



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:09 AM UTC

PDB ID : 3CCV / pdb_00003ccv
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2616A
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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

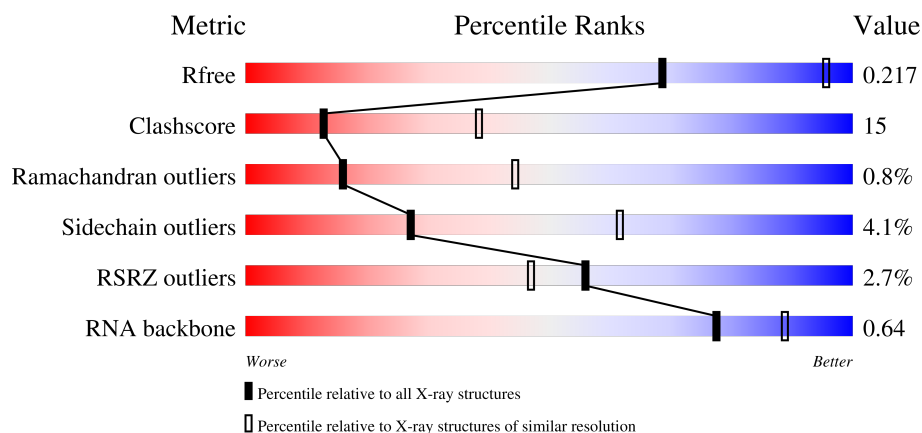
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	2% 65% 29% 5%
2	B	338	% 60% 35% .
3	C	246	68% 28% .
4	D	177	16% 48% 27% . 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
33	CL	J	8801	-	-	X	-
34	SR	0	9006	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99121 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			59019	26349	10873	19052	2745			

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

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

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	0	87	Total	Mg	0	0
			87	87		
32	9	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (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	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	0	10	Total Cl 10 10	0	0

- Molecule 34 is STRONTIUM ION (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	Y	1	Total Sr 1 1	0	0
34	1	2	Total Sr 2 2	0	0
34	3	1	Total Sr 1 1	0	0
34	0	94	Total Sr 94 94	0	0

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

- Molecule 38 is water.

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

Continued on next page...

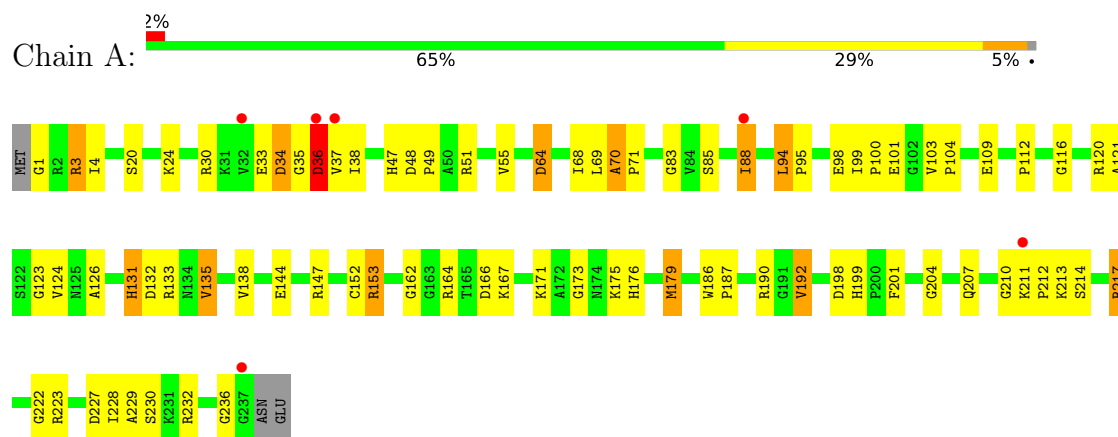
Continued from previous page...

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

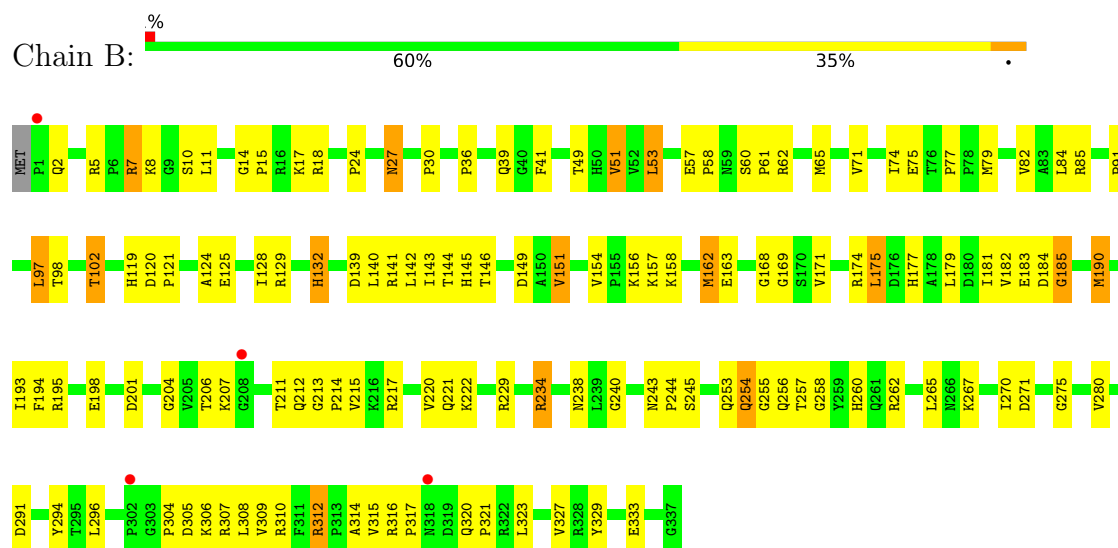
3 Residue-property plots [i](#)

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

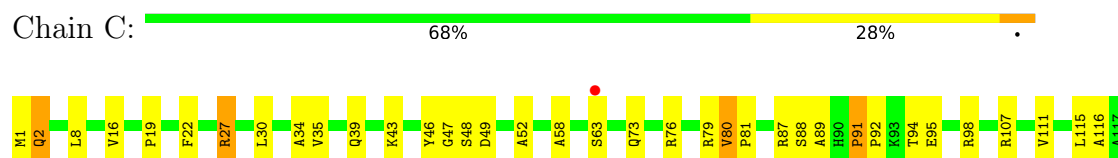
• Molecule 1: 50S ribosomal protein L2P



• Molecule 2: 50S ribosomal protein L3P

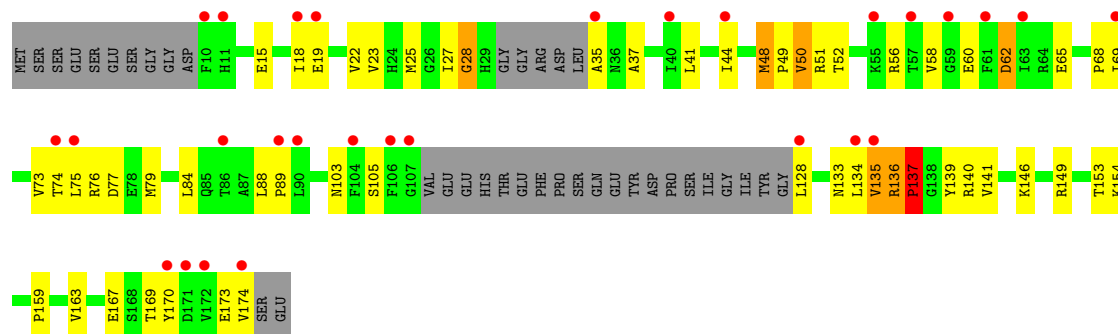


• Molecule 3: 50S ribosomal protein L4P

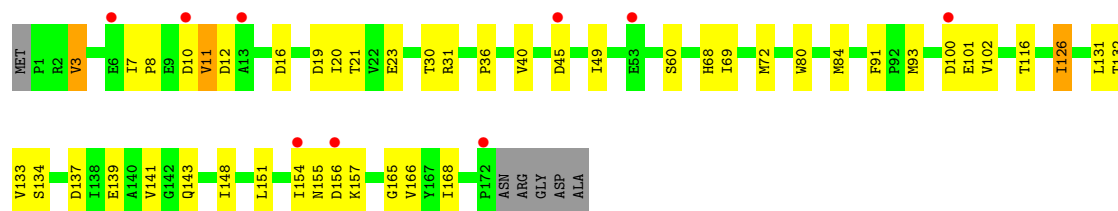




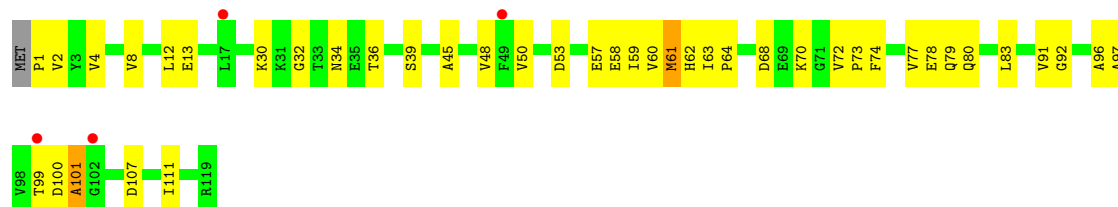
• Molecule 4: 50S ribosomal protein L5P



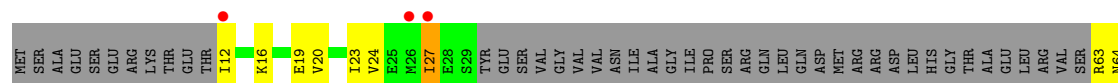
• Molecule 5: 50S ribosomal protein L6P



• Molecule 6: 50S ribosomal protein L7Ae

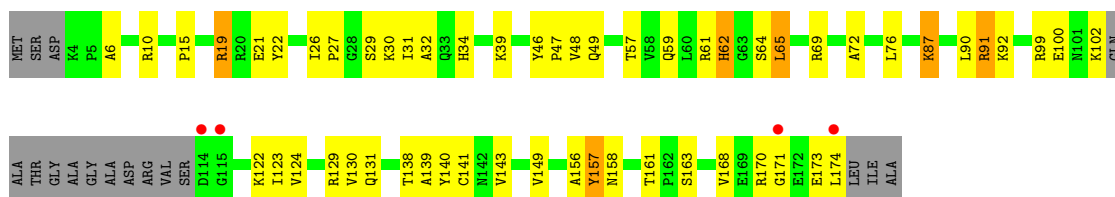


• Molecule 7: 50S ribosomal protein L10E

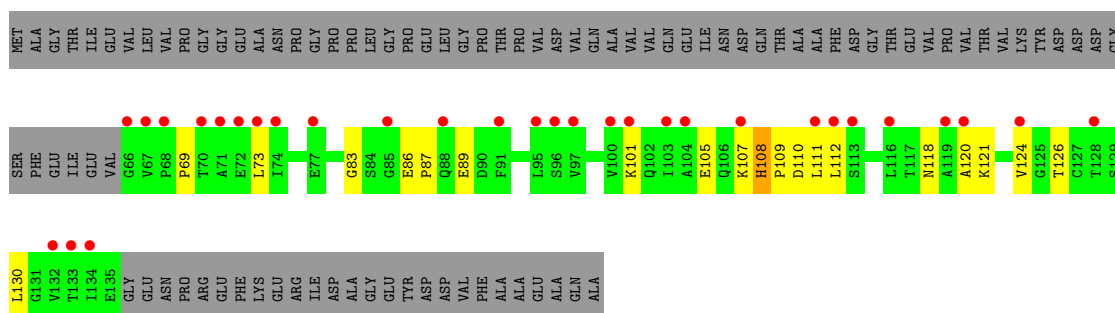




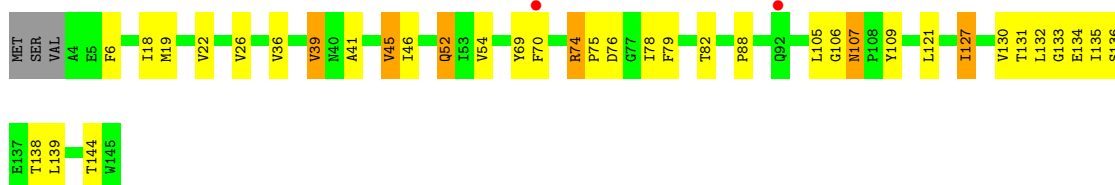
- Molecule 8: 50S ribosomal protein L10e



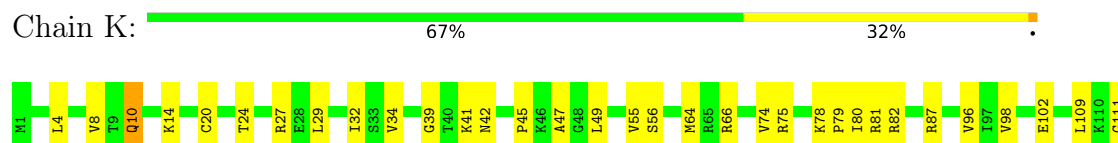
- Molecule 9: 50S ribosomal protein L11P



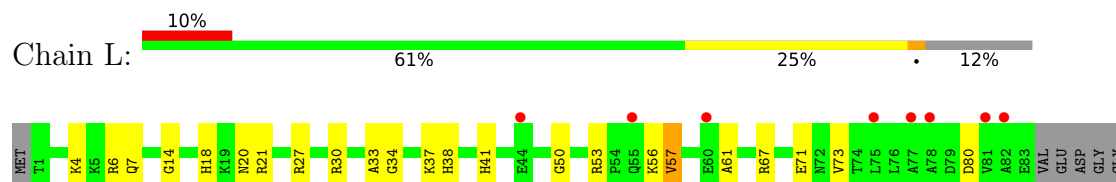
- Molecule 10: 50S ribosomal protein L13P



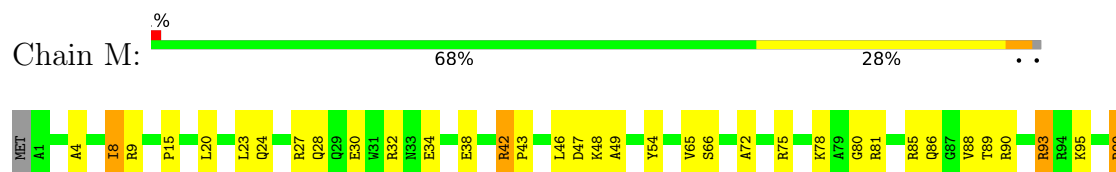
- Molecule 11: 50S ribosomal protein L14P



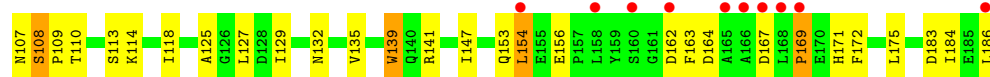
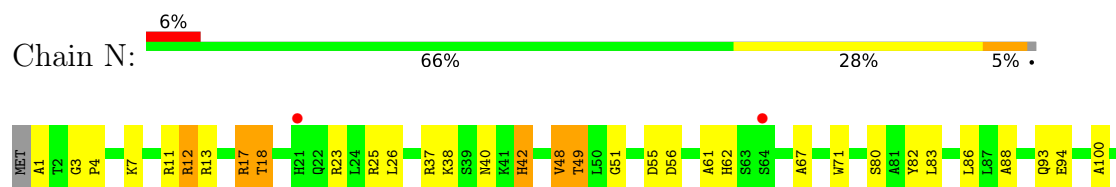
- Molecule 12: 50S ribosomal protein L15P



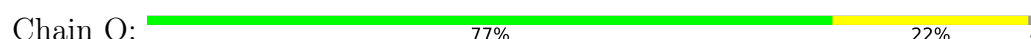
- Molecule 13: 50S ribosomal protein L15e



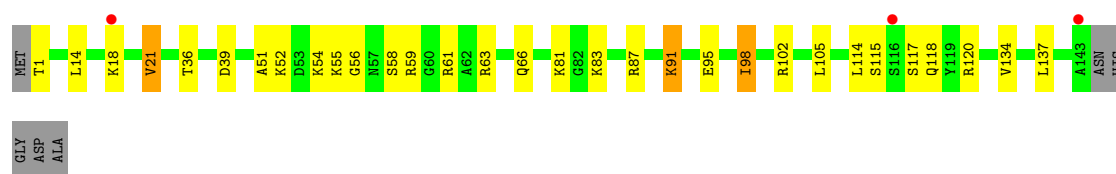
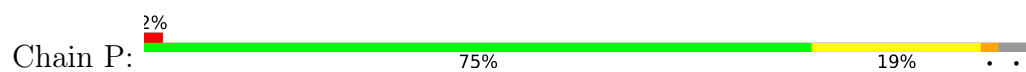
- Molecule 14: 50S ribosomal protein L18P



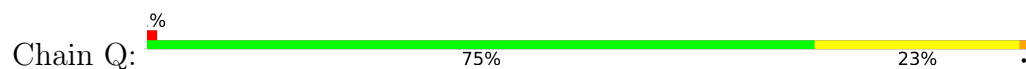
- Molecule 15: 50S ribosomal protein L18e



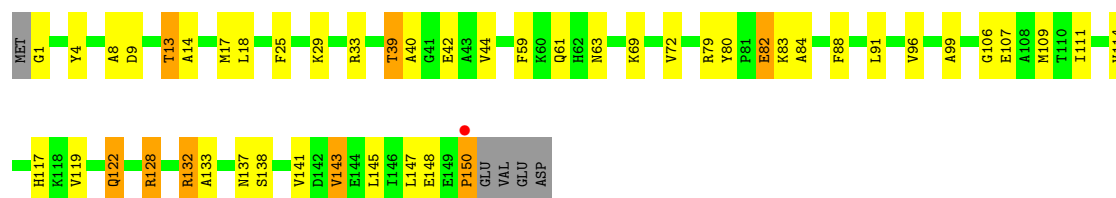
- Molecule 16: 50S ribosomal protein L19e



- Molecule 17: 50S ribosomal protein L21e



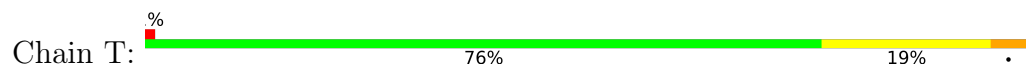
- Molecule 18: 50S ribosomal protein L22P



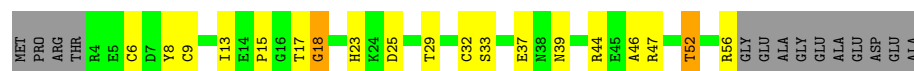
- Molecule 19: 50S ribosomal protein L23P



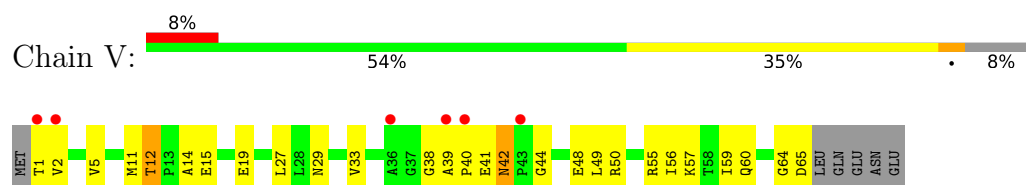
- Molecule 20: 50S ribosomal protein L24P



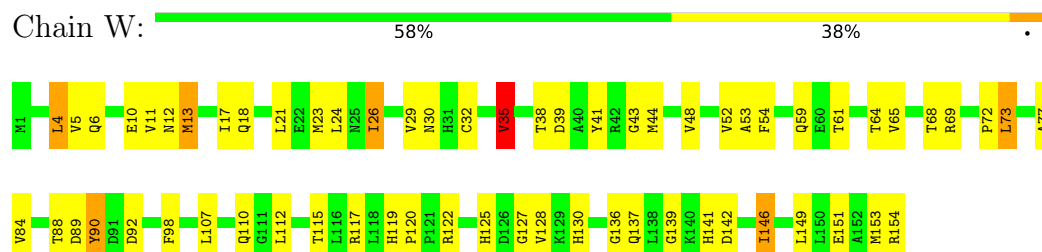
- Molecule 21: 50S ribosomal protein L24e



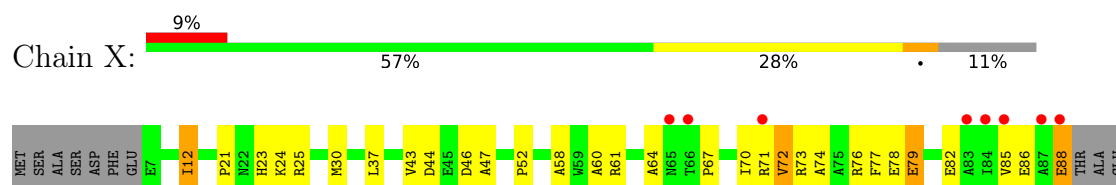
- Molecule 22: 50S ribosomal protein L29P



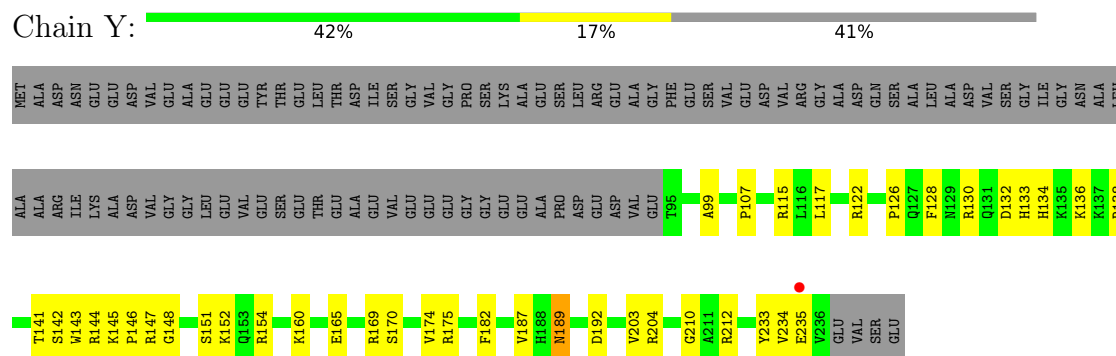
- Molecule 23: 50S ribosomal protein L30P



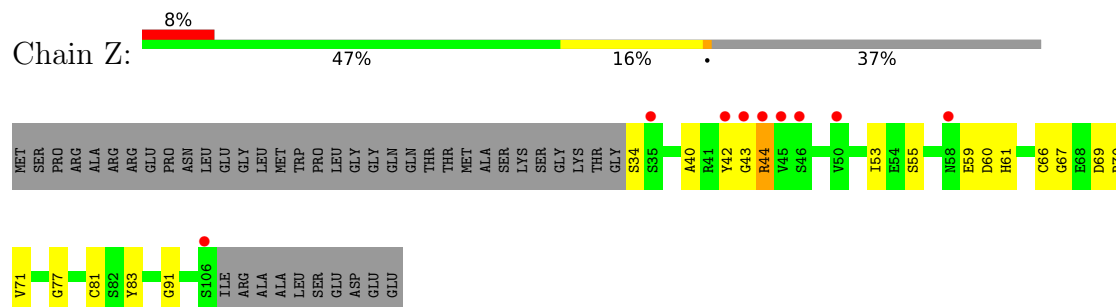
- Molecule 24: 50S ribosomal protein L31e



- Molecule 25: 50S ribosomal protein L32e

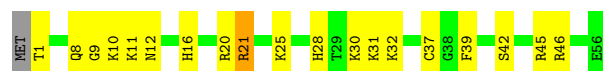


- Molecule 26: 50S ribosomal protein L37Ae

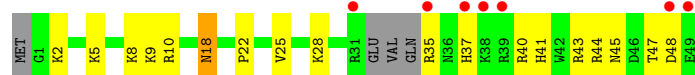


- Molecule 27: 50S ribosomal protein L37e

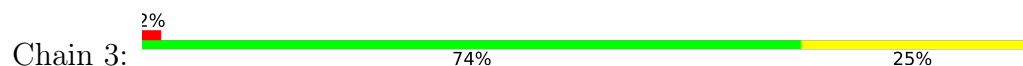




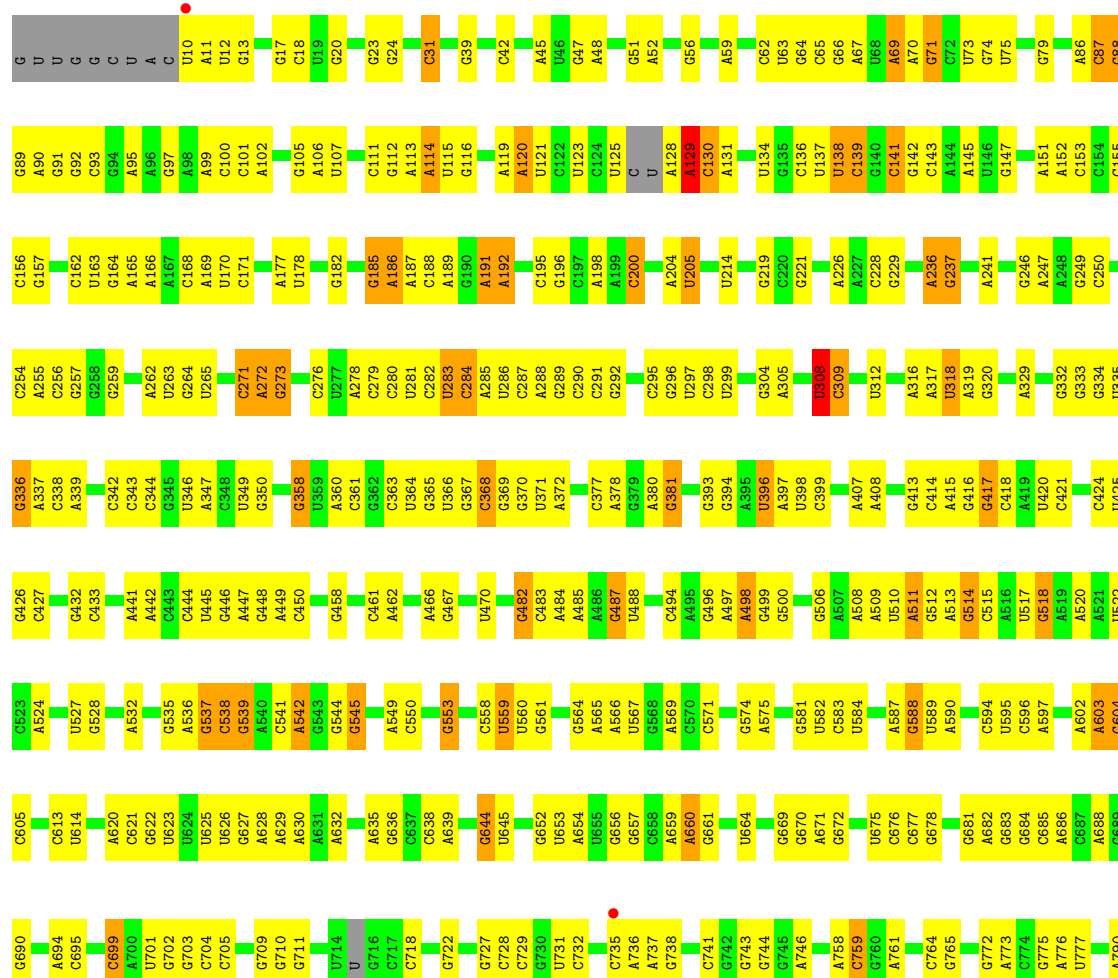
- Molecule 28: 50S ribosomal protein L39e



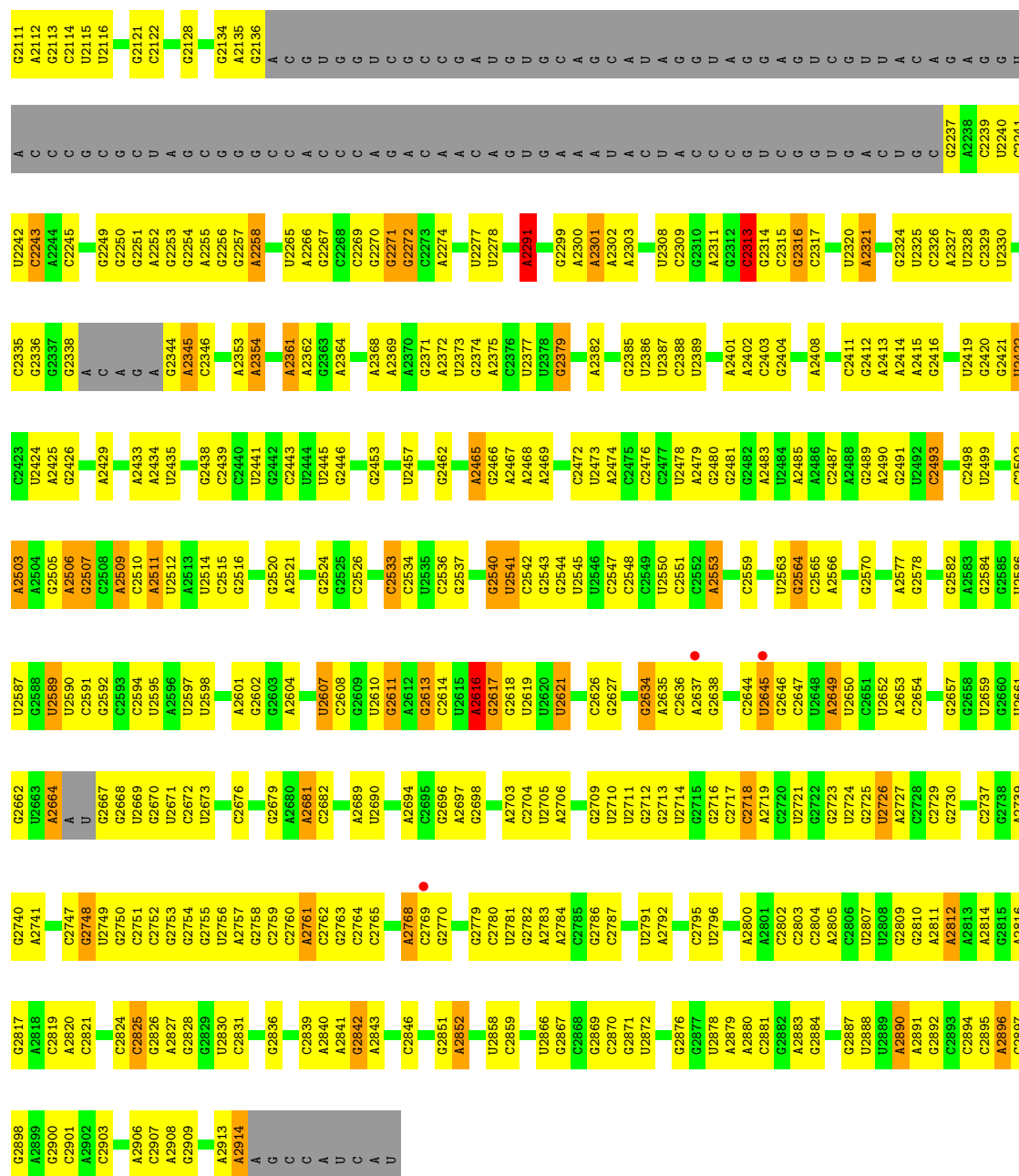
- Molecule 29: 50S ribosomal protein L44E



