



wwPDB EM Map/Model Validation Report ⓘ

Oct 3, 2016 – 04:35 PM EDT

PDB ID : 5GAG
EMDB ID: : EMD-8003
Title : RNC in complex with SRP-SR in the closed state
Authors : Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.
Deposited on : 2015-11-26
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

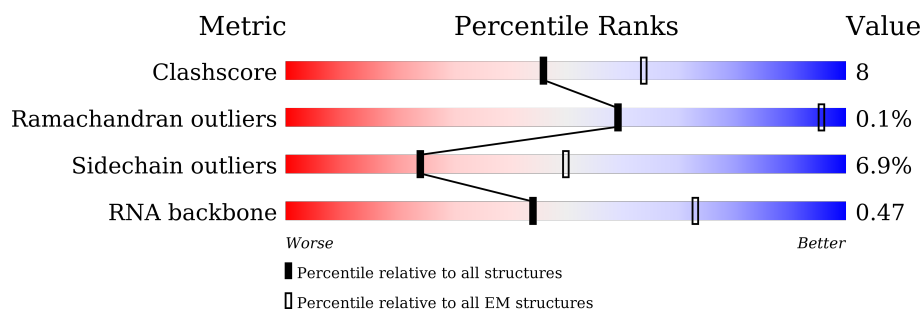
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	113	18% 17% . 62%
2	2	3	67% 33%
3	A	2903	58% 34% 6% ..
4	B	120	68% 30% .
5	C	273	70% 25% . .
6	D	209	73% 24% .
7	E	201	78% 21%
8	F	179	63% 32% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	G	177	
10	H	149	
11	I	165	
12	J	142	
13	K	142	
14	L	123	
15	M	144	
16	N	136	
17	O	127	
18	P	117	
19	Q	115	
20	R	118	
21	S	103	
22	T	110	
23	U	100	
24	V	104	
25	W	94	
26	X	85	
27	Y	78	
28	Z	63	
29	a	59	
30	b	57	
31	c	55	
32	d	46	
33	e	65	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	f	38	<div><div></div><div>100%</div></div>
35	i	450	<div><div></div><div>26%</div><div></div><div>72%</div></div>
36	k	18	<div><div></div><div>100%</div></div>

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 94031 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 SRP 4.5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	43	Total	C	N	O	P	0	0
			926	413	174	296	43		

- Molecule 2 is a RNA chain called tRNA CCAend.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	2883	Total	C	N	O	P	0	0
			61902	27613	11397	20009	2883		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	125	Total	C	N	O	S	0	0
			946	599	169	175	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	85	VAL	SER	conflict	UNP P0A7J3
I	86	THR	MET	conflict	UNP P0A7J3

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	95	Total	C	N	O	S	0	0
			757	479	141	136	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	V	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	51	Total	C	N	O	0	0
			414	266	76	72		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a protein called Signal recognition particle protein Ffh.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	126	Total	C	N	O	S	0	0
			916	575	169	161	11		

- Molecule 36 is a protein called 1A9L SS.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	18	Total	C	N	O	S	0	0
			137	94	20	22	1		

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	D	1	Total	Mg	0
			1	1	
37	B	12	Total	Mg	0
			12	12	
37	b	1	Total	Mg	0
			1	1	
37	C	2	Total	Mg	0
			2	2	
37	A	411	Total	Mg	0
			411	411	
37	O	1	Total	Mg	0
			1	1	
37	2	1	Total	Mg	0
			1	1	
37	Y	1	Total	Mg	0
			1	1	
37	R	1	Total	Mg	0
			1	1	

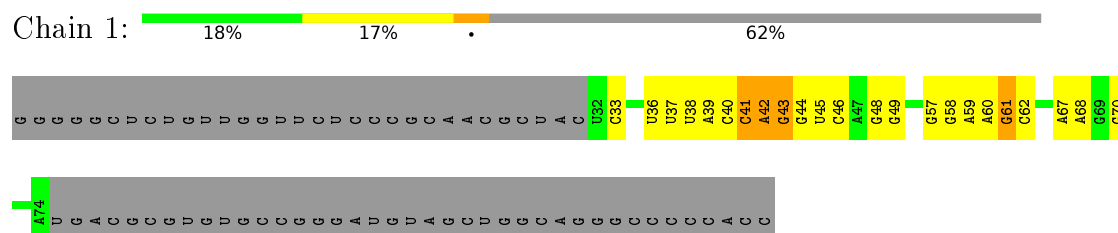
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	f	1	Total	Zn	0
			1	1	

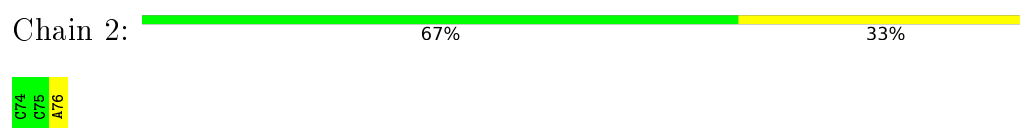
3 Residue-property plots

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. 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. 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.

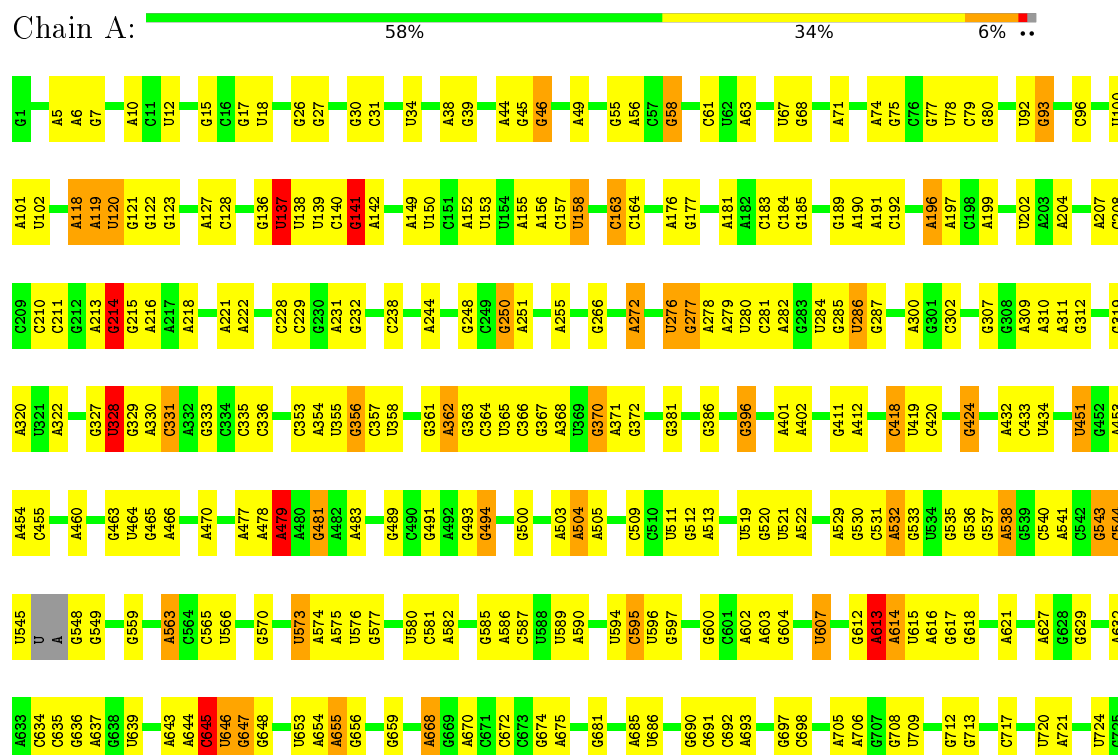
• Molecule 1: SRP 4.5S RNA



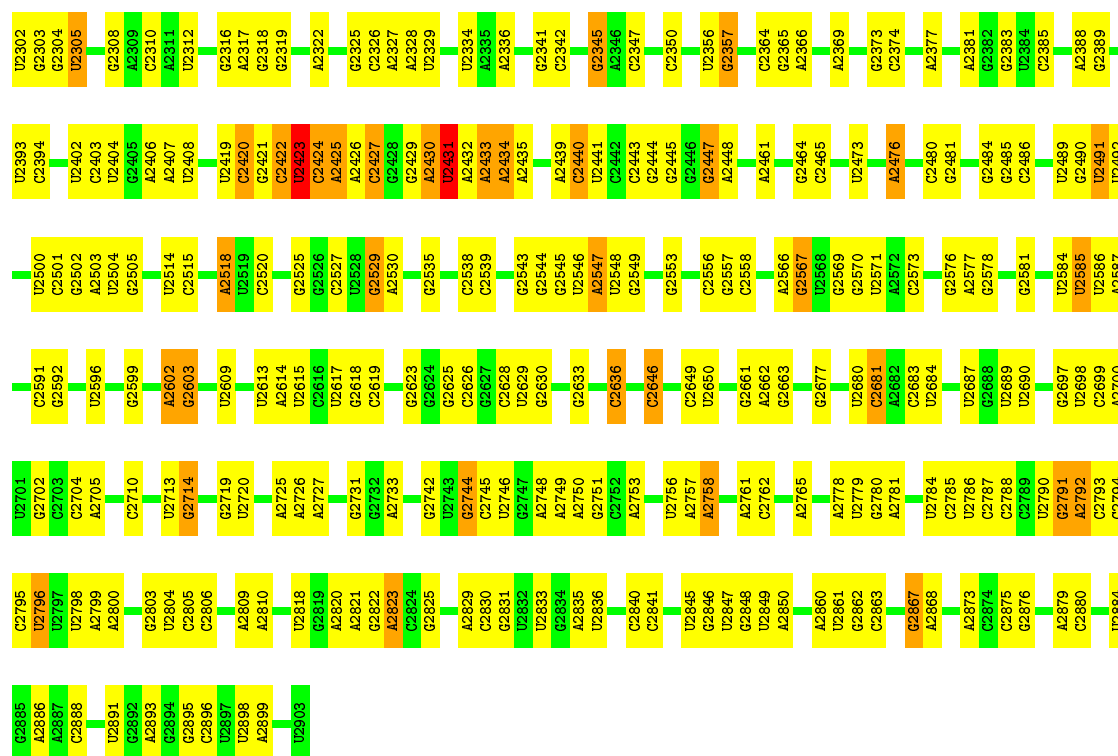
• Molecule 2: tRNA CCAend



• Molecule 3: 23S rRNA

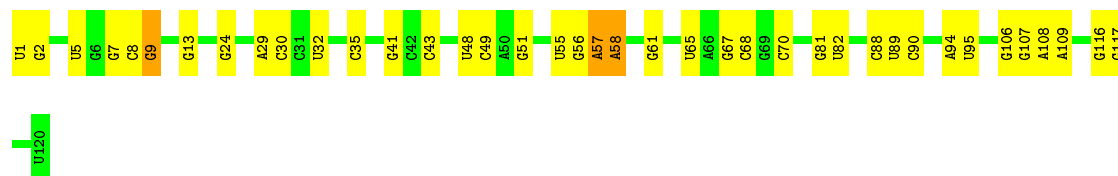


G2217	C2145	A2062	C1962	U1859	U1758	G1631	G1524		A1342	G1206	A1103	A1020	G914	U828	G726
G2221	C2146	G2069	U1963	G1860	A1759	U1636	A1525	A1439	G1343	C1207	C1104	A1021	C915	U831	A727
G2222	A2070	A2070	C1964	A1866	C1764	A1637	G1526	U1440	U1344	C1208	U1105	G1022	C922	G832	G728
G2223	G2148	A2071	A1966	A1867	C1764	C1638	G1527	G1441	U1345	U1209	G1106	U1023	C922	U832	G729
G2224	U2149	C2072	G1967	G1869	A1773	G1643	G1528	U1442	G1346	G1212	G1107	G1024	A927	A833	A730
A2225	C2150	C2073	G1968	A1870	G1776	G1643	G1529	U1443	A1347			G1025		G834	
G2228	G2152	U2075	A1969	A1871	G1776		A1532	G1444	U1352	G1218	G1110	G1026	U832	U839	G738
U2229	C2153	A2076	A1970	A1872	U1779	U1647	C1533	G1445	A1353		G1111	A1027	A933	C840	U741
G2230	A2154	G2078	U1971	G1873	U1779	U1648	U1534	G1448	A1354	G1223	G1112	A1028	A934	U834	A742
U2231	U2155	C2078	G1972	C1874	G1649	G1649	A1535	G1449	G1355	U1224	U1119	U1033	C935	G843	A743
G2232	U2156	U2086	G1973	G1875	A1783	G1653	C1536	G1450	G1358	G1227	U1130	G1038	A936	A844	U747
U2233	G2157	G2087	U1974	A1784	G1653		G1537	G1451	G1359		G1131	A1039	C937	A845	U747
G2234	C2158	A2088	U1982	U1880	C1656		G1538	G1452	G1361	G1236	U1132	A1046	G942	U847	G748
G2238	G2159	C2092	U1987	C1881	U1659		U1539	A1453	C1362	A1237	A1133	G1047	A943	U848	A753
G2239	C2160	G2093	G1988	A1791	G1659		G1543	G1456	A1365	G1238	C1134	G1047	A849	U754	U754
	G2162		A1889	A1890	A1664		A1544	U1457	A1366		C1135		C946		G757
U2243	A2163	A2097	U1991	U1900	A1665		G1546	G1459	G1369	G1252	G1139	G1056	G956	G857	
U2244	C2164	A2101	G1992	U1796	U1665		C1547	U1460	C1253		C1140	A1057	C957	G858	A764
U2245	U2165	G2102	U1993	G1799	G1674		U1548	C1461	C1370	A1253	C1141	G1064	U958	U860	C765
G2246	A2166	C2103	G1903	C1800	G1674		A1549	C1462	G1256		U1141	U1065	A959	U766	U766
A2247	U2167	C2104	G1904	A1801	A1677		A1553	C1463	G1377	G1266	A1142	U1060	A960	A863	U767
G2248	G2168	C1997	C1905	A1802	A1678		A1554	G1464	A1378		A1143	U1061	C961	G864	
U2249	A2169	U2105	G1996	A1802	A1678		U1554	G1465	U1379		A1144	G1062	G962	G864	
G2250	A2170	U2106	C1999	A1808	G1682		A1566	U1466	A1383	G1271	C1153	G1063	C963	G869	G774
	A2171	G2107	G1910	G1811	G1687		U1566	U1467	A1384	A1272	C1154	C1064	C964	U870	G775
G2256	U2172	A2108	G1911	G1811	G1687		A1570	U1468	A1385	G1278	G1155	U1066	U967	U871	G776
A2173	A2173		U1912	G1814	A1698		A1571	A1470	C1386	G1279	A1155	U1066	C968	U872	G777
C2174	C2174		A1912	A1815	A1698		A1572	G1471	A1387		C1164	A1069		C873	G780
	C2177		A	G1816	G1702		A1578	U1474	A1387	U1282	A1165	A1070	A973	A878	A783
C2178	C2178		C	G1817	G1702		U1578	U1475	A1395	G1283	A1166	G1071	G974	G879	A783
C2179	C2179		U1917	U1818	U1709		U1578	G1476	A1395	G1293	C1167	C1072	A975	G880	G784
	U2182		U1917	U1819	G1710		G1581	G1478	A1403	U1294	G1172	G1075	G976	G881	G785
U2186	U2186		U1923	U1820	G1715		C1582		A1408		U1173	C1076	A880	G882	A789
G2271	G2271		C1924	U1825	G1715		A1583	G1482	U1408	C1297	U	C1077	A981	U	U790
A2272	A2272		U1924	G1826	U1720		U1584	U1482	U1409		A	U1078	C982	C	C791
A2274	G2276		A1927	U1827	G1721		C1585	C1489	G1410	G1300	U	C1079	A983	A	
G2275	U2187		G1928	G1828	A1722		A1586	A1490	A1301	A1301	G1177	A1080	A984	U	A794
G2277	U2187		A2032	A1829	G1722		G1587	G1491	A1413	A1302	G1182	U1081	C985	C	G797
A2278	G2190		G1929	A1829	U1729		G1588	G1492	C1414	A1308	U1183	U1082	C986	C	
G2279	A2191		G1930	C1833	C1730		U1589	C1493	C1414		U1184	U1083	C987	C	
G2280	U2192		A1932	G1842	G1731		A1590	A1494	G1416	G1317	G1187	A1084	C995	A	A800
A2281	C2282		G1935	C1843	G1732		A1591	A1495	C1417		U1188	A1085	A996	C	G805
C2283	C2196		U1937	G1843	G1733		C1592	U1496	G1421	A1321	U1188	G1087	A996	C	C806
G2286	U2197		G1936	C1843	G1733		U1592	U1497	G1422		A1189	U1087	A1000	U894	U807
A2287	A2198		A1937	G1846	G1738		A1603	C1498	G1423	G1324	G1195	A1083	A1001	U896	
	U2203		A1938	A1847	A1739		C1606	A1508	U1424	U1325	G1196	G1093	G1002	A896	C812
G2290	G2204		U1939	A1848	G1740		C1607	A1509	G1425	U1326	C1197	U813	U1002	C897	U813
U2291	C2205		G1849	G1850	G1750		A1608	G1510	G1426	A1327	G1197	A1096	C1007	A899	C814
U2292	G2209		A1953	G1850	U1751		G1613	A1427	A1427	G1331	U1198	U1097	A1008	U806	C815
	C2055		U1955	A1853	C1752		A1614	G1511	C1428	G1332	U1199	A1098	A1009	U806	C816
A2297	A2211		U1956	A1854	G1753		A1515		G1432	G1332	U1203	G1099	U1012	A910	A819
A2298	A2212		C2056	A1854	G1753		A1522	U1523	G1432	U1340	A1204	C1100	C1013	A911	U827
U2299	C2215		A2060	G1857	G1756		C1617		A1433	U1340	A1204	C1100	C1013	A911	U827
C2300	G2216		G2061	A1858	A1757				A1434	G1341	A1205	C1102			



