



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

Sep 18, 2017 – 05:40 AM EDT

PDB ID : 5KCS  
EMDB ID: : EMD-8238  
Title : Cryo-EM structure of the Escherichia coli 70S ribosome in complex with antibiotic Evernimycin, mRNA, TetM and P-site tRNA at 3.9Å resolution  
Authors : Arenz, S.; Juetten, M.F.; Graf, M.; Nguyen, F.; Huter, P.; Polikanov, Y.S.; Blanchard, S.C.; Wilson, D.N.  
Deposited on : unknown  
Resolution : 3.90 Å(reported)

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  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

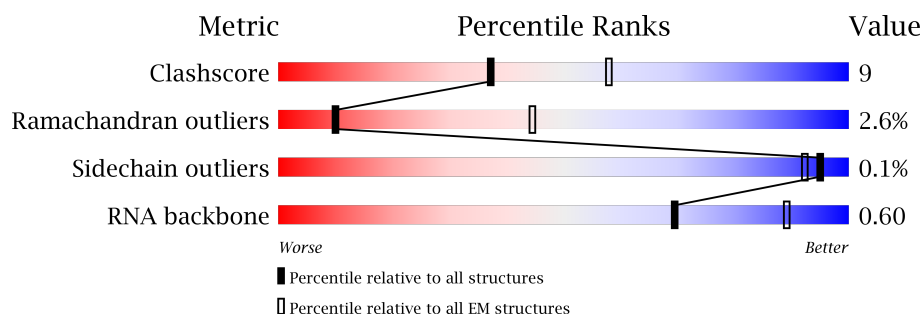
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 Å.

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




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	1A	2904	54% 40% 7%
2	1B	120	63% 31% 6%
3	1D	273	64% 34% .
4	1E	209	72% 28%
5	1F	201	73% 27%
6	1G	179	71% 27% ..
7	1H	177	85% 15% .
8	1L	121	57% 43%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	1I	149	
10	1J	165	
11	1K	142	
12	1N	142	
13	1O	123	
14	1P	144	
15	1Q	136	
16	1R	127	
17	1S	117	
18	1T	115	
19	1U	118	
20	1V	103	
21	1W	110	
22	1X	100	
23	1Y	104	
24	1Z	94	
25	10	85	
26	11	78	
27	12	63	
28	13	59	
29	14	70	
30	15	57	
31	16	55	
32	17	46	
33	18	65	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	19	38	
35	1a	1539	
36	1b	241	
37	1c	233	
38	1d	206	
39	1e	167	
40	1f	135	
41	1g	179	
42	1h	130	
43	1i	130	
44	1j	103	
45	1k	129	
46	1l	124	
47	1m	118	
48	1n	101	
49	1o	89	
50	1p	82	
51	1q	84	
52	1r	75	
53	1s	92	
54	1t	87	
55	1u	71	
56	1v	60	
57	1w	639	
58	1x	77	

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 148945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	2900	Total	C	N	O	P	0	0
			62276	27788	11459	20129	2900		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1847	G	A	conflict	GB 802133627

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1D	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1E	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1F	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1G	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1H	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	1L	69	Total	C	N	O	0	0
			276	138	69	69		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1N	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1O	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1P	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1Q	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1R	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	1S	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1T	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	1U	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1V	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1W	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1X	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1Y	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1Z	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	10	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	11	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 27 is a protein called 50S ribosomal protein L29.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	12	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	13	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	14	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	15	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
31	16	50	Total	C	N	O	0	0
			409	263	75	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	17	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	18	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	19	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	1r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	1v	9	Total	C	N	O	P	0	0
			192	86	35	62	9		

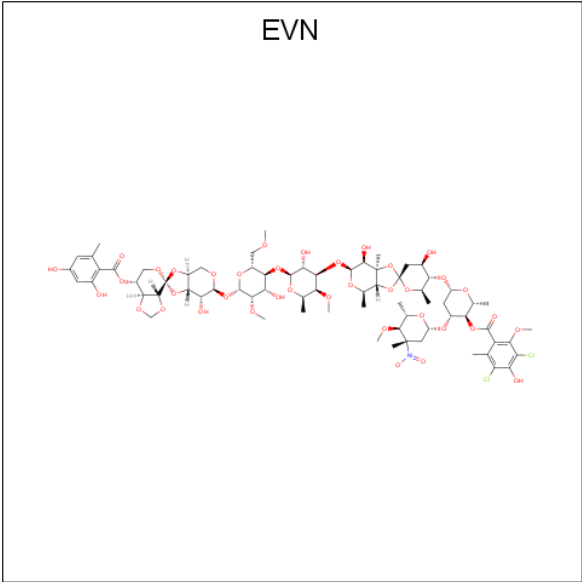
- Molecule 57 is a protein called Tetracycline resistance protein TetM from transposon Tn916.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	1w	639	Total	C	N	O		0	0
			2590	1308	640	642			

- Molecule 58 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	1x	73	Total	C	N	O	P	0	0
			1567	699	285	510	73		

- Molecule 59 is (2R,3R,4R,6S)-6-{{(2R,3aR,4R,4'R,5'S,6S,6'R,7S,7aR)-6-{{(2S,3R,4R,5S,6R)-2-{{[(2R,3S,4S,5S,6S)-6-{{(2R,3aS,3a'R,6S,7R,7'R,7aS,7a'S)-7'-[(2,4-dihydroxy-6-methylbenzoyl)oxy]-7-hydroxyoctahydro-4H-2,4'-spirobi[[1,3]dioxolo[4,5-c]pyran]-6-yl}oxy)-4-hydroxy-5-methoxy-2-(methoxymethyl)tetrahydro-2H-pyran-3-yl}oxy}-3-hydroxy-5-methoxy-6-methyltetrahydro-2H-pyran-4-yl}oxy}-4',7-dihydroxy-4,6',7a-trimethyloctahydro-4H-spiro[1,3-dioxolo[4,5-c]pyran-2,2'-pyran]-5'-yl}oxy}-4-{{(2R,4S,5R,6S)-5-methoxy-4,6-dimethyl-4-nitrotetrahydro-2H-pyran-2-yl}oxy}-2-methyltetrahydro-2H-pyran-3-yl 3,5-dichloro-4-hydroxy-2-methoxy-6-methylbenzoate (non-preferred name) (three-letter code: EVN) (formula: C<sub>70</sub>H<sub>97</sub>Cl<sub>2</sub>NO<sub>38</sub>).

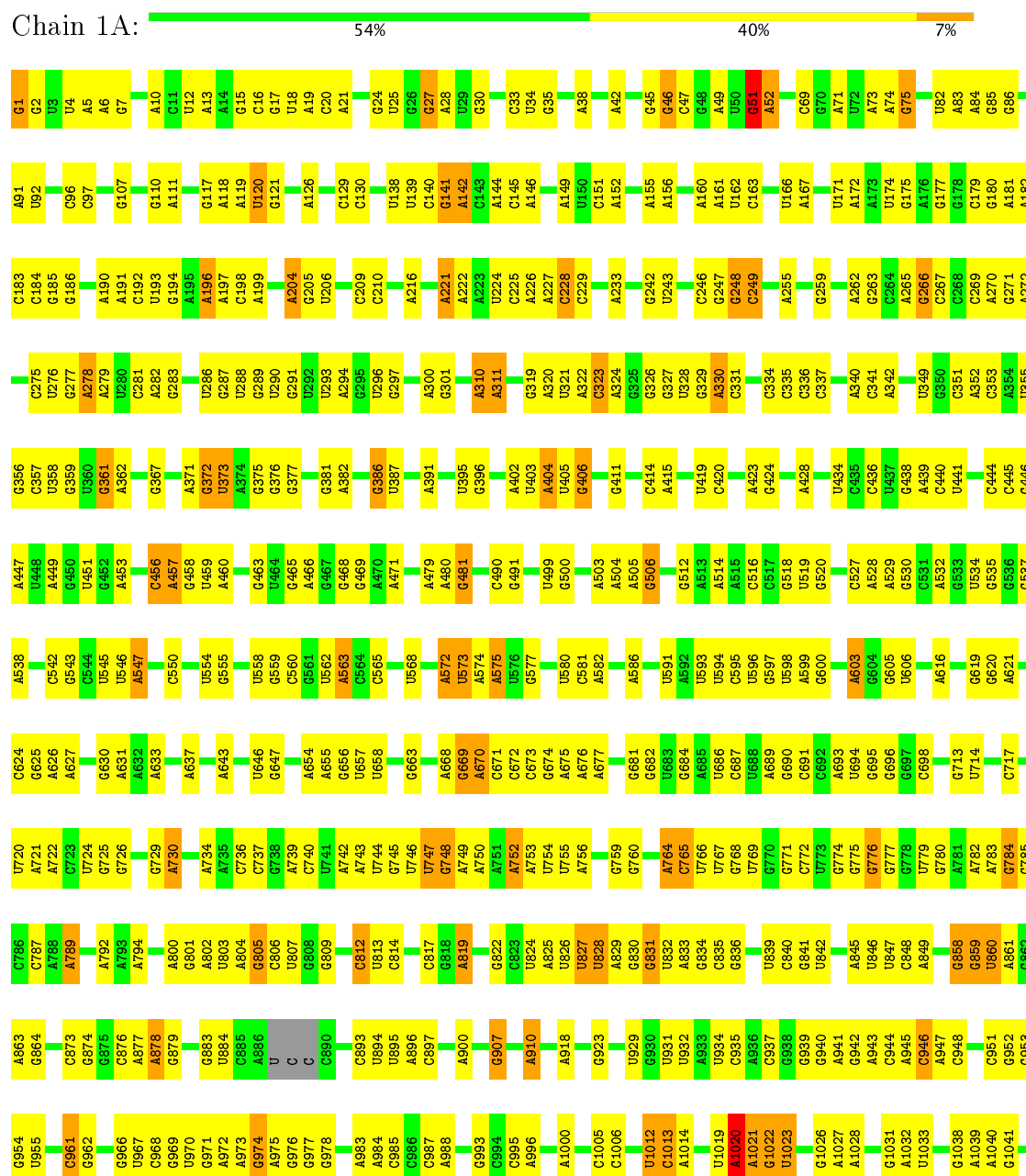


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
59	1A	1	111	70	2	1	38	0

### 3 Residue-property plots

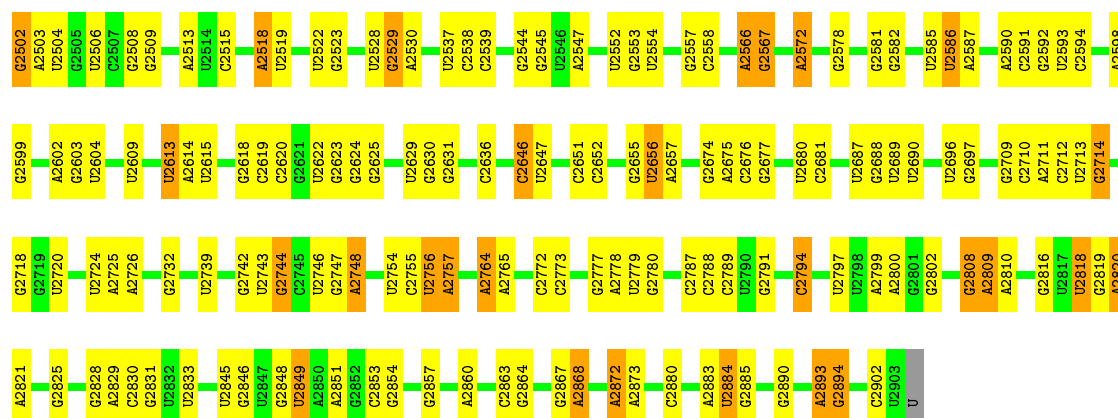
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

#### • Molecule 1: 23S Ribosomal RNA



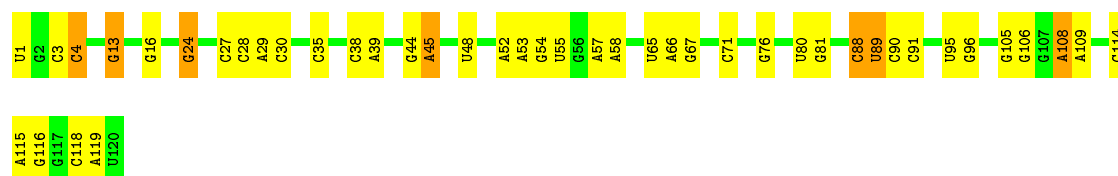
G2421	A2346	U2259	C2146	A2062	G1972	G1897	A1808	A1598	G1516	C1417	U1326	A1247	G1131	A1046
C2422	C2347	C2260	A2147	A2063	G1972	U1896	A1809	A1599	G1517	G1418	A1327	G1248	U1132	G1047
C2423	U2348	C2261	G2162	U2068	A1981	A1899	A1810	A1602	G1517	A1419	A1328	U1249	A1132	A1048
C2424	C2349	C2262	C2163	G2069	U1991	A1900	G1814	A1603	G1524	A1420	U1329	G1250	A1133	
A2425	C2350		C2164	A2070	U1992	A1901	G1815	C1606	A1528	G1421	G1330	G1251	C1135	C1053
C2427	G2353	A2267	A2170	C2072	U1993	C1906	G1816	C1611	A1529	G1422	G1331	G1252	C1054	A1054
G2428	C2354	A2268	A2171	C2073	U1994	G1906	G1817	C1612	A1530	G1423	G1332	A1253	G1055	G1056
G2429	C2355	G2270	A2172	U2074	C1996	C1909	G1818	G1613	C1533	C1428	A1336	G1256	U1141	U1058
A2430	U2356	G2271	U2172	U2074	C1997	G1910	A1819	A1614	U1534	G1429	G1337	C1261	C1146	G1059
U2431	G2357		A2173	U2075	C1998	G1910	A1820	C1615	A1535	A1430	U1340	C1261	A1147	U1060
A2432	A2358	G2276	U2189	A2080	G2002	A1913	A1821	G1738	A1536	A1431	G1341	A1264	U1142	U1061
A2433	C2359	G2277	G2190	U2081	A2005	C1914	G1822	G1740	G1537	G1432	A1342	A1265	G1154	G1062
A2434	G2360	A2278	A2191	A2082	G2004	U1915	G1823		U1538	A1433	G1343	A1266	A1155	C1063
G2435	G2361	G2280	U2192	G2083	A2005	A1916	G1824	U1618	U1539	A1434	U1344	U1267		U1064
G2436		A2281	G2193	C2086	U2008	U1917	G1825	A1745	U1540	G1435	G1345	A1268	C1158	U1065
G2437	C2364	G2282	U2194	U2086	C2008	A1918	G1826	A1635	C1541	U1442	G1346	A1269	U1066	U1066
	G2365	U2087	U2195	G2087	A2009	A1919	G1827	U1636	U1542	U1443	A1347	C1270	A1165	A1067
C2440	A2369	A2088		A2088	G2010		G1828	A1637	G1543	U1443		G1271	G1166	G1068
U2441	C2285		A2198		U2011	C1924	A1829	C1646	A1549	G1448	C1351	A1272	C1167	A1069
C2442	G2286	G2093	A2199	G2093	G2012	C1925	G1830	U1647	A1549	G1449	U1352	U1273	U1174	U1070
C2443	A2287	C2012	C2200	A2094	A2013	U1926	G1831	U1648	G1555	G1450	A1353	A1274	A1175	C1071
G2445	A2095	A2095	G2201	A2095	A2013	A1927	U1758		C1556	C1451	G1354		U1176	C1072
G2446	C2374	C2096	U2202	C2096	A2020	G1928	G1835	G1651	C1557	G1452	G1355	G1278	G1177	C1075
G2447	G2375	A2097	U2203	A2097	C2021	G1929	G1836	U1762	C1558	C1453	G1356	G1279		C1076
A2448	A2377	U2098	G2204	U2098	U2022	G1930	A1931	G1763	C1559	C1454	G1357			
	A2378				C2023	U1931	G1837	U1759	C1560	G1454	G1362	G1283	U1179	C1079
A2453	A2297	A2298	A2211	A2101	G2027	G1935	G1843		C1561	C1461	G1363	A1286	U1180	A1080
G2454	A2298		A2212	G2102	U2028	A1936	G1844	G1766	U1562	U1563	G1364	A1287	U1181	
	U2305		C2213	C2103	G2029	U1937	G1845		C1564	A1469	A1365	G1288	U1182	A1084
A2461	A2309		C2215	C2104	U2030	A1938		G1658	U1565	A1470	A1366	G1289	U1183	
C2462	C2313	C2313	G2221	G2110	A2031	U1939	G1849	G1659	C1566	G1475	A1367	C1290	G1187	A1088
C2463	A2314	A2314	C2222	G2111	G2032	U1939	G1850	G1660	G1567	G1475	G1368	C1291	U1188	A1089
C2464	G2315	U2113	G2223	G2112	A2033	U1940	G1851	G1661	U1568	U1481	A1378	G1292	U1189	G1092
C2465		U2143	G2224	G2113	U2034	C1941	A1858		A1569	G1482	U1379	G1296	G1190	G1093
C2466					G2035			A1664	U1570				G1191	U1094
G2470	G2319	G2116	A2225	G2116	C2036	U1944	G1863	G1667	A1571	U1485	G1382	G1300	U1199	A1095
A2471	U2320	A2117	C2226	A2118	U2039	G1945	U1864		A1572	U1486	A1383	A1301	U1205	A1096
G2472		U2118		G2119	U2040	G1949	U1865	C1670	A1573	A1490	U1394	A1307	A1206	U1097
C2475	G2325	U2131	U2233	G2120	U2041	G1954	U1866	U1671	A1579	A1491	U1397	A1308	G1210	A1098
A2476	C2326	G2121	G2234	G2120	A2042	U1955	G1869	A1672	U1580	G1492	U1398	G1309	G1211	G1099
U2477	A2327	G2121	G2235	G2121	C2043	U1956	C1870	G1674	G1581	C1493	C1399	G1310	G1212	C1104
U2478	A2328	U2237	U2236	G2122	G2043	C1957	A1871	C1675	G1585	A1494	U1400		A1213	U1105
C2480	G2329	G2237	G2237	G2123	C2043	C1958	G1872	A1676	C1588	G1501	G1401	U1313	G1214	
U2484	U2330	G2238	G2238	G2124	G2048	A1960	G1875		A1588		U1405	C1315	U1119	
G2484	G2331	U2131	A2241	U2132	G2049	C1961	G1876	G1681	G1587	A1504	U1406	U1316	G1218	G1110
G2485	C2332	G2138	G2242	G2138	A2054	C1962	G1877	G1682	U1588	A1505	U1407	U1317	G1219	A1111
C2486	A2333	U2139	U2245	U2139	C2055	U1963	G1878	G1684	U1589	U1506	G1408	U1318	G1225	G1112
G2487	U2334	G2140	G2246	G2139	G2056	G1964	U1882	G1797	A1591	C1507	U1409	C1319	U1225	
G2488	G2410	G2410	G2246	U2139	G2057	U1968	U1883	A1689	G1592	A1508	U1409	C1320	U1119	
U2489	A2411	G2411	G2246	G2139	G2057	U1968	G1884	A1690	U1593	A1509	A1321	A1321	G1236	
G2496	G2415	C2339	G2250	G2141	A2058	C1967			U1594	G1510	U1411	A1322	A1237	G1125
A2497	C2416	A2340	G2251	G2141	A2059	G1968			C1595		U1415	G1323	G1238	
C2498	C2417		G2252	A2142	A2059	A1969			U1596	G1514	A1515	G1324	G1239	
C2499	A2418		U2257	G2143	A2060	A1970			A1596					
U2500	U2419		G2258	G2144	A2060	A1971			A1597					
C2501	C2420				C2061	U1971	G1896							





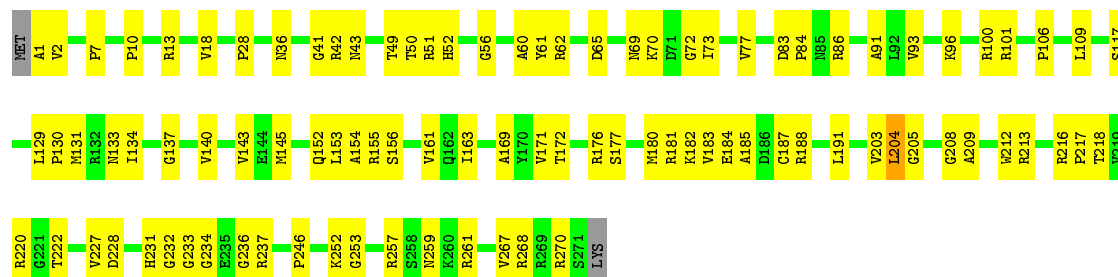
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 63% 31% 6%



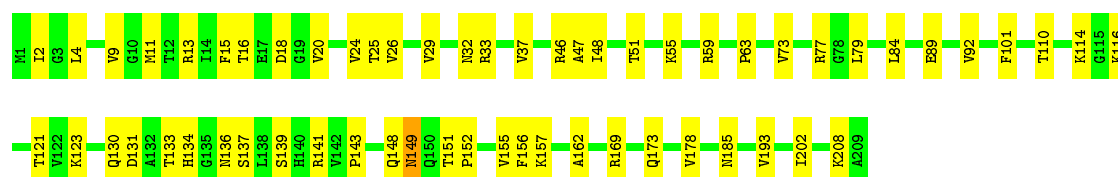
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 64% 34% 2%



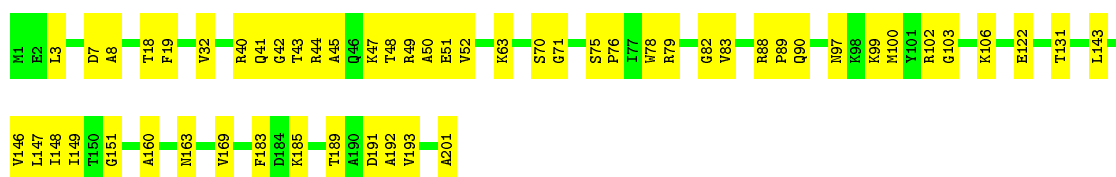
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 72% 28% 0%



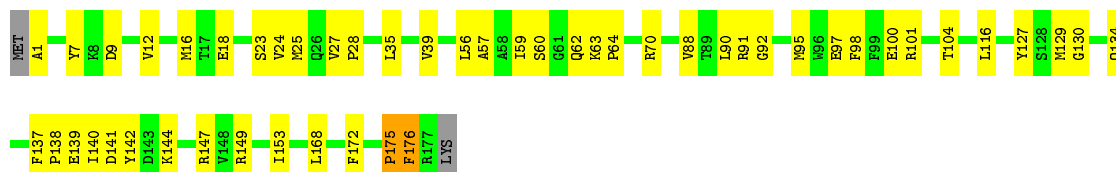
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 73% 27% 0%



- Molecule 6: 50S ribosomal protein L5

Chain 1G: 71% 27% ..



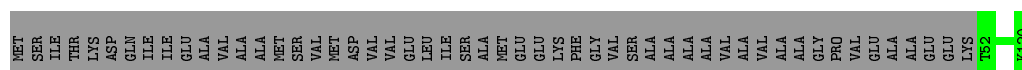
- Molecule 7: 50S ribosomal protein L6

Chain 1H: 85% 15% .



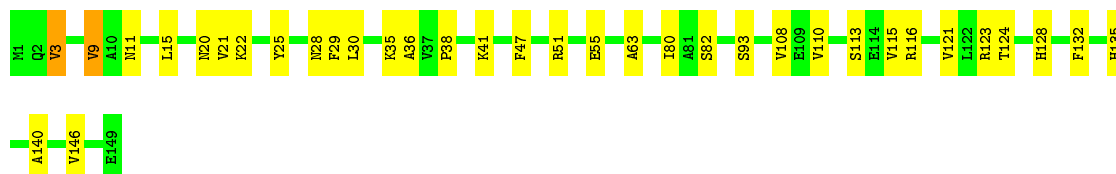
- Molecule 8: 50S ribosomal protein L7/L12

Chain 1L: 57% 43%



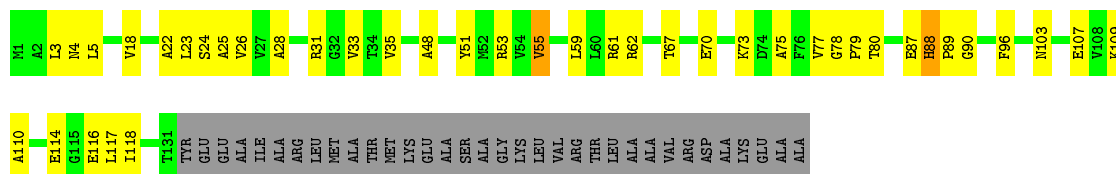
- Molecule 9: 50S ribosomal protein L9

Chain 1I: 77% 22% .