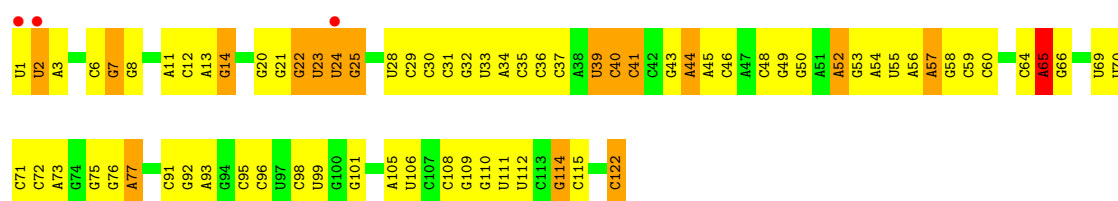
- Molecule 30: 23S RIBOSOMAL RNA



U2008	G1926	A1938	A1742	A1641	C1553	A1471	G1385	G1295	C1213	G1143	U1056	C	A875	A791
G2009	G1926	A1839	G1743	A1642	C1553	C1472	G1386	U1298	G1214	G1149	A1057	C	A876	G792
A2010	A1927	A1840	G1752	G1649	A1559	U1473	G1387	G1299	G1215	A1150	A1058	G	A877	A793
G2011		C1841		C1650	U	A1474		G1300	G1216	A1151	G1059	C	G878	U794
U2012	A1930	A1845	A1755	G1655	C1562	G1475	G1391	U1304	U1218	A1152	A882	U	A796	G795
G2013	A1931	U1945	G1756	U1654	C1565	C1477	A1392	U1305	U1219	G1153	U1066	C	A797	A797
A2022	C1940	G1849	G1760	G1655	C1566	U1478	C1395	U1306	U1220	G1154	A1067	C	C803	C803
A2030	A1941	U1850	G1761	A1656	C1567		C1396	A1307		G1155		G	C804	C804
C2031	A1942	G1850	U1761	G1665	G1567	A1482	C1397	A1308	G1224	G1158	G1072	A	A895	G805
U2032	C1943	G1851	C1762	G1666	U1568	C1483	C1398	U1309	C1225	G1159	G1074	A	A896	A806
G2033	A1852	C1853	C1763	U1569	U1569	G1484	A1399	U1310		G1160	G1075	G	A897	A807
U2034	C1946	C1854	U1766	A1667	U1574	A1485	C1400	G1311	C1229	A1161	G1076	G	C898	A808
G1947	G1948	U1855	U1767	U1668	C1574	A1486	G1401	G1312	A1230	G1162	G1077	A	C899	A809
G1948		C1856	A1767	G1669	C1575	A1494	A1406	A1313	U1234	G1163	A1078	G		G810
A2039		A1857	C1769	A1670	U1577	C1495	A1407	A1314	U1237	U1164	A1079	U	G902	A811
G2044	G1951	U1677	U1770	U1583	U1577	A1496	A1408	G1315	U1244	G1165	C1080	C	C905	A812
A		A1678	U1771	C1584		G1497	G1409	G1316	A1246	A1166	A1081	G		C813
C		C1679	C1772	C1585					C1238	G1167		G	A912	C814
U		A1773	G1774	C1586		A1501	G1415	A1321	G1239	C1168	C1084	C	A912	U815
A		A1778	G1774	C1587		A1502	G1416	G1322	A1242	U1170	G1087	A	C920	G816
U		U1779	G1774	U1587		A1503	G1417	G1322	C1243	A1171	A1088	C	G921	G817
G		A1685	G1774	G1588		U1505	U1418	A1326	C1245	G1172		A	A923	G820
A		C1686	G1774	G1589		U1506	U1419		A1246	A1173		C999	U821	U821
C		C1687	G1774				U1422	C1331	U1249	A1174		C1000	C822	U823
C		C1692	G1774	C1593		U1511	A1423	C1332	C1250	G1175		C1001	U827	A827
C		C1692	G1774	C1594		G1512	A1424	C1334	C1251	U1180		A1006	G834	G834
U1964	U1964	A1701	C1787	C1595		A1515	A1425	C1334	A1252	A1181		A1007	U835	U835
C1965	U1966	U1702	G1789	U1596		U1516	C1426	G1339	C1268	C1182		C1008	A840	U840
U1966		U1702	G1790	A1597		C1517	A1427	G1340	G1269	C1183		U1009	G941	G941
G1970	G1970	G1706	U1791	U1598			G1430	A1341		C1184		C1010	U942	A841
G1971	G1971	G1707		A1603		G1520	G1430	C1342	A1261	U1185		A1013	A943	A943
U1972	U1972	G1707		G1604		C1521	A1434	C1343	G1260	U1187		A1014	G944	G944
A1973	A1973	A1710		G1605		A1522	U1435		U1266	A1188		C1015	U945	U945
G1974	G1974	A1711		A1606		G1523	U1436	A1352	C1267	U1189		U1016	C847	C847
C1975	C1975	A1712		A1607		U1524	U1436	C1353	G1268	A1190		A1016	C848	C848
G1976	G1976	A1713		C1613		G1525	U1440	C1360	C1269	A1191		G1021	U947	U947
G1977	G1977	C1714		G1614		A1526	G1441	C1360	G1269	A1192		A1022	U948	U948
G1979	G1979	C1715		A1615		A1527	G1442	G1363	C1273	A1193		C1023	U950	U950
C2088	C2088	A1716		A1616		G1528	G1443	G1364	A1274	A1194		G1024	A951	A951
A2089	A2089	A1717		C1617		G1529	G1444	C1365	U1274				G952	G853
G2090	G2090	U1722		G1622			G1445	C1366	C1275	U1198		G1027	G953	G854
U1905	U1905	G1723		C1623		G1535	U1446	G1370		A1199		U1028	G958	U855
C1906	C1906	U1724		A1624		C1536	U1447	U1371	U1278	A1200		U1029	G959	G856
U1907	U1907	C1725		U1625		U1537	U1447	A1372	A1280	C1201		G958	A857	A857
G1908	G1908	U1725		A1626		C1538	C1451	G1373	C1281	A1202		U1041	U858	U858
A1909	A1909	G1730		A1627		U1539	C1451	C1374		G1203			G960	
U1915	U1915	G1731		G1627			C1456	G1374	A1286	C1204			A961	U862
C1916	C1916	A1732		A1632		G1543	U1457	A1375	U1287	A1199		C1044	G963	G863
G1917	G1917	A1733		C1633		U1544	U1457	G1376	A1287	A1205		G1045	G968	G868
U1918	U1918	G1734		G1634		C1545	U1461	C1377	U1288	A1207		C1046	G969	G869
A1919	A1919	C1735		G1634		G1546	C1462	G1378	G1289	C1208		U1336	U970	U970
C1920	C1920	U1735		U1635		A1547	C1463	C1379	G1290	C1209		G1137	G	G
A1921	A1921	G1739		G1636		U1548	U1464	A1379	A1291	G1210		G1138	U	U
U1922	U1922	U1740		A1637		C1549	C1464	U1380		G1211		C1140	G	G
G2110	G2110	U1741				G1552	A1470	C1384	A1294	C1212			U	U



• 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	211.75Å 299.01Å 574.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 2.90 49.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (49.99-2.90) 92.1 (49.99-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.175 , 0.225 0.171 , 0.217	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.0	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	0.94	EDS
Total number of atoms	99121	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

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

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, SR, NA, PSU, MG, CL, OMG, UR3, K, CD, 1MA

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	0.43	0/1786	1.01	9/2408 (0.4%)
2	B	0.41	0/2690	1.03	17/3652 (0.5%)
3	C	0.46	0/1885	0.99	8/2552 (0.3%)
4	D	0.41	0/1111	0.98	8/1498 (0.5%)
5	E	0.40	0/1382	0.88	1/1880 (0.1%)
6	F	0.40	0/901	0.95	4/1224 (0.3%)
7	G	0.37	0/241	0.89	1/324 (0.3%)
8	H	0.40	0/1302	0.97	4/1743 (0.2%)
9	I	0.38	0/526	0.91	0/716
10	J	0.42	0/1136	0.96	2/1530 (0.1%)
11	K	0.42	0/1004	0.99	2/1351 (0.1%)
12	L	0.38	0/1130	0.96	5/1509 (0.3%)
13	M	0.43	0/1582	0.92	6/2116 (0.3%)
14	N	0.38	0/1474	1.08	12/1999 (0.6%)
15	O	0.44	0/874	0.95	5/1181 (0.4%)
16	P	0.39	0/1147	0.83	0/1528
17	Q	0.42	0/749	1.04	5/1005 (0.5%)
18	R	1.29	7/1172 (0.6%)	1.39	9/1578 (0.6%)
19	S	0.38	0/648	0.88	2/875 (0.2%)
20	T	0.40	0/958	1.02	8/1289 (0.6%)
21	U	0.40	0/417	0.84	1/562 (0.2%)
22	V	0.41	0/502	0.96	2/675 (0.3%)
23	W	0.48	0/1219	0.99	3/1655 (0.2%)
24	X	0.44	0/664	1.01	4/895 (0.4%)
25	Y	0.44	0/1146	0.93	1/1536 (0.1%)
26	Z	0.39	0/584	0.97	1/781 (0.1%)
27	1	0.44	0/438	0.89	1/578 (0.2%)
28	2	0.40	0/401	0.79	0/529
29	3	0.38	0/771	0.84	4/1024 (0.4%)
30	0	0.38	0/65956	0.60	17/102865 (0.0%)
31	9	0.37	0/2904	0.58	2/4526 (0.0%)
All	All	0.41	7/98700 (0.0%)	0.73	144/147584 (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
18	R	1	0
23	W	0	1
30	0	0	29
All	All	1	30

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.50	2.87	1.49
18	R	150	PRO	CA-C	-17.28	1.16	1.52
18	R	150	PRO	CG-CD	13.49	1.96	1.50
18	R	150	PRO	N-CA	13.02	1.66	1.47
18	R	150	PRO	C-O	11.74	1.47	1.23
18	R	150	PRO	N-CD	10.77	1.62	1.47
18	R	150	PRO	CA-CB	7.67	1.68	1.53

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-28.63	55.71	110.10
18	R	150	PRO	N-CA-C	-20.10	61.85	112.10
18	R	150	PRO	N-CA-CB	12.27	116.50	103.00
18	R	150	PRO	CA-N-CD	12.05	128.87	112.00
14	N	163	PHE	N-CA-C	-11.78	98.71	113.55
17	Q	17	LYS	N-CA-C	-9.35	98.34	109.93
20	T	52	ARG	N-CA-C	8.30	124.22	113.18
1	A	222	GLY	N-CA-C	-8.02	105.00	113.58
4	D	136	ARG	CA-C-N	7.96	129.79	119.84
4	D	136	ARG	C-N-CA	7.96	129.79	119.84
2	B	175	LEU	N-CA-C	-7.86	102.66	111.14
2	B	222	LYS	N-CA-C	-7.78	98.37	110.42
3	C	236	THR	N-CA-C	-7.51	99.36	110.48
4	D	15	GLU	CA-C-N	7.15	128.78	119.84
4	D	15	GLU	C-N-CA	7.15	128.78	119.84
14	N	169	PRO	N-CA-C	-7.02	105.08	113.86
20	T	3	GLN	CA-C-N	6.95	126.47	119.24
20	T	3	GLN	C-N-CA	6.95	126.47	119.24
1	A	133	ARG	N-CA-C	-6.87	104.93	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	141	VAL	N-CA-C	6.86	118.36	108.48
1	A	166	ASP	N-CA-C	6.80	119.53	111.71
24	X	77	PHE	N-CA-C	6.78	116.82	107.73
2	B	265	LEU	N-CA-C	6.61	119.25	110.53
7	G	27	ILE	N-CA-C	-6.57	106.58	111.90
23	W	35	VAL	N-CA-C	6.57	115.43	107.61
14	N	51	GLY	CA-C-N	6.52	126.75	119.32
14	N	51	GLY	C-N-CA	6.52	126.75	119.32
30	O	1942	A	C5'-C4'-C3'	6.49	125.73	116.00
14	N	42	HIS	N-CA-C	6.45	118.98	109.69
20	T	54	ASP	N-CA-C	-6.43	105.40	113.18
31	9	39	U	N1-C1'-C2'	6.42	121.63	112.00
18	R	150	PRO	CA-CB-CG	-6.41	92.32	104.50
30	O	1504	A	N9-C1'-C2'	6.41	121.62	112.00
8	H	163	SER	N-CA-C	-6.41	101.90	110.55
18	R	150	PRO	CA-C-O	-6.40	99.79	119.00
25	Y	143	TRP	N-CA-C	6.38	119.53	109.96
8	H	10	ARG	N-CA-C	6.36	118.21	111.28
4	D	170	TYR	N-CA-C	6.34	120.40	111.52
27	1	21	ARG	N-CA-C	6.34	119.14	111.40
14	N	48	VAL	N-CA-C	6.29	116.97	108.17
13	M	89	THR	N-CA-C	6.25	119.07	111.82
6	F	79	GLN	N-CA-C	6.13	119.39	109.40
19	S	27	ALA	N-CA-C	-6.10	98.78	108.73
3	C	192	ILE	N-CA-C	6.09	116.94	108.89
3	C	134	ASP	N-CA-C	-6.06	104.87	112.93
29	3	55	VAL	CA-C-N	6.06	127.41	119.84
29	3	55	VAL	C-N-CA	6.06	127.41	119.84
30	O	2726	U	N1-C1'-C2'	6.05	121.08	112.00
30	O	1120	U	C5'-C4'-C3'	-5.93	107.11	116.00
2	B	120	ASP	CA-C-N	5.91	125.61	119.05
2	B	120	ASP	C-N-CA	5.91	125.61	119.05
8	H	161	THR	N-CA-C	5.87	120.88	113.25
29	3	43	ASN	N-CA-C	5.86	120.12	113.15
10	J	107	ASN	CA-C-N	5.86	125.47	119.56
10	J	107	ASN	C-N-CA	5.86	125.47	119.56
3	C	89	ALA	N-CA-C	5.85	118.16	111.02
30	O	1592	G	N9-C1'-C2'	5.85	120.78	112.00
12	L	7	GLN	N-CA-C	5.83	118.58	111.82
30	O	834	G	C2'-C3'-O3'	-5.80	105.00	113.70
30	O	2316	G	C5'-C4'-C3'	-5.79	106.52	115.20
2	B	151	VAL	CA-C-N	5.79	125.32	119.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	151	VAL	C-N-CA	5.79	125.32	119.19
4	D	135	VAL	N-CA-C	5.78	114.75	107.70
3	C	175	LYS	N-CA-C	5.78	118.21	110.35
3	C	219	ASN	N-CA-C	5.76	118.24	109.95
2	B	193	ILE	N-CA-C	5.74	116.55	111.90
6	F	8	VAL	CA-C-N	5.70	125.63	119.76
6	F	8	VAL	C-N-CA	5.70	125.63	119.76
1	A	135	VAL	N-CA-C	5.69	116.87	108.45
15	O	4	ASN	CA-C-N	5.69	125.36	119.05
15	O	4	ASN	C-N-CA	5.69	125.36	119.05
2	B	143	ILE	N-CA-C	-5.66	102.22	109.30
24	X	12	ILE	N-CA-C	5.64	113.46	107.76
30	0	2291	A	N9-C1'-C2'	5.63	120.44	112.00
15	O	43	VAL	N-CA-C	5.62	116.39	108.36
17	Q	49	ASN	N-CA-C	5.60	118.81	110.52
22	V	42	ASN	CA-C-N	5.60	126.84	119.84
22	V	42	ASN	C-N-CA	5.60	126.84	119.84
14	N	108	SER	CA-C-N	5.59	126.83	119.84
14	N	108	SER	C-N-CA	5.59	126.83	119.84
15	O	69	VAL	N-CA-C	5.58	116.52	108.48
2	B	102	THR	N-CA-C	5.56	115.75	108.07
1	A	70	ALA	N-CA-C	5.55	117.66	109.50
30	0	921	G	N9-C1'-C2'	5.54	120.31	112.00
17	Q	84	ILE	N-CA-C	5.53	115.91	108.17
1	A	64	ASP	N-CA-C	5.52	117.71	109.59
12	L	145	LEU	N-CA-C	-5.50	105.20	111.14
3	C	80	VAL	CA-C-N	5.49	126.70	119.84
3	C	80	VAL	C-N-CA	5.49	126.70	119.84
29	3	67	LEU	N-CA-C	5.48	118.01	109.52
12	L	73	VAL	N-CA-C	5.46	115.67	110.42
1	A	228	ILE	N-CA-C	5.44	116.02	108.84
2	B	82	VAL	N-CA-C	5.42	117.87	111.09
13	M	125	ARG	N-CA-C	5.41	121.08	113.02
11	K	111	GLY	CA-C-N	5.38	125.38	120.21
11	K	111	GLY	C-N-CA	5.38	125.38	120.21
30	0	2301	A	N9-C1'-C2'	5.38	120.08	112.00
17	Q	47	VAL	CA-C-N	5.38	124.72	118.85
17	Q	47	VAL	C-N-CA	5.38	124.72	118.85
2	B	323	LEU	N-CA-C	5.31	117.57	110.35
26	Z	42	TYR	N-CA-C	5.30	122.09	110.80
5	E	11	VAL	N-CA-C	5.29	117.17	108.97
14	N	3	GLY	CA-C-N	5.27	124.60	118.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	3	GLY	C-N-CA	5.27	124.60	118.85
30	O	920	C	C2'-C3'-O3'	-5.27	105.79	113.70
2	B	157	LYS	N-CA-C	-5.27	107.51	114.31
12	L	20	ASN	N-CA-C	5.27	119.21	111.04
30	O	2291	A	C4'-C3'-O3'	-5.27	105.10	113.00
1	A	24	LYS	N-CA-C	5.23	119.14	111.04
18	R	137	ASN	N-CA-C	5.22	118.51	110.42
24	X	60	ALA	N-CA-C	5.22	117.37	111.11
30	O	308	U	C2'-C3'-O3'	-5.19	105.92	113.70
20	T	78	THR	N-CA-C	5.18	117.28	109.41
19	S	66	VAL	N-CA-C	5.17	115.54	107.99
4	D	137	PRO	N-CA-C	5.16	123.10	112.47
30	O	2313	C	C5'-C4'-C3'	5.16	123.73	116.00
4	D	77	ASP	CB-CA-C	-5.15	110.65	116.63
2	B	213	GLY	CA-C-N	5.15	124.76	119.05
2	B	213	GLY	C-N-CA	5.15	124.76	119.05
14	N	153	GLN	N-CA-C	-5.14	102.73	110.70
21	U	18	GLY	N-CA-C	5.14	120.84	112.61
31	9	65	A	N9-C1'-C2'	5.14	119.71	112.00
12	L	57	VAL	N-CA-C	-5.14	107.97	112.90
2	B	154	VAL	CA-C-N	5.13	124.75	119.05
2	B	154	VAL	C-N-CA	5.13	124.75	119.05
15	O	66	GLY	N-CA-C	5.13	125.35	113.18
6	F	62	HIS	N-CA-C	5.13	117.77	111.82
20	T	14	ALA	CA-C-N	5.10	125.37	119.92
20	T	14	ALA	C-N-CA	5.10	125.37	119.92
30	O	2616	A	C2'-C3'-O3'	-5.09	101.86	109.50
20	T	72	ILE	N-CA-C	5.09	117.35	108.95
30	O	138	U	C2'-C3'-O3'	-5.08	106.09	113.70
24	X	79	GLU	N-CA-C	5.07	116.50	111.07
18	R	122	GLN	N-CA-C	-5.05	99.57	108.20
1	A	213	LYS	N-CA-C	5.04	117.66	111.82
30	O	129	A	C2'-C3'-O3'	5.04	121.25	113.70
13	M	8	ILE	N-CA-C	-5.03	105.64	110.72
8	H	143	VAL	N-CA-C	5.02	115.63	110.36
23	W	35	VAL	CA-C-N	5.02	124.92	119.85
23	W	35	VAL	C-N-CA	5.02	124.92	119.85
14	N	18	THR	N-CA-C	5.01	116.56	108.34
13	M	42	ARG	CA-C-N	5.01	124.92	119.76
13	M	42	ARG	C-N-CA	5.01	124.92	119.76
13	M	121	GLY	N-CA-C	5.00	119.17	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain
30	0	1430	G	Sidechain
30	0	1819	G	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	205	U	Sidechain
30	0	221	G	Sidechain
30	0	2308	U	Sidechain
30	0	2313	C	Sidechain
30	0	246	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2607	U	Sidechain
30	0	2673	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	795	G	Sidechain
30	0	817	G	Sidechain
30	0	868	G	Sidechain
30	0	952	G	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	74	0
2	B	2625	0	2532	111	0
3	C	1860	0	1813	56	0
4	D	1094	0	1085	39	0
5	E	1357	0	1266	37	0
6	F	890	0	843	29	0
7	G	240	0	231	9	0
8	H	1282	0	1292	40	0
9	I	519	0	500	21	0
10	J	1120	0	1098	42	0
11	K	994	0	1027	41	0
12	L	1118	0	1076	38	0
13	M	1558	0	1573	52	0
14	N	1445	0	1401	54	0
15	O	865	0	873	23	0
16	P	1136	0	1123	25	0
17	Q	735	0	729	18	0
18	R	1149	0	1122	43	0
19	S	641	0	605	13	0
20	T	950	0	924	22	0
21	U	410	0	364	17	0
22	V	499	0	511	21	0
23	W	1196	0	1137	70	0
24	X	654	0	653	23	0
25	Y	1130	0	1133	40	0
26	Z	573	0	531	15	0
27	1	431	0	426	25	0
28	2	396	0	413	17	0
29	3	755	0	728	15	0
30	0	59019	0	29809	1377	0
31	9	2599	0	1325	96	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	10	0	0	1	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	94	0	0	0	0
34	1	2	0	0	0	0
34	3	1	0	0	0	0
34	9	2	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	67	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5910	0	0	205	0
38	1	54	0	0	6	0
38	2	44	0	0	1	0
38	3	69	0	0	2	0
38	9	142	0	0	10	0
38	A	112	0	0	7	0
38	B	149	0	0	12	0
38	C	185	0	0	17	0
38	D	49	0	0	4	0
38	E	45	0	0	4	0
38	F	26	0	0	3	0
38	G	17	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	67	0	0	4	0
38	I	8	0	0	1	0
38	J	51	0	0	2	0
38	K	51	0	0	2	0
38	L	89	0	0	8	0
38	M	133	0	0	4	0
38	N	61	0	0	7	0
38	O	39	0	0	3	0
38	P	62	0	0	1	0
38	Q	45	0	0	2	0
38	R	81	0	0	4	0
38	S	32	0	0	3	0
38	T	35	0	0	3	0
38	U	29	0	0	2	0
38	V	15	0	0	2	0
38	W	67	0	0	6	0
38	X	26	0	0	4	0
38	Y	98	0	0	5	0
38	Z	32	0	0	1	0
All	All	99121	0	59909	2259	0

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

All (2259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.43
30:0:1160:G:C5'	30:0:1161:A:H5'	1.74	1.18
30:0:871:G:C8	30:0:871:G:H5'	1.80	1.15
30:0:1160:G:H5'	30:0:1161:A:C5'	1.74	1.15
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.12
30:0:871:G:H5'	30:0:871:G:H8	1.07	1.11
14:N:37:ARG:NH1	31:9:6:C:H5''	1.63	1.09
30:0:1559:A:H1'	38:0:5862:HOH:O	1.53	1.08
30:0:1205:U:H2'	30:0:1206:U:H5''	1.31	1.07
30:0:2717:C:C2'	30:0:2718:C:H5''	1.84	1.07
30:0:1701:A:H4'	30:0:1702:U:H5''	1.38	1.05
30:0:2717:C:H2'	30:0:2718:C:H5''	1.34	1.05
31:9:56:A:C2'	31:9:57:A:H5''	1.86	1.05
31:9:56:A:H2'	31:9:57:A:H5''	1.08	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:3:THR:HG22	30:0:656:G:H5'	1.37	1.02
30:0:2291:A:C8	30:0:2309:C:H5'	1.95	1.02
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.41	1.01
31:9:76:G:H3'	31:9:77:A:H5''	1.41	1.00
10:J:82:THR:HG23	30:0:1242:A:H5'	1.41	0.98
30:0:282:C:H1'	30:0:368:C:N4	1.79	0.98
30:0:1666:C:O2'	30:0:1667:A:H5''	1.64	0.98
30:0:1474:C:H6	30:0:1474:C:H5'	1.29	0.97
30:0:545:G:H5'	30:0:545:G:H8	1.24	0.97
13:M:171:ARG:HD3	30:0:156:C:H5''	1.44	0.96
30:0:1187:U:HO2'	30:0:1189:A:H2	0.98	0.96
2:B:162:MET:HE3	2:B:310:ARG:HD3	1.48	0.95
30:0:870:G:H2'	30:0:871:G:H5''	1.48	0.95
30:0:1625:U:H4'	38:0:4666:HOH:O	1.67	0.95
30:0:871:G:H8	30:0:871:G:C5'	1.81	0.94
11:K:10:GLN:HE21	11:K:10:GLN:H	1.06	0.93
4:D:154:LYS:H	4:D:154:LYS:HD2	1.34	0.93
30:0:1205:U:H2'	30:0:1206:U:C5'	1.99	0.93
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.82	0.92
30:0:2812:A:H2	30:0:2814:A:H62	1.11	0.92
30:0:1116:U:O2'	30:0:1118:A:H2	1.51	0.92
30:0:542:A:H5'	30:0:542:A:H8	1.35	0.92
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.10	0.92
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.49	0.92
30:0:506:G:H22	30:0:509:A:C5'	1.82	0.92
3:C:236:THR:HG22	3:C:239:ALA:H	1.31	0.91
30:0:2010:A:H2'	38:0:5957:HOH:O	1.69	0.91
30:0:2533:C:H5'	30:0:2533:C:H6	1.34	0.90
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.54	0.90
30:0:69:A:H5'	30:0:69:A:C8	2.07	0.90
30:0:1184:C:H1'	38:0:7462:HOH:O	1.71	0.90
30:0:877:G:H5'	30:0:878:G:OP1	1.72	0.90
30:0:1603:A:H5'	30:0:1605:G:O4'	1.71	0.90
16:P:115:SER:H	16:P:118:GLN:HE21	1.18	0.90
15:O:3:THR:CG2	30:0:656:G:H5'	2.02	0.89
30:0:381:G:H5''	38:0:4318:HOH:O	1.72	0.89
30:0:853:C:H3'	38:0:4550:HOH:O	1.72	0.89
30:0:2908:A:H2'	30:0:2909:G:O4'	1.73	0.89
30:0:1474:C:H5'	30:0:1474:C:C6	2.09	0.88
30:0:282:C:O2'	30:0:283:U:H5'	1.73	0.88
30:0:2541:U:H5'	30:0:2541:U:H6	1.37	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.18	0.88
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.56	0.88
30:0:541:C:H2'	30:0:542:A:H5''	1.55	0.88
30:0:272:A:H3'	38:0:7525:HOH:O	1.74	0.88
30:0:541:C:C2'	30:0:542:A:H5''	2.04	0.88
30:0:69:A:H5'	30:0:69:A:H8	1.39	0.87
30:0:1878:G:H1'	38:0:6119:HOH:O	1.74	0.87
30:0:2783:A:H3'	38:0:5234:HOH:O	1.75	0.87
2:B:238:ASN:HD22	2:B:240:GLY:H	1.22	0.87
30:0:1667:A:H8	30:0:1667:A:H5'	1.39	0.86
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.57	0.86
30:0:1835:U:H5	30:0:1840:A:N7	1.74	0.86
30:0:1118:A:H8	30:0:1118:A:H3'	1.39	0.86
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.58	0.85
30:0:2644:C:O2'	30:0:2645:U:H5'	1.76	0.85
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.58	0.85
30:0:1205:U:C2'	30:0:1206:U:H5''	2.06	0.85
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.59	0.85
30:0:1979:G:H2'	38:0:3289:HOH:O	1.73	0.85
28:2:18:ASN:HD21	28:2:40:ARG:H	1.24	0.84
30:0:1118:A:H3'	30:0:1118:A:C8	2.11	0.84
14:N:37:ARG:HH12	31:9:6:C:H5''	1.43	0.84
30:0:1666:C:C2'	30:0:1667:A:H5''	2.07	0.84
30:0:2506:A:O2'	30:0:2507:G:H8	1.59	0.84
30:0:1372:A:H3'	38:0:7186:HOH:O	1.78	0.84
3:C:1:MET:HG2	3:C:2:GLN:H	1.42	0.84
30:0:2769:C:C2'	30:0:2770:G:H5'	2.08	0.84
31:9:92:G:H2'	31:9:93:A:C8	2.13	0.84
30:0:1183:C:N4	30:0:1184:C:H41	1.76	0.83
30:0:182:G:H5'	38:0:5160:HOH:O	1.79	0.83
30:0:2635:A:O2'	30:0:2636:C:H5'	1.79	0.83
31:9:29:C:H2'	31:9:30:C:H5'	1.60	0.83
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.59	0.83
30:0:559:U:H6	30:0:559:U:H5'	1.43	0.83
30:0:506:G:H22	30:0:509:A:H5'	1.44	0.82
23:W:88:THR:HB	38:W:6679:HOH:O	1.78	0.82
30:0:1119:G:H22	30:0:1246:A:H2	1.25	0.82
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.25	0.82
30:0:1701:A:H5'	38:0:6284:HOH:O	1.80	0.82
30:0:545:G:H5'	30:0:545:G:C8	2.12	0.82
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2586:U:H3	30:0:2592:G:H22	1.26	0.81
11:K:39:GLY:HA2	38:0:5223:HOH:O	1.79	0.81
31:9:14:G:H5'	31:9:14:G:H8	1.45	0.81
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.63	0.81
30:0:2502:C:C2'	30:0:2503:A:H5'	2.11	0.81
30:0:2502:C:H2'	30:0:2503:A:H5'	1.61	0.81
30:0:2506:A:HO2'	30:0:2507:G:H8	0.83	0.81
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.62	0.81
30:0:1119:G:N2	30:0:1246:A:C2	2.48	0.80
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.77	0.80
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.46	0.80
30:0:1175:G:H1'	30:0:1193:A:H2'	1.63	0.80
30:0:363:C:H1'	38:0:5282:HOH:O	1.82	0.80
30:0:2896:A:H5''	38:0:6099:HOH:O	1.81	0.80
30:0:283:U:H5	30:0:284:C:N3	1.79	0.80
30:0:1206:U:H5'	30:0:1206:U:H6	1.45	0.80
28:2:41:HIS:H	28:2:45:ASN:HD22	1.29	0.80
30:0:1160:G:H5'	30:0:1161:A:H5'	0.87	0.80
30:0:603:A:H5''	30:0:604:G:OP1	1.81	0.80
30:0:1973:A:H5'	30:0:1973:A:H8	1.45	0.80
30:0:1603:A:H5''	30:0:1605:G:H5'	1.63	0.79
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.62	0.79
30:0:541:C:H2'	30:0:542:A:C5'	2.12	0.79
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.64	0.79
2:B:62:ARG:HA	2:B:65:MET:HE3	1.63	0.79
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.17	0.78
27:1:1:THR:HA	38:0:9358:HOH:O	1.83	0.78
30:0:281:U:O2'	30:0:282:C:H5'	1.83	0.78
14:N:113:SER:HB2	38:N:8855:HOH:O	1.82	0.78
30:0:2644:C:H2'	38:0:4596:HOH:O	1.83	0.78
15:O:47:ARG:HH11	15:O:47:ARG:HG3	1.47	0.78
21:U:9:CYS:HA	21:U:52:THR:HG22	1.64	0.78
30:0:1183:C:H42	30:0:1184:C:H41	1.32	0.78
30:0:2795:C:O2'	30:0:2796:U:H5'	1.83	0.78
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.63	0.78
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.84	0.78
30:0:236:A:H4'	30:0:237:G:H5'	1.66	0.78
30:0:1189:A:H1'	30:0:1209:C:O4'	1.84	0.78
30:0:558:C:O2'	30:0:559:U:H5''	1.84	0.77
30:0:2748:G:H5'	38:0:7537:HOH:O	1.83	0.77
30:0:1300:G:H1'	38:0:4684:HOH:O	1.83	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:117:SER:HB3	30:0:1593:C:OP1	1.84	0.77
30:0:1116:U:H3	30:0:1246:A:H62	1.31	0.77
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.77
12:L:133:VAL:HA	38:L:8876:HOH:O	1.84	0.77
30:0:2769:C:O2'	30:0:2770:G:H5'	1.83	0.77
30:0:871:G:C8	30:0:871:G:C5'	2.60	0.77
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.22	0.77
30:0:1183:C:H2'	38:0:6244:HOH:O	1.85	0.77
31:9:49:G:H5''	38:9:9087:HOH:O	1.84	0.77
2:B:206:THR:HG21	30:0:2716:G:H5''	1.68	0.76
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.65	0.76
30:0:2578:G:H5'	30:0:2578:G:H8	1.51	0.76
14:N:141:ARG:HH21	31:9:48:C:H4'	1.50	0.76
30:0:1209:C:H2'	30:0:1210:G:H8	1.51	0.76
30:0:192:A:H5'	38:0:7639:HOH:O	1.86	0.76
8:H:29:SER:HA	8:H:62:HIS:HD2	1.50	0.76
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.69	0.75
30:0:2533:C:H5'	30:0:2533:C:C6	2.20	0.75
30:0:2748:G:H1'	38:0:7896:HOH:O	1.85	0.75
30:0:567:U:H5''	38:0:5289:HOH:O	1.87	0.75
30:0:506:G:H22	30:0:509:A:H5''	1.51	0.75
30:0:1189:A:H1'	30:0:1209:C:C1'	2.15	0.75
30:0:847:C:H4'	38:0:3748:HOH:O	1.87	0.75
30:0:1790:C:H2'	30:0:1791:U:H6	1.52	0.75
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.15	0.74
1:A:35:GLY:O	1:A:36:ASP:HB3	1.86	0.74
30:0:1120:U:H5'	30:0:1121:G:OP2	1.86	0.74
30:0:1701:A:H4'	30:0:1702:U:C5'	2.17	0.74
30:0:558:C:C2'	30:0:559:U:H5''	2.17	0.74
30:0:1666:C:H2'	30:0:1667:A:C5'	2.16	0.74
30:0:2487:C:H5	38:0:4889:HOH:O	1.71	0.74
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.03	0.74
30:0:1080:C:H4'	30:0:1081:A:OP1	1.87	0.74
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.88	0.74
30:0:870:G:C2'	30:0:871:G:H5''	2.16	0.74
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.23	0.74
30:0:2637:A:H4'	38:0:6063:HOH:O	1.87	0.74
30:0:2717:C:H2'	30:0:2718:C:C5'	2.14	0.74
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.70	0.73
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.70	0.73
30:0:544:G:H2'	30:0:545:G:H5''	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1441:G:O2'	30:0:1442:A:H5'	1.88	0.73
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.71	0.73
30:0:1189:A:H3'	38:0:7676:HOH:O	1.86	0.73
30:0:2541:U:H5'	30:0:2541:U:C6	2.23	0.73
30:0:2787:C:H5	38:0:4633:HOH:O	1.72	0.73
30:0:1641:A:H2'	30:0:1642:A:H5'	1.69	0.73
30:0:2717:C:O2'	30:0:2718:C:H5''	1.89	0.73
30:0:1666:C:H2'	30:0:1667:A:H5'	1.71	0.73
30:0:2524:G:H21	30:0:2526:C:N4	1.86	0.73
30:0:2679:G:H2'	30:0:2681:A:OP2	1.89	0.73
4:D:25:MET:HE2	4:D:41:LEU:HG	1.71	0.73
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.70	0.73
22:V:1:THR:HG23	22:V:2:VAL:H	1.54	0.73
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.70	0.73
30:0:1701:A:H5''	30:0:1702:U:H3'	1.71	0.73
30:0:271:C:H41	30:0:378:A:H2	1.33	0.73
30:0:2420:G:O2'	30:0:2421:G:H5'	1.88	0.73
30:0:396:U:H1'	38:0:7622:HOH:O	1.88	0.72
30:0:1118:A:H62	30:0:1244:U:H3	1.36	0.72
23:W:149:LEU:HG	23:W:153:MET:HE2	1.70	0.72
30:0:1525:G:H5'	30:0:1526:A:OP2	1.89	0.72
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.71	0.72
30:0:2102:G:H2'	38:0:7763:HOH:O	1.87	0.72
4:D:103:ASN:ND2	4:D:134:LEU:H	1.88	0.72
30:0:827:A:H1'	38:0:6214:HOH:O	1.89	0.72
30:0:2254:G:H1'	38:0:5534:HOH:O	1.89	0.72
30:0:2644:C:HO2'	30:0:2645:U:H6	1.36	0.72
30:0:1632:A:H2'	30:0:1633:C:H5'	1.72	0.71
10:J:19:MET:HE2	10:J:79:PHE:HA	1.73	0.71
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.25	0.71
30:0:1441:G:H1'	38:0:7761:HOH:O	1.90	0.71
3:C:139:VAL:HG13	38:C:8659:HOH:O	1.90	0.71
30:0:280:C:H2'	30:0:281:U:O4'	1.91	0.71
30:0:2769:C:H2'	30:0:2770:G:H5'	1.73	0.71
13:M:95:LYS:HE2	30:0:157:G:H4'	1.73	0.71
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.71
30:0:31:C:H4'	38:0:7421:HOH:O	1.91	0.70
30:0:2491:G:H1'	38:0:6868:HOH:O	1.90	0.70
30:0:2577:A:H8	38:0:9598:HOH:O	1.74	0.70
30:0:1730:G:H5'	30:0:1731:C:C5	2.27	0.70
30:0:2505:G:O2'	30:0:2506:A:H5'	1.92	0.70