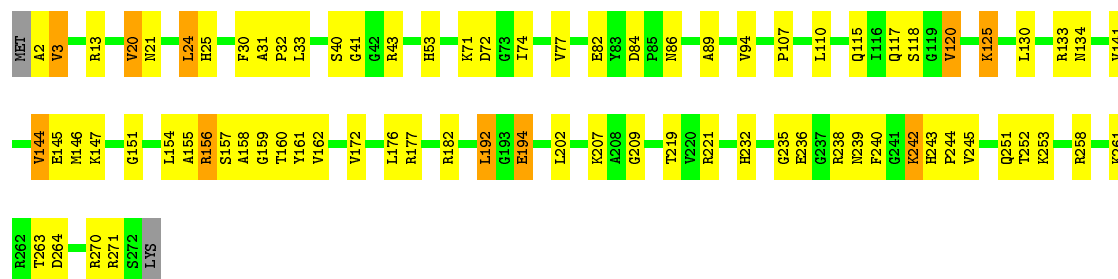
• Molecule 4: 5S rRNA

Chain B: 68% 30%



• Molecule 5: 50S ribosomal protein L2

Chain C: 70% 25%



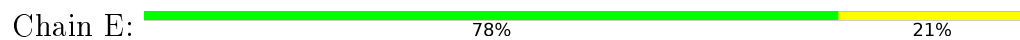
• Molecule 6: 50S ribosomal protein L3

Chain D: 73% 24%

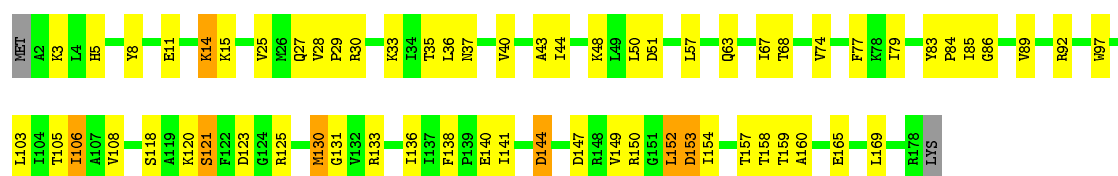




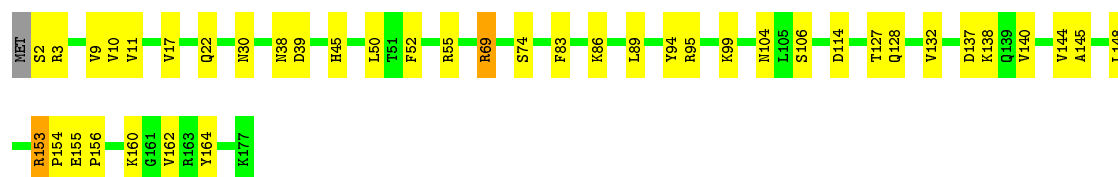
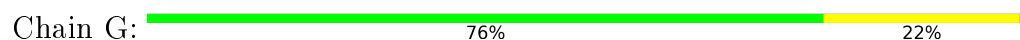
• Molecule 7: 50S ribosomal protein L4



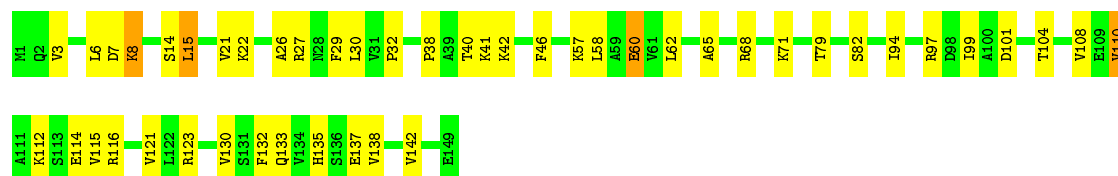
• Molecule 8: 50S ribosomal protein L5



• Molecule 9: 50S ribosomal protein L6

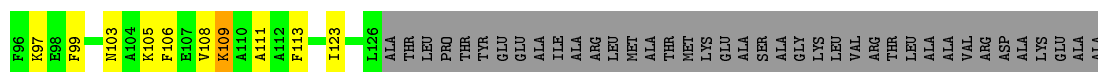


• Molecule 10: 50S ribosomal protein L9



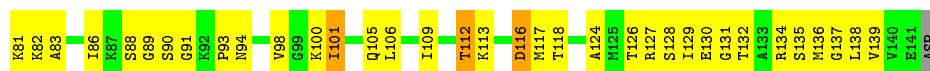
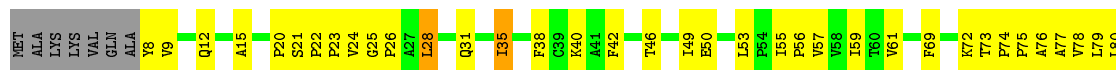
• Molecule 11: 50S ribosomal protein L10





- Molecule 12: 50S ribosomal protein L11

Chain J: 44% 46% 6%



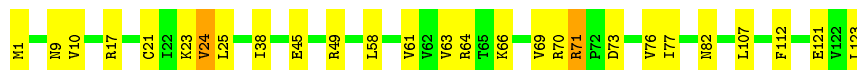
- Molecule 13: 50S ribosomal protein L13

Chain K: 73% 25% 2%



- Molecule 14: 50S ribosomal protein L14

Chain L: 78% 20% 2%



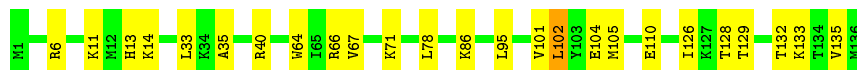
- Molecule 15: 50S ribosomal protein L15

Chain M: 77% 22% 1%



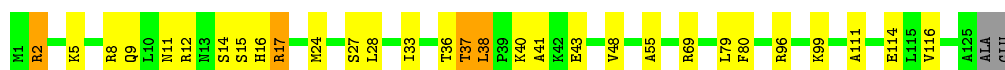
- Molecule 16: 50S ribosomal protein L16

Chain N: 82% 18% 0%

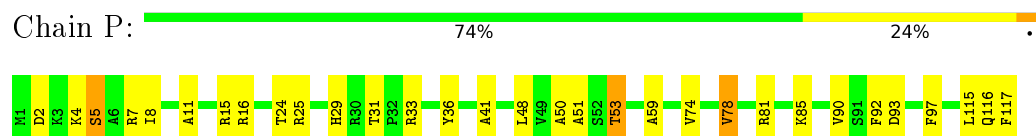


- Molecule 17: 50S ribosomal protein L17

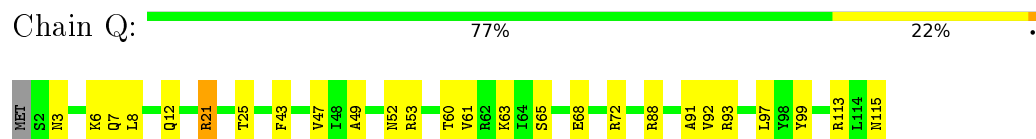
Chain O: 75% 20% 5%



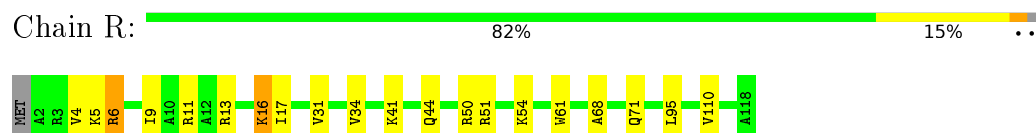
- Molecule 18: 50S ribosomal protein L18



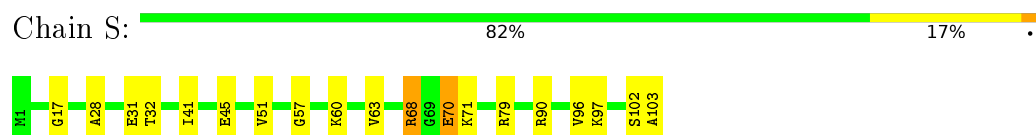
- Molecule 19: 50S ribosomal protein L19



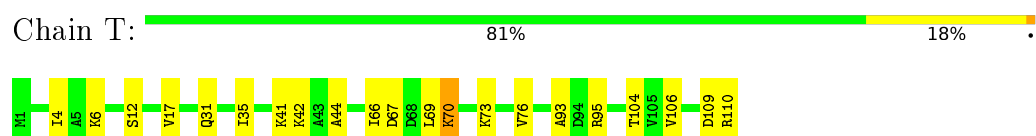
- Molecule 20: 50S ribosomal protein L20



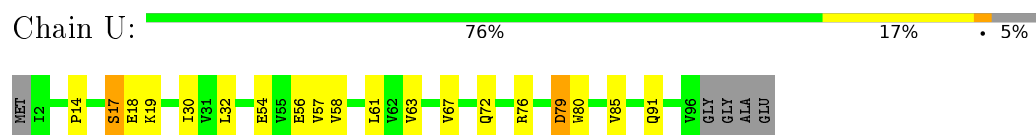
- Molecule 21: 50S ribosomal protein L21



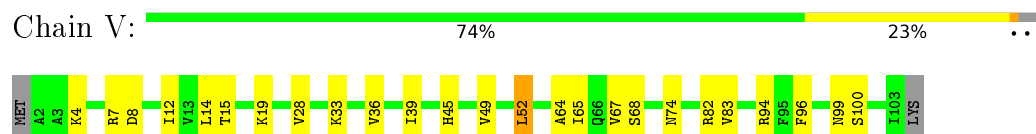
- Molecule 22: 50S ribosomal protein L22




- Molecule 23: 50S ribosomal protein L23



- Molecule 24: 50S ribosomal protein L24



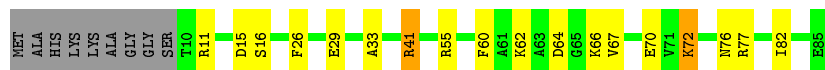
- Molecule 25: 50S ribosomal protein L25

Chain W:  82% 15% .



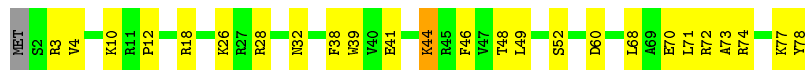
- Molecule 26: 50S ribosomal protein L27

Chain X:  68% 19% . 11%



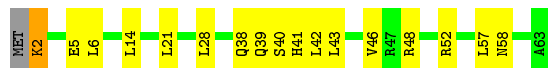
- Molecule 27: 50S ribosomal protein L28

Chain Y:  67% 31% ..



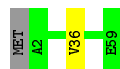
- Molecule 28: 50S ribosomal protein L29

Chain Z:  71% 25% ..




- Molecule 29: 50S ribosomal protein L30

Chain a:  97% ..



- Molecule 30: 50S ribosomal protein L32

Chain b:  86% 12% .



- Molecule 31: 50S ribosomal protein L33

Chain c:  87% 5% 7%

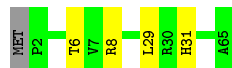


- Molecule 32: 50S ribosomal protein L34

Chain d:  87% 13%



- Molecule 33: 50S ribosomal protein L35

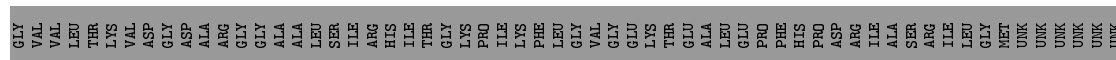


- Molecule 34: 50S ribosomal protein L36



There are no outlier residues recorded for this chain.

- Molecule 35: Signal recognition particle protein Ffh



- Molecule 36: 1A9L SS



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	75942	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.87	0/1037	1.34	8/1616 (0.5%)
10	H	0.47	0/1121	0.57	0/1515
11	I	0.58	0/958	0.62	0/1292
12	J	0.65	0/993	0.69	1/1341 (0.1%)
13	K	0.42	0/1152	0.55	0/1551
14	L	0.43	0/955	0.60	0/1279
15	M	0.40	0/1062	0.59	0/1413
16	N	0.43	0/1093	0.56	0/1460
17	O	0.45	0/1006	0.61	0/1345
18	P	0.40	0/910	0.56	0/1219
19	Q	0.42	0/929	0.56	0/1242
2	2	0.43	0/68	1.05	0/103
20	R	0.51	1/960 (0.1%)	0.56	0/1278
21	S	0.42	0/829	0.61	0/1107
22	T	0.46	0/864	0.67	0/1156
23	U	0.47	0/764	0.60	0/1021
24	V	0.42	0/788	0.57	0/1051
25	W	0.38	0/766	0.53	0/1025
26	X	0.45	0/587	0.58	0/776
27	Y	0.43	0/635	0.56	0/848
28	Z	0.43	0/502	0.60	0/667
29	a	0.37	0/453	0.55	0/605
3	A	0.63	8/69329 (0.0%)	1.10	112/108152 (0.1%)
30	b	0.45	0/450	0.64	0/599
31	c	0.40	0/421	0.58	0/561
32	d	0.42	0/380	0.60	0/498
33	e	0.41	0/513	0.58	0/676
34	f	0.45	0/303	0.56	0/397
35	i	0.46	0/672	0.57	0/883
36	k	0.74	0/137	0.85	0/186
4	B	0.48	0/2872	0.97	0/4478
5	C	0.42	0/2122	0.60	0/2852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
6	D	0.43	0/1586	0.60	0/2134
7	E	0.41	0/1571	0.59	0/2113
8	F	0.39	0/1435	0.53	0/1926
9	G	0.39	0/1343	0.58	0/1816
All	All	0.58	9/101566 (0.0%)	1.00	121/152181 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
35	i	0	1
5	C	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1490	A	N9-C4	6.41	1.41	1.37
3	A	2117	A	N9-C4	6.03	1.41	1.37
3	A	1070	A	N9-C4	5.99	1.41	1.37
3	A	2158	A	N9-C4	5.74	1.41	1.37
3	A	2114	A	N9-C4	5.67	1.41	1.37
3	A	1321	A	N9-C4	5.42	1.41	1.37
3	A	1853	A	N9-C4	-5.36	1.34	1.37
20	R	61	TRP	CB-CG	-5.24	1.40	1.50
3	A	1088	A	N9-C4	5.07	1.40	1.37

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1490	A	C8-N9-C4	-10.42	101.63	105.80
3	A	2422	C	O4'-C1'-N1	8.66	115.13	108.20
3	A	2427	C	C6-N1-C2	-8.57	116.87	120.30
3	A	2160	C	C6-N1-C2	-8.50	116.90	120.30
3	A	2423	U	C6-N1-C2	-8.23	116.06	121.00
3	A	1072	C	C6-N1-C2	-8.15	117.04	120.30
3	A	1490	A	N7-C8-N9	7.75	117.67	113.80
3	A	1584	U	C2-N1-C1'	7.72	126.96	117.70
3	A	1970	A	C8-N9-C4	-7.31	102.88	105.80
1	1	62	C	C6-N1-C2	-7.24	117.41	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1052	C	C5-C6-N1	7.24	124.62	121.00
3	A	2422	C	C6-N1-C2	-7.23	117.41	120.30
3	A	1533	C	C5-C6-N1	7.23	124.61	121.00
3	A	995	C	C6-N1-C2	7.11	123.15	120.30
3	A	2153	C	C6-N1-C2	-7.11	117.46	120.30
3	A	1917	U	C2-N1-C1'	6.97	126.07	117.70
1	1	42	A	C4-N9-C1'	6.71	138.39	126.30
3	A	2160	C	C5-C6-N1	6.69	124.34	121.00
3	A	2431	U	C5-C4-O4	6.57	129.84	125.90
3	A	280	U	OP2-P-O3'	6.53	119.56	105.20
1	1	42	A	O4'-C1'-N9	6.48	113.38	108.20
3	A	1533	C	C6-N1-C2	-6.47	117.71	120.30
3	A	645	C	C2-N1-C1'	6.44	125.88	118.80
3	A	1584	U	N1-C2-O2	6.40	127.28	122.80
3	A	1164	C	C6-N1-C2	-6.34	117.76	120.30
3	A	141	G	N7-C8-N9	6.33	116.27	113.10
3	A	1065	U	C6-N1-C2	-6.23	117.26	121.00
3	A	1072	C	C5-C6-N1	6.19	124.09	121.00
3	A	2796	U	C5-C6-N1	6.18	125.79	122.70
3	A	1308	A	N1-C6-N6	-6.08	114.95	118.60
3	A	2177	C	C6-N1-C2	-6.07	117.87	120.30
3	A	1065	U	C5-C6-N1	6.04	125.72	122.70
3	A	1434	A	O4'-C1'-N9	6.00	113.00	108.20
3	A	1297	C	C6-N1-C2	-5.93	117.93	120.30
3	A	613	A	P-O3'-C3'	5.93	126.82	119.70
3	A	2423	U	C5-C6-N1	5.92	125.66	122.70
3	A	2145	C	C6-N1-C2	-5.90	117.94	120.30
3	A	2003	A	C8-N9-C4	-5.88	103.45	105.80
3	A	2422	C	N1-C2-O2	5.88	122.42	118.90
3	A	479	A	O4'-C1'-N9	5.85	112.88	108.20
3	A	1064	C	C6-N1-C2	-5.84	117.96	120.30
3	A	2122	U	C5-C6-N1	5.84	125.62	122.70
3	A	1172	C	C5-C6-N1	5.82	123.91	121.00
3	A	645	C	C6-N1-C2	-5.78	117.99	120.30
3	A	906	U	C5-C4-O4	5.78	129.37	125.90
3	A	748	G	O4'-C1'-N9	5.78	112.82	108.20
1	1	42	A	C8-N9-C1'	-5.72	117.41	127.70
3	A	2233	U	N3-C2-O2	-5.71	118.20	122.20
3	A	214	G	N3-C4-C5	-5.71	125.75	128.60
3	A	774	G	C4-C5-N7	5.70	113.08	110.80
3	A	1853	A	C8-N9-C4	5.70	108.08	105.80
3	A	1471	G	C8-N9-C4	5.69	108.68	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	58	G	N3-C4-C5	-5.66	125.77	128.60
3	A	137	U	C5-C4-O4	-5.66	122.50	125.90
3	A	2447	G	C8-N9-C4	5.62	108.65	106.40
1	1	42	A	N7-C8-N9	5.61	116.60	113.80
3	A	2103	C	C6-N1-C2	-5.60	118.06	120.30
3	A	748	G	N3-C4-C5	-5.60	125.80	128.60
3	A	776	G	C4-N9-C1'	5.60	133.78	126.50
3	A	2431	U	N3-C2-O2	-5.58	118.29	122.20
3	A	1341	G	C4-C5-N7	5.58	113.03	110.80
3	A	1341	G	N9-C4-C5	-5.56	103.18	105.40
3	A	1776	G	N3-C4-C5	-5.55	125.83	128.60
3	A	1756	G	C4-N9-C1'	-5.53	119.32	126.50
3	A	2556	C	C6-N1-C2	-5.52	118.09	120.30
3	A	280	U	P-O3'-C3'	5.51	126.32	119.70
3	A	2422	C	N3-C2-O2	-5.50	118.05	121.90
3	A	1358	G	C4-C5-N7	5.43	112.97	110.80
3	A	418	C	C6-N1-C2	-5.41	118.14	120.30
3	A	783	A	C8-N9-C4	-5.40	103.64	105.80
3	A	776	G	C8-N9-C4	-5.39	104.24	106.40
3	A	2681	C	C6-N1-C2	5.39	122.46	120.30
3	A	937	C	C6-N1-C2	-5.39	118.14	120.30
3	A	1102	C	C6-N1-C2	-5.38	118.15	120.30
3	A	202	U	N1-C2-O2	5.37	126.56	122.80
3	A	2155	U	C5-C6-N1	5.37	125.39	122.70
3	A	2500	U	C5-C6-N1	-5.37	120.02	122.70
3	A	2174	C	C6-N1-C2	-5.37	118.15	120.30
3	A	1617	C	C6-N1-C2	5.36	122.44	120.30
3	A	1187	G	C4-N9-C1'	5.35	133.46	126.50
3	A	776	G	O4'-C1'-N9	5.35	112.48	108.20
3	A	2850	A	C8-N9-C4	-5.34	103.66	105.80
3	A	1631	G	N1-C6-O6	5.33	123.10	119.90
3	A	776	G	N3-C4-C5	-5.28	125.96	128.60
3	A	2117	A	C8-N9-C4	-5.28	103.69	105.80
3	A	783	A	C2-N3-C4	5.27	113.24	110.60
3	A	1871	A	C8-N9-C4	-5.27	103.69	105.80
3	A	741	U	C5-C6-N1	-5.26	120.07	122.70
3	A	1936	A	N1-C6-N6	5.24	121.74	118.60
3	A	141	G	C8-N9-C4	-5.21	104.32	106.40
3	A	1251	C	C6-N1-C2	5.21	122.38	120.30
3	A	2168	G	C8-N9-C4	-5.20	104.32	106.40
3	A	1917	U	C6-N1-C1'	-5.19	113.93	121.20
3	A	1533	C	C2-N3-C4	5.18	122.49	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	61	G	C8-N9-C4	-5.18	104.33	106.40
3	A	190	A	C8-N9-C4	-5.17	103.73	105.80
3	A	238	C	C6-N1-C2	-5.17	118.23	120.30
3	A	1584	U	C6-N1-C1'	-5.15	113.99	121.20
3	A	1066	U	C5-C6-N1	5.14	125.27	122.70
3	A	1172	C	C6-N1-C2	-5.14	118.24	120.30
3	A	280	U	OP1-P-O3'	-5.14	93.90	105.20
3	A	2277	G	C8-N9-C4	-5.12	104.35	106.40
3	A	964	C	C6-N1-C2	5.12	122.35	120.30
3	A	897	C	N1-C2-O2	5.12	121.97	118.90
3	A	2078	C	C6-N1-C2	-5.12	118.25	120.30
3	A	2465	C	C2-N3-C4	-5.11	117.34	119.90
3	A	595	C	C6-N1-C2	5.11	122.34	120.30
3	A	1144	A	N1-C2-N3	5.10	131.85	129.30
3	A	1938	A	O4'-C1'-N9	5.10	112.28	108.20
3	A	2806	C	C6-N1-C2	-5.10	118.26	120.30
1	1	42	A	C6-C5-N7	-5.10	128.73	132.30
3	A	1779	U	C5-C6-N1	5.09	125.25	122.70
3	A	2150	C	C6-N1-C2	-5.07	118.27	120.30
3	A	1874	C	C6-N1-C2	-5.07	118.27	120.30
3	A	1133	A	O4'-C1'-N9	5.06	112.25	108.20
12	J	116	ASP	N-CA-C	5.06	124.65	111.00
3	A	2233	U	N1-C2-O2	5.05	126.33	122.80
1	1	68	A	C8-N9-C4	-5.04	103.78	105.80
3	A	1682	G	C8-N9-C4	-5.04	104.39	106.40
3	A	1849	G	N7-C8-N9	5.02	115.61	113.10
3	A	328	U	C6-N1-C2	5.01	124.01	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
35	i	367	UNK	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	1	926	0	467	10	0
2	2	62	0	34	0	0
3	A	61902	0	31133	666	0
4	B	2569	0	1301	22	0
5	C	2083	0	2154	49	0
6	D	1565	0	1616	37	0
7	E	1552	0	1619	31	0
8	F	1411	0	1444	41	0
9	G	1323	0	1371	25	0
10	H	1110	0	1148	30	0
11	I	946	0	978	31	0
12	J	979	0	1028	56	0
13	K	1129	0	1162	26	0
14	L	946	0	1023	18	0
15	M	1053	0	1129	22	0
16	N	1074	0	1157	12	0
17	O	993	0	1034	21	0
18	P	900	0	935	24	0
19	Q	917	0	962	17	0
20	R	947	0	1019	13	0
21	S	816	0	839	11	0
22	T	857	0	922	10	0
23	U	757	0	817	9	0
24	V	780	0	831	12	0
25	W	753	0	780	8	0
26	X	580	0	594	13	0
27	Y	625	0	652	16	0
28	Z	501	0	531	14	0
29	a	449	0	488	0	0
30	b	444	0	458	0	0
31	c	414	0	442	0	0
32	d	377	0	418	0	0
33	e	504	0	572	0	0
34	f	302	0	340	0	0
35	i	916	0	943	0	0
36	k	137	0	168	0	0
37	2	1	0	0	0	0
37	A	411	0	0	0	0
37	B	12	0	0	0	0
37	C	2	0	0	0	0
37	D	1	0	0	0	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	Y	1	0	0	0	0
37	b	1	0	0	0	0
38	f	1	0	0	0	0
All	All	94031	0	62509	1121	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 8.

