



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 11:04 AM UTC

PDB ID : 3CCL / pdb_00003ccl
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation U2535C. Density for Anisomycin is visible but not included in model.
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:

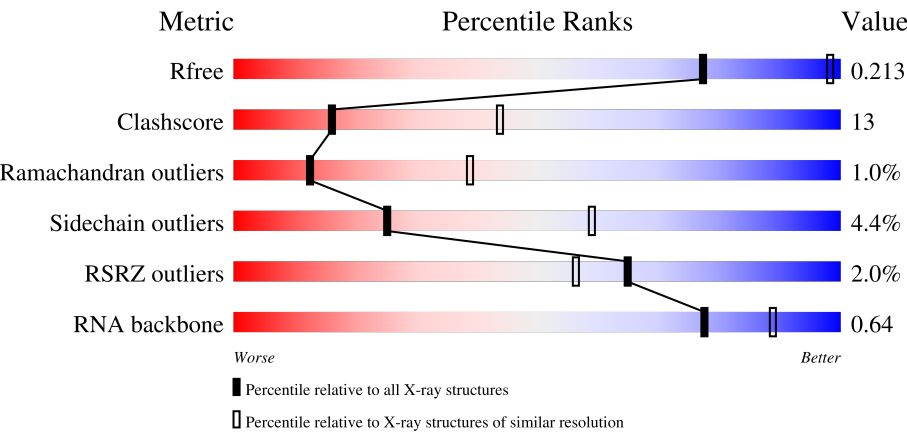
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	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% 70% 24% 5%
2	B	338	% 62% 34% .
3	C	246	% 68% 28% .
4	D	177	11% 43% 33% . 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
35	NA	0	8518	-	-	-	X
35	NA	9	8572	-	-	-	X

2 Entry composition [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10874	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	1	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	0	93	Total Sr 93 93	0	0
34	9	3	Total Sr 3 3	0	0

- 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	116	Total	O	0	0
			116	116		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	B	141	Total 141	O 141	0	0
38	C	170	Total 170	O 170	0	0
38	D	44	Total 44	O 44	0	0
38	E	45	Total 45	O 45	0	0
38	F	27	Total 27	O 27	0	0
38	G	19	Total 19	O 19	0	0
38	H	63	Total 63	O 63	0	0
38	I	8	Total 8	O 8	0	0
38	J	53	Total 53	O 53	0	0
38	K	56	Total 56	O 56	0	0
38	L	85	Total 85	O 85	0	0
38	M	123	Total 123	O 123	0	0
38	N	55	Total 55	O 55	0	0
38	O	43	Total 43	O 43	0	0
38	P	67	Total 67	O 67	0	0
38	Q	50	Total 50	O 50	0	0
38	R	85	Total 85	O 85	0	0
38	S	33	Total 33	O 33	0	0
38	T	34	Total 34	O 34	0	0
38	U	27	Total 27	O 27	0	0
38	V	13	Total 13	O 13	0	0

Continued on next page...

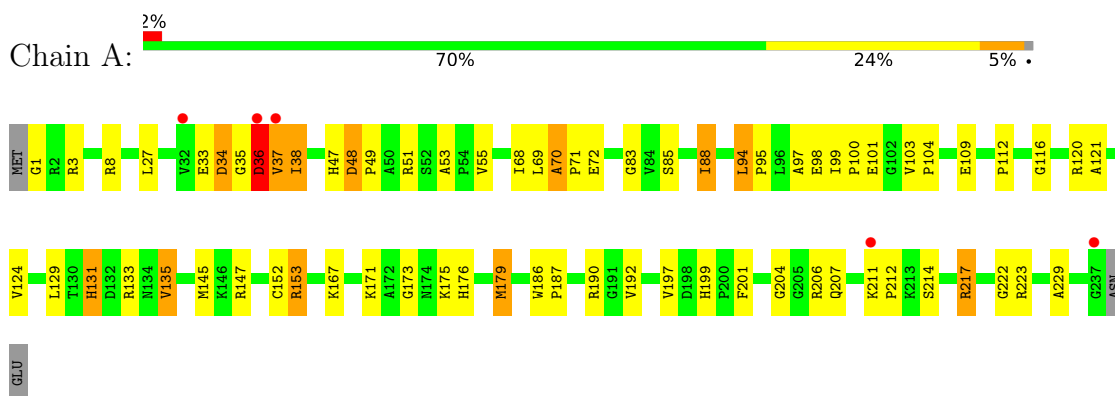
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	W	69	Total 69	O 69	0	0
38	X	25	Total 25	O 25	0	0
38	Y	95	Total 95	O 95	0	0
38	Z	26	Total 26	O 26	0	0
38	1	63	Total 63	O 63	0	0
38	2	50	Total 50	O 50	0	0
38	3	62	Total 62	O 62	0	0
38	0	5929	Total 5929	O 5929	0	0
38	9	147	Total 147	O 147	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.

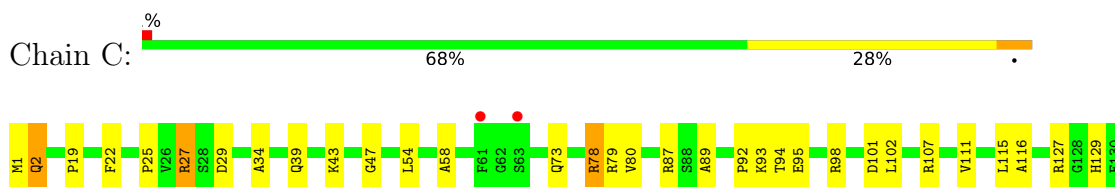
• Molecule 1: 50S ribosomal protein L2P



• Molecule 2: 50S ribosomal protein L3P

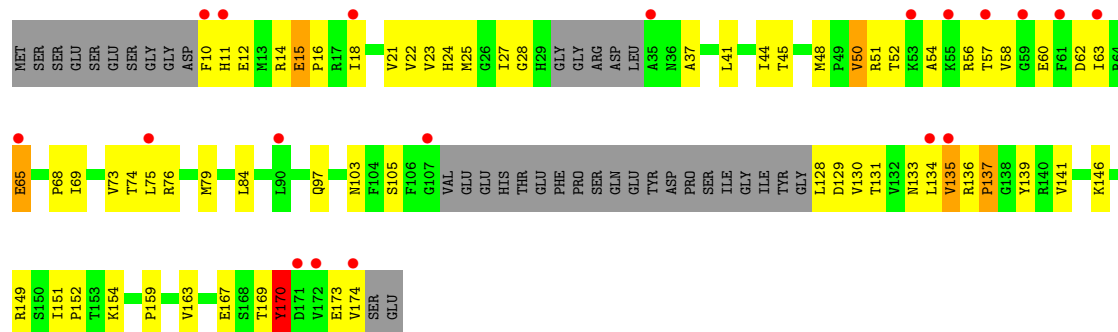
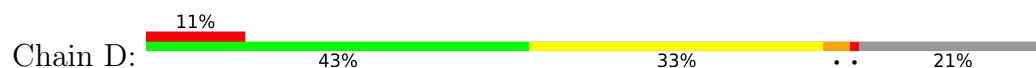


• Molecule 3: 50S ribosomal protein L4P

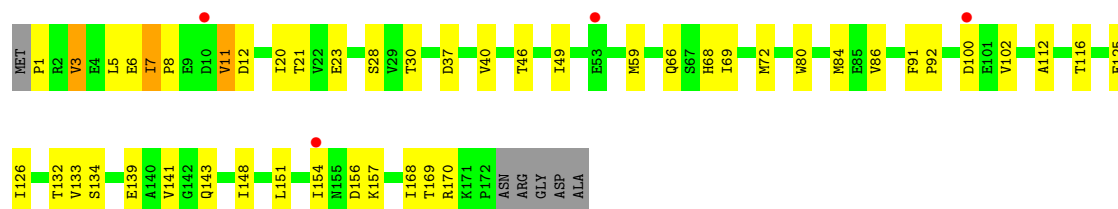




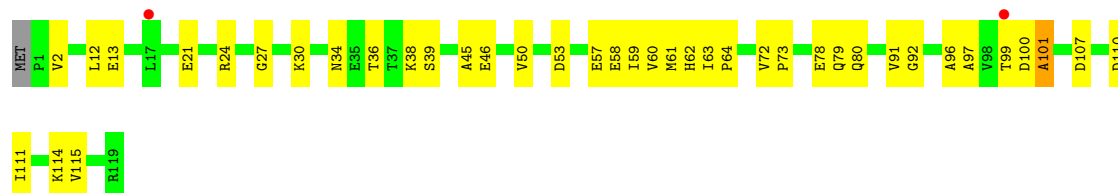
• Molecule 4: 50S ribosomal protein L5P



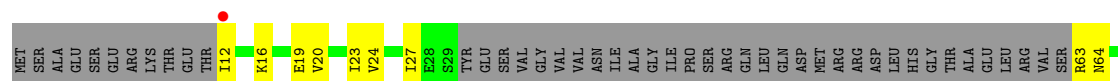
• Molecule 5: 50S ribosomal protein L6P



• Molecule 6: 50S ribosomal protein L7Ae

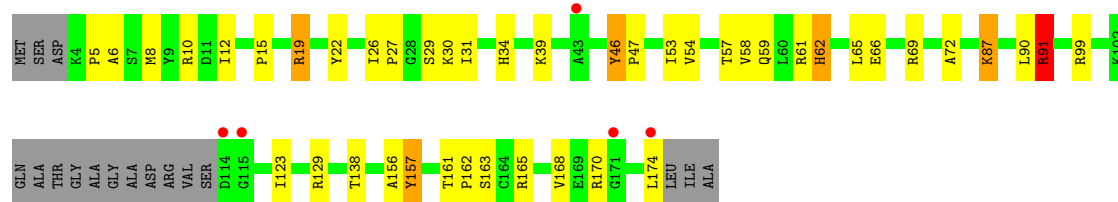


• Molecule 7: 50S ribosomal protein L10E

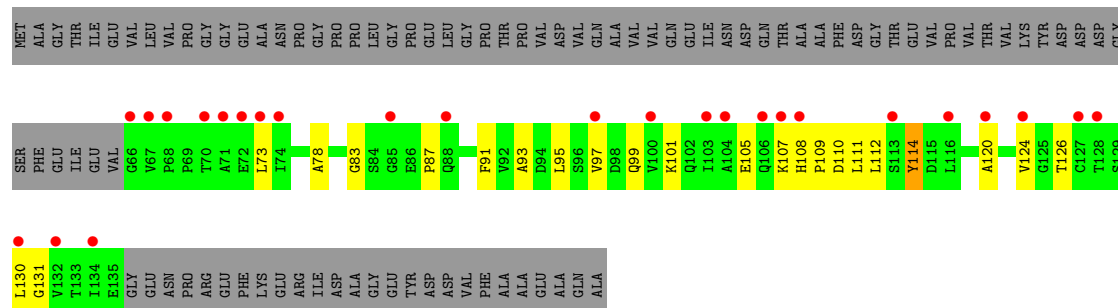




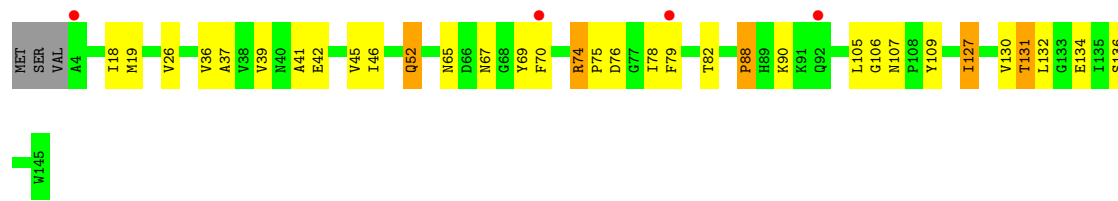
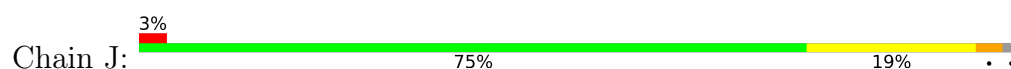
• Molecule 8: 50S ribosomal protein L10e



• Molecule 9: 50S ribosomal protein L11P



• Molecule 10: 50S ribosomal protein L13P



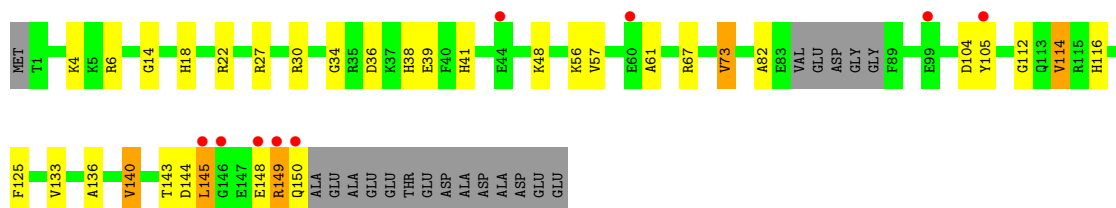
• Molecule 11: 50S ribosomal protein L14P

Chain K:  73% 23% .



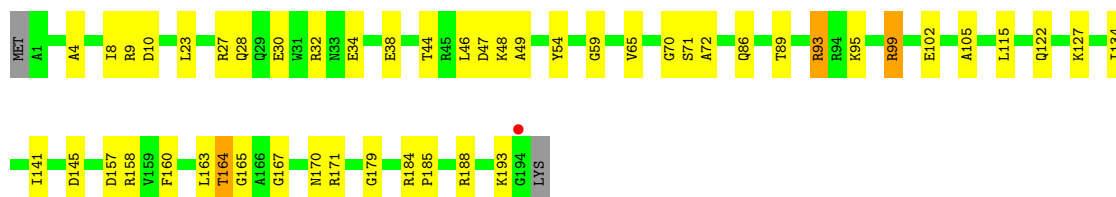
- Molecule 12: 50S ribosomal protein L15P

Chain L:  5% 67% 18% 12% .



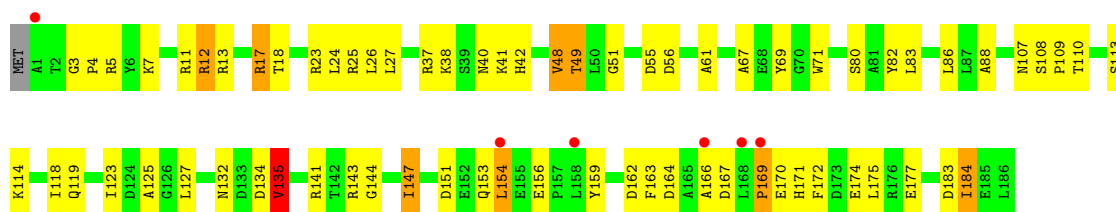
- Molecule 13: 50S ribosomal protein L15e

Chain M:  74% 23% ..



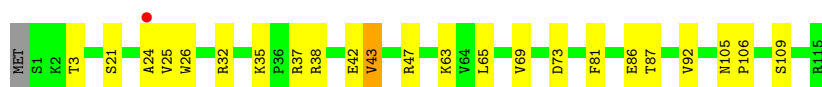
- Molecule 14: 50S ribosomal protein L18P

Chain N:  3% 62% 33% ..

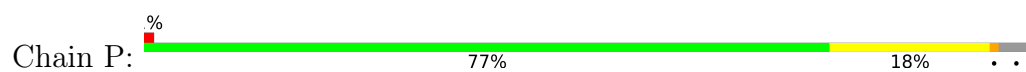


- Molecule 15: 50S ribosomal protein L18e

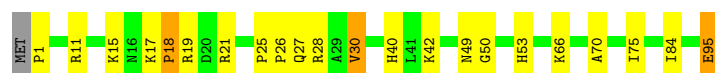
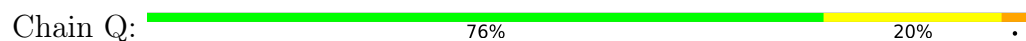
Chain O:  79% 19% ..



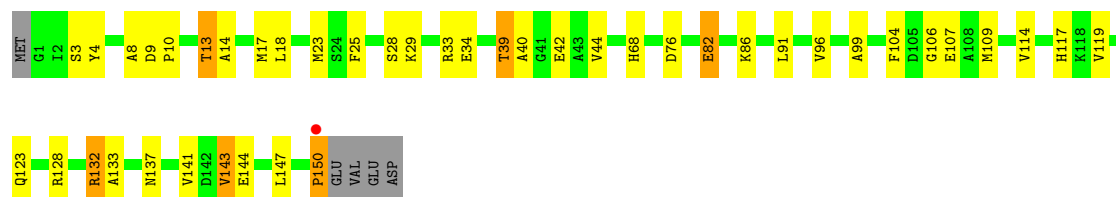
- Molecule 16: 50S ribosomal protein L19e



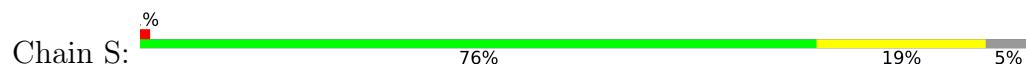
- Molecule 17: 50S ribosomal protein L21e



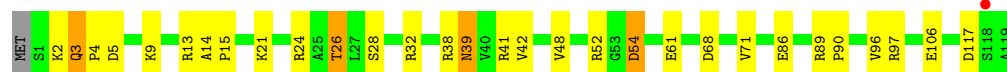
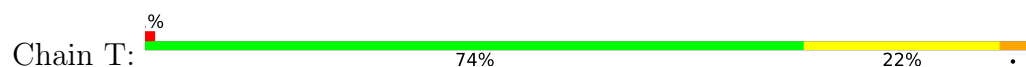
- Molecule 18: 50S ribosomal protein L22P



- Molecule 19: 50S ribosomal protein L23P



- Molecule 20: 50S ribosomal protein L24P

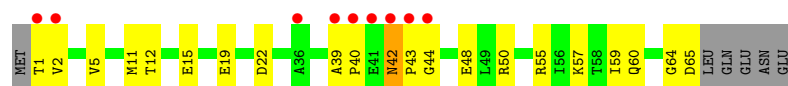


- Molecule 21: 50S ribosomal protein L24e

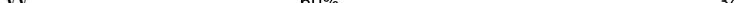


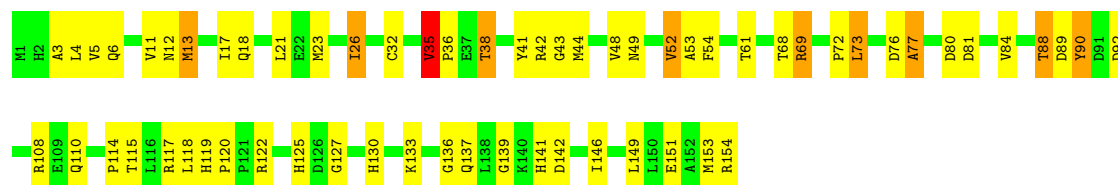
- Molecule 22: 50S ribosomal protein L29P



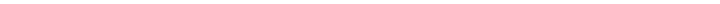


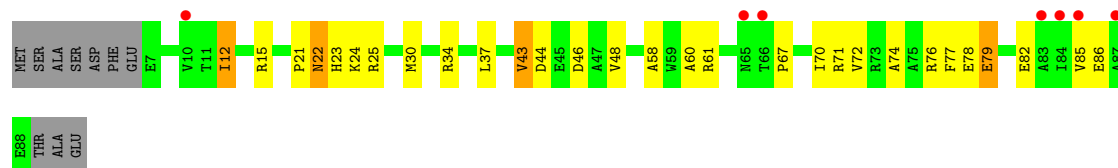
- Molecule 23: 50S ribosomal protein L30P

Chain W:  60% 34% 6%



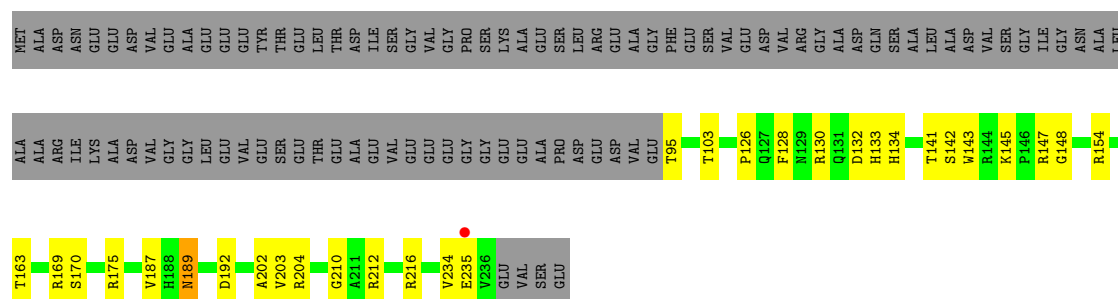
- Molecule 24: 50S ribosomal protein L31e

Chain X: 

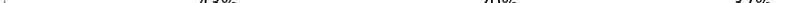


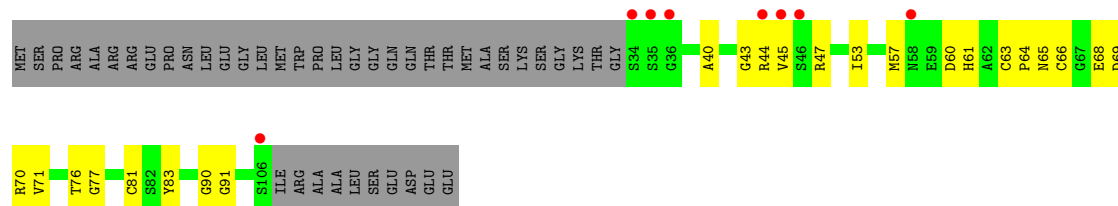
- Molecule 25: 50S ribosomal protein L32e

Chain Y:  46% 12% 41%



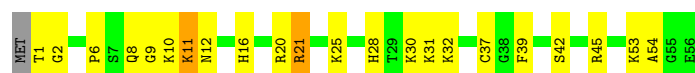
- Molecule 26: 50S ribosomal protein L37Ae

Chain Z: 



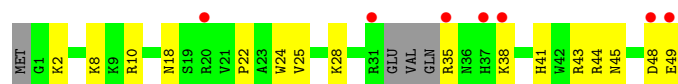
- Molecule 27: 50S ribosomal protein L37e

Chain 1: 



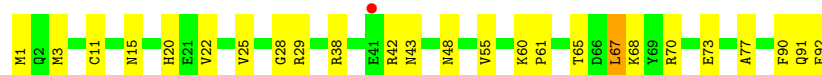
- Molecule 28: 50S ribosomal protein L39e

Chain 2: 



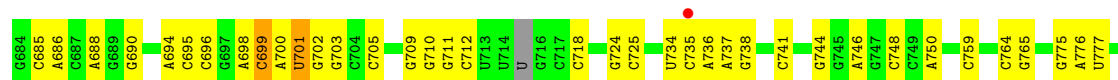
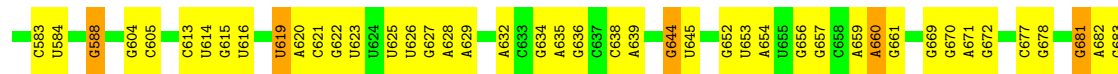
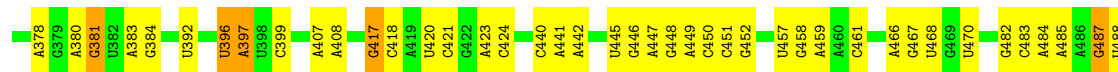
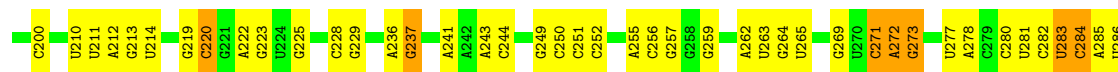
- Molecule 29: 50S ribosomal protein L44E

Chain 3: 

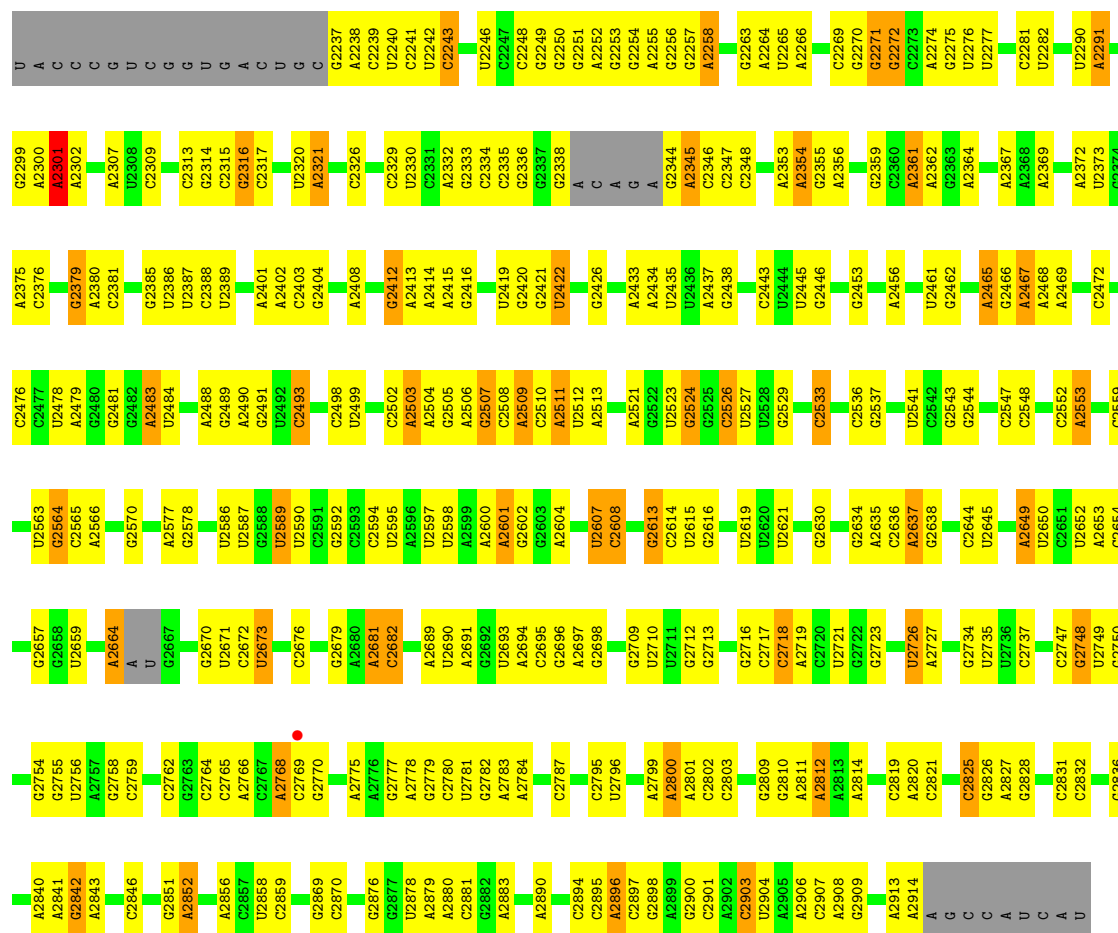


- Molecule 30: 23S RIBOSOMAL RNA

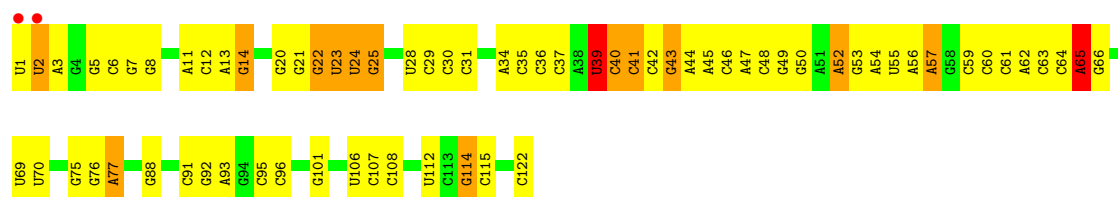
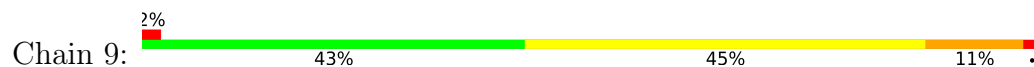
Chain 0: 