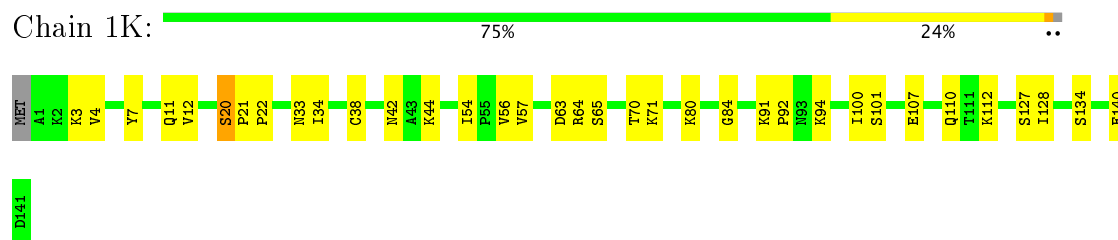


- Molecule 10: 50S ribosomal protein L10

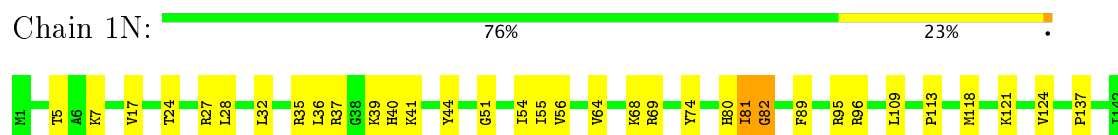
Chain 1J: 55% 24% 21%



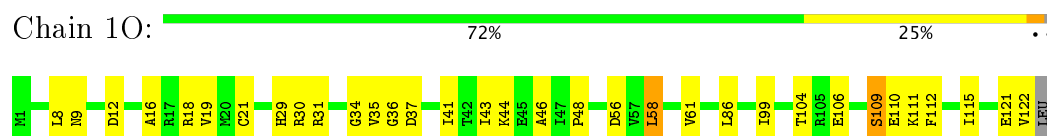
- Molecule 11: 50S ribosomal protein L11



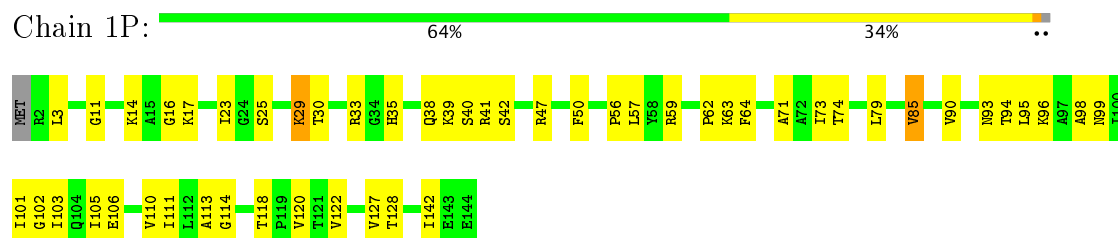
- Molecule 12: 50S ribosomal protein L13



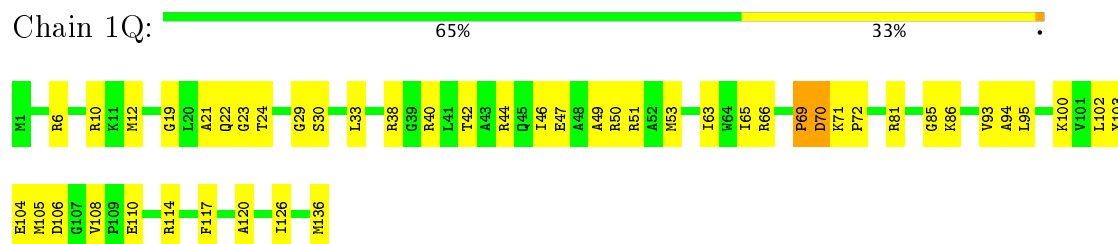
- Molecule 13: 50S ribosomal protein L14



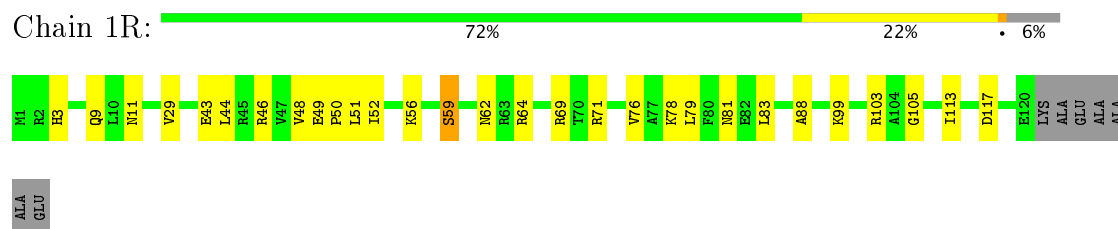
- Molecule 14: 50S ribosomal protein L15




- Molecule 15: 50S ribosomal protein L16



- Molecule 16: 50S ribosomal protein L17




- Molecule 17: 50S ribosomal protein L18

Chain 1S:  86% 13%




- Molecule 18: 50S ribosomal protein L19

Chain 1T:  86% 13%




- Molecule 19: 50S ribosomal protein L20

Chain 1U:  79% 20%




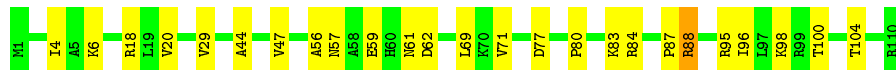
- Molecule 20: 50S ribosomal protein L21

Chain 1V:  76% 24%



- Molecule 21: 50S ribosomal protein L22

Chain 1W:  77% 22%



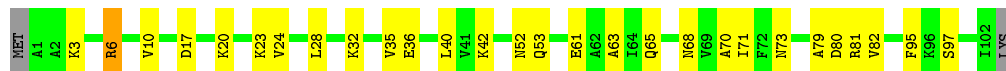
- Molecule 22: 50S ribosomal protein L23

Chain 1X:  73% 19% 7%

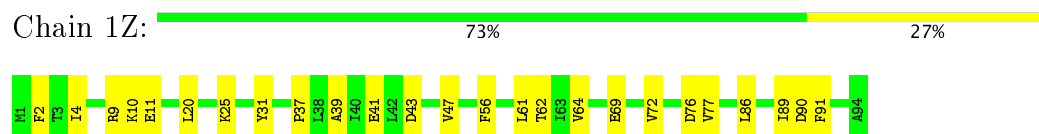


- Molecule 23: 50S ribosomal protein L24

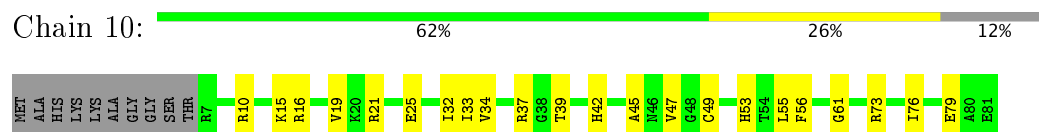
Chain 1Y:  71% 26%



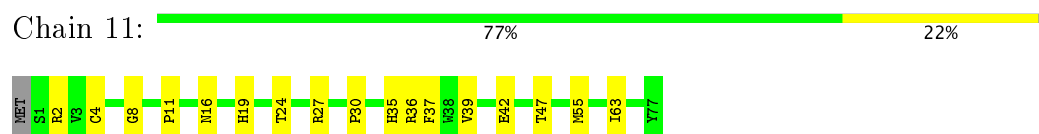
- Molecule 24: 50S ribosomal protein L25



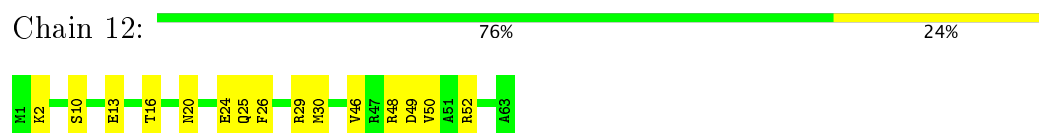
- Molecule 25: 50S ribosomal protein L27



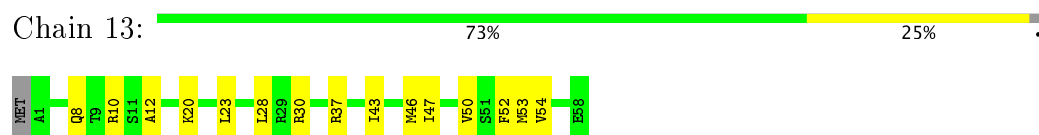
- Molecule 26: 50S ribosomal protein L28



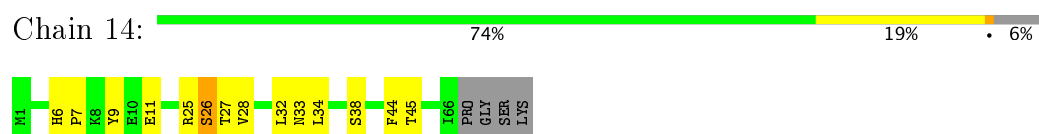
- Molecule 27: 50S ribosomal protein L29



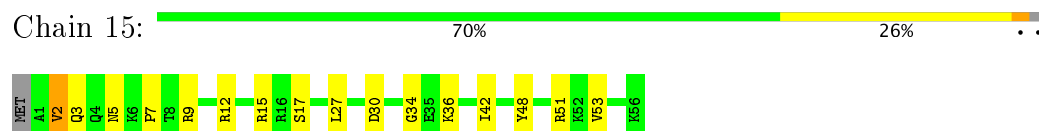
- Molecule 28: 50S ribosomal protein L30



- Molecule 29: 50S ribosomal protein L31



- Molecule 30: 50S ribosomal protein L32

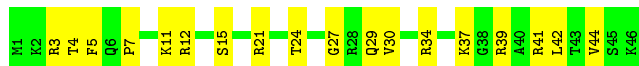


- Molecule 31: 50S ribosomal protein L33

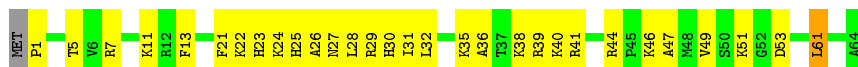




- Molecule 32: 50S ribosomal protein L34



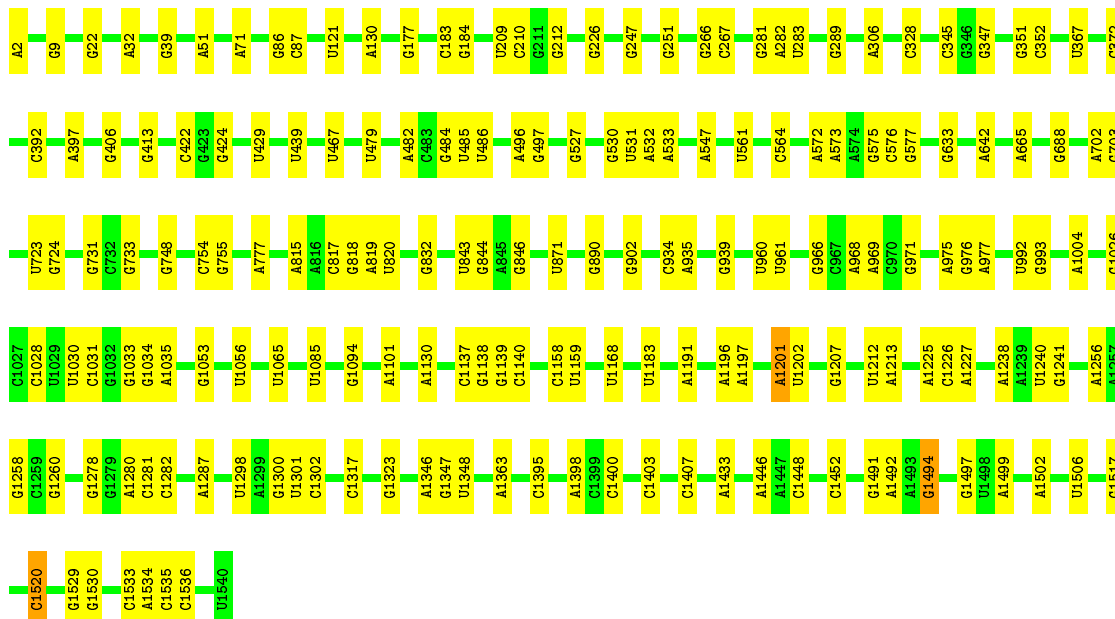
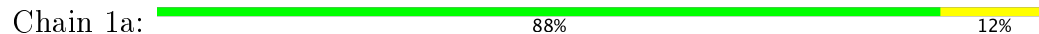
- Molecule 33: 50S ribosomal protein L35



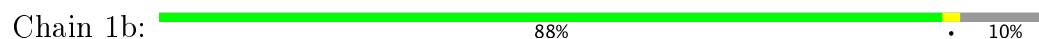
- Molecule 34: 50S ribosomal protein L36



- Molecule 35: 16S Ribosomal RNA



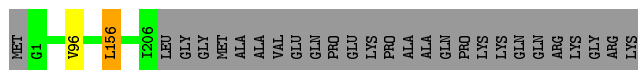
- Molecule 36: 30S ribosomal protein S2





- Molecule 37: 30S ribosomal protein S3

Chain 1c: 88% 12%



- Molecule 38: 30S ribosomal protein S4

Chain 1d: 98%



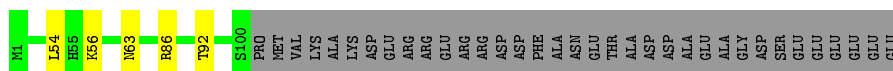
- Molecule 39: 30S ribosomal protein S5

Chain 1e: 89% 5% 6%



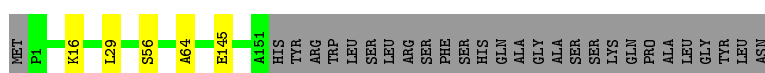
- Molecule 40: 30S ribosomal protein S6

Chain 1f: 70% 26%



- Molecule 41: 30S ribosomal protein S7

Chain 1g: 82% 16%



- Molecule 42: 30S ribosomal protein S8

Chain 1h: 98%




- Molecule 43: 30S ribosomal protein S9

Chain 1i: 93% 5%




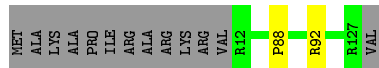
- Molecule 44: 30S ribosomal protein S10

Chain 1j:  89% 6% 5%



- Molecule 45: 30S ribosomal protein S11

Chain 1k:  88% 10%



- Molecule 46: 30S ribosomal protein S12

Chain 1l:  94% 6%



- Molecule 47: 30S ribosomal protein S13

Chain 1m:  94% 5% 1%



- Molecule 48: 30S ribosomal protein S14

Chain 1n:  92% 7% 1%



- Molecule 49: 30S ribosomal protein S15

Chain 1o:  94% 5% 1%



- Molecule 50: 30S ribosomal protein S16

Chain 1p:  99%




- Molecule 51: 30S ribosomal protein S17



Chain 1q:  92% • 5%




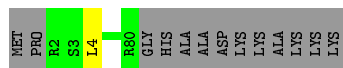
- Molecule 52: 30S ribosomal protein S18

Chain 1r:  83% • 13%



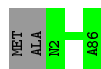
- Molecule 53: 30S ribosomal protein S19

Chain 1s:  85% • 14%




- Molecule 54: 30S ribosomal protein S20

Chain 1t:  98% •



- Molecule 55: 30S ribosomal protein S21

Chain 1u:  82% • 8% 8%



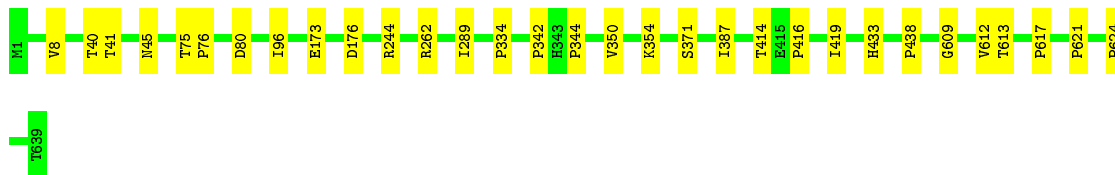
- Molecule 56: mRNA

Chain 1v:  13% • 85%

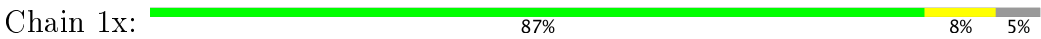


- Molecule 57: Tetracycline resistance protein TetM from transposon Tn916

Chain 1w:  95% 5%



- Molecule 58: P-site tRNA



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	78186	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 ( $e^-/\text{\AA}^2$ )	28	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (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: 5MU, OMC, OMG, OMU, EVN, MA6, G7M, H2U, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, 3TD, 7MG, 1MG, 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	1A	0.19	1/69174 (0.0%)	0.69	11/107910 (0.0%)
10	1J	0.29	0/1001	0.47	0/1350
11	1K	0.27	0/1046	0.44	0/1410
12	1N	0.25	0/1152	0.42	0/1551
13	1O	0.26	0/947	0.45	0/1268
14	1P	0.27	0/1054	0.45	0/1403
15	1Q	0.30	0/1093	0.49	0/1460
16	1R	0.25	0/973	0.41	0/1301
17	1S	0.26	0/902	0.39	0/1209
18	1T	0.26	0/929	0.46	0/1242
19	1U	0.25	0/960	0.35	0/1278
2	1B	0.26	1/2873 (0.0%)	0.68	0/4478
20	1V	0.27	0/829	0.45	0/1107
21	1W	0.26	0/864	0.44	0/1156
22	1X	0.26	0/744	0.42	0/994
23	1Y	0.27	0/787	0.45	0/1051
24	1Z	0.28	0/766	0.42	0/1025
25	10	0.27	0/582	0.42	0/769
26	11	0.25	0/635	0.41	0/848
27	12	0.24	0/510	0.40	0/677
28	13	0.24	0/453	0.45	0/605
29	14	0.28	0/531	0.43	0/709
3	1D	0.28	0/2121	0.47	0/2852
30	15	0.24	0/450	0.43	0/599
31	16	0.26	0/416	0.43	0/554
32	17	0.25	0/380	0.43	0/498
33	18	0.26	0/513	0.44	0/676
34	19	0.25	0/303	0.40	0/397
35	1a	0.19	1/36701 (0.0%)	0.70	13/57246 (0.0%)
36	1b	0.26	0/1735	0.41	0/2338
37	1c	0.26	0/1651	0.44	0/2225

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
38	1d	0.26	0/1665	0.42	0/2227
39	1e	0.26	0/1154	0.44	0/1554
4	1E	0.27	0/1586	0.46	0/2134
40	1f	0.25	0/835	0.43	0/1128
41	1g	0.26	0/1195	0.42	0/1602
42	1h	0.26	0/989	0.46	0/1326
43	1i	0.26	0/1034	0.45	0/1375
44	1j	0.25	0/796	0.47	0/1077
45	1k	0.26	0/885	0.43	0/1195
46	1l	0.26	0/969	0.46	0/1300
47	1m	0.25	0/892	0.43	0/1193
48	1n	0.26	0/806	0.43	0/1074
49	1o	0.24	0/722	0.38	0/964
5	1F	0.25	0/1571	0.41	0/2113
50	1p	0.26	0/659	0.42	0/884
51	1q	0.28	0/657	0.46	0/881
52	1r	0.26	0/511	0.42	0/689
53	1s	0.25	0/652	0.40	0/877
54	1t	0.26	0/671	0.37	0/888
55	1u	0.38	1/500 (0.2%)	0.40	0/668
56	1v	0.53	0/214	1.10	3/331 (0.9%)
57	1w	0.26	0/2594	0.47	0/3251
58	1x	0.36	1/1656 (0.1%)	0.72	0/2575
6	1G	0.27	0/1434	0.42	0/1926
7	1H	0.26	0/1343	0.44	0/1816
8	1L	0.25	0/275	0.43	0/342
9	1I	0.27	0/1122	0.43	0/1515
All	All	0.22	5/160462 (0.0%)	0.63	27/239091 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1x	1	A	OP3-P	-10.60	1.48	1.61
35	1a	2	A	OP3-P	-10.55	1.48	1.61
2	1B	1	U	OP3-P	-10.46	1.48	1.61
1	1A	1	G	OP3-P	-10.44	1.48	1.61
55	1u	9	GLU	C-N	5.99	1.45	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1a	754	C	C2-N1-C1'	8.93	128.63	118.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1a	754	C	N1-C2-O2	8.83	124.20	118.90
35	1a	1158	C	C2-N1-C1'	8.63	128.30	118.80
35	1a	1158	C	N1-C2-O2	8.58	124.05	118.90
1	1A	2884	U	C2-N1-C1'	7.77	127.02	117.70
1	1A	1313	U	C2-N1-C1'	7.42	126.60	117.70
1	1A	1313	U	N1-C2-O2	7.38	127.97	122.80
35	1a	1158	C	N3-C2-O2	-7.25	116.83	121.90
1	1A	2884	U	N1-C2-O2	7.06	127.74	122.80
1	1A	1313	U	N3-C2-O2	-6.98	117.32	122.20
56	1v	25	A	C2-N3-C4	-6.92	107.14	110.60
35	1a	754	C	N3-C2-O2	-6.85	117.10	121.90
1	1A	2884	U	N3-C2-O2	-6.54	117.62	122.20
35	1a	754	C	C6-N1-C1'	-6.44	113.07	120.80
35	1a	1158	C	C6-N1-C2	-6.35	117.76	120.30
1	1A	1378	A	OP1-P-O3'	5.98	118.36	105.20
1	1A	51	G	OP2-P-O3'	5.87	118.12	105.20
35	1a	1158	C	C6-N1-C1'	-5.77	113.87	120.80
1	1A	752	A	OP2-P-O3'	5.55	117.42	105.20
56	1v	25	A	C5-N7-C8	-5.37	101.22	103.90
35	1a	1494	G	N3-C4-C5	5.29	131.24	128.60
35	1a	1520	C	C2-N3-C4	5.20	122.50	119.90
1	1A	752	A	P-O3'-C3'	5.15	125.89	119.70
35	1a	754	C	C6-N1-C2	-5.14	118.24	120.30
56	1v	25	A	N3-C4-C5	5.08	130.36	126.80
35	1a	1201	A	P-O3'-C3'	5.04	125.74	119.70
1	1A	1020	A	P-O3'-C3'	5.01	125.72	119.70

There are no chirality outliers.

There are no planarity outliers.

## 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	1A	62276	0	31344	905	0
2	1B	2570	0	1301	26	0
3	1D	2082	0	2157	78	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1E	1565	0	1616	47	0
5	1F	1552	0	1619	38	0
6	1G	1410	0	1447	37	0
7	1H	1323	0	1374	17	0
8	1L	276	0	79	0	0
9	1I	1111	0	1148	22	0
10	1J	988	0	1025	24	0
11	1K	1032	0	1088	17	0
12	1N	1129	0	1162	26	0
13	1O	938	0	1012	22	0
14	1P	1045	0	1117	40	0
15	1Q	1074	0	1157	33	0
16	1R	960	0	1000	21	0
17	1S	892	0	923	9	0
18	1T	917	0	965	13	0
19	1U	947	0	1022	19	0
20	1V	816	0	839	17	0
21	1W	857	0	922	21	0
22	1X	738	0	807	12	0
23	1Y	779	0	834	19	0
24	1Z	753	0	780	16	0
25	10	575	0	592	19	0
26	11	625	0	655	15	0
27	12	509	0	543	10	0
28	13	449	0	491	9	0
29	14	522	0	522	12	0
30	15	444	0	461	12	0
31	16	409	0	440	9	0
32	17	377	0	418	22	0
33	18	504	0	574	25	0
34	19	302	0	343	9	0
35	1a	33029	0	16644	0	0
36	1b	1704	0	1732	0	0
37	1c	1624	0	1699	0	0
38	1d	1643	0	1710	0	0
39	1e	1141	0	1170	0	0
40	1f	817	0	808	0	0
41	1g	1181	0	1240	0	0
42	1h	979	0	1034	0	0
43	1i	1022	0	1070	0	0
44	1j	786	0	828	0	0
45	1k	869	0	878	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1l	955	0	1019	0	0
47	1m	883	0	944	0	0
48	1n	794	0	833	0	0
49	1o	714	0	737	0	0
50	1p	649	0	666	0	0
51	1q	648	0	691	0	0
52	1r	504	0	502	0	0
53	1s	637	0	665	0	0
54	1t	665	0	714	0	0
55	1u	495	0	486	0	0
56	1v	192	0	98	0	0
57	1w	2590	0	731	0	0
58	1x	1567	0	798	0	0
59	1A	111	0	0	0	0
All	All	148945	0	99474	1397	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 9.

All (1397) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:827:U:H2'	1:1A:2068:U:O2	1.20	1.28
1:1A:827:U:C2'	1:1A:2068:U:O2	1.98	1.12
1:1A:827:U:H2'	1:1A:2068:U:C2	1.97	1.00
1:1A:776:G:H22	1:1A:2072:C:H5'	1.35	0.89
6:1G:140:ILE:HG22	6:1G:142:TYR:H	1.43	0.84
2:1B:30:C:H1'	2:1B:57:A:H61	1.41	0.83
14:1P:62:PRO:HB2	33:18:29:ARG:HH11	1.44	0.83
1:1A:297:G:N2	1:1A:300:A:OP2	12.98	0.82
1:1A:1613:G:H4'	32:17:3:ARG:HE	1.46	0.80
13:1O:19:VAL:HG12	13:1O:43:ILE:HA	1.62	0.80
5:1F:146:VAL:HG12	5:1F:185:LYS:HB2	1.64	0.79
1:1A:38:A:H4'	5:1F:45:ALA:HB3	1.63	0.79
1:1A:807:U:OP2	14:1P:41:ARG:NH1	2.15	0.79
1:1A:1798:U:H5''	3:1D:257:ARG:HB2	1.64	0.78
1:1A:2598:A:H5''	3:1D:233:GLY:HA3	1.65	0.78
1:1A:1032:A:H1'	34:19:23:ILE:HD13	1.66	0.78
1:1A:198:C:H1'	1:1A:2434:A:H61	1.49	0.77
1:1A:827:U:C2'	1:1A:2068:U:C2	2.63	0.77
1:1A:676:A:N6	1:1A:713:G:O6	92.59	0.77