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	1.35	0.70
4:D:105:SER:OG	30:0:2338:G:H1'	1.90	0.70
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.92	0.70
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.74	0.70
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.70
30:0:2073:G:OP2	30:0:2490:A:H5'	1.92	0.70
30:0:2812:A:H1'	38:0:5787:HOH:O	1.92	0.70
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.74	0.70
1:A:51:ARG:HB2	38:A:9063:HOH:O	1.91	0.70
13:M:171:ARG:CD	30:0:156:C:H5''	2.20	0.69
38:C:8676:HOH:O	30:0:2100:A:H5'	1.92	0.69
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.74	0.69
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.32	0.69
30:0:1838:U:O2'	30:0:2644:C:H5'	1.92	0.69
30:0:2135:A:O2'	30:0:2136:G:H5'	1.92	0.69
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.74	0.69
30:0:285:A:H2'	30:0:286:U:O4'	1.92	0.69
30:0:1634:G:H3'	38:0:3891:HOH:O	1.93	0.69
30:0:2004:U:H4'	38:0:5307:HOH:O	1.92	0.69
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.03	0.69
30:0:558:C:H2'	30:0:559:U:C5'	2.23	0.69
30:0:681:G:N3	30:0:681:G:H5'	2.08	0.69
30:0:2670:G:O2'	30:0:2671:U:H5'	1.92	0.69
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.57	0.69
30:0:1377:C:H5'	30:0:1377:C:H6	1.58	0.69
30:0:1451:C:H5'	30:0:1505:U:C5	2.28	0.69
30:0:1666:C:C2'	30:0:1667:A:C5'	2.70	0.69
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.88	0.69
30:0:1835:U:C5	30:0:1840:A:N7	2.59	0.69
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.08	0.68
30:0:2563:U:H2'	30:0:2565:C:O5'	1.93	0.68
24:X:78:GLU:HB3	38:X:5564:HOH:O	1.94	0.68
16:P:115:SER:H	16:P:118:GLN:NE2	1.88	0.68
30:0:960:G:N3	30:0:960:G:H2'	2.09	0.68
30:0:1667:A:H5'	30:0:1667:A:C8	2.27	0.68
30:0:2851:G:O2'	30:0:2852:A:H5'	1.94	0.68
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.08	0.68
30:0:812:A:H1'	38:0:3955:HOH:O	1.93	0.68
30:0:2005:G:H3'	30:0:2005:G:OP2	1.94	0.68
1:A:199:HIS:HD2	1:A:201:PHE:H	1.41	0.68
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:47:ARG:HG3	38:U:4381:HOH:O	1.94	0.68
30:0:138:U:H5''	30:0:139:C:OP2	1.94	0.68
30:0:2111:G:H1'	38:0:9049:HOH:O	1.93	0.68
20:T:2:LYS:HG2	30:0:447:A:OP1	1.93	0.68
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.75	0.68
30:0:564:G:H1'	38:0:6310:HOH:O	1.92	0.68
30:0:1528:A:H2'	30:0:1529:G:O4'	1.94	0.68
30:0:2659:U:H5''	38:0:4123:HOH:O	1.93	0.68
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.75	0.67
30:0:1730:G:H5''	30:0:1731:C:H6	1.59	0.67
30:0:2827:A:H2'	30:0:2828:G:O4'	1.94	0.67
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.74	0.67
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.76	0.67
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.60	0.67
18:R:150:PRO:CG	18:R:150:PRO:O	2.42	0.67
30:0:1562:C:O2	30:0:1562:C:H2'	1.94	0.67
30:0:1182:C:H1'	30:0:1192:A:H8	1.60	0.67
3:C:236:THR:HA	38:C:8662:HOH:O	1.95	0.67
30:0:299:U:H5'	38:0:7336:HOH:O	1.93	0.67
3:C:236:THR:HG22	3:C:239:ALA:N	2.09	0.67
14:N:37:ARG:NH1	31:9:6:C:C5'	2.52	0.67
23:W:80:ASP:O	23:W:84:VAL:HG23	1.94	0.67
29:3:48:ASN:HD21	30:0:2468:A:H61	1.43	0.67
30:0:130:C:H2'	38:0:3158:HOH:O	1.95	0.67
30:0:544:G:C2'	30:0:545:G:H5''	2.24	0.67
31:9:75:G:H1	31:9:106:U:H3	1.42	0.67
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.95	0.67
30:0:2852:A:H5''	38:0:5236:HOH:O	1.94	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.29	0.66
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.77	0.66
30:0:292:G:H2'	30:0:358:G:N2	2.10	0.66
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.76	0.66
22:V:42:ASN:HB3	38:V:7247:HOH:O	1.95	0.66
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.95	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.42	0.66
30:0:2524:G:H21	30:0:2526:C:H41	1.44	0.66
30:0:1189:A:O2'	30:0:1208:C:H2'	1.96	0.66
30:0:848:C:H5'	38:0:7271:HOH:O	1.94	0.66
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.60	0.66
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.59	0.66
33:0:8813:CL:CL	38:0:4684:HOH:O	2.51	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:23:U:O2'	31:9:24:U:H4'	1.96	0.66
30:0:1118:A:C8	30:0:1118:A:C3'	2.75	0.66
14:N:110:THR:HB	14:N:113:SER:OG	1.95	0.66
30:0:1834:C:H2'	30:0:1840:A:N6	2.10	0.66
26:Z:34:SER:HA	30:0:797:A:H5'	1.76	0.65
30:0:441:A:H1'	30:0:442:A:N7	2.12	0.65
31:9:92:G:H2'	31:9:93:A:H8	1.61	0.65
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.61	0.65
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.11	0.65
23:W:59:GLN:HE22	23:W:98:PHE:HB2	1.62	0.65
30:0:2812:A:C2	30:0:2814:A:N6	2.62	0.65
13:M:164:THR:HG22	13:M:167:GLY:H	1.59	0.65
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.78	0.65
30:0:482:G:H4'	30:0:508:A:N1	2.12	0.65
30:0:2755:G:H1'	38:0:4683:HOH:O	1.97	0.65
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.78	0.65
3:C:140:VAL:HB	38:C:8662:HOH:O	1.97	0.65
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.79	0.65
6:F:96:ALA:HA	38:F:3111:HOH:O	1.96	0.65
30:0:2878:U:H2'	30:0:2879:A:O4'	1.96	0.65
30:0:2748:G:H2'	38:0:7537:HOH:O	1.96	0.65
30:0:2769:C:H2'	30:0:2770:G:C5'	2.25	0.65
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.79	0.65
30:0:841:A:H5''	38:0:6907:HOH:O	1.96	0.65
31:9:14:G:H5'	31:9:14:G:C8	2.30	0.65
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.78	0.65
30:0:1477:C:H5'	30:0:1868:G:C5'	2.27	0.65
30:0:1741:U:H5'	30:0:1742:A:OP1	1.96	0.65
30:0:2559:C:H4'	38:0:7254:HOH:O	1.97	0.65
30:0:1278:A:H4'	30:0:1279:U:C4	2.32	0.65
30:0:558:C:H2'	30:0:559:U:H5'	1.79	0.64
30:0:1649:G:H1'	38:0:5533:HOH:O	1.97	0.64
30:0:2756:U:N3	30:0:2896:A:H2	1.95	0.64
3:C:184:ARG:NH2	30:0:450:C:OP1	2.30	0.64
30:0:711:G:H1'	38:0:7093:HOH:O	1.96	0.64
30:0:2768:A:H2'	30:0:2769:C:O4'	1.96	0.64
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.80	0.64
19:S:43:GLU:HB3	38:S:8989:HOH:O	1.97	0.64
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.61	0.64
10:J:41:ALA:HB3	38:J:5907:HOH:O	1.96	0.64
30:0:308:U:H5'	30:0:309:C:OP1	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2256:G:O2'	30:0:2257:G:H5'	1.98	0.64
23:W:26:ILE:HB	38:W:5420:HOH:O	1.96	0.64
30:0:1166:A:H61	30:0:1180:U:H3	1.45	0.64
30:0:1741:U:O2'	30:0:2723:G:H4'	1.98	0.64
30:0:2894:C:O2'	30:0:2895:C:H5'	1.98	0.64
2:B:98:THR:HG22	30:0:2820:A:OP1	1.98	0.64
38:Z:8707:HOH:O	30:0:1886:A:H4'	1.97	0.64
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.33	0.64
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.33	0.64
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.13	0.64
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.80	0.64
12:L:114:VAL:HG11	38:L:8876:HOH:O	1.97	0.64
10:J:82:THR:CG2	30:0:1242:A:H5'	2.21	0.64
11:K:66:ARG:HH22	30:0:1994:A:P	2.21	0.64
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.80	0.64
30:0:559:U:H5'	30:0:559:U:C6	2.29	0.64
30:0:1603:A:C5'	30:0:1605:G:H5'	2.28	0.64
4:D:23:VAL:HG22	4:D:73:VAL:HB	1.80	0.63
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.33	0.63
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.06	0.63
3:C:174:ILE:HD11	30:0:338:C:H4'	1.80	0.63
30:0:1790:C:H2'	30:0:1791:U:C6	2.32	0.63
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.63	0.63
30:0:1183:C:N3	30:0:1184:C:C5	2.67	0.63
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.28	0.63
31:9:49:G:H2'	31:9:50:G:O4'	1.98	0.63
12:L:18:HIS:HD2	30:0:902:G:N7	1.97	0.63
13:M:86:GLN:NE2	30:0:2274:A:H1'	2.14	0.63
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.46	0.63
30:0:542:A:H5'	30:0:542:A:C8	2.24	0.63
5:E:137:ASP:O	5:E:141:VAL:HG23	1.99	0.63
38:N:8844:HOH:O	31:9:7:G:H5'	1.98	0.63
30:0:71:G:H8	38:0:3908:HOH:O	1.81	0.63
30:0:123:U:H5'	38:0:6657:HOH:O	1.97	0.63
30:0:247:A:H2'	38:0:3920:HOH:O	1.99	0.63
30:0:1187:U:H2'	38:0:6893:HOH:O	1.99	0.63
30:0:1189:A:H1'	30:0:1209:C:H1'	1.79	0.63
9:I:126:THR:O	9:I:130:LEU:HG	1.99	0.62
17:Q:25:PRO:HB2	38:Q:4350:HOH:O	1.99	0.62
30:0:2345:A:H3'	30:0:2346:C:C6	2.34	0.62
30:0:200:C:H2'	38:0:3440:HOH:O	1.97	0.62