A2074	C1853	C1750	C1652	U1435	U1350	C1245	C1168	C1068	A790
A2081	C1854	C1751	A1653	C1436	G1351	A1246	U1169	C1069	A791
G2082	C1855	G1752	U1654	G1441	C1554	U1249	A1171	A1070	G792
A2083	C1856	G1753	A1655	A1442	C1555	C1250	G1172	G1071	G800
C2088	A1857	A1759	A1656	U1446	U1358	A1261	A1173	U858	U801
A2089	A1858	G1760	A1657	U1447	U1359	U1268	A1174	G808	A807
G2090	G1863	U1761	A1658	U1450	C1360	G1269	G1175	C899	A808
C2091	G1868	C1762	A1659	C1451	C1366	U1270	U1180	U903	G809
G2092	G1871	C1763	U1661	C1451	C1366	C1273	U1181	U904	C905
A2096	U1871	U1766	U1668	U1461	A1372	A1278	A1182	A912	A812
A2101	C1872	C1767	U1677	C1462	G1373	U1279	C1183	G	C813
G2102	G1873	C1768	A1678	C1474	C1374	A1280	U1185	A1097	G814
A2103	G1877	U1770	A1679	C1474	C1375	U1289	U1186	A1098	U815
C2104	U1878	U1771	C1679	A1476	G1376	A1291	A1187	C1186	G816
C2105	U1879	C1772	A1682	C1477	C1377	A1287	U1188	G920	G817
C2106	G1883	G1773	G1683	U1478	G1378	U1288	A1189	A922	G921
	A1884	C1774	A1684	C1482	A1381	G1289	U1190	A923	G820
	A1886	U1779	C1685	C1483	U1380	G1290	U1191	A926	U821
	G1886	A1778	C1686	G1484	G1382	A1291	A1192	U932	U822
	U1897	C1787	C1687	A1485	U1383	G1300	A1193	A1006	U823
	U1897	U1788	C1692	A1485	G1384	G1295	A1194	A1007	G824
	U1903	G1789	G1697	A1487	G1385	A1296	U1198	A939	U825
	A1904	C1790	C1700	U1488	G1387	U1297	A1199	G940	U826
	U1905	U1791	A1701	C1495	G1391	G1299	U1200	G941	U827
	G1905	G1795	U1702	C1495	A1392	G1300	G1201	A1009	G834
	A1909	A1796	U1706	U1503	A1393	U1304	A1202	A943	U835
	A1919	U1797	G1706	A1504	C1394	C1305	A1203	A944	G836
	C1920	C1798	G1707	U1505	U1395	U1306	G1204	U945	U840
	A1921	G1805	A1710	U1506	C1396	A1307	A1207	U947	A843
	A1922	G1806	A1711	C1513	G1397	A1308	U1208	G950	A846
	G1925	C1818	C1714	C1514	A1399	G1311	G1209	A951	C847
	G1926	G1819	C1715	A1515	C1400	G1312	G1210	G952	C848
	A1927	G1820	A1717	U1516	G1401	A1313	G1211	G953	C853
	C1940	U1825	U1722	G1520	A1407	U1314	G1212	G958	G854
	A1941	C1826	G1723	A1522	U1408	A1321	G1216	C959	A857
	A1942	A1829	U1724	G1523	G1409	G1322	G1221	A961	U858
	C1943	C1830	C1725	U1524	A1413	G1325	U149	C962	A861
	G1947	C1834	G1730	G1525	A1414	A1328	A1150	C963	
	G1948	U1835	C1731	A1526	G1415	A1328	G1151	G968	A867
	G1949	U1835	A1732	A1527	U1419	A1231	A1154	G969	G868
	G1950	U1838	A1733	A1528	U1419	A1232	G1155	U970	G869
	U1951	A1839	C1734	G1535	U1422	G1331	G1159	G	G870
	U	C1840	U1736	G1536	C1423	G1332	A1160	U	G871
	A	A1840	A1736	A1637	A1424	C1334	U1237	U	U872
	A	A1845	G1739	A1641	C1426	G1339	A1161	U	A875
	C	U1846	U1740	C1642	C1426	G1340	G1162	C	A876
	U	A1847	U1741	C1643	G1430	A1341	U1164	G	G877
	A	G1848	U1742	U1644	G1430	C1342	G1165	C	G878
	U		U1742	U1645	A1434	C1343	A1166	C	G879
	G		G1743	G1546	A1434	G1344	U1244	U	C880



● 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	213.16Å 300.03Å 576.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 2.90 49.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.98-2.90) 92.0 (49.98-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.171 , 0.220 0.167 , 0.213	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: MG, OMG, SR, CD, PSU, OMU, NA, CL, 1MA, K, UR3

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	0.99	6/2408 (0.2%)
2	B	0.42	0/2690	1.02	20/3652 (0.5%)
3	C	0.45	0/1885	0.99	9/2552 (0.4%)
4	D	0.41	0/1111	1.01	6/1498 (0.4%)
5	E	0.40	0/1382	0.90	4/1880 (0.2%)
6	F	0.40	0/901	0.98	2/1224 (0.2%)
7	G	0.36	0/241	0.81	0/324
8	H	0.39	0/1302	0.96	8/1743 (0.5%)
9	I	0.39	0/526	0.87	0/716
10	J	0.42	0/1136	0.93	2/1530 (0.1%)
11	K	0.41	0/1004	0.98	3/1351 (0.2%)
12	L	0.37	0/1130	0.94	2/1509 (0.1%)
13	M	0.44	0/1582	0.92	2/2116 (0.1%)
14	N	0.38	0/1474	1.08	12/1999 (0.6%)
15	O	0.42	0/874	0.93	2/1181 (0.2%)
16	P	0.40	0/1147	0.83	0/1528
17	Q	0.40	0/749	0.99	3/1005 (0.3%)
18	R	1.29	7/1172 (0.6%)	1.40	11/1578 (0.7%)
19	S	0.38	0/648	0.86	1/875 (0.1%)
20	T	0.41	0/958	1.04	6/1289 (0.5%)
21	U	0.40	0/417	0.88	1/562 (0.2%)
22	V	0.39	0/502	0.96	2/675 (0.3%)
23	W	0.49	0/1219	0.99	4/1655 (0.2%)
24	X	0.46	0/664	1.03	6/895 (0.7%)
25	Y	0.45	0/1146	0.96	2/1536 (0.1%)
26	Z	0.40	0/584	0.94	0/781
27	1	0.42	0/438	0.89	3/578 (0.5%)
28	2	0.43	0/401	0.86	1/529 (0.2%)
29	3	0.39	0/771	0.82	4/1024 (0.4%)
30	0	0.38	0/65957	0.60	17/102867 (0.0%)
31	9	0.37	0/2904	0.59	2/4526 (0.0%)
All	All	0.41	7/98701 (0.0%)	0.72	141/147586 (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	28
31	9	0	1
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	27.35	2.86	1.49
18	R	150	PRO	CA-C	-17.43	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	11.73	1.47	1.23
18	R	150	PRO	N-CD	10.80	1.62	1.47
18	R	150	PRO	CA-CB	7.67	1.68	1.53

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-28.56	55.83	110.10
18	R	150	PRO	N-CA-C	-20.18	61.65	112.10
18	R	150	PRO	N-CA-CB	12.24	116.46	103.00
18	R	150	PRO	CA-N-CD	12.08	128.92	112.00
14	N	163	PHE	N-CA-C	-11.31	99.30	113.55
4	D	136	ARG	CA-C-N	8.11	129.97	119.84
4	D	136	ARG	C-N-CA	8.11	129.97	119.84
5	E	11	VAL	N-CA-C	7.92	118.68	110.05
24	X	22	ASN	N-CA-C	7.74	120.69	111.33
20	T	52	ARG	N-CA-C	7.64	123.33	114.62
4	D	15	GLU	CA-C-N	7.49	129.21	119.84
4	D	15	GLU	C-N-CA	7.49	129.21	119.84
1	A	70	ALA	N-CA-C	7.40	118.97	109.65
17	Q	17	LYS	N-CA-C	-7.22	100.11	110.08
24	X	77	PHE	N-CA-C	7.19	117.36	107.73
20	T	54	ASP	N-CA-C	-7.16	104.52	113.18
13	M	89	THR	N-CA-C	7.13	119.05	111.28
14	N	135	VAL	N-CA-C	-7.09	105.71	113.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	323	LEU	N-CA-C	7.07	119.43	110.24
14	N	51	GLY	CA-C-N	7.06	127.66	119.47
14	N	51	GLY	C-N-CA	7.06	127.66	119.47
25	Y	143	TRP	N-CA-C	7.06	120.55	109.96
8	H	10	ARG	N-CA-C	6.98	118.89	111.28
20	T	3	GLN	CA-C-N	6.84	126.36	119.24
20	T	3	GLN	C-N-CA	6.84	126.36	119.24
30	O	1120	U	C5'-C4'-C3'	-6.81	105.78	116.00
18	R	123	GLN	N-CA-C	6.77	120.53	109.76
23	W	35	VAL	N-CA-C	6.76	115.26	107.89
6	F	62	HIS	N-CA-C	6.71	119.60	111.82
1	A	222	GLY	N-CA-C	-6.63	106.03	113.79
2	B	175	LEU	N-CA-C	-6.61	104.00	111.14
20	T	89	ARG	CA-C-N	6.57	126.59	119.89
20	T	89	ARG	C-N-CA	6.57	126.59	119.89
30	O	1942	A	C5'-C4'-C3'	6.57	125.85	116.00
14	N	169	PRO	N-CA-C	-6.55	105.97	114.03
14	N	13	ARG	N-CA-C	-6.48	105.02	113.12
30	O	1592	G	N9-C1'-C2'	6.45	121.67	112.00
2	B	154	VAL	CA-C-N	6.45	125.67	118.97
2	B	154	VAL	C-N-CA	6.45	125.67	118.97
18	R	150	PRO	CA-C-O	-6.41	99.79	119.00
4	D	170	TYR	N-CA-C	6.40	120.71	111.56
31	9	39	U	N1-C1'-C2'	6.38	121.57	112.00
18	R	150	PRO	CA-CB-CG	-6.36	92.42	104.50
8	H	161	THR	N-CA-C	6.34	121.50	113.25
2	B	151	VAL	CA-C-N	6.28	125.69	118.85
2	B	151	VAL	C-N-CA	6.28	125.69	118.85
3	C	89	ALA	N-CA-C	6.27	118.67	111.02
2	B	222	LYS	N-CA-C	-6.24	100.75	110.42
14	N	42	HIS	N-CA-C	6.21	118.63	109.69
22	V	42	ASN	CA-C-N	6.18	127.56	119.84
22	V	42	ASN	C-N-CA	6.18	127.56	119.84
14	N	3	GLY	CA-C-N	6.16	125.72	119.19
14	N	3	GLY	C-N-CA	6.16	125.72	119.19
4	D	135	VAL	N-CA-C	6.13	115.18	107.70
27	1	21	ARG	N-CA-C	6.13	118.88	111.40
30	O	1504	A	N9-C1'-C2'	6.10	121.15	112.00
3	C	219	ASN	N-CA-C	6.04	118.39	109.69
2	B	265	LEU	N-CA-C	6.02	118.67	110.55
2	B	157	LYS	N-CA-C	-5.98	106.53	113.88
12	L	145	LEU	N-CA-C	-5.96	104.86	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	205	ARG	N-CA-C	5.92	119.33	111.75
30	0	1979	G	C4'-C3'-O3'	-5.91	104.14	113.00
3	C	134	ASP	N-CA-C	-5.91	106.11	113.55
30	0	2726	U	N1-C1'-C2'	5.89	120.83	112.00
8	H	163	SER	N-CA-C	-5.85	101.82	110.48
30	0	2291	A	N9-C1'-C2'	5.84	120.75	112.00
12	L	73	VAL	N-CA-C	5.80	115.99	110.42
21	U	50	GLU	N-CA-C	5.80	119.18	111.75
30	0	2301	A	N9-C1'-C2'	5.76	120.65	112.00
2	B	120	ASP	CA-C-N	5.75	125.29	119.19
2	B	120	ASP	C-N-CA	5.75	125.29	119.19
18	R	137	ASN	N-CA-C	5.73	118.89	110.59
28	2	24	TRP	N-CA-C	5.72	118.28	111.71
3	C	78	ARG	N-CA-C	5.70	116.07	108.38
1	A	48	ASP	CA-C-N	5.69	125.54	119.28
1	A	48	ASP	C-N-CA	5.69	125.54	119.28
30	0	834	G	C2'-C3'-O3'	-5.69	105.17	113.70
5	E	112	ALA	CA-C-N	5.62	125.38	119.76
5	E	112	ALA	C-N-CA	5.62	125.38	119.76
24	X	12	ILE	CB-CA-C	-5.62	104.70	110.71
30	0	920	C	C2'-C3'-O3'	-5.62	105.28	113.70
2	B	158	LYS	CA-C-N	5.58	125.89	119.92
2	B	158	LYS	C-N-CA	5.58	125.89	119.92
11	K	122	GLY	N-CA-C	5.56	119.37	112.64
1	A	135	VAL	N-CA-C	5.55	116.67	108.45
24	X	79	GLU	N-CA-C	5.55	117.77	111.11
11	K	8	VAL	N-CA-C	5.51	115.89	108.17
30	0	1979	G	N9-C1'-C2'	5.47	120.21	112.00
29	3	43	ASN	N-CA-C	5.47	119.82	113.20
18	R	34	GLU	N-CA-C	5.46	117.32	111.36
3	C	244	ALA	N-CA-C	5.46	117.23	111.28
18	R	141	VAL	N-CA-C	5.46	117.19	108.89
29	3	67	LEU	N-CA-C	5.45	118.46	109.85
18	R	76	ASP	N-CA-C	5.45	119.92	112.68
27	1	11	LYS	N-CA-C	5.43	118.03	109.39
30	0	2316	G	C5'-C4'-C3'	-5.43	107.06	115.20
15	O	43	VAL	N-CA-C	5.42	115.76	108.17
2	B	22	GLU	N-CA-C	-5.41	106.18	112.89
23	W	69	ARG	N-CA-C	5.40	120.74	113.72
17	Q	49	ASN	N-CA-C	5.40	117.84	110.55
14	N	48	VAL	N-CA-C	5.35	116.29	108.53
1	A	133	ARG	N-CA-C	-5.32	106.64	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	80	VAL	CA-C-N	5.31	125.37	119.32
3	C	80	VAL	C-N-CA	5.31	125.37	119.32
24	X	12	ILE	N-CA-C	5.30	113.12	107.76
8	H	53	ILE	N-CA-C	5.28	115.70	107.99
23	W	118	LEU	N-CA-C	5.27	116.89	110.41
19	S	27	ALA	N-CA-C	-5.27	100.14	108.73
27	1	54	ALA	N-CA-C	5.26	117.69	111.33
15	O	69	VAL	N-CA-C	5.25	116.14	108.53
8	H	58	VAL	N-CA-C	5.22	114.90	108.53
8	H	91	ARG	N-CA-C	5.22	119.37	112.89
30	0	1819	G	C5'-C4'-C3'	5.21	123.82	116.00
6	F	79	GLN	N-CA-C	5.20	117.96	109.59
31	9	65	A	N9-C1'-C2'	5.20	119.80	112.00
3	C	177	GLY	N-CA-C	5.20	117.34	112.04
14	N	153	GLN	N-CA-C	-5.19	102.66	110.70
30	0	921	G	N9-C1'-C2'	5.17	119.76	112.00
5	E	37	ASP	N-CA-C	5.17	119.17	112.86
30	0	2673	U	N1-C1'-C2'	5.15	119.73	112.00
2	B	217	ARG	N-CA-C	5.15	116.97	111.36
25	Y	202	ALA	N-CA-C	-5.14	102.58	110.14
10	J	88	PRO	N-CA-C	-5.12	105.57	112.48
17	Q	84	ILE	N-CA-C	5.12	115.34	108.17
13	M	70	GLY	N-CA-C	5.11	120.37	112.45
10	J	67	ASN	N-CA-C	-5.10	105.81	111.36
2	B	303	GLY	CA-C-N	5.08	126.34	120.85
2	B	303	GLY	C-N-CA	5.08	126.34	120.85
8	H	46	TYR	CA-C-N	5.08	124.39	118.85
8	H	46	TYR	C-N-CA	5.08	124.39	118.85
2	B	2	GLN	CA-C-N	5.06	125.05	119.89
2	B	2	GLN	C-N-CA	5.06	125.05	119.89
29	3	55	VAL	CA-C-N	5.05	126.16	119.84
29	3	55	VAL	C-N-CA	5.05	126.16	119.84
2	B	230	GLN	N-CA-C	5.05	118.70	112.54
14	N	162	ASP	N-CA-C	5.05	117.48	109.96
24	X	60	ALA	N-CA-C	5.03	117.14	111.11
11	K	74	VAL	N-CA-C	5.02	116.13	111.81
30	0	1878	G	O4'-C1'-C2'	-5.02	102.58	107.60
23	W	142	ASP	N-CA-C	-5.02	103.78	110.55
30	0	1261	A	N9-C1'-C2'	5.01	119.52	112.00

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	131	A	Sidechain
30	0	1430	G	Sidechain
30	0	1592	G	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1970	G	Sidechain
30	0	220	C	Sidechain
30	0	2301	A	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2524	G	Sidechain
30	0	2552	C	Sidechain
30	0	2607	U	Sidechain
30	0	2673	U	Sidechain
30	0	2842	G	Sidechain
30	0	333	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	888	U	Sidechain
31	9	39	U	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	65	0
2	B	2625	0	2533	90	0
3	C	1860	0	1813	59	0
4	D	1094	0	1085	48	0
5	E	1357	0	1266	32	0
6	F	890	0	843	27	0
7	G	240	0	231	8	0
8	H	1282	0	1292	34	0
9	I	519	0	500	23	0
10	J	1120	0	1098	34	0
11	K	994	0	1027	33	0
12	L	1118	0	1076	29	0
13	M	1558	0	1573	43	0
14	N	1445	0	1401	51	0
15	O	865	0	873	18	0
16	P	1136	0	1123	24	0
17	Q	735	0	729	21	0
18	R	1149	0	1122	37	0
19	S	641	0	605	10	0
20	T	950	0	924	21	0
21	U	410	0	364	8	0
22	V	499	0	511	18	0
23	W	1196	0	1137	63	0
24	X	654	0	653	19	0
25	Y	1130	0	1133	24	0
26	Z	573	0	532	15	0
27	1	431	0	426	24	0
28	2	396	0	413	15	0
29	3	755	0	728	19	0
30	0	59020	0	29811	1166	0
31	9	2599	0	1325	101	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	4	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	1	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	93	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	67	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5929	0	0	185	0
38	1	63	0	0	4	0
38	2	50	0	0	1	0
38	3	62	0	0	3	0
38	9	147	0	0	7	0
38	A	116	0	0	5	0
38	B	141	0	0	12	0
38	C	170	0	0	13	0
38	D	44	0	0	3	0
38	E	45	0	0	2	0
38	F	27	0	0	2	0
38	G	19	0	0	1	0
38	H	63	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	I	8	0	0	3	0
38	J	53	0	0	1	0
38	K	56	0	0	5	0
38	L	85	0	0	6	0
38	M	123	0	0	2	0
38	N	55	0	0	5	0
38	O	43	0	0	3	0
38	P	67	0	0	2	0
38	Q	50	0	0	3	0
38	R	85	0	0	1	0
38	S	33	0	0	2	0
38	T	34	0	0	2	0
38	U	27	0	0	2	0
38	V	13	0	0	2	0
38	W	69	0	0	4	0
38	X	25	0	0	2	0
38	Y	95	0	0	5	0
38	Z	26	0	0	3	0
All	All	99122	0	59913	1971	0

