	19	GLU	2.6
21	U	37	GLU	2.6
30	0	1194	A	2.6
30	0	1233	A	2.6
30	0	1437	A	2.6
30	0	1712	A	2.6
30	0	2099	A	2.6
30	0	2291	A	2.6
30	0	2361	A	2.6
30	0	2622	A	2.6
30	0	2811	A	2.6
31	9	57	A	2.6
28	2	45	ASN	2.6
29	3	48	ASN	2.6
1	A	14	SER	2.6
2	B	220	VAL	2.6
10	J	101	VAL	2.6
11	K	16	SER	2.6
14	N	35	VAL	2.6
14	N	64	SER	2.6
19	S	52	VAL	2.6
23	W	5	VAL	2.6
2	B	58	PRO	2.6
18	R	139	PRO	2.6
19	S	64	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	N	2	THR	2.6
3	C	45	ASP	2.6
3	C	198	ASP	2.6
30	0	31	C	2.6
30	0	162	C	2.6
30	0	889	C	2.6
30	0	890	C	2.6
30	0	1421	C	2.6
30	0	1584	C	2.6
30	0	1720	C	2.6
30	0	1721	C	2.6
30	0	2122	C	2.6
30	0	2427	C	2.6
30	0	2496	C	2.6
30	0	2519	C	2.6
30	0	2769	C	2.6
30	0	2850	C	2.6
30	0	2912	C	2.6
17	Q	43	ILE	2.6
20	T	72	ILE	2.6
5	E	18	LEU	2.6
12	L	145	LEU	2.6
13	M	7	TYR	2.6
19	S	24	LEU	2.6
26	Z	86	TYR	2.6
1	A	47	HIS	2.6
2	B	322	ARG	2.6
6	F	119	ARG	2.6
16	P	139	ARG	2.6
20	T	73	HIS	2.6
24	X	36	HIS	2.6
28	2	10	ARG	2.6
2	B	157	LYS	2.6
22	V	47	LYS	2.6
30	0	1985	U	2.6
30	0	2027	U	2.6
30	0	2116	U	2.6
30	0	2290	U	2.6
30	0	2693	U	2.6
30	0	2705	U	2.6
5	E	14	GLU	2.6
12	L	83	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	X	20	GLU	2.6
2	B	255	GLY	2.6
30	0	1743	G	2.6
30	0	1744	G	2.6
30	0	1884	G	2.6
30	0	2374	G	2.6
30	0	2611	G	2.6
30	0	2642	G	2.6
30	0	2698	G	2.6
30	0	2772	G	2.6
31	9	32	G	2.6
1	A	25	ALA	2.6
1	A	121	ALA	2.6
2	B	154	VAL	2.6
2	B	214	PRO	2.6
3	C	52	ALA	2.6
3	C	68	ALA	2.6
13	M	166	ALA	2.6
18	R	40	ALA	2.6
22	V	5	VAL	2.6
28	2	22	PRO	2.6
29	3	4	PRO	2.6
5	E	122	THR	2.6
11	K	107	THR	2.6
12	L	58	GLN	2.6
14	N	71	TRP	2.6
16	P	133	SER	2.6
19	S	21	GLN	2.6
23	W	64	THR	2.6
23	W	102	SER	2.6
25	Y	98	GLN	2.6
25	Y	103	THR	2.6
29	3	30	GLN	2.6
23	W	148	ASP	2.6
24	X	44	ASP	2.6
30	0	317	A	2.6
30	0	843	A	2.6
30	0	1487	A	2.6
30	0	1991	A	2.6
30	0	1994	A	2.6
30	0	2252	A	2.6
30	0	2368	A	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2532	A	2.6
8	H	8	MET	2.6
8	H	80	LEU	2.6
10	J	105	LEU	2.6
30	0	240	C	2.6
30	0	1105	C	2.6
30	0	1212	C	2.6
30	0	1343	C	2.6
30	0	1377	C	2.6
30	0	1675	C	2.6
30	0	1734	C	2.6
30	0	1738	C	2.6
30	0	1893	C	2.6
5	E	82	TYR	2.6
16	P	71	TYR	2.6
1	A	131	HIS	2.6
16	P	83	LYS	2.6
5	E	98	GLU	2.6
2	B	213	GLY	2.6
6	F	88	GLY	2.6
1	A	220	PRO	2.6
30	0	268	U	2.6
30	0	751	U	2.6
30	0	837	U	2.6
30	0	855	U	2.6
30	0	2904	U	2.6
3	C	204	ALA	2.6
3	C	235	PHE	2.6
4	D	98	PHE	2.6
6	F	87	ALA	2.6
18	R	129	ALA	2.6
20	T	88	PRO	2.6
24	X	60	ALA	2.6
1	A	93	THR	2.5
5	E	51	SER	2.5
6	F	36	THR	2.5
7	G	29	SER	2.5
9	I	82	THR	2.5
10	J	136	SER	2.5
25	Y	95	THR	2.5
29	3	2	GLN	2.6
12	L	101	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	104	ASP	2.5
30	0	257	G	2.5
30	0	417	G	2.5
30	0	636	G	2.5
30	0	1387	G	2.5
30	0	1806	G	2.5
30	0	2121	G	2.5
30	0	2428	G	2.5
30	0	2643	G	2.5
30	0	2712	G	2.5
30	0	2887	G	2.5
31	9	66	G	2.5
31	9	68	G	2.5
10	J	83	ILE	2.5
11	K	49	LEU	2.5
23	W	138	LEU	2.5
30	0	242	A	2.5
30	0	261	A	2.5
30	0	340	A	2.5
30	0	1247	A	2.5
30	0	1381	A	2.5
30	0	1427	A	2.5
30	0	1522	A	2.5
30	0	1658	A	2.5
30	0	2038	A	2.5
30	0	2380	A	2.5
30	0	2576	A	2.5
30	0	2599	A	2.5
30	0	2827	A	2.5
1	A	206	ARG	2.5
1	A	223	ARG	2.5
2	B	328	ARG	2.5
12	L	37	LYS	2.5
13	M	42	ARG	2.5
14	N	17	ARG	2.5
17	Q	15	LYS	2.5
5	E	17	HIS	2.5
28	2	41	HIS	2.5
8	H	22	TYR	2.5
13	M	118	TYR	2.5
1	A	72	GLU	2.5
9	I	86	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	J	58	GLU	2.5
21	U	14	GLU	2.5
30	0	139	C	2.5
30	0	228	C	2.5
30	0	480	C	2.5
30	0	851	C	2.5
30	0	1148	C	2.5
30	0	1209	C	2.5
30	0	1495	C	2.5
30	0	1982	C	2.5
30	0	2593	C	2.5
31	9	95	C	2.5
31	9	96	C	2.5
1	A	63	GLY	2.5
4	D	46	GLY	2.5
8	H	28	GLY	2.5
2	B	315	VAL	2.5
5	E	113	PRO	2.5
8	H	130	VAL	2.5
18	R	58	PRO	2.5
19	S	8	PRO	2.5
1	A	119	ALA	2.5
11	K	76	GLN	2.5
12	L	89	PHE	2.5
13	M	28	GLN	2.5
25	Y	131	GLN	2.5
19	S	48	THR	2.5
26	Z	65	ASN	2.5
27	1	15	THR	2.5
2	B	190	MET	2.5
5	E	72	MET	2.5
5	E	84	MET	2.5
30	0	374	U	2.5
30	0	623	U	2.5
30	0	1001	U	2.5
30	0	1488	U	2.5
30	0	1677	U	2.5
30	0	1766	U	2.5
30	0	1918	U	2.5
30	0	2539	U	2.5
3	C	167	ASP	2.5
9	I	98	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	S	30	ASP	2.5
8	H	123	ILE	2.5
13	M	97	ILE	2.5
5	E	32	ARG	2.5
12	L	3	LYS	2.5
12	L	130	ARG	2.5
12	L	142	LEU	2.5
13	M	112	LEU	2.5
13	M	147	LEU	2.5
16	P	20	ARG	2.5
12	L	43	HIS	2.5
30	0	28	G	2.5
30	0	50	G	2.5
30	0	77	G	2.5
30	0	877	G	2.5
30	0	1210	G	2.5
30	0	1214	G	2.5
30	0	1223	G	2.5
30	0	1438	G	2.5
30	0	1556	G	2.5
30	0	2082	G	2.5
30	0	2579	G	2.5
31	9	84	G	2.5
9	I	135	GLU	2.5
10	J	71	TYR	2.5
30	0	191	A	2.5
30	0	511	A	2.5
30	0	590	A	2.5
30	0	1527	A	2.5
30	0	1573	A	2.5
30	0	1616	A	2.5
30	0	1637	A	2.5
30	0	1742	A	2.5
30	0	2600	A	2.5
31	9	54	A	2.5
31	9	85	A	2.5
3	C	64	GLY	2.5
13	M	18	GLY	2.5
13	M	165	GLY	2.5
13	M	172	GLY	2.5
2	B	61	PRO	2.5
18	R	10	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	95	VAL	2.5
18	R	6	VAL	2.5
7	G	70	ALA	2.5
10	J	4	ALA	2.5
