



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 30, 2020 – 01:21 PM EST

PDB ID : 6V3B  
EMDB ID: : EMD-21032  
Title : Cryo-EM structure of the Acinetobacter baumannii Ribosome: 70S in Empty state  
Authors : Morgan, C.E.; Yu, E.W.  
Deposited on : 2019-11-25  
Resolution : 2.91 Å(reported)  
Based on PDB ID : 5AFI

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

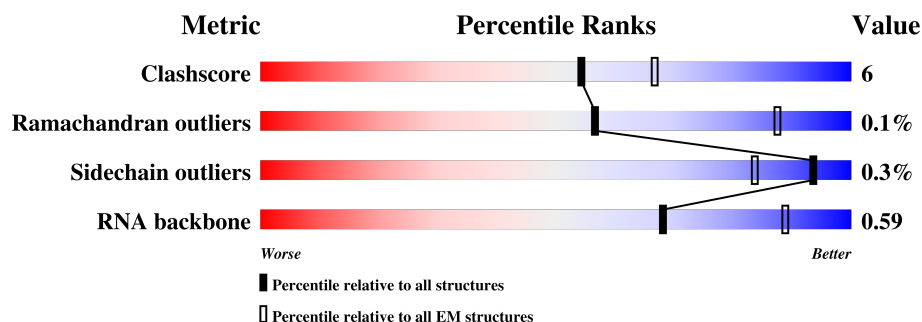
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.91 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.








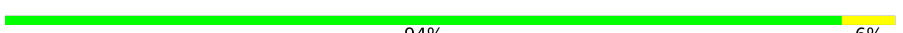



















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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  $\geq 3$ , 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	0	51	92% 8%
2	1	44	86% 14%
3	2	64	77% 17% . . .
4	3	38	92% 8%
5	AN1	2918	64% 30% 5% .
6	B	115	53% 37% 9% .
7	C	274	89% 10% .
8	D	212	92% 8%

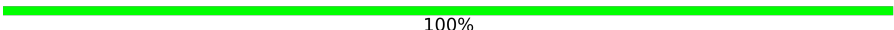
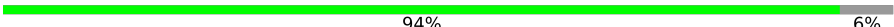


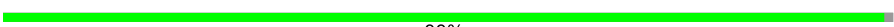









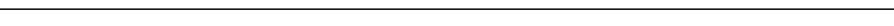


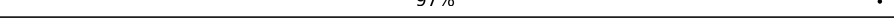
*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26	V	85	
27	W	78	
28	X	65	
29	Y	58	
30	Z	61	
31	sN1	1544	
32	b	250	
33	c	250	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
34	d	208	 100%
35	e	165	 94% 6%
36	f	127	 74% 26%
37	g	156	 89% 10%
38	h	131	 99% .
39	i	128	 98% ..
40	j	103	 97% .
41	k	128	 91% 9%
42	l	124	 98% .
43	m	118	 97% .
44	n	101	 99% .
45	o	89	 99% .
46	p	101	 81% 18%
47	q	85	 94% 6%
48	r	75	 71% 29%
49	s	91	 90% 10%
50	t	88	 97% .
51	u	71	 28% 70%

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 140290 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 protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			363	222	85	54	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AN1	2892	Total	C	N	O	P	0	0
			62023	27689	11345	20098	2891		

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	270	Total	C	N	O	S	0	0
			2096	1291	434	363	8		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	186	Total	C	N	O	S	0	0
			1419	893	265	257	4		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1381	877	247	249	8		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	174	Total	C	N	O	S	0	0
			1318	832	236	249	1		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	122	Total	C	N	O	S	0	0
			946	592	180	169	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	146	Total	C	N	O	S	0	0
			1089	673	215	200	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	137	Total	C	N	O	S	0	0
			1087	687	210	185	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			942	590	186	163	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total	C	N	O	S	0	0
			857	528	173	155	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	117	Total	C	N	O	0	0
			919	578	177	164		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	103	Total	C	N	O	S	0	0
			807	506	155	143	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	109	Total	C	N	O	S	0	0
			826	514	158	150	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	90	Total	C	N	O		0	0
			702	447	127	128			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	100	Total	C	N	O		0	0
			749	465	139	145			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	97	Total	C	N	O	S	0	0
			760	477	143	139	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	80	Total	C	N	O	S	0	0
			598	370	115	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	77	Total	C	N	O	S	0	0
			632	395	130	105	2		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	62	Total	C	N	O	S	0	0
			498	308	96	93	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	58	Total	C	N	O	S	0	0
			463	286	88	85	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	55	Total	C	N	O	S	0	0
			456	271	102	82	1		

- Molecule 31 is a RNA chain called 16s Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	sN1	1528	Total	C	N	O	P	0	0
			32782	14631	5994	10630	1527		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	225	Total	C	N	O	S	0	0
			1769	1110	328	325	6		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	215	Total	C	N	O	S	0	0
			1690	1065	318	299	8		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1631	1017	313	299	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	94	Total	C	N	O	S	0	0
			793	499	147	143	4		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	141	Total	C	N	O	S	0	0
			1111	696	210	199	6		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	130	Total	C	N	O	S	0	0
			985	615	177	187	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	127	Total	C	N	O	S	0	0
			995	621	198	175	1		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	100	Total	C	N	O	S	0	0
			801	500	150	148	3		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	117	Total	C	N	O	S	0	0
			862	535	167	159	1		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	122	Total	C	N	O	S	0	0
			945	580	193	167	5		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	115	Total	C	N	O	S	0	0
			903	558	184	158	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			705	434	144	126	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	83	Total	C	N	O	S	0	0
			649	406	129	113	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	80	Total	C	N	O	S	0	0
			630	396	118	115	1		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	53	Total	C	N	O	0	0
			438	282	75	81		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			646	412	125	107	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	85	Total	C	N	O	S	0	0
			658	406	138	112	2		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	u	21	Total	C	N	O	0	0
			182	115	37	30		

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	3	1	Total	Zn	0
			1	1	

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	AN1	52	Total	Mg	0
			52	52	
53	sN1	41	Total	Mg	0
			41	41	

- Molecule 54 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
54	AN1	1	Total	Na	0
			1	1	

- Molecule 55 is water.

Mol	Chain	Residues	Atoms		AltConf
55	3	1	Total	O	0
			1	1	
55	AN1	253	Total	O	0
			253	253	

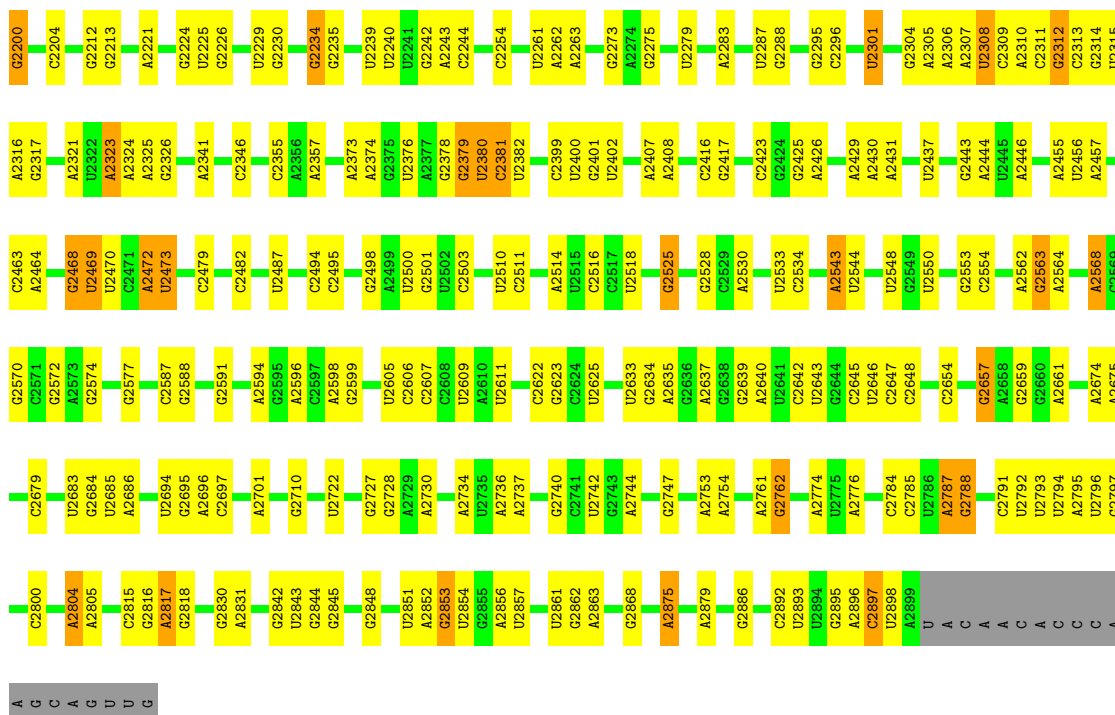
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
55	B	5	Total 5	O 5	0
55	C	3	Total 3	O 3	0
55	D	3	Total 3	O 3	0
55	E	2	Total 2	O 2	0
55	K	3	Total 3	O 3	0
55	M	1	Total 1	O 1	0
55	P	1	Total 1	O 1	0
55	Q	3	Total 3	O 3	0
55	R	1	Total 1	O 1	0
55	V	2	Total 2	O 2	0
55	Y	1	Total 1	O 1	0
55	Z	1	Total 1	O 1	0
55	sN1	107	Total 107	O 107	0
55	g	1	Total 1	O 1	0
55	h	1	Total 1	O 1	0
55	i	2	Total 2	O 2	0
55	m	2	Total 2	O 2	0
55	n	1	Total 1	O 1	0
55	s	3	Total 3	O 3	0
55	t	1	Total 1	O 1	0

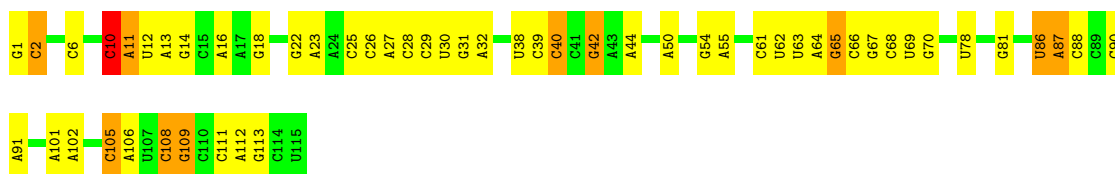


A2122	G2028	A1914	U1826	U1712	A1564	U1477	A1381	G1242	U1078	A976	A861	U745	A625	G517	U359
G2123	A2029	A1915	G1827	U1713	A1567	G1478	U1382	A1242	U1079	A977	G862	A750	G626	C518	A364
G2124	U2030	C1916	C1828	G1714	A1568	U1479	A1387	G1245	A1080	A978	C963	A750	A627	A519	U365
	C2039	G1917	C1829	G1715	A1569	U1480	A1387	G1245	A1081	C979	C963	A754	A630	G521	G366
U2127	G2048	G1918	U1830	G1717	A1570	U1481	U1388	A1248	A1082	A980	G873	A755	A631	C526	A367
G2129	G2049	U1919	G1831	G1718	A1571	U1482	U1389	A1248	A1083	A981	C874	A756	A632	A527	C368
A2130	A2050	C1920	G1835	U1719	U1574	U1485	A1390	G1251	A1084	A993	C875	A757	A633	A528	G370
A2131	G2051	U1921	G1836	U1720	U1575	G1486	U1407	G1252	A1085	A994	U875	A758	A634	A529	C371
G2132	G2052	A1922	U1837	C1726	A1577	C1488	A1408	A1287	A1086	A997	U876	A759	A635	C530	U372
C2133		A1923	G1842	G1727	U1578	U1489	A1409	A1288	A1087	A998	G877	A760	A636	A531	A373
	A2066	G1924	A1843	U1730	U1579	A1490	U1412	A1270	C1089	A999	G878	A761	A637		
A2137	G2057	G1925	G1844	C1731	U1580	A1491	G1413	A1271	C1090	U1004	G879	A762	A638		
A2138		U1932	U1846	G1734	A1581		A1414	G1272	A1091	A1005	G880	A763	A639		
	A2058	A1933	U1847	U1735	U1582	G1498	U1415	G1273	A1095	A1006	G881		A644		
	C2059	A1934	U1848	C1736	U1583	G1499	A1416	G1274	A1096	U1007	U882		A645		
	G2060	U1935	U1849	G1737	A1584	U1500	G1417	G1275	G1097	U1008	C983		A646		
C2061	C2061	U1936	U1850	U1738	U1585	U1501	G1418	U1276	A1100	U1009	A884		A647		
G2065	G2065	C1937	U1851	G1742	U1586	C1502	G1421	U1277	A1101	C1010	C887		A648		
A2066	A2066	U1938	U1852	A1743	C1503	U1503	A1422	G1287	C1101	A1011	C888		A649		
A2067	C2067	U1939	U1853	C1744	A1591	U1504	C1423	U1288	U1102	G1023	C889		A650		
C2068	G1863	U1940	G1745	U1745	A1592	U1505	G1424	U1289	A1103	A1024	A890		A651		
G2150	G2069	U1941	G1746	G1746	A1593	A1506	A1425	A1296	G1104	A1025	A891		A652		
U2070	U2070	C1943	G1749	G1749	A1594	G1510	G1426	A1297	A1108	C1026	A892		A653		
U2071	U2071	U1944	C1750	C1750	C1603	G1511	A1427	G1303	A1109	G1027	A893		A654		
U2072	U2072	G1950	U1866	U1751	C1604	G1512	A1428	G1304	U1110	G1028	C995		A655		
A2154	U1951	U1951	A1867	G1752	A1606	U1519	C1432	G1305	G1112	A1029	C996		A656		
	U1959	U1959	C1870	G1759	A1616	G1521	A1436	U1308	G1113	U1032	A894		A657		
C2077	A2078	G1960	U1871	G1760	G1617	C1522	A1437	C1310	G1121	A1036	A903		A658		
U2157	U2157	C1961	A1872	G1761	G1617	C1523	U1438	G1311	U1129	A1037	U904		A659		
U2158	G2089	U1962	C1875	C1767	A1623	U1526	A1439	G1312	A1130	G1038	A908		A660		
U2159	A2090	C1963	U1876	A1768	A1624	U1527	G1440	G1313	G1131	G1039	A909		A661		
C2161	A2091	U1964	C1877	U1769	A1624	U1528	C1441	A1316	C1040	G693	C803		A662		
U2163	U2093	U1965	U1878	U1775	G1634	U1529	C1442	U1324	A1132	A1041	A899		A663		
G2164	U2094	U1966	U1879	A1776	A1635	U1530	C1443	U1325	G1133	U1042	C900		A664		
A2165	U2095	G1968	G1880		A1635	U1531	G1444	U1326	G1134	U1043	A903		A665		
A2166	G2096	U1978	A1885	A1780	C1642	U1532	G1445	G1336	A1140	G1044	A904		A666		
A2167	A2097	U1979	C1888	U1792	U1645	U1533	U1448	U1337	U1148	G1053	U905		A667		
U2168	C2098	U1980	C1889	U1793	U1646	U1534	U1449	C1340	G1149	A1054	G926		A668		
A2169	C2099	G1983	C1890	C1793	U1647	U1535	U1450	U1341	U1150	U1057	C927		A669		
C2171	U2104	U1984	A1895	G1796	A1662	U1536	U1451	A1348	U1167	U1058	C928		A670		
A2172	U2105	C1992	U1899	A1797	U1663	U1537	U1452	A1349	U1170	U1059	U929		A671		
G2173	G2106	U1993	C1899	A1798	G1665	U1538	G1462	G1356	U1171	G1060	A938		A672		
C2174	U2107	A2010	G1902	A1799	G1666	U1539	A1463	C1357	U1172	G1061	A939		A673		
G2175	G2108	A2011	C1903	A1804	G1672	U1540	A1464	C1358	U1173	U1062	A940		A674		
U2176	U2109	A2012	C1904	U1805	U1679	U1541	A1465	G1359	G1179	U1063	A941		A675		
G2177	G2111	U2018	C1905	A1806	G1680	U1542	G1466	A1360	U1180	U1064	A942		A676		
G2178	G2112	G2020	G1906	G1807	U1681	U1543	G1467	A1361	U1181	A1065	A943		A677		
	A2113	C2021	U1907	U1808	U1682	U1544	A1468	G1362	U1182	U1066	A944		A678		
U2184	U2185	G2022	U1908	G1812	A1682	U1545	A1469	G1363	U1183	A1067	A945		A679		
G2185	G2186	U2023	A1909	U1813	U1683	U1546	G1470	A1373	A1199	A1068	A946		A680		
A2187	A2187	G2116	U1910	G1814	U1684	U1547	G1471	U1374	A1200	A1069	A947		A681		
G2188	G2188	G2026	U1911	A1817	U1685	U1548	G1472	U1375	A1201	A1070	A948		A682		
	A2190	A2027	A1912	G1818	G1708	U1549	G1473	U1376	G1230	C1076	A970		A683		
	G2120	G2026	A1913	U1819	G1708	U1550	G1474	A1378	G1231	C1077	A971		A684		
A2194	G2121	G2121	U1913	A1825	A1825	U1551	A1476	A1379					A685		