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

All (1971) 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
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.13
30:0:1160:G:C5'	30:0:1161:A:H5'	1.77	1.12
30:0:871:G:C8	30:0:871:G:H5'	1.84	1.11
30:0:871:G:H5'	30:0:871:G:H8	1.09	1.10
31:9:56:A:H2'	31:9:57:A:H5''	1.31	1.10
14:N:37:ARG:NH1	31:9:6:C:H5''	1.63	1.09
13:M:171:ARG:HD3	30:0:156:C:H5''	1.33	1.09
30:0:1160:G:H5'	30:0:1161:A:C5'	1.82	1.09
31:9:76:G:H3'	31:9:77:A:H5''	1.36	1.06
30:0:545:G:H5'	30:0:545:G:H8	1.19	1.06
30:0:1205:U:H2'	30:0:1206:U:H5''	1.32	1.04
30:0:1160:G:H5'	30:0:1161:A:H5'	1.03	1.02
30:0:1701:A:H4'	30:0:1702:U:H5''	1.42	1.01
2:B:62:ARG:HA	2:B:65:MET:HE3	1.37	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:82:THR:HG23	30:0:1242:A:H5'	1.39	1.01
15:O:3:THR:HG22	30:0:656:G:H5'	1.41	1.01
30:0:2717:C:C2'	30:0:2718:C:H5''	1.92	0.99
30:0:1979:G:H2'	38:0:3301:HOH:O	1.61	0.98
31:9:29:C:H2'	31:9:30:C:H5'	1.44	0.98
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.46	0.97
11:K:10:GLN:HE21	11:K:10:GLN:H	0.95	0.95
30:0:182:G:H5'	38:0:5168:HOH:O	1.67	0.95
30:0:1666:C:O2'	30:0:1667:A:H5''	1.67	0.94
30:0:1118:A:H8	30:0:1118:A:H3'	1.30	0.94
30:0:2717:C:H2'	30:0:2718:C:H5''	1.50	0.94
30:0:381:G:H5''	38:0:4330:HOH:O	1.67	0.93
30:0:1187:U:HO2'	30:0:1189:A:H2	1.01	0.93
30:0:1205:U:H2'	30:0:1206:U:C5'	1.99	0.93
30:0:1118:A:H3'	30:0:1118:A:C8	2.03	0.93
30:0:1603:A:H5'	30:0:1605:G:O4'	1.67	0.92
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.47	0.92
30:0:1634:G:H3'	38:0:3907:HOH:O	1.70	0.91
30:0:282:C:H1'	30:0:368:C:N4	1.84	0.91
16:P:115:SER:H	16:P:118:GLN:HE21	1.03	0.91
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.85	0.91
30:0:271:C:H41	30:0:378:A:H2	1.17	0.90
2:B:162:MET:SD	2:B:310:ARG:HD3	2.11	0.90
30:0:559:U:H6	30:0:559:U:H5'	1.35	0.90
30:0:545:G:H5'	30:0:545:G:C8	2.05	0.90
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.20	0.90
30:0:871:G:H8	30:0:871:G:C5'	1.85	0.90
30:0:542:A:H5'	30:0:542:A:H8	1.36	0.90
31:9:14:G:H5'	31:9:14:G:H8	1.37	0.90
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.55	0.89
31:9:56:A:C2'	31:9:57:A:H5''	2.03	0.89
30:0:1119:G:H22	30:0:1246:A:H2	1.20	0.89
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.89
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.17	0.88
30:0:1632:A:H2'	30:0:1633:C:H5'	1.56	0.88
30:0:2508:C:H2'	38:0:6764:HOH:O	1.73	0.87
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.87
4:D:25:MET:HE2	4:D:41:LEU:HG	1.57	0.86
30:0:558:C:C2'	30:0:559:U:H5''	2.05	0.86
30:0:506:G:H22	30:0:509:A:H5'	1.40	0.86
30:0:1205:U:C2'	30:0:1206:U:H5''	2.05	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.73	0.86
30:0:1184:C:H1'	38:0:7480:HOH:O	1.74	0.86
30:0:2507:G:H2'	30:0:2510:C:H42	1.41	0.86
30:0:541:C:C2'	30:0:542:A:H5''	2.06	0.86
30:0:2908:A:H2'	30:0:2909:G:O4'	1.76	0.86
30:0:1189:A:H1'	30:0:1209:C:O4'	1.76	0.85
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.58	0.85
30:0:1183:C:H2'	38:0:6249:HOH:O	1.76	0.85
16:P:117:SER:HB3	30:0:1593:C:OP1	1.75	0.85
30:0:1667:A:H8	30:0:1667:A:H5'	1.41	0.85
30:0:541:C:H2'	30:0:542:A:H5''	1.58	0.85
30:0:2717:C:O2'	30:0:2718:C:H5''	1.77	0.85
30:0:2586:U:H3	30:0:2592:G:H22	1.22	0.84
30:0:2291:A:C8	30:0:2309:C:H5'	2.12	0.84
2:B:238:ASN:HD22	2:B:240:GLY:H	1.24	0.84
38:O:7674:HOH:O	30:0:653:U:H5''	1.77	0.84
30:0:1206:U:H5'	30:0:1206:U:H6	1.41	0.84
30:0:2710:U:H1'	38:0:7632:HOH:O	1.77	0.84
30:0:2506:A:HO2'	30:0:2507:G:H8	1.21	0.84
31:9:2:U:OP2	31:9:3:A:H5'	1.78	0.84
30:0:1474:C:H6	30:0:1474:C:H5'	1.43	0.83
4:D:154:LYS:H	4:D:154:LYS:HD2	1.43	0.83
18:R:29:LYS:HE2	30:0:524:A:C5'	2.08	0.83
30:0:558:C:O2'	30:0:559:U:H5''	1.78	0.83
30:0:1474:C:H5'	30:0:1474:C:C6	2.13	0.83
30:0:506:G:H22	30:0:509:A:C5'	1.92	0.83
30:0:877:G:H5'	30:0:878:G:OP1	1.79	0.83
30:0:1119:G:N2	30:0:1246:A:C2	2.46	0.82
30:0:1116:U:O2'	30:0:1118:A:H2	1.62	0.82
14:N:37:ARG:HH12	31:9:6:C:H5''	1.43	0.82
18:R:29:LYS:HE2	30:0:524:A:H5''	1.59	0.82
23:W:149:LEU:HG	23:W:153:MET:HE2	1.62	0.82
30:0:1116:U:H3	30:0:1246:A:H62	1.24	0.82
30:0:283:U:H5	30:0:284:C:N3	1.78	0.81
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.27	0.81
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.62	0.81
30:0:69:A:H5'	30:0:69:A:C8	2.15	0.81
30:0:1878:G:H1'	38:0:6126:HOH:O	1.77	0.81
30:0:2852:A:H5''	38:0:5244:HOH:O	1.80	0.81
15:O:3:THR:CG2	30:0:656:G:H5'	2.10	0.81
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:541:C:H2'	30:0:542:A:C5'	2.11	0.81
30:0:1116:U:HO2'	30:0:1118:A:H2	0.82	0.81
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.63	0.80
30:0:2529:G:H3'	38:0:7197:HOH:O	1.80	0.80
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.62	0.79
30:0:2506:A:O2'	30:0:2507:G:H8	1.64	0.79
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.63	0.79
11:K:10:GLN:H	11:K:10:GLN:NE2	1.79	0.79
30:0:2502:C:C2'	30:0:2503:A:H5'	2.13	0.78
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.65	0.78
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.64	0.78
11:K:39:GLY:HA2	38:0:5232:HOH:O	1.83	0.78
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.18	0.78
30:0:2578:G:H5'	30:0:2578:G:H8	1.48	0.78
30:0:1632:A:C2'	30:0:1633:C:H5'	2.13	0.78
3:C:236:THR:HG22	3:C:239:ALA:H	1.46	0.78
30:0:2256:G:O2'	30:0:2257:G:H5'	1.82	0.78
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.66	0.78
30:0:282:C:O2'	30:0:283:U:H5'	1.84	0.78
14:N:113:SER:HB2	38:N:8849:HOH:O	1.84	0.77
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.67	0.77
30:0:2526:C:C6	30:0:2526:C:H5'	2.19	0.77
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.65	0.77
30:0:1300:G:H1'	38:0:4694:HOH:O	1.83	0.77
30:0:2635:A:O2'	30:0:2636:C:H5'	1.84	0.77
13:M:164:THR:HG22	13:M:167:GLY:H	1.50	0.77
30:0:272:A:H3'	38:0:7542:HOH:O	1.84	0.77
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.66	0.77
30:0:396:U:H1'	38:0:7640:HOH:O	1.85	0.77
30:0:2502:C:H2'	30:0:2503:A:H5'	1.65	0.77
30:0:2608:C:H3'	38:0:7824:HOH:O	1.85	0.77
31:9:14:G:H5'	31:9:14:G:C8	2.19	0.77
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.67	0.76
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.76
30:0:69:A:H5'	30:0:69:A:H8	1.50	0.76
30:0:1118:A:H62	30:0:1244:U:H3	1.31	0.76
30:0:1701:A:H5'	38:0:6290:HOH:O	1.83	0.76
30:0:2783:A:H3'	38:0:5242:HOH:O	1.83	0.76
30:0:2812:A:H2	30:0:2814:A:H62	1.31	0.76
30:0:2679:G:H2'	30:0:2681:A:OP2	1.86	0.76
31:9:54:A:O2'	31:9:55:U:H5'	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1372:A:H3'	38:0:7202:HOH:O	1.86	0.76
30:0:2403:C:H5'	38:0:6033:HOH:O	1.84	0.76
22:V:1:THR:HB	30:0:93:C:H5''	1.68	0.76
30:0:192:A:H5'	38:0:7655:HOH:O	1.85	0.76
30:0:1603:A:H5''	30:0:1605:G:H5'	1.68	0.75
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.69	0.75
6:F:91:VAL:HG12	6:F:92:GLY:H	1.52	0.75
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.51	0.75
30:0:1172:G:H5''	38:0:7271:HOH:O	1.85	0.75
30:0:558:C:H2'	30:0:559:U:C5'	2.17	0.74
30:0:1701:A:H4'	30:0:1702:U:C5'	2.15	0.74
3:C:1:MET:HG2	3:C:2:GLN:H	1.51	0.74
30:0:2748:G:H5'	38:0:7554:HOH:O	1.87	0.74
30:0:2768:A:O2'	30:0:2769:C:H5'	1.87	0.74
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.69	0.74
30:0:2420:G:O2'	30:0:2421:G:H5'	1.86	0.74
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.70	0.74
30:0:2717:C:H2'	30:0:2718:C:C5'	2.18	0.74
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.03	0.74
30:0:2404:G:H5''	38:0:5222:HOH:O	1.88	0.74
18:R:25:PHE:CE2	18:R:29:LYS:HE3	2.23	0.73
11:K:10:GLN:HE21	11:K:10:GLN:N	1.79	0.73
33:0:8812:CL:CL	38:0:5135:HOH:O	2.41	0.73
22:V:1:THR:HG23	22:V:2:VAL:H	1.53	0.73
30:0:1666:C:H2'	30:0:1667:A:H5'	1.70	0.73
1:A:211:LYS:HB2	38:A:9082:HOH:O	1.87	0.73
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.54	0.73
29:3:65:THR:HG22	29:3:67:LEU:HG	1.69	0.73
30:0:2004:U:H4'	38:0:5316:HOH:O	1.88	0.73
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.87	0.73
30:0:138:U:H5''	30:0:139:C:OP2	1.88	0.73
15:O:47:ARG:HH11	15:O:47:ARG:HG3	1.53	0.73
30:0:2896:A:H5''	38:0:6105:HOH:O	1.87	0.73
38:Z:8707:HOH:O	30:0:1886:A:H4'	1.89	0.73
3:C:139:VAL:HG13	38:C:8644:HOH:O	1.88	0.73
30:0:1666:C:C2'	30:0:1667:A:H5''	2.19	0.72
30:0:1641:A:H2'	30:0:1642:A:H5'	1.71	0.72
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.88	0.72
30:0:2765:C:H4'	38:0:5531:HOH:O	1.88	0.72
22:V:50:ARG:NH1	30:0:56:G:H5''	2.04	0.72
30:0:870:G:C2'	30:0:871:G:H5''	2.18	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:41:HIS:H	28:2:45:ASN:HD22	1.35	0.72
30:0:1118:A:C8	30:0:1118:A:C3'	2.69	0.72
30:0:2256:G:C2'	30:0:2257:G:H5'	2.18	0.72
30:0:468:U:H3'	38:0:7580:HOH:O	1.89	0.72
30:0:827:A:H1'	38:0:6220:HOH:O	1.88	0.72
30:0:871:G:C8	30:0:871:G:C5'	2.64	0.72
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.24	0.72
20:T:9:LYS:HE2	20:T:13:ARG:NH1	2.04	0.72
22:V:50:ARG:HH12	30:0:56:G:H5''	1.55	0.72
30:0:1187:U:O2'	30:0:1189:A:H2	1.71	0.72
30:0:1201:C:H5''	38:0:6238:HOH:O	1.89	0.72
30:0:2769:C:C2'	30:0:2770:G:H5'	2.20	0.72
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.04	0.71
33:0:8813:CL:CL	38:0:4694:HOH:O	2.45	0.71
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.55	0.71
30:0:1183:C:N4	30:0:1184:C:H41	1.87	0.71
30:0:1525:G:H5'	30:0:1526:A:OP2	1.91	0.71
30:0:2491:G:H1'	38:0:6878:HOH:O	1.89	0.71
31:9:29:C:C2'	31:9:30:C:H5'	2.18	0.71
30:0:1189:A:H3'	38:0:7693:HOH:O	1.90	0.71
30:0:1741:U:H5'	30:0:1742:A:OP1	1.90	0.71
30:0:2372:A:H2'	30:0:2373:U:H6	1.56	0.70
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.21	0.70
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.92	0.70
2:B:206:THR:HG21	30:0:2716:G:H5''	1.73	0.70
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.57	0.70
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.70
30:0:2659:U:H5''	38:0:4138:HOH:O	1.92	0.70
31:9:20:G:O2'	31:9:21:G:H5'	1.91	0.70
30:0:2637:A:H5'	38:0:9281:HOH:O	1.92	0.70
31:9:92:G:H2'	31:9:93:A:C8	2.27	0.70
30:0:567:U:H5''	38:0:5297:HOH:O	1.92	0.70
30:0:1973:A:H5'	30:0:1973:A:H8	1.57	0.69
30:0:1835:U:C5	30:0:1840:A:N7	2.59	0.69
30:0:1750:C:H5''	38:0:3676:HOH:O	1.91	0.69
24:X:71:ARG:HD3	38:X:2171:HOH:O	1.91	0.69
30:0:380:A:H2'	38:0:7240:HOH:O	1.92	0.69
30:0:544:G:H2'	30:0:545:G:H5''	1.74	0.69
30:0:2010:A:H2'	38:0:5965:HOH:O	1.91	0.69
7:G:12:ILE:HG23	38:0:5468:HOH:O	1.93	0.69
30:0:281:U:O2'	30:0:282:C:H5'	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.23	0.69
16:P:115:SER:H	16:P:118:GLN:NE2	1.85	0.69
1:A:51:ARG:HB2	38:A:9066:HOH:O	1.91	0.69
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.75	0.69
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.73	0.69
30:0:1441:G:O2'	30:0:1442:A:H5'	1.91	0.69
30:0:1377:C:H5'	30:0:1377:C:H6	1.58	0.69
30:0:2251:G:H2'	30:0:2252:A:C8	2.28	0.69
27:1:25:LYS:HD2	28:2:49:GLU:H	1.58	0.68
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.91	0.68
30:0:1666:C:H2'	30:0:1667:A:C5'	2.22	0.68
30:0:2111:G:H1'	38:0:9053:HOH:O	1.92	0.68
30:0:2768:A:H2'	30:0:2769:C:O4'	1.93	0.68
30:0:2563:U:H2'	30:0:2565:C:O5'	1.94	0.68
3:C:174:ILE:HD11	30:0:338:C:H4'	1.75	0.68
13:M:23:LEU:HD13	13:M:27:ARG:HH21	1.57	0.68
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.75	0.68
30:0:1183:C:H42	30:0:1184:C:H41	1.42	0.68
12:L:133:VAL:HA	38:L:8874:HOH:O	1.92	0.68
30:0:1603:A:C5'	30:0:1605:G:H5'	2.23	0.68
6:F:91:VAL:HG12	6:F:92:GLY:N	2.09	0.68
14:N:141:ARG:HH21	31:9:48:C:H4'	1.58	0.68
30:0:2453:G:H3'	38:0:5927:HOH:O	1.94	0.68
14:N:80:SER:HB2	38:N:8830:HOH:O	1.93	0.68
30:0:558:C:H2'	30:0:559:U:H5''	1.72	0.67
30:0:2256:G:H2'	30:0:2257:G:C5'	2.23	0.67
31:9:39:U:H1'	31:9:44:A:H61	1.59	0.67
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.75	0.67
31:9:23:U:O2'	31:9:24:U:H4'	1.94	0.67
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.60	0.67
1:A:36:ASP:HB2	1:A:85:SER:H	1.60	0.67
18:R:150:PRO:CG	18:R:150:PRO:O	2.41	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.28	0.67
30:0:285:A:H2'	30:0:286:U:O4'	1.95	0.67
30:0:1730:G:H5'	30:0:1731:C:C5	2.30	0.67
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.77	0.66
23:W:88:THR:HG22	23:W:89:ASP:H	1.60	0.66
30:0:1834:C:H2'	30:0:1840:A:N6	2.09	0.66
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.76	0.66
30:0:125:U:H2'	38:0:3776:HOH:O	1.94	0.66
30:0:853:C:H3'	38:0:4563:HOH:O	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2237:G:H1'	38:0:4866:HOH:O	1.94	0.66
30:0:2509:A:OP2	30:0:2510:C:H5	1.78	0.66
30:0:1524:U:OP1	30:0:1524:U:H4'	1.95	0.66
30:0:2256:G:H2'	30:0:2257:G:H5'	1.77	0.66
30:0:2372:A:H2'	30:0:2373:U:C6	2.30	0.66
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.76	0.66
21:U:14:GLU:O	21:U:17:THR:HB	1.95	0.66
30:0:1120:U:H5'	30:0:1121:G:OP2	1.95	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.42	0.66
31:9:22:G:H5'	31:9:23:U:OP1	1.94	0.66
30:0:31:C:H2'	38:0:7702:HOH:O	1.95	0.66
30:0:1667:A:H5'	30:0:1667:A:C8	2.29	0.66
30:0:2498:C:O2'	30:0:2499:U:H5'	1.94	0.66
30:0:2836:G:H1'	38:0:6850:HOH:O	1.95	0.66
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.76	0.66
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.77	0.66
8:H:29:SER:HA	8:H:62:HIS:HD2	1.60	0.66
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.31	0.66
10:J:82:THR:CG2	30:0:1242:A:H5'	2.21	0.66
23:W:26:ILE:HB	38:W:5420:HOH:O	1.95	0.66
30:0:2320:U:H4'	30:0:2321:A:O4'	1.95	0.66
30:0:283:U:C5	30:0:284:C:N3	2.63	0.66
30:0:544:G:C2'	30:0:545:G:H5''	2.26	0.66
30:0:1562:C:O2	30:0:1562:C:H2'	1.95	0.66
30:0:1819:G:H2'	30:0:1820:G:H4'	1.76	0.66
30:0:2505:G:C2'	30:0:2506:A:H5'	2.25	0.66
30:0:2505:G:O2'	30:0:2506:A:H5'	1.95	0.66
30:0:485:A:N3	30:0:487:G:H5''	2.10	0.65
30:0:2748:G:H1'	38:0:7914:HOH:O	1.95	0.65
30:0:2795:C:O2'	30:0:2796:U:H5'	1.96	0.65
1:A:35:GLY:O	1:A:36:ASP:HB3	1.96	0.65
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.62	0.65
13:M:171:ARG:CD	30:0:156:C:H5''	2.18	0.65
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.78	0.65
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.96	0.65
30:0:1477:C:H5'	30:0:1868:G:C5'	2.26	0.65
30:0:1666:C:C2'	30:0:1667:A:C5'	2.74	0.65
30:0:836:G:H5''	38:0:9288:HOH:O	1.95	0.65
30:0:2766:A:H5'	38:0:9565:HOH:O	1.97	0.65
23:W:44:MET:HE2	30:0:944:G:H21	1.61	0.65
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.31	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:74:ARG:O	10:J:78:ILE:HG12	1.97	0.65
29:3:48:ASN:HD21	30:0:2468:A:H61	1.43	0.65
10:J:19:MET:HE2	10:J:79:PHE:HA	1.77	0.64
23:W:13:MET:HE2	23:W:18:GLN:HA	1.78	0.64
30:0:558:C:C2'	30:0:559:U:C5'	2.75	0.64
30:0:960:G:H3'	30:0:960:G:N3	2.12	0.64
30:0:1741:U:O2'	30:0:2723:G:H4'	1.97	0.64
30:0:1183:C:H2'	30:0:1183:C:O2	1.95	0.64
30:0:1279:U:O2	30:0:1279:U:H2'	1.95	0.64
30:0:281:U:H2'	30:0:282:C:O4'	1.96	0.64
31:9:31:C:H1'	38:9:9014:HOH:O	1.96	0.64
18:R:29:LYS:HE2	30:0:524:A:H5'	1.79	0.64
19:S:43:GLU:HB3	38:S:8991:HOH:O	1.97	0.64
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.80	0.64
10:J:107:ASN:ND2	10:J:109:TYR:H	1.96	0.64
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.10	0.64
2:B:190:MET:HE2	2:B:194:PHE:HD1	1.63	0.64
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.63	0.64
30:0:814:G:H4'	38:0:3141:HOH:O	1.98	0.64
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.79	0.64
29:3:73:GLU:HB3	38:3:9049:HOH:O	1.97	0.64
30:0:564:G:H1'	38:0:6317:HOH:O	1.97	0.64
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.80	0.64
30:0:2481:G:H5''	38:0:4558:HOH:O	1.97	0.64
30:0:1701:A:H5''	30:0:1702:U:H3'	1.80	0.64
30:0:2827:A:H2'	30:0:2828:G:O4'	1.98	0.64
14:N:37:ARG:NH1	31:9:6:C:C5'	2.52	0.63
18:R:9:ASP:O	18:R:13:THR:HB	1.98	0.63
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.27	0.63
3:C:184:ARG:NH2	30:0:450:C:OP1	2.32	0.63
14:N:11:ARG:HD3	31:9:114:G:O6	1.99	0.63
30:0:12:U:H2'	30:0:13:G:H5'	1.80	0.63
30:0:1058:A:H2'	30:0:1060:C:H5''	1.78	0.63
12:L:41:HIS:HD2	30:0:926:A:O2'	1.80	0.63
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.81	0.63
38:I:1549:HOH:O	30:0:1180:U:H1'	1.97	0.63
18:R:117:HIS:HD2	30:0:20:G:H21	1.45	0.63
3:C:140:VAL:HB	38:C:8647:HOH:O	1.99	0.63
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.28	0.63
30:0:2768:A:H5''	38:0:4438:HOH:O	1.98	0.63
30:0:1243:C:H3'	38:0:4848:HOH:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1166:A:OP1	30:0:1174:A:H4'	1.99	0.62
30:0:2509:A:H2'	30:0:2510:C:O4'	1.99	0.62
30:0:671:A:O2'	30:0:672:G:H2'	1.99	0.62
30:0:1185:U:H5'	38:0:7480:HOH:O	1.99	0.62
30:0:2426:G:H1'	38:0:6098:HOH:O	1.99	0.62
30:0:2781:U:H2'	30:0:2782:G:H5'	1.79	0.62
27:1:8:GLN:HE22	27:1:11:LYS:NZ	1.97	0.62
30:0:371:U:H2'	30:0:372:A:H8	1.65	0.62
30:0:848:C:H5'	38:0:7283:HOH:O	1.99	0.62
30:0:1527:A:H1'	30:0:1528:A:C8	2.34	0.62
31:9:49:G:O2'	31:9:50:G:H5'	1.99	0.62
31:9:114:G:H2'	31:9:115:C:C6	2.35	0.62
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.80	0.62
5:E:69:ILE:HA	5:E:72:MET:HE3	1.80	0.62
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.82	0.62
12:L:136:ALA:HB3	38:L:8874:HOH:O	2.00	0.62
30:0:559:U:H5'	30:0:559:U:C6	2.26	0.62
31:9:39:U:H3'	31:9:40:C:H5''	1.82	0.62
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.39	0.62
30:0:2316:G:H4'	38:0:6098:HOH:O	2.00	0.62
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.81	0.62
27:1:28:HIS:HE1	30:0:776:A:OP1	1.83	0.62
30:0:1398:G:O2'	30:0:1399:A:H5'	2.00	0.62
30:0:378:A:H1'	38:0:3510:HOH:O	1.98	0.62
30:0:542:A:H5'	30:0:542:A:C8	2.25	0.62
30:0:681:G:N3	30:0:681:G:H5'	2.15	0.62
30:0:1278:A:H4'	30:0:1279:U:C4	2.34	0.62
30:0:2748:G:H2'	38:0:7554:HOH:O	1.98	0.62
38:B:9095:HOH:O	30:0:2672:C:H1'	2.00	0.61
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.81	0.61
30:0:1603:A:H5'	30:0:1605:G:C4'	2.30	0.61
30:0:2597:U:H2'	30:0:2598:U:H5'	1.81	0.61
30:0:1185:U:H2'	30:0:1186:C:C6	2.35	0.61
30:0:2781:U:C2'	30:0:2782:G:H5'	2.30	0.61
30:0:128:A:O2'	30:0:129:A:H5'	2.00	0.61
30:0:2300:A:H4'	30:0:2301:A:O5'	2.01	0.61
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.65	0.61
30:0:1342:C:C2'	30:0:1343:C:H5'	2.30	0.61
30:0:2252:A:C5	30:0:2253:G:H1'	2.34	0.61
30:0:2769:C:H2'	30:0:2770:G:H5'	1.82	0.61
30:0:2851:G:O2'	30:0:2852:A:H5'	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:110:ASP:O	30:0:1163:G:H5'	2.01	0.61
23:W:81:ASP:OD1	23:W:92:ASP:HB2	1.99	0.61
30:0:138:U:OP2	30:0:139:C:H5	1.83	0.61
30:0:1166:A:H61	30:0:1180:U:H3	1.46	0.61
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.98	0.61
30:0:308:U:H5'	30:0:309:C:OP1	1.99	0.61
30:0:558:C:H2'	30:0:559:U:H5'	1.82	0.61
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.83	0.61
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.00	0.61
30:0:255:A:H2'	30:0:256:C:H6	1.64	0.61
30:0:2507:G:H2'	30:0:2510:C:N4	2.12	0.61
23:W:61:THR:HG23	23:W:151:GLU:HG3	1.83	0.61
30:0:2894:C:O2'	30:0:2895:C:H5'	2.01	0.61
13:M:164:THR:HG22	13:M:167:GLY:N	2.15	0.61
30:0:1171:A:H2'	30:0:1172:G:H5'	1.81	0.61
30:0:2419:U:H5''	30:0:2420:G:H5'	1.83	0.61
31:9:1:U:O3'	31:9:3:A:H5''	2.01	0.61
28:2:41:HIS:HD2	28:2:44:ARG:H	1.49	0.60
30:0:1878:G:O2'	30:0:1879:U:C6	2.52	0.60
2:B:294:TYR:HE2	38:B:9111:HOH:O	1.84	0.60
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.81	0.60
13:M:145:ASP:HB2	38:M:8862:HOH:O	1.99	0.60
30:0:2344:G:H2'	30:0:2344:G:N3	2.16	0.60
30:0:2718:C:H6	30:0:2718:C:H5'	1.66	0.60
2:B:264:GLU:HG2	2:B:267:LYS:HE2	1.83	0.60
18:R:128:ARG:NH2	30:0:2054:A:N3	2.49	0.60
30:0:2616:G:H1'	38:0:9433:HOH:O	2.00	0.60
31:9:49:G:H2'	31:9:50:G:O4'	2.01	0.60
30:0:1080:C:H4'	30:0:1081:A:OP1	2.01	0.60
30:0:1174:A:C5	30:0:1201:C:H4'	2.36	0.60
30:0:1192:A:H3'	30:0:1193:A:H5'	1.83	0.60
1:A:199:HIS:CD2	1:A:201:PHE:H	2.19	0.60
4:D:58:VAL:HB	4:D:62:ASP:HB2	1.83	0.60
4:D:103:ASN:ND2	4:D:134:LEU:H	1.99	0.60
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.83	0.60
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.83	0.60
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.94	0.60
30:0:1730:G:H5''	30:0:1731:C:H6	1.65	0.60
30:0:1766:U:O2	30:0:1778:A:H5'	2.01	0.60
30:0:1972:U:H2'	30:0:1973:A:C5'	2.31	0.60
18:R:39:THR:HG22	18:R:42:GLU:H	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:10:LYS:HG3	38:1:8981:HOH:O	2.01	0.60
30:0:2900:G:H2'	30:0:2901:C:O4'	2.01	0.60
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.67	0.60
17:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.01	0.60
30:0:1182:C:H1'	30:0:1192:A:H8	1.67	0.60
1:A:48:ASP:HB3	38:A:9066:HOH:O	2.02	0.60
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.42	0.60
30:0:1119:G:N2	30:0:1246:A:H2	1.92	0.60
30:0:1730:G:H5''	30:0:1731:C:C6	2.37	0.60
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.50	0.59
30:0:515:C:H5''	38:0:5654:HOH:O	2.01	0.59
30:0:1116:U:O2'	30:0:1118:A:C2	2.46	0.59
30:0:1528:A:H2'	30:0:1529:G:O4'	2.02	0.59
31:9:64:C:C2'	31:9:65:A:H5'	2.32	0.59
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.02	0.59
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.83	0.59
30:0:2505:G:H2'	30:0:2506:A:H5'	1.84	0.59
30:0:659:A:H5''	38:0:7111:HOH:O	2.03	0.59
30:0:1641:A:C2'	30:0:1642:A:H5'	2.32	0.59
10:J:107:ASN:C	10:J:107:ASN:HD22	2.09	0.59
30:0:2472:C:O2'	30:0:2634:G:H4'	2.03	0.59
30:0:2637:A:H4'	38:0:6071:HOH:O	2.02	0.59
30:0:1189:A:O2'	30:0:1208:C:H2'	2.03	0.59
31:9:49:G:H5''	38:9:9092:HOH:O	2.02	0.59
31:9:64:C:H2'	31:9:65:A:H5'	1.84	0.59
1:A:36:ASP:CB	1:A:85:SER:H	2.16	0.59
12:L:41:HIS:CD2	30:0:926:A:O2'	2.56	0.59
22:V:39:ALA:N	22:V:40:PRO:HD2	2.17	0.59
30:0:1189:A:H1'	30:0:1209:C:C1'	2.32	0.59
30:0:2613:G:O2'	30:0:2614:C:H5'	2.03	0.59
31:9:54:A:C2'	31:9:55:U:H5'	2.32	0.59
24:X:43:VAL:HG12	24:X:44:ASP:H	1.66	0.59
4:D:48:MET:HE2	31:9:41:C:H5''	1.83	0.59
5:E:84:MET:HG2	5:E:168:ILE:HA	1.85	0.59
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.18	0.59
27:1:9:GLY:HA2	30:0:1687:C:O2	2.03	0.59
5:E:143:GLN:NE2	30:0:2779:G:H21	2.00	0.59
30:0:960:G:N3	30:0:960:G:C2'	2.65	0.59
30:0:2089:A:O2'	30:0:2090:G:H5'	2.03	0.59
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.84	0.59
23:W:13:MET:HE2	23:W:18:GLN:CA	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.84	0.59
30:0:583:C:H2'	30:0:584:U:H6	1.68	0.59
30:0:2802:C:H2'	30:0:2803:C:H6	1.68	0.59
30:0:1200:A:H3'	38:0:5763:HOH:O	2.03	0.58
23:W:139:GLY:O	23:W:141:HIS:HD2	1.86	0.58
31:9:76:G:C3'	31:9:77:A:H5''	2.24	0.58
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.38	0.58
30:0:807:A:O2'	30:0:808:A:H5'	2.03	0.58
30:0:2526:C:H5'	30:0:2526:C:H6	1.64	0.58
31:9:1:U:H4'	31:9:3:A:OP1	2.03	0.58
30:0:1730:G:C5'	30:0:1731:C:C6	2.86	0.58
30:0:1942:A:O2'	30:0:1943:C:H5'	2.02	0.58
31:9:2:U:H4'	38:9:9104:HOH:O	2.02	0.58
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.85	0.58
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.18	0.58
8:H:168:VAL:HG13	38:H:210:HOH:O	2.03	0.58
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.68	0.58
23:W:44:MET:CE	30:0:944:G:H21	2.16	0.58
30:0:1183:C:N3	30:0:1184:C:C5	2.72	0.58
30:0:2421:G:H1'	38:0:7033:HOH:O	2.03	0.58
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.84	0.58
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.84	0.58
