



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:33 PM GMT

PDB ID : 4WCE
Title : The crystal structure of the large ribosomal subunit of Staphylococcus aureus
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.
Deposited on : 2014-09-04
Resolution : 3.53 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

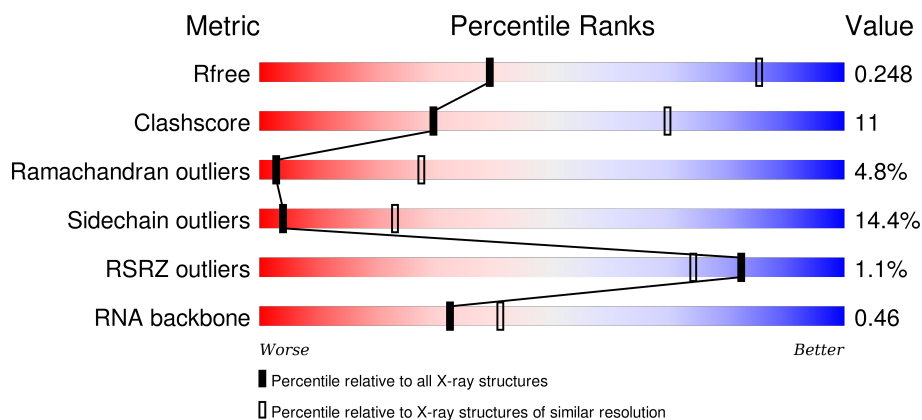
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 Å.

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










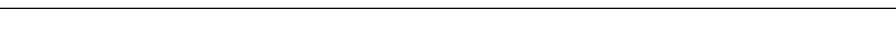
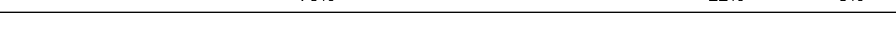
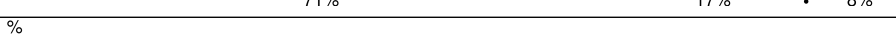
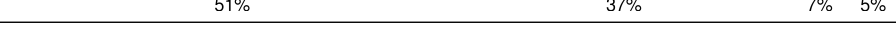









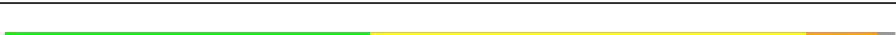
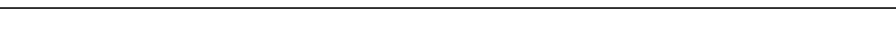
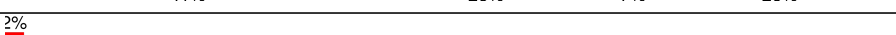

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1089 (3.64-3.40)
Clashscore	102246	1197 (3.64-3.40)
Ramachandran outliers	100387	1159 (3.64-3.40)
Sidechain outliers	100360	1160 (3.64-3.40)
RSRZ outliers	91569	1096 (3.64-3.40)
RNA backbone	2183	1051 (4.22-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	X	2923	
2	Y	114	
3	A	277	
4	B	220	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MPD	X	3002	-	-	-	X
29	MPD	X	3006	-	-	-	X
29	MPD	X	3007	-	-	-	X
29	MPD	X	3008	-	-	-	X
29	MPD	X	3009	-	-	-	X
29	MPD	X	3010	-	-	-	X
29	MPD	Z	101	-	-	-	X
30	MN	X	3012	-	-	-	X
30	MN	X	3047	-	-	-	X
30	MN	X	3055	-	-	-	X
30	MN	X	3153	-	-	-	X
30	MN	X	3154	-	-	-	X
30	MN	X	3166	-	-	-	X
30	MN	X	3196	-	-	-	X
30	MN	X	3197	-	-	-	X
30	MN	X	3210	-	-	-	X
30	MN	X	3213	-	-	-	X
30	MN	X	3225	-	-	-	X
30	MN	X	3230	-	-	-	X
30	MN	X	3242	-	-	-	X
30	MN	X	3252	-	-	-	X
30	MN	X	3255	-	-	-	X
30	MN	X	3260	-	-	-	X
30	MN	X	3265	-	-	-	X
30	MN	X	3271	-	-	-	X
30	MN	X	3272	-	-	-	X
30	MN	X	3273	-	-	-	X
30	MN	X	3278	-	-	-	X
30	MN	X	3279	-	-	-	X
30	MN	X	3280	-	-	-	X
30	MN	X	3283	-	-	-	X
30	MN	X	3286	-	-	-	X
31	MG	X	3030	-	-	-	X
31	MG	X	3092	-	-	-	X
31	MG	X	3103	-	-	-	X
31	MG	X	3174	-	-	-	X
33	SPD	X	3312	-	-	-	X
33	SPD	X	3313	-	-	-	X
33	SPD	X	3314	-	-	-	X
33	SPD	X	3315	-	-	-	X
34	EOH	X	3316	-	-	-	X
34	EOH	X	3318	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	EOH	X	3322	-	-	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 81909 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 RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2708	Total	C	N	O	P	0	0	0
			58077	25928	10647	18794	2708			

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	114	Total	C	N	O	P	0	0	0
			2430	1086	436	794	114			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	269	Total	C	N	O	S	0	0	0
			1686	1024	333	324	5			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1558	976	291	286	5			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1320	818	249	251	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	166	Total	C	N	O	S	0	0	0
			866	523	166	175	2			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	156	Total	C	N	O	S	0	0	0
			970	596	177	195	2			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1106	693	204	206	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			884	548	167	165	4			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			859	527	170	161	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	141	Total	C	N	O	S	0	0	0
			1068	684	198	183	3			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			908	557	177	173	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	110	Total	C	N	O	0	0	0
			705	433	137	135			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O			
			826	521	164	141	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S			
			932	587	187	154	4	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	102	Total	C	N	O	S			
			751	477	138	135	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S			
			862	537	164	158	3	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	89	Total	C	N	O	S			
			626	394	113	116	3	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	100	Total	C	N	O	S			
			683	424	127	131	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S			
			1097	690	191	214	2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			568	352	110	106			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	46	Total	C	N	O	0	0	0
			300	182	65	53			

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	0	0	0
			486	299	89	98			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	58	Total	C	N	O	S	0	0	0
			449	279	84	85	1			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	43	Total	C	N	O	S	0	0	0
			339	208	70	57	4			

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			362	222	86	53	1			

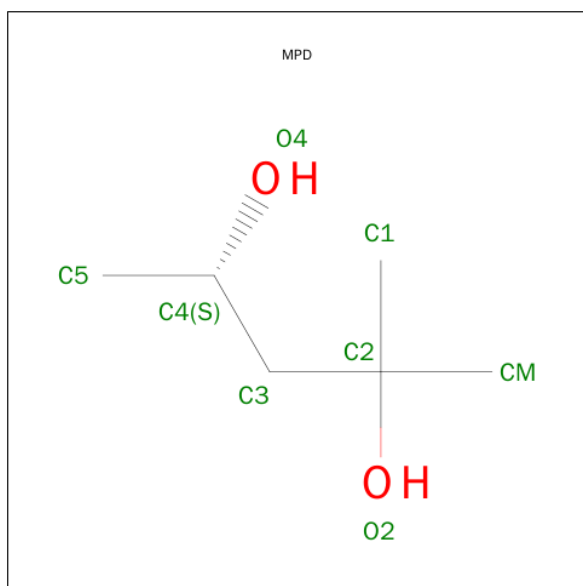
- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			420	260	84	74	2			

- Molecule 28 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			277	173	58	41	5			

- Molecule 29 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		
29	X	1	Total	C	O	0	0
			8	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	X	1	Total	C	O	0	0
			8	6	2		
29	Z	1	Total	C	O	0	0
			8	6	2		

- Molecule 30 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	J	1	Total	Mn	0	0
			1	1		
30	B	1	Total	Mn	0	0
			1	1		
30	I	2	Total	Mn	0	0
			2	2		
30	X	223	Total	Mn	0	0
			223	223		
30	R	2	Total	Mn	0	0
			2	2		
30	Y	2	Total	Mn	0	0
			2	2		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

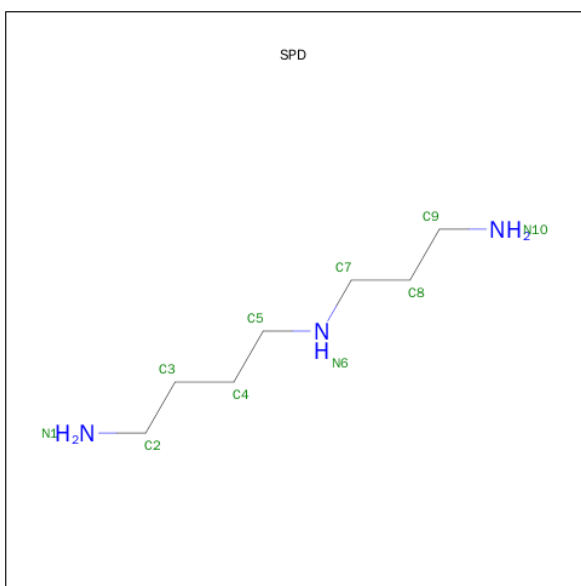
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	G	3	Total	Mg	0	0
			3	3		
31	B	2	Total	Mg	0	0
			2	2		
31	I	1	Total	Mg	0	0
			1	1		
31	C	1	Total	Mg	0	0
			1	1		
31	X	80	Total	Mg	0	0
			80	80		
31	O	1	Total	Mg	0	0
			1	1		
31	Y	3	Total	Mg	0	0
			3	3		

- Molecule 32 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 33 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



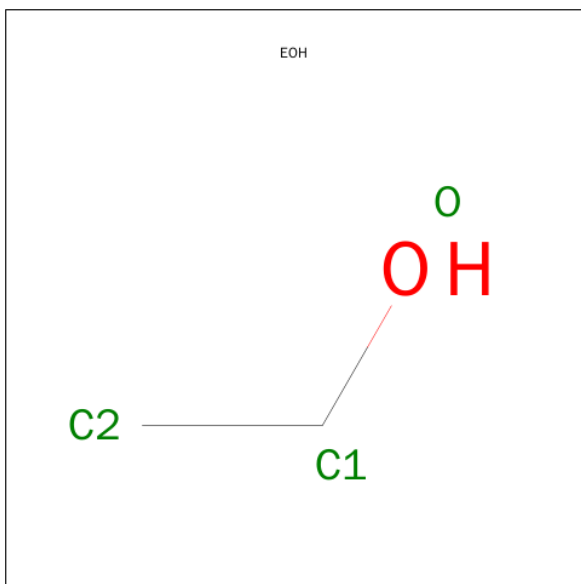
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		

- Molecule 34 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).

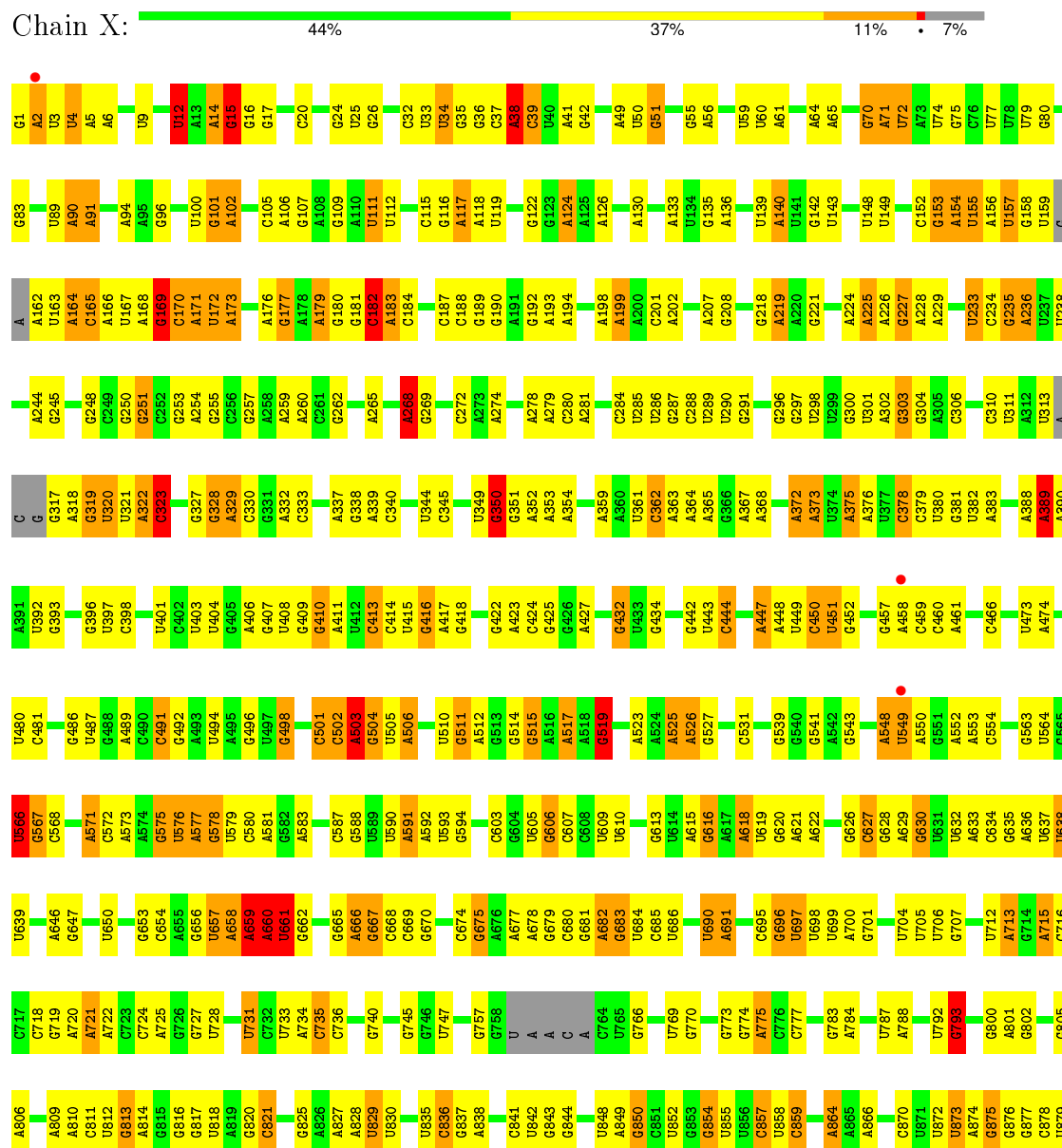


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		

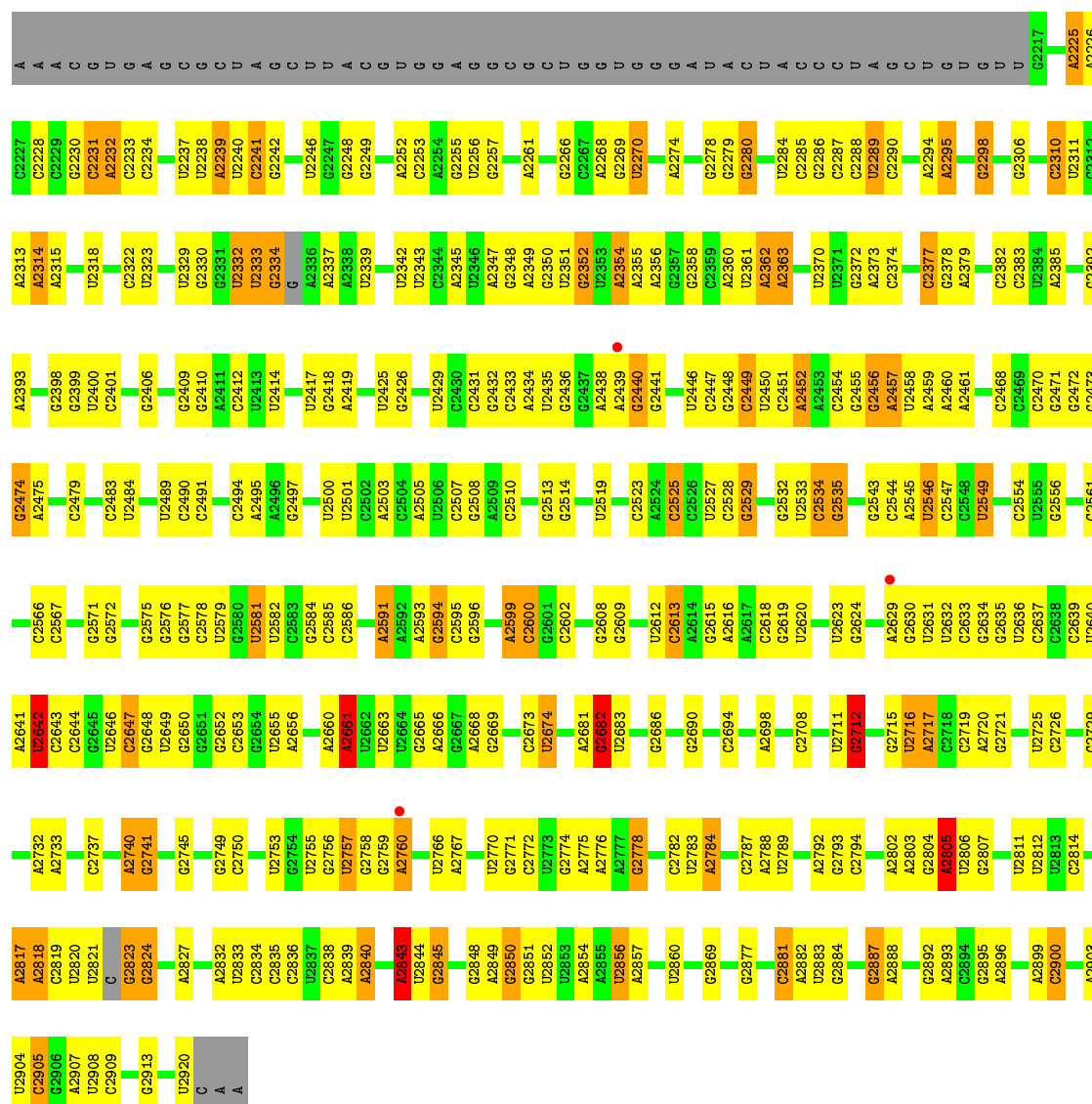
3 Residue-property plots

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

• Molecule 1: 23S rRNA

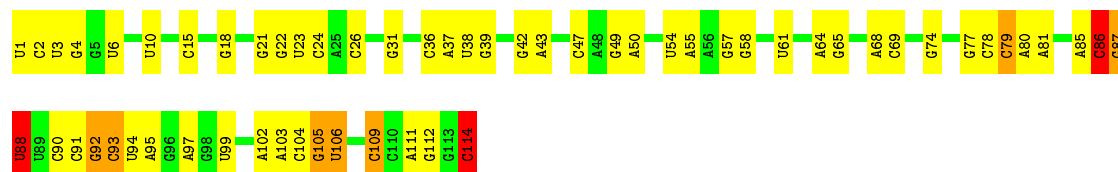


G2088	A1997	A1916	C1833	G1759	A1653	G1518	U1451		U1301	U1209	A		A1059	G966	A880
A2089	A1998	C1922	G1834	G1760	G1657	U1519	C1452	A1379	G1302	C1213	A		U1060	C967	A887
C2093	A1999	A1923	U1835	G1761	G1658	A	G1453	G1380	G1303	G1214	G		U1061	U970	G888
G2094	G1999	G1924	A1836	U1762		A1521	U1454	U1381	G1304	U1215	A		U1063	U971	U889
U2095	G2007		A1837	U1763	G1661	G1523	U	G1382	U1305	U	G		A1064	G890	G890
G2096	A2008	C1929	U1843	U1764	A1662	C1524	U	G1384	G1306	U1217	U		A1065	A891	A891
U2101	U2009	G1930	G1844	A1765	G1663	U	A1459	G1385	G1309	G1218	G		U1066	U892	U892
U2102	G2012	G1931	U1845	C1766	G1664	G1526	A		A1310	G1219	C		U1067	A985	U895
C2013	G2013	C1932	U1846	C1768	U1680	A1527	U1460	U1389	A1311	A	G		G1068	U896	U896
U2106	G2014	G1933	U1847	C1769	U1681	U1529	G1462	A1391	A1312	A1222	U		G1069	A897	A897
G2107		C1934	A1848	C1770	C1682	A1530	A1463	G1392	G1313	G1225	A		A1070	U898	U898
U2018	U2018	C		A1771	U1683	U	U1464		A1314	G1226	U		A1071	A993	A993
C2111	U2019	C	G1851	G1772	U1684	A1592		G1395	C1315		A		A1072	U995	A902
U2020	U2020	G	U1854	G1775	A1684	G1593	G1466	G1396	G1316	A1227	A		U1077	G996	G903
U2021	U2021	U	U1855	A1776	G1687	A	G1467		A1228	U1228	G		U1078	G997	A903
A2024	A2024	A	A1856	A1777	U1688	G1595	G1468	C1400	G1323	G1229	U		U1079	G998	G904
G2027	G2027	C	C1857	C1781	G1689	G1597	A1469	G1401	A1324	G1230	U		U1080	U999	U905
U2119	U2027	U	U1857	A1782	A1690	U1598	G1470	A1402	U1325	U1240			G1086	A906	A906
G2121	A2031	A	C1864	A1787	G1691	G1599	A1471	G1405	C1326	A1241			U1087	U1001	G907
A2122	A2032	U	C1865	U1788	G1692	A	C1472		G1327	U1242			U1088	U1002	
A2123	A2032	U	G1867	A1789	G1693	U1603	G1476	G1408	C1328	U1243			U1089	A1004	A911
U2119	G2036	A	U1868	G1790	G1694	G1604	U1477	U1409	G1329	U1244			U1090	G1005	U916
G2126	G2037	G	G1869	G1791	G1695	A1605	A1478	G1411	U1330	U1245			U1091	G1006	
G	A2040	U	C1870	C1792	A1696	U1609		G1412	C1335	G1257			U1092	U1007	G822
G	A2047	C	G1875	C1793	A1699	G1610	A1481	G1413	G1336	U1258			U1093	G1008	A923
A	G2048	C	A1876	U1794	U1701	C1612	G1487	G1414	A1337	G1273			U1094	G1009	G924
C	U2049	U	U1877	A1795	C1702	G1613	A1488	A1415	U1338	A1264			U1095	U1013	G925
G	A2050	A	A1880	U1796	U1703	U1614	A1489	U1416	U1339	U1265			U1096	G1015	G
G	C2051	G	U1885	A1800	A1708	G1615	U1490	G1417	G1340	C1268			U1097	G1016	G
C	C2052	U	A1886	G1803	A1709	A1616	C1491	U1421		A1269			U1098	A1017	C
U	U2053	U	G1887	U1806	G1710	U	U1492	A1422	G1347	U1272			U1099	A1018	C
U	G2056	U	U1888	U1807	G1711	A	G1493	C1423	U1348	G1274			U	A1023	C
C	A2057	C	G1889	U1808	G1718	G1555	G1494	A1424	U1349	G1275			U	A1024	C
C	C2058	U	U1890	U1809	G1719	G1556	C1495	G1425	U1350	U1276			U	A1025	C
G	C2059	U	U1891	U1810	G1720	C1557	G1496	G1429	C1351	G1277			U	G1026	C
A	A2060	U	U1892	U1811	A1721	U1558	U1498	U1430	G1352	C1278			U	A1027	C
G	U2061	U	A1893	A1812	C1730	G1559	U1499	U1431	A1353	C1279			U	G1028	G
A	G2062	A	G1894	A1813	U1731	A1560	U1500	U1432	G1354	U1280			U	A1029	C
U	C2063	U	U1895	A1814	U1732	G1561	G1501	U1433	G1355	U1281			U	G1030	G
A	A2064	C	U1896	C1815	U1733	C1562	A1502	U1434	G1356	A1282			U	U	
G	C2070	U	U	A1816	U1737	U1563	U1503	C1435	A1358	G1182			U	G1033	G942
U	C2071	U	C	C1817	C1738	G1564	U1504	C1436	A1359	G1183			U	A1034	C943
A	G2077	U	G1900	A1818	G1739	U1565	G1505	U1437	A1284	C1184			U	A1037	A945
G	A2078	U	C1901	G1819	G1740	G1566	G1506	U1438	G1360	U1185			U	A1038	A946
G	C2079	U	G1902	U1823		U1567	A1507	U1439	U1366	A1187			U	C1039	U947
A	U2078	U	G1903	C1824	A1744	U1568	C1508	A1440	C1367	A1188			U	U948	U948
A	G2080	U	U1904	U1825	A1745	G1569	G1509	C1441	G1368	A1189			U	A955	A955
C	A2081	U	G1905	U1826	G1746	U1640	U1510	C1442	G1369	A1195			U	A956	A956
C	C2082	U	U1906	G1827	G1747	G1572	C1511	G1445	C1370	A1196			U	U1043	C959
U	G2083	U	A1908	U1828	U1755	A1573	U1512	U1446	C1371	G1197			U	C960	C960
U	G2084	U	C1909	A1829	U1756	G1574	A1513	A1447	C1372	G1198			U	G961	G961
U		U	U1911	A1830	U1757	A1575	A1514	U1448	U1373	A1199			U	A1053	
G	A2087	U	A1912	A1831	G1650	A1576	G1515	U1449	G1374	A1200			U	U1056	U964
		U			C1651	A1577	C1516	A1450	G1375	A1208			U	U1058	G965
		G			A1652	A1578	A1517		G1376						



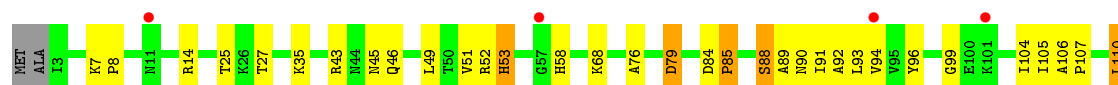
• Molecule 2: 5S rRNA

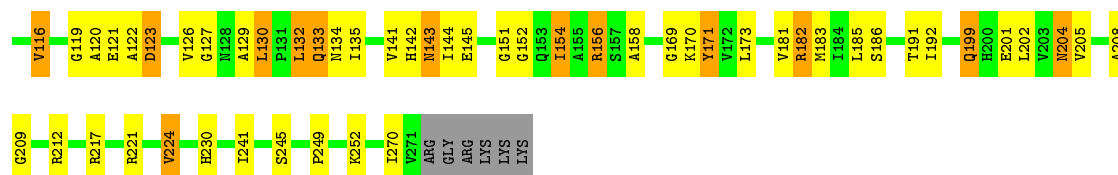
Chain Y: 48% 43% 6%



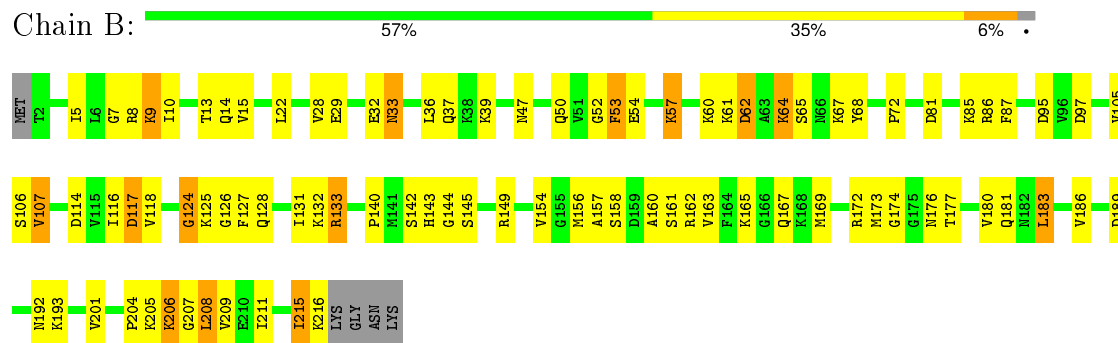
• Molecule 3: 50S ribosomal protein L2

Chain A: 66% 24% 6%

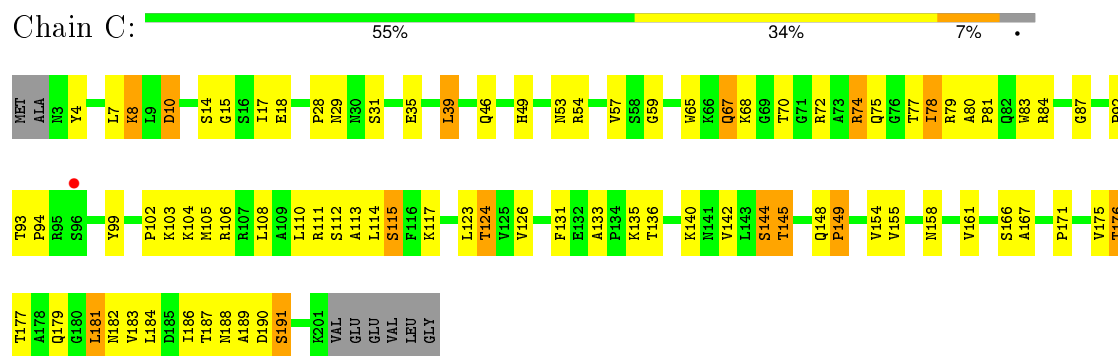




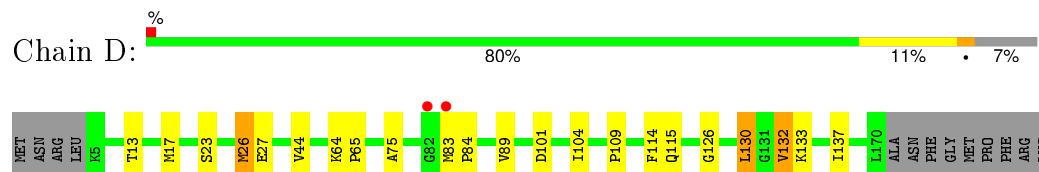
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4