• Molecule 6: 5s ribosomal RNA

Chain B: 53% 37% 9%



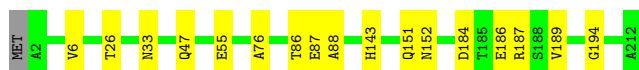
• Molecule 7: 50S ribosomal protein L2

Chain C: 89% 10%



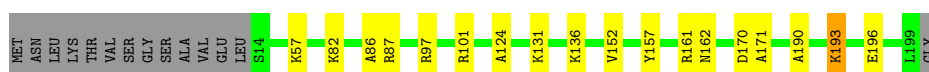
• Molecule 8: 50S ribosomal protein L3

Chain D: 92% 8%



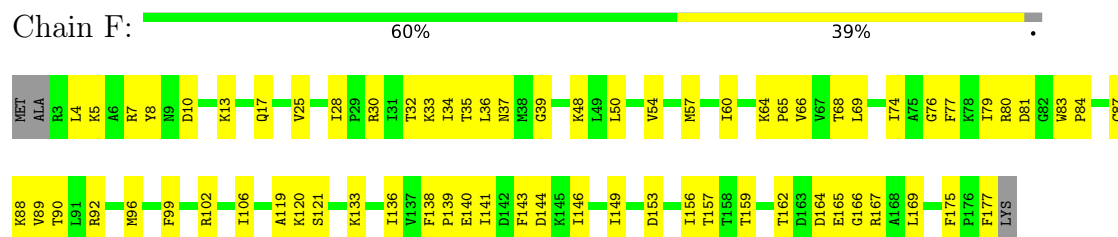
• Molecule 9: 50S ribosomal protein L4

Chain E: 84% 9% 7%

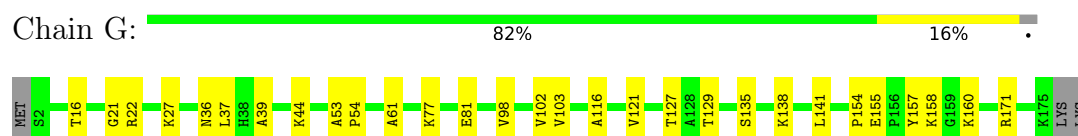




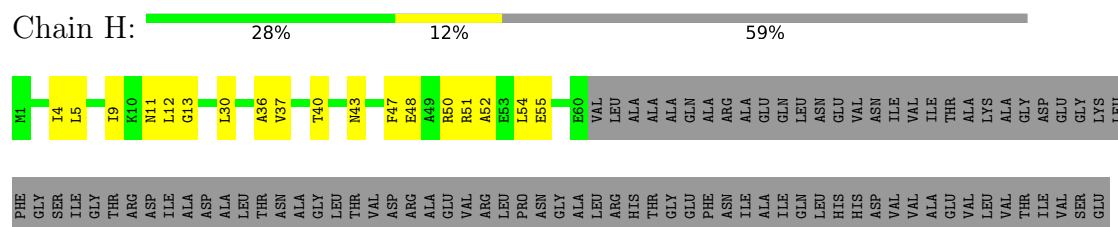
- Molecule 10: 50S ribosomal protein L5



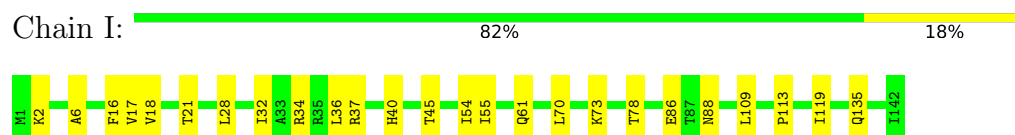
- Molecule 11: 50S ribosomal protein L6



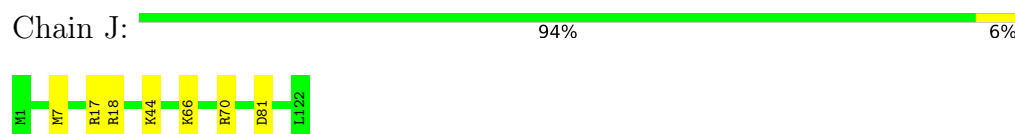
- Molecule 12: 50S ribosomal protein L9



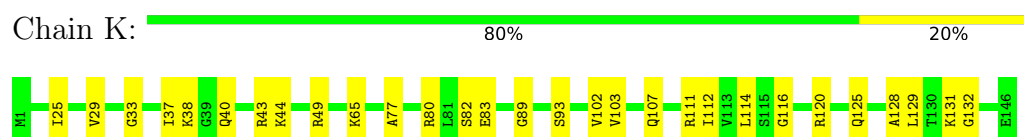
- Molecule 13: 50S ribosomal protein L13



- Molecule 14: 50S ribosomal protein L14



- Molecule 15: 50S ribosomal protein L15



- Molecule 16: 50S ribosomal protein L16





- Molecule 17: 50S ribosomal protein L17

Chain M: 90% 6% 5%



- Molecule 18: 50S ribosomal protein L18

Chain N: 84% 14% .



- Molecule 19: 50S ribosomal protein L19

Chain O: 84% 12% .



- Molecule 20: 50S ribosomal protein L20

Chain P: 91% 8% .



- Molecule 21: 50S ribosomal protein L21

Chain Q: 84% 16%



- Molecule 22: 50S ribosomal protein L22

Chain R: 93% 7%




- Molecule 23: 50S ribosomal protein L23

Chain S: 73% 12% 15%




- Molecule 24: 50S ribosomal protein L24

Chain T:  83% 12% 5%



- Molecule 25: 50S ribosomal protein L25

Chain U:  84% 15% .




- Molecule 26: 50S ribosomal protein L27

Chain V:  87% 7% 6%




- Molecule 27: 50S ribosomal protein L28

Chain W:  90% 9% .




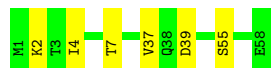
- Molecule 28: 50S ribosomal protein L29

Chain X:  83% 12% 5%



- Molecule 29: 50S ribosomal protein L30

Chain Y:  90% 10%




- Molecule 30: 50S ribosomal protein L32

Chain Z:  77% 13% 10%



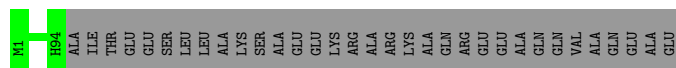
- Molecule 31: 16s Ribosomal RNA

Chain sN1:  85% 14% .


WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

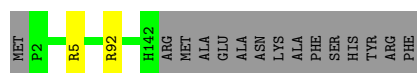
 **EMDataBank**  
Unified Data Resource for 3DEM

Chain f:  74% 26%



- Molecule 37: 30S ribosomal protein S7

Chain g:  89% 10%



- Molecule 38: 30S ribosomal protein S8

Chain h:  99%



- Molecule 39: 30S ribosomal protein S9

Chain i:  98%



- Molecule 40: 30S ribosomal protein S10

Chain j:  97%



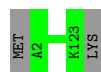
- Molecule 41: 30S ribosomal protein S11

Chain k:  91% 9%



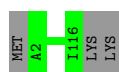
- Molecule 42: 30S ribosomal protein S12

Chain l:  98%



- Molecule 43: 30S ribosomal protein S13

Chain m:  97%



- Molecule 44: 30S ribosomal protein S14

Chain n: 99%



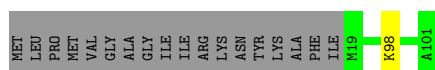
- Molecule 45: 30S ribosomal protein S15

Chain o: 99%



- Molecule 46: 30S ribosomal protein S16

Chain p: 81% 18%



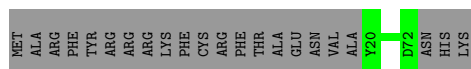
- Molecule 47: 30S ribosomal protein S17

Chain q: 94% 6%



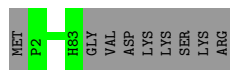
- Molecule 48: 30S ribosomal protein S18

Chain r: 71% 29%



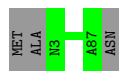
- Molecule 49: 30S ribosomal protein S19

Chain s: 90% 10%

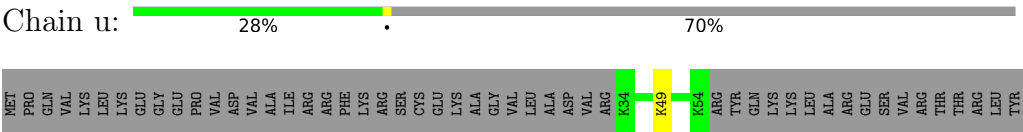


- Molecule 50: 30S ribosomal protein S20

Chain t: 97%



● Molecule 51: 30S ribosomal protein S21



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66318	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, 5MU, ZN, OMG, OMU, MA6, NA, MG, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, 7MG, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 2$	RMSZ	# $ Z  > 2$
1	O	0.24	0/434	0.42	0/573
10	F	0.26	0/1401	0.51	0/1877
11	G	0.26	0/1337	0.43	0/1807
12	H	0.26	0/461	0.51	0/616
13	I	0.25	0/1151	0.40	0/1551
14	J	0.24	0/956	0.45	0/1286
15	K	0.24	0/1097	0.44	0/1461
16	L	0.24	0/1104	0.43	0/1475
17	M	0.24	0/956	0.41	0/1282
18	N	0.24	0/865	0.43	0/1156
19	O	0.24	0/931	0.43	0/1249
2	1	0.23	0/367	0.38	0/481
20	P	0.25	0/947	0.34	0/1262
21	Q	0.23	0/818	0.45	0/1094
22	R	0.23	0/831	0.40	0/1113
23	S	0.25	0/708	0.42	0/947
24	T	0.24	0/753	0.48	0/1010
25	U	0.24	0/770	0.42	0/1036
26	V	0.25	0/606	0.46	0/810
27	W	0.23	0/642	0.43	0/856
28	X	0.23	0/499	0.37	0/662
29	Y	0.23	0/468	0.42	0/624
3	2	0.24	0/515	0.53	1/678 (0.1%)
30	Z	0.23	0/462	0.41	0/615
31	sN1	0.18	0/36476	0.75	6/56895 (0.0%)
32	b	0.26	0/1799	0.49	0/2429
33	c	0.24	0/1714	0.42	0/2304
34	d	0.24	0/1653	0.40	0/2213
35	e	0.24	0/1141	0.43	0/1537
36	f	0.24	0/808	0.48	0/1089
37	g	0.24	0/1127	0.39	0/1511
38	h	0.24	0/993	0.42	0/1331

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	i	0.24	0/1006	0.42	0/1346
4	3	0.23	0/296	0.47	0/389
40	j	0.23	0/811	0.42	0/1096
41	k	0.25	0/878	0.44	0/1189
42	l	0.25	0/958	0.47	0/1284
43	m	0.23	0/913	0.41	0/1226
44	n	0.24	0/803	0.38	0/1071
45	o	0.23	0/715	0.35	0/958
46	p	0.24	0/660	0.41	0/886
47	q	0.22	0/637	0.44	0/858
48	r	0.25	0/445	0.45	0/601
49	s	0.23	0/664	0.39	0/897
5	AN1	0.22	0/69101	0.77	20/107780 (0.0%)
50	t	0.25	0/664	0.36	0/885
51	u	0.30	0/184	0.54	0/240
6	B	0.20	0/2739	0.80	3/4266 (0.1%)
7	C	0.24	0/2136	0.43	0/2869
8	D	0.25	0/1590	0.45	0/2142
9	E	0.24	0/1440	0.41	0/1944
All	All	0.22	0/151430	0.69	30/226757 (0.0%)

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
12	H	0	1
3	2	0	1
All	All	0	2

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	sN1	415	C	N3-C2-O2	-7.48	116.66	121.90
31	sN1	1095	C	N1-C2-O2	6.81	122.99	118.90
31	sN1	1095	C	N3-C2-O2	-6.72	117.20	121.90
5	AN1	788	U	C2-N1-C1'	6.71	125.76	117.70
3	2	32	LEU	CA-CB-CG	6.66	130.62	115.30
5	AN1	1308	U	C2-N1-C1'	6.63	125.66	117.70
5	AN1	2170	C	N1-C2-O2	6.09	122.55	118.90

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	10	C	N1-C2-O2	5.80	122.38	118.90
5	AN1	1889	C	N3-C2-O2	-5.78	117.86	121.90
5	AN1	1308	U	N1-C2-O2	5.77	126.84	122.80
5	AN1	2170	C	N3-C2-O2	-5.69	117.92	121.90
5	AN1	1603	C	N3-C2-O2	-5.64	117.95	121.90
5	AN1	788	U	N1-C2-O2	5.54	126.68	122.80
5	AN1	2116	G	N1-C6-O6	-5.52	116.59	119.90
5	AN1	912	C	C2-N1-C1'	5.51	124.86	118.80
5	AN1	715	C	N1-C2-O2	5.51	122.20	118.90
5	AN1	2473	U	C2-N1-C1'	5.46	124.25	117.70
6	B	10	C	C2-N1-C1'	5.37	124.71	118.80
5	AN1	715	C	C2-N1-C1'	5.34	124.67	118.80
5	AN1	1603	C	N1-C2-O2	5.32	122.09	118.90
5	AN1	1308	U	N3-C2-O2	-5.28	118.50	122.20
31	sN1	1122	U	C2-N1-C1'	5.28	124.03	117.70
5	AN1	2175	C	C2-N1-C1'	5.24	124.56	118.80
5	AN1	368	C	OP2-P-O3'	5.19	116.61	105.20
31	sN1	751	C	C2-N1-C1'	5.18	124.50	118.80
31	sN1	1155	C	C2-N1-C1'	5.11	124.42	118.80
5	AN1	788	U	N3-C2-O2	-5.08	118.64	122.20
5	AN1	1889	C	N1-C2-O2	5.05	121.93	118.90
5	AN1	368	C	P-O3'-C3'	5.02	125.73	119.70
6	B	1	G	C4-N9-C1'	5.02	133.03	126.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	30	HIS	Peptide
12	H	47	PHE	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	0	427	0	462	2	0
2	1	363	0	401	6	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	509	0	566	12	0
4	3	295	0	326	2	0
5	AN1	62023	0	31194	497	0
6	B	2450	0	1241	44	0
7	C	2096	0	2157	19	0
8	D	1572	0	1610	12	0
9	E	1419	0	1464	16	0
10	F	1381	0	1433	53	0
11	G	1318	0	1373	19	0
12	H	458	0	480	12	0
13	I	1125	0	1148	16	0
14	J	946	0	1007	5	0
15	K	1089	0	1159	17	0
16	L	1087	0	1162	6	0
17	M	942	0	987	5	0
18	N	857	0	899	10	0
19	O	919	0	973	9	0
20	P	934	0	997	7	0
21	Q	807	0	842	14	0
22	R	826	0	894	6	0
23	S	702	0	756	10	0
24	T	749	0	797	9	0
25	U	760	0	783	11	0
26	V	598	0	600	4	0
27	W	632	0	667	6	0
28	X	498	0	537	6	0
29	Y	463	0	488	3	0
30	Z	456	0	448	6	0
31	sN1	32782	0	16507	0	0
32	b	1769	0	1787	0	0
33	c	1690	0	1774	0	0
34	d	1631	0	1691	0	0
35	e	1129	0	1174	0	0
36	f	793	0	788	0	0
37	g	1111	0	1163	0	0
38	h	985	0	1047	0	0
39	i	995	0	1053	0	0
40	j	801	0	832	0	0
41	k	862	0	877	0	0
42	l	945	0	996	0	0
43	m	903	0	962	0	0
44	n	792	0	833	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	o	705	0	712	0	0
46	p	649	0	660	0	0
47	q	630	0	678	0	0
48	r	438	0	456	0	0
49	s	646	0	663	0	0
50	t	658	0	710	0	0
51	u	182	0	198	0	0
52	3	1	0	0	0	0
53	AN1	52	0	0	0	0
53	sN1	41	0	0	0	0
54	AN1	1	0	0	0	0
55	3	1	0	0	0	0
55	AN1	253	0	0	2	0
55	B	5	0	0	1	0
55	C	3	0	0	0	0
55	D	3	0	0	0	0
55	E	2	0	0	0	0
55	K	3	0	0	0	0
55	M	1	0	0	0	0
55	P	1	0	0	1	0
55	Q	3	0	0	0	0
55	R	1	0	0	0	0
55	V	2	0	0	0	0
55	Y	1	0	0	0	0
55	Z	1	0	0	0	0
55	g	1	0	0	0	0
55	h	1	0	0	0	0
55	i	2	0	0	0	0
55	m	2	0	0	0	0
55	n	1	0	0	0	0
55	s	3	0	0	0	0
55	sN1	107	0	0	0	0
55	t	1	0	0	0	0
All	All	140290	0	93412	768	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 6.

All (768) 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)
5:AN1:1462:G:H1	5:AN1:1520:A:N6	1.43	1.16
5:AN1:2096:G:H1	5:AN1:2185:U:H3	0.91	0.90
6:B:70:G:H21	6:B:101:A:H62	1.11	0.89
6:B:2:C:O2	6:B:113:G:N2	2.08	0.86
10:F:146:ILE:HD12	10:F:149:ILE:HD11	1.59	0.84
5:AN1:1846:G:N2	5:AN1:1888:C:O2	2.11	0.82
5:AN1:873:G:N1	5:AN1:900:C:N3	2.30	0.79
5:AN1:1713:U:H3	5:AN1:1739:G:H1	1.30	0.79
6:B:70:G:N2	6:B:101:A:H62	1.80	0.79
5:AN1:873:G:N2	5:AN1:900:C:O2	2.16	0.79
3:2:30:HIS:O	3:2:32:LEU:N	2.16	0.78
10:F:120:LYS:HG3	10:F:121:SER:H	1.48	0.78
18:N:82:LYS:NZ	18:N:112:GLY:O	2.15	0.78
5:AN1:1595:A:H5''	5:AN1:1596:A:H5'	1.66	0.77
1:0:29:LYS:HB3	1:0:47:GLU:HB3	1.67	0.77
6:B:18:G:N1	6:B:61:C:N3	2.29	0.77
5:AN1:2311:C:HO2'	5:AN1:2312:G:H8	1.31	0.76
7:C:5:LYS:NZ	7:C:14:ARG:O	2.17	0.76
6:B:2:C:N3	6:B:113:G:N1	2.31	0.75
5:AN1:1862:A:H61	5:AN1:1871:G:H2'	1.52	0.75
5:AN1:875:U:O2	5:AN1:898:A:N7	2.19	0.75
5:AN1:1036:A:H61	5:AN1:1113:G:H1	1.32	0.74
5:AN1:879:G:H2'	5:AN1:880:G:H8	1.52	0.74
17:M:32:GLU:HG2	17:M:115:LEU:HD12	1.71	0.73
6:B:18:G:N2	6:B:61:C:O2	2.15	0.73
5:AN1:878:G:H2'	5:AN1:879:G:H8	1.54	0.72
5:AN1:2301:U:H3	10:F:39:GLY:H	1.35	0.72
5:AN1:2159:U:OP1	5:AN1:2161:C:N4	2.23	0.71
6:B:70:G:H21	6:B:101:A:N6	1.86	0.71
5:AN1:2787:A:HO2'	5:AN1:2788:G:H8	1.35	0.71
5:AN1:474:C:O2	5:AN1:478:A:N6	2.23	0.71
5:AN1:1749:G:N2	5:AN1:1752:G:OP2	2.23	0.70
10:F:80:ARG:H	10:F:83:TRP:HD1	1.39	0.70
3:2:28:LYS:HA	3:2:32:LEU:HD11	1.74	0.70
5:AN1:829:G:O2'	15:K:40:GLN:NE2	2.25	0.69
5:AN1:1041:A:O2'	5:AN1:1108:A:N6	2.25	0.69
5:AN1:342:A:O2'	9:E:161:ARG:NH1	2.26	0.69
5:AN1:711:G:H8	5:AN1:716:A:H62	1.41	0.68
12:H:48:GLU:O	12:H:52:ALA:HB3	1.93	0.68
9:E:193:LYS:HA	9:E:196:GLU:HG2	1.74	0.68
5:AN1:1528:G:O2'	5:AN1:1536:A:N1	2.26	0.67
5:AN1:1662:A:H61	5:AN1:1992:C:H42	1.43	0.67