30:0:90:A:H2'	30:0:91:G:O4'	2.02	0.58
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.85	0.58
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.04	0.58
30:0:644:G:H5'	30:0:644:G:N3	2.19	0.58
30:0:1175:G:H1'	30:0:1193:A:H2'	1.84	0.58
30:0:1187:U:H2'	38:0:6907:HOH:O	2.04	0.58
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.84	0.58
3:C:174:ILE:CD1	30:0:338:C:H4'	2.33	0.58
14:N:37:ARG:HH11	31:9:6:C:H5''	1.65	0.58
8:H:174:LEU:HA	38:H:220:HOH:O	2.02	0.58
21:U:17:THR:HG22	21:U:18:GLY:N	2.19	0.58
30:0:1174:A:C6	30:0:1201:C:H4'	2.39	0.58
2:B:258:GLY:H	2:B:260:HIS:CE1	2.21	0.58
9:I:126:THR:O	9:I:130:LEU:HG	2.03	0.58
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.85	0.57
31:9:107:C:O2'	31:9:108:C:H5'	2.04	0.57
2:B:98:THR:HG22	30:0:2820:A:OP1	2.04	0.57
30:0:952:G:N3	30:0:2302:A:H2'	2.19	0.57
30:0:2589:U:H2'	30:0:2590:U:C6	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2712:G:H5'	38:0:5232:HOH:O	2.03	0.57
30:0:2769:C:O2'	30:0:2770:G:H5'	2.04	0.57
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.20	0.57
30:0:420:U:H2'	30:0:421:C:C6	2.39	0.57
30:0:2756:U:H3	30:0:2896:A:H2	1.48	0.57
31:9:29:C:H2'	31:9:30:C:C5'	2.28	0.57
4:D:52:THR:HG21	30:0:2346:C:O2'	2.04	0.57
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.34	0.57
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.19	0.57
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.04	0.57
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.68	0.57
30:0:185:G:H4'	30:0:186:A:OP1	2.05	0.57
30:0:272:A:H5'	30:0:273:G:OP2	2.03	0.57
30:0:541:C:H2'	30:0:542:A:H5'	1.86	0.57
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.04	0.57
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.03	0.57
17:Q:27:GLN:HE21	31:9:8:G:H4'	1.70	0.57
30:0:280:C:H2'	30:0:281:U:O4'	2.04	0.57
30:0:559:U:H6	30:0:559:U:C5'	2.12	0.57
30:0:2135:A:O2'	30:0:2136:G:H5'	2.04	0.57
13:M:28:GLN:O	13:M:32:ARG:HG3	2.04	0.57
18:R:39:THR:HG23	18:R:107:GLU:O	2.04	0.57
30:0:10:U:O4	30:0:532:A:OP2	2.23	0.57
30:0:2604:A:H5'	38:0:5798:HOH:O	2.04	0.57
30:0:2787:C:H5	38:0:4643:HOH:O	1.86	0.57
1:A:36:ASP:O	1:A:38:ILE:N	2.38	0.57
12:L:4:LYS:HE2	30:0:645:U:OP2	2.05	0.57
30:0:1171:A:C2'	30:0:1172:G:H5'	2.35	0.57
30:0:1377:C:H5'	30:0:1377:C:C6	2.40	0.57
30:0:1942:A:H3'	38:0:7360:HOH:O	2.03	0.57
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.86	0.57
30:0:1016:U:H1'	38:0:3667:HOH:O	2.04	0.57
31:9:75:G:H1	31:9:106:U:H3	1.53	0.57
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.87	0.57
3:C:188:ARG:HD3	38:C:8559:HOH:O	2.04	0.57
30:0:1741:U:HO2'	30:0:2723:G:H4'	1.70	0.57
31:9:39:U:H1'	31:9:44:A:N6	2.19	0.57
2:B:264:GLU:HG2	2:B:267:LYS:CE	2.35	0.57
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.42	0.57
30:0:228:C:H2'	30:0:229:G:H5'	1.86	0.57
30:0:960:G:N3	30:0:960:G:H2'	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2005:G:H3'	30:0:2005:G:OP2	2.05	0.57
30:0:2488:A:H1'	38:0:9096:HOH:O	2.03	0.57
30:0:2559:C:H4'	38:0:7268:HOH:O	2.05	0.57
1:A:99:ILE:O	1:A:131:HIS:HE1	1.88	0.56
3:C:1:MET:HG2	3:C:2:GLN:N	2.19	0.56
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.35	0.56
30:0:711:G:H1'	38:0:7108:HOH:O	2.04	0.56
30:0:941:G:C5	30:0:942:U:C4	2.93	0.56
30:0:1304:U:H2'	30:0:1305:C:C6	2.40	0.56
30:0:1838:U:O2'	30:0:2644:C:H5'	2.05	0.56
30:0:2578:G:H5'	30:0:2578:G:C8	2.36	0.56
4:D:25:MET:CE	4:D:37:ALA:HB1	2.35	0.56
12:L:143:THR:HG22	12:L:144:ASP:N	2.20	0.56
29:3:70:ARG:HB3	38:3:9059:HOH:O	2.04	0.56
30:0:1632:A:C3'	30:0:1633:C:H5'	2.35	0.56
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.86	0.56
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.05	0.56
11:K:66:ARG:HH22	30:0:1994:A:P	2.29	0.56
30:0:1474:C:H6	30:0:1474:C:C5'	2.15	0.56
30:0:1947:G:N2	30:0:1966:U:C2	2.73	0.56
2:B:125:GLU:O	2:B:129:ARG:HG3	2.06	0.56
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.69	0.56
20:T:2:LYS:HG2	30:0:447:A:OP1	2.05	0.56
16:P:143:ALA:HA	38:P:192:HOH:O	2.04	0.56
27:1:42:SER:HB2	38:1:8956:HOH:O	2.05	0.56
30:0:31:C:H4'	38:0:7437:HOH:O	2.06	0.56
30:0:506:G:N2	30:0:509:A:H5'	2.18	0.56
30:0:1209:C:H2'	30:0:1210:G:H8	1.70	0.56
30:0:2032:U:H2'	30:0:2033:G:C5'	2.36	0.56
31:9:13:A:O2'	31:9:14:G:H5''	2.06	0.56
30:0:363:C:O2'	30:0:364:U:H5'	2.06	0.56
30:0:368:C:H2'	30:0:369:G:H5'	1.88	0.56
30:0:876:A:H2'	30:0:876:A:N3	2.21	0.56
1:A:199:HIS:HD2	1:A:201:PHE:H	1.54	0.56
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.71	0.56
27:1:16:HIS:HD2	30:0:470:U:O2'	1.88	0.56
1:A:153:ARG:HB2	1:A:153:ARG:HH11	1.70	0.55
9:I:120:ALA:O	9:I:124:VAL:HG23	2.06	0.55
30:0:119:A:H2'	30:0:120:A:H5''	1.87	0.55
30:0:1904:A:H2'	30:0:1905:U:O4'	2.05	0.55
30:0:1972:U:H2'	30:0:1973:A:H5''	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.69	0.55
10:J:107:ASN:HD22	10:J:109:TYR:H	1.54	0.55
25:Y:212:ARG:HD2	38:Y:8900:HOH:O	2.07	0.55
30:0:2064:U:H5'	30:0:2652:U:H4'	1.88	0.55
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.89	0.55
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.06	0.55
28:2:10:ARG:NH2	30:0:121:U:OP2	2.35	0.55
30:0:821:U:H3'	38:0:3780:HOH:O	2.07	0.55
4:D:159:PRO:O	4:D:163:VAL:HG23	2.05	0.55
30:0:2781:U:H2'	30:0:2782:G:C5'	2.36	0.55
14:N:132:ASN:HD22	30:0:2413:A:H4'	1.72	0.55
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.87	0.55
30:0:168:C:O5'	30:0:168:C:H6	1.89	0.55
30:0:396:U:O2'	30:0:418:C:H4'	2.07	0.55
30:0:407:A:H5'	38:0:6032:HOH:O	2.06	0.55
30:0:2254:G:H1'	38:0:5546:HOH:O	2.07	0.55
30:0:2840:A:H3'	38:0:7659:HOH:O	2.05	0.55
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.88	0.55
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.88	0.55
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.06	0.55
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.89	0.55
29:3:15:ASN:O	30:0:2408:A:H4'	2.06	0.55
30:0:660:A:H4'	30:0:661:G:O5'	2.07	0.55
30:0:711:G:C2	30:0:718:C:C2	2.95	0.55
30:0:1060:C:H6	30:0:1060:C:H5'	1.72	0.55
3:C:132:ASP:HB3	38:C:8560:HOH:O	2.06	0.55
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.89	0.55
30:0:1132:A:N6	30:0:1229:C:H2'	2.22	0.55
30:0:1596:U:H2'	30:0:1598:A:OP2	2.07	0.55
4:D:65:GLU:HA	38:D:6752:HOH:O	2.05	0.55
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.89	0.55
7:G:64:ASN:HD22	7:G:64:ASN:N	2.04	0.55
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.89	0.55
27:1:1:THR:HA	38:1:8958:HOH:O	2.06	0.55
30:0:2510:C:H5'	30:0:2511:A:OP2	2.07	0.55
31:9:24:U:H3'	31:9:25:G:C5'	2.37	0.55
31:9:55:U:H4'	31:9:56:A:C8	2.42	0.55
30:0:1538:C:O2'	30:0:1539:U:H5'	2.06	0.55
2:B:145:HIS:HD2	2:B:146:THR:O	1.90	0.55
7:G:23:ILE:O	7:G:27:ILE:HG13	2.06	0.55
13:M:95:LYS:HE2	30:0:157:G:H4'	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:4:TYR:CE1	18:R:17:MET:HE2	2.41	0.55
1:A:121:ALA:O	1:A:124:VAL:HG22	2.07	0.54
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.90	0.54
12:L:150:GLN:HB3	38:L:8869:HOH:O	2.06	0.54
30:0:2577:A:H8	38:0:9602:HOH:O	1.89	0.54
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.38	0.54
30:0:2083:A:H3'	38:0:7590:HOH:O	2.07	0.54
2:B:27:ASN:HD22	2:B:27:ASN:H	1.56	0.54
30:0:1154:A:H2'	30:0:1155:G:C8	2.42	0.54
30:0:1291:A:H2	38:0:5300:HOH:O	1.89	0.54
30:0:1523:G:C5	30:0:1524:U:C4	2.96	0.54
30:0:2878:U:H2'	30:0:2879:A:O4'	2.06	0.54
31:9:59:C:O5'	31:9:59:C:H6	1.90	0.54
26:Z:40:ALA:HA	30:0:1773:G:C8	2.42	0.54
30:0:292:G:H2'	30:0:358:G:N2	2.23	0.54
30:0:812:A:H1'	38:0:3969:HOH:O	2.06	0.54
30:0:1202:A:H2'	30:0:1203:G:O4'	2.07	0.54
30:0:2256:G:C2'	30:0:2257:G:C5'	2.84	0.54
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.38	0.54
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.89	0.54
31:9:52:A:O2'	31:9:53:G:H5'	2.08	0.54
3:C:154:VAL:O	3:C:158:GLU:HG3	2.07	0.54
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.22	0.54
30:0:241:A:C2	30:0:378:A:H4'	2.42	0.54
30:0:1477:C:H5'	30:0:1868:G:H5'	1.89	0.54
17:Q:27:GLN:HE21	31:9:8:G:C5'	2.20	0.54
30:0:282:C:H1'	30:0:368:C:H41	1.72	0.54
30:0:441:A:H1'	30:0:442:A:N7	2.23	0.54
30:0:1342:C:O2'	30:0:1343:C:H5'	2.07	0.54
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.08	0.54
12:L:73:VAL:HG21	12:L:116:HIS:CE1	2.42	0.54
14:N:154:LEU:C	14:N:156:GLU:H	2.14	0.54
25:Y:204:ARG:HH22	30:0:553:G:P	2.31	0.54
31:9:3:A:H2	31:9:21:G:N3	2.06	0.54
1:A:33:GLU:H	1:A:33:GLU:CD	2.15	0.54
3:C:218:VAL:HG12	38:C:8620:HOH:O	2.07	0.54
7:G:16:LYS:O	7:G:20:VAL:HG23	2.08	0.54
18:R:68:HIS:O	30:0:2842:G:H5'	2.08	0.54
1:A:112:PRO:HD3	1:A:152:CYS:SG	2.48	0.54
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.88	0.54
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:143:THR:HG22	12:L:144:ASP:H	1.71	0.54
19:S:33:SER:O	19:S:37:VAL:HG23	2.07	0.54
4:D:105:SER:OG	30:0:2338:G:H1'	2.07	0.53
18:R:132:ARG:HG2	18:R:133:ALA:N	2.23	0.53
3:C:236:THR:HA	38:C:8647:HOH:O	2.08	0.53
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.90	0.53
10:J:39:VAL:HG13	10:J:106:GLY:O	2.08	0.53
13:M:30:GLU:O	13:M:34:GLU:HG3	2.09	0.53
15:O:73:ASP:HA	15:O:92:VAL:O	2.08	0.53
18:R:150:PRO:CG	18:R:150:PRO:CB	2.86	0.53
30:0:2670:G:O2'	30:0:2671:U:H5'	2.07	0.53
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.91	0.53
30:0:1586:G:O2'	30:0:1587:U:H5'	2.08	0.53
30:0:1819:G:H2'	30:0:1820:G:C4'	2.39	0.53
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.23	0.53
30:0:136:C:H2'	30:0:137:U:O4'	2.08	0.53
30:0:488:U:H2'	38:0:4019:HOH:O	2.08	0.53
30:0:1373:G:H1'	38:0:6143:HOH:O	2.08	0.53
30:0:1919:A:H4'	38:0:4862:HOH:O	2.07	0.53
30:0:2064:U:H5'	30:0:2652:U:O3'	2.08	0.53
30:0:2842:G:H2'	30:0:2843:A:H5'	1.90	0.53
30:0:1339:G:C6	30:0:1340:G:N1	2.77	0.53
30:0:1592:G:H2'	30:0:1593:C:H6	1.72	0.53
14:N:144:GLY:O	14:N:147:ILE:HG23	2.08	0.53
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.91	0.53
30:0:1205:U:C2'	30:0:1206:U:C5'	2.76	0.53
30:0:1451:C:H5'	30:0:1505:U:C5	2.43	0.53
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.43	0.53
30:0:2502:C:H2'	30:0:2503:A:C5'	2.37	0.53
31:9:24:U:H3'	31:9:25:G:H5'	1.91	0.53
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.91	0.53
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.44	0.53
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.74	0.53
4:D:154:LYS:HD2	4:D:154:LYS:N	2.16	0.53
22:V:55:ARG:O	22:V:59:ILE:HG12	2.09	0.53
30:0:544:G:C3'	30:0:545:G:H5''	2.39	0.53
30:0:920:C:H5''	30:0:921:G:O5'	2.09	0.53
30:0:1135:G:H5'	38:0:5935:HOH:O	2.07	0.53
30:0:2250:G:H2'	30:0:2251:G:O4'	2.09	0.53
30:0:2769:C:H2'	30:0:2770:G:C5'	2.39	0.53
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.74	0.53
30:0:299:U:H5'	38:0:7349:HOH:O	2.08	0.53
30:0:510:U:H6	38:0:7450:HOH:O	1.92	0.53
30:0:635:A:H2'	30:0:636:G:H5''	1.90	0.53
9:I:108:HIS:H	9:I:109:PRO:HD2	1.74	0.53
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.57	0.53
23:W:154:ARG:NH1	30:0:588:G:O6	2.42	0.53
30:0:282:C:O2'	30:0:283:U:C5'	2.56	0.53
30:0:513:A:N3	38:0:3668:HOH:O	2.34	0.53
30:0:820:G:H3'	38:0:3058:HOH:O	2.08	0.53
30:0:1066:U:H2'	30:0:1067:A:C8	2.42	0.53
30:0:1166:A:P	30:0:1174:A:H4'	2.49	0.53
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.52
27:1:16:HIS:HE1	30:0:775:G:OP1	1.92	0.52
30:0:284:C:OP2	30:0:284:C:C6	2.62	0.52
30:0:958:G:H2'	30:0:959:C:C6	2.43	0.52
2:B:254:GLN:HG2	2:B:255:GLY:N	2.24	0.52
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.90	0.52
5:E:11:VAL:HG12	5:E:12:ASP:N	2.24	0.52
30:0:1819:G:H2'	30:0:1820:G:C5'	2.39	0.52
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.91	0.52
10:J:41:ALA:HB3	38:J:5907:HOH:O	2.09	0.52
23:W:23:MET:HE1	30:0:944:G:C8	2.44	0.52
25:Y:216:ARG:HD2	38:Y:8870:HOH:O	2.08	0.52
30:0:1787:C:H4'	30:0:2883:A:O4'	2.09	0.52
30:0:2356:A:H5'	38:0:5644:HOH:O	2.09	0.52
31:9:91:C:H2'	31:9:92:G:O4'	2.09	0.52
5:E:6:GLU:HG2	5:E:46:THR:HG22	1.92	0.52
14:N:5:ARG:NH1	30:0:1010:C:OP1	2.42	0.52
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.09	0.52
30:0:255:A:H2'	30:0:256:C:C6	2.45	0.52
30:0:920:C:H4'	30:0:921:G:C2	2.44	0.52
30:0:1268:C:O2'	30:0:1269:G:H5'	2.08	0.52
2:B:36:PRO:HG3	2:B:169:GLY:H	1.75	0.52
13:M:158:ARG:HB2	13:M:163:LEU:HB2	1.91	0.52
15:O:32:ARG:O	15:O:32:ARG:HD3	2.09	0.52
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.44	0.52
30:0:1181:A:N1	30:0:1192:A:O2'	2.43	0.52
30:0:1515:A:H2'	30:0:1516:U:C6	2.44	0.52
30:0:1624:A:H5'	30:0:1626:A:O4'	2.09	0.52
30:0:2263:G:H1'	38:0:6631:HOH:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2291:A:N9	30:0:2309:C:H5'	2.25	0.52
30:0:2478:U:O2'	30:0:2479:A:H5'	2.09	0.52
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.91	0.52
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.91	0.52
30:0:120:A:H2'	30:0:120:A:N3	2.25	0.52
30:0:1314:U:H2'	38:0:5880:HOH:O	2.09	0.52
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.92	0.52
30:0:1342:C:H2'	30:0:1343:C:H5'	1.92	0.52
30:0:2103:A:H2'	30:0:2104:C:H5'	1.92	0.52
30:0:2445:U:H2'	30:0:2446:G:H8	1.75	0.52
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.10	0.52
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.44	0.52
30:0:1679:C:H5'	38:0:9331:HOH:O	2.10	0.52
30:0:1972:U:C2'	30:0:1973:A:H5''	2.39	0.52
30:0:2359:G:H3'	38:0:5698:HOH:O	2.10	0.52
30:0:2756:U:N3	30:0:2896:A:H2	2.08	0.52
31:9:45:A:H2'	31:9:46:C:H6	1.75	0.52
6:F:21:GLU:O	6:F:24:ARG:HG2	2.09	0.52
17:Q:19:ARG:HH21	31:9:11:A:P	2.33	0.52
22:V:64:GLY:O	22:V:65:ASP:HB2	2.09	0.52
30:0:694:A:H2'	30:0:695:C:H5'	1.90	0.52
30:0:1170:U:H2'	30:0:1172:G:OP2	2.09	0.52
30:0:1730:G:C5'	30:0:1731:C:C5	2.93	0.52
30:0:2326:C:H4'	30:0:2412:G:H4'	1.92	0.52
30:0:2756:U:N3	30:0:2896:A:C2	2.74	0.52
30:0:2769:C:H2'	30:0:2770:G:O4'	2.09	0.52
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.91	0.52
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.91	0.52
3:C:43:LYS:HG2	30:0:449:A:N7	2.25	0.52
30:0:567:U:H5''	38:0:6408:HOH:O	2.08	0.52
30:0:2764:C:O2'	30:0:2765:C:H5'	2.09	0.52
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.10	0.51
13:M:188:ARG:NH1	30:0:154:C:H3'	2.24	0.51
14:N:37:ARG:HD3	33:N:8807:CL:CL	2.47	0.51
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.40	0.51
30:0:497:A:H2'	30:0:498:A:C5'	2.40	0.51
30:0:541:C:O2'	30:0:542:A:H5''	2.10	0.51
30:0:613:C:H2'	30:0:614:U:H6	1.74	0.51
30:0:619:U:H3'	38:0:3289:HOH:O	2.09	0.51
30:0:1477:C:O2'	30:0:1478:U:H5'	2.10	0.51
30:0:2105:C:H2'	30:0:2106:C:C6	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2524:G:H21	30:0:2526:C:N4	2.08	0.51
13:M:188:ARG:HD3	30:0:155:C:OP2	2.09	0.51
16:P:115:SER:OG	16:P:118:GLN:HG3	2.10	0.51
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.40	0.51
30:0:65:C:O2'	30:0:66:G:H5'	2.10	0.51
30:0:2269:C:C2'	30:0:2270:G:H5'	2.40	0.51
30:0:2768:A:H3'	30:0:2768:A:N3	2.25	0.51
31:9:2:U:C4'	38:9:9104:HOH:O	2.57	0.51
12:L:61:ALA:HB2	12:L:105:TYR:CE2	2.45	0.51
13:M:179:GLY:O	30:0:399:C:H5'	2.10	0.51
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.91	0.51
18:R:23:MET:HE3	18:R:28:SER:OG	2.10	0.51
30:0:506:G:H22	30:0:509:A:H5''	1.73	0.51
30:0:812:A:H2'	30:0:813:C:C6	2.45	0.51
30:0:1131:G:C6	30:0:1230:A:C4	2.99	0.51
30:0:1592:G:H2'	30:0:1593:C:C6	2.45	0.51
30:0:1878:G:C1'	38:0:6126:HOH:O	2.44	0.51
3:C:153:VAL:O	3:C:157:LEU:HG	2.10	0.51
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.26	0.51
19:S:11:THR:H	19:S:14:ALA:HB3	1.75	0.51
26:Z:57:MET:HE3	38:0:6288:HOH:O	2.09	0.51
30:0:447:A:O2'	30:0:448:G:H5'	2.11	0.51
30:0:1029:U:O2'	30:0:1273:C:OP1	2.25	0.51
30:0:1447:U:H3'	30:0:1506:U:O2	2.11	0.51
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.76	0.51
30:0:256:C:H2'	30:0:257:G:O4'	2.10	0.51
30:0:445:U:H2'	30:0:446:G:H8	1.75	0.51
30:0:512:G:O3'	30:0:513:A:H8	1.92	0.51
30:0:1080:C:O5'	30:0:1080:C:H6	1.94	0.51
30:0:1730:G:H5'	30:0:1731:C:H5	1.74	0.51
30:0:2445:U:H2'	30:0:2446:G:C8	2.46	0.51
30:0:2717:C:C2'	30:0:2718:C:C5'	2.75	0.51
31:9:12:C:H5'	31:9:70:U:O4'	2.11	0.51
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.93	0.51
12:L:14:GLY:O	30:0:1295:G:H5''	2.10	0.51
12:L:149:ARG:O	12:L:150:GLN:HB2	2.10	0.51
23:W:125:HIS:CD2	23:W:127:GLY:H	2.29	0.51
30:0:228:C:C2'	30:0:229:G:H5'	2.41	0.51
30:0:318:U:H5'	30:0:339:A:C2	2.46	0.51
30:0:690:G:H4'	30:0:741:C:O2	2.11	0.51
30:0:1535:G:H2'	30:0:1536:C:C6	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.91	0.51
23:W:139:GLY:O	23:W:141:HIS:CD2	2.64	0.51
30:0:545:G:H8	30:0:545:G:C5'	2.06	0.51
30:0:1015:C:H2'	30:0:1016:U:H6	1.75	0.51
30:0:1422:U:H2'	30:0:1423:C:C6	2.45	0.51
30:0:1973:A:H2'	30:0:1974:G:O4'	2.10	0.51
30:0:2401:A:H2'	30:0:2402:A:C8	2.46	0.51
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.11	0.51
6:F:101:ALA:HA	38:F:5413:HOH:O	2.10	0.51
28:2:35:ARG:HB2	38:2:2691:HOH:O	2.09	0.51
30:0:968:G:C2	30:0:1001:U:O2	2.63	0.51
31:9:1:U:O3'	31:9:3:A:C5'	2.58	0.51
2:B:85:ARG:NH1	38:B:9095:HOH:O	2.44	0.51
16:P:1:THR:O	30:0:1396:C:H1'	2.11	0.51
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.93	0.51
27:1:25:LYS:HD2	28:2:49:GLU:N	2.23	0.51
30:0:483:C:C4	30:0:484:A:C6	2.99	0.51
30:0:1160:G:H5''	30:0:1161:A:H5'	1.84	0.51
30:0:1183:C:C2	30:0:1184:C:C5	2.99	0.51
30:0:2326:C:H4'	30:0:2412:G:C4'	2.41	0.51
3:C:95:GLU:HG3	38:C:8672:HOH:O	2.12	0.50
14:N:4:PRO:HG3	31:9:69:U:OP1	2.11	0.50
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.92	0.50
30:0:101:C:H2'	30:0:102:A:H8	1.76	0.50
30:0:407:A:H3'	38:0:4473:HOH:O	2.10	0.50
30:0:1139:U:H2'	30:0:1140:C:C6	2.46	0.50
30:0:1268:C:H2'	30:0:1269:G:H8	1.76	0.50
30:0:2754:G:H2'	30:0:2755:G:O4'	2.11	0.50
1:A:51:ARG:NH1	1:A:120:ARG:O	2.44	0.50
3:C:236:THR:HG22	3:C:239:ALA:N	2.20	0.50
8:H:69:ARG:HD3	38:H:229:HOH:O	2.11	0.50
9:I:95:LEU:HD22	9:I:99:GLN:HB3	1.93	0.50
30:0:951:A:C2'	30:0:952:G:H5'	2.41	0.50
30:0:1193:A:C2	30:0:1194:A:N6	2.79	0.50
30:0:1739:G:O2'	30:0:1740:U:H5'	2.11	0.50
2:B:214:PRO:HD2	38:B:8990:HOH:O	2.11	0.50
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.93	0.50
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.08	0.50
27:1:2:GLY:O	27:1:6:PRO:HG2	2.11	0.50
30:0:899:C:H5'	38:0:3209:HOH:O	2.12	0.50
30:0:1160:G:H5'	30:0:1161:A:C4'	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1878:G:O2'	30:0:1879:U:H6	1.95	0.50
31:9:76:G:H3'	31:9:77:A:C5'	2.24	0.50
2:B:305:ASP:O	2:B:306:LYS:HB2	2.12	0.50
12:L:143:THR:HG21	38:L:8838:HOH:O	2.10	0.50
29:3:29:ARG:NH2	30:0:1925:G:H5'	2.26	0.50
30:0:185:G:H4'	30:0:186:A:H4'	1.93	0.50
30:0:271:C:C2	30:0:273:G:O4'	2.64	0.50
30:0:700:A:H5''	30:0:701:U:H5'	1.93	0.50
30:0:737:A:H2'	30:0:738:G:O4'	2.10	0.50
30:0:960:G:N3	30:0:960:G:C3'	2.74	0.50
30:0:1118:A:H8	30:0:1119:G:H5''	1.75	0.50
30:0:1183:C:O2	30:0:1183:C:C2'	2.60	0.50
30:0:1878:G:O2'	30:0:1879:U:P	2.70	0.50
30:0:2269:C:H2'	30:0:2270:G:H5'	1.93	0.50
2:B:217:ARG:CG	2:B:257:THR:HG22	2.38	0.50
2:B:310:ARG:HB3	38:B:9109:HOH:O	2.11	0.50
3:C:214:THR:HG23	38:C:8633:HOH:O	2.11	0.50
8:H:170:ARG:HD2	38:H:190:HOH:O	2.11	0.50
12:L:27:ARG:HH21	12:L:30:ARG:HG2	1.77	0.50
14:N:37:ARG:NH1	31:9:6:C:OP1	2.44	0.50
20:T:54:ASP:OD2	30:0:316:A:H5'	2.11	0.50
30:0:661:G:C5	30:0:686:A:C2	3.00	0.50
30:0:1289:C:O2'	30:0:1290:G:H5'	2.12	0.50
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.93	0.50
7:G:20:VAL:O	7:G:24:VAL:HG23	2.12	0.50
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.45	0.50
19:S:77:VAL:O	19:S:80:ARG:HG2	2.12	0.50
30:0:440:C:H2'	30:0:441:A:C8	2.47	0.50
30:0:947:U:H2'	30:0:948:G:C8	2.47	0.50
30:0:1181:A:H2'	30:0:1182:C:H5'	1.94	0.50
30:0:1244:U:H4'	30:0:1246:A:O4'	2.11	0.50
30:0:2276:U:H2'	30:0:2277:U:C6	2.46	0.50
31:9:5:G:O2'	31:9:6:C:H5'	2.11	0.50
31:9:95:C:O2'	31:9:96:C:H5'	2.12	0.50
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.42	0.50
18:R:33:ARG:NH1	38:R:8950:HOH:O	2.45	0.50
20:T:28:SER:O	20:T:32:ARG:HG3	2.11	0.50
30:0:137:U:OP1	30:0:259:G:O2'	2.30	0.50
30:0:1166:A:C6	30:0:1181:A:C2	2.99	0.50
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.50
2:B:275:GLY:O	2:B:291:ASP:HA	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.92	0.50
30:0:1056:U:H2'	30:0:1057:A:O4'	2.12	0.50
30:0:2511:A:H4'	38:0:5478:HOH:O	2.12	0.50
4:D:48:MET:HE2	31:9:41:C:C5'	2.41	0.50
15:O:37:ARG:HD2	30:0:656:G:OP2	2.12	0.50
23:W:80:ASP:O	23:W:84:VAL:HG23	2.10	0.50
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.77	0.50
30:0:182:G:H5''	38:0:3733:HOH:O	2.12	0.50
30:0:541:C:C2'	30:0:542:A:C5'	2.78	0.50
30:0:816:G:C6	30:0:817:G:N1	2.80	0.50
30:0:877:G:C5'	30:0:878:G:OP1	2.57	0.50
30:0:1185:U:H2'	30:0:1186:C:H6	1.77	0.50
30:0:2010:A:C2'	38:0:5965:HOH:O	2.55	0.50
14:N:110:THR:HB	14:N:113:SER:OG	2.12	0.49
30:0:1211:G:H2'	30:0:1212:C:H6	1.77	0.49
30:0:1743:G:N7	38:0:9265:HOH:O	2.35	0.49
2:B:212:GLN:HA	30:0:1733:A:H4'	1.93	0.49
30:0:364:U:H2'	30:0:365:G:O4'	2.12	0.49
30:0:509:A:H2'	38:0:7099:HOH:O	2.11	0.49
30:0:1588:G:C6	30:0:1589:G:N1	2.81	0.49
30:0:1657:A:H2'	30:0:1658:A:C8	2.47	0.49
30:0:1972:U:H2'	30:0:1973:A:H5'	1.93	0.49
30:0:2414:A:H2'	30:0:2415:A:C8	2.47	0.49
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.93	0.49
22:V:1:THR:CB	30:0:93:C:H5''	2.40	0.49
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.11	0.49
28:2:38:LYS:HE3	38:0:4239:HOH:O	2.12	0.49
30:0:2851:G:C2'	30:0:2852:A:H5'	2.43	0.49
31:9:59:C:H2'	31:9:60:C:C6	2.47	0.49
2:B:41:PHE:HB3	2:B:190:MET:CE	2.43	0.49
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.93	0.49
5:E:133:VAL:HG12	5:E:141:VAL:HG13	1.94	0.49
20:T:5:ASP:O	20:T:9:LYS:HB2	2.13	0.49
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.95	0.49
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.93	0.49
30:0:1625:U:H6	30:0:1625:U:H3'	1.75	0.49
30:0:1856:C:H5'	30:0:1858:A:O4'	2.12	0.49
30:0:1903:U:O2'	30:0:1904:A:N7	2.42	0.49
11:K:27:ARG:HD2	38:K:3442:HOH:O	2.11	0.49
11:K:63:GLU:HG2	38:K:6344:HOH:O	2.11	0.49
18:R:40:ALA:O	18:R:44:VAL:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:669:G:O2'	30:0:670:G:H5'	2.12	0.49
30:0:1762:C:H2'	30:0:1763:C:H6	1.77	0.49
30:0:1790:C:H2'	30:0:1791:U:H6	1.76	0.49
30:0:1838:U:H3'	38:0:5533:HOH:O	2.12	0.49
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.95	0.49
30:0:407:A:H2'	30:0:408:A:C8	2.48	0.49
30:0:1503:U:H2'	30:0:1504:A:O4'	2.11	0.49
30:0:1545:C:H2'	30:0:1546:G:O4'	2.12	0.49
30:0:1940:C:H4'	38:0:7360:HOH:O	2.12	0.49
30:0:2493:C:O2	30:0:2493:C:H2'	2.11	0.49
30:0:2709:G:N2	38:0:7632:HOH:O	2.46	0.49
2:B:238:ASN:HD22	2:B:240:GLY:N	2.02	0.49
14:N:169:PRO:O	14:N:172:PHE:HB3	2.13	0.49
30:0:876:A:N3	30:0:876:A:C2'	2.76	0.49
30:0:2271:G:N3	30:0:2271:G:H2'	2.27	0.49
30:0:2345:A:H3'	30:0:2346:C:C6	2.47	0.49
30:0:2435:U:H1'	38:0:5440:HOH:O	2.13	0.49
3:C:78:ARG:HH11	3:C:78:ARG:HG3	1.78	0.49
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.27	0.49
30:0:702:G:O2'	30:0:703:G:H5'	2.13	0.49
30:0:734:U:O2'	30:0:736:A:N7	2.39	0.49
30:0:1391:G:H2'	30:0:1392:A:H5'	1.95	0.49
31:9:3:A:C2	31:9:21:G:N3	2.81	0.49
31:9:3:A:N6	31:9:22:G:H1'	2.28	0.49
1:A:186:TRP:CG	1:A:187:PRO:HA	2.48	0.49
2:B:244:PRO:HB3	30:0:1234:U:N3	2.27	0.49
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.94	0.49
8:H:30:LYS:H	8:H:62:HIS:CD2	2.30	0.49
15:O:25:VAL:HG12	30:0:709:G:O2'	2.11	0.49