10	J	98	PHE	2.5
13	M	26	GLN	2.5
30	0	110	C	2.5
30	0	122	C	2.5
30	0	1008	C	2.5
30	0	1396	C	2.5
30	0	1861	C	2.5
30	0	1920	C	2.5
30	0	1936	C	2.5
30	0	2835	C	2.5
22	V	12	THR	2.5
1	A	178	LYS	2.5
10	J	7	ASP	2.5
16	P	91	LYS	2.5
18	R	60	LYS	2.5
12	L	53	ARG	2.5
13	M	73	ARG	2.5
13	M	133	LEU	2.5
14	N	143	ARG	2.5
15	O	115	ARG	2.5
29	3	80	ARG	2.5
30	0	649	U	2.5
30	0	1380	U	2.5
30	0	1418	U	2.5
30	0	2063	U	2.5
30	0	2107	U	2.5
30	0	2378	U	2.5
30	0	2607	U	2.5
30	0	2714	U	2.5
30	0	2721	U	2.5
17	Q	8	GLU	2.5
18	R	7	GLU	2.5
13	M	16	GLY	2.5
13	M	110	PRO	2.5
7	G	20	VAL	2.5
11	K	34	VAL	2.5
30	0	255	A	2.5
30	0	812	A	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	841	A	2.5
30	0	868	G	2.5
30	0	924	G	2.5
30	0	1402	G	2.5
30	0	1406	A	2.5
30	0	1465	A	2.5
30	0	1496	A	2.5
30	0	2272	G	2.5
30	0	2505	G	2.5
30	0	2646	G	2.5
30	0	2689	A	2.5
30	0	2800	A	2.5
30	0	2875	A	2.5
30	0	2914	A	2.5
6	F	95	ALA	2.5
6	F	96	ALA	2.5
15	O	18	ALA	2.5
23	W	67	ALA	2.5
29	3	39	GLN	2.5
29	3	90	PHE	2.5
18	R	13	THR	2.5
1	A	106	CYS	2.5
15	O	35	LYS	2.5
17	Q	17	LYS	2.5
5	E	28	SER	2.5
8	H	31	ILE	2.5
9	I	96	SER	2.5
14	N	60	SER	2.5
14	N	83	LEU	2.5
29	3	36	ILE	2.5
1	A	166	ASP	2.5
3	C	170	ASP	2.5
30	0	260	C	2.5
30	0	847	C	2.5
30	0	1469	C	2.5
30	0	1545	C	2.5
30	0	1644	C	2.5
30	0	1687	C	2.5
30	0	2036	C	2.5
30	0	2536	C	2.5
30	0	2654	C	2.5
30	0	2672	C	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2717	C	2.5
30	0	2833	C	2.5
31	9	40	C	2.5
12	L	116	HIS	2.5
8	H	66	GLU	2.5
9	I	105	GLU	2.5
29	3	21	GLU	2.5
29	3	73	GLU	2.5
30	0	559	U	2.5
30	0	1122	U	2.5
30	0	1244	U	2.5
30	0	1696	U	2.5
30	0	1903	U	2.5
30	0	2789	U	2.5
30	0	2853	U	2.5
30	0	2872	U	2.5
3	C	10	GLY	2.5
14	N	3	GLY	2.5
1	A	150	PRO	2.5
3	C	1	MET	2.5
13	M	15	PRO	2.5
2	B	127	GLN	2.5
3	C	234	VAL	2.5
10	J	38	VAL	2.5
12	L	113	GLN	2.5
15	O	113	VAL	2.5
24	X	48	VAL	2.5
2	B	228	ALA	2.5
3	C	159	ALA	2.5
13	M	21	ALA	2.5
17	Q	52	PHE	2.5
27	1	18	LYS	2.4
27	1	25	LYS	2.4
12	L	63	THR	2.4
2	B	266	ASN	2.4
13	M	90	ARG	2.4
30	0	780	A	2.4
30	0	1845	A	2.4
30	0	2332	A	2.4
30	0	2856	A	2.4
2	B	269	LEU	2.4
13	M	23	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	N	90	LEU	2.4
20	T	1	SER	2.4
25	Y	180	SER	2.4
30	0	219	G	2.4
30	0	324	G	2.4
30	0	738	G	2.4
30	0	2823	G	2.4
4	D	145	ASP	2.4
12	L	102	ASP	2.4
13	M	12	TRP	2.4
19	S	17	ASP	2.4
1	A	98	GLU	2.4
2	B	104	GLU	2.4
2	B	274	GLU	2.4
6	F	58	GLU	2.4
6	F	116	GLU	2.4
9	I	81	GLU	2.4
22	V	48	GLU	2.4
30	0	341	C	2.4
30	0	1157	C	2.4
30	0	1553	C	2.4
30	0	1793	C	2.4
30	0	2346	C	2.4
31	9	42	C	2.4
30	0	626	U	2.4
30	0	1279	U	2.4
30	0	1531	U	2.4
30	0	2610	U	2.4
13	M	185	PRO	2.4
1	A	117	LYS	2.4
1	A	167	LYS	2.4
6	F	80	GLN	2.4
15	O	74	VAL	2.4
28	2	25	VAL	2.4
2	B	86	ALA	2.4
10	J	129	PHE	2.4
18	R	88	PHE	2.4
19	S	27	ALA	2.4
25	Y	211	ALA	2.4
2	B	112	THR	2.4
11	K	75	ARG	2.4
20	T	89	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	H	70	LEU	2.4
28	2	11	LEU	2.4
5	E	134	SER	2.4
12	L	26	HIS	2.4
27	1	16	HIS	2.4
2	B	173	ASP	2.4
3	C	165	ASP	2.4
10	J	110	ASP	2.4
20	T	54	ASP	2.4
21	U	53	ASP	2.4
30	0	630	A	2.4
30	0	806	A	2.4
30	0	844	A	2.4
30	0	1294	A	2.4
30	0	1356	A	2.4
30	0	1502	A	2.4
30	0	2375	A	2.4
30	0	2906	A	2.4
31	9	34	A	2.4
4	D	92	GLU	2.4
26	Z	56	GLU	2.4
30	0	66	G	2.4
30	0	71	G	2.4
30	0	274	G	2.4
30	0	1269	G	2.4
30	0	1295	G	2.4
30	0	1364	G	2.4
30	0	1621	G	2.4
30	0	1719	G	2.4
30	0	2125	G	2.4
30	0	2482	G	2.4
30	0	2892	G	2.4
31	9	92	G	2.4
1	A	209	PRO	2.4
8	H	25	GLY	2.4
8	H	63	GLY	2.4
8	H	87	LYS	2.4
1	A	76	VAL	2.4
1	A	170	VAL	2.4
3	C	218	VAL	2.4
13	M	114	VAL	2.4
20	T	22	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	53	C	2.4
30	0	245	C	2.4
30	0	1245	C	2.4
30	0	1558	C	2.4
30	0	1940	C	2.4
30	0	2472	C	2.4
30	0	2707	C	2.4
2	B	174	ARG	2.4
3	C	58	ALA	2.4
12	L	11	ARG	2.4
17	Q	93	ARG	2.4
28	2	12	ALA	2.4
30	0	286	U	2.4
30	0	402	U	2.4
30	0	1128	U	2.4
30	0	1500	U	2.4
30	0	1741	U	2.4
30	0	2590	U	2.4
29	3	84	ARG	2.4
2	B	250	THR	2.4
15	O	70	LEU	2.4
22	V	42	ASN	2.4
25	Y	188	HIS	2.4
4	D	105	SER	2.4
13	M	83	SER	2.4
2	B	120	ASP	2.4
5	E	101	GLU	2.4
8	H	169	GLU	2.4
11	K	28	GLU	2.4
14	N	151	ASP	2.4
20	T	58	GLU	2.4
21	U	41	ASP	2.4
18	R	109	MET	2.4
11	K	52	LYS	2.4
30	0	160	A	2.4
30	0	262	A	2.4
30	0	380	A	2.4
30	0	1098	A	2.4
30	0	1188	A	2.4
30	0	1664	A	2.4
30	0	2135	A	2.4
30	0	2566	A	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	35	GLY	2.4
2	B	168	GLY	2.4
5	E	165	GLY	2.4
18	R	78	GLY	2.4
27	1	9	GLY	2.4
1	A	7	GLN	2.4
2	B	94	GLN	2.4
2	B	82	VAL	2.4
2	B	100	VAL	2.4
10	J	10	VAL	2.4
10	J	26	VAL	2.4
1	A	22	ARG	2.4
1	A	120	ARG	2.4
2	B	26	PHE	2.4
2	B	235	ARG	2.4
3	C	46	TYR	2.4
10	J	84	ARG	2.4
14	N	5	ARG	2.4
21	U	40	ALA	2.4
29	3	77	ALA	2.4
30	0	641	G	2.4
30	0	1074	G	2.4
30	0	1094	G	2.4
30	0	1138	G	2.4
30	0	1611	G	2.4
30	0	1629	G	2.4
30	0	1773	G	2.4
30	0	1902	G	2.4
30	0	2310	G	2.4
30	0	2459	G	2.4
30	0	2574	G	2.4
3	C	207	LEU	2.4
23	W	150	LEU	2.4
4	D	86	THR	2.4