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1N:80:HIS:O	12:1N:82:GLY:N	2.17	0.76
1:1A:574:A:N6	1:1A:2034:U:OP1	2.19	0.76
1:1A:2420:C:H2'	1:1A:2421:G:H8	1.51	0.75
1:1A:2394:C:H5''	14:1P:63:LYS:HE3	1.68	0.75
1:1A:466:A:OP1	32:17:34:ARG:NH1	2.20	0.74
18:1T:59:THR:HG22	18:1T:72:VAL:HG12	1.69	0.74
1:1A:1266:G:N2	1:1A:1269:A:OP2	12.94	0.74
1:1A:275:C:O2	1:1A:362:A:N6	2.20	0.74
1:1A:1568:G:OP2	3:1D:62:ARG:NH2	2.15	0.74
1:1A:2484:G:OP1	15:1Q:44:ARG:NH2	2.21	0.73
1:1A:1992:G:N2	1:1A:1996:C:O2'	2.22	0.73
24:1Z:9:ARG:HD3	24:1Z:39:ALA:HB1	1.70	0.73
1:1A:320:A:N3	5:1F:163:ASN:ND2	2.36	0.73
1:1A:1054:A:H61	1:1A:1105:U:H3	1.37	0.73
9:1I:80:ILE:HD12	9:1I:146:VAL:HG22	1.71	0.72
4:1E:15:PHE:H	18:1T:11:GLN:HE22	1.37	0.72
1:1A:1796:U:H2'	1:1A:1797:G:H8	1.55	0.72
1:1A:621:A:OP2	14:1P:99:ASN:ND2	2.23	0.72
1:1A:2478:A:H5'	34:19:32:LYS:HE3	1.72	0.72
1:1A:668:A:H2'	1:1A:670:A:H62	1.55	0.71
1:1A:1759:A:HO2'	1:1A:2714:G:HO2'	1.29	0.71
1:1A:1364:G:N2	1:1A:1367:A:OP2	2.22	0.71
1:1A:690:G:H1	1:1A:772:C:H42	1.39	0.71
1:1A:2581:G:N2	1:1A:2581:G:OP2	2.24	0.71
1:1A:2063:C:N4	1:1A:2501:C:O2	2.24	0.71
25:10:33:ILE:HG22	25:10:34:VAL:HG23	1.72	0.71
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.09	0.70
10:1J:73:LYS:HB3	10:1J:117:LEU:HD11	1.72	0.70
1:1A:1072:C:N3	1:1A:1092:C:N4	2.39	0.70
1:1A:698:C:O2'	1:1A:734:A:N6	2.23	0.70
14:1P:23:ILE:HD13	20:1V:84:ARG:HH22	1.55	0.70
1:1A:2251:OMG:OP1	15:1Q:81:ARG:NH1	2.23	0.70
1:1A:291:G:H1	1:1A:349:U:H3	1.39	0.70
5:1F:75:SER:HB3	5:1F:78:TRP:HD1	1.57	0.70
13:1O:29:HIS:CE1	13:1O:31:ARG:HH12	2.10	0.70
1:1A:1837:C:O2'	1:1A:1927:A:N3	2.25	0.70
13:1O:21:CYS:HA	13:1O:41:ILE:HG22	1.73	0.69
13:1O:112:PHE:HD1	13:1O:115:ILE:HD12	1.58	0.69
1:1A:1799:G:N2	1:1A:1819:A:OP2	2.20	0.69
1:1A:192:C:O2'	1:1A:802:A:N3	2.23	0.69
1:1A:1416:G:O2'	1:1A:1587:G:N2	2.26	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:17:15:SER:O	32:17:21:ARG:NH2	2.25	0.69
1:1A:1614:A:H61	21:1W:88:ARG:H	1.41	0.69
1:1A:1992:G:O2'	1:1A:1997:C:N4	2.26	0.69
1:1A:910:A:H62	15:1Q:12:MET:HA	1.58	0.69
13:1O:121:GLU:HG2	13:1O:122:VAL:HG23	1.73	0.68
6:1G:134:GLN:NE2	6:1G:149:ARG:O	2.26	0.68
22:1X:1:MET:HG3	22:1X:3:ARG:H	1.58	0.68
1:1A:1787:A:OP1	3:1D:237:ARG:NH2	2.26	0.68
1:1A:2279:G:HO2'	1:1A:2327:A:HO2'	1.28	0.68
1:1A:1501:G:OP1	3:1D:100:ARG:NH2	2.26	0.68
1:1A:674:G:H5''	5:1F:71:GLY:H	1.58	0.68
6:1G:1:ALA:N	6:1G:97:GLU:OE1	2.28	0.67
1:1A:465:G:OP1	32:17:12:ARG:NH1	2.25	0.67
5:1F:45:ALA:HB2	5:1F:89:PRO:HD3	1.76	0.67
20:1V:34:GLU:HG2	20:1V:60:LYS:HG2	1.74	0.67
1:1A:518:G:OP1	21:1W:18:ARG:NH1	2.25	0.67
1:1A:669:G:N2	1:1A:672:C:OP1	2.27	0.67
1:1A:1945:G:N2	1:1A:1963:U:O4	2.27	0.67
1:1A:51:G:H4'	1:1A:52:A:H5'	1.76	0.67
1:1A:1158:C:H5''	28:13:30:ARG:HD2	1.75	0.67
1:1A:190:A:H5''	1:1A:204:A:H61	1.60	0.67
10:1J:33:VAL:HG12	10:1J:35:VAL:H	1.59	0.67
13:1O:9:ASN:OD1	13:1O:18:ARG:NH1	2.28	0.67
29:14:26:SER:OG	29:14:27:THR:N	2.27	0.67
1:1A:1309:G:H4'	32:17:7:PRO:HG2	1.75	0.67
1:1A:658:U:O2'	5:1F:97:ASN:OD1	2.12	0.67
4:1E:110:THR:HB	4:1E:202:ILE:HB	1.76	0.67
1:1A:1046:A:H4'	10:1J:61:ARG:HB3	1.77	0.67
13:1O:43:ILE:HD12	13:1O:56:ASP:HB2	1.77	0.67
16:1R:43:GLU:OE2	16:1R:46:ARG:NH2	2.28	0.67
1:1A:2118:U:O2	1:1A:2145:C:N4	2.28	0.66
1:1A:45:G:H5''	1:1A:46:G:H5'	1.76	0.66
1:1A:1022:G:N2	1:1A:1023:U:O4	2.28	0.66
13:1O:30:ARG:NH2	13:1O:37:ASP:OD2	2.25	0.66
14:1P:93:ASN:O	14:1P:95:LEU:N	2.29	0.66
1:1A:2618:G:H21	4:1E:155:VAL:HG21	1.60	0.66
1:1A:2591:C:H2'	1:1A:2592:G:H8	1.61	0.66
1:1A:953:G:H2'	1:1A:954:G:H8	1.61	0.66
1:1A:1394:U:H4'	1:1A:1603:A:H4'	1.78	0.65
1:1A:568:U:H1'	1:1A:2030:6MZ:H9C1	1.78	0.65
1:1A:993:G:OP2	19:1U:50:ARG:NH2	2.27	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:807:U:H1'	1:1A:2445:2MG:OP1	1.96	0.65
1:1A:1378:A:H4'	1:1A:1379:U:OP1	1.97	0.65
1:1A:2523:G:HO2'	1:1A:2764:A:HO2'	1.44	0.65
1:1A:1060:U:H5'	1:1A:1062:G:H5'	1.79	0.65
1:1A:2656:U:H2'	1:1A:2657:A:H8	1.62	0.65
1:1A:2816:G:H5''	16:1R:99:LYS:HE2	1.77	0.65
1:1A:1670:C:O2	4:1E:134:HIS:NE2	2.30	0.65
1:1A:2418:A:OP1	33:18:44:ARG:NH2	2.30	0.65
1:1A:1824:G:H5''	3:1D:51:ARG:HH21	1.61	0.65
24:1Z:64:VAL:HG22	24:1Z:69:GLU:HG2	1.79	0.65
1:1A:1787:A:H5''	3:1D:237:ARG:HH21	1.62	0.64
1:1A:1365:A:O4'	26:11:27:ARG:NH2	2.29	0.64
28:13:12:ALA:HB1	28:13:20:LYS:HG2	1.79	0.64
1:1A:2688:G:N1	1:1A:2720:U:OP2	2.28	0.64
21:1W:57:ASN:OD1	21:1W:61:ASN:ND2	2.30	0.64
1:1A:2305:U:H5''	6:1G:130:GLY:HA3	1.80	0.64
7:1H:94:ARG:HB2	7:1H:105:SER:HB2	1.80	0.64
5:1F:76:PRO:HA	5:1F:82:GLY:HA3	1.78	0.64
25:10:15:LYS:HG3	25:10:37:ARG:HH22	1.63	0.64
32:17:39:ARG:HG2	32:17:41:ARG:H	1.62	0.64
1:1A:624:C:O2'	1:1A:657:U:OP1	2.16	0.64
5:1F:41:GLN:NE2	5:1F:43:THR:OG1	2.31	0.64
15:1Q:66:ARG:NH1	15:1Q:104:GLU:OE2	2.31	0.63
12:1N:32:LEU:HD22	12:1N:54:ILE:HG21	1.80	0.63
22:1X:23:ALA:O	22:1X:28:ASN:N	2.31	0.63
1:1A:1418:G:N1	1:1A:1579:A:OP2	2.26	0.63
1:1A:743:A:O2'	1:1A:1659:G:OP1	2.16	0.63
6:1G:57:ALA:HB1	29:14:7:PRO:HG3	1.80	0.63
1:1A:1784:A:O2'	1:1A:1981:A:N7	2.27	0.63
1:1A:806:C:O2	1:1A:2444:G:O2'	2.15	0.63
16:1R:44:LEU:HD23	16:1R:113:ILE:HD13	1.80	0.63
29:14:11:GLU:HA	29:14:25:ARG:HA	1.81	0.63
1:1A:445:C:O2'	1:1A:449:A:N3	2.29	0.63
1:1A:471:A:OP1	5:1F:79:ARG:NH1	2.29	0.63
25:10:21:ARG:HB2	25:10:33:ILE:HG23	1.81	0.63
26:11:36:ARG:HA	26:11:47:THR:HA	1.80	0.62
1:1A:1423:G:H2'	1:1A:1424:G:H8	1.64	0.62
1:1A:745:1MG:O2'	1:1A:748:G:H1'	1.98	0.62
1:1A:750:A:OP1	1:1A:1615:C:N4	2.29	0.62
1:1A:225:C:H2'	1:1A:226:A:O4'	1.99	0.62
1:1A:824:U:O2'	1:1A:2358:A:N6	2.32	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:77:VAL:HG22	3:1D:93:VAL:HG22	1.81	0.62
1:1A:210:C:OP1	32:17:29:GLN:NE2	2.32	0.62
1:1A:1309:G:O2'	1:1A:1611:C:O2'	2.17	0.62
2:1B:116:G:H5'	17:1S:55:GLU:HG2	1.82	0.62
29:14:28:VAL:HG11	29:14:32:LEU:HD13	1.79	0.62
31:16:26:LYS:NZ	31:16:30:PRO:O	2.32	0.62
1:1A:749:A:H5'	1:1A:1271:G:H1'	1.80	0.62
1:1A:1323:C:N4	1:1A:1324:G:O6	2.32	0.62
17:1S:108:ASP:OD1	17:1S:111:ARG:NH1	2.32	0.62
1:1A:1656:C:OP1	4:1E:141:ARG:NE	2.20	0.62
1:1A:1835:2MG:H2'	1:1A:1836:C:C6	2.33	0.62
23:1Y:28:LEU:HD12	23:1Y:32:LYS:HB2	1.81	0.62
1:1A:684:G:OP1	32:17:21:ARG:NH1	2.31	0.62
1:1A:572:A:H61	1:1A:2029:G:H21	1.48	0.62
1:1A:2057:G:H1'	30:15:2:VAL:HG21	1.81	0.62
1:1A:2298:A:OP1	6:1G:70:ARG:NH2	2.31	0.62
1:1A:784:G:C5	3:1D:227:VAL:HG11	2.35	0.62
1:1A:1813:G:O2'	3:1D:49:THR:OG1	2.10	0.62
6:1G:56:LEU:HB2	6:1G:64:PRO:HG3	1.81	0.62
13:1O:58:LEU:HD11	13:1O:86:LEU:HD22	1.81	0.62
1:1A:1199:U:H1'	19:1U:3:VAL:HG22	1.82	0.62
2:1B:76:G:OP1	24:1Z:9:ARG:NH2	2.29	0.62
1:1A:1905:C:N4	1:1A:1969:A:OP2	2.32	0.61
22:1X:3:ARG:HH12	22:1X:7:LEU:HD21	1.64	0.61
1:1A:2357:G:N2	1:1A:2360:G:OP2	2.24	0.61
11:1K:11:GLN:NE2	11:1K:54:ILE:O	2.33	0.61
12:1N:17:VAL:HG23	12:1N:137:PRO:HB2	1.82	0.61
1:1A:1800:C:OP1	3:1D:257:ARG:NH2	2.33	0.61
1:1A:2853:C:H2'	1:1A:2854:G:H8	1.65	0.61
1:1A:987:C:O2'	1:1A:1000:A:N3	2.32	0.61
14:1P:33:ARG:NH2	14:1P:39:LYS:O	2.32	0.61
1:1A:527:C:N4	1:1A:2777:G:O2'	2.33	0.61
1:1A:451:U:O2	1:1A:453:A:N6	2.32	0.61
16:1R:79:LEU:HD23	16:1R:83:LEU:HD12	1.83	0.61
1:1A:2260:C:HO2'	1:1A:2388:A:HO2'	1.47	0.61
1:1A:499:U:H5''	23:1Y:42:LYS:HE2	1.81	0.61
9:1I:28:ASN:OD1	26:11:35:HIS:NE2	2.30	0.61
1:1A:1341:G:OP1	1:1A:1602:U:O2'	2.18	0.61
1:1A:166:U:H2'	1:1A:167:A:H8	2.38	0.61
1:1A:1363:C:O2'	1:1A:1809:A:N3	2.34	0.61
22:1X:14:PRO:HD3	27:12:30:MET:HG3	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Z:86:LEU:HD13	24:1Z:89:ILE:HD11	1.81	0.61
1:1A:772:C:O2	3:1D:42:ARG:NH1	2.35	0.60
10:1J:88:HIS:HB2	10:1J:89:PRO:HD3	1.83	0.60
33:18:32:LEU:HB3	33:18:40:LYS:HD3	1.82	0.60
1:1A:605:G:OP1	5:1F:99:LYS:NZ	2.34	0.60
6:1G:97:GLU:OE2	29:14:25:ARG:N	2.31	0.60
1:1A:581:C:H2'	1:1A:582:A:C8	2.37	0.60
4:1E:110:THR:O	4:1E:202:ILE:N	2.23	0.60
1:1A:1765:U:H2'	1:1A:1766:G:H8	1.65	0.60
1:1A:1998:A:OP2	4:1E:141:ARG:NH1	2.34	0.60
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.37	0.60
1:1A:2831:G:OP2	4:1E:59:ARG:NH1	2.33	0.60
1:1A:594:U:H2'	1:1A:595:C:C6	2.36	0.60
1:1A:2420:C:H2'	1:1A:2421:G:C8	2.36	0.60
9:1I:124:THR:O	9:1I:128:HIS:NE2	2.32	0.60
24:1Z:25:LYS:HG2	24:1Z:43:ASP:HA	1.82	0.60
1:1A:2788:C:O2'	1:1A:2809:A:N3	2.32	0.60
1:1A:28:A:O2'	1:1A:296:U:OP1	48.88	0.60
27:12:24:GLU:HB3	27:12:46:VAL:HG21	1.83	0.60
31:16:3:GLY:O	31:16:5:ARG:N	2.33	0.60
1:1A:789:A:H5'	32:17:4:THR:HG21	1.82	0.60
1:1A:1615:C:OP2	1:1A:1617:C:N4	2.35	0.60
1:1A:2101:A:H2'	1:1A:2102:G:H8	1.66	0.60
21:1W:56:ALA:HA	21:1W:59:GLU:HG2	1.82	0.60
1:1A:834:G:O2'	1:1A:2358:A:O2'	2.10	0.60
17:1S:33:ARG:HG2	17:1S:34:HIS:CD2	2.37	0.60
4:1E:130:GLN:OE1	4:1E:139:SER:OG	2.20	0.59
18:1T:52:ARG:H	18:1T:56:SER:HB3	1.68	0.59
1:1A:2420:C:H5''	31:16:7:LYS:HD2	1.84	0.59
5:1F:75:SER:HB3	5:1F:78:TRP:CD1	2.36	0.59
31:16:36:LYS:HG3	31:16:47:ILE:HG13	1.82	0.59
1:1A:269:C:H2'	1:1A:270:A:H8	1.66	0.59
1:1A:563:A:N3	19:1U:36:GLN:NE2	2.49	0.59
1:1A:1818:U:H5'	3:1D:156:SER:HB2	1.85	0.59
1:1A:1660:G:H2'	1:1A:1661:G:H8	1.67	0.59
2:1B:28:C:H2'	2:1B:29:A:C8	2.37	0.59
3:1D:56:GLY:HA2	3:1D:212:TRP:HA	1.83	0.59
1:1A:30:G:O2'	1:1A:1214:A:N3	2.35	0.59
1:1A:1310:G:H1'	1:1A:1611:C:H5''	1.84	0.59
6:1G:35:LEU:HB2	6:1G:88:VAL:HB	1.85	0.59
27:12:16:THR:O	27:12:20:ASN:ND2	2.34	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2033:A:O2'	1:1A:2035:G:OP1	2.18	0.59
1:1A:2444:G:H2'	1:1A:2445:2MG:O4'	2.02	0.59
1:1A:1062:G:N2	11:1K:134:SER:OG	2.35	0.59
24:1Z:77:VAL:HG23	24:1Z:89:ILE:HG12	1.84	0.59
26:11:39:VAL:HG12	26:11:42:GLU:H	1.68	0.59
1:1A:1031:G:H2'	1:1A:1032:A:C8	2.37	0.59
1:1A:1031:G:H2'	1:1A:1032:A:H8	1.68	0.59
1:1A:2528:U:O2'	1:1A:2530:A:OP1	2.18	0.59
1:1A:2431:U:N3	1:1A:2434:A:OP2	2.26	0.59
1:1A:955:PSU:H5'	15:1Q:86:LYS:HD3	1.84	0.59
1:1A:1528:A:N6	1:1A:1543:G:O2'	2.36	0.59
6:1G:28:PRO:HB2	6:1G:168:LEU:HD22	1.85	0.59
14:1P:29:LYS:HG2	14:1P:30:THR:HG23	1.84	0.59
11:1K:44:LYS:HE2	11:1K:70:THR:HG21	1.85	0.58
1:1A:1022:G:H4'	1:1A:1023:U:O5'	2.03	0.58
1:1A:69:C:O2	1:1A:73:A:O2'	2.18	0.58
1:1A:931:U:O2	1:1A:1167:C:O2'	2.16	0.58
1:1A:2260:C:N4	25:10:10:ARG:HD2	2.17	0.58
1:1A:1423:G:H2'	1:1A:1424:G:C8	2.38	0.58
1:1A:1801:A:N6	1:1A:2201:G:O2'	2.36	0.58
10:1J:103:ASN:HA	10:1J:107:GLU:HB3	1.83	0.58
23:1Y:40:LEU:HD23	23:1Y:61:GLU:HG3	1.84	0.58
1:1A:2339:C:H2'	1:1A:2340:A:C8	2.39	0.58
6:1G:1:ALA:N	6:1G:100:GLU:OE1	2.36	0.58
6:1G:62:GLN:HE22	6:1G:90:LEU:HB3	1.69	0.58
1:1A:1323:C:OP1	21:1W:98:LYS:NZ	2.37	0.58
1:1A:2346:A:O2'	31:16:37:LYS:NZ	2.37	0.58
1:1A:2200:C:OP1	26:11:36:ARG:N	2.33	0.57
14:1P:96:LYS:HD3	14:1P:103:ILE:HA	1.85	0.57
1:1A:2189:U:H2'	1:1A:2190:G:C8	2.40	0.57
1:1A:575:A:OP2	1:1A:2499:C:O2'	2.21	0.57
1:1A:2260:C:H42	25:10:10:ARG:HD2	1.68	0.57
1:1A:698:C:OP1	1:1A:1634:A:N6	2.21	0.57
21:1W:29:VAL:HG22	21:1W:71:VAL:HG23	1.85	0.57
21:1W:29:VAL:HG21	21:1W:69:LEU:HG	1.87	0.57
1:1A:1765:U:H2'	1:1A:1766:G:C8	2.39	0.57
1:1A:2508:G:H2'	1:1A:2509:G:H8	1.70	0.57
4:1E:15:PHE:H	18:1T:11:GLN:NE2	2.02	0.57
27:12:2:LYS:HB3	27:12:52:ARG:HD3	1.86	0.57
5:1F:88:ARG:O	5:1F:90:GLN:N	2.37	0.57
1:1A:1469:A:H2'	1:1A:1470:A:C8	2.39	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:46:ARG:NH2	4:1E:89:GLU:OE1	2.37	0.57
26:11:16:ASN:N	26:11:24:THR:O	2.36	0.57
1:1A:1352:U:O2'	1:1A:1570:A:N3	2.34	0.57
1:1A:2283:C:OP1	31:16:3:GLY:N	2.38	0.57
4:1E:156:PHE:HB3	12:1N:81:ILE:HG13	1.87	0.57
6:1G:141:ASP:HB2	6:1G:144:LYS:HD3	1.87	0.57
14:1P:62:PRO:HD3	33:18:26:ALA:HB2	1.85	0.57
1:1A:1961:C:OP2	1:1A:1962:5MC:HM52	2.05	0.56
1:1A:2743:U:O2'	7:1H:152:ARG:NH1	2.38	0.56
1:1A:1309:G:HO2'	1:1A:1611:C:HO2'	1.51	0.56
3:1D:41:GLY:O	3:1D:49:THR:OG1	2.20	0.56
1:1A:444:C:OP2	5:1F:44:ARG:NH2	2.38	0.56
1:1A:1154:G:OP2	19:1U:57:ARG:NH1	2.36	0.56
1:1A:1818:U:C5	3:1D:155:ARG:HD3	2.40	0.56
1:1A:647:G:N2	1:1A:2350:C:O2'	2.38	0.56
1:1A:1296:G:OP1	1:1A:2709:G:O2'	2.21	0.56
1:1A:463:G:N2	1:1A:465:G:H3'	2.21	0.56
15:1Q:49:ALA:O	15:1Q:53:MET:HG2	2.06	0.56
18:1T:70:GLU:OE2	18:1T:100:ARG:NH1	2.38	0.56
1:1A:2853:C:H2'	1:1A:2854:G:C8	2.39	0.56
1:1A:742:A:H2'	1:1A:743:A:C8	2.41	0.56
1:1A:970:U:H2'	1:1A:971:G:H8	1.70	0.56
11:1K:38:CYS:O	11:1K:42:ASN:ND2	2.34	0.56
1:1A:197:A:H4'	1:1A:2069:G7M:OP2	2.05	0.56
3:1D:137:GLY:H	3:1D:163:ILE:HB	1.69	0.56
1:1A:1820:U:H5	3:1D:176:ARG:HH21	1.53	0.56
20:1V:31:GLU:HG3	20:1V:32:THR:H	1.71	0.56
1:1A:2443:C:H2'	1:1A:2444:G:C8	2.40	0.56
1:1A:2030:6MZ:N3	1:1A:2499:C:H5''	2.20	0.56
1:1A:546:U:H2'	1:1A:547:A:H4'	1.87	0.56
13:1O:8:LEU:HB2	13:1O:19:VAL:HG23	1.88	0.56
20:1V:61:ALA:HB1	20:1V:96:VAL:HB	1.87	0.56
5:1F:7:ASP:OD1	5:1F:8:ALA:N	2.36	0.56
33:18:28:LEU:HA	33:18:32:LEU:HD21	1.87	0.56
1:1A:1799:G:O5'	1:1A:1819:A:N6	2.39	0.56
1:1A:878:A:H3'	1:1A:879:G:H8	1.71	0.56
1:1A:2087:G:H2'	1:1A:2088:A:C8	2.41	0.56
1:1A:2399:G:N2	1:1A:2417:C:N3	2.52	0.56
1:1A:774:G:H1'	1:1A:777:G:H21	1.69	0.56
3:1D:171:VAL:N	3:1D:183:VAL:O	2.38	0.56
1:1A:558:U:H2'	1:1A:559:G:H8	1.72	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:48:ALA:HB3	10:1J:51:TYR:HE2	1.71	0.55
1:1A:2391:G:O2'	1:1A:2392:A:O5'	2.20	0.55
1:1A:2893:A:H5''	1:1A:2894:G:H5'	1.87	0.55
1:1A:247:G:O2'	1:1A:386:G:N1	2.40	0.55
3:1D:153:LEU:HD11	3:1D:181:ARG:NH2	2.21	0.55
1:1A:2529:G:H4'	7:1H:174:LYS:HG3	1.88	0.55
1:1A:694:U:H3	1:1A:768:G:H1	1.53	0.55
1:1A:771:G:OP2	32:17:11:LYS:NZ	2.40	0.55
30:15:27:LEU:HD23	30:15:36:LYS:HB3	1.88	0.55
1:1A:2830:C:O2'	1:1A:2883:A:N1	2.37	0.55
3:1D:204:LEU:HD22	3:1D:209:ALA:HB1	1.87	0.55
1:1A:1796:U:H2'	1:1A:1797:G:C8	2.40	0.55
1:1A:1844:C:H2'	1:1A:1845:G:H8	1.71	0.55
1:1A:2461:A:N6	1:1A:2488:G:O6	2.40	0.55
1:1A:599:A:H2'	1:1A:600:G:H8	1.71	0.55
4:1E:47:ALA:HA	4:1E:84:LEU:HG	1.88	0.55
33:18:22:LYS:HB2	33:18:46:LYS:HB3	1.87	0.55
1:1A:2075:U:OP2	1:1A:2238:G:O2'	2.24	0.55
1:1A:690:G:N2	1:1A:772:C:N3	2.54	0.55
1:1A:166:U:H2'	1:1A:167:A:C8	2.98	0.55
1:1A:676:A:H62	1:1A:802:A:H61	1.55	0.55
16:1R:51:LEU:HD21	16:1R:69:ARG:HD2	1.89	0.55
23:1Y:52:ASN:OD1	23:1Y:53:GLN:N	2.40	0.55
1:1A:747:5MU:H71	1:1A:2613:U:C4	2.42	0.55
31:16:18:HIS:HE1	31:16:20:TYR:CZ	2.25	0.55
1:1A:2198:A:C2	9:1I:29:PHE:HB2	2.42	0.55
10:1J:53:ARG:HB3	10:1J:55:VAL:HG13	1.89	0.55
14:1P:33:ARG:HD2	14:1P:40:SER:HA	1.89	0.55
15:1Q:69:PRO:HA	15:1Q:94:ALA:HB2	1.88	0.55
1:1A:827:U:O2'	1:1A:2068:U:O2	2.26	0.54
1:1A:290:U:H2'	1:1A:291:G:H8	1.72	0.54
1:1A:75:G:OP1	27:12:48:ARG:NH2	2.40	0.54
3:1D:180:MET:HB2	3:1D:267:VAL:HB	1.89	0.54
1:1A:538:A:H4'	12:1N:7:LYS:HG2	1.89	0.54
1:1A:2027:G:H1	1:1A:2036:C:H42	1.56	0.54
1:1A:2343:U:HO2'	1:1A:2373:G:HO2'	1.53	0.54
1:1A:247:G:HO2'	1:1A:386:G:H1	1.52	0.54
1:1A:351:C:H2'	1:1A:352:A:C8	2.42	0.54
3:1D:184:GLU:HB3	3:1D:187:CYS:SG	2.47	0.54
6:1G:64:PRO:HB3	6:1G:88:VAL:HG22	1.90	0.54
1:1A:177:G:N2	1:1A:177:G:OP2	2.30	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:106:PRO:HG2	3:1D:109:LEU:HB2	1.88	0.54
1:1A:1261:C:OP2	21:1W:83:LYS:NZ	2.31	0.54
1:1A:2748:A:H5'	7:1H:3:VAL:HG21	1.88	0.54
1:1A:783:A:H2'	1:1A:784:G:H4'	1.89	0.54
1:1A:321:U:H5''	5:1F:131:THR:HG23	1.89	0.54
6:1G:147:ARG:HG3	6:1G:149:ARG:H	1.72	0.54
20:1V:69:GLY:N	20:1V:91:GLN:O	2.34	0.54
1:1A:434:U:O2'	1:1A:436:C:N4	2.40	0.54
1:1A:2744:G:N2	7:1H:142:GLN:OE1	2.34	0.54
1:1A:2282:G:N2	1:1A:2390:U:O2	2.39	0.54
1:1A:586:A:N1	1:1A:809:G:O2'	2.37	0.54
1:1A:674:G:H5''	5:1F:71:GLY:N	2.21	0.54
1:1A:939:G:H2'	1:1A:940:G:H8	1.72	0.54
2:1B:29:A:O2'	2:1B:58:A:N1	2.37	0.54
21:1W:83:LYS:O	21:1W:84:ARG:NH2	2.37	0.54
27:12:26:PHE:HD1	27:12:29:ARG:HH11	1.56	0.54
1:1A:1013:C:H2'	1:1A:1014:A:H8	1.72	0.54
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.43	0.54
12:1N:40:HIS:CE1	12:1N:41:LYS:HG3	2.42	0.54
1:1A:144:A:H4'	22:1X:2:ILE:HD11	1.90	0.54
1:1A:1012:U:O2	12:1N:27:ARG:NH1	2.40	0.54
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.22	0.54
1:1A:351:C:H2'	1:1A:352:A:H8	1.72	0.54
12:1N:56:VAL:HB	12:1N:124:VAL:HG12	1.89	0.54
1:1A:1094:U:N3	1:1A:1097:U:OP2	2.35	0.54
1:1A:631:A:OP2	33:18:22:LYS:NZ	2.37	0.54
12:1N:35:ARG:HB2	12:1N:54:ILE:HD11	1.90	0.54
7:1H:88:LEU:HD23	7:1H:93:TYR:HB3	1.90	0.54
1:1A:4:U:H2'	1:1A:5:A:H8	1.73	0.53
1:1A:690:G:H21	3:1D:42:ARG:HH12	1.55	0.53
15:1Q:21:ALA:HB1	15:1Q:100:LYS:HD3	1.88	0.53
2:1B:95:U:H2'	2:1B:96:G:H8	1.74	0.53
5:1F:103:GLY:HA2	5:1F:106:LYS:HD3	1.91	0.53
15:1Q:46:ILE:O	15:1Q:50:ARG:HB2	2.07	0.53
24:1Z:76:ASP:HB3	24:1Z:90:ASP:HB2	1.91	0.53
1:1A:804:A:H2'	1:1A:806:C:C4	2.43	0.53
7:1H:104:LEU:HB2	7:1H:112:VAL:HB	1.89	0.53
20:1V:32:THR:OG1	20:1V:61:ALA:O	2.21	0.53
20:1V:76:LYS:HB2	20:1V:85:LYS:HB3	1.89	0.53
23:1Y:17:ASP:HB3	23:1Y:20:LYS:HD2	1.89	0.53
1:1A:2271:G:H5'	25:10:16:ARG:HD3	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1264:A:H5'	30:15:7:PRO:HG2	1.91	0.53
1:1A:1363:C:H2'	1:1A:1364:G:H8	1.74	0.53
3:1D:169:ALA:O	3:1D:185:ALA:N	2.41	0.53
3:1D:36:ASN:HD22	3:1D:61:TYR:HB2	1.73	0.53
20:1V:98:ILE:HG22	20:1V:100:GLY:H	1.73	0.53
1:1A:2335:A:HO2'	1:1A:2336:A:H8	1.57	0.53
1:1A:568:U:H4'	1:1A:945:A:N6	2.23	0.53
14:1P:56:PRO:HD2	14:1P:59:ARG:HD3	1.90	0.53
15:1Q:105:MET:SD	15:1Q:108:VAL:HG21	2.48	0.53
15:1Q:40:ARG:HB2	15:1Q:93:VAL:HB	1.90	0.53
1:1A:1450:G:H21	1:1A:1452:G:H1	1.56	0.53
1:1A:1844:C:H2'	1:1A:1845:G:C8	2.44	0.53
1:1A:248:G:O2'	1:1A:2432:A:OP1	2.17	0.53
1:1A:598:U:H2'	1:1A:599:A:C8	2.44	0.53
1:1A:1490:A:H62	3:1D:96:LYS:HB3	1.74	0.53
34:19:11:CYS:SG	34:19:33:HIS:ND1	2.70	0.53
34:19:36:ARG:HG2	34:19:37:GLN:H	1.74	0.53
1:1A:1530:G:H22	1:1A:1542:U:H1'	1.73	0.53
1:1A:1814:G:H4'	3:1D:50:THR:HG21	1.90	0.53
1:1A:1055:G:H1	1:1A:1104:C:H42	1.56	0.53
1:1A:744:U:H5''	1:1A:1658:C:H5''	1.91	0.53
1:1A:2002:G:OP2	16:1R:9:GLN:NE2	2.42	0.53
3:1D:69:ASN:HA	3:1D:188:ARG:HH12	1.73	0.53
1:1A:2276:G:OP2	15:1Q:85:GLY:N	2.42	0.53
15:1Q:12:MET:O	15:1Q:86:LYS:NZ	2.42	0.53
27:12:49:ASP:OD1	27:12:52:ARG:NH2	2.42	0.52
1:1A:1028:A:H61	1:1A:1125:G:H2'	1.74	0.52
1:1A:1320:C:HO2'	1:1A:1321:A:H8	1.56	0.52
1:1A:1365:A:OP1	26:11:2:ARG:NH1	2.35	0.52
1:1A:2022:U:O4	30:15:5:ASN:ND2	2.42	0.52
1:1A:968:C:H2'	1:1A:969:G:H8	1.74	0.52
33:18:13:PHE:HB3	33:18:21:PHE:HB3	1.90	0.52
1:1A:1068:G:N2	1:1A:1095:A:O2'	2.41	0.52
1:1A:1316:U:H2'	1:1A:1317:G:H8	1.74	0.52
1:1A:1916:A:H2'	1:1A:1917:PSU:O4'	2.10	0.52
1:1A:2189:U:H2'	1:1A:2190:G:H8	1.75	0.52
1:1A:1129:A:O2'	1:1A:2515:C:O2	2.25	0.52
1:1A:4:U:H2'	1:1A:5:A:C8	2.45	0.52
1:1A:835:C:H2'	1:1A:836:G:H8	1.74	0.52
9:1I:47:PHE:HA	9:1I:51:ARG:HB2	1.91	0.52
1:1A:1320:C:N4	1:1A:1330:C:OP2	2.41	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1501:G:P	3:1D:100:ARG:HH22	2.32	0.52
6:1G:59:ILE:O	6:1G:101:ARG:NH1	2.42	0.52
1:1A:1187:G:N2	1:1A:1188:U:O4	2.42	0.52
1:1A:1283:G:N1	1:1A:1286:A:OP2	2.41	0.52
1:1A:1954:G:O2'	1:1A:1956:U:O4	2.23	0.52
1:1A:2120:G:H2'	1:1A:2121:G:C8	2.45	0.52
1:1A:2280:G:H2'	1:1A:2281:A:C8	2.44	0.52
1:1A:15:G:H4'	30:15:17:SER:HB3	1.92	0.52
1:1A:1038:G:H2'	1:1A:1039:A:C8	2.45	0.52
1:1A:754:U:O2'	1:1A:1618:6MZ:H2	2.09	0.52
31:16:5:ARG:HG2	31:16:23:THR:HB	1.91	0.52
33:18:21:PHE:O	33:18:49:VAL:HG23	2.09	0.52
1:1A:1796:U:H3	1:1A:1823:G:H1	1.56	0.52
1:1A:559:G:N3	19:1U:55:GLN:NE2	2.55	0.52
1:1A:690:G:N2	3:1D:42:ARG:HH12	2.07	0.52
14:1P:101:ILE:HB	14:1P:105:ILE:HG13	1.90	0.52
14:1P:79:LEU:HD12	14:1P:114:GLY:H	1.73	0.52
33:18:5:THR:HG23	33:18:61:LEU:HA	1.91	0.52
1:1A:2333:A:OP1	25:10:73:ARG:NH2	2.36	0.52
1:1A:1924:C:H2'	1:1A:1925:C:C6	2.44	0.52
1:1A:2372:U:H2'	1:1A:2373:G:H8	1.74	0.52
1:1A:970:U:H2'	1:1A:971:G:C8	2.45	0.52
1:1A:2280:G:H2'	1:1A:2281:A:H8	1.75	0.52
1:1A:747:5MU:H71	1:1A:2613:U:C5	2.44	0.52
1:1A:500:G:N1	1:1A:503:A:OP2	2.43	0.52
15:1Q:19:GLY:O	15:1Q:38:ARG:NH1	2.40	0.52
15:1Q:53:MET:HE2	15:1Q:63:ILE:HD13	1.91	0.52
28:13:53:MET:HG3	28:13:54:VAL:HG13	1.93	0.52
1:1A:2101:A:H2'	1:1A:2102:G:C8	2.45	0.52
1:1A:573:U:O2'	1:1A:575:A:OP1	2.22	0.52
1:1A:720:U:H2'	1:1A:721:A:C8	2.44	0.52
1:1A:597:G:O2'	14:1P:11:GLY:O	2.26	0.52
1:1A:1517:G:N3	1:1A:1919:A:O2'	103.21	0.51
1:1A:1693:U:H3'	1:1A:1694:C:H6	1.75	0.51
1:1A:918:A:N3	2:1B:80:U:O2'	2.37	0.51
1:1A:973:A:H5'	1:1A:1188:U:H1'	1.91	0.51
4:1E:16:THR:OG1	4:1E:20:VAL:O	2.22	0.51
20:1V:68:ARG:HB2	20:1V:90:ARG:HH21	1.76	0.51
6:1G:63:LYS:H	29:14:6:HIS:CE1	2.29	0.51
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.10	0.51
1:1A:1827:U:H5	3:1D:220:ARG:HD3	1.75	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:10:55:LEU:HD12	25:10:76:ILE:HD12	1.93	0.51
1:1A:1291:C:H2'	1:1A:1292:G:H8	1.75	0.51
1:1A:1808:A:H3'	1:1A:1809:A:H8	1.76	0.51
1:1A:415:A:O2'	1:1A:1866:A:OP1	2.29	0.51
1:1A:767:U:H2'	1:1A:768:G:H8	1.76	0.51
16:1R:76:VAL:HA	16:1R:79:LEU:HD12	1.91	0.51
21:1W:62:ASP:N	21:1W:62:ASP:OD1	2.42	0.51
23:1Y:10:VAL:HA	23:1Y:71:ILE:HA	1.91	0.51
1:1A:2757:A:OP1	34:19:20:ASP:N	2.42	0.51
1:1A:1675:C:O2	4:1E:133:THR:OG1	2.28	0.51
1:1A:2508:G:H2'	1:1A:2509:G:C8	2.46	0.51
1:1A:2857:G:N2	1:1A:2860:A:OP2	2.35	0.51
1:1A:290:U:H2'	1:1A:291:G:C8	2.45	0.51
1:1A:962:G:O2'	1:1A:2496:C:O2'	2.29	0.51
1:1A:1509:A:H2'	1:1A:1510:G:C8	2.45	0.51
1:1A:1858:A:N6	1:1A:1884:G:O2'	2.43	0.51
1:1A:414:C:O3'	1:1A:1878:G:N2	2.44	0.51
1:1A:445:C:N4	1:1A:446:G:O6	2.44	0.51
1:1A:883:G:N2	1:1A:893:C:O2	2.29	0.51
9:1I:80:ILE:HG22	9:1I:82:SER:H	1.74	0.51
1:1A:2470:G:O6	1:1A:2476:A:O2'	2.23	0.51
1:1A:518:G:OP2	30:15:12:ARG:NH2	2.34	0.51
1:1A:538:A:H5''	12:1N:7:LYS:HE3	1.93	0.51
18:1T:47:ILE:O	18:1T:96:LEU:N	2.44	0.51
19:1U:17:LEU:HA	19:1U:20:ALA:HB3	1.92	0.51
1:1A:910:A:N3	1:1A:2264:C:O2'	2.36	0.51
15:1Q:33:LEU:HD23	15:1Q:103:TYR:HD2	1.76	0.51
1:1A:2361:G:O3'	33:18:27:ASN:ND2	2.44	0.51
13:1O:29:HIS:O	13:1O:29:HIS:ND1	2.43	0.51
1:1A:1566:A:O2'	1:1A:1568:G:N2	2.44	0.51
1:1A:2020:A:H61	1:1A:2034:U:H3	1.57	0.51
1:1A:2440:C:H5''	1:1A:2587:A:H4'	1.93	0.51
1:1A:1225:G:H5'	20:1V:88:GLY:H	1.75	0.51
1:1A:233:A:H61	1:1A:428:A:H61	1.59	0.51
4:1E:4:LEU:HD23	4:1E:32:ASN:HD22	1.76	0.51
1:1A:1019:U:H3	1:1A:1142:A:H62	1.57	0.50
1:1A:1432:G:H2'	1:1A:1433:A:C8	2.46	0.50
1:1A:2039:U:H2'	1:1A:2040:G:H8	1.76	0.50
1:1A:2238:G:N2	1:1A:2238:G:OP2	2.44	0.50
1:1A:24:G:H2'	1:1A:25:U:C6	2.46	0.50
1:1A:951:C:H2'	1:1A:952:G:H8	1.76	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1028:A:N3	1:1A:2486:C:O2'	2.39	0.50
1:1A:414:C:H2'	1:1A:415:A:C8	2.47	0.50
1:1A:776:G:N2	1:1A:802:A:OP2	23.96	0.50
2:1B:24:G:N2	2:1B:27:C:N3	2.58	0.50
3:1D:77:VAL:HA	3:1D:93:VAL:HA	1.94	0.50
6:1G:7:TYR:OH	6:1G:28:PRO:O	2.23	0.50
22:1X:13:ALA:H	22:1X:33:LYS:HB2	1.77	0.50
1:1A:13:A:O2'	1:1A:15:G:N7	2.39	0.50
1:1A:1567:G:H3'	3:1D:84:PRO:HG3	1.92	0.50
2:1B:45:A:O4'	6:1G:91:ARG:NH2	2.44	0.50
10:1J:59:LEU:HB3	10:1J:62:ARG:HB3	1.92	0.50
1:1A:2820:A:H4'	16:1R:3:HIS:CD2	2.46	0.50
1:1A:619:G:H3'	1:1A:620:G:H21	1.77	0.50
1:1A:2258:C:O2'	1:1A:2427:C:OP2	2.25	0.50
1:1A:2443:C:H2'	1:1A:2444:G:H8	1.77	0.50
1:1A:328:U:H4'	23:1Y:65:GLN:HG3	1.94	0.50
1:1A:775:G:H4'	1:1A:776:G:O5'	2.10	0.50
3:1D:129:LEU:HD13	3:1D:133:ASN:HB2	1.92	0.50
3:1D:51:ARG:HH22	3:1D:246:PRO:HG2	1.75	0.50
1:1A:819:A:H3'	1:1A:973:A:H61	1.75	0.50
4:1E:25:THR:HG21	4:1E:193:VAL:HG21	1.94	0.50
6:1G:116:LEU:HD13	6:1G:175:PRO:HG2	1.94	0.50
13:1O:16:ALA:HA	13:1O:46:ALA:HA	1.94	0.50
14:1P:79:LEU:H	14:1P:113:ALA:HB3	1.77	0.50
1:1A:2221:G:H2'	1:1A:2222:C:C6	2.46	0.50
1:1A:2472:G:H2'	1:1A:2475:C:H42	1.77	0.50
1:1A:266:G:O6	1:1A:270:A:N6	12.88	0.50
1:1A:516:C:OP1	30:15:9:ARG:NH1	2.44	0.50
1:1A:803:U:O4	1:1A:804:A:N6	2.45	0.50
5:1F:97:ASN:HB2	5:1F:100:MET:HG3	1.93	0.50
1:1A:119:A:H4'	1:1A:120:U:H5'	1.93	0.50
1:1A:1930:G:HO2'	1:1A:1931:U:H6	1.59	0.50
1:1A:1059:G:H5'	1:1A:1060:U:OP2	2.12	0.50
1:1A:1597:A:H5''	1:1A:1598:A:H5'	1.93	0.50
1:1A:1949:G:H1	1:1A:1957:C:H42	1.60	0.50
1:1A:259:G:O2'	1:1A:621:A:O2'	2.26	0.50
1:1A:1:G:H1	1:1A:2902:C:H42	1.58	0.50
3:1D:70:LYS:HB3	3:1D:73:ILE:HD12	1.94	0.50
1:1A:1190:G:H2'	1:1A:1191:G:C8	2.47	0.49
1:1A:2002:G:H5''	16:1R:9:GLN:HE21	1.77	0.49
1:1A:2270:A:H2'	1:1A:2271:G:O4'	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:729:G:H5''	1:1A:730:A:H5''	1.94	0.49
2:1B:114:C:H2'	2:1B:115:A:C8	2.47	0.49
10:1J:3:LEU:HD12	10:1J:5:LEU:H	1.76	0.49
1:1A:2696:U:H2'	1:1A:2697:G:H8	1.77	0.49
1:1A:2808:G:O2'	1:1A:2809:A:H8	1.94	0.49
4:1E:51:THR:HB	4:1E:79:LEU:HD23	1.94	0.49
5:1F:47:LYS:HB2	5:1F:51:GLU:HB2	1.94	0.49
1:1A:1415:U:H3	1:1A:1587:G:H1	1.60	0.49
1:1A:1818:U:H4'	1:1A:1821:A:H1'	1.93	0.49
1:1A:2345:G:H4'	1:1A:2346:A:H3'	1.93	0.49
2:1B:105:G:H2'	2:1B:106:G:H8	1.77	0.49
2:1B:118:C:H2'	2:1B:119:A:H8	1.78	0.49
3:1D:143:VAL:HB	3:1D:153:LEU:HB2	1.94	0.49
5:1F:49:ARG:HD2	5:1F:76:PRO:HD3	1.94	0.49
9:1I:63:ALA:HB1	9:1I:135:HIS:HE2	1.77	0.49
13:1O:19:VAL:HA	13:1O:44:LYS:H	1.77	0.49
25:10:61:GLY:HA3	25:10:79:GLU:O	2.13	0.49
1:1A:249:C:O2	33:18:11:LYS:NZ	2.45	0.49
1:1A:18:U:OP1	19:1U:25:GLY:N	2.44	0.49
1:1A:1899:A:H4'	1:1A:1901:A:H5''	1.94	0.49
1:1A:2059:A:C8	1:1A:2503:2MA:HM23	2.47	0.49
1:1A:2566:A:H4'	1:1A:2567:G:O5'	2.11	0.49
1:1A:655:A:H4'	1:1A:656:G:H5'	1.92	0.49
1:1A:946:C:H2'	1:1A:947:A:H8	1.77	0.49
1:1A:1528:A:OP2	1:1A:1543:G:N2	2.46	0.49
1:1A:2284:A:H1'	1:1A:2325:G:N1	2.27	0.49
1:1A:2059:A:N6	1:1A:2503:2MA:H2'	2.27	0.49
1:1A:2732:G:P	4:1E:208:LYS:HZ3	2.35	0.49
3:1D:72:GLY:N	3:1D:117:SER:O	2.35	0.49
3:1D:2:VAL:HG13	3:1D:18:VAL:HG22	1.95	0.49
21:1W:80:PRO:O	21:1W:100:THR:OG1	2.28	0.49
25:10:19:VAL:HG13	25:10:34:VAL:HG22	1.94	0.49
1:1A:1693:U:O2'	3:1D:13:ARG:NH1	2.45	0.49
1:1A:1752:C:H2'	1:1A:1753:G:C8	2.48	0.49
1:1A:1871:A:H8	1:1A:1872:A:C8	2.30	0.49
1:1A:191:A:H2'	1:1A:192:C:C6	2.47	0.49
1:1A:2061:G:HO2'	1:1A:2063:C:H5	1.61	0.49
1:1A:2496:C:N3	1:1A:2498:OMC:N4	2.60	0.49
1:1A:341:C:H2'	1:1A:342:A:C8	2.48	0.49
1:1A:839:U:H3	1:1A:939:G:H1	1.59	0.49
1:1A:939:G:H2'	1:1A:940:G:C8	2.48	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2257:U:O4	1:1A:2258:C:N4	2.46	0.49
2:1B:48:U:H5'	17:1S:98:GLN:HB3	1.94	0.49
11:1K:63:ASP:O	11:1K:65:SER:N	2.46	0.49
1:1A:1320:C:O2'	1:1A:1321:A:H8	1.96	0.49
1:1A:151:C:H2'	1:1A:152:A:H8	1.78	0.49
1:1A:2331:G:H4'	25:10:39:THR:H	1.78	0.49
1:1A:2417:C:H2'	1:1A:2418:A:C8	2.48	0.49
1:1A:2651:C:H2'	1:1A:2652:C:C6	2.48	0.49
1:1A:373:U:H1'	1:1A:423:A:N3	2.27	0.49
1:1A:860:U:H2'	1:1A:861:A:H8	1.76	0.49
1:1A:907:G:N2	15:1Q:70:ASP:OD2	2.46	0.49
3:1D:65:ASP:HB2	3:1D:101:ARG:HB3	1.95	0.49
1:1A:768:G:N2	1:1A:1379:U:O2'	2.45	0.49
1:1A:185:G:H2'	1:1A:186:G:H8	1.78	0.49
1:1A:2245:U:H5''	1:1A:2246:G:H5'	1.94	0.49
1:1A:832:U:H2'	1:1A:833:A:C8	2.47	0.49
1:1A:784:G:C6	3:1D:227:VAL:HG11	2.47	0.49
6:1G:56:LEU:O	6:1G:60:SER:OG	2.19	0.49
7:1H:68:ARG:HH12	7:1H:72:ASN:ND2	2.10	0.49
20:1V:68:ARG:HH11	20:1V:90:ARG:HB2	1.78	0.49
2:1B:76:G:P	24:1Z:9:ARG:HH22	2.35	0.49
1:1A:1930:G:N1	1:1A:1968:G:N7	2.61	0.49
1:1A:2082:A:H2'	1:1A:2083:G:O4'	2.12	0.49
1:1A:2141:G:H2'	1:1A:2142:A:H8	1.77	0.49
1:1A:2326:C:O2'	1:1A:2327:A:OP1	2.29	0.49
1:1A:2489:U:O2'	1:1A:2518:A:N6	2.46	0.49
1:1A:2845:U:H2'	1:1A:2846:G:C8	2.47	0.49
1:1A:606:U:H4'	1:1A:658:U:O2'	2.13	0.49
11:1K:107:GLU:O	11:1K:110:GLN:NE2	2.44	0.49
1:1A:1181:U:H2'	1:1A:1182:G:H8	1.78	0.48
1:1A:1407:G:H2'	1:1A:1408:G:H8	1.78	0.48
1:1A:2011:U:H2'	1:1A:2012:G:O4'	2.12	0.48
1:1A:693:A:O2'	1:1A:1353:A:N3	2.45	0.48
1:1A:721:A:H2'	1:1A:722:A:C8	2.47	0.48
15:1Q:12:MET:HG2	15:1Q:72:PRO:HG2	1.95	0.48
28:13:8:GLN:HB2	28:13:28:LEU:HD13	1.95	0.48
1:1A:1266:G:N2	1:1A:1267:U:O4	2.30	0.48
1:1A:1415:U:H2'	1:1A:1416:G:H4'	1.95	0.48
1:1A:1682:G:C4	1:1A:1757:A:H1'	2.47	0.48
1:1A:1794:A:H2'	1:1A:1795:C:C6	2.47	0.48
1:1A:2039:U:H2'	1:1A:2040:G:C8	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2233:U:H2'	1:1A:2234:G:H8	1.78	0.48
1:1A:2258:C:C4	1:1A:2426:A:H5'	2.47	0.48
1:1A:2431:U:O2'	1:1A:2433:A:N7	2.40	0.48
1:1A:2794:C:H42	1:1A:2802:G:H1	1.59	0.48
1:1A:514:A:N3	1:1A:581:C:O2'	2.44	0.48
1:1A:534:U:H2'	1:1A:535:G:H8	1.77	0.48
1:1A:977:G:H2'	1:1A:978:G:H8	1.78	0.48
5:1F:143:LEU:HB3	5:1F:146:VAL:HG11	1.95	0.48
17:1S:39:VAL:N	17:1S:49:VAL:O	2.38	0.48
23:1Y:3:LYS:HB3	23:1Y:82:VAL:HG21	1.96	0.48
1:1A:2418:A:P	33:18:44:ARG:HH21	2.36	0.48
1:1A:2120:G:H2'	1:1A:2121:G:H8	1.77	0.48
1:1A:599:A:H2'	1:1A:600:G:C8	2.48	0.48
1:1A:765:C:H2'	1:1A:766:U:H6	1.77	0.48
1:1A:877:A:O2'	1:1A:900:A:N6	2.47	0.48
2:1B:88:C:O2'	2:1B:89:U:O5'	2.23	0.48
4:1E:24:VAL:HG12	4:1E:178:VAL:HG21	1.94	0.48
6:1G:12:VAL:O	6:1G:16:MET:HG2	2.14	0.48
11:1K:20:SER:HB3	11:1K:21:PRO:HD3	1.95	0.48
1:1A:581:C:H2'	1:1A:582:A:H8	1.76	0.48
1:1A:663:G:H5''	14:1P:17:LYS:HD3	1.94	0.48
1:1A:966:G:H2'	1:1A:967:U:C6	2.48	0.48
2:1B:28:C:H2'	2:1B:29:A:H8	1.78	0.48
2:1B:55:U:HO2'	6:1G:23:SER:HG	1.61	0.48
3:1D:140:VAL:HG12	3:1D:191:LEU:HD23	1.94	0.48
11:1K:91:LYS:HG3	11:1K:94:LYS:HE2	1.95	0.48
14:1P:73:ILE:HD12	14:1P:106:GLU:HB2	1.95	0.48
14:1P:71:ALA:O	14:1P:74:THR:HG22	2.14	0.48
28:13:23:LEU:HD21	28:13:53:MET:SD	2.53	0.48
33:18:25:HIS:CE1	33:18:47:ALA:HB2	2.48	0.48
1:1A:1355:G:H2'	1:1A:1356:G:H8	1.79	0.48
1:1A:2374:C:N4	1:1A:2375:G:O6	2.46	0.48
11:1K:33:ASN:OD1	11:1K:34:ILE:N	2.46	0.48
32:17:30:VAL:O	32:17:34:ARG:HG2	2.13	0.48
1:1A:1775:U:H2'	1:1A:1776:G:O4'	2.12	0.48
1:1A:1836:C:H2'	1:1A:1837:C:H6	1.79	0.48
1:1A:2313:C:H2'	1:1A:2314:A:C8	2.48	0.48
1:1A:633:A:O2'	1:1A:2404:U:OP1	2.29	0.48
1:1A:630:G:N2	1:1A:633:A:OP2	2.38	0.48
7:1H:21:GLN:NE2	7:1H:40:VAL:O	2.34	0.48
1:1A:2623:G:H2'	1:1A:2624:G:C8	2.49	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2724:U:H2'	1:1A:2725:A:C8	2.49	0.48
6:1G:9:ASP:OD1	6:1G:9:ASP:N	2.46	0.48
1:1A:1777:U:H3	1:1A:1787:A:H61	1.60	0.48
1:1A:813:U:H2'	1:1A:814:C:C6	2.49	0.48
3:1D:106:PRO:HD2	3:1D:109:LEU:HD22	1.95	0.48
1:1A:729:G:N2	3:1D:10:PRO:O	2.47	0.48
14:1P:57:LEU:HD22	33:18:53:ASP:HB3	1.95	0.48
17:1S:40:ILE:HG12	17:1S:47:VAL:HG12	1.96	0.48
19:1U:111:LYS:HB2	20:1V:48:LYS:HD2	1.95	0.48
19:1U:68:ALA:HB1	19:1U:73:ILE:HG23	1.94	0.48
1:1A:1278:C:H2'	1:1A:1279:G:H8	1.79	0.48
1:1A:2051:A:H2'	1:1A:2578:G:OP1	2.13	0.48
1:1A:2286:G:H4'	1:1A:2287:A:O5'	2.13	0.48
1:1A:672:C:H2'	1:1A:673:C:C6	2.49	0.48
1:1A:696:G:N2	1:1A:767:U:H1'	2.29	0.48
1:1A:832:U:H5'	14:1P:38:GLN:HB3	1.96	0.48
1:1A:85:G:OP1	23:1Y:6:ARG:N	2.46	0.48
10:1J:59:LEU:HG	10:1J:61:ARG:H	1.79	0.48
14:1P:30:THR:HG21	14:1P:35:HIS:CD2	2.49	0.48
1:1A:465:G:P	32:17:12:ARG:HH12	2.36	0.48
1:1A:1636:U:H2'	1:1A:1637:A:C8	2.49	0.48
1:1A:1826:G:O2'	1:1A:1971:U:OP2	2.18	0.48
1:1A:2593:U:H2'	1:1A:2594:C:C6	2.49	0.48
1:1A:2696:U:H2'	1:1A:2697:G:C8	2.49	0.48
9:1I:132:PHE:HB2	9:1I:140:ALA:HB3	1.96	0.48
13:1O:34:GLY:O	13:1O:36:GLY:N	2.45	0.48
7:1H:41:GLU:HB2	7:1H:54:ARG:HB2	1.95	0.47
11:1K:57:VAL:HG23	11:1K:71:LYS:HZ2	1.78	0.47
19:1U:87:VAL:HG12	19:1U:89:ILE:H	1.79	0.47
1:1A:151:C:H2'	1:1A:152:A:C8	2.49	0.47
1:1A:2052:A:H2'	1:1A:2053:G:H8	1.78	0.47
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.49	0.47
1:1A:2297:A:N6	1:1A:2319:G:H1'	2.29	0.47