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	2.32	0.62
30:0:2426:G:H1'	38:0:6092:HOH:O	1.98	0.62
30:0:2637:A:H5'	38:0:4930:HOH:O	1.99	0.62
3:C:174:ILE:CD1	30:0:338:C:H4'	2.30	0.62
30:0:1632:A:C2'	30:0:1633:C:H5'	2.29	0.62
30:0:2481:G:H5''	38:0:4543:HOH:O	1.98	0.62
4:D:159:PRO:O	4:D:163:VAL:HG23	2.00	0.62
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.29	0.62
30:0:371:U:H2'	30:0:372:A:H8	1.65	0.62
30:0:1249:U:H2'	30:0:1250:C:C6	2.34	0.62
30:0:2320:U:H4'	30:0:2321:A:O4'	1.99	0.62
30:0:2478:U:O2'	30:0:2479:A:H5'	1.99	0.62
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.27	0.62
28:2:35:ARG:HB2	38:2:2691:HOH:O	1.98	0.62
30:0:583:C:H2'	30:0:584:U:H6	1.64	0.62
30:0:1132:A:N6	30:0:1229:C:H2'	2.14	0.62
30:0:1730:G:C5'	30:0:1731:C:C6	2.82	0.62
15:O:25:VAL:HG12	30:0:709:G:O2'	1.99	0.62
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.81	0.62
30:0:960:G:N3	30:0:960:G:C2'	2.63	0.62
2:B:254:GLN:HG2	2:B:255:GLY:N	2.14	0.62
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.95	0.62
6:F:91:VAL:HG12	6:F:92:GLY:N	2.15	0.61
10:J:131:THR:HB	10:J:134:GLU:HG3	1.81	0.61
16:P:59:ARG:HH22	16:P:66:GLN:NE2	1.98	0.61
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.81	0.61
23:W:13:MET:HE2	23:W:18:GLN:HA	1.80	0.61
30:0:363:C:O2'	30:0:364:U:H5'	2.00	0.61
30:0:1942:A:H3'	38:0:7346:HOH:O	1.99	0.61
30:0:2541:U:H6	30:0:2541:U:C5'	2.09	0.61
30:0:2644:C:O2'	30:0:2645:U:H6	1.83	0.61
31:9:39:U:H1'	31:9:44:A:H61	1.65	0.61
31:9:58:G:C8	31:9:59:C:C5	2.88	0.61
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.63	0.61
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.82	0.61
30:0:2241:C:O2'	30:0:2242:U:H5'	2.00	0.61
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.29	0.61
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.80	0.61
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.64	0.61
30:0:635:A:H2'	30:0:636:G:H5''	1.82	0.61
30:0:1172:G:H1'	38:0:4974:HOH:O	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2768:A:O2'	30:0:2769:C:H5'	2.00	0.61
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.81	0.61
30:0:1474:C:H6	30:0:1474:C:C5'	2.07	0.61
1:A:109:GLU:HG2	1:A:116:GLY:H	1.65	0.61
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.31	0.61
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.83	0.61
11:K:10:GLN:HE21	11:K:10:GLN:N	1.89	0.61
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.81	0.61
29:3:15:ASN:O	30:0:2408:A:H4'	2.01	0.61
30:0:558:C:C2'	30:0:559:U:C5'	2.79	0.61
30:0:1185:U:H5'	38:0:7462:HOH:O	1.99	0.61
30:0:2604:A:H5'	38:0:5788:HOH:O	2.01	0.61
3:C:1:MET:HG2	3:C:2:GLN:N	2.15	0.61
11:K:49:LEU:HD23	11:K:80:ILE:HD13	1.83	0.61
30:0:407:A:H5'	38:0:6024:HOH:O	2.00	0.61
1:A:36:ASP:O	1:A:38:ILE:N	2.33	0.61
12:L:6:ARG:HD3	30:0:1299:G:O6	1.99	0.61
20:T:61:GLU:HG2	38:T:3851:HOH:O	1.98	0.61
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.66	0.61
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.84	0.60
30:0:1202:A:C2'	30:0:1203:G:H5'	2.31	0.60
26:Z:34:SER:CB	30:0:797:A:H4'	2.30	0.60
30:0:514:G:H4'	38:0:5644:HOH:O	2.00	0.60
30:0:1377:C:H5'	30:0:1377:C:C6	2.36	0.60
30:0:2781:U:C2'	30:0:2782:G:H5'	2.31	0.60
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.66	0.60
27:1:8:GLN:HE22	27:1:11:LYS:NZ	1.98	0.60
30:0:969:G:H1	30:0:999:C:N4	1.98	0.60
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.84	0.60
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.36	0.60
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.83	0.60
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.84	0.60
30:0:644:G:H5'	30:0:644:G:N3	2.16	0.60
30:0:1819:G:H2'	30:0:1820:G:H4'	1.81	0.60
30:0:2414:A:H2'	30:0:2415:A:C8	2.35	0.60
1:A:199:HIS:CD2	1:A:201:PHE:H	2.18	0.60
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.83	0.60
25:Y:204:ARG:HH22	30:0:553:G:P	2.25	0.60
30:0:120:A:H2'	30:0:120:A:N3	2.16	0.60
2:B:71:VAL:HG11	2:B:296:LEU:HB3	1.81	0.60
10:J:39:VAL:HG22	10:J:106:GLY:O	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:625:U:H5''	30:0:1044:C:N4	2.16	0.60
30:0:920:C:H5''	30:0:921:G:O5'	2.02	0.60
30:0:1202:A:O2'	30:0:1203:G:H5'	2.01	0.60
30:0:1342:C:C2'	30:0:1343:C:H5'	2.30	0.60
30:0:1730:G:H5''	30:0:1731:C:C6	2.36	0.60
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.02	0.60
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.01	0.60
18:R:39:THR:HG22	18:R:42:GLU:H	1.67	0.60
26:Z:40:ALA:HA	30:0:1773:G:C8	2.37	0.60
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.41	0.60
30:0:746:A:H5'	38:0:5514:HOH:O	2.02	0.60
14:N:40:ASN:ND2	31:9:28:U:H5''	2.17	0.60
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.32	0.60
30:0:1393:A:H2'	30:0:1394:C:C6	2.37	0.60
30:0:2869:G:H2'	30:0:2870:C:C6	2.36	0.60
1:A:33:GLU:H	1:A:33:GLU:CD	2.10	0.59
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.36	0.59
18:R:128:ARG:NH2	30:0:2054:A:N3	2.50	0.59
27:1:16:HIS:HD2	30:0:470:U:O2'	1.83	0.59
30:0:669:G:O2'	30:0:670:G:H5'	2.02	0.59
30:0:31:C:H2'	38:0:7684:HOH:O	2.02	0.59
30:0:515:C:H5''	38:0:5644:HOH:O	2.01	0.59
30:0:2524:G:N2	30:0:2526:C:H41	2.00	0.59
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.83	0.59
30:0:283:U:C5	30:0:284:C:N3	2.67	0.59
30:0:1457:U:H5	38:0:7872:HOH:O	1.84	0.59
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.84	0.59
9:I:120:ALA:O	9:I:124:VAL:HG23	2.02	0.59
12:L:41:HIS:CD2	30:0:926:A:O2'	2.56	0.59
18:R:39:THR:HG23	18:R:107:GLU:O	2.02	0.59
20:T:9:LYS:HD3	38:0:3750:HOH:O	2.02	0.59
30:0:128:A:O2'	30:0:129:A:H5'	2.02	0.59
30:0:2498:C:O2'	30:0:2499:U:H5'	2.02	0.59
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.84	0.59
30:0:1425:G:O2'	30:0:1426:C:H5'	2.02	0.59
30:0:2403:C:H5'	38:0:6025:HOH:O	2.02	0.59
30:0:2756:U:N3	30:0:2896:A:C2	2.63	0.59
2:B:36:PRO:HG3	2:B:169:GLY:H	1.67	0.59
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.01	0.59
31:9:13:A:O2'	31:9:14:G:H5''	2.03	0.59
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:134:GLU:HG3	38:L:8857:HOH:O	2.03	0.59
30:0:1183:C:H42	30:0:1184:C:N4	2.00	0.59
30:0:1268:C:O2'	30:0:1269:G:H5'	2.01	0.59
1:A:99:ILE:O	1:A:131:HIS:HE1	1.86	0.59
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.84	0.59
30:0:1426:C:H2'	38:0:9591:HOH:O	2.03	0.59
30:0:2419:U:H5''	30:0:2420:G:H5'	1.83	0.59
30:0:2505:G:C2'	30:0:2506:A:H5'	2.33	0.59
2:B:294:TYR:HE2	38:B:9117:HOH:O	1.85	0.59
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.38	0.59
20:T:9:LYS:HB2	38:0:7421:HOH:O	2.01	0.59
27:1:28:HIS:HE1	30:0:776:A:OP1	1.86	0.58
30:0:807:A:O2'	30:0:808:A:H5'	2.03	0.58
31:9:2:U:OP2	31:9:3:A:H5'	2.03	0.58
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.18	0.58
30:0:2344:G:H2'	30:0:2344:G:N3	2.18	0.58
30:0:2637:A:C5'	38:0:4930:HOH:O	2.50	0.58
30:0:2781:U:H2'	30:0:2782:G:H5'	1.84	0.58
30:0:2900:G:H2'	30:0:2901:C:O4'	2.03	0.58
1:A:48:ASP:HB3	38:A:9063:HOH:O	2.02	0.58
11:K:8:VAL:HG13	11:K:80:ILE:HG22	1.84	0.58
18:R:29:LYS:HD3	30:0:524:A:H5''	1.85	0.58
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.84	0.58
22:V:44:GLY:HA3	30:0:92:G:H4'	1.85	0.58
23:W:52:VAL:HG22	23:W:53:ALA:H	1.68	0.58
30:0:1201:C:H5''	38:0:6233:HOH:O	2.02	0.58
31:9:1:U:H5''	31:9:3:A:OP1	2.03	0.58
14:N:11:ARG:HD3	31:9:114:G:O6	2.03	0.58
15:O:42:GLU:HB2	38:O:2176:HOH:O	2.02	0.58
30:0:1230:A:H8	30:0:1230:A:OP1	1.85	0.58
30:0:1942:A:O2'	30:0:1943:C:H5'	2.03	0.58
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.85	0.58
30:0:485:A:N3	30:0:487:G:H5''	2.19	0.58
30:0:2335:C:H2'	30:0:2336:G:C8	2.38	0.58
14:N:141:ARG:NH2	31:9:48:C:H4'	2.19	0.58
30:0:2533:C:H6	30:0:2533:C:C5'	2.12	0.58
12:L:30:ARG:HD3	30:0:164:G:H4'	1.86	0.58
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.86	0.58
20:T:41:ARG:HG2	20:T:41:ARG:HH11	1.66	0.58
30:0:1211:G:H2'	30:0:1212:C:H6	1.69	0.58
30:0:1649:G:O2'	30:0:1650:C:H5'	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:179:GLY:O	30:0:399:C:H5'	2.04	0.58
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.85	0.58
18:R:4:TYR:CE1	18:R:17:MET:HE2	2.39	0.58
30:0:1015:C:H2'	30:0:1016:U:H6	1.67	0.58
30:0:2445:U:H2'	30:0:2446:G:C8	2.39	0.58
30:0:2802:C:H2'	30:0:2803:C:H6	1.68	0.58
1:A:212:PRO:HB2	38:A:9024:HOH:O	2.04	0.58
2:B:145:HIS:HD2	2:B:146:THR:O	1.87	0.58
13:M:163:LEU:HD21	30:0:188:C:H5''	1.86	0.58
30:0:2032:U:H2'	30:0:2033:G:C5'	2.34	0.58
1:A:55:VAL:HG23	1:A:68:ILE:O	2.04	0.57
2:B:190:MET:HE2	2:B:194:PHE:HD1	1.69	0.57
30:0:1165:G:O2'	30:0:1174:A:H1'	2.04	0.57
30:0:1207:A:C8	30:0:1208:C:C5	2.92	0.57
30:0:1856:C:H5'	30:0:1858:A:O4'	2.04	0.57
30:0:1596:U:H2'	30:0:1598:A:OP2	2.03	0.57
30:0:1947:G:N2	30:0:1966:U:C2	2.71	0.57
9:I:110:ASP:O	30:0:1163:G:H5'	2.04	0.57
30:0:705:C:O2	30:0:705:C:H2'	2.04	0.57
30:0:1015:C:H2'	30:0:1016:U:C6	2.39	0.57
30:0:1181:A:H2'	30:0:1182:C:H5'	1.86	0.57
30:0:1741:U:HO2'	30:0:2723:G:H4'	1.68	0.57
30:0:1819:G:H2'	30:0:1820:G:C5'	2.34	0.57
30:0:1903:U:O2'	30:0:1904:A:N7	2.38	0.57
30:0:2472:C:O2'	30:0:2634:G:H4'	2.03	0.57
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.86	0.57
21:U:17:THR:HG22	21:U:18:GLY:N	2.18	0.57
30:0:1307:A:H2'	30:0:1308:A:C8	2.39	0.57
30:0:1463:U:H2'	30:0:1464:C:C6	2.39	0.57
30:0:1477:C:O2'	30:0:1478:U:H5'	2.04	0.57
30:0:2851:G:C2'	30:0:2852:A:H5'	2.34	0.57
22:V:1:THR:HB	30:0:93:C:H5''	1.86	0.57
22:V:38:GLY:O	22:V:41:GLU:HG3	2.05	0.57
30:0:2251:G:H2'	30:0:2252:A:C8	2.40	0.57
4:D:25:MET:CE	4:D:37:ALA:HB1	2.35	0.57
30:0:255:A:H2'	30:0:256:C:H6	1.68	0.57
30:0:264:G:H1'	30:0:265:U:H5	1.70	0.57
30:0:2415:A:H2'	30:0:2416:G:H5'	1.86	0.57
2:B:125:GLU:O	2:B:129:ARG:HG3	2.04	0.57
30:0:876:A:H2'	30:0:876:A:N3	2.19	0.57
30:0:1138:G:H4'	38:0:5706:HOH:O	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2689:A:H2'	30:0:2690:U:H5'	1.87	0.57
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.39	0.57
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.35	0.57
30:0:941:G:C5	30:0:942:U:C4	2.93	0.57
30:0:1588:G:C6	30:0:1589:G:N1	2.73	0.57
1:A:121:ALA:O	1:A:124:VAL:HG22	2.05	0.57
38:B:9100:HOH:O	30:0:2672:C:H1'	2.05	0.57
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.34	0.57
25:Y:235:GLU:CD	25:Y:235:GLU:H	2.11	0.57
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.37	0.57
30:0:823:U:H3'	38:0:4446:HOH:O	2.03	0.57
30:0:1044:C:H5''	38:0:9025:HOH:O	2.05	0.57
30:0:1174:A:C5	30:0:1201:C:H4'	2.39	0.57
30:0:1603:A:H5'	30:0:1605:G:C4'	2.34	0.57
30:0:2134:G:N2	30:0:2242:U:C2	2.73	0.57
30:0:2291:A:N9	30:0:2309:C:H5'	2.19	0.57
30:0:2509:A:H2'	30:0:2510:C:O4'	2.05	0.57
2:B:140:LEU:HA	38:B:9048:HOH:O	2.05	0.57
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.87	0.57
30:0:694:A:H2'	30:0:695:C:H5'	1.86	0.57
31:9:22:G:H5'	31:9:23:U:OP1	2.05	0.57
5:E:132:THR:HB	38:E:2227:HOH:O	2.05	0.56
30:0:821:U:H3'	38:0:3765:HOH:O	2.05	0.56
30:0:834:G:H3'	30:0:835:U:H4'	1.87	0.56
3:C:188:ARG:HD3	38:C:8564:HOH:O	2.05	0.56
30:0:821:U:H2'	30:0:822:C:H6	1.70	0.56
30:0:2710:U:H1'	38:0:7616:HOH:O	2.04	0.56
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.34	0.56
10:J:74:ARG:O	10:J:78:ILE:HG12	2.05	0.56
17:Q:19:ARG:HH21	31:9:11:A:P	2.27	0.56
30:0:671:A:O2'	30:0:672:G:H2'	2.05	0.56
30:0:952:G:N3	30:0:2302:A:H2'	2.20	0.56
30:0:1135:G:H5'	38:0:5927:HOH:O	2.05	0.56
30:0:1641:A:C2'	30:0:1642:A:H5'	2.35	0.56
31:9:29:C:C2'	31:9:30:C:H5'	2.33	0.56
17:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.04	0.56
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.69	0.56
30:0:308:U:C4	30:0:342:C:H1'	2.41	0.56
5:E:143:GLN:NE2	30:0:2779:G:H21	2.04	0.56
30:0:1160:G:O2'	30:0:1190:G:H1'	2.06	0.56
30:0:1279:U:O2	30:0:1279:U:H2'	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.87	0.56
27:1:20:ARG:HG2	30:0:111:C:O2'	2.06	0.56
30:0:316:A:N3	30:0:336:G:O2'	2.37	0.56
23:W:13:MET:HE2	23:W:18:GLN:CA	2.36	0.56
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.87	0.56
30:0:2256:G:H2'	30:0:2257:G:C5'	2.35	0.56
9:I:108:HIS:H	9:I:109:PRO:HD2	1.71	0.56
23:W:139:GLY:O	23:W:141:HIS:HD2	1.89	0.56
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.88	0.56
30:0:10:U:O4	30:0:532:A:OP2	2.23	0.56
31:9:76:G:C3'	31:9:77:A:H5''	2.28	0.56
1:A:36:ASP:HB2	1:A:85:SER:H	1.71	0.56
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.71	0.56
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.88	0.56
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.05	0.56
23:W:125:HIS:NE2	30:0:1097:A:H5''	2.21	0.56
30:0:282:C:O2'	30:0:283:U:C5'	2.50	0.56
30:0:1592:G:H2'	30:0:1593:C:C6	2.41	0.56
30:0:1768:C:H2'	30:0:1769:C:O4'	2.06	0.56
30:0:2880:A:H2'	30:0:2881:C:H5'	1.88	0.56
2:B:85:ARG:NH1	38:B:9100:HOH:O	2.39	0.56
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.33	0.56
14:N:37:ARG:NH1	31:9:6:C:OP1	2.38	0.56
14:N:169:PRO:O	14:N:172:PHE:HB3	2.06	0.56
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.88	0.56
31:9:64:C:C2'	31:9:65:A:H5'	2.36	0.56
2:B:27:ASN:HD22	2:B:27:ASN:H	1.54	0.55
19:S:76:GLU:HB3	38:S:8991:HOH:O	2.05	0.55
30:0:816:G:C6	30:0:817:G:N1	2.74	0.55
30:0:1118:A:H8	30:0:1119:G:H5''	1.71	0.55
30:0:2703:A:H2'	30:0:2704:C:H6	1.71	0.55
31:9:64:C:H2'	31:9:65:A:H5'	1.88	0.55
8:H:48:VAL:HA	8:H:170:ARG:O	2.05	0.55
30:0:1163:G:H1	30:0:1184:C:N4	2.03	0.55
30:0:1588:G:C6	30:0:1589:G:C6	2.94	0.55
30:0:1595:G:O2'	30:0:1596:U:H5'	2.06	0.55
30:0:2269:C:C2'	30:0:2270:G:H5'	2.37	0.55
30:0:2645:U:C6	30:0:2645:U:OP2	2.60	0.55
30:0:2802:C:H2'	30:0:2803:C:C6	2.41	0.55
28:2:10:ARG:NH2	30:0:121:U:OP2	2.40	0.55
30:0:1119:G:N2	30:0:1246:A:H2	1.97	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1477:C:H5'	30:0:1868:G:H5''	1.88	0.55
30:0:2256:G:C2'	30:0:2257:G:H5'	2.35	0.55
5:E:84:MET:HG2	5:E:168:ILE:HA	1.88	0.55
23:W:88:THR:HG22	23:W:89:ASP:H	1.71	0.55
30:0:407:A:H3'	38:0:4460:HOH:O	2.06	0.55
30:0:735:C:H2'	30:0:736:A:H5'	1.87	0.55
30:0:1878:G:O2'	30:0:1879:U:C6	2.58	0.55
31:9:39:U:H3'	31:9:40:C:H5''	1.88	0.55
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.88	0.55
30:0:652:G:H8	38:0:3009:HOH:O	1.89	0.55
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.06	0.55
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.88	0.55
30:0:272:A:H5'	30:0:273:G:OP2	2.07	0.55
30:0:1377:C:H6	30:0:1377:C:C5'	2.18	0.55
2:B:275:GLY:O	2:B:291:ASP:HA	2.07	0.55
30:0:810:G:H2'	30:0:811:C:C6	2.42	0.55
30:0:2626:C:H2'	30:0:2627:G:C8	2.42	0.55
4:D:154:LYS:HD2	4:D:154:LYS:N	2.15	0.55
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.71	0.55
27:1:46:ARG:HA	38:1:8971:HOH:O	2.05	0.55
28:2:18:ASN:ND2	28:2:40:ARG:H	2.01	0.55
30:0:581:G:O2'	30:0:582:U:H5'	2.06	0.55
30:0:877:G:C5'	30:0:878:G:OP1	2.52	0.55
31:9:12:C:H5'	31:9:70:U:O4'	2.06	0.55
31:9:39:U:H1'	31:9:44:A:N6	2.21	0.55
31:9:49:G:O2'	31:9:50:G:H5'	2.07	0.55
1:A:223:ARG:HD2	30:0:2272:G:OP1	2.07	0.55
38:O:7674:HOH:O	30:0:935:G:H5'	2.05	0.55
22:V:50:ARG:HH12	30:0:56:G:H5''	1.70	0.55
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.35	0.55
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.90	0.55
23:W:38:THR:HG22	23:W:39:ASP:N	2.22	0.55
30:0:2502:C:H2'	30:0:2503:A:C5'	2.36	0.55
31:9:28:U:H2'	31:9:29:C:C6	2.41	0.55
31:9:91:C:H2'	31:9:92:G:O4'	2.07	0.55
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.07	0.54
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.89	0.54
22:V:50:ARG:NH1	30:0:56:G:H5''	2.22	0.54
30:0:271:C:C2	30:0:273:G:O4'	2.60	0.54
30:0:567:U:H5''	38:0:6401:HOH:O	2.06	0.54
30:0:1174:A:C6	30:0:1201:C:H4'	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1209:C:H2'	30:0:1210:G:C8	2.36	0.54
30:0:2697:A:H2'	30:0:2698:G:O4'	2.07	0.54
31:9:1:U:H4'	31:9:3:A:OP1	2.07	0.54
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.19	0.54
30:0:204:A:H2'	30:0:205:U:H5'	1.88	0.54
30:0:1291:A:H2	38:0:5292:HOH:O	1.89	0.54
30:0:2616:A:H4'	30:0:2617:G:OP1	2.06	0.54
30:0:2718:C:H6	30:0:2718:C:H5'	1.73	0.54
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.89	0.54
23:W:154:ARG:NH1	30:0:588:G:O6	2.40	0.54
27:1:9:GLY:HA2	30:0:1687:C:O2	2.07	0.54
30:0:999:C:O2'	30:0:1000:C:H5'	2.07	0.54
30:0:1172:G:H5''	38:0:7257:HOH:O	2.07	0.54
21:U:9:CYS:HA	21:U:52:THR:CG2	2.35	0.54
21:U:17:THR:HG22	21:U:18:GLY:H	1.72	0.54
30:0:1484:G:H2'	38:0:9103:HOH:O	2.08	0.54
30:0:2564:G:OP2	30:0:2565:C:H5''	2.06	0.54
2:B:267:LYS:HD3	38:0:9562:HOH:O	2.06	0.54
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.22	0.54
11:K:27:ARG:HD2	38:K:3442:HOH:O	2.07	0.54
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.55	0.54
17:Q:7:LEU:HD12	30:0:2424:U:H1'	1.89	0.54
8:H:168:VAL:HG13	38:H:213:HOH:O	2.08	0.54
14:N:80:SER:HB2	38:N:8833:HOH:O	2.07	0.54
30:0:1175:G:H1'	30:0:1193:A:C2'	2.36	0.54
30:0:1559:A:OP2	30:0:1559:A:H8	1.88	0.54
30:0:1766:U:O2	30:0:1778:A:H5'	2.08	0.54
15:O:37:ARG:HD2	30:0:656:G:OP2	2.08	0.54
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.89	0.54
30:0:65:C:O2'	30:0:66:G:H5'	2.07	0.54
2:B:211:THR:HG23	30:0:2840:A:OP1	2.08	0.54
5:E:10:ASP:HA	38:E:6017:HOH:O	2.06	0.54
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.90	0.54
8:H:64:SER:OG	30:0:2520:G:H5'	2.07	0.54
19:S:33:SER:O	19:S:37:VAL:HG23	2.08	0.54
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.89	0.54
27:1:37:CYS:SG	27:1:39:PHE:HB2	2.48	0.54
30:0:958:G:H2'	30:0:959:C:C6	2.42	0.54
30:0:1131:G:C6	30:0:1230:A:C4	2.96	0.54
30:0:1183:C:C2	30:0:1184:C:C5	2.96	0.54
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:20:VAL:O	7:G:24:VAL:HG23	2.08	0.54
14:N:132:ASN:O	14:N:135:VAL:HG12	2.08	0.54
30:0:2269:C:O2'	30:0:2270:G:H5'	2.07	0.54
30:0:420:U:H2'	30:0:421:C:C6	2.44	0.53
30:0:549:A:O2'	30:0:550:C:H5'	2.08	0.53
31:9:34:A:H2'	31:9:35:C:O4'	2.08	0.53
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.73	0.53
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.23	0.53
13:M:28:GLN:O	13:M:32:ARG:HG3	2.08	0.53
30:0:90:A:H2'	30:0:91:G:O4'	2.08	0.53
30:0:961:A:H4'	38:0:6768:HOH:O	2.07	0.53
30:0:1730:G:H5'	30:0:1731:C:H5	1.73	0.53
30:0:2070:G:H2'	30:0:2072:G:OP1	2.08	0.53
30:0:2345:A:H3'	30:0:2346:C:H6	1.71	0.53
30:0:2705:U:H2'	30:0:2706:A:C8	2.43	0.53
31:9:1:U:O3'	31:9:3:A:H5''	2.08	0.53
3:C:95:GLU:HG3	38:C:8688:HOH:O	2.07	0.53
5:E:68:HIS:O	5:E:72:MET:HG3	2.09	0.53
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.90	0.53
22:V:55:ARG:O	22:V:59:ILE:HG12	2.08	0.53
23:W:44:MET:HE2	30:0:944:G:H21	1.72	0.53
23:W:125:HIS:HB2	23:W:137:GLN:HG2	1.90	0.53
30:0:255:A:H2'	30:0:256:C:C6	2.44	0.53
30:0:1505:U:H1'	38:0:7584:HOH:O	2.07	0.53
30:0:1615:A:H5'	38:0:4180:HOH:O	2.09	0.53
30:0:1622:G:H2'	30:0:1623:C:H5'	1.90	0.53
30:0:2826:G:C6	30:0:2913:A:N6	2.75	0.53
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.91	0.53
8:H:174:LEU:HD21	30:0:1220:U:H4'	1.89	0.53
12:L:41:HIS:HD2	30:0:926:A:O2'	1.90	0.53
13:M:188:ARG:HD3	30:0:155:C:OP2	2.08	0.53
14:N:114:LYS:O	14:N:118:ILE:HG13	2.07	0.53
30:0:297:U:H2'	30:0:298:C:C6	2.43	0.53
30:0:318:U:H5'	30:0:339:A:C2	2.44	0.53
30:0:484:A:N1	30:0:506:G:H4'	2.23	0.53
30:0:1838:U:H3'	38:0:5521:HOH:O	2.09	0.53
30:0:2597:U:H2'	30:0:2598:U:H5'	1.90	0.53
31:9:20:G:O2'	31:9:21:G:H5'	2.08	0.53
10:J:107:ASN:C	10:J:107:ASN:HD22	2.16	0.53
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.90	0.53
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2243:C:H5''	38:0:3745:HOH:O	2.07	0.53
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.72	0.53
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.09	0.53
30:0:281:U:C2'	30:0:282:C:H5'	2.39	0.53
30:0:1878:G:O2'	30:0:1879:U:P	2.67	0.53
30:0:2371:G:H5'	38:0:5010:HOH:O	2.07	0.53
5:E:69:ILE:HA	5:E:72:MET:CE	2.39	0.53
13:M:164:THR:HB	38:M:8819:HOH:O	2.08	0.53
28:2:28:LYS:O	30:0:87:C:H2'	2.09	0.53
30:0:319:A:H4'	30:0:338:C:C4	2.44	0.53
30:0:1483:C:O2'	30:0:1484:G:H5'	2.09	0.53
30:0:1592:G:H2'	30:0:1593:C:H6	1.71	0.53
30:0:1921:A:O2'	30:0:1922:A:H5'	2.09	0.53
30:0:1972:U:H2'	30:0:1973:A:C5'	2.38	0.53
31:9:24:U:H3'	31:9:25:G:C5'	2.39	0.53
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.72	0.53
30:0:256:C:H2'	30:0:257:G:O4'	2.09	0.53
30:0:506:G:N2	30:0:509:A:H5''	2.22	0.53
30:0:2301:A:H5''	30:0:2302:A:H5'	1.91	0.53
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.07	0.53
28:2:41:HIS:HD2	28:2:44:ARG:H	1.56	0.53
30:0:522:U:O2'	30:0:1366:C:H5'	2.08	0.53
30:0:1202:A:H2'	30:0:1203:G:C5'	2.39	0.53
30:0:1795:G:H2'	30:0:1796:A:O4'	2.09	0.53
3:C:63:SER:OG	30:0:2101:A:H2'	2.09	0.52
22:V:39:ALA:N	22:V:40:PRO:HD2	2.24	0.52
27:1:45:ARG:NH2	38:1:8976:HOH:O	2.38	0.52
30:0:396:U:O2'	30:0:418:C:H4'	2.08	0.52
30:0:413:G:H2'	30:0:414:C:C6	2.44	0.52
30:0:1342:C:H2'	30:0:1343:C:H5'	1.91	0.52
30:0:1535:G:H2'	30:0:1536:C:C6	2.44	0.52
12:L:37:LYS:HE2	30:0:2466:G:OP2	2.09	0.52
30:0:1201:C:H2'	30:0:1202:A:H5'	1.91	0.52
30:0:1603:A:C5'	30:0:1605:G:O4'	2.53	0.52
30:0:1878:G:C1'	38:0:6119:HOH:O	2.42	0.52
30:0:2507:G:H2'	30:0:2510:C:H42	1.74	0.52
3:C:2:GLN:HB3	38:C:8534:HOH:O	2.09	0.52
3:C:218:VAL:HG12	38:C:8634:HOH:O	2.08	0.52
8:H:69:ARG:HD3	38:H:233:HOH:O	2.10	0.52
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.90	0.52
22:V:64:GLY:O	22:V:65:ASP:HB2	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.90	0.52
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.92	0.52
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.90	0.52
30:0:1213:C:O2'	30:0:1214:G:H5'	2.10	0.52
30:0:1268:C:H2'	30:0:1269:G:H8	1.75	0.52
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.10	0.52
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.90	0.52
13:M:75:ARG:HH11	30:0:1864:C:H5	1.56	0.52
18:R:33:ARG:NH1	38:R:8946:HOH:O	2.43	0.52
28:2:40:ARG:HD2	28:2:47:THR:HG22	1.91	0.52
30:0:613:C:H2'	30:0:614:U:H6	1.75	0.52
30:0:1855:G:H4'	30:0:1856:C:O5'	2.09	0.52
31:9:56:A:H2'	31:9:57:A:C5'	2.05	0.52
1:A:186:TRP:CG	1:A:187:PRO:HA	2.45	0.52
5:E:80:TRP:O	5:E:134:SER:HA	2.09	0.52
14:N:93:GLN:HA	14:N:93:GLN:HE21	1.74	0.52
30:0:137:U:H2'	30:0:139:C:C5	2.45	0.52
30:0:1183:C:H2'	30:0:1183:C:O2	2.08	0.52
30:0:1497:G:H4'	30:0:1627:G:O2'	2.09	0.52
30:0:1679:C:H5'	38:0:9325:HOH:O	2.08	0.52
30:0:2300:A:H4'	30:0:2301:A:O5'	2.10	0.52
30:0:2433:A:H2'	30:0:2434:A:C8	2.44	0.52
30:0:2613:G:O2'	30:0:2614:C:H5'	2.09	0.52
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.89	0.52
12:L:148:GLU:HA	38:L:8875:HOH:O	2.08	0.52
13:M:30:GLU:O	13:M:34:GLU:HG3	2.10	0.52
23:W:119:HIS:HD2	23:W:120:PRO:O	1.93	0.52
25:Y:146:PRO:O	25:Y:154:ARG:HG3	2.10	0.52
30:0:2445:U:H2'	30:0:2446:G:H8	1.74	0.52
30:0:2469:A:H1'	38:0:3237:HOH:O	2.08	0.52
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.92	0.52
2:B:238:ASN:HD22	2:B:240:GLY:N	2.00	0.52
2:B:320:GLN:NE2	2:B:321:PRO:HD2	2.24	0.52
3:C:107:ARG:O	3:C:111:VAL:HG23	2.10	0.52
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.25	0.52
18:R:117:HIS:HD2	30:0:20:G:H21	1.56	0.52
20:T:38:ARG:NH1	38:T:6217:HOH:O	2.42	0.52
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.09	0.52
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.58	0.52
30:0:603:A:H1'	30:0:605:C:C2	2.44	0.52
30:0:1309:U:O2'	30:0:1310:U:H5'	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1342:C:O2'	30:0:1343:C:H5'	2.09	0.52
30:0:2256:G:H2'	30:0:2257:G:H5'	1.92	0.52
30:0:2781:U:O2'	30:0:2782:G:H5'	2.08	0.52
2:B:271:ASP:HB3	2:B:296:LEU:HD12	1.91	0.52
4:D:52:THR:HG21	30:0:2346:C:O2'	2.10	0.52
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.88	0.52
16:P:58:SER:HB3	38:0:5627:HOH:O	2.10	0.52
25:Y:142:SER:OG	30:0:1331:G:OP2	2.27	0.52
30:0:645:U:O2	30:0:761:A:H2	1.92	0.52
30:0:905:C:H3'	38:0:5190:HOH:O	2.08	0.52
30:0:1202:A:H2'	30:0:1203:G:H5'	1.91	0.52
30:0:1527:A:H1'	30:0:1528:A:C8	2.45	0.52
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.92	0.52
31:9:52:A:O2'	31:9:53:G:H5'	2.10	0.52
31:9:110:G:C5	31:9:111:U:C5	2.97	0.52
1:A:171:LYS:HB2	30:0:820:G:C5	2.45	0.52
2:B:158:LYS:HD3	30:0:2846:C:OP1	2.10	0.52
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.10	0.52
6:F:57:GLU:O	6:F:61:MET:HG3	2.09	0.52
12:L:143:THR:HG21	38:L:8841:HOH:O	2.09	0.52
16:P:115:SER:N	16:P:118:GLN:HE21	1.97	0.52
21:U:9:CYS:CA	21:U:52:THR:HG22	2.39	0.52
30:0:559:U:H6	30:0:559:U:C5'	2.17	0.52
30:0:1207:A:C8	30:0:1208:C:C6	2.98	0.52
30:0:1477:C:C5'	30:0:1868:G:H5''	2.39	0.52
30:0:1825:U:O2'	30:0:1826:C:H5'	2.10	0.52
30:0:2269:C:H2'	30:0:2270:G:C5'	2.40	0.52
30:0:2836:G:H1'	38:0:6838:HOH:O	2.09	0.52
2:B:41:PHE:HB3	2:B:190:MET:CE	2.40	0.52
9:I:69:PRO:HA	30:0:1164:U:OP1	2.10	0.52
18:R:40:ALA:O	18:R:44:VAL:HG23	2.10	0.52
24:X:43:VAL:HG12	24:X:44:ASP:N	2.25	0.52
30:0:177:A:H2'	30:0:178:U:O4'	2.09	0.52
30:0:538:C:H5''	30:0:539:G:C8	2.45	0.52
30:0:1636:G:O2'	30:0:1637:A:H5'	2.09	0.52
30:0:1857:A:H5''	38:0:6701:HOH:O	2.10	0.52
30:0:2072:G:C6	30:0:2533:C:H1'	2.45	0.52
30:0:2781:U:H2'	30:0:2782:G:C5'	2.39	0.52
4:D:65:GLU:HA	38:D:6752:HOH:O	2.09	0.51
15:O:3:THR:HG22	30:0:656:G:C5'	2.26	0.51
30:0:12:U:H2'	30:0:13:G:H5'	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:912:A:C4	30:0:1294:A:C2	2.97	0.51
30:0:1419:U:H2'	30:0:1685:A:C2	2.45	0.51
30:0:1589:G:H4'	38:0:6857:HOH:O	2.10	0.51
30:0:2830:U:O2'	30:0:2831:C:H5'	2.09	0.51
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.26	0.51
30:0:24:G:N2	30:0:518:G:H1'	2.25	0.51
30:0:497:A:H2'	30:0:498:A:C5'	2.41	0.51
30:0:1058:A:H2'	30:0:1060:C:H5''	1.91	0.51
30:0:1165:G:H4'	30:0:1174:A:O2'	2.10	0.51
30:0:1762:C:H2'	30:0:1763:C:H6	1.76	0.51
1:A:51:ARG:NH1	1:A:120:ARG:O	2.43	0.51
1:A:210:GLY:HA3	38:A:9046:HOH:O	2.08	0.51
27:1:25:LYS:HD2	28:2:48:ASP:HA	1.92	0.51
29:3:70:ARG:HB3	38:3:8997:HOH:O	2.09	0.51
30:0:304:G:H1'	30:0:347:A:N6	2.25	0.51
30:0:558:C:H2'	30:0:559:U:H5''	1.87	0.51
30:0:661:G:C5	30:0:686:A:C2	2.99	0.51
30:0:1188:A:C6	30:0:1189:A:C6	2.98	0.51
30:0:2064:U:H5'	30:0:2652:U:H4'	1.93	0.51
30:0:2435:U:H1'	38:0:5428:HOH:O	2.11	0.51
31:9:52:A:H2'	31:9:53:G:O4'	2.09	0.51
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.91	0.51
20:T:68:ASP:HB2	38:0:5658:HOH:O	2.10	0.51
30:0:119:A:H2'	30:0:120:A:H5''	1.92	0.51
30:0:1565:C:O2'	30:0:1566:C:H5'	2.10	0.51
30:0:1976:G:H1'	30:0:2005:G:N2	2.26	0.51
30:0:2689:A:C2'	30:0:2690:U:H5'	2.39	0.51
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.76	0.51
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.39	0.51
29:3:3:MET:O	29:3:90:PHE:HA	2.10	0.51
30:0:64:G:H2'	30:0:65:C:O4'	2.11	0.51
30:0:380:A:H2'	38:0:7225:HOH:O	2.10	0.51
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.40	0.51
30:0:42:C:H1'	38:0:4676:HOH:O	2.10	0.51
30:0:204:A:C2'	30:0:205:U:H5'	2.40	0.51
30:0:677:C:O2'	30:0:678:G:H5'	2.10	0.51
30:0:2421:G:H3'	30:0:2422:U:C5'	2.40	0.51
30:0:2421:G:H3'	30:0:2422:U:H5''	1.92	0.51
8:H:61:ARG:HG3	38:0:4972:HOH:O	2.10	0.51
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.93	0.51
14:N:154:LEU:C	14:N:156:GLU:H	2.18	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:85:VAL:HG12	24:X:86:GLU:N	2.26	0.51
25:Y:133:HIS:HD2	38:Y:9065:HOH:O	1.93	0.51
30:0:1029:U:O2'	30:0:1273:C:OP1	2.27	0.51
30:0:1730:G:C5'	30:0:1731:C:H6	2.23	0.51
2:B:212:GLN:HA	30:0:1733:A:H4'	1.91	0.51
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.92	0.51
18:R:59:PHE:O	18:R:63:ASN:HB3	2.11	0.51
20:T:97:ARG:NH2	30:0:309:C:OP1	2.44	0.51
30:0:407:A:H8	38:0:4460:HOH:O	1.94	0.51
30:0:537:G:O4'	30:0:538:C:C5	2.64	0.51
30:0:589:U:H2'	30:0:590:A:H8	1.75	0.51
30:0:1925:G:O2'	30:0:1926:G:H5'	2.11	0.51
30:0:2105:C:H2'	30:0:2106:C:C6	2.46	0.51
3:C:214:THR:HG23	38:C:8648:HOH:O	2.10	0.51
7:G:12:ILE:HG23	38:0:5457:HOH:O	2.09	0.51
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.46	0.51
30:0:1622:G:C2'	30:0:1623:C:H5'	2.41	0.51
7:G:64:ASN:HD22	7:G:64:ASN:N	2.09	0.51
12:L:92:ASP:HA	12:L:121:ILE:HB	1.91	0.51
23:W:119:HIS:HE1	38:0:9554:HOH:O	1.93	0.51
30:0:1252:A:H2'	30:0:1253:C:O4'	2.11	0.51
30:0:1482:A:O2'	30:0:1483:C:H5'	2.11	0.51
30:0:1819:G:H2'	30:0:1820:G:C4'	2.41	0.51
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.44	0.50
5:E:84:MET:HE1	5:E:148:ILE:CD1	2.41	0.50
12:L:143:THR:HG22	12:L:144:ASP:N	2.27	0.50
16:P:83:LYS:HG2	30:0:793:A:H5''	1.93	0.50
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.92	0.50
30:0:567:U:C5'	38:0:6401:HOH:O	2.59	0.50
30:0:1205:U:C2'	30:0:1206:U:C5'	2.77	0.50
30:0:1321:A:H2'	30:0:1322:G:C8	2.47	0.50
30:0:2717:C:C2'	30:0:2718:C:C5'	2.75	0.50
2:B:132:HIS:NE2	2:B:171:VAL:HG23	2.27	0.50
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.44	0.50
25:Y:212:ARG:HD2	38:Y:9085:HOH:O	2.09	0.50
30:0:1173:A:H4'	30:0:1174:A:C8	2.45	0.50
30:0:1191:A:C2	30:0:1207:A:C2	2.99	0.50
30:0:1386:G:O2'	30:0:1387:G:H5'	2.12	0.50
30:0:1684:A:O2'	30:0:1685:A:H5''	2.12	0.50
30:0:1762:C:O2'	30:0:1763:C:H5'	2.12	0.50
30:0:1778:A:H2'	30:0:1779:A:H5'	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1915:U:O2'	30:0:1916:C:H5'	2.11	0.50
30:0:2769:C:H2'	30:0:2770:G:O4'	2.11	0.50
1:A:112:PRO:HD3	1:A:152:CYS:SG	2.51	0.50
2:B:102:THR:HG21	2:B:182:VAL:O	2.11	0.50
4:D:103:ASN:HD22	4:D:134:LEU:H	1.59	0.50
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.11	0.50