8	H	12	ILE	2.4
8	H	77	ILE	2.4
22	V	28	LEU	2.4
12	L	12	THR	2.4
30	0	68	U	2.4
30	0	399	C	2.4
30	0	403	C	2.4
30	0	438	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	778	C	2.4
30	0	1102	C	2.4
30	0	1967	U	2.4
30	0	2086	C	2.4
30	0	2247	C	2.4
30	0	2411	C	2.4
30	0	2640	U	2.4
28	2	36	ASN	2.4
5	E	6	GLU	2.4
12	L	32	ASP	2.4
19	S	59	ASP	2.4
23	W	16	ASP	2.4
8	H	41	LYS	2.4
2	B	96	PRO	2.4
1	A	73	GLY	2.4
14	N	70	GLY	2.4
18	R	74	GLY	2.4
16	P	28	GLN	2.4
1	A	51	ARG	2.4
6	F	29	VAL	2.4
11	K	96	VAL	2.4
18	R	50	VAL	2.4
18	R	72	VAL	2.4
20	T	62	VAL	2.4
28	2	40	ARG	2.4
29	3	6	ARG	2.4
30	0	148	A	2.4
30	0	1369	A	2.4
30	0	1448	A	2.4
30	0	2083	A	2.4
30	0	2511	A	2.4
26	Z	51	ALA	2.4
4	D	157	LEU	2.3
23	W	73	LEU	2.3
1	A	21	HIS	2.3
4	D	24	HIS	2.3
21	U	48	ASN	2.3
30	0	17	G	2.3
30	0	112	G	2.3
30	0	135	G	2.3
30	0	379	G	2.3
30	0	496	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	531	G	2.3
30	0	740	G	2.3
6	F	13	GLU	2.3
10	J	99	GLU	2.3
17	Q	37	GLU	2.3
30	0	1062	U	2.3
30	0	1382	G	2.3
30	0	1757	U	2.3
30	0	2069	U	2.3
30	0	2093	G	2.3
30	0	2499	U	2.3
30	0	2531	U	2.3
30	0	2632	G	2.3
30	0	2656	G	2.3
30	0	2669	U	2.3
30	0	2670	G	2.3
30	0	2798	G	2.3
30	0	2909	G	2.3
31	9	86	G	2.3
2	B	65	MET	2.3
29	3	33	MET	2.3
5	E	54	ASP	2.3
5	E	137	ASP	2.3
8	H	51	SER	2.3
18	R	17	MET	2.3
10	J	128	LYS	2.3
17	Q	44	ASP	2.3
30	0	443	C	2.3
30	0	491	C	2.3
30	0	530	C	2.3
30	0	1360	C	2.3
30	0	1455	C	2.3
30	0	2259	C	2.3
30	0	2294	C	2.3
30	0	2895	C	2.3
1	A	19	PRO	2.3
2	B	325	PRO	2.3
17	Q	45	PRO	2.3
23	W	120	PRO	2.3
29	3	56	PRO	2.3
6	F	102	GLY	2.3
1	A	9	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	H	135	GLN	2.3
17	Q	78	GLY	2.3
20	T	57	GLY	2.3
1	A	219	ALA	2.3
18	R	47	LEU	2.3
20	T	31	LEU	2.3
22	V	54	ALA	2.3
15	O	89	ILE	2.3
14	N	20	TYR	2.3
6	F	62	HIS	2.3
8	H	75	HIS	2.3
14	N	57	THR	2.3
30	0	429	A	2.3
30	0	1572	A	2.3
30	0	1747	A	2.3
30	0	1973	A	2.3
30	0	2085	A	2.3
30	0	2321	A	2.3
30	0	2467	A	2.3
30	0	2488	A	2.3
31	9	77	A	2.3
6	F	34	ASN	2.3
1	A	87	GLU	2.3
2	B	224	LYS	2.3
2	B	326	GLU	2.3
6	F	117	GLU	2.3
11	K	70	GLU	2.3
17	Q	81	GLU	2.3
24	X	86	GLU	2.3
27	1	31	LYS	2.3
12	L	17	SER	2.3
15	O	13	ASP	2.3
18	R	73	ASP	2.3
30	0	27	U	2.3
30	0	1234	U	2.3
30	0	1509	U	2.3
30	0	2563	U	2.3
2	B	218	TRP	2.3
13	M	31	TRP	2.3
30	0	353	G	2.3
30	0	579	G	2.3
30	0	716	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1837	G	2.3
30	0	2124	G	2.3
30	0	2293	G	2.3
30	0	2491	G	2.3
30	0	2763	G	2.3
30	0	2771	G	2.3
30	0	2842	G	2.3
3	C	178	GLN	2.3
8	H	10	ARG	2.3
13	M	155	GLN	2.3
13	M	177	GLY	2.3
18	R	120	GLY	2.3
21	U	4	ARG	2.3
26	Z	104	ARG	2.3
30	0	42	C	2.3
30	0	586	C	2.3
30	0	687	C	2.3
30	0	910	C	2.3
30	0	1735	C	2.3
30	0	2313	C	2.3
30	0	2790	C	2.3
30	0	2797	C	2.3
31	9	26	C	2.3
2	B	73	VAL	2.3
2	B	166	VAL	2.3
2	B	290	VAL	2.3
14	N	115	VAL	2.3
17	Q	29	ALA	2.3
18	R	30	ALA	2.3
23	W	118	LEU	2.3
29	3	67	LEU	2.3
29	3	9	THR	2.3
4	D	154	LYS	2.3
10	J	19	MET	2.3
11	K	59	LYS	2.3
23	W	153	MET	2.3
8	H	158	ASN	2.3
23	W	60	GLU	2.3
24	X	80	GLU	2.3
30	0	737	A	2.3
30	0	895	A	2.3
30	0	912	A	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2761	A	2.3
30	0	2814	A	2.3
1	A	122	SER	2.3
12	L	49	SER	2.3
18	R	85	SER	2.3
18	R	127	PRO	2.3
19	S	19	ASP	2.3
1	A	65	ARG	2.3
7	G	63	ARG	2.3
22	V	45	ARG	2.3
23	W	57	PRO	2.3
2	B	283	GLY	2.3
11	K	15	GLY	2.3
13	M	59	GLY	2.3
29	3	18	GLN	2.3
30	0	614	U	2.3
30	0	966	U	2.3
30	0	2003	U	2.3
30	0	2282	U	2.3
18	R	96	VAL	2.3
23	W	7	LEU	2.3
12	L	64	ILE	2.3
14	N	100	ALA	2.3
15	O	12	ALA	2.3
18	R	8	ALA	2.3
5	E	74	HIS	2.3
30	0	64	G	2.3
30	0	159	G	2.3
30	0	190	G	2.3
30	0	235	C	2.3
30	0	238	C	2.3
30	0	276	C	2.3
30	0	315	G	2.3
30	0	338	C	2.3
30	0	490	C	2.3
30	0	833	G	2.3
30	0	1216	G	2.3
30	0	1398	G	2.3
30	0	1894	C	2.3
30	0	1908	G	2.3
30	0	2114	C	2.3
30	0	2262	C	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2326	C	2.3
30	0	2385	G	2.3
30	0	2522	G	2.3
30	0	2609	G	2.3
30	0	2638	G	2.3
30	0	2782	G	2.3
30	0	2881	C	2.3
30	0	2911	C	2.3
31	9	49	G	2.3
31	9	53	G	2.3
3	C	94	THR	2.3
3	C	233	THR	2.3
4	D	25	MET	2.3
27	1	1	THR	2.3
3	C	6	TYR	2.3
10	J	114	GLU	2.3
11	K	13	GLU	2.3
25	Y	104	GLU	2.3
10	J	67	ASN	2.3
11	K	42	ASN	2.3
1	A	100	PRO	2.3
2	B	165	ARG	2.3
2	B	321	PRO	2.3
5	E	8	PRO	2.3
6	F	42	ARG	2.3
8	H	85	ASP	2.3
10	J	100	SER	2.3
10	J	108	PRO	2.3
13	M	76	ARG	2.3
14	N	134	ASP	2.3
17	Q	6	PRO	2.3
8	H	96	GLN	2.3
1	A	203	GLY	2.3
4	D	70	GLY	2.3
9	I	131	GLY	2.3
17	Q	50	GLY	2.3
23	W	111	GLY	2.3
30	0	70	A	2.3
30	0	177	A	2.3
30	0	241	A	2.3
30	0	513	A	2.3
30	0	520	A	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1236	A	2.3
30	0	2497	A	2.3
30	0	2902	A	2.3
27	1	50	TRP	2.3
7	G	24	VAL	2.3
2	B	203	ALA	2.2
19	S	32	ALA	2.2
28	2	6	ALA	2.2
28	2	23	ALA	2.2
29	3	11	CYS	2.2
30	0	176	U	2.2
30	0	1095	U	2.2
30	0	1205	U	2.2
30	0	1249	U	2.2
30	0	1740	U	2.2
30	0	2064	U	2.2
30	0	2424	U	2.2
16	P	36	THR	2.2
8	H	55	GLU	2.2
12	L	59	GLU	2.2
18	R	46	TYR	2.2