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.49
30:0:951:A:O2'	30:0:952:G:H5'	2.13	0.49
30:0:1149:U:H5''	30:0:1151:G:O4'	2.13	0.49
30:0:2649:A:H5'	30:0:2649:A:H8	1.77	0.49
30:0:2880:A:H2'	30:0:2881:C:H5'	1.95	0.49
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.94	0.49
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.95	0.49
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.23	0.49
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.12	0.49
30:0:297:U:H2'	30:0:298:C:C6	2.48	0.49
30:0:815:U:O2'	30:0:1598:A:H4'	2.12	0.49
30:0:2387:U:H2'	30:0:2388:C:C6	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2802:C:H2'	30:0:2803:C:C6	2.46	0.49
30:0:2908:A:O5'	30:0:2908:A:H8	1.94	0.49
24:X:85:VAL:HG12	24:X:86:GLU:N	2.28	0.48
30:0:1118:A:C8	30:0:1119:G:H5''	2.47	0.48
30:0:2353:A:H4'	30:0:2354:A:O5'	2.13	0.48
31:9:56:A:C3'	31:9:57:A:H5''	2.43	0.48
31:9:63:C:O2'	31:9:64:C:H5'	2.13	0.48
4:D:62:ASP:HA	38:D:4233:HOH:O	2.14	0.48
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.95	0.48
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.95	0.48
30:0:1159:G:H1	30:0:1208:C:H42	1.61	0.48
30:0:2335:C:H2'	30:0:2336:G:C8	2.48	0.48
30:0:2420:G:H2'	30:0:2421:G:C8	2.48	0.48
30:0:2697:A:H2'	30:0:2698:G:O4'	2.13	0.48
31:9:2:U:P	31:9:3:A:H5'	2.53	0.48
9:I:78:ALA:HB1	9:I:93:ALA:HB1	1.95	0.48
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.28	0.48
23:W:38:THR:O	23:W:42:ARG:HB2	2.13	0.48
30:0:1181:A:C2'	30:0:1182:C:H5'	2.43	0.48
30:0:1477:C:H5'	30:0:1868:G:H5''	1.94	0.48
30:0:2781:U:O2'	30:0:2782:G:H5'	2.13	0.48
17:Q:1:PRO:HA	30:0:2299:G:O6	2.13	0.48
17:Q:50:GLY:HA2	38:0:6033:HOH:O	2.12	0.48
22:V:12:THR:HG22	22:V:15:GLU:CG	2.39	0.48
30:0:947:U:H2'	30:0:948:G:H8	1.78	0.48
30:0:1119:G:N2	30:0:1246:A:N1	2.61	0.48
30:0:1419:U:H2'	30:0:1685:A:C2	2.48	0.48
2:B:18:ARG:HE	2:B:256:GLN:NE2	2.11	0.48
4:D:170:TYR:CD1	4:D:170:TYR:N	2.81	0.48
8:H:34:HIS:HD2	8:H:90:LEU:O	1.96	0.48
9:I:87:PRO:HB3	38:I:6825:HOH:O	2.13	0.48
10:J:130:VAL:HG12	10:J:131:THR:N	2.28	0.48
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.95	0.48
23:W:90:TYR:N	23:W:90:TYR:CD1	2.80	0.48
30:0:1221:G:C8	38:0:5995:HOH:O	2.55	0.48
30:0:1523:G:H2'	30:0:1524:U:C6	2.48	0.48
30:0:2134:G:C6	30:0:2258:A:C8	3.02	0.48
30:0:2419:U:H5''	30:0:2420:G:C5'	2.42	0.48
30:0:2825:C:H4'	30:0:2826:G:O5'	2.13	0.48
30:0:2842:G:C2'	30:0:2843:A:H5'	2.43	0.48
2:B:17:LYS:O	2:B:260:HIS:HD2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:ARG:HD3	38:0:3517:HOH:O	2.14	0.48
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.39	0.48
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.95	0.48
30:0:482:G:H4'	30:0:508:A:N1	2.29	0.48
30:0:1206:U:C5'	30:0:1206:U:H6	2.18	0.48
30:0:1513:C:O2'	30:0:1514:C:H5'	2.13	0.48
13:M:167:GLY:O	13:M:171:ARG:HG3	2.13	0.48
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.95	0.48
20:T:68:ASP:HB2	38:0:5667:HOH:O	2.12	0.48
30:0:2335:C:H2'	30:0:2336:G:H8	1.77	0.48
30:0:2896:A:N3	30:0:2896:A:H2'	2.29	0.48
1:A:36:ASP:HA	1:A:83:GLY:HA3	1.96	0.48
7:G:19:GLU:O	7:G:23:ILE:HG13	2.14	0.48
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.78	0.48
10:J:74:ARG:HH11	10:J:74:ARG:CB	2.25	0.48
16:P:13:VAL:HG21	16:P:41:ARG:HG2	1.96	0.48
19:S:57:THR:C	19:S:59:ASP:H	2.22	0.48
30:0:535:G:C6	30:0:2064:U:C5	3.01	0.48
30:0:2001:G:O2'	30:0:2002:C:H5'	2.13	0.48
30:0:2598:U:O2	30:0:2600:A:H8	1.97	0.48
6:F:91:VAL:CG1	6:F:92:GLY:H	2.25	0.48
13:M:164:THR:HG23	13:M:165:GLY:N	2.29	0.48
29:3:91:GLN:O	29:3:92:GLU:HB2	2.14	0.48
30:0:130:C:H2'	38:0:3167:HOH:O	2.14	0.48
30:0:2415:A:H2'	30:0:2416:G:H5'	1.96	0.48
30:0:2506:A:N6	30:0:2511:A:O2'	2.46	0.48
30:0:2587:OMU:H5	38:0:7497:HOH:O	2.12	0.48
30:0:2649:A:H5'	30:0:2649:A:C8	2.49	0.48
2:B:14:GLY:HA2	2:B:15:PRO:C	2.39	0.48
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.73	0.48
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.78	0.48
13:M:163:LEU:HD21	30:0:188:C:H5''	1.96	0.48
14:N:119:GLN:O	14:N:123:ILE:HG13	2.14	0.48
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.96	0.48
23:W:23:MET:O	30:0:1025:C:H5'	2.14	0.48
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.95	0.48
30:0:834:G:H4'	30:0:835:U:OP2	2.13	0.48
30:0:1562:C:O2	30:0:1562:C:C2'	2.62	0.48
1:A:212:PRO:HA	30:0:1943:C:O4'	2.14	0.47
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.95	0.47
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:22:ARG:HG2	38:0:9996:HOH:O	2.14	0.47
14:N:11:ARG:NH1	31:9:8:G:O6	2.47	0.47
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.95	0.47
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.96	0.47
23:W:4:LEU:HD22	23:W:52:VAL:CG2	2.44	0.47
25:Y:210:GLY:N	30:0:1313:A:H5''	2.29	0.47
30:0:821:U:H2'	30:0:822:C:H6	1.79	0.47
30:0:1130:U:H2'	30:0:1131:G:O4'	2.13	0.47
30:0:1209:C:O2'	30:0:1210:G:H5'	2.13	0.47
30:0:1947:G:N2	30:0:1966:U:N3	2.61	0.47
2:B:5:ARG:HD2	2:B:8:LYS:NZ	2.30	0.47
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.49	0.47
3:C:246:ARG:NE	38:C:8620:HOH:O	2.40	0.47
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.14	0.47
18:R:114:VAL:HA	18:R:144:GLU:O	2.14	0.47
23:W:119:HIS:HE1	38:0:9557:HOH:O	1.97	0.47
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.14	0.47
30:0:407:A:H8	38:0:4473:HOH:O	1.98	0.47
30:0:523:C:H2'	30:0:524:A:C8	2.50	0.47
30:0:1161:A:O5'	30:0:1161:A:H8	1.96	0.47
30:0:2334:C:O2'	30:0:2335:C:H5'	2.14	0.47
1:A:33:GLU:O	1:A:34:ASP:HB2	2.14	0.47
3:C:22:PHE:HA	3:C:116:ALA:HA	1.96	0.47
3:C:233:THR:HG22	3:C:234:VAL:N	2.29	0.47
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.11	0.47
5:E:21:THR:HG23	5:E:30:THR:OG1	2.14	0.47
6:F:58:GLU:HA	6:F:61:MET:HE2	1.96	0.47
13:M:47:ASP:CG	13:M:48:LYS:N	2.72	0.47
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.39	0.47
30:0:567:U:C5'	38:0:6408:HOH:O	2.63	0.47
30:0:823:U:H3'	38:0:4459:HOH:O	2.14	0.47
30:0:920:C:H5'	30:0:921:G:C4	2.49	0.47
30:0:1762:C:H2'	30:0:1763:C:C6	2.50	0.47
30:0:1768:C:H2'	30:0:1769:C:O4'	2.14	0.47
30:0:2112:A:H2'	30:0:2113:G:C8	2.49	0.47
30:0:2589:U:H2'	30:0:2590:U:H6	1.77	0.47
31:9:47:A:C2	31:9:48:C:C2	3.02	0.47
3:C:136:VAL:HG22	3:C:137:PRO:HA	1.97	0.47
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.48	0.47
30:0:1343:C:H2'	30:0:1344:G:O5'	2.15	0.47
30:0:2420:G:H2'	30:0:2421:G:H8	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:114:G:H2'	31:9:115:C:H6	1.78	0.47
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.80	0.47
1:A:171:LYS:HB2	30:0:820:G:C6	2.50	0.47
8:H:66:GLU:HA	38:H:229:HOH:O	2.13	0.47
10:J:90:LYS:HB2	33:J:8802:CL:CL	2.52	0.47
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.49	0.47
14:N:132:ASN:O	14:N:135:VAL:HG12	2.15	0.47
14:N:164:ASP:CG	14:N:167:ASP:HA	2.39	0.47
23:W:52:VAL:HG22	23:W:53:ALA:H	1.80	0.47
23:W:115:THR:HG23	38:W:5420:HOH:O	2.15	0.47
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.47
30:0:523:C:H2'	30:0:524:A:H8	1.80	0.47
30:0:1450:C:H5''	38:0:9621:HOH:O	2.15	0.47
30:0:1589:G:N2	30:0:1605:G:H1'	2.29	0.47
30:0:1615:A:H5'	38:0:4194:HOH:O	2.14	0.47
30:0:2587:OMU:O5'	30:0:2587:OMU:H6	2.14	0.47
1:A:8:ARG:HG2	38:A:9016:HOH:O	2.14	0.47
10:J:131:THR:HB	10:J:134:GLU:HG3	1.96	0.47
23:W:125:HIS:HD2	23:W:127:GLY:H	1.62	0.47
29:3:3:MET:O	29:3:90:PHE:HA	2.15	0.47
30:0:101:C:H2'	30:0:102:A:C8	2.50	0.47
30:0:222:A:H2'	30:0:223:G:O4'	2.14	0.47
30:0:308:U:C4	30:0:342:C:H1'	2.49	0.47
30:0:312:U:C2	30:0:320:G:N2	2.83	0.47
30:0:2526:C:C6	30:0:2526:C:C5'	2.95	0.47
30:0:2637:A:C5'	38:0:4941:HOH:O	2.62	0.47
30:0:2691:A:H5'	30:0:2693:U:H1'	1.96	0.47
6:F:91:VAL:HG11	30:0:262:A:OP2	2.14	0.47
8:H:54:VAL:HG13	8:H:162:PRO:HG3	1.97	0.47
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.80	0.47
30:0:251:C:H2'	30:0:252:C:H6	1.80	0.47
30:0:304:G:H1'	30:0:347:A:N6	2.29	0.47
30:0:625:U:H5''	30:0:1044:C:N4	2.30	0.47
30:0:1682:A:H5''	38:0:9463:HOH:O	2.14	0.47
30:0:2241:C:O2'	30:0:2242:U:H5'	2.15	0.47
30:0:2269:C:H2'	30:0:2270:G:C5'	2.45	0.47
30:0:2506:A:O2'	30:0:2507:G:C8	2.50	0.47
31:9:1:U:C4'	31:9:3:A:OP1	2.62	0.47
2:B:132:HIS:NE2	2:B:171:VAL:HG23	2.28	0.47
30:0:545:G:C8	30:0:545:G:C5'	2.88	0.47
30:0:629:A:C2	30:0:2074:A:C2	3.03	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:685:C:O2	30:0:748:C:H4'	2.15	0.47
30:0:1165:G:H4'	30:0:1174:A:O2'	2.15	0.47
30:0:1632:A:H2'	30:0:1633:C:C5'	2.39	0.47
30:0:1667:A:H2'	30:0:1668:U:C6	2.50	0.47
30:0:2000:G:O2'	30:0:2001:G:H5'	2.15	0.47
31:9:42:C:H5'	31:9:43:G:OP2	2.15	0.47
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.30	0.47
10:J:36:VAL:HG12	10:J:37:ALA:N	2.30	0.47
10:J:42:GLU:O	10:J:131:THR:HG23	2.15	0.47
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.96	0.47
13:M:9:ARG:HD2	30:0:380:A:OP2	2.15	0.47
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.30	0.47
30:0:264:G:H1'	30:0:265:U:H5	1.80	0.47
30:0:295:C:H2'	30:0:296:G:O4'	2.15	0.47
30:0:638:C:H2'	30:0:639:A:C8	2.50	0.47
30:0:1167:G:H2'	30:0:1168:C:O4'	2.15	0.47
30:0:2073:G:OP2	30:0:2490:A:H5'	2.15	0.47
4:D:141:VAL:HG21	31:9:57:A:H8	1.80	0.46
10:J:19:MET:HE1	10:J:78:ILE:HG22	1.96	0.46
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.97	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.14	0.46
30:0:677:C:O2'	30:0:678:G:H5'	2.15	0.46
30:0:1321:A:H2'	30:0:1322:G:C8	2.50	0.46
31:9:3:A:OP2	31:9:25:G:N2	2.47	0.46
31:9:7:G:H5'	38:9:9100:HOH:O	2.16	0.46
1:A:53:ALA:HB3	38:A:9066:HOH:O	2.15	0.46
2:B:298:LYS:HG2	38:0:5531:HOH:O	2.15	0.46
11:K:41:LYS:O	11:K:42:ASN:HB2	2.15	0.46
17:Q:75:ILE:HB	38:Q:6286:HOH:O	2.15	0.46
23:W:119:HIS:HD2	23:W:120:PRO:O	1.98	0.46
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.51	0.46
25:Y:210:GLY:H	30:0:1313:A:H5''	1.80	0.46
30:0:853:C:H2'	30:0:854:G:O4'	2.15	0.46
30:0:1180:U:O2'	30:0:1181:A:H5'	2.15	0.46
30:0:1477:C:C5'	30:0:1868:G:H5''	2.45	0.46
30:0:1805:G:H2'	30:0:1806:G:H8	1.79	0.46
30:0:2566:A:C2	30:0:2696:G:O4'	2.68	0.46
31:9:45:A:C5	31:9:46:C:C5	3.02	0.46
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.97	0.46
8:H:5:PRO:HD2	8:H:8:MET:SD	2.55	0.46
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.95	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.41	0.46
14:N:17:ARG:HB3	14:N:17:ARG:HH11	1.80	0.46
29:3:38:ARG:HB3	29:3:42:ARG:HH12	1.81	0.46
30:0:255:A:C5	30:0:256:C:C5	3.02	0.46
30:0:319:A:H4'	30:0:338:C:C4	2.50	0.46
1:A:204:GLY:N	30:0:2634:G:OP2	2.47	0.46
3:C:19:PRO:HG2	3:C:22:PHE:CD1	2.51	0.46
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.47	0.46
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.97	0.46
17:Q:27:GLN:HE21	31:9:8:G:H5''	1.80	0.46
20:T:26:THR:HA	20:T:39:ASN:HB3	1.97	0.46
29:3:29:ARG:NH2	30:0:1925:G:C5'	2.79	0.46
30:0:800:G:H2'	30:0:801:U:C6	2.50	0.46
30:0:1139:U:H2'	30:0:1140:C:H6	1.80	0.46
30:0:1925:G:O2'	30:0:1926:G:H5'	2.16	0.46
30:0:2249:G:C2	30:0:2253:G:C6	3.04	0.46
30:0:2250:G:C2	30:0:2251:G:H1'	2.51	0.46
30:0:2831:C:C2'	30:0:2832:C:H5'	2.45	0.46
31:9:65:A:N6	31:9:112:U:C6	2.83	0.46
3:C:206:ASN:HB2	30:0:329:A:OP2	2.16	0.46
8:H:31:ILE:HG23	38:H:229:HOH:O	2.15	0.46
9:I:107:LYS:HB3	9:I:110:ASP:HB2	1.97	0.46
12:L:6:ARG:HD3	30:0:1299:G:O6	2.15	0.46
30:0:369:G:H2'	30:0:370:G:H8	1.81	0.46
30:0:1393:A:H2'	30:0:1394:C:C6	2.51	0.46
30:0:2869:G:H2'	30:0:2870:C:C6	2.50	0.46
31:9:55:U:H4'	31:9:56:A:H8	1.80	0.46
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.75	0.46
6:F:96:ALA:HA	38:F:3111:HOH:O	2.15	0.46
13:M:27:ARG:HH12	13:M:44:THR:CG2	2.28	0.46
16:P:120:ARG:NH1	30:0:1594:C:C5	2.84	0.46
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.15	0.46
30:0:158:A:H3'	38:0:7573:HOH:O	2.15	0.46
30:0:255:A:C4	30:0:256:C:C6	3.04	0.46
30:0:365:G:C6	30:0:366:U:C4	3.04	0.46
30:0:622:G:O2'	30:0:623:U:H5'	2.15	0.46
30:0:736:A:H2'	30:0:737:A:O4'	2.16	0.46
30:0:1211:G:H2'	30:0:1212:C:C6	2.50	0.46
30:0:1641:A:H2'	30:0:1642:A:C5'	2.44	0.46
30:0:1942:A:H4'	38:0:9046:HOH:O	2.16	0.46
30:0:2826:G:C6	30:0:2913:A:N6	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:25:MET:HE1	4:D:37:ALA:HB1	1.98	0.46
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.98	0.46
12:L:18:HIS:HB2	30:0:903:U:O4	2.16	0.46
13:M:184:ARG:HG3	13:M:185:PRO:HA	1.98	0.46
30:0:451:C:O2'	30:0:452:G:H5'	2.16	0.46
30:0:2379:G:N7	30:0:2408:A:N1	2.64	0.46
30:0:2433:A:H2'	30:0:2434:A:C8	2.50	0.46
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.46
30:0:2895:C:H2'	38:0:9573:HOH:O	2.15	0.46
13:M:27:ARG:NH1	13:M:44:THR:CG2	2.78	0.46
26:Z:76:THR:HG21	30:0:1652:C:H4'	1.96	0.46
30:0:1603:A:H5''	30:0:1604:G:H3'	1.98	0.46
30:0:1825:U:O2'	30:0:1826:C:H5'	2.15	0.46
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.30	0.46
30:0:366:U:H2'	30:0:367:G:O4'	2.16	0.46
30:0:466:A:H2'	30:0:467:G:O4'	2.15	0.46
30:0:1015:C:O5'	30:0:1015:C:H6	1.98	0.46
30:0:1506:U:H6	30:0:1506:U:H5'	1.81	0.46
31:9:45:A:H2'	31:9:46:C:C6	2.51	0.46
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.16	0.46
4:D:103:ASN:HD22	4:D:134:LEU:H	1.60	0.46
8:H:165:ARG:HD2	38:H:231:HOH:O	2.16	0.46
15:O:24:ALA:HB3	30:0:710:G:OP1	2.16	0.46
16:P:120:ARG:NH2	16:P:123:TYR:CD2	2.83	0.46
23:W:21:LEU:O	23:W:26:ILE:HG23	2.16	0.46
30:0:958:G:O2'	30:0:959:C:H5'	2.15	0.46
30:0:1180:U:H2'	30:0:1181:A:O4'	2.16	0.46
30:0:1622:G:H2'	30:0:1623:C:H5'	1.98	0.46
30:0:1684:A:O2'	30:0:1685:A:H5''	2.16	0.46
30:0:1714:C:O2'	30:0:1715:C:H5'	2.16	0.46
30:0:1774:G:H1'	38:0:4551:HOH:O	2.14	0.46
30:0:2361:A:H2'	30:0:2362:A:C8	2.49	0.46
31:9:52:A:H2'	31:9:53:G:O4'	2.16	0.46
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.16	0.45
14:N:82:TYR:C	14:N:82:TYR:CD2	2.93	0.45
15:O:63:LYS:NZ	30:0:659:A:N7	2.53	0.45
16:P:40:VAL:O	16:P:44:VAL:HG23	2.17	0.45
30:0:417:G:P	38:0:7432:HOH:O	2.74	0.45
30:0:735:C:C5	30:0:736:A:N3	2.84	0.45
30:0:1165:G:H1'	30:0:1174:A:H1'	1.97	0.45
30:0:1202:A:O2'	30:0:1203:G:H5'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1278:A:H2'	30:0:1280:A:C8	2.51	0.45
30:0:1523:G:C6	30:0:1524:U:C4	3.04	0.45
30:0:2355:G:H5'	30:0:2356:A:OP2	2.16	0.45
30:0:2869:G:H2'	30:0:2870:C:H6	1.81	0.45
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.49	0.45
3:C:79:ARG:O	3:C:87:ARG:HG2	2.16	0.45
9:I:114:TYR:CD1	9:I:114:TYR:N	2.84	0.45
20:T:38:ARG:NH1	38:0:6693:HOH:O	2.42	0.45
24:X:43:VAL:HG12	24:X:44:ASP:N	2.30	0.45
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.31	0.45
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.51	0.45
30:0:24:G:N2	30:0:518:G:H1'	2.31	0.45
30:0:64:G:H2'	30:0:65:C:O4'	2.16	0.45
30:0:236:A:H4'	30:0:237:G:OP1	2.15	0.45
30:0:271:C:N4	30:0:378:A:C2	2.71	0.45
30:0:496:G:H3'	38:0:7681:HOH:O	2.15	0.45
30:0:711:G:O2'	30:0:712:C:H5'	2.17	0.45
31:9:106:U:O2'	31:9:107:C:H5'	2.15	0.45
2:B:26:PHE:HE1	38:B:9109:HOH:O	1.99	0.45
3:C:233:THR:HG22	3:C:234:VAL:H	1.81	0.45
4:D:170:TYR:N	4:D:170:TYR:HD1	2.14	0.45
5:E:1:PRO:HG2	5:E:59:MET:SD	2.56	0.45
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.97	0.45
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.50	0.45
15:O:25:VAL:HG23	15:O:26:TRP:N	2.31	0.45
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.30	0.45
20:T:21:LYS:HA	20:T:24:ARG:HG3	1.99	0.45
21:U:17:THR:CG2	21:U:18:GLY:N	2.79	0.45
23:W:73:LEU:HD12	23:W:73:LEU:HA	1.80	0.45
30:0:105:G:O2'	30:0:106:A:H5'	2.16	0.45
30:0:1201:C:H2'	30:0:1202:A:H5'	1.98	0.45
30:0:1883:U:C2'	30:0:1884:G:H5'	2.46	0.45
30:0:1909:A:N1	30:0:2128:G:H1'	2.31	0.45
30:0:2092:G:H2'	30:0:2613:G:OP1	2.16	0.45
30:0:2467:A:O2'	30:0:2468:A:H2'	2.17	0.45
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.97	0.45
8:H:157:TYR:CD1	8:H:157:TYR:C	2.94	0.45
30:0:210:U:H2'	30:0:211:U:C6	2.51	0.45
30:0:1015:C:H2'	30:0:1016:U:C6	2.51	0.45
31:9:2:U:OP2	31:9:2:U:H4'	2.16	0.45
3:C:236:THR:CG2	3:C:239:ALA:H	2.21	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.46	0.45
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.98	0.45
27:1:25:LYS:O	27:1:25:LYS:HG2	2.17	0.45
30:0:843:A:C2	30:0:846:A:C8	3.04	0.45
30:0:1001:U:O2'	30:0:1002:G:H5'	2.17	0.45
30:0:1268:C:H2'	30:0:1269:G:C8	2.52	0.45
30:0:1834:C:H2'	30:0:1840:A:H62	1.82	0.45
30:0:1855:G:H4'	30:0:1856:C:O5'	2.16	0.45
30:0:2895:C:O2'	30:0:2896:A:H5''	2.16	0.45
1:A:199:HIS:HD2	1:A:201:PHE:HB2	1.82	0.45
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.81	0.45
4:D:141:VAL:HG21	31:9:57:A:C8	2.51	0.45
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.52	0.45
25:Y:133:HIS:HD2	38:Y:8881:HOH:O	1.98	0.45
28:2:48:ASP:O	28:2:49:GLU:HB2	2.17	0.45
30:0:423:A:C5	30:0:424:C:C5	3.05	0.45
30:0:682:A:H2'	30:0:683:G:O4'	2.16	0.45
30:0:945:U:H2'	30:0:946:C:C6	2.52	0.45
30:0:1634:G:C3'	38:0:3907:HOH:O	2.46	0.45
30:0:2314:G:C2'	30:0:2315:C:H5'	2.47	0.45
30:0:2456:A:H5'	38:0:5702:HOH:O	2.17	0.45
30:0:2664:A:H8	30:0:2664:A:OP1	1.99	0.45
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.50	0.45
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.83	0.45
23:W:13:MET:CE	23:W:17:ILE:HG22	2.47	0.45
27:1:8:GLN:HE22	27:1:11:LYS:HZ1	1.63	0.45
30:0:73:U:O2'	30:0:74:G:H5'	2.17	0.45
30:0:482:G:O4'	30:0:511:A:C2	2.69	0.45
30:0:1183:C:H42	30:0:1184:C:N4	2.10	0.45
30:0:1379:A:H1'	38:0:9695:HOH:O	2.16	0.45
30:0:1386:G:O2'	30:0:1387:G:H5'	2.17	0.45
30:0:1624:A:H4'	30:0:1626:A:H5''	1.99	0.45
30:0:2506:A:C4	38:0:6063:HOH:O	2.67	0.45
30:0:2681:A:H4'	30:0:2682:C:OP1	2.16	0.45
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.49	0.45
2:B:223:ARG:HG3	2:B:232:TRP:O	2.17	0.45
12:L:61:ALA:HB2	12:L:105:TYR:CZ	2.52	0.45
14:N:40:ASN:ND2	31:9:28:U:H5''	2.31	0.45
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.99	0.45
18:R:104:PHE:HB3	18:R:109:MET:HE2	1.99	0.45
30:0:670:G:H2'	30:0:671:A:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1014:A:H2'	30:0:1015:C:H5'	1.99	0.45
30:0:1484:G:H2'	38:0:9106:HOH:O	2.17	0.45
5:E:84:MET:HE2	5:E:133:VAL:HG23	1.99	0.45
5:E:154:ILE:HD11	5:E:157:LYS:NZ	2.32	0.45
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.47	0.45
13:M:49:ALA:C	13:M:54:TYR:HB3	2.41	0.45
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.16	0.45
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.16	0.45
30:0:1221:G:H8	38:0:5995:HOH:O	1.95	0.45
30:0:1400:C:O2'	30:0:1401:G:H5'	2.17	0.45
30:0:2248:C:C4	30:0:2249:G:N7	2.85	0.45
30:0:2727:A:C6	30:0:2756:U:C2	3.05	0.45
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.47	0.45
11:K:34:VAL:HB	38:K:7169:HOH:O	2.17	0.45
27:1:20:ARG:HG2	30:0:111:C:O2'	2.17	0.45
30:0:441:A:H8	30:0:441:A:O5'	1.99	0.45
30:0:861:A:H4'	30:0:1697:G:H4'	1.99	0.45
30:0:1191:A:C2	30:0:1207:A:C2	3.05	0.45
30:0:1279:U:O2	30:0:1279:U:C2'	2.64	0.45
30:0:1425:G:O2'	30:0:1426:C:H5'	2.17	0.45
30:0:1537:C:H1'	38:0:6597:HOH:O	2.16	0.45
30:0:2002:C:H2'	30:0:2003:U:H5'	1.99	0.45
30:0:2256:G:HO2'	30:0:2257:G:H5'	1.78	0.45
30:0:2819:C:H2'	30:0:2820:A:C8	2.51	0.45
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.82	0.44
12:L:36:ASP:HB2	38:L:8836:HOH:O	2.17	0.44
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.18	0.44
24:X:74:ALA:HB2	24:X:85:VAL:HG13	2.00	0.44
30:0:107:U:H2'	30:0:108:U:H5'	1.99	0.44
30:0:128:A:C8	30:0:128:A:H3'	2.52	0.44
30:0:1333:U:H2'	30:0:1334:C:C6	2.52	0.44
30:0:1771:U:O2'	30:0:1773:G:N7	2.50	0.44
30:0:2072:G:C6	30:0:2533:C:H1'	2.52	0.44
30:0:2483:A:H4'	30:0:2484:U:OP2	2.17	0.44
30:0:2812:A:H1'	38:0:5796:HOH:O	2.17	0.44
31:9:36:C:C5	31:9:37:C:C5	3.05	0.44
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.99	0.44
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.80	0.44
20:T:9:LYS:HD2	38:0:3766:HOH:O	2.16	0.44
23:W:4:LEU:O	23:W:32:CYS:HA	2.17	0.44
30:0:213:G:N2	30:0:225:G:H2'	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:368:C:C2'	30:0:369:G:H5'	2.47	0.44
30:0:506:G:N2	30:0:509:A:C5'	2.72	0.44
30:0:790:A:H1'	30:0:1710:A:H2'	1.99	0.44
30:0:905:C:H3'	38:0:5198:HOH:O	2.17	0.44
30:0:1759:A:N3	30:0:1818:C:H2'	2.33	0.44
30:0:2329:C:O2'	30:0:2330:U:H5'	2.17	0.44
30:0:2543:G:H2'	30:0:2544:G:O4'	2.17	0.44
30:0:2689:A:H2'	30:0:2690:U:H5'	1.99	0.44
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.31	0.44
13:M:86:GLN:NE2	30:0:2274:A:H1'	2.32	0.44
13:M:164:THR:CG2	13:M:167:GLY:H	2.27	0.44
20:T:9:LYS:HG3	38:0:7437:HOH:O	2.16	0.44
21:U:33:SER:O	21:U:37:GLU:HG3	2.16	0.44
30:0:343:C:O2'	30:0:344:C:H5'	2.17	0.44
30:0:579:G:H2'	30:0:580:A:C8	2.52	0.44
30:0:1522:A:C2	30:0:1665:G:C6	3.05	0.44
30:0:1545:C:H1'	30:0:1641:A:N6	2.33	0.44
30:0:2511:A:H2'	30:0:2512:U:O4'	2.17	0.44
31:9:39:U:C2'	31:9:40:C:OP1	2.65	0.44
1:A:109:GLU:HG2	1:A:116:GLY:N	2.33	0.44
1:A:223:ARG:HD2	30:0:2272:G:OP1	2.17	0.44
2:B:75:GLU:C	2:B:77:PRO:HD3	2.43	0.44
2:B:320:GLN:NE2	2:B:321:PRO:HD2	2.29	0.44
3:C:236:THR:HG22	3:C:239:ALA:CB	2.47	0.44
5:E:169:THR:HG22	5:E:170:ARG:HG3	2.00	0.44
17:Q:95:GLU:HA	30:0:949:U:H4'	1.99	0.44
30:0:281:U:H5	38:0:7606:HOH:O	2.01	0.44
30:0:999:C:O2'	30:0:1000:C:H5'	2.18	0.44
30:0:1622:G:C2'	30:0:1623:C:H5'	2.47	0.44
30:0:2239:C:H2'	30:0:2240:U:C6	2.53	0.44
30:0:2375:A:H2'	30:0:2376:C:C6	2.53	0.44
30:0:2775:A:C6	30:0:2799:A:C8	3.06	0.44
2:B:211:THR:HG21	38:0:7469:HOH:O	2.17	0.44
38:C:8546:HOH:O	30:0:457:U:H4'	2.17	0.44
6:F:57:GLU:O	6:F:61:MET:HG3	2.18	0.44
13:M:164:THR:HB	38:M:8819:HOH:O	2.18	0.44
14:N:141:ARG:NH2	31:9:48:C:H4'	2.27	0.44
14:N:143:ARG:HE	14:N:143:ARG:HB3	1.61	0.44
19:S:57:THR:HG22	19:S:58:MET:N	2.32	0.44
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.01	0.44
30:0:249:G:O2'	30:0:250:C:H5'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2238:A:O2'	30:0:2239:C:H5'	2.17	0.44
30:0:2858:U:H2'	30:0:2859:C:O4'	2.16	0.44
2:B:280:VAL:HG13	2:B:333:GLU:O	2.18	0.44
11:K:87:ARG:NE	38:0:5721:HOH:O	2.50	0.44
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.98	0.44
30:0:277:U:O2'	30:0:278:A:H5'	2.18	0.44
30:0:1790:C:H2'	30:0:1791:U:C6	2.51	0.44
30:0:1973:A:H5'	30:0:1973:A:C8	2.44	0.44
30:0:2800:A:H5'	30:0:2801:A:OP2	2.18	0.44
30:0:2812:A:N7	38:0:7529:HOH:O	2.36	0.44
31:9:1:U:H5''	31:9:3:A:OP1	2.18	0.44
4:D:57:THR:HG23	4:D:63:ILE:HA	2.00	0.44
7:G:63:ARG:N	38:G:2569:HOH:O	2.50	0.44
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.64	0.44
23:W:122:ARG:NH2	38:0:5297:HOH:O	2.49	0.44
23:W:133:LYS:HG3	38:W:5904:HOH:O	2.18	0.44
30:0:302:A:O2'	30:0:303:C:H5'	2.17	0.44
30:0:371:U:H2'	30:0:372:A:C8	2.48	0.44
30:0:636:G:H1'	30:0:2058:G:C4	2.53	0.44
30:0:1434:A:H2'	30:0:1436:C:C5	2.53	0.44
30:0:1592:G:O2'	30:0:1593:C:O4'	2.33	0.44
30:0:1593:C:H1'	38:0:6112:HOH:O	2.17	0.44
30:0:1950:G:H2'	30:0:1951:G:C8	2.53	0.44
30:0:2653:A:H2'	30:0:2654:C:C6	2.53	0.44
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.53	0.44
4:D:76:ARG:NE	31:9:44:A:O4'	2.51	0.44
7:G:63:ARG:O	7:G:67:LEU:HG	2.17	0.44
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.98	0.44
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.32	0.44
30:0:289:G:O2'	30:0:290:C:H5'	2.17	0.44
30:0:291:C:H2'	30:0:292:G:O4'	2.18	0.44
30:0:790:A:H2'	30:0:791:A:O4'	2.17	0.44
30:0:1067:A:H3'	38:0:4304:HOH:O	2.17	0.44
30:0:1191:A:H2	30:0:1206:U:H3	1.65	0.44
30:0:2252:A:C6	30:0:2253:G:H1'	2.53	0.44
30:0:2718:C:H5'	30:0:2718:C:C6	2.50	0.44
30:0:2831:C:H2'	30:0:2832:C:H5'	1.99	0.44