All (1121) 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)
12:J:86:ILE:HD13	12:J:138:LEU:HD21	1.51	0.93
3:A:276:U:O2	3:A:278:A:N6	2.03	0.91
3:A:2584:U:H3'	3:A:2585:U:H5''	1.52	0.89
3:A:2304:G:H22	3:A:2312:U:H3	1.18	0.88
3:A:2128:G:H1	3:A:2160:C:H42	1.19	0.88
3:A:2305:U:H5''	8:F:131:GLY:HA3	1.58	0.86
4:B:43:C:O2	8:F:92:ARG:NH2	2.09	0.84
3:A:1069:A:H4'	3:A:1070:A:H5''	1.58	0.83
3:A:2107:G:H1	3:A:2182:U:H3	1.25	0.81
3:A:362:A:H3'	3:A:363:G:H8	1.44	0.81
3:A:1753:G:OP1	19:Q:93:ARG:NH1	2.12	0.81
3:A:545:U:N3	3:A:548:G:O6	2.13	0.81
8:F:158:THR:HG22	8:F:160:ALA:H	1.46	0.79
3:A:617:G:OP1	7:E:102:ARG:NH2	2.15	0.79
3:A:284:U:H3	3:A:356:G:H1	1.27	0.78
3:A:1848:A:H3'	3:A:1849:G:H8	1.49	0.78
3:A:1869:G:N2	3:A:1871:A:O2'	2.17	0.77
15:M:78:ARG:HG2	15:M:113:ALA:HB3	1.66	0.77
3:A:2122:U:OP1	3:A:2168:G:N2	2.17	0.77
3:A:2310:C:H2'	8:F:77:PHE:HE2	1.49	0.77
16:N:13:HIS:O	16:N:71:LYS:NZ	2.18	0.77
17:O:96:ARG:HH12	17:O:116:VAL:HG13	1.50	0.76
3:A:585:G:N7	20:R:6:ARG:NH1	2.34	0.75
3:A:1342:A:O2'	3:A:1344:U:OP2	2.05	0.74
3:A:1818:U:OP2	5:C:156:ARG:NH1	2.20	0.74
8:F:67:ILE:HD12	8:F:84:PRO:HB3	1.69	0.74
3:A:2102:G:N2	3:A:2187:U:O2	2.21	0.74
3:A:1653:G:H3'	17:O:2:ARG:HG3	1.70	0.73
7:E:97:ASN:OD1	7:E:97:ASN:N	2.22	0.72
3:A:2128:G:H1	3:A:2160:C:N4	1.87	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:882:G:H1	3:A:894:U:H3	1.36	0.72
3:A:1466:U:HO2'	3:A:1546:G:HO2'	1.37	0.72
13:K:131:ASN:N	13:K:131:ASN:OD1	2.23	0.72
5:C:107:PRO:HD2	5:C:110:LEU:HD22	1.70	0.71
10:H:110:VAL:HG11	10:H:132:PHE:CD2	2.25	0.71
28:Z:2:LYS:HD2	28:Z:6:LEU:HD11	1.73	0.71
13:K:31:GLU:OE1	13:K:34:ARG:NH1	2.23	0.71
3:A:1664:A:H61	3:A:1996:C:H42	1.39	0.71
3:A:2830:C:H5''	6:D:56:LYS:HE3	1.72	0.71
11:I:50:VAL:HG22	11:I:85:VAL:HG13	1.73	0.70
3:A:545:U:O2	3:A:548:G:N1	2.19	0.70
18:P:5:SER:HA	18:P:8:ILE:HD12	1.74	0.69
3:A:2788:C:O2'	3:A:2809:A:N3	2.24	0.69
3:A:2134:A:H1'	3:A:2159:G:H21	1.58	0.69
17:O:96:ARG:HH22	17:O:116:VAL:HA	1.58	0.69
3:A:742:A:H2'	3:A:743:A:C8	2.27	0.69
11:I:27:VAL:HG22	11:I:82:ILE:HG22	1.74	0.69
3:A:807:U:OP2	15:M:41:ARG:NH1	2.26	0.68
3:A:2130:U:O2'	3:A:2133:G:O2'	2.11	0.68
3:A:281:C:H2'	3:A:282:A:H8	1.59	0.68
21:S:17:GLY:HA2	21:S:97:LYS:HE3	1.74	0.68
3:A:1490:A:H8	3:A:1491:G:N7	1.92	0.68
3:A:2584:U:H3'	3:A:2585:U:C5'	2.23	0.68
3:A:1534:U:O2'	3:A:1537:G:O6	2.10	0.67
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.76	0.67
18:P:41:ALA:HB2	18:P:48:LEU:HD21	1.75	0.67
3:A:1105:U:H2'	3:A:1106:G:C8	2.29	0.67
17:O:14:SER:HA	17:O:17:ARG:HH11	1.59	0.67
3:A:1060:U:OP2	12:J:113:LYS:NZ	2.27	0.67
3:A:2119:A:N6	3:A:2167:U:O2	2.27	0.67
6:D:12:THR:OG1	6:D:13:ARG:N	2.28	0.67
3:A:2086:U:H2'	3:A:2087:G:C8	2.30	0.67
28:Z:28:LEU:HD13	28:Z:43:LEU:HD23	1.77	0.67
3:A:276:U:O2'	3:A:278:A:N7	2.22	0.67
3:A:45:G:H5''	3:A:46:G:H5'	1.76	0.66
1:I:60:A:H2'	1:I:61:G:O4'	1.96	0.66
3:A:355:U:H2'	3:A:356:G:C8	2.30	0.66
25:W:20:LEU:HD23	25:W:25:LYS:HB2	1.77	0.66
3:A:833:A:H2'	3:A:834:G:C8	2.31	0.66
13:K:140:LEU:HD11	13:K:142:ILE:HD13	1.78	0.66
3:A:2848:G:O2'	3:A:2867:G:N2	2.20	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:42:LYS:HG2	10:H:46:PHE:HE2	1.61	0.65
3:A:636:G:N1	15:M:76:GLU:OE2	2.28	0.65
9:G:22:GLN:HE21	9:G:39:ASP:HA	1.59	0.65
3:A:1464:G:H2'	3:A:1465:G:H8	1.61	0.65
7:E:1:MET:HG3	7:E:14:VAL:HG23	1.78	0.65
11:I:57:ASN:ND2	11:I:76:PHE:O	2.30	0.65
27:Y:72:ARG:HG3	27:Y:78:TYR:HE2	1.61	0.65
28:Z:28:LEU:HD11	28:Z:42:LEU:HB3	1.77	0.65
7:E:21:ARG:HD3	7:E:106:LYS:HB3	1.77	0.65
8:F:44:ILE:HG21	8:F:79:ILE:HG22	1.79	0.65
10:H:82:SER:HB2	10:H:94:ILE:HD11	1.79	0.65
16:N:11:LYS:HD3	16:N:86:LYS:HG2	1.78	0.65
3:A:833:A:H2'	3:A:834:G:H8	1.62	0.65
3:A:1528:A:OP2	3:A:1543:G:N2	2.27	0.65
3:A:2162:G:H5''	3:A:2171:A:H2'	1.78	0.65
3:A:668:A:H2'	3:A:670:A:H62	1.63	0.64
3:A:1266:G:O2'	3:A:2012:G:O6	2.15	0.64
16:N:66:ARG:NH1	16:N:104:GLU:OE1	2.30	0.64
8:F:36:LEU:HD22	8:F:154:ILE:HD13	1.79	0.64
3:A:396:G:OP2	27:Y:10:LYS:NZ	2.31	0.64
3:A:1827:U:OP2	5:C:221:ARG:NH1	2.31	0.64
5:C:258:ARG:NH2	5:C:263:THR:OG1	2.27	0.64
5:C:270:ARG:HH21	5:C:271:ARG:HH12	1.45	0.63
22:T:73:LYS:HB2	22:T:106:VAL:HB	1.81	0.63
22:T:109:ASP:OD1	22:T:110:ARG:N	2.32	0.63
25:W:51:GLN:OE1	25:W:57:TYR:OH	2.17	0.63
3:A:1796:U:H2'	3:A:1797:G:H8	1.63	0.63
3:A:2039:U:H2'	3:A:2040:G:C8	2.34	0.63
3:A:2822:G:O6	17:O:2:ARG:NH1	2.31	0.63
8:F:40:VAL:HG11	8:F:43:ALA:HB2	1.80	0.63
3:A:370:G:O2'	3:A:424:G:OP1	2.14	0.62
3:A:942:G:H2'	3:A:943:A:H8	1.64	0.62
11:I:26:VAL:HG13	11:I:111:ALA:HB2	1.81	0.62
23:U:56:GLU:HG2	23:U:57:VAL:HG12	1.79	0.62
3:A:1495:A:H2'	3:A:1496:A:C8	2.34	0.62
3:A:720:U:H2'	3:A:721:A:C8	2.35	0.62
8:F:74:VAL:HG22	8:F:79:ILE:HD11	1.81	0.62
5:C:3:VAL:HG11	5:C:202:LEU:HD23	1.81	0.62
3:A:2430:A:N3	3:A:2430:A:H2'	2.14	0.62
4:B:116:G:H2'	4:B:117:G:H8	1.65	0.62
3:A:362:A:H3'	3:A:363:G:C8	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1973:G:H2'	3:A:1974:C:C6	2.35	0.62
3:A:196:A:OP2	15:M:47:ARG:NH1	2.31	0.62
3:A:1614:A:N1	22:T:93:ALA:HB2	2.14	0.62
3:A:790:U:H5'	3:A:791:C:OP2	1.99	0.62
3:A:2861:U:H2'	3:A:2862:G:H8	1.65	0.61
3:A:2476:A:H2	3:A:2481:G:H1	1.47	0.61
4:B:1:U:H2'	4:B:2:G:H8	1.66	0.61
28:Z:38:GLN:HG3	28:Z:39:GLN:HG3	1.82	0.61
3:A:1028:A:N3	3:A:2486:C:O2'	2.26	0.61
3:A:1796:U:H2'	3:A:1797:G:C8	2.35	0.61
10:H:116:ARG:HH21	10:H:133:GLN:HB3	1.64	0.61
3:A:1199:U:H1'	20:R:4:VAL:HG22	1.82	0.61
27:Y:71:LEU:HD23	27:Y:78:TYR:HB3	1.82	0.61
5:C:2:ALA:N	5:C:20:VAL:O	2.33	0.61
3:A:1462:C:HO2'	3:A:2702:G:HO2'	1.45	0.61
24:V:49:VAL:HG12	24:V:52:LEU:H	1.66	0.61
3:A:1873:G:H2'	3:A:1874:C:H6	1.66	0.61
3:A:675:A:OP1	7:E:58:LYS:NZ	2.33	0.61
12:J:53:LEU:HD11	12:J:82:LYS:HD2	1.82	0.61
12:J:75:PRO:HD2	12:J:78:VAL:HB	1.82	0.60
3:A:645:C:O2'	3:A:646:U:OP1	2.18	0.60
3:A:1224:U:OP2	21:S:68:ARG:NH1	2.33	0.60
3:A:1482:G:H1'	3:A:1509:A:H61	1.66	0.60
3:A:2636:C:O2'	6:D:45:TYR:OH	2.18	0.60
3:A:284:U:O2	3:A:356:G:N2	2.29	0.60
3:A:910:A:H2'	3:A:911:A:C8	2.37	0.60
4:B:116:G:H2'	4:B:117:G:C8	2.37	0.60
3:A:2209:G:H1	3:A:2215:C:H42	1.50	0.60
3:A:357:C:H2'	3:A:358:U:C6	2.35	0.60
3:A:576:U:H2'	3:A:577:G:C8	2.37	0.60
3:A:2680:U:H5'	6:D:194:PRO:HA	1.83	0.60
3:A:1105:U:H2'	3:A:1106:G:H8	1.64	0.60
3:A:1606:C:H5'	3:A:1607:C:OP1	2.02	0.59
3:A:2087:G:H2'	3:A:2088:A:H8	1.67	0.59
3:A:2135:A:N6	3:A:2156:G:O2'	2.34	0.59
3:A:2303:G:O2'	8:F:121:SER:O	2.20	0.59
3:A:2753:A:O2'	8:F:15:LYS:NZ	106.13	0.59
3:A:2704:C:H2'	3:A:2705:A:O4'	2.02	0.59
3:A:2799:A:O2'	3:A:2800:A:H5''	2.01	0.59
12:J:38:PHE:HE1	12:J:57:VAL:HG21	1.68	0.59
3:A:2543:G:H2'	3:A:2544:G:H8	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:286:U:H2'	3:A:287:G:C8	2.37	0.59
3:A:776:G:O2'	3:A:777:G:OP1	2.21	0.59
15:M:95:LEU:HD22	15:M:100:ILE:HD12	1.84	0.59
24:V:74:ASN:HD21	24:V:99:ASN:HD21	1.51	0.59
3:A:1848:A:H3'	3:A:1849:G:C8	2.36	0.59
3:A:2163:A:OP1	3:A:2170:A:O2'	2.21	0.58
3:A:2543:G:H2'	3:A:2544:G:C8	2.38	0.58
15:M:79:LEU:HD11	15:M:112:LEU:HD12	1.83	0.58
6:D:148:GLN:N	6:D:148:GLN:OE1	2.36	0.58
28:Z:39:GLN:HB3	28:Z:41:HIS:CE1	2.37	0.58
10:H:99:ILE:HD13	10:H:130:VAL:HG21	1.83	0.58
11:I:60:LEU:O	11:I:64:VAL:HB	2.03	0.58
3:A:191:A:H2'	3:A:192:C:C6	2.38	0.58
3:A:1973:G:H2'	3:A:1974:C:H6	1.67	0.58
11:I:39:THR:HG22	11:I:43:LYS:HE3	1.85	0.58
3:A:1930:G:N2	3:A:1968:G:H2'	2.18	0.58
3:A:614:A:O2'	3:A:616:A:N7	2.36	0.58
10:H:27:ARG:NH2	27:Y:60:ASP:OD2	2.37	0.58
11:I:93:ALA:O	11:I:97:LYS:NZ	2.36	0.58
12:J:38:PHE:CD1	12:J:59:ILE:HD11	2.38	0.58
8:F:160:ALA:HB1	8:F:165:GLU:HB2	1.85	0.58
13:K:12:LYS:O	13:K:41:LYS:NZ	2.36	0.58
3:A:489:G:N2	3:A:1321:A:OP1	2.27	0.58
3:A:1721:G:HO2'	3:A:1722:A:H8	1.50	0.58
3:A:197:A:N6	3:A:2430:A:O2'	2.37	0.58
3:A:2461:A:H1'	3:A:2492:U:C2	2.39	0.58
5:C:144:VAL:HB	5:C:154:LEU:HB2	1.86	0.58
15:M:2:ARG:HB2	15:M:5:THR:HG23	1.86	0.57
3:A:381:G:OP1	27:Y:18:ARG:NH2	2.37	0.57
3:A:2683:C:H4'	6:D:13:ARG:HH12	1.69	0.57
13:K:117:ALA:HA	13:K:120:ARG:NH2	2.19	0.57
3:A:2074:U:H2'	3:A:2075:U:C6	2.39	0.57
3:A:319:G:H2'	3:A:320:A:O4'	2.03	0.57
3:A:1509:A:HO2'	3:A:1510:G:H8	1.53	0.57
3:A:277:G:H4'	3:A:278:A:N7	2.19	0.57
3:A:1062:G:N2	12:J:93:PRO:HG2	2.19	0.57
3:A:2310:C:H2'	8:F:77:PHE:CE2	2.37	0.57
6:D:186:LEU:HD13	19:Q:8:LEU:HD11	1.86	0.57
8:F:144:ASP:OD1	8:F:144:ASP:N	2.38	0.57
19:Q:91:ALA:HB2	19:Q:113:ARG:HA	1.87	0.57
6:D:196:ALA:O	6:D:199:SER:OG	2.13	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1:MET:N	6:D:1:MET:SD	5.28	0.57
6:D:33:ARG:NH2	6:D:74:GLU:O	2.38	0.57
3:A:2273:A:H2'	3:A:2274:A:C8	2.40	0.57
18:P:51:ALA:HB3	18:P:78:VAL:HG13	1.87	0.57
3:A:310:A:H5''	24:V:15:THR:HG23	1.86	0.56
6:D:4:LEU:HD13	6:D:29:VAL:HG11	1.87	0.56
8:F:138:PHE:HB3	8:F:140:GLU:OE1	2.04	0.56
22:T:6:LYS:HG2	22:T:104:THR:HG23	1.87	0.56
3:A:563:A:OP2	21:S:79:ARG:NH2	2.39	0.56
21:S:28:ALA:HB3	21:S:31:GLU:HG3	1.87	0.56
3:A:2087:G:H2'	3:A:2088:A:C8	2.40	0.56
3:A:2861:U:H2'	3:A:2862:G:C8	2.41	0.56
3:A:742:A:H2'	3:A:743:A:H8	1.68	0.56
27:Y:32:ASN:O	27:Y:52:SER:HA	2.05	0.56
3:A:2127:G:O2'	3:A:2128:G:O4'	2.24	0.56
4:B:29:A:H2'	4:B:30:C:C6	2.40	0.56
3:A:1386:C:H2'	3:A:1387:A:C8	2.41	0.56
10:H:68:ARG:HA	10:H:71:LYS:HD2	1.86	0.56
3:A:2602:A:H4'	3:A:2603:G:O5'	2.06	0.56
3:A:2845:U:H5''	19:Q:52:ASN:O	2.05	0.56
3:A:300:A:N3	3:A:319:G:H1'	2.21	0.56
4:B:1:U:H2'	4:B:2:G:C8	2.40	0.56
4:B:8:C:O3'	18:P:25:ARG:NH1	2.39	0.56
5:C:41:GLY:O	5:C:43:ARG:NH1	2.38	0.56
3:A:612:G:HO2'	3:A:614:A:H2	1.54	0.56
3:A:1709:U:H2'	3:A:1710:G:H8	1.71	0.55
3:A:612:G:N2	3:A:614:A:O2'	2.39	0.55
3:A:1799:G:C5	5:C:176:LEU:HD13	2.41	0.55
3:A:2423:U:H2'	3:A:2424:C:C1'	2.36	0.55
6:D:97:SER:OG	6:D:98:VAL:N	2.37	0.55
3:A:1909:C:H2'	3:A:1910:G:C8	2.41	0.55
3:A:30:G:OP2	20:R:5:LYS:NZ	2.26	0.55
8:F:5:HIS:HB2	8:F:97:TRP:CD1	2.42	0.55
3:A:1987:A:H2'	3:A:1988:G:H8	1.71	0.55
3:A:2491:U:C5'	3:A:2570:G:H5''	2.36	0.55
3:A:602:A:HO2'	3:A:604:G:HO2'	1.55	0.55
4:B:7:G:H5''	18:P:29:HIS:CE1	2.42	0.55
14:L:77:ILE:HG12	19:Q:72:ARG:HG3	1.87	0.55
3:A:2298:A:H2'	3:A:2299:U:O4'	2.06	0.55
3:A:958:U:OP2	16:N:14:LYS:NZ	2.40	0.55
13:K:88:THR:N	13:K:91:GLU:OE2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:483:A:O4'	24:V:45:HIS:HB3	2.07	0.55
17:O:15:SER:OG	17:O:16:HIS:N	2.40	0.55
3:A:2158:A:H4'	3:A:2159:G:O5'	2.06	0.54
3:A:600:G:OP1	7:E:24:ASN:ND2	2.40	0.54
11:I:8:LYS:HD3	11:I:56:ARG:HH12	1.71	0.54
12:J:50:GLU:HG3	12:J:82:LYS:NZ	2.21	0.54
3:A:1063:G:N2	12:J:91:GLY:O	2.40	0.54
3:A:645:C:H3'	3:A:647:G:N7	2.22	0.54
12:J:73:THR:OG1	12:J:113:LYS:HE3	2.07	0.54
3:A:1203:U:H5'	15:M:3:LEU:HD12	1.89	0.54
11:I:3:LEU:HB2	11:I:56:ARG:HH22	1.73	0.54
3:A:2341:G:H2'	3:A:2342:C:O4'	2.07	0.54
3:A:477:A:H2'	3:A:478:A:C8	2.43	0.54
11:I:8:LYS:HD3	11:I:56:ARG:NH1	2.23	0.54
3:A:1607:C:O2'	3:A:1608:A:OP1	2.24	0.54
3:A:983:A:H62	3:A:984:A:N6	2.06	0.54
12:J:59:ILE:HD13	12:J:69:PHE:HB3	1.90	0.54
3:A:2683:C:O2	14:L:70:ARG:NH2	2.37	0.54
3:A:1709:U:H2'	3:A:1710:G:C8	2.43	0.54
3:A:1751:U:H2'	3:A:1752:C:C6	2.42	0.54
3:A:1789:A:OP1	5:C:221:ARG:HG3	2.08	0.54
3:A:2151:U:H2'	3:A:2152:G:C8	2.43	0.54
3:A:860:U:H1'	3:A:2268:A:H5'	1.88	0.54
6:D:108:ASP:OD1	6:D:174:SER:N	2.36	0.54
18:P:53:THR:O	18:P:59:ALA:HB2	2.08	0.54
3:A:596:U:H2'	3:A:597:G:H8	1.72	0.53
3:A:644:A:H2'	3:A:645:C:O4'	2.08	0.53
3:A:812:C:H4'	20:R:13:ARG:HH11	1.73	0.53
3:A:1026:G:H2'	3:A:1027:A:H8	1.73	0.53
3:A:322:A:OP2	7:E:163:ASN:HB2	2.09	0.53
12:J:83:ALA:O	12:J:105:GLN:NE2	2.41	0.53
3:A:2107:G:N2	3:A:2182:U:O2	2.40	0.53
9:G:153:ARG:HG2	9:G:154:PRO:HD2	1.89	0.53
3:A:2570:G:H2'	3:A:2571:U:O4'	2.08	0.53
3:A:843:G:H1	3:A:935:C:H42	1.56	0.53
12:J:79:LEU:HB3	12:J:109:ILE:HG12	1.89	0.53
3:A:1528:A:N6	3:A:1529:G:N3	2.57	0.53
3:A:2520:C:C6	3:A:2567:G:H1'	2.42	0.53
14:L:63:VAL:HG23	14:L:64:ARG:HG3	1.91	0.53
3:A:2744:G:H2'	3:A:2745:C:H6	1.74	0.53
6:D:109:VAL:HG22	6:D:203:VAL:HG13	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2423:U:H2'	3:A:2424:C:O4'	2.08	0.53
3:A:2751:G:P	9:G:3:ARG:HH11	2.31	0.53
10:H:7:ASP:OD1	10:H:8:LYS:N	2.41	0.53
3:A:493:G:H2'	3:A:494:G:O4'	2.09	0.53
5:C:21:ASN:HB3	5:C:24:LEU:HD22	1.90	0.53
3:A:2821:A:H4'	6:D:167:ASN:ND2	2.23	0.53
6:D:207:VAL:HG13	6:D:208:LYS:HG3	1.91	0.53
8:F:25:VAL:O	8:F:28:VAL:HG12	2.09	0.53
3:A:1077:A:H1'	12:J:93:PRO:HB2	1.90	0.53
3:A:2290:G:H2'	3:A:2291:U:O4'	2.09	0.53
3:A:2538:C:H2'	3:A:2539:C:C6	2.44	0.53
3:A:674:G:H5''	7:E:71:GLY:N	2.24	0.53
3:A:697:G:H2'	3:A:698:C:C6	2.44	0.53
6:D:125:TRP:CD1	6:D:160:LYS:HB3	2.44	0.53
3:A:1133:A:H4'	3:A:1134:A:H5''	1.91	0.52
3:A:1141:U:H4'	3:A:1142:A:O4'	2.09	0.52
6:D:71:ALA:HB3	6:D:73:VAL:HG22	1.91	0.52
10:H:104:THR:HA	10:H:108:VAL:O	2.09	0.52
17:O:38:LEU:HD13	17:O:111:ALA:HB2	1.90	0.52