12:L:97:VAL:HG12	12:L:98:GLU:O	2.12	0.50
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.93	0.50
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.92	0.50
30:0:711:G:C2	30:0:718:C:C2	3.00	0.50
30:0:940:G:C5	30:0:1027:G:C2	3.00	0.50
30:0:1158:G:O2'	30:0:1159:G:H5'	2.11	0.50
30:0:1667:A:H2'	30:0:1668:U:C6	2.45	0.50
30:0:2385:G:H2'	30:0:2386:U:C6	2.47	0.50
38:M:8837:HOH:O	30:0:169:A:H5''	2.12	0.50
18:R:132:ARG:HG2	18:R:133:ALA:N	2.24	0.50
21:U:39:ASN:ND2	21:U:44:ARG:HH11	2.08	0.50
23:W:43:GLY:HA3	30:0:945:U:O2'	2.11	0.50
30:0:735:C:C2'	30:0:736:A:H5'	2.41	0.50
30:0:1130:U:H2'	30:0:1131:G:O4'	2.11	0.50
30:0:1187:U:O2'	30:0:1189:A:H2	1.79	0.50
30:0:1304:U:H2'	30:0:1305:C:C6	2.46	0.50
30:0:2089:A:O2'	30:0:2090:G:H5'	2.11	0.50
30:0:2250:G:N2	30:0:2251:G:H1'	2.27	0.50
30:0:2584:G:H4'	38:0:7115:HOH:O	2.10	0.50
30:0:2667:G:H1'	30:0:2914:A:N3	2.26	0.50
31:9:3:A:H2	31:9:21:G:N3	2.09	0.50
3:C:22:PHE:HA	3:C:116:ALA:HA	1.92	0.50
15:O:25:VAL:HG23	15:O:26:TRP:N	2.27	0.50
18:R:150:PRO:CG	18:R:150:PRO:CB	2.87	0.50
30:0:17:G:H2'	30:0:18:C:C6	2.47	0.50
30:0:282:C:H1'	30:0:368:C:H41	1.71	0.50
30:0:559:U:C5	30:0:560:U:C5	3.00	0.50
30:0:2724:U:H2'	30:0:2725:G:O4'	2.11	0.50
1:A:33:GLU:O	1:A:34:ASP:HB2	2.10	0.50
3:C:79:ARG:O	3:C:87:ARG:HG2	2.11	0.50
9:I:89:GLU:OE2	30:0:1181:A:H5'	2.11	0.50
17:Q:95:GLU:HA	30:0:949:U:H4'	1.93	0.50
25:Y:151:SER:HB3	25:Y:154:ARG:HB2	1.92	0.50
30:0:69:A:C8	30:0:69:A:C5'	2.90	0.50
30:0:332:G:O2'	30:0:333:G:H5'	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1333:U:H2'	30:0:1334:C:C6	2.47	0.50
31:9:55:U:H5'	38:9:9135:HOH:O	2.11	0.50
1:A:109:GLU:HG2	1:A:116:GLY:N	2.26	0.50
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.92	0.50
10:J:107:ASN:HD22	10:J:109:TYR:H	1.58	0.50
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.93	0.50
26:Z:34:SER:HB3	30:0:797:A:H4'	1.93	0.50
30:0:1200:A:H3'	38:0:5754:HOH:O	2.11	0.50
30:0:1422:U:H2'	30:0:1423:C:C6	2.47	0.50
30:0:2372:A:H2'	30:0:2373:U:H6	1.77	0.50
30:0:2710:U:H2'	30:0:2711:U:C6	2.46	0.50
30:0:638:C:H2'	30:0:639:A:C8	2.47	0.50
30:0:920:C:H4'	30:0:921:G:C2	2.45	0.50
30:0:1170:U:H2'	30:0:1172:G:OP2	2.11	0.50
30:0:1380:U:H5'	38:0:9218:HOH:O	2.12	0.50
30:0:1762:C:H2'	30:0:1763:C:C6	2.47	0.50
30:0:2252:A:C5	30:0:2253:G:H1'	2.47	0.50
2:B:258:GLY:H	2:B:260:HIS:CE1	2.29	0.50
22:V:12:THR:HG23	22:V:14:ALA:H	1.77	0.50
30:0:876:A:N3	30:0:876:A:C2'	2.75	0.50
31:9:24:U:H3'	31:9:25:G:H5'	1.94	0.50
4:D:50:VAL:HG13	31:9:41:C:O4'	2.12	0.49
6:F:91:VAL:HG11	30:0:262:A:OP2	2.11	0.49
11:K:49:LEU:CD2	11:K:80:ILE:HD13	2.42	0.49
11:K:55:VAL:HG12	11:K:56:SER:N	2.27	0.49
30:0:136:C:H2'	30:0:137:U:O4'	2.12	0.49
30:0:2871:G:H2'	30:0:2872:U:C6	2.47	0.49
31:9:55:U:H4'	31:9:56:A:C8	2.47	0.49
8:H:34:HIS:HD2	8:H:90:LEU:O	1.95	0.49
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.46	0.49
23:W:61:THR:HG23	23:W:151:GLU:HG3	1.94	0.49
30:0:488:U:H2'	38:0:4004:HOH:O	2.12	0.49
30:0:1165:G:O2'	30:0:1174:A:C1'	2.60	0.49
30:0:1211:G:H2'	30:0:1212:C:C6	2.47	0.49
30:0:2534:C:H1'	38:0:3491:HOH:O	2.11	0.49
2:B:91:PRO:HA	10:J:144:THR:OG1	2.12	0.49
4:D:76:ARG:NE	31:9:44:A:O4'	2.44	0.49
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.13	0.49
18:R:9:ASP:O	18:R:13:THR:HB	2.11	0.49
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.42	0.49
38:R:8953:HOH:O	30:0:1370:G:H5''	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.76	0.49
30:0:559:U:H2'	30:0:560:U:O4'	2.12	0.49
30:0:790:A:H1'	30:0:1710:A:H2'	1.94	0.49
30:0:1186:C:N4	30:0:1187:U:C4	2.81	0.49
2:B:244:PRO:HB3	30:0:1234:U:N3	2.27	0.49
5:E:69:ILE:HA	5:E:72:MET:HE3	1.94	0.49
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.27	0.49
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.10	0.49
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.47	0.49
18:R:128:ARG:NH2	30:0:2054:A:C2	2.80	0.49
30:0:69:A:H8	30:0:69:A:C5'	2.17	0.49
30:0:947:U:O2'	30:0:948:G:H5'	2.13	0.49
30:0:1181:A:N1	30:0:1192:A:O2'	2.42	0.49
30:0:1286:A:H5''	30:0:1287:A:OP1	2.13	0.49
30:0:1309:U:C2'	30:0:1310:U:H5'	2.43	0.49
30:0:1515:A:H2'	30:0:1516:U:C6	2.48	0.49
30:0:1524:U:OP1	30:0:1524:U:H4'	2.12	0.49
30:0:1972:U:C2'	30:0:1973:A:H5''	2.42	0.49
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.13	0.49
14:N:1:ALA:HB2	31:9:14:G:O2'	2.13	0.49
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.49
30:0:483:C:C4	30:0:484:A:C6	3.01	0.49
30:0:968:G:C2	30:0:1001:U:O2	2.66	0.49
30:0:1193:A:C2	30:0:1194:A:N6	2.80	0.49
30:0:2326:C:H4'	30:0:2412:G:C4'	2.43	0.49
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.38	0.49
5:E:126:ILE:HB	5:E:131:LEU:HD23	1.94	0.49
30:0:920:C:H5'	30:0:921:G:C4	2.48	0.49
30:0:1056:U:H2'	30:0:1057:A:O4'	2.12	0.49
30:0:1119:G:N2	30:0:1246:A:N1	2.60	0.49
30:0:1245:C:O5'	30:0:1245:C:H6	1.96	0.49
30:0:1278:A:H2'	30:0:1280:A:C8	2.48	0.49
2:B:17:LYS:O	2:B:260:HIS:HD2	1.95	0.49
2:B:243:ASN:HA	2:B:244:PRO:C	2.38	0.49
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.94	0.49
11:K:130:MET:SD	21:U:25:ASP:O	2.70	0.49
19:S:57:THR:HG22	19:S:58:MET:N	2.28	0.49
30:0:371:U:H2'	30:0:372:A:C8	2.47	0.49
30:0:899:C:H5'	38:0:3199:HOH:O	2.13	0.49
30:0:1706:G:H1'	30:0:1712:A:H61	1.78	0.49
30:0:1909:A:N1	30:0:2128:G:H1'	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2269:C:H2'	30:0:2270:G:H5'	1.94	0.49
30:0:2541:U:O2'	30:0:2542:C:H5'	2.13	0.49
31:9:56:A:C3'	31:9:57:A:H5''	2.42	0.49
1:A:179:MET:HG2	1:A:186:TRP:CB	2.43	0.49
2:B:79:MET:HE3	2:B:144:THR:HG21	1.95	0.49
6:F:107:ASP:O	6:F:111:ILE:HG13	2.12	0.49
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.12	0.49
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.76	0.49
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.13	0.49
14:N:17:ARG:HB3	14:N:17:ARG:HH11	1.78	0.49
30:0:1849:G:H1'	30:0:2011:A:N1	2.28	0.49
30:0:2869:G:H2'	30:0:2870:C:H6	1.78	0.49
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.43	0.49
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.45	0.49
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.94	0.49
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.28	0.49
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.42	0.49
15:O:24:ALA:HB3	30:0:710:G:OP1	2.13	0.49
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.47	0.49
30:0:2121:G:O2'	30:0:2122:C:H5'	2.13	0.49
2:B:206:THR:HG21	30:0:2716:G:C5'	2.40	0.49
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.94	0.49
13:M:78:LYS:HD3	38:0:7679:HOH:O	2.13	0.49
14:N:4:PRO:HG3	31:9:69:U:OP1	2.13	0.49
20:T:53:GLY:HA3	38:0:6800:HOH:O	2.12	0.49
30:0:226:A:H1'	30:0:393:G:C5	2.48	0.49
30:0:1066:U:H2'	30:0:1067:A:C8	2.48	0.49
30:0:1506:U:H6	30:0:1506:U:H5'	1.77	0.49
30:0:2271:G:N3	30:0:2271:G:H2'	2.28	0.49
30:0:2512:U:H4'	30:0:2514:U:O4	2.12	0.49
13:M:167:GLY:O	13:M:171:ARG:HG3	2.13	0.48
19:S:11:THR:H	19:S:14:ALA:HB3	1.77	0.48
19:S:57:THR:HG23	38:S:8979:HOH:O	2.11	0.48
30:0:191:A:C4	30:0:237:G:N7	2.81	0.48
30:0:1118:A:C8	30:0:1119:G:H5''	2.48	0.48
30:0:1545:C:H2'	30:0:1546:G:O4'	2.13	0.48
30:0:2645:U:H1'	38:0:9305:HOH:O	2.13	0.48
30:0:2664:A:H8	30:0:2664:A:OP1	1.96	0.48
30:0:2836:G:H5''	38:0:5165:HOH:O	2.12	0.48
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.78	0.48
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1116:U:O2'	30:0:1118:A:C2	2.39	0.48
30:0:1447:U:H3'	30:0:1506:U:O2	2.13	0.48
30:0:1477:C:H5'	30:0:1868:G:H5'	1.94	0.48
30:0:1972:U:H2'	30:0:1973:A:H5''	1.94	0.48
30:0:2326:C:H4'	30:0:2412:G:H4'	1.95	0.48
30:0:2329:C:O2'	30:0:2330:U:H5'	2.13	0.48
30:0:2379:G:N7	30:0:2408:A:N1	2.61	0.48
31:9:3:A:OP2	31:9:25:G:N2	2.45	0.48
3:C:43:LYS:HG2	30:0:449:A:N7	2.28	0.48
4:D:141:VAL:HG21	31:9:57:A:H8	1.78	0.48
23:W:4:LEU:O	23:W:32:CYS:HA	2.13	0.48
30:0:10:U:C4	30:0:532:A:C8	3.01	0.48
30:0:59:A:H5'	38:0:4330:HOH:O	2.12	0.48
30:0:447:A:O2'	30:0:448:G:H5'	2.13	0.48
30:0:1013:A:H1'	38:0:9158:HOH:O	2.13	0.48
30:0:2102:G:H1'	30:0:2103:A:N7	2.29	0.48
30:0:2816:A:H5''	30:0:2817:G:H5'	1.96	0.48
2:B:139:ASP:HB2	38:B:8995:HOH:O	2.12	0.48
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.77	0.48
12:L:34:GLY:HA2	38:0:5408:HOH:O	2.12	0.48
16:P:115:SER:OG	16:P:118:GLN:HG3	2.13	0.48
23:W:139:GLY:O	23:W:141:HIS:CD2	2.66	0.48
30:0:1185:U:H2'	30:0:1186:C:C6	2.48	0.48
30:0:1589:G:N2	30:0:1605:G:H1'	2.27	0.48
30:0:1667:A:C2	30:0:1668:U:C2	3.02	0.48
30:0:2420:G:H2'	30:0:2421:G:H8	1.79	0.48
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.96	0.48
2:B:119:HIS:O	2:B:121:PRO:HD3	2.13	0.48
5:E:84:MET:HE1	5:E:148:ILE:HD12	1.96	0.48
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.94	0.48
13:M:171:ARG:NH2	30:0:189:A:OP1	2.47	0.48
23:W:88:THR:HG22	23:W:90:TYR:CD1	2.48	0.48
30:0:228:C:H2'	30:0:229:G:H5'	1.94	0.48
30:0:541:C:O2'	30:0:542:A:H5''	2.14	0.48
30:0:699:C:H6	30:0:744:G:O4'	1.96	0.48
30:0:1520:G:C6	30:0:1521:C:N4	2.82	0.48
30:0:1522:A:C2	30:0:1665:G:C6	3.02	0.48
30:0:2374:G:H2'	30:0:2375:A:C8	2.48	0.48
30:0:2493:C:O2	30:0:2493:C:H2'	2.13	0.48
16:P:1:THR:O	30:0:1396:C:H1'	2.14	0.48
20:T:106:GLU:HG3	38:T:4913:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:499:G:O2'	30:0:500:G:H5'	2.13	0.48
30:0:536:A:H3'	38:0:5049:HOH:O	2.14	0.48
30:0:2372:A:H2'	30:0:2373:U:C6	2.48	0.48
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.13	0.48
5:E:101:GLU:HB2	5:E:116:THR:O	2.14	0.48
27:1:45:ARG:HB3	38:1:8967:HOH:O	2.14	0.48
30:0:346:U:H4'	38:0:6842:HOH:O	2.13	0.48
30:0:834:G:H4'	30:0:835:U:OP2	2.13	0.48
30:0:1594:C:O2'	30:0:1607:A:H4'	2.13	0.48
30:0:1739:G:O2'	30:0:1740:U:H5'	2.13	0.48
30:0:2387:U:H2'	30:0:2388:C:C6	2.48	0.48
25:Y:189:ASN:C	25:Y:189:ASN:HD22	2.21	0.48
30:0:291:C:H2'	30:0:292:G:O4'	2.14	0.48
30:0:312:U:C2	30:0:320:G:N2	2.82	0.48
30:0:1130:U:H5'	38:0:7668:HOH:O	2.13	0.48
30:0:1314:U:H5''	30:0:1316:G:O4'	2.13	0.48
31:9:1:U:C4'	31:9:3:A:OP1	2.60	0.48
31:9:45:A:C5	31:9:46:C:C5	3.02	0.48
1:A:3:ARG:HD3	30:0:870:G:OP2	2.13	0.48
1:A:126:ALA:HB1	1:A:138:VAL:CG1	2.44	0.48
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.94	0.48
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.29	0.48
30:0:289:G:O2'	30:0:290:C:H5'	2.14	0.48
30:0:304:G:H1'	30:0:347:A:H61	1.78	0.48
30:0:545:G:H8	30:0:545:G:C5'	2.12	0.48
30:0:2255:A:O2'	30:0:2256:G:H5'	2.14	0.48
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.49	0.48
14:N:110:THR:HB	14:N:113:SER:HG	1.76	0.48
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.96	0.48
27:1:12:ASN:O	30:0:1415:G:H5'	2.14	0.48
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.44	0.48
30:0:466:A:H2'	30:0:467:G:O4'	2.13	0.48
30:0:625:U:H3'	38:0:3250:HOH:O	2.13	0.48
30:0:820:G:H5'	30:0:821:U:H5'	1.95	0.48
30:0:1423:C:O2'	30:0:1424:A:H5'	2.14	0.48
30:0:1593:C:H1'	38:0:6105:HOH:O	2.14	0.48
30:0:2090:G:H2'	30:0:2091:G:C8	2.48	0.48
30:0:2840:A:H3'	38:0:7643:HOH:O	2.13	0.48
2:B:162:MET:HE3	2:B:310:ARG:CD	2.32	0.47
23:W:122:ARG:NH2	38:0:5289:HOH:O	2.46	0.47
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:106:A:H2'	30:0:107:U:O4'	2.14	0.47
30:0:541:C:C2'	30:0:542:A:C5'	2.79	0.47
30:0:736:A:H2'	30:0:737:A:O4'	2.14	0.47
30:0:1028:U:H1'	38:0:3639:HOH:O	2.14	0.47
31:9:110:G:C6	31:9:111:U:C5	3.02	0.47
4:D:51:ARG:NH1	4:D:68:PRO:HB3	2.29	0.47
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.29	0.47
16:P:87:ARG:HG2	38:P:185:HOH:O	2.14	0.47
23:W:23:MET:HE1	30:0:944:G:C8	2.49	0.47
30:0:185:G:O3'	30:0:186:A:H4'	2.14	0.47
30:0:559:U:C6	30:0:559:U:C3'	2.97	0.47
30:0:602:A:O2'	30:0:605:C:H4'	2.13	0.47
30:0:722:G:H22	30:0:938:G:P	2.37	0.47
30:0:1787:C:H4'	30:0:2883:A:O4'	2.14	0.47
6:F:59:ILE:CD1	30:0:263:U:C2	2.98	0.47
8:H:158:ASN:ND2	30:0:2502:C:H4'	2.30	0.47
14:N:100:ALA:O	14:N:129:ILE:HG23	2.13	0.47
22:V:12:THR:HG22	22:V:15:GLU:H	1.77	0.47
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.49	0.47
30:0:946:C:O2'	30:0:947:U:H5'	2.14	0.47
30:0:1181:A:H2'	30:0:1182:C:C5'	2.44	0.47
30:0:1181:A:C2'	30:0:1182:C:H5'	2.43	0.47
30:0:1456:C:H2'	30:0:1457:U:C6	2.49	0.47
30:0:1562:C:O2	30:0:1562:C:C2'	2.61	0.47
30:0:2032:U:O2'	30:0:2033:G:H5''	2.14	0.47
30:0:2134:G:C6	30:0:2258:A:C8	3.02	0.47
30:0:2266:A:H2'	30:0:2267:G:C8	2.49	0.47
30:0:2541:U:H3'	38:0:9060:HOH:O	2.14	0.47
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.50	0.47
30:0:968:G:O2'	30:0:969:G:H5'	2.14	0.47
30:0:1588:G:C5	30:0:1589:G:C6	3.03	0.47
30:0:1890:U:H4'	30:0:2010:A:C6	2.50	0.47
31:9:71:C:H2'	31:9:72:C:H6	1.79	0.47
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.96	0.47
8:H:31:ILE:HD11	8:H:65:LEU:HD23	1.96	0.47
23:W:64:THR:O	23:W:68:THR:HG22	2.14	0.47
25:Y:210:GLY:H	30:0:1313:A:H5''	1.78	0.47
30:0:168:C:O5'	30:0:168:C:H6	1.97	0.47
30:0:305:A:C5	30:0:329:A:C2	3.03	0.47
30:0:1137:G:H1'	38:0:3876:HOH:O	2.14	0.47
30:0:1183:C:N3	30:0:1184:C:N4	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1206:U:H2'	30:0:1207:A:O4'	2.14	0.47
30:0:2000:G:O2'	30:0:2001:G:H5'	2.15	0.47
30:0:2001:G:O2'	30:0:2002:C:H5'	2.14	0.47
30:0:2712:G:O2'	30:0:2713:G:H5'	2.14	0.47
31:9:65:A:N6	31:9:112:U:C6	2.82	0.47
11:K:81:ARG:HD3	11:K:87:ARG:NH2	2.30	0.47
30:0:138:U:OP2	30:0:139:C:H5	1.98	0.47
30:0:1153:C:N3	30:0:2786:G:O6	2.48	0.47
30:0:1406:A:H4'	30:0:1407:A:H5''	1.96	0.47
30:0:1823:G:O2'	30:0:1824:C:H5'	2.14	0.47
30:0:2335:C:H2'	30:0:2336:G:H8	1.78	0.47
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.48	0.47
2:B:14:GLY:HA2	2:B:15:PRO:C	2.39	0.47
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.32	0.47
11:K:41:LYS:O	11:K:42:ASN:HB2	2.15	0.47
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.95	0.47
13:M:49:ALA:C	13:M:54:TYR:HB3	2.39	0.47
16:P:59:ARG:O	16:P:63:ARG:HG3	2.15	0.47
19:S:77:VAL:O	19:S:80:ARG:HG2	2.15	0.47
20:T:26:THR:HA	20:T:39:ASN:HB3	1.95	0.47
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.13	0.47
25:Y:136:LYS:HE2	25:Y:138:ARG:NH1	2.28	0.47
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.95	0.47
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.15	0.47
30:0:283:U:C5	30:0:284:C:C4	3.03	0.47
30:0:527:U:H2'	30:0:528:G:C8	2.49	0.47
30:0:560:U:H2'	30:0:561:G:H8	1.79	0.47
30:0:814:G:H4'	38:0:3130:HOH:O	2.15	0.47
30:0:844:A:C6	30:0:882:A:C6	3.03	0.47
30:0:969:G:H1	30:0:999:C:H42	1.61	0.47
30:0:1400:C:O2'	30:0:1401:G:H5'	2.15	0.47
30:0:1548:U:O2'	30:0:1549:C:H5'	2.14	0.47
30:0:2074:A:H2'	38:0:3533:HOH:O	2.14	0.47
30:0:2239:C:O2'	30:0:2240:U:H5'	2.14	0.47
30:0:2361:A:H2'	30:0:2362:A:C8	2.49	0.47
30:0:2649:A:H5'	30:0:2649:A:C8	2.50	0.47
30:0:2871:G:H2'	30:0:2872:U:H6	1.79	0.47
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.04	0.47
18:R:122:GLN:HB3	18:R:138:SER:HB2	1.95	0.47
30:0:249:G:O2'	30:0:250:C:H5'	2.15	0.47
30:0:810:G:H2'	30:0:811:C:H6	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:853:C:H2'	30:0:854:G:O4'	2.14	0.47
30:0:1904:A:H2'	30:0:1905:U:O4'	2.15	0.47
30:0:2506:A:N6	30:0:2511:A:O2'	2.43	0.47
10:J:127:ILE:CG2	33:J:8801:CL:CL	2.96	0.47
14:N:147:ILE:HB	38:9:9087:HOH:O	2.15	0.47
25:Y:144:ARG:CZ	38:Y:9096:HOH:O	2.62	0.47
30:0:290:C:O2'	30:0:291:C:H5'	2.14	0.47
30:0:1014:A:H2'	30:0:1015:C:H5'	1.96	0.47
30:0:1377:C:H1'	38:0:9039:HOH:O	2.15	0.47
30:0:1942:A:H2'	30:0:1943:C:H6	1.79	0.47
2:B:144:THR:HB	38:B:9092:HOH:O	2.14	0.47
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.44	0.47
10:J:6:PHE:HB3	10:J:109:TYR:OH	2.15	0.47
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.96	0.47
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.50	0.47
14:N:162:ASP:HA	38:N:8830:HOH:O	2.15	0.47
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.50	0.47
30:0:1970:G:H2'	30:0:1970:G:N3	2.30	0.47
30:0:2649:A:H5'	30:0:2649:A:H8	1.79	0.47
3:C:95:GLU:CD	3:C:95:GLU:H	2.23	0.46
3:C:168:ARG:NH2	3:C:190:ALA:O	2.48	0.46
10:J:131:THR:HG22	10:J:133:GLY:N	2.30	0.46
12:L:27:ARG:HH21	12:L:30:ARG:HG2	1.80	0.46
14:N:82:TYR:C	14:N:82:TYR:CD2	2.93	0.46
16:P:91:LYS:O	16:P:95:GLU:HG3	2.15	0.46
16:P:114:LEU:HA	16:P:118:GLN:NE2	2.30	0.46
30:0:17:G:H2'	30:0:18:C:H6	1.79	0.46
30:0:254:C:O2	30:0:254:C:H2'	2.14	0.46
30:0:364:U:H2'	30:0:365:G:O4'	2.15	0.46
30:0:1149:U:C5	30:0:1215:A:C5	3.04	0.46
30:0:1760:G:H5'	30:0:1818:C:O2'	2.15	0.46
31:9:3:A:C2	31:9:21:G:N3	2.83	0.46
18:R:111:ILE:HG23	18:R:145:LEU:CD1	2.46	0.46
25:Y:189:ASN:ND2	25:Y:192:ASP:H	2.13	0.46
27:1:16:HIS:HE1	30:0:775:G:OP1	1.98	0.46
27:1:42:SER:HB2	38:1:8956:HOH:O	2.14	0.46
30:0:1379:A:H1'	38:0:9689:HOH:O	2.15	0.46
31:9:76:G:H3'	31:9:77:A:C5'	2.28	0.46
12:L:30:ARG:NH2	38:L:8823:HOH:O	2.44	0.46
13:M:169:ARG:NH2	38:M:8849:HOH:O	2.48	0.46
15:O:65:LEU:HD13	30:0:746:A:C6	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:13:MET:CE	23:W:17:ILE:HG22	2.46	0.46
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.45	0.46
30:0:162:C:H2'	30:0:163:U:H5'	1.97	0.46
30:0:1244:U:H4'	30:0:1246:A:O4'	2.16	0.46
30:0:1820:G:C6	30:0:2030:A:C2	3.04	0.46
30:0:1940:C:H4'	38:0:7346:HOH:O	2.16	0.46
30:0:2858:U:H2'	30:0:2859:C:O4'	2.15	0.46
31:9:1:U:O3'	31:9:3:A:C5'	2.63	0.46
4:D:25:MET:HE1	4:D:37:ALA:HB1	1.96	0.46
4:D:167:GLU:C	4:D:169:THR:H	2.23	0.46
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	1.98	0.46
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.46
30:0:95:A:H5''	30:0:97:G:O4'	2.14	0.46
30:0:152:A:H2'	30:0:153:C:C6	2.50	0.46
30:0:764:C:H2'	30:0:765:G:O4'	2.15	0.46
30:0:1268:C:H2'	30:0:1269:G:C8	2.50	0.46
30:0:1511:U:O2'	30:0:1512:G:H5'	2.15	0.46
30:0:1921:A:C6	30:0:1922:A:C2	3.04	0.46
30:0:2064:U:H4'	30:0:2653:A:OP1	2.14	0.46
30:0:2578:G:H5'	30:0:2578:G:C8	2.39	0.46
1:A:36:ASP:CB	1:A:85:SER:H	2.29	0.46
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.79	0.46
2:B:162:MET:CE	2:B:310:ARG:HD3	2.33	0.46
3:C:39:GLN:O	3:C:43:LYS:HD3	2.16	0.46
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.96	0.46
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.48	0.46
24:X:71:ARG:HD3	38:X:2171:HOH:O	2.16	0.46
27:1:1:THR:HB	38:0:7140:HOH:O	2.15	0.46
30:0:89:G:H4'	38:0:4766:HOH:O	2.16	0.46
30:0:255:A:C5	30:0:256:C:C4	3.04	0.46
30:0:1021:G:O2'	30:0:1022:A:H5'	2.16	0.46
30:0:1339:G:C6	30:0:1340:G:N1	2.84	0.46
30:0:2420:G:H2'	30:0:2421:G:C8	2.51	0.46
30:0:2783:A:H2'	30:0:2784:A:C8	2.50	0.46
30:0:2839:C:H2'	30:0:2840:A:H5''	1.96	0.46
31:9:33:U:H2'	38:9:9066:HOH:O	2.15	0.46
31:9:58:G:H3'	31:9:59:C:C6	2.49	0.46
2:B:280:VAL:HG13	2:B:333:GLU:O	2.16	0.46
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.50	0.46
3:C:132:ASP:HB3	38:C:8567:HOH:O	2.16	0.46
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:44:ARG:HD3	38:0:6937:HOH:O	2.15	0.46
30:0:125:U:H2'	38:0:3761:HOH:O	2.15	0.46
30:0:282:C:C2'	30:0:283:U:H5'	2.45	0.46
30:0:1087:G:H4'	30:0:1088:A:OP1	2.15	0.46
30:0:1845:A:O2'	30:0:1846:U:H5'	2.15	0.46
30:0:2617:G:N3	30:0:2617:G:H2'	2.30	0.46
2:B:260:HIS:HE1	38:0:5167:HOH:O	1.97	0.46
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.98	0.46
3:C:46:TYR:CE1	30:0:450:C:H4'	2.50	0.46
4:D:52:THR:CG2	30:0:2346:C:H4'	2.45	0.46
7:G:16:LYS:O	7:G:20:VAL:HG23	2.16	0.46
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.48	0.46
30:0:407:A:H2'	30:0:408:A:C8	2.51	0.46
30:0:704:C:H2'	30:0:705:C:H6	1.81	0.46
30:0:1044:C:H5	38:0:6604:HOH:O	1.98	0.46
30:0:1166:A:H2'	30:0:1166:A:N3	2.31	0.46
30:0:1840:A:H4'	30:0:1841:C:O5'	2.16	0.46
30:0:1878:G:O2'	30:0:1879:U:OP2	2.33	0.46
30:0:2795:C:HO2'	30:0:2796:U:H5'	1.80	0.46
3:C:48:SER:HB3	30:0:1352:A:N1	2.31	0.46
5:E:143:GLN:HE22	30:0:2779:G:H21	1.63	0.46
8:H:157:TYR:CD1	8:H:157:TYR:C	2.94	0.46
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.98	0.46
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.98	0.46
13:M:81:ARG:HG3	13:M:85:ARG:HB2	1.97	0.46
13:M:159:VAL:HG13	13:M:160:PHE:N	2.31	0.46
19:S:45:TYR:O	19:S:80:ARG:NH2	2.49	0.46
19:S:57:THR:C	19:S:59:ASP:H	2.24	0.46
23:W:10:GLU:HB2	23:W:18:GLN:NE2	2.31	0.46
24:X:85:VAL:HG12	24:X:86:GLU:H	1.80	0.46
30:0:1730:G:C5'	30:0:1731:C:C5	2.95	0.46
30:0:2032:U:H2'	30:0:2033:G:H5'	1.97	0.46
30:0:2353:A:H4'	30:0:2354:A:O5'	2.16	0.46
11:K:74:VAL:HG13	11:K:113:ILE:HG12	1.98	0.46
13:M:145:ASP:HB2	38:M:8864:HOH:O	2.15	0.46
30:0:772:G:H2'	30:0:773:A:O4'	2.16	0.46
30:0:862:U:H2'	30:0:863:G:H8	1.80	0.46
30:0:1052:G:H2'	30:0:1052:G:N3	2.30	0.46
30:0:1834:C:H2'	30:0:1840:A:H62	1.81	0.46
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.51	0.46
3:C:197:SER:HB3	38:C:8579:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:233:THR:HG22	3:C:234:VAL:N	2.31	0.46
14:N:94:GLU:HG3	14:N:186:LEU:HD12	1.98	0.46
30:0:424:C:H2'	30:0:425:U:C6	2.51	0.46
30:0:571:C:O5'	30:0:571:C:H6	1.99	0.46
30:0:699:C:H2'	30:0:744:G:N3	2.31	0.46
30:0:2002:C:H2'	30:0:2003:U:H5'	1.97	0.46
30:0:2250:G:H2'	30:0:2251:G:O4'	2.16	0.46
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.46
30:0:2906:A:H5'	30:0:2907:C:O4'	2.16	0.46
31:9:36:C:C5	31:9:37:C:C5	3.04	0.46
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.97	0.45
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.31	0.45
3:C:27:ARG:HG2	3:C:30:LEU:HG	1.98	0.45
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.98	0.45
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.46	0.45
7:G:23:ILE:O	7:G:27:ILE:HG13	2.16	0.45
8:H:91:ARG:O	30:0:1003:U:H4'	2.16	0.45
10:J:39:VAL:HG22	10:J:107:ASN:HA	1.98	0.45
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.45	0.45
12:L:18:HIS:CD2	30:0:902:G:N7	2.82	0.45
30:0:1154:A:H2'	30:0:1155:G:C8	2.51	0.45
30:0:2505:G:H2'	30:0:2506:A:H5'	1.97	0.45
31:9:58:G:H3'	31:9:59:C:C5	2.51	0.45
2:B:305:ASP:O	2:B:306:LYS:HB2	2.17	0.45
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.96	0.45
7:G:67:LEU:O	7:G:71:LEU:HG	2.15	0.45
13:M:9:ARG:HD2	30:0:380:A:OP2	2.15	0.45
23:W:24:LEU:O	23:W:26:ILE:HG22	2.16	0.45
30:0:559:U:C6	30:0:559:U:H3'	2.51	0.45
30:0:1080:C:O5'	30:0:1080:C:H6	1.99	0.45
30:0:1626:A:H2'	30:0:1627:G:C5'	2.47	0.45
30:0:2112:A:H2'	30:0:2113:G:C8	2.51	0.45
30:0:2473:U:O3'	30:0:2474:A:H3'	2.16	0.45
30:0:2756:U:C2	30:0:2896:A:H2	2.33	0.45
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.40	0.45
8:H:31:ILE:HG23	38:H:233:HOH:O	2.16	0.45
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.98	0.45
11:K:114:ALA:HB3	11:K:117:VAL:HG23	1.99	0.45
12:L:18:HIS:HB3	38:0:9150:HOH:O	2.15	0.45
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.51	0.45
30:0:366:U:H2'	30:0:367:G:O4'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1185:U:C5'	38:0:7462:HOH:O	2.62	0.45
30:0:2506:A:O2'	30:0:2507:G:O5'	2.35	0.45
30:0:2511:A:H2'	30:0:2512:U:O4'	2.16	0.45
30:0:2825:C:H4'	30:0:2826:G:O5'	2.16	0.45
31:9:114:G:H2'	31:9:115:C:C6	2.52	0.45
2:B:27:ASN:HD21	30:0:2807:U:P	2.39	0.45
3:C:129:HIS:CE1	3:C:232:LEU:H	2.35	0.45
12:L:67:ARG:O	12:L:71:GLU:HG3	2.17	0.45
19:S:37:VAL:O	19:S:41:VAL:HG23	2.16	0.45
25:Y:148:GLY:HA3	30:0:622:G:P	2.56	0.45
30:0:214:U:H5'	38:0:6139:HOH:O	2.15	0.45
30:0:297:U:H2'	30:0:298:C:H6	1.80	0.45
30:0:816:G:H5'	30:0:1598:A:H4'	1.98	0.45
30:0:1850:U:H2'	30:0:1851:G:H8	1.80	0.45
31:9:55:U:H4'	31:9:56:A:H8	1.81	0.45
1:A:164:ARG:NH2	30:0:1877:G:OP1	2.49	0.45
4:D:140:ARG:HH11	4:D:140:ARG:HG3	1.80	0.45
10:J:52:GLN:HE22	30:0:1119:G:H8	1.65	0.45
15:O:21:SER:OG	15:O:106:PRO:HB2	2.15	0.45
17:Q:32:GLU:O	17:Q:93:ARG:NH2	2.50	0.45
20:T:54:ASP:OD2	30:0:316:A:H5'	2.16	0.45
25:Y:122:ARG:NH2	38:Y:9019:HOH:O	2.49	0.45
30:0:432:G:O2'	30:0:433:C:H5'	2.16	0.45
30:0:513:A:N3	38:0:3653:HOH:O	2.36	0.45
30:0:702:G:O2'	30:0:703:G:H5'	2.16	0.45
30:0:1182:C:C1'	30:0:1192:A:H8	2.28	0.45
30:0:2250:G:C2	30:0:2251:G:H1'	2.50	0.45
30:0:2740:G:H2'	30:0:2741:A:O4'	2.16	0.45
4:D:49:PRO:HA	4:D:73:VAL:HG22	1.99	0.45
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.51	0.45
30:0:101:C:H2'	30:0:102:A:C8	2.51	0.45
30:0:652:G:H2'	30:0:653:U:O4'	2.16	0.45
30:0:1100:G:O2'	30:0:1107:A:N1	2.48	0.45
30:0:1789:G:H2'	30:0:1790:C:O5'	2.16	0.45
30:0:2439:C:H5'	38:0:5486:HOH:O	2.17	0.45
30:0:2644:C:H4'	38:0:9154:HOH:O	2.16	0.45
12:L:30:ARG:HD2	30:0:164:G:H5'	1.99	0.45
13:M:47:ASP:CG	13:M:48:LYS:N	2.75	0.45
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.99	0.45
20:T:79:LEU:HG	20:T:89:ARG:HB2	1.98	0.45
24:X:25:ARG:HD2	38:X:5356:HOH:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:415:A:O2'	30:0:416:G:H5'	2.17	0.45
30:0:1198:U:C6	30:0:1200:A:OP2	2.70	0.45
30:0:2415:A:C2'	30:0:2416:G:H5'	2.46	0.45
30:0:2637:A:H5'	38:0:9275:HOH:O	2.16	0.45
2:B:256:GLN:HG2	38:B:9125:HOH:O	2.16	0.45
6:F:91:VAL:HG12	6:F:92:GLY:H	1.79	0.45
8:H:157:TYR:C	8:H:157:TYR:HD1	2.25	0.45
12:L:57:VAL:O	12:L:57:VAL:HG12	2.17	0.45
13:M:164:THR:CG2	13:M:165:GLY:N	2.79	0.45
23:W:122:ARG:HG3	23:W:122:ARG:HH11	1.81	0.45
30:0:113:A:OP2	30:0:114:A:H2'	2.17	0.45
30:0:1015:C:O5'	30:0:1015:C:H6	1.99	0.45
30:0:1209:C:C2	30:0:1210:G:C8	3.05	0.45
30:0:2032:U:C2'	30:0:2033:G:C5'	2.95	0.45
30:0:2324:G:N2	30:0:2377:U:H1'	2.32	0.45
30:0:2566:A:C2	30:0:2696:G:O4'	2.70	0.45
1:A:232:ARG:NH2	1:A:236:GLY:O	2.50	0.45
4:D:48:MET:HB3	31:9:41:C:H4'	1.99	0.45
12:L:150:GLN:HB3	38:L:8872:HOH:O	2.16	0.45
15:O:35:LYS:HD3	38:0:4615:HOH:O	2.17	0.45
16:P:36:THR:O	16:P:39:ASP:HB2	2.17	0.45
23:W:11:VAL:O	23:W:12:ASN:HB2	2.17	0.45
23:W:119:HIS:CG	38:0:5289:HOH:O	2.70	0.45
30:0:587:A:H5''	38:0:7285:HOH:O	2.16	0.45
30:0:690:G:H4'	30:0:741:C:O2	2.17	0.45
30:0:1006:A:N1	30:0:2311:A:H1'	2.31	0.45
30:0:1117:A:C2	30:0:1244:U:C2	3.05	0.45
30:0:2361:A:H5'	30:0:2361:A:H8	1.82	0.45
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.99	0.45
1:A:211:LYS:HB2	38:A:9077:HOH:O	2.16	0.45
2:B:75:GLU:C	2:B:77:PRO:HD3	2.42	0.45
2:B:214:PRO:HD2	38:0:9075:HOH:O	2.15	0.45
2:B:215:VAL:HA	2:B:220:VAL:HG22	1.98	0.45
2:B:229:ARG:HD2	38:0:9108:HOH:O	2.17	0.45
3:C:49:ASP:HB3	3:C:52:ALA:HB2	1.99	0.45
30:0:629:A:H2'	30:0:630:A:O4'	2.17	0.45
30:0:737:A:H2'	30:0:738:G:O4'	2.17	0.45
30:0:1171:A:H2'	30:0:1172:G:H5'	1.98	0.45
30:0:1543:G:N1	30:0:1641:A:OP2	2.40	0.45
2:B:177:HIS:O	2:B:181:ILE:HG13	2.17	0.44
3:C:138:VAL:HG11	3:C:160:LEU:HD13	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:112:LEU:HG	30:0:1162:G:O2'	2.17	0.44
18:R:29:LYS:HD2	38:R:8943:HOH:O	2.16	0.44
24:X:25:ARG:HD3	24:X:64:ALA:O	2.16	0.44
30:0:105:G:O2'	30:0:106:A:H5'	2.17	0.44
30:0:1163:G:H2'	30:0:1164:U:C5	2.52	0.44
30:0:1188:A:N6	30:0:1189:A:N6	2.65	0.44
30:0:1224:G:H2'	30:0:1225:C:C6	2.51	0.44
30:0:2114:C:O2'	30:0:2115:U:H5'	2.17	0.44
30:0:2325:U:O2'	30:0:2411:C:H1'	2.16	0.44
31:9:35:C:H5''	38:9:9076:HOH:O	2.17	0.44
2:B:217:ARG:CG	2:B:257:THR:HG22	2.47	0.44
8:H:30:LYS:H	8:H:62:HIS:CD2	2.35	0.44
12:L:14:GLY:O	30:0:1295:G:H5''	2.17	0.44
12:L:33:ALA:HB3	38:L:8896:HOH:O	2.16	0.44
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.46	0.44
16:P:55:LYS:HG2	16:P:56:GLY:N	2.31	0.44
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.99	0.44
30:0:134:U:C2	30:0:145:A:C2	3.06	0.44
30:0:137:U:OP1	30:0:259:G:O2'	2.33	0.44
30:0:195:C:H2'	30:0:196:G:H5'	1.99	0.44
30:0:541:C:H2'	30:0:542:A:H5'	1.91	0.44
30:0:699:C:C2	30:0:743:G:N2	2.85	0.44
30:0:727:G:H3'	30:0:728:C:H6	1.82	0.44
30:0:820:G:O2'	30:0:856:G:H4'	2.18	0.44
30:0:1398:G:O2'	30:0:1399:A:H5'	2.18	0.44
30:0:1501:A:H4'	38:0:5597:HOH:O	2.17	0.44
30:0:1592:G:O2'	30:0:1593:C:O5'	2.35	0.44
30:0:1992:U:H2'	30:0:1994:A:OP2	2.17	0.44
2:B:198:GLU:HA	38:B:9126:HOH:O	2.17	0.44
6:F:101:ALA:HA	38:F:5413:HOH:O	2.16	0.44
15:O:25:VAL:CG1	30:0:710:G:H5'	2.48	0.44
24:X:73:ARG:NH1	24:X:88:GLU:HB2	2.33	0.44
30:0:283:U:H5	30:0:284:C:C4	2.33	0.44
30:0:660:A:H4'	30:0:661:G:O5'	2.18	0.44
30:0:1206:U:C5'	30:0:1206:U:H6	2.22	0.44
30:0:1583:U:H2'	30:0:1584:C:O4'	2.18	0.44
30:0:1702:U:H1'	38:0:5772:HOH:O	2.18	0.44
30:0:2509:A:OP2	30:0:2510:C:H5	2.00	0.44
30:0:2753:G:O2'	30:0:2754:G:H5'	2.18	0.44
2:B:253:GLN:OE1	30:0:2090:G:N2	2.51	0.44
10:J:45:VAL:HG11	10:J:121:LEU:HD22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:210:GLY:N	30:0:1313:A:H5''	2.33	0.44
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.17	0.44
28:2:37:HIS:CE1	30:0:462:A:C8	3.06	0.44
30:0:295:C:H2'	30:0:296:G:O4'	2.17	0.44
30:0:535:G:C5	30:0:2063:U:C4	3.05	0.44
30:0:790:A:H2'	30:0:791:A:O4'	2.18	0.44
30:0:999:C:H2'	30:0:1000:C:O4'	2.17	0.44
30:0:1166:A:OP1	30:0:1174:A:H4'	2.16	0.44
30:0:1249:U:H2'	30:0:1250:C:H6	1.79	0.44
30:0:1714:C:O2'	30:0:1715:C:H5'	2.17	0.44
30:0:2003:U:H4'	30:0:2004:U:H5	1.83	0.44
30:0:2245:C:H6	30:0:2245:C:O5'	2.00	0.44
30:0:2401:A:H2'	30:0:2402:A:C8	2.52	0.44
30:0:2657:G:O2'	30:0:2842:G:N7	2.47	0.44
1:A:144:GLU:OE2	30:0:1855:G:H8	2.00	0.44
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.01	0.44
3:C:80:VAL:HA	3:C:81:PRO:HD3	1.84	0.44
8:H:76:LEU:HD21	8:H:149:VAL:HA	1.98	0.44
10:J:130:VAL:HG12	10:J:131:THR:N	2.33	0.44
12:L:4:LYS:HE2	30:0:645:U:OP2	2.18	0.44
17:Q:1:PRO:HA	30:0:2299:G:O6	2.17	0.44
30:0:73:U:O2'	30:0:74:G:H5'	2.18	0.44
30:0:545:G:C8	30:0:545:G:C5'	2.94	0.44
30:0:694:A:C2'	30:0:695:C:H5'	2.47	0.44
30:0:1163:G:N2	38:0:4726:HOH:O	2.49	0.44
30:0:1183:C:H41	30:0:1192:A:P	2.40	0.44
30:0:1434:A:H2'	30:0:1436:C:C5	2.52	0.44
1:A:167:LYS:HB2	26:Z:53:ILE:HD13	1.99	0.44