1:1A:2680:U:O2'	4:1E:11:MET:SD	2.72	0.47
10:1J:67:THR:HG21	10:1J:75:ALA:HB2	1.96	0.47
23:1Y:73:ASN:HA	23:1Y:95:PHE:CE1	2.49	0.47
32:17:3:ARG:HG3	32:17:5:PHE:H	1.80	0.47
1:1A:1836:C:H2'	1:1A:1837:C:C6	2.49	0.47
1:1A:1993:U:H4'	4:1E:133:THR:HG21	1.95	0.47
1:1A:2453:A:H2'	1:1A:2454:G:H8	1.79	0.47
2:1B:3:C:H3'	2:1B:4:C:H5''	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:80:U:H2'	2:1B:81:G:H8	1.79	0.47
9:1I:51:ARG:HA	9:1I:55:GLU:HB2	1.97	0.47
23:1Y:80:ASP:OD2	23:1Y:95:PHE:HB3	2.14	0.47
27:12:25:GLN:HE21	27:12:50:VAL:HG21	1.79	0.47
1:1A:1071:G:H1'	1:1A:1089:A:N7	2.29	0.47
1:1A:1141:U:H4'	1:1A:1142:A:O4'	2.14	0.47
13:1O:12:ASP:HB3	13:1O:99:ILE:HG12	1.96	0.47
20:1V:14:VAL:HG21	20:1V:98:ILE:HG13	1.95	0.47
24:1Z:76:ASP:OD1	24:1Z:77:VAL:N	2.48	0.47
25:10:42:HIS:CD2	25:10:73:ARG:HB2	2.49	0.47
1:1A:1494:A:H2	1:1A:1579:A:H1'	1.80	0.47
1:1A:1792:G:O2'	1:1A:1830:C:OP1	2.29	0.47
1:1A:331:C:H41	1:1A:1210:G:N2	2.12	0.47
1:1A:558:U:H2'	1:1A:559:G:C8	2.49	0.47
1:1A:724:U:H2'	1:1A:725:G:O4'	2.14	0.47
5:1F:52:VAL:HG21	5:1F:82:GLY:H	1.78	0.47
1:1A:2746:U:H5''	7:1H:137:LYS:HE2	1.95	0.47
32:17:34:ARG:NH2	32:17:41:ARG:O	2.48	0.47
1:1A:1005:C:H2'	1:1A:1006:C:C6	2.49	0.47
1:1A:1562:U:H2'	1:1A:1563:U:C6	2.48	0.47
1:1A:1636:U:H2'	1:1A:1637:A:H8	1.79	0.47
1:1A:196:A:OP2	14:1P:47:ARG:NH1	2.47	0.47
10:1J:77:VAL:HG13	10:1J:114:GLU:OE2	2.15	0.47
23:1Y:24:VAL:HA	23:1Y:35:VAL:HG22	1.96	0.47
32:17:37:LYS:NZ	32:17:39:ARG:HH21	2.13	0.47
1:1A:1182:G:H5'	1:1A:1183:U:OP1	6.04	0.47
1:1A:824:U:HO2'	1:1A:2358:A:N6	2.13	0.47
1:1A:2417:C:H2'	1:1A:2418:A:H8	1.80	0.47
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.49	0.47
1:1A:2773:C:OP1	4:1E:169:ARG:NH2	2.48	0.47
1:1A:2819:G:H2'	1:1A:2821:A:N7	2.30	0.47
1:1A:780:G:O2'	1:1A:783:A:N6	2.44	0.47
3:1D:172:THR:HA	3:1D:182:LYS:HA	1.97	0.47
15:1Q:22:GLN:O	15:1Q:24:THR:N	2.48	0.47
1:1A:2851:A:O3'	16:1R:64:ARG:NH2	2.48	0.47
1:1A:1187:G:H5''	20:1V:83:TYR:CZ	2.48	0.47
1:1A:1751:U:H2'	1:1A:1752:C:C6	2.50	0.47
1:1A:2259:U:O2	1:1A:2282:G:N2	2.45	0.47
1:1A:1863:G:H4'	1:1A:2411:A:H4'	1.96	0.47
1:1A:742:A:H2'	1:1A:743:A:H8	1.80	0.47
1:1A:828:U:O4	1:1A:858:G:N2	40.81	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:937:C:OP2	33:18:51:LYS:NZ	2.47	0.47
1:1A:129:C:H2'	1:1A:130:C:C6	2.49	0.47
1:1A:171:U:H2'	1:1A:172:A:H8	1.80	0.47
1:1A:179:C:H2'	1:1A:180:G:C8	2.50	0.47
1:1A:2809:A:H2'	1:1A:2810:A:C8	2.49	0.47
1:1A:534:U:H2'	1:1A:535:G:C8	2.50	0.47
1:1A:690:G:H2'	1:1A:691:C:C6	2.50	0.47
14:1P:110:VAL:HG21	14:1P:127:VAL:HG22	1.97	0.47
14:1P:85:VAL:HG13	14:1P:98:ALA:HB2	1.97	0.47
18:1T:26:GLU:HA	18:1T:43:GLU:HA	1.96	0.47
1:1A:227:A:C2	1:1A:228:C:H1'	2.50	0.47
1:1A:259:G:HO2'	1:1A:621:A:HO2'	1.56	0.47
1:1A:682:G:O6	1:1A:794:A:N6	2.48	0.47
15:1Q:30:SER:OG	15:1Q:106:ASP:OD1	2.24	0.47
1:1A:789:A:N6	32:17:3:ARG:HH12	2.13	0.47
1:1A:1048:A:OP2	1:1A:1110:G:N2	2.48	0.47
1:1A:1218:G:OP2	19:1U:14:LYS:NZ	2.41	0.47
1:1A:1571:A:H2'	1:1A:1572:A:C8	2.50	0.47
1:1A:271:G:H1'	1:1A:272:A:C8	2.50	0.47
4:1E:121:THR:HG21	4:1E:143:PRO:HB3	1.97	0.47
9:1I:20:ASN:OD1	9:1I:21:VAL:N	2.48	0.47
3:1D:130:PRO:HA	3:1D:188:ARG:HA	1.98	0.46
9:1I:3:VAL:HA	9:1I:38:PRO:HA	1.96	0.46
30:15:51:ARG:HD2	30:15:53:VAL:HG12	1.97	0.46
1:1A:1808:A:H3'	1:1A:1809:A:C8	2.51	0.46
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.51	0.46
1:1A:2314:A:H2'	1:1A:2315:G:C8	2.50	0.46
1:1A:2339:C:H2'	1:1A:2340:A:H8	1.79	0.46
3:1D:259:ASN:O	3:1D:261:ARG:N	2.41	0.46
3:1D:267:VAL:HG12	3:1D:268:ARG:HG2	1.96	0.46
15:1Q:102:LEU:HD11	15:1Q:126:ILE:HD11	1.97	0.46
1:1A:2522:U:O2'	1:1A:2647:U:OP1	2.26	0.46
1:1A:839:U:H2'	1:1A:840:C:C6	2.51	0.46
4:1E:29:VAL:O	4:1E:185:ASN:HB3	2.14	0.46
1:1A:2357:G:P	25:10:16:ARG:HE	2.39	0.46
1:1A:1190:G:H2'	1:1A:1191:G:H8	1.80	0.46
1:1A:528:A:C2	1:1A:2042:A:H2'	2.51	0.46
1:1A:2194:U:H2'	1:1A:2195:U:C6	2.50	0.46
1:1A:2267:A:H5''	1:1A:2268:A:H5'	1.98	0.46
1:1A:537:G:H22	1:1A:555:G:H2'	1.80	0.46
1:1A:565:C:N4	1:1A:575:A:H61	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1Q:29:GLY:HA2	15:1Q:106:ASP:HB2	1.97	0.46
1:1A:2146:C:H4'	1:1A:2147:A:C5	2.50	0.46
1:1A:336:C:H2'	1:1A:337:C:C6	2.51	0.46
1:1A:355:U:H2'	1:1A:356:G:H8	1.80	0.46
1:1A:948:C:O2	1:1A:984:A:O2'	2.14	0.46
6:1G:129:MET:HG2	6:1G:153:ILE:HB	1.96	0.46
1:1A:2144:G:O2'	1:1A:2147:A:N1	2.45	0.46
1:1A:968:C:H2'	1:1A:969:G:C8	2.51	0.46
2:1B:38:C:H2'	2:1B:39:A:C8	2.50	0.46
2:1B:71:C:H42	2:1B:105:G:H1	1.64	0.46
21:1W:20:VAL:HG11	21:1W:44:ALA:HA	1.98	0.46
1:1A:1146:C:H2'	1:1A:1147:A:C8	2.50	0.46
1:1A:1238:G:H2'	1:1A:1239:G:H8	1.80	0.46
1:1A:1843:C:H42	1:1A:1897:G:H1	1.63	0.46
1:1A:1667:G:N2	1:1A:1992:G:OP2	2.47	0.46
1:1A:233:A:N6	1:1A:428:A:H61	2.13	0.46
1:1A:438:G:H2'	1:1A:439:A:C8	2.51	0.46
1:1A:453:A:N3	1:1A:457:A:O2'	2.46	0.46
3:1D:137:GLY:HA2	3:1D:163:ILE:O	2.15	0.46
15:1Q:47:GLU:OE2	15:1Q:51:ARG:NE	2.47	0.46
1:1A:1345:C:H2'	1:1A:1346:G:H8	1.81	0.46
1:1A:1397:U:N3	1:1A:1602:U:O2	2.49	0.46
1:1A:1672:A:C2	1:1A:2582:G:H5'	2.51	0.46
1:1A:18:U:H2'	1:1A:19:A:C8	2.51	0.46
1:1A:807:U:H4'	1:1A:2446:G:OP1	2.16	0.46
1:1A:2519:U:H5'	1:1A:2567:G:H21	1.80	0.46
1:1A:440:C:H2'	1:1A:441:U:C6	2.51	0.46
1:1A:863:A:H2'	1:1A:864:G:C8	2.50	0.46
1:1A:942:G:H2'	1:1A:943:A:O4'	2.15	0.46
15:1Q:110:GLU:OE2	15:1Q:114:ARG:NH1	2.49	0.46
6:1G:97:GLU:HG2	29:14:25:ARG:HB2	1.98	0.46
1:1A:160:A:H2'	1:1A:161:A:C8	2.50	0.46
1:1A:2845:U:O3'	18:1T:52:ARG:NH1	2.49	0.46
1:1A:334:C:OP1	1:1A:335:C:N4	2.48	0.46
1:1A:357:C:H2'	1:1A:358:U:C6	2.51	0.46
1:1A:2572:A:OP2	4:1E:149:ASN:HB3	2.16	0.46
5:1F:48:THR:OG1	5:1F:51:GLU:OE1	2.22	0.46
11:1K:4:VAL:HA	11:1K:7:TYR:CE2	2.51	0.46
13:1O:109:SER:O	13:1O:111:LYS:N	2.49	0.46
16:1R:29:VAL:HG13	16:1R:83:LEU:HD11	1.98	0.46
33:18:38:LYS:HG3	33:18:41:ARG:HH11	1.81	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:976:G:O2'	1:1A:1155:A:O2'	2.20	0.46
1:1A:2828:G:H2'	1:1A:2829:A:H8	1.80	0.46
2:1B:13:G:N2	2:1B:16:G:O2'	2.49	0.46
22:1X:37:ASP:O	22:1X:81:LYS:NZ	2.45	0.46
1:1A:1935:G:N2	1:1A:1964:G:O4'	2.45	0.45
1:1A:2557:G:H2'	1:1A:2558:C:C6	2.51	0.45
1:1A:2818:U:H2'	1:1A:2819:G:C8	2.51	0.45
1:1A:281:C:N3	1:1A:359:G:N2	2.63	0.45
4:1E:151:THR:HB	4:1E:152:PRO:HD3	1.98	0.45
9:1I:30:LEU:HA	9:1I:35:LYS:HB2	1.98	0.45
30:15:30:ASP:HB3	30:15:34:GLY:H	1.81	0.45
1:1A:2336:A:N3	1:1A:2385:C:H1'	2.31	0.45
1:1A:2884:U:H2'	1:1A:2885:G:H8	1.82	0.45
1:1A:326:G:H2'	1:1A:327:G:C8	2.51	0.45
1:1A:341:C:H2'	1:1A:342:A:H8	1.81	0.45
1:1A:625:G:H2'	1:1A:626:A:C8	2.50	0.45
1:1A:805:G:N2	1:1A:829:A:OP1	2.50	0.45
1:1A:2060:A:H3'	5:1F:63:LYS:NZ	2.31	0.45
12:1N:36:LEU:HD22	12:1N:121:LYS:HB2	1.98	0.45
6:1G:104:THR:HA	29:14:38:SER:HB3	1.98	0.45
1:1A:1514:G:O2'	1:1A:1557:C:O2'	2.24	0.45
1:1A:1:G:H2'	1:1A:2:G:H8	1.82	0.45
1:1A:560:C:O2'	19:1U:47:ARG:NH2	2.49	0.45
3:1D:51:ARG:HH12	3:1D:246:PRO:HG2	1.82	0.45
1:1A:1485:U:H2'	1:1A:1486:U:C6	2.50	0.45
1:1A:2400:G:H1	1:1A:2416:C:H42	1.64	0.45
1:1A:2615:U:C2	30:15:3:GLN:HA	2.51	0.45
1:1A:2651:C:H2'	1:1A:2652:C:H6	1.82	0.45
1:1A:395:U:H2'	1:1A:396:G:C8	2.52	0.45
1:1A:405:U:O4	3:1D:1:ALA:N	100.79	0.45
1:1A:876:C:H2'	1:1A:877:A:O4'	2.16	0.45
1:1A:972:A:OP2	1:1A:973:A:O2'	2.27	0.45
5:1F:189:THR:HG22	5:1F:191:ASP:H	1.80	0.45
1:1A:2251:OMG:H1'	1:1A:2251:OMG:HM22	1.62	0.45
1:1A:286:U:H2'	1:1A:287:G:C8	2.51	0.45
1:1A:355:U:H2'	1:1A:356:G:C8	2.51	0.45
1:1A:46:G:H2'	1:1A:47:C:C6	2.51	0.45
1:1A:764:A:H5'	3:1D:208:GLY:HA3	1.99	0.45
1:1A:801:G:C8	5:1F:50:ALA:HB2	2.51	0.45
12:1N:95:ARG:HG2	12:1N:96:ARG:HG2	1.97	0.45
14:1P:127:VAL:HG21	14:1P:142:ILE:HG21	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:17:24:THR:HG23	32:17:27:GLY:H	1.82	0.45
1:1A:126:A:N6	32:17:42:LEU:HD23	2.32	0.45
1:1A:1026:G:H2'	1:1A:1027:A:H8	1.81	0.45
1:1A:1326:U:H2'	1:1A:1327:A:C8	2.52	0.45
1:1A:1363:C:H2'	1:1A:1364:G:C8	2.50	0.45
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.52	0.45
1:1A:2622:U:O2'	1:1A:2825:G:N7	2.50	0.45
1:1A:519:U:H2'	1:1A:520:G:H8	1.81	0.45
2:1B:52:A:N6	17:1S:33:ARG:HB2	2.31	0.45
3:1D:203:VAL:O	3:1D:205:GLY:N	2.49	0.45
9:1I:113:SER:O	9:1I:116:ARG:NH1	2.36	0.45
10:1J:24:SER:HB2	10:1J:116:GLU:HG3	1.99	0.45
1:1A:1288:G:OP2	1:1A:1288:G:N2	2.30	0.45
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.16	0.45
1:1A:376:G:H2'	1:1A:377:G:C8	2.91	0.45
1:1A:819:A:H5'	1:1A:973:A:N1	2.31	0.45
4:1E:16:THR:OG1	4:1E:18:ASP:OD1	2.35	0.45
9:1I:108:VAL:HG12	9:1I:110:VAL:H	1.82	0.45
1:1A:1343:G:H4'	9:1I:123:ARG:HB2	77.65	0.45
11:1K:112:LYS:HE2	11:1K:128:ILE:HD13	1.99	0.45
1:1A:1422:G:OP1	13:1O:48:PRO:HG3	97.11	0.45
15:1Q:30:SER:N	15:1Q:105:MET:O	2.50	0.45
32:17:12:ARG:HE	32:17:44:VAL:HG21	1.81	0.45
1:1A:1103:A:H3'	1:1A:1104:C:H5''	1.98	0.45
1:1A:1882:U:H2'	1:1A:1883:U:C6	2.51	0.45
1:1A:2742:G:OP2	34:19:24:ARG:NH1	2.50	0.45
1:1A:1825:U:H1'	3:1D:252:LYS:HE3	1.98	0.45
4:1E:13:ARG:HH11	18:1T:55:HIS:HA	1.82	0.45
1:1A:1345:C:H2'	1:1A:1346:G:C8	2.52	0.45
1:1A:2236:U:H2'	1:1A:2237:G:O4'	2.17	0.45
1:1A:460:A:H62	1:1A:469:G:H21	1.64	0.45
1:1A:18:U:O2'	1:1A:554:U:OP1	2.35	0.45
1:1A:774:G:O2'	1:1A:777:G:N3	2.46	0.45
3:1D:52:HIS:HA	3:1D:216:ARG:HB3	1.98	0.45
5:1F:18:THR:HG23	5:1F:106:LYS:HG2	1.98	0.45
15:1Q:40:ARG:HB3	15:1Q:95:LEU:HD23	1.99	0.45
1:1A:1251:C:H5''	19:1U:5:ARG:NH2	2.32	0.45
1:1A:1434:A:H2'	1:1A:1435:G:C8	2.52	0.45
1:1A:1481:U:H2'	1:1A:1482:G:C8	7.06	0.45
1:1A:1783:A:N1	1:1A:2587:A:H2'	2.32	0.45
3:1D:154:ALA:HB2	3:1D:161:VAL:HG23	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2590:A:H5''	3:1D:237:ARG:NE	2.32	0.45
7:1H:37:ASN:OD1	7:1H:38:ASP:N	2.50	0.45
11:1K:101:SER:HA	11:1K:140:GLU:H	1.82	0.45
24:1Z:2:PHE:O	24:1Z:62:THR:OG1	2.26	0.45
27:12:10:SER:HA	27:12:13:GLU:HG2	1.99	0.44
1:1A:171:U:H2'	1:1A:172:A:C8	2.52	0.44
1:1A:1813:G:O6	1:1A:1814:G:N1	2.50	0.44
3:1D:70:LYS:HD2	3:1D:73:ILE:HD12	1.98	0.44
7:1H:97:VAL:HG22	7:1H:102:ILE:HG23	1.98	0.44
1:1A:1046:A:H62	10:1J:4:ASN:HD21	1.65	0.44
1:1A:1410:G:H2'	1:1A:1411:U:C6	2.53	0.44
1:1A:1506:U:H2'	1:1A:1507:C:C6	2.52	0.44
1:1A:1475:G:H4'	1:1A:1689:A:H4'	68.47	0.44
1:1A:1721:G:HO2'	1:1A:1722:A:H8	1.60	0.44
1:1A:1849:G:H2'	1:1A:1850:G:H8	1.82	0.44
1:1A:961:C:O2	1:1A:2031:A:N6	2.50	0.44
1:1A:2328:A:H2'	1:1A:2329:U:C6	2.52	0.44
1:1A:320:A:H4'	1:1A:322:A:N7	2.32	0.44
3:1D:83:ASP:HB3	3:1D:86:ARG:HB2	1.98	0.44
4:1E:55:LYS:HE2	4:1E:77:ARG:HA	1.99	0.44
15:1Q:42:THR:HG22	15:1Q:93:VAL:HG12	2.00	0.44
1:1A:574:A:H2	1:1A:2032:G:O2'	2.00	0.44
1:1A:2893:A:H4'	1:1A:2894:G:C4	2.52	0.44
1:1A:554:U:H2'	1:1A:555:G:O4'	2.17	0.44
7:1H:68:ARG:HH12	7:1H:72:ASN:HD22	1.65	0.44
10:1J:78:GLY:N	10:1J:79:PRO:HD2	2.31	0.44
1:1A:1130:U:O2'	1:1A:1131:G:OP1	2.29	0.44
1:1A:2674:G:H2'	1:1A:2675:A:C8	2.53	0.44
1:1A:277:G:H4'	1:1A:278:A:N7	2.33	0.44
1:1A:2808:G:H2'	1:1A:2890:G:O6	2.18	0.44
1:1A:1791:A:H5''	3:1D:204:LEU:HD12	1.99	0.44
12:1N:36:LEU:O	12:1N:51:GLY:HA3	2.18	0.44
15:1Q:105:MET:HB2	15:1Q:117:PHE:CZ	2.53	0.44
20:1V:79:ARG:O	20:1V:81:LYS:N	2.44	0.44
1:1A:1940:U:H4'	1:1A:1941:C:O5'	2.16	0.44
1:1A:1361:G:HO2'	1:1A:2215:C:HO2'	1.62	0.44
2:1B:65:U:H3'	2:1B:108:A:H61	1.82	0.44
1:1A:1061:U:N3	11:1K:11:GLN:O	2.50	0.44
20:1V:68:ARG:NH1	20:1V:90:ARG:HB2	2.33	0.44
23:1Y:3:LYS:HD3	23:1Y:82:VAL:HB	1.98	0.44
1:1A:1022:G:H1'	1:1A:1023:U:OP2	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2032:G:N2	4:1E:151:THR:OG1	2.50	0.44
1:1A:2061:G:H5''	1:1A:2503:2MA:HM22	2.00	0.44
1:1A:2297:A:OP2	1:1A:2297:A:H8	2.00	0.44
1:1A:2335:A:H2'	1:1A:2336:A:H2'	1.99	0.44
1:1A:2624:G:H2'	1:1A:2625:G:H8	1.83	0.44
1:1A:944:C:H5''	1:1A:945:A:H5'	1.99	0.44
1:1A:2599:G:N7	3:1D:234:GLY:HA2	2.32	0.44
14:1P:90:VAL:HB	14:1P:122:VAL:HA	1.99	0.44
21:1W:6:LYS:HA	21:1W:104:THR:HA	1.99	0.44
1:1A:1401:G:H8	1:1A:1401:G:O5'	2.61	0.44
1:1A:174:U:H2'	1:1A:175:G:C8	2.53	0.44
1:1A:2068:U:H5'	1:1A:2069:G7M:OP1	2.18	0.44
3:1D:204:LEU:HD21	3:1D:213:ARG:HH21	1.83	0.44
4:1E:33:ARG:HD3	4:1E:73:VAL:HB	2.00	0.44
28:13:10:ARG:NH2	28:13:52:PHE:O	2.51	0.44
1:1A:1612:C:H4'	32:17:7:PRO:HD3	1.99	0.44
1:1A:1869:G:H2'	1:1A:1871:A:OP1	2.17	0.44
1:1A:1931:U:H2'	1:1A:1932:A:H8	1.81	0.44
1:1A:2772:C:H5'	4:1E:173:GLN:HE21	1.83	0.44
2:1B:118:C:H2'	2:1B:119:A:C8	2.53	0.44
1:1A:2052:A:O2'	4:1E:149:ASN:O	2.35	0.44
1:1A:1653:G:O6	16:1R:11:ASN:N	2.51	0.44
33:18:36:ALA:HB3	33:18:39:ARG:HG3	2.00	0.44
1:1A:1795:C:O2'	1:1A:1901:A:OP2	2.24	0.44
1:1A:2544:G:H2'	1:1A:2545:G:H8	1.83	0.44
1:1A:674:G:H2'	1:1A:675:A:C8	4.71	0.44
1:1A:775:G:H2'	1:1A:776:G:H8	6.70	0.44
3:1D:131:MET:HG2	3:1D:134:ILE:HD12	1.99	0.44
6:1G:116:LEU:HD23	6:1G:127:TYR:OH	2.18	0.44
2:1B:54:G:N2	6:1G:25:MET:SD	2.85	0.44
6:1G:39:VAL:HG23	6:1G:149:ARG:HD3	2.00	0.44
15:1Q:50:ARG:HD2	15:1Q:65:ILE:HD11	2.00	0.44
1:1A:1278:C:H2'	1:1A:1279:G:C8	2.53	0.43
1:1A:1307:A:N6	1:1A:1606:C:O2'	2.51	0.43
1:1A:1316:U:H2'	1:1A:1317:G:C8	2.52	0.43
1:1A:1682:G:C5	1:1A:1757:A:H1'	2.52	0.43
1:1A:1799:G:P	1:1A:1819:A:H61	2.41	0.43
1:1A:736:C:H2'	1:1A:737:C:C6	2.81	0.43
1:1A:780:G:N2	3:1D:228:ASP:OD2	2.48	0.43
5:1F:102:ARG:HH12	5:1F:201:ALA:HB3	1.83	0.43
10:1J:107:GLU:O	10:1J:109:LYS:N	2.48	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1N:28:LEU:O	12:1N:32:LEU:HG	2.18	0.43
1:1A:1652:A:N6	16:1R:11:ASN:OD1	2.49	0.43
22:1X:6:ARG:O	22:1X:10:VAL:HG23	2.18	0.43
29:14:44:PHE:CD1	29:14:45:THR:HG23	2.53	0.43
1:1A:330:A:H1'	1:1A:1210:G:C6	2.53	0.43
1:1A:1382:G:H4'	1:1A:1573:G:C2	2.52	0.43
1:1A:1613:G:C2	1:1A:1617:C:C2	3.05	0.43
1:1A:690:G:H1	1:1A:772:C:N4	2.10	0.43
20:1V:79:ARG:C	20:1V:81:LYS:H	2.21	0.43
1:1A:1419:A:H61	1:1A:1494:A:H61	1.65	0.43
1:1A:160:A:H2'	1:1A:161:A:O4'	2.73	0.43
1:1A:1681:G:H1'	1:1A:1762:A:H2'	2.01	0.43
1:1A:2756:U:H1'	1:1A:2757:A:H5''	2.01	0.43
1:1A:82:U:O4	1:1A:83:A:N6	2.52	0.43
1:1A:951:C:H2'	1:1A:952:G:C8	2.53	0.43
6:1G:35:LEU:HD21	6:1G:98:PHE:CZ	2.53	0.43
1:1A:1248:G:C6	19:1U:2:ARG:HD2	2.53	0.43
23:1Y:70:ALA:HB3	23:1Y:79:ALA:HB1	2.00	0.43
6:1G:139:GLU:HA	29:14:28:VAL:HG22	2.00	0.43
1:1A:1268:A:H62	1:1A:2012:G:H21	1.64	0.43
1:1A:1909:C:H2'	1:1A:1910:G:H8	1.84	0.43
1:1A:2059:A:H2'	1:1A:2503:2MA:HM23	2.00	0.43
1:1A:2681:C:OP2	4:1E:114:LYS:NZ	2.52	0.43
1:1A:2747:G:H1	1:1A:2754:U:H2'	1.83	0.43
1:1A:2755:C:O2'	1:1A:2756:U:H2'	2.18	0.43
1:1A:283:G:H1	1:1A:357:C:H42	1.65	0.43
4:1E:131:ASP:O	4:1E:136:ASN:ND2	2.44	0.43
4:1E:4:LEU:HB2	4:1E:101:PHE:CZ	2.53	0.43
5:1F:32:VAL:HG21	14:1P:3:LEU:HD11	2.00	0.43
10:1J:23:LEU:HB3	10:1J:87:GLU:OE1	2.19	0.43
13:1O:16:ALA:HB3	13:1O:86:LEU:HD11	2.01	0.43
14:1P:14:LYS:O	14:1P:16:GLY:N	2.51	0.43
19:1U:95:ALA:O	19:1U:99:VAL:HG23	2.18	0.43
21:1W:83:LYS:HG2	21:1W:95:ARG:NH1	2.34	0.43
1:1A:107:G:O3'	1:1A:293:U:O2'	2.36	0.43
1:1A:110:G:H2'	1:1A:111:A:H8	1.83	0.43
1:1A:1346:G:H2'	1:1A:1347:A:H8	1.83	0.43
1:1A:193:U:H2'	1:1A:194:G:H8	1.84	0.43
1:1A:2463:C:H2'	1:1A:2464:G:C8	2.53	0.43
1:1A:953:G:H2'	1:1A:954:G:C8	2.48	0.43
9:1I:115:VAL:HG21	10:1J:62:ARG:HB2	190.14	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1O:61:VAL:HG21	13:1O:112:PHE:CE1	2.53	0.43
1:1A:1099:G:H2'	1:1A:1100:C:O4'	2.87	0.43
1:1A:1365:A:OP2	26:11:2:ARG:N	2.41	0.43
1:1A:1809:A:H2'	1:1A:1810:A:C8	2.54	0.43
1:1A:755:U:H2'	1:1A:756:A:C8	2.54	0.43
4:1E:133:THR:HG23	4:1E:134:HIS:CD2	2.53	0.43
1:1A:2787:C:H1'	4:1E:63:PRO:HG3	2.00	0.43
4:1E:9:VAL:O	4:1E:26:VAL:HB	2.18	0.43
21:1W:77:ASP:N	21:1W:77:ASP:OD1	2.50	0.43
1:1A:1005:C:H2'	1:1A:1006:C:H6	1.82	0.43
1:1A:1318:U:H2'	1:1A:1319:C:C6	2.54	0.43
1:1A:1365:A:O5'	26:11:27:ARG:NH2	2.49	0.43
1:1A:20:C:H2'	1:1A:21:A:C8	2.53	0.43
1:1A:2410:G:H2'	1:1A:2411:A:O4'	2.19	0.43
1:1A:593:U:H2'	1:1A:594:U:C6	2.54	0.43
4:1E:121:THR:HG23	4:1E:162:ALA:HB2	2.01	0.43
4:1E:116:LYS:HB3	4:1E:123:LYS:HZ1	1.82	0.43
4:1E:157:LYS:O	12:1N:81:ILE:HB	2.17	0.43
19:1U:20:ALA:HA	19:1U:23:TYR:CE2	2.53	0.43
1:1A:591:U:H1'	33:18:1:PRO:H2	1.83	0.43
1:1A:1301:A:H2'	1:1A:1301:A:N3	2.34	0.43
1:1A:1683:U:H2'	1:1A:1684:G:C8	2.53	0.43
1:1A:1790:C:OP2	1:1A:1828:G:N1	2.47	0.43
1:1A:2710:C:H2'	1:1A:2711:A:C8	2.54	0.43
1:1A:281:C:H2'	1:1A:282:A:H8	1.84	0.43
1:1A:714:U:N3	1:1A:717:C:OP2	2.50	0.43
6:1G:92:GLY:O	6:1G:95:MET:HG2	2.19	0.43
7:1H:88:LEU:HG	7:1H:161:VAL:HG22	2.01	0.43
13:1O:29:HIS:HE1	13:1O:31:ARG:HH12	1.63	0.43
1:1A:456:C:H2'	22:1X:73:ARG:HH22	1.82	0.43
26:11:37:PHE:HZ	26:11:55:MET:HG2	1.84	0.43
32:17:34:ARG:HB2	32:17:42:LEU:HD12	2.01	0.43
1:1A:1340:U:H4'	1:1A:1394:U:O2'	2.19	0.43
1:1A:1491:G:H2'	1:1A:1492:G:C8	2.53	0.43
1:1A:155:A:H2'	1:1A:156:A:C8	2.54	0.43
1:1A:1595:C:H2'	1:1A:1596:A:C8	2.54	0.43
1:1A:1882:U:H2'	1:1A:1883:U:H6	1.84	0.43
1:1A:190:A:H5''	1:1A:204:A:N6	2.30	0.43
1:1A:2353:G:H2'	1:1A:2354:C:O4'	2.19	0.43
1:1A:2061:G:H2'	1:1A:2501:C:O2'	2.19	0.43
1:1A:2630:G:H2'	1:1A:2631:G:C8	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:603:A:N6	1:1A:655:A:O4'	2.51	0.43
1:1A:209:C:H4'	1:1A:681:G:H4'	1.99	0.43
3:1D:209:ALA:HA	3:1D:212:TRP:CZ2	2.54	0.43
10:1J:26:VAL:HG21	10:1J:114:GLU:HG2	2.01	0.43
10:1J:79:PRO:O	10:1J:80:THR:OG1	2.30	0.43
1:1A:831:G:O2'	14:1P:38:GLN:OE1	2.35	0.43
28:13:43:ILE:O	28:13:47:ILE:HG13	2.19	0.43
1:1A:1020:A:H4'	1:1A:1021:A:O5'	2.18	0.43
1:1A:1213:A:N6	1:1A:1236:G:H1'	2.34	0.43
1:1A:1565:C:O2'	1:1A:1566:A:H8	2.02	0.43
1:1A:16:C:H2'	1:1A:17:G:H8	1.84	0.43
1:1A:1834:U:O2'	1:1A:1969:A:H3'	2.18	0.43
1:1A:221:A:N1	1:1A:265:A:O2'	2.48	0.43
1:1A:2591:C:C2	1:1A:2592:G:C8	3.07	0.43
1:1A:2073:C:O2'	1:1A:2598:A:O2'	2.32	0.43
1:1A:2630:G:H2'	1:1A:2631:G:H8	1.84	0.43
1:1A:319:G:H2'	1:1A:320:A:C8	3.33	0.43
1:1A:537:G:H4'	12:1N:5:THR:HG21	2.00	0.43
1:1A:832:U:P	14:1P:38:GLN:H	2.41	0.43
16:1R:49:GLU:HB2	16:1R:50:PRO:HD3	2.00	0.43
21:1W:88:ARG:HA	21:1W:88:ARG:HD2	1.76	0.43
1:1A:1183:U:H2'	1:1A:1184:U:C6	2.53	0.42
1:1A:2140:G:H2'	1:1A:2141:G:C8	2.53	0.42
1:1A:2200:C:H2'	1:1A:2201:G:H8	1.83	0.42
1:1A:2437:G:O2'	1:1A:2599:G:H4'	2.19	0.42
1:1A:404:A:H1'	1:1A:406:G:C4	2.54	0.42
1:1A:934:U:H2'	1:1A:935:C:C6	2.54	0.42
12:1N:74:TYR:HE2	12:1N:89:PHE:HD1	1.68	0.42
16:1R:48:VAL:O	16:1R:52:ILE:HG13	2.19	0.42
21:1W:84:ARG:HB2	21:1W:96:ILE:HG13	2.01	0.42
25:10:42:HIS:CD2	25:10:73:ARG:HD3	2.54	0.42
26:11:4:CYS:HB3	26:11:8:GLY:H	1.84	0.42
1:1A:2539:C:H5'	34:19:3:VAL:HG11	2.01	0.42
1:1A:1336:A:H2'	1:1A:1337:G:C8	2.54	0.42
1:1A:1539:U:H2'	1:1A:1540:G:C8	2.53	0.42
1:1A:1565:C:O2'	1:1A:1566:A:H2'	2.19	0.42
1:1A:2137:U:H2'	1:1A:2138:G:C8	2.54	0.42
1:1A:27:G:N2	1:1A:512:G:H1'	2.33	0.42
6:1G:137:PHE:HA	6:1G:138:PRO:HD3	1.91	0.42
9:1I:9:VAL:HG12	9:1I:11:ASN:H	1.82	0.42
16:1R:69:ARG:O	16:1R:71:ARG:N	2.47	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:776:G:N2	1:1A:2072:C:H5'	2.16	0.42
1:1A:2872:A:H2'	1:1A:2873:A:C8	2.54	0.42
1:1A:372:G:O2'	1:1A:373:U:O5'	2.31	0.42
1:1A:438:G:H2'	1:1A:439:A:H8	1.84	0.42
1:1A:596:U:H2'	1:1A:597:G:H8	1.84	0.42
1:1A:643:A:N1	1:1A:2369:A:O2'	2.49	0.42
1:1A:671:C:H2'	1:1A:672:C:C6	2.55	0.42
5:1F:151:GLY:N	5:1F:192:ALA:HB2	2.33	0.42
1:1A:2746:U:H1'	7:1H:138:GLN:HE22	1.85	0.42
13:1O:104:THR:HG22	13:1O:106:GLU:H	1.84	0.42
21:1W:4:ILE:HD12	21:1W:6:LYS:HE3	2.01	0.42
1:1A:1272:A:O2'	1:1A:1274:A:OP1	2.29	0.42
1:1A:1592:C:H2'	1:1A:1593:A:C8	2.55	0.42
1:1A:1822:C:H2'	1:1A:1823:G:C8	2.55	0.42
1:1A:1833:C:O2'	1:1A:1969:A:N1	2.37	0.42
1:1A:2052:A:H2'	1:1A:2053:G:C8	2.54	0.42
1:1A:2286:G:H4'	1:1A:2287:A:O4'	2.19	0.42
1:1A:2687:U:H2'	1:1A:2688:G:O4'	2.20	0.42
1:1A:2884:U:H2'	1:1A:2885:G:C8	2.54	0.42
1:1A:375:G:H2'	1:1A:376:G:C8	2.54	0.42
1:1A:402:A:H2'	1:1A:403:U:O4'	2.19	0.42
1:1A:563:A:N6	1:1A:577:G:O6	2.52	0.42
3:1D:222:THR:O	3:1D:232:GLY:HA2	2.19	0.42
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.54	0.42
3:1D:7:PRO:HB3	3:1D:13:ARG:HG3	2.00	0.42
4:1E:2:ILE:HD13	4:1E:48:ILE:HD11	2.01	0.42
9:1I:25:TYR:O	9:1I:29:PHE:HB3	2.19	0.42
14:1P:62:PRO:HG2	33:18:24:LYS:HB3	2.02	0.42
15:1Q:50:ARG:CD	15:1Q:65:ILE:HD11	2.50	0.42
21:1W:44:ALA:HA	21:1W:47:VAL:HG12	2.01	0.42
30:15:42:ILE:HG22	30:15:48:TYR:HB2	2.01	0.42
1:1A:1020:A:H1'	1:1A:1021:A:OP2	2.20	0.42
1:1A:1442:U:H2'	1:1A:1443:U:C6	2.54	0.42
1:1A:1744:A:H3'	1:1A:1745:A:H8	1.83	0.42
1:1A:1939:5MU:OP1	1:1A:2604:PSU:O2'	2.35	0.42
1:1A:2103:C:H2'	1:1A:2104:C:C6	2.55	0.42
1:1A:2192:U:H2'	1:1A:2193:G:C8	2.55	0.42
1:1A:288:U:H2'	1:1A:289:G:H8	1.85	0.42
1:1A:326:G:H2'	1:1A:327:G:H8	1.84	0.42
1:1A:52:A:OP2	1:1A:52:A:H8	2.02	0.42
1:1A:668:A:N3	1:1A:670:A:N6	2.68	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:858:G:O2'	1:1A:859:G:OP1	2.33	0.42
5:1F:70:SER:HB2	5:1F:78:TRP:HZ2	1.85	0.42
9:1I:30:LEU:HB3	9:1I:36:ALA:HB3	2.01	0.42
10:1J:18:VAL:HG11	10:1J:70:GLU:HB3	2.00	0.42
31:16:7:LYS:HA	31:16:23:THR:HA	2.00	0.42
34:19:7:VAL:HG11	34:19:37:GLN:O	2.20	0.42
1:1A:1326:U:H2'	1:1A:1327:A:H8	1.85	0.42
1:1A:1675:C:H2'	1:1A:1676:A:O4'	2.18	0.42
1:1A:1549:A:O3'	1:1A:1740:G:N2	2.53	0.42
1:1A:929:U:H4'	28:13:37:ARG:NH2	2.35	0.42
5:1F:131:THR:HG22	5:1F:160:ALA:HA	2.02	0.42
6:1G:7:TYR:HB2	6:1G:172:PHE:HZ	1.84	0.42
12:1N:64:VAL:HB	12:1N:68:LYS:HE3	2.01	0.42
16:1R:59:SER:OG	16:1R:62:ASN:OD1	2.24	0.42
23:1Y:36:GLU:HA	23:1Y:61:GLU:HG2	2.00	0.42
26:11:39:VAL:HG22	26:11:63:ILE:HG12	2.02	0.42
1:1A:262:A:H2'	1:1A:263:G:O4'	2.19	0.42
1:1A:381:G:H2'	1:1A:382:A:C8	2.55	0.42
1:1A:970:U:C2	1:1A:971:G:C8	3.08	0.42
33:18:30:HIS:ND1	33:18:31:ILE:HG13	2.35	0.42
1:1A:2008:C:H2'	1:1A:2009:A:C8	2.55	0.42
1:1A:2020:A:N6	1:1A:2034:U:H3	2.16	0.42
1:1A:468:G:O6	32:17:39:ARG:NH2	2.47	0.42
1:1A:745:1MG:HN21	1:1A:745:1MG:HM11	1.73	0.42
3:1D:43:ASN:HB3	3:1D:49:THR:HG21	2.01	0.42
5:1F:147:LEU:HB2	5:1F:183:PHE:CD2	2.55	0.42
9:1I:93:SER:HB3	9:1I:121:VAL:HB	2.01	0.42
17:1S:51:ALA:HB3	17:1S:78:VAL:HG22	2.01	0.42
23:1Y:23:LYS:O	23:1Y:35:VAL:HG13	2.20	0.42
1:1A:2619:C:H2'	1:1A:2620:C:H6	1.84	0.42
12:1N:69:ARG:HA	12:1N:89:PHE:HD2	1.85	0.42
1:1A:300:A:P	23:1Y:81:ARG:HH12	2.42	0.42
1:1A:1801:A:H5''	1:1A:2203:U:H2'	2.02	0.41
1:1A:674:G:H1	1:1A:806:C:H42	1.67	0.41
1:1A:774:G:N2	1:1A:787:C:O2'	2.53	0.41
1:1A:873:C:H2'	1:1A:874:G:C8	2.54	0.41
5:1F:148:ILE:HB	5:1F:169:VAL:HG22	2.00	0.41
13:1O:41:ILE:HG13	13:1O:58:LEU:O	2.20	0.41
15:1Q:53:MET:HB3	15:1Q:120:ALA:HB2	2.01	0.41
19:1U:97:ILE:HG22	19:1U:105:PHE:HB2	2.02	0.41
1:1A:1054:A:OP1	10:1J:31:ARG:NH1	2.45	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1265:A:N1	1:1A:2013:A:H5''	2.35	0.41
1:1A:1407:G:H2'	1:1A:1408:G:C8	2.54	0.41
1:1A:1428:C:C4	1:1A:1569:A:H5''	2.55	0.41
1:1A:1589:U:H2'	1:1A:1590:A:C8	2.55	0.41
1:1A:1909:C:H2'	1:1A:1910:G:C8	2.55	0.41
1:1A:2427:C:H5'	1:1A:2429:G:H5'	2.02	0.41
1:1A:2544:G:H2'	1:1A:2545:G:C8	2.55	0.41
1:1A:672:C:H5	14:1P:42:SER:HB2	1.85	0.41
1:1A:806:C:H3'	14:1P:41:ARG:HH11	1.85	0.41
1:1A:848:C:H2'	1:1A:849:A:C8	2.56	0.41
4:1E:136:ASN:OD1	4:1E:137:SER:N	2.53	0.41
12:1N:17:VAL:HG22	12:1N:55:ILE:HB	2.02	0.41
12:1N:44:TYR:O	19:1U:63:ARG:NE	2.52	0.41
22:1X:80:TRP:CZ3	22:1X:82:LYS:HD2	2.55	0.41
1:1A:2466:C:OP1	34:19:4:ARG:HB3	2.20	0.41
1:1A:121:G:H4'	1:1A:149:A:H5'	2.02	0.41
1:1A:1320:C:O2'	1:1A:1321:A:H5''	2.21	0.41
1:1A:1592:C:H2'	1:1A:1593:A:H8	1.84	0.41
1:1A:224:U:O4	1:1A:419:U:O2'	2.38	0.41
1:1A:2430:A:H5'	1:1A:2431:U:OP2	2.20	0.41
1:1A:2619:C:H2'	1:1A:2620:C:C6	2.55	0.41
1:1A:2674:G:H2'	1:1A:2675:A:H8	1.85	0.41
1:1A:281:C:H2'	1:1A:282:A:C8	2.54	0.41
1:1A:2863:C:H2'	1:1A:2864:G:H8	1.85	0.41
1:1A:279:A:N6	1:1A:361:G:H1'	2.35	0.41
1:1A:729:G:N3	1:1A:729:G:H3'	2.35	0.41
3:1D:60:ALA:HB3	3:1D:62:ARG:HH12	1.85	0.41
10:1J:25:ALA:HB2	10:1J:96:PHE:CD1	2.55	0.41
12:1N:37:ARG:HD3	12:1N:39:LYS:HD2	2.01	0.41
23:1Y:32:LYS:HB3	23:1Y:63:ALA:HB1	2.02	0.41
24:1Z:10:LYS:HG3	24:1Z:11:GLU:HG3	2.02	0.41
24:1Z:4:ILE:HD13	24:1Z:47:VAL:HG22	2.02	0.41
1:1A:1013:C:H2'	1:1A:1014:A:C8	2.53	0.41
1:1A:145:C:H2'	1:1A:146:A:C8	2.55	0.41
1:1A:185:G:H2'	1:1A:186:G:C8	2.55	0.41
1:1A:196:A:N1	14:1P:50:PHE:HZ	2.18	0.41
1:1A:952:G:O2'	1:1A:2267:A:H1'	2.21	0.41
1:1A:2408:U:H2'	1:1A:2409:G:H8	1.85	0.41
1:1A:689:A:N3	1:1A:779:U:O2'	2.52	0.41
1:1A:764:A:H2	3:1D:217:PRO:HG2	1.85	0.41
5:1F:40:ARG:HG2	5:1F:42:GLY:H	1.84	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:28:ALA:H	10:1J:110:ALA:HA	1.85	0.41
14:1P:96:LYS:HG3	14:1P:102:GLY:O	2.20	0.41
14:1P:62:PRO:HB2	33:18:29:ARG:NH1	2.25	0.41
28:13:46:MET:O	28:13:50:VAL:HG22	2.21	0.41
14:1P:64:PHE:CZ	33:18:23:HIS:HA	2.56	0.41
1:1A:1346:G:H2'	1:1A:1347:A:C8	2.55	0.41
1:1A:184:C:H2'	1:1A:185:G:C8	2.56	0.41
1:1A:2004:G:H2'	1:1A:2005:A:O4'	2.20	0.41
1:1A:2143:C:H2'	1:1A:2144:G:C8	2.55	0.41
1:1A:2291:U:H2'	1:1A:2292:U:C6	2.55	0.41
1:1A:246:C:N4	33:18:7:ARG:HG3	2.36	0.41
1:1A:2676:C:H2'	1:1A:2677:G:C8	2.54	0.41
1:1A:2788:C:H2'	1:1A:2789:C:C6	2.55	0.41
1:1A:563:A:H61	1:1A:884:U:H3	104.99	0.41
1:1A:974:G:H1'	1:1A:975:A:C8	2.56	0.41
3:1D:28:PRO:HG3	3:1D:62:ARG:NH2	2.35	0.41
5:1F:3:LEU:HD21	5:1F:19:PHE:CE2	2.55	0.41
15:1Q:40:ARG:H	15:1Q:40:ARG:HG2	1.40	0.41
15:1Q:71:LYS:HB3	15:1Q:93:VAL:O	2.20	0.41
24:1Z:56:PHE:CE1	24:1Z:61:LEU:HD21	2.56	0.41
26:11:11:PRO:HG3	26:11:30:PRO:HD2	2.03	0.41
1:1A:141:G:N2	1:1A:142:A:N3	2.69	0.41
1:1A:2048:G:H2'	1:1A:2049:G:O4'	2.21	0.41
1:1A:310:A:H2'	1:1A:311:A:H5''	2.02	0.41
1:1A:322:A:H5'	1:1A:340:A:H1'	2.03	0.41
1:1A:33:C:O2	1:1A:447:A:N6	2.53	0.41
1:1A:580:U:H2'	1:1A:581:C:C6	2.56	0.41
1:1A:739:A:N3	1:1A:740:C:N4	2.69	0.41
1:1A:768:G:C6	1:1A:769:U:C4	3.09	0.41
1:1A:841:G:C2	1:1A:842:U:C2	3.09	0.41
12:1N:24:THR:HB	12:1N:27:ARG:HB2	2.02	0.41
16:1R:103:ARG:HG2	16:1R:105:GLY:H	1.84	0.41
16:1R:56:LYS:NZ	16:1R:88:ALA:HA	2.35	0.41
18:1T:102:ARG:HD3	18:1T:106:ALA:HB1	2.01	0.41
1:1A:1808:A:C6	26:11:27:ARG:HD2	2.56	0.41
1:1A:1080:A:H1'	11:1K:127:SER:HA	2.01	0.41
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.56	0.41
1:1A:975:A:H62	1:1A:988:A:H2	1.69	0.41
1:1A:923:G:H4'	25:10:25:GLU:HG3	2.01	0.41
29:14:9:TYR:CE2	29:14:25:ARG:HD3	2.56	0.41
1:1A:1131:G:N2	1:1A:1132:U:O4	2.45	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1291:C:H2'	1:1A:1292:G:C8	2.54	0.41
1:1A:2052:A:C2	1:1A:2618:G:H1'	2.56	0.41
1:1A:2283:C:C5	1:1A:2389:G:H2'	2.55	0.41
1:1A:2623:G:H2'	1:1A:2624:G:H8	1.86	0.41
1:1A:2624:G:H2'	1:1A:2625:G:C8	2.56	0.41
1:1A:825:A:H2'	1:1A:826:U:C6	2.56	0.41
3:1D:77:VAL:HG13	3:1D:91:ALA:HB1	2.02	0.41
16:1R:78:LYS:HE2	16:1R:83:LEU:HD21	2.01	0.41
22:1X:23:ALA:HB1	22:1X:29:THR:HB	2.02	0.41
1:1A:1351:C:H2'	1:1A:1352:U:C6	2.56	0.41
1:1A:179:C:H2'	1:1A:180:G:H8	1.85	0.41
1:1A:2060:A:C6	1:1A:2502:G:C2	3.09	0.41
3:1D:177:SER:O	3:1D:270:ARG:HG3	2.21	0.41
4:1E:148:GLN:HB2	4:1E:152:PRO:HG2	2.03	0.41
9:1I:121:VAL:HG23	9:1I:123:ARG:HG3	2.03	0.41
21:1W:84:ARG:HG3	21:1W:98:LYS:HE3	2.02	0.41
1:1A:2355:G:H1'	25:10:32:ILE:HD12	2.03	0.41
1:1A:1530:G:N2	1:1A:1542:U:H1'	2.36	0.41
1:1A:198:C:H1'	1:1A:2434:A:N6	2.27	0.41
1:1A:2365:G:H4'	25:10:56:PHE:CZ	2.55	0.41
1:1A:481:G:OP1	1:1A:481:G:H4'	2.21	0.41
1:1A:647:G:N2	1:1A:2350:C:O3'	2.54	0.41
1:1A:812:C:H2'	1:1A:813:U:H6	1.86	0.41
11:1K:11:GLN:NE2	11:1K:56:VAL:HG12	2.36	0.41
14:1P:118:THR:O	14:1P:120:VAL:N	2.54	0.41
1:1A:2068:U:H6	1:1A:2068:U:H5''	1.86	0.41
1:1A:2137:U:H2'	1:1A:2138:G:H8	1.86	0.41
7:1H:136:ASP:OD2	7:1H:138:GLN:HB3	2.21	0.41
11:1K:80:LYS:O	11:1K:84:GLY:N	2.54	0.41
1:1A:117:G:O6	1:1A:289:G:H1'	45.19	0.40
1:1A:817:C:H42	1:1A:1190:G:H1	1.69	0.40
1:1A:1429:G:H2'	1:1A:1430:G:C8	2.56	0.40
1:1A:1689:A:H2'	1:1A:1690:A:C8	2.56	0.40
1:1A:1915:3TD:H3'	1:1A:1916:A:H8	1.86	0.40
1:1A:1:G:H1	1:1A:2902:C:N4	2.17	0.40
1:1A:562:U:H2'	1:1A:572:A:O4'	2.21	0.40
1:1A:720:U:H2'	1:1A:721:A:H8	1.85	0.40
1:1A:759:G:H2'	1:1A:760:G:H8	1.86	0.40
3:1D:52:HIS:CE1	3:1D:218:THR:HA	2.56	0.40
16:1R:79:LEU:O	16:1R:81:ASN:N	2.49	0.40
18:1T:47:ILE:HB	18:1T:96:LEU:HB2	2.03	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1X:15:HIS:HE1	22:1X:17:SER:HB3	1.85	0.40
24:1Z:72:VAL:HB	24:1Z:91:PHE:HB3	2.03	0.40
25:10:49:CYS:SG	25:10:53:HIS:HA	2.60	0.40
33:18:31:ILE:O	33:18:35:LYS:NZ	2.44	0.40
1:1A:110:G:H2'	1:1A:111:A:C8	2.56	0.40
1:1A:1132:U:H2'	1:1A:1133:A:C8	2.57	0.40
1:1A:1448:G:H2'	1:1A:1449:G:C8	2.56	0.40
1:1A:729:G:H2'	1:1A:1775:U:H1'	2.03	0.40
1:1A:182:A:H2'	1:1A:183:C:C6	2.55	0.40
1:1A:1958:C:H2'	1:1A:1959:G:H8	1.86	0.40
1:1A:1827:U:OP1	1:1A:1971:U:H4'	2.21	0.40
1:1A:2146:C:H4'	1:1A:2147:A:C4	2.56	0.40
1:1A:2333:A:H4'	1:1A:2334:U:O5'	2.21	0.40
1:1A:372:G:H4'	1:1A:373:U:H5'	2.03	0.40
1:1A:827:U:OP2	1:1A:828:U:N3	2.55	0.40
1:1A:558:U:OP2	12:1N:113:PRO:HD2	2.22	0.40
24:1Z:20:LEU:HD11	24:1Z:41:GLU:HG3	2.03	0.40
1:1A:2080:A:OP1	26:11:19:HIS:HB3	2.21	0.40
27:12:26:PHE:HD1	27:12:29:ARG:NH1	2.20	0.40
1:1A:323:C:H2'	1:1A:1205:A:N1	2.37	0.40
1:1A:1654:A:H2'	1:1A:1655:A:C8	2.56	0.40
1:1A:1874:C:H2'	1:1A:1875:G:O4'	2.21	0.40
1:1A:2343:U:O2'	1:1A:2373:G:O2'	2.30	0.40
1:1A:269:C:H2'	1:1A:270:A:C8	2.50	0.40
1:1A:2848:G:O2'	1:1A:2868:A:N6	2.54	0.40
1:1A:376:G:H2'	1:1A:377:G:H8	2.05	0.40
1:1A:481:G:O2'	1:1A:506:G:N2	2.54	0.40
1:1A:814:C:H1'	1:1A:1225:G:H21	1.86	0.40
1:1A:873:C:H2'	1:1A:874:G:H8	1.87	0.40
1:1A:96:C:H2'	1:1A:97:C:C6	2.57	0.40
3:1D:145:MET:HG2	3:1D:152:GLN:HG3	2.04	0.40
4:1E:37:VAL:HG23	4:1E:92:VAL:HG22	2.02	0.40
1:1A:2093:G:OP2	9:1I:22:LYS:HD3	2.21	0.40
12:1N:109:LEU:HD22	12:1N:118:MET:SD	2.61	0.40
1:1A:2849:U:OP1	18:1T:92:ARG:HB2	2.22	0.40
1:1A:1614:A:N1	21:1W:87:PRO:HA	2.36	0.40
24:1Z:31:TYR:HB3	24:1Z:37:PRO:HB3	2.02	0.40
1:1A:1040:A:H2'	1:1A:1041:G:C8	2.56	0.40
1:1A:1289:C:H2'	1:1A:1290:C:C6	2.56	0.40
1:1A:2050:C:N4	1:1A:2051:A:N1	2.69	0.40
1:1A:2200:C:H2'	1:1A:2201:G:C8	2.57	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2241:A:H2'	1:1A:2242:G:C8	2.56	0.40
1:1A:2399:G:H2'	1:1A:2400:G:C8	2.57	0.40
1:1A:2415:G:C6	1:1A:2416:C:C4	3.09	0.40
1:1A:2464:G:C2	1:1A:2487:G:C2	3.10	0.40
1:1A:2586:U:H2'	1:1A:2587:A:C8	2.56	0.40
1:1A:419:U:H2'	1:1A:420:C:C6	2.56	0.40
1:1A:755:U:O4	1:1A:756:A:N6	2.55	0.40
1:1A:813:U:C4	14:1P:25:SER:HA	2.56	0.40
5:1F:189:THR:O	5:1F:193:VAL:HG23	2.22	0.40
6:1G:24:VAL:O	6:1G:27:VAL:HG12	2.22	0.40
12:1N:80:HIS:ND1	12:1N:81:ILE:HG22	2.36	0.40
17:1S:26:LEU:HD13	17:1S:39:VAL:HG22	2.04	0.40
23:1Y:65:GLN:HB2	23:1Y:68:ASN:OD1	2.21	0.40
25:10:45:ALA:O	25:10:47:VAL:HG23	2.22	0.40
29:14:33:ASN:OD1	29:14:34:LEU:N	2.54	0.40
30:15:12:ARG:HG3	30:15:15:ARG:NH1	2.36	0.40
1:1A:1165:A:H2'	1:1A:1166:G:C8	2.56	0.40
1:1A:1363:C:C2	1:1A:1364:G:C8	3.09	0.40
1:1A:1837:C:H2'	1:1A:1899:A:H61	1.85	0.40
1:1A:19:A:H5''	19:1U:21:LYS:HG2	2.02	0.40
1:1A:227:A:H1'	1:1A:229:C:C4	2.56	0.40
1:1A:2720:U:OP1	18:1T:52:ARG:NH2	2.52	0.40
1:1A:6:A:H2'	1:1A:7:G:C8	2.56	0.40
1:1A:894:U:H2'	1:1A:895:U:O4'	2.22	0.40
6:1G:176:PHE:HD1	6:1G:176:PHE:HA	1.77	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
3	1D	269/273 (98%)	242 (90%)	23 (9%)	4 (2%)	12 54