5:C:53:HIS:CE1	5:C:219:THR:HG23	2.44	0.52
9:G:86:LYS:HG2	9:G:132:VAL:HG22	1.91	0.52
11:I:41:LEU:HD22	11:I:99:PHE:CD2	2.44	0.52
17:O:37:THR:HG23	17:O:40:LYS:HD2	1.89	0.52
3:A:464:U:H2'	3:A:465:G:O4'	2.08	0.52
3:A:207:A:H2'	3:A:208:C:O4'	2.10	0.52
4:B:106:G:H2'	4:B:107:G:O4'	2.09	0.52
18:P:7:ARG:HD2	18:P:97:PHE:CZ	2.44	0.52
21:S:68:ARG:NH2	21:S:90:ARG:HD3	2.24	0.52
3:A:878:A:H5'	3:A:879:G:OP2	2.09	0.52
21:S:57:GLY:HA2	21:S:102:SER:O	2.09	0.52
3:A:367:G:H3'	3:A:368:A:H8	1.75	0.52
3:A:55:G:H2'	3:A:56:A:H8	1.73	0.52
12:J:21:SER:O	12:J:26:PRO:HD2	2.09	0.52
3:A:839:U:H2'	3:A:840:C:C6	2.45	0.52
8:F:29:PRO:HB2	8:F:169:LEU:HD22	1.92	0.52
26:X:70:GLU:HG3	26:X:72:LYS:HG3	1.92	0.52
3:A:1223:G:C6	3:A:1227:G:C6	2.98	0.52
3:A:1880:U:H2'	3:A:1881:C:C6	2.45	0.52
3:A:2291:U:H2'	3:A:2292:U:C6	2.45	0.52
3:A:2051:A:N6	3:A:2614:A:O2'	2.40	0.52
3:A:2795:C:H2'	3:A:2796:U:H6	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:98:GLU:OE1	13:K:98:GLU:N	2.31	0.52
3:A:2548:U:O2	14:L:23:LYS:NZ	2.43	0.52
3:A:2697:G:H2'	3:A:2698:U:O4'	2.10	0.52
13:K:125:TYR:OH	13:K:132:HIS:NE2	2.42	0.52
3:A:136:G:H2'	3:A:137:U:O4'	2.09	0.51
3:A:1866:A:N6	3:A:1875:G:O2'	2.43	0.51
3:A:213:A:O2'	3:A:214:G:H5'	2.09	0.51
3:A:2491:U:H5''	3:A:2570:G:H5''	1.93	0.51
10:H:62:LEU:HD22	10:H:137:GLU:OE1	2.11	0.51
3:A:2070:A:C2	3:A:2071:A:C4	2.97	0.51
3:A:2216:G:H2'	3:A:2217:G:C8	2.46	0.51
12:J:127:ARG:HA	12:J:130:GLU:HB2	1.92	0.51
3:A:1386:C:H2'	3:A:1387:A:H8	1.76	0.51
3:A:2126:A:H61	3:A:2163:A:H5'	1.75	0.51
3:A:479:A:N3	3:A:481:G:H5''	2.25	0.51
27:Y:3:ARG:O	27:Y:12:PRO:HD3	2.10	0.51
3:A:141:G:H3'	3:A:141:G:H8	1.75	0.51
3:A:1783:A:N1	3:A:2587:A:H2'	2.25	0.51
3:A:708:G:N2	3:A:724:U:H1'	2.25	0.51
3:A:2271:G:H2'	3:A:2272:U:C6	2.45	0.51
3:A:613:A:O2'	3:A:614:A:O5'	2.26	0.51
3:A:2810:A:H5''	6:D:62:LYS:NZ	2.26	0.51
6:D:26:VAL:HG22	6:D:188:LEU:HD22	1.93	0.51
6:D:56:LYS:HB2	6:D:59:ARG:HB2	1.92	0.51
12:J:89:GLY:HA2	12:J:98:VAL:HG21	1.93	0.51
12:J:94:ASN:H	12:J:137:GLY:HA2	1.75	0.51
4:B:9:G:P	18:P:25:ARG:HH12	2.34	0.51
16:N:35:ALA:HB2	16:N:102:LEU:HD21	1.92	0.51
3:A:155:A:H2'	3:A:156:A:C8	2.45	0.51
3:A:2245:U:H5''	3:A:2246:G:H5'	1.92	0.51
7:E:138:LEU:HD22	7:E:143:LEU:HB2	1.93	0.51
3:A:2060:A:H3'	7:E:63:LYS:HZ1	1.75	0.51
17:O:24:MET:HE1	17:O:40:LYS:HD3	1.93	0.51
3:A:1508:A:O2'	3:A:1509:A:O4'	2.19	0.51
3:A:2625:G:H2'	3:A:2626:C:O4'	2.11	0.51
3:A:2684:U:H4'	14:L:76:VAL:HG21	1.91	0.51
3:A:586:A:H5'	7:E:84:THR:HG21	1.93	0.51
5:C:117:GLN:HG2	5:C:118:SER:N	2.26	0.51
5:C:161:TYR:HB3	5:C:194:GLU:HB3	1.92	0.51
5:C:245:VAL:HG12	5:C:251:GLN:HA	1.92	0.51
3:A:1416:G:N2	3:A:1582:C:O2	2.35	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:27:VAL:HG13	11:I:80:THR:HG23	1.93	0.51
11:I:38:MET:O	11:I:42:ARG:HG2	2.09	0.51
25:W:2:PHE:HB2	25:W:61:LEU:HD22	1.93	0.51
3:A:1251:C:OP2	20:R:6:ARG:NH2	2.43	0.50
3:A:335:C:H2'	3:A:336:C:H6	1.76	0.50
10:H:135:HIS:HB3	10:H:138:VAL:HB	1.92	0.50
3:A:1297:C:OP1	3:A:2710:C:H4'	2.10	0.50
22:T:41:LYS:HB2	22:T:44:ALA:HB2	1.93	0.50
3:A:2283:C:C2	3:A:2389:G:C2	2.99	0.50
3:A:2538:C:H2'	3:A:2539:C:H6	1.76	0.50
3:A:1536:C:H4'	3:A:1537:G:H5''	1.94	0.50
3:A:2327:A:H2'	3:A:2328:A:C8	2.47	0.50
12:J:53:LEU:HD21	12:J:82:LYS:HB3	1.92	0.50
6:D:152:PRO:HG3	6:D:156:PHE:CZ	2.45	0.50
12:J:25:GLY:HA2	12:J:35:ILE:HD11	1.92	0.50
3:A:2039:U:H2'	3:A:2040:G:H8	1.77	0.50
3:A:2318:G:C6	3:A:2319:G:N1	2.79	0.50
3:A:419:U:H2'	3:A:420:C:C6	2.46	0.50
3:A:647:G:H2'	3:A:648:G:C8	2.46	0.50
3:A:1636:U:H2'	3:A:1637:A:C8	2.46	0.50
3:A:2793:C:O2	3:A:2803:G:N2	2.19	0.50
3:A:6:A:H2'	3:A:7:G:C8	2.47	0.50
3:A:2037:A:H2'	3:A:2038:G:C8	2.47	0.50
4:B:48:U:H2'	4:B:49:C:H6	1.77	0.50
12:J:113:LYS:HG3	12:J:129:ILE:HD11	1.94	0.50
17:O:14:SER:HA	17:O:17:ARG:NH1	2.27	0.50
3:A:1413:A:H2'	3:A:1414:C:O4'	2.12	0.50
3:A:2122:U:OP2	3:A:2169:A:O2'	2.29	0.50
3:A:2758:A:O2'	9:G:38:ASN:ND2	2.45	0.50
9:G:94:TYR:HA	9:G:106:SER:O	2.11	0.50
12:J:28:LEU:HD12	12:J:59:ILE:HG21	1.93	0.50
13:K:31:GLU:HG3	13:K:142:ILE:HG13	1.93	0.50
19:Q:49:ALA:HB3	19:Q:60:THR:HB	1.94	0.50
3:A:1873:G:H2'	3:A:1874:C:C6	2.46	0.49
3:A:2051:A:C2	3:A:2614:A:C2	3.01	0.49
24:V:4:LYS:O	24:V:94:ARG:NH2	2.45	0.49
26:X:15:ASP:OD1	26:X:16:SER:N	2.42	0.49
3:A:1474:U:C4	3:A:1475:G:C6	3.01	0.49
3:A:2221:G:OP1	10:H:112:LYS:NZ	2.43	0.49
3:A:2230:G:H2'	3:A:2231:U:H6	1.78	0.49
3:A:2366:A:H4'	26:X:62:LYS:HE3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1278:C:H2'	3:A:1279:G:C8	2.47	0.49
3:A:2115:G:H2'	3:A:2117:A:C8	2.47	0.49
3:A:2230:G:H2'	3:A:2231:U:C6	2.48	0.49
3:A:543:G:H5'	3:A:544:C:OP2	2.12	0.49
12:J:22:PRO:HB2	12:J:23:PRO:HD3	1.94	0.49
3:A:1636:U:H2'	3:A:1637:A:H8	1.78	0.49
3:A:1880:U:H2'	3:A:1881:C:H6	1.78	0.49
3:A:2040:G:H2'	3:A:2041:U:O4'	2.13	0.49
3:A:2849:U:H4'	3:A:2868:A:C2	2.48	0.49
3:A:766:U:H2'	3:A:767:U:C6	2.48	0.49
8:F:118:SER:OG	8:F:120:LYS:HG3	2.13	0.49
3:A:1324:G:O2'	3:A:1326:U:OP2	2.25	0.49
3:A:1432:G:H2'	3:A:1433:A:C8	2.46	0.49
3:A:1469:A:H2'	3:A:1470:A:C8	2.47	0.49
3:A:963:U:H2'	3:A:964:C:C6	2.47	0.49
3:A:2591:C:OP1	5:C:238:ARG:NH1	2.45	0.49
15:M:57:LEU:O	15:M:61:LEU:HG	2.12	0.49
3:A:1682:G:C8	3:A:1757:A:C2	3.01	0.49
9:G:17:VAL:HG11	9:G:50:LEU:HD21	1.94	0.49
3:A:1545:A:H2'	3:A:1546:G:O4'	2.13	0.49
3:A:565:C:H4'	3:A:1253:A:N6	2.28	0.49
5:C:71:LYS:HG2	5:C:74:ILE:HD12	1.94	0.49
11:I:99:PHE:HD2	11:I:106:PHE:HZ	1.60	0.49
12:J:73:THR:HB	12:J:112:THR:HG22	1.95	0.49
3:A:1293:C:H2'	3:A:1294:U:O4'	2.13	0.49
3:A:690:G:O2'	5:C:43:ARG:NH2	2.46	0.49
5:C:84:ASP:OD1	5:C:86:ASN:ND2	2.43	0.49
25:W:15:GLY:O	25:W:19:ARG:HG3	2.13	0.49
1:1:59:A:H2'	1:1:60:A:C8	2.48	0.48
1:1:49:G:H1	1:1:60:A:H61	1.59	0.48
3:A:1069:A:C2	3:A:1096:A:H5''	2.48	0.48
3:A:122:G:H2'	3:A:123:G:O4'	2.13	0.48
3:A:1827:U:H2'	3:A:1828:G:O4'	2.13	0.48
8:F:136:ILE:HA	8:F:141:ILE:HG21	1.95	0.48
18:P:4:LYS:HG3	18:P:7:ARG:HH21	1.78	0.48
3:A:2356:U:H2'	3:A:2357:G:O4'	2.13	0.48
3:A:2649:C:H2'	3:A:2650:U:C6	2.48	0.48
3:A:2862:G:H2'	3:A:2863:C:C6	2.48	0.48
6:D:105:LYS:NZ	6:D:105:LYS:HB3	2.28	0.48
6:D:48:ILE:HG23	6:D:84:LEU:HD11	1.94	0.48
17:O:38:LEU:HD21	17:O:99:LYS:HG2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2300:C:H2'	3:A:2301:C:C6	2.47	0.48
3:A:573:U:O2'	3:A:574:A:H3'	2.14	0.48
10:H:15:LEU:HD23	10:H:15:LEU:H	1.78	0.48
11:I:60:LEU:HB3	11:I:76:PHE:CZ	2.48	0.48
17:O:12:ARG:HE	17:O:16:HIS:CE1	2.31	0.48
3:A:2720:U:OP1	19:Q:53:ARG:NH2	2.46	0.48
3:A:2316:G:H4'	8:F:125:ARG:NE	2.29	0.48
3:A:1081:U:H4'	12:J:124:ALA:HB1	1.96	0.48
3:A:743:A:O2'	3:A:1659:G:OP1	2.29	0.48
3:A:2282:G:C6	3:A:2425:A:C2	3.02	0.48
3:A:2780:G:OP2	13:K:120:ARG:NE	2.24	0.48
3:A:312:G:H5'	3:A:331:C:O2'	2.14	0.48
3:A:38:A:H2'	3:A:39:G:O4'	2.14	0.48
3:A:956:G:N2	3:A:960:A:OP2	2.45	0.48
3:A:1183:U:H2'	3:A:1184:U:C6	2.48	0.48
3:A:2117:A:N6	3:A:2171:A:H61	2.11	0.48
3:A:2514:U:H2'	3:A:2515:C:C6	2.48	0.48
8:F:103:LEU:HG	8:F:108:VAL:HG23	1.95	0.48
9:G:137:ASP:HB3	9:G:140:VAL:HB	1.96	0.48
3:A:1441:G:H2'	3:A:1442:U:C6	2.49	0.48
3:A:1490:A:C8	3:A:1491:G:N7	2.78	0.48
3:A:2133:G:H21	3:A:2158:A:H62	1.62	0.48
3:A:2784:U:H2'	3:A:2785:C:H6	1.79	0.48
3:A:873:C:H4'	16:N:64:TRP:CD1	2.48	0.48
3:A:967:U:H2'	3:A:968:C:C6	2.49	0.48
5:C:30:PHE:HD2	5:C:33:LEU:HG	1.78	0.48
14:L:10:VAL:HG23	14:L:17:ARG:O	2.13	0.48
3:A:1859:U:H2'	3:A:1860:G:C8	2.48	0.48
3:A:463:G:N2	3:A:466:A:OP2	2.45	0.48
5:C:117:GLN:HG2	5:C:118:SER:H	1.79	0.48
3:A:1063:G:H5'	12:J:77:ALA:HB1	1.94	0.48
3:A:1450:G:C6	3:A:1451:C:N4	2.82	0.48
3:A:2056:G:N3	3:A:2056:G:H2'	2.29	0.48
3:A:871:U:H2'	3:A:872:U:C6	2.49	0.48
6:D:121:THR:HG21	6:D:143:PRO:HG3	1.95	0.48
7:E:21:ARG:HD3	7:E:106:LYS:CB	2.43	0.48
3:A:2713:U:H3'	3:A:2714:G:H5''	1.95	0.48
3:A:589:U:H2'	3:A:590:A:C8	2.49	0.48
11:I:43:LYS:HE2	12:J:118:THR:HA	1.96	0.48
22:T:31:GLN:O	22:T:35:ILE:HG13	2.14	0.48
3:A:228:C:H4'	3:A:229:C:H5''	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2461:A:H1'	3:A:2492:U:N3	2.28	0.47
11:I:103:ASN:HB3	11:I:105:LYS:HD2	1.95	0.47
24:V:4:LYS:HD3	24:V:83:VAL:HB	1.95	0.47
24:V:96:PHE:O	24:V:100:SER:HA	2.14	0.47
3:A:1869:G:H2'	3:A:1871:A:N7	2.29	0.47
3:A:570:G:H2'	3:A:2030:A:C8	2.49	0.47
15:M:39:LYS:HE3	15:M:39:LYS:HB2	1.63	0.47
3:A:1571:A:H2'	3:A:1572:A:C8	2.49	0.47
3:A:2831:G:OP1	6:D:56:LYS:NZ	2.44	0.47
6:D:7:LYS:HB3	6:D:7:LYS:HE2	1.51	0.47
8:F:40:VAL:HG21	8:F:50:LEU:HD13	1.96	0.47
23:U:17:SER:OG	23:U:19:LYS:N	2.47	0.47
3:A:185:G:H4'	3:A:218:A:H4'	1.97	0.47
3:A:2491:U:H5'	3:A:2570:G:H5''	1.96	0.47
3:A:2786:U:H2'	3:A:2787:C:H6	1.78	0.47
3:A:2846:G:H2'	3:A:2847:U:O4'	2.15	0.47
3:A:2683:C:H4'	6:D:13:ARG:NH1	2.29	0.47
7:E:164:LEU:HD23	7:E:164:LEU:HA	1.74	0.47
1:I:40:C:H3'	1:I:41:C:H5''	1.97	0.47
3:A:141:G:H3'	3:A:141:G:C8	2.50	0.47
3:A:1452:G:H22	3:A:1457:U:H2'	1.79	0.47
3:A:2419:U:H2'	3:A:2420:C:C6	2.49	0.47
3:A:2602:A:H4'	3:A:2603:G:C5'	2.45	0.47
11:I:43:LYS:HG2	11:I:46:ARG:HH22	1.79	0.47
11:I:58:THR:HA	11:I:61:ARG:HD2	1.96	0.47
15:M:57:LEU:HD13	15:M:60:ARG:NH1	2.29	0.47
3:A:1076:C:H2'	3:A:1077:A:C8	2.49	0.47
3:A:1527:G:N1	3:A:1544:A:OP2	2.43	0.47
3:A:2121:G:H1	3:A:2177:C:H42	1.61	0.47
3:A:2790:U:H5'	3:A:2893:A:N7	2.29	0.47
3:A:327:G:C2	3:A:328:U:C2	3.02	0.47
3:A:1653:G:O6	17:O:11:ASN:ND2	2.48	0.47
3:A:1456:G:C6	3:A:1457:U:C4	3.03	0.47
3:A:2364:C:H2'	3:A:2365:G:O4'	2.14	0.47
3:A:2473:U:OP1	3:A:2529:G:N2	2.46	0.47
3:A:1750:G:O2'	3:A:2860:A:N1	2.42	0.47
3:A:44:A:C6	3:A:45:G:C5	3.03	0.47
3:A:521:U:H2'	3:A:522:A:C8	2.49	0.47
3:A:61:C:H5'	28:Z:43:LEU:HD12	1.95	0.47
3:A:691:C:H2'	3:A:692:C:C6	2.49	0.47
6:D:124:ARG:NH1	6:D:161:MET:O	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:34:VAL:HG23	6:D:94:GLN:O	2.15	0.47
10:H:82:SER:CB	10:H:94:ILE:HD11	2.43	0.47
26:X:41:ARG:HD3	26:X:41:ARG:HA	1.44	0.47
3:A:2116:G:O6	3:A:2171:A:N6	2.44	0.47
3:A:2786:U:H2'	3:A:2787:C:C6	2.49	0.47
3:A:780:G:H8	3:A:780:G:O5'	1.97	0.47
3:A:77:G:H2'	3:A:78:U:O4'	2.15	0.47
7:E:67:ARG:HB3	7:E:67:ARG:HE	1.29	0.47
12:J:100:LYS:HB3	12:J:139:VAL:HG23	1.97	0.47
3:A:2699:C:H2'	3:A:2700:A:O4'	2.15	0.47
10:H:40:THR:HG22	10:H:41:LYS:H	1.80	0.47
11:I:41:LEU:HD11	11:I:95:LEU:HG	1.97	0.47
11:I:51:TYR:HB3	11:I:84:TYR:HB2	1.95	0.47
12:J:72:LYS:HB3	12:J:116:ASP:OD2	2.15	0.47
18:P:16:ARG:HA	18:P:16:ARG:HD3	1.74	0.47
3:A:513:A:O2'	20:R:11:ARG:NH1	2.47	0.47
3:A:1872:A:H2'	3:A:1873:G:O4'	2.15	0.47
3:A:1953:A:N1	3:A:2549:G:O2'	2.43	0.47
3:A:2247:A:H2'	3:A:2248:C:H6	1.80	0.47
3:A:720:U:H2'	3:A:721:A:H8	1.79	0.47
23:U:67:VAL:HG22	23:U:76:ARG:HD2	1.97	0.47
3:A:1589:U:H2'	3:A:1590:A:H8	1.79	0.46
3:A:1800:C:H5'	5:C:146:MET:HE1	1.96	0.46
3:A:2271:G:H2'	3:A:2272:U:H6	1.80	0.46
3:A:2592:G:C2	3:A:2603:G:C2	3.03	0.46
3:A:728:G:H4'	5:C:13:ARG:HD3	1.97	0.46
12:J:28:LEU:HG	12:J:28:LEU:O	2.16	0.46
15:M:56:PRO:HG2	15:M:59:ARG:HG3	1.97	0.46
21:S:63:VAL:HA	21:S:96:VAL:HG12	1.96	0.46
24:V:14:LEU:O	24:V:19:LYS:HG3	2.15	0.46
3:A:691:C:H2'	3:A:692:C:H6	1.81	0.46
24:V:36:VAL:HB	24:V:39:ILE:HB	1.95	0.46
3:A:594:U:H2'	3:A:595:C:C6	2.51	0.46
9:G:99:LYS:NZ	9:G:104:ASN:OD1	2.48	0.46
19:Q:47:VAL:HG22	19:Q:61:VAL:HG22	1.97	0.46
3:A:1331:G:O2'	3:A:1332:G:H5'	2.14	0.46
3:A:1468:U:H2'	3:A:1522:A:N6	2.30	0.46
3:A:1799:G:C4	5:C:176:LEU:HD13	2.51	0.46
3:A:1110:G:HO2'	3:A:1111:A:H8	1.64	0.46
3:A:2795:C:H2'	3:A:2796:U:C6	2.50	0.46
3:A:987:C:O2'	3:A:1000:A:N3	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1104:C:H2'	3:A:1105:U:H6	1.81	0.46
3:A:2125:G:O2'	3:A:2173:A:N6	2.40	0.46
3:A:2403:C:H2'	3:A:2404:U:H6	1.81	0.46
3:A:983:A:H62	3:A:984:A:H62	1.63	0.46
3:A:2619:C:H5''	6:D:157:LYS:HA	1.96	0.46
22:T:70:LYS:HB2	22:T:70:LYS:NZ	2.31	0.46
24:V:33:LYS:HD3	24:V:64:ALA:HB1	1.98	0.46
3:A:521:U:H2'	3:A:522:A:H8	1.80	0.46
3:A:1820:U:C4	5:C:159:GLY:HA3	2.51	0.46
13:K:78:THR:HG23	13:K:83:GLY:O	2.16	0.46
23:U:17:SER:OG	23:U:18:GLU:N	2.49	0.46
3:A:1084:A:H2'	3:A:1085:A:C8	2.51	0.46
3:A:2557:G:H2'	3:A:2558:C:C6	2.51	0.46
3:A:2784:U:H2'	3:A:2785:C:C6	2.50	0.46
3:A:880:G:N2	3:A:898:C:C2	2.84	0.46
3:A:898:C:H2'	3:A:899:A:O4'	2.16	0.46
5:C:31:ALA:HB3	5:C:32:PRO:HD3	1.97	0.46
11:I:3:LEU:HD12	11:I:56:ARG:NH2	2.30	0.46
12:J:106:LEU:HB3	12:J:126:THR:HG23	1.98	0.46
3:A:1038:G:H2'	3:A:1039:A:H8	1.80	0.46
3:A:1077:A:N1	3:A:1088:A:H2'	2.31	0.46
3:A:813:U:C2	3:A:1195:G:N2	2.84	0.46
3:A:127:A:H5''	3:A:128:C:O4'	2.16	0.46
3:A:136:G:C6	3:A:137:U:C4	3.04	0.46
3:A:1414:C:H2'	3:A:1415:U:O4'	2.16	0.46
3:A:1987:A:H2'	3:A:1988:G:C8	2.51	0.46
3:A:2196:C:H2'	3:A:2197:U:C6	2.50	0.46
3:A:2544:G:H1'	3:A:2646:C:H5'	1.97	0.46
3:A:2793:C:H2'	3:A:2794:C:C6	2.51	0.46
9:G:94:TYR:OH	9:G:160:LYS:NZ	2.49	0.46
10:H:57:LYS:O	10:H:60:GLU:HG3	2.16	0.46