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:52:G:H5'	5:AN1:53:G:H5'	1.76	0.67
5:AN1:293:U:H3	5:AN1:351:G:H1	1.41	0.67
5:AN1:364:A:OP2	5:AN1:424:G:O2'	2.13	0.67
5:AN1:2301:U:O2'	10:F:133:LYS:NZ	2.27	0.66
5:AN1:879:G:O6	5:AN1:893:U:O2	2.12	0.66
23:S:3:ASN:HD21	23:S:48:LYS:HE2	1.61	0.66
21:Q:16:GLU:HG3	21:Q:101:ILE:HG13	1.78	0.66
2:1:7:PRO:HB2	5:AN1:1304:G:H4'	1.77	0.66
11:G:54:PRO:HB3	11:G:61:ALA:HB1	1.77	0.65
5:AN1:1413:G:N2	5:AN1:1577:A:OP2	2.30	0.65
5:AN1:195:G:H5'	27:W:14:VAL:HG21	1.77	0.65
5:AN1:1647:G:O2'	17:M:106:ASP:OD2	2.14	0.65
5:AN1:1361:A:OP1	27:W:2:SER:OG	2.15	0.65
5:AN1:198:A:H3'	5:AN1:199:G:H21	1.61	0.65
5:AN1:2804:A:O2'	5:AN1:2886:G:O6	2.14	0.65
5:AN1:294:U:H3	5:AN1:350:G:H22	1.44	0.65
5:AN1:93:G:HO2'	5:AN1:111:U:HO2'	1.41	0.65
5:AN1:2130:A:OP2	5:AN1:2152:G:N1	2.30	0.65
5:AN1:70:A:H61	5:AN1:98:A:H61	1.45	0.65
6:B:108:C:H2'	6:B:109:G:H8	1.60	0.64
5:AN1:2879:A:OP2	30:Z:49:ARG:NH1	2.31	0.64
5:AN1:2130:A:H62	5:AN1:2153:G:H4'	1.62	0.64
30:Z:25:ASN:OD1	30:Z:38:ARG:NH2	2.31	0.64
5:AN1:1750:C:H5	19:O:97:ARG:HH11	1.45	0.63
21:Q:42:VAL:HG22	21:Q:47:ILE:HG23	1.79	0.63
5:AN1:280:A:H2	5:AN1:364:A:H62	1.47	0.63
10:F:143:PHE:HB2	17:M:71:ARG:HD2	174.90	0.63
5:AN1:1775:U:OP2	5:AN1:1780:A:N6	2.27	0.62
5:AN1:2324:A:H2'	5:AN1:2325:A:C8	2.34	0.62
5:AN1:1587:U:H2'	5:AN1:1588:A:H8	1.64	0.62
5:AN1:2309:C:O4'	10:F:37:ASN:ND2	2.33	0.62
10:F:32:THR:OG1	10:F:157:THR:O	2.16	0.62
5:AN1:527:A:H5'	13:I:113:PRO:HG3	1.82	0.62
10:F:34:ILE:HG12	10:F:156:ILE:HG22	1.82	0.61
10:F:74:ILE:HG22	10:F:76:GLY:H	1.65	0.61
2:1:30:VAL:HG22	2:1:33:ARG:HH11	1.65	0.61
24:T:38:ASN:HB3	24:T:61:ALA:HB3	1.81	0.61
5:AN1:2287:U:H2'	5:AN1:2288:G:C8	2.35	0.61
7:C:230:HIS:HD2	7:C:232:HIS:H	1.48	0.61
5:AN1:877:G:H2'	5:AN1:878:G:C8	2.36	0.61
12:H:48:GLU:O	12:H:52:ALA:CB	2.49	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:11:ALA:H	22:R:100:THR:HG23	1.65	0.61
9:E:124:ALA:O	9:E:136:LYS:NZ	2.33	0.60
5:AN1:843:G:O2'	5:AN1:845:A:N7	2.33	0.60
5:AN1:2107:U:O2	5:AN1:2111:G:N2	2.33	0.60
5:AN1:2111:G:O2'	5:AN1:2113:A:N7	2.34	0.60
11:G:121:VAL:HG22	11:G:135:SER:HB2	1.82	0.60
5:AN1:570:A:OP2	21:Q:80:ARG:NH2	2.33	0.60
8:D:6:VAL:H	8:D:33:ASN:HD21	1.48	0.60
5:AN1:846:U:H2'	5:AN1:847:A:H8	1.66	0.60
10:F:136:ILE:HG13	10:F:138:PHE:HD1	1.66	0.60
5:AN1:1111:C:H2'	5:AN1:1112:G:C8	2.36	0.60
5:AN1:673:A:OP1	9:E:57:LYS:NZ	2.35	0.59
10:F:69:LEU:HA	10:F:84:PRO:HA	1.83	0.59
19:O:4:LYS:O	19:O:9:GLN:NE2	2.36	0.59
5:AN1:168:A:H3'	5:AN1:169:U:H5''	1.84	0.59
5:AN1:1535:U:H2'	5:AN1:1536:A:H8	1.67	0.59
5:AN1:2401:G:O2'	5:AN1:2407:A:N6	2.36	0.59
5:AN1:955:U:O2'	6:B:86:U:O4	2.19	0.59
5:AN1:2577:G:OP2	5:AN1:2577:G:N2	2.34	0.58
6:B:18:G:O6	6:B:61:C:N4	2.32	0.58
5:AN1:2596:A:N6	7:C:236:GLU:OE1	2.36	0.58
3:2:30:HIS:O	3:2:32:LEU:HD22	2.04	0.58
5:AN1:1533:U:N3	5:AN1:1534:G:N3	2.47	0.58
3:2:24:LYS:NZ	3:2:46:CYS:SG	2.77	0.58
5:AN1:719:A:H2'	5:AN1:720:A:C8	2.38	0.58
5:AN1:1719:U:O4	5:AN1:1734:G:N2	2.37	0.58
5:AN1:84:U:OP1	28:X:52:ARG:NH2	2.37	0.58
6:B:12:U:OP2	6:B:68:C:O2'	2.22	0.58
14:J:7:MET:HB3	14:J:18:ARG:HH11	1.68	0.58
5:AN1:2301:U:H4'	10:F:133:LYS:HE2	1.85	0.58
5:AN1:879:G:N2	5:AN1:893:U:O2'	2.32	0.58
8:D:47:GLN:NE2	8:D:87:GLU:OE1	2.36	0.58
5:AN1:410:G:OP2	5:AN1:2402:U:O2'	2.22	0.58
5:AN1:274:C:HO2'	5:AN1:280:A:H8	1.52	0.57
5:AN1:2166:A:H2'	5:AN1:2167:A:H5''	1.85	0.57
5:AN1:2077:C:H2'	5:AN1:2078:A:H8	1.68	0.57
5:AN1:2309:C:H5''	10:F:88:LYS:HD2	1.86	0.57
10:F:87:CYS:SG	10:F:88:LYS:N	2.76	0.57
16:L:51:ARG:HG3	16:L:66:ILE:HD11	1.85	0.57
5:AN1:518:C:H2'	5:AN1:519:A:H8	1.68	0.57
10:F:138:PHE:O	10:F:140:GLU:N	2.37	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:303:C:H5''	5:AN1:336:U:H2'	1.86	0.57
5:AN1:719:A:H2'	5:AN1:720:A:H8	1.70	0.57
10:F:10:ASP:OD1	10:F:13:LYS:NZ	2.38	0.57
5:AN1:1111:C:H2'	5:AN1:1112:G:H8	1.68	0.57
5:AN1:2309:C:H2'	5:AN1:2310:A:H8	1.68	0.57
11:G:21:GLY:O	11:G:22:ARG:NH2	2.38	0.57
18:N:71:THR:HG22	18:N:104:ALA:HB1	1.87	0.56
3:2:31:ILE:O	3:2:33:THR:N	2.39	0.56
5:AN1:2151:U:OP2	5:AN1:2153:G:N2	2.38	0.56
5:AN1:878:G:H2'	5:AN1:879:G:C8	2.37	0.56
3:2:6:THR:HG22	3:2:62:PRO:HD2	1.88	0.56
5:AN1:1462:G:H1	5:AN1:1520:A:H61	0.66	0.56
5:AN1:516:C:OP2	30:Z:10:ARG:NH2	2.39	0.56
24:T:45:LYS:HD2	24:T:46:PRO:HD2	1.86	0.56
29:Y:2:LYS:O	29:Y:39:ASP:N	2.31	0.56
5:AN1:2315:U:H2'	5:AN1:2317:G:H1	1.70	0.56
5:AN1:1713:U:O2	5:AN1:1739:G:N2	2.31	0.56
5:AN1:2784:C:O2'	5:AN1:2805:A:N3	2.37	0.56
23:S:29:GLN:OE1	23:S:90:GLN:NE2	2.31	0.56
5:AN1:1310:C:O2'	5:AN1:1387:A:N3	2.33	0.56
6:B:64:A:H61	6:B:105:C:H2'	1.71	0.56
10:F:80:ARG:HG2	10:F:81:ASP:H	1.71	0.56
5:AN1:2701:A:O2'	5:AN1:2848:G:OP1	2.22	0.56
5:AN1:579:C:H2'	5:AN1:580:A:H8	1.71	0.56
21:Q:51:ALA:HB3	21:Q:52:PRO:HD3	1.88	0.56
5:AN1:1717:G:N2	5:AN1:1734:G:O2'	2.38	0.55
5:AN1:1535:U:H2'	5:AN1:1536:A:C8	2.41	0.55
5:AN1:167:A:N3	5:AN1:2204:C:O2'	2.38	0.55
5:AN1:877:G:H2'	5:AN1:878:G:H8	1.70	0.55
15:K:102:VAL:HG23	15:K:103:VAL:HG23	1.89	0.55
18:N:51:GLN:O	18:N:80:ARG:NH2	2.39	0.55
5:AN1:322:G:N7	9:E:131:LYS:NZ	2.54	0.55
9:E:97:ARG:HD3	9:E:101:ARG:HH21	1.71	0.55
5:AN1:2119:G:N2	5:AN1:2120:G:O6	2.39	0.55
5:AN1:2654:C:H5''	11:G:158:LYS:HE3	1.88	0.55
10:F:17:GLN:HE22	10:F:25:VAL:HA	1.71	0.55
15:K:114:LEU:HD22	15:K:132:GLY:HA3	1.87	0.55
5:AN1:1276:G:H2'	5:AN1:1277:U:C6	2.42	0.55
5:AN1:2587:C:H2'	5:AN1:2588:G:H8	1.72	0.55
8:D:86:THR:HG22	8:D:88:ALA:H	1.71	0.55
23:S:7:TYR:O	28:X:29:ARG:NH1	2.39	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:1842:G:H2'	5:AN1:1843:A:C8	2.42	0.55
5:AN1:2242:G:H2'	5:AN1:2243:A:H8	1.72	0.55
5:AN1:579:C:H2'	5:AN1:580:A:C8	2.43	0.55
5:AN1:2254:C:O2'	5:AN1:2423:C:OP2	2.25	0.54
5:AN1:2123:G:H2'	5:AN1:2124:G:C8	2.43	0.54
5:AN1:1870:C:H3'	5:AN1:1871:G:H4'	1.90	0.54
5:AN1:1310:C:H2'	5:AN1:1311:A:H8	1.73	0.54
5:AN1:2568:A:H2'	8:D:152:ASN:HD21	1.71	0.54
30:Z:46:GLY:O	30:Z:53:LEU:N	2.38	0.54
5:AN1:1462:G:N2	5:AN1:1520:A:N1	2.41	0.54
5:AN1:552:U:H2'	5:AN1:553:G:O4'	2.07	0.54
5:AN1:881:G:H2'	5:AN1:882:U:H6	1.73	0.54
18:N:19:ILE:HG21	18:N:26:ARG:HB3	1.89	0.54
5:AN1:1348:A:H2'	5:AN1:1349:A:H8	1.73	0.54
5:AN1:520:U:H2'	5:AN1:521:G:H8	1.72	0.54
24:T:27:VAL:HG22	24:T:32:VAL:HG12	1.89	0.54
5:AN1:1919:U:H2'	5:AN1:1920:C:C6	2.44	0.53
5:AN1:1932:A:H2	5:AN1:1939:U:H3	1.56	0.53
5:AN1:805:U:OP2	15:K:43:ARG:NH2	2.39	0.53
5:AN1:1526:C:N4	5:AN1:1538:A:N3	2.55	0.53
5:AN1:2468:G:N2	5:AN1:2469:U:O2'	2.42	0.53
5:AN1:2734:A:N1	5:AN1:2762:G:O6	2.41	0.53
5:AN1:2479:C:H1'	16:L:52:ARG:HH12	1.72	0.53
23:S:55:VAL:HG23	23:S:87:LYS:HG2	1.90	0.53
5:AN1:2242:G:H2'	5:AN1:2243:A:C8	2.44	0.53
5:AN1:2528:G:N2	5:AN1:2659:G:O2'	2.41	0.53
23:S:53:GLU:CD	23:S:53:GLU:H	2.11	0.53
5:AN1:1911:3TD:N1	5:AN1:1938:C:O2	2.36	0.53
10:F:5:LYS:HG3	10:F:7:ARG:H	1.73	0.53
5:AN1:86:C:H2'	5:AN1:87:G:H8	1.74	0.53
5:AN1:2308:U:H2'	10:F:37:ASN:HD21	1.73	0.53
10:F:162:THR:HG22	10:F:164:ASP:H	1.74	0.52
5:AN1:1311:A:H2'	5:AN1:1312:G:H8	1.74	0.52
5:AN1:499:G:N1	5:AN1:502:A:OP2	2.37	0.52
5:AN1:627:A:N3	5:AN1:637:U:O2'	2.42	0.52
5:AN1:862:G:H2'	5:AN1:863:C:C6	2.45	0.52
20:P:105:ALA:HA	21:Q:47:ILE:HD13	1.91	0.52
5:AN1:1387:A:N6	23:S:17:GLU:OE1	2.39	0.52
10:F:5:LYS:H	10:F:8:TYR:HB2	1.75	0.52
11:G:22:ARG:HH11	11:G:39:ALA:HA	1.74	0.52
21:Q:32:THR:HA	21:Q:62:GLU:HA	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:30:HIS:C	3:2:32:LEU:H	2.09	0.52
5:AN1:1025:A:H2'	5:AN1:1026:A:C8	2.45	0.52
5:AN1:1083:A:H1'	5:AN1:1100:A:H61	1.74	0.52
5:AN1:1306:G:OP2	5:AN1:1306:G:N2	2.36	0.52
5:AN1:2049:G:H5'	8:D:152:ASN:O	2.10	0.52
5:AN1:2325:A:H2'	5:AN1:2326:G:C8	2.45	0.52
5:AN1:2067:A:H2'	5:AN1:2068:C:C6	2.44	0.52
5:AN1:35:A:H61	5:AN1:511:G:H1'	1.73	0.52
15:K:89:GLY:O	15:K:120:ARG:NH2	2.42	0.52
19:O:34:LYS:HE3	19:O:83:VAL:HA	1.91	0.52
10:F:83:TRP:HE3	10:F:84:PRO:HD2	1.74	0.52
5:AN1:1442:C:O2'	5:AN1:1542:A:N3	2.43	0.52
5:AN1:462:G:N2	5:AN1:465:A:OP2	2.32	0.52
5:AN1:1430:G:H2'	5:AN1:1431:G:C8	2.45	0.52
5:AN1:2091:A:OP1	12:H:11:ASN:ND2	2.42	0.52
5:AN1:1413:G:O2'	5:AN1:1577:A:N6	2.43	0.52
5:AN1:2229:U:H2'	5:AN1:2230:G:C8	2.45	0.52
7:C:6:CYS:SG	7:C:18:LYS:NZ	2.83	0.52
20:P:28:ARG:NH1	55:P:201:HOH:O	2.40	0.51
5:AN1:1199:A:H4'	5:AN1:1200:A:H5'	1.92	0.51
5:AN1:1412:C:H3'	5:AN1:1413:G:H8	1.74	0.51
27:W:76:GLN:HB3	27:W:78:ILE:HG23	1.92	0.51
6:B:64:A:N6	6:B:105:C:H2'	2.25	0.51
19:O:2:SER:OG	19:O:3:GLY:N	2.43	0.51
21:Q:50:GLY:H	21:Q:54:VAL:HG22	1.75	0.51
5:AN1:2171:C:H2'	5:AN1:2172:A:N7	2.24	0.51
5:AN1:2852:A:H2'	5:AN1:2853:G:O4'	2.11	0.51
12:H:9:ILE:HD13	12:H:12:LEU:HD11	1.92	0.51
24:T:46:PRO:HB3	24:T:54:GLY:H	1.76	0.51
5:AN1:510:U:H4'	5:AN1:1230:G:H4'	1.93	0.51
5:AN1:1487:G:H5''	5:AN1:1488:C:H5''	1.92	0.51
5:AN1:1528:G:N2	5:AN1:1535:U:O4	2.44	0.51
6:B:108:C:H2'	6:B:109:G:C8	2.44	0.51
15:K:77:ALA:HB2	15:K:107:GLN:HE21	1.76	0.51
5:AN1:1103:A:N6	5:AN1:1104:G:O6	2.44	0.51
5:AN1:2137:A:H2	5:AN1:2138:A:H62	1.57	0.51
5:AN1:2116:G:H5''	5:AN1:2164:G:H22	1.76	0.51
5:AN1:714:A:C5	5:AN1:715:C:H1'	2.45	0.51
5:AN1:9:G:H2'	5:AN1:10:U:C6	2.46	0.51
5:AN1:158:U:H2'	5:AN1:159:G:H8	1.75	0.51
5:AN1:2591:G:N2	5:AN1:2594:A:OP2	2.32	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:22:G:O2'	6:B:25:C:N4	2.44	0.51
5:AN1:12:A:H2'	5:AN1:13:A:C8	2.45	0.51
5:AN1:293:U:O4	5:AN1:351:G:O6	2.28	0.51
4:3:18:ARG:HE	4:3:21:GLY:HA2	1.75	0.50
5:AN1:1108:A:H8	5:AN1:1109:G:H4'	1.75	0.50
5:AN1:1356:G:H2'	5:AN1:1357:C:C6	2.46	0.50
6:B:108:C:O2'	6:B:109:G:OP1	2.26	0.50
10:F:4:LEU:HD12	10:F:8:TYR:HB3	1.92	0.50
25:U:11:ARG:HH21	25:U:31:PRO:HB3	1.76	0.50
5:AN1:879:G:H2'	5:AN1:880:G:C8	2.39	0.50
5:AN1:1591:C:H2'	5:AN1:1592:A:C8	2.47	0.50
5:AN1:372:U:H2'	5:AN1:373:A:H8	1.75	0.50
11:G:44:LYS:NZ	11:G:53:ALA:HB3	2.27	0.50
28:X:30:MET:O	28:X:34:THR:HG23	2.10	0.50
5:AN1:2287:U:H2'	5:AN1:2288:G:H8	1.77	0.50
7:C:159:GLY:H	7:C:195:VAL:HB	1.77	0.50
18:N:67:ILE:O	18:N:71:THR:HG23	2.12	0.50
5:AN1:1680:G:H2'	5:AN1:1681:U:C6	2.46	0.50
5:AN1:2853:G:N1	5:AN1:2856:A:OP2	2.42	0.50
10:F:166:GLY:O	10:F:169:LEU:HG	2.12	0.50
5:AN1:1095:A:H2'	5:AN1:1096:G:H8	1.75	0.50
5:AN1:1844:A:H5''	5:AN1:1845:G:OP1	2.12	0.50
5:AN1:887:C:H3'	5:AN1:888:C:H5''	1.93	0.50
13:I:6:ALA:H	13:I:45:THR:HG21	1.77	0.50
5:AN1:1767:C:H2'	5:AN1:1768:A:H8	1.77	0.50
5:AN1:2639:G:H2'	5:AN1:2640:A:H8	1.76	0.50
7:C:24:LEU:HD13	7:C:83:TYR:HB2	1.93	0.50
5:AN1:34:G:H22	5:AN1:511:G:H2'	1.77	0.50
13:I:18:VAL:HG11	13:I:28:LEU:HD11	1.94	0.50
5:AN1:1421:G:OP2	5:AN1:1422:A:O2'	2.28	0.50
5:AN1:1798:A:H2'	5:AN1:1799:A:C8	2.46	0.50
5:AN1:727:G:OP1	7:C:13:ARG:HG2	2.12	0.50
5:AN1:1827:G:H2'	5:AN1:1828:C:C6	2.47	0.49
5:AN1:2105:U:OP1	5:AN1:2145:U:N3	2.29	0.49
5:AN1:2212:G:H2'	5:AN1:2213:G:H8	1.77	0.49
10:F:66:VAL:HG13	10:F:68:THR:OG1	2.12	0.49
5:AN1:2115:A:H2'	5:AN1:2165:A:H2	1.76	0.49
5:AN1:580:A:H2'	5:AN1:581:G:C8	2.47	0.49
5:AN1:70:A:H61	5:AN1:98:A:N6	2.09	0.49
6:B:16:A:H1'	6:B:65:G:N2	2.27	0.49
7:C:137:ILE:HD11	7:C:167:ARG:HG2	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2172:A:H2'	5:AN1:2173:C:C6	2.47	0.49
5:AN1:413:C:H2'	5:AN1:414:A:C8	2.47	0.49
6:B:26:C:H2'	6:B:27:A:C8	2.47	0.49
21:Q:59:VAL:HG22	21:Q:101:ILE:HG23	1.93	0.49
5:AN1:1010:C:H2'	5:AN1:1011:A:H8	1.78	0.49
5:AN1:1438:C:H2'	5:AN1:1439:A:H8	1.77	0.49
5:AN1:1767:C:H2'	5:AN1:1768:A:C8	2.48	0.49
5:AN1:184:G:H3'	5:AN1:185:G:H8	1.77	0.49
5:AN1:2225:U:H2'	5:AN1:2226:G:H8	1.77	0.49
5:AN1:678:A:H2'	5:AN1:679:G:C8	2.47	0.49
9:E:86:ALA:O	9:E:87:ARG:NH1	2.44	0.49
5:AN1:413:C:H2'	5:AN1:414:A:H8	1.78	0.49
5:AN1:879:G:C6	5:AN1:893:U:O2	2.65	0.49
5:AN1:1053:G:H21	5:AN1:1101:C:H41	1.60	0.49
5:AN1:1411:G:H2'	5:AN1:1412:C:C6	2.47	0.49
5:AN1:1500:A:O2'	5:AN1:1502:U:O4'	2.30	0.49
5:AN1:1591:C:H2'	5:AN1:1592:A:H8	1.76	0.49
9:E:190:ALA:O	9:E:193:LYS:HG3	2.11	0.49
16:L:112:ASP:O	16:L:116:GLU:HG3	2.12	0.49
5:AN1:1273:C:H2'	5:AN1:1274:G:H8	1.78	0.49
5:AN1:2637:A:H5''	13:I:78:THR:HG21	1.95	0.49
5:AN1:35:A:N6	5:AN1:511:G:O2'	2.46	0.49
16:L:20:LEU:HD23	16:L:99:PRO:HG2	1.94	0.49
15:K:111:ARG:HG2	15:K:128:ALA:HB3	1.94	0.49
5:AN1:1588:A:H2'	5:AN1:1589:C:H6	1.78	0.48
5:AN1:2309:C:H2'	5:AN1:2310:A:C8	2.47	0.48
22:R:10:ALA:HB1	22:R:46:LEU:HD13	1.95	0.48
5:AN1:520:U:H2'	5:AN1:521:G:C8	2.48	0.48
5:AN1:873:G:O6	5:AN1:900:C:N4	2.34	0.48
5:AN1:322:G:N3	9:E:162:ASN:ND2	2.61	0.48
30:Z:52:GLN:NE2	30:Z:53:LEU:O	2.46	0.48
9:E:170:ASP:OD1	9:E:171:ALA:N	2.45	0.48
15:K:112:ILE:HB	15:K:129:LEU:HD23	1.95	0.48
5:AN1:1348:A:H2'	5:AN1:1349:A:C8	2.47	0.48
5:AN1:1792:U:H2'	5:AN1:1793:C:C6	2.48	0.48
5:AN1:2311:C:O2'	5:AN1:2312:G:H8	1.94	0.48
5:AN1:844:A:H61	5:AN1:929:C:H1'	1.79	0.48
5:AN1:1589:C:H2'	5:AN1:1590:A:H8	1.78	0.48
5:AN1:2694:U:H2'	5:AN1:2695:G:C8	2.48	0.48
10:F:140:GLU:HG2	10:F:141:ILE:H	1.78	0.48
5:AN1:1517:G:OP2	5:AN1:1518:A:O2'	2.24	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2060:C:H2'	5:AN1:2061:C:C6	2.49	0.48
5:AN1:308:U:H2'	5:AN1:309:G:O4'	2.14	0.48
20:P:82:GLY:O	20:P:86:ALA:N	2.45	0.48
5:AN1:2161:C:N4	5:AN1:2162:U:O4	2.47	0.48
5:AN1:2229:U:H2'	5:AN1:2230:G:H8	1.78	0.48
5:AN1:2563:G:H2'	5:AN1:2564:A:C8	2.49	0.48
5:AN1:2787:A:O2'	5:AN1:2788:G:H8	1.96	0.48
5:AN1:2818:G:O6	17:M:2:ARG:NH1	2.44	0.48
7:C:230:HIS:CD2	7:C:232:HIS:H	2.31	0.48
10:F:140:GLU:HG2	10:F:141:ILE:N	2.28	0.48
5:AN1:1879:U:H2'	5:AN1:1880:G:O4'	2.14	0.48
5:AN1:1938:C:OP2	5:AN1:1939:U:O2'	2.23	0.48
5:AN1:2123:G:N2	5:AN1:2158:G:O6	2.46	0.48
5:AN1:2147:C:O2	5:AN1:2148:C:N4	2.47	0.48
5:AN1:2674:A:H2'	5:AN1:2675:A:C8	2.48	0.48
11:G:158:LYS:HD2	11:G:160:LYS:HD2	1.96	0.48
13:I:17:VAL:HG22	13:I:55:ILE:HB	1.96	0.48
28:X:18:LEU:HB2	28:X:53:ILE:HG21	1.94	0.48
5:AN1:1081:A:O3'	5:AN1:1102:U:O2'	2.31	0.48
5:AN1:1427:G:H2'	5:AN1:1428:A:C8	2.48	0.48
6:B:28:C:H2'	6:B:29:C:O4'	2.14	0.48
5:AN1:1797:A:OP2	7:C:150:LYS:NZ	2.46	0.48
10:F:17:GLN:NE2	10:F:28:ILE:HD11	2.29	0.48
12:H:4:ILE:N	12:H:37:VAL:O	2.42	0.48
5:AN1:1054:A:N6	5:AN1:1084:G:OP2	2.46	0.48
5:AN1:1087:A:H2'	5:AN1:1088:G:C8	2.48	0.48
5:AN1:2324:A:H2'	5:AN1:2325:A:H8	1.75	0.48
5:AN1:1521:G:H2'	5:AN1:1522:C:C6	2.49	0.47
5:AN1:2166:A:H2'	5:AN1:2166:A:N3	2.28	0.47
10:F:119:ALA:O	10:F:167:ARG:NH1	2.45	0.47
10:F:33:LYS:HE2	10:F:92:ARG:HH12	1.79	0.47
5:AN1:2727:G:H2'	5:AN1:2728:G:C8	2.50	0.47
5:AN1:2843:U:H2'	5:AN1:2844:G:O4'	2.14	0.47
6:B:29:C:H2'	6:B:30:U:C5	2.49	0.47
10:F:57:MET:HA	10:F:60:ILE:HB	1.95	0.47
19:O:17:LYS:HD3	19:O:80:HIS:HA	1.96	0.47
5:AN1:1921:C:H2'	5:AN1:1922:U:C6	2.49	0.47
5:AN1:2570:G:H1'	8:D:151:GLN:HG3	1.96	0.47
6:B:61:C:H2'	6:B:62:U:C6	2.48	0.47
6:B:68:C:H2'	6:B:69:U:H6	1.79	0.47
5:AN1:2048:A:O3'	8:D:152:ASN:HA	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:155:GLU:HG2	11:G:157:TYR:H	1.79	0.47
18:N:59:LEU:HD21	18:N:72:LYS:HB3	1.96	0.47
5:AN1:107:U:OP1	5:AN1:108:U:O2'	2.27	0.47
7:C:53:HIS:HA	7:C:217:ARG:HB2	1.96	0.47
5:AN1:1108:A:H2'	5:AN1:1109:G:H4'	1.95	0.47
5:AN1:1730:U:H2'	5:AN1:1731:C:C6	2.49	0.47
5:AN1:665:U:H2'	5:AN1:666:A:O4'	2.13	0.47
10:F:87:CYS:SG	10:F:89:VAL:HG23	2.55	0.47
18:N:3:GLU:HB2	18:N:6:GLN:HG2	1.95	0.47
5:AN1:2070:U:H2'	5:AN1:2071:U:C6	2.49	0.47
2:1:29:GLN:NE2	5:AN1:217:C:OP1	2.47	0.47
5:AN1:1430:G:H2'	5:AN1:1431:G:H8	1.80	0.47
5:AN1:663:U:H2'	5:AN1:664:A:H8	1.78	0.47
6:B:11:A:O2'	6:B:13:A:OP2	2.27	0.47
5:AN1:1662:A:H61	5:AN1:1992:C:N4	2.09	0.47
5:AN1:2622:C:H2'	5:AN1:2623:G:C8	2.50	0.47
5:AN1:970:A:H5'	5:AN1:1183:U:H1'	1.97	0.47
18:N:82:LYS:NZ	18:N:113:GLY:HA3	2.30	0.47
5:AN1:12:A:H2'	5:AN1:13:A:H8	1.80	0.47
5:AN1:1475:C:H2'	5:AN1:1476:A:C8	2.50	0.47
5:AN1:43:G:N3	5:AN1:449:G:O2'	2.47	0.47
20:P:104:VAL:HG12	21:Q:47:ILE:HD11	1.95	0.47
3:2:16:ALA:HB2	3:2:64:ILE:HG13	1.97	0.47
5:AN1:2072:U:OP2	5:AN1:2234:G:N2	2.40	0.47
5:AN1:591:U:H2'	5:AN1:592:U:C6	2.50	0.47
15:K:37:ILE:HG22	15:K:38:LYS:H	1.80	0.47
19:O:56:ARG:O	19:O:60:SER:OG	2.32	0.47
24:T:2:ALA:HA	24:T:81:VAL:HB	1.95	0.47
26:V:83:GLU:N	26:V:83:GLU:OE1	2.48	0.47
5:AN1:498:U:H2'	5:AN1:499:G:O4'	2.15	0.47
23:S:49:LEU:HD13	28:X:26:PHE:CZ	2.50	0.47
5:AN1:309:G:N1	5:AN1:312:A:OP2	2.43	0.46
14:J:66:LYS:HE2	14:J:81:ASP:HA	1.97	0.46
25:U:40:GLU:O	25:U:97:ARG:NH2	2.35	0.46
5:AN1:199:G:N2	5:AN1:199:G:OP2	2.48	0.46
5:AN1:2543:A:H2'	5:AN1:2544:U:C6	2.49	0.46
5:AN1:2645:C:H2'	5:AN1:2646:U:H6	1.80	0.46
5:AN1:762:A:H5'	7:C:209:GLY:HA2	1.97	0.46
5:AN1:1004:C:OP1	13:I:37:ARG:NH1	2.48	0.46
5:AN1:1025:A:N3	5:AN1:2482:C:O2'	2.40	0.46
5:AN1:2306:A:H2'	5:AN1:2307:A:H5''	1.96	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:587:U:H2'	5:AN1:588:A:H8	1.80	0.46
6:B:90:C:OP1	25:U:26:ARG:NH2	2.49	0.46
7:C:21:HIS:ND1	7:C:90:HIS:HE1	2.14	0.46
5:AN1:13:A:O2'	13:I:135:GLN:NE2	2.48	0.46
25:U:47:GLU:HB3	25:U:50:GLU:HG2	1.97	0.46
11:G:102:VAL:HG12	11:G:116:ALA:HA	1.96	0.46
5:AN1:1078:U:H2'	5:AN1:1079:U:C5	2.49	0.46
5:AN1:1878:U:H2'	5:AN1:1879:U:C6	2.50	0.46
5:AN1:2106:G:O5'	5:AN1:2114:U:H2'	2.14	0.46
5:AN1:578:U:H2'	5:AN1:579:C:C6	2.50	0.46
13:I:34:ARG:HH22	13:I:40:HIS:HB3	1.80	0.46
5:AN1:1437:U:H2'	5:AN1:1438:C:H6	1.80	0.46
5:AN1:1479:U:O4	5:AN1:1480:A:N6	2.44	0.46
5:AN1:2119:G:H1'	5:AN1:2172:A:C2	2.51	0.46
3:2:18:ALA:HB2	5:AN1:626:G:H5'	1.97	0.46
11:G:22:ARG:NH1	11:G:39:ALA:HA	2.30	0.46
16:L:60:ARG:HD2	16:L:60:ARG:HA	1.84	0.46
5:AN1:1490:A:H2'	5:AN1:1491:A:H8	1.79	0.46
5:AN1:2287:U:OP1	5:AN1:2376:U:O2'	2.32	0.46
5:AN1:2683:U:H2'	5:AN1:2684:G:O4'	2.16	0.46
6:B:27:A:H2'	6:B:28:C:C6	2.51	0.46
25:U:84:HIS:HD2	25:U:87:LYS:H	1.63	0.46
27:W:15:GLY:HA3	27:W:29:PHE:HE1	1.80	0.46
5:AN1:1437:U:H2'	5:AN1:1438:C:C6	2.51	0.46
5:AN1:2111:G:H4'	5:AN1:2113:A:H62	1.81	0.46
5:AN1:909:A:H8	5:AN1:2273:G:H21	1.62	0.46
5:AN1:844:A:N6	5:AN1:929:C:O2'	2.49	0.46
10:F:30:ARG:H	10:F:159:THR:HB	1.81	0.46
5:AN1:1490:A:H2'	5:AN1:1491:A:C8	2.51	0.46
5:AN1:1828:C:H2'	5:AN1:1829:C:O4'	2.16	0.46
5:AN1:2104:U:O2	5:AN1:2177:G:N2	2.47	0.46
5:AN1:2533:U:H2'	5:AN1:2534:C:H6	1.81	0.46
5:AN1:493:G:H21	22:R:57:ASN:HD21	1.64	0.46
11:G:16:THR:HB	11:G:27:LYS:HE3	1.98	0.46
5:AN1:203:A:OP2	15:K:49:ARG:NH2	2.49	0.46
22:R:22:ASP:OD1	22:R:25:ARG:NH2	2.30	0.46
5:AN1:1588:A:H2'	5:AN1:1589:C:C6	2.51	0.45
5:AN1:2830:G:H2'	5:AN1:2875:A:H61	1.81	0.45
6:B:38:U:N3	6:B:42:G:OP2	2.37	0.45
19:O:103:LEU:HD23	19:O:106:LEU:HD12	1.98	0.45
5:AN1:1356:G:H2'	5:AN1:1357:C:H6	1.79	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:358:A:HO2'	5:AN1:359:U:H6	1.65	0.45
15:K:93:SER:HB2	15:K:125:GLN:HE21	1.82	0.45