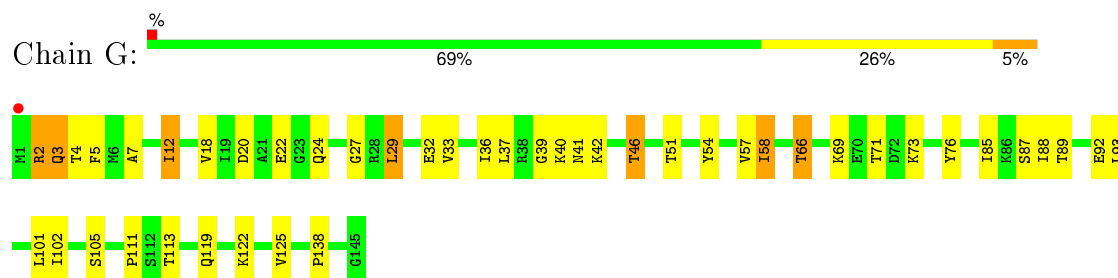
• Molecule 6: 50S ribosomal protein L5



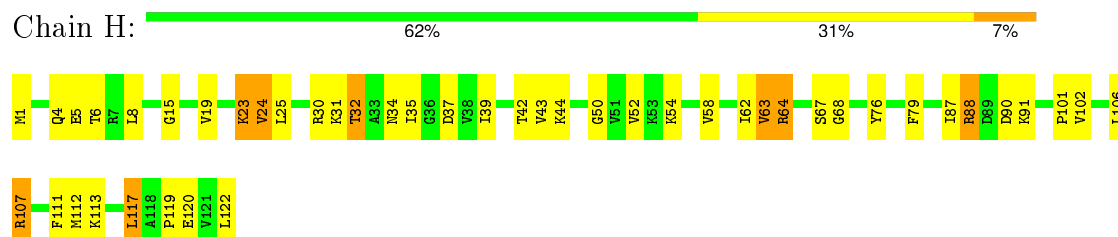
• Molecule 7: 50S ribosomal protein L6



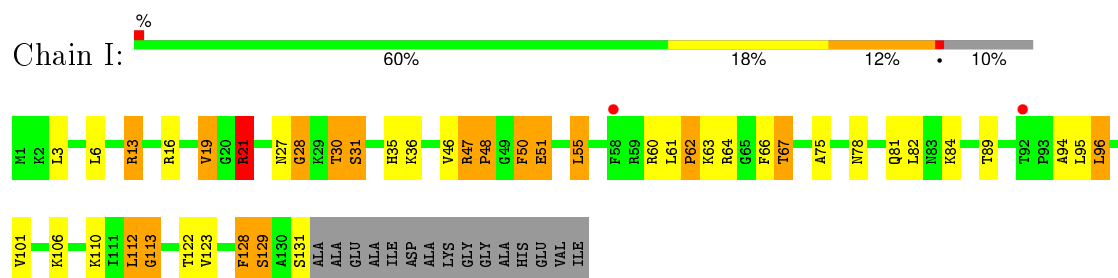
• Molecule 8: 50S ribosomal protein L13



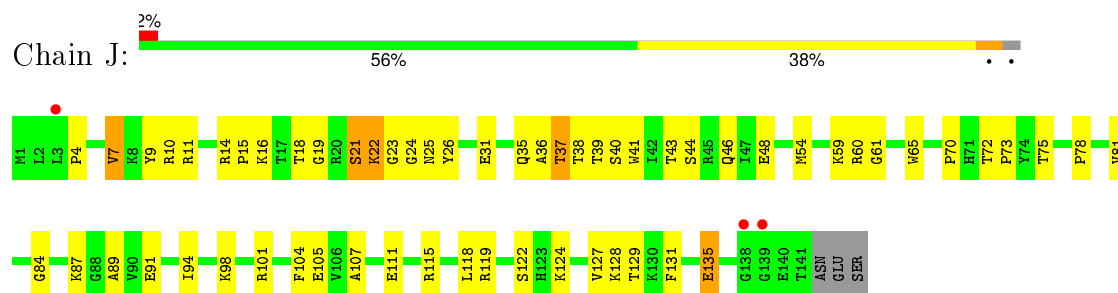
- Molecule 9: 50S ribosomal protein L14



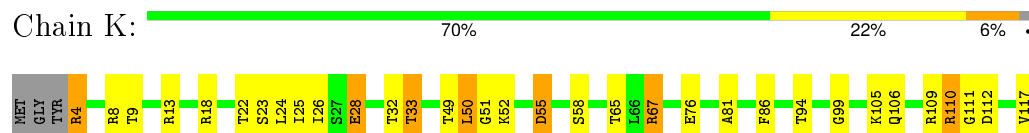
- Molecule 10: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L17

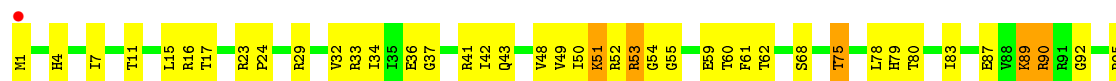


- Molecule 13: 50S ribosomal protein L18

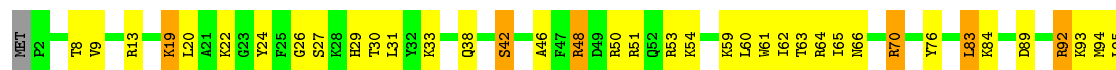




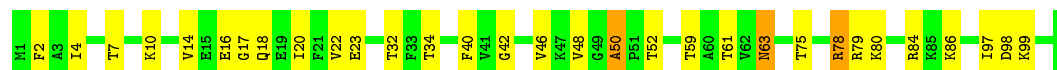
- Molecule 14: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L23

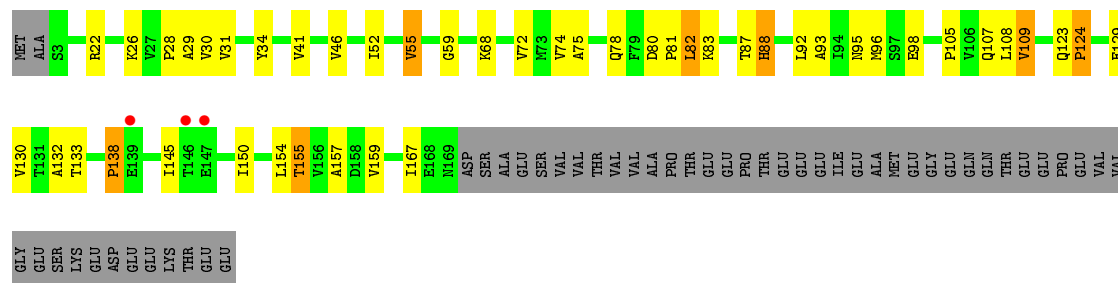


- Molecule 19: 50S ribosomal protein L24

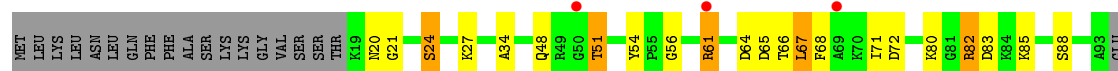




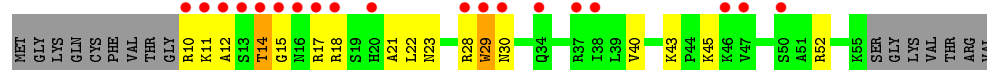
• Molecule 20: 50S ribosomal protein L25



• Molecule 21: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L28



• Molecule 23: 50S ribosomal protein L29

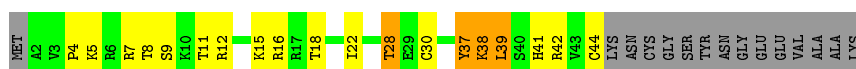


• Molecule 24: 50S ribosomal protein L30



• Molecule 25: 50S ribosomal protein L32





- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	279.76Å 279.76Å 872.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.74 – 3.53 49.74 – 3.53	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.74-3.53) 96.0 (49.74-3.53)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.246 0.206 , 0.248	Depositor DCC
R_{free} test set	11858 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	108.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 236666 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	81909	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.29% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MN, EOH, MPD, EPE, SPD

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	X	0.64	12/65032 (0.0%)	1.16	279/101388 (0.3%)
2	Y	0.56	0/2717	1.14	17/4232 (0.4%)
3	A	0.25	0/1717	0.55	0/2361
4	B	0.32	0/1581	0.62	0/2129
5	C	0.48	0/1338	0.72	0/1831
6	D	0.23	0/869	0.48	0/1205
7	E	0.27	0/982	0.51	0/1354
8	G	0.37	0/1128	0.58	0/1525
9	H	0.28	0/891	0.53	0/1203
10	I	0.58	0/868	0.91	1/1172 (0.1%)
11	J	0.30	0/1092	0.54	0/1473
12	K	0.31	0/911	0.59	0/1219
13	L	0.25	0/711	0.54	0/970
14	M	0.51	0/838	0.76	0/1132
15	N	0.38	0/944	0.59	0/1252
16	O	0.30	0/761	0.58	1/1022 (0.1%)
17	P	0.55	0/870	0.78	0/1171
18	Q	0.40	0/633	0.66	0/859
19	R	0.27	0/688	0.59	0/930
20	S	0.28	0/1109	0.58	0/1522
21	T	0.26	0/574	0.48	0/763
22	U	0.28	0/305	0.55	0/419
23	V	0.29	0/487	0.53	0/654
24	W	0.54	0/451	0.69	0/607
25	Z	0.48	0/345	0.67	0/460
26	2	0.47	0/366	0.65	0/480
27	3	0.32	0/424	0.66	0/566
28	4	0.39	0/280	0.63	0/371
All	All	0.59	12/88912 (0.0%)	1.07	298/134270 (0.2%)

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
3	A	0	1
7	E	0	1
27	3	0	1
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1289	A	N9-C4	-8.14	1.32	1.37
1	X	1065	A	N9-C4	-6.85	1.33	1.37
1	X	350	G	N9-C4	6.79	1.43	1.38
1	X	2845	G	N9-C4	-6.28	1.32	1.38
1	X	1186	A	N9-C4	-6.07	1.34	1.37
1	X	659	A	N9-C4	6.06	1.41	1.37
1	X	721	A	C5-C6	-5.68	1.35	1.41
1	X	2081	A	N9-C4	-5.66	1.34	1.37
1	X	721	A	N9-C4	-5.65	1.34	1.37
1	X	1027	A	N9-C4	-5.28	1.34	1.37
1	X	1004	A	N9-C4	-5.23	1.34	1.37
1	X	1065	A	C5-C6	-5.11	1.36	1.41

All (298) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2845	G	N3-C4-C5	11.31	134.26	128.60
1	X	955	A	N1-C6-N6	11.28	125.37	118.60
1	X	350	G	N3-C4-C5	-10.89	123.15	128.60
2	Y	86	C	N3-C2-O2	-10.49	114.56	121.90
1	X	1065	A	C2-N3-C4	-9.90	105.65	110.60
1	X	515	G	C4-C5-N7	9.80	114.72	110.80
1	X	2845	G	C2-N3-C4	-9.76	107.02	111.90
1	X	721	A	C2-N3-C4	-9.38	105.91	110.60
1	X	575	G	C2-N3-C4	9.21	116.51	111.90
1	X	2523	C	C6-N1-C2	9.07	123.93	120.30
1	X	1186	A	C2-N3-C4	-9.01	106.09	110.60
2	Y	86	C	N1-C2-O2	9.00	124.30	118.90
2	Y	93	C	N3-C2-O2	-8.86	115.70	121.90
1	X	515	G	C5-N7-C8	-8.72	99.94	104.30
1	X	350	G	C4-N9-C1'	8.55	137.62	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1806	U	C5-C6-N1	-8.50	118.45	122.70
2	Y	86	C	C2-N1-C1'	8.44	128.08	118.80
1	X	515	G	C6-C5-N7	-8.33	125.40	130.40
1	X	1289	A	C2-N3-C4	-8.28	106.46	110.60
1	X	2081	A	C2-N3-C4	-8.26	106.47	110.60
1	X	721	A	C5-N7-C8	-8.25	99.77	103.90
1	X	955	A	C5-C6-N6	-8.22	117.12	123.70
1	X	350	G	N3-C4-N9	8.20	130.92	126.00
1	X	1030	C	C6-N1-C2	8.09	123.53	120.30
1	X	12	U	C2-N1-C1'	7.99	127.29	117.70
1	X	2544	C	C6-N1-C2	7.99	123.50	120.30
1	X	12	U	N3-C2-O2	-7.98	116.62	122.20
1	X	515	G	N7-C8-N9	7.96	117.08	113.10
1	X	496	G	N1-C6-O6	7.90	124.64	119.90
1	X	2845	G	C4-C5-N7	7.81	113.92	110.80
1	X	2845	G	N3-C4-N9	-7.79	121.33	126.00
1	X	1065	A	C5-N7-C8	-7.72	100.04	103.90
1	X	2081	A	N1-C6-N6	7.67	123.20	118.60
1	X	350	G	C8-N9-C4	-7.61	103.36	106.40
1	X	2062	G	C5-C6-O6	-7.56	124.06	128.60
1	X	660	A	P-O3'-C3'	7.54	128.75	119.70
1	X	721	A	C4-C5-N7	7.52	114.46	110.70
2	Y	93	C	N1-C2-O2	7.49	123.39	118.90
1	X	1294	G	C4-N9-C1'	7.47	136.22	126.50
1	X	721	A	N1-C6-N6	7.46	123.08	118.60
1	X	955	A	N9-C4-C5	-7.46	102.82	105.80
1	X	1491	C	C6-N1-C2	-7.44	117.32	120.30
1	X	1395	G	N3-C4-C5	-7.43	124.88	128.60
1	X	2642	U	C2-N1-C1'	7.35	126.52	117.70
1	X	515	G	C5-C6-O6	-7.27	124.24	128.60
1	X	2845	G	N1-C6-O6	7.24	124.25	119.90
1	X	1180	G	N1-C6-O6	7.23	124.24	119.90
1	X	568	C	C6-N1-C2	7.23	123.19	120.30
1	X	2071	C	C6-N1-C2	-7.20	117.42	120.30
2	Y	88	U	N3-C2-O2	-7.13	117.21	122.20
1	X	12	U	N1-C2-O2	7.11	127.78	122.80
1	X	1289	A	C5-N7-C8	-7.07	100.36	103.90
1	X	2483	C	C6-N1-C2	7.07	123.13	120.30
1	X	2479	C	C2-N1-C1'	7.07	126.57	118.80
1	X	1017	A	C8-N9-C4	-7.06	102.98	105.80
1	X	1065	A	N1-C6-N6	7.03	122.82	118.60
2	Y	92	G	N3-C4-C5	7.01	132.11	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	21	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	X	1516	C	C6-N1-C2	-6.97	117.51	120.30
1	X	2036	G	O5'-P-OP2	-6.94	99.45	105.70
1	X	2845	G	C5-N7-C8	-6.93	100.83	104.30
1	X	2716	U	C2-N1-C1'	-6.90	109.42	117.70
1	X	591	A	N1-C6-N6	6.89	122.73	118.60
1	X	1289	A	O4'-C1'-N9	-6.89	102.69	108.20
1	X	2062	G	N1-C6-O6	6.88	124.03	119.90
2	Y	93	C	C6-N1-C2	-6.84	117.56	120.30
1	X	1360	G	N1-C6-O6	6.83	124.00	119.90
1	X	503	A	C5-N7-C8	-6.82	100.49	103.90
1	X	515	G	N1-C6-O6	6.81	123.99	119.90
1	X	571	A	N1-C6-N6	-6.77	114.54	118.60
1	X	793	G	O5'-P-OP2	-6.75	99.62	105.70
1	X	504	G	C4-C5-N7	-6.72	108.11	110.80
1	X	2608	G	N1-C6-O6	-6.72	115.87	119.90
1	X	2772	C	C6-N1-C2	6.69	122.98	120.30
1	X	1294	G	C8-N9-C1'	-6.69	118.31	127.00
1	X	1350	U	C2-N1-C1'	6.64	125.66	117.70
1	X	519	G	O5'-P-OP2	-6.62	99.74	105.70
1	X	657	U	C2-N1-C1'	6.61	125.63	117.70
1	X	2566	C	C6-N1-C2	6.59	122.94	120.30
1	X	1395	G	N3-C4-N9	6.59	129.95	126.00
1	X	1395	G	C4-N9-C1'	6.58	135.06	126.50
1	X	1200	A	N1-C6-N6	6.57	122.54	118.60
2	Y	109	C	N3-C2-O2	-6.55	117.32	121.90
1	X	1968	C	C6-N1-C2	-6.54	117.69	120.30
1	X	34	U	N1-C2-O2	6.53	127.37	122.80
1	X	376	A	C8-N9-C4	-6.51	103.19	105.80
1	X	2716	U	C5-C4-O4	6.51	129.81	125.90
1	X	657	U	C6-N1-C1'	-6.49	112.11	121.20
1	X	2881	C	C6-N1-C2	-6.49	117.70	120.30
1	X	2591	A	C8-N9-C4	-6.46	103.22	105.80
1	X	661	U	C5-C6-N1	6.46	125.93	122.70
1	X	2535	G	N1-C6-O6	6.45	123.77	119.90
1	X	2845	G	N3-C2-N2	-6.43	115.40	119.90
1	X	657	U	N1-C2-O2	6.42	127.29	122.80
1	X	1335	C	C6-N1-C2	-6.42	117.73	120.30
1	X	2546	U	C2-N1-C1'	-6.41	110.00	117.70
2	Y	86	C	C6-N1-C1'	-6.41	113.11	120.80
1	X	659	A	O4'-C1'-N9	6.39	113.31	108.20
1	X	1149	U	N1-C2-O2	6.38	127.26	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1304	G	C8-N9-C4	6.36	108.94	106.40
1	X	2716	U	N3-C4-O4	-6.34	114.96	119.40
1	X	1291	A	O5'-P-OP2	-6.34	100.00	105.70
1	X	496	G	C6-C5-N7	-6.33	126.60	130.40
1	X	515	G	O4'-C1'-N9	6.32	113.26	108.20
1	X	656	G	C8-N9-C4	-6.32	103.87	106.40
2	Y	109	C	C6-N1-C2	-6.30	117.78	120.30
1	X	2600	C	N1-C2-O2	6.26	122.66	118.90
1	X	38	A	O5'-P-OP1	-6.25	100.07	105.70
1	X	2058	A	N9-C4-C5	6.25	108.30	105.80
1	X	2805	A	O5'-P-OP2	-6.24	100.08	105.70
1	X	2613	C	C6-N1-C2	-6.23	117.81	120.30
2	Y	99	U	N3-C2-O2	-6.23	117.84	122.20
1	X	854	G	C8-N9-C4	-6.21	103.92	106.40
1	X	498	G	N9-C4-C5	-6.20	102.92	105.40
1	X	350	G	C8-N9-C1'	-6.18	118.97	127.00
1	X	389	A	C8-N9-C4	-6.17	103.33	105.80
1	X	1250	G	O4'-C1'-N9	6.15	113.12	108.20
1	X	1661	C	C6-N1-C2	6.14	122.76	120.30
1	X	2708	C	C6-N1-C2	6.14	122.76	120.30
1	X	955	A	C6-C5-N7	-6.13	128.00	132.30
1	X	1065	A	N7-C8-N9	6.12	116.86	113.80
1	X	2474	G	C6-C5-N7	-6.12	126.73	130.40
1	X	2479	C	N1-C2-O2	6.11	122.57	118.90
1	X	2647	C	C6-N1-C2	-6.11	117.86	120.30
1	X	2048	G	C2-N3-C4	6.10	114.95	111.90
1	X	2474	G	N9-C4-C5	-6.09	102.96	105.40
1	X	1721	A	N1-C6-N6	-6.06	114.97	118.60
1	X	1371	U	N1-C2-O2	-6.03	118.58	122.80
1	X	548	A	O4'-C1'-N9	6.03	113.02	108.20
1	X	721	A	N3-C4-C5	6.02	131.02	126.80
1	X	1149	U	N3-C2-O2	-5.99	118.00	122.20
1	X	591	A	O5'-P-OP1	-5.99	100.31	105.70
1	X	1079	U	C6-N1-C2	-5.97	117.42	121.00
1	X	607	C	C6-N1-C2	-5.94	117.92	120.30
1	X	531	C	C6-N1-C2	-5.94	117.92	120.30
1	X	1499	U	N3-C2-O2	-5.90	118.07	122.20
1	X	1568	U	P-O3'-C3'	5.90	126.78	119.70
1	X	491	C	C6-N1-C2	-5.89	117.94	120.30
1	X	491	C	C5-C6-N1	5.89	123.94	121.00
1	X	1466	G	C4-N9-C1'	5.89	134.15	126.50
1	X	2843	A	O5'-P-OP2	-5.89	100.40	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1065	A	C6-C5-N7	-5.87	128.19	132.30
1	X	1561	G	C8-N9-C4	-5.84	104.06	106.40
1	X	503	A	C4-C5-N7	5.82	113.61	110.70
1	X	511	G	C8-N9-C4	-5.82	104.07	106.40
1	X	350	G	C2-N3-C4	5.82	114.81	111.90
1	X	2058	A	N1-C6-N6	-5.80	115.12	118.60
2	Y	92	G	N3-C4-N9	-5.79	122.53	126.00
1	X	1289	A	N3-C4-C5	5.78	130.85	126.80
1	X	2474	G	N1-C6-O6	5.76	123.36	119.90
1	X	890	G	N3-C4-C5	5.75	131.47	128.60
1	X	2674	U	C6-N1-C2	5.75	124.45	121.00
1	X	2844	U	N1-C2-O2	-5.75	118.78	122.80
1	X	1368	C	C6-N1-C2	5.74	122.60	120.30
1	X	1200	A	C5-C6-N6	-5.73	119.12	123.70
1	X	505	U	C2-N1-C1'	5.73	124.57	117.70
1	X	2280	G	C6-C5-N7	-5.72	126.97	130.40
2	Y	106	U	N3-C2-O2	-5.71	118.20	122.20
1	X	1042	C	C6-N1-C2	5.71	122.58	120.30
1	X	875	G	N1-C6-O6	-5.69	116.49	119.90
1	X	1144	C	C6-N1-C2	-5.69	118.03	120.30
2	Y	114	C	N1-C2-O2	5.64	122.28	118.90
1	X	2909	C	C6-N1-C2	-5.62	118.05	120.30
1	X	1065	A	C4-C5-N7	5.62	113.51	110.70
1	X	2290	C	C6-N1-C2	-5.61	118.06	120.30
1	X	34	U	C2-N1-C1'	5.60	124.42	117.70
1	X	2081	A	N1-C2-N3	5.60	132.10	129.30
1	X	2278	G	C6-C5-N7	-5.59	127.04	130.40
1	X	955	A	C4-C5-N7	5.55	113.47	110.70
1	X	2905	C	C6-N1-C2	-5.55	118.08	120.30
1	X	1360	G	C4-C5-N7	5.54	113.02	110.80
1	X	1068	G	N1-C6-O6	5.54	123.22	119.90
1	X	199	A	O5'-P-OP1	-5.53	100.72	105.70
1	X	1351	C	C5-C6-N1	5.53	123.76	121.00
1	X	1186	A	N1-C6-N6	5.52	121.91	118.60
1	X	721	A	C6-C5-N7	-5.52	128.44	132.30
1	X	2757	U	C6-N1-C2	-5.52	117.69	121.00
1	X	515	G	C8-N9-C4	-5.51	104.20	106.40
1	X	836	C	C6-N1-C2	5.51	122.50	120.30
1	X	661	U	C2-N1-C1'	5.51	124.31	117.70
1	X	1721	A	N9-C4-C5	5.50	108.00	105.80
1	X	34	U	C6-N1-C1'	-5.50	113.50	121.20
1	X	1492	G	C8-N9-C4	-5.50	104.20	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2310	C	C6-N1-C2	-5.49	118.10	120.30
1	X	116	G	N3-C4-C5	-5.49	125.86	128.60
1	X	2012	G	N1-C6-O6	-5.48	116.61	119.90
1	X	1230	G	N7-C8-N9	-5.48	110.36	113.10
1	X	2523	C	C5-C6-N1	-5.48	118.26	121.00
1	X	696	G	O5'-P-OP1	5.47	117.27	110.70
1	X	2036	G	O5'-P-OP1	5.47	117.27	110.70
1	X	1370	C	N3-C4-C5	5.47	124.09	121.90
1	X	2637	C	C6-N1-C2	5.47	122.49	120.30
1	X	268	A	O4'-C1'-N9	5.46	112.57	108.20
1	X	2803	A	OP1-P-O3'	5.46	117.20	105.20
1	X	389	A	N7-C8-N9	5.45	116.53	113.80
1	X	2491	C	C6-N1-C2	5.45	122.48	120.30
1	X	707	G	N3-C4-N9	5.44	129.26	126.00
1	X	1304	G	N7-C8-N9	-5.44	110.38	113.10
1	X	1277	C	C6-N1-C2	-5.43	118.13	120.30
1	X	1721	A	C5-C6-N6	5.43	128.04	123.70
1	X	2052	C	C6-N1-C2	-5.42	118.13	120.30
1	X	323	C	C6-N1-C2	-5.42	118.13	120.30
1	X	1350	U	N3-C2-O2	-5.42	118.41	122.20
1	X	1702	C	C6-N1-C2	5.39	122.46	120.30
2	Y	105	G	C2-N3-C4	-5.38	109.21	111.90
1	X	503	A	N1-C6-N6	5.38	121.83	118.60
1	X	955	A	N3-C4-N9	5.37	131.69	127.40
1	X	2755	U	C6-N1-C2	-5.36	117.78	121.00
1	X	169	G	O4'-C1'-N9	5.36	112.49	108.20
1	X	2027	G	C8-N9-C4	5.36	108.54	106.40
1	X	1042	C	N3-C4-C5	5.35	124.04	121.90
1	X	2599	A	C8-N9-C4	5.35	107.94	105.80
1	X	515	G	C4-N9-C1'	5.34	133.45	126.50
1	X	1506	C	N1-C2-O2	5.34	122.11	118.90
1	X	2642	U	C6-N1-C1'	-5.34	113.73	121.20
1	X	2756	G	N3-C4-C5	-5.33	125.93	128.60
1	X	1524	C	C6-N1-C2	-5.33	118.17	120.30
1	X	496	G	C8-N9-C1'	-5.32	120.08	127.00
1	X	2682	G	O4'-C1'-N9	5.32	112.45	108.20
1	X	2712	G	N3-C2-N2	-5.32	116.18	119.90
1	X	2549	U	N3-C4-O4	5.31	123.12	119.40
1	X	378	C	C6-N1-C2	-5.31	118.18	120.30
1	X	2599	A	N9-C4-C5	-5.30	103.68	105.80
1	X	1360	G	C5-C6-O6	-5.30	125.42	128.60
1	X	1179	C	C6-N1-C2	5.30	122.42	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	660	A	OP1-P-O3'	5.29	116.84	105.20
1	X	1016	G	N1-C6-O6	-5.29	116.73	119.90
1	X	659	A	C2-N3-C4	5.28	113.24	110.60
1	X	1664	G	N1-C6-O6	5.28	123.07	119.90
1	X	1230	G	C8-N9-C4	5.28	108.51	106.40
1	X	2655	U	N3-C4-O4	5.28	123.09	119.40
2	Y	79	C	C5-C4-N4	-5.28	116.51	120.20
1	X	1395	G	C8-N9-C1'	-5.28	120.14	127.00
1	X	2062	G	C4-C5-N7	5.27	112.91	110.80
1	X	2527	U	OP2-P-O3'	5.27	116.79	105.20
1	X	1229	G	OP2-P-O3'	5.27	116.78	105.20
16	O	50	ALA	C-N-CD	5.25	139.44	128.40
1	X	15	G	C8-N9-C4	5.25	108.50	106.40
1	X	16	G	C4-C5-C6	5.25	121.95	118.80
1	X	1091	G	P-O3'-C3'	5.25	126.00	119.70
1	X	576	U	O5'-P-OP2	-5.24	100.98	105.70
1	X	2479	C	N3-C2-O2	-5.24	118.23	121.90
1	X	372	A	C8-N9-C4	5.23	107.89	105.80
1	X	859	C	C6-N1-C2	-5.23	118.21	120.30
1	X	2535	G	C5-C6-O6	-5.23	125.46	128.60
1	X	1661	C	C2-N1-C1'	-5.22	113.06	118.80
1	X	2599	A	N1-C6-N6	5.22	121.73	118.60
1	X	199	A	C8-N9-C4	-5.21	103.72	105.80
1	X	2661	A	N1-C6-N6	-5.20	115.48	118.60
1	X	504	G	N3-C4-C5	-5.20	126.00	128.60
1	X	728	U	C6-N1-C2	-5.20	117.88	121.00
1	X	2716	U	C6-N1-C1'	5.19	128.47	121.20
1	X	182	C	N1-C2-O2	5.19	122.01	118.90
1	X	1079	U	N3-C2-O2	-5.19	118.57	122.20
1	X	2740	A	N1-C6-N6	5.18	121.71	118.60
1	X	1149	U	C2-N1-C1'	5.18	123.91	117.70
1	X	1186	A	C5-N7-C8	-5.16	101.32	103.90
1	X	2278	G	N1-C6-O6	5.16	123.00	119.90
1	X	875	G	C5-C6-O6	5.16	131.69	128.60
1	X	102	A	N1-C6-N6	5.15	121.69	118.60
1	X	985	A	O5'-P-OP1	-5.15	101.07	105.70
1	X	1708	A	C8-N9-C4	-5.14	103.74	105.80
1	X	2053	U	N3-C4-O4	5.14	123.00	119.40
1	X	20	C	C5-C4-N4	-5.14	116.60	120.20
1	X	1294	G	N3-C4-N9	5.14	129.08	126.00
1	X	2510	C	C6-N1-C2	-5.13	118.25	120.30
1	X	498	G	C4-C5-N7	5.13	112.85	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	880	A	N1-C6-N6	5.13	121.68	118.60
1	X	591	A	C5-C6-N6	-5.12	119.61	123.70
1	X	1968	C	C2-N1-C1'	5.11	124.42	118.80
1	X	1006	G	N3-C2-N2	-5.09	116.34	119.90
1	X	2905	C	C5-C6-N1	5.07	123.54	121.00
1	X	2479	C	C6-N1-C2	-5.07	118.27	120.30
1	X	875	G	C4-C5-N7	-5.07	108.77	110.80
1	X	362	C	C6-N1-C2	-5.07	118.27	120.30
1	X	552	A	N1-C6-N6	5.07	121.64	118.60
1	X	675	G	N1-C6-O6	5.07	122.94	119.90
1	X	2064	A	C8-N9-C4	-5.07	103.77	105.80
1	X	517	A	C8-N9-C4	5.06	107.82	105.80
1	X	1351	C	C2-N1-C1'	5.06	124.36	118.80
1	X	1758	A	C8-N9-C4	-5.05	103.78	105.80
1	X	638	U	N1-C2-O2	5.05	126.33	122.80
1	X	1065	A	C8-N9-C4	-5.05	103.78	105.80
1	X	2546	U	N3-C4-O4	-5.04	115.87	119.40
1	X	36	G	N3-C4-N9	5.04	129.03	126.00
1	X	2014	G	O5'-P-OP2	-5.04	101.16	105.70
1	X	376	A	N7-C8-N9	5.04	116.32	113.80
1	X	2639	C	N3-C4-C5	5.03	123.91	121.90
1	X	2836	C	N3-C4-C5	-5.03	119.89	121.90
1	X	1064	A	C8-N9-C4	5.02	107.81	105.80
1	X	12	U	C6-N1-C1'	-5.02	114.17	121.20
1	X	2298	G	N9-C4-C5	-5.02	103.39	105.40
1	X	350	G	C5-C6-N1	5.02	114.01	111.50
1	X	1312	A	OP1-P-O3'	5.02	116.23	105.20
1	X	656	G	N7-C8-N9	5.01	115.60	113.10
1	X	566	U	O4'-C1'-N1	5.00	112.20	108.20
1	X	2893	A	O4'-C1'-N9	5.00	112.20	108.20
1	X	568	C	C5-C6-N1	-5.00	118.50	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	3	24	ARG	Peptide
3	A	52	ARG	Peptide
7	E	119	GLU	Peptide

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	X	58077	0	29209	849	0
2	Y	2430	0	1229	48	0
3	A	1686	0	1350	48	0
4	B	1558	0	1545	60	0
5	C	1320	0	1171	54	0
6	D	866	0	470	8	0
7	E	970	0	741	23	0
8	G	1106	0	1072	31	0
9	H	884	0	902	26	0
10	I	859	0	772	37	0
11	J	1068	0	1078	42	0
12	K	908	0	935	28	0
13	L	705	0	589	10	0
14	M	826	0	831	41	0
15	N	932	0	995	37	0
16	O	751	0	743	14	0
17	P	862	0	920	37	0
18	Q	626	0	567	21	0
19	R	683	0	661	21	0
20	S	1097	0	956	18	0
21	T	568	0	575	11	0
22	U	300	0	231	9	0
23	V	486	0	469	6	0
24	W	449	0	490	25	0
25	Z	339	0	350	19	0
26	2	362	0	398	14	0
27	3	420	0	405	7	0
28	4	277	0	301	17	0
29	X	88	0	154	14	0
29	Z	8	0	14	0	0
30	B	1	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	R	2	0	0	0	0
30	X	223	0	0	0	0
30	Y	2	0	0	0	0
31	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	C	1	0	0	0	0
31	G	3	0	0	0	0
31	I	1	0	0	0	0
31	O	1	0	0	0	0
31	X	80	0	0	0	0
31	Y	3	0	0	0	0
32	X	15	0	17	0	0
33	X	40	0	76	0	0
34	X	21	0	42	0	0
All	All	81909	0	50258	1401	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 11.