11:K:66:ARG:HH12	30:0:1992:U:H3'	1.82	0.44
16:P:120:ARG:NH1	30:0:1594:C:C5	2.86	0.44
26:Z:44:ARG:HB2	30:0:1886:A:O2'	2.18	0.44
27:1:25:LYS:O	27:1:25:LYS:HG2	2.18	0.44
30:0:758:A:H2'	30:0:759:C:O4'	2.17	0.44
30:0:1163:G:C2	30:0:1184:C:N3	2.86	0.44
30:0:1191:A:H2	30:0:1206:U:H3	1.64	0.44
30:0:1444:G:O2'	30:0:1502:A:N1	2.41	0.44
30:0:1755:A:H2'	30:0:1756:G:O4'	2.18	0.44
30:0:1805:G:O2'	30:0:1806:G:H5'	2.17	0.44
30:0:1871:U:O4'	30:0:1873:G:C8	2.71	0.44
30:0:2846:C:H4'	38:0:5080:HOH:O	2.18	0.44
31:9:31:C:H2'	31:9:32:G:O4'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:VAL:CG1	2:B:53:LEU:HD13	2.46	0.44
2:B:75:GLU:OE2	2:B:151:VAL:HG13	2.18	0.44
4:D:25:MET:HE2	4:D:41:LEU:CG	2.42	0.44
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.17	0.44
11:K:41:LYS:HA	30:0:2582:G:O3'	2.18	0.44
15:O:32:ARG:O	15:O:32:ARG:HD3	2.17	0.44
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.32	0.44
25:Y:165:GLU:HB3	38:0:6704:HOH:O	2.17	0.44
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.52	0.44
30:0:241:A:N1	30:0:378:A:H4'	2.33	0.44
30:0:506:G:N2	30:0:509:A:C5'	2.66	0.44
30:0:603:A:H4'	30:0:604:G:O5'	2.17	0.44
30:0:1016:U:O2'	30:0:2303:A:N7	2.40	0.44
30:0:1972:U:H2'	30:0:1973:A:H5'	1.99	0.44
30:0:2064:U:H5'	30:0:2652:U:O3'	2.18	0.44
30:0:2104:C:O2	30:0:2485:A:N1	2.51	0.44
30:0:2895:C:H2'	38:0:9570:HOH:O	2.18	0.44
31:9:1:U:C5'	31:9:3:A:OP1	2.65	0.44
1:A:95:PRO:HA	1:A:153:ARG:HA	2.00	0.44
4:D:62:ASP:HA	38:D:4233:HOH:O	2.18	0.44
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.51	0.44
8:H:57:THR:HG23	8:H:131:GLN:HA	2.00	0.44
14:N:108:SER:HA	14:N:109:PRO:HD3	1.75	0.44
30:0:512:G:O3'	30:0:513:A:H8	2.00	0.44
30:0:574:G:O2'	30:0:575:A:H5'	2.18	0.44
30:0:731:U:H2'	30:0:732:C:C6	2.53	0.44
30:0:1051:C:H2'	30:0:1052:G:O4'	2.18	0.44
30:0:1143:G:C6	30:0:1221:G:C6	3.06	0.44
30:0:1702:U:H5'	38:0:3421:HOH:O	2.16	0.44
2:B:124:ALA:O	2:B:128:ILE:HG13	2.18	0.44
3:C:16:VAL:HG21	38:C:8641:HOH:O	2.17	0.44
9:I:101:LYS:O	9:I:105:GLU:HG3	2.18	0.44
13:M:86:GLN:HE22	30:0:2274:A:H1'	1.83	0.44
20:T:23:VAL:HG23	20:T:41:ARG:HG3	1.98	0.44
30:0:494:C:H2'	30:0:496:G:OP2	2.17	0.44
30:0:596:C:H2'	30:0:597:A:C8	2.52	0.44
30:0:596:C:H2'	30:0:597:A:H8	1.83	0.44
30:0:1116:U:HO2'	30:0:1118:A:H2	0.68	0.44
30:0:1819:G:C2'	30:0:1820:G:H5'	2.47	0.44
30:0:2073:G:H5''	38:0:3823:HOH:O	2.17	0.44
30:0:2249:G:C2	30:0:2253:G:C6	3.06	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2328:U:C4	30:0:2329:C:C5	3.06	0.44
30:0:2891:A:C2	30:0:2892:G:C4	3.06	0.44
30:0:2908:A:O5'	30:0:2908:A:H8	2.00	0.44
31:9:39:U:C2'	31:9:40:C:OP1	2.66	0.44
1:A:223:ARG:NH1	38:A:8985:HOH:O	2.50	0.43
2:B:315:VAL:HG23	2:B:316:ARG:HG2	2.00	0.43
9:I:87:PRO:HB3	38:I:6825:HOH:O	2.18	0.43
16:P:81:LYS:HG2	38:0:9538:HOH:O	2.18	0.43
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.99	0.43
30:0:88:G:H8	30:0:88:G:H5'	1.83	0.43
30:0:276:C:H6	30:0:276:C:O5'	2.01	0.43
30:0:1586:G:O2'	30:0:1587:U:H5'	2.18	0.43
30:0:2314:G:C2'	30:0:2315:C:H5'	2.48	0.43
30:0:2515:C:H2'	30:0:2516:G:O4'	2.18	0.43
30:0:2544:G:H2'	30:0:2545:U:O4'	2.18	0.43
30:0:2662:G:N3	30:0:2816:A:H2	2.16	0.43
30:0:2896:A:N3	30:0:2896:A:H2'	2.32	0.43
2:B:24:PRO:HG2	2:B:204:GLY:HA2	2.00	0.43
3:C:88:SER:HB3	3:C:91:PRO:HB3	2.01	0.43
10:J:131:THR:HG22	10:J:133:GLY:H	1.82	0.43
10:J:135:ILE:O	10:J:139:LEU:HG	2.18	0.43
14:N:18:THR:HG21	38:N:8844:HOH:O	2.17	0.43
30:0:482:G:O4'	30:0:511:A:C2	2.70	0.43
30:0:506:G:N2	30:0:509:A:H5'	2.23	0.43
30:0:1504:A:H5'	38:0:4414:HOH:O	2.18	0.43
30:0:1568:G:O2'	30:0:1569:U:H5'	2.18	0.43
30:0:1797:A:H2'	30:0:1799:G:O5'	2.18	0.43
30:0:1996:U:O2'	30:0:1997:A:H5'	2.18	0.43
30:0:2524:G:H5''	38:0:4731:HOH:O	2.18	0.43
30:0:2705:U:H2'	30:0:2706:A:H8	1.82	0.43
2:B:185:GLY:HA2	38:B:9099:HOH:O	2.17	0.43
2:B:215:VAL:HB	38:B:9086:HOH:O	2.18	0.43
8:H:91:ARG:NH1	8:H:138:THR:OG1	2.47	0.43
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.99	0.43
11:K:74:VAL:HG21	11:K:96:VAL:HG23	1.99	0.43
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.18	0.43
20:T:52:ARG:O	30:0:317:A:OP1	2.35	0.43
23:W:21:LEU:O	23:W:26:ILE:HG23	2.19	0.43
38:3:8961:HOH:O	30:0:2382:A:H5'	2.17	0.43
30:0:398:U:H2'	30:0:399:C:C6	2.53	0.43
30:0:629:A:C2	30:0:2074:A:C2	3.06	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:675:U:H2'	30:0:676:C:H5'	2.00	0.43
30:0:806:A:H2'	30:0:807:A:O4'	2.19	0.43
30:0:875:A:H5'	30:0:876:A:N7	2.33	0.43
30:0:960:G:N3	30:0:960:G:H3'	2.33	0.43
30:0:1163:G:N2	30:0:1184:C:N3	2.66	0.43
30:0:1167:G:H2'	30:0:1168:C:O4'	2.18	0.43
30:0:1538:C:O2'	30:0:1539:U:H5'	2.17	0.43
30:0:2115:U:H2'	30:0:2116:U:C6	2.53	0.43
30:0:2887:G:H2'	30:0:2888:U:C6	2.53	0.43
6:F:68:ASP:C	6:F:70:LYS:H	2.26	0.43
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.81	0.43
15:O:105:ASN:HD21	15:O:109:SER:N	2.16	0.43
19:S:49:VAL:HG13	19:S:66:VAL:HG13	2.00	0.43
23:W:115:THR:HG23	38:W:5420:HOH:O	2.19	0.43
30:0:1079:A:H4'	30:0:2078:U:H5'	2.00	0.43
30:0:2067:A:H2'	30:0:2068:G:O4'	2.18	0.43
30:0:2653:A:H2'	30:0:2654:C:C6	2.54	0.43
5:E:126:ILE:HB	5:E:131:LEU:CD2	2.48	0.43
6:F:77:VAL:HG21	6:F:83:LEU:HD13	1.99	0.43
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.83	0.43
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.19	0.43
26:Z:55:SER:O	26:Z:59:GLU:HG3	2.17	0.43
28:2:5:LYS:O	28:2:9:LYS:HG3	2.18	0.43
30:0:255:A:C5	30:0:256:C:C5	3.06	0.43
30:0:368:C:H2'	30:0:369:G:H5'	2.00	0.43
30:0:445:U:H2'	30:0:446:G:H8	1.84	0.43
30:0:699:C:C6	30:0:744:G:O4'	2.71	0.43
30:0:1127:C:C5	30:0:1128:U:C4	3.06	0.43
30:0:1333:U:H2'	30:0:1334:C:H6	1.83	0.43
30:0:1890:U:H1'	38:0:5957:HOH:O	2.18	0.43
30:0:2265:U:H2'	30:0:2266:A:C8	2.53	0.43
30:0:2543:G:O3'	30:0:2590:U:H5'	2.19	0.43
4:D:41:LEU:HA	4:D:44:ILE:HG22	2.00	0.43
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.54	0.43
14:N:38:LYS:HD2	14:N:114:LYS:HE3	2.01	0.43
16:P:134:VAL:O	16:P:137:LEU:HB3	2.19	0.43
21:U:6:CYS:HA	21:U:13:ILE:HD11	2.01	0.43
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.19	0.43
30:0:426:G:H2'	30:0:427:C:O4'	2.18	0.43
30:0:565:A:C6	30:0:566:A:C6	3.07	0.43
30:0:821:U:H2'	30:0:822:C:C6	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1425:G:C2'	30:0:1426:C:H5'	2.48	0.43
30:0:1850:U:O4'	30:0:1941:A:C2	2.71	0.43
30:0:2072:G:N2	38:0:6868:HOH:O	2.51	0.43
30:0:2403:C:H2'	30:0:2404:G:O5'	2.18	0.43
31:9:98:C:O2'	31:9:99:U:H5'	2.19	0.43
1:A:123:GLY:HA3	1:A:162:GLY:HA2	1.99	0.43
2:B:5:ARG:NH1	30:0:2547:C:OP2	2.52	0.43
6:F:91:VAL:CG1	6:F:92:GLY:N	2.81	0.43
12:L:6:ARG:NH1	30:0:1299:G:N7	2.66	0.43
23:W:130:HIS:O	23:W:136:GLY:HA3	2.18	0.43
25:Y:107:PRO:HB3	25:Y:182:PHE:CD2	2.53	0.43
30:0:170:U:H2'	30:0:171:C:H5'	1.98	0.43
30:0:807:A:H2'	30:0:808:A:O4'	2.19	0.43
30:0:1250:C:O2'	30:0:1251:C:H5'	2.18	0.43
30:0:1427:A:H61	30:0:1440:U:H1'	1.82	0.43
30:0:1773:G:N2	30:0:1774:G:C8	2.86	0.43
30:0:1819:G:O2'	30:0:1820:G:H5'	2.18	0.43
18:R:99:ALA:HB1	18:R:109:MET:CE	2.30	0.43
23:W:107:LEU:O	23:W:112:LEU:HB2	2.18	0.43
24:X:76:ARG:HG3	24:X:76:ARG:NH1	2.31	0.43
26:Z:43:GLY:HA2	30:0:1771:U:O2	2.19	0.43
30:0:163:U:O3'	30:0:896:C:H4'	2.19	0.43
30:0:684:G:H2'	30:0:685:C:C6	2.54	0.43
30:0:1474:C:C6	30:0:1474:C:C5'	2.90	0.43
30:0:1634:G:H2'	30:0:1635:U:C6	2.53	0.43
30:0:2256:G:C2'	30:0:2257:G:C5'	2.97	0.43
30:0:2543:G:H2'	30:0:2544:G:O4'	2.18	0.43
31:9:105:A:H2'	31:9:106:U:O4'	2.18	0.43
5:E:11:VAL:HG12	5:E:12:ASP:N	2.34	0.43
5:E:19:ASP:HA	5:E:31:ARG:O	2.19	0.43
8:H:49:GLN:HG3	8:H:140:TYR:CE2	2.54	0.43
22:V:29:ASN:O	22:V:33:VAL:HG23	2.18	0.43
30:0:111:C:O2'	30:0:112:G:H5'	2.19	0.43
30:0:1167:G:C2	30:0:1168:C:C2	3.07	0.43
30:0:1463:U:H2'	30:0:1464:C:H6	1.83	0.43
30:0:2661:U:H3	30:0:2812:A:H62	1.65	0.43
31:9:54:A:C2	31:9:55:U:N3	2.87	0.43
1:A:101:GLU:HG2	38:A:9034:HOH:O	2.18	0.43
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.47	0.43
12:L:33:ALA:HB2	30:0:165:A:H5''	1.99	0.43
22:V:56:ILE:O	22:V:60:GLN:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:71:ARG:HD2	38:X:7542:HOH:O	2.18	0.43
25:Y:189:ASN:ND2	25:Y:192:ASP:N	2.66	0.43
30:0:111:C:C2'	30:0:112:G:H5'	2.49	0.43
30:0:162:C:O2'	30:0:895:A:N3	2.48	0.43
30:0:544:G:C3'	30:0:545:G:H5''	2.48	0.43
30:0:1023:C:O2'	30:0:1024:G:H5'	2.19	0.43
30:0:1517:C:O2	30:0:1670:A:C2	2.72	0.43
30:0:1682:A:H5''	38:0:9456:HOH:O	2.19	0.43
30:0:2079:G:H2'	30:0:2080:G:O4'	2.19	0.43
30:0:2540:G:H5''	38:0:4662:HOH:O	2.19	0.43
30:0:2757:A:H2'	30:0:2758:G:O4'	2.18	0.43
7:G:19:GLU:O	7:G:23:ILE:HG13	2.19	0.42
10:J:107:ASN:ND2	10:J:109:TYR:H	2.16	0.42
14:N:37:ARG:HH11	31:9:6:C:H5''	1.71	0.42
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.92	0.42
27:1:28:HIS:HD2	27:1:30:LYS:H	1.65	0.42
30:0:699:C:C2	30:0:744:G:C2	3.06	0.42
30:0:702:G:C2	30:0:703:G:C8	3.07	0.42
30:0:920:C:H4'	30:0:921:G:N2	2.34	0.42
30:0:1461:U:H2'	30:0:1462:C:C6	2.54	0.42
30:0:1503:U:H2'	30:0:1504:A:O4'	2.19	0.42
30:0:1576:G:H2'	30:0:1577:U:O4'	2.19	0.42
30:0:2102:G:C2'	38:0:7763:HOH:O	2.59	0.42
30:0:2610:U:H3'	38:0:7521:HOH:O	2.18	0.42
30:0:2668:G:H2'	30:0:2669:U:C6	2.54	0.42
1:A:4:ILE:HG22	1:A:198:ASP:O	2.19	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.18	0.42
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.52	0.42
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.49	0.42
12:L:61:ALA:HB2	12:L:105:TYR:CZ	2.54	0.42
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.19	0.42
23:W:4:LEU:HD13	23:W:52:VAL:HG21	2.01	0.42
29:3:48:ASN:ND2	29:3:50:GLY:H	2.17	0.42
30:0:62:C:C4	30:0:63:U:C4	3.07	0.42
30:0:142:G:O2'	30:0:143:C:H5'	2.18	0.42
30:0:343:C:O2'	30:0:344:C:H5'	2.19	0.42
30:0:512:G:H5''	30:0:515:C:H1'	2.00	0.42
30:0:682:A:H2'	30:0:683:G:O4'	2.18	0.42
30:0:705:C:O2	30:0:705:C:C2'	2.67	0.42
30:0:946:C:H2'	30:0:947:U:H6	1.83	0.42
30:0:1166:A:H1'	30:0:1192:A:C2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1181:A:C2	30:0:1192:A:C8	3.06	0.42
30:0:2054:A:H5'	38:0:4901:HOH:O	2.18	0.42
30:0:2635:A:C2'	30:0:2636:C:H5'	2.49	0.42
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.87	0.42
5:E:21:THR:HG23	5:E:30:THR:OG1	2.18	0.42
10:J:19:MET:CE	10:J:132:LEU:HD11	2.41	0.42
14:N:132:ASN:HD22	30:0:2413:A:H4'	1.83	0.42
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.19	0.42
23:W:65:VAL:HA	23:W:68:THR:HG22	2.00	0.42
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.01	0.42
30:0:729:C:C2	30:0:743:G:C2	3.07	0.42
30:0:2474:A:N7	30:0:2621:PSU:H4'	2.34	0.42
30:0:2646:G:C5	30:0:2647:C:C5	3.07	0.42
30:0:2809:G:H2'	30:0:2810:G:O4'	2.20	0.42
31:9:95:C:O2'	31:9:96:C:H5'	2.20	0.42
31:9:108:C:H2'	31:9:109:G:C8	2.53	0.42
2:B:53:LEU:HD21	2:B:270:ILE:HD12	2.00	0.42
3:C:140:VAL:HG12	3:C:141:SER:N	2.34	0.42
8:H:123:ILE:HD12	8:H:123:ILE:N	2.34	0.42
8:H:141:CYS:HB2	38:H:197:HOH:O	2.20	0.42
10:J:39:VAL:CG2	10:J:107:ASN:HA	2.49	0.42
13:M:93:ARG:HD2	30:0:1470:A:OP1	2.19	0.42
14:N:42:HIS:CG	14:N:62:HIS:HE1	2.37	0.42
18:R:109:MET:HG2	18:R:148:GLU:C	2.45	0.42
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.31	0.42
24:X:43:VAL:HG12	24:X:44:ASP:H	1.83	0.42
25:Y:152:LYS:CB	25:Y:160:LYS:HG3	2.49	0.42
25:Y:154:ARG:NH2	30:0:1072:G:OP2	2.53	0.42
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.33	0.42
30:0:51:G:O2'	30:0:52:A:H5'	2.20	0.42
30:0:349:U:O2'	30:0:350:G:H5'	2.19	0.42
30:0:622:G:O2'	30:0:623:U:H5'	2.20	0.42
30:0:1298:U:H2'	30:0:1299:G:C8	2.54	0.42
30:0:1947:G:H2'	30:0:1948:G:H8	1.84	0.42
1:A:186:TRP:CD1	1:A:187:PRO:HA	2.55	0.42
2:B:84:LEU:HD23	2:B:142:LEU:HD23	2.02	0.42
3:C:35:VAL:HG21	3:C:227:GLY:HA2	2.01	0.42
4:D:135:VAL:HG22	4:D:136:ARG:N	2.34	0.42
6:F:99:THR:HG23	6:F:99:THR:O	2.19	0.42
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.34	0.42
14:N:71:TRP:HB2	38:N:8836:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:18:LEU:HD12	18:R:143:VAL:HG11	2.01	0.42
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.18	0.42
30:0:39:G:N2	30:0:444:C:C2	2.88	0.42
30:0:1416:G:C2'	30:0:1417:G:H5'	2.50	0.42
30:0:1616:A:H5''	30:0:1617:C:OP1	2.19	0.42
30:0:1706:G:C6	30:0:1707:G:C6	3.08	0.42
30:0:2237:G:H1'	38:0:4856:HOH:O	2.18	0.42
30:0:2316:G:H4'	38:0:6092:HOH:O	2.19	0.42
30:0:2429:A:H4'	38:0:7729:HOH:O	2.19	0.42
30:0:2626:C:H2'	30:0:2627:G:H8	1.84	0.42
1:A:36:ASP:HA	1:A:83:GLY:HA3	2.01	0.42
2:B:60:SER:HA	2:B:61:PRO:HD3	1.87	0.42
9:I:118:ASN:HB3	30:0:1185:U:H5''	2.01	0.42
22:V:11:MET:HE1	22:V:19:GLU:HG2	2.01	0.42
30:0:360:A:H2'	30:0:361:C:O4'	2.19	0.42
30:0:567:U:O5'	30:0:567:U:H6	2.03	0.42
30:0:664:U:O4	30:0:681:G:H5''	2.20	0.42
30:0:851:C:O2	30:0:2022:A:H2	2.03	0.42
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.42
30:0:1850:U:H2'	30:0:1851:G:C8	2.55	0.42
30:0:1973:A:H2'	30:0:1974:G:O4'	2.19	0.42
30:0:2002:C:C2'	30:0:2003:U:H5'	2.49	0.42
30:0:2004:U:H6	30:0:2004:U:P	2.43	0.42
30:0:2709:G:N2	38:0:7616:HOH:O	2.51	0.42
30:0:2751:C:H2'	30:0:2752:C:H6	1.84	0.42
30:0:2883:A:H2'	30:0:2884:G:O4'	2.19	0.42
1:A:88:ILE:O	1:A:88:ILE:HG22	2.20	0.42
2:B:18:ARG:HG3	2:B:256:GLN:HG3	2.02	0.42
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.02	0.42
2:B:258:GLY:HA2	38:0:4005:HOH:O	2.20	0.42
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.20	0.42
5:E:7:ILE:HG22	5:E:45:ASP:O	2.19	0.42
10:J:22:VAL:O	10:J:26:VAL:HG23	2.20	0.42
13:M:42:ARG:HA	13:M:43:PRO:HD3	1.87	0.42
18:R:84:ALA:O	18:R:88:PHE:HD1	2.02	0.42
28:2:2:LYS:HG3	30:0:1486:A:C5	2.54	0.42
30:0:128:A:C8	30:0:128:A:H3'	2.54	0.42
30:0:130:C:H5'	38:0:5216:HOH:O	2.19	0.42
30:0:187:A:H3'	30:0:188:C:C6	2.55	0.42
30:0:236:A:H4'	30:0:237:G:OP1	2.19	0.42
30:0:417:G:P	38:0:7414:HOH:O	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1058:A:H2'	30:0:1060:C:C5'	2.50	0.42
30:0:1139:U:H2'	30:0:1140:C:C6	2.54	0.42
30:0:1917:G:C6	30:0:1918:U:C4	3.07	0.42
30:0:1942:A:H2'	30:0:1943:C:C6	2.55	0.42
30:0:2645:U:O2'	30:0:2646:G:P	2.78	0.42
30:0:2761:A:C4	30:0:2763:G:C8	3.07	0.42
3:C:236:THR:HG21	38:C:8579:HOH:O	2.20	0.42
3:C:242:GLU:HB2	38:C:8587:HOH:O	2.19	0.42
5:E:11:VAL:HG13	5:E:23:GLU:O	2.19	0.42
5:E:60:SER:OG	30:0:2784:A:H1'	2.20	0.42
15:O:29:VAL:HG11	15:O:98:LEU:HD21	2.01	0.42
20:T:24:ARG:HH21	20:T:39:ASN:ND2	2.16	0.42
23:W:44:MET:CE	30:0:944:G:H21	2.33	0.42
25:Y:138:ARG:HD3	30:0:638:C:OP2	2.20	0.42
27:1:10:LYS:HG3	38:1:8981:HOH:O	2.19	0.42
30:0:309:C:O2	30:0:309:C:H2'	2.19	0.42
30:0:377:C:H5	38:0:3302:HOH:O	2.01	0.42
30:0:1060:C:H6	30:0:1060:C:H5'	1.85	0.42
30:0:1191:A:N3	30:0:1207:A:C2	2.87	0.42
30:0:1214:G:H4'	38:0:4747:HOH:O	2.19	0.42
30:0:1907:U:O2'	30:0:1908:G:H5'	2.20	0.42
31:9:31:C:C2	31:9:50:G:N2	2.88	0.42
1:A:103:VAL:HA	1:A:104:PRO:HD3	1.86	0.42
8:H:139:ALA:HB3	8:H:149:VAL:HG21	2.02	0.42
9:I:87:PRO:C	9:I:89:GLU:H	2.27	0.42
13:M:15:PRO:HA	13:M:20:LEU:HD23	2.02	0.42
13:M:80:GLY:O	13:M:81:ARG:HD3	2.20	0.42
13:M:122:GLN:HB2	13:M:126:GLN:O	2.20	0.42
15:O:39:THR:O	15:O:115:ARG:NH2	2.53	0.42
30:0:241:A:C2	30:0:378:A:H4'	2.54	0.42
30:0:569:A:H5''	30:0:587:A:N1	2.35	0.42
30:0:999:C:C2'	30:0:1000:C:H5'	2.49	0.42
30:0:1008:C:O2'	30:0:1009:U:H5'	2.20	0.42
30:0:1159:G:H1	30:0:1208:C:H42	1.68	0.42
30:0:1520:G:C6	30:0:1521:C:C4	3.07	0.42
30:0:1789:G:C2'	30:0:1790:C:O5'	2.68	0.42
30:0:1903:U:O2'	30:0:1904:A:C8	2.68	0.42
31:9:73:A:N1	31:9:108:C:O2	2.53	0.42
3:C:206:ASN:HB2	30:0:329:A:OP2	2.20	0.42
5:E:7:ILE:HA	5:E:8:PRO:HD3	1.95	0.42
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:24:THR:HB	11:K:64:MET:HE2	2.01	0.42
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.02	0.42
14:N:171:HIS:CE1	38:N:8861:HOH:O	2.71	0.42
18:R:69:LYS:HB2	18:R:72:VAL:HG23	2.02	0.42
22:V:1:THR:CG2	22:V:2:VAL:H	2.25	0.42
23:W:29:VAL:O	23:W:30:ASN:HB2	2.19	0.42
25:Y:141:THR:HG23	38:Y:9073:HOH:O	2.19	0.42
30:0:365:G:C6	30:0:366:U:C4	3.08	0.42
30:0:699:C:C6	30:0:744:G:C4	3.08	0.42
30:0:1130:U:H2'	30:0:1131:G:C4'	2.50	0.42
30:0:1373:G:H4'	38:0:5286:HOH:O	2.20	0.42
30:0:1494:A:C4	30:0:1495:C:C5	3.08	0.42
30:0:2553:A:H2'	30:0:2553:A:N3	2.35	0.42
30:0:2739:A:C6	30:0:2740:G:C5	3.08	0.42
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.49	0.41
6:F:83:LEU:HD12	6:F:83:LEU:HA	1.91	0.41
20:T:41:ARG:HG2	20:T:41:ARG:NH1	2.34	0.41
30:0:45:A:N6	30:0:147:G:C4	2.88	0.41
30:0:116:G:H1'	30:0:129:A:N3	2.35	0.41
30:0:424:C:H2'	30:0:425:U:H6	1.85	0.41
30:0:939:A:C2	30:0:1027:G:N3	2.88	0.41
30:0:941:G:C6	30:0:942:U:C4	3.08	0.41
30:0:1183:C:N3	30:0:1184:C:C4	2.88	0.41
30:0:1207:A:N6	38:0:5631:HOH:O	2.53	0.41
30:0:1375:A:C2'	30:0:1376:G:H5'	2.50	0.41
30:0:1416:G:H2'	30:0:1417:G:H5'	2.01	0.41
30:0:1574:C:O5'	30:0:1574:C:H6	2.03	0.41
30:0:1771:U:O2'	30:0:1773:G:N7	2.52	0.41
30:0:1926:G:H2'	30:0:1927:A:C8	2.55	0.41
30:0:2256:G:H2'	30:0:2257:G:O5'	2.19	0.41
30:0:2425:A:H5'	30:0:2426:G:OP2	2.20	0.41
30:0:2541:U:H5''	38:0:5398:HOH:O	2.20	0.41
30:0:2587:OMU:O5'	30:0:2587:OMU:H6	2.19	0.41
30:0:2616:A:C4'	30:0:2617:G:OP1	2.67	0.41
5:E:84:MET:HE2	5:E:133:VAL:CG2	2.50	0.41
8:H:102:LYS:HD3	8:H:122:LYS:HD3	2.02	0.41
11:K:109:LEU:CD1	11:K:113:ILE:HD11	2.50	0.41
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.56	0.41
30:0:131:A:OP2	30:0:141:C:H5	2.03	0.41
30:0:803:C:O2'	30:0:804:C:H5'	2.21	0.41
30:0:1001:U:O2'	30:0:1002:G:H5'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1202:A:H2'	30:0:1203:G:O4'	2.20	0.41
30:0:2509:A:OP2	30:0:2510:C:C5	2.73	0.41
30:0:2591:C:H2'	30:0:2592:G:O4'	2.20	0.41
30:0:2611:G:H5'	30:0:2613:G:C8	2.55	0.41
30:0:2866:U:H4'	30:0:2867:G:H5'	2.01	0.41
31:9:2:U:C1'	38:9:9099:HOH:O	2.67	0.41
31:9:2:U:H1'	38:9:9099:HOH:O	2.19	0.41
1:A:212:PRO:HA	30:0:1943:C:O4'	2.19	0.41
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.50	0.41
4:D:58:VAL:HG12	4:D:60:GLU:HG2	2.01	0.41
5:E:93:MET:HE1	5:E:165:GLY:N	2.35	0.41
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.20	0.41
18:R:106:GLY:HA2	18:R:109:MET:HE3	2.02	0.41
23:W:73:LEU:HD12	23:W:73:LEU:HA	1.77	0.41
23:W:125:HIS:CD2	23:W:127:GLY:H	2.38	0.41
24:X:73:ARG:HH12	24:X:88:GLU:HB2	1.85	0.41
25:Y:189:ASN:HD22	25:Y:192:ASP:H	1.67	0.41
30:0:862:U:H2'	30:0:863:G:C8	2.55	0.41
30:0:1191:A:H2'	30:0:1193:A:H5'	2.02	0.41
30:0:1391:G:H2'	30:0:1392:A:H5'	2.02	0.41
30:0:1946:C:H2'	30:0:1971:G:C8	2.55	0.41
30:0:2361:A:H2'	30:0:2362:A:O4'	2.20	0.41
30:0:2438:G:H2'	30:0:2439:C:C6	2.55	0.41
30:0:2729:C:O2'	30:0:2730:G:H5'	2.19	0.41
2:B:62:ARG:HA	2:B:65:MET:CE	2.41	0.41
3:C:240:LEU:HB2	38:C:8659:HOH:O	2.20	0.41
10:J:75:PRO:HD3	10:J:136:SER:OG	2.20	0.41
14:N:4:PRO:HB2	30:0:1010:C:H4'	2.02	0.41
15:O:38:ARG:HD3	30:0:654:A:OP2	2.20	0.41
17:Q:7:LEU:HD12	30:0:2424:U:C1'	2.50	0.41
20:T:26:THR:HG23	20:T:97:ARG:HG3	2.02	0.41
21:U:23:HIS:NE2	21:U:29:THR:OG1	2.41	0.41
22:V:44:GLY:O	22:V:48:GLU:HG2	2.21	0.41
29:3:69:TYR:HB2	29:3:78:HIS:CE1	2.55	0.41
30:0:23:G:H1'	30:0:520:A:N6	2.36	0.41
30:0:1398:G:H2'	30:0:1399:A:C8	2.55	0.41
30:0:1576:G:H2'	30:0:1577:U:C6	2.55	0.41
30:0:1613:C:H2'	30:0:1614:G:O4'	2.20	0.41
30:0:1940:C:H1'	38:0:9375:HOH:O	2.20	0.41
30:0:2880:A:C2'	30:0:2881:C:H5'	2.50	0.41
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:SER:HA	1:A:227:ASP:O	2.21	0.41
6:F:72:VAL:HA	6:F:73:PRO:HD3	1.86	0.41
14:N:147:ILE:HD12	38:9:9087:HOH:O	2.20	0.41
18:R:39:THR:HB	18:R:42:GLU:HG3	2.02	0.41
23:W:38:THR:HG22	23:W:39:ASP:H	1.86	0.41
30:0:370:G:N2	30:0:371:U:C2	2.89	0.41
30:0:946:C:H2'	30:0:947:U:C6	2.54	0.41
30:0:1327:G:C6	30:0:1331:G:C6	3.09	0.41
30:0:2737:C:H2'	38:0:6141:HOH:O	2.21	0.41
31:9:2:U:OP2	31:9:2:U:H4'	2.21	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.92	0.41
4:D:88:LEU:HB2	4:D:89:PRO:HD3	2.02	0.41
6:F:32:GLY:N	38:F:3111:HOH:O	2.53	0.41
8:H:92:LYS:HG3	8:H:130:VAL:HG22	2.02	0.41
13:M:24:GLN:NE2	13:M:24:GLN:HA	2.35	0.41
18:R:61:GLN:CD	38:R:8943:HOH:O	2.64	0.41
18:R:80:TYR:O	30:0:2050:G:H5''	2.20	0.41
25:Y:145:LYS:O	25:Y:147:ARG:HG2	2.20	0.41
29:3:38:ARG:HD2	30:0:396:U:OP2	2.20	0.41
30:0:334:G:H2'	30:0:335:U:O4'	2.20	0.41
30:0:659:A:H5''	38:0:7096:HOH:O	2.19	0.41
30:0:1259:A:N1	30:0:1261:A:H1'	2.35	0.41
30:0:1311:G:C2	30:0:1312:G:C8	3.08	0.41
30:0:1471:A:H2'	30:0:1472:C:C6	2.55	0.41
30:0:2088:C:H1'	30:0:2841:A:N1	2.36	0.41
30:0:2506:A:H62	30:0:2511:A:HO2'	1.66	0.41
1:A:20:SER:HB3	30:0:1872:C:H5	1.85	0.41
2:B:174:ARG:HA	2:B:177:HIS:HB3	2.03	0.41
38:D:7597:HOH:O	31:9:56:A:H2	2.04	0.41
6:F:1:PRO:H3	6:F:4:VAL:HG23	1.86	0.41
10:J:52:GLN:NE2	30:0:1119:G:H8	2.18	0.41
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.41
16:P:18:LYS:O	16:P:21:VAL:HG13	2.20	0.41
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.20	0.41
18:R:114:VAL:HG13	18:R:114:VAL:O	2.21	0.41
20:T:77:VAL:HG11	20:T:91:LEU:HD11	2.03	0.41
24:X:43:VAL:HG12	24:X:47:ALA:HB3	2.01	0.41
25:Y:151:SER:HB3	25:Y:154:ARG:CB	2.50	0.41
29:3:69:TYR:CZ	29:3:80:ARG:HD2	2.55	0.41
29:3:91:GLN:O	29:3:92:GLU:HB2	2.20	0.41
30:0:99:A:C8	30:0:100:C:C5	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:517:U:C2'	30:0:518:G:H5'	2.50	0.41
30:0:1076:G:C2	30:0:1084:C:C2	3.08	0.41
30:0:1982:C:H2'	30:0:1983:C:O4'	2.20	0.41
30:0:2083:A:H3'	38:0:7573:HOH:O	2.20	0.41
30:0:2102:G:N2	30:0:2104:C:C6	2.89	0.41
30:0:2480:G:O2'	30:0:2481:G:H5'	2.21	0.41
30:0:2526:C:H6	30:0:2526:C:H3'	1.85	0.41
30:0:2764:C:H2'	30:0:2765:C:H6	1.84	0.41
2:B:53:LEU:HD11	2:B:327:VAL:HG22	2.02	0.41
2:B:97:LEU:O	2:B:98:THR:HG23	2.21	0.41
6:F:50:VAL:CG2	6:F:63:ILE:HG21	2.51	0.41
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.51	0.41
18:R:1:GLY:HA2	18:R:119:VAL:HG21	2.02	0.41
30:0:10:U:O4	30:0:532:A:H8	2.04	0.41
30:0:79:G:N2	30:0:97:G:H1'	2.36	0.41
30:0:278:A:C6	30:0:279:C:C4	3.09	0.41
30:0:626:U:C4	30:0:627:G:C6	3.08	0.41
30:0:1626:A:C2'	30:0:1627:G:H5'	2.51	0.41
30:0:1896:G:C6	30:0:1897:U:C4	3.09	0.41
30:0:2607:U:H4'	38:0:9440:HOH:O	2.21	0.41
31:9:1:U:O3'	31:9:3:A:OP1	2.39	0.41
2:B:10:SER:HB2	30:0:2714:U:H4'	2.02	0.41
4:D:35:ALA:C	4:D:37:ALA:H	2.29	0.41
4:D:88:LEU:N	4:D:89:PRO:CD	2.83	0.41
5:E:166:VAL:HG12	38:E:3134:HOH:O	2.21	0.41
14:N:38:LYS:HE3	14:N:38:LYS:HB2	1.81	0.41
15:O:14:LEU:HD23	15:O:102:ILE:HD11	2.03	0.41
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.69	0.41
18:R:99:ALA:CB	18:R:109:MET:HE1	2.31	0.41
23:W:80:ASP:HB2	38:W:3312:HOH:O	2.21	0.41
27:1:28:HIS:O	27:1:32:LYS:N	2.47	0.41
30:0:196:G:H1'	30:0:198:A:N7	2.35	0.41
30:0:287:C:H2'	30:0:288:A:C8	2.56	0.41
30:0:393:G:C6	30:0:394:G:C6	3.09	0.41
30:0:812:A:H2'	30:0:813:C:C6	2.55	0.41
30:0:812:A:H2'	30:0:813:C:O4'	2.21	0.41
30:0:1074:G:H4'	30:0:1260:G:C6	2.56	0.41
30:0:1275:C:N3	30:0:1281:C:N4	2.69	0.41
30:0:1406:A:H4'	30:0:1407:A:C5'	2.51	0.41
30:0:1445:G:N2	30:0:1678:A:H1'	2.36	0.41
30:0:1552:G:H2'	30:0:1553:C:C6	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1632:A:C3'	30:0:1633:C:H5'	2.51	0.41
30:0:1783:A:O2'	30:0:1784:U:H5'	2.21	0.41
30:0:1964:U:O2	30:0:1964:U:H2'	2.21	0.41
1:A:204:GLY:N	30:0:2634:G:OP2	2.53	0.41
2:B:57:GLU:HA	2:B:58:PRO:HD2	1.91	0.41
2:B:85:ARG:NH1	30:0:2671:U:O2	2.54	0.41
2:B:211:THR:HG21	38:0:7451:HOH:O	2.21	0.41
5:E:49:ILE:HD11	5:E:69:ILE:HD12	2.03	0.41
8:H:100:GLU:HB3	8:H:124:VAL:HG11	2.02	0.41
10:J:105:LEU:HD23	38:J:5907:HOH:O	2.21	0.41
14:N:13:ARG:NH1	30:0:2368:A:C6	2.89	0.41
17:Q:50:GLY:HA2	38:0:6025:HOH:O	2.20	0.41
18:R:79:ARG:HB3	30:0:2050:G:OP1	2.21	0.41
21:U:6:CYS:C	21:U:8:TYR:H	2.28	0.41
21:U:33:SER:O	21:U:37:GLU:HG3	2.21	0.41
30:0:74:G:O2'	30:0:75:U:H5'	2.20	0.41
30:0:594:C:C4	30:0:595:U:C4	3.09	0.41
30:0:1084:C:H6	30:0:1084:C:O5'	2.04	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.34	0.41
30:0:1363:G:H2'	30:0:1364:G:C8	2.56	0.41
30:0:1587:U:H2'	30:0:1588:G:O4'	2.21	0.41
30:0:1641:A:H2'	30:0:1642:A:C5'	2.45	0.41
30:0:1712:A:H2'	30:0:1713:G:O4'	2.20	0.41
30:0:1743:G:H1'	38:0:4892:HOH:O	2.20	0.41
30:0:1930:A:H2'	30:0:1931:A:C8	2.55	0.41
30:0:2277:U:O2'	30:0:2278:U:H5'	2.21	0.41
30:0:2804:C:H2'	30:0:2805:A:O4'	2.21	0.41
30:0:2842:G:H2'	30:0:2843:A:H5'	2.02	0.41
31:9:58:G:N7	31:9:59:C:C4	2.89	0.41
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.54	0.40
3:C:214:THR:HG21	38:C:8608:HOH:O	2.20	0.40
4:D:18:ILE:HD13	4:D:84:LEU:HD12	2.03	0.40
12:L:121:ILE:HG12	12:L:141:GLU:HB2	2.04	0.40
12:L:129:ALA:O	12:L:133:VAL:HG23	2.21	0.40
18:R:82:GLU:HG3	18:R:83:LYS:N	2.35	0.40
22:V:5:VAL:HG23	38:V:2271:HOH:O	2.20	0.40
22:V:27:LEU:HA	22:V:49:LEU:HD13	2.02	0.40
29:3:38:ARG:HH11	30:0:396:U:P	2.43	0.40
29:3:79:LEU:HD13	30:0:2457:U:H1'	2.04	0.40
30:0:11:A:H5'	30:0:12:U:OP2	2.20	0.40
30:0:228:C:C2'	30:0:229:G:H5'	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1041:U:H4'	30:0:1295:G:H5'	2.03	0.40
30:0:1760:G:C2	30:0:1813:U:O4'	2.74	0.40
30:0:1917:G:C5	30:0:1918:U:C4	3.09	0.40
30:0:2072:G:O2'	30:0:2489:G:N2	2.53	0.40
30:0:2617:G:C2	30:0:2618:G:C8	3.09	0.40
1:A:173:GLY:O	1:A:176:HIS:HB3	2.21	0.40
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.36	0.40
2:B:310:ARG:HD2	38:B:9115:HOH:O	2.21	0.40
12:L:50:GLY:C	30:0:2453:G:H4'	2.46	0.40
14:N:23:ARG:HG2	14:N:23:ARG:HH11	1.87	0.40
16:P:14:LEU:HD13	16:P:51:ALA:HB2	2.03	0.40
30:0:17:G:O2'	30:0:18:C:H5'	2.20	0.40
30:0:42:C:H3'	38:0:4165:HOH:O	2.21	0.40
30:0:79:G:H22	30:0:97:G:H1'	1.86	0.40
30:0:844:A:C6	30:0:882:A:C5	3.08	0.40
30:0:1014:A:H5''	31:9:101:G:O2'	2.21	0.40
30:0:1215:A:O3'	30:0:1216:G:C4'	2.69	0.40
30:0:1819:G:C2'	30:0:1820:G:C5'	2.99	0.40
30:0:2712:G:H5'	38:0:5223:HOH:O	2.20	0.40
30:0:2712:G:P	38:0:5223:HOH:O	2.80	0.40
30:0:2791:U:H1'	30:0:2792:A:H5''	2.03	0.40
30:0:2820:A:H2'	30:0:2821:C:C6	2.55	0.40
1:A:94:LEU:HD12	1:A:98:GLU:CB	2.43	0.40
2:B:7:ARG:HH11	2:B:7:ARG:CG	2.35	0.40
3:C:135:GLU:HB3	38:C:8582:HOH:O	2.20	0.40
13:M:118:TYR:CZ	13:M:130:GLU:HB2	2.56	0.40
14:N:93:GLN:HA	14:N:93:GLN:NE2	2.35	0.40
30:0:47:G:N3	30:0:114:A:C2	2.90	0.40
30:0:517:U:H2'	30:0:518:G:H5'	2.03	0.40
30:0:1102:C:H5	38:0:3487:HOH:O	2.04	0.40
30:0:1183:C:O2	30:0:1183:C:C2'	2.70	0.40
30:0:1624:A:H5'	30:0:1626:A:O4'	2.20	0.40
30:0:2004:U:H2'	30:0:2005:G:OP1	2.22	0.40
30:0:2039:A:H4'	30:0:2760:C:O2'	2.22	0.40
30:0:2252:A:H2'	30:0:2253:G:H5'	2.03	0.40
30:0:2550:U:O2'	30:0:2551:C:H5'	2.20	0.40
30:0:2819:C:H2'	30:0:2820:A:C8	2.55	0.40
30:0:2897:C:H2'	30:0:2898:G:H8	1.85	0.40
1:A:132:ASP:HB3	1:A:135:VAL:H	1.87	0.40
1:A:230:SER:HB2	30:0:1852:A:H4'	2.04	0.40
2:B:245:SER:HB3	30:0:2094:G:H4'	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:64:ASN:N	7:G:64:ASN:ND2	2.69	0.40
20:T:52:ARG:HB2	20:T:95:ASN:HB3	2.02	0.40
23:W:88:THR:HG22	23:W:89:ASP:N	2.34	0.40
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.56	0.40
27:1:10:LYS:N	38:1:8981:HOH:O	2.50	0.40
30:0:101:C:H2'	30:0:102:A:H8	1.87	0.40
30:0:129:A:H4'	30:0:130:C:OP1	2.21	0.40
30:0:249:G:H2'	30:0:250:C:H6	1.86	0.40
30:0:445:U:H2'	30:0:446:G:C8	2.57	0.40
30:0:694:A:H4'	30:0:2441:U:OP1	2.21	0.40
30:0:1139:U:H2'	30:0:1140:C:H6	1.85	0.40
30:0:1544:U:H2'	30:0:1545:C:H6	1.87	0.40
30:0:2758:G:H2'	30:0:2759:C:C6	2.56	0.40
31:9:59:C:H2'	31:9:60:C:C6	2.56	0.40
31:9:122:C:C6	38:9:9043:HOH:O	2.71	0.40
1:A:171:LYS:HB2	30:0:820:G:C6	2.57	0.40
2:B:149:ASP:HB2	38:B:9049:HOH:O	2.21	0.40
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.70	0.40
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.68	0.40
30:0:272:A:N1	30:0:369:G:H5''	2.36	0.40
30:0:517:U:H1'	38:0:7571:HOH:O	2.20	0.40
30:0:951:A:O2'	30:0:952:G:H5'	2.21	0.40
30:0:1116:U:C2'	30:0:1118:A:C2	3.05	0.40
30:0:1217:G:C2	30:0:1218:U:C2	3.09	0.40
30:0:1472:C:H6	30:0:1472:C:O5'	2.04	0.40
30:0:1589:G:H22	30:0:1605:G:H1'	1.85	0.40
30:0:2327:A:H2'	30:0:2328:U:O4'	2.21	0.40
30:0:2491:G:C1'	38:0:6868:HOH:O	2.59	0.40
30:0:2824:C:H5''	30:0:2825:C:H5'	2.03	0.40
31:9:8:G:H5'	38:9:9103:HOH:O	2.21	0.40
31:9:65:A:C6	31:9:112:U:C5	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	212 (90%)	19 (8%)	4 (2%)	7	26
2	B	335/338 (99%)	308 (92%)	24 (7%)	3 (1%)	14	41
3	C	244/246 (99%)	228 (93%)	15 (6%)	1 (0%)	30	59
4	D	134/177 (76%)	112 (84%)	18 (13%)	4 (3%)	3	14
5	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
6	F	117/120 (98%)	106 (91%)	8 (7%)	3 (3%)	4	17
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	9	32
9	I	68/162 (42%)	55 (81%)	11 (16%)	2 (3%)	3	15
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
11	K	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	16	44
12	L	141/165 (86%)	126 (89%)	12 (8%)	3 (2%)	5	21
13	M	192/196 (98%)	185 (96%)	6 (3%)	1 (0%)	24	54
14	N	184/187 (98%)	169 (92%)	11 (6%)	4 (2%)	5	20
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
17	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
18	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
19	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
20	T	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
21	U	51/67 (76%)	46 (90%)	5 (10%)	0	100	100
22	V	63/71 (89%)	59 (94%)	4 (6%)	0	100	100
23	W	152/154 (99%)	146 (96%)	6 (4%)	0	100	100
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	9	32
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
26	Z	71/116 (61%)	63 (89%)	7 (10%)	1 (1%)	9	30
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	11	36
All	All	3705/4472 (83%)	3451 (93%)	223 (6%)	31 (1%)	16	44