5:AN1:1862:A:H2'	5:AN1:1863:G:C8	2.51	0.45
5:AN1:2096:G:O6	5:AN1:2185:U:O4	2.35	0.45
3:2:13:ARG:HD2	15:K:65:LYS:HG2	1.97	0.45
5:AN1:1381:A:H2'	5:AN1:1382:U:C6	2.51	0.45
5:AN1:1681:U:H2'	5:AN1:1682:A:C8	2.52	0.45
5:AN1:1681:U:H2'	5:AN1:1682:A:H8	1.82	0.45
5:AN1:1923:A:H2'	5:AN1:1924:A:C8	2.52	0.45
13:I:73:LYS:HD3	13:I:86:GLU:OE2	2.16	0.45
25:U:94:ASP:N	25:U:94:ASP:OD1	2.47	0.45
26:V:11:LYS:O	26:V:14:ARG:NH1	2.41	0.45
5:AN1:1793:C:O2'	7:C:257:THR:OG1	2.35	0.45
5:AN1:86:C:H2'	5:AN1:87:G:C8	2.52	0.45
11:G:77:LYS:O	11:G:81:GLU:HG3	2.17	0.45
26:V:37:ILE:HG22	26:V:38:VAL:HG23	1.97	0.45
5:AN1:1311:A:H2'	5:AN1:1312:G:C8	2.52	0.45
5:AN1:1478:G:H2'	5:AN1:1479:U:C6	2.52	0.45
5:AN1:2200:G:OP2	7:C:147:LYS:NZ	2.45	0.45
5:AN1:395:G:OP2	27:W:10:LYS:NZ	2.41	0.45
5:AN1:475:G:N1	5:AN1:478:A:OP2	2.44	0.45
5:AN1:1846:G:H2'	5:AN1:1847:U:C6	2.52	0.45
5:AN1:2622:C:H2'	5:AN1:2623:G:H8	1.82	0.45
14:J:17:ARG:HD3	14:J:17:ARG:HA	1.76	0.45
5:AN1:1467:G:O6	5:AN1:1468:A:N6	2.50	0.45
5:AN1:2021:C:H2'	5:AN1:2022:U:C6	2.52	0.45
5:AN1:2373:A:H2'	5:AN1:2374:A:C8	2.51	0.45
5:AN1:2026:6MZ:H2	5:AN1:2495:C:H5''	1.99	0.45
5:AN1:291:G:O2'	5:AN1:292:U:H5''	2.17	0.45
10:F:77:PHE:CE2	10:F:79:ILE:HG12	2.52	0.45
12:H:9:ILE:HB	12:H:12:LEU:HG	1.98	0.45
5:AN1:1680:G:H2'	5:AN1:1681:U:H6	1.81	0.45
5:AN1:636:G:H2'	5:AN1:637:U:C6	2.52	0.45
5:AN1:342:A:HO2'	9:E:161:ARG:HH12	1.63	0.45
5:AN1:2169:A:H2'	5:AN1:2170:C:C5	2.52	0.45
29:Y:4:ILE:HB	29:Y:37:VAL:HG23	1.99	0.45
5:AN1:1470:G:H5''	5:AN1:1510:G:O6	2.17	0.44
5:AN1:713:A:H2'	5:AN1:714:A:O4'	2.17	0.44
10:F:120:LYS:HG3	10:F:121:SER:N	2.24	0.44
5:AN1:2312:G:H2'	5:AN1:2313:C:C6	2.52	0.44
5:AN1:2674:A:H2'	5:AN1:2675:A:H8	1.83	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:144:ASP:O	10:F:146:ILE:HG23	2.17	0.44
23:S:67:LYS:NZ	23:S:76:ARG:HE	2.15	0.44
25:U:9:GLN:O	25:U:45:THR:N	2.43	0.44
5:AN1:664:A:H2'	5:AN1:665:U:C6	2.52	0.44
5:AN1:1089:C:H3'	5:AN1:1090:G:H8	1.83	0.44
5:AN1:1303:A:N7	55:AN1:3135:HOH:O	2.36	0.44
5:AN1:1562:C:H2'	5:AN1:1563:C:C6	2.53	0.44
5:AN1:1583:C:H3'	5:AN1:1584:A:H8	1.82	0.44
5:AN1:307:C:H2'	5:AN1:308:U:C6	2.52	0.44
5:AN1:372:U:H2'	5:AN1:373:A:C8	2.51	0.44
7:C:205:LEU:HB3	7:C:210:ALA:HB3	1.99	0.44
5:AN1:1475:C:H2'	5:AN1:1476:A:H8	1.83	0.44
5:AN1:1961:C:H5''	5:AN1:1962:A:H2'	2.00	0.44
5:AN1:2295:G:H2'	5:AN1:2296:C:C6	2.53	0.44
5:AN1:2323:A:H2'	5:AN1:2324:A:C8	2.52	0.44
5:AN1:2815:C:H2'	5:AN1:2817:A:N7	2.33	0.44
5:AN1:849:C:H2'	5:AN1:850:A:H8	1.82	0.44
6:B:68:C:H2'	6:B:69:U:C6	2.53	0.44
5:AN1:1412:C:H3'	5:AN1:1413:G:C8	2.53	0.44
5:AN1:1561:U:H2'	5:AN1:1562:C:C6	2.52	0.44
5:AN1:2107:U:O4'	5:AN1:2114:U:O2'	2.35	0.44
5:AN1:2176:U:H2'	5:AN1:2177:G:C8	2.52	0.44
5:AN1:2185:U:H2'	5:AN1:2186:G:H8	1.83	0.44
5:AN1:553:G:HO2'	5:AN1:554:A:H8	1.64	0.44
5:AN1:606:A:H2'	5:AN1:607:A:C8	2.53	0.44
5:AN1:861:A:H2'	5:AN1:862:G:C8	2.53	0.44
5:AN1:997:A:H2'	5:AN1:998:A:C8	2.52	0.44
10:F:99:PHE:HD1	10:F:102:ARG:HH11	1.66	0.44
12:H:40:THR:OG1	12:H:43:ASN:ND2	2.50	0.44
22:R:65:ASP:N	22:R:65:ASP:OD1	2.51	0.44
5:AN1:67:G:C6	5:AN1:81:A:C6	3.05	0.44
5:AN1:873:G:H2'	5:AN1:874:C:C6	2.53	0.44
6:B:87:A:H2'	16:L:18:THR:HG22	1.99	0.44
5:AN1:1634:G:H2'	5:AN1:1635:A:C8	2.53	0.44
5:AN1:2587:C:H2'	5:AN1:2588:G:C8	2.53	0.44
5:AN1:2594:A:H5''	7:C:234:GLY:HA3	1.99	0.44
5:AN1:1743:A:H2'	5:AN1:1744:C:C6	2.53	0.44
5:AN1:1876:U:H2'	5:AN1:1877:C:C6	2.53	0.44
5:AN1:2169:A:H2'	5:AN1:2170:C:C6	2.53	0.44
5:AN1:2301:U:C5	10:F:153:ASP:HB2	2.53	0.44
5:AN1:2747:G:N2	5:AN1:2747:G:OP1	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:580:A:H2'	5:AN1:581:G:H8	1.82	0.44
5:AN1:720:A:H2'	5:AN1:721:C:C6	2.53	0.44
8:D:55:GLU:HA	8:D:76:ALA:O	2.18	0.44
10:F:162:THR:HB	10:F:165:GLU:HG3	2.00	0.44
12:H:50:ARG:NH1	12:H:54:LEU:HD22	2.33	0.44
12:H:5:LEU:CD1	12:H:13:GLY:HA3	2.48	0.44
13:I:109:LEU:HD12	13:I:119:ILE:HD13	2.00	0.44
20:P:78:ARG:HD3	20:P:78:ARG:HA	1.77	0.44
5:AN1:181:C:H2'	5:AN1:182:A:H8	1.83	0.43
5:AN1:2262:A:H4'	5:AN1:2263:A:N3	2.33	0.43
5:AN1:2896:A:H2'	5:AN1:2897:C:C6	2.53	0.43
5:AN1:596:U:H2'	5:AN1:597:A:C8	2.53	0.43
6:B:26:C:H2'	6:B:27:A:H8	1.83	0.43
5:AN1:2734:A:H2	5:AN1:2762:G:H1	1.66	0.43
10:F:34:ILE:HD12	10:F:96:MET:HB2	2.00	0.43
5:AN1:1310:C:H2'	5:AN1:1311:A:C8	2.52	0.43
5:AN1:2170:C:H2'	5:AN1:2171:C:O4'	2.18	0.43
5:AN1:2510:U:H2'	5:AN1:2511:C:C6	2.53	0.43
5:AN1:2861:U:OP2	5:AN1:2862:G:O2'	2.23	0.43
5:AN1:720:A:H2'	5:AN1:721:C:H6	1.82	0.43
6:B:22:G:O6	6:B:54:G:O2'	2.35	0.43
14:J:44:LYS:HA	14:J:44:LYS:HD3	1.82	0.43
15:K:80:ARG:HB2	15:K:83:GLU:HG3	2.00	0.43
24:T:5:LYS:N	24:T:8:ASP:OD2	2.36	0.43
5:AN1:2172:A:O2'	5:AN1:2173:C:O4'	2.32	0.43
5:AN1:2187:A:H2'	5:AN1:2188:G:C8	2.53	0.43
5:AN1:278:U:H3	5:AN1:366:G:H22	1.66	0.43
5:AN1:695:G:H2'	5:AN1:696:C:C6	2.54	0.43
6:B:6:C:O3'	18:N:26:ARG:NH2	2.45	0.43
20:P:81:ASP:OD1	20:P:85:LYS:NZ	2.51	0.43
5:AN1:1038:G:N1	5:AN1:1039:G:O6	2.52	0.43
5:AN1:158:U:H2'	5:AN1:159:G:C8	2.54	0.43
5:AN1:2239:U:H2'	5:AN1:2240:U:C6	2.54	0.43
5:AN1:2463:C:H2'	5:AN1:2464:A:O4'	2.18	0.43
5:AN1:2639:G:H2'	5:AN1:2640:A:C8	2.53	0.43
5:AN1:758:G:H2'	5:AN1:759:A:O4'	2.17	0.43
6:B:28:C:H1'	6:B:55:A:H61	1.82	0.43
15:K:29:VAL:HG12	15:K:33:GLY:HA2	2.01	0.43
5:AN1:563:C:P	21:Q:80:ARG:H	2.41	0.43
25:U:84:HIS:CD2	25:U:86:ALA:H	2.36	0.43
5:AN1:2010:A:H2'	5:AN1:2011:A:C8	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:2066:A:H2'	5:AN1:2067:A:H8	1.84	0.43
5:AN1:611:U:H5''	5:AN1:612:A:C8	2.54	0.43
6:B:54:G:H4'	6:B:55:A:H8	1.84	0.43
8:D:184:ASP:HB3	8:D:189:VAL:HG22	2.00	0.43
13:I:16:PHE:HB2	13:I:54:ILE:HD13	2.01	0.43
5:AN1:2679:C:O2	14:J:70:ARG:NH2	2.51	0.43
20:P:43:GLY:HA3	21:Q:75:ILE:HD12	2.00	0.43
5:AN1:2379:G:O2'	5:AN1:2380:U:OP1	2.33	0.43
5:AN1:2533:U:H2'	5:AN1:2534:C:C6	2.53	0.43
6:B:10:C:C5	26:V:74:GLN:HB3	2.54	0.43
5:AN1:1382:U:H5'	5:AN1:1464:A:H1'	2.00	0.43
5:AN1:568:G:H2'	5:AN1:2026:6MZ:N7	2.34	0.43
5:AN1:587:U:H2'	5:AN1:588:A:C8	2.54	0.43
10:F:35:THR:HA	10:F:90:THR:HA	2.01	0.43
12:H:51:ARG:HE	12:H:55:GLU:HG2	1.84	0.43
5:AN1:1679:G:N2	5:AN1:1759:G:OP2	2.41	0.43
5:AN1:413:C:H1'	5:AN1:1860:U:H1'	2.00	0.43
5:AN1:631:A:O2'	5:AN1:2400:U:OP1	2.35	0.43
5:AN1:301:A:N3	5:AN1:321:C:O2'	2.45	0.43
10:F:120:LYS:CG	10:F:121:SER:H	2.22	0.43
13:I:21:THR:HA	13:I:61:GLN:HB3	2.01	0.43
24:T:46:PRO:HD3	24:T:54:GLY:HA3	2.00	0.43
5:AN1:1078:U:H2'	5:AN1:1079:U:H5	1.83	0.43
5:AN1:1590:A:H2'	5:AN1:1591:C:H6	1.84	0.43
5:AN1:2309:C:O3'	10:F:88:LYS:NZ	2.38	0.43
5:AN1:2795:A:H2'	5:AN1:2797:G:OP2	2.18	0.43
5:AN1:67:G:C2	5:AN1:68:A:N6	2.87	0.43
5:AN1:569:U:H3'	21:Q:80:ARG:NH2	2.34	0.43
25:U:76:VAL:HG12	25:U:97:ARG:HA	2.01	0.43
2:1:1:MET:N	5:AN1:1617:G:H21	2.16	0.42
5:AN1:298:U:H2'	5:AN1:299:G:C8	2.54	0.42
5:AN1:502:A:H4'	5:AN1:504:A:H5''	2.01	0.42
5:AN1:93:G:O2'	5:AN1:111:U:O2'	2.23	0.42
9:E:152:VAL:HG11	9:E:157:TYR:CZ	2.53	0.42
11:G:154:PRO:HA	11:G:160:LYS:O	2.19	0.42
5:AN1:1287:G:H2'	5:AN1:1288:U:C6	2.55	0.42
5:AN1:2093:U:H2'	5:AN1:2094:U:C6	2.54	0.42
5:AN1:2416:C:H2'	5:AN1:2417:G:H8	1.84	0.42
5:AN1:2456:U:C2	5:AN1:2457:A:C8	3.07	0.42
6:B:111:C:H2'	6:B:112:A:H8	1.84	0.42
6:B:81:G:O6	6:B:91:A:N6	2.52	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:40:C:OP1	10:F:64:LYS:NZ	2.53	0.42
29:Y:7:THR:HG23	29:Y:55:SER:HB3	2.01	0.42
5:AN1:2109:U:O4	5:AN1:2163:U:O2'	2.38	0.42
5:AN1:1587:U:H2'	5:AN1:1588:A:C8	2.50	0.42
5:AN1:1861:U:H2'	5:AN1:1862:A:C8	2.54	0.42
5:AN1:2110:A:H3'	5:AN1:2111:G:H8	1.84	0.42
5:AN1:2553:G:H2'	5:AN1:2554:C:C6	2.54	0.42
5:AN1:2696:A:H2'	5:AN1:2697:C:C6	2.54	0.42
5:AN1:69:U:H2'	5:AN1:70:A:H8	1.84	0.42
5:AN1:831:A:H2'	5:AN1:832:G:C8	2.54	0.42
6:B:13:A:H5''	6:B:105:C:C2	2.54	0.42
6:B:88:C:OP2	55:B:201:HOH:O	2.22	0.42
5:AN1:1908:A:H2	5:AN1:1913:PSU:HN3	1.66	0.42
5:AN1:2098:C:H2'	5:AN1:2099:C:O4'	2.19	0.42
5:AN1:9:G:H2'	5:AN1:10:U:H6	1.82	0.42
7:C:258:ARG:NH2	7:C:260:ASN:O	2.53	0.42
10:F:36:LEU:N	10:F:89:VAL:O	2.37	0.42
23:S:53:GLU:HG2	23:S:87:LYS:H	1.85	0.42
25:U:40:GLU:HG2	25:U:41:PRO:O	2.20	0.42
2:1:1:MET:HE1	5:AN1:750:A:H3'	2.02	0.42
7:C:6:CYS:SG	7:C:13:ARG:NH2	2.90	0.42
9:E:152:VAL:HG11	9:E:157:TYR:CE1	2.54	0.42
5:AN1:2110:A:H3'	5:AN1:2111:G:C8	2.54	0.42
5:AN1:2381:C:H2'	5:AN1:2382:U:C6	2.55	0.42
5:AN1:2633:U:H2'	5:AN1:2634:G:O4'	2.20	0.42
5:AN1:2518:U:O2'	5:AN1:2643:U:OP1	2.26	0.42
5:AN1:2657:G:H8	5:AN1:2657:G:OP2	2.02	0.42
5:AN1:2784:C:H2'	5:AN1:2785:C:C6	2.54	0.42
5:AN1:826:U:H2'	5:AN1:827:A:C8	2.55	0.42
24:T:42:LYS:NZ	24:T:43:HIS:O	2.50	0.42
24:T:5:LYS:HE2	24:T:5:LYS:HB3	1.84	0.42
5:AN1:1835:G:C2	5:AN1:1836:G:C8	3.07	0.42
5:AN1:2472:A:H61	5:AN1:2525:G:H2'	1.85	0.42
5:AN1:2647:C:H2'	5:AN1:2648:C:C6	2.55	0.42
5:AN1:353:C:H2'	5:AN1:354:A:H8	1.85	0.42
5:AN1:754:A:H2'	5:AN1:755:G:O4'	2.19	0.42
5:AN1:856:G:H3'	5:AN1:857:G:C8	2.55	0.42
11:G:127:THR:HG22	11:G:129:THR:H	1.84	0.42
15:K:82:SER:OG	15:K:116:GLY:HA3	2.20	0.42
1:O:22:ASN:HD21	1:O:24:ARG:CZ	2.33	0.42
5:AN1:1482:C:N4	5:AN1:1498:G:H1	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:32:LEU:HD12	3:2:35:LYS:HD2	2.01	0.42
5:AN1:1296:A:H2	5:AN1:1624:A:H2	1.68	0.42
5:AN1:292:U:H2'	5:AN1:293:U:C6	2.55	0.42
5:AN1:612:A:H5'	5:AN1:614:A:C6	2.55	0.42
5:AN1:976:A:H2'	5:AN1:979:C:H41	1.85	0.42
5:AN1:1359:G:N7	27:W:2:SER:N	2.68	0.42
5:AN1:1441:C:H2'	5:AN1:1442:C:H6	1.85	0.41
5:AN1:1862:A:H2	5:AN1:1872:A:C8	2.38	0.41
5:AN1:1942:U:H2'	5:AN1:1943:C:H6	1.85	0.41
5:AN1:2736:A:H2'	5:AN1:2737:A:C8	2.55	0.41
5:AN1:309:G:N2	5:AN1:311:G:H3'	2.35	0.41
5:AN1:718:U:O2'	5:AN1:719:A:H8	2.03	0.41
6:B:101:A:H2'	6:B:102:A:O4'	2.20	0.41
23:S:2:ASN:ND2	28:X:19:ASP:OD1	2.52	0.41
4:3:2:LYS:HB2	4:3:2:LYS:HE3	1.92	0.41
5:AN1:103:U:H2'	5:AN1:104:C:O4'	2.20	0.41
5:AN1:1590:A:H2'	5:AN1:1591:C:C6	2.55	0.41
5:AN1:2243:A:H2'	5:AN1:2244:C:H6	1.86	0.41
5:AN1:2572:G:H5'	5:AN1:2574:G:N7	2.35	0.41
11:G:98:VAL:HG22	11:G:103:VAL:HG23	2.00	0.41
5:AN1:1749:G:H5''	19:O:96:ARG:HD3	2.02	0.41
5:AN1:1804:A:H2'	5:AN1:1805:A:C8	2.55	0.41
5:AN1:34:G:N2	5:AN1:511:G:H2'	2.35	0.41
5:AN1:67:G:O6	5:AN1:81:A:N6	2.52	0.41
5:AN1:86:C:C2	5:AN1:87:G:C8	3.08	0.41
5:AN1:880:G:C6	5:AN1:893:U:H1'	2.55	0.41
10:F:50:LEU:O	10:F:54:VAL:HG13	2.21	0.41
11:G:36:ASN:OD1	11:G:37:LEU:N	2.50	0.41
5:AN1:1041:A:H1'	5:AN1:1108:A:H62	1.85	0.41
5:AN1:1665:G:O2'	5:AN1:1987:U:O4	2.28	0.41
5:AN1:2892:C:H2'	5:AN1:2893:U:C6	2.55	0.41
5:AN1:707:U:H2'	5:AN1:708:U:C6	2.56	0.41
5:AN1:881:G:H2'	5:AN1:882:U:C6	2.55	0.41
5:AN1:903:A:H3'	5:AN1:904:U:H5''	2.01	0.41
9:E:97:ARG:HG2	9:E:101:ARG:HE	1.84	0.41
11:G:135:SER:HB3	11:G:141:LEU:HB2	2.03	0.41
12:H:30:LEU:HB3	12:H:36:ALA:HB3	2.02	0.41
13:I:32:ILE:O	13:I:36:LEU:HB2	2.20	0.41
5:AN1:1464:A:H2'	5:AN1:1465:A:C8	2.55	0.41
5:AN1:2122:A:H2	5:AN1:2159:U:H3	1.68	0.41
5:AN1:597:A:H2'	5:AN1:598:G:H8	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:630:A:H2'	5:AN1:631:A:C8	2.56	0.41
5:AN1:1569:A:H2'	5:AN1:1570:A:C8	2.56	0.41
5:AN1:1708:G:H4'	5:AN1:2854:U:O2	2.20	0.41
5:AN1:298:U:H2'	5:AN1:299:G:H8	1.86	0.41
5:AN1:981:A:N3	5:AN1:981:A:H2'	2.36	0.41
6:B:66:C:H2'	6:B:67:G:O4'	2.21	0.41
5:AN1:2645:C:H2'	5:AN1:2646:U:C6	2.55	0.41
5:AN1:2842:G:H2'	5:AN1:2843:U:C6	2.56	0.41
5:AN1:25:C:O2'	5:AN1:552:U:OP1	2.37	0.41
10:F:102:ARG:O	10:F:106:ILE:HG12	2.21	0.41
18:N:74:GLY:O	18:N:77:ILE:HG22	2.21	0.41
3:2:31:ILE:H	3:2:31:ILE:HG13	1.40	0.41
5:AN1:1065:G:O6	5:AN1:1066:A:N6	2.53	0.41
5:AN1:1407:U:O4	5:AN1:1408:A:N6	2.53	0.41
5:AN1:176:U:H2'	5:AN1:177:G:H8	1.85	0.41
5:AN1:1911:3TD:OP1	5:AN1:1911:3TD:O3'	2.38	0.41
5:AN1:239:G:OP2	5:AN1:239:G:H8	2.04	0.41
5:AN1:249:G:N2	5:AN1:262:A:OP2	2.48	0.41
10:F:36:LEU:HB2	10:F:89:VAL:HB	2.03	0.41
13:I:70:LEU:HA	13:I:88:ASN:HD21	1.86	0.41
5:AN1:1589:C:H2'	5:AN1:1590:A:C8	2.55	0.41
5:AN1:1844:A:H4'	5:AN1:1845:G:H8	1.85	0.41
5:AN1:518:C:H2'	5:AN1:519:A:C8	2.53	0.41
5:AN1:794:C:H2'	5:AN1:795:U:C6	2.56	0.41
55:AN1:3126:HOH:O	8:D:143:HIS:NE2	2.36	0.41
19:O:99:LYS:HA	19:O:99:LYS:HD3	1.87	0.41
5:AN1:1389:U:H2'	5:AN1:1390:A:O4'	2.21	0.41
5:AN1:1817:A:H2'	5:AN1:1818:G:H8	1.85	0.41
5:AN1:2895:G:C6	5:AN1:2896:A:N6	2.89	0.41
5:AN1:876:A:H3'	5:AN1:877:G:C8	2.56	0.41
6:B:40:C:H1'	10:F:64:LYS:O	2.21	0.41
8:D:186:GLU:OE2	8:D:187:ARG:HG3	2.20	0.41
5:AN1:324:A:OP2	9:E:162:ASN:HB2	2.20	0.41
21:Q:33:ILE:N	21:Q:61:ALA:O	2.34	0.41
5:AN1:1876:U:H2'	5:AN1:1877:C:H6	1.85	0.41
5:AN1:74:U:C2	5:AN1:75:G:C8	3.09	0.41
10:F:175:PHE:HB3	10:F:177:PHE:HD1	1.85	0.41
13:I:119:ILE:HD12	13:I:119:ILE:HA	1.93	0.41
25:U:84:HIS:CD2	25:U:87:LYS:H	2.39	0.41
5:AN1:1029:A:H2'	5:AN1:1030:U:C6	2.56	0.40
5:AN1:1296:A:H2	5:AN1:1624:A:C2	2.40	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AN1:1424:G:H2'	5:AN1:1425:G:H8	1.85	0.40
5:AN1:1549:U:H2'	5:AN1:1550:G:O4'	2.20	0.40
5:AN1:2224:G:H2'	5:AN1:2225:U:C6	2.56	0.40
5:AN1:944:A:H2'	5:AN1:945:C:C6	2.56	0.40
15:K:25:ILE:HG12	21:Q:82:HIS:CE1	2.56	0.40
5:AN1:727:G:O2'	5:AN1:761:G:H4'	2.22	0.40
8:D:26:THR:OG1	8:D:194:GLY:O	2.39	0.40
13:I:2:LYS:HB3	13:I:2:LYS:HE2	1.79	0.40
15:K:131:LYS:HG3	15:K:132:GLY:H	1.86	0.40
5:AN1:493:G:N2	22:R:57:ASN:HD21	2.19	0.40
5:AN1:1381:A:H2'	5:AN1:1382:U:H6	1.86	0.40
5:AN1:181:C:H2'	5:AN1:182:A:C8	2.57	0.40
5:AN1:182:A:H2'	5:AN1:183:A:C8	2.57	0.40
12:H:50:ARG:HH12	12:H:54:LEU:HD22	1.86	0.40
17:M:72:ASN:HB3	17:M:75:THR:HB	2.03	0.40
2:1:3:ARG:HD3	2:1:3:ARG:HA	1.90	0.40
5:AN1:1623:C:H2'	5:AN1:1624:A:O4'	2.21	0.40
5:AN1:2096:G:N2	5:AN1:2185:U:O2	2.32	0.40
5:AN1:2791:C:H2'	5:AN1:2792:U:C6	2.56	0.40
9:E:82:LYS:HE2	9:E:82:LYS:HB3	1.85	0.40
5:AN1:2742:U:H5''	11:G:138:LYS:HD2	2.04	0.40
11:G:157:TYR:O	11:G:171:ARG:NH1	2.50	0.40
5:AN1:1436:A:H2'	5:AN1:1437:U:C6	2.57	0.40
5:AN1:812:C:H2'	5:AN1:813:C:H6	1.86	0.40
5:AN1:916:A:N3	6:B:78:U:O2'	2.47	0.40
5:AN1:976:A:H2'	5:AN1:979:C:N4	2.35	0.40
6:B:62:U:H2'	6:B:63:U:C5	2.57	0.40
10:F:65:PRO:HA	10:F:89:VAL:HG22	2.02	0.40
30:Z:38:ARG:HB3	30:Z:41:HIS:HB2	2.02	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	
1	0	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
2	1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
3	2	61/64 (95%)	58 (95%)	1 (2%)	2 (3%)	4	16
4	3	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	C	268/274 (98%)	260 (97%)	8 (3%)	0	100	100
8	D	209/212 (99%)	203 (97%)	6 (3%)	0	100	100
9	E	184/200 (92%)	184 (100%)	0	0	100	100
10	F	173/178 (97%)	151 (87%)	21 (12%)	1 (1%)	27	60
11	G	172/177 (97%)	166 (96%)	6 (4%)	0	100	100
12	H	58/148 (39%)	55 (95%)	3 (5%)	0	100	100
13	I	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
14	J	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
15	K	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
16	L	135/137 (98%)	134 (99%)	1 (1%)	0	100	100
17	M	117/125 (94%)	116 (99%)	1 (1%)	0	100	100
18	N	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
19	O	115/122 (94%)	111 (96%)	4 (4%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
22	R	107/109 (98%)	107 (100%)	0	0	100	100
23	S	88/106 (83%)	85 (97%)	3 (3%)	0	100	100
24	T	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
25	U	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
26	V	78/85 (92%)	78 (100%)	0	0	100	100
27	W	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
28	X	60/65 (92%)	58 (97%)	2 (3%)	0	100	100
29	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	Z	53/61 (87%)	51 (96%)	2 (4%)	0	100	100
32	b	223/250 (89%)	211 (95%)	12 (5%)	0	100	100
33	c	213/250 (85%)	204 (96%)	9 (4%)	0	100	100
34	d	205/208 (99%)	204 (100%)	1 (0%)	0	100	100
35	e	153/165 (93%)	152 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	f	92/127 (72%)	88 (96%)	4 (4%)	0	100	100
37	g	139/156 (89%)	137 (99%)	2 (1%)	0	100	100
38	h	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
39	i	125/128 (98%)	123 (98%)	2 (2%)	0	100	100
40	j	98/103 (95%)	93 (95%)	5 (5%)	0	100	100
41	k	115/128 (90%)	109 (95%)	6 (5%)	0	100	100
42	l	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
45	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
46	p	81/101 (80%)	80 (99%)	1 (1%)	0	100	100
47	q	78/85 (92%)	77 (99%)	1 (1%)	0	100	100
48	r	51/75 (68%)	51 (100%)	0	0	100	100
49	s	80/91 (88%)	80 (100%)	0	0	100	100
50	t	83/88 (94%)	83 (100%)	0	0	100	100
51	u	19/71 (27%)	16 (84%)	3 (16%)	0	100	100
All	All	5361/5872 (91%)	5203 (97%)	155 (3%)	3 (0%)	56	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	31	ILE
3	2	32	LEU
10	F	139	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
1	0	47/47 (100%)	47 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	216/220 (98%)	216 (100%)	0	100	100
8	D	166/167 (99%)	166 (100%)	0	100	100
9	E	144/155 (93%)	143 (99%)	1 (1%)	85	96
10	F	145/147 (99%)	144 (99%)	1 (1%)	85	96
11	G	139/142 (98%)	139 (100%)	0	100	100
12	H	45/112 (40%)	45 (100%)	0	100	100
13	I	118/118 (100%)	118 (100%)	0	100	100
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	108/108 (100%)	107 (99%)	1 (1%)	81	94
16	L	113/113 (100%)	113 (100%)	0	100	100
17	M	96/101 (95%)	96 (100%)	0	100	100
18	N	83/85 (98%)	83 (100%)	0	100	100
19	O	99/102 (97%)	99 (100%)	0	100	100
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	76/87 (87%)	76 (100%)	0	100	100
24	T	82/85 (96%)	82 (100%)	0	100	100
25	U	79/80 (99%)	79 (100%)	0	100	100
26	V	60/64 (94%)	60 (100%)	0	100	100
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	54/56 (96%)	54 (100%)	0	100	100
29	Y	54/54 (100%)	54 (100%)	0	100	100
30	Z	47/50 (94%)	47 (100%)	0	100	100
32	b	185/200 (92%)	182 (98%)	3 (2%)	65	88
33	c	175/198 (88%)	174 (99%)	1 (1%)	87	96
34	d	170/171 (99%)	170 (100%)	0	100	100
35	e	113/120 (94%)	113 (100%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	f	86/111 (78%)	86 (100%)	0	100	100
37	g	116/128 (91%)	114 (98%)	2 (2%)	63	87
38	h	108/109 (99%)	108 (100%)	0	100	100
39	i	99/100 (99%)	98 (99%)	1 (1%)	78	93
40	j	89/91 (98%)	89 (100%)	0	100	100
41	k	88/98 (90%)	88 (100%)	0	100	100
42	l	104/106 (98%)	104 (100%)	0	100	100
43	m	95/98 (97%)	95 (100%)	0	100	100
44	n	81/82 (99%)	81 (100%)	0	100	100
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	62 (98%)	1 (2%)	65	88
47	q	72/76 (95%)	72 (100%)	0	100	100
48	r	47/66 (71%)	47 (100%)	0	100	100
49	s	70/78 (90%)	70 (100%)	0	100	100
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	18/62 (29%)	17 (94%)	1 (6%)	23	54
All	All	4436/4756 (93%)	4424 (100%)	12 (0%)	93	98