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	1E	207/209 (99%)	187 (90%)	19 (9%)	1 (0%)	32	73
5	1F	199/201 (99%)	185 (93%)	11 (6%)	3 (2%)	12	54
6	1G	175/179 (98%)	153 (87%)	19 (11%)	3 (2%)	11	52
7	1H	174/177 (98%)	154 (88%)	18 (10%)	2 (1%)	17	60
8	1L	67/121 (55%)	64 (96%)	3 (4%)	0	100	100
9	1I	147/149 (99%)	130 (88%)	13 (9%)	4 (3%)	6	43
10	1J	129/165 (78%)	101 (78%)	23 (18%)	5 (4%)	3	35
11	1K	139/142 (98%)	118 (85%)	14 (10%)	7 (5%)	2	29
12	1N	140/142 (99%)	132 (94%)	6 (4%)	2 (1%)	13	55
13	1O	120/123 (98%)	106 (88%)	11 (9%)	3 (2%)	6	44
14	1P	141/144 (98%)	120 (85%)	16 (11%)	5 (4%)	4	38
15	1Q	134/136 (98%)	120 (90%)	9 (7%)	5 (4%)	4	36
16	1R	118/127 (93%)	103 (87%)	13 (11%)	2 (2%)	11	52
17	1S	114/117 (97%)	103 (90%)	9 (8%)	2 (2%)	10	51
18	1T	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
19	1U	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
20	1V	101/103 (98%)	89 (88%)	8 (8%)	4 (4%)	3	34
21	1W	108/110 (98%)	96 (89%)	12 (11%)	0	100	100
22	1X	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	8	47
23	1Y	100/104 (96%)	86 (86%)	12 (12%)	2 (2%)	9	49
24	1Z	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
25	10	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
26	11	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
27	12	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
28	13	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
29	14	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	11	53
30	15	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	9	50
31	16	48/55 (87%)	42 (88%)	5 (10%)	1 (2%)	8	48
32	17	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
33	18	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
34	19	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	6	43