3:A:1069:A:H4'	3:A:1070:A:C5'	2.37	0.46
3:A:1441:G:H2'	3:A:1442:U:H6	1.81	0.46
3:A:1826:G:C5	3:A:1827:U:C5	3.04	0.46
3:A:2875:C:H2'	3:A:2876:G:H8	1.81	0.46
3:A:674:G:H5''	7:E:71:GLY:H	1.81	0.46
3:A:1278:C:H2'	3:A:1279:G:H8	1.81	0.45
3:A:191:A:H2'	3:A:192:C:H6	1.79	0.45
3:A:2424:C:H5'	3:A:2425:A:H5'	1.96	0.45
3:A:2581:G:H2'	3:A:2581:G:N3	2.30	0.45
3:A:878:A:N6	3:A:899:A:O2'	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:819:A:H5''	3:A:973:A:N1	2.31	0.45
18:P:2:ASP:O	18:P:5:SER:OG	2.31	0.45
3:A:1106:G:H2'	3:A:1107:G:H8	1.81	0.45
3:A:1188:U:O2'	3:A:1189:A:H5'	2.16	0.45
3:A:1510:G:H2'	3:A:1511:G:C8	2.51	0.45
7:E:134:LEU:HD23	7:E:164:LEU:HD12	1.98	0.45
9:G:9:VAL:HB	9:G:50:LEU:HB2	1.98	0.45
18:P:15:ARG:HG2	18:P:93:ASP:OD2	2.16	0.45
3:A:1361:G:H2'	3:A:1362:C:C6	2.52	0.45
3:A:157:C:H2'	3:A:158:U:O4'	2.16	0.45
3:A:2423:U:H2'	3:A:2424:C:H1'	1.96	0.45
3:A:366:C:H2'	3:A:367:G:O4'	2.16	0.45
4:B:48:U:H2'	4:B:49:C:C6	2.51	0.45
5:C:145:GLU:HG2	5:C:151:GLY:C	2.36	0.45
8:F:5:HIS:HB2	8:F:97:TRP:CG	2.51	0.45
12:J:76:ALA:HB2	12:J:129:ILE:HD13	1.96	0.45
23:U:14:PRO:HA	23:U:32:LEU:HD23	1.97	0.45
3:A:1047:G:N2	3:A:1110:G:H2'	2.31	0.45
3:A:1464:G:H2'	3:A:1465:G:C8	2.47	0.45
3:A:1687:G:H1'	3:A:1702:G:N2	2.32	0.45
3:A:2069:G:C2	3:A:2070:A:C8	3.04	0.45
3:A:2316:G:H4'	8:F:125:ARG:CZ	2.47	0.45
3:A:741:U:H2'	3:A:742:A:C8	2.52	0.45
3:A:857:G:H2'	3:A:858:G:O4'	2.17	0.45
7:E:168:ASP:OD2	7:E:170:ARG:NH1	2.49	0.45
12:J:132:THR:O	12:J:136:MET:HG2	2.15	0.45
27:Y:48:THR:O	27:Y:49:LEU:HD23	2.16	0.45
3:A:1354:A:H2'	3:A:1355:G:O4'	2.16	0.45
3:A:1427:A:H4'	3:A:1428:C:O4'	2.17	0.45
3:A:1638:C:H1'	3:A:2698:U:O2'	2.17	0.45
3:A:2114:A:C2	3:A:2166:U:H2'	2.52	0.45
3:A:2301:C:H2'	3:A:2302:U:C6	2.52	0.45
3:A:2259:U:C4	3:A:2427:C:N4	2.84	0.45
3:A:1999:C:O2	3:A:2687:U:O2'	2.32	0.45
3:A:697:G:C6	3:A:698:C:N4	2.85	0.45
5:C:240:PHE:O	5:C:242:LYS:HE2	2.17	0.45
17:O:28:LEU:HD23	17:O:48:VAL:HG21	1.98	0.45
3:A:118:A:OP2	3:A:119:A:H2'	2.17	0.45
3:A:1346:G:H2'	3:A:1347:A:H8	1.82	0.45
3:A:1425:G:H2'	3:A:1426:G:O4'	2.17	0.45
3:A:2133:G:H21	3:A:2158:A:N6	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2209:G:N2	3:A:2215:C:N3	2.57	0.45
3:A:2246:G:H2'	3:A:2247:A:C8	2.52	0.45
3:A:2393:U:H2'	3:A:2394:C:O4'	2.17	0.45
3:A:647:G:H2'	3:A:648:G:H8	1.82	0.45
4:B:57:A:H2'	4:B:58:A:C8	2.51	0.45
5:C:243:HIS:HA	5:C:244:PRO:HD3	1.81	0.45
8:F:130:MET:HE3	8:F:130:MET:HB2	1.90	0.45
12:J:80:LEU:HD23	12:J:101:ILE:HG21	1.99	0.45
20:R:41:LYS:HD2	20:R:44:GLN:OE1	2.16	0.45
3:A:1538:G:H2'	3:A:1539:U:C6	2.52	0.45
3:A:1570:A:C6	3:A:1571:A:C6	3.05	0.45
3:A:2233:U:H2'	3:A:2234:G:C8	2.52	0.45
3:A:272:A:H61	3:A:365:U:H3	1.65	0.45
9:G:155:GLU:HB2	9:G:156:PRO:HD2	1.99	0.45
3:A:2749:A:OP1	9:G:2:SER:N	2.50	0.45
14:L:66:LYS:HB3	14:L:66:LYS:HE2	1.71	0.45
3:A:1093:G:H1'	3:A:1099:G:N2	2.32	0.45
3:A:2256:G:N2	3:A:2275:C:C4	2.84	0.45
3:A:2898:U:H2'	3:A:2899:A:C8	2.52	0.45
3:A:960:A:H5''	3:A:961:C:OP1	2.17	0.45
7:E:138:LEU:HA	7:E:138:LEU:HD23	1.80	0.45
18:P:92:PHE:HB2	18:P:117:PHE:CD1	2.51	0.45
27:Y:41:GLU:O	27:Y:44:LYS:HD2	2.17	0.45
3:A:364:C:H2'	3:A:365:U:C6	2.52	0.45
3:A:519:U:H2'	3:A:520:G:H8	1.81	0.45
3:A:532:A:H2'	3:A:532:A:N3	2.31	0.45
3:A:613:A:C8	3:A:613:A:OP1	2.70	0.45
3:A:708:G:H2'	3:A:709:U:H6	1.81	0.45
3:A:77:G:OP1	28:Z:52:ARG:NH2	2.50	0.45
3:A:814:C:H2'	3:A:815:C:C6	2.52	0.45
18:P:31:THR:HG22	18:P:33:ARG:H	1.82	0.45
28:Z:28:LEU:HD23	28:Z:28:LEU:HA	1.67	0.45
3:A:753:A:H2'	3:A:754:U:H6	1.81	0.45
7:E:19:PHE:HB3	7:E:113:VAL:HG21	1.98	0.45
10:H:115:VAL:HG22	10:H:132:PHE:CE2	2.51	0.45
12:J:9:VAL:HG11	12:J:31:GLN:HG3	1.99	0.45
28:Z:21:LEU:HD22	28:Z:46:VAL:HG13	1.98	0.45
3:A:1425:G:H2'	3:A:1426:G:C8	2.52	0.44
3:A:1433:A:N1	3:A:1434:A:N6	2.65	0.44
3:A:1448:G:H2'	3:A:1449:G:O4'	2.17	0.44
3:A:1494:A:H2'	3:A:1495:A:C8	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1869:G:C2	3:A:1873:G:C6	3.05	0.44
12:J:130:GLU:HB3	12:J:134:ARG:CZ	2.47	0.44
14:L:38:ILE:HD11	14:L:112:PHE:HZ	1.80	0.44
17:O:12:ARG:NE	17:O:16:HIS:CE1	2.85	0.44
3:A:1009:A:N3	3:A:1153:C:O2'	2.48	0.44
3:A:1385:A:C6	3:A:1403:A:C5	3.06	0.44
3:A:1846:G:N2	3:A:1848:A:H62	2.15	0.44
3:A:460:A:C2	3:A:470:A:C4	3.06	0.44
8:F:44:ILE:HG22	8:F:83:TYR:HD2	1.81	0.44
3:A:210:C:H2'	3:A:211:C:C6	2.53	0.44
3:A:848:C:H2'	3:A:849:A:C8	2.51	0.44
3:A:764:A:H5''	5:C:209:GLY:HA2	1.98	0.44
10:H:110:VAL:HG12	10:H:114:GLU:HB2	1.99	0.44
14:L:71:ARG:HA	14:L:71:ARG:HD3	1.40	0.44
21:S:70:GLU:HG3	21:S:71:LYS:N	2.31	0.44
22:T:4:ILE:HG23	22:T:106:VAL:HG22	1.98	0.44
3:A:1038:G:H2'	3:A:1039:A:C8	2.53	0.44
3:A:1060:U:C2	3:A:1062:G:H5'	2.53	0.44
3:A:1900:A:N1	3:A:1970:A:C6	2.86	0.44
3:A:2577:A:H5''	3:A:2578:G:H5'	1.98	0.44
3:A:2617:U:H2'	3:A:2618:G:O4'	2.18	0.44
3:A:511:U:C5	3:A:512:G:C5	3.05	0.44
3:A:845:A:H61	3:A:932:U:H3	1.65	0.44
8:F:105:THR:HG22	8:F:106:ILE:HG12	1.99	0.44
10:H:8:LYS:HB2	10:H:14:SER:HA	1.98	0.44
10:H:6:LEU:O	10:H:15:LEU:HB3	2.17	0.44
11:I:29:ASP:CG	11:I:79:PRO:HG2	2.38	0.44
14:L:17:ARG:HB2	14:L:45:GLU:HB2	2.00	0.44
3:A:1410:G:H1	3:A:1592:C:H42	1.66	0.44
3:A:2547:A:H2'	3:A:2548:U:C6	2.52	0.44
3:A:705:A:H2'	3:A:706:A:O4'	2.17	0.44
12:J:53:LEU:HD21	12:J:82:LYS:HD2	2.00	0.44
3:A:2377:A:O2'	18:P:117:PHE:O	2.31	0.44
3:A:2365:G:OP1	26:X:55:ARG:HG2	2.17	0.44
26:X:62:LYS:HE2	26:X:62:LYS:HB3	1.84	0.44
3:A:1444:G:H2'	3:A:1445:G:H8	1.81	0.44
3:A:2725:A:N7	3:A:2727:A:C5	2.86	0.44
3:A:2791:G:H2'	3:A:2792:A:O4'	2.18	0.44
3:A:540:C:H2'	3:A:541:A:H8	1.82	0.44
3:A:976:G:HO2'	3:A:1155:A:HO2'	1.59	0.44
3:A:2312:U:O2	8:F:37:ASN:ND2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:97:ARG:HB2	10:H:112:LYS:HD2	2.00	0.44
19:Q:25:THR:HB	19:Q:88:ARG:HG2	1.98	0.44
3:A:2139:U:H2'	3:A:2140:G:H8	1.82	0.44
3:A:2228:G:H2'	3:A:2229:U:C6	2.52	0.44
13:K:125:TYR:HH	13:K:132:HIS:CD2	2.34	0.44
14:L:121:GLU:OE1	14:L:123:LEU:HD21	2.18	0.44
16:N:126:ILE:O	16:N:128:THR:HG23	2.18	0.44
3:A:2316:G:H2'	3:A:2317:A:H8	1.83	0.44
3:A:629:G:H1'	3:A:639:U:O2'	2.17	0.44
8:F:5:HIS:O	8:F:8:TYR:HB3	2.17	0.44
14:L:23:LYS:HG3	14:L:24:VAL:N	2.32	0.44
3:A:1075:C:H2'	3:A:1076:C:C6	2.52	0.44
3:A:1721:G:C6	3:A:1738:G:C6	3.05	0.44
3:A:2172:U:H4'	3:A:2173:A:H5'	1.98	0.44
3:A:2431:U:H5	3:A:2433:A:H5''	1.83	0.44
3:A:2792:A:H61	3:A:2804:U:H3	1.66	0.44
3:A:1820:U:OP1	5:C:177:ARG:HG2	2.18	0.44
3:A:2823:A:OP1	6:D:118:PHE:HB2	2.18	0.44
10:H:32:PRO:HA	27:Y:39:TRP:CD1	2.53	0.44
12:J:15:ALA:O	12:J:46:THR:OG1	2.23	0.44
21:S:68:ARG:HB3	21:S:90:ARG:HB3	1.99	0.44
3:A:1062:G:H8	3:A:1062:G:O5'	2.01	0.43
3:A:1088:A:N6	12:J:135:SER:HB3	2.33	0.43
3:A:1847:A:HO2'	3:A:1848:A:H8	1.66	0.43
3:A:2302:U:H2'	3:A:2303:G:H8	1.83	0.43
3:A:596:U:H2'	3:A:597:G:C8	2.52	0.43
3:A:879:G:H22	3:A:899:A:H1'	1.83	0.43
5:C:25:HIS:HB3	5:C:82:GLU:HG2	1.99	0.43
6:D:99:GLU:OE2	6:D:182:ALA:HB2	2.18	0.43
7:E:159:LEU:HA	7:E:159:LEU:HD23	1.83	0.43
9:G:89:LEU:HG	9:G:162:VAL:HG22	1.99	0.43
18:P:50:ALA:O	18:P:81:ARG:NH2	2.50	0.43
3:A:2114:A:C2	3:A:2115:G:H1'	2.53	0.43
3:A:2662:A:H2'	3:A:2663:G:O4'	2.17	0.43
3:A:319:G:N2	3:A:333:G:H1'	2.33	0.43
3:A:433:C:H2'	3:A:434:U:C6	2.53	0.43
3:A:580:U:H2'	3:A:581:C:C6	2.53	0.43
5:C:30:PHE:CD2	5:C:33:LEU:HG	2.53	0.43
9:G:52:PHE:CE1	9:G:69:ARG:HA	2.52	0.43
12:J:49:ILE:HD12	12:J:74:PRO:HD3	2.00	0.43
12:J:50:GLU:HG3	12:J:82:LYS:HZ1	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:27:LEU:O	15:M:31:GLY:HA2	2.18	0.43
16:N:40:ARG:HG2	16:N:95:LEU:CD2	2.48	0.43
18:P:115:LEU:HD12	18:P:115:LEU:HA	1.86	0.43
18:P:24:THR:HG22	18:P:90:VAL:HG12	2.00	0.43
19:Q:3:ASN:HA	19:Q:6:LYS:HB3	1.98	0.43
3:A:2744:G:C6	3:A:2761:A:C6	3.06	0.43
3:A:183:C:O2'	3:A:432:A:N3	2.51	0.43
3:A:6:A:H2'	3:A:7:G:H8	1.83	0.43
5:C:155:ALA:HB2	5:C:162:VAL:HG23	1.98	0.43
8:F:63:GLN:HE21	8:F:89:VAL:HG13	1.83	0.43
15:M:55:MET:O	15:M:60:ARG:HD3	2.18	0.43
20:R:50:ARG:O	20:R:54:LYS:NZ	2.42	0.43
3:A:1923:U:H2'	3:A:1924:C:C6	2.53	0.43
3:A:2443:C:H2'	3:A:2444:G:C8	2.54	0.43
8:F:33:LYS:HG3	8:F:157:THR:HB	2.00	0.43
3:A:1056:G:N1	3:A:1102:C:OP2	2.38	0.43
3:A:2328:A:H2'	3:A:2329:U:C6	2.54	0.43
3:A:2545:G:H2'	3:A:2546:U:O4'	2.17	0.43
12:J:42:PHE:CE1	12:J:46:THR:HG21	2.53	0.43
13:K:32:LEU:O	13:K:36:LEU:HG	2.78	0.43
3:A:1814:G:OP1	5:C:40:SER:OG	2.36	0.43
3:A:1827:U:H5'	3:A:1971:U:H5'	1.99	0.43
3:A:2135:A:H1'	3:A:2159:G:O2'	2.18	0.43
3:A:2489:U:C4	3:A:2490:G:C6	3.06	0.43
3:A:26:G:C6	3:A:27:G:N1	2.87	0.43
3:A:2895:G:H2'	3:A:2896:C:C6	2.53	0.43
3:A:61:C:C5'	28:Z:43:LEU:HD12	2.49	0.43
9:G:83:PHE:CE2	9:G:138:LYS:HB2	2.53	0.43
11:I:53:ARG:HE	11:I:55:VAL:HG22	1.84	0.43
15:M:109:LYS:HE3	15:M:126:ARG:HB3	2.00	0.43
16:N:33:LEU:HD12	16:N:129:THR:O	2.19	0.43
3:A:1026:G:H2'	3:A:1027:A:C8	2.53	0.43
3:A:1301:A:H4'	3:A:1302:A:OP1	2.19	0.43
3:A:1587:G:H2'	3:A:1588:G:H8	1.83	0.43
3:A:1881:C:H2'	3:A:1882:U:O4'	2.17	0.43
3:A:1931:U:H2'	3:A:1932:A:H8	1.83	0.43
3:A:1972:G:C2	3:A:1973:G:N7	2.86	0.43
3:A:2373:G:H2'	3:A:2374:C:C6	2.53	0.43
5:C:261:LYS:HA	5:C:264:ASP:OD2	2.19	0.43
17:O:36:THR:HG23	17:O:41:ALA:HB2	2.01	0.43
27:Y:39:TRP:HZ2	27:Y:44:LYS:HZ3	1.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:22:GLN:NE2	9:G:55:ARG:HH12	2.17	0.43
16:N:66:ARG:HB2	16:N:101:VAL:O	2.18	0.43
18:P:11:ALA:O	18:P:15:ARG:HG3	2.19	0.43
18:P:29:HIS:HB3	18:P:36:TYR:HB2	2.00	0.43
23:U:58:VAL:HG22	23:U:85:VAL:HG22	2.00	0.43
26:X:33:ALA:N	26:X:64:ASP:OD1	2.50	0.43
3:A:1444:G:H2'	3:A:1445:G:C8	2.53	0.43
7:E:5:LEU:HD23	7:E:122:GLU:HG2	2.01	0.43
14:L:66:LYS:N	14:L:82:ASN:OD1	2.46	0.43
3:A:1385:A:H1'	3:A:1386:C:C6	2.54	0.43
3:A:1739:A:H2'	3:A:1740:G:O4'	2.19	0.43
3:A:2073:C:H2'	3:A:2074:U:H6	1.84	0.43
3:A:2127:G:H21	3:A:2173:A:H1'	1.84	0.43
3:A:2128:G:H21	3:A:2173:A:H4'	1.83	0.43
3:A:2503:A:H4'	3:A:2504:U:OP1	2.19	0.43
3:A:2840:C:H2'	3:A:2841:C:C6	2.54	0.43
5:C:120:VAL:HG12	5:C:134:ASN:HD21	1.84	0.43
3:A:764:A:H5''	5:C:209:GLY:CA	2.49	0.43
8:F:123:ASP:CG	8:F:125:ARG:H	2.22	0.43
10:H:101:ASP:HA	10:H:104:THR:OG1	2.19	0.43
17:O:33:ILE:HD12	17:O:114:GLU:HB3	2.01	0.43
19:Q:113:ARG:HG2	19:Q:115:ASN:OD1	2.19	0.43
1:1:49:G:N2	1:1:60:A:N1	2.65	0.42
3:A:1355:G:C6	3:A:1377:G:N2	2.87	0.42
3:A:1638:C:O2	3:A:2698:U:O2'	2.36	0.42
3:A:307:G:N2	3:A:309:A:H3'	2.34	0.42
3:A:335:C:H5''	24:V:82:ARG:HD3	2.01	0.42
3:A:655:A:H4'	3:A:656:G:H5'	2.00	0.42
3:A:815:C:H2'	3:A:816:C:C6	2.53	0.42
3:A:863:A:H2'	3:A:864:G:H8	1.84	0.42
6:D:68:PHE:CE1	6:D:79:LEU:HD21	2.54	0.42
7:E:149:ILE:HB	7:E:188:MET:HG2	2.02	0.42
12:J:12:GLN:HA	12:J:56:PRO:HA	2.00	0.42
16:N:35:ALA:HA	16:N:128:THR:HG22	2.00	0.42
18:P:85:LYS:HB3	18:P:85:LYS:HE2	1.68	0.42
18:P:4:LYS:O	18:P:8:ILE:HG13	2.19	0.42
3:A:1052:C:O5'	3:A:1052:C:H6	2.02	0.42
3:A:176:A:C5	3:A:177:G:C6	3.07	0.42
3:A:2530:A:C6	9:G:156:PRO:HG3	2.54	0.42
3:A:401:A:H2'	3:A:402:A:C8	2.55	0.42
3:A:536:G:H2'	3:A:537:G:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:235:GLY:HA3	5:C:239:ASN:HB2	2.01	0.42
10:H:29:PHE:O	10:H:32:PRO:HD2	2.19	0.42
12:J:42:PHE:CE1	12:J:57:VAL:HB	2.54	0.42
12:J:74:PRO:HA	12:J:75:PRO:HD3	1.91	0.42
13:K:110:PRO:O	13:K:115:GLY:HA3	2.19	0.42
27:Y:70:GLU:HA	27:Y:73:ALA:HB3	2.01	0.42
3:A:1007:C:OP1	13:K:39:LYS:NZ	2.52	0.42
3:A:1177:G:O5'	3:A:1177:G:H8	2.01	0.42
3:A:1526:C:H2'	3:A:1527:G:O4'	2.19	0.42
3:A:1757:A:H8	3:A:1757:A:O5'	2.02	0.42
3:A:1954:G:H1'	3:A:1956:U:O4	2.20	0.42
3:A:2439:A:H4'	3:A:2440:C:H5''	2.00	0.42
3:A:2628:C:O2'	3:A:2781:A:H2'	2.19	0.42
3:A:776:G:HO2'	3:A:777:G:P	2.40	0.42
20:R:31:VAL:HG12	20:R:34:VAL:H	1.83	0.42
3:A:2103:C:O2	3:A:2186:G:N1	2.42	0.42
3:A:2069:G:N2	3:A:2443:C:C2	2.87	0.42
3:A:251:A:O5'	3:A:251:A:H8	2.02	0.42
3:A:418:C:H2'	3:A:419:U:O4'	2.19	0.42
3:A:843:G:H1	3:A:935:C:N4	2.17	0.42
4:B:32:U:C2	4:B:51:G:N2	2.87	0.42
13:K:21:THR:HG23	13:K:61:LYS:HB3	2.01	0.42
3:A:149:A:H2'	3:A:150:U:O4'	2.19	0.42
3:A:1439:A:C2	3:A:1553:A:C5	3.07	0.42
3:A:2577:A:H2'	3:A:2614:A:N6	2.34	0.42
3:A:55:G:H2'	3:A:56:A:C8	2.53	0.42
5:C:141:VAL:HG12	5:C:192:LEU:HD13	2.01	0.42
4:B:57:A:O4'	8:F:27:GLN:HG2	2.20	0.42
12:J:81:LYS:HG3	12:J:136:MET:HE1	2.01	0.42
15:M:135:ILE:HB	15:M:142:ILE:HD11	2.01	0.42
17:O:9:GLN:HA	17:O:17:ARG:NH2	2.33	0.42
3:A:1079:C:O2	12:J:131:GLY:HA3	2.18	0.42
3:A:1799:G:H4'	3:A:1800:C:O5'	2.20	0.42
3:A:1869:G:H3'	3:A:1870:C:H5''	2.02	0.42
3:A:2071:A:H2'	3:A:2072:C:C6	2.54	0.42
3:A:634:C:H2'	3:A:635:C:C6	2.55	0.42
7:E:112:LEU:HA	7:E:112:LEU:HD23	1.91	0.42
13:K:16:TYR:HD2	13:K:140:LEU:HB2	1.83	0.42
20:R:68:ALA:O	20:R:71:GLN:HB2	2.19	0.42
25:W:41:GLU:O	25:W:42:LEU:HD23	2.19	0.42
3:A:61:C:O4'	28:Z:40:SER:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1064:C:H2'	3:A:1065:U:O4'	2.19	0.42