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	E	193	LYS
10	F	48	LYS
15	K	44	LYS
32	b	128	PHE
32	b	133	LYS
32	b	147	GLU
33	c	45	LYS
37	g	5	ARG
37	g	92	ARG
39	i	104	ARG
46	p	98	LYS
51	u	49	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	19	ASN
3	2	50	HIS
7	C	48	HIS
7	C	58	HIS
7	C	60	GLN
7	C	90	HIS
7	C	117	GLN
7	C	230	HIS
7	C	243	GLN
8	D	47	GLN
8	D	50	GLN
8	D	108	GLN
8	D	153	GLN
9	E	96	ASN
9	E	114	GLN
9	E	165	HIS
10	F	17	GLN
11	G	19	GLN
11	G	106	ASN
12	H	43	ASN
13	I	13	HIS
13	I	40	HIS
13	I	135	GLN
14	J	59	ASN
15	K	40	GLN
15	K	56	GLN
15	K	107	GLN
15	K	125	GLN
18	N	39	GLN
19	O	13	ASN
19	O	78	GLN
20	P	11	HIS
21	Q	48	GLN
21	Q	87	GLN
22	R	37	ASN
22	R	57	ASN
22	R	60	HIS
25	U	16	GLN
25	U	75	ASN
25	U	84	HIS
27	W	6	GLN
27	W	36	HIS
28	X	61	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	Z	4	GLN
30	Z	41	HIS
32	b	60	ASN
32	b	80	ASN
32	b	85	GLN
32	b	105	ASN
33	c	6	HIS
33	c	19	ASN
34	d	42	HIS
34	d	102	ASN
34	d	118	GLN
34	d	138	GLN
34	d	154	GLN
35	e	121	ASN
35	e	131	ASN
36	f	11	HIS
36	f	35	GLN
36	f	94	HIS
37	g	32	GLN
38	h	86	GLN
39	i	73	GLN
39	i	79	HIS
40	j	56	HIS
40	j	58	ASN
41	k	49	GLN
45	o	37	ASN
45	o	42	HIS
46	p	44	ASN
47	q	32	HIS
49	s	52	HIS
50	t	13	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	sN1	1524/1544 (98%)	212 (13%)	0
5	AN1	2888/2918 (98%)	493 (17%)	10 (0%)
6	B	114/115 (99%)	18 (15%)	1 (0%)
All	All	4526/4577 (98%)	723 (15%)	11 (0%)