All (1401) 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)
1:X:2231:C:HO2'	1:X:2232:A:H8	1.06	0.97
2:Y:80:A:H61	2:Y:91:C:H42	1.05	0.94
2:Y:79:C:H42	2:Y:92:G:H1	1.06	0.94
1:X:1487:G:H1	1:X:1597:U:H3	1.17	0.93
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.52	0.90
2:Y:15:C:H42	2:Y:105:G:H21	1.19	0.88
8:G:87:SER:O	8:G:89:THR:N	2.09	0.86
1:X:65:A:N1	1:X:90:A:N6	2.26	0.84
28:4:25:VAL:HG22	28:4:34:GLN:HB2	1.59	0.83
1:X:2850:G:H5'	4:B:67:LYS:HE3	1.58	0.83
5:C:7:LEU:HD21	5:C:126:VAL:H	1.42	0.82
1:X:864:A:OP2	1:X:1226:G:N2	2.09	0.82
1:X:1448:U:H3'	1:X:1449:A:H5''	1.62	0.82
19:R:6:GLY:HA2	19:R:23:VAL:HG22	1.61	0.81
1:X:1522:G:H1	1:X:1558:U:H3	1.28	0.81
1:X:268:A:N6	1:X:473:U:O2'	2.14	0.80
1:X:1323:A:O2'	1:X:1325:U:OP2	1.98	0.80
1:X:2432:G:OP1	10:I:63:LYS:NZ	2.14	0.80
1:X:1492:G:N2	1:X:1508:C:N3	2.31	0.78
9:H:63:VAL:HG21	9:H:102:VAL:HG22	1.64	0.78
1:X:627:C:OP2	29:X:3007:MPD:O2	2.01	0.78
1:X:878:C:H1'	10:I:48:PRO:HB3	1.66	0.78
1:X:498:G:H21	1:X:503:A:H8	1.31	0.77
1:X:2314:A:O2'	1:X:2315:A:H2'	1.85	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:77:G:H1	2:Y:94:U:H3	1.30	0.77
1:X:1513:A:H3'	1:X:1514:A:H8	1.49	0.77
1:X:1518:G:H1	1:X:1562:C:H42	1.30	0.77
4:B:117:ASP:HB3	4:B:181:GLN:HA	1.66	0.76
1:X:2852:U:OP1	4:B:61:LYS:NZ	2.17	0.76
1:X:1250:G:O2'	1:X:1275:A:N6	2.18	0.76
2:Y:18:G:H1	2:Y:61:U:H3	1.32	0.76
1:X:1781:C:H5	14:M:96:ARG:HH22	1.31	0.76
18:Q:55:ILE:HG13	18:Q:78:ALA:HB2	1.67	0.76
1:X:1851:G:OP2	3:A:53:HIS:NE2	2.18	0.76
1:X:1063:U:H3	1:X:1186:A:H62	1.34	0.76
1:X:1515:G:H1	1:X:1565:U:H3	1.34	0.76
1:X:459:C:O2'	1:X:1907:U:O2'	2.04	0.76
1:X:501:C:H3'	1:X:502:C:H5''	1.67	0.76
2:Y:15:C:H42	2:Y:105:G:N2	1.83	0.75
4:B:67:LYS:HA	4:B:86:ARG:HH22	1.49	0.75
1:X:1894:G:O6	1:X:1902:G:N2	2.19	0.75
1:X:1501:G:H22	1:X:2729:G:H22	1.31	0.75
1:X:304:G:H1	1:X:413:C:H42	1.34	0.75
1:X:2228:C:O2	1:X:2249:G:N2	2.19	0.74
2:Y:78:C:N3	2:Y:93:C:N4	2.34	0.74
3:A:89:ALA:HB2	3:A:158:ALA:HA	1.68	0.74
2:Y:81:A:H61	2:Y:90:C:H42	1.31	0.74
3:A:68:LYS:HA	3:A:151:GLY:HA2	1.69	0.74
1:X:1512:U:H2'	1:X:1513:A:C8	2.23	0.73
1:X:2649:U:O2'	1:X:2845:G:N2	2.21	0.73
1:X:193:A:OP2	22:U:28:ARG:NH2	2.21	0.73
15:N:61:TRP:CE2	15:N:93:LYS:HB2	2.24	0.73
20:S:133:THR:HG21	20:S:159:VAL:HB	1.70	0.73
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.71	0.73
24:W:26:LEU:HD21	24:W:46:GLN:HB3	1.71	0.72
1:X:1683:U:H2'	1:X:1684:A:H5''	1.70	0.72
4:B:158:SER:O	4:B:161:SER:OG	2.07	0.72
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.70	0.72
2:Y:31:G:H1	2:Y:47:C:H42	1.37	0.72
4:B:33:ASN:HB3	4:B:105:VAL:HG22	1.71	0.72
2:Y:69:C:H42	2:Y:102:A:H61	1.38	0.72
18:Q:13:THR:HG23	18:Q:16:SER:HB3	1.71	0.72
1:X:1563:U:H2'	1:X:1564:G:H8	1.55	0.72
13:L:36:SER:OG	13:L:37:ASN:N	2.23	0.71
23:V:45:THR:HA	23:V:48:LYS:HD2	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1490:G:O2'	1:X:1491:C:O4'	2.09	0.71
1:X:1845:U:H5''	3:A:156:ARG:HB2	1.71	0.71
1:X:657:U:O4	1:X:659:A:N6	2.24	0.71
10:I:112:LEU:HD22	10:I:112:LEU:H	1.56	0.70
2:Y:15:C:N4	2:Y:105:G:H21	1.89	0.70
1:X:427:A:H5''	22:U:18:ARG:HE	1.56	0.70
1:X:2650:G:O5'	1:X:2845:G:N2	2.24	0.70
1:X:2883:U:H2'	1:X:2884:G:H8	1.55	0.70
28:4:27:CYS:HB3	28:4:32:HIS:HB2	1.71	0.70
19:R:80:ARG:NH1	19:R:95:LYS:O	2.24	0.70
28:4:27:CYS:SG	28:4:32:HIS:ND1	2.65	0.70
2:Y:79:C:N4	2:Y:92:G:H1	1.87	0.70
11:J:40:SER:HB3	11:J:127:VAL:HG22	1.73	0.70
19:R:3:ILE:HG13	19:R:4:LYS:HG2	1.74	0.70
1:X:735:C:O2'	1:X:825:G:OP1	2.08	0.69
14:M:102:LEU:O	14:M:103:ARG:NH2	2.24	0.69
1:X:736:C:OP1	3:A:217:ARG:NH1	2.25	0.69
1:X:37:C:H2'	1:X:38:A:C8	2.28	0.69
1:X:2711:U:OP2	14:M:53:ARG:NH1	2.25	0.69
1:X:1563:U:H2'	1:X:1564:G:C8	2.27	0.69
3:A:209:GLY:HA2	3:A:212:ARG:HB2	1.75	0.69
1:X:2051:C:H2'	1:X:2052:C:H6	1.58	0.69
13:L:45:ILE:HG23	13:L:52:THR:HG22	1.74	0.69
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.75	0.69
5:C:166:SER:OG	5:C:167:ALA:N	2.26	0.69
1:X:503:A:H2	1:X:517:A:H62	1.41	0.69
1:X:2804:G:H5''	1:X:2805:A:H5'	1.74	0.68
1:X:1492:G:N7	1:X:1493:U:H5	1.91	0.68
1:X:2495:A:OP1	11:J:119:ARG:NH2	2.27	0.68
20:S:22:ARG:HH21	20:S:28:PRO:HG3	1.58	0.68
7:E:102:ASP:H	7:E:115:ILE:HD13	1.59	0.68
2:Y:80:A:N6	2:Y:91:C:H42	1.87	0.68
17:P:2:GLU:HG3	17:P:109:ASP:H	1.57	0.68
5:C:133:ALA:HB1	5:C:135:LYS:H	1.58	0.68
1:X:1998:A:O2'	1:X:1999:G:OP1	2.11	0.67
1:X:1472:C:N4	1:X:1617:A:OP2	2.27	0.67
1:X:1521:A:H61	1:X:1560:A:H1'	1.59	0.67
1:X:1250:G:H2'	1:X:1274:G:N2	2.08	0.67
1:X:2817:A:O2'	1:X:2818:A:OP2	2.13	0.67
1:X:922:G:H22	1:X:944:G:H1	1.43	0.67
1:X:83:G:H21	1:X:102:A:H2	1.41	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:351:G:O2'	19:R:15:LYS:NZ	2.28	0.67
1:X:2835:C:H1'	25:Z:39:LEU:HD23	1.75	0.67
12:K:24:LEU:O	12:K:28:GLU:N	2.28	0.67
5:C:103:LYS:HA	5:C:106:ARG:NE	2.10	0.67
9:H:87:ILE:HD11	9:H:91:LYS:HA	1.77	0.67
1:X:2673:C:OP2	1:X:2759:G:O2'	2.12	0.67
15:N:27:SER:HB2	15:N:31:LEU:HG	1.76	0.67
8:G:2:ARG:HG3	8:G:3:GLN:H	1.59	0.67
14:M:105:LEU:O	14:M:106:ARG:NH1	2.27	0.67
1:X:2419:A:H2	1:X:2451:C:H42	1.41	0.66
1:X:1591:G:OP2	1:X:1591:G:N2	2.28	0.66
1:X:787:U:H2'	1:X:788:A:C8	2.31	0.66
18:Q:58:TYR:HB2	18:Q:75:ARG:HB2	1.76	0.66
1:X:1931:G:H1	1:X:1957:G:H22	1.43	0.66
1:X:721:A:H8	1:X:2096:G:H21	1.41	0.66
1:X:1491:C:O2	1:X:1492:G:N2	2.29	0.66
1:X:1575:A:H2'	1:X:1576:A:H5'	1.76	0.66
1:X:2360:A:H5'	1:X:2362:A:H1'	1.77	0.66
1:X:2554:C:H5''	28:4:30:PRO:HB3	1.76	0.66
11:J:22:LYS:HE3	11:J:23:GLY:H	1.61	0.66
1:X:388:A:H1'	1:X:389:A:H2	1.61	0.66
28:4:9:PRO:HB3	28:4:14:CYS:HB2	1.78	0.65
1:X:2313:A:H4'	1:X:2314:A:O4'	1.97	0.65
2:Y:6:U:OP1	13:L:11:ARG:NH2	2.25	0.65
1:X:1490:G:O2'	1:X:1491:C:O5'	2.14	0.65
1:X:2330:G:H4'	6:D:114:PHE:HA	1.78	0.65
1:X:877:G:H2'	1:X:878:C:C6	2.32	0.65
1:X:1513:A:H3'	1:X:1514:A:C8	2.31	0.65
1:X:1523:G:N2	1:X:1557:C:N3	2.42	0.64
1:X:24:G:O2'	17:P:78:GLU:O	2.14	0.64
19:R:10:LYS:HE3	19:R:18:GLY:HA2	1.78	0.64
1:X:665:G:H4'	1:X:666:A:H5''	1.79	0.64
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.11	0.64
1:X:700:A:H4'	1:X:701:G:H5'	1.80	0.64
1:X:17:G:OP1	25:Z:11:THR:HG22	1.97	0.64
1:X:1337:A:H4'	1:X:1338:U:H5''	1.79	0.64
25:Z:38:LYS:HZ2	25:Z:38:LYS:HB2	1.62	0.64
1:X:2860:U:H5''	12:K:49:THR:HG21	1.80	0.64
9:H:19:VAL:HG12	9:H:43:VAL:HA	1.80	0.64
1:X:1395:G:N2	1:X:1395:G:OP2	2.28	0.64
10:I:51:GLU:H	10:I:51:GLU:CD	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1523:G:H1	1:X:1557:C:H42	1.45	0.64
29:X:3003:MPD:HO4	29:X:3003:MPD:HO2	1.43	0.64
1:X:1826:G:N2	1:X:1845:U:O2'	2.31	0.63
5:C:108:LEU:O	5:C:112:SER:OG	2.09	0.63
28:4:27:CYS:O	28:4:29:ASN:N	2.31	0.63
1:X:1467:G:O2'	1:X:1543:G:O2'	2.14	0.63
15:N:92:ARG:O	15:N:93:LYS:HB3	1.97	0.63
21:T:61:ARG:NH1	21:T:65:ASP:OD1	2.32	0.63
1:X:1498:U:HO2'	1:X:1499:U:H5	1.47	0.63
1:X:1065:A:H3'	1:X:1065:A:C8	2.34	0.63
1:X:637:U:H2'	1:X:638:U:C6	2.33	0.63
1:X:2112:C:H42	1:X:2261:A:H61	1.46	0.63
1:X:460:C:O2	1:X:1891:U:O2'	2.17	0.63
1:X:280:C:H2'	1:X:281:A:H8	1.63	0.63
1:X:2717:A:H62	12:K:13:ARG:HD2	1.64	0.63
1:X:444:C:H41	22:U:52:ARG:HH12	1.46	0.63
14:M:15:LEU:HD22	14:M:79:HIS:CE1	2.34	0.63
5:C:14:SER:OG	5:C:15:GLY:N	2.31	0.62
1:X:2354:A:H2'	1:X:2355:A:C8	2.34	0.62
1:X:1769:C:N4	1:X:1770:C:H41	1.98	0.62
3:A:92:ALA:H	3:A:106:ALA:HB2	1.64	0.62
24:W:19:GLN:O	24:W:23:VAL:HG23	1.98	0.62
1:X:904:G:O2'	1:X:961:G:O6	2.16	0.62
9:H:15:GLY:HA3	9:H:50:GLY:HA3	1.80	0.62
9:H:76:TYR:HB2	14:M:75:THR:HG23	1.80	0.62
1:X:79:U:H2'	1:X:389:A:H8	1.65	0.62
18:Q:49:LYS:HD3	18:Q:50:VAL:N	2.15	0.62
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.82	0.62
8:G:89:THR:HG21	8:G:93:LEU:HD12	1.82	0.62
1:X:262:G:H21	1:X:666:A:H8	1.48	0.62
1:X:2018:U:O2'	1:X:2019:G:H5'	2.00	0.62
1:X:2619:G:H2'	1:X:2620:U:O4'	2.00	0.62
1:X:2749:G:H2'	1:X:2750:C:C6	2.35	0.62
1:X:606:G:OP2	16:O:78:ARG:NH2	2.32	0.61
3:A:123:ASP:OD1	3:A:123:ASP:N	2.33	0.61
5:C:140:LYS:HA	5:C:142:VAL:HG12	1.82	0.61
14:M:23:ARG:HH21	14:M:23:ARG:HG3	1.64	0.61
22:U:21:ALA:O	22:U:23:ASN:N	2.33	0.61
9:H:34:ASN:ND2	9:H:68:GLY:O	2.31	0.61
1:X:903:G:OP2	21:T:85:LYS:NZ	2.34	0.61
1:X:1737:U:O2'	3:A:14:ARG:NH2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:105:LYS:HB2	25:Z:41:HIS:HA	1.82	0.61
1:X:1:G:H3'	1:X:2:A:H4'	1.83	0.61
1:X:956:A:C6	11:J:11:ARG:HD3	2.35	0.61
3:A:199:GLN:HG3	3:A:202:LEU:HB2	1.83	0.61
11:J:31:GLU:H	11:J:107:ALA:HB2	1.64	0.61
3:A:133:GLN:HG3	3:A:186:SER:HB3	1.83	0.61
5:C:77:THR:HG22	5:C:79:ARG:H	1.66	0.61
1:X:1510:U:O4	1:X:1572:G:N2	2.33	0.61
1:X:1415:A:O2'	1:X:1417:G:N7	2.29	0.61
4:B:116:ILE:HD12	4:B:211:ILE:HG23	1.83	0.61
11:J:111:GLU:OE2	11:J:115:ARG:NH1	2.32	0.61
1:X:2120:G:H21	1:X:2225:A:H62	1.48	0.61
4:B:118:VAL:HG12	4:B:211:ILE:HA	1.82	0.61
1:X:2050:A:H5'	1:X:2644:C:H4'	1.82	0.60
1:X:1816:A:OP2	3:A:221:ARG:NH1	2.31	0.60
19:R:40:ILE:HG23	19:R:61:ALA:HB2	1.82	0.60
1:X:2776:A:H4'	7:E:62:ARG:HG3	1.84	0.60
1:X:1567:A:H5''	1:X:1568:U:H2'	1.82	0.60
1:X:2370:U:O2'	1:X:2400:U:O2'	2.14	0.60
1:X:613:G:H2'	1:X:2057:A:N7	2.16	0.60
1:X:1465:G:H2'	1:X:1466:G:C8	2.36	0.60
1:X:2470:C:H2'	1:X:2471:G:H8	1.65	0.60
1:X:1289:A:N7	29:X:3007:MPD:H11	2.16	0.60
1:X:615:A:OP2	16:O:79:ARG:NH2	2.34	0.60
11:J:36:ALA:HA	11:J:129:THR:HG22	1.84	0.60
24:W:50:VAL:HB	24:W:53:LEU:HD11	1.82	0.60
1:X:1512:U:H2'	1:X:1513:A:H8	1.64	0.60
11:J:65:TRP:HB2	11:J:105:GLU:HG3	1.84	0.60
1:X:1514:A:N6	1:X:1566:G:H1	1.99	0.60
1:X:1250:G:H2'	1:X:1274:G:H22	1.65	0.60
1:X:2682:G:O2'	1:X:2683:U:H5	1.84	0.60
4:B:8:ARG:NH1	4:B:206:LYS:O	2.35	0.60
1:X:857:C:HO2'	1:X:1264:A:HO2'	1.50	0.60
1:X:683:G:C6	1:X:696:G:C6	2.90	0.60
2:Y:80:A:H61	2:Y:91:C:N4	1.88	0.60
1:X:1056:U:OP2	15:N:70:ARG:NH2	2.35	0.60
24:W:22:THR:HG23	24:W:46:GLN:HG2	1.84	0.59
1:X:2089:A:OP1	29:X:3003:MPD:O2	2.14	0.59
1:X:2355:A:H2'	1:X:2356:A:C8	2.37	0.59
1:X:858:U:H2'	1:X:859:C:C6	2.37	0.59
9:H:31:LYS:HG3	9:H:32:THR:HG22	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:44:ARG:HG2	23:V:48:LYS:HE3	1.84	0.59
1:X:2431:C:H42	1:X:2440:G:H1	1.51	0.59
1:X:2351:U:H3	1:X:2358:G:H1	1.49	0.59
1:X:1527:A:H2'	1:X:1528:G:H5'	1.83	0.59
1:X:2845:G:O6	4:B:172:ARG:NH2	2.35	0.59
1:X:38:A:O2'	1:X:39:C:OP1	2.17	0.59
1:X:2358:G:O2'	1:X:2363:A:N1	2.32	0.59
5:C:190:ASP:OD1	5:C:191:SER:N	2.31	0.59
1:X:1658:A:H61	17:P:88:ARG:H	1.50	0.59
28:4:35:ARG:HG2	28:4:37:GLY:H	1.67	0.59
7:E:53:VAL:HA	7:E:66:GLY:HA2	1.82	0.59
1:X:1765:A:O2'	1:X:1766:C:O4'	2.19	0.59
1:X:1487:G:N2	1:X:1597:U:O2	2.36	0.59
1:X:2089:A:OP1	29:X:3003:MPD:O4	2.21	0.59
1:X:683:G:C6	1:X:696:G:N1	2.70	0.59
19:R:11:VAL:HA	19:R:67:ASN:HB3	1.83	0.59
1:X:2883:U:H2'	1:X:2884:G:C8	2.37	0.59
1:X:1208:A:H2'	1:X:1209:U:C6	2.38	0.59
14:M:55:GLY:H	14:M:59:GLU:HG3	1.67	0.59
1:X:1440:A:HO2'	1:X:1514:A:HO2'	1.47	0.59
7:E:133:VAL:HG11	7:E:141:VAL:HG13	1.85	0.59
1:X:1568:U:O2'	1:X:1569:G:OP2	2.20	0.59
1:X:1072:A:N3	1:X:2513:G:O2'	2.33	0.59
5:C:4:TYR:HA	5:C:18:GLU:HA	1.84	0.59
17:P:73:GLU:HG2	17:P:106:VAL:HB	1.83	0.59
1:X:218:G:H4'	1:X:219:A:H4'	1.85	0.59
1:X:2051:C:H2'	1:X:2052:C:C6	2.36	0.58
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.85	0.58
12:K:23:SER:HA	12:K:26:ILE:HD12	1.85	0.58
1:X:1300:G:OP2	17:P:99:ARG:NH2	2.35	0.58
3:A:119:GLY:O	3:A:121:GLU:N	2.35	0.58
26:2:20:ARG:HB2	26:2:20:ARG:NH1	2.18	0.58
1:X:666:A:H2'	1:X:667:G:H5'	1.85	0.58
17:P:61:ASN:HB2	17:P:62:TYR:CE1	2.38	0.58
1:X:1465:G:H2'	1:X:1466:G:H8	1.68	0.58
20:S:28:PRO:O	20:S:88:HIS:HA	2.03	0.58
1:X:1565:U:H2'	1:X:1566:G:C8	2.39	0.58
8:G:111:PRO:HB2	8:G:113:THR:HG23	1.84	0.58
1:X:1395:G:O2'	1:X:1410:A:N6	2.37	0.58
17:P:86:ARG:HG3	17:P:87:PRO:HD2	1.86	0.58
1:X:15:G:O2'	25:Z:18:THR:HG21	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:14:THR:OG1	22:U:15:GLY:N	2.36	0.58
1:X:1197:C:OP1	15:N:92:ARG:NH2	2.37	0.58
1:X:659:A:H1'	1:X:660:A:H5'	1.86	0.58
1:X:2905:C:H42	25:Z:39:LEU:HG	1.69	0.57
1:X:2856:U:H2'	1:X:2857:A:C8	2.39	0.57
20:S:107:GLN:HA	20:S:138:PRO:HD2	1.86	0.57
1:X:1423:C:O2'	1:X:1512:U:O2	2.16	0.57
1:X:460:C:H2'	1:X:461:A:H8	1.67	0.57
17:P:4:LYS:HB2	17:P:106:VAL:HG22	1.85	0.57
28:4:16:VAL:HG22	28:4:25:VAL:HG12	1.85	0.57
2:Y:74:G:H22	2:Y:97:A:H61	1.51	0.57
1:X:1041:G:OP1	15:N:92:ARG:HG2	2.04	0.57
1:X:956:A:C5	11:J:11:ARG:HD3	2.39	0.57
1:X:1491:C:O2	1:X:1509:G:N2	2.37	0.57
1:X:2059:G:H22	1:X:2599:A:H5'	1.69	0.57
1:X:2618:C:H2'	1:X:2619:G:C8	2.40	0.57
24:W:6:ILE:HD12	24:W:56:VAL:HG12	1.85	0.57
2:Y:22:G:N2	2:Y:26:C:N3	2.53	0.57
1:X:1424:A:H2'	1:X:1425:G:C8	2.39	0.57
1:X:2470:C:H2'	1:X:2471:G:C8	2.39	0.57
10:I:3:LEU:HA	10:I:6:LEU:HD21	1.87	0.57
1:X:1962:G:H1'	1:X:1991:G:N2	2.20	0.57
20:S:81:PRO:O	20:S:83:LYS:N	2.36	0.57
1:X:1761:G:O2'	1:X:1762:U:O4'	2.22	0.57
3:A:169:GLY:O	3:A:171:TYR:N	2.37	0.56
13:L:89:ILE:HG23	13:L:90:LYS:H	1.68	0.56
1:X:1614:A:O4'	1:X:1615:G:N2	2.38	0.56
1:X:677:A:H4'	10:I:60:ARG:HH22	1.70	0.56
1:X:1424:A:H2'	1:X:1425:G:H8	1.69	0.56
1:X:327:G:O2'	1:X:328:G:H8	1.89	0.56
1:X:1257:G:OP2	15:N:19:LYS:NZ	2.32	0.56
1:X:1293:U:H5''	1:X:1294:G:H5''	1.85	0.56
22:U:43:LYS:O	22:U:45:LYS:N	2.33	0.56
1:X:1353:A:H2'	1:X:1354:G:C8	2.41	0.56
11:J:4:PRO:HG2	11:J:48:GLU:HG2	1.87	0.56
8:G:20:ASP:HA	8:G:58:ILE:HG22	1.87	0.56
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.38	0.56
1:X:1835:U:H2'	1:X:1836:A:H5''	1.86	0.56
1:X:183:A:H5'	1:X:481:C:H1'	1.86	0.56
1:X:684:U:H2'	1:X:685:C:C6	2.40	0.56
7:E:23:HIS:HA	7:E:28:GLY:HA3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:111:ARG:O	5:C:115:SER:OG	2.20	0.56
1:X:1281:U:H2'	1:X:1282:A:H8	1.71	0.56
1:X:1352:C:H2'	1:X:1353:A:C8	2.41	0.56
8:G:18:VAL:HG23	8:G:138:PRO:HB2	1.87	0.56
1:X:2007:G:O2'	1:X:2009:U:OP2	2.23	0.56
1:X:1637:A:O2'	1:X:1638:G:O4'	2.23	0.56
1:X:1450:A:H5''	1:X:1451:U:H5	1.70	0.56
3:A:116:VAL:HG13	3:A:127:GLY:HA3	1.88	0.56
1:X:2060:A:O2'	1:X:2062:G:OP2	2.19	0.56
1:X:622:A:H62	29:X:3011:MPD:H52	1.69	0.56
1:X:501:C:H3'	1:X:502:C:C5'	2.35	0.56
4:B:95:ASP:O	4:B:97:ASP:N	2.39	0.56
10:I:28:GLY:H	10:I:30:THR:H	1.52	0.56
1:X:38:A:H2'	1:X:39:C:O4'	2.06	0.56
1:X:1016:G:H3'	1:X:1017:A:H5''	1.87	0.56
1:X:501:C:N3	1:X:519:G:H5'	2.21	0.56
1:X:1065:A:H3'	1:X:1065:A:H8	1.70	0.56
5:C:136:THR:HG22	5:C:140:LYS:NZ	2.20	0.56
1:X:2887:G:O2'	1:X:2888:A:OP2	2.22	0.56
1:X:2358:G:H4'	21:T:51:THR:H	1.71	0.56
12:K:18:ARG:NE	12:K:65:THR:O	2.38	0.56
1:X:1813:A:H1'	1:X:1965:A:N6	2.20	0.56
24:W:4:LEU:HB3	24:W:58:GLU:HB2	1.87	0.56
1:X:731:U:O5'	26:2:12:LYS:NZ	2.36	0.56
1:X:955:A:C4	11:J:15:PRO:HG3	2.41	0.56
14:M:106:ARG:HA	14:M:106:ARG:CZ	2.36	0.55
1:X:1466:G:H3'	1:X:1467:G:H5''	1.87	0.55
11:J:22:LYS:HD3	11:J:101:ARG:HB2	1.88	0.55
1:X:1359:A:N1	1:X:1370:C:O2'	2.37	0.55
18:Q:64:ARG:HA	18:Q:69:GLN:HA	1.88	0.55
2:Y:36:C:H2'	2:Y:37:A:H8	1.71	0.55
16:O:78:ARG:O	16:O:80:LYS:N	2.39	0.55
1:X:1515:G:N2	1:X:1565:U:O2	2.35	0.55
14:M:106:ARG:HA	14:M:106:ARG:NE	2.21	0.55
1:X:1281:U:H2'	1:X:1282:A:C8	2.42	0.55
6:D:132:VAL:HG22	6:D:133:LYS:H	1.70	0.55
8:G:76:TYR:HB3	8:G:85:ILE:HD11	1.89	0.55
11:J:39:THR:HG23	11:J:98:LYS:HA	1.88	0.55
24:W:4:LEU:HA	24:W:58:GLU:HG3	1.89	0.55
1:X:1280:U:H2'	1:X:1281:U:C6	2.41	0.55
1:X:916:U:H5'	11:J:7:VAL:HG12	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1825:U:H3	1:X:1848:A:H61	1.55	0.55
1:X:422:G:H2'	1:X:423:A:C8	2.42	0.55
5:C:114:LEU:HG	5:C:181:LEU:HD11	1.89	0.55
1:X:322:A:H2'	1:X:323:C:H5'	1.89	0.55
5:C:158:ASN:HA	5:C:161:VAL:HG22	1.89	0.55
1:X:2599:A:N7	4:B:158:SER:HB3	2.22	0.55
1:X:2725:U:H2'	1:X:2726:C:C6	2.42	0.55
15:N:94:MET:O	15:N:98:ILE:HG12	2.07	0.55
1:X:1492:G:N2	1:X:1508:C:C4	2.75	0.55
1:X:658:A:H3'	1:X:659:A:C5'	2.37	0.55
1:X:153:G:C6	1:X:177:G:C6	2.95	0.55
1:X:706:U:H1'	10:I:13:ARG:HA	1.89	0.54
4:B:132:LYS:HG2	4:B:173:MET:HE1	1.88	0.54
1:X:1806:U:H5	1:X:1811:A:N7	2.05	0.54
12:K:50:LEU:HD22	12:K:58:SER:HB2	1.89	0.54
1:X:333:C:H42	1:X:393:G:H1	1.55	0.54
11:J:14:ARG:HD2	11:J:73:PRO:HD2	1.89	0.54
1:X:680:C:O2'	1:X:684:U:OP1	2.24	0.54
1:X:245:G:O2'	1:X:257:G:O6	2.17	0.54
1:X:2446:U:H2'	1:X:2447:C:C6	2.43	0.54
10:I:21:ARG:HG2	10:I:21:ARG:HH11	1.73	0.54
15:N:105:ALA:HB1	16:O:40:PHE:HZ	1.70	0.54
1:X:1340:G:P	29:X:3005:MPD:H32	2.48	0.54
1:X:226:A:O2'	1:X:466:C:O2	2.25	0.54
1:X:2811:U:H2'	1:X:2812:U:H6	1.72	0.54
14:M:78:LEU:HB3	14:M:79:HIS:HD2	1.72	0.54
1:X:2749:G:H2'	1:X:2750:C:H6	1.72	0.54
1:X:1544:G:O2'	3:A:99:GLY:O	2.18	0.54
7:E:95:ARG:HA	7:E:104:ILE:HA	1.88	0.54
16:O:14:VAL:HG12	16:O:20:ILE:HG21	1.90	0.54
1:X:690:U:H4'	1:X:691:A:OP2	2.07	0.54
17:P:30:ALA:HA	17:P:33:ILE:HD12	1.89	0.54
1:X:1523:G:H1	1:X:1557:C:N4	2.05	0.54
15:N:83:LEU:HD23	15:N:113:ALA:HB2	1.90	0.54
7:E:102:ASP:N	7:E:115:ILE:HD13	2.23	0.54
1:X:1875:A:H2'	1:X:1876:G:O4'	2.08	0.54
5:C:10:ASP:OD1	5:C:10:ASP:N	2.41	0.54
1:X:37:C:H2'	1:X:38:A:H8	1.70	0.54
11:J:43:THR:HG22	11:J:46:GLN:CD	2.28	0.54
1:X:718:C:H5''	5:C:81:PRO:HD2	1.89	0.54
1:X:1514:A:H2'	1:X:1515:G:H5'	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1242:A:H4'	10:I:3:LEU:HD23	1.89	0.54
1:X:1340:G:OP1	29:X:3005:MPD:O4	2.19	0.54
1:X:100:U:H3'	1:X:101:G:H5'	1.90	0.54
19:R:86:VAL:O	19:R:90:LYS:HB2	2.08	0.54
2:Y:91:C:H2'	2:Y:92:G:H8	1.71	0.54
1:X:1410:A:H2'	1:X:1411:G:O4'	2.07	0.54
1:X:1644:C:P	18:Q:76:ARG:HH22	2.30	0.54
1:X:1347:G:OP2	26:2:10:LYS:HE2	2.08	0.54
1:X:2507:C:C2'	1:X:2508:G:H5'	2.38	0.54
9:H:1:MET:N	9:H:67:SER:OG	2.40	0.54
1:X:1213:C:H42	1:X:1219:G:H1	1.56	0.54
1:X:629:A:H62	1:X:1289:A:H2	1.55	0.53
3:A:88:SER:HB2	3:A:158:ALA:HB2	1.90	0.53
1:X:2081:A:C2	1:X:2643:C:N3	2.76	0.53
18:Q:5:ASP:OD1	18:Q:5:ASP:N	2.41	0.53
7:E:89:LEU:HD11	7:E:94:TYR:HA	1.90	0.53
1:X:2268:A:H2'	1:X:2269:G:C8	2.43	0.53
1:X:2784:A:N1	7:E:67:THR:HG21	2.23	0.53
1:X:1514:A:N6	1:X:1566:G:H22	2.06	0.53
1:X:2241:C:H2'	1:X:2242:G:O4'	2.09	0.53
1:X:460:C:H2'	1:X:461:A:C8	2.42	0.53
1:X:379:C:C2	1:X:380:U:C5	2.96	0.53
1:X:1391:A:H2'	1:X:1392:G:O4'	2.08	0.53
1:X:1888:U:O4	1:X:1910:G:N2	2.42	0.53
2:Y:91:C:H2'	2:Y:92:G:C8	2.42	0.53
1:X:712:U:H2'	1:X:713:A:O4'	2.09	0.53
1:X:1097:U:O4	1:X:1098:A:N6	2.42	0.53
1:X:329:A:N6	1:X:398:C:H42	2.06	0.53
28:4:24:MET:HG3	28:4:34:GLN:O	2.08	0.53
1:X:1290:G:OP2	15:N:13:ARG:NH2	2.41	0.53
1:X:257:G:N7	27:3:5:LYS:HE3	2.24	0.53
3:A:142:HIS:N	3:A:191:THR:O	2.40	0.53
1:X:1091:G:H2'	1:X:1154:G:H1	1.74	0.53
1:X:1395:G:C6	1:X:1408:G:N7	2.77	0.53
12:K:23:SER:O	12:K:25:ILE:N	2.40	0.53
1:X:1630:A:H2'	1:X:1631:G:H5'	1.91	0.53
11:J:59:LYS:O	11:J:61:GLY:N	2.42	0.53
1:X:1540:U:H1'	1:X:1625:U:H4'	1.90	0.53
1:X:2255:G:H2'	1:X:2256:U:H6	1.72	0.53
1:X:2120:G:H21	1:X:2225:A:N6	2.07	0.53
4:B:125:LYS:HB2	4:B:173:MET:HB3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:75:ALA:HB2	20:S:92:LEU:HB2	1.90	0.53
1:X:946:A:H2'	1:X:947:U:H5'	1.91	0.53
1:X:2774:G:O2'	7:E:67:THR:HG22	2.09	0.53
1:X:1072:A:N6	1:X:1169:G:H2'	2.24	0.53
1:X:1460:U:H3	1:X:1628:A:N6	2.07	0.53
1:X:1501:G:N2	1:X:2729:G:H22	2.03	0.53
1:X:1313:G:OP2	1:X:1689:G:O2'	2.20	0.53
1:X:1186:A:C4	1:X:1188:A:C8	2.97	0.52
1:X:55:G:H2'	1:X:56:A:H8	1.72	0.52
1:X:587:C:O2'	1:X:588:G:H5'	2.09	0.52
1:X:774:G:H5'	1:X:775:A:H5''	1.91	0.52
1:X:2725:U:H2'	1:X:2726:C:H6	1.74	0.52
1:X:233:U:O2'	1:X:234:C:H5'	2.10	0.52
1:X:955:A:C6	11:J:15:PRO:HD3	2.45	0.52
1:X:2294:A:H5''	1:X:2295:A:H5'	1.90	0.52
1:X:2047:A:H5'	25:Z:9:SER:HB3	1.91	0.52
1:X:154:A:O2'	1:X:155:U:H5''	2.09	0.52
1:X:2385:A:N1	10:I:50:PHE:HZ	2.08	0.52
2:Y:65:G:O6	2:Y:105:G:N2	2.33	0.52
24:W:4:LEU:HD13	24:W:6:ILE:HD11	1.92	0.52
1:X:179:A:OP2	1:X:179:A:H8	1.91	0.52
1:X:79:U:HO2'	1:X:389:A:H8	1.57	0.52
1:X:2646:U:OP1	4:B:165:LYS:NZ	2.30	0.52
19:R:56:ILE:HB	19:R:58:GLU:HG2	1.91	0.52
1:X:339:A:H2'	1:X:340:C:C6	2.45	0.52
9:H:120:GLU:N	9:H:120:GLU:OE1	2.43	0.52
1:X:1013:U:O3'	24:W:14:GLY:HA2	2.09	0.52
1:X:897:A:H2'	1:X:898:U:H6	1.75	0.52
1:X:2314:A:H2	1:X:2373:A:H62	1.58	0.52
1:X:1472:C:O2'	1:X:1616:A:OP2	2.24	0.52
3:A:142:HIS:CE1	3:A:143:ASN:HB2	2.44	0.52
10:I:78:ASN:ND2	10:I:106:LYS:O	2.43	0.52
15:N:26:GLY:O	15:N:29:HIS:ND1	2.43	0.52
1:X:489:A:N3	1:X:1240:U:H1'	2.23	0.52
1:X:1864:C:O2'	1:X:1955:A:N3	2.38	0.52
1:X:632:U:H2'	1:X:633:A:C8	2.45	0.52
3:A:132:LEU:H	3:A:134:ASN:H	1.58	0.52
1:X:142:G:N2	1:X:1640:U:O3'	2.38	0.52
1:X:1053:A:N3	1:X:1197:C:O2'	2.41	0.52
22:U:10:ARG:NH1	22:U:11:LYS:O	2.43	0.52
1:X:83:G:N2	1:X:102:A:H2	2.06	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:11:ARG:HA	17:P:100:THR:HG22	1.92	0.51
7:E:136:ILE:HG13	7:E:137:SER:H	1.75	0.51
15:N:61:TRP:CD2	15:N:93:LYS:HB2	2.45	0.51
11:J:44:SER:HB3	11:J:70:PRO:HG3	1.92	0.51
24:W:40:ASN:HB2	24:W:43:ILE:H	1.75	0.51
1:X:2694:C:N3	7:E:110:SER:OG	2.43	0.51
1:X:1767:G:HO2'	1:X:1768:C:H6	1.57	0.51
1:X:2895:G:N2	14:M:1:MET:HA	2.25	0.51
24:W:50:VAL:HB	24:W:53:LEU:CD1	2.41	0.51
1:X:1651:C:OP1	29:X:3005:MPD:O2	2.22	0.51
1:X:947:U:H2'	1:X:948:U:C6	2.45	0.51
1:X:1460:U:H3	1:X:1628:A:H61	1.56	0.51
1:X:2459:A:H2'	1:X:2460:A:C8	2.46	0.51
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.92	0.51
1:X:874:A:N7	1:X:2274:A:O2'	2.43	0.51
1:X:2783:U:H3'	28:4:19:ARG:O	2.10	0.51
1:X:1039:C:O2'	15:N:93:LYS:NZ	2.44	0.51
1:X:1575:A:H2'	1:X:1576:A:C5'	2.40	0.51
1:X:2759:G:H3'	1:X:2760:A:O4'	2.10	0.51
17:P:20:VAL:HG21	17:P:43:SER:HB2	1.93	0.51
28:4:19:ARG:HG3	28:4:24:MET:SD	2.51	0.51
8:G:32:GLU:O	8:G:36:ILE:HG12	2.11	0.51
1:X:1185:U:H2'	8:G:66:THR:HG21	1.92	0.51
1:X:637:U:H2'	1:X:638:U:H6	1.74	0.51
1:X:1599:G:OP1	1:X:1761:G:N2	2.44	0.51
1:X:1452:C:O2	1:X:1631:G:N2	2.43	0.51
19:R:24:ILE:O	19:R:34:VAL:HB	2.10	0.51
8:G:7:ALA:H	8:G:46:THR:HG21	1.76	0.51
1:X:1329:G:H2'	1:X:1330:U:C6	2.45	0.51
1:X:1700:C:H2'	1:X:1701:U:C6	2.46	0.51
1:X:1094:A:C2	1:X:2778:G:C5	2.98	0.51
6:D:23:SER:N	6:D:27:GLU:OE1	2.43	0.51
1:X:124:A:C6	26:2:11:ARG:HD3	2.46	0.51
1:X:581:A:H5'	15:N:53:ARG:HD3	1.93	0.51
1:X:658:A:H3'	1:X:659:A:H5''	1.92	0.51
14:M:51:LYS:HD2	14:M:53:ARG:HG2	1.93	0.51
1:X:2286:G:C6	1:X:2287:C:C4	2.99	0.51
1:X:1796:A:O2'	1:X:1985:C:OP1	2.24	0.51
1:X:2534:C:C2	1:X:2535:G:C8	2.99	0.51
2:Y:87:G:N1	11:J:39:THR:O	2.45	0.50
1:X:650:U:H3	1:X:666:A:H2	1.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:59:GLY:HA3	5:C:79:ARG:HG3	1.94	0.50
1:X:2895:G:H21	14:M:1:MET:HA	1.76	0.50
1:X:704:U:H2'	1:X:705:U:O4'	2.11	0.50
1:X:2425:U:H2'	1:X:2426:G:C8	2.46	0.50
1:X:2732:A:H2'	1:X:2733:A:O4'	2.10	0.50
1:X:2856:U:H2'	1:X:2857:A:H8	1.76	0.50
5:C:179:GLN:O	5:C:183:VAL:HG12	2.11	0.50
1:X:1833:C:H2'	1:X:1834:G:H8	1.77	0.50
1:X:793:G:C8	17:P:89:ALA:HB1	2.47	0.50
1:X:1197:C:H2'	1:X:1198:G:O4'	2.11	0.50
11:J:10:ARG:O	11:J:11:ARG:HG3	2.10	0.50
1:X:2037:G:OP2	17:P:41:LYS:NZ	2.33	0.50
1:X:1867:G:C8	1:X:1954:A:C2	2.99	0.50
1:X:1561:G:H8	1:X:1562:C:C6	2.29	0.50
1:X:1846:A:H4'	1:X:1847:U:H5''	1.92	0.50
1:X:2473:G:H2'	1:X:2474:G:H5''	1.92	0.50
1:X:2549:U:O2'	1:X:2674:U:OP1	2.15	0.50
1:X:407:G:H2'	1:X:408:U:C6	2.46	0.50
1:X:1303:A:H8	1:X:1303:A:OP1	1.95	0.50
1:X:2602:C:H5'	4:B:157:ALA:HB2	1.94	0.50
14:M:102:LEU:O	14:M:103:ARG:CZ	2.60	0.50
1:X:2869:G:OP1	14:M:95:ARG:NH1	2.45	0.50
8:G:57:VAL:HB	8:G:125:VAL:HG13	1.94	0.50
28:4:2:LYS:HG2	28:4:4:ARG:HD2	1.93	0.50
1:X:1423:C:H2'	1:X:1424:A:C8	2.47	0.50
1:X:679:G:H2'	1:X:680:C:C6	2.46	0.50
1:X:1450:A:N6	1:X:1635:A:H62	2.09	0.50
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.45	0.50
1:X:841:C:H2'	1:X:842:U:C6	2.46	0.50
1:X:450:C:H4'	1:X:451:U:H5'	1.94	0.50
1:X:157:U:H2'	1:X:158:G:H8	1.77	0.50
1:X:168:A:H2	1:X:169:G:C2	2.29	0.50
10:I:21:ARG:CG	10:I:21:ARG:HH11	2.24	0.50
1:X:2903:A:C5'	1:X:2904:U:H5'	2.42	0.50
18:Q:17:SER:HA	18:Q:20:MET:HE2	1.93	0.50
1:X:788:A:O2'	1:X:1703:U:OP1	2.26	0.50
1:X:719:G:O2'	5:C:74:ARG:HG3	2.12	0.50
1:X:381:G:N2	1:X:382:U:H1'	2.27	0.50
1:X:1023:A:H2'	1:X:1026:C:H42	1.75	0.50
1:X:1817:C:H2'	1:X:1818:A:C5	2.47	0.50
7:E:87:LEU:HD23	7:E:164:TYR:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:5:PHE:O	15:N:64:ARG:NH2	2.45	0.50
1:X:1775:G:H2'	1:X:1776:A:C8	2.47	0.49
26:2:16:VAL:H	26:2:21:LYS:HG3	1.76	0.49
1:X:89:U:H3	1:X:90:A:H62	1.57	0.49
1:X:665:G:H4'	1:X:666:A:C5'	2.41	0.49
1:X:1382:C:N4	1:X:1383:G:O6	2.45	0.49
1:X:620:G:H2'	1:X:621:A:C8	2.47	0.49
1:X:1229:G:OP1	10:I:31:SER:HA	2.13	0.49
1:X:1091:G:O2'	1:X:1092:A:O5'	2.25	0.49
5:C:29:ASN:HB3	5:C:108:LEU:HD11	1.94	0.49
10:I:60:ARG:HB3	10:I:60:ARG:CZ	2.43	0.49
1:X:2770:U:OP1	28:4:33:LYS:NZ	2.44	0.49
1:X:1379:A:O2'	1:X:1381:U:OP2	2.19	0.49
1:X:396:G:H2'	1:X:397:U:H5'	1.94	0.49
14:M:16:ARG:HH12	14:M:83:ILE:HG22	1.77	0.49
1:X:319:G:N3	1:X:319:G:H2'	2.27	0.49
4:B:133:ARG:NH1	4:B:172:ARG:O	2.45	0.49
1:X:734:A:H2'	1:X:735:C:C6	2.48	0.49
1:X:677:A:H2'	1:X:678:A:C8	2.46	0.49
1:X:627:C:OP2	29:X:3007:MPD:H4	2.13	0.49
1:X:1065:A:H62	1:X:1185:U:H3	1.60	0.49
15:N:59:LYS:O	15:N:63:THR:HG23	2.12	0.49
1:X:2255:G:H2'	1:X:2256:U:C6	2.47	0.49
1:X:272:C:H42	1:X:416:G:H1	1.60	0.49
4:B:142:SER:HG	4:B:143:HIS:HD1	1.60	0.49
7:E:106:ASN:O	7:E:108:GLY:N	2.45	0.49
12:K:110:ARG:HG3	12:K:111:GLY:N	2.28	0.49
19:R:64:HIS:O	19:R:66:SER:N	2.46	0.49
1:X:850:G:O4'	10:I:36:LYS:HE3	2.12	0.49
1:X:1487:G:O6	1:X:1596:G:N1	2.46	0.49
1:X:327:G:O2'	1:X:328:G:O5'	2.31	0.49
1:X:1700:C:H2'	1:X:1701:U:H6	1.76	0.49
1:X:1315:C:H2'	1:X:1316:G:H8	1.77	0.49
5:C:7:LEU:HD21	5:C:126:VAL:N	2.21	0.49
1:X:378:C:H2'	1:X:379:C:H6	1.76	0.49
17:P:69:LEU:HD22	17:P:107:VAL:HG12	1.95	0.49
4:B:163:VAL:HG13	4:B:167:GLN:HG3	1.94	0.49
1:X:2372:G:H1'	1:X:2409:G:H5'	1.94	0.49
25:Z:28:THR:HG23	25:Z:37:TYR:CD1	2.47	0.49
12:K:28:GLU:HG3	12:K:121:LEU:HD11	1.95	0.49
17:P:11:ARG:NE	17:P:11:ARG:O	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:5:PHE:HD2	15:N:100:ILE:HD13	1.76	0.49
14:M:24:PRO:HA	14:M:49:VAL:HG12	1.94	0.49
1:X:2774:G:O6	1:X:2782:C:H5''	2.13	0.49
2:Y:57:G:H3'	2:Y:58:G:H8	1.78	0.49
1:X:379:C:H2'	1:X:380:U:C6	2.48	0.49
1:X:1867:G:C2	1:X:1868:U:C2	3.00	0.49
1:X:1381:U:O2'	1:X:1421:A:H2'	2.11	0.49
9:H:44:LYS:O	9:H:54:LYS:HE2	2.12	0.49
17:P:13:ALA:HB1	17:P:14:PRO:HD2	1.95	0.49
1:X:352:A:H5'	19:R:15:LYS:HG3	1.94	0.49
1:X:2377:C:H2'	1:X:2378:G:O4'	2.12	0.49
1:X:630:G:P	10:I:21:ARG:HH22	2.35	0.49
1:X:1806:U:C5	1:X:1811:A:N7	2.80	0.49
1:X:2543:G:C4	1:X:2596:G:N2	2.81	0.49
1:X:2079:G:O2'	4:B:160:ALA:O	2.29	0.49
1:X:1494:G:C8	1:X:1495:C:H5	2.31	0.49
1:X:615:A:H5''	1:X:616:G:OP2	2.13	0.48
1:X:805:G:H4'	1:X:1803:G:OP1	2.13	0.48
1:X:274:A:N3	1:X:414:C:O2'	2.45	0.48
1:X:828:A:H2'	1:X:828:A:N3	2.27	0.48
1:X:2332:U:H2'	1:X:2333:U:H5'	1.95	0.48
1:X:1331:C:O2'	12:K:67:ARG:HG3	2.13	0.48
15:N:98:ILE:HD11	16:O:4:ILE:HD11	1.93	0.48
12:K:55:ASP:OD1	12:K:55:ASP:N	2.45	0.48
2:Y:86:C:H3'	2:Y:86:C:O2	2.13	0.48
1:X:1698:A:H1'	1:X:2843:A:H5'	1.94	0.48
1:X:79:U:C2'	1:X:389:A:H8	2.25	0.48
1:X:460:C:H1'	1:X:1891:U:O2'	2.12	0.48
4:B:116:ILE:HG12	4:B:183:LEU:O	2.14	0.48
1:X:379:C:H2'	1:X:380:U:H6	1.79	0.48
1:X:1886:A:H3'	1:X:1887:G:H8	1.77	0.48
1:X:1818:A:H4'	3:A:205:VAL:HB	1.94	0.48
19:R:8:ASN:HA	19:R:22:LYS:HG2	1.96	0.48
1:X:2101:U:H2'	1:X:2102:U:C6	2.49	0.48
1:X:810:A:H2'	1:X:811:C:C6	2.48	0.48
1:X:2788:A:H2'	1:X:2789:U:C6	2.48	0.48
1:X:674:C:N4	1:X:675:G:O6	2.46	0.48
3:A:43:ARG:HD3	3:A:49:LEU:HA	1.96	0.48
1:X:12:U:H2'	1:X:12:U:O2	2.13	0.48
1:X:1491:C:C2	1:X:1492:G:C2	3.01	0.48
11:J:22:LYS:HD2	11:J:98:LYS:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1400:C:O2'	1:X:1836:A:H1'	2.14	0.48
16:O:18:GLN:O	16:O:97:ILE:HG12	2.13	0.48
1:X:548:A:H4'	1:X:549:U:H5''	1.94	0.48
1:X:1521:A:O2'	1:X:1522:G:OP1	2.30	0.48
1:X:1492:G:N3	1:X:1593:G:N2	2.62	0.48
1:X:1091:G:H2'	1:X:1154:G:N1	2.28	0.48
1:X:2717:A:H5''	12:K:4:ARG:HH21	1.79	0.48
1:X:685:C:H2'	1:X:686:U:C6	2.48	0.48
1:X:897:A:H2'	1:X:898:U:C6	2.47	0.48
17:P:40:ASN:O	17:P:41:LYS:HD2	2.12	0.48
5:C:123:LEU:O	5:C:188:ASN:HA	2.13	0.48
1:X:424:C:N4	1:X:425:G:O6	2.46	0.48
13:L:30:ARG:N	13:L:45:ILE:O	2.46	0.48
1:X:2494:C:H2'	1:X:2495:A:O4'	2.14	0.48
1:X:32:C:O2'	1:X:33:U:H5'	2.13	0.48
22:U:29:TRP:CG	22:U:30:ASN:N	2.76	0.48
17:P:36:LEU:HD13	17:P:48:GLU:HA	1.95	0.48
2:Y:90:C:H2'	2:Y:91:C:C6	2.49	0.48
1:X:1510:U:H2'	1:X:1511:C:C6	2.48	0.48
1:X:1833:C:H2'	1:X:1834:G:C8	2.49	0.48
12:K:32:THR:HG22	12:K:33:THR:N	2.29	0.48
1:X:526:A:H4'	19:R:42:LYS:HB2	1.96	0.48
1:X:2382:C:C4	1:X:2383:C:C4	3.01	0.48
1:X:1295:C:H4'	5:C:83:TRP:CE3	2.48	0.48
8:G:12:ILE:HD11	8:G:51:THR:HA	1.96	0.48
4:B:189:ASP:OD1	4:B:192:ASN:N	2.38	0.48
10:I:19:VAL:HG22	10:I:27:ASN:HB3	1.96	0.48
1:X:1218:G:H2'	1:X:1219:G:C8	2.49	0.48
10:I:95:LEU:HD12	10:I:96:LEU:N	2.29	0.48
1:X:1922:C:H2'	1:X:1923:A:H8	1.77	0.48
1:X:1059:A:H2'	1:X:1060:U:C6	2.49	0.48
20:S:155:THR:HG22	20:S:159:VAL:HG13	1.95	0.48
24:W:6:ILE:CD1	24:W:56:VAL:HG12	2.44	0.48
23:V:63:GLU:HA	23:V:66:LYS:HG3	1.94	0.48
1:X:1819:G:O2'	1:X:1857:C:OP1	2.24	0.48
1:X:1574:G:H2'	1:X:1575:A:O4'	2.14	0.48
2:Y:6:U:H3	2:Y:109:C:H42	1.61	0.48
1:X:280:C:H2'	1:X:281:A:C8	2.44	0.48
25:Z:15:LYS:O	25:Z:18:THR:HG23	2.14	0.48
1:X:1494:G:HO2'	1:X:1495:C:C5'	2.26	0.48
4:B:154:VAL:HG21	4:B:169:MET:HE3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:49:G:C6	2:Y:50:A:C6	3.02	0.48
1:X:1710:G:O3'	9:H:6:THR:HG23	2.13	0.48
8:G:69:LYS:HG2	8:G:73:LYS:HB2	1.96	0.48
4:B:205:LYS:O	4:B:207:GLY:N	2.46	0.48
11:J:22:LYS:HE2	11:J:101:ARG:CZ	2.44	0.47
5:C:8:LYS:HA	5:C:14:SER:H	1.79	0.47
1:X:680:C:H2'	1:X:681:G:O4'	2.14	0.47
1:X:626:G:N2	1:X:1296:C:C2	2.82	0.47
1:X:302:A:HO2'	1:X:303:G:H8	1.62	0.47
1:X:1609:U:H2'	1:X:1610:G:C8	2.49	0.47
1:X:1302:G:OP1	25:Z:16:ARG:NH2	2.37	0.47
1:X:575:G:N3	1:X:575:G:H2'	2.29	0.47
1:X:1521:A:HO2'	1:X:1522:G:P	2.36	0.47
1:X:2811:U:H2'	1:X:2812:U:C6	2.49	0.47
11:J:22:LYS:HG2	11:J:101:ARG:HB2	1.96	0.47
1:X:1013:U:H2'	1:X:1014:U:C6	2.49	0.47
1:X:1694:A:O3'	12:K:33:THR:HG21	2.14	0.47
1:X:2632:U:H2'	1:X:2633:C:C6	2.49	0.47
1:X:2311:U:H1'	1:X:2352:G:N2	2.28	0.47
20:S:55:VAL:HB	20:S:59:GLY:HA3	1.96	0.47
4:B:53:PHE:CG	4:B:54:GLU:N	2.81	0.47
14:M:54:GLY:HA3	14:M:59:GLU:HA	1.96	0.47
1:X:1346:G:H4'	26:2:8:PRO:HG2	1.97	0.47
1:X:1985:C:H2'	1:X:1986:G:H8	1.78	0.47
13:L:95:ASP:O	13:L:97:GLY:N	2.47	0.47
21:T:20:ASN:OD1	21:T:21:GLY:N	2.47	0.47
7:E:75:MET:O	7:E:79:VAL:HB	2.15	0.47
1:X:1869:G:H2'	1:X:1870:C:C6	2.50	0.47
7:E:103:LEU:H	7:E:115:ILE:HD11	1.79	0.47
1:X:24:G:H2'	1:X:25:U:H6	1.80	0.47
1:X:2903:A:H5''	1:X:2904:U:H5'	1.96	0.47
1:X:250:G:H4'	1:X:432:G:C4	2.49	0.47
17:P:6:VAL:HG22	17:P:104:THR:HG23	1.95	0.47
1:X:1183:G:H5'	8:G:105:SER:OG	2.15	0.47