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.82	0.44
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.43	0.44
8:H:157:TYR:C	8:H:157:TYR:HD1	2.26	0.44
10:J:107:ASN:ND2	10:J:107:ASN:C	2.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.18	0.44
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.99	0.44
23:W:13:MET:HE1	23:W:21:LEU:HD12	2.00	0.44
25:Y:142:SER:OG	30:0:1331:G:OP2	2.32	0.44
30:0:567:U:O2'	30:0:568:G:H5'	2.17	0.44
30:0:699:C:H6	30:0:744:G:O4'	2.01	0.44
30:0:705:C:O2	30:0:705:C:H2'	2.17	0.44
30:0:1044:C:H5''	38:0:9029:HOH:O	2.18	0.44
30:0:1181:A:H2'	30:0:1182:C:C5'	2.48	0.44
30:0:1202:A:C2'	30:0:1203:G:H5'	2.48	0.44
30:0:1603:A:C5'	30:0:1605:G:C5'	2.95	0.44
30:0:2064:U:H4'	30:0:2653:A:OP1	2.17	0.44
30:0:2264:A:H2'	30:0:2265:U:C6	2.53	0.44
1:A:97:ALA:HA	1:A:131:HIS:NE2	2.33	0.43
3:C:168:ARG:NH2	3:C:190:ALA:O	2.51	0.43
8:H:87:LYS:NZ	8:H:87:LYS:HB2	2.33	0.43
15:O:65:LEU:HD13	30:0:746:A:C6	2.53	0.43
25:Y:141:THR:HG23	38:Y:8888:HOH:O	2.18	0.43
28:2:41:HIS:CD2	28:2:44:ARG:H	2.33	0.43
30:0:47:G:N3	30:0:114:A:C2	2.86	0.43
30:0:129:A:H4'	30:0:130:C:OP1	2.18	0.43
30:0:825:U:H5''	30:0:826:U:OP1	2.18	0.43
30:0:1127:C:C5	30:0:1128:U:C4	3.06	0.43
30:0:1163:G:C2	30:0:1184:C:N3	2.86	0.43
30:0:2598:U:O2	30:0:2600:A:C8	2.71	0.43
4:D:154:LYS:H	4:D:154:LYS:CD	2.24	0.43
6:F:91:VAL:CG1	6:F:92:GLY:N	2.78	0.43
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.45	0.43
14:N:114:LYS:O	14:N:118:ILE:HG13	2.18	0.43
18:R:128:ARG:NH2	30:0:2054:A:C2	2.86	0.43
30:0:134:U:C2	30:0:145:A:C2	3.07	0.43
30:0:677:C:P	38:0:7147:HOH:O	2.75	0.43
30:0:1552:G:N2	30:0:1634:G:H1'	2.33	0.43
30:0:1947:G:H2'	30:0:1948:G:H8	1.82	0.43
30:0:2379:G:H5'	30:0:2381:C:O4'	2.18	0.43
30:0:2421:G:H3'	30:0:2422:U:C5'	2.47	0.43
30:0:2488:A:H2'	30:0:2489:G:O4'	2.19	0.43
30:0:2566:A:H2	30:0:2695:C:O2	2.01	0.43
31:9:35:C:H5''	38:9:9080:HOH:O	2.17	0.43
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.83	0.43
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:80:TRP:O	5:E:134:SER:HA	2.18	0.43
12:L:48:LYS:HE2	30:0:220:C:C2	2.53	0.43
22:V:44:GLY:HA3	30:0:92:G:H4'	1.99	0.43
30:0:484:A:N1	30:0:506:G:H4'	2.33	0.43
30:0:1115:U:O2'	30:0:1116:U:H5'	2.18	0.43
30:0:1762:C:O2'	30:0:1763:C:H5'	2.17	0.43
30:0:2607:U:H4'	38:0:9448:HOH:O	2.18	0.43
9:I:111:LEU:CD2	30:0:1163:G:H4'	2.45	0.43
14:N:41:LYS:HD3	38:9:9063:HOH:O	2.19	0.43
16:P:7:LYS:HG2	16:P:23:PHE:CE2	2.54	0.43
25:Y:189:ASN:C	25:Y:189:ASN:HD22	2.27	0.43
30:0:17:G:H2'	30:0:18:C:H6	1.82	0.43
30:0:1245:C:O5'	30:0:1245:C:H6	2.01	0.43
30:0:1395:C:H2'	30:0:1396:C:C6	2.53	0.43
30:0:1700:C:H5''	30:0:1701:A:OP2	2.18	0.43
30:0:2256:G:H2'	30:0:2257:G:O5'	2.17	0.43
33:0:8814:CL:CL	38:0:7753:HOH:O	2.59	0.43
31:9:34:A:H2'	31:9:35:C:O4'	2.18	0.43
1:A:55:VAL:HG23	1:A:68:ILE:O	2.19	0.43
1:A:95:PRO:HA	1:A:153:ARG:HA	1.99	0.43
1:A:103:VAL:HA	1:A:104:PRO:HD3	1.83	0.43
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.52	0.43
2:B:198:GLU:HA	38:B:9119:HOH:O	2.19	0.43
2:B:271:ASP:HB3	2:B:296:LEU:HD12	1.99	0.43
3:C:93:LYS:O	3:C:98:ARG:NH2	2.51	0.43
4:D:50:VAL:HG13	31:9:41:C:O4'	2.18	0.43
6:F:59:ILE:HD13	30:0:263:U:O4'	2.18	0.43
8:H:61:ARG:HG3	38:0:4984:HOH:O	2.17	0.43
11:K:115:ARG:HG3	11:K:116:GLU:N	2.34	0.43
13:M:157:ASP:HB3	13:M:160:PHE:HD1	1.84	0.43
24:X:15:ARG:HH22	30:0:2856:A:P	2.41	0.43
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.65	0.43
30:0:522:U:O2'	30:0:1366:C:H5'	2.18	0.43
30:0:559:U:H2'	30:0:560:U:O4'	2.18	0.43
30:0:1896:G:C6	30:0:1897:U:C4	3.07	0.43
30:0:1964:U:O2	30:0:1964:U:H2'	2.17	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.96	0.43
30:0:2504:A:H2'	30:0:2505:G:H5'	2.00	0.43
4:D:167:GLU:C	4:D:169:THR:H	2.26	0.43
12:L:39:GLU:HG2	30:0:926:A:C4'	2.48	0.43
13:M:193:LYS:HB3	30:0:392:U:H4'	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:151:ASP:OD1	14:N:166:ALA:HA	2.19	0.43
23:W:125:HIS:HB2	23:W:137:GLN:HG2	2.00	0.43
25:Y:216:ARG:NH1	38:Y:8833:HOH:O	2.51	0.43
30:0:542:A:H2'	30:0:543:G:O4'	2.18	0.43
30:0:570:C:H2'	30:0:571:C:H5'	2.01	0.43
30:0:1063:G:H8	38:0:9865:HOH:O	2.01	0.43
30:0:1187:U:C2	30:0:1189:A:OP2	2.72	0.43
30:0:1702:U:H5'	38:0:3432:HOH:O	2.18	0.43
30:0:2070:G:H2'	30:0:2072:G:OP1	2.19	0.43
30:0:2437:A:H2'	30:0:2438:G:C8	2.54	0.43
30:0:2906:A:H5'	30:0:2907:C:O4'	2.19	0.43
31:9:28:U:H2'	31:9:29:C:C6	2.54	0.43
1:A:179:MET:HG2	1:A:186:TRP:CB	2.49	0.43
2:B:87:TYR:HD1	38:B:9041:HOH:O	2.01	0.43
3:C:25:PRO:HG2	38:C:8523:HOH:O	2.18	0.43
3:C:54:LEU:HD23	3:C:79:ARG:HG3	2.00	0.43
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.54	0.43
30:0:17:G:H2'	30:0:18:C:C6	2.53	0.43
30:0:37:A:H2'	30:0:38:G:C8	2.54	0.43
30:0:243:A:H61	30:0:269:G:H1'	1.83	0.43
30:0:969:G:H1	30:0:999:C:H42	1.66	0.43
30:0:1198:U:C6	30:0:1200:A:OP2	2.72	0.43
30:0:2115:U:H2'	30:0:2116:U:C6	2.53	0.43
30:0:2587:OMU:H2'	30:0:2589:U:H5''	2.00	0.43
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.43
2:B:248:ARG:NH1	38:B:9080:HOH:O	2.50	0.43
2:B:297:VAL:HB	38:B:9070:HOH:O	2.19	0.43
3:C:173:LYS:HE3	30:0:1311:G:O6	2.18	0.43
4:D:10:PHE:CG	4:D:11:HIS:N	2.87	0.43
6:F:72:VAL:HA	6:F:73:PRO:HD3	1.85	0.43
14:N:108:SER:HA	14:N:109:PRO:HD3	1.78	0.43
16:P:133:SER:HA	38:0:3512:HOH:O	2.18	0.43
28:2:28:LYS:O	30:0:87:C:H2'	2.18	0.43
30:0:652:G:H8	38:0:3020:HOH:O	2.00	0.43
30:0:734:U:H2'	30:0:736:A:OP2	2.19	0.43
30:0:886:A:OP2	30:0:2113:G:H5'	2.19	0.43
30:0:947:U:O2'	30:0:948:G:H5'	2.19	0.43
30:0:1163:G:H1	30:0:1184:C:N4	2.16	0.43
30:0:1553:C:H2'	30:0:1554:C:H6	1.84	0.43
30:0:1588:G:C6	30:0:1589:G:C6	3.07	0.43
30:0:2134:G:N2	30:0:2242:U:C2	2.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:PHE:HB3	2:B:190:MET:HE3	2.01	0.43
2:B:79:MET:HE3	2:B:144:THR:HG21	2.00	0.43
3:C:170:ASP:OD2	30:0:330:C:H5	2.01	0.43
27:1:37:CYS:SG	27:1:39:PHE:HB2	2.59	0.43
30:0:129:A:O2'	30:0:131:A:OP1	2.36	0.43
30:0:297:U:H1'	38:0:3947:HOH:O	2.18	0.43
30:0:735:C:C5	30:0:736:A:C2	3.06	0.43
30:0:792:G:H4'	38:0:3424:HOH:O	2.19	0.43
30:0:1186:C:N4	30:0:1187:U:C4	2.87	0.43
30:0:1942:A:H2'	30:0:1943:C:H6	1.83	0.43
31:9:1:U:O3'	31:9:3:A:OP1	2.36	0.43
31:9:106:U:O5'	31:9:106:U:H6	2.01	0.43
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.54	0.43
13:M:171:ARG:NH2	30:0:189:A:OP1	2.51	0.43
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.34	0.43
30:0:397:A:O2'	30:0:417:G:N3	2.43	0.43
30:0:1883:U:O2'	30:0:1884:G:H5'	2.19	0.43
30:0:2712:G:O2'	30:0:2713:G:H5'	2.19	0.43
30:0:2820:A:H2'	30:0:2821:C:C6	2.54	0.43
30:0:2842:G:H2'	30:0:2843:A:C5'	2.48	0.43
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.34	0.42
3:C:236:THR:HG22	3:C:239:ALA:HB2	2.01	0.42
5:E:69:ILE:HA	5:E:72:MET:CE	2.48	0.42
14:N:23:ARG:O	14:N:27:LEU:HG	2.18	0.42
14:N:171:HIS:CE1	38:N:8855:HOH:O	2.72	0.42
15:O:81:PHE:HB2	15:O:86:GLU:HB2	2.01	0.42
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.54	0.42
21:U:4:ARG:N	38:U:5334:HOH:O	2.52	0.42
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.46	0.42
26:Z:47:ARG:NH1	38:Z:8704:HOH:O	2.50	0.42
27:1:28:HIS:HD2	27:1:30:LYS:H	1.66	0.42
30:0:212:A:O4'	30:0:214:U:C6	2.72	0.42
30:0:282:C:O2'	30:0:283:U:C4'	2.67	0.42
30:0:305:A:C5	30:0:329:A:C2	3.07	0.42
30:0:1052:G:N3	30:0:1052:G:H2'	2.33	0.42
30:0:1965:C:O5'	30:0:1965:C:H6	2.02	0.42
30:0:2756:U:C2	30:0:2896:A:H2	2.37	0.42
30:0:2783:A:H2'	30:0:2784:A:C8	2.54	0.42
3:C:184:ARG:NH1	30:0:1306:U:OP1	2.51	0.42
3:C:237:GLU:HA	38:C:8626:HOH:O	2.18	0.42
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:128:A:O2'	30:0:129:A:C5'	2.67	0.42
30:0:162:C:H2'	30:0:163:U:H5'	2.02	0.42
30:0:834:G:H3'	30:0:835:U:H4'	2.01	0.42
30:0:867:A:H2	30:0:880:C:O2	2.02	0.42
30:0:1706:G:C5	30:0:1707:G:C6	3.07	0.42
30:0:1921:A:C6	30:0:1922:A:C2	3.08	0.42
30:0:2332:A:H3'	30:0:2333:G:H8	1.84	0.42
2:B:74:ILE:HG13	38:B:9070:HOH:O	2.17	0.42
2:B:238:ASN:ND2	2:B:240:GLY:H	2.04	0.42
14:N:69:TYR:CE2	14:N:184:ILE:HD11	2.55	0.42
19:S:57:THR:HG23	38:S:8979:HOH:O	2.19	0.42
30:0:31:C:C4'	38:0:7437:HOH:O	2.66	0.42
30:0:128:A:C8	30:0:128:A:C3'	3.02	0.42
30:0:932:U:H1'	30:0:1296:A:H1'	2.00	0.42
30:0:1249:U:H2'	30:0:1250:C:C6	2.54	0.42
30:0:1350:U:H4'	38:0:5134:HOH:O	2.18	0.42
30:0:1461:U:H2'	30:0:1462:C:C6	2.54	0.42
30:0:2121:G:O2'	30:0:2122:C:H5'	2.19	0.42
30:0:2347:C:H2'	30:0:2348:C:H6	1.83	0.42
6:F:59:ILE:CD1	30:0:263:U:C2	3.02	0.42
6:F:110:ASP:O	6:F:114:LYS:HG3	2.20	0.42
15:O:105:ASN:HD21	15:O:109:SER:N	2.17	0.42
29:3:11:CYS:HB2	29:3:20:HIS:HE1	1.85	0.42
30:0:40:C:O5'	30:0:40:C:H6	2.02	0.42
30:0:699:C:C2	30:0:744:G:C2	3.07	0.42
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.42
30:0:1613:C:H2'	30:0:1614:G:O4'	2.19	0.42
30:0:1741:U:C4	30:0:2033:G:C8	3.07	0.42
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.20	0.42
10:J:75:PRO:HD3	10:J:136:SER:OG	2.20	0.42
14:N:71:TRP:HB2	38:N:8833:HOH:O	2.19	0.42
16:P:87:ARG:HG2	38:P:188:HOH:O	2.18	0.42
18:R:3:SER:HB2	30:0:20:G:O3'	2.19	0.42
23:W:4:LEU:HD23	23:W:4:LEU:HA	1.83	0.42
30:0:74:G:H2'	30:0:75:U:C6	2.54	0.42
30:0:177:A:H2'	30:0:178:U:O4'	2.19	0.42
30:0:1020:A:H1'	38:0:7242:HOH:O	2.19	0.42
30:0:2032:U:O2'	30:0:2033:G:H5''	2.20	0.42
30:0:2801:A:H2'	30:0:2801:A:N3	2.34	0.42
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.55	0.42
24:X:78:GLU:HB3	38:X:5564:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.19	0.42
30:0:69:A:C8	30:0:69:A:C5'	2.96	0.42
30:0:316:A:N3	30:0:336:G:O2'	2.46	0.42
30:0:1081:A:H5''	38:0:3159:HOH:O	2.19	0.42
30:0:1482:A:O2'	30:0:1483:C:H5'	2.20	0.42
30:0:1495:C:H1'	30:0:1573:A:H1'	2.02	0.42
30:0:1760:G:H5'	30:0:1818:C:O2'	2.20	0.42
30:0:2089:A:C2'	30:0:2090:G:H5'	2.49	0.42
30:0:2657:G:O2'	30:0:2842:G:N7	2.47	0.42
30:0:2754:G:C2'	30:0:2755:G:H5'	2.49	0.42
2:B:56:ASP:HB2	2:B:322:ARG:HE	1.85	0.42
4:D:18:ILE:HD13	4:D:84:LEU:HD12	2.01	0.42
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.85	0.42
17:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.20	0.42
22:V:11:MET:HE1	22:V:19:GLU:HG2	2.01	0.42
30:0:1735:C:O2'	30:0:1736:A:H5'	2.19	0.42
30:0:2523:U:O2'	30:0:2524:G:H5'	2.20	0.42
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.84	0.42
4:D:21:VAL:HA	4:D:131:THR:O	2.19	0.42
8:H:91:ARG:NH1	8:H:138:THR:OG1	2.50	0.42
11:K:29:LEU:HD22	11:K:55:VAL:HG11	2.02	0.42
18:R:82:GLU:O	18:R:86:LYS:HG3	2.19	0.42
28:2:41:HIS:HB3	28:2:44:ARG:HB2	2.02	0.42
30:0:113:A:OP2	30:0:114:A:H2'	2.19	0.42
30:0:445:U:H2'	30:0:446:G:C8	2.54	0.42
30:0:583:C:H2'	30:0:584:U:C6	2.50	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.48	0.42
30:0:2265:U:H2'	30:0:2266:A:C8	2.55	0.42
30:0:2421:G:H3'	30:0:2422:U:H5''	2.02	0.42
30:0:2600:A:H2'	30:0:2601:A:O4'	2.19	0.42
30:0:2809:G:H2'	30:0:2810:G:O4'	2.20	0.42
1:A:206:ARG:NH2	30:0:2630:G:O6	2.53	0.42
6:F:107:ASP:O	6:F:111:ILE:HG13	2.19	0.42
6:F:111:ILE:O	6:F:115:VAL:HG23	2.20	0.42
9:I:114:TYR:N	9:I:114:TYR:HD1	2.17	0.42
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.42
14:N:37:ARG:NH2	38:N:8828:HOH:O	2.51	0.42
14:N:159:TYR:HE1	31:9:50:G:H5''	1.85	0.42
16:P:13:VAL:HG13	16:P:14:LEU:N	2.35	0.42
19:S:37:VAL:O	19:S:41:VAL:HG23	2.20	0.42
20:T:41:ARG:NH1	20:T:42:VAL:O	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:2:LYS:HG3	30:0:1486:A:C5	2.55	0.42
30:0:1307:A:H2'	30:0:1308:A:C8	2.55	0.42
30:0:1562:C:N4	38:0:5872:HOH:O	2.52	0.42
30:0:1603:A:H5'	30:0:1605:G:C5'	2.49	0.42
30:0:1644:C:O2'	30:0:1645:U:H5'	2.19	0.42
30:0:1878:G:O2'	30:0:1879:U:OP2	2.38	0.42
30:0:2255:A:O2'	30:0:2256:G:H5'	2.20	0.42
2:B:5:ARG:NH1	30:0:2547:C:OP2	2.53	0.42
2:B:18:ARG:HG3	2:B:256:GLN:HG3	2.01	0.42
3:C:111:VAL:HB	38:C:8522:HOH:O	2.20	0.42
5:E:84:MET:HE1	5:E:148:ILE:CD1	2.50	0.42
8:H:12:ILE:HD12	8:H:57:THR:HG22	2.02	0.42
20:T:97:ARG:NH2	30:0:308:U:H5'	2.35	0.42
30:0:634:G:O2'	30:0:1358:A:OP1	2.35	0.42
30:0:912:A:C4	30:0:1294:A:C2	3.07	0.42
30:0:1398:G:H2'	30:0:1399:A:C8	2.55	0.42
30:0:1788:U:C2	30:0:1805:G:N2	2.88	0.42
30:0:2032:U:C2'	30:0:2033:G:C5'	2.98	0.42
30:0:2461:U:O2	30:0:2466:G:H1'	2.19	0.42
30:0:2553:A:H2'	30:0:2553:A:N3	2.34	0.42
30:0:2758:G:H2'	30:0:2759:C:C6	2.55	0.42
4:D:131:THR:HG21	30:0:2348:C:H1'	2.01	0.41
6:F:38:LYS:HE3	30:0:244:C:OP2	2.20	0.41
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.43	0.41
18:R:9:ASP:HA	18:R:10:PRO:HD2	1.90	0.41
22:V:44:GLY:O	22:V:48:GLU:HG2	2.20	0.41
23:W:11:VAL:O	23:W:12:ASN:HB2	2.20	0.41
27:1:45:ARG:HB3	38:1:8967:HOH:O	2.20	0.41
30:0:12:U:C2'	30:0:13:G:H5'	2.49	0.41
30:0:1845:A:O2'	30:0:1846:U:H5'	2.19	0.41
30:0:1942:A:C4'	38:0:9046:HOH:O	2.67	0.41
30:0:2290:U:H2'	38:0:7148:HOH:O	2.19	0.41
3:C:39:GLN:O	3:C:43:LYS:HD3	2.19	0.41
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.92	0.41
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.02	0.41
22:V:1:THR:HG23	22:V:2:VAL:HG23	2.02	0.41
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.56	0.41
24:X:34:ARG:NH1	24:X:48:VAL:O	2.51	0.41
26:Z:63:CYS:HA	26:Z:64:PRO:HD3	1.91	0.41
29:3:70:ARG:HD3	38:3:9059:HOH:O	2.19	0.41
30:0:297:U:H2'	30:0:298:C:H6	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:351:A:O2'	30:0:352:A:H5'	2.20	0.41
30:0:488:U:C2'	38:0:4019:HOH:O	2.67	0.41
30:0:1598:A:N6	33:0:8815:CL:CL	2.90	0.41
30:0:1636:G:O2'	30:0:1637:A:H5'	2.20	0.41
31:9:5:G:C2'	31:9:6:C:H5'	2.49	0.41
1:A:129:LEU:HD12	1:A:145:MET:HE1	2.02	0.41
4:D:76:ARG:NH1	31:9:42:C:O2	2.50	0.41
10:J:88:PRO:HD3	30:0:1104:C:H4'	2.01	0.41
24:X:22:ASN:HA	24:X:25:ARG:HG3	2.02	0.41
30:0:383:A:H2'	30:0:384:G:O4'	2.19	0.41
30:0:941:G:C6	30:0:942:U:C4	3.08	0.41
30:0:1375:A:C2'	30:0:1376:G:H5'	2.50	0.41
30:0:2088:C:H1'	30:0:2841:A:N1	2.35	0.41
30:0:2090:G:H2'	30:0:2091:G:C8	2.55	0.41
31:9:49:G:C2'	31:9:50:G:H5'	2.50	0.41
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.20	0.41
1:A:167:LYS:HB2	26:Z:53:ILE:HD13	2.02	0.41
1:A:214:SER:HB2	38:0:4377:HOH:O	2.20	0.41
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.33	0.41
4:D:12:GLU:C	4:D:14:ARG:H	2.29	0.41
13:M:59:GLY:HA3	13:M:141:ILE:HD12	2.02	0.41
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.85	0.41
23:W:3:ALA:O	23:W:54:PHE:HA	2.20	0.41
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.03	0.41
30:0:1625:U:H3'	30:0:1625:U:C6	2.54	0.41
30:0:1706:G:C6	30:0:1707:G:C6	3.09	0.41
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.50	0.41
11:K:37:TYR:HB3	38:K:7169:HOH:O	2.20	0.41
12:L:114:VAL:HG11	38:L:8874:HOH:O	2.20	0.41
15:O:21:SER:OG	15:O:106:PRO:HB2	2.20	0.41
23:W:43:GLY:HA3	30:0:945:U:O2'	2.20	0.41
23:W:76:ASP:O	23:W:77:ALA:C	2.63	0.41
27:1:12:ASN:O	30:0:1415:G:H5'	2.20	0.41
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.20	0.41
30:0:69:A:H2'	30:0:70:A:OP2	2.20	0.41
30:0:423:A:C4	30:0:424:C:C6	3.09	0.41
30:0:724:G:O2'	30:0:725:C:H5'	2.21	0.41
30:0:920:C:H4'	30:0:921:G:N2	2.35	0.41
30:0:1069:C:H2'	30:0:1070:A:O4'	2.21	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.35	0.41
30:0:2274:A:O2'	30:0:2275:G:H5'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2385:G:H2'	30:0:2386:U:C6	2.56	0.41
30:0:2635:A:C2'	30:0:2636:C:H5'	2.50	0.41
1:A:1:GLY:HA2	1:A:197:VAL:HG23	2.03	0.41
1:A:173:GLY:O	1:A:176:HIS:HB3	2.19	0.41
1:A:179:MET:HA	1:A:179:MET:HE3	2.01	0.41
3:C:107:ARG:O	3:C:111:VAL:HG23	2.21	0.41
30:0:307:G:H3'	38:0:6693:HOH:O	2.21	0.41
30:0:1193:A:H2	30:0:1194:A:N6	2.16	0.41
30:0:1413:A:H2'	30:0:1414:A:O4'	2.20	0.41
30:0:1483:C:O2'	30:0:1484:G:H5'	2.21	0.41
30:0:1594:C:O2'	30:0:1607:A:H4'	2.20	0.41
30:0:1787:C:O2'	30:0:1788:U:H5'	2.20	0.41
30:0:2281:C:C2'	30:0:2282:U:H5'	2.50	0.41
30:0:2505:G:H2'	30:0:2506:A:C5'	2.48	0.41
30:0:2506:A:O2'	30:0:2507:G:P	2.79	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.20	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.85	0.41
2:B:233:ARG:HG2	2:B:233:ARG:NH1	2.35	0.41
3:C:101:ASP:HB2	30:0:750:A:O3'	2.21	0.41
4:D:128:LEU:N	38:D:6007:HOH:O	2.53	0.41
30:0:309:C:O2	30:0:309:C:H2'	2.20	0.41
30:0:459:A:H4'	38:0:9460:HOH:O	2.20	0.41
30:0:571:C:O5'	30:0:571:C:H6	2.04	0.41
30:0:736:A:H8	38:0:7219:HOH:O	2.03	0.41
30:0:1381:A:N3	30:0:1382:G:H1'	2.36	0.41
30:0:1926:G:H2'	30:0:1927:A:H8	1.86	0.41
30:0:2032:U:H2'	30:0:2033:G:H5'	2.03	0.41
30:0:2903:C:O2'	30:0:2904:U:H5'	2.21	0.41
2:B:243:ASN:HA	2:B:244:PRO:C	2.44	0.41
9:I:101:LYS:O	9:I:105:GLU:HG3	2.20	0.41
30:0:764:C:H2'	30:0:765:G:O4'	2.20	0.41
30:0:962:C:H2'	30:0:963:C:H5'	2.03	0.41
30:0:1829:A:H2'	30:0:1830:C:H5'	2.03	0.41
30:0:1926:G:H2'	30:0:1927:A:C8	2.55	0.41
2:B:60:SER:HA	2:B:61:PRO:HD3	1.87	0.41
2:B:101:TRP:HB2	2:B:119:HIS:CD2	2.56	0.41
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.08	0.41
5:E:7:ILE:HG13	5:E:11:VAL:HB	2.03	0.41
5:E:68:HIS:CE1	38:E:5919:HOH:O	2.74	0.41
5:E:125:GLU:HB2	5:E:132:THR:HG23	2.03	0.41
12:L:6:ARG:NH1	30:0:1299:G:N7	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:59:ARG:O	16:P:63:ARG:HG3	2.21	0.41
22:V:5:VAL:HG23	38:V:2271:HOH:O	2.20	0.41
23:W:119:HIS:CG	38:0:5297:HOH:O	2.74	0.41
27:1:28:HIS:O	27:1:32:LYS:N	2.48	0.41
29:3:38:ARG:NH1	30:0:396:U:C2	2.89	0.41
30:0:243:A:H61	30:0:269:G:C1'	2.34	0.41
30:0:535:G:O6	30:0:2064:U:C6	2.74	0.41
30:0:653:U:H2'	30:0:654:A:C8	2.55	0.41
30:0:1159:G:H2'	30:0:1160:G:O4'	2.21	0.41
30:0:1298:U:H2'	30:0:1299:G:C8	2.56	0.41
30:0:1520:G:C6	30:0:1521:C:C4	3.08	0.41
30:0:1625:U:C6	30:0:1625:U:C3'	3.04	0.41
30:0:1626:A:H2'	30:0:1627:G:O4'	2.21	0.41
30:0:1634:G:H2'	30:0:1635:U:C6	2.56	0.41
30:0:2314:G:H2'	30:0:2315:C:H5'	2.03	0.41
30:0:2316:G:H8	38:0:5663:HOH:O	2.03	0.41
30:0:2354:A:C2	30:0:2367:A:C8	3.09	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.39	0.41
31:9:61:C:H2'	31:9:62:A:H8	1.85	0.41
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.56	0.41
2:B:225:GLY:HA3	38:B:9027:HOH:O	2.21	0.41
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.90	0.41
18:R:18:LEU:HG	18:R:91:LEU:HD13	2.03	0.41
20:T:106:GLU:HG3	38:T:4913:HOH:O	2.21	0.41
30:0:491:C:O2'	30:0:492:C:H5'	2.21	0.41
30:0:506:G:N1	30:0:509:A:OP2	2.54	0.41
30:0:615:G:H2'	30:0:616:U:C6	2.56	0.41
30:0:694:A:C2'	30:0:695:C:H5'	2.51	0.41
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.41
30:0:1795:G:H2'	30:0:1796:A:O4'	2.21	0.41
30:0:1857:A:N1	30:0:2246:U:O2'	2.51	0.41
30:0:1871:U:O4'	30:0:1873:G:C8	2.74	0.41
30:0:1903:U:O2'	30:0:1904:A:C8	2.72	0.41
30:0:2754:G:O2'	30:0:2755:G:H5'	2.20	0.41
30:0:2765:C:H2'	30:0:2766:A:C8	2.56	0.41
1:A:109:GLU:HG2	1:A:116:GLY:H	1.85	0.40
3:C:131:PHE:CD2	3:C:131:PHE:N	2.89	0.40
9:I:112:LEU:HG	30:0:1162:G:O2'	2.21	0.40
22:V:39:ALA:N	22:V:40:PRO:CD	2.84	0.40
23:W:130:HIS:NE2	31:9:88:G:OP1	2.50	0.40
23:W:130:HIS:O	23:W:136:GLY:HA3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.45	0.40
30:0:106:A:H2'	30:0:107:U:O4'	2.21	0.40
30:0:213:G:HO2'	30:0:214:U:P	2.44	0.40
30:0:304:G:H1'	30:0:347:A:H61	1.86	0.40
30:0:626:U:C4	30:0:627:G:C6	3.09	0.40
30:0:1116:U:C2	30:0:1246:A:N6	2.89	0.40
30:0:1205:U:H2'	30:0:1206:U:H5'	1.94	0.40
30:0:1375:A:H2'	30:0:1376:G:H5'	2.04	0.40
30:0:1555:G:H4'	30:0:1630:A:H2	1.86	0.40
30:0:2112:A:H2'	30:0:2113:G:H8	1.85	0.40
30:0:2491:G:C1'	38:0:6878:HOH:O	2.58	0.40
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.88	0.40
1:A:88:ILE:O	1:A:88:ILE:HG22	2.21	0.40
11:K:125:ALA:C	11:K:127:ALA:H	2.30	0.40
14:N:170:GLU:O	14:N:174:GLU:HG3	2.20	0.40
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.53	0.40
20:T:9:LYS:HE2	20:T:13:ARG:HH12	1.84	0.40
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.83	0.40
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.21	0.40
30:0:423:A:H2'	30:0:424:C:H6	1.87	0.40
30:0:499:G:O2'	30:0:500:G:H5'	2.21	0.40
30:0:1992:U:H2'	30:0:1994:A:OP2	2.20	0.40
30:0:2564:G:OP2	30:0:2565:C:H5''	2.21	0.40
3:C:102:LEU:HD12	3:C:102:LEU:HA	1.91	0.40
3:C:193:LEU:HD12	3:C:211:ASP:O	2.21	0.40
25:Y:145:LYS:O	25:Y:147:ARG:HG2	2.21	0.40
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.21	0.40
27:1:21:ARG:HD2	27:1:39:PHE:HB2	2.04	0.40
30:0:553:G:O4'	30:0:1325:G:H5'	2.22	0.40
30:0:570:C:O5'	30:0:570:C:H6	2.04	0.40
30:0:821:U:H2'	30:0:822:C:C6	2.57	0.40
30:0:1062:U:O2'	30:0:2307:A:N3	2.48	0.40
30:0:1761:U:H2'	30:0:1762:C:C6	2.55	0.40
30:0:1947:G:H2'	30:0:1948:G:C8	2.56	0.40
30:0:2614:C:O2'	30:0:2615:U:H5'	2.21	0.40
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.85	0.40
2:B:229:ARG:HD2	38:0:9111:HOH:O	2.20	0.40
4:D:22:VAL:HA	4:D:73:VAL:O	2.21	0.40
4:D:23:VAL:HG12	4:D:130:VAL:HG22	2.03	0.40
5:E:68:HIS:O	5:E:72:MET:HG3	2.22	0.40
9:I:130:LEU:HA	38:I:6825:HOH:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:145:LEU:O	12:L:148:GLU:HG3	2.21	0.40
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.22	0.40
18:R:18:LEU:HD12	18:R:143:VAL:HG11	2.03	0.40
18:R:114:VAL:HG13	18:R:114:VAL:O	2.22	0.40
25:Y:148:GLY:HA3	30:0:622:G:P	2.62	0.40
26:Z:45:VAL:HG12	38:Z:8713:HOH:O	2.21	0.40
29:3:1:MET:HE1	30:0:2380:A:N1	2.36	0.40
30:0:138:U:OP2	30:0:139:C:C5	2.70	0.40
30:0:503:G:H2'	30:0:504:G:H8	1.87	0.40
30:0:939:A:N1	30:0:1027:G:O2'	2.50	0.40
30:0:1014:A:H5''	31:9:101:G:O2'	2.22	0.40
30:0:1311:G:C2	30:0:1312:G:C8	3.09	0.40
30:0:2032:U:H2'	30:0:2033:G:H5''	2.03	0.40
30:0:2135:A:O4'	30:0:2243:C:N4	2.54	0.40
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.85	0.40
2:B:267:LYS:HD3	38:0:9565:HOH:O	2.22	0.40
13:M:188:ARG:HH11	30:0:154:C:H3'	1.86	0.40
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.86	0.40
16:P:94:TRP:CZ2	16:P:98:ILE:HG13	2.57	0.40
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.85	0.40
27:1:53:LYS:HD3	27:1:53:LYS:HA	1.91	0.40
30:0:214:U:H5'	38:0:6146:HOH:O	2.22	0.40
30:0:695:C:H2'	30:0:696:C:C6	2.57	0.40
30:0:812:A:H2'	30:0:813:C:O4'	2.21	0.40
30:0:1236:A:H2'	30:0:1237:U:O4'	2.22	0.40
30:0:1773:G:N2	30:0:1774:G:C8	2.90	0.40
30:0:2509:A:C2	30:0:2510:C:H1'	2.56	0.40
30:0:2734:G:O2'	30:0:2735:U:H5'	2.22	0.40
30:0:2897:C:O2'	30:0:2898:G:H5'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	211 (90%)	18 (8%)	6 (3%)	4	17
2	B	335/338 (99%)	306 (91%)	25 (8%)	4 (1%)	10	34
3	C	244/246 (99%)	224 (92%)	19 (8%)	1 (0%)	30	59
4	D	134/177 (76%)	113 (84%)	16 (12%)	5 (4%)	2	11
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
6	F	117/120 (98%)	106 (91%)	8 (7%)	3 (3%)	4	17
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	147 (94%)	8 (5%)	1 (1%)	21	51
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	8	28
10	J	140/145 (97%)	130 (93%)	9 (6%)	1 (1%)	18	48
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	16	44
12	L	141/165 (86%)	125 (89%)	14 (10%)	2 (1%)	9	30
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	24	54
14	N	184/187 (98%)	169 (92%)	12 (6%)	3 (2%)	7	27
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	141 (100%)	0	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	110 (94%)	7 (6%)	0	100	100
21	U	51/67 (76%)	45 (88%)	5 (10%)	1 (2%)	6	22
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	7	27
23	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	9	32
24	X	80/92 (87%)	75 (94%)	4 (5%)	1 (1%)	9	32
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
26	Z	71/116 (61%)	62 (87%)	7 (10%)	2 (3%)	4	15
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3705/4472 (83%)	3447 (93%)	222 (6%)	36 (1%)	12	39