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
6	F	101	ALA
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
1	A	34	ASP
4	D	27	ILE
12	L	80	ASP
12	L	149	ARG
24	X	70	ILE
26	Z	44	ARG
1	A	36	ASP
1	A	88	ILE
2	B	2	GLN
3	C	8	LEU
6	F	100	ASP
8	H	19	ARG
11	K	127	ALA
12	L	21	ARG
14	N	139	TRP
2	B	184	ASP
4	D	56	ARG
2	B	185	GLY
6	F	61	MET
9	I	108	HIS
9	I	83	GLY
29	3	56	PRO
8	H	171	GLY
4	D	28	GLY
13	M	88	VAL

5.3.2 Protein sidechains ⓘ

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%)	167 (93%)	12 (7%)	15	43
2	B	282/283 (100%)	266 (94%)	16 (6%)	18	49
3	C	193/193 (100%)	177 (92%)	16 (8%)	10	32
4	D	117/148 (79%)	110 (94%)	7 (6%)	17	47
5	E	152/156 (97%)	145 (95%)	7 (5%)	24	57
6	F	93/94 (99%)	92 (99%)	1 (1%)	65	88
7	G	27/282 (10%)	26 (96%)	1 (4%)	30	64
8	H	134/145 (92%)	127 (95%)	7 (5%)	21	52
9	I	58/130 (45%)	58 (100%)	0	100	100
10	J	118/121 (98%)	112 (95%)	6 (5%)	21	53
11	K	106/106 (100%)	105 (99%)	1 (1%)	70	90
12	L	113/127 (89%)	108 (96%)	5 (4%)	25	59
13	M	158/160 (99%)	154 (98%)	4 (2%)	42	74
14	N	149/150 (99%)	144 (97%)	5 (3%)	32	66
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	109 (96%)	4 (4%)	32	66
17	Q	79/80 (99%)	77 (98%)	2 (2%)	42	74
18	R	117/122 (96%)	111 (95%)	6 (5%)	21	53
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	99 (94%)	6 (6%)	18	49
21	U	44/53 (83%)	43 (98%)	1 (2%)	44	76
22	V	51/57 (90%)	50 (98%)	1 (2%)	48	78
23	W	130/130 (100%)	122 (94%)	8 (6%)	16	46
24	X	66/74 (89%)	60 (91%)	6 (9%)	9	28
25	Y	120/196 (61%)	118 (98%)	2 (2%)	53	82
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	43	75
29	3	79/79 (100%)	78 (99%)	1 (1%)	61	86
All	All	3095/3646 (85%)	2969 (96%)	126 (4%)	27	61

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	36	ASP
1	A	64	ASP
1	A	69	LEU
1	A	94	LEU
1	A	131	HIS
1	A	153	ARG
1	A	175	LYS
1	A	179	MET
1	A	192	VAL
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN
2	B	49	THR
2	B	51	VAL
2	B	53	LEU
2	B	97	LEU
2	B	132	HIS
2	B	162	MET
2	B	175	LEU
2	B	190	MET
2	B	195	ARG
2	B	234	ARG
2	B	254	GLN
2	B	308	LEU
2	B	312	ARG
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	91	PRO
3	C	94	THR
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	202	THR
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	240	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	243	VAL
4	D	19	GLU
4	D	48	MET
4	D	50	VAL
4	D	62	ASP
4	D	137	PRO
4	D	149	ARG
4	D	153	THR
5	E	3	VAL
5	E	16	ASP
5	E	36	PRO
5	E	102	VAL
5	E	126	ILE
5	E	155	ASN
5	E	156	ASP
6	F	12	LEU
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
8	H	173	GLU
10	J	39	VAL
10	J	45	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	127	ILE
11	K	10	GLN
12	L	99	GLU
12	L	101	ASP
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	164	THR
14	N	12	ARG
14	N	17	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	26	LEU
14	N	49	THR
14	N	127	LEU
16	P	21	VAL
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	95	GLU
18	R	13	THR
18	R	39	THR
18	R	82	GLU
18	R	128	ARG
18	R	132	ARG
18	R	143	VAL
20	T	26	THR
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	96	VAL
20	T	117	ASP
21	U	52	THR
22	V	12	THR
23	W	4	LEU
23	W	13	MET
23	W	26	ILE
23	W	35	VAL
23	W	73	LEU
23	W	128	VAL
23	W	142	ASP
23	W	146	ILE
24	X	12	ILE
24	X	46	ASP
24	X	52	PRO
24	X	72	VAL
24	X	79	GLU
24	X	88	GLU
25	Y	189	ASN
25	Y	203	VAL
28	2	18	ASN
29	3	56	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	125	ASN
1	A	199	HIS
1	A	218	ASN
2	B	2	GLN
2	B	27	ASN
2	B	145	HIS
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	67	GLN
3	C	73	GLN
3	C	129	HIS
4	D	103	ASN
5	E	106	ASN
5	E	119	HIS
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	49	GLN
8	H	59	GLN
8	H	62	HIS
8	H	131	GLN
8	H	142	ASN
9	I	118	ASN
10	J	25	GLN
10	J	29	GLN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	42	ASN
12	L	18	HIS
12	L	41	HIS
13	M	24	GLN
13	M	58	GLN
13	M	170	ASN
14	N	21	HIS
14	N	93	GLN
14	N	107	ASN
14	N	140	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	89	ASN
16	P	118	GLN
17	Q	40	HIS
18	R	22	GLN
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
18	R	122	GLN
18	R	123	GLN
19	S	44	GLN
19	S	53	ASN
19	S	55	GLN
19	S	56	ASN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	60	GLN
23	W	18	GLN
23	W	27	HIS
23	W	28	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
24	X	36	HIS
25	Y	119	GLN
25	Y	129	ASN
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
26	Z	61	HIS
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	17	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	13	HIS
29	3	20	HIS
29	3	30	GLN
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	25 (0%)
31	9	121/122 (99%)	17 (14%)	2 (1%)
All	All	2866/3045 (94%)	259 (9%)	27 (0%)

All (259) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	185	G
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	236	A
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	368	C
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1161	A
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1331	G
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1475	G
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1559	A
30	0	1592	G
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1731	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1965	C
30	0	1971	G
30	0	1973	A
30	0	1979	G
30	0	1996	U
30	0	2004	U
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2103	A
30	0	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2465	A
30	0	2467	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2540	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2611	G
30	0	2613	G
30	0	2617	G
30	0	2634	G
30	0	2638	G
30	0	2645	U
30	0	2649	A
30	0	2650	U
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2718	C
30	0	2719	A
30	0	2726	U
30	0	2727	A
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	603	A
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1237	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1246	A
30	0	1352	A
30	0	1474	C
30	0	1506	U
30	0	1692	C
30	0	1730	G
30	0	2313	C
30	0	2467	A
30	0	2536	C
30	0	2616	A
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
31	9	43	G
31	9	65	A

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

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	1.54	2 (11%)	21,30,33	1.45	3 (14%)
30	OMG	0	2588	30	23,26,27	0.32	0	32,38,41	0.39	0
30	OMU	0	2587	30,35	19,22,23	0.32	0	25,31,34	0.36	0
30	1MA	0	628	30,35	21,25,26	0.72	1 (4%)	30,37,40	0.75	1 (3%)
30	UR3	0	2619	30	19,22,23	0.46	0	26,32,35	0.67	1 (3%)

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	OMG	0	2588	30	-	0/9/27/28	0/3/3/3
30	OMU	0	2587	30,35	-	0/9/27/28	0/2/2/2
30	1MA	0	628	30,35	-	2/7/25/26	0/3/3/3
30	UR3	0	2619	30	-	0/7/25/26	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	4.98	1.43	1.36
30	0	2621	PSU	C6-C5	2.74	1.38	1.35
30	0	628	1MA	C6-N6	2.50	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	3.76	120.71	118.17
30	0	2621	PSU	C6-N1-C2	-3.22	119.70	122.69
30	0	2621	PSU	O2-C2-N1	3.12	126.00	122.79
30	0	628	1MA	N1-C2-N3	2.81	129.33	126.00
30	0	2619	UR3	C4-N3-C2	2.78	126.82	124.58