4:B:14:GLN:NE2	4:B:22:LEU:HD21	2.30	0.47
1:X:1151:G:H2'	1:X:1152:U:C6	2.49	0.47
1:X:2111:C:H2'	1:X:2112:C:H6	1.78	0.47
1:X:51:G:H1'	1:X:117:A:H61	1.78	0.47
1:X:1182:G:H2'	1:X:1183:G:O4'	2.14	0.47
1:X:187:C:H2'	1:X:188:C:C6	2.50	0.47
17:P:9:THR:HG22	17:P:80:PRO:HD2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:105:PRO:HD2	20:S:123:GLN:O	2.15	0.47
1:X:870:C:H4'	1:X:2455:G:N7	2.28	0.47
1:X:136:A:H61	1:X:143:U:H3	1.62	0.47
1:X:1973:U:H2'	1:X:1974:C:C6	2.49	0.47
1:X:638:U:H2'	1:X:639:U:C6	2.48	0.47
1:X:605:U:O2	1:X:615:A:H1'	2.15	0.47
1:X:719:G:O2'	5:C:67:GLN:OE1	2.29	0.47
1:X:1818:A:N6	1:X:1855:G:O2'	2.47	0.47
17:P:24:ILE:HD11	17:P:36:LEU:HG	1.96	0.47
1:X:813:G:H2'	1:X:814:A:C8	2.50	0.47
1:X:2122:A:H2'	1:X:2123:A:C8	2.50	0.47
7:E:45:GLN:N	7:E:45:GLN:OE1	2.48	0.47
1:X:1376:G:OP1	18:Q:13:THR:HG21	2.14	0.47
1:X:2905:C:N4	25:Z:39:LEU:HG	2.29	0.47
1:X:70:G:N2	1:X:71:A:N1	2.63	0.47
1:X:71:A:H4'	1:X:72:U:H5''	1.95	0.47
14:M:78:LEU:HB3	14:M:79:HIS:CD2	2.50	0.47
2:Y:21:G:N1	2:Y:22:G:O6	2.48	0.47
1:X:1353:A:H2'	1:X:1354:G:H8	1.79	0.47
1:X:1651:C:H5''	1:X:1652:A:H5'	1.96	0.47
1:X:2334:G:O2'	1:X:2337:A:N6	2.30	0.47
1:X:769:U:H2'	1:X:770:G:O4'	2.14	0.47
12:K:51:GLY:HA2	12:K:86:PHE:CZ	2.49	0.47
14:M:102:LEU:HA	14:M:102:LEU:HD13	1.54	0.47
1:X:1931:G:H1	1:X:1957:G:N2	2.12	0.47
1:X:1373:U:H2'	1:X:1374:G:C8	2.50	0.47
1:X:183:A:OP2	1:X:183:A:H3'	2.15	0.47
1:X:2425:U:H2'	1:X:2426:G:H8	1.80	0.47
1:X:1815:C:H5''	3:A:224:VAL:HG11	1.97	0.47
14:M:29:ARG:HH11	14:M:89:LYS:NZ	2.13	0.47
1:X:510:U:H5'	26:2:6:TYR:CD1	2.49	0.47
1:X:5:A:H2'	1:X:6:A:C8	2.50	0.47
10:I:60:ARG:HB3	10:I:60:ARG:NH1	2.30	0.47
1:X:1279:C:H2'	1:X:1280:U:H6	1.79	0.47
1:X:2438:A:H2'	1:X:2439:A:C8	2.50	0.47
6:D:13:THR:O	6:D:17:MET:HB2	2.15	0.47
1:X:1487:G:C6	1:X:1596:G:N1	2.83	0.47
1:X:1448:U:H3'	1:X:1449:A:C5'	2.41	0.47
1:X:1893:A:N6	1:X:1902:G:O2'	2.48	0.47
1:X:353:A:O2'	1:X:354:A:H2'	2.15	0.47
1:X:1854:U:H2'	1:X:1855:G:O4'	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:811:C:N4	1:X:812:U:O4	2.48	0.47
10:I:96:LEU:HB2	10:I:113:GLY:O	2.15	0.47
1:X:1793:C:H2'	1:X:1794:C:H6	1.80	0.47
1:X:2817:A:HO2'	1:X:2818:A:P	2.36	0.46
1:X:682:A:H4'	1:X:683:G:H5'	1.96	0.46
17:P:14:PRO:O	17:P:18:ARG:HG3	2.15	0.46
19:R:26:THR:HA	19:R:33:VAL:HA	1.97	0.46
1:X:2782:C:H3'	28:4:19:ARG:NH2	2.30	0.46
1:X:24:G:H2'	1:X:25:U:C6	2.51	0.46
24:W:51:LYS:NZ	24:W:56:VAL:H	2.13	0.46
1:X:1437:U:H2'	1:X:1438:G:O4'	2.16	0.46
1:X:1468:G:H2'	1:X:1469:G:O4'	2.16	0.46
1:X:2881:C:H2'	1:X:2882:A:H8	1.80	0.46
1:X:494:U:H1'	5:C:84:ARG:HG3	1.97	0.46
1:X:2093:C:C2'	1:X:2094:G:H5'	2.46	0.46
1:X:1053:A:H5''	15:N:63:THR:HG22	1.97	0.46
24:W:15:ARG:HD2	24:W:53:LEU:HD23	1.96	0.46
1:X:1352:C:H42	1:X:1374:G:H1	1.62	0.46
1:X:140:A:O2'	1:X:1446:U:H5'	2.15	0.46
4:B:9:LYS:O	4:B:28:VAL:HA	2.15	0.46
17:P:5:ALA:HB3	17:P:54:ALA:HB2	1.97	0.46
5:C:104:LYS:HE2	5:C:104:LYS:HB3	1.61	0.46
16:O:2:PHE:CE1	16:O:42:GLY:HA3	2.51	0.46
1:X:2419:A:H2	1:X:2451:C:N4	2.12	0.46
4:B:7:GLY:HA2	4:B:53:PHE:CZ	2.50	0.46
5:C:113:ALA:HB3	5:C:181:LEU:HD13	1.97	0.46
1:X:747:U:H3	1:X:775:A:H61	1.62	0.46
1:X:1611:C:H2'	1:X:1612:C:C6	2.51	0.46
1:X:1268:C:H2'	1:X:1269:A:C8	2.51	0.46
1:X:566:U:H2'	1:X:567:G:N7	2.31	0.46
6:D:101:ASP:HA	6:D:130:LEU:HD11	1.98	0.46
11:J:37:THR:HG22	20:S:82:LEU:HD23	1.98	0.46
1:X:2111:C:H2'	1:X:2112:C:C6	2.50	0.46
10:I:21:ARG:HG2	10:I:21:ARG:NH1	2.30	0.46
1:X:234:C:O2'	1:X:235:G:O4'	2.26	0.46
1:X:1295:C:H5'	5:C:75:GLN:NE2	2.29	0.46
3:A:91:ILE:HB	3:A:104:ILE:O	2.16	0.46
17:P:86:ARG:HG3	17:P:87:PRO:CD	2.45	0.46
1:X:1038:C:OP2	15:N:54:LYS:NZ	2.49	0.46
1:X:2740:A:H3'	1:X:2741:G:H5''	1.96	0.46
1:X:2349:A:H2'	1:X:2350:G:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:906:A:H2'	1:X:907:G:O4'	2.15	0.46
1:X:788:A:OP1	4:B:144:GLY:HA2	2.16	0.46
1:X:1451:U:H2'	1:X:1452:C:C6	2.51	0.46
1:X:1438:G:H2'	1:X:1439:U:C6	2.50	0.46
1:X:2642:U:N1	25:Z:4:PRO:HA	2.30	0.46
1:X:1441:C:H2'	1:X:1442:C:H6	1.80	0.46
1:X:198:A:N6	1:X:201:C:OP2	2.46	0.46
17:P:7:ALA:HB1	17:P:10:ILE:HD11	1.98	0.46
5:C:145:THR:HG21	5:C:186:ILE:HG13	1.97	0.46
2:Y:94:U:H2'	2:Y:95:A:O4'	2.16	0.46
1:X:1065:A:C3'	1:X:1065:A:C8	2.96	0.46
1:X:1053:A:OP2	8:G:40:LYS:NZ	2.46	0.46
24:W:26:LEU:HB2	24:W:28:LEU:HD12	1.97	0.46
25:Z:38:LYS:H	25:Z:38:LYS:NZ	2.14	0.46
1:X:1241:A:H2'	1:X:1242:A:C8	2.49	0.46
1:X:1450:A:H5''	1:X:1451:U:C5	2.48	0.46
17:P:50:VAL:HG12	17:P:105:ILE:HD12	1.97	0.46
1:X:506:A:N1	1:X:515:G:H8	2.14	0.46
14:M:92:GLY:HA2	14:M:110:ALA:HA	1.97	0.46
1:X:409:G:N2	1:X:411:A:H61	2.14	0.46
1:X:2860:U:C5'	12:K:49:THR:HG21	2.45	0.46
1:X:2507:C:H2'	1:X:2508:G:H5'	1.98	0.46
1:X:2077:C:H1'	4:B:169:MET:HE1	1.98	0.46
1:X:1003:A:N3	1:X:2484:U:O2'	2.43	0.46
1:X:720:A:C8	1:X:849:A:C6	3.04	0.46
26:2:13:HIS:O	26:2:17:HIS:HB2	2.16	0.46
28:4:27:CYS:O	28:4:29:ASN:ND2	2.47	0.46
24:W:51:LYS:HZ1	24:W:55:THR:HA	1.81	0.46
8:G:20:ASP:OD2	8:G:22:GLU:HG2	2.15	0.46
12:K:55:ASP:O	12:K:58:SER:OG	2.26	0.46
7:E:87:LEU:HB2	7:E:131:VAL:HG23	1.98	0.46
14:M:99:LEU:HA	14:M:101:TYR:CE1	2.50	0.46
21:T:82:ARG:NH2	21:T:83:ASP:HB3	2.31	0.46
1:X:2833:U:H2'	1:X:2834:C:H6	1.81	0.46
1:X:997:G:N2	1:X:1008:C:O2	2.32	0.46
1:X:1034:A:N6	1:X:1225:G:H1'	2.31	0.46
18:Q:74:LYS:HG3	18:Q:74:LYS:H	1.48	0.46
1:X:1289:A:H5''	15:N:13:ARG:HH12	1.80	0.45
1:X:318:A:C6	1:X:319:G:H1'	2.51	0.45
1:X:1916:A:H1'	1:X:2114:G:H5'	1.98	0.45
1:X:1476:G:H2'	1:X:1477:U:C6	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:149:PRO:HD2	5:C:187:THR:HA	1.98	0.45
1:X:1390:A:OP2	1:X:1414:G:N1	2.38	0.45
1:X:628:G:N7	29:X:3007:MPD:H13	2.32	0.45
1:X:1422:A:O2'	1:X:1423:C:O4'	2.21	0.45
25:Z:28:THR:CG2	25:Z:39:LEU:HD12	2.46	0.45
18:Q:75:ARG:HD3	18:Q:75:ARG:HA	1.71	0.45
11:J:14:ARG:HD3	11:J:72:THR:HG22	1.98	0.45
17:P:33:ILE:O	17:P:37:LYS:HB2	2.15	0.45
1:X:1699:A:H1'	4:B:127:PHE:CD1	2.51	0.45
1:X:181:G:H2'	1:X:182:C:O4'	2.16	0.45
1:X:1385:G:C2	1:X:1643:C:N3	2.84	0.45
1:X:668:C:H2'	1:X:669:C:C6	2.52	0.45
14:M:4:HIS:HB2	14:M:7:ILE:HB	1.98	0.45
1:X:170:C:H2'	1:X:171:A:C8	2.51	0.45
1:X:416:G:OP2	1:X:416:G:H8	1.98	0.45
10:I:128:PHE:HD2	10:I:129:SER:H	1.63	0.45
1:X:189:G:H2'	1:X:190:G:H8	1.80	0.45
1:X:603:C:O2	15:N:48:ARG:NH1	2.49	0.45
19:R:77:GLU:HA	19:R:78:PRO:HD3	1.78	0.45
4:B:107:VAL:HG21	4:B:193:LYS:HA	1.97	0.45
1:X:718:C:OP1	5:C:54:ARG:NH1	2.47	0.45
1:X:2392:G:H4'	21:T:68:PHE:CZ	2.51	0.45
18:Q:34:ASN:O	18:Q:38:VAL:HG23	2.17	0.45
1:X:61:A:C5	1:X:94:A:C2	3.04	0.45
2:Y:87:G:H22	11:J:38:THR:HB	1.81	0.45
1:X:169:G:O2'	1:X:170:C:O5'	2.34	0.45
4:B:53:PHE:O	4:B:85:LYS:HD2	2.16	0.45
1:X:695:C:N4	1:X:696:G:C6	2.85	0.45
1:X:2581:U:H2'	1:X:2582:U:C6	2.52	0.45
1:X:2457:A:H2'	1:X:2457:A:N3	2.32	0.45
1:X:579:U:H5'	15:N:42:SER:OG	2.17	0.45
4:B:61:LYS:HD2	4:B:68:TYR:CZ	2.52	0.45
1:X:1092:A:N6	1:X:1155:A:C4	2.84	0.45
1:X:677:A:H4'	10:I:60:ARG:NH2	2.30	0.45
1:X:1644:C:OP1	18:Q:76:ARG:NH2	2.49	0.45
1:X:1628:A:OP1	1:X:1628:A:H4'	2.16	0.45
17:P:24:ILE:HD13	17:P:24:ILE:HA	1.74	0.45
1:X:2284:U:O2'	1:X:2285:C:H5'	2.16	0.45
20:S:29:ALA:HB3	20:S:41:VAL:HG23	1.99	0.45
1:X:879:U:H2'	1:X:880:A:H8	1.81	0.45
1:X:806:A:OP2	1:X:806:A:H8	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2833:U:H2'	1:X:2834:C:C6	2.51	0.45
1:X:725:A:OP1	1:X:821:C:N4	2.50	0.45
12:K:52:LYS:HD2	12:K:94:THR:HA	1.99	0.45
2:Y:64:A:N6	2:Y:104:C:H2'	2.31	0.45
1:X:2435:U:H2'	1:X:2436:G:C8	2.51	0.45
1:X:2494:C:O2	11:J:124:LYS:NZ	2.41	0.45
1:X:388:A:H1'	1:X:389:A:C2	2.46	0.45
1:X:685:C:H2'	1:X:686:U:H6	1.82	0.45
1:X:1461:C:H2'	1:X:1462:G:O4'	2.17	0.45
1:X:1867:G:C8	1:X:1954:A:H2	2.34	0.45
1:X:410:G:H21	1:X:411:A:H62	1.65	0.45
15:N:65:ILE:HD11	15:N:95:LEU:HB3	1.98	0.45
1:X:1290:G:C2	1:X:1291:A:C2	3.04	0.45
28:4:11:CYS:HB2	28:4:32:HIS:CE1	2.51	0.45
1:X:1092:A:HO2'	1:X:1093:C:H6	1.63	0.45
1:X:684:U:C2	1:X:696:G:N2	2.85	0.45
2:Y:21:G:H22	2:Y:58:G:H1	1.65	0.45
1:X:1352:C:H2'	1:X:1353:A:H8	1.82	0.45
1:X:630:G:C6	10:I:30:THR:HG21	2.52	0.45
8:G:102:ILE:HB	8:G:125:VAL:HG11	1.99	0.45
4:B:126:GLY:O	4:B:128:GLN:HG2	2.17	0.45
1:X:1089:C:H4'	1:X:1090:A:H5''	1.99	0.45
11:J:118:LEU:HD12	11:J:131:PHE:HD1	1.82	0.45
1:X:2418:G:C6	1:X:2454:C:H1'	2.52	0.45
21:T:54:TYR:HD2	21:T:80:LYS:HE3	1.82	0.45
1:X:2623:U:H2'	1:X:2624:G:O4'	2.16	0.45
1:X:1422:A:O2'	1:X:1423:C:O5'	2.34	0.45
8:G:5:PHE:CD2	15:N:100:ILE:HD13	2.51	0.45
1:X:1315:C:OP1	12:K:32:THR:HG23	2.17	0.45
1:X:674:C:H2'	1:X:675:G:C8	2.51	0.45
24:W:11:SER:OG	24:W:13:ILE:HG13	2.17	0.45
1:X:2031:G:C6	1:X:2032:A:C4	3.05	0.45
5:C:39:LEU:HD12	5:C:39:LEU:O	2.17	0.45
1:X:111:U:H5'	1:X:112:U:OP2	2.17	0.45
1:X:2851:G:C8	4:B:64:LYS:HG3	2.52	0.45
1:X:1185:U:H4'	1:X:1186:A:O4'	2.18	0.44
9:H:64:ARG:HA	9:H:79:PHE:CD2	2.52	0.44
1:X:2887:G:C4	14:M:23:ARG:NH1	2.85	0.44
2:Y:86:C:N4	2:Y:88:U:C2	2.85	0.44
4:B:14:GLN:HB3	4:B:22:LEU:HD11	1.98	0.44
9:H:107:ARG:HB2	9:H:107:ARG:HH11	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:55:LEU:HA	10:I:55:LEU:HD23	1.79	0.44
1:X:1492:G:N7	1:X:1493:U:C5	2.79	0.44
1:X:2599:A:O2'	1:X:2602:C:OP1	2.35	0.44
2:Y:102:A:H2'	2:Y:103:A:H8	1.82	0.44
1:X:1845:U:OP2	3:A:156:ARG:HD2	2.17	0.44
5:C:57:VAL:O	5:C:59:GLY:N	2.50	0.44
1:X:1357:G:C2	1:X:1366:U:H5'	2.52	0.44
1:X:1340:G:OP2	29:X:3005:MPD:H32	2.17	0.44
14:M:29:ARG:HB2	14:M:87:GLU:HB2	1.99	0.44
1:X:344:U:H1'	1:X:345:C:C6	2.52	0.44
24:W:5:GLN:HG3	24:W:36:VAL:HG22	2.00	0.44
18:Q:50:VAL:HG13	18:Q:51:ALA:H	1.82	0.44
15:N:19:LYS:HA	15:N:19:LYS:HD2	1.68	0.44
1:X:1886:A:N6	1:X:1910:G:O2'	2.49	0.44
1:X:2577:G:C6	1:X:2578:C:C4	3.06	0.44
18:Q:46:PHE:CD1	18:Q:87:ILE:HD13	2.52	0.44
1:X:1687:G:C6	1:X:1688:U:C4	3.05	0.44
2:Y:3:U:H3	2:Y:112:G:H1	1.65	0.44
1:X:1494:G:O2'	1:X:1495:C:H6	2.01	0.44
3:A:76:ALA:HB2	3:A:96:TYR:HD1	1.83	0.44
1:X:1306:A:C2	1:X:2040:A:C4	3.06	0.44
1:X:854:G:C6	1:X:855:U:C4	3.05	0.44
1:X:1506:C:H2'	1:X:1507:A:C8	2.52	0.44
1:X:55:G:O2'	1:X:126:A:N1	2.43	0.44
1:X:2088:G:H2'	1:X:2528:C:O2'	2.17	0.44
17:P:41:LYS:HE3	17:P:41:LYS:HB3	1.78	0.44
1:X:2079:G:H4'	4:B:156:MET:O	2.17	0.44
1:X:1184:C:H5'	8:G:27:GLY:HA3	1.99	0.44
1:X:2634:G:H2'	1:X:2635:G:O4'	2.18	0.44
1:X:970:U:H3'	1:X:970:U:OP1	2.17	0.44
1:X:1471:A:H1'	1:X:1472:C:C5	2.53	0.44
1:X:1167:C:H2'	1:X:1168:C:H6	1.83	0.44
1:X:228:A:N6	1:X:234:C:H42	2.15	0.44
5:C:80:ALA:HB3	5:C:83:TRP:CD1	2.53	0.44
1:X:1477:U:H2'	1:X:1478:A:C8	2.53	0.44
13:L:31:LEU:HD12	13:L:44:ILE:HG12	2.00	0.44
1:X:304:G:N2	1:X:413:C:N3	2.47	0.44
10:I:112:LEU:HD13	10:I:131:SER:HA	2.00	0.44
1:X:1542:C:H3'	1:X:1543:G:H5''	1.98	0.44
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.18	0.44
1:X:1292:A:H5''	1:X:1293:U:H5'	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:72:THR:O	11:J:94:ILE:N	2.47	0.44
16:O:20:ILE:HD13	16:O:97:ILE:HD11	1.99	0.44
1:X:2757:U:H2'	1:X:2758:G:H8	1.83	0.44
1:X:2668:A:H2'	1:X:2669:G:H8	1.82	0.44
1:X:2575:G:N3	9:H:23:LYS:HE2	2.32	0.44
5:C:70:THR:HG22	5:C:72:ARG:HG3	1.99	0.44
2:Y:90:C:H2'	2:Y:91:C:H6	1.83	0.44
4:B:57:LYS:HD2	4:B:68:TYR:CE1	2.52	0.44
1:X:895:U:O2	24:W:46:GLN:NE2	2.50	0.44
2:Y:4:G:H1	2:Y:111:A:H62	1.64	0.44
18:Q:49:LYS:HD3	18:Q:50:VAL:H	1.83	0.44
1:X:661:U:O2'	1:X:662:G:OP2	2.34	0.44
26:2:31:VAL:O	26:2:35:ARG:HG3	2.18	0.44
1:X:3:U:H2'	1:X:4:U:C6	2.53	0.44
14:M:34:ILE:HB	14:M:41:ARG:O	2.18	0.44
1:X:1429:G:C6	1:X:1430:A:N6	2.86	0.44
1:X:2279:G:H2'	1:X:2280:G:C8	2.53	0.44
14:M:96:ARG:HA	14:M:96:ARG:HD3	1.58	0.44
2:Y:21:G:H1	2:Y:58:G:H1	1.66	0.44
1:X:677:A:C4'	10:I:60:ARG:HH22	2.31	0.44
1:X:1446:U:O2	1:X:1638:G:N2	2.51	0.44
1:X:1346:G:OP1	26:2:10:LYS:HG3	2.18	0.44
1:X:713:A:H2'	1:X:715:A:H62	1.83	0.44
3:A:143:ASN:ND2	3:A:143:ASN:O	2.47	0.44
7:E:121:ILE:HD11	7:E:136:ILE:HG12	1.99	0.44
1:X:319:G:N2	1:X:320:U:O3'	2.50	0.44
4:B:9:LYS:HD3	4:B:205:LYS:H	1.82	0.44
1:X:2348:G:H5''	1:X:2349:A:OP2	2.17	0.44
1:X:172:U:H2'	1:X:173:A:H8	1.82	0.44
3:A:182:ARG:HB2	3:A:270:ILE:HA	2.00	0.44
2:Y:114:C:H6	2:Y:114:C:H2'	1.57	0.44
1:X:351:G:H2'	1:X:352:A:O4'	2.18	0.43
4:B:5:ILE:HG13	4:B:211:ILE:HB	2.00	0.43
19:R:38:VAL:O	19:R:61:ALA:N	2.35	0.43
15:N:46:ALA:O	15:N:50:ARG:HG3	2.17	0.43
1:X:339:A:H2'	1:X:340:C:H6	1.82	0.43
1:X:578:G:C5	1:X:579:U:C4	3.05	0.43
1:X:2571:G:H2'	1:X:2572:G:H8	1.81	0.43
9:H:24:VAL:HB	9:H:30:ARG:HD2	2.00	0.43
9:H:35:ILE:HD13	9:H:62:ILE:HG22	1.99	0.43
20:S:78:GLN:HB2	20:S:87:THR:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:72:ASP:OD1	19:R:72:ASP:N	2.51	0.43
1:X:1504:U:H6	1:X:1504:U:H2'	1.63	0.43
1:X:1518:G:N2	1:X:1562:C:N3	2.49	0.43
1:X:1781:C:H2'	1:X:1782:A:O4'	2.18	0.43
1:X:660:A:N3	1:X:660:A:O4'	2.49	0.43
1:X:1931:G:O2'	1:X:1955:A:N6	2.51	0.43
2:Y:87:G:N3	2:Y:87:G:H2'	2.32	0.43
1:X:306:C:H42	1:X:409:G:H1	1.67	0.43
4:B:131:ILE:HD11	4:B:149:ARG:NH2	2.34	0.43
1:X:1371:U:H2'	1:X:1372:C:C6	2.53	0.43
1:X:1746:G:C2	1:X:1747:G:N7	2.86	0.43
1:X:59:U:C2	1:X:74:U:H5	2.36	0.43
12:K:105:LYS:O	25:Z:42:ARG:N	2.39	0.43
1:X:1441:C:H2'	1:X:1442:C:C6	2.52	0.43
1:X:843:G:H2'	1:X:844:G:C8	2.53	0.43
1:X:2448:G:H5''	1:X:2449:C:OP2	2.17	0.43
11:J:22:LYS:HA	11:J:98:LYS:HB2	2.00	0.43
2:Y:74:G:H1	2:Y:97:A:H62	1.66	0.43
1:X:158:G:H2'	1:X:158:G:N3	2.32	0.43
4:B:140:PRO:HG2	4:B:145:SER:HB2	2.01	0.43
1:X:487:U:O2'	5:C:46:GLN:NE2	2.50	0.43
4:B:37:GLN:HE21	4:B:39:LYS:HG3	1.84	0.43
5:C:110:LEU:HD23	5:C:110:LEU:HA	1.74	0.43
21:T:71:ILE:HG12	21:T:72:ASP:N	2.34	0.43
3:A:201:GLU:HG3	3:A:202:LEU:HD12	1.98	0.43
1:X:1494:G:C8	1:X:1495:C:C5	3.07	0.43
1:X:259:A:H2'	1:X:260:A:C8	2.53	0.43
14:M:89:LYS:HB2	14:M:90:ARG:H	1.63	0.43
1:X:800:G:H2'	1:X:801:A:H8	1.84	0.43
1:X:2567:C:O2	1:X:2767:A:H2	2.02	0.43
1:X:2489:U:H2'	1:X:2490:C:O4'	2.19	0.43
13:L:2:ILE:HG12	13:L:3:SER:H	1.84	0.43
9:H:113:LYS:O	9:H:117:LEU:HB2	2.18	0.43
1:X:1518:G:H1	1:X:1562:C:N4	2.07	0.43
1:X:1521:A:N7	1:X:1561:G:N1	2.67	0.43
1:X:2712:G:P	14:M:51:LYS:HZ1	2.41	0.43
1:X:1092:A:O2'	1:X:1093:C:H6	2.02	0.43
1:X:2760:A:N1	4:B:216:LYS:HB2	2.34	0.43
1:X:1930:G:C5	1:X:1931:G:N7	2.87	0.43
1:X:2289:U:OP1	1:X:2414:U:O2'	2.30	0.43
1:X:2646:U:H2'	1:X:2647:C:H6	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:354:A:C8	1:X:375:A:C5	3.07	0.43
1:X:1700:C:C2	1:X:1701:U:C5	3.06	0.43
4:B:37:GLN:NE2	4:B:39:LYS:HE3	2.34	0.43
1:X:251:G:N7	1:X:253:G:H1'	2.34	0.43
1:X:2106:U:H2'	1:X:2107:G:O4'	2.18	0.43
1:X:817:G:H2'	1:X:818:U:H6	1.84	0.43
1:X:1039:C:O2	8:G:4:THR:OG1	2.31	0.43
1:X:1576:A:N3	1:X:1577:G:C8	2.86	0.43
1:X:1092:A:N6	1:X:1155:A:C2	2.86	0.43
11:J:38:THR:HG23	11:J:128:LYS:HB3	1.99	0.43
1:X:1510:U:O2'	1:X:1511:C:O5'	2.36	0.43
5:C:177:THR:HB	5:C:179:GLN:OE1	2.18	0.43
1:X:1383:G:N2	1:X:1644:C:O2	2.49	0.43
11:J:59:LYS:HD3	11:J:59:LYS:HA	1.74	0.43
1:X:618:A:O2'	1:X:619:U:H5'	2.19	0.43
20:S:95:ASN:OD1	20:S:96:MET:N	2.52	0.43
9:H:88:ARG:O	9:H:90:ASP:N	2.46	0.43
25:Z:8:THR:HG22	25:Z:12:ARG:HB3	2.01	0.43
9:H:102:VAL:O	9:H:122:LEU:N	2.51	0.43
1:X:1514:A:C2'	1:X:1515:G:H5'	2.49	0.43
14:M:62:THR:OG1	14:M:75:THR:HB	2.19	0.43
4:B:160:ALA:C	4:B:162:ARG:H	2.22	0.43
1:X:828:A:H2'	1:X:829:U:H4'	2.00	0.43
1:X:1286:G:H5'	5:C:92:PRO:HD3	2.01	0.43
1:X:999:U:H5''	11:J:87:LYS:HD3	2.00	0.43
13:L:73:ALA:HB1	13:L:107:ALA:HB2	2.01	0.43
5:C:182:ASN:OD1	5:C:182:ASN:N	2.49	0.43
19:R:80:ARG:NH2	19:R:96:LYS:HA	2.33	0.43
8:G:2:ARG:HG3	8:G:3:GLN:N	2.31	0.43
8:G:42:LYS:HE2	8:G:51:THR:O	2.18	0.43
4:B:37:GLN:HB3	4:B:50:GLN:HB3	2.01	0.43
1:X:995:U:H2'	1:X:996:G:C8	2.54	0.43
11:J:54:MET:HE1	11:J:104:PHE:CD1	2.54	0.43
3:A:145:GLU:HA	3:A:152:GLY:HA2	2.01	0.43
6:D:64:LYS:HA	6:D:65:PRO:HD2	1.79	0.43
1:X:296:G:C6	1:X:297:G:C2	3.07	0.43
1:X:49:A:H4'	1:X:50:U:H5''	2.01	0.43
1:X:106:A:H2'	1:X:107:G:H8	1.83	0.43
10:I:62:PRO:O	10:I:63:LYS:HG3	2.19	0.43
1:X:2805:A:H8	1:X:2805:A:H5''	1.84	0.43
1:X:1498:U:O2'	1:X:1499:U:H5	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1880:A:H1'	1:X:2261:A:H5'	2.01	0.43
1:X:2507:C:O2'	1:X:2508:G:H5'	2.19	0.43
1:X:349:U:H2'	1:X:350:G:O4'	2.19	0.43
1:X:164:A:O2'	1:X:165:C:H5'	2.19	0.43
1:X:2907:A:H2'	1:X:2908:U:C6	2.54	0.43
1:X:2652:G:H2'	1:X:2653:C:C6	2.54	0.43
1:X:265:A:H5'	1:X:653:G:O2'	2.19	0.43
1:X:2839:A:O2'	1:X:2840:A:H5''	2.18	0.43
1:X:902:A:H61	1:X:965:G:H1	1.67	0.43
1:X:2318:U:O2'	1:X:2401:C:O2	2.31	0.43
20:S:80:ASP:OD2	20:S:83:LYS:HB2	2.19	0.42
1:X:317:G:H2'	1:X:318:A:O4'	2.19	0.42
17:P:24:ILE:HD12	17:P:32:ALA:HB1	2.00	0.42
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.54	0.42
21:T:56:GLY:HA3	21:T:88:SER:HB3	2.01	0.42
1:X:539:G:OP1	17:P:8:ARG:NH1	2.50	0.42
1:X:192:G:H2'	1:X:208:G:N2	2.34	0.42
8:G:29:LEU:O	8:G:33:VAL:HG23	2.19	0.42
5:C:78:ILE:HD13	5:C:78:ILE:H	1.83	0.42
1:X:90:A:O2'	1:X:91:A:O4'	2.37	0.42
10:I:61:LEU:HA	10:I:62:PRO:HD3	1.85	0.42
9:H:106:LEU:HD22	9:H:111:PHE:HB2	2.01	0.42
24:W:52:HIS:CD2	24:W:53:LEU:HG	2.53	0.42
1:X:1314:A:H2'	1:X:1315:C:C6	2.54	0.42
8:G:12:ILE:CD1	8:G:51:THR:HA	2.50	0.42
3:A:76:ALA:HB2	3:A:96:TYR:CD1	2.53	0.42
9:H:24:VAL:HA	9:H:39:ILE:HG22	2.01	0.42
10:I:81:GLN:CB	10:I:110:LYS:H	2.32	0.42
17:P:95:ALA:O	17:P:96:ILE:HG13	2.18	0.42
1:X:889:U:H3'	1:X:890:G:C8	2.54	0.42
1:X:889:U:H3'	1:X:890:G:H8	1.85	0.42
1:X:1490:G:H1'	1:X:1491:C:OP1	2.19	0.42
15:N:61:TRP:CZ2	15:N:93:LYS:HD2	2.54	0.42
26:2:20:ARG:HB2	26:2:20:ARG:HH11	1.82	0.42
1:X:1526:G:N2	1:X:1549:C:N3	2.66	0.42
1:X:1923:A:H2'	1:X:1924:G:C8	2.54	0.42
1:X:1819:G:H5''	3:A:204:ASN:HB2	2.01	0.42
1:X:250:G:H4'	1:X:432:G:C5	2.54	0.42
1:X:189:G:H2'	1:X:190:G:C8	2.54	0.42
4:B:62:ASP:OD1	4:B:62:ASP:N	2.52	0.42
1:X:2823:G:H2'	1:X:2824:G:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:78:LEU:CB	14:M:79:HIS:HD2	2.31	0.42
1:X:2289:U:H4'	1:X:2355:A:C2	2.53	0.42
1:X:1711:G:N2	1:X:2018:U:H2'	2.34	0.42
1:X:695:C:N4	1:X:696:G:O6	2.49	0.42
1:X:1208:A:H2'	1:X:1209:U:H6	1.84	0.42
1:X:1762:U:H5'	1:X:1763:U:OP2	2.19	0.42
1:X:1279:C:H2'	1:X:1280:U:C6	2.54	0.42
1:X:1631:G:O2'	1:X:1632:A:OP2	2.32	0.42
1:X:158:G:H2'	1:X:159:U:H5'	2.01	0.42
4:B:39:LYS:O	4:B:47:ASN:HA	2.19	0.42
20:S:108:LEU:HB3	20:S:109:VAL:H	1.74	0.42
8:G:54:TYR:CE1	8:G:122:LYS:HG2	2.54	0.42
1:X:2900:C:O2	12:K:99:GLY:HA3	2.19	0.42
1:X:1326:C:H2'	1:X:1327:C:C6	2.54	0.42
21:T:48:GLN:HE22	21:T:67:LEU:HD22	1.84	0.42
3:A:84:ASP:OD1	3:A:85:PRO:HD2	2.20	0.42
1:X:502:C:H5	18:Q:68:TYR:CD1	2.37	0.42
1:X:2360:A:C5'	1:X:2362:A:H1'	2.47	0.42
1:X:1765:A:H2'	1:X:1765:A:N3	2.34	0.42
7:E:121:ILE:HD11	7:E:136:ILE:CG1	2.50	0.42
1:X:854:G:C4	1:X:855:U:C5	3.07	0.42
1:X:2668:A:H2'	1:X:2669:G:C8	2.54	0.42
1:X:14:A:C6	1:X:571:A:C2	3.08	0.42
15:N:62:ILE:HG23	15:N:76:TYR:CZ	2.55	0.42
15:N:66:ASN:HA	15:N:76:TYR:HB2	2.01	0.42
1:X:1024:A:C6	1:X:1025:A:N1	2.87	0.42
3:A:133:GLN:CD	3:A:133:GLN:H	2.23	0.42
1:X:2058:A:C6	1:X:2525:C:H1'	2.54	0.42
10:I:19:VAL:HG21	10:I:30:THR:HG23	2.02	0.42
1:X:148:U:H2'	1:X:149:U:C6	2.54	0.42
3:A:142:HIS:NE2	3:A:191:THR:HB	2.35	0.42
9:H:88:ARG:C	9:H:90:ASP:H	2.22	0.42
27:3:32:LEU:HB3	27:3:33:PHE:CE1	2.55	0.42
1:X:41:A:H2'	1:X:42:G:C8	2.55	0.42
1:X:2615:G:H2'	1:X:2616:A:O4'	2.19	0.42
14:M:98:LYS:HD3	14:M:98:LYS:HA	1.83	0.42
1:X:1149:U:H2'	1:X:1149:U:O2	2.18	0.42
1:X:2372:G:H4'	1:X:2373:A:H5''	2.01	0.42
1:X:162:A:H5''	1:X:163:U:H2'	2.00	0.42
3:A:7:LYS:HA	3:A:8:PRO:HD3	1.84	0.42
1:X:1567:A:OP2	1:X:1568:U:O2'	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:22:THR:OG1	12:K:67:ARG:HB2	2.19	0.42
2:Y:57:G:H3'	2:Y:58:G:C8	2.53	0.42
1:X:1356:G:C5	1:X:1357:G:C6	3.08	0.42
1:X:1352:C:N3	1:X:1374:G:N2	2.56	0.42
1:X:874:A:H5'	1:X:876:G:N7	2.35	0.42
1:X:619:U:H4'	1:X:2529:G:C8	2.54	0.42
3:A:144:ILE:HB	3:A:154:ILE:HD12	2.02	0.42
1:X:1929:C:H5''	3:A:241:ILE:HG13	2.02	0.42
5:C:93:THR:HB	5:C:94:PRO:HD2	2.01	0.42
3:A:122:ALA:HA	3:A:130:LEU:HD12	2.00	0.42
1:X:2287:C:H2'	1:X:2288:C:H6	1.84	0.42
18:Q:50:VAL:O	18:Q:82:LEU:HA	2.19	0.42
24:W:51:LYS:NZ	24:W:55:THR:HA	2.35	0.42
1:X:1834:G:N1	1:X:1835:U:H1'	2.34	0.42
1:X:1312:A:N3	1:X:1313:G:H1'	2.35	0.42
1:X:272:C:N3	1:X:416:G:N2	2.63	0.42
20:S:123:GLN:HB2	20:S:124:PRO:HD3	2.01	0.42
15:N:51:ARG:O	15:N:54:LYS:HB2	2.20	0.42
1:X:995:U:P	2:Y:85:A:H61	2.43	0.42
1:X:1432:A:C6	1:X:1435:C:C2	3.07	0.42
1:X:1070:A:H1'	1:X:1178:C:H41	1.85	0.42
2:Y:55:A:C4	6:D:26:MET:HB3	2.54	0.42
1:X:1000:G:N2	1:X:1004:A:OP2	2.45	0.42
3:A:173:LEU:HA	3:A:183:MET:HA	2.02	0.42
16:O:22:VAL:HG22	16:O:23:GLU:H	1.85	0.42
1:X:1889:G:C6	1:X:1908:A:C6	3.08	0.42
1:X:864:A:C4	1:X:1228:A:C2	3.07	0.42
1:X:1901:C:O2'	1:X:1902:G:O5'	2.25	0.42
11:J:22:LYS:HG3	11:J:24:GLY:H	1.85	0.42
3:A:171:TYR:HB3	3:A:185:LEU:HA	2.01	0.42
1:X:407:G:H2'	1:X:408:U:H6	1.83	0.42
10:I:95:LEU:HD12	10:I:96:LEU:H	1.85	0.42
1:X:514:G:C2'	1:X:515:G:H5'	2.49	0.42
1:X:2571:G:H2'	1:X:2572:G:C8	2.55	0.42
4:B:36:LEU:N	4:B:50:GLN:O	2.52	0.42
20:S:108:LEU:HD23	20:S:108:LEU:HA	1.94	0.42
1:X:2719:C:H2'	1:X:2720:A:O4'	2.19	0.42
3:A:79:ASP:OD2	3:A:93:LEU:HD23	2.20	0.42
11:J:78:PRO:HB2	11:J:81:VAL:HG21	2.01	0.42
19:R:4:LYS:HB3	19:R:4:LYS:NZ	2.35	0.42
24:W:16:PRO:HD2	24:W:19:GLN:CD	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:615:A:N6	1:X:616:G:C6	2.87	0.42
1:X:1886:A:H3'	1:X:1887:G:C8	2.53	0.42
1:X:1830:A:C8	1:X:1831:A:C8	3.07	0.42
1:X:2322:C:H2'	1:X:2323:U:H6	1.85	0.42
1:X:1680:U:H2'	1:X:1681:U:C6	2.55	0.42
11:J:18:THR:OG1	11:J:19:GLY:N	2.53	0.42
1:X:2051:C:C2	1:X:2052:C:C5	3.08	0.41
1:X:616:G:N2	1:X:2058:A:OP1	2.45	0.41
17:P:86:ARG:NH1	17:P:86:ARG:HB2	2.35	0.41
1:X:1760:G:C2	1:X:1761:G:N7	2.88	0.41
1:X:1357:G:N2	1:X:1366:U:H5'	2.35	0.41
18:Q:57:ASN:OD1	18:Q:76:ARG:HG2	2.20	0.41
1:X:235:G:HO2'	1:X:236:A:C5'	2.34	0.41
1:X:2456:G:H5''	1:X:2457:A:OP2	2.20	0.41
1:X:367:A:H2'	1:X:368:A:O4'	2.20	0.41
1:X:373:A:H2	1:X:1248:U:H2'	1.85	0.41
5:C:124:THR:HA	5:C:189:ALA:O	2.20	0.41
8:G:40:LYS:O	8:G:41:ASN:HB2	2.20	0.41
9:H:91:LYS:HD2	9:H:111:PHE:CZ	2.55	0.41
1:X:2379:A:C4	1:X:2393:A:C2	3.08	0.41
1:X:873:U:H4'	1:X:876:G:N1	2.36	0.41
1:X:2585:C:H2'	1:X:2586:C:O4'	2.20	0.41
1:X:2279:G:H2'	1:X:2280:G:H8	1.85	0.41
1:X:253:G:C6	1:X:254:A:C6	3.08	0.41
1:X:2814:C:H1'	4:B:72:PRO:HG3	2.02	0.41
3:A:105:ILE:O	3:A:107:PRO:HD3	2.20	0.41
15:N:114:LYS:O	15:N:117:LEU:HB2	2.20	0.41
1:X:2660:A:H2'	1:X:2661:A:O4'	2.20	0.41
1:X:2089:A:OP2	29:X:3003:MPD:HM1	2.20	0.41
1:X:2288:C:C2'	1:X:2289:U:H5'	2.50	0.41
4:B:52:GLY:HA3	4:B:85:LYS:HG3	2.02	0.41
1:X:1650:G:H5''	1:X:1651:C:OP1	2.19	0.41
12:K:109:ARG:HD2	12:K:112:ASP:OD1	2.21	0.41
1:X:1817:C:O2'	3:A:208:ALA:HB2	2.21	0.41
11:J:118:LEU:HD12	11:J:131:PHE:CD1	2.55	0.41
5:C:117:LYS:NZ	5:C:182:ASN:HA	2.35	0.41
8:G:119:GLN:HA	8:G:122:LYS:HD3	2.00	0.41
1:X:609:U:H2'	1:X:610:U:O4'	2.20	0.41
1:X:1963:A:OP2	1:X:1988:C:N4	2.54	0.41
14:M:50:ILE:HD13	14:M:50:ILE:HA	1.82	0.41
1:X:733:U:O2'	1:X:734:A:H5'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1013:U:OP1	24:W:17:GLU:HG2	2.19	0.41
1:X:361:U:H2'	1:X:362:C:H6	1.85	0.41
10:I:16:ARG:HG2	10:I:16:ARG:H	1.60	0.41
2:Y:81:A:N1	2:Y:90:C:N3	2.69	0.41
5:C:28:PRO:HB3	5:C:112:SER:O	2.20	0.41
5:C:142:VAL:HG13	5:C:144:SER:HB2	2.02	0.41
1:X:302:A:N6	1:X:450:C:C2	2.89	0.41
1:X:2418:G:O6	1:X:2452:A:H5''	2.20	0.41
5:C:39:LEU:HD11	5:C:99:TYR:O	2.21	0.41
27:3:20:GLY:O	27:3:45:ARG:HA	2.21	0.41
1:X:278:A:N1	1:X:279:A:N6	2.68	0.41
7:E:41:MET:O	7:E:43:PHE:N	2.42	0.41
1:X:2793:G:C2	1:X:2794:C:C6	3.09	0.41
20:S:72:VAL:HG12	20:S:93:ALA:HA	2.02	0.41
4:B:208:LEU:HA	4:B:208:LEU:HD12	1.76	0.41
1:X:1906:C:H2'	1:X:1907:U:O4'	2.21	0.41
5:C:53:ASN:O	5:C:57:VAL:HG23	2.21	0.41
1:X:2725:U:C2	1:X:2726:C:C5	3.09	0.41
1:X:619:U:H2'	1:X:620:G:C8	2.55	0.41
8:G:39:GLY:HA3	8:G:51:THR:HG23	2.01	0.41
14:M:50:ILE:HG23	14:M:50:ILE:HD12	1.86	0.41
1:X:1086:G:C6	1:X:1158:G:C6	3.09	0.41
14:M:33:ARG:HA	14:M:42:ILE:HG12	2.01	0.41
1:X:745:G:H1	1:X:777:C:H42	1.68	0.41
1:X:2342:U:H2'	1:X:2343:U:C6	2.54	0.41
27:3:59:LYS:HA	27:3:59:LYS:HD3	1.90	0.41
1:X:1515:G:N2	1:X:1516:C:C2	2.89	0.41
3:A:8:PRO:HB3	3:A:14:ARG:HB2	2.02	0.41
1:X:696:G:H2'	1:X:697:U:C6	2.55	0.41
1:X:696:G:H2'	1:X:697:U:H6	1.86	0.41
1:X:2311:U:H1'	1:X:2352:G:C2	2.56	0.41
1:X:800:G:H2'	1:X:801:A:C8	2.56	0.41
10:I:66:PHE:HB3	10:I:67:THR:H	1.68	0.41
1:X:442:G:O2'	1:X:443:U:H5'	2.19	0.41
1:X:268:A:O2'	1:X:269:G:H4'	2.21	0.41
1:X:1290:G:N3	15:N:33:LYS:HE2	2.36	0.41
14:M:51:LYS:O	14:M:61:PHE:HA	2.21	0.41
1:X:2256:U:H2'	1:X:2257:G:C8	2.55	0.41
1:X:1438:G:H2'	1:X:1439:U:H6	1.86	0.41
5:C:184:LEU:O	5:C:186:ILE:N	2.51	0.41
1:X:306:C:O2	1:X:411:A:N6	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:344:U:C2	1:X:345:C:C5	3.09	0.41
1:X:2757:U:H2'	1:X:2758:G:C8	2.56	0.41
1:X:1272:U:H2'	1:X:1273:G:O4'	2.21	0.41
1:X:1823:U:H2'	1:X:1824:C:C6	2.56	0.41
1:X:2594:G:H2'	1:X:2595:C:C6	2.55	0.41
1:X:511:G:C6	1:X:512:A:N6	2.89	0.41
1:X:1959:A:H2'	1:X:1960:G:O4'	2.21	0.41
1:X:2665:G:C4	1:X:2802:A:C2	3.08	0.41
1:X:1491:C:H4'	1:X:1593:G:H5''	2.02	0.41
2:Y:68:A:N1	2:Y:103:A:N1	2.68	0.41
13:L:30:ARG:HD3	13:L:91:GLU:HG3	2.02	0.41
1:X:25:U:H2'	1:X:26:G:O4'	2.21	0.41
1:X:1410:A:H4'	1:X:2239:A:H1'	2.02	0.41
4:B:118:VAL:HG21	4:B:201:VAL:HG12	2.02	0.41
1:X:2120:G:N2	1:X:2225:A:H62	2.17	0.41
1:X:1658:A:H8	1:X:1658:A:P	2.44	0.41
12:K:22:THR:O	12:K:26:ILE:HG13	2.21	0.41
1:X:1356:G:O2'	1:X:1357:G:H5'	2.21	0.41
1:X:514:G:H2'	1:X:515:G:H5'	2.02	0.41
11:J:75:THR:HG21	11:J:87:LYS:HE2	2.03	0.41
6:D:65:PRO:HD2	6:D:83:MET:HA	2.03	0.41
5:C:102:PRO:HB2	5:C:105:MET:HG3	2.03	0.41
1:X:447:A:H2'	1:X:448:A:O4'	2.21	0.41
18:Q:36:THR:O	18:Q:40:MET:HG2	2.20	0.41
1:X:365:A:C5	1:X:383:A:C2	3.09	0.41
1:X:105:C:O2	1:X:337:A:O2'	2.38	0.41
1:X:225:A:N6	1:X:227:G:C2	2.89	0.41
1:X:363:A:H4'	1:X:365:A:C8	2.56	0.41
23:V:25:LEU:HA	23:V:28:LEU:HD12	2.02	0.41
23:V:25:LEU:HB2	23:V:46:VAL:HG11	2.03	0.41
1:X:1445:C:C2	1:X:1639:G:N2	2.89	0.41
1:X:77:U:OP1	23:V:52:ARG:HD2	2.21	0.41
26:2:3:LYS:HE3	26:2:3:LYS:HB2	1.81	0.41
1:X:577:A:N3	1:X:577:A:H2'	2.34	0.41
10:I:47:ARG:HA	10:I:48:PRO:HD3	1.85	0.41
7:E:103:LEU:H	7:E:115:ILE:CD1	2.34	0.41
4:B:8:ARG:NH2	4:B:54:GLU:OE2	2.53	0.41
1:X:946:A:C2'	1:X:947:U:H5'	2.51	0.41
1:X:1983:U:H1'	1:X:2579:U:OP1	2.21	0.41
22:U:17:ARG:O	22:U:29:TRP:HD1	2.04	0.41
3:A:230:HIS:CD2	3:A:249:PRO:HG3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:563:G:H2'	1:X:564:U:C6	2.55	0.41
28:4:14:CYS:SG	28:4:32:HIS:ND1	2.74	0.40
25:Z:39:LEU:O	25:Z:41:HIS:ND1	2.46	0.40
1:X:1241:A:C6	1:X:1242:A:C6	3.09	0.40
1:X:713:A:OP2	29:X:3008:MPD:HM3	2.20	0.40
15:N:60:LEU:O	15:N:64:ARG:HD2	2.21	0.40
1:X:135:G:C2	1:X:136:A:C8	3.09	0.40
1:X:579:U:H2'	1:X:580:C:C6	2.55	0.40
1:X:724:C:H2'	1:X:725:A:C8	2.56	0.40
1:X:1681:U:H5'	1:X:1787:A:O2'	2.21	0.40
1:X:634:C:HO2'	27:3:2:PRO:N	2.18	0.40
1:X:635:G:C2	1:X:636:A:C8	3.09	0.40
2:Y:1:U:O2'	2:Y:2:C:OP2	2.33	0.40
1:X:852:U:O2'	1:X:2087:A:N1	2.53	0.40
27:3:56:LYS:HE3	27:3:56:LYS:HB2	1.87	0.40
17:P:1:MET:HG2	17:P:2:GLU:OE2	2.20	0.40
12:K:106:GLN:H	12:K:117:VAL:HA	1.84	0.40
4:B:215:ILE:O	4:B:216:LYS:HG2	2.21	0.40
19:R:11:VAL:HA	19:R:67:ASN:CB	2.48	0.40
1:X:1168:C:H2'	1:X:1169:G:O4'	2.21	0.40
3:A:142:HIS:CD2	3:A:191:THR:HB	2.55	0.40
1:X:1313:G:N7	1:X:1689:G:C2	2.89	0.40
1:X:2848:G:O2'	1:X:2849:A:H5'	2.22	0.40
1:X:2584:G:H2'	1:X:2585:C:C6	2.57	0.40
1:X:810:A:H2'	1:X:811:C:H6	1.86	0.40
1:X:525:A:H4'	1:X:526:A:OP1	2.20	0.40
14:M:34:ILE:CD1	14:M:43:GLN:HB2	2.52	0.40
7:E:19:PHE:HB3	7:E:20:ASP:H	1.58	0.40
17:P:19:LEU:HD22	25:Z:22:ILE:HG23	2.04	0.40
16:O:32:THR:HG22	16:O:61:THR:HA	2.03	0.40
1:X:221:G:N2	1:X:238:U:H4'	2.36	0.40
5:C:57:VAL:HG21	5:C:87:GLY:HA2	2.04	0.40
1:X:616:G:O6	1:X:2056:G:O2'	2.25	0.40
17:P:72:LYS:N	17:P:106:VAL:O	2.54	0.40
24:W:51:LYS:HZ2	24:W:56:VAL:H	1.69	0.40
3:A:129:ALA:HA	3:A:191:THR:HA	2.02	0.40
1:X:1460:U:C2'	1:X:1461:C:H5'	2.51	0.40
8:G:33:VAL:O	8:G:37:LEU:HG	2.22	0.40
1:X:1326:C:H2'	1:X:1327:C:H6	1.86	0.40
27:3:32:LEU:HD22	27:3:33:PHE:CE1	2.56	0.40
15:N:24:TYR:CE2	15:N:38:GLN:HG3	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2686:G:O5'	1:X:2686:G:H8	2.04	0.40
25:Z:28:THR:HG21	25:Z:39:LEU:HD12	2.02	0.40
2:Y:87:G:N2	11:J:38:THR:HB	2.36	0.40
1:X:2329:U:H2'	1:X:2330:G:C8	2.56	0.40
1:X:1825:U:C4	1:X:1846:A:C2	3.09	0.40
1:X:793:G:H5''	17:P:89:ALA:HB2	2.03	0.40
1:X:854:G:C5	1:X:855:U:C5	3.09	0.40
10:I:66:PHE:CD1	10:I:94:ALA:HB3	2.56	0.40
1:X:1730:C:H2'	1:X:1731:G:O4'	2.21	0.40
9:H:64:ARG:HD3	9:H:101:PRO:HG2	2.03	0.40
14:M:23:ARG:NH2	14:M:23:ARG:HG3	2.32	0.40
1:X:1016:G:C3'	1:X:1017:A:H5''	2.49	0.40
5:C:177:THR:O	5:C:181:LEU:HB2	2.22	0.40
16:O:17:GLY:H	16:O:97:ILE:HB	1.86	0.40
1:X:2269:G:H2'	1:X:2270:U:O4'	2.21	0.40
1:X:2757:U:O2'	1:X:2758:G:H5'	2.21	0.40
11:J:75:THR:HG21	11:J:87:LYS:HB3	2.02	0.40
1:X:2720:A:H2'	1:X:2721:G:H8	1.86	0.40
24:W:8:LEU:HD23	24:W:31:THR:HA	2.03	0.40
1:X:1663:G:HO2'	26:2:2:VAL:N	2.20	0.40
1:X:967:C:O2'	21:T:34:ALA:HB2	2.21	0.40
1:X:491:C:N4	1:X:492:G:O6	2.55	0.40
1:X:122:G:O3'	1:X:1413:C:H4'	2.22	0.40
16:O:63:ASN:OD1	16:O:63:ASN:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	1 19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	213/220 (97%)	182 (85%)	18 (8%)	13 (6%)	2	21
5	C	197/207 (95%)	169 (86%)	20 (10%)	8 (4%)	3	33
6	D	164/179 (92%)	134 (82%)	19 (12%)	11 (7%)	1	19
7	E	154/178 (86%)	112 (73%)	27 (18%)	15 (10%)	1	10
8	G	143/145 (99%)	129 (90%)	12 (8%)	2 (1%)	14	57
9	H	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	7	45
10	I	129/146 (88%)	91 (70%)	25 (19%)	13 (10%)	1	9
11	J	139/144 (96%)	124 (89%)	9 (6%)	6 (4%)	3	31
12	K	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	21	67
13	L	108/119 (91%)	88 (82%)	15 (14%)	5 (5%)	3	29
14	M	108/116 (93%)	93 (86%)	11 (10%)	4 (4%)	4	36
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	4	33
17	P	110/117 (94%)	107 (97%)	3 (3%)	0	100	100
18	Q	87/91 (96%)	78 (90%)	7 (8%)	2 (2%)	8	47
19	R	98/105 (93%)	76 (78%)	18 (18%)	4 (4%)	3	33
20	S	165/217 (76%)	130 (79%)	19 (12%)	16 (10%)	1	10
21	T	73/94 (78%)	65 (89%)	7 (10%)	1 (1%)	14	57
22	U	44/62 (71%)	31 (70%)	9 (20%)	4 (9%)	1	11
23	V	63/69 (91%)	58 (92%)	4 (6%)	1 (2%)	12	54
24	W	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
25	Z	41/58 (71%)	38 (93%)	3 (7%)	0	100	100
26	2	42/45 (93%)	38 (90%)	2 (5%)	2 (5%)	3	28
27	3	58/66 (88%)	46 (79%)	4 (7%)	8 (14%)	0	4
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	6	42
All	All	2945/3215 (92%)	2499 (85%)	304 (10%)	142 (5%)	3	28