3:A:152:A:H2'	3:A:153:U:C6	2.54	0.42
3:A:1967:C:C4	3:A:1968:G:C5	3.07	0.42
3:A:2790:U:H4'	3:A:2791:G:OP1	2.20	0.42
3:A:356:G:H2'	3:A:357:C:O4'	2.20	0.42
3:A:607:U:OP1	7:E:97:ASN:HA	2.19	0.42
8:F:152:LEU:HD23	8:F:153:ASP:N	2.35	0.42
8:F:30:ARG:NH2	8:F:159:THR:HG21	2.35	0.42
12:J:56:PRO:HD3	12:J:75:PRO:HD3	2.02	0.42
15:M:95:LEU:HB2	15:M:101:ILE:HD11	2.01	0.42
3:A:1064:C:H5''	12:J:88:SER:HB2	2.00	0.42
3:A:1853:A:H2'	3:A:1854:A:C8	2.54	0.42
3:A:2209:G:H1	3:A:2215:C:N4	2.14	0.42
3:A:5:A:H2'	3:A:6:A:C8	2.55	0.42
3:A:672:C:O5'	3:A:672:C:H6	2.03	0.42
3:A:845:A:N3	3:A:845:A:H3'	2.35	0.42
3:A:980:A:N6	3:A:981:A:N1	2.67	0.42
4:B:7:G:H2'	4:B:8:C:H6	1.85	0.42
5:C:133:ARG:HD2	10:H:123:ARG:NH1	2.34	0.42
3:A:2599:G:C8	5:C:236:GLU:HB2	2.55	0.42
15:M:135:ILE:HG22	15:M:140:GLY:HA3	2.02	0.42
19:Q:21:ARG:HG3	19:Q:113:ARG:HH12	1.84	0.42
25:W:82:TYR:N	25:W:82:TYR:CD1	2.88	0.42
1:I:44:G:C6	1:I:45:U:C4	3.07	0.42
3:A:1020:A:C2	3:A:1141:U:C2	3.08	0.42
3:A:1206:G:H2'	3:A:1207:C:C6	2.55	0.42
3:A:1825:U:H2'	3:A:1826:G:C8	2.55	0.42
3:A:2165:C:H2'	3:A:2166:U:O4'	2.20	0.42
3:A:2591:C:H2'	3:A:2592:G:C8	2.54	0.42
6:D:14:ILE:HD13	19:Q:12:GLN:NE2	2.34	0.42
6:D:56:LYS:O	6:D:60:VAL:HG23	2.20	0.42
11:I:64:VAL:HG22	11:I:69:PHE:HB2	2.01	0.42
11:I:3:LEU:HD22	11:I:7:ASP:HB3	2.00	0.42
13:K:117:ALA:HA	13:K:120:ARG:HH21	1.84	0.42
23:U:79:ASP:OD1	23:U:79:ASP:N	2.52	0.42
3:A:1208:C:C4	3:A:1209:U:C4	3.08	0.42
3:A:1369:G:C6	3:A:1370:C:C4	3.08	0.42
3:A:2191:A:C6	3:A:2192:U:C4	3.08	0.42
5:C:270:ARG:HH21	5:C:271:ARG:NH1	2.16	0.42
9:G:94:TYR:O	9:G:95:ARG:NH1	2.49	0.42
10:H:29:PHE:C	10:H:32:PRO:HD2	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:538:A:H5'	13:K:7:LYS:HE2	2.01	0.42
13:K:95:ARG:HG2	13:K:96:ARG:N	2.35	0.42
14:L:1:MET:HB3	14:L:1:MET:HE3	1.90	0.42
23:U:54:GLU:HB2	23:U:91:GLN:HE21	1.85	0.42
1:1:43:G:C2	1:1:67:A:C8	3.08	0.41
3:A:189:G:OP2	27:Y:26:LYS:NZ	2.53	0.41
3:A:2027:G:C4	3:A:2028:U:C5	3.08	0.41
3:A:2433:A:H5'	3:A:2434:A:P	2.60	0.41
3:A:613:A:H1'	3:A:614:A:H5'	2.02	0.41
3:A:636:G:OP2	15:M:109:LYS:NZ	2.45	0.41
7:E:48:THR:HG22	7:E:86:ALA:HB3	2.02	0.41
11:I:29:ASP:HB3	11:I:106:PHE:HB2	2.01	0.41
11:I:64:VAL:HG22	11:I:69:PHE:CB	2.50	0.41
22:T:66:ILE:HA	22:T:69:LEU:HD12	2.01	0.41
3:A:136:G:N1	3:A:137:U:C4	2.89	0.41
3:A:1394:U:H4'	3:A:1603:A:H4'	2.01	0.41
3:A:2028:U:H2'	3:A:2029:G:C8	2.55	0.41
3:A:815:C:H2'	3:A:816:C:H6	1.83	0.41
3:A:983:A:N6	3:A:984:A:H62	2.18	0.41
7:E:106:LYS:HE2	7:E:200:LEU:HB3	2.03	0.41
3:A:1205:A:C5	7:E:165:HIS:CD2	3.07	0.41
12:J:24:VAL:HG13	12:J:25:GLY:N	2.35	0.41
3:A:7:G:H1'	13:K:135:GLN:NE2	2.34	0.41
14:L:25:LEU:HD12	14:L:38:ILE:HG22	2.02	0.41
3:A:2334:U:C4	18:P:16:ARG:HG3	2.55	0.41
27:Y:77:LYS:HD2	27:Y:77:LYS:HA	1.88	0.41
3:A:1056:G:O2'	3:A:1086:A:H1'	2.20	0.41
3:A:1720:U:H2'	3:A:1721:G:O4'	2.21	0.41
3:A:244:A:C2	3:A:255:A:C4	3.09	0.41
3:A:783:A:C5	3:A:785:G:H1'	2.54	0.41
4:B:5:U:OP1	4:B:61:G:O2'	2.27	0.41
4:B:7:G:H2'	4:B:8:C:C6	2.54	0.41
5:C:192:LEU:HD13	5:C:192:LEU:HA	1.78	0.41
7:E:88:ARG:HA	7:E:88:ARG:HD3	1.76	0.41
9:G:144:VAL:O	9:G:148:LEU:HG	2.19	0.41
9:G:22:GLN:NE2	9:G:39:ASP:HA	2.32	0.41
11:I:75:ALA:O	11:I:109:LYS:NZ	2.38	0.41
12:J:74:PRO:HG2	12:J:79:LEU:HD21	2.01	0.41
3:A:1139:G:H5''	13:K:72:LYS:NZ	2.35	0.41
3:A:1665:A:H1'	14:L:1:MET:HE2	2.01	0.41
19:Q:8:LEU:HD23	19:Q:8:LEU:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1408:G:C6	3:A:1409:U:C4	3.08	0.41
3:A:1421:G:C2	3:A:1422:G:C8	3.09	0.41
3:A:17:G:H2'	3:A:18:U:C6	2.55	0.41
3:A:511:U:O4	3:A:512:G:N1	2.54	0.41
3:A:581:C:H2'	3:A:582:A:C8	2.55	0.41
3:A:753:A:H2'	3:A:754:U:C6	2.55	0.41
5:C:252:THR:OG1	5:C:253:LYS:N	2.53	0.41
12:J:59:ILE:HG22	12:J:61:VAL:HG12	2.02	0.41
12:J:8:TYR:N	12:J:61:VAL:HG13	2.36	0.41
14:L:107:LEU:O	14:L:112:PHE:HB2	2.21	0.41
18:P:74:VAL:O	18:P:78:VAL:HG22	2.20	0.41
19:Q:97:LEU:O	19:Q:99:TYR:N	2.54	0.41
26:X:29:GLU:O	26:X:66:LYS:HA	2.21	0.41
1:1:49:G:H1	1:1:60:A:N6	2.19	0.41
3:A:1935:G:H1'	3:A:1964:G:N2	2.35	0.41
3:A:2116:G:C6	3:A:2171:A:N6	2.89	0.41
3:A:2680:U:O2'	3:A:2681:C:H5'	2.21	0.41
21:S:32:THR:HG21	21:S:60:LYS:NZ	2.36	0.41
3:A:1020:A:N1	3:A:1141:U:H1'	2.35	0.41
3:A:121:G:H4'	3:A:149:A:H5'	2.01	0.41
3:A:1326:U:H2'	3:A:1327:A:H8	1.85	0.41
3:A:1677:A:H3'	3:A:1678:A:H8	1.86	0.41
3:A:1889:A:H2'	3:A:1890:A:C8	2.54	0.41
3:A:1937:A:N7	3:A:1939:U:H2'	2.35	0.41
3:A:1266:G:N2	3:A:2012:G:H2'	2.36	0.41
3:A:2804:U:H2'	3:A:2805:C:C6	2.56	0.41
3:A:712:G:H2'	3:A:713:G:O4'	2.21	0.41
3:A:784:G:H5'	3:A:785:G:OP1	2.21	0.41
4:B:57:A:H2'	4:B:58:A:O4'	2.20	0.41
8:F:11:GLU:O	8:F:14:LYS:HD3	2.20	0.41
8:F:48:LYS:HE2	8:F:48:LYS:HB2	1.79	0.41
3:A:2530:A:N6	9:G:156:PRO:HG3	2.36	0.41
16:N:133:LYS:HB3	16:N:133:LYS:HE3	1.77	0.41
20:R:13:ARG:O	20:R:16:LYS:HB3	2.20	0.41
25:W:80:HIS:N	25:W:87:GLN:HG2	2.36	0.41
3:A:1021:A:H3'	3:A:1021:A:N3	2.35	0.41
3:A:1282:U:H2'	3:A:1283:G:O4'	2.20	0.41
3:A:1340:U:H4'	3:A:1341:G:OP2	2.21	0.41
3:A:2102:G:H1	3:A:2187:U:H3	1.69	0.41
3:A:2102:G:C2	3:A:2187:U:O2	2.74	0.41
3:A:2316:G:H2'	3:A:2317:A:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2484:G:C2	3:A:2485:G:C8	3.09	0.41
3:A:67:U:C2	3:A:68:G:C8	3.09	0.41
7:E:116:ASP:O	7:E:185:LYS:NZ	2.54	0.41
10:H:65:ALA:CB	10:H:135:HIS:HB2	2.51	0.41
14:L:17:ARG:HD3	14:L:17:ARG:HA	1.60	0.41
17:O:55:ALA:HA	17:O:80:PHE:CE2	2.56	0.41
19:Q:43:PHE:CE2	19:Q:63:LYS:HE2	2.56	0.41
26:X:67:VAL:HA	26:X:82:ILE:HD13	2.03	0.41
27:Y:38:PHE:O	27:Y:46:PHE:HA	2.21	0.41
3:A:1467:U:H5	3:A:1546:G:H2'	1.86	0.41
3:A:1467:U:C4	3:A:1468:U:C5	3.09	0.41
3:A:184:C:H2'	3:A:185:G:C8	2.55	0.41
3:A:231:A:N6	3:A:232:G:C2	2.89	0.41
3:A:2403:C:H2'	3:A:2404:U:C6	2.56	0.41
3:A:250:G:C6	3:A:251:A:C6	3.07	0.41
3:A:632:A:H4'	15:M:68:SER:HB2	2.02	0.41
3:A:196:A:O2'	3:A:805:G:O6	2.33	0.41
3:A:932:U:O2'	3:A:934:U:O4	2.36	0.41
4:B:65:U:C4	4:B:108:A:C4	3.09	0.41
4:B:81:G:H2'	4:B:82:U:C6	2.56	0.41
8:F:147:ASP:OD1	8:F:150:ARG:NH2	2.54	0.41
12:J:20:PRO:O	12:J:24:VAL:HG12	2.21	0.41
3:A:582:A:H5''	20:R:11:ARG:NH2	2.36	0.41
23:U:63:VAL:HG21	23:U:80:TRP:CZ2	2.55	0.41
24:V:7:ARG:O	24:V:8:ASP:HB2	2.20	0.41
3:A:163:C:H2'	3:A:164:C:C6	2.56	0.41
3:A:807:U:O2'	3:A:2060:A:N1	2.53	0.41
8:F:68:THR:N	8:F:86:GLY:O	2.54	0.41
3:A:566:U:OP1	15:M:29:LYS:HD2	2.21	0.41
26:X:15:ASP:CG	26:X:16:SER:H	2.24	0.41
27:Y:74:ARG:HB2	27:Y:74:ARG:HE	1.59	0.41
3:A:1022:G:C6	3:A:1140:C:C5	3.09	0.41
3:A:2821:A:C2	3:A:2822:G:C4	3.09	0.41
3:A:2829:A:C6	3:A:2830:C:C4	3.09	0.41
3:A:30:G:H2'	3:A:31:C:C6	2.55	0.41
3:A:370:G:H4'	3:A:371:A:OP2	2.21	0.41
3:A:92:U:C5	3:A:93:G:C5	3.09	0.41
8:F:35:THR:O	8:F:36:LEU:HD23	2.21	0.41
26:X:82:ILE:HD13	26:X:82:ILE:HA	1.85	0.41
28:Z:57:LEU:HD23	28:Z:57:LEU:HA	1.94	0.41
3:A:1581:G:C5	3:A:1582:C:C4	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1842:G:C2	3:A:1843:C:C2	3.09	0.41
3:A:1664:A:N6	3:A:1996:C:H42	2.13	0.41
3:A:2345:G:C5	3:A:2381:A:C2	3.09	0.41
3:A:2719:G:O2'	3:A:2720:U:H5'	2.21	0.41
3:A:2677:G:C2	3:A:2731:G:C2	3.08	0.41
3:A:451:U:C2	3:A:453:A:N7	2.89	0.41
3:A:503:A:H4'	3:A:504:A:C5'	2.50	0.41
3:A:613:A:O2'	3:A:614:A:H2'	2.21	0.41
3:A:643:A:N1	3:A:2369:A:O2'	2.49	0.41
3:A:2746:U:H4'	9:G:138:LYS:HG2	2.02	0.41
11:I:14:GLU:O	11:I:18:VAL:HG23	2.21	0.41
1:1:49:G:C6	1:1:61:G:N2	2.89	0.40
3:A:1613:G:C2	3:A:1617:C:C2	3.09	0.40
3:A:1826:G:C6	3:A:1827:U:C4	3.09	0.40
3:A:1969:A:O2'	3:A:1972:G:N3	2.53	0.40
3:A:2150:C:H2'	3:A:2151:U:O4'	2.20	0.40
3:A:2286:G:H4'	3:A:2287:A:O4'	2.21	0.40
3:A:741:U:H2'	3:A:742:A:H8	1.86	0.40
5:C:115:GLN:O	5:C:125:LYS:NZ	2.54	0.40
7:E:57:LYS:HA	7:E:57:LYS:HD2	1.79	0.40
3:A:659:G:O5'	7:E:95:LYS:HD3	2.21	0.40
10:H:42:LYS:HG2	10:H:46:PHE:CE2	2.49	0.40
12:J:109:ILE:HG22	12:J:129:ILE:HD12	2.03	0.40
1:1:48:G:H3'	1:1:49:G:H8	1.86	0.40
3:A:120:U:C2	3:A:149:A:C6	3.10	0.40
3:A:1859:U:H2'	3:A:1860:G:H8	1.86	0.40
3:A:2000:C:OP1	17:O:5:LYS:NZ	2.49	0.40
3:A:2898:U:H2'	3:A:2899:A:H8	1.86	0.40
3:A:535:G:C6	3:A:559:G:C6	3.09	0.40
4:B:94:A:C5	4:B:95:U:C4	3.09	0.40
13:K:88:THR:HG23	13:K:91:GLU:OE1	2.21	0.40
25:W:40:ILE:HD12	25:W:42:LEU:HD21	2.03	0.40
28:Z:39:GLN:HB3	28:Z:41:HIS:ND1	2.35	0.40
3:A:2075:U:H4'	3:A:2596:U:O2	2.22	0.40
3:A:2407:A:H2'	3:A:2408:U:C6	2.56	0.40
3:A:2518:A:N3	3:A:2518:A:H2'	2.36	0.40
3:A:500:G:N1	3:A:503:A:OP2	2.52	0.40
9:G:95:ARG:HD2	9:G:128:GLN:HB3	2.03	0.40
10:H:26:ALA:HA	10:H:30:LEU:HB2	2.04	0.40
13:K:13:ARG:HB3	13:K:53:TYR:HE1	1.87	0.40
28:Z:42:LEU:HD23	28:Z:42:LEU:HA	1.71	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1903:G:N3	3:A:1904:G:C8	2.90	0.40
3:A:2365:G:H4'	26:X:60:PHE:CE1	2.56	0.40
3:A:2662:A:O5'	3:A:2662:A:H8	2.04	0.40
3:A:613:A:H8	3:A:613:A:OP1	2.05	0.40
3:A:681:G:C2	3:A:797:G:C2	3.10	0.40
6:D:201:LEU:HD23	6:D:201:LEU:HA	1.83	0.40
9:G:145:ALA:HB1	9:G:164:TYR:HE1	1.85	0.40
13:K:109:LEU:HD23	13:K:109:LEU:HA	1.96	0.40
13:K:7:LYS:HA	13:K:8:PRO:HD3	1.74	0.40
15:M:90:VAL:HG13	15:M:95:LEU:HD21	2.03	0.40
20:R:95:LEU:HA	20:R:95:LEU:HD23	1.84	0.40
21:S:41:ILE:HD13	21:S:103:ALA:HA	2.02	0.40
22:T:17:VAL:HG12	22:T:76:VAL:HG21	2.03	0.40
3:A:922:C:H1'	26:X:26:PHE:CD1	2.57	0.40
3:A:1086:A:H4'	3:A:1103:A:C2	2.57	0.40
3:A:1365:A:C6	3:A:1366:A:C5	3.10	0.40
3:A:1548:A:H2'	3:A:1549:A:C8	2.56	0.40
3:A:2750:A:H8	3:A:2750:A:OP1	2.04	0.40
3:A:570:G:H2'	3:A:2030:A:N7	2.37	0.40
5:C:157:SER:HB3	5:C:160:THR:HG21	2.03	0.40
5:C:89:ALA:HA	5:C:158:ALA:HB2	2.04	0.40
11:I:85:VAL:HG21	11:I:90:GLY:O	2.21	0.40
12:J:113:LYS:HG3	12:J:129:ILE:CD1	2.52	0.40
17:O:8:ARG:HG3	17:O:43:GLU:OE1	2.21	0.40
19:Q:63:LYS:HE3	19:Q:65:SER:OG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
5	C	269/273 (98%)	262 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	D	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
7	E	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	34	77
8	F	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
9	G	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
10	H	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
11	I	123/165 (74%)	113 (92%)	9 (7%)	1 (1%)	24	70
12	J	132/142 (93%)	125 (95%)	7 (5%)	0	100	100
13	K	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
14	L	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
17	O	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
20	R	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
23	U	93/100 (93%)	89 (96%)	4 (4%)	0	100	100
24	V	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
26	X	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
28	Z	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
29	a	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
30	b	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
31	c	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
33	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100
35	i	84/450 (19%)	84 (100%)	0	0	100	100
36	k	16/18 (89%)	12 (75%)	4 (25%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3532/4042 (87%)	3424 (97%)	106 (3%)	2 (0%)	59 90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	E	6	LYS
11	I	108	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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
5	C	216/218 (99%)	198 (92%)	18 (8%)	14 52
6	D	164/164 (100%)	155 (94%)	9 (6%)	27 68
7	E	165/165 (100%)	157 (95%)	8 (5%)	31 71
8	F	148/150 (99%)	135 (91%)	13 (9%)	12 50
9	G	137/138 (99%)	128 (93%)	9 (7%)	21 62
10	H	114/114 (100%)	104 (91%)	10 (9%)	12 50
11	I	95/123 (77%)	90 (95%)	5 (5%)	28 69
12	J	104/110 (94%)	95 (91%)	9 (9%)	13 50
13	K	116/116 (100%)	106 (91%)	10 (9%)	13 51
14	L	104/104 (100%)	95 (91%)	9 (9%)	13 50
15	M	103/103 (100%)	99 (96%)	4 (4%)	39 75
16	N	109/109 (100%)	101 (93%)	8 (7%)	17 58
17	O	102/103 (99%)	95 (93%)	7 (7%)	19 60
18	P	87/87 (100%)	83 (95%)	4 (5%)	33 72
19	Q	99/100 (99%)	95 (96%)	4 (4%)	38 75
20	R	89/90 (99%)	83 (93%)	6 (7%)	20 62
21	S	84/84 (100%)	80 (95%)	4 (5%)	31 71
22	T	93/93 (100%)	88 (95%)	5 (5%)	27 68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	82/84 (98%)	77 (94%)	5 (6%)	23	65
24	V	83/85 (98%)	77 (93%)	6 (7%)	18	58
25	W	78/78 (100%)	72 (92%)	6 (8%)	16	56
26	X	57/63 (90%)	52 (91%)	5 (9%)	12	50
27	Y	67/68 (98%)	63 (94%)	4 (6%)	24	65
28	Z	54/55 (98%)	49 (91%)	5 (9%)	11	47
29	a	48/49 (98%)	47 (98%)	1 (2%)	61	86
30	b	47/48 (98%)	40 (85%)	7 (15%)	4	26
31	c	45/49 (92%)	42 (93%)	3 (7%)	20	62
32	d	38/38 (100%)	32 (84%)	6 (16%)	3	23
33	e	51/52 (98%)	47 (92%)	4 (8%)	16	55
34	f	34/34 (100%)	34 (100%)	0	100	100
35	i	71/313 (23%)	65 (92%)	6 (8%)	13	52
36	k	17/17 (100%)	17 (100%)	0	100	100
All	All	2901/3204 (90%)	2701 (93%)	200 (7%)	24	60