All (36) 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	27	LEU
8	H	19	ARG
1	A	34	ASP
10	J	65	ASN
23	W	49	ASN
23	W	77	ALA
26	Z	44	ARG
1	A	36	ASP
2	B	2	GLN
2	B	185	GLY
4	D	65	GLU
11	K	127	ALA
12	L	149	ARG
13	M	71	SER
24	X	70	ILE
26	Z	65	ASN
2	B	184	ASP
4	D	56	ARG
6	F	100	ASP
12	L	82	ALA
21	U	55	ALA
22	V	43	PRO
1	A	69	LEU
3	C	201	SER
4	D	27	ILE
4	D	97	GLN
9	I	83	GLY
1	A	88	ILE
2	B	169	GLY
6	F	27	GLY

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	169 (94%)	10 (6%)	19	50
2	B	282/283 (100%)	263 (93%)	19 (7%)	15	43
3	C	193/193 (100%)	177 (92%)	16 (8%)	10	32
4	D	117/148 (79%)	112 (96%)	5 (4%)	26	60
5	E	152/156 (97%)	146 (96%)	6 (4%)	28	63
6	F	93/94 (99%)	91 (98%)	2 (2%)	45	77
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	129 (96%)	5 (4%)	30	64
9	I	58/130 (45%)	57 (98%)	1 (2%)	53	82
10	J	118/121 (98%)	112 (95%)	6 (5%)	21	53
11	K	106/106 (100%)	103 (97%)	3 (3%)	38	72
12	L	113/127 (89%)	110 (97%)	3 (3%)	39	73
13	M	158/160 (99%)	152 (96%)	6 (4%)	29	64
14	N	149/150 (99%)	140 (94%)	9 (6%)	17	47
15	O	93/94 (99%)	91 (98%)	2 (2%)	45	77
16	P	113/117 (97%)	110 (97%)	3 (3%)	39	73
17	Q	79/80 (99%)	75 (95%)	4 (5%)	21	53
18	R	117/122 (96%)	111 (95%)	6 (5%)	21	53
19	S	71/74 (96%)	70 (99%)	1 (1%)	59	85
20	T	105/106 (99%)	99 (94%)	6 (6%)	18	49
21	U	44/53 (83%)	42 (96%)	2 (4%)	24	58
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%)	62 (94%)	4 (6%)	17	46
25	Y	120/196 (61%)	114 (95%)	6 (5%)	22	53
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%)	2959 (96%)	136 (4%)	25	59

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

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	37	VAL
1	A	38	ILE
1	A	94	LEU
1	A	131	HIS
1	A	153	ARG
1	A	175	LYS
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	16	ARG
2	B	27	ASN
2	B	49	THR
2	B	71	VAL
2	B	97	LEU
2	B	98	THR
2	B	103	ASP
2	B	108	GLU
2	B	175	LEU
2	B	190	MET
2	B	195	ARG
2	B	234	ARG
2	B	248	ARG
2	B	251	VAL
2	B	254	GLN
2	B	264	GLU
2	B	277	GLU
3	C	2	GLN
3	C	27	ARG
3	C	94	THR
3	C	136	VAL
3	C	151	GLN
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	237	GLU
3	C	240	LEU
3	C	243	VAL
4	D	24	HIS
4	D	50	VAL
4	D	137	PRO
4	D	149	ARG
4	D	170	TYR
5	E	3	VAL
5	E	7	ILE
5	E	86	VAL
5	E	102	VAL
5	E	126	ILE
5	E	156	ASP
6	F	12	LEU
6	F	46	GLU
8	H	62	HIS
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
9	I	114	TYR
10	J	45	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	127	ILE
10	J	131	THR
11	K	10	GLN
11	K	98	VAL
11	K	119	GLN
12	L	104	ASP
12	L	114	VAL
12	L	140	VAL
13	M	10	ASP
13	M	46	LEU
13	M	93	ARG
13	M	99	ARG
13	M	115	LEU
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
14	N	134	ASP
14	N	135	VAL
14	N	147	ILE
14	N	177	GLU
15	O	43	VAL
15	O	87	THR
16	P	21	VAL
16	P	52	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	18	PRO
17	Q	30	VAL
17	Q	95	GLU
18	R	13	THR
18	R	39	THR
18	R	82	GLU
18	R	119	VAL
18	R	132	ARG
18	R	143	VAL
19	S	10	VAL
20	T	26	THR
20	T	39	ASN
20	T	48	VAL
20	T	86	GLU
20	T	96	VAL
20	T	117	ASP
21	U	28	THR
21	U	47	ARG
22	V	22	ASP
23	W	13	MET
23	W	26	ILE
23	W	35	VAL
23	W	38	THR
23	W	52	VAL
23	W	73	LEU
23	W	88	THR
23	W	146	ILE
24	X	12	ILE
24	X	43	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	X	46	ASP
24	X	79	GLU
25	Y	95	THR
25	Y	103	THR
25	Y	154	ARG
25	Y	163	THR
25	Y	189	ASN
25	Y	203	VAL
28	2	18	ASN
29	3	22	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) 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	221	GLN
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
3	C	2	GLN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	103	ASN
5	E	106	ASN
5	E	119	HIS
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	40	GLN
8	H	59	GLN
8	H	62	HIS
8	H	131	GLN
10	J	52	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	107	ASN
10	J	126	ASN
10	J	142	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
11	K	119	GLN
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	142	GLN
13	M	170	ASN
14	N	93	GLN
14	N	107	ASN
14	N	132	ASN
14	N	140	GLN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	89	ASN
16	P	118	GLN
17	Q	27	GLN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	102	GLN
18	R	113	HIS
18	R	117	HIS
19	S	44	GLN
19	S	53	ASN
19	S	55	GLN
20	T	39	ASN
20	T	73	HIS
21	U	39	ASN
21	U	48	ASN
22	V	4	HIS
22	V	60	GLN
23	W	6	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	98	GLN
25	Y	119	GLN
25	Y	133	HIS
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	36	ASN
28	2	37	HIS
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	13	HIS
29	3	15	ASN
29	3	20	HIS
29	3	48	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	244 (8%)	27 (0%)
31	9	121/122 (99%)	15 (12%)	1 (0%)
All	All	2866/3045 (94%)	259 (9%)	28 (0%)