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	1b	216/241 (90%)	187 (87%)	24 (11%)	5 (2%)	7	46
37	1c	204/233 (88%)	190 (93%)	12 (6%)	2 (1%)	18	61
38	1d	203/206 (98%)	179 (88%)	20 (10%)	4 (2%)	9	49
39	1e	155/167 (93%)	136 (88%)	11 (7%)	8 (5%)	2	28
40	1f	98/135 (73%)	87 (89%)	6 (6%)	5 (5%)	2	28
41	1g	149/179 (83%)	129 (87%)	15 (10%)	5 (3%)	4	39
42	1h	127/130 (98%)	115 (91%)	11 (9%)	1 (1%)	22	65
43	1i	125/130 (96%)	107 (86%)	12 (10%)	6 (5%)	2	30
44	1j	96/103 (93%)	80 (83%)	10 (10%)	6 (6%)	1	24
45	1k	114/129 (88%)	98 (86%)	14 (12%)	2 (2%)	10	51
46	1l	121/124 (98%)	100 (83%)	14 (12%)	7 (6%)	2	26
47	1m	112/118 (95%)	102 (91%)	7 (6%)	3 (3%)	6	43
48	1n	98/101 (97%)	83 (85%)	9 (9%)	6 (6%)	2	25
49	1o	86/89 (97%)	76 (88%)	6 (7%)	4 (5%)	3	30
50	1p	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	14	57
51	1q	78/84 (93%)	65 (83%)	10 (13%)	3 (4%)	4	35
52	1r	63/75 (84%)	57 (90%)	3 (5%)	3 (5%)	2	30
53	1s	77/92 (84%)	70 (91%)	6 (8%)	1 (1%)	14	57
54	1t	83/87 (95%)	78 (94%)	5 (6%)	0	100	100
55	1u	63/71 (89%)	45 (71%)	11 (18%)	7 (11%)	0	10
57	1w	637/639 (100%)	548 (86%)	58 (9%)	31 (5%)	2	29
All	All	6550/6980 (94%)	5803 (89%)	577 (9%)	170 (3%)	10	44