All (723) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	AN1	10	U
5	AN1	41	U
5	AN1	50	G
5	AN1	53	G
5	AN1	58	G
5	AN1	59	A
5	AN1	67	G
5	AN1	68	A
5	AN1	69	U
5	AN1	78	A
5	AN1	81	A
5	AN1	82	G
5	AN1	86	C
5	AN1	98	A
5	AN1	101	U
5	AN1	102	A
5	AN1	106	U
5	AN1	107	U
5	AN1	108	U
5	AN1	125	A
5	AN1	127	U
5	AN1	146	U
5	AN1	147	A
5	AN1	169	U
5	AN1	170	A
5	AN1	172	A
5	AN1	188	A
5	AN1	203	A
5	AN1	206	A
5	AN1	223	A
5	AN1	229	A
5	AN1	232	C
5	AN1	235	U
5	AN1	236	U
5	AN1	255	G
5	AN1	257	G
5	AN1	259	G
5	AN1	262	A
5	AN1	271	C
5	AN1	272	A
5	AN1	273	G
5	AN1	279	U
5	AN1	280	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	AN1	283	U
5	AN1	284	U
5	AN1	285	A
5	AN1	291	G
5	AN1	293	U
5	AN1	303	C
5	AN1	313	A
5	AN1	331	G
5	AN1	332	A
5	AN1	336	U
5	AN1	345	C
5	AN1	351	G
5	AN1	356	A
5	AN1	357	C
5	AN1	359	U
5	AN1	366	G
5	AN1	368	C
5	AN1	369	G
5	AN1	371	G
5	AN1	385	G
5	AN1	386	U
5	AN1	395	G
5	AN1	403	A
5	AN1	410	G
5	AN1	423	G
5	AN1	434	C
5	AN1	455	C
5	AN1	479	A
5	AN1	480	G
5	AN1	504	A
5	AN1	508	C
5	AN1	509	C
5	AN1	526	C
5	AN1	529	G
5	AN1	530	C
5	AN1	531	A
5	AN1	543	U
5	AN1	544	U
5	AN1	545	C
5	AN1	547	U
5	AN1	554	A
5	AN1	561	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
5	AN1	564	U
5	AN1	571	U
5	AN1	573	A
5	AN1	601	A
5	AN1	612	A
5	AN1	625	A
5	AN1	635	A
5	AN1	637	U
5	AN1	643	U
5	AN1	644	A
5	AN1	651	U
5	AN1	652	U
5	AN1	656	U
5	AN1	657	G
5	AN1	666	A
5	AN1	667	G
5	AN1	668	A
5	AN1	684	U
5	AN1	692	U
5	AN1	693	G
5	AN1	711	G
5	AN1	712	U
5	AN1	713	A
5	AN1	714	A
5	AN1	719	A
5	AN1	724	G
5	AN1	727	G
5	AN1	728	A
5	AN1	745	U
5	AN1	762	A
5	AN1	763	C
5	AN1	773	G
5	AN1	774	G
5	AN1	780	A
5	AN1	782	G
5	AN1	783	G
5	AN1	787	A
5	AN1	803	G
5	AN1	810	C
5	AN1	817	A
5	AN1	825	U
5	AN1	828	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	AN1	843	G
5	AN1	855	G
5	AN1	857	G
5	AN1	880	G
5	AN1	883	C
5	AN1	884	A
5	AN1	888	C
5	AN1	889	G
5	AN1	890	A
5	AN1	894	A
5	AN1	895	C
5	AN1	899	A
5	AN1	903	A
5	AN1	904	U
5	AN1	908	A
5	AN1	926	G
5	AN1	929	C
5	AN1	930	U
5	AN1	938	A
5	AN1	942	A
5	AN1	943	G
5	AN1	955	U
5	AN1	958	C
5	AN1	971	G
5	AN1	977	A
5	AN1	980	A
5	AN1	993	A
5	AN1	1006	A
5	AN1	1009	U
5	AN1	1010	C
5	AN1	1023	G
5	AN1	1028	G
5	AN1	1032	U
5	AN1	1036	A
5	AN1	1037	A
5	AN1	1039	G
5	AN1	1040	C
5	AN1	1041	A
5	AN1	1042	U
5	AN1	1043	A
5	AN1	1044	G
5	AN1	1054	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	AN1	1057	U
5	AN1	1058	U
5	AN1	1059	G
5	AN1	1061	C
5	AN1	1063	U
5	AN1	1067	A
5	AN1	1070	A
5	AN1	1076	C
5	AN1	1078	U
5	AN1	1081	A
5	AN1	1082	A
5	AN1	1085	A
5	AN1	1086	A
5	AN1	1091	U
5	AN1	1101	C
5	AN1	1108	A
5	AN1	1109	G
5	AN1	1110	U
5	AN1	1121	G
5	AN1	1129	U
5	AN1	1130	A
5	AN1	1131	A
5	AN1	1132	C
5	AN1	1140	A
5	AN1	1148	U
5	AN1	1149	G
5	AN1	1167	U
5	AN1	1170	U
5	AN1	1171	U
5	AN1	1172	U
5	AN1	1173	G
5	AN1	1179	G
5	AN1	1200	A
5	AN1	1201	G
5	AN1	1231	G
5	AN1	1242	A
5	AN1	1245	G
5	AN1	1248	A
5	AN1	1251	G
5	AN1	1267	A
5	AN1	1270	A
5	AN1	1296	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	AN1	1316	A
5	AN1	1324	U
5	AN1	1336	G
5	AN1	1340	C
5	AN1	1360	A
5	AN1	1363	G
5	AN1	1373	A
5	AN1	1374	U
5	AN1	1378	A
5	AN1	1390	A
5	AN1	1407	U
5	AN1	1408	A
5	AN1	1411	G
5	AN1	1414	A
5	AN1	1415	U
5	AN1	1423	C
5	AN1	1428	A
5	AN1	1432	C
5	AN1	1447	G
5	AN1	1448	U
5	AN1	1453	U
5	AN1	1455	U
5	AN1	1456	C
5	AN1	1469	U
5	AN1	1470	G
5	AN1	1473	G
5	AN1	1477	U
5	AN1	1485	A
5	AN1	1501	C
5	AN1	1502	U
5	AN1	1504	U
5	AN1	1505	A
5	AN1	1510	G
5	AN1	1520	A
5	AN1	1530	A
5	AN1	1531	C
5	AN1	1533	U
5	AN1	1534	G
5	AN1	1539	G
5	AN1	1540	C
5	AN1	1541	G
5	AN1	1542	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	AN1	1544	G
5	AN1	1545	U
5	AN1	1564	A
5	AN1	1567	A
5	AN1	1574	U
5	AN1	1582	U
5	AN1	1583	C
5	AN1	1605	G
5	AN1	1606	A
5	AN1	1616	A
5	AN1	1642	C
5	AN1	1645	U
5	AN1	1646	U
5	AN1	1672	G
5	AN1	1691	U
5	AN1	1712	U
5	AN1	1713	U
5	AN1	1714	G
5	AN1	1717	G
5	AN1	1725	U
5	AN1	1726	C
5	AN1	1731	C
5	AN1	1742	G
5	AN1	1746	G
5	AN1	1760	G
5	AN1	1769	A
5	AN1	1776	A
5	AN1	1780	A
5	AN1	1796	C
5	AN1	1797	A
5	AN1	1798	A
5	AN1	1805	A
5	AN1	1807	G
5	AN1	1812	C
5	AN1	1825	A
5	AN1	1829	C
5	AN1	1830	U
5	AN1	1831	G
5	AN1	1844	A
5	AN1	1845	G
5	AN1	1855	U
5	AN1	1861	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	AN1	1864	C
5	AN1	1866	U
5	AN1	1867	A
5	AN1	1871	G
5	AN1	1872	A
5	AN1	1875	C
5	AN1	1885	A
5	AN1	1895	A
5	AN1	1899	G
5	AN1	1902	G
5	AN1	1904	C
5	AN1	1905	C
5	AN1	1907	PSU
5	AN1	1909	A
5	AN1	1910	C
5	AN1	1915	A
5	AN1	1917	G
5	AN1	1918	G
5	AN1	1921	C
5	AN1	1923	A
5	AN1	1925	G
5	AN1	1926	G
5	AN1	1932	A
5	AN1	1933	A
5	AN1	1934	A
5	AN1	1936	U
5	AN1	1950	G
5	AN1	1951	U
5	AN1	1959	U
5	AN1	1960	G
5	AN1	1963	C
5	AN1	1966	A
5	AN1	1967	U
5	AN1	1968	G
5	AN1	1978	U
5	AN1	1987	U
5	AN1	1989	U
5	AN1	1993	C
5	AN1	2018	U
5	AN1	2019	C
5	AN1	2025	G
5	AN1	2027	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	AN1	2029	A
5	AN1	2030	U
5	AN1	2039	C
5	AN1	2051	C
5	AN1	2052	G
5	AN1	2056	A
5	AN1	2057	G
5	AN1	2058	A
5	AN1	2065	7MG
5	AN1	2089	G
5	AN1	2092	C
5	AN1	2104	U
5	AN1	2106	G
5	AN1	2107	U
5	AN1	2108	G
5	AN1	2111	G
5	AN1	2112	G
5	AN1	2113	A
5	AN1	2114	U
5	AN1	2115	A
5	AN1	2116	G
5	AN1	2120	G
5	AN1	2121	G
5	AN1	2122	A
5	AN1	2123	G
5	AN1	2127	U
5	AN1	2128	U
5	AN1	2129	G
5	AN1	2131	A
5	AN1	2133	C
5	AN1	2142	U
5	AN1	2143	A
5	AN1	2145	U
5	AN1	2146	U
5	AN1	2148	C
5	AN1	2149	A
5	AN1	2152	G
5	AN1	2153	G
5	AN1	2154	A
5	AN1	2157	C
5	AN1	2158	G
5	AN1	2162	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	AN1	2166	A
5	AN1	2167	A
5	AN1	2168	U
5	AN1	2169	A
5	AN1	2171	C
5	AN1	2172	A
5	AN1	2174	C
5	AN1	2178	G
5	AN1	2184	U
5	AN1	2185	U
5	AN1	2188	G
5	AN1	2194	A
5	AN1	2200	G
5	AN1	2221	A
5	AN1	2234	G
5	AN1	2235	G
5	AN1	2261	U
5	AN1	2275	G
5	AN1	2279	U
5	AN1	2283	A
5	AN1	2301	U
5	AN1	2304	G
5	AN1	2305	A
5	AN1	2308	U
5	AN1	2312	G
5	AN1	2314	G
5	AN1	2316	A
5	AN1	2321	A
5	AN1	2323	A
5	AN1	2341	A
5	AN1	2346	C
5	AN1	2355	C
5	AN1	2357	A
5	AN1	2378	G
5	AN1	2379	G
5	AN1	2380	U
5	AN1	2381	C
5	AN1	2399	C
5	AN1	2408	A
5	AN1	2425	G
5	AN1	2426	A
5	AN1	2429	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
5	AN1	2430	A
5	AN1	2431	A
5	AN1	2437	U
5	AN1	2443	G
5	AN1	2444	A
5	AN1	2446	A
5	AN1	2455	A
5	AN1	2468	G
5	AN1	2469	U
5	AN1	2470	U
5	AN1	2472	A
5	AN1	2473	U
5	AN1	2487	U
5	AN1	2494	C
5	AN1	2498	G
5	AN1	2500	PSU
5	AN1	2501	G
5	AN1	2503	C
5	AN1	2514	A
5	AN1	2516	C
5	AN1	2525	G
5	AN1	2530	A
5	AN1	2543	A
5	AN1	2548	OMU
5	AN1	2550	U
5	AN1	2562	A
5	AN1	2563	G
5	AN1	2568	A
5	AN1	2598	A
5	AN1	2599	G
5	AN1	2605	U
5	AN1	2606	C
5	AN1	2607	C
5	AN1	2609	U
5	AN1	2611	U
5	AN1	2625	U
5	AN1	2635	A
5	AN1	2642	C
5	AN1	2657	G
5	AN1	2661	A
5	AN1	2685	U
5	AN1	2686	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	AN1	2710	G
5	AN1	2722	U
5	AN1	2730	A
5	AN1	2740	G
5	AN1	2744	A
5	AN1	2753	A
5	AN1	2754	A
5	AN1	2761	A
5	AN1	2762	G
5	AN1	2774	A
5	AN1	2776	A
5	AN1	2787	A
5	AN1	2788	G
5	AN1	2793	U
5	AN1	2794	U
5	AN1	2796	U
5	AN1	2800	C
5	AN1	2804	A
5	AN1	2816	G
5	AN1	2817	A
5	AN1	2831	A
5	AN1	2845	G
5	AN1	2851	U
5	AN1	2853	G
5	AN1	2857	U
5	AN1	2863	A
5	AN1	2868	G
5	AN1	2875	A
5	AN1	2897	C
5	AN1	2898	U
6	B	2	C
6	B	10	C
6	B	11	A
6	B	14	G
6	B	23	A
6	B	31	G
6	B	32	A
6	B	39	C
6	B	40	C
6	B	42	G
6	B	44	A
6	B	50	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	B	65	G
6	B	86	U
6	B	87	A
6	B	105	C
6	B	106	A
6	B	109	G
31	sN1	6	C
31	sN1	11	G
31	sN1	33	G
31	sN1	41	G
31	sN1	49	C
31	sN1	50	U
31	sN1	53	A
31	sN1	56	C
31	sN1	57	A
31	sN1	64	U
31	sN1	80	A
31	sN1	86	C
31	sN1	87	U
31	sN1	90	C
31	sN1	91	G
31	sN1	94	C
31	sN1	97	A
31	sN1	105	A
31	sN1	107	G
31	sN1	126	A
31	sN1	127	U
31	sN1	140	G
31	sN1	157	A
31	sN1	170	A
31	sN1	184	A
31	sN1	186	G
31	sN1	193	A
31	sN1	204	U
31	sN1	205	U
31	sN1	206	C
31	sN1	212	U
31	sN1	216	G
31	sN1	236	C
31	sN1	241	U
31	sN1	243	G
31	sN1	247	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
31	sN1	262	G
31	sN1	263	C
31	sN1	285	G
31	sN1	289	G
31	sN1	302	A
31	sN1	324	C
31	sN1	326	C
31	sN1	340	A
31	sN1	341	C
31	sN1	348	C
31	sN1	359	A
31	sN1	363	U
31	sN1	368	C
31	sN1	369	A
31	sN1	388	C
31	sN1	393	A
31	sN1	402	G
31	sN1	407	A
31	sN1	408	A
31	sN1	409	G
31	sN1	425	U
31	sN1	463	U
31	sN1	474	A
31	sN1	475	G
31	sN1	476	U
31	sN1	478	G
31	sN1	479	A
31	sN1	481	G
31	sN1	482	U
31	sN1	493	A
31	sN1	494	U
31	sN1	505	U
31	sN1	506	A
31	sN1	507	A
31	sN1	508	C
31	sN1	515	C
31	sN1	521	G
31	sN1	522	C
31	sN1	524	7MG
31	sN1	527	G
31	sN1	544	A
31	sN1	556	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
31	sN1	561	C
31	sN1	567	G
31	sN1	569	A
31	sN1	570	A
31	sN1	572	G
31	sN1	573	C
31	sN1	574	G
31	sN1	593	A
31	sN1	615	C
31	sN1	630	G
31	sN1	639	A
31	sN1	650	A
31	sN1	662	A
31	sN1	684	A
31	sN1	685	G
31	sN1	692	A
31	sN1	699	A
31	sN1	700	G
31	sN1	714	U
31	sN1	720	U
31	sN1	721	G
31	sN1	728	G
31	sN1	745	U
31	sN1	752	G
31	sN1	774	A
31	sN1	790	U
31	sN1	791	A
31	sN1	812	A
31	sN1	814	C
31	sN1	839	U
31	sN1	840	U
31	sN1	841	G
31	sN1	842	A
31	sN1	843	G
31	sN1	899	G
31	sN1	923	G
31	sN1	931	C
31	sN1	932	A
31	sN1	957	U
31	sN1	958	U
31	sN1	966	A
31	sN1	968	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
31	sN1	972	A
31	sN1	973	G
31	sN1	974	A
31	sN1	989	U
31	sN1	990	G
31	sN1	991	A
31	sN1	992	C
31	sN1	993	A
31	sN1	998	A
31	sN1	1001	A
31	sN1	1003	C
31	sN1	1007	C
31	sN1	1008	C
31	sN1	1010	G
31	sN1	1016	G
31	sN1	1023	G
31	sN1	1025	C
31	sN1	1026	U
31	sN1	1028	C
31	sN1	1029	G
31	sN1	1030	G
31	sN1	1041	A
31	sN1	1042	C
31	sN1	1050	G
31	sN1	1051	C
31	sN1	1061	G
31	sN1	1062	U
31	sN1	1069	G
31	sN1	1083	U
31	sN1	1084	G
31	sN1	1086	G
31	sN1	1091	G
31	sN1	1092	U
31	sN1	1095	C
31	sN1	1098	A
31	sN1	1123	U
31	sN1	1124	G
31	sN1	1131	U
31	sN1	1134	C
31	sN1	1136	G
31	sN1	1156	U
31	sN1	1157	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
31	sN1	1161	G
31	sN1	1164	A
31	sN1	1165	C
31	sN1	1169	C
31	sN1	1180	C
31	sN1	1181	G
31	sN1	1182	G
31	sN1	1188	A
31	sN1	1193	A
31	sN1	1194	A
31	sN1	1209	U
31	sN1	1210	A
31	sN1	1217	G
31	sN1	1224	A
31	sN1	1235	A
31	sN1	1247	A
31	sN1	1255	G
31	sN1	1257	U
31	sN1	1259	C
31	sN1	1277	A
31	sN1	1284	A
31	sN1	1295	U
31	sN1	1297	G
31	sN1	1299	C
31	sN1	1302	G
31	sN1	1317	C
31	sN1	1360	A
31	sN1	1378	U
31	sN1	1380	C
31	sN1	1385	C
31	sN1	1394	C
31	sN1	1395	A
31	sN1	1398	G
31	sN1	1402	G
31	sN1	1404	C
31	sN1	1425	A
31	sN1	1427	C
31	sN1	1444	A
31	sN1	1448	C
31	sN1	1449	A
31	sN1	1450	A
31	sN1	1488	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
31	sN1	1490	A
31	sN1	1491	G
31	sN1	1496	A
31	sN1	1499	A
31	sN1	1503	U
31	sN1	1517	C
31	sN1	1526	G
31	sN1	1527	G