All (259) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	130	C
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	187	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	605	C
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	698	A
30	0	701	U
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1151	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1205	U
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	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	1488	U
30	0	1505	U
30	0	1506	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1562	C
30	0	1592	G
30	0	1617	C
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
30	0	1732	A
30	0	1752	G
30	0	1778	A
30	0	1779	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	1968	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2004	U
30	0	2006	C
30	0	2008	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2317	C
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2465	A
30	0	2469	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2513	A
30	0	2526	C
30	0	2527	U
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2637	A
30	0	2638	G
30	0	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	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	52	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	604	G
30	0	644	G
30	0	681	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	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1377	C
30	0	1474	C
30	0	1506	U
30	0	1692	C
30	0	1979	G
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2726	U
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
30	PSU	0	2621	30	18,21,22	1.50	2 (11%)	21,30,33	1.43	3 (14%)
30	OMG	0	2588	30	23,26,27	0.27	0	32,38,41	0.37	0
30	1MA	0	628	30	21,25,26	0.73	1 (4%)	30,37,40	0.71	1 (3%)
30	OMU	0	2587	30	19,22,23	0.31	0	25,31,34	0.38	0
30	UR3	0	2619	30	19,22,23	0.45	0	26,32,35	0.72	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	1MA	0	628	30	-	2/7/25/26	0/3/3/3
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2
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	4.86	1.43	1.36
30	0	2621	PSU	C6-C5	2.55	1.38	1.35
30	0	628	1MA	C6-N6	2.46	1.33	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	3.80	120.74	118.17
30	0	2621	PSU	C6-N1-C2	-3.12	119.79	122.69
30	0	2619	UR3	C4-N3-C2	2.91	126.92	124.58
30	0	2621	PSU	O2-C2-N1	2.91	125.78	122.79
30	0	628	1MA	N1-C2-N3	2.84	129.37	126.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.07	5 (2%) 63 54	35, 59, 97, 117	0
2	B	337/338 (99%)	-0.02	2 (0%) 85 81	36, 60, 90, 100	0
3	C	246/246 (100%)	-0.20	2 (0%) 82 77	30, 51, 75, 89	0
4	D	140/177 (79%)	1.19	19 (13%) 7 5	73, 108, 135, 146	0
5	E	172/178 (96%)	0.14	4 (2%) 61 52	51, 74, 96, 104	0
6	F	119/120 (99%)	0.31	2 (1%) 69 61	55, 78, 111, 125	0
7	G	29/348 (8%)	0.89	2 (6%) 23 18	83, 103, 109, 112	0
8	H	160/177 (90%)	0.19	5 (3%) 51 42	50, 73, 106, 113	0
9	I	70/162 (43%)	1.93	26 (37%) 1 0	137, 156, 173, 174	0
10	J	142/145 (97%)	-0.01	4 (2%) 55 46	41, 58, 78, 97	0
11	K	132/132 (100%)	-0.35	0 100 100	40, 55, 79, 82	0
12	L	145/165 (87%)	0.34	9 (6%) 26 21	34, 73, 123, 136	0
13	M	194/196 (98%)	-0.22	1 (0%) 87 83	35, 50, 66, 73	0
14	N	186/187 (99%)	0.36	6 (3%) 50 41	52, 75, 123, 135	0
15	O	115/116 (99%)	-0.03	1 (0%) 81 75	45, 61, 78, 84	0
16	P	143/149 (95%)	0.02	1 (0%) 84 79	46, 61, 77, 84	0
17	Q	95/96 (98%)	-0.13	0 100 100	44, 55, 71, 86	0
18	R	150/155 (96%)	-0.33	1 (0%) 84 79	39, 52, 71, 86	0
19	S	81/85 (95%)	-0.05	1 (1%) 76 69	49, 65, 86, 98	0
20	T	119/120 (99%)	0.04	1 (0%) 82 77	47, 62, 89, 123	0
21	U	53/67 (79%)	-0.16	0 100 100	48, 62, 79, 88	0
22	V	65/71 (91%)	0.53	9 (13%) 6 5	55, 80, 129, 134	0
23	W	154/154 (100%)	-0.06	0 100 100	41, 57, 74, 88	0
24	X	82/92 (89%)	0.35	7 (8%) 16 14	49, 67, 90, 108	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%)	-0.26	1 (0%) 84 79	31, 50, 73, 94	0
26	Z	73/116 (62%)	0.81	8 (10%) 10 9	63, 87, 101, 106	0
27	1	56/57 (98%)	-0.65	0 100 100	32, 39, 45, 53	0
28	2	46/50 (92%)	0.62	7 (15%) 5 4	41, 69, 104, 115	0
29	3	92/92 (100%)	-0.13	1 (1%) 78 71	44, 68, 81, 91	0
30	0	2749/2923 (94%)	-0.72	4 (0%) 92 90	28, 53, 96, 172	0
31	9	122/122 (100%)	-0.37	2 (1%) 70 62	45, 74, 96, 153	0
All	All	6646/7517 (88%)	-0.25	131 (1%) 65 56	28, 58, 108, 174	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	7.4
26	Z	46	SER	6.0
9	I	128	THR	5.6
4	D	10	PHE	5.1
9	I	104	ALA	5.0
4	D	63	ILE	5.0
9	I	71	ALA	4.9
9	I	74	ILE	4.6
26	Z	106	SER	4.6
9	I	66	GLY	4.3
22	V	39	ALA	4.2
28	2	49	GLU	4.1
22	V	43	PRO	4.0
4	D	174	VAL	4.0
9	I	134	ILE	3.9
12	L	60	GLU	3.9
28	2	38	LYS	3.9
5	E	53	GLU	3.7
28	2	35	ARG	3.7
22	V	40	PRO	3.7
22	V	2	VAL	3.7
4	D	90	LEU	3.6
9	I	113	SER	3.6
4	D	18	ILE	3.6
9	I	124	VAL	3.6
9	I	106	GLN	3.5
9	I	120	ALA	3.5
26	Z	35	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	100	VAL	3.4
9	I	132	VAL	3.4
4	D	35	ALA	3.4
1	A	37	VAL	3.3
9	I	67	VAL	3.3
4	D	55	LYS	3.3
4	D	107	GLY	3.3
7	G	12	ILE	3.3
4	D	57	THR	3.3
8	H	171	GLY	3.3
12	L	148	GLU	3.2
14	N	168	LEU	3.2
8	H	114	ASP	3.1
6	F	99	THR	3.1
24	X	83	ALA	3.0
5	E	154	ILE	3.0
8	H	174	LEU	3.0
14	N	154	LEU	3.0
24	X	66	THR	3.0
1	A	36	ASP	3.0
1	A	32	VAL	3.0
9	I	70	THR	3.0
24	X	87	ALA	3.0
9	I	97	VAL	3.0
9	I	72	GLU	2.9
30	O	735	C	2.9
8	H	115	GLY	2.9
19	S	81	ILE	2.9
4	D	134	LEU	2.8
9	I	73	LEU	2.8
10	J	92	GLN	2.8
10	J	70	PHE	2.8
30	O	2769	C	2.8
26	Z	44	ARG	2.8
29	3	41	GLU	2.8
7	G	71	LEU	2.8
22	V	42	ASN	2.8
9	I	68	PRO	2.8
24	X	85	VAL	2.7
28	2	37	HIS	2.7
4	D	59	GLY	2.7
14	N	166	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	1	PRO	2.6
13	M	194	GLY	2.6
10	J	4	ALA	2.6
12	L	149	ARG	2.6
12	L	146	GLY	2.6
25	Y	235	GLU	2.6
9	I	116	LEU	2.6
10	J	79	PHE	2.6
4	D	65	GLU	2.5
16	P	143	ALA	2.5
24	X	65	ASN	2.5
30	O	10	U	2.5
4	D	135	VAL	2.5
12	L	150	GLN	2.5
14	N	1	ALA	2.5
22	V	41	GLU	2.5
9	I	127	CYS	2.5
9	I	108	HIS	2.5
6	F	17	LEU	2.5
26	Z	45	VAL	2.4
22	V	44	GLY	2.4
14	N	158	LEU	2.4
28	2	48	ASP	2.4
4	D	171	ASP	2.4
8	H	43	ALA	2.3
31	9	2	U	2.3
1	A	211	LYS	2.3
4	D	61	PHE	2.3
24	X	84	ILE	2.3
14	N	169	PRO	2.3
2	B	34	GLY	2.3
4	D	53	LYS	2.3
20	T	118	SER	2.3
26	Z	34	SER	2.3
1	A	237	GLY	2.3
4	D	75	LEU	2.2
26	Z	58	ASN	2.2
5	E	10	ASP	2.2
28	2	31	ARG	2.2
24	X	10	VAL	2.2
4	D	11	HIS	2.2
9	I	85	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	145	LEU	2.2
12	L	99	GLU	2.2
22	V	36	ALA	2.2
31	9	1	U	2.2
4	D	172	VAL	2.2
18	R	150	PRO	2.2
12	L	105	TYR	2.2
15	O	24	ALA	2.2
3	C	63	SER	2.1
9	I	88	GLN	2.1
3	C	61	PHE	2.1
12	L	44	GLU	2.1
30	0	1199	A	2.1
9	I	107	LYS	2.1
28	2	20	ARG	2.0
9	I	130	LEU	2.0
26	Z	36	GLY	2.0
9	I	103	ILE	2.0
5	E	100	ASP	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	1MA	0	628	23/24	0.98	0.06	35,38,38,39	0
30	OMU	0	2587	21/22	0.98	0.06	40,43,46,49	0
30	OMG	0	2588	24/25	0.98	0.06	38,42,43,43	0
30	UR3	0	2619	21/22	0.98	0.06	43,45,48,49	0
30	PSU	0	2621	20/21	0.98	0.06	35,38,47,48	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
34	SR	0	9006	1/1	0.50	0.29	200,200,200,200	0
35	NA	0	8518	1/1	0.65	0.48	94,94,94,94	0
35	NA	0	8525	1/1	0.66	0.22	78,78,78,78	0
34	SR	0	8976	1/1	0.73	0.19	200,200,200,200	0
34	SR	9	8980	1/1	0.76	0.12	200,200,200,200	0
35	NA	9	8572	1/1	0.76	0.46	111,111,111,111	0
35	NA	0	8571	1/1	0.78	0.16	77,77,77,77	0
34	SR	0	8919	1/1	0.78	0.15	192,192,192,192	0
34	SR	0	8991	1/1	0.79	0.17	197,197,197,197	0
35	NA	J	8538	1/1	0.79	0.18	60,60,60,60	0
34	SR	0	9001	1/1	0.80	0.12	173,173,173,173	0
35	NA	0	8559	1/1	0.82	0.29	76,76,76,76	0
35	NA	0	8562	1/1	0.82	0.31	74,74,74,74	0
34	SR	0	8938	1/1	0.83	0.11	192,192,192,192	0
34	SR	0	8983	1/1	0.83	0.20	195,195,195,195	0
34	SR	0	8947	1/1	0.83	0.14	200,200,200,200	0
34	SR	0	8993	1/1	0.83	0.12	182,182,182,182	0
34	SR	0	8996	1/1	0.83	0.28	200,200,200,200	0
34	SR	A	8977	1/1	0.84	0.08	161,161,161,161	0
34	SR	0	8979	1/1	0.84	0.13	198,198,198,198	0
34	SR	0	8994	1/1	0.85	0.31	200,200,200,200	0
34	SR	0	8971	1/1	0.85	0.12	180,180,180,180	0
35	NA	0	8564	1/1	0.86	0.15	81,81,81,81	0
34	SR	0	8959	1/1	0.86	0.08	174,174,174,174	0
35	NA	0	8573	1/1	0.86	0.12	77,77,77,77	0
35	NA	0	8554	1/1	0.86	0.38	78,78,78,78	0
34	SR	0	8997	1/1	0.87	0.21	200,200,200,200	0
32	MG	0	8049	1/1	0.87	0.19	68,68,68,68	0
35	NA	0	8522	1/1	0.87	0.24	83,83,83,83	0
32	MG	A	8051	1/1	0.87	0.12	72,72,72,72	0
35	NA	0	8550	1/1	0.87	0.21	61,61,61,61	0
34	SR	B	8987	1/1	0.87	0.35	200,200,200,200	0
32	MG	0	8040	1/1	0.88	0.26	96,96,96,96	0
35	NA	0	8502	1/1	0.88	0.21	65,65,65,65	0
35	NA	0	8561	1/1	0.88	0.47	78,78,78,78	0
34	SR	0	8922	1/1	0.88	0.20	170,170,170,170	0
34	SR	0	9002	1/1	0.88	0.15	184,184,184,184	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	8080	1/1	0.88	0.08	69,69,69,69	0
35	NA	0	8546	1/1	0.88	0.28	112,112,112,112	0
34	SR	0	8988	1/1	0.88	0.07	173,173,173,173	0
35	NA	0	8570	1/1	0.89	0.14	60,60,60,60	0
35	NA	0	8514	1/1	0.89	0.18	48,48,48,48	0
35	NA	0	8556	1/1	0.89	0.36	49,49,49,49	0
35	NA	0	8574	1/1	0.89	0.35	55,55,55,55	0
35	NA	0	8575	1/1	0.89	0.35	86,86,86,86	0
35	NA	9	8543	1/1	0.89	0.28	49,49,49,49	0
34	SR	9	9003	1/1	0.89	0.09	170,170,170,170	0
32	MG	0	8071	1/1	0.90	0.24	71,71,71,71	0
34	SR	0	9004	1/1	0.90	0.40	200,200,200,200	0
34	SR	0	8933	1/1	0.90	0.16	150,150,150,150	0
35	NA	0	8565	1/1	0.90	0.20	68,68,68,68	0
35	NA	0	8569	1/1	0.90	0.14	54,54,54,54	0
35	NA	0	8536	1/1	0.90	0.08	65,65,65,65	0
32	MG	0	8073	1/1	0.90	0.31	83,83,83,83	0
35	NA	0	8548	1/1	0.90	0.18	55,55,55,55	0
34	SR	0	8944	1/1	0.90	0.15	182,182,182,182	0
32	MG	0	8033	1/1	0.90	0.11	49,49,49,49	0
34	SR	0	9000	1/1	0.90	0.22	177,177,177,177	0
34	SR	0	8951	1/1	0.90	0.08	142,142,142,142	0
34	SR	B	8950	1/1	0.91	0.10	132,132,132,132	0
34	SR	0	8939	1/1	0.91	0.10	160,160,160,160	0
34	SR	0	8998	1/1	0.91	0.17	175,175,175,175	0
35	NA	0	8537	1/1	0.91	0.07	41,41,41,41	0
35	NA	0	8544	1/1	0.91	0.34	75,75,75,75	0
34	SR	0	8969	1/1	0.91	0.23	160,160,160,160	0
34	SR	0	8927	1/1	0.91	0.12	151,151,151,151	0
35	NA	0	8509	1/1	0.91	0.15	69,69,69,69	0
35	NA	0	8511	1/1	0.91	0.13	59,59,59,59	0
34	SR	0	8975	1/1	0.91	0.11	135,135,135,135	0
35	NA	0	8557	1/1	0.91	0.09	52,52,52,52	0
34	SR	0	8920	1/1	0.91	0.12	134,134,134,134	0
34	SR	0	8970	1/1	0.92	0.07	128,128,128,128	0
32	MG	0	8037	1/1	0.92	0.25	90,90,90,90	0
32	MG	0	8060	1/1	0.92	0.12	61,61,61,61	0
34	SR	0	8958	1/1	0.92	0.08	123,123,123,123	0
32	MG	0	8063	1/1	0.92	0.20	71,71,71,71	0
34	SR	0	8981	1/1	0.92	0.15	153,153,153,153	0
34	SR	0	8915	1/1	0.92	0.09	131,131,131,131	0
34	SR	0	8986	1/1	0.92	0.14	200,200,200,200	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8506	1/1	0.92	0.11	68,68,68,68	0
35	NA	0	8563	1/1	0.92	0.51	94,94,94,94	0
35	NA	0	8553	1/1	0.93	0.13	68,68,68,68	0
34	SR	0	8924	1/1	0.93	0.15	135,135,135,135	0
35	NA	0	8555	1/1	0.93	0.16	51,51,51,51	0
32	MG	0	8081	1/1	0.93	0.13	74,74,74,74	0
34	SR	0	8955	1/1	0.93	0.16	200,200,200,200	0
34	SR	0	8956	1/1	0.93	0.08	155,155,155,155	0
34	SR	0	8957	1/1	0.93	0.19	196,196,196,196	0
35	NA	0	8516	1/1	0.93	0.10	42,42,42,42	0
34	SR	0	8982	1/1	0.93	0.30	200,200,200,200	0
32	MG	0	8092	1/1	0.93	0.09	67,67,67,67	0
34	SR	0	8984	1/1	0.93	0.07	123,123,123,123	0
35	NA	0	8529	1/1	0.93	0.11	45,45,45,45	0
34	SR	0	8985	1/1	0.93	0.12	143,143,143,143	0
33	CL	0	8822	1/1	0.93	0.34	106,106,106,106	0
34	SR	0	9007	1/1	0.93	0.39	200,200,200,200	0
32	MG	0	8039	1/1	0.93	0.18	77,77,77,77	0
35	NA	0	8547	1/1	0.93	0.18	54,54,54,54	0
34	SR	0	8989	1/1	0.93	0.15	185,185,185,185	0
32	MG	T	8057	1/1	0.93	0.19	65,65,65,65	0
33	CL	J	8801	1/1	0.94	0.13	79,79,79,79	0
33	CL	0	8816	1/1	0.94	0.12	85,85,85,85	0
35	NA	0	8549	1/1	0.94	0.14	58,58,58,58	0
35	NA	S	8510	1/1	0.94	0.07	49,49,49,49	0
34	SR	0	8992	1/1	0.94	0.21	137,137,137,137	0
35	NA	0	8505	1/1	0.94	0.39	49,49,49,49	0
32	MG	0	8031	1/1	0.94	0.05	72,72,72,72	0
34	SR	0	8973	1/1	0.94	0.08	137,137,137,137	0
34	SR	0	8995	1/1	0.94	0.11	140,140,140,140	0
35	NA	0	8512	1/1	0.94	0.17	56,56,56,56	0
35	NA	0	8560	1/1	0.94	0.18	83,83,83,83	0
34	SR	0	8953	1/1	0.94	0.12	157,157,157,157	0
34	SR	A	8929	1/1	0.94	0.18	137,137,137,137	0
32	MG	0	8089	1/1	0.94	0.08	57,57,57,57	0
35	NA	0	8520	1/1	0.94	0.15	53,53,53,53	0
32	MG	0	8091	1/1	0.94	0.07	62,62,62,62	0
32	MG	0	8038	1/1	0.94	0.07	75,75,75,75	0
35	NA	0	8526	1/1	0.94	0.08	57,57,57,57	0
32	MG	9	8074	1/1	0.94	0.14	77,77,77,77	0
34	SR	0	8960	1/1	0.94	0.07	150,150,150,150	0
34	SR	0	8964	1/1	0.94	0.08	139,139,139,139	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	8541	1/1	0.94	0.11	69,69,69,69	0
34	SR	0	8967	1/1	0.94	0.07	132,132,132,132	0
34	SR	0	8968	1/1	0.94	0.11	165,165,165,165	0
32	MG	0	8064	1/1	0.95	0.06	37,37,37,37	0
33	CL	N	8807	1/1	0.95	0.11	71,71,71,71	0
35	NA	0	8524	1/1	0.95	0.08	58,58,58,58	0
32	MG	0	8083	1/1	0.95	0.18	73,73,73,73	0
32	MG	0	8035	1/1	0.95	0.13	68,68,68,68	0
35	NA	0	8528	1/1	0.95	0.08	58,58,58,58	0
34	SR	0	8954	1/1	0.95	0.10	112,112,112,112	0
35	NA	0	8533	1/1	0.95	0.14	67,67,67,67	0
32	MG	0	8090	1/1	0.95	0.08	62,62,62,62	0
34	SR	0	8974	1/1	0.95	0.10	149,149,149,149	0
32	MG	0	8036	1/1	0.95	0.13	50,50,50,50	0
35	NA	0	8566	1/1	0.95	0.13	60,60,60,60	0
35	NA	0	8568	1/1	0.95	0.14	50,50,50,50	0
34	SR	0	8928	1/1	0.95	0.07	135,135,135,135	0
32	MG	0	8077	1/1	0.95	0.07	49,49,49,49	0
32	MG	0	8030	1/1	0.95	0.22	69,69,69,69	0
34	SR	F	9005	1/1	0.95	0.08	134,134,134,134	0
34	SR	0	8962	1/1	0.95	0.10	175,175,175,175	0
34	SR	0	8963	1/1	0.95	0.06	134,134,134,134	0
35	NA	0	8551	1/1	0.95	0.09	59,59,59,59	0
34	SR	0	8941	1/1	0.95	0.07	116,116,116,116	0
37	K	0	8401	1/1	0.95	0.10	74,74,74,74	0
32	MG	0	8067	1/1	0.96	0.04	34,34,34,34	0
34	SR	0	8946	1/1	0.96	0.07	122,122,122,122	0
35	NA	0	8507	1/1	0.96	0.06	42,42,42,42	0
34	SR	3	8999	1/1	0.96	0.06	106,106,106,106	0
34	SR	0	8972	1/1	0.96	0.17	141,141,141,141	0
35	NA	0	8552	1/1	0.96	0.10	72,72,72,72	0
33	CL	L	8810	1/1	0.96	0.07	61,61,61,61	0
34	SR	0	8916	1/1	0.96	0.08	113,113,113,113	0
34	SR	0	8917	1/1	0.96	0.07	111,111,111,111	0
32	MG	0	8085	1/1	0.96	0.13	73,73,73,73	0
33	CL	O	8808	1/1	0.96	0.09	81,81,81,81	0
35	NA	0	8521	1/1	0.96	0.09	65,65,65,65	0
33	CL	0	8813	1/1	0.96	0.05	61,61,61,61	0
35	NA	0	8523	1/1	0.96	0.10	45,45,45,45	0
33	CL	0	8815	1/1	0.96	0.08	78,78,78,78	0
34	SR	0	8926	1/1	0.96	0.08	127,127,127,127	0
32	MG	0	8053	1/1	0.96	0.07	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8527	1/1	0.96	0.17	71,71,71,71	0
32	MG	0	8029	1/1	0.96	0.18	48,48,48,48	0
35	NA	0	8567	1/1	0.96	0.23	80,80,80,80	0
32	MG	0	8032	1/1	0.96	0.05	46,46,46,46	0
35	NA	0	8530	1/1	0.96	0.10	55,55,55,55	0
35	NA	C	8503	1/1	0.96	0.06	44,44,44,44	0
35	NA	0	8534	1/1	0.96	0.09	42,42,42,42	0
35	NA	0	8535	1/1	0.96	0.13	53,53,53,53	0
32	MG	0	8052	1/1	0.96	0.07	52,52,52,52	0
35	NA	Q	8540	1/1	0.96	0.11	60,60,60,60	0
35	NA	R	8532	1/1	0.96	0.09	46,46,46,46	0
32	MG	0	8066	1/1	0.96	0.13	76,76,76,76	0
33	CL	B	8819	1/1	0.96	0.14	54,54,54,54	0
37	K	0	8402	1/1	0.96	0.10	87,87,87,87	0
35	NA	0	8545	1/1	0.97	0.12	41,41,41,41	0
34	SR	0	8921	1/1	0.97	0.05	92,92,92,92	0
32	MG	0	8059	1/1	0.97	0.05	59,59,59,59	0
32	MG	0	8078	1/1	0.97	0.10	61,61,61,61	0
35	NA	0	8508	1/1	0.97	0.10	39,39,39,39	0
32	MG	0	8047	1/1	0.97	0.13	65,65,65,65	0
32	MG	0	8093	1/1	0.97	0.04	35,35,35,35	0
32	MG	B	8042	1/1	0.97	0.12	50,50,50,50	0
35	NA	0	8513	1/1	0.97	0.08	58,58,58,58	0
34	SR	0	8965	1/1	0.97	0.07	124,124,124,124	0
35	NA	0	8515	1/1	0.97	0.05	37,37,37,37	0
34	SR	0	8931	1/1	0.97	0.06	117,117,117,117	0
35	NA	0	8517	1/1	0.97	0.07	36,36,36,36	0
35	NA	0	8558	1/1	0.97	0.11	50,50,50,50	0
34	SR	A	8930	1/1	0.97	0.04	104,104,104,104	0
34	SR	0	8934	1/1	0.97	0.12	130,130,130,130	0
33	CL	A	8809	1/1	0.97	0.14	74,74,74,74	0
32	MG	0	8082	1/1	0.97	0.08	69,69,69,69	0
32	MG	0	8072	1/1	0.97	0.05	53,53,53,53	0
33	CL	J	8821	1/1	0.97	0.11	71,71,71,71	0
34	SR	S	8961	1/1	0.97	0.06	122,122,122,122	0
34	SR	1	8952	1/1	0.97	0.05	91,91,91,91	0
34	SR	9	8978	1/1	0.97	0.05	133,133,133,133	0
34	SR	0	8948	1/1	0.97	0.06	102,102,102,102	0
34	SR	0	8949	1/1	0.97	0.08	119,119,119,119	0
32	MG	0	8056	1/1	0.97	0.09	51,51,51,51	0
32	MG	0	8087	1/1	0.97	0.05	47,47,47,47	0
35	NA	M	8539	1/1	0.97	0.08	34,34,34,34	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	8076	1/1	0.97	0.06	42,42,42,42	0
33	CL	Y	8820	1/1	0.97	0.08	51,51,51,51	0
33	CL	0	8803	1/1	0.97	0.09	62,62,62,62	0
35	NA	0	8501	1/1	0.97	0.12	44,44,44,44	0
35	NA	0	8542	1/1	0.97	0.25	66,66,66,66	0
33	CL	0	8805	1/1	0.97	0.06	67,67,67,67	0
32	MG	0	8034	1/1	0.98	0.04	45,45,45,45	0
33	CL	0	8817	1/1	0.98	0.03	65,65,65,65	0
34	SR	0	8923	1/1	0.98	0.04	116,116,116,116	0
33	CL	J	8802	1/1	0.98	0.07	76,76,76,76	0
34	SR	0	8925	1/1	0.98	0.07	91,91,91,91	0
32	MG	0	8088	1/1	0.98	0.04	42,42,42,42	0
32	MG	0	8026	1/1	0.98	0.03	37,37,37,37	0
33	CL	M	8818	1/1	0.98	0.07	47,47,47,47	0
35	NA	0	8519	1/1	0.98	0.04	50,50,50,50	0
32	MG	K	8054	1/1	0.98	0.07	50,50,50,50	0
34	SR	0	8966	1/1	0.98	0.05	111,111,111,111	0
32	MG	0	8079	1/1	0.98	0.05	55,55,55,55	0
32	MG	0	8055	1/1	0.98	0.09	46,46,46,46	0
34	SR	0	8936	1/1	0.98	0.04	94,94,94,94	0
34	SR	0	8937	1/1	0.98	0.05	115,115,115,115	0
34	SR	R	8912	1/1	0.98	0.05	86,86,86,86	0
33	CL	3	8804	1/1	0.98	0.05	67,67,67,67	0
32	MG	0	8044	1/1	0.98	0.04	53,53,53,53	0
34	SR	0	8942	1/1	0.98	0.05	133,133,133,133	0
34	SR	0	8943	1/1	0.98	0.07	117,117,117,117	0
32	MG	0	8046	1/1	0.98	0.05	41,41,41,41	0
34	SR	0	8945	1/1	0.98	0.06	112,112,112,112	0
34	SR	0	8908	1/1	0.98	0.05	110,110,110,110	0
34	SR	0	8911	1/1	0.98	0.04	85,85,85,85	0
34	SR	0	8914	1/1	0.98	0.13	110,110,110,110	0
33	CL	0	8811	1/1	0.98	0.11	68,68,68,68	0
33	CL	0	8812	1/1	0.98	0.07	54,54,54,54	0
32	MG	0	8024	1/1	0.98	0.06	55,55,55,55	0
33	CL	0	8814	1/1	0.98	0.08	60,60,60,60	0
32	MG	0	8075	1/1	0.98	0.04	46,46,46,46	0
34	SR	0	8990	1/1	0.98	0.06	137,137,137,137	0
32	MG	0	8050	1/1	0.99	0.05	37,37,37,37	0
32	MG	0	8002	1/1	0.99	0.05	32,32,32,32	0
32	MG	0	8003	1/1	0.99	0.08	34,34,34,34	0
32	MG	0	8005	1/1	0.99	0.05	33,33,33,33	0
32	MG	0	8084	1/1	0.99	0.09	37,37,37,37	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	8006	1/1	0.99	0.04	30,30,30,30	0
32	MG	0	8058	1/1	0.99	0.04	23,23,23,23	0
32	MG	0	8007	1/1	0.99	0.04	38,38,38,38	0
32	MG	0	8008	1/1	0.99	0.08	27,27,27,27	0
32	MG	0	8061	1/1	0.99	0.06	30,30,30,30	0
32	MG	0	8062	1/1	0.99	0.07	50,50,50,50	0
35	NA	0	8504	1/1	0.99	0.05	37,37,37,37	0
34	SR	0	8935	1/1	0.99	0.04	80,80,80,80	0
32	MG	0	8010	1/1	0.99	0.03	35,35,35,35	0
32	MG	0	8012	1/1	0.99	0.03	25,25,25,25	0
32	MG	0	8015	1/1	0.99	0.06	36,36,36,36	0
32	MG	0	8016	1/1	0.99	0.07	60,60,60,60	0
34	SR	0	8940	1/1	0.99	0.04	93,93,93,93	0
32	MG	0	8068	1/1	0.99	0.06	54,54,54,54	0
32	MG	0	8069	1/1	0.99	0.07	72,72,72,72	0
34	SR	1	8913	1/1	0.99	0.04	96,96,96,96	0
32	MG	0	8070	1/1	0.99	0.03	45,45,45,45	0
34	SR	3	8932	1/1	0.99	0.02	79,79,79,79	0
32	MG	0	8017	1/1	0.99	0.09	25,25,25,25	0
34	SR	0	8901	1/1	0.99	0.03	85,85,85,85	0
34	SR	0	8904	1/1	0.99	0.08	66,66,66,66	0
34	SR	0	8905	1/1	0.99	0.14	68,68,68,68	0
32	MG	0	8018	1/1	0.99	0.10	46,46,46,46	0
34	SR	0	8909	1/1	0.99	0.05	85,85,85,85	0
34	SR	0	8910	1/1	0.99	0.05	101,101,101,101	0
32	MG	0	8043	1/1	0.99	0.06	49,49,49,49	0
32	MG	0	8020	1/1	0.99	0.11	43,43,43,43	0
32	MG	Y	8086	1/1	0.99	0.03	46,46,46,46	0
33	CL	R	8806	1/1	0.99	0.04	52,52,52,52	0
32	MG	0	8001	1/1	0.99	0.02	33,33,33,33	0
34	SR	0	8918	1/1	0.99	0.07	85,85,85,85	0
32	MG	0	8048	1/1	0.99	0.08	26,26,26,26	0
35	NA	0	8531	1/1	0.99	0.09	44,44,44,44	0
36	CD	O	8705	1/1	0.99	0.05	94,94,94,94	0
36	CD	Z	8703	1/1	0.99	0.02	91,91,91,91	0
32	MG	0	8027	1/1	0.99	0.03	49,49,49,49	0
34	SR	0	9008	1/1	0.99	0.04	89,89,89,89	0
32	MG	0	8004	1/1	1.00	0.04	30,30,30,30	0
32	MG	0	8025	1/1	1.00	0.01	35,35,35,35	0
32	MG	0	8011	1/1	1.00	0.02	33,33,33,33	0
32	MG	0	8009	1/1	1.00	0.08	29,29,29,29	0
32	MG	0	8028	1/1	1.00	0.04	27,27,27,27	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	8013	1/1	1.00	0.02	30,30,30,30	0
34	SR	0	8902	1/1	1.00	0.02	66,66,66,66	0
34	SR	0	8903	1/1	1.00	0.10	58,58,58,58	0
32	MG	0	8041	1/1	1.00	0.05	31,31,31,31	0
32	MG	0	8019	1/1	1.00	0.04	27,27,27,27	0
34	SR	0	8906	1/1	1.00	0.05	60,60,60,60	0
34	SR	0	8907	1/1	1.00	0.03	56,56,56,56	0
32	MG	0	8014	1/1	1.00	0.07	35,35,35,35	0
32	MG	0	8045	1/1	1.00	0.04	35,35,35,35	0
32	MG	0	8021	1/1	1.00	0.04	30,30,30,30	0
36	CD	U	8701	1/1	1.00	0.01	72,72,72,72	0
32	MG	0	8022	1/1	1.00	0.05	32,32,32,32	0
36	CD	1	8702	1/1	1.00	0.05	65,65,65,65	0
36	CD	3	8704	1/1	1.00	0.03	81,81,81,81	0
32	MG	0	8023	1/1	1.00	0.03	32,32,32,32	0
32	MG	0	8065	1/1	1.00	0.02	49,49,49,49	0

6.5 Other polymers

There are no such residues in this entry.