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	18	GLU
7	1H	108	PHE
11	1K	22	PRO
11	1K	92	PRO
12	1N	81	ILE
14	1P	85	VAL
15	1Q	6	ARG
20	1V	55	ASP
37	1c	96	VAL

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
37	1c	156	LEU
39	1e	122	VAL
40	1f	92	THR
41	1g	16	LYS
43	1i	90	ASP
52	1r	17	VAL
57	1w	8	VAL
57	1w	76	PRO
57	1w	96	ILE
57	1w	176	ASP
57	1w	334	PRO
57	1w	342	PRO
57	1w	344	PRO
57	1w	416	PRO
57	1w	433	HIS
57	1w	438	PRO
57	1w	612	VAL
57	1w	617	PRO
57	1w	624	PRO
9	1I	9	VAL
10	1J	55	VAL
10	1J	90	GLY
11	1K	12	VAL
11	1K	64	ARG
12	1N	82	GLY
14	1P	111	ILE
14	1P	128	THR
15	1Q	10	ARG
15	1Q	23	GLY
20	1V	43	ASN
22	1X	71	GLY
23	1Y	6	ARG
38	1d	26	ALA
38	1d	152	SER
41	1g	29	LEU
41	1g	145	GLU
42	1h	74	ILE
43	1i	57	VAL
43	1i	120	ALA
44	1j	57	VAL
45	1k	88	PRO
46	1l	33	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
47	1m	6	ILE
48	1n	35	ASN
48	1n	54	ASP
55	1u	12	ASP
55	1u	32	ARG
57	1w	80	ASP
3	1D	204	LEU
11	1K	20	SER
14	1P	94	THR
16	1R	59	SER
16	1R	117	ASP
17	1S	66	GLY
23	1Y	97	SER
36	1b	71	THR
41	1g	56	SER
41	1g	64	ALA
43	1i	13	SER
43	1i	125	GLN
44	1j	35	GLN
44	1j	75	ASP
45	1k	92	ARG
46	1l	23	LEU
46	1l	76	HIS
47	1m	113	LYS
48	1n	3	LYS
48	1n	38	ASP
49	1o	2	LEU
49	1o	45	HIS
51	1q	49	ASN
52	1r	18	GLN
55	1u	30	GLU
55	1u	37	TYR
57	1w	40	THR
57	1w	262	ARG
3	1D	231	HIS
5	1F	83	VAL
5	1F	122	GLU
6	1G	176	PHE
9	1I	41	LYS
10	1J	22	ALA
10	1J	88	HIS
11	1K	100	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	1O	109	SER
13	1O	110	GLU
14	1P	29	LYS
17	1S	100	HIS
22	1X	37	ASP
29	14	26	SER
31	16	45	HIS
34	19	29	ALA
36	1b	11	ALA
36	1b	126	ASP
38	1d	166	LYS
38	1d	191	SER
39	1e	53	ARG
39	1e	98	ALA
40	1f	54	LEU
40	1f	56	LYS
40	1f	63	ASN
40	1f	86	ARG
44	1j	29	ALA
46	1l	2	THR
46	1l	35	ARG
49	1o	13	GLU
50	1p	8	ARG
53	1s	4	LEU
55	1u	34	ARG
55	1u	65	ARG
57	1w	45	ASN
57	1w	173	GLU
57	1w	244	ARG
57	1w	289	ILE
57	1w	354	LYS
57	1w	414	THR
57	1w	609	GLY
4	1E	149	ASN
5	1F	149	ILE
7	1H	45	ALA
9	1I	3	VAL
9	1I	15	LEU
10	1J	118	ILE
15	1Q	70	ASP
20	1V	53	PHE
30	15	2	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
36	1b	19	THR
39	1e	23	THR
39	1e	77	ASN
39	1e	121	ASN
44	1j	33	GLY
46	1l	42	LYS
46	1l	88	ASP
48	1n	23	LYS
48	1n	100	SER
49	1o	87	ARG
51	1q	17	GLU
52	1r	46	THR
57	1w	350	VAL
57	1w	371	SER
57	1w	419	ILE
57	1w	613	THR
11	1K	3	LYS
20	1V	54	VAL
36	1b	87	ASP
39	1e	102	THR
43	1i	9	GLY
57	1w	41	THR
15	1Q	69	PRO
51	1q	20	ILE
57	1w	75	THR
3	1D	236	GLY
3	1D	253	GLY
39	1e	93	VAL
44	1j	41	PRO
57	1w	621	PRO
13	1O	35	VAL
47	1m	9	PRO
6	1G	175	PRO
55	1u	9	GLU
57	1w	387	ILE

### 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	
3	1D	216/218 (99%)	216 (100%)	0	100	100
4	1E	164/164 (100%)	164 (100%)	0	100	100
5	1F	165/165 (100%)	165 (100%)	0	100	100
6	1G	148/150 (99%)	148 (100%)	0	100	100
7	1H	137/138 (99%)	137 (100%)	0	100	100
9	1I	114/114 (100%)	114 (100%)	0	100	100
10	1J	100/123 (81%)	100 (100%)	0	100	100
11	1K	109/110 (99%)	109 (100%)	0	100	100
12	1N	116/116 (100%)	116 (100%)	0	100	100
13	1O	103/104 (99%)	102 (99%)	1 (1%)	80	90
14	1P	102/103 (99%)	102 (100%)	0	100	100
15	1Q	109/109 (100%)	108 (99%)	1 (1%)	82	92
16	1R	100/103 (97%)	100 (100%)	0	100	100
17	1S	86/87 (99%)	86 (100%)	0	100	100
18	1T	99/100 (99%)	99 (100%)	0	100	100
19	1U	89/90 (99%)	89 (100%)	0	100	100
20	1V	84/84 (100%)	84 (100%)	0	100	100
21	1W	93/93 (100%)	92 (99%)	1 (1%)	78	89
22	1X	80/84 (95%)	80 (100%)	0	100	100
23	1Y	83/85 (98%)	83 (100%)	0	100	100
24	1Z	78/78 (100%)	78 (100%)	0	100	100
25	10	57/63 (90%)	57 (100%)	0	100	100
26	11	67/68 (98%)	67 (100%)	0	100	100
27	12	55/55 (100%)	55 (100%)	0	100	100
28	13	48/49 (98%)	48 (100%)	0	100	100
29	14	59/62 (95%)	59 (100%)	0	100	100
30	15	47/48 (98%)	47 (100%)	0	100	100
31	16	45/49 (92%)	45 (100%)	0	100	100
32	17	38/38 (100%)	38 (100%)	0	100	100
33	18	51/52 (98%)	50 (98%)	1 (2%)	60	83
34	19	34/34 (100%)	34 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	1b	180/199 (90%)	180 (100%)	0	100	100
37	1c	170/190 (90%)	169 (99%)	1 (1%)	89	95
38	1d	172/173 (99%)	172 (100%)	0	100	100
39	1e	114/126 (90%)	114 (100%)	0	100	100
40	1f	87/116 (75%)	87 (100%)	0	100	100
41	1g	124/147 (84%)	124 (100%)	0	100	100
42	1h	104/105 (99%)	104 (100%)	0	100	100
43	1i	105/107 (98%)	105 (100%)	0	100	100
44	1j	86/90 (96%)	86 (100%)	0	100	100
45	1k	89/99 (90%)	89 (100%)	0	100	100
46	1l	103/104 (99%)	103 (100%)	0	100	100
47	1m	92/96 (96%)	92 (100%)	0	100	100
48	1n	79/84 (94%)	78 (99%)	1 (1%)	73	88
49	1o	76/77 (99%)	76 (100%)	0	100	100
50	1p	65/65 (100%)	65 (100%)	0	100	100
51	1q	74/78 (95%)	74 (100%)	0	100	100
52	1r	48/65 (74%)	48 (100%)	0	100	100
53	1s	70/79 (89%)	70 (100%)	0	100	100
54	1t	65/66 (98%)	65 (100%)	0	100	100
55	1u	44/61 (72%)	44 (100%)	0	100	100
57	1w	6/576 (1%)	6 (100%)	0	100	100
All	All	4829/5639 (86%)	4823 (100%)	6 (0%)	95	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	1O	58	LEU
15	1Q	136	MET
21	1W	88	ARG
33	18	61	LEU
37	1c	156	LEU
48	1n	34	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	36	ASN
3	1D	45	ASN
3	1D	85	ASN
3	1D	225	ASN
4	1E	32	ASN
4	1E	49	GLN
4	1E	150	GLN
4	1E	173	GLN
5	1F	41	GLN
6	1G	4	HIS
7	1H	44	HIS
7	1H	72	ASN
7	1H	103	ASN
7	1H	138	GLN
10	1J	4	ASN
10	1J	88	HIS
12	1N	40	HIS
13	1O	3	GLN
15	1Q	13	HIS
16	1R	9	GLN
18	1T	2	ASN
18	1T	11	GLN
21	1W	7	HIS
21	1W	40	ASN
21	1W	61	ASN
22	1X	15	HIS
24	1Z	87	GLN
25	10	42	HIS
26	11	16	ASN
27	12	25	GLN
27	12	27	ASN
31	16	18	HIS
36	1b	18	GLN
36	1b	41	ASN
38	1d	125	ASN
38	1d	197	HIS
39	1e	145	ASN
40	1f	11	HIS
40	1f	58	HIS
41	1g	141	HIS
42	1h	3	GLN
42	1h	20	ASN
44	1j	70	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
49	1o	39	GLN
50	1p	79	ASN
51	1q	30	HIS
53	1s	51	HIS
53	1s	55	GLN
53	1s	68	HIS
54	1t	2	ASN
54	1t	60	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2894/2904 (99%)	424 (14%)	33 (1%)
2	1B	119/120 (99%)	14 (11%)	2 (1%)
35	1a	1535/1539 (99%)	179 (11%)	0
56	1v	8/60 (13%)	0	0
58	1x	70/77 (90%)	5 (7%)	0
All	All	4626/4700 (98%)	622 (13%)	35 (0%)

All (622) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	A
1	1A	12	U
1	1A	27	G
1	1A	34	U
1	1A	35	G
1	1A	42	A
1	1A	46	G
1	1A	49	A
1	1A	51	G
1	1A	52	A
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	91	A
1	1A	92	U
1	1A	118	A
1	1A	120	U
1	1A	138	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	139	U
1	1A	140	C
1	1A	141	G
1	1A	142	A
1	1A	162	U
1	1A	163	C
1	1A	181	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	206	U
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	228	C
1	1A	242	G
1	1A	243	U
1	1A	248	G
1	1A	249	C
1	1A	255	A
1	1A	266	G
1	1A	267	C
1	1A	276	U
1	1A	278	A
1	1A	294	A
1	1A	301	G
1	1A	310	A
1	1A	311	A
1	1A	323	C
1	1A	324	A
1	1A	329	G
1	1A	330	A
1	1A	353	C
1	1A	361	G
1	1A	367	G
1	1A	371	A
1	1A	372	G
1	1A	373	U
1	1A	386	G
1	1A	387	U
1	1A	391	A
1	1A	404	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	406	G
1	1A	411	G
1	1A	424	G
1	1A	456	C
1	1A	457	A
1	1A	458	G
1	1A	459	U
1	1A	480	A
1	1A	481	G
1	1A	491	G
1	1A	504	A
1	1A	505	A
1	1A	506	G
1	1A	529	A
1	1A	530	G
1	1A	532	A
1	1A	542	C
1	1A	543	G
1	1A	545	U
1	1A	547	A
1	1A	550	C
1	1A	563	A
1	1A	572	A
1	1A	573	U
1	1A	575	A
1	1A	603	A
1	1A	616	A
1	1A	627	A
1	1A	637	A
1	1A	646	U
1	1A	654	A
1	1A	669	G
1	1A	670	A
1	1A	677	A
1	1A	686	U
1	1A	687	C
1	1A	695	G
1	1A	726	G
1	1A	730	A
1	1A	746	PSU
1	1A	747	5MU
1	1A	748	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	752	A
1	1A	753	A
1	1A	764	A
1	1A	765	C
1	1A	776	G
1	1A	782	A
1	1A	784	G
1	1A	785	G
1	1A	789	A
1	1A	792	A
1	1A	800	A
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	822	G
1	1A	827	U
1	1A	828	U
1	1A	830	G
1	1A	831	G
1	1A	845	A
1	1A	846	U
1	1A	847	U
1	1A	858	G
1	1A	859	G
1	1A	860	U
1	1A	878	A
1	1A	896	A
1	1A	897	C
1	1A	907	G
1	1A	910	A
1	1A	932	U
1	1A	941	A
1	1A	946	C
1	1A	961	C
1	1A	974	G
1	1A	983	A
1	1A	985	C
1	1A	995	C
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1021	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1022	G
1	1A	1023	U
1	1A	1033	U
1	1A	1046	A
1	1A	1047	G
1	1A	1053	C
1	1A	1054	A
1	1A	1057	A
1	1A	1060	U
1	1A	1061	U
1	1A	1062	G
1	1A	1064	C
1	1A	1065	U
1	1A	1066	U
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1075	C
1	1A	1076	C
1	1A	1079	C
1	1A	1084	A
1	1A	1088	A
1	1A	1104	C
1	1A	1111	A
1	1A	1112	G
1	1A	1119	U
1	1A	1130	U
1	1A	1131	G
1	1A	1132	U
1	1A	1133	A
1	1A	1135	C
1	1A	1143	A
1	1A	1174	U
1	1A	1175	A
1	1A	1176	U
1	1A	1177	G
1	1A	1179	G
1	1A	1180	U
1	1A	1206	G
1	1A	1212	G
1	1A	1247	A
1	1A	1248	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1250	G
1	1A	1251	C
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1300	G
1	1A	1301	A
1	1A	1314	C
1	1A	1321	A
1	1A	1329	U
1	1A	1332	G
1	1A	1341	G
1	1A	1345	C
1	1A	1365	A
1	1A	1368	G
1	1A	1378	A
1	1A	1379	U
1	1A	1383	A
1	1A	1416	G
1	1A	1419	A
1	1A	1420	A
1	1A	1428	C
1	1A	1454	C
1	1A	1461	C
1	1A	1482	G
1	1A	1490	A
1	1A	1491	G
1	1A	1504	A
1	1A	1515	A
1	1A	1524	G
1	1A	1533	C
1	1A	1535	A
1	1A	1536	C
1	1A	1537	G
1	1A	1555	G
1	1A	1559	U
1	1A	1560	G
1	1A	1565	C
1	1A	1567	G
1	1A	1569	A
1	1A	1581	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1585	C
1	1A	1611	C
1	1A	1634	A
1	1A	1646	C
1	1A	1647	U
1	1A	1648	U
1	1A	1651	G
1	1A	1654	A
1	1A	1664	A
1	1A	1670	C
1	1A	1674	G
1	1A	1694	C
1	1A	1695	G
1	1A	1715	G
1	1A	1729	U
1	1A	1730	C
1	1A	1732	C
1	1A	1738	G
1	1A	1758	U
1	1A	1764	C
1	1A	1773	A
1	1A	1780	A
1	1A	1781	U
1	1A	1784	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	A
1	1A	1802	A
1	1A	1808	A
1	1A	1816	C
1	1A	1829	A
1	1A	1833	C
1	1A	1834	U
1	1A	1871	A
1	1A	1890	A
1	1A	1896	G
1	1A	1901	A
1	1A	1906	G
1	1A	1913	A
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1937	A
1	1A	1938	A
1	1A	1940	U
1	1A	1941	C
1	1A	1944	U
1	1A	1955	U
1	1A	1962	5MC
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	U
1	1A	1972	G
1	1A	1991	U
1	1A	1993	U
1	1A	1997	C
1	1A	2021	C
1	1A	2022	U
1	1A	2023	C
1	1A	2031	A
1	1A	2033	A
1	1A	2043	C
1	1A	2049	G
1	1A	2052	A
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2068	U
1	1A	2069	G7M
1	1A	2070	A
1	1A	2072	C
1	1A	2093	G
1	1A	2095	A
1	1A	2096	C
1	1A	2098	U
1	1A	2110	G
1	1A	2111	U
1	1A	2112	G
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2119	A
1	1A	2127	G
1	1A	2131	U
1	1A	2132	U
1	1A	2133	G
1	1A	2145	C
1	1A	2162	G
1	1A	2164	C
1	1A	2170	A
1	1A	2172	U
1	1A	2173	A
1	1A	2192	U
1	1A	2198	A
1	1A	2204	G
1	1A	2211	A
1	1A	2213	U
1	1A	2225	A
1	1A	2226	C
1	1A	2238	G
1	1A	2250	G
1	1A	2251	OMG
1	1A	2252	G
1	1A	2278	A
1	1A	2283	C
1	1A	2287	A
1	1A	2305	U
1	1A	2309	A
1	1A	2320	U
1	1A	2327	A
1	1A	2334	U
1	1A	2335	A
1	1A	2350	C
1	1A	2354	C
1	1A	2361	G
1	1A	2383	G
1	1A	2385	C
1	1A	2391	G
1	1A	2392	A
1	1A	2402	U
1	1A	2407	A
1	1A	2423	U
1	1A	2424	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2426	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2441	U
1	1A	2445	2MG
1	1A	2448	A
1	1A	2476	A
1	1A	2484	G
1	1A	2499	C
1	1A	2502	G
1	1A	2504	PSU
1	1A	2506	U
1	1A	2513	A
1	1A	2518	A
1	1A	2529	G
1	1A	2547	A
1	1A	2552	OMU
1	1A	2553	G
1	1A	2554	U
1	1A	2567	G
1	1A	2572	A
1	1A	2585	U
1	1A	2586	U
1	1A	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2613	U
1	1A	2614	A
1	1A	2629	U
1	1A	2636	C
1	1A	2646	C
1	1A	2655	G
1	1A	2656	U
1	1A	2689	U
1	1A	2690	U
1	1A	2712	C
1	1A	2713	U
1	1A	2714	G
1	1A	2718	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2726	A
1	1A	2739	U
1	1A	2744	G
1	1A	2748	A
1	1A	2757	A
1	1A	2764	A
1	1A	2765	A
1	1A	2778	A
1	1A	2779	U
1	1A	2780	G
1	1A	2791	G
1	1A	2794	C
1	1A	2797	U
1	1A	2799	A
1	1A	2800	A
1	1A	2808	G
1	1A	2809	A
1	1A	2818	U
1	1A	2820	A
1	1A	2833	U
1	1A	2849	U
1	1A	2867	G
1	1A	2868	A
1	1A	2872	A
1	1A	2880	C
1	1A	2893	A
1	1A	2894	G
2	1B	4	C
2	1B	13	G
2	1B	24	G
2	1B	35	C
2	1B	44	G
2	1B	45	A
2	1B	53	A
2	1B	67	G
2	1B	88	C
2	1B	89	U
2	1B	90	C
2	1B	91	C
2	1B	108	A
2	1B	109	A
35	1a	9	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
35	1a	22	G
35	1a	32	A
35	1a	39	G
35	1a	51	A
35	1a	71	A
35	1a	86	G
35	1a	87	C
35	1a	121	U
35	1a	130	A
35	1a	177	G
35	1a	183	C
35	1a	184	G
35	1a	209	U
35	1a	210	C
35	1a	212	G
35	1a	226	G
35	1a	247	G
35	1a	251	G
35	1a	266	G
35	1a	267	C
35	1a	281	G
35	1a	282	A
35	1a	283	U
35	1a	289	G
35	1a	306	A
35	1a	328	C
35	1a	345	C
35	1a	347	G
35	1a	351	G
35	1a	352	C
35	1a	367	U
35	1a	372	C
35	1a	392	C
35	1a	397	A
35	1a	406	G
35	1a	413	G
35	1a	422	C
35	1a	424	G
35	1a	429	U
35	1a	439	U
35	1a	467	U
35	1a	479	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
35	1a	482	A
35	1a	484	G
35	1a	485	U
35	1a	486	U
35	1a	496	A
35	1a	497	G
35	1a	527	7MG
35	1a	530	G
35	1a	531	U
35	1a	532	A
35	1a	533	A
35	1a	547	A
35	1a	561	U
35	1a	564	C
35	1a	572	A
35	1a	573	A
35	1a	575	G
35	1a	576	C
35	1a	577	G
35	1a	633	G
35	1a	642	A
35	1a	665	A
35	1a	688	G
35	1a	702	A
35	1a	703	G
35	1a	723	U
35	1a	724	G
35	1a	731	G
35	1a	733	G
35	1a	748	G
35	1a	755	G
35	1a	777	A
35	1a	815	A
35	1a	817	C
35	1a	818	G
35	1a	819	A
35	1a	820	U
35	1a	832	G
35	1a	843	U
35	1a	844	G
35	1a	846	G
35	1a	871	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
35	1a	890	G
35	1a	902	G
35	1a	934	C
35	1a	935	A
35	1a	939	G
35	1a	960	U
35	1a	961	U
35	1a	966	2MG
35	1a	968	A
35	1a	969	A
35	1a	971	G
35	1a	975	A
35	1a	976	G
35	1a	977	A
35	1a	992	U
35	1a	993	G
35	1a	1004	A
35	1a	1026	G
35	1a	1028	C
35	1a	1030	U
35	1a	1031	C
35	1a	1033	G
35	1a	1034	G
35	1a	1035	A
35	1a	1053	G
35	1a	1056	U
35	1a	1065	U
35	1a	1085	U
35	1a	1094	G
35	1a	1101	A
35	1a	1130	A
35	1a	1137	C
35	1a	1138	G
35	1a	1139	G
35	1a	1140	C
35	1a	1159	U
35	1a	1168	U
35	1a	1183	U
35	1a	1191	A
35	1a	1196	A
35	1a	1197	A
35	1a	1201	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
35	1a	1202	U
35	1a	1207	2MG
35	1a	1212	U
35	1a	1213	A
35	1a	1225	A
35	1a	1226	C
35	1a	1227	A
35	1a	1238	A
35	1a	1240	U
35	1a	1241	G
35	1a	1256	A
35	1a	1258	G
35	1a	1260	G
35	1a	1278	G
35	1a	1280	A
35	1a	1281	C
35	1a	1282	C
35	1a	1287	A
35	1a	1298	U
35	1a	1300	G
35	1a	1301	U
35	1a	1302	C
35	1a	1317	C
35	1a	1323	G
35	1a	1346	A
35	1a	1347	G
35	1a	1348	U
35	1a	1363	A
35	1a	1395	C
35	1a	1398	A
35	1a	1400	C
35	1a	1403	C
35	1a	1407	5MC
35	1a	1433	A
35	1a	1446	A
35	1a	1448	C
35	1a	1452	C
35	1a	1491	G
35	1a	1492	A
35	1a	1494	G
35	1a	1497	G
35	1a	1499	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
35	1a	1502	A
35	1a	1506	U
35	1a	1517	G
35	1a	1520	C
35	1a	1529	G
35	1a	1530	G
35	1a	1533	C
35	1a	1534	A
35	1a	1535	C
35	1a	1536	C
58	1x	9	A
58	1x	19	G
58	1x	22	G
58	1x	47	U
58	1x	67	A