30	0	323	C	2.2
30	0	893	C	2.2
30	0	1428	C	2.2
30	0	1554	C	2.2
30	0	1816	C	2.2
30	0	1935	C	2.2
30	0	2261	C	2.2
30	0	2720	C	2.2
30	0	2824	C	2.2
30	0	2873	C	2.2
13	M	137	ASN	2.2
13	M	143	ASN	2.2
30	0	809	G	2.2
30	0	1121	G	2.2
30	0	1241	G	2.2
30	0	1619	G	2.2
30	0	1688	G	2.2
30	0	2073	G	2.2
30	0	2110	G	2.2
30	0	2357	G	2.2
30	0	2715	G	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	J	93	ARG	2.2
12	L	8	ARG	2.2
13	M	39	ARG	2.2
25	Y	227	ARG	2.2
26	Z	105	ARG	2.2
2	B	252	PRO	2.2
14	N	109	PRO	2.2
1	A	127	GLN	2.2
1	A	149	ASP	2.2
3	C	2	GLN	2.2
3	C	161	ASP	2.2
6	F	7	ASP	2.2
11	K	33	SER	2.2
11	K	119	GLN	2.2
13	M	157	ASP	2.2
20	T	68	ASP	2.2
25	Y	162	ASP	2.2
27	1	7	SER	2.2
28	2	46	ASP	2.2
29	3	66	ASP	2.2
2	B	210	GLY	2.2
3	C	53	GLY	2.2
13	M	162	GLY	2.2
5	E	161	VAL	2.2
8	H	136	LEU	2.2
20	T	77	VAL	2.2
1	A	146	LYS	2.2
3	C	3	ALA	2.2
5	E	56	ALA	2.2
6	F	10	ALA	2.2
8	H	92	LYS	2.2
13	M	91	ILE	2.2
14	N	7	LYS	2.2
18	R	59	PHE	2.2
30	0	1106	A	2.2
30	0	2067	A	2.2
30	0	2238	A	2.2
30	0	2356	A	2.2
30	0	2816	A	2.2
30	0	2841	A	2.2
31	9	3	A	2.2
5	E	93	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	H	128	ALA	2.2
16	P	11	ALA	2.2
17	Q	70	ALA	2.2
22	V	30	ALA	2.2
2	B	72	THR	2.2
2	B	295	THR	2.2
4	D	169	THR	2.2
5	E	77	THR	2.2
5	E	152	THR	2.2
6	F	65	GLU	2.2
14	N	72	GLU	2.2
25	Y	184	GLU	2.2
26	Z	102	THR	2.2
30	0	609	U	2.2
30	0	1583	U	2.2
30	0	1673	U	2.2
30	0	1915	U	2.2
30	0	2240	U	2.2
31	9	111	U	2.2
6	F	3	TYR	2.2
10	J	104	TYR	2.2
29	3	69	TYR	2.2
1	A	195	ASN	2.2
4	D	14	ARG	2.2
4	D	56	ARG	2.2
4	D	140	ARG	2.2
12	L	21	ARG	2.2
14	N	37	ARG	2.2
22	V	29	ASN	2.2
1	A	141	PRO	2.2
2	B	293	PRO	2.2
10	J	72	PRO	2.2
30	0	58	C	2.2
30	0	101	C	2.2
30	0	1083	C	2.2
30	0	1085	C	2.2
30	0	1906	C	2.2
30	0	2066	C	2.2
30	0	2281	C	2.2
2	B	170	SER	2.2
5	E	12	ASP	2.2
11	K	126	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	S	33	SER	2.2
14	N	34	LEU	2.2
16	P	43	LEU	2.2
17	Q	7	LEU	2.2
23	W	24	LEU	2.2
23	W	34	LEU	2.2
30	0	47	G	2.2
30	0	221	G	2.2
30	0	622	G	2.2
30	0	765	G	2.2
30	0	938	G	2.2
30	0	952	G	2.2
30	0	953	G	2.2
30	0	1048	G	2.2
30	0	1093	G	2.2
30	0	1443	G	2.2
30	0	2399	G	2.2
30	0	2639	G	2.2
30	0	2700	G	2.2
31	9	22	G	2.2
31	9	109	G	2.2
2	B	215	VAL	2.2
3	C	154	VAL	2.2
5	E	29	VAL	2.2
10	J	80	LYS	2.2
18	R	69	LYS	2.2
18	R	118	LYS	2.2
20	T	42	VAL	2.2
25	Y	228	VAL	2.2
3	C	163	HIS	2.2
10	J	78	ILE	2.2
27	1	28	HIS	2.2
3	C	77	ALA	2.2
5	E	140	ALA	2.2
10	J	8	ALA	2.2
18	R	77	ALA	2.2
1	A	152	CYS	2.2
9	I	89	GLU	2.2
11	K	91	GLU	2.2
14	N	18	THR	2.2
30	0	166	A	2.2
30	0	243	A	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	419	A	2.2
30	0	460	A	2.2
30	0	635	A	2.2
30	0	688	A	2.2
30	0	819	A	2.2
30	0	1501	A	2.2
30	0	1733	A	2.2
30	0	2074	A	2.2
30	0	2793	A	2.2
1	A	8	ARG	2.2
6	F	24	ARG	2.2
26	Z	41	ARG	2.2
30	0	22	U	2.2
30	0	137	U	2.2
30	0	1383	U	2.2
30	0	1883	U	2.2
30	0	1897	U	2.2
30	0	2550	U	2.2
30	0	2554	U	2.2
30	0	2648	U	2.2
8	H	142	ASN	2.2
8	H	15	PRO	2.2
5	E	15	GLN	2.2
1	A	12	GLY	2.2
2	B	208	GLY	2.2
2	B	291	ASP	2.2
5	E	37	ASP	2.2
8	H	78	LYS	2.2
10	J	113	GLY	2.2
15	O	88	LYS	2.2
19	S	10	VAL	2.2
3	C	194	PHE	2.2
17	Q	53	HIS	2.2
18	R	75	TRP	2.2
24	X	33	ILE	2.2
30	0	1011	C	2.2
30	0	1084	C	2.2
30	0	2243	C	2.2
30	0	2298	C	2.2
30	0	2317	C	2.2
30	0	2676	C	2.2
31	9	91	C	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	J	23	ALA	2.2
20	T	70	ALA	2.2
18	R	148	GLU	2.2
23	W	22	GLU	2.2
24	X	79	GLU	2.2
30	0	336	G	2.2
30	0	386	G	2.2
30	0	469	G	2.2
30	0	601	G	2.2
30	0	902	G	2.2
30	0	1065	G	2.2
30	0	1339	G	2.2
30	0	1370	G	2.2
30	0	1444	G	2.2
30	0	2136	G	2.2
30	0	2284	G	2.2
2	B	49	THR	2.2
13	M	92	THR	2.2
13	M	183	THR	2.2
23	W	68	THR	2.2
26	Z	97	THR	2.2
13	M	50	ARG	2.2
18	R	79	ARG	2.2
25	Y	216	ARG	2.2
8	H	47	PRO	2.2
10	J	107	ASN	2.2
30	0	113	A	2.2
30	0	236	A	2.2
30	0	1097	A	2.2
30	0	1242	A	2.2
30	0	2675	A	2.2
30	0	2775	A	2.2
31	9	45	A	2.2
19	S	55	GLN	2.2
8	H	159	LYS	2.2
18	R	126	LYS	2.2
29	3	34	LYS	2.2
30	0	1368	U	2.2
30	0	1371	U	2.2
30	0	1846	U	2.2
30	0	2004	U	2.2
30	0	2120	U	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2435	U	2.2
30	0	2598	U	2.2
2	B	299	GLY	2.2
12	L	120	LEU	2.2
27	1	2	GLY	2.2
1	A	194	MET	2.2
24	X	51	ASP	2.2
25	Y	132	ASP	2.2
1	A	137	VAL	2.2
2	B	188	HIS	2.2
11	K	57	VAL	2.2
15	O	59	VAL	2.2
2	B	242	TRP	2.1
4	D	164	ALA	2.1
8	H	146	ALA	2.1
24	X	57	ALA	2.1
1	A	28	GLU	2.1
11	K	2	GLU	2.1
11	K	100	GLU	2.1
18	R	20	GLU	2.1
23	W	86	GLU	2.1
24	X	45	GLU	2.1
1	A	164	ARG	2.1
1	A	235	ARG	2.1
12	L	67	ARG	2.1
16	P	41	ARG	2.1
18	R	19	ARG	2.1
18	R	132	ARG	2.1
19	S	31	ARG	2.1
27	1	17	THR	2.1
30	0	156	C	2.1
30	0	303	C	2.1
30	0	368	C	2.1
30	0	483	C	2.1
30	0	749	C	2.1
30	0	1384	C	2.1
30	0	1990	C	2.1
23	W	121	PRO	2.1
30	0	51	G	2.1
30	0	175	G	2.1
30	0	345	G	2.1
30	0	618	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	634	G	2.1
30	0	1108	G	2.1
30	0	1425	G	2.1
30	0	1557	G	2.1
30	0	2134	G	2.1
30	0	2543	G	2.1