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	3	VAL
5	C	20	VAL
5	C	24	LEU
5	C	72	ASP
5	C	77	VAL
5	C	94	VAL
5	C	120	VAL
5	C	125	LYS
5	C	130	LEU
5	C	144	VAL
5	C	147	LYS
5	C	156	ARG
5	C	172	VAL
5	C	182	ARG
5	C	192	LEU
5	C	194	GLU
5	C	207	LYS
5	C	242	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	12	THR
6	D	13	ARG
6	D	18	ASP
6	D	22	ILE
6	D	24	VAL
6	D	62	LYS
6	D	97	SER
6	D	128	ARG
6	D	203	VAL
7	E	7	ASP
7	E	65	THR
7	E	72	SER
7	E	73	ILE
7	E	97	ASN
7	E	105	LEU
7	E	125	SER
7	E	162	ARG
8	F	3	LYS
8	F	14	LYS
8	F	51	ASP
8	F	57	LEU
8	F	85	ILE
8	F	106	ILE
8	F	121	SER
8	F	130	MET
8	F	133	ARG
8	F	144	ASP
8	F	149	VAL
8	F	152	LEU
8	F	153	ASP
9	G	10	VAL
9	G	11	VAL
9	G	30	ASN
9	G	45	HIS
9	G	69	ARG
9	G	74	SER
9	G	114	ASP
9	G	127	THR
9	G	153	ARG
10	H	8	LYS
10	H	15	LEU
10	H	21	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	H	22	LYS
10	H	58	LEU
10	H	60	GLU
10	H	79	THR
10	H	110	VAL
10	H	121	VAL
10	H	142	VAL
11	I	85	VAL
11	I	88	HIS
11	I	109	LYS
11	I	113	PHE
11	I	123	ILE
12	J	28	LEU
12	J	35	ILE
12	J	40	LYS
12	J	55	ILE
12	J	90	SER
12	J	101	ILE
12	J	112	THR
12	J	117	MET
12	J	128	SER
13	K	17	VAL
13	K	28	LEU
13	K	34	ARG
13	K	40	HIS
13	K	64	VAL
13	K	69	ARG
13	K	88	THR
13	K	91	GLU
13	K	124	VAL
13	K	131	ASN
14	L	9	ASN
14	L	21	CYS
14	L	24	VAL
14	L	49	ARG
14	L	58	LEU
14	L	61	VAL
14	L	69	VAL
14	L	71	ARG
14	L	73	ASP
15	M	7	SER
15	M	59	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	M	67	THR
15	M	116	VAL
16	N	6	ARG
16	N	67	VAL
16	N	78	LEU
16	N	102	LEU
16	N	105	MET
16	N	110	GLU
16	N	132	THR
16	N	135	VAL
17	O	2	ARG
17	O	17	ARG
17	O	27	SER
17	O	37	THR
17	O	38	LEU
17	O	69	ARG
17	O	79	LEU
18	P	5	SER
18	P	53	THR
18	P	78	VAL
18	P	116	GLN
19	Q	7	GLN
19	Q	21	ARG
19	Q	68	GLU
19	Q	92	VAL
20	R	6	ARG
20	R	9	ILE
20	R	16	LYS
20	R	17	ILE
20	R	51	ARG
20	R	110	VAL
21	S	45	GLU
21	S	51	VAL
21	S	68	ARG
21	S	70	GLU
22	T	12	SER
22	T	42	LYS
22	T	67	ASP
22	T	70	LYS
22	T	95	ARG
23	U	17	SER
23	U	30	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	U	61	LEU
23	U	72	GLN
23	U	79	ASP
24	V	12	ILE
24	V	28	VAL
24	V	52	LEU
24	V	65	ILE
24	V	67	VAL
24	V	68	SER
25	W	20	LEU
25	W	25	LYS
25	W	41	GLU
25	W	65	VAL
25	W	76	ASP
25	W	92	VAL
26	X	11	ARG
26	X	41	ARG
26	X	72	LYS
26	X	76	ASN
26	X	77	ARG
27	Y	4	VAL
27	Y	28	ARG
27	Y	44	LYS
27	Y	68	LEU
28	Z	2	LYS
28	Z	5	GLU
28	Z	14	LEU
28	Z	48	ARG
28	Z	58	ASN
29	a	36	VAL
30	b	5	GLN
30	b	9	THR
30	b	26	THR
30	b	28	LEU
30	b	32	LYS
30	b	43	ILE
30	b	52	ARG
31	c	5	ILE
31	c	6	ARG
31	c	46	HIS
32	d	1	MET
32	d	12	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	d	22	MET
32	d	24	THR
32	d	25	LYS
32	d	41	ARG
33	e	6	THR
33	e	8	ARG
33	e	29	LEU
33	e	31	HIS
35	i	337	GLN
35	i	369	ASP
35	i	379	ILE
35	i	421	ASP
35	i	425	ARG
35	i	430	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
5	C	134	ASN
5	C	251	GLN
6	D	140	HIS
7	E	90	GLN
7	E	136	GLN
7	E	165	HIS
8	F	5	HIS
8	F	63	GLN
8	F	81	GLN
9	G	22	GLN
9	G	38	ASN
9	G	111	HIS
9	G	143	GLN
10	H	33	GLN
12	J	31	GLN
12	J	111	GLN
16	N	3	GLN
16	N	13	HIS
17	O	11	ASN
17	O	62	ASN
18	P	29	HIS
18	P	100	HIS
19	Q	7	GLN
20	R	14	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R	37	GLN
22	T	7	HIS
24	V	74	ASN
26	X	46	HIS
28	Z	39	GLN
30	b	5	GLN
30	b	19	HIS
35	i	381	ASN
36	k	29	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	42/113 (37%)	12 (28%)	0
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	488 (16%)	17 (0%)
4	B	119/120 (99%)	16 (13%)	0
All	All	3041/3139 (96%)	517 (17%)	17 (0%)