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	AN1	355	C
5	AN1	356	A
5	AN1	368	C
5	AN1	478	A
5	AN1	782	G
5	AN1	893	U
5	AN1	1171	U
5	AN1	1538	A
5	AN1	2170	C
5	AN1	2379	G
6	B	108	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PSU	AN1	1907	5	16,21,22	1.13	1 (6%)	20,30,33	3.12	6 (30%)
5	3TD	AN1	1911	5	16,22,23	3.24	6 (37%)	19,32,35	1.55	3 (15%)
5	PSU	AN1	1913	5	16,21,22	1.06	1 (6%)	20,30,33	3.21	7 (35%)
5	5MU	AN1	1935	5	13,22,23	1.61	2 (15%)	14,32,35	3.00	2 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	6MZ	AN1	2026	5	17,25,26	1.99	3 (17%)	15,36,39	4.27	5 (33%)
5	7MG	AN1	2065	5	20,26,27	4.45	10 (50%)	24,39,42	1.77	6 (25%)
5	OMG	AN1	2247	5	18,26,27	3.50	7 (38%)	22,38,41	1.81	4 (18%)
5	2MG	AN1	2441	5	18,26,27	4.57	7 (38%)	19,38,41	2.20	8 (42%)
5	PSU	AN1	2453	5	16,21,22	1.11	2 (12%)	20,30,33	3.05	6 (30%)
5	2MA	AN1	2499	5,53	16,25,26	4.15	5 (31%)	17,37,40	2.48	5 (29%)
5	PSU	AN1	2500	5	16,21,22	1.15	2 (12%)	20,30,33	3.15	6 (30%)
5	OMU	AN1	2548	5	14,22,23	3.51	5 (35%)	17,31,34	0.63	0
5	PSU	AN1	2576	5	16,21,22	1.13	2 (12%)	20,30,33	3.06	6 (30%)
5	PSU	AN1	2601	5	16,21,22	1.11	1 (6%)	20,30,33	3.15	6 (30%)
5	PSU	AN1	952	5	16,21,22	1.14	2 (12%)	20,30,33	3.07	6 (30%)
31	2MG	sN1	1204	31	18,26,27	4.60	7 (38%)	19,38,41	2.29	8 (42%)
31	4OC	sN1	1399	31	16,23,24	3.46	6 (37%)	20,32,35	1.09	1 (5%)
31	UR3	sN1	1495	31	13,22,23	3.21	3 (23%)	15,32,35	0.66	0
31	MA6	sN1	1515	31	16,26,27	1.07	2 (12%)	16,38,41	4.13	3 (18%)
31	MA6	sN1	1516	31	16,26,27	1.07	2 (12%)	16,38,41	4.24	3 (18%)
31	PSU	sN1	513	31	16,21,22	1.06	1 (6%)	20,30,33	3.34	6 (30%)
31	7MG	sN1	524	31	20,26,27	4.54	10 (50%)	24,39,42	1.77	6 (25%)
31	2MG	sN1	963	31	18,26,27	4.66	7 (38%)	19,38,41	2.28	8 (42%)
31	5MC	sN1	964	31	14,22,23	3.23	5 (35%)	17,32,35	1.34	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	AN1	1907	5	-	1/7/25/26	0/2/2/2
5	3TD	AN1	1911	5	-	3/7/25/26	0/2/2/2
5	PSU	AN1	1913	5	-	4/7/25/26	0/2/2/2
5	5MU	AN1	1935	5	-	0/3/25/26	0/2/2/2
5	6MZ	AN1	2026	5	-	2/5/27/28	0/3/3/3
5	7MG	AN1	2065	5	-	3/7/37/38	0/3/3/3
5	OMG	AN1	2247	5	-	0/5/27/28	0/3/3/3
5	2MG	AN1	2441	5	-	1/5/27/28	0/3/3/3
5	PSU	AN1	2453	5	-	0/7/25/26	0/2/2/2
5	2MA	AN1	2499	5,53	-	2/3/25/26	0/3/3/3