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	51	VAL
3	A	120	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	126	VAL
3	A	141	VAL
3	A	154	ILE
4	B	9	LYS
4	B	10	ILE
4	B	208	LEU
5	C	154	VAL
6	D	84	PRO
6	D	104	ILE
6	D	109	PRO
6	D	137	ILE
7	E	55	PRO
7	E	107	VAL
7	E	171	ARG
8	G	88	ILE
10	I	13	ARG
10	I	46	VAL
10	I	48	PRO
10	I	62	PRO
10	I	75	ALA
10	I	101	VAL
12	K	81	ALA
13	L	90	LYS
13	L	100	LEU
16	O	50	ALA
19	R	76	ASN
20	S	34	TYR
20	S	130	VAL
20	S	145	ILE
22	U	22	LEU
27	3	54	ASP
3	A	170	LYS
3	A	192	ILE
3	A	224	VAL
4	B	32	GLU
4	B	53	PHE
4	B	60	LYS
5	C	131	PHE
5	C	145	THR
6	D	44	VAL
6	D	115	GLN
6	D	126	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	E	50	ILE
7	E	52	VAL
7	E	59	LYS
9	H	25	LEU
10	I	64	ARG
10	I	113	GLY
11	J	21	SER
11	J	84	GLY
11	J	135	GLU
13	L	89	ILE
14	M	89	LYS
16	O	52	THR
16	O	99	LYS
18	Q	50	VAL
20	S	109	VAL
20	S	129	GLU
20	S	132	ALA
22	U	14	THR
22	U	40	VAL
26	2	16	VAL
27	3	25	SER
28	4	28	GLU
3	A	110	LEU
3	A	132	LEU
4	B	106	SER
4	B	186	VAL
4	B	206	LYS
6	D	75	ALA
6	D	130	LEU
7	E	24	VAL
7	E	35	ARG
7	E	51	GLU
7	E	134	GLU
8	G	2	ARG
9	H	119	PRO
10	I	129	SER
11	J	60	ARG
13	L	96	ARG
14	M	36	GLU
18	Q	86	SER
19	R	65	VAL
19	R	74	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	S	82	LEU
20	S	88	HIS
20	S	98	GLU
20	S	138	PRO
20	S	150	ILE
21	T	24	SER
27	3	29	THR
3	A	25	THR
3	A	245	SER
3	A	252	LYS
4	B	176	ASN
5	C	171	PRO
5	C	191	SER
6	D	89	VAL
7	E	33	LEU
7	E	36	THR
7	E	116	LYS
7	E	121	ILE
7	E	172	LYS
9	H	64	ARG
10	I	30	THR
10	I	128	PHE
11	J	89	ALA
14	M	108	LYS
16	O	16	GLU
19	R	77	GLU
20	S	68	LYS
20	S	157	ALA
20	S	167	ILE
22	U	12	ALA
23	V	12	SER
26	2	6	TYR
27	3	18	ALA
27	3	46	LYS
3	A	35	LYS
3	A	135	ILE
3	A	156	ARG
4	B	204	PRO
4	B	209	VAL
5	C	175	VAL
10	I	28	GLY
10	I	35	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	L	65	THR
27	3	28	PHE
27	3	34	ALA
4	B	124	GLY
5	C	176	THR
6	D	132	VAL
11	J	25	ASN
27	3	45	ARG
14	M	37	GLY
20	S	124	PRO
3	A	85	PRO
20	S	74	VAL
5	C	149	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	120/224 (54%)	101 (84%)	19 (16%)	3	19
4	B	153/177 (86%)	136 (89%)	17 (11%)	8	35
5	C	106/169 (63%)	88 (83%)	18 (17%)	2	15
6	D	18/158 (11%)	17 (94%)	1 (6%)	26	66
7	E	67/155 (43%)	58 (87%)	9 (13%)	5	26
8	G	111/123 (90%)	101 (91%)	10 (9%)	12	47
9	H	91/100 (91%)	78 (86%)	13 (14%)	4	24
10	I	67/112 (60%)	52 (78%)	15 (22%)	1	6
11	J	103/119 (87%)	91 (88%)	12 (12%)	7	32
12	K	91/102 (89%)	81 (89%)	10 (11%)	8	36
13	L	47/95 (50%)	39 (83%)	8 (17%)	2	15
14	M	80/102 (78%)	66 (82%)	14 (18%)	2	14
15	N	93/98 (95%)	79 (85%)	14 (15%)	3	21
16	O	71/86 (83%)	60 (84%)	11 (16%)	3	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	P	91/94 (97%)	84 (92%)	7 (8%)	16	54
18	Q	53/82 (65%)	39 (74%)	14 (26%)	0	4
19	R	63/90 (70%)	46 (73%)	17 (27%)	0	4
20	S	91/190 (48%)	83 (91%)	8 (9%)	12	48
21	T	56/75 (75%)	48 (86%)	8 (14%)	4	24
22	U	18/52 (35%)	17 (94%)	1 (6%)	26	66
23	V	47/62 (76%)	42 (89%)	5 (11%)	8	38
24	W	52/53 (98%)	40 (77%)	12 (23%)	1	6
25	Z	38/51 (74%)	30 (79%)	8 (21%)	1	8
26	2	37/40 (92%)	32 (86%)	5 (14%)	5	26
27	3	37/57 (65%)	33 (89%)	4 (11%)	8	37
28	4	30/35 (86%)	27 (90%)	3 (10%)	9	41
All	All	1831/2701 (68%)	1568 (86%)	263 (14%)	4	23