30	0	2794	G	2.1
31	9	19	G	2.1
31	9	76	G	2.1
5	E	106	ASN	2.1
7	G	17	GLN	2.1
8	H	150	LYS	2.1
13	M	19	GLN	2.1
21	U	38	ASN	2.1
23	W	41	TYR	2.1
11	K	4	LEU	2.1
14	N	102	LEU	2.1
18	R	130	MET	2.1
18	R	147	LEU	2.1
22	V	11	MET	2.1
1	A	83	GLY	2.1
1	A	113	GLY	2.1
2	B	288	GLY	2.1
30	0	187	A	2.1
30	0	248	A	2.1
30	0	620	A	2.1
30	0	965	A	2.1
30	0	1078	A	2.1
30	0	2060	A	2.1
30	0	2327	A	2.1
30	0	2468	A	2.1
30	0	2513	A	2.1
30	0	2899	A	2.1
6	F	48	VAL	2.1
10	J	9	ASP	2.1
10	J	53	ILE	2.1
10	J	103	VAL	2.1
12	L	66	VAL	2.1
22	V	56	ILE	2.1
25	Y	217	ILE	2.1
30	0	398	U	2.1
30	0	517	U	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1266	U	2.1
30	0	1519	U	2.1
30	0	2265	U	2.1
30	0	2458	U	2.1
30	0	2650	U	2.1
10	J	30	ALA	2.1
19	S	14	ALA	2.1
27	1	54	ALA	2.1
8	H	173	GLU	2.1
10	J	15	ARG	2.1
24	X	49	ARG	2.1
1	A	41	THR	2.1
13	M	13	LYS	2.1
13	M	74	LYS	2.1
14	N	31	LYS	2.1
18	R	56	PRO	2.1
23	W	140	LYS	2.1
26	Z	101	LYS	2.1
30	0	515	C	2.1
30	0	557	C	2.1
2	B	243	ASN	2.1
2	B	320	GLN	2.1
25	Y	230	ASN	2.1
26	Z	74	GLN	2.1
30	0	1889	C	2.1
30	0	2061	C	2.1
30	0	2351	C	2.1
30	0	2575	C	2.1
5	E	83	GLY	2.1
6	F	27	GLY	2.1
23	W	136	GLY	2.1
25	Y	148	GLY	2.1
28	2	37	HIS	2.1
2	B	276	ASP	2.1
3	C	132	ASP	2.1
6	F	107	ASP	2.1
10	J	45	VAL	2.1
13	M	61	ILE	2.1
13	M	146	ASP	2.1
16	P	13	VAL	2.1
18	R	2	ILE	2.1
24	X	9	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
27	1	33	VAL	2.1
30	0	150	G	2.1
30	0	273	G	2.1
30	0	428	G	2.1
30	0	512	G	2.1
30	0	572	G	2.1
30	0	873	G	2.1
30	0	964	G	2.1
30	0	1110	G	2.1
30	0	1113	G	2.1
30	0	2256	G	2.1
30	0	2257	G	2.1
30	0	2286	G	2.1
26	Z	92	SER	2.1
16	P	51	ALA	2.1
3	C	158	GLU	2.1
5	E	110	GLU	2.1
30	0	43	U	2.1
30	0	63	U	2.1
30	0	73	U	2.1
30	0	98	A	2.1
30	0	121	U	2.1
30	0	205	U	2.1
30	0	215	A	2.1
30	0	463	A	2.1
30	0	489	A	2.1
30	0	495	A	2.1
30	0	507	A	2.1
30	0	522	U	2.1
30	0	673	U	2.1
30	0	876	A	2.1
30	0	1117	A	2.1
30	0	1124	A	2.1
30	0	1149	U	2.1
30	0	1358	A	2.1
30	0	1432	U	2.1
30	0	1447	U	2.1
30	0	2089	A	2.1
30	0	2095	A	2.1
30	0	2129	U	2.1
30	0	2300	A	2.1
30	0	2402	A	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2673	U	2.1
30	0	2677	A	2.1
30	0	2888	U	2.1
30	0	2913	A	2.1
31	9	39	U	2.1
31	9	65	A	2.1
2	B	229	ARG	2.1
4	D	51	ARG	2.1
13	M	104	ARG	2.1
20	T	52	ARG	2.1
3	C	12	THR	2.1
18	R	39	THR	2.1
1	A	171	LYS	2.1
3	C	123	LEU	2.1
7	G	67	LEU	2.1
23	W	116	LEU	2.1
7	G	64	ASN	2.1
18	R	94	ASN	2.1
1	A	208	HIS	2.1
2	B	167	GLY	2.1
10	J	69	TYR	2.1
10	J	133	GLY	2.1
21	U	16	GLY	2.1
24	X	40	HIS	2.1
25	Y	225	GLY	2.1
2	B	182	VAL	2.1
6	F	22	VAL	2.1
14	N	48	VAL	2.1
21	U	13	ILE	2.1
25	Y	190	VAL	2.1
30	0	298	C	2.1
30	0	421	C	2.1
30	0	494	C	2.1
30	0	558	C	2.1
30	0	585	C	2.1
30	0	1250	C	2.1
30	0	1613	C	2.1
30	0	1987	C	2.1
30	0	2071	C	2.1
30	0	2450	C	2.1
30	0	2498	C	2.1
30	0	2780	C	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	2795	C	2.1
31	9	41	C	2.1
20	T	116	ASP	2.1
25	Y	199	ASP	2.1
2	B	88	GLU	2.1
2	B	310	ARG	2.1
3	C	246	ARG	2.1
12	L	71	GLU	2.1
14	N	44	ARG	2.1
24	X	61	ARG	2.1
29	3	42	ARG	2.1
24	X	24	LYS	2.1
28	2	13	LYS	2.1
30	0	21	G	2.1
30	0	94	G	2.1
30	0	149	G	2.1
30	0	249	G	2.1
30	0	266	G	2.1
30	0	503	G	2.1
30	0	739	G	2.1
30	0	1063	G	2.1
30	0	1159	G	2.1
30	0	1322	G	2.1
30	0	1385	G	2.1
30	0	1416	G	2.1
30	0	2634	G	2.1
30	0	2855	G	2.1
31	9	7	G	2.1
2	B	211	THR	2.1
19	S	54	THR	2.1
30	0	90	A	2.1
30	0	247	A	2.1
30	0	625	U	2.1
30	0	1367	A	2.1
30	0	2690	U	2.1
30	0	2807	U	2.1
30	0	2820	A	2.1
30	0	2838	A	2.1
31	9	38	A	2.1
31	9	106	U	2.1
2	B	317	PRO	2.1
23	W	137	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	265	LEU	2.1
14	N	106	LEU	2.1
25	Y	229	LEU	2.1
14	N	54	GLY	2.1
23	W	43	GLY	2.1
6	F	40	ILE	2.1
18	R	51	ILE	2.1
24	X	31	ILE	2.1
25	Y	233	TYR	2.1
4	D	156	ARG	2.0
18	R	9	ASP	2.0
18	R	54	ASP	2.0
18	R	142	ASP	2.0
20	T	100	ASP	2.0
4	D	167	GLU	2.0
6	F	18	GLU	2.0
13	M	140	ALA	2.0
14	N	170	GLU	2.0
20	T	108	ARG	2.0
5	E	67	SER	2.0
6	F	51	ALA	2.0
14	N	39	SER	2.0
24	X	29	ALA	2.0
24	X	47	ALA	2.0
27	1	44	LYS	2.0
30	0	251	C	2.0
30	0	361	C	2.0
30	0	1015	C	2.0
30	0	2803	C	2.0
30	0	2821	C	2.0
31	9	30	C	2.0
13	M	164	THR	2.0
20	T	82	THR	2.0
2	B	78	PRO	2.0
3	C	151	GLN	2.0
4	D	97	GLN	2.0
10	J	139	LEU	2.0
13	M	58	GLN	2.0
14	N	179	LEU	2.0
20	T	103	LEU	2.0
30	0	125	U	2.0
30	0	142	G	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	184	G	2.0
30	0	225	G	2.0
30	0	362	G	2.0
30	0	452	G	2.0
30	0	475	G	2.0
30	0	549	A	2.0
30	0	885	G	2.0
30	0	892	G	2.0
30	0	1089	G	2.0
30	0	1090	A	2.0
30	0	1158	G	2.0
30	0	1859	A	2.0
30	0	1904	A	2.0
30	0	2123	A	2.0
30	0	2271	G	2.0
30	0	2433	A	2.0
30	0	2604	A	2.0
30	0	2679	G	2.0
31	9	21	G	2.0
13	M	14	ASN	2.0
22	V	44	GLY	2.0
14	N	82	TYR	2.0
27	1	48	TYR	2.0
2	B	129	ARG	2.0
11	K	121	PHE	2.0
13	M	64	ARG	2.0
14	N	176	ARG	2.0
25	Y	154	ARG	2.0
2	B	56	ASP	2.0
2	B	187	GLU	2.0
2	B	198	GLU	2.0
3	C	126	ASP	2.0
6	F	103	GLU	2.0
11	K	51	ASP	2.0
12	L	124	ASP	2.0
10	J	73	LYS	2.0
28	2	5	LYS	2.0