All (517) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	C
1	1	36	U
1	1	37	U
1	1	38	U
1	1	39	A
1	1	41	C
1	1	42	A
1	1	43	G
1	1	46	C
1	1	57	G
1	1	58	G
1	1	70	G
2	2	76	A
3	A	10	A
3	A	12	U
3	A	15	G
3	A	34	U
3	A	46	G
3	A	49	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	58	G
3	A	63	A
3	A	71	A
3	A	74	A
3	A	75	G
3	A	79	C
3	A	80	G
3	A	93	G
3	A	96	C
3	A	101	A
3	A	102	U
3	A	118	A
3	A	119	A
3	A	120	U
3	A	137	U
3	A	138	U
3	A	139	U
3	A	140	C
3	A	141	G
3	A	142	A
3	A	158	U
3	A	163	C
3	A	181	A
3	A	196	A
3	A	199	A
3	A	204	A
3	A	214	G
3	A	215	G
3	A	216	A
3	A	221	A
3	A	222	A
3	A	248	G
3	A	250	G
3	A	266	G
3	A	272	A
3	A	276	U
3	A	277	G
3	A	279	A
3	A	285	G
3	A	286	U
3	A	302	C
3	A	311	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	328	U
3	A	329	G
3	A	330	A
3	A	331	C
3	A	353	C
3	A	354	A
3	A	356	G
3	A	361	G
3	A	362	A
3	A	370	G
3	A	372	G
3	A	386	G
3	A	396	G
3	A	411	G
3	A	412	A
3	A	424	G
3	A	451	U
3	A	454	A
3	A	455	C
3	A	479	A
3	A	481	G
3	A	491	G
3	A	494	G
3	A	504	A
3	A	505	A
3	A	509	C
3	A	529	A
3	A	530	G
3	A	531	C
3	A	532	A
3	A	533	G
3	A	538	A
3	A	543	G
3	A	544	C
3	A	549	G
3	A	563	A
3	A	573	U
3	A	575	A
3	A	587	C
3	A	603	A
3	A	607	U
3	A	613	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	614	A
3	A	615	U
3	A	618	G
3	A	621	A
3	A	627	A
3	A	637	A
3	A	645	C
3	A	646	U
3	A	647	G
3	A	653	U
3	A	654	A
3	A	655	A
3	A	668	A
3	A	685	A
3	A	686	U
3	A	693	A
3	A	717	C
3	A	726	G
3	A	729	G
3	A	730	A
3	A	738	G
3	A	747	U
3	A	748	G
3	A	757	G
3	A	764	A
3	A	775	G
3	A	776	G
3	A	777	G
3	A	782	A
3	A	784	G
3	A	785	G
3	A	789	A
3	A	790	U
3	A	791	C
3	A	794	A
3	A	800	A
3	A	805	G
3	A	812	C
3	A	827	U
3	A	828	U
3	A	831	G
3	A	845	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	846	U
3	A	858	G
3	A	859	G
3	A	869	G
3	A	878	A
3	A	896	A
3	A	899	A
3	A	910	A
3	A	914	G
3	A	915	C
3	A	927	A
3	A	932	U
3	A	935	C
3	A	946	C
3	A	961	C
3	A	973	A
3	A	974	G
3	A	983	A
3	A	985	C
3	A	996	A
3	A	1002	G
3	A	1012	U
3	A	1013	C
3	A	1022	G
3	A	1023	U
3	A	1025	G
3	A	1026	G
3	A	1027	A
3	A	1033	U
3	A	1046	A
3	A	1057	A
3	A	1070	A
3	A	1083	U
3	A	1084	A
3	A	1087	G
3	A	1088	A
3	A	1097	U
3	A	1101	U
3	A	1111	A
3	A	1112	G
3	A	1119	U
3	A	1130	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1132	U
3	A	1133	A
3	A	1135	C
3	A	1136	G
3	A	1141	U
3	A	1142	A
3	A	1165	A
3	A	1167	C
3	A	1173	U
3	A	1182	G
3	A	1197	G
3	A	1212	G
3	A	1218	G
3	A	1224	U
3	A	1236	G
3	A	1238	G
3	A	1252	G
3	A	1253	A
3	A	1256	G
3	A	1271	G
3	A	1272	A
3	A	1294	U
3	A	1300	G
3	A	1301	A
3	A	1317	G
3	A	1321	A
3	A	1332	G
3	A	1345	C
3	A	1352	U
3	A	1365	A
3	A	1379	U
3	A	1383	A
3	A	1386	C
3	A	1395	A
3	A	1416	G
3	A	1417	C
3	A	1424	G
3	A	1428	C
3	A	1434	A
3	A	1449	G
3	A	1451	C
3	A	1452	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1453	A
3	A	1458	U
3	A	1460	U
3	A	1478	G
3	A	1482	G
3	A	1489	C
3	A	1490	A
3	A	1491	G
3	A	1493	C
3	A	1494	A
3	A	1495	A
3	A	1497	U
3	A	1498	C
3	A	1509	A
3	A	1510	G
3	A	1515	A
3	A	1524	G
3	A	1529	G
3	A	1532	A
3	A	1533	C
3	A	1535	A
3	A	1537	G
3	A	1546	G
3	A	1554	U
3	A	1566	A
3	A	1569	A
3	A	1578	U
3	A	1581	G
3	A	1583	A
3	A	1584	U
3	A	1585	C
3	A	1607	C
3	A	1608	A
3	A	1643	G
3	A	1647	U
3	A	1648	U
3	A	1649	G
3	A	1656	C
3	A	1674	G
3	A	1677	A
3	A	1698	A
3	A	1715	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1729	U
3	A	1730	C
3	A	1731	G
3	A	1732	C
3	A	1733	G
3	A	1738	G
3	A	1756	G
3	A	1758	U
3	A	1759	A
3	A	1764	C
3	A	1773	A
3	A	1784	A
3	A	1791	A
3	A	1800	C
3	A	1801	A
3	A	1802	A
3	A	1808	A
3	A	1811	G
3	A	1816	C
3	A	1829	A
3	A	1833	C
3	A	1847	A
3	A	1848	A
3	A	1849	G
3	A	1850	G
3	A	1857	G
3	A	1870	C
3	A	1871	A
3	A	1872	A
3	A	1889	A
3	A	1906	G
3	A	1927	A
3	A	1929	G
3	A	1937	A
3	A	1939	U
3	A	1955	U
3	A	1960	A
3	A	1962	C
3	A	1964	G
3	A	1966	A
3	A	1967	C
3	A	1970	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1971	U
3	A	1972	G
3	A	1982	U
3	A	1991	U
3	A	1993	U
3	A	1997	C
3	A	2023	C
3	A	2027	G
3	A	2030	A
3	A	2031	A
3	A	2033	A
3	A	2043	C
3	A	2049	G
3	A	2050	C
3	A	2055	C
3	A	2056	G
3	A	2060	A
3	A	2061	G
3	A	2062	A
3	A	2069	G
3	A	2092	U
3	A	2093	G
3	A	2097	A
3	A	2101	A
3	A	2103	C
3	A	2105	U
3	A	2106	U
3	A	2108	A
3	A	2111	U
3	A	2112	G
3	A	2113	U
3	A	2114	A
3	A	2116	G
3	A	2117	A
3	A	2118	U
3	A	2119	A
3	A	2120	G
3	A	2123	G
3	A	2125	G
3	A	2126	A
3	A	2128	G
3	A	2131	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2132	U
3	A	2133	G
3	A	2134	A
3	A	2137	U
3	A	2145	C
3	A	2146	C
3	A	2147	A
3	A	2148	G
3	A	2149	U
3	A	2158	A
3	A	2159	G
3	A	2160	C
3	A	2161	C
3	A	2163	A
3	A	2164	C
3	A	2165	C
3	A	2167	U
3	A	2168	G
3	A	2169	A
3	A	2170	A
3	A	2171	A
3	A	2172	U
3	A	2173	A
3	A	2177	C
3	A	2178	C
3	A	2179	C
3	A	2185	U
3	A	2187	U
3	A	2190	G
3	A	2198	A
3	A	2203	U
3	A	2204	G
3	A	2211	A
3	A	2212	A
3	A	2223	G
3	A	2225	A
3	A	2238	G
3	A	2239	G
3	A	2243	U
3	A	2250	G
3	A	2259	U
3	A	2279	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2280	G
3	A	2283	C
3	A	2287	A
3	A	2297	A
3	A	2301	C
3	A	2305	U
3	A	2308	G
3	A	2322	A
3	A	2325	G
3	A	2326	C
3	A	2336	A
3	A	2345	G
3	A	2347	C
3	A	2350	C
3	A	2357	G
3	A	2383	G
3	A	2385	C
3	A	2388	A
3	A	2402	U
3	A	2406	A
3	A	2420	C
3	A	2421	G
3	A	2422	C
3	A	2423	U
3	A	2424	C
3	A	2425	A
3	A	2426	A
3	A	2429	G
3	A	2430	A
3	A	2431	U
3	A	2432	A
3	A	2433	A
3	A	2434	A
3	A	2435	A
3	A	2440	C
3	A	2441	U
3	A	2445	G
3	A	2447	G
3	A	2448	A
3	A	2464	G
3	A	2476	A
3	A	2480	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2491	U
3	A	2501	C
3	A	2502	G
3	A	2505	G
3	A	2518	A
3	A	2525	G
3	A	2527	C
3	A	2529	G
3	A	2535	G
3	A	2547	A
3	A	2553	G
3	A	2566	A
3	A	2567	G
3	A	2569	G
3	A	2573	C
3	A	2576	G
3	A	2585	U
3	A	2586	U
3	A	2602	A
3	A	2603	G
3	A	2609	U
3	A	2613	U
3	A	2615	U
3	A	2623	G
3	A	2629	U
3	A	2630	G
3	A	2633	G
3	A	2636	C
3	A	2646	C
3	A	2661	G
3	A	2689	U
3	A	2690	U
3	A	2714	G
3	A	2726	A
3	A	2733	A
3	A	2742	G
3	A	2744	G
3	A	2748	A
3	A	2757	A
3	A	2758	A
3	A	2762	C
3	A	2765	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	2778	A
3	A	2779	U
3	A	2791	G
3	A	2792	A
3	A	2798	U
3	A	2818	U
3	A	2820	A
3	A	2823	A
3	A	2825	G
3	A	2833	U
3	A	2835	A
3	A	2836	U
3	A	2867	G
3	A	2873	A
3	A	2879	A
3	A	2880	C
3	A	2884	U
3	A	2886	A
3	A	2888	C
3	A	2891	U
4	B	9	G
4	B	13	G
4	B	24	G
4	B	35	C
4	B	41	G
4	B	55	U
4	B	56	G
4	B	57	A
4	B	58	A
4	B	67	G
4	B	68	C
4	B	70	C
4	B	88	C
4	B	89	U
4	B	90	C
4	B	109	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	100	U
3	A	613	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	627	A
3	A	645	C
3	A	653	U
3	A	784	G
3	A	805	G
3	A	1110	G
3	A	1344	U
3	A	1494	A
3	A	1730	C
3	A	2127	G
3	A	2158	A
3	A	2422	C
3	A	2430	A
3	A	2602	A
3	A	2756	U

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 432 ligands modelled in this entry, 432 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.