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	45	ASN
3	A	46	GLN
3	A	53	HIS
3	A	58	HIS
3	A	79	ASP
3	A	88	SER
3	A	90	ASN
3	A	94	VAL
3	A	110	LEU
3	A	116	VAL
3	A	123	ASP
3	A	130	LEU
3	A	133	GLN
3	A	143	ASN
3	A	171	TYR
3	A	181	VAL
3	A	182	ARG
3	A	199	GLN
3	A	204	ASN
4	B	13	THR
4	B	15	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	29	GLU
4	B	33	ASN
4	B	57	LYS
4	B	62	ASP
4	B	64	LYS
4	B	65	SER
4	B	81	ASP
4	B	107	VAL
4	B	114	ASP
4	B	117	ASP
4	B	133	ARG
4	B	177	THR
4	B	180	VAL
4	B	183	LEU
4	B	215	ILE
5	C	8	LYS
5	C	10	ASP
5	C	17	ILE
5	C	31	SER
5	C	35	GLU
5	C	39	LEU
5	C	49	HIS
5	C	67	GLN
5	C	68	LYS
5	C	74	ARG
5	C	78	ILE
5	C	115	SER
5	C	124	THR
5	C	144	SER
5	C	148	GLN
5	C	155	VAL
5	C	176	THR
5	C	181	LEU
6	D	26	MET
7	E	38	ASN
7	E	58	SER
7	E	61	ASP
7	E	79	VAL
7	E	89	LEU
7	E	92	VAL
7	E	115	ILE
7	E	131	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	E	139	GLU
8	G	3	GLN
8	G	12	ILE
8	G	24	GLN
8	G	29	LEU
8	G	46	THR
8	G	58	ILE
8	G	66	THR
8	G	71	THR
8	G	92	GLU
8	G	101	LEU
9	H	8	LEU
9	H	23	LYS
9	H	24	VAL
9	H	32	THR
9	H	37	ASP
9	H	42	THR
9	H	52	VAL
9	H	58	VAL
9	H	63	VAL
9	H	88	ARG
9	H	107	ARG
9	H	112	MET
9	H	117	LEU
10	I	19	VAL
10	I	21	ARG
10	I	31	SER
10	I	47	ARG
10	I	50	PHE
10	I	51	GLU
10	I	55	LEU
10	I	67	THR
10	I	82	LEU
10	I	84	LYS
10	I	89	THR
10	I	96	LEU
10	I	112	LEU
10	I	122	THR
10	I	123	VAL
11	J	7	VAL
11	J	9	TYR
11	J	16	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	J	21	SER
11	J	22	LYS
11	J	26	TYR
11	J	35	GLN
11	J	37	THR
11	J	41	TRP
11	J	91	GLU
11	J	122	SER
11	J	135	GLU
12	K	4	ARG
12	K	8	ARG
12	K	9	THR
12	K	28	GLU
12	K	33	THR
12	K	50	LEU
12	K	55	ASP
12	K	67	ARG
12	K	76	GLU
12	K	110	ARG
13	L	36	SER
13	L	41	TYR
13	L	45	ILE
13	L	46	ASP
13	L	53	LEU
13	L	91	GLU
13	L	92	ILE
13	L	99	TYR
14	M	11	THR
14	M	17	THR
14	M	32	VAL
14	M	48	VAL
14	M	51	LYS
14	M	52	ARG
14	M	53	ARG
14	M	60	THR
14	M	75	THR
14	M	80	THR
14	M	90	ARG
14	M	102	LEU
14	M	103	ARG
14	M	106	ARG
15	N	8	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	N	9	VAL
15	N	19	LYS
15	N	20	LEU
15	N	22	LYS
15	N	30	THR
15	N	42	SER
15	N	48	ARG
15	N	70	ARG
15	N	83	LEU
15	N	84	LYS
15	N	89	ASP
15	N	92	ARG
15	N	96	SER
16	O	7	THR
16	O	10	LYS
16	O	34	THR
16	O	48	VAL
16	O	59	THR
16	O	63	ASN
16	O	75	THR
16	O	78	ARG
16	O	84	ARG
16	O	86	LYS
16	O	98	ASP
17	P	2	GLU
17	P	11	ARG
17	P	19	LEU
17	P	38	LEU
17	P	62	TYR
17	P	81	THR
17	P	109	ASP
18	Q	5	ASP
18	Q	6	ILE
18	Q	12	ILE
18	Q	13	THR
18	Q	27	PHE
18	Q	28	ASP
18	Q	40	MET
18	Q	49	LYS
18	Q	58	TYR
18	Q	68	TYR
18	Q	72	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	Q	76	ARG
18	Q	87	ILE
18	Q	88	ASP
19	R	3	ILE
19	R	9	VAL
19	R	11	VAL
19	R	24	ILE
19	R	32	ARG
19	R	33	VAL
19	R	36	GLU
19	R	43	LYS
19	R	48	THR
19	R	56	ILE
19	R	59	THR
19	R	60	GLU
19	R	68	VAL
19	R	72	ASP
19	R	80	ARG
19	R	90	LYS
19	R	100	GLU
20	S	26	LYS
20	S	30	VAL
20	S	31	VAL
20	S	46	VAL
20	S	52	ILE
20	S	55	VAL
20	S	154	LEU
20	S	155	THR
21	T	24	SER
21	T	27	LYS
21	T	51	THR
21	T	61	ARG
21	T	64	ASP
21	T	66	THR
21	T	67	LEU
21	T	82	ARG
22	U	29	TRP
23	V	30	PHE
23	V	32	LEU
23	V	37	LEU
23	V	38	GLU
23	V	52	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	W	1	MET
24	W	3	LYS
24	W	4	LEU
24	W	5	GLN
24	W	9	THR
24	W	12	VAL
24	W	15	ARG
24	W	18	THR
24	W	43	ILE
24	W	48	ASN
24	W	53	LEU
24	W	54	VAL
25	Z	5	LYS
25	Z	7	ARG
25	Z	28	THR
25	Z	30	CYS
25	Z	37	TYR
25	Z	38	LYS
25	Z	39	LEU
25	Z	44	CYS
26	2	2	VAL
26	2	5	THR
26	2	23	MET
26	2	42	VAL
26	2	44	SER
27	3	6	THR
27	3	29	THR
27	3	44	LEU
27	3	50	VAL
28	4	24	MET
28	4	26	ILE
28	4	29	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2691/2923 (92%)	627 (23%)	18 (0%)
2	Y	113/114 (99%)	13 (11%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2804/3037 (92%)	640 (22%)	18 (0%)