16	P	115	SER	2.0
10	J	82	THR	2.0
15	O	26	TRP	2.0
19	S	18	MET	2.0
1	A	54	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	95	PRO	2.0
2	B	261	GLN	2.0
6	F	55	GLN	2.0
18	R	61	GLN	2.0
18	R	145	LEU	2.0
30	0	82	C	2.0
30	0	906	C	2.0
30	0	1080	C	2.0
30	0	1365	C	2.0
30	0	2559	C	2.0
30	0	2819	C	2.0
30	0	2844	C	2.0
8	H	50	ILE	2.0
14	N	129	ILE	2.0
18	R	103	GLY	2.0
22	V	8	ILE	2.0
25	Y	129	ASN	2.0
30	0	172	U	2.0
30	0	647	U	2.0
30	0	840	U	2.0
30	0	1748	U	2.0
30	0	1817	U	2.0
30	0	2034	U	2.0
30	0	2473	U	2.0
1	A	225	VAL	2.0
5	E	170	ARG	2.0
19	S	41	VAL	2.0
25	Y	155	ARG	2.0
30	0	603	A	2.0
30	0	2010	A	2.0
30	0	2429	A	2.0
30	0	2447	A	2.0
30	0	2553	A	2.0
30	0	2805	A	2.0
31	9	93	A	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	OMU	0	2587	21/22	0.75	0.23	31,33,34,36	0
30	OMG	0	2588	24/25	0.83	0.19	30,31,35,36	0
30	UR3	0	2619	21/22	0.83	0.18	33,35,38,43	0
30	1MA	0	628	23/24	0.88	0.16	25,27,30,31	0
30	PSU	0	2621	20/21	0.89	0.16	30,32,37,37	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	9001	1/1	0.30	0.21	169,169,169,169	0
32	MG	0	8067	1/1	0.36	0.14	33,33,33,33	0
32	MG	0	8082	1/1	0.38	0.24	76,76,76,76	0
32	MG	0	8063	1/1	0.38	0.41	98,98,98,98	0
35	NA	0	8533	1/1	0.40	0.21	65,65,65,65	0
35	NA	0	8535	1/1	0.40	0.18	35,35,35,35	0
32	MG	0	8089	1/1	0.41	0.28	53,53,53,53	0
35	NA	0	8562	1/1	0.43	0.30	67,67,67,67	0
34	SR	0	9006	1/1	0.45	0.24	200,200,200,200	0
35	NA	0	8571	1/1	0.45	0.17	72,72,72,72	0
35	NA	0	8548	1/1	0.46	0.48	66,66,66,66	0
34	SR	0	8979	1/1	0.48	0.24	200,200,200,200	0
32	MG	Y	8086	1/1	0.50	0.20	40,40,40,40	0
34	SR	0	8919	1/1	0.51	0.25	144,144,144,144	0
34	SR	0	8944	1/1	0.51	0.25	148,148,148,148	0
35	NA	0	8517	1/1	0.52	0.29	38,38,38,38	0
32	MG	0	8092	1/1	0.52	0.21	40,40,40,40	0
34	SR	0	8988	1/1	0.53	0.20	144,144,144,144	0
34	SR	0	8971	1/1	0.54	0.27	172,172,172,172	0
35	NA	0	8518	1/1	0.55	0.41	76,76,76,76	0
34	SR	9	8968	1/1	0.55	0.23	178,178,178,178	0
35	NA	0	8570	1/1	0.55	0.28	40,40,40,40	0
34	SR	0	8996	1/1	0.55	0.33	200,200,200,200	0
32	MG	0	8033	1/1	0.56	0.25	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8035	1/1	0.56	0.27	58,58,58,58	0
35	NA	0	8558	1/1	0.58	0.21	36,36,36,36	0
34	SR	F	9005	1/1	0.59	0.18	130,130,130,130	0
32	MG	0	8066	1/1	0.60	0.15	53,53,53,53	0
34	SR	0	8947	1/1	0.60	0.31	160,160,160,160	0
32	MG	0	8044	1/1	0.60	0.15	40,40,40,40	0
32	MG	0	8079	1/1	0.60	0.34	67,67,67,67	0
32	MG	0	8017	1/1	0.60	0.13	29,29,29,29	0
34	SR	0	8938	1/1	0.60	0.20	175,175,175,175	0
32	MG	0	8010	1/1	0.61	0.13	34,34,34,34	0
32	MG	0	8071	1/1	0.61	0.24	56,56,56,56	0
35	NA	0	8509	1/1	0.61	0.17	64,64,64,64	0
32	MG	T	8057	1/1	0.62	0.20	54,54,54,54	0
34	SR	0	8967	1/1	0.62	0.25	145,145,145,145	0
32	MG	0	8055	1/1	0.62	0.12	28,28,28,28	0
35	NA	0	8557	1/1	0.62	0.34	57,57,57,57	0
33	CL	0	8814	1/1	0.63	0.47	62,62,62,62	0
35	NA	0	8561	1/1	0.64	0.42	71,71,71,71	0
34	SR	0	8983	1/1	0.64	0.19	183,183,183,183	0
34	SR	0	8957	1/1	0.64	0.19	200,200,200,200	0
34	SR	0	8993	1/1	0.64	0.34	173,173,173,173	0
32	MG	0	8083	1/1	0.65	0.12	30,30,30,30	0
34	SR	B	8987	1/1	0.65	0.33	200,200,200,200	0
34	SR	0	9000	1/1	0.65	0.24	171,171,171,171	0
32	MG	0	8049	1/1	0.65	0.18	53,53,53,53	0
32	MG	0	8062	1/1	0.65	0.24	68,68,68,68	0
34	SR	0	8965	1/1	0.65	0.20	125,125,125,125	0
35	NA	0	8574	1/1	0.65	0.29	63,63,63,63	0
35	NA	0	8508	1/1	0.66	0.27	54,54,54,54	0
32	MG	0	8038	1/1	0.66	0.14	74,74,74,74	0
33	CL	A	8809	1/1	0.66	0.28	65,65,65,65	0
34	SR	0	8991	1/1	0.66	0.19	176,176,176,176	0
35	NA	0	8566	1/1	0.66	0.62	40,40,40,40	0
34	SR	9	8980	1/1	0.66	0.26	154,154,154,154	0
35	NA	0	8502	1/1	0.66	0.21	78,78,78,78	0
35	NA	0	8506	1/1	0.66	0.23	74,74,74,74	0
32	MG	0	8065	1/1	0.67	0.14	37,37,37,37	0
35	NA	0	8560	1/1	0.67	0.31	58,58,58,58	0
35	NA	0	8525	1/1	0.67	0.23	91,91,91,91	0
34	SR	0	8997	1/1	0.67	0.37	189,189,189,189	0
34	SR	A	8977	1/1	0.68	0.20	147,147,147,147	0
34	SR	0	9004	1/1	0.68	0.29	200,200,200,200	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8573	1/1	0.68	0.20	78,78,78,78	0
35	NA	0	8526	1/1	0.68	0.18	31,31,31,31	0
34	SR	S	8961	1/1	0.69	0.22	124,124,124,124	0
35	NA	0	8523	1/1	0.69	0.26	62,62,62,62	0
34	SR	0	8954	1/1	0.69	0.17	94,94,94,94	0
34	SR	9	8978	1/1	0.69	0.20	150,150,150,150	0
35	NA	0	8565	1/1	0.69	0.26	65,65,65,65	0
35	NA	0	8501	1/1	0.70	0.18	30,30,30,30	0
34	SR	0	8953	1/1	0.70	0.19	130,130,130,130	0
34	SR	0	8960	1/1	0.70	0.20	138,138,138,138	0
34	SR	0	8964	1/1	0.70	0.19	131,131,131,131	0
32	MG	0	8036	1/1	0.70	0.13	40,40,40,40	0
35	NA	R	8532	1/1	0.70	0.23	58,58,58,58	0
35	NA	9	8572	1/1	0.70	0.40	88,88,88,88	0
35	NA	0	8521	1/1	0.71	0.15	42,42,42,42	0
34	SR	0	8903	1/1	0.71	0.16	53,53,53,53	0
35	NA	0	8529	1/1	0.71	0.16	35,35,35,35	0
34	SR	0	8958	1/1	0.72	0.14	99,99,99,99	0
34	SR	3	8999	1/1	0.72	0.17	95,95,95,95	0
33	CL	0	8812	1/1	0.73	0.20	35,35,35,35	0