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	AN1	2500	5	-	0/7/25/26	0/2/2/2
5	OMU	AN1	2548	5	-	2/5/27/28	0/2/2/2
5	PSU	AN1	2576	5	-	0/7/25/26	0/2/2/2
5	PSU	AN1	2601	5	-	0/7/25/26	0/2/2/2
5	PSU	AN1	952	5	-	0/7/25/26	0/2/2/2
31	2MG	sN1	1204	31	-	0/5/27/28	0/3/3/3
31	4OC	sN1	1399	31	-	2/7/29/30	0/2/2/2
31	UR3	sN1	1495	31	-	2/3/25/26	0/2/2/2
31	MA6	sN1	1515	31	-	0/7/29/30	0/3/3/3
31	MA6	sN1	1516	31	-	3/7/29/30	0/3/3/3
31	PSU	sN1	513	31	-	0/7/25/26	0/2/2/2
31	7MG	sN1	524	31	-	3/7/37/38	0/3/3/3
31	2MG	sN1	963	31	-	0/5/27/28	0/3/3/3
31	5MC	sN1	964	31	-	0/3/25/26	0/2/2/2

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	sN1	963	2MG	C2-N2	13.83	1.45	1.34
31	sN1	1204	2MG	C2-N2	13.56	1.45	1.34
5	AN1	2441	2MG	C2-N2	13.47	1.45	1.34
31	sN1	524	7MG	C4-N3	10.59	1.47	1.34
5	AN1	2065	7MG	C4-N3	10.43	1.47	1.34
31	sN1	524	7MG	C6-C5	9.67	1.52	1.41
5	AN1	2065	7MG	C6-C5	9.23	1.52	1.41
5	AN1	2499	2MA	C4-N3	9.16	1.50	1.35
31	sN1	963	2MG	C4-N3	8.83	1.49	1.35
31	sN1	1204	2MG	C4-N3	8.73	1.49	1.35
5	AN1	2441	2MG	C4-N3	8.73	1.49	1.35
5	AN1	2247	OMG	C4-N3	8.49	1.49	1.35
31	sN1	1495	UR3	C6-N1	8.08	1.46	1.35
5	AN1	2499	2MA	C6-C5	8.06	1.54	1.41
31	sN1	1399	4OC	C6-N1	7.91	1.46	1.35
5	AN1	2499	2MA	C2-N3	7.53	1.46	1.34
5	AN1	2548	OMU	C4-N3	7.49	1.46	1.33
5	AN1	1911	3TD	C6-C5	7.37	1.49	1.38
5	AN1	2548	OMU	C6-N1	7.11	1.45	1.35
31	sN1	963	2MG	C6-C5	7.08	1.53	1.41
5	AN1	2441	2MG	C6-C5	7.05	1.53	1.41
31	sN1	1204	2MG	C6-C5	7.04	1.53	1.41
31	sN1	964	5MC	C4-N3	7.00	1.45	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AN1	2247	OMG	C6-C5	6.84	1.53	1.41
31	sN1	524	7MG	C2-N3	6.81	1.47	1.35
31	sN1	524	7MG	C6-N1	6.81	1.44	1.33
5	AN1	2065	7MG	C6-N1	6.77	1.44	1.33
5	AN1	2065	7MG	C2-N3	6.76	1.47	1.35
5	AN1	2026	6MZ	C6-N6	6.75	1.45	1.35
5	AN1	2065	7MG	C2-N1	6.57	1.47	1.35
31	sN1	524	7MG	C2-N1	6.56	1.47	1.35
5	AN1	2499	2MA	C2-N1	6.11	1.44	1.34
5	AN1	2247	OMG	C6-N1	6.05	1.43	1.33
31	sN1	963	2MG	C6-N1	6.03	1.43	1.33
31	sN1	524	7MG	C2-N2	5.97	1.46	1.33
31	sN1	1204	2MG	C6-N1	5.96	1.43	1.33
5	AN1	2548	OMU	C2-N3	5.94	1.49	1.38
5	AN1	2065	7MG	C2-N2	5.89	1.45	1.33
31	sN1	1495	UR3	C6-C5	5.82	1.50	1.38
5	AN1	2441	2MG	C6-N1	5.79	1.43	1.33
5	AN1	1911	3TD	C2-N1	5.75	1.49	1.38
31	sN1	964	5MC	C5-C4	5.63	1.49	1.41
5	AN1	1911	3TD	C4-N3	5.58	1.46	1.38
5	AN1	1911	3TD	C6-N1	5.51	1.46	1.34
31	sN1	1399	4OC	C2-N3	5.43	1.48	1.38
31	sN1	964	5MC	C2-N3	5.41	1.48	1.38
31	sN1	1399	4OC	C4-N3	5.36	1.44	1.34
31	sN1	1495	UR3	C4-N3	5.31	1.46	1.38
31	sN1	1399	4OC	C6-C5	5.27	1.49	1.38
5	AN1	2499	2MA	C6-N1	4.86	1.44	1.34
5	AN1	2247	OMG	C2-N2	4.86	1.43	1.33
5	AN1	2247	OMG	C2-N1	4.76	1.43	1.35
5	AN1	2548	OMU	C6-C5	4.66	1.48	1.38
31	sN1	1399	4OC	C4-N4	4.65	1.46	1.36
31	sN1	964	5MC	C4-N4	4.48	1.45	1.34
5	AN1	1935	5MU	C4-N3	-4.43	1.25	1.33
31	sN1	1399	4OC	C5-C4	4.22	1.49	1.39
31	sN1	963	2MG	C2-N3	3.85	1.46	1.34
31	sN1	1204	2MG	C2-N3	3.81	1.46	1.34
5	AN1	2441	2MG	C2-N3	3.76	1.46	1.34
31	sN1	524	7MG	C4-N9	3.69	1.44	1.38
5	AN1	2065	7MG	C4-N9	3.44	1.44	1.38
31	sN1	964	5MC	C6-C5	3.43	1.49	1.40
31	sN1	1204	2MG	C2-N1	3.13	1.44	1.34
31	sN1	963	2MG	C2-N1	3.13	1.44	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AN1	2441	2MG	C2-N1	3.09	1.44	1.34
5	AN1	1913	PSU	C4-N3	3.06	1.38	1.33
5	AN1	1907	PSU	C4-N3	3.03	1.38	1.33
31	sN1	513	PSU	C4-N3	3.00	1.38	1.33
5	AN1	2601	PSU	C4-N3	2.92	1.38	1.33
5	AN1	2500	PSU	C4-N3	2.91	1.38	1.33
5	AN1	952	PSU	C4-N3	2.90	1.38	1.33
5	AN1	2026	6MZ	C5-C4	-2.89	1.34	1.40
5	AN1	2576	PSU	C4-N3	2.87	1.38	1.33
5	AN1	2453	PSU	C4-N3	2.85	1.38	1.33
31	sN1	1515	MA6	C5-C4	-2.85	1.34	1.40
31	sN1	1516	MA6	C5-C4	-2.81	1.34	1.40
31	sN1	524	7MG	C5-C4	2.81	1.44	1.38
5	AN1	1911	3TD	C5-C1'	-2.67	1.50	1.52
5	AN1	2065	7MG	C5-C4	2.65	1.43	1.38
5	AN1	1935	5MU	O4-C4	-2.57	1.18	1.24
5	AN1	2247	OMG	C2-N3	2.53	1.46	1.35
31	sN1	1515	MA6	C2-N3	2.51	1.36	1.32
31	sN1	1516	MA6	C2-N3	2.49	1.36	1.32
5	AN1	2247	OMG	O6-C6	-2.48	1.18	1.24
31	sN1	524	7MG	C8-N9	2.36	1.51	1.45
5	AN1	2065	7MG	O6-C6	-2.33	1.18	1.24
5	AN1	2548	OMU	O4-C4	-2.29	1.18	1.24
31	sN1	1204	2MG	O6-C6	-2.29	1.18	1.24
5	AN1	2441	2MG	O6-C6	-2.28	1.18	1.24
5	AN1	1911	3TD	O4-C4	-2.28	1.18	1.24
5	AN1	2065	7MG	C8-N9	2.27	1.51	1.45
31	sN1	963	2MG	O6-C6	-2.26	1.18	1.24
5	AN1	2026	6MZ	C2-N3	2.25	1.35	1.32
31	sN1	524	7MG	O6-C6	-2.21	1.19	1.24
5	AN1	952	PSU	C5-C1'	-2.08	1.50	1.52
5	AN1	2453	PSU	O4'-C1'	-2.05	1.41	1.44
5	AN1	2576	PSU	C5-C1'	-2.01	1.50	1.52
5	AN1	2500	PSU	C5-C1'	-2.01	1.50	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	sN1	1516	MA6	N1-C6-N6	-14.29	102.02	117.06
31	sN1	1515	MA6	N1-C6-N6	-13.87	102.46	117.06
5	AN1	2026	6MZ	C1'-N9-C4	-13.25	103.75	126.64
31	sN1	513	PSU	N1-C2-N3	-11.39	119.38	128.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AN1	1913	PSU	N1-C2-N3	-10.62	119.99	128.43
5	AN1	2601	PSU	N1-C2-N3	-10.44	120.13	128.43
5	AN1	1907	PSU	N1-C2-N3	-10.35	120.20	128.43
5	AN1	2500	PSU	N1-C2-N3	-10.34	120.21	128.43
5	AN1	2453	PSU	N1-C2-N3	-10.32	120.22	128.43
5	AN1	2576	PSU	N1-C2-N3	-10.25	120.28	128.43
5	AN1	952	PSU	N1-C2-N3	-10.21	120.31	128.43
5	AN1	1935	5MU	C5-C6-N1	-8.59	112.85	122.15
5	AN1	2026	6MZ	C5-C6-N6	7.48	132.74	120.37
5	AN1	2499	2MA	C1'-N9-C4	7.02	138.76	126.64
5	AN1	1935	5MU	C4-N3-C2	6.98	121.03	115.14
31	sN1	1516	MA6	C5-C6-N6	6.97	138.17	122.58
31	sN1	1515	MA6	C5-C6-N6	6.87	137.93	122.58
31	sN1	513	PSU	C4-N3-C2	6.58	120.69	115.14
5	AN1	1913	PSU	C4-N3-C2	5.96	120.17	115.14
5	AN1	1907	PSU	C4-N3-C2	5.61	119.88	115.14
5	AN1	2500	PSU	C4-N3-C2	5.56	119.83	115.14
5	AN1	2576	PSU	C4-N3-C2	5.52	119.81	115.14
5	AN1	2601	PSU	C4-N3-C2	5.45	119.74	115.14
31	sN1	1515	MA6	N3-C2-N1	-5.36	120.05	128.68
5	AN1	2247	OMG	N3-C2-N1	-5.34	120.02	127.25
31	sN1	1516	MA6	N3-C2-N1	-5.34	120.07	128.68
5	AN1	952	PSU	C4-N3-C2	5.29	119.61	115.14
5	AN1	2453	PSU	C4-N3-C2	5.26	119.58	115.14
5	AN1	2499	2MA	C2-N3-C4	5.14	119.73	115.53
5	AN1	2026	6MZ	N3-C2-N1	-5.08	120.49	128.68
5	AN1	1913	PSU	C5-C4-N3	-4.48	119.59	125.36
5	AN1	2576	PSU	C5-C4-N3	-4.48	119.59	125.36
5	AN1	1907	PSU	C5-C4-N3	-4.46	119.62	125.36
5	AN1	2441	2MG	C2-N3-C4	4.45	120.33	115.28
5	AN1	2500	PSU	C5-C4-N3	-4.43	119.65	125.36
31	sN1	1204	2MG	C1'-N9-C4	-4.41	119.01	126.64
31	sN1	513	PSU	C5-C4-N3	-4.34	119.78	125.36
31	sN1	963	2MG	C1'-N9-C4	-4.33	119.16	126.64
31	sN1	963	2MG	C2-N3-C4	4.32	120.18	115.28
5	AN1	952	PSU	C5-C4-N3	-4.31	119.81	125.36
5	AN1	2601	PSU	C5-C4-N3	-4.28	119.85	125.36
5	AN1	2453	PSU	C5-C4-N3	-4.23	119.91	125.36
31	sN1	1204	2MG	C2-N3-C4	4.23	120.08	115.28
5	AN1	2247	OMG	C2-N3-C4	4.17	120.12	115.36
31	sN1	963	2MG	N3-C2-N1	-4.02	119.96	126.22
5	AN1	2065	7MG	C6-C5-C4	4.00	119.49	115.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	sN1	1204	2MG	N3-C2-N1	-3.96	120.06	126.22
31	sN1	524	7MG	C6-C5-C4	3.92	119.41	115.20
5	AN1	2441	2MG	N3-C2-N1	-3.90	120.16	126.22
31	sN1	964	5MC	C2-N3-C4	3.85	120.31	115.92
31	sN1	524	7MG	C5-C4-N3	-3.67	120.34	126.47
31	sN1	1399	4OC	CM4-N4-C4	-3.66	119.78	122.95
5	AN1	1911	3TD	C5-C6-N1	-3.65	119.86	124.44
5	AN1	2065	7MG	C5-C4-N3	-3.63	120.42	126.47
5	AN1	2441	2MG	C1'-N9-C4	-3.61	120.40	126.64
5	AN1	2500	PSU	C5-C1'-C2'	-3.45	109.17	115.32
5	AN1	2065	7MG	N1-C2-N3	-3.39	120.05	125.42
5	AN1	2453	PSU	C5-C6-N1	-3.38	120.21	124.44
31	sN1	524	7MG	N1-C2-N3	-3.35	120.11	125.42
5	AN1	952	PSU	C5-C6-N1	-3.34	120.25	124.44
5	AN1	2576	PSU	C5-C6-N1	-3.32	120.28	124.44
31	sN1	1204	2MG	N2-C2-N1	3.30	120.13	116.96
31	sN1	513	PSU	C6-N1-C2	3.30	120.58	115.32
5	AN1	2601	PSU	C6-N1-C2	3.28	120.55	115.32
5	AN1	2601	PSU	C5-C6-N1	-3.28	120.33	124.44
5	AN1	2453	PSU	C6-N1-C2	3.26	120.52	115.32
31	sN1	963	2MG	N2-C2-N1	3.24	120.07	116.96
5	AN1	952	PSU	C6-N1-C2	3.23	120.47	115.32
5	AN1	2500	PSU	C5-C6-N1	-3.23	120.39	124.44
5	AN1	1907	PSU	C5-C6-N1	-3.22	120.40	124.44
31	sN1	1204	2MG	CM2-N2-C2	-3.21	119.71	123.59
5	AN1	2601	PSU	C5-C1'-C2'	-3.20	109.61	115.32
5	AN1	2576	PSU	C6-N1-C2	3.20	120.42	115.32
5	AN1	1907	PSU	C6-N1-C2	3.20	120.41	115.32
5	AN1	2500	PSU	C6-N1-C2	3.19	120.40	115.32
5	AN1	1911	3TD	C6-N1-C2	3.14	120.33	115.32
5	AN1	2499	2MA	N3-C2-N1	-3.14	119.83	125.70
31	sN1	963	2MG	N2-C2-N3	3.13	119.97	116.96
5	AN1	1913	PSU	C6-N1-C2	3.12	120.30	115.32
5	AN1	2441	2MG	CM2-N2-C2	-3.11	119.84	123.59
5	AN1	2441	2MG	N2-C2-N1	3.10	119.94	116.96
5	AN1	2441	2MG	N2-C2-N3	3.06	119.90	116.96
5	AN1	1911	3TD	C5-C1'-C2'	-3.02	109.93	115.32
31	sN1	1204	2MG	N2-C2-N3	2.96	119.81	116.96
31	sN1	513	PSU	C5-C6-N1	-2.93	120.76	124.44
31	sN1	963	2MG	CM2-N2-C2	-2.93	120.05	123.59
31	sN1	524	7MG	C5-C4-N9	2.93	110.40	106.29
31	sN1	524	7MG	C6-N1-C2	2.85	120.12	116.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AN1	2026	6MZ	C2-N1-C6	2.84	119.14	116.62
5	AN1	1907	PSU	C5-C1'-C2'	-2.83	110.27	115.32
5	AN1	2065	7MG	C6-N1-C2	2.81	120.07	116.06
5	AN1	1913	PSU	C5-C6-N1	-2.80	120.93	124.44
5	AN1	2065	7MG	C5-C4-N9	2.79	110.21	106.29
5	AN1	952	PSU	C5-C1'-C2'	-2.76	110.40	115.32
5	AN1	2499	2MA	C5-C6-N1	-2.76	120.08	123.10
5	AN1	1913	PSU	O4'-C1'-C5	2.58	113.92	109.93
31	sN1	963	2MG	C6-N1-C2	2.51	119.67	115.18
31	sN1	963	2MG	C5-C6-N1	-2.48	120.02	123.47
5	AN1	2247	OMG	C6-N1-C2	2.48	119.59	116.06
5	AN1	2441	2MG	C5-C6-N1	-2.46	120.05	123.47
5	AN1	2247	OMG	C5-C6-N1	-2.45	120.06	123.47
31	sN1	1204	2MG	C6-N1-C2	2.45	119.56	115.18
31	sN1	1204	2MG	C5-C6-N1	-2.42	120.10	123.47
5	AN1	2441	2MG	C6-N1-C2	2.38	119.45	115.18
31	sN1	524	7MG	C2-N3-C4	2.25	120.22	113.94
5	AN1	2065	7MG	C2-N3-C4	2.22	120.16	113.94
31	sN1	513	PSU	O4'-C1'-C2'	2.10	108.06	104.66
5	AN1	2499	2MA	CM2-C2-N1	2.09	120.44	117.16
5	AN1	2026	6MZ	C9-N6-C6	-2.07	121.09	122.87
31	sN1	964	5MC	N4-C4-N3	2.07	119.98	117.03
31	sN1	964	5MC	C5-C6-N1	-2.06	119.92	122.15
5	AN1	1913	PSU	O4'-C1'-C2'	2.03	107.94	104.66
5	AN1	2453	PSU	O4'-C1'-C2'	2.01	107.92	104.66
5	AN1	2576	PSU	O4'-C1'-C2'	2.00	107.91	104.66

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AN1	1913	PSU	O4'-C1'-C5-C4
5	AN1	1913	PSU	O4'-C1'-C5-C6
5	AN1	2548	OMU	C3'-C4'-C5'-O5'
5	AN1	2548	OMU	O4'-C4'-C5'-O5'
31	sN1	1516	MA6	C5-C6-N6-C9
31	sN1	524	7MG	C3'-C4'-C5'-O5'
5	AN1	2026	6MZ	O4'-C4'-C5'-O5'
5	AN1	2026	6MZ	C3'-C4'-C5'-O5'
5	AN1	2499	2MA	O4'-C4'-C5'-O5'
5	AN1	2499	2MA	C3'-C4'-C5'-O5'
5	AN1	1911	3TD	C3'-C4'-C5'-O5'

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	AN1	1911	3TD	O4'-C4'-C5'-O5'
31	sN1	1399	4OC	O4'-C4'-C5'-O5'
31	sN1	524	7MG	O4'-C4'-C5'-O5'
31	sN1	1516	MA6	C5-C6-N6-C10
31	sN1	1495	UR3	O4'-C4'-C5'-O5'
5	AN1	1913	PSU	O4'-C4'-C5'-O5'
31	sN1	1516	MA6	N1-C6-N6-C9
31	sN1	1399	4OC	C3'-C4'-C5'-O5'
5	AN1	1911	3TD	C4'-C5'-O5'-P
5	AN1	1907	PSU	C4'-C5'-O5'-P
31	sN1	524	7MG	C4'-C5'-O5'-P
5	AN1	2065	7MG	O4'-C4'-C5'-O5'
31	sN1	1495	UR3	C3'-C4'-C5'-O5'
5	AN1	2441	2MG	C3'-C4'-C5'-O5'
5	AN1	2065	7MG	C4'-C5'-O5'-P
5	AN1	1913	PSU	C3'-C4'-C5'-O5'
5	AN1	2065	7MG	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AN1	1911	3TD	2	0
5	AN1	1913	PSU	1	0
5	AN1	2026	6MZ	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 95 ligands modelled in this entry, 95 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.