All (640) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	4	U
1	X	9	U
1	X	12	U
1	X	14	A
1	X	15	G
1	X	34	U
1	X	35	G
1	X	39	C
1	X	51	G
1	X	60	U
1	X	64	A
1	X	70	G
1	X	71	A
1	X	72	U
1	X	75	G
1	X	80	G
1	X	90	A
1	X	91	A
1	X	96	G
1	X	101	G
1	X	109	G
1	X	111	U
1	X	115	C
1	X	117	A
1	X	118	A
1	X	119	U
1	X	124	A
1	X	130	A
1	X	133	A
1	X	139	U
1	X	140	A
1	X	152	C
1	X	153	G
1	X	154	A
1	X	155	U
1	X	156	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	157	U
1	X	164	A
1	X	165	C
1	X	166	A
1	X	167	U
1	X	169	G
1	X	170	C
1	X	171	A
1	X	172	U
1	X	173	A
1	X	176	A
1	X	177	G
1	X	179	A
1	X	180	G
1	X	182	C
1	X	183	A
1	X	184	C
1	X	194	A
1	X	199	A
1	X	202	A
1	X	207	A
1	X	219	A
1	X	224	A
1	X	225	A
1	X	227	G
1	X	229	A
1	X	233	U
1	X	235	G
1	X	236	A
1	X	244	A
1	X	248	G
1	X	251	G
1	X	255	G
1	X	268	A
1	X	284	C
1	X	285	U
1	X	286	U
1	X	287	G
1	X	288	C
1	X	289	U
1	X	290	U
1	X	291	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	298	U
1	X	300	G
1	X	301	U
1	X	303	G
1	X	310	C
1	X	311	U
1	X	313	U
1	X	319	G
1	X	320	U
1	X	321	U
1	X	322	A
1	X	323	C
1	X	328	G
1	X	329	A
1	X	330	C
1	X	332	A
1	X	338	G
1	X	350	G
1	X	359	A
1	X	364	A
1	X	372	A
1	X	373	A
1	X	375	A
1	X	389	A
1	X	390	A
1	X	392	U
1	X	401	U
1	X	403	U
1	X	404	U
1	X	406	A
1	X	410	G
1	X	413	C
1	X	415	U
1	X	416	G
1	X	417	A
1	X	418	G
1	X	432	G
1	X	434	G
1	X	444	C
1	X	447	A
1	X	449	U
1	X	450	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	451	U
1	X	452	G
1	X	457	G
1	X	458	A
1	X	474	A
1	X	480	U
1	X	486	G
1	X	501	C
1	X	502	C
1	X	503	A
1	X	504	G
1	X	506	A
1	X	519	G
1	X	523	A
1	X	526	A
1	X	527	G
1	X	541	G
1	X	543	G
1	X	549	U
1	X	550	A
1	X	553	A
1	X	554	C
1	X	566	U
1	X	567	G
1	X	572	C
1	X	573	A
1	X	576	U
1	X	577	A
1	X	578	G
1	X	583	A
1	X	590	U
1	X	591	A
1	X	592	A
1	X	593	U
1	X	594	G
1	X	606	G
1	X	616	G
1	X	618	A
1	X	627	C
1	X	630	G
1	X	646	A
1	X	647	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	654	C
1	X	658	A
1	X	659	A
1	X	660	A
1	X	661	U
1	X	666	A
1	X	667	G
1	X	670	G
1	X	682	A
1	X	683	G
1	X	690	U
1	X	691	A
1	X	697	U
1	X	698	U
1	X	699	U
1	X	713	A
1	X	715	A
1	X	716	C
1	X	722	A
1	X	727	G
1	X	731	U
1	X	735	C
1	X	740	G
1	X	757	G
1	X	766	G
1	X	773	G
1	X	775	A
1	X	783	G
1	X	784	A
1	X	792	U
1	X	793	G
1	X	802	G
1	X	809	A
1	X	813	G
1	X	816	G
1	X	820	G
1	X	821	C
1	X	827	A
1	X	829	U
1	X	830	U
1	X	835	U
1	X	836	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	837	G
1	X	838	A
1	X	848	U
1	X	850	G
1	X	857	C
1	X	864	A
1	X	866	A
1	X	872	U
1	X	873	U
1	X	875	G
1	X	887	A
1	X	892	U
1	X	904	G
1	X	911	A
1	X	922	G
1	X	923	A
1	X	924	G
1	X	943	C
1	X	944	G
1	X	947	U
1	X	955	A
1	X	959	C
1	X	964	U
1	X	970	U
1	X	971	U
1	X	977	A
1	X	985	A
1	X	989	A
1	X	990	G
1	X	1001	A
1	X	1005	G
1	X	1017	A
1	X	1018	A
1	X	1027	A
1	X	1029	C
1	X	1033	G
1	X	1034	A
1	X	1040	A
1	X	1043	U
1	X	1056	U
1	X	1057	A
1	X	1061	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1064	A
1	X	1066	G
1	X	1067	U
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1078	G
1	X	1086	G
1	X	1087	C
1	X	1089	C
1	X	1091	G
1	X	1092	A
1	X	1093	C
1	X	1145	U
1	X	1146	C
1	X	1147	A
1	X	1148	C
1	X	1150	A
1	X	1151	G
1	X	1154	G
1	X	1155	A
1	X	1156	G
1	X	1172	A
1	X	1176	U
1	X	1178	C
1	X	1179	C
1	X	1180	G
1	X	1186	A
1	X	1195	A
1	X	1200	A
1	X	1213	C
1	X	1215	U
1	X	1218	G
1	X	1222	A
1	X	1250	G
1	X	1276	G
1	X	1278	G
1	X	1284	A
1	X	1285	A
1	X	1286	G
1	X	1291	A
1	X	1293	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1294	G
1	X	1309	G
1	X	1310	A
1	X	1311	A
1	X	1313	G
1	X	1324	A
1	X	1337	A
1	X	1338	U
1	X	1339	U
1	X	1349	U
1	X	1366	U
1	X	1382	C
1	X	1389	U
1	X	1401	G
1	X	1402	A
1	X	1405	G
1	X	1415	A
1	X	1416	U
1	X	1421	A
1	X	1422	A
1	X	1432	A
1	X	1433	U
1	X	1437	U
1	X	1448	U
1	X	1449	A
1	X	1450	A
1	X	1451	U
1	X	1452	C
1	X	1453	G
1	X	1454	U
1	X	1461	C
1	X	1462	G
1	X	1463	A
1	X	1464	U
1	X	1465	G
1	X	1466	G
1	X	1467	G
1	X	1471	A
1	X	1472	C
1	X	1481	A
1	X	1489	A
1	X	1490	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1491	C
1	X	1492	G
1	X	1493	U
1	X	1494	G
1	X	1495	C
1	X	1496	G
1	X	1497	A
1	X	1498	U
1	X	1503	U
1	X	1504	U
1	X	1505	G
1	X	1508	C
1	X	1509	G
1	X	1510	U
1	X	1511	C
1	X	1512	U
1	X	1513	A
1	X	1514	A
1	X	1515	G
1	X	1516	C
1	X	1519	U
1	X	1522	G
1	X	1524	C
1	X	1527	A
1	X	1528	G
1	X	1529	U
1	X	1541	C
1	X	1542	C
1	X	1543	G
1	X	1544	G
1	X	1546	A
1	X	1547	C
1	X	1548	U
1	X	1550	G
1	X	1556	G
1	X	1557	C
1	X	1561	G
1	X	1568	U
1	X	1569	G
1	X	1573	A
1	X	1575	A
1	X	1576	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1577	G
1	X	1592	A
1	X	1593	G
1	X	1594	U
1	X	1599	G
1	X	1603	U
1	X	1605	A
1	X	1613	G
1	X	1616	A
1	X	1623	U
1	X	1625	U
1	X	1628	A
1	X	1629	U
1	X	1630	A
1	X	1631	G
1	X	1632	A
1	X	1636	U
1	X	1637	A
1	X	1638	G
1	X	1650	G
1	X	1652	A
1	X	1653	A
1	X	1657	G
1	X	1662	A
1	X	1683	U
1	X	1684	A
1	X	1690	A
1	X	1691	G
1	X	1692	C
1	X	1695	G
1	X	1718	G
1	X	1732	U
1	X	1738	C
1	X	1739	G
1	X	1740	G
1	X	1744	A
1	X	1745	A
1	X	1746	G
1	X	1755	U
1	X	1756	U
1	X	1757	U
1	X	1760	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1761	G
1	X	1762	U
1	X	1763	U
1	X	1765	A
1	X	1766	C
1	X	1768	C
1	X	1770	C
1	X	1771	A
1	X	1772	G
1	X	1789	A
1	X	1790	G
1	X	1791	G
1	X	1800	A
1	X	1808	U
1	X	1818	A
1	X	1826	G
1	X	1827	C
1	X	1828	U
1	X	1829	A
1	X	1835	U
1	X	1836	A
1	X	1837	A
1	X	1843	U
1	X	1847	U
1	X	1848	A
1	X	1856	A
1	X	1865	C
1	X	1875	A
1	X	1885	G
1	X	1902	G
1	X	1908	A
1	X	1909	C
1	X	1911	A
1	X	1912	A
1	X	1930	G
1	X	1932	C
1	X	1933	G
1	X	1953	U
1	X	1954	A
1	X	1955	A
1	X	1963	A
1	X	1964	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1965	A
1	X	1982	U
1	X	1987	A
1	X	1994	C
1	X	1997	A
1	X	1998	A
1	X	1999	G
1	X	2009	U
1	X	2018	U
1	X	2019	G
1	X	2020	U
1	X	2024	A
1	X	2050	A
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2070	C
1	X	2078	A
1	X	2079	G
1	X	2082	C
1	X	2083	G
1	X	2084	G
1	X	2087	A
1	X	2088	G
1	X	2089	A
1	X	2094	G
1	X	2096	G
1	X	2107	G
1	X	2119	U
1	X	2225	A
1	X	2226	A
1	X	2230	G
1	X	2231	C
1	X	2232	A
1	X	2233	C
1	X	2234	C
1	X	2237	U
1	X	2238	U
1	X	2239	A
1	X	2240	U
1	X	2241	C
1	X	2246	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2248	G
1	X	2252	A
1	X	2253	C
1	X	2266	G
1	X	2270	U
1	X	2289	U
1	X	2295	A
1	X	2298	G
1	X	2306	G
1	X	2310	C
1	X	2314	A
1	X	2332	U
1	X	2333	U
1	X	2334	G
1	X	2339	U
1	X	2345	A
1	X	2347	A
1	X	2352	G
1	X	2354	A
1	X	2361	U
1	X	2362	A
1	X	2363	A
1	X	2374	C
1	X	2377	C
1	X	2398	G
1	X	2399	G
1	X	2406	G
1	X	2410	G
1	X	2412	C
1	X	2417	U
1	X	2429	U
1	X	2433	C
1	X	2434	A
1	X	2440	G
1	X	2441	G
1	X	2449	C
1	X	2450	U
1	X	2452	A
1	X	2456	G
1	X	2457	A
1	X	2458	U
1	X	2461	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2468	C
1	X	2472	G
1	X	2475	A
1	X	2497	G
1	X	2500	U
1	X	2501	U
1	X	2503	A
1	X	2505	A
1	X	2514	G
1	X	2519	U
1	X	2525	C
1	X	2529	G
1	X	2532	G
1	X	2533	U
1	X	2534	C
1	X	2545	A
1	X	2546	U
1	X	2547	C
1	X	2556	G
1	X	2561	C
1	X	2576	G
1	X	2581	U
1	X	2591	A
1	X	2593	A
1	X	2594	G
1	X	2600	C
1	X	2609	G
1	X	2612	U
1	X	2613	C
1	X	2629	A
1	X	2630	G
1	X	2631	U
1	X	2636	U
1	X	2640	U
1	X	2641	A
1	X	2642	U
1	X	2648	G
1	X	2656	A
1	X	2661	A
1	X	2663	U
1	X	2666	A
1	X	2681	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2682	G
1	X	2690	G
1	X	2698	A
1	X	2712	G
1	X	2715	G
1	X	2716	U
1	X	2717	A
1	X	2737	C
1	X	2741	G
1	X	2745	G
1	X	2753	U
1	X	2760	A
1	X	2766	U
1	X	2771	G
1	X	2775	A
1	X	2778	G
1	X	2784	A
1	X	2787	C
1	X	2792	A
1	X	2805	A
1	X	2806	U
1	X	2807	G
1	X	2817	A
1	X	2818	A
1	X	2819	C
1	X	2820	U
1	X	2821	U
1	X	2824	G
1	X	2827	A
1	X	2832	A
1	X	2838	C
1	X	2840	A
1	X	2843	A
1	X	2850	G
1	X	2854	A
1	X	2856	U
1	X	2877	G
1	X	2887	G
1	X	2892	G
1	X	2896	A
1	X	2899	A
1	X	2900	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2913	G
1	X	2920	U
2	Y	10	U
2	Y	23	U
2	Y	24	C
2	Y	38	U
2	Y	39	G
2	Y	42	G
2	Y	43	A
2	Y	54	U
2	Y	86	C
2	Y	87	G
2	Y	88	U
2	Y	106	U
2	Y	114	C