32	MG	0	8040	1/1	0.73	0.22	69,69,69,69	0
32	MG	0	8034	1/1	0.73	0.15	28,28,28,28	0
34	SR	0	8974	1/1	0.73	0.41	155,155,155,155	0
35	NA	0	8559	1/1	0.73	0.26	74,74,74,74	0
35	NA	C	8503	1/1	0.74	0.14	32,32,32,32	0
34	SR	0	8920	1/1	0.74	0.23	106,106,106,106	0
34	SR	0	8926	1/1	0.74	0.20	145,145,145,145	0
34	SR	0	8918	1/1	0.74	0.15	73,73,73,73	0
34	SR	0	8959	1/1	0.74	0.14	142,142,142,142	0
34	SR	B	8950	1/1	0.75	0.20	108,108,108,108	0
34	SR	0	8911	1/1	0.75	0.14	70,70,70,70	0
32	MG	0	8037	1/1	0.75	0.40	77,77,77,77	0
34	SR	0	8982	1/1	0.75	0.34	186,186,186,186	0
32	MG	B	8042	1/1	0.75	0.19	48,48,48,48	0
34	SR	0	8985	1/1	0.75	0.17	137,137,137,137	0
33	CL	0	8816	1/1	0.75	0.17	62,62,62,62	0
35	NA	9	8543	1/1	0.75	0.22	53,53,53,53	0
32	MG	0	8018	1/1	0.75	0.18	37,37,37,37	0
35	NA	0	8553	1/1	0.76	0.39	70,70,70,70	0
32	MG	0	8001	1/1	0.76	0.10	27,27,27,27	0
34	SR	0	8989	1/1	0.76	0.26	182,182,182,182	0
34	SR	0	8937	1/1	0.76	0.15	101,101,101,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	8905	1/1	0.76	0.15	55,55,55,55	0
35	NA	0	8546	1/1	0.76	0.33	57,57,57,57	0
32	MG	0	8081	1/1	0.76	0.15	48,48,48,48	0
35	NA	0	8563	1/1	0.76	0.28	70,70,70,70	0
33	CL	N	8807	1/1	0.77	0.19	59,59,59,59	0
35	NA	0	8511	1/1	0.77	0.17	54,54,54,54	0
34	SR	0	8928	1/1	0.77	0.19	167,167,167,167	0
33	CL	J	8802	1/1	0.77	0.13	70,70,70,70	0
35	NA	0	8520	1/1	0.77	0.10	55,55,55,55	0
34	SR	A	8929	1/1	0.77	0.22	135,135,135,135	0
34	SR	0	8923	1/1	0.78	0.12	104,104,104,104	0
35	NA	0	8507	1/1	0.78	0.19	39,39,39,39	0
34	SR	0	8972	1/1	0.78	0.26	159,159,159,159	0
32	MG	0	8053	1/1	0.78	0.13	44,44,44,44	0
34	SR	3	8932	1/1	0.78	0.10	68,68,68,68	0
35	NA	0	8569	1/1	0.78	0.41	64,64,64,64	0
33	CL	0	8803	1/1	0.78	0.18	40,40,40,40	0
35	NA	M	8539	1/1	0.78	0.15	30,30,30,30	0
34	SR	0	8955	1/1	0.78	0.26	174,174,174,174	0
35	NA	S	8510	1/1	0.78	0.12	26,26,26,26	0
34	SR	0	8966	1/1	0.78	0.15	97,97,97,97	0
34	SR	0	8922	1/1	0.78	0.20	177,177,177,177	0
34	SR	0	8925	1/1	0.79	0.14	90,90,90,90	0
33	CL	R	8806	1/1	0.79	0.20	43,43,43,43	0
32	MG	0	8013	1/1	0.79	0.13	29,29,29,29	0
32	MG	0	8080	1/1	0.79	0.12	58,58,58,58	0
34	SR	0	8901	1/1	0.79	0.13	78,78,78,78	0
35	NA	0	8512	1/1	0.79	0.24	51,51,51,51	0
35	NA	0	8514	1/1	0.79	0.26	52,52,52,52	0
34	SR	0	8939	1/1	0.79	0.18	129,129,129,129	0
34	SR	0	8942	1/1	0.79	0.17	109,109,109,109	0
32	MG	0	8075	1/1	0.79	0.23	36,36,36,36	0
34	SR	0	9002	1/1	0.79	0.27	170,170,170,170	0
32	MG	0	8090	1/1	0.79	0.18	45,45,45,45	0
35	NA	0	8564	1/1	0.80	0.28	67,67,67,67	0
35	NA	0	8552	1/1	0.80	0.22	47,47,47,47	0
32	MG	9	8074	1/1	0.80	0.13	73,73,73,73	0
33	CL	0	8820	1/1	0.80	0.15	39,39,39,39	0
34	SR	0	8994	1/1	0.80	0.27	188,188,188,188	0
32	MG	0	8039	1/1	0.80	0.23	55,55,55,55	0
34	SR	0	8951	1/1	0.80	0.13	139,139,139,139	0
32	MG	0	8087	1/1	0.80	0.11	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	SR	9	9003	1/1	0.80	0.17	157,157,157,157	0
32	MG	0	8088	1/1	0.80	0.09	26,26,26,26	0
35	NA	0	8551	1/1	0.81	0.40	39,39,39,39	0
34	SR	0	8921	1/1	0.81	0.12	74,74,74,74	0
32	MG	K	8054	1/1	0.81	0.16	29,29,29,29	0
35	NA	0	8567	1/1	0.81	0.32	57,57,57,57	0
35	NA	0	8528	1/1	0.81	0.23	51,51,51,51	0
34	SR	R	8912	1/1	0.81	0.11	80,80,80,80	0
34	SR	0	8990	1/1	0.81	0.23	109,109,109,109	0
32	MG	0	8011	1/1	0.81	0.13	31,31,31,31	0
35	NA	0	8544	1/1	0.81	0.25	59,59,59,59	0
35	NA	0	8522	1/1	0.81	0.19	57,57,57,57	0
32	MG	A	8051	1/1	0.81	0.18	64,64,64,64	0
36	CD	U	8701	1/1	0.81	0.13	60,60,60,60	0
37	K	0	8401	1/1	0.81	0.49	149,149,149,149	0
37	K	0	8402	1/1	0.81	0.23	63,63,63,63	0
35	NA	0	8534	1/1	0.82	0.12	35,35,35,35	0
34	SR	0	9008	1/1	0.82	0.12	89,89,89,89	0
34	SR	0	8976	1/1	0.82	0.24	173,173,173,173	0
34	SR	0	8936	1/1	0.82	0.15	86,86,86,86	0
34	SR	0	8970	1/1	0.82	0.14	121,121,121,121	0
35	NA	0	8549	1/1	0.82	0.31	42,42,42,42	0
34	SR	0	8924	1/1	0.82	0.16	140,140,140,140	0
34	SR	0	8943	1/1	0.82	0.18	113,113,113,113	0
35	NA	0	8519	1/1	0.82	0.31	35,35,35,35	0
34	SR	0	8914	1/1	0.82	0.17	105,105,105,105	0
34	SR	0	8956	1/1	0.83	0.15	167,167,167,167	0
32	MG	0	8061	1/1	0.83	0.16	29,29,29,29	0
32	MG	0	8014	1/1	0.83	0.12	15,15,15,15	0
32	MG	0	8085	1/1	0.83	0.32	82,82,82,82	0
32	MG	0	8077	1/1	0.83	0.15	24,24,24,24	0
35	NA	0	8524	1/1	0.83	0.23	56,56,56,56	0
34	SR	0	8917	1/1	0.83	0.20	114,114,114,114	0
32	MG	0	8016	1/1	0.83	0.11	36,36,36,36	0
32	MG	0	8068	1/1	0.83	0.32	58,58,58,58	0
35	NA	0	8513	1/1	0.83	0.23	44,44,44,44	0
35	NA	0	8530	1/1	0.83	0.29	59,59,59,59	0
35	NA	Q	8540	1/1	0.83	0.23	46,46,46,46	0
36	CD	Z	8703	1/1	0.83	0.11	64,64,64,64	0
32	MG	0	8069	1/1	0.83	0.40	61,61,61,61	0
34	SR	0	8902	1/1	0.83	0.13	54,54,54,54	0
35	NA	0	8541	1/1	0.84	0.31	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8026	1/1	0.84	0.12	35,35,35,35	0
32	MG	0	8028	1/1	0.84	0.09	23,23,23,23	0
34	SR	0	8909	1/1	0.84	0.15	88,88,88,88	0
35	NA	0	8575	1/1	0.84	0.31	72,72,72,72	0