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.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no 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%)	-0.01	6 (2%) 58 48	25, 49, 89, 109	0
2	B	337/338 (99%)	0.13	4 (1%) 76 69	27, 54, 81, 92	0
3	C	246/246 (100%)	-0.17	1 (0%) 88 85	22, 42, 65, 77	0
4	D	140/177 (79%)	1.43	28 (20%) 3 2	65, 101, 125, 137	0
5	E	172/178 (96%)	0.33	9 (5%) 33 26	45, 70, 92, 97	0
6	F	119/120 (99%)	0.45	4 (3%) 48 39	48, 69, 99, 116	0
7	G	29/348 (8%)	1.16	5 (17%) 4 3	76, 95, 103, 106	0
8	H	160/177 (90%)	0.20	4 (2%) 58 48	41, 59, 97, 103	0
9	I	70/162 (43%)	2.07	31 (44%) 0 0	127, 146, 165, 166	0
10	J	142/145 (97%)	0.02	2 (1%) 73 65	38, 51, 72, 91	0
11	K	132/132 (100%)	-0.17	0 100 100	35, 50, 74, 84	0
12	L	145/165 (87%)	0.47	17 (11%) 9 8	25, 64, 110, 127	0
13	M	194/196 (98%)	-0.25	1 (0%) 87 83	28, 40, 57, 65	0
14	N	186/187 (99%)	0.60	12 (6%) 25 20	41, 66, 114, 123	0
15	O	115/116 (99%)	0.12	0 100 100	34, 53, 72, 76	0
16	P	143/149 (95%)	0.12	3 (2%) 63 54	37, 54, 69, 79	0
17	Q	95/96 (98%)	-0.04	1 (1%) 78 71	36, 46, 62, 76	0
18	R	150/155 (96%)	-0.30	1 (0%) 84 79	30, 44, 65, 81	0
19	S	81/85 (95%)	0.04	2 (2%) 58 48	41, 56, 78, 89	0
20	T	119/120 (99%)	0.17	1 (0%) 82 77	39, 54, 83, 110	0
21	U	53/67 (79%)	-0.02	0 100 100	42, 55, 75, 83	0
22	V	65/71 (91%)	0.45	6 (9%) 14 12	44, 70, 119, 125	0
23	W	154/154 (100%)	0.03	0 100 100	36, 50, 67, 80	0
24	X	82/92 (89%)	0.48	8 (9%) 13 11	43, 60, 86, 101	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.18	1 (0%) 84 79	24, 42, 67, 88	0
26	Z	73/116 (62%)	0.90	9 (12%) 8 7	55, 77, 92, 98	0
27	1	56/57 (98%)	-0.67	0 100 100	25, 30, 37, 43	0
28	2	46/50 (92%)	0.66	7 (15%) 5 4	31, 61, 91, 101	0
29	3	92/92 (100%)	0.13	2 (2%) 62 53	36, 63, 77, 90	0
30	0	2749/2923 (94%)	-0.65	9 (0%) 90 87	19, 44, 88, 164	0
31	9	122/122 (100%)	-0.16	3 (2%) 58 48	37, 67, 89, 147	0
All	All	6646/7517 (88%)	-0.16	177 (2%) 56 47	19, 51, 100, 166	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	128	THR	6.6
4	D	10	PHE	5.7
26	Z	46	SER	5.6
9	I	74	ILE	5.4
22	V	40	PRO	5.3
30	0	2645	U	5.2
22	V	1	THR	4.9
26	Z	106	SER	4.8
4	D	63	ILE	4.6
9	I	134	ILE	4.5
28	2	49	GLU	4.5
22	V	39	ALA	4.4
4	D	174	VAL	4.4
31	9	1	U	4.2
4	D	18	ILE	4.2
9	I	100	VAL	4.2
14	N	154	LEU	4.2
14	N	168	LEU	4.1
4	D	107	GLY	4.0
28	2	35	ARG	4.0
9	I	113	SER	3.9
5	E	53	GLU	3.9
9	I	104	ALA	3.8
9	I	71	ALA	3.7
24	X	87	ALA	3.7
26	Z	35	SER	3.6
22	V	2	VAL	3.5
12	L	99	GLU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	Y	235	GLU	3.5
8	H	171	GLY	3.4
8	H	114	ASP	3.4
7	G	12	ILE	3.4
9	I	67	VAL	3.4
5	E	154	ILE	3.4
9	I	70	THR	3.3
1	A	37	VAL	3.3
22	V	43	PRO	3.2
4	D	75	LEU	3.2
12	L	60	GLU	3.2
28	2	39	ARG	3.2
9	I	66	GLY	3.2
4	D	35	ALA	3.2
2	B	208	GLY	3.2
9	I	85	GLY	3.2
9	I	95	LEU	3.1
9	I	120	ALA	3.1
4	D	55	LYS	3.1
28	2	38	LYS	3.1
1	A	36	ASP	3.1
9	I	97	VAL	3.1
9	I	73	LEU	3.1
4	D	172	VAL	3.0
10	J	92	GLN	3.0
12	L	82	ALA	3.0
14	N	166	ALA	3.0
9	I	72	GLU	3.0
10	J	70	PHE	3.0
14	N	158	LEU	2.9
3	C	63	SER	2.9
4	D	74	THR	2.9
24	X	83	ALA	2.9
7	G	71	LEU	2.9
26	Z	58	ASN	2.9
31	9	2	U	2.8
30	0	2769	C	2.8
4	D	59	GLY	2.8
30	0	2637	A	2.8
12	L	149	ARG	2.8
24	X	85	VAL	2.8
4	D	61	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	H	174	LEU	2.8
9	I	88	GLN	2.8
30	O	10	U	2.8
7	G	26	MET	2.8
12	L	148	GLU	2.7
19	S	81	ILE	2.7
5	E	100	ASP	2.7
2	B	1	PRO	2.7
1	A	32	VAL	2.7
9	I	107	LYS	2.7
24	X	65	ASN	2.7
18	R	150	PRO	2.7
9	I	91	PHE	2.7
4	D	57	THR	2.7
29	3	82	GLY	2.7
24	X	88	GLU	2.7
8	H	115	GLY	2.6
4	D	90	LEU	2.6
5	E	45	ASP	2.6
4	D	171	ASP	2.6
12	L	78	ALA	2.6
14	N	160	SER	2.6
9	I	133	THR	2.6
4	D	135	VAL	2.6
9	I	124	VAL	2.6
30	O	960	G	2.5
30	O	1198	U	2.5
1	A	211	LYS	2.5
4	D	40	ILE	2.5
4	D	44	ILE	2.5
30	O	1165	G	2.5
20	T	117	ASP	2.5
30	O	735	C	2.5
13	M	194	GLY	2.5
28	2	37	HIS	2.5
14	N	162	ASP	2.4
9	I	111	LEU	2.4
9	I	132	VAL	2.4
4	D	104	PHE	2.4
4	D	106	PHE	2.4
24	X	66	THR	2.4
4	D	11	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	9	24	U	2.4
26	Z	50	VAL	2.4
30	0	1199	A	2.4
14	N	64	SER	2.4
6	F	17	LEU	2.4
9	I	101	LYS	2.3
26	Z	45	VAL	2.3
4	D	134	LEU	2.3
14	N	21	HIS	2.3
4	D	86	THR	2.3
24	X	84	ILE	2.3
7	G	27	ILE	2.3
26	Z	44	ARG	2.3
9	I	68	PRO	2.3
12	L	97	VAL	2.3
14	N	169	PRO	2.3
6	F	49	PHE	2.3
6	F	99	THR	2.3
26	Z	43	GLY	2.3
9	I	119	ALA	2.2
16	P	143	ALA	2.2
28	2	31	ARG	2.2
12	L	146	GLY	2.2
5	E	6	GLU	2.2
9	I	112	LEU	2.2
9	I	116	LEU	2.2
12	L	44	GLU	2.2
1	A	88	ILE	2.2
12	L	55	GLN	2.2
12	L	150	GLN	2.2
14	N	167	ASP	2.2
12	L	105	TYR	2.2
19	S	20	PHE	2.2
2	B	318	ASN	2.2
14	N	186	LEU	2.2
16	P	116	SER	2.2
4	D	89	PRO	2.1
28	2	48	ASP	2.1
1	A	237	GLY	2.1
26	Z	42	TYR	2.1
16	P	18	LYS	2.1
7	G	73	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	75	LEU	2.1
12	L	77	ALA	2.1
9	I	96	SER	2.1
12	L	145	LEU	2.1
4	D	170	TYR	2.1
9	I	103	ILE	2.1
5	E	172	PRO	2.1
6	F	102	GLY	2.1
4	D	69	ILE	2.1
14	N	165	ALA	2.1
22	V	36	ALA	2.1
2	B	302	PRO	2.0
17	Q	12	GLY	2.0
24	X	71	ARG	2.0
5	E	13	ALA	2.0
12	L	102	ASP	2.0
4	D	128	LEU	2.0
4	D	19	GLU	2.0
5	E	10	ASP	2.0
5	E	156	ASP	2.0
9	I	77	GLU	2.0
29	3	41	GLU	2.0
12	L	81	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	UR3	0	2619	21/22	0.96	0.08	45,48,53,54	0
30	PSU	0	2621	20/21	0.97	0.07	26,30,50,51	0
30	OMG	0	2588	24/25	0.98	0.07	30,35,38,40	0
30	1MA	0	628	23/24	0.98	0.07	28,29,31,32	0
30	OMU	0	2587	21/22	0.98	0.06	32,36,38,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	NA	0	8525	1/1	0.47	0.30	83,83,83,83	0
35	NA	0	8502	1/1	0.73	0.16	51,51,51,51	0
34	SR	0	9006	1/1	0.74	0.42	200,200,200,200	0
34	SR	9	9003	1/1	0.76	0.12	171,171,171,171	0
34	SR	0	9001	1/1	0.77	0.14	176,176,176,176	0
34	SR	0	8976	1/1	0.78	0.18	194,194,194,194	0
35	NA	0	8556	1/1	0.78	0.38	55,55,55,55	0
34	SR	0	8971	1/1	0.79	0.16	175,175,175,175	0
34	SR	0	8983	1/1	0.79	0.23	177,177,177,177	0
35	NA	0	8554	1/1	0.79	0.35	69,69,69,69	0
34	SR	0	8993	1/1	0.79	0.14	173,173,173,173	0
34	SR	0	8990	1/1	0.80	0.23	173,173,173,173	0
34	SR	0	8991	1/1	0.80	0.14	186,186,186,186	0
34	SR	0	9004	1/1	0.80	0.39	200,200,200,200	0
34	SR	Y	9002	1/1	0.81	0.19	188,188,188,188	0
34	SR	0	8919	1/1	0.81	0.17	178,178,178,178	0
34	SR	0	8979	1/1	0.82	0.18	198,198,198,198	0
34	SR	0	8955	1/1	0.82	0.22	198,198,198,198	0
35	NA	0	8522	1/1	0.82	0.19	67,67,67,67	0
35	NA	0	8561	1/1	0.82	0.44	77,77,77,77	0
34	SR	0	8997	1/1	0.83	0.29	194,194,194,194	0
32	MG	0	8063	1/1	0.84	0.27	90,90,90,90	0
32	MG	A	8051	1/1	0.84	0.12	60,60,60,60	0
35	NA	0	8514	1/1	0.84	0.14	48,48,48,48	0
35	NA	0	8557	1/1	0.84	0.17	57,57,57,57	0
32	MG	T	8057	1/1	0.84	0.24	66,66,66,66	0
35	NA	0	8564	1/1	0.84	0.14	70,70,70,70	0
35	NA	0	8571	1/1	0.84	0.15	61,61,61,61	0
34	SR	0	8922	1/1	0.85	0.17	155,155,155,155	0
35	NA	0	8518	1/1	0.85	0.39	82,82,82,82	0
34	SR	0	8988	1/1	0.86	0.09	162,162,162,162	0
34	SR	9	8980	1/1	0.86	0.11	158,158,158,158	0
32	MG	0	8078	1/1	0.87	0.29	76,76,76,76	0
34	SR	0	8938	1/1	0.87	0.12	165,165,165,165	0
35	NA	0	8548	1/1	0.87	0.14	42,42,42,42	0
35	NA	0	8574	1/1	0.87	0.32	52,52,52,52	0
37	K	0	8401	1/1	0.87	0.14	93,93,93,93	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	8989	1/1	0.88	0.17	159,159,159,159	0
35	NA	0	8570	1/1	0.88	0.11	48,48,48,48	0
35	NA	0	8559	1/1	0.88	0.29	67,67,67,67	0
34	SR	A	8977	1/1	0.88	0.08	154,154,154,154	0
35	NA	0	8562	1/1	0.88	0.31	55,55,55,55	0
34	SR	B	8950	1/1	0.89	0.12	114,114,114,114	0
32	MG	0	8082	1/1	0.89	0.12	73,73,73,73	0
34	SR	0	8944	1/1	0.89	0.13	175,175,175,175	0
34	SR	0	8982	1/1	0.89	0.24	197,197,197,197	0
34	SR	0	8951	1/1	0.89	0.07	144,144,144,144	0
32	MG	0	8066	1/1	0.89	0.34	80,80,80,80	0
35	NA	0	8549	1/1	0.89	0.17	51,51,51,51	0
34	SR	0	8957	1/1	0.89	0.21	200,200,200,200	0
35	NA	9	8572	1/1	0.89	0.24	80,80,80,80	0
34	SR	0	8959	1/1	0.89	0.09	159,159,159,159	0
35	NA	0	8558	1/1	0.90	0.17	45,45,45,45	0
32	MG	0	8038	1/1	0.90	0.07	66,66,66,66	0
34	SR	0	8975	1/1	0.90	0.10	137,137,137,137	0
34	SR	0	8933	1/1	0.90	0.14	141,141,141,141	0
32	MG	0	8039	1/1	0.90	0.21	67,67,67,67	0
34	SR	0	8920	1/1	0.90	0.09	112,112,112,112	0
35	NA	0	8553	1/1	0.90	0.15	52,52,52,52	0
34	SR	0	8996	1/1	0.90	0.19	200,200,200,200	0
35	NA	0	8506	1/1	0.90	0.11	63,63,63,63	0
34	SR	0	8968	1/1	0.90	0.13	161,161,161,161	0
35	NA	0	8520	1/1	0.91	0.12	40,40,40,40	0
34	SR	0	8928	1/1	0.91	0.09	139,139,139,139	0
32	MG	0	8089	1/1	0.91	0.10	42,42,42,42	0
35	NA	0	8575	1/1	0.91	0.34	83,83,83,83	0
35	NA	0	8546	1/1	0.91	0.25	82,82,82,82	0
34	SR	0	9000	1/1	0.91	0.20	165,165,165,165	0
34	SR	0	8992	1/1	0.92	0.19	133,133,133,133	0
34	SR	0	8974	1/1	0.92	0.14	158,158,158,158	0
34	SR	0	8947	1/1	0.92	0.12	162,162,162,162	0
34	SR	0	8927	1/1	0.92	0.14	170,170,170,170	0
34	SR	0	8953	1/1	0.92	0.15	160,160,160,160	0
32	MG	9	8074	1/1	0.92	0.20	75,75,75,75	0
35	NA	0	8544	1/1	0.92	0.27	60,60,60,60	0
35	NA	0	8565	1/1	0.92	0.14	57,57,57,57	0
34	SR	0	8956	1/1	0.92	0.09	138,138,138,138	0
33	CL	J	8802	1/1	0.92	0.09	66,66,66,66	0
32	MG	0	8073	1/1	0.92	0.26	74,74,74,74	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	8550	1/1	0.92	0.12	53,53,53,53	0
35	NA	9	8543	1/1	0.92	0.24	44,44,44,44	0
34	SR	0	8939	1/1	0.92	0.13	145,145,145,145	0
32	MG	0	8080	1/1	0.92	0.06	66,66,66,66	0
35	NA	Q	8540	1/1	0.93	0.13	58,58,58,58	0
34	SR	B	8987	1/1	0.93	0.26	200,200,200,200	0
34	SR	0	8994	1/1	0.93	0.25	192,192,192,192	0
35	NA	0	8509	1/1	0.93	0.15	63,63,63,63	0
35	NA	0	8511	1/1	0.93	0.11	56,56,56,56	0
35	NA	0	8513	1/1	0.93	0.12	42,42,42,42	0
34	SR	0	8962	1/1	0.93	0.16	155,155,155,155	0
34	SR	F	9005	1/1	0.93	0.09	132,132,132,132	0
34	SR	0	8986	1/1	0.93	0.17	200,200,200,200	0
35	NA	0	8521	1/1	0.93	0.09	50,50,50,50	0
34	SR	0	8970	1/1	0.93	0.06	123,123,123,123	0
32	MG	0	8071	1/1	0.93	0.22	50,50,50,50	0
35	NA	0	8529	1/1	0.93	0.14	39,39,39,39	0
35	NA	0	8535	1/1	0.93	0.19	55,55,55,55	0
35	NA	0	8537	1/1	0.93	0.06	38,38,38,38	0
35	NA	0	8541	1/1	0.93	0.13	61,61,61,61	0
32	MG	0	8033	1/1	0.93	0.12	49,49,49,49	0
32	MG	0	8067	1/1	0.93	0.06	50,50,50,50	0
32	MG	0	8090	1/1	0.93	0.10	55,55,55,55	0
32	MG	0	8081	1/1	0.94	0.14	74,74,74,74	0
34	SR	0	8998	1/1	0.94	0.15	172,172,172,172	0
33	CL	J	8801	1/1	0.94	0.12	71,71,71,71	0
34	SR	0	8973	1/1	0.94	0.07	121,121,121,121	0
32	MG	0	8037	1/1	0.94	0.17	59,59,59,59	0
33	CL	Y	8820	1/1	0.94	0.07	40,40,40,40	0
35	NA	0	8566	1/1	0.94	0.21	71,71,71,71	0
35	NA	0	8567	1/1	0.94	0.29	72,72,72,72	0
34	SR	0	9007	1/1	0.94	0.29	191,191,191,191	0
33	CL	0	8822	1/1	0.94	0.39	83,83,83,83	0
35	NA	0	8573	1/1	0.94	0.08	61,61,61,61	0
34	SR	0	8964	1/1	0.94	0.07	124,124,124,124	0
34	SR	0	8967	1/1	0.94	0.07	131,131,131,131	0
35	NA	0	8555	1/1	0.94	0.17	53,53,53,53	0
34	SR	0	8915	1/1	0.94	0.08	110,110,110,110	0
35	NA	0	8534	1/1	0.94	0.24	64,64,64,64	0
34	SR	0	8985	1/1	0.95	0.11	124,124,124,124	0
34	SR	S	8961	1/1	0.95	0.07	128,128,128,128	0
34	SR	0	8969	1/1	0.95	0.28	164,164,164,164	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	CL	A	8809	1/1	0.95	0.12	65,65,65,65	0
32	MG	0	8044	1/1	0.95	0.06	45,45,45,45	0
35	NA	0	8528	1/1	0.95	0.05	44,44,44,44	0
35	NA	0	8560	1/1	0.95	0.17	85,85,85,85	0
34	SR	0	8934	1/1	0.95	0.12	117,117,117,117	0
35	NA	0	8533	1/1	0.95	0.12	55,55,55,55	0
35	NA	0	8563	1/1	0.95	0.25	67,67,67,67	0
32	MG	0	8092	1/1	0.95	0.14	66,66,66,66	0
35	NA	J	8538	1/1	0.95	0.09	43,43,43,43	0
34	SR	0	8958	1/1	0.95	0.06	97,97,97,97	0
32	MG	0	8072	1/1	0.95	0.09	43,43,43,43	0
35	NA	0	8568	1/1	0.95	0.19	36,36,36,36	0
35	NA	0	8569	1/1	0.95	0.08	44,44,44,44	0
34	SR	0	8995	1/1	0.95	0.07	136,136,136,136	0
34	SR	0	8942	1/1	0.95	0.07	115,115,115,115	0
35	NA	0	8547	1/1	0.95	0.22	60,60,60,60	0
33	CL	0	8815	1/1	0.95	0.10	67,67,67,67	0
34	SR	0	8926	1/1	0.95	0.08	122,122,122,122	0
34	SR	0	8999	1/1	0.95	0.07	93,93,93,93	0
35	NA	0	8552	1/1	0.95	0.16	72,72,72,72	0
35	NA	0	8516	1/1	0.95	0.09	45,45,45,45	0
34	SR	0	8981	1/1	0.96	0.12	171,171,171,171	0
32	MG	0	8083	1/1	0.96	0.07	37,37,37,37	0
35	NA	0	8501	1/1	0.96	0.11	33,33,33,33	0
34	SR	0	8945	1/1	0.96	0.08	107,107,107,107	0
35	NA	0	8505	1/1	0.96	0.20	34,34,34,34	0
32	MG	0	8016	1/1	0.96	0.10	50,50,50,50	0
32	MG	0	8024	1/1	0.96	0.10	52,52,52,52	0
32	MG	0	8091	1/1	0.96	0.09	51,51,51,51	0
32	MG	0	8069	1/1	0.96	0.08	57,57,57,57	0
32	MG	0	8029	1/1	0.96	0.19	46,46,46,46	0
34	SR	0	8916	1/1	0.96	0.08	104,104,104,104	0
34	SR	0	8917	1/1	0.96	0.07	111,111,111,111	0
32	MG	0	8031	1/1	0.96	0.07	57,57,57,57	0
32	MG	0	8049	1/1	0.96	0.12	58,58,58,58	0
32	MG	0	8077	1/1	0.96	0.10	35,35,35,35	0
35	NA	0	8524	1/1	0.96	0.04	52,52,52,52	0
34	SR	0	8965	1/1	0.96	0.07	121,121,121,121	0
34	SR	0	8924	1/1	0.96	0.14	133,133,133,133	0
33	CL	J	8821	1/1	0.96	0.07	60,60,60,60	0
35	NA	0	8531	1/1	0.96	0.11	41,41,41,41	0
33	CL	L	8810	1/1	0.96	0.10	52,52,52,52	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	8055	1/1	0.96	0.07	30,30,30,30	0
34	SR	0	8931	1/1	0.96	0.07	110,110,110,110	0
35	NA	0	8536	1/1	0.96	0.08	47,47,47,47	0
32	MG	0	8056	1/1	0.96	0.10	41,41,41,41	0
32	MG	B	8042	1/1	0.96	0.09	44,44,44,44	0
34	SR	A	8929	1/1	0.96	0.17	130,130,130,130	0
34	SR	A	8930	1/1	0.96	0.05	110,110,110,110	0
32	MG	0	8064	1/1	0.96	0.06	41,41,41,41	0
37	K	0	8402	1/1	0.96	0.13	67,67,67,67	0
34	SR	0	8972	1/1	0.97	0.14	127,127,127,127	0
32	MG	0	8093	1/1	0.97	0.04	27,27,27,27	0
34	SR	0	8943	1/1	0.97	0.06	99,99,99,99	0
35	NA	0	8542	1/1	0.97	0.09	48,48,48,48	0
34	SR	0	8914	1/1	0.97	0.11	121,121,121,121	0
35	NA	C	8503	1/1	0.97	0.06	27,27,27,27	0
33	CL	3	8804	1/1	0.97	0.05	58,58,58,58	0
35	NA	M	8539	1/1	0.97	0.08	26,26,26,26	0
34	SR	0	8978	1/1	0.97	0.04	119,119,119,119	0
35	NA	R	8532	1/1	0.97	0.09	45,45,45,45	0
35	NA	0	8551	1/1	0.97	0.08	38,38,38,38	0
35	NA	S	8510	1/1	0.97	0.04	27,27,27,27	0
34	SR	0	8946	1/1	0.97	0.05	99,99,99,99	0
33	CL	0	8803	1/1	0.97	0.06	52,52,52,52	0
34	SR	0	8949	1/1	0.97	0.07	104,104,104,104	0
33	CL	0	8805	1/1	0.97	0.05	53,53,53,53	0
35	NA	0	8507	1/1	0.97	0.05	32,32,32,32	0
35	NA	0	8508	1/1	0.97	0.07	43,43,43,43	0
33	CL	0	8811	1/1	0.97	0.09	63,63,63,63	0
34	SR	0	8954	1/1	0.97	0.06	100,100,100,100	0
33	CL	0	8813	1/1	0.97	0.06	46,46,46,46	0
32	MG	0	8010	1/1	0.97	0.04	48,48,48,48	0
33	CL	0	8816	1/1	0.97	0.17	67,67,67,67	0
34	SR	0	8925	1/1	0.97	0.07	87,87,87,87	0
35	NA	0	8519	1/1	0.97	0.08	39,39,39,39	0
32	MG	0	8085	1/1	0.97	0.13	80,80,80,80	0
32	MG	0	8060	1/1	0.97	0.06	43,43,43,43	0
34	SR	0	8963	1/1	0.97	0.05	131,131,131,131	0
32	MG	0	8035	1/1	0.97	0.13	43,43,43,43	0
32	MG	0	8006	1/1	0.97	0.05	21,21,21,21	0
35	NA	0	8526	1/1	0.97	0.08	39,39,39,39	0
34	SR	0	8966	1/1	0.97	0.06	100,100,100,100	0
32	MG	0	8017	1/1	0.97	0.07	23,23,23,23	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	8530	1/1	0.97	0.08	41,41,41,41	0
33	CL	M	8818	1/1	0.97	0.06	44,44,44,44	0
33	CL	N	8807	1/1	0.97	0.07	71,71,71,71	0
33	CL	O	8808	1/1	0.97	0.14	73,73,73,73	0
34	SR	0	8941	1/1	0.97	0.06	104,104,104,104	0
32	MG	0	8068	1/1	0.98	0.07	52,52,52,52	0
32	MG	0	8030	1/1	0.98	0.18	72,72,72,72	0
32	MG	0	8070	1/1	0.98	0.05	43,43,43,43	0
33	CL	0	8812	1/1	0.98	0.04	45,45,45,45	0
34	SR	0	8921	1/1	0.98	0.04	77,77,77,77	0
32	MG	0	8052	1/1	0.98	0.04	39,39,39,39	0
33	CL	0	8814	1/1	0.98	0.11	50,50,50,50	0
34	SR	0	8960	1/1	0.98	0.06	134,134,134,134	0
35	NA	0	8515	1/1	0.98	0.06	35,35,35,35	0
32	MG	0	8053	1/1	0.98	0.03	38,38,38,38	0
32	MG	0	8036	1/1	0.98	0.07	46,46,46,46	0
33	CL	0	8817	1/1	0.98	0.04	51,51,51,51	0
32	MG	0	8075	1/1	0.98	0.04	39,39,39,39	0
33	CL	B	8819	1/1	0.98	0.14	51,51,51,51	0
32	MG	0	8076	1/1	0.98	0.05	39,39,39,39	0
35	NA	0	8523	1/1	0.98	0.07	46,46,46,46	0
32	MG	0	8007	1/1	0.98	0.04	43,43,43,43	0
34	SR	0	8935	1/1	0.98	0.05	80,80,80,80	0
34	SR	0	8937	1/1	0.98	0.05	102,102,102,102	0
35	NA	0	8527	1/1	0.98	0.13	47,47,47,47	0
32	MG	0	8059	1/1	0.98	0.08	50,50,50,50	0
32	MG	0	8079	1/1	0.98	0.05	39,39,39,39	0
32	MG	0	8032	1/1	0.98	0.06	44,44,44,44	0
32	MG	K	8054	1/1	0.98	0.04	37,37,37,37	0
32	MG	0	8040	1/1	0.98	0.06	80,80,80,80	0
34	SR	1	8952	1/1	0.98	0.03	79,79,79,79	0
34	SR	0	8908	1/1	0.98	0.04	83,83,83,83	0
34	SR	0	8910	1/1	0.98	0.05	99,99,99,99	0
34	SR	0	8911	1/1	0.98	0.04	75,75,75,75	0
32	MG	0	8034	1/1	0.98	0.04	38,38,38,38	0
32	MG	0	8046	1/1	0.98	0.12	44,44,44,44	0
36	CD	O	8705	1/1	0.98	0.05	84,84,84,84	0
34	SR	0	8984	1/1	0.98	0.06	114,114,114,114	0
35	NA	0	8545	1/1	0.98	0.08	38,38,38,38	0
33	CL	R	8806	1/1	0.99	0.04	47,47,47,47	0
32	MG	0	8005	1/1	0.99	0.06	31,31,31,31	0
32	MG	Y	8086	1/1	0.99	0.03	35,35,35,35	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	8018	1/1	0.99	0.05	27,27,27,27	0
32	MG	0	8062	1/1	0.99	0.07	44,44,44,44	0
34	SR	0	9008	1/1	0.99	0.03	84,84,84,84	0
34	SR	0	8918	1/1	0.99	0.06	79,79,79,79	0
32	MG	0	8084	1/1	0.99	0.09	29,29,29,29	0
32	MG	0	8020	1/1	0.99	0.09	36,36,36,36	0
32	MG	0	8087	1/1	0.99	0.02	31,31,31,31	0
32	MG	0	8088	1/1	0.99	0.05	32,32,32,32	0
34	SR	0	8923	1/1	0.99	0.03	87,87,87,87	0
32	MG	0	8022	1/1	0.99	0.08	31,31,31,31	0
32	MG	0	8065	1/1	0.99	0.03	33,33,33,33	0
32	MG	0	8001	1/1	0.99	0.03	30,30,30,30	0
32	MG	0	8025	1/1	0.99	0.03	27,27,27,27	0
35	NA	0	8504	1/1	0.99	0.06	31,31,31,31	0
32	MG	0	8043	1/1	0.99	0.07	43,43,43,43	0
32	MG	0	8027	1/1	0.99	0.03	31,31,31,31	0
32	MG	0	8045	1/1	0.99	0.05	35,35,35,35	0
32	MG	0	8008	1/1	0.99	0.04	24,24,24,24	0
32	MG	0	8047	1/1	0.99	0.09	50,50,50,50	0
34	SR	0	8936	1/1	0.99	0.05	91,91,91,91	0
35	NA	0	8512	1/1	0.99	0.14	45,45,45,45	0
32	MG	0	8048	1/1	0.99	0.06	22,22,22,22	0
34	SR	R	8912	1/1	0.99	0.06	83,83,83,83	0
32	MG	0	8003	1/1	0.99	0.06	26,26,26,26	0
34	SR	0	8940	1/1	0.99	0.03	78,78,78,78	0
35	NA	0	8517	1/1	0.99	0.11	46,46,46,46	0
32	MG	0	8050	1/1	0.99	0.04	28,28,28,28	0
34	SR	1	8913	1/1	0.99	0.05	91,91,91,91	0
32	MG	0	8012	1/1	0.99	0.04	22,22,22,22	0
34	SR	3	8932	1/1	0.99	0.03	74,74,74,74	0
34	SR	0	8901	1/1	0.99	0.04	84,84,84,84	0
34	SR	0	8902	1/1	0.99	0.02	37,37,37,37	0
34	SR	0	8904	1/1	0.99	0.07	55,55,55,55	0
34	SR	0	8948	1/1	0.99	0.04	88,88,88,88	0
34	SR	0	8905	1/1	0.99	0.12	69,69,69,69	0
34	SR	0	8906	1/1	0.99	0.05	53,53,53,53	0
34	SR	0	8907	1/1	0.99	0.02	43,43,43,43	0
32	MG	0	8013	1/1	0.99	0.02	21,21,21,21	0
36	CD	Z	8703	1/1	0.99	0.02	83,83,83,83	0
36	CD	1	8702	1/1	0.99	0.03	60,60,60,60	0
34	SR	0	8909	1/1	0.99	0.06	86,86,86,86	0
32	MG	0	8015	1/1	0.99	0.04	31,31,31,31	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	8041	1/1	1.00	0.06	29,29,29,29	0
32	MG	0	8021	1/1	1.00	0.06	32,32,32,32	0
32	MG	0	8058	1/1	1.00	0.04	16,16,16,16	0
32	MG	0	8002	1/1	1.00	0.02	30,30,30,30	0
32	MG	0	8023	1/1	1.00	0.03	26,26,26,26	0
32	MG	0	8061	1/1	1.00	0.06	25,25,25,25	0
32	MG	0	8011	1/1	1.00	0.01	23,23,23,23	0
32	MG	0	8004	1/1	1.00	0.05	25,25,25,25	0
34	SR	0	8903	1/1	1.00	0.07	53,53,53,53	0
32	MG	0	8026	1/1	1.00	0.05	33,33,33,33	0
36	CD	U	8701	1/1	1.00	0.01	62,62,62,62	0
32	MG	0	8009	1/1	1.00	0.09	28,28,28,28	0
32	MG	0	8028	1/1	1.00	0.05	24,24,24,24	0
36	CD	3	8704	1/1	1.00	0.03	76,76,76,76	0
32	MG	0	8019	1/1	1.00	0.05	19,19,19,19	0
32	MG	0	8014	1/1	1.00	0.07	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.