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	38	A
1	X	90	A
1	X	165	C
1	X	373	A
1	X	525	A
1	X	660	A
1	X	1091	G
1	X	1490	G
1	X	1503	U
1	X	1510	U
1	X	1521	A
1	X	1526	G
1	X	1568	U
1	X	1575	A
1	X	1576	A
1	X	1901	C
1	X	2457	A
1	X	2823	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 346 ligands modelled in this entry, 322 are monoatomic - leaving 24 for Mogul analysis.

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	$\# Z > 2$
29	MPD	X	3001	-	6,7,7	0.31	0	6,10,10	0.34	0
29	MPD	X	3002	-	6,7,7	0.48	0	6,10,10	0.24	0
29	MPD	X	3003	-	6,7,7	0.30	0	6,10,10	0.38	0
29	MPD	X	3004	-	6,7,7	0.42	0	6,10,10	0.11	0
29	MPD	X	3005	-	6,7,7	0.44	0	6,10,10	0.16	0
29	MPD	X	3006	-	6,7,7	0.34	0	6,10,10	0.10	0
29	MPD	X	3007	-	6,7,7	0.23	0	6,10,10	0.43	0
29	MPD	X	3008	-	6,7,7	0.44	0	6,10,10	0.15	0
29	MPD	X	3009	-	6,7,7	0.42	0	6,10,10	0.13	0
29	MPD	X	3010	-	6,7,7	0.36	0	6,10,10	0.16	0
29	MPD	X	3011	-	6,7,7	0.58	0	6,10,10	0.36	0
32	EPE	X	3311	-	15,15,15	1.20	1 (6%)	19,20,20	0.63	1 (5%)
33	SPD	X	3312	-	9,9,9	0.29	0	8,8,8	0.37	0
33	SPD	X	3313	-	9,9,9	0.21	0	8,8,8	0.30	0
33	SPD	X	3314	-	9,9,9	0.17	0	8,8,8	0.22	0
33	SPD	X	3315	-	9,9,9	0.25	0	8,8,8	0.26	0
34	EOH	X	3316	-	2,2,2	0.65	0	1,1,1	0.42	0
34	EOH	X	3317	-	2,2,2	0.53	0	1,1,1	0.65	0
34	EOH	X	3318	-	2,2,2	0.56	0	1,1,1	0.64	0
34	EOH	X	3319	-	2,2,2	0.49	0	1,1,1	0.75	0
34	EOH	X	3320	-	2,2,2	0.57	0	1,1,1	0.62	0
34	EOH	X	3321	-	2,2,2	0.57	0	1,1,1	0.61	0
34	EOH	X	3322	-	2,2,2	0.53	0	1,1,1	0.65	0
29	MPD	Z	101	-	6,7,7	0.29	0	6,10,10	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	MPD	X	3001	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3002	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3003	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3004	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3005	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3006	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3007	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3008	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3009	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3010	-	-	0/5/5/5	0/0/0/0
29	MPD	X	3011	-	-	0/5/5/5	0/0/0/0
32	EPE	X	3311	-	-	0/9/19/19	0/1/1/1
33	SPD	X	3312	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3313	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3314	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3315	-	-	0/7/7/7	0/0/0/0
34	EOH	X	3316	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3317	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3318	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3319	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3320	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3321	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3322	-	-	0/0/0/0	0/0/0/0
29	MPD	Z	101	-	-	0/5/5/5	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	3311	EPE	C10-S	-4.42	1.70	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	3311	EPE	O1S-S-C10	-2.19	105.32	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	3003	MPD	4	0
29	X	3005	MPD	4	0
29	X	3007	MPD	4	0
29	X	3008	MPD	1	0
29	X	3011	MPD	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	X	2708/2923 (92%)	-0.47	9 (0%) 94 91	11, 51, 139, 230	0
2	Y	114/114 (100%)	-0.66	0 100 100	22, 67, 115, 151	0
3	A	269/277 (97%)	-0.24	4 (1%) 76 68	43, 74, 106, 136	0
4	B	215/220 (97%)	-0.32	0 100 100	12, 28, 66, 97	0
5	C	199/207 (96%)	-0.53	1 (0%) 91 88	12, 35, 71, 107	0
6	D	166/179 (92%)	-0.41	2 (1%) 81 73	80, 102, 132, 150	0
7	E	156/178 (87%)	-0.25	3 (1%) 70 61	61, 86, 120, 131	0
8	G	145/145 (100%)	-0.28	1 (0%) 89 83	9, 26, 58, 114	0
9	H	122/122 (100%)	-0.39	0 100 100	17, 41, 74, 102	0
10	I	131/146 (89%)	-0.11	2 (1%) 76 68	14, 47, 91, 108	0
11	J	141/144 (97%)	-0.04	3 (2%) 67 58	25, 43, 97, 121	0
12	K	119/122 (97%)	-0.44	0 100 100	14, 37, 86, 97	0
13	L	110/119 (92%)	-0.50	0 100 100	39, 62, 92, 111	0
14	M	110/116 (94%)	-0.48	1 (0%) 85 78	23, 43, 89, 115	0
15	N	116/118 (98%)	-0.54	0 100 100	6, 21, 59, 69	0
16	O	102/102 (100%)	-0.57	0 100 100	7, 35, 75, 92	0
17	P	112/117 (95%)	-0.35	0 100 100	7, 21, 86, 125	0
18	Q	89/91 (97%)	-0.23	1 (1%) 82 74	39, 60, 93, 108	0
19	R	100/105 (95%)	0.18	3 (3%) 54 43	43, 66, 122, 142	0
20	S	167/217 (76%)	-0.19	3 (1%) 71 63	42, 61, 120, 130	0
21	T	75/94 (79%)	0.20	3 (4%) 42 33	21, 39, 81, 102	0
22	U	46/62 (74%)	1.90	19 (41%) 0 0	60, 91, 122, 130	0
23	V	65/69 (94%)	-0.29	0 100 100	48, 71, 105, 119	0
24	W	58/59 (98%)	-0.11	0 100 100	12, 24, 72, 108	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	43/58 (74%)	-0.39	0 100 100	11, 20, 99, 127	0
26	2	44/45 (97%)	0.01	1 (2%) 64 54	19, 41, 73, 93	0
27	3	60/66 (90%)	-0.43	0 100 100	10, 32, 69, 83	0
28	4	37/37 (100%)	1.54	10 (27%) 1 1	39, 60, 89, 103	0
All	All	5819/6252 (93%)	-0.35	66 (1%) 82 74	6, 51, 123, 230	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	13	SER	6.3
22	U	12	ALA	6.1
22	U	14	THR	5.3
22	U	11	LYS	5.1
20	S	146	THR	4.1
22	U	17	ARG	4.1
22	U	38	ILE	4.0
22	U	30	ASN	3.9
1	X	1148	C	3.7
28	4	12	GLU	3.7
6	D	82	GLY	3.5
22	U	28	ARG	3.4
22	U	15	GLY	3.4
11	J	3	LEU	3.4
28	4	36	GLN	3.2
22	U	47	VAL	3.1
18	Q	27	PHE	3.0
1	X	2	A	3.0
22	U	16	ASN	3.0
26	2	2	VAL	2.8
14	M	1	MET	2.8
11	J	138	GLY	2.7
19	R	88	GLY	2.7
28	4	30	PRO	2.7
22	U	37	ARG	2.6
1	X	942	C	2.6
3	A	11	ASN	2.6
22	U	10	ARG	2.5
3	A	57	GLY	2.4
20	S	147	GLU	2.4
21	T	50	GLY	2.4
28	4	24	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	4	34	GLN	2.4
22	U	50	SER	2.4
28	4	29	ASN	2.4
1	X	1147	A	2.3
8	G	1	MET	2.3
1	X	458	A	2.3
1	X	2439	A	2.3
1	X	2629	A	2.3
22	U	20	HIS	2.3
11	J	139	GLY	2.3
22	U	46	LYS	2.3
22	U	18	ARG	2.3
7	E	55	PRO	2.2
7	E	90	VAL	2.2
1	X	549	U	2.2
22	U	29	TRP	2.2
3	A	101	LYS	2.2
5	C	96	SER	2.2
28	4	7	VAL	2.1
19	R	54	GLY	2.1
28	4	13	LYS	2.1
7	E	164	TYR	2.1
28	4	3	VAL	2.1
3	A	94	VAL	2.1
21	T	69	ALA	2.1
6	D	83	MET	2.1
19	R	55	GLY	2.1
10	I	58	PHE	2.1
28	4	25	VAL	2.0
20	S	139	GLU	2.0
1	X	2760	A	2.0
22	U	34	GLN	2.0
10	I	92	THR	2.0
21	T	61	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
34	EOH	X	3322	3/3	0.91	0.47	20.99	34,34,34,34	0
30	MN	X	3255	1/1	0.92	0.56	17.42	35,35,35,35	0
30	MN	X	3252	1/1	0.96	0.30	14.07	17,17,17,17	0
30	MN	X	3260	1/1	0.96	0.30	11.96	40,40,40,40	0
30	MN	X	3225	1/1	0.96	0.41	11.40	41,41,41,41	0
34	EOH	X	3318	3/3	0.83	0.27	10.92	47,47,47,47	0
31	MG	X	3103	1/1	0.92	0.44	10.10	3,3,3,3	0
30	MN	X	3286	1/1	0.99	0.31	8.64	57,57,57,57	0
30	MN	X	3272	1/1	0.98	0.36	8.18	44,44,44,44	0
33	SPD	X	3312	10/10	0.77	0.30	8.12	47,47,47,47	0
30	MN	X	3283	1/1	0.98	0.34	6.85	14,14,14,14	0
29	MPD	X	3010	8/8	0.81	0.33	6.52	87,87,87,87	0
30	MN	X	3242	1/1	0.97	0.30	6.46	22,22,22,22	0
33	SPD	X	3314	10/10	0.87	0.48	6.36	26,26,26,26	0
29	MPD	X	3002	8/8	0.83	0.32	6.23	45,45,45,45	0
29	MPD	Z	101	8/8	0.90	0.35	6.23	48,48,48,48	0
29	MPD	X	3008	8/8	0.79	0.35	6.21	70,70,70,70	0
30	MN	X	3230	1/1	0.92	0.28	6.04	65,65,65,65	0
31	MG	X	3174	1/1	0.88	0.31	5.63	5,5,5,5	0
30	MN	X	3196	1/1	0.96	0.33	5.55	51,51,51,51	0
30	MN	X	3012	1/1	0.97	0.31	5.46	19,19,19,19	0
29	MPD	X	3009	8/8	0.92	0.14	5.29	76,76,76,76	0
30	MN	X	3197	1/1	0.98	0.24	5.25	34,34,34,34	0
30	MN	X	3166	1/1	0.97	0.23	5.19	62,62,62,62	0
30	MN	X	3280	1/1	0.98	0.27	5.13	39,39,39,39	0
34	EOH	X	3316	3/3	0.85	0.40	5.10	10,10,10,10	0
30	MN	X	3273	1/1	0.89	0.27	4.94	41,41,41,41	0
29	MPD	X	3007	8/8	0.96	0.28	4.75	9,9,9,9	0
31	MG	X	3092	1/1	0.96	0.14	4.69	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3055	1/1	0.61	0.21	4.49	94,94,94,94	0
30	MN	X	3278	1/1	0.97	0.30	4.35	35,35,35,35	0
30	MN	X	3153	1/1	0.95	0.29	4.14	95,95,95,95	0
31	MG	X	3030	1/1	0.97	0.21	3.66	15,15,15,15	0
30	MN	X	3271	1/1	0.99	0.25	3.54	17,17,17,17	0
29	MPD	X	3006	8/8	0.85	0.18	3.50	88,88,88,88	0
30	MN	X	3279	1/1	0.99	0.25	3.47	25,25,25,25	0
33	SPD	X	3313	10/10	0.86	0.29	2.90	30,30,30,30	0
30	MN	X	3047	1/1	0.97	0.20	2.79	69,69,69,69	0
30	MN	X	3210	1/1	0.98	0.20	2.58	57,57,57,57	0
33	SPD	X	3315	10/10	0.84	0.31	2.56	46,46,46,46	0
30	MN	X	3265	1/1	0.95	0.24	2.40	43,43,43,43	0
30	MN	X	3154	1/1	0.99	0.22	2.10	40,40,40,40	0
30	MN	X	3213	1/1	0.71	0.23	2.09	95,95,95,95	0
30	MN	X	3257	1/1	0.99	0.23	1.94	25,25,25,25	0
30	MN	X	3185	1/1	0.99	0.21	1.93	28,28,28,28	0
30	MN	X	3258	1/1	0.96	0.22	1.61	35,35,35,35	0
29	MPD	X	3011	8/8	0.85	0.24	1.48	39,39,39,39	0
30	MN	X	3269	1/1	0.93	0.24	1.33	36,36,36,36	0
30	MN	X	3198	1/1	0.99	0.20	1.18	64,64,64,64	0
30	MN	X	3256	1/1	0.98	0.22	1.18	13,13,13,13	0
30	MN	X	3246	1/1	0.99	0.19	1.11	13,13,13,13	0
30	MN	X	3224	1/1	0.94	0.25	1.03	53,53,53,53	0
30	MN	X	3227	1/1	0.92	0.17	1.02	57,57,57,57	0
32	EPE	X	3311	15/15	0.95	0.18	0.87	57,57,57,57	0
31	MG	X	3080	1/1	0.97	0.19	0.73	33,33,33,33	0
30	MN	X	3244	1/1	0.90	0.18	0.68	57,57,57,57	0
30	MN	X	3231	1/1	0.93	0.24	0.66	74,74,74,74	0
30	MN	X	3251	1/1	0.98	0.19	0.65	8,8,8,8	0
30	MN	X	3078	1/1	0.97	0.20	0.63	78,78,78,78	0
29	MPD	X	3004	8/8	0.92	0.34	0.50	73,73,73,73	0
30	MN	X	3167	1/1	0.99	0.20	0.46	57,57,57,57	0
29	MPD	X	3005	8/8	0.94	0.17	0.46	65,65,65,65	0
30	MN	X	3164	1/1	0.98	0.23	0.43	48,48,48,48	0
30	MN	X	3324	1/1	0.96	0.18	0.38	12,12,12,12	0
30	MN	X	3140	1/1	0.82	0.16	0.30	71,71,71,71	0
29	MPD	X	3001	8/8	0.94	0.14	0.22	33,33,33,33	0
30	MN	X	3157	1/1	0.94	0.22	0.12	68,68,68,68	0
30	MN	X	3163	1/1	0.98	0.16	-0.03	61,61,61,61	0
31	MG	X	3082	1/1	0.88	0.17	-0.06	31,31,31,31	0
31	MG	X	3176	1/1	0.95	0.16	-0.20	14,14,14,14	0
30	MN	X	3058	1/1	0.91	0.15	-0.20	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	MPD	X	3003	8/8	0.97	0.19	-0.23	21,21,21,21	0
30	MN	X	3281	1/1	0.96	0.17	-0.25	40,40,40,40	0
30	MN	J	201	1/1	0.79	0.20	-0.45	78,78,78,78	0
30	MN	X	3326	1/1	0.99	0.18	-0.46	57,57,57,57	0
30	MN	X	3277	1/1	0.98	0.17	-0.59	35,35,35,35	0
30	MN	X	3171	1/1	0.95	0.15	-0.73	86,86,86,86	0
30	MN	X	3274	1/1	0.98	0.10	-0.84	36,36,36,36	0
31	MG	X	3088	1/1	0.97	0.13	-0.85	36,36,36,36	0
31	MG	X	3310	1/1	0.94	0.13	-0.88	15,15,15,15	0
30	MN	X	3150	1/1	0.99	0.13	-0.95	50,50,50,50	0
30	MN	X	3062	1/1	0.99	0.16	-0.96	42,42,42,42	0
30	MN	R	201	1/1	0.96	0.10	-1.00	63,63,63,63	0
30	MN	X	3147	1/1	0.97	0.12	-1.02	82,82,82,82	0
30	MN	X	3061	1/1	0.93	0.12	-1.19	63,63,63,63	0
30	MN	X	3159	1/1	0.97	0.15	-1.20	42,42,42,42	0
30	MN	X	3112	1/1	0.96	0.06	-1.46	54,54,54,54	0
31	MG	B	302	1/1	0.98	0.11	-1.47	4,4,4,4	0
30	MN	X	3323	1/1	0.97	0.15	-1.53	42,42,42,42	0
30	MN	X	3229	1/1	0.93	0.13	-1.63	79,79,79,79	0
30	MN	X	3063	1/1	0.93	0.12	-1.68	60,60,60,60	0
31	MG	X	3037	1/1	0.96	0.12	-1.78	11,11,11,11	0
30	MN	X	3170	1/1	0.97	0.10	-1.93	54,54,54,54	0
30	MN	X	3288	1/1	0.91	0.11	-2.29	55,55,55,55	0
31	MG	X	3036	1/1	0.95	0.14	-	8,8,8,8	0
30	MN	X	3057	1/1	0.71	0.20	-	71,71,71,71	0
30	MN	X	3129	1/1	0.94	0.08	-	73,73,73,73	0
31	MG	X	3100	1/1	0.93	0.21	-	17,17,17,17	0
31	MG	X	3032	1/1	0.94	0.25	-	21,21,21,21	0
31	MG	X	3096	1/1	0.98	0.24	-	9,9,9,9	0
30	MN	X	3015	1/1	0.74	0.38	-	75,75,75,75	0
30	MN	X	3200	1/1	0.99	0.26	-	37,37,37,37	0
30	MN	X	3053	1/1	0.63	0.54	-	89,89,89,89	0
31	MG	X	3081	1/1	0.98	0.07	-	36,36,36,36	0
30	MN	X	3189	1/1	0.99	0.30	-	64,64,64,64	0
31	MG	X	3093	1/1	0.84	0.27	-	21,21,21,21	0
30	MN	X	3051	1/1	0.98	0.18	-	67,67,67,67	0
30	MN	X	3259	1/1	0.96	0.15	-	13,13,13,13	0
30	MN	X	3264	1/1	0.99	0.34	-	52,52,52,52	0
30	MN	X	3247	1/1	0.99	0.25	-	25,25,25,25	0
30	MN	X	3218	1/1	0.94	0.31	-	65,65,65,65	0
30	MN	X	3250	1/1	0.91	0.27	-	80,80,80,80	0
30	MN	X	3216	1/1	0.88	0.19	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3017	1/1	0.98	0.36	-	103,103,103,103	0
31	MG	X	3300	1/1	0.91	0.17	-	11,11,11,11	0
31	MG	X	3035	1/1	0.89	0.33	-	23,23,23,23	0
30	MN	X	3162	1/1	0.94	0.31	-	43,43,43,43	0
30	MN	X	3191	1/1	0.94	0.15	-	51,51,51,51	0
30	MN	X	3066	1/1	0.79	0.12	-	56,56,56,56	0
31	MG	X	3306	1/1	0.96	0.07	-	29,29,29,29	0
31	MG	C	301	1/1	0.90	0.26	-	2,2,2,2	0
31	MG	X	3020	1/1	0.97	0.25	-	20,20,20,20	0
30	MN	I	202	1/1	0.84	0.25	-	64,64,64,64	0
31	MG	X	3108	1/1	0.94	0.10	-	12,12,12,12	0
30	MN	X	3160	1/1	0.94	0.18	-	45,45,45,45	0
30	MN	X	3155	1/1	0.90	0.39	-	87,87,87,87	0
30	MN	X	3193	1/1	0.97	0.18	-	33,33,33,33	0
31	MG	X	3104	1/1	0.96	0.32	-	28,28,28,28	0
31	MG	X	3018	1/1	0.93	0.47	-	15,15,15,15	0
30	MN	X	3065	1/1	0.92	0.10	-	60,60,60,60	0
30	MN	X	3165	1/1	0.97	0.16	-	63,63,63,63	0
30	MN	X	3121	1/1	0.78	0.31	-	88,88,88,88	0
30	MN	X	3261	1/1	0.95	0.16	-	30,30,30,30	0
31	MG	X	3298	1/1	0.82	1.02	-	23,23,23,23	0
31	MG	Y	203	1/1	0.87	0.76	-	21,21,21,21	0
31	MG	X	3094	1/1	0.98	0.16	-	5,5,5,5	0
31	MG	X	3038	1/1	0.91	0.29	-	23,23,23,23	0
31	MG	X	3136	1/1	0.93	0.34	-	27,27,27,27	0
30	MN	X	3132	1/1	0.67	0.16	-	97,97,97,97	0
30	MN	X	3181	1/1	0.97	0.19	-	39,39,39,39	0
30	MN	X	3111	1/1	0.80	0.13	-	99,99,99,99	0
31	MG	X	3304	1/1	0.94	0.78	-	15,15,15,15	0
30	MN	X	3183	1/1	0.88	0.15	-	41,41,41,41	0
31	MG	X	3013	1/1	0.76	0.83	-	30,30,30,30	0
30	MN	X	3138	1/1	0.83	0.10	-	112,112,112,112	0
30	MN	X	3222	1/1	0.73	0.36	-	71,71,71,71	0
30	MN	X	3134	1/1	0.91	0.18	-	58,58,58,58	0
31	MG	X	3173	1/1	0.71	1.12	-	26,26,26,26	0
30	MN	X	3151	1/1	0.97	0.17	-	44,44,44,44	0
30	MN	X	3243	1/1	0.99	0.42	-	28,28,28,28	0
30	MN	X	3076	1/1	0.82	0.10	-	74,74,74,74	0
31	MG	X	3089	1/1	0.94	0.15	-	13,13,13,13	0
30	MN	X	3235	1/1	0.98	0.39	-	40,40,40,40	0
30	MN	X	3179	1/1	0.95	0.21	-	83,83,83,83	0
30	MN	X	3024	1/1	0.97	0.43	-	107,107,107,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3044	1/1	0.70	0.24	-	94,94,94,94	0
30	MN	X	3270	1/1	0.99	0.16	-	30,30,30,30	0
31	MG	X	3137	1/1	0.80	0.91	-	17,17,17,17	0
30	MN	Y	202	1/1	0.88	0.14	-	57,57,57,57	0
31	MG	O	201	1/1	0.92	0.28	-	7,7,7,7	0
30	MN	X	3177	1/1	0.95	0.21	-	82,82,82,82	0
30	MN	X	3180	1/1	0.96	0.54	-	76,76,76,76	0
31	MG	X	3023	1/1	0.78	0.29	-	37,37,37,37	0
31	MG	X	3307	1/1	0.96	0.04	-	21,21,21,21	0
30	MN	X	3234	1/1	0.99	0.18	-	17,17,17,17	0
30	MN	X	3049	1/1	0.96	0.39	-	82,82,82,82	0
30	MN	X	3043	1/1	0.98	0.11	-	61,61,61,61	0
31	MG	X	3101	1/1	0.98	0.35	-	9,9,9,9	0
30	MN	X	3118	1/1	0.87	0.31	-	101,101,101,101	0
31	MG	X	3102	1/1	0.96	0.34	-	6,6,6,6	0
31	MG	I	201	1/1	0.92	0.27	-	0,0,0,0	0
30	MN	X	3126	1/1	0.81	0.24	-	77,77,77,77	0
30	MN	X	3124	1/1	0.81	0.11	-	77,77,77,77	0
30	MN	X	3206	1/1	0.96	0.45	-	57,57,57,57	0
30	MN	R	202	1/1	0.96	0.23	-	58,58,58,58	0
30	MN	X	3071	1/1	0.96	0.08	-	69,69,69,69	0
30	MN	X	3130	1/1	0.81	0.13	-	102,102,102,102	0
30	MN	X	3073	1/1	0.88	0.14	-	86,86,86,86	0
30	MN	X	3050	1/1	0.74	0.47	-	99,99,99,99	0
31	MG	X	3295	1/1	0.94	0.68	-	18,18,18,18	0
30	MN	X	3046	1/1	0.93	0.30	-	94,94,94,94	0
31	MG	X	3116	1/1	0.99	0.14	-	20,20,20,20	0
31	MG	X	3099	1/1	0.94	0.14	-	26,26,26,26	0
31	MG	X	3114	1/1	0.82	0.57	-	36,36,36,36	0
30	MN	X	3161	1/1	0.97	0.23	-	46,46,46,46	0
31	MG	X	3029	1/1	0.97	0.39	-	19,19,19,19	0
31	MG	X	3095	1/1	0.84	0.34	-	26,26,26,26	0
30	MN	X	3169	1/1	0.89	0.68	-	78,78,78,78	0
30	MN	X	3214	1/1	0.98	0.11	-	81,81,81,81	0
30	MN	X	3133	1/1	0.73	0.32	-	98,98,98,98	0
30	MN	X	3068	1/1	0.87	0.22	-	70,70,70,70	0
30	MN	X	3119	1/1	0.93	0.15	-	63,63,63,63	0
31	MG	Y	205	1/1	0.88	0.14	-	12,12,12,12	0
30	MN	X	3239	1/1	0.97	0.36	-	15,15,15,15	0
30	MN	X	3048	1/1	0.95	0.10	-	59,59,59,59	0
31	MG	X	3172	1/1	0.87	0.80	-	27,27,27,27	0
31	MG	G	203	1/1	0.46	0.33	-	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3142	1/1	0.95	0.39	-	72,72,72,72	0
30	MN	X	3208	1/1	0.94	0.25	-	37,37,37,37	0
30	MN	X	3067	1/1	0.91	0.19	-	51,51,51,51	0
30	MN	X	3236	1/1	0.97	0.15	-	36,36,36,36	0
30	MN	X	3064	1/1	0.99	0.14	-	68,68,68,68	0
30	MN	X	3117	1/1	0.92	0.25	-	80,80,80,80	0
30	MN	X	3204	1/1	0.97	0.16	-	21,21,21,21	0
30	MN	X	3143	1/1	0.78	0.18	-	94,94,94,94	0
30	MN	X	3152	1/1	0.97	0.29	-	68,68,68,68	0
31	MG	X	3034	1/1	0.73	0.39	-	18,18,18,18	0
30	MN	X	3190	1/1	0.99	0.41	-	59,59,59,59	0
31	MG	X	3031	1/1	0.89	0.33	-	11,11,11,11	0
31	MG	X	3109	1/1	0.83	0.70	-	24,24,24,24	0
30	MN	X	3139	1/1	0.99	0.29	-	97,97,97,97	0
30	MN	X	3074	1/1	0.89	0.06	-	78,78,78,78	0
30	MN	X	3287	1/1	0.97	0.31	-	78,78,78,78	0
30	MN	X	3070	1/1	0.95	0.10	-	78,78,78,78	0
31	MG	X	3106	1/1	0.85	0.22	-	37,37,37,37	0
30	MN	X	3215	1/1	0.99	0.28	-	26,26,26,26	0
30	MN	X	3202	1/1	0.93	0.23	-	54,54,54,54	0
31	MG	X	3309	1/1	0.93	0.24	-	20,20,20,20	0
30	MN	X	3263	1/1	0.94	0.33	-	52,52,52,52	0
30	MN	X	3188	1/1	0.94	0.45	-	87,87,87,87	0
30	MN	X	3146	1/1	0.90	0.23	-	101,101,101,101	0
31	MG	X	3115	1/1	0.91	0.72	-	1,1,1,1	1
30	MN	X	3158	1/1	0.84	0.22	-	62,62,62,62	0
31	MG	X	3107	1/1	0.91	0.58	-	18,18,18,18	0
30	MN	X	3293	1/1	0.81	0.19	-	70,70,70,70	0
30	MN	B	303	1/1	0.70	0.74	-	102,102,102,102	0
30	MN	X	3226	1/1	0.92	0.33	-	89,89,89,89	0
30	MN	X	3120	1/1	0.96	0.17	-	55,55,55,55	0
31	MG	X	3294	1/1	0.86	0.34	-	37,37,37,37	0
31	MG	X	3087	1/1	0.95	0.32	-	51,51,51,51	0
30	MN	X	3211	1/1	0.93	0.20	-	60,60,60,60	0
30	MN	X	3056	1/1	0.99	0.19	-	61,61,61,61	0
30	MN	X	3249	1/1	0.99	0.20	-	51,51,51,51	0
30	MN	X	3285	1/1	0.98	0.22	-	85,85,85,85	0
30	MN	X	3199	1/1	0.92	0.36	-	51,51,51,51	0
31	MG	X	3026	1/1	0.91	0.60	-	18,18,18,18	0
31	MG	X	3302	1/1	0.87	0.31	-	20,20,20,20	0
30	MN	X	3127	1/1	0.90	0.13	-	44,44,44,44	0
30	MN	X	3233	1/1	0.92	0.26	-	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	MN	X	3262	1/1	0.96	0.22	-	50,50,50,50	0
30	MN	X	3228	1/1	0.96	0.34	-	85,85,85,85	0
30	MN	X	3168	1/1	0.73	0.21	-	74,74,74,74	0
31	MG	X	3019	1/1	0.93	0.25	-	15,15,15,15	0
30	MN	X	3128	1/1	0.79	0.16	-	84,84,84,84	0
30	MN	X	3045	1/1	0.99	0.28	-	3,3,3,3	0
30	MN	X	3141	1/1	0.97	0.35	-	69,69,69,69	0
30	MN	X	3268	1/1	0.86	0.29	-	27,27,27,27	0
30	MN	X	3220	1/1	0.81	0.43	-	68,68,68,68	0
30	MN	X	3072	1/1	0.93	0.17	-	80,80,80,80	0
30	MN	X	3245	1/1	0.99	0.21	-	28,28,28,28	0
30	MN	Y	204	1/1	0.97	0.11	-	63,63,63,63	0
31	MG	X	3039	1/1	0.88	0.30	-	7,7,7,7	0
34	EOH	X	3317	3/3	0.71	0.52	-	46,46,46,46	0
30	MN	X	3125	1/1	0.85	0.33	-	79,79,79,79	0
30	MN	X	3241	1/1	0.97	0.28	-	20,20,20,20	0
30	MN	X	3131	1/1	0.85	0.49	-	89,89,89,89	0
30	MN	X	3221	1/1	0.94	0.12	-	46,46,46,46	0
31	MG	X	3033	1/1	0.98	0.20	-	19,19,19,19	0
30	MN	X	3240	1/1	0.96	0.19	-	28,28,28,28	0
30	MN	X	3182	1/1	0.77	0.38	-	107,107,107,107	0
31	MG	X	3305	1/1	0.90	0.92	-	15,15,15,15	0
30	MN	X	3025	1/1	0.96	0.21	-	52,52,52,52	0
30	MN	X	3014	1/1	0.97	0.20	-	12,12,12,12	0
30	MN	X	3276	1/1	0.88	0.17	-	42,42,42,42	0
30	MN	X	3187	1/1	0.94	0.28	-	74,74,74,74	0
30	MN	X	3282	1/1	0.97	0.21	-	49,49,49,49	0
31	MG	X	3175	1/1	0.80	0.30	-	0,0,0,0	0
30	MN	X	3041	1/1	0.90	0.22	-	84,84,84,84	0
30	MN	X	3135	1/1	0.83	0.15	-	94,94,94,94	0
30	MN	X	3060	1/1	0.98	0.15	-	51,51,51,51	0
31	MG	X	3016	1/1	0.74	0.38	-	23,23,23,23	0
30	MN	X	3205	1/1	0.98	0.27	-	61,61,61,61	0
31	MG	X	3105	1/1	0.95	0.25	-	35,35,35,35	0
30	MN	X	3195	1/1	0.98	0.21	-	30,30,30,30	0
30	MN	X	3149	1/1	0.93	0.28	-	94,94,94,94	0
30	MN	X	3156	1/1	0.95	0.22	-	53,53,53,53	0
30	MN	X	3291	1/1	0.93	0.52	-	94,94,94,94	0
30	MN	X	3219	1/1	0.97	0.31	-	53,53,53,53	0
30	MN	X	3059	1/1	0.84	0.10	-	61,61,61,61	0
30	MN	X	3122	1/1	0.84	0.50	-	89,89,89,89	0
31	MG	X	3144	1/1	0.96	0.19	-	8,8,8,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	3297	1/1	0.92	0.31	-	5,5,5,5	0
30	MN	X	3209	1/1	0.94	0.20	-	24,24,24,24	0
31	MG	X	3303	1/1	0.94	0.25	-	4,4,4,4	0
30	MN	X	3186	1/1	0.92	0.29	-	51,51,51,51	0
30	MN	X	3290	1/1	0.90	0.18	-	89,89,89,89	0
31	MG	X	3022	1/1	0.91	0.60	-	25,25,25,25	0
30	MN	X	3238	1/1	0.98	0.22	-	34,34,34,34	0
31	MG	X	3021	1/1	0.95	0.18	-	21,21,21,21	0
30	MN	X	3148	1/1	0.75	0.25	-	79,79,79,79	0
30	MN	X	3275	1/1	0.99	0.18	-	30,30,30,30	0
30	MN	X	3292	1/1	0.97	0.28	-	99,99,99,99	0
30	MN	X	3267	1/1	0.94	0.31	-	48,48,48,48	0
31	MG	X	3097	1/1	0.91	0.22	-	14,14,14,14	0
30	MN	X	3178	1/1	0.92	0.46	-	78,78,78,78	0
31	MG	X	3028	1/1	0.91	0.29	-	34,34,34,34	0
30	MN	X	3232	1/1	0.98	0.30	-	55,55,55,55	0
30	MN	X	3042	1/1	0.84	0.11	-	104,104,104,104	0
30	MN	X	3253	1/1	0.97	0.34	-	26,26,26,26	0
30	MN	X	3052	1/1	0.83	0.21	-	71,71,71,71	0
30	MN	X	3207	1/1	0.92	0.44	-	62,62,62,62	0
30	MN	X	3075	1/1	0.97	0.11	-	76,76,76,76	0
30	MN	X	3145	1/1	0.99	0.16	-	51,51,51,51	0
34	EOH	X	3320	3/3	0.88	0.28	-	28,28,28,28	0
30	MN	X	3308	1/1	0.39	0.74	-	92,92,92,92	0
34	EOH	X	3321	3/3	0.88	0.31	-	18,18,18,18	0
30	MN	X	3217	1/1	0.98	0.27	-	38,38,38,38	0
30	MN	X	3223	1/1	0.89	0.24	-	60,60,60,60	0
31	MG	X	3085	1/1	0.91	0.21	-	9,9,9,9	0
30	MN	X	3212	1/1	0.97	0.26	-	56,56,56,56	0
30	MN	X	3069	1/1	0.94	0.14	-	68,68,68,68	0
30	MN	X	3110	1/1	0.95	0.13	-	96,96,96,96	0
30	MN	X	3325	1/1	0.95	0.22	-	59,59,59,59	0
31	MG	X	3299	1/1	0.93	0.26	-	5,5,5,5	0
34	EOH	X	3319	3/3	0.90	0.19	-	47,47,47,47	0
31	MG	G	201	1/1	0.86	0.20	-	19,19,19,19	0
30	MN	X	3040	1/1	0.95	0.19	-	74,74,74,74	0
31	MG	Y	201	1/1	0.88	0.11	-	34,34,34,34	0
31	MG	X	3113	1/1	0.65	1.07	-	45,45,45,45	0
30	MN	X	3289	1/1	0.97	0.28	-	57,57,57,57	0
30	MN	X	3237	1/1	0.99	0.23	-	47,47,47,47	0
30	MN	X	3123	1/1	0.83	0.42	-	97,97,97,97	0
31	MG	X	3296	1/1	0.96	0.48	-	9,9,9,9	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	3091	1/1	0.96	0.44	-	30,30,30,30	0
30	MN	X	3090	1/1	0.84	0.35	-	96,96,96,96	0
30	MN	I	203	1/1	0.97	0.22	-	33,33,33,33	0
30	MN	X	3184	1/1	0.94	0.36	-	88,88,88,88	0
31	MG	X	3098	1/1	0.91	0.33	-	14,14,14,14	0
31	MG	X	3083	1/1	0.71	0.34	-	37,37,37,37	0
31	MG	X	3079	1/1	0.84	0.74	-	27,27,27,27	0
30	MN	X	3266	1/1	0.97	0.18	-	22,22,22,22	0
30	MN	X	3201	1/1	0.99	0.20	-	40,40,40,40	0
30	MN	X	3054	1/1	0.94	0.28	-	86,86,86,86	0
30	MN	X	3194	1/1	0.96	0.17	-	31,31,31,31	0
30	MN	X	3284	1/1	0.99	0.15	-	21,21,21,21	0
31	MG	X	3301	1/1	0.99	0.13	-	8,8,8,8	0
31	MG	G	202	1/1	0.94	0.37	-	12,12,12,12	0
31	MG	X	3086	1/1	0.96	0.10	-	26,26,26,26	0
31	MG	X	3084	1/1	0.76	0.14	-	14,14,14,14	0
30	MN	X	3254	1/1	0.83	0.23	-	48,48,48,48	0
31	MG	B	301	1/1	0.89	0.14	-	0,0,0,0	0
30	MN	X	3203	1/1	0.98	0.37	-	27,27,27,27	0
31	MG	X	3027	1/1	0.94	0.19	-	29,29,29,29	0
30	MN	X	3077	1/1	0.98	0.20	-	78,78,78,78	0
30	MN	X	3248	1/1	0.99	0.28	-	37,37,37,37	0
30	MN	X	3192	1/1	0.90	0.32	-	84,84,84,84	0

6.5 Other polymers

There are no such residues in this entry.