32	MG	0	8009	1/1	0.84	0.12	29,29,29,29	0
32	MG	A	8050	1/1	0.84	0.10	48,48,48,48	0
34	SR	0	8915	1/1	0.84	0.16	114,114,114,114	0
32	MG	0	8059	1/1	0.84	0.10	33,33,33,33	0
32	MG	0	8021	1/1	0.84	0.16	32,32,32,32	0
34	SR	0	8946	1/1	0.84	0.16	110,110,110,110	0
32	MG	0	8046	1/1	0.85	0.09	28,28,28,28	0
35	NA	0	8547	1/1	0.85	0.30	36,36,36,36	0
35	NA	0	8516	1/1	0.85	0.21	31,31,31,31	0
33	CL	0	8815	1/1	0.85	0.15	66,66,66,66	0
34	SR	0	8934	1/1	0.85	0.14	100,100,100,100	0
33	CL	0	8822	1/1	0.86	0.26	80,80,80,80	0
34	SR	0	8910	1/1	0.86	0.23	87,87,87,87	0
34	SR	0	9007	1/1	0.86	0.44	181,181,181,181	0
33	CL	J	8821	1/1	0.86	0.19	63,63,63,63	0
33	CL	M	8818	1/1	0.86	0.12	30,30,30,30	0
34	SR	0	8992	1/1	0.86	0.17	123,123,123,123	0
32	MG	0	8045	1/1	0.86	0.10	29,29,29,29	0
34	SR	0	8940	1/1	0.86	0.14	79,79,79,79	0
32	MG	0	8072	1/1	0.86	0.10	68,68,68,68	0
33	CL	0	8817	1/1	0.86	0.12	60,60,60,60	0
34	SR	0	8998	1/1	0.86	0.22	134,134,134,134	0
34	SR	0	8927	1/1	0.86	0.18	167,167,167,167	0
35	NA	0	8537	1/1	0.86	0.10	39,39,39,39	0
32	MG	0	8022	1/1	0.86	0.12	24,24,24,24	0
34	SR	0	8933	1/1	0.86	0.17	134,134,134,134	0
35	NA	0	8556	1/1	0.87	0.32	35,35,35,35	0
32	MG	0	8070	1/1	0.87	0.16	65,65,65,65	0
32	MG	0	8064	1/1	0.87	0.10	37,37,37,37	0
34	SR	A	8930	1/1	0.87	0.14	87,87,87,87	0
32	MG	0	8078	1/1	0.87	0.20	41,41,41,41	0
35	NA	J	8538	1/1	0.87	0.17	58,58,58,58	0
34	SR	0	8935	1/1	0.87	0.11	75,75,75,75	0
35	NA	0	8531	1/1	0.87	0.15	33,33,33,33	0
36	CD	O	8705	1/1	0.87	0.10	81,81,81,81	0
35	NA	0	8550	1/1	0.87	0.16	42,42,42,42	0
32	MG	0	8060	1/1	0.87	0.11	42,42,42,42	0
34	SR	0	8963	1/1	0.87	0.09	177,177,177,177	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	8973	1/1	0.87	0.09	124,124,124,124	0
34	SR	0	8931	1/1	0.88	0.13	108,108,108,108	0
35	NA	0	8515	1/1	0.88	0.11	33,33,33,33	0
34	SR	1	8913	1/1	0.88	0.12	82,82,82,82	0
34	SR	0	8981	1/1	0.88	0.15	140,140,140,140	0
32	MG	0	8030	1/1	0.88	0.22	53,53,53,53	0
32	MG	0	8015	1/1	0.88	0.17	36,36,36,36	0
34	SR	0	8969	1/1	0.88	0.30	143,143,143,143	0
34	SR	0	8949	1/1	0.89	0.11	105,105,105,105	0
33	CL	B	8819	1/1	0.89	0.16	49,49,49,49	0
33	CL	J	8801	1/1	0.89	0.16	65,65,65,65	0
32	MG	0	8032	1/1	0.89	0.08	29,29,29,29	0
34	SR	1	8952	1/1	0.89	0.14	70,70,70,70	0
33	CL	0	8813	1/1	0.89	0.18	45,45,45,45	0
32	MG	0	8020	1/1	0.89	0.11	37,37,37,37	0
34	SR	0	8916	1/1	0.89	0.11	107,107,107,107	0
34	SR	0	8975	1/1	0.89	0.17	146,146,146,146	0
32	MG	0	8004	1/1	0.89	0.09	26,26,26,26	0
32	MG	0	8041	1/1	0.89	0.09	21,21,21,21	0
34	SR	0	8962	1/1	0.89	0.38	157,157,157,157	0
33	CL	Q	8811	1/1	0.89	0.15	57,57,57,57	0
35	NA	0	8542	1/1	0.89	0.17	53,53,53,53	0
34	SR	0	8904	1/1	0.89	0.10	49,49,49,49	0
34	SR	0	8948	1/1	0.89	0.13	101,101,101,101	0
32	MG	0	8093	1/1	0.90	0.12	35,35,35,35	0
34	SR	0	8906	1/1	0.90	0.08	51,51,51,51	0
34	SR	0	8907	1/1	0.90	0.09	58,58,58,58	0
32	MG	0	8052	1/1	0.90	0.14	40,40,40,40	0
32	MG	0	8056	1/1	0.90	0.14	48,48,48,48	0
34	SR	0	8986	1/1	0.90	0.22	200,200,200,200	0
36	CD	1	8702	1/1	0.90	0.09	53,53,53,53	0
32	MG	0	8005	1/1	0.90	0.14	25,25,25,25	0
35	NA	0	8505	1/1	0.90	0.35	36,36,36,36	0
33	CL	0	8805	1/1	0.91	0.09	50,50,50,50	0
32	MG	0	8073	1/1	0.91	0.13	57,57,57,57	0
34	SR	0	8945	1/1	0.91	0.14	113,113,113,113	0
34	SR	0	8995	1/1	0.91	0.14	140,140,140,140	0
33	CL	L	8810	1/1	0.91	0.12	57,57,57,57	0
35	NA	0	8554	1/1	0.91	0.29	50,50,50,50	0
33	CL	O	8808	1/1	0.91	0.13	63,63,63,63	0
35	NA	0	8536	1/1	0.91	0.07	43,43,43,43	0
35	NA	0	8555	1/1	0.92	0.17	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8504	1/1	0.92	0.18	39,39,39,39	0
32	MG	0	8025	1/1	0.92	0.07	16,16,16,16	0
32	MG	0	8031	1/1	0.92	0.08	45,45,45,45	0
32	MG	0	8003	1/1	0.92	0.10	28,28,28,28	0
34	SR	0	8984	1/1	0.92	0.09	106,106,106,106	0
32	MG	0	8024	1/1	0.92	0.15	50,50,50,50	0
35	NA	0	8545	1/1	0.92	0.17	30,30,30,30	0
32	MG	0	8029	1/1	0.92	0.19	40,40,40,40	0
34	SR	0	8941	1/1	0.93	0.11	104,104,104,104	0
32	MG	0	8091	1/1	0.93	0.13	43,43,43,43	0
32	MG	0	8023	1/1	0.93	0.09	27,27,27,27	0
32	MG	0	8019	1/1	0.93	0.12	24,24,24,24	0
33	CL	3	8804	1/1	0.93	0.10	58,58,58,58	0
34	SR	0	8908	1/1	0.94	0.12	87,87,87,87	0
32	MG	0	8076	1/1	0.94	0.13	29,29,29,29	0
35	NA	0	8527	1/1	0.94	0.17	43,43,43,43	0
32	MG	0	8043	1/1	0.94	0.12	47,47,47,47	0
32	MG	0	8007	1/1	0.95	0.07	28,28,28,28	0
35	NA	0	8568	1/1	0.96	0.10	37,37,37,37	0
36	CD	3	8704	1/1	0.96	0.06	62,62,62,62	0
32	MG	0	8058	1/1	0.96	0.08	18,18,18,18	0
32	MG	0	8048	1/1	0.96	0.13	20,20,20,20	0
32	MG	0	8002	1/1	0.97	0.04	26,26,26,26	0
32	MG	0	8027	1/1	0.97	0.08	35,35,35,35	0
32	MG	0	8008	1/1	0.97	0.22	18,18,18,18	0
32	MG	0	8084	1/1	0.97	0.11	30,30,30,30	0
32	MG	0	8006	1/1	0.97	0.06	34,34,34,34	0
32	MG	0	8047	1/1	0.98	0.10	45,45,45,45	0
32	MG	0	8012	1/1	0.99	0.05	16,16,16,16	0

6.5 Other polymers

There are no such residues in this entry.