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	51	G
1	1A	86	G
1	1A	204	A
1	1A	242	G
1	1A	372	G
1	1A	458	G
1	1A	479	A
1	1A	490	C
1	1A	747	5MU
1	1A	752	A
1	1A	858	G
1	1A	859	G
1	1A	1020	A
1	1A	1022	G
1	1A	1070	A
1	1A	1111	A
1	1A	1130	U
1	1A	1182	G
1	1A	1190	G
1	1A	1300	G
1	1A	1378	A
1	1A	1399	C
1	1A	1432	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1940	U
1	1A	2251	OMG
1	1A	2286	G
1	1A	2326	C
1	1A	2333	A
1	1A	2391	G
1	1A	2566	A
1	1A	2655	G
1	1A	2756	U
1	1A	2808	G
2	1B	66	A
2	1B	88	C

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

39 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$
1	6MZ	1A	1618	1	18,25,26	0.98	1 (5%)	16,36,39	2.64	4 (25%)
1	2MG	1A	1835	1	19,26,27	1.19	2 (10%)	20,38,41	2.23	7 (35%)
1	PSU	1A	1911	1	16,21,22	1.45	1 (6%)	20,30,33	3.23	7 (35%)
1	3TD	1A	1915	1	16,22,23	1.55	3 (18%)	19,32,35	1.91	4 (21%)
1	PSU	1A	1917	1	16,21,22	1.35	1 (6%)	20,30,33	3.22	7 (35%)
1	5MU	1A	1939	1	14,22,23	0.70	1 (7%)	16,32,35	2.18	3 (18%)
1	5MC	1A	1962	1	15,22,23	1.45	1 (6%)	17,32,35	0.99	1 (5%)
1	6MZ	1A	2030	1	18,25,26	1.01	1 (5%)	16,36,39	2.92	4 (25%)
1	G7M	1A	2069	1	19,26,27	1.12	1 (5%)	19,39,42	2.00	4 (21%)
1	OMG	1A	2251	1,58	18,26,27	1.21	2 (11%)	22,38,41	2.27	6 (27%)
1	2MG	1A	2445	1	19,26,27	1.18	2 (10%)	20,38,41	2.23	7 (35%)
1	H2U	1A	2449	1	17,21,22	1.19	2 (11%)	21,30,33	1.68	4 (19%)
1	PSU	1A	2457	1	16,21,22	1.33	1 (6%)	20,30,33	3.17	8 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMC	1A	2498	1	15,22,23	0.72	0	19,31,34	0.97	1 (5%)
1	2MA	1A	2503	1	18,25,26	1.62	3 (16%)	17,37,40	2.07	2 (11%)
1	PSU	1A	2504	1	16,21,22	1.46	1 (6%)	20,30,33	3.23	6 (30%)
1	OMU	1A	2552	1	14,22,23	0.84	0	18,31,34	1.91	1 (5%)
1	PSU	1A	2580	1	16,21,22	1.38	1 (6%)	20,30,33	3.18	7 (35%)
1	PSU	1A	2604	1	16,21,22	1.42	1 (6%)	20,30,33	3.25	7 (35%)
1	PSU	1A	2605	1	16,21,22	1.29	1 (6%)	20,30,33	3.22	6 (30%)
1	1MG	1A	745	1	18,26,27	1.52	3 (16%)	18,39,42	1.73	3 (16%)
1	PSU	1A	746	1	16,21,22	1.49	2 (12%)	20,30,33	3.70	7 (35%)
1	5MU	1A	747	1	14,22,23	0.75	0	16,32,35	2.38	6 (37%)
1	PSU	1A	955	1	16,21,22	1.39	1 (6%)	20,30,33	3.22	6 (30%)
35	2MG	1a	1207	35	19,26,27	1.20	2 (10%)	20,38,41	2.16	5 (25%)
35	4OC	1a	1402	35	16,23,24	0.78	0	19,32,35	1.12	2 (10%)
35	5MC	1a	1407	35	15,22,23	1.38	1 (6%)	17,32,35	1.02	2 (11%)
35	UR3	1a	1498	35	14,22,23	0.73	0	16,32,35	0.83	0
35	2MG	1a	1516	35	19,26,27	1.43	3 (15%)	20,38,41	2.38	8 (40%)
35	MA6	1a	1518	35	16,26,27	1.05	1 (6%)	18,38,41	2.47	7 (38%)
35	MA6	1a	1519	35	16,26,27	1.01	1 (6%)	18,38,41	2.40	7 (38%)
35	PSU	1a	516	35	16,21,22	1.38	1 (6%)	20,30,33	3.20	6 (30%)
35	7MG	1a	527	35	20,26,27	1.71	2 (10%)	22,39,42	2.57	4 (18%)
35	2MG	1a	966	35	19,26,27	1.24	2 (10%)	20,38,41	2.23	7 (35%)
35	5MC	1a	967	35	15,22,23	1.51	1 (6%)	17,32,35	1.10	2 (11%)
58	7MG	1x	46	58	20,26,27	1.67	2 (10%)	22,39,42	3.00	7 (31%)
58	5MU	1x	54	58	14,22,23	0.70	0	16,32,35	2.20	3 (18%)
58	PSU	1x	55	58	16,21,22	1.24	1 (6%)	20,30,33	3.31	7 (35%)
58	PSU	1x	65	58	16,21,22	1.55	2 (12%)	20,30,33	3.52	7 (35%)

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
1	6MZ	1A	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	1A	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	3TD	1A	1915	1	-	0/7/25/26	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/3/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/3/25/26	0/2/2/2
1	6MZ	1A	2030	1	-	0/5/27/28	0/3/3/3
1	G7M	1A	2069	1	-	0/3/25/26	0/3/3/3
1	OMG	1A	2251	1,58	-	0/5/27/28	0/3/3/3
1	2MG	1A	2445	1	-	0/5/27/28	0/3/3/3
1	H2U	1A	2449	1	-	0/7/38/39	0/2/2/2
1	PSU	1A	2457	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	2498	1	-	0/5/27/28	0/2/2/2
1	2MA	1A	2503	1	-	0/3/25/26	0/3/3/3
1	PSU	1A	2504	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/5/27/28	0/2/2/2
1	PSU	1A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2604	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	1A	745	1	-	0/3/25/26	0/3/3/3
1	PSU	1A	746	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	747	1	-	0/3/25/26	0/2/2/2
1	PSU	1A	955	1	-	0/7/25/26	0/2/2/2
35	2MG	1a	1207	35	-	0/5/27/28	0/3/3/3
35	4OC	1a	1402	35	-	0/7/29/30	0/2/2/2
35	5MC	1a	1407	35	-	0/3/25/26	0/2/2/2
35	UR3	1a	1498	35	-	0/3/25/26	0/2/2/2
35	2MG	1a	1516	35	-	0/5/27/28	0/3/3/3
35	MA6	1a	1518	35	-	0/7/29/30	0/3/3/3
35	MA6	1a	1519	35	-	0/7/29/30	0/3/3/3
35	PSU	1a	516	35	-	0/7/25/26	0/2/2/2
35	7MG	1a	527	35	-	0/7/37/38	0/3/3/3
35	2MG	1a	966	35	-	0/5/27/28	0/3/3/3
35	5MC	1a	967	35	-	0/3/25/26	0/2/2/2
58	7MG	1x	46	58	-	0/7/37/38	0/3/3/3
58	5MU	1x	54	58	-	0/3/25/26	0/2/2/2
58	PSU	1x	55	58	-	0/7/25/26	0/2/2/2
58	PSU	1x	65	58	-	0/7/25/26	0/2/2/2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1x	65	PSU	C5-C1'	-4.70	1.48	1.52
1	1A	2504	PSU	C5-C1'	-4.66	1.48	1.52
1	1A	1911	PSU	C5-C1'	-4.62	1.48	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2604	PSU	C5-C1'	-4.52	1.48	1.52
35	1a	516	PSU	C5-C1'	-4.37	1.48	1.52
1	1A	955	PSU	C5-C1'	-4.35	1.48	1.52
1	1A	2580	PSU	C5-C1'	-4.35	1.48	1.52
1	1A	1917	PSU	C5-C1'	-4.23	1.48	1.52
1	1A	2457	PSU	C5-C1'	-4.10	1.48	1.52
1	1A	746	PSU	C5-C1'	-3.97	1.48	1.52
1	1A	2605	PSU	C5-C1'	-3.86	1.48	1.52
1	1A	1915	3TD	C5-C1'	-3.71	1.49	1.52
58	1x	55	PSU	C5-C1'	-3.68	1.49	1.52
1	1A	746	PSU	O4'-C1'	-3.29	1.39	1.44
1	1A	1915	3TD	C4-N3	-2.99	1.33	1.38
1	1A	2449	H2U	C2-N3	-2.84	1.32	1.38
1	1A	1915	3TD	O4'-C1'	-2.77	1.40	1.44
1	1A	2449	H2U	C4-N3	-2.77	1.33	1.37
58	1x	65	PSU	O4'-C1'	-2.59	1.40	1.44
1	1A	1939	5MU	C2-N3	-2.10	1.34	1.38
1	1A	745	1MG	C6-N1	2.27	1.41	1.38
35	1a	1516	2MG	C2-N2	2.38	1.36	1.34
1	1A	2251	OMG	C5-C4	2.84	1.46	1.40
35	1a	1207	2MG	C5-C4	2.99	1.47	1.40
1	1A	1835	2MG	C5-C4	3.02	1.47	1.40
1	1A	2445	2MG	C5-C4	3.06	1.47	1.40
1	1A	1618	6MZ	C5-C4	3.08	1.47	1.40
35	1a	966	2MG	C5-C4	3.11	1.47	1.40
35	1a	1519	MA6	C5-C4	3.16	1.47	1.40
35	1a	1518	MA6	C5-C4	3.16	1.47	1.40
35	1a	527	7MG	C5-C4	3.19	1.47	1.39
1	1A	2503	2MA	C5-C4	3.22	1.47	1.40
35	1a	1516	2MG	C5-C4	3.28	1.47	1.40
1	1A	2030	6MZ	C5-C4	3.33	1.48	1.40
35	1a	1207	2MG	C6-C5	3.36	1.47	1.41
58	1x	46	7MG	C5-C4	3.37	1.48	1.39
1	1A	745	1MG	C5-C4	3.39	1.48	1.40
1	1A	2445	2MG	C6-C5	3.40	1.47	1.41
35	1a	966	2MG	C6-C5	3.40	1.47	1.41
1	1A	2251	OMG	C6-C5	3.47	1.48	1.41
1	1A	2503	2MA	C6-N6	3.52	1.35	1.27
1	1A	2069	G7M	C6-C5	3.58	1.48	1.41
1	1A	1835	2MG	C6-C5	3.58	1.48	1.41
35	1a	1516	2MG	C6-C5	3.97	1.48	1.41
1	1A	745	1MG	C6-C5	4.23	1.48	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2503	2MA	C6-C5	4.38	1.48	1.41
35	1a	1407	5MC	C5-C4	4.74	1.48	1.41
1	1A	1962	5MC	C5-C4	4.99	1.48	1.41
35	1a	967	5MC	C5-C4	5.20	1.49	1.41
58	1x	46	7MG	C6-C5	5.67	1.48	1.41
35	1a	527	7MG	C6-C5	5.93	1.48	1.41

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	746	PSU	N1-C2-N3	-9.38	121.65	128.40
58	1x	65	PSU	N1-C2-N3	-8.99	121.93	128.40
58	1x	55	PSU	N1-C2-N3	-8.97	121.95	128.40
1	1A	746	PSU	C5-C4-N3	-8.86	118.16	125.43
1	1A	2605	PSU	N1-C2-N3	-8.85	122.04	128.40
1	1A	1917	PSU	N1-C2-N3	-8.77	122.09	128.40
58	1x	65	PSU	C5-C4-N3	-8.74	118.26	125.43
1	1A	2604	PSU	N1-C2-N3	-8.54	122.26	128.40
1	1A	2504	PSU	N1-C2-N3	-8.53	122.27	128.40
1	1A	955	PSU	N1-C2-N3	-8.50	122.29	128.40
1	1A	1911	PSU	N1-C2-N3	-8.49	122.29	128.40
35	1a	516	PSU	N1-C2-N3	-8.48	122.30	128.40
1	1A	2580	PSU	N1-C2-N3	-8.29	122.43	128.40
1	1A	2457	PSU	N1-C2-N3	-8.19	122.51	128.40
1	1A	2604	PSU	C5-C4-N3	-7.69	119.12	125.43
58	1x	55	PSU	C5-C4-N3	-7.62	119.18	125.43
1	1A	2580	PSU	C5-C4-N3	-7.55	119.23	125.43
1	1A	1911	PSU	C5-C4-N3	-7.48	119.30	125.43
1	1A	2457	PSU	C5-C4-N3	-7.42	119.34	125.43
1	1A	955	PSU	C5-C4-N3	-7.41	119.35	125.43
1	1A	1917	PSU	C5-C4-N3	-7.40	119.36	125.43
35	1a	516	PSU	C5-C4-N3	-7.38	119.38	125.43
1	1A	2605	PSU	C5-C4-N3	-7.29	119.45	125.43
1	1A	2504	PSU	C5-C4-N3	-7.27	119.47	125.43
35	1a	1519	MA6	N3-C2-N1	-6.26	123.41	128.86
35	1a	1518	MA6	N3-C2-N1	-6.12	123.53	128.86
1	1A	2030	6MZ	C9-N6-C6	-5.73	117.94	122.85
58	1x	46	7MG	C5-C4-N3	-5.55	117.21	126.47
1	1A	747	5MU	C5-C4-N3	-5.40	119.29	125.24
58	1x	54	5MU	C5-C4-N3	-5.37	119.32	125.24
1	1A	2030	6MZ	N3-C2-N1	-5.36	124.19	128.86
1	1A	1939	5MU	C5-C4-N3	-5.35	119.35	125.24

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2069	G7M	C5-C6-N1	-5.03	116.32	123.48
1	1A	1618	6MZ	N3-C2-N1	-4.92	124.57	128.86
58	1x	46	7MG	C5-C6-N1	-4.86	115.74	123.37
35	1a	527	7MG	C5-C4-N3	-4.77	118.52	126.47
1	1A	2449	H2U	C4-N3-C2	-4.58	121.89	125.81
1	1A	1915	3TD	C5-C6-N1	-4.42	118.66	124.39
35	1a	1516	2MG	C5-C6-N1	-4.41	117.20	123.48
35	1a	527	7MG	C5-C6-N1	-4.41	116.45	123.37
1	1A	2251	OMG	C6-C5-C4	-4.22	116.64	120.84
35	1a	1516	2MG	C6-C5-C4	-4.15	116.71	120.84
35	1a	966	2MG	C5-C6-N1	-4.08	117.67	123.48
1	1A	2457	PSU	C5-C6-N1	-4.06	119.13	124.39
1	1A	2445	2MG	C5-C6-N1	-4.00	117.80	123.48
1	1A	1618	6MZ	C9-N6-C6	-3.96	119.46	122.85
1	1A	2251	OMG	C5-C6-N1	-3.95	117.86	123.48
1	1A	2504	PSU	C5-C6-N1	-3.92	119.31	124.39
1	1A	1835	2MG	C6-C5-C4	-3.88	116.98	120.84
1	1A	2605	PSU	C5-C6-N1	-3.87	119.38	124.39
1	1A	747	5MU	C5-C6-N1	-3.87	117.97	122.15
35	1a	1519	MA6	C10-N6-C6	-3.86	107.83	119.51
35	1a	1518	MA6	C4-C5-N7	-3.85	105.69	109.41
1	1A	2580	PSU	C5-C6-N1	-3.84	119.41	124.39
1	1A	2445	2MG	C6-C5-C4	-3.83	117.03	120.84
1	1A	1917	PSU	C5-C6-N1	-3.83	119.43	124.39
1	1A	2504	PSU	C5-C1'-C2'	-3.83	108.95	115.55
35	1a	1207	2MG	C5-C6-N1	-3.82	118.04	123.48
1	1A	1911	PSU	C5-C1'-C2'	-3.80	109.00	115.55
58	1x	65	PSU	C5-C6-N1	-3.73	119.56	124.39
35	1a	1207	2MG	C6-C5-C4	-3.71	117.16	120.84
35	1a	516	PSU	C5-C6-N1	-3.68	119.61	124.39
1	1A	1835	2MG	C5-C6-N1	-3.65	118.28	123.48
1	1A	746	PSU	C5-C6-N1	-3.63	119.68	124.39
1	1A	1911	PSU	C5-C6-N1	-3.62	119.69	124.39
1	1A	2604	PSU	C5-C6-N1	-3.62	119.70	124.39
1	1A	2030	6MZ	C4-C5-N7	-3.56	105.97	109.41
1	1A	955	PSU	C5-C6-N1	-3.54	119.80	124.39
1	1A	2503	2MA	C4-C5-N7	-3.50	106.03	109.41
35	1a	1516	2MG	CM2-N2-C2	-3.49	119.39	123.63
1	1A	955	PSU	C5-C1'-C2'	-3.47	109.56	115.55
1	1A	2251	OMG	N3-C2-N1	-3.47	122.39	127.46
35	1a	1519	MA6	C4-C5-N7	-3.44	106.09	109.41
35	1a	966	2MG	C6-C5-C4	-3.43	117.43	120.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1a	1518	MA6	C10-N6-C6	-3.37	109.32	119.51
1	1A	2604	PSU	C5-C1'-C2'	-3.35	109.78	115.55
1	1A	746	PSU	O4'-C1'-C5	-3.32	104.79	109.93
58	1x	55	PSU	C5-C6-N1	-3.24	120.18	124.39
1	1A	1835	2MG	CM2-N2-C2	-3.18	119.76	123.63
35	1a	1207	2MG	CM2-N2-C2	-3.15	119.80	123.63
35	1a	516	PSU	C5-C1'-C2'	-3.11	110.18	115.55
1	1A	1939	5MU	C5-C6-N1	-2.95	118.96	122.15
1	1A	2580	PSU	C5-C1'-C2'	-2.94	110.48	115.55
1	1A	2445	2MG	CM2-N2-C2	-2.92	120.07	123.63
35	1a	1518	MA6	C10-N6-C9	-2.91	106.61	116.03
1	1A	1835	2MG	C4-C5-N7	-2.87	106.63	109.41
1	1A	1618	6MZ	C4-C5-N7	-2.87	106.64	109.41
1	1A	2449	H2U	O2-C2-N1	-2.85	119.55	123.12
1	1A	2251	OMG	C4-C5-N7	-2.84	106.67	109.41
58	1x	65	PSU	C5-C1'-C2'	-2.75	110.81	115.55
1	1A	745	1MG	C4-C5-N7	-2.69	106.81	109.41
1	1A	2069	G7M	N3-C2-N1	-2.57	123.71	127.46
1	1A	2445	2MG	C4-C5-N7	-2.45	107.04	109.41
1	1A	2498	OMC	CM2-O2'-C2'	-2.45	107.85	114.54
35	1a	1519	MA6	C9-N6-C6	-2.44	112.13	119.51
35	1a	1519	MA6	C10-N6-C9	-2.43	108.18	116.03
35	1a	1516	2MG	N3-C2-N1	-2.41	122.58	126.23
35	1a	1402	4OC	CM4-N4-C4	-2.41	120.86	122.94
35	1a	1407	5MC	C5-C6-N1	-2.39	119.56	122.15
35	1a	966	2MG	C4-C5-N7	-2.37	107.12	109.41
35	1a	967	5MC	C5-C6-N1	-2.32	119.64	122.15
1	1A	745	1MG	C6-C5-C4	-2.29	118.34	119.92
58	1x	46	7MG	C5-C4-N9	-2.24	103.05	106.31
35	1a	1402	4OC	C5-C4-N3	-2.22	119.50	123.21
35	1a	966	2MG	N3-C2-N1	-2.20	122.90	126.23
58	1x	54	5MU	C5-C6-N1	-2.20	119.77	122.15
1	1A	1917	PSU	C5-C1'-C2'	-2.19	111.77	115.55
35	1a	1516	2MG	C4-C5-N7	-2.17	107.31	109.41
35	1a	1518	MA6	C9-N6-C6	-2.09	113.20	119.51
1	1A	747	5MU	C5M-C5-C4	-2.07	117.78	120.17
1	1A	2445	2MG	N3-C2-N1	-2.06	123.12	126.23
1	1A	2457	PSU	C5-C1'-C2'	-2.01	112.09	115.55
58	1x	55	PSU	O4'-C1'-C5	2.00	113.03	109.93
1	1A	747	5MU	C2'-C3'-C4'	2.02	106.55	102.62
35	1a	1407	5MC	N4-C4-N3	2.02	119.99	117.00
1	1A	1917	PSU	O4'-C1'-C2'	2.02	107.70	104.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2604	PSU	O4'-C1'-C2'	2.02	107.70	104.45
1	1A	1915	3TD	C3'-C2'-C1'	2.04	104.28	101.93
1	1A	2449	H2U	C5-C4-N3	2.04	118.75	116.72
1	1A	2605	PSU	O4'-C1'-C2'	2.06	107.76	104.45
58	1x	46	7MG	C2-N3-C4	2.07	119.75	113.95
1	1A	1911	PSU	O4'-C1'-C2'	2.09	107.81	104.45
1	1A	2580	PSU	O4'-C1'-C2'	2.09	107.81	104.45
1	1A	747	5MU	C4'-O4'-C1'	2.10	112.00	109.77
1	1A	2457	PSU	O4'-C1'-C2'	2.12	107.86	104.45
35	1a	1519	MA6	N1-C6-N6	2.13	119.26	117.00
58	1x	55	PSU	O4'-C1'-C2'	2.17	107.94	104.45
35	1a	1516	2MG	N2-C2-N3	2.17	119.07	116.95
35	1a	1518	MA6	N1-C6-N6	2.19	119.32	117.00
58	1x	46	7MG	C4-N9-C1'	2.24	131.99	126.58
1	1A	1835	2MG	N2-C2-N3	2.31	119.19	116.95
1	1A	2457	PSU	O4'-C1'-C5	2.33	113.54	109.93
1	1A	1962	5MC	N4-C4-N3	2.39	120.53	117.00
35	1a	967	5MC	N4-C4-N3	2.62	120.88	117.00
58	1x	65	PSU	O4'-C1'-C2'	2.77	108.90	104.45
1	1A	746	PSU	O4'-C1'-C2'	2.90	109.10	104.45
35	1a	966	2MG	N2-C2-N3	3.09	119.95	116.95
1	1A	1915	3TD	O4'-C1'-C2'	3.39	109.90	104.45
1	1A	2449	H2U	N3-C2-N1	3.79	120.50	116.73
58	1x	55	PSU	C6-N1-C2	3.79	121.43	115.36
1	1A	2604	PSU	C6-N1-C2	3.87	121.56	115.36
1	1A	1911	PSU	C6-N1-C2	3.88	121.58	115.36
1	1A	955	PSU	C6-N1-C2	3.89	121.59	115.36
35	1a	1207	2MG	C6-N1-C2	3.91	122.18	115.18
1	1A	2580	PSU	C6-N1-C2	3.93	121.66	115.36
1	1A	1835	2MG	C6-N1-C2	3.94	122.24	115.18
58	1x	65	PSU	C6-N1-C2	4.00	121.77	115.36
35	1a	516	PSU	C6-N1-C2	4.03	121.81	115.36
1	1A	2605	PSU	C6-N1-C2	4.04	121.82	115.36
1	1A	746	PSU	C6-N1-C2	4.04	121.82	115.36
1	1A	2504	PSU	C6-N1-C2	4.04	121.83	115.36
1	1A	1917	PSU	C6-N1-C2	4.07	121.87	115.36
1	1A	2457	PSU	C6-N1-C2	4.09	121.90	115.36
1	1A	2445	2MG	C6-N1-C2	4.12	122.56	115.18
35	1a	1518	MA6	C2-N1-C6	4.20	122.13	111.82
35	1a	1519	MA6	C2-N1-C6	4.23	122.21	111.82
1	1A	2069	G7M	C6-N1-C2	4.30	122.25	116.06
35	1a	966	2MG	C6-N1-C2	4.30	122.89	115.18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1915	3TD	C6-N1-C2	4.33	122.28	115.36
1	1A	2445	2MG	C2-N3-C4	4.36	120.09	115.11
35	1a	1207	2MG	C2-N3-C4	4.38	120.11	115.11
35	1a	966	2MG	C2-N3-C4	4.44	120.18	115.11
1	1A	2069	G7M	C2-N3-C4	4.44	120.35	115.16
35	1a	527	7MG	C6-N1-C2	4.47	122.50	116.06
35	1a	1516	2MG	C6-N1-C2	4.53	123.30	115.18
58	1x	46	7MG	C6-N1-C2	4.55	122.61	116.06
35	1a	1516	2MG	C2-N3-C4	4.61	120.38	115.11
1	1A	2251	OMG	C6-N1-C2	4.70	122.82	116.06
1	1A	1835	2MG	C2-N3-C4	4.71	120.48	115.11
1	1A	2251	OMG	C2-N3-C4	4.82	120.78	115.16
1	1A	2457	PSU	C4-N3-C2	5.06	119.59	115.16
1	1A	747	5MU	C4-N3-C2	5.22	119.72	115.16
1	1A	2504	PSU	C4-N3-C2	5.30	119.80	115.16
1	1A	2580	PSU	C4-N3-C2	5.31	119.80	115.16
35	1a	516	PSU	C4-N3-C2	5.37	119.86	115.16
1	1A	1911	PSU	C4-N3-C2	5.42	119.90	115.16
1	1A	1917	PSU	C4-N3-C2	5.52	119.99	115.16
1	1A	955	PSU	C4-N3-C2	5.54	120.01	115.16
1	1A	2604	PSU	C4-N3-C2	5.57	120.03	115.16
1	1A	2605	PSU	C4-N3-C2	5.61	120.06	115.16
1	1A	1939	5MU	C4-N3-C2	5.84	120.27	115.16
1	1A	745	1MG	C2-N3-C4	5.87	122.02	115.16
58	1x	55	PSU	C4-N3-C2	6.08	120.47	115.16
58	1x	65	PSU	C4-N3-C2	6.29	120.66	115.16
58	1x	54	5MU	C4-N3-C2	6.31	120.68	115.16
1	1A	746	PSU	C4-N3-C2	6.74	121.05	115.16
1	1A	2503	2MA	C2-N3-C4	7.05	121.51	115.41
1	1A	2552	OMU	C4-N3-C2	7.11	120.24	114.13
1	1A	2030	6MZ	C2-N1-C6	7.58	121.47	116.53
1	1A	1618	6MZ	C2-N1-C6	7.67	121.53	116.53
35	1a	527	7MG	N3-C4-N9	8.44	137.76	126.98
58	1x	46	7MG	N3-C4-N9	9.99	139.74	126.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1618	6MZ	1	0
1	1A	1835	2MG	1	0
1	1A	1915	3TD	1	0
1	1A	1917	PSU	1	0
1	1A	1939	5MU	1	0
1	1A	1962	5MC	1	0
1	1A	2030	6MZ	2	0
1	1A	2069	G7M	2	0
1	1A	2251	OMG	2	0
1	1A	2445	2MG	2	0
1	1A	2498	OMC	1	0
1	1A	2503	2MA	4	0
1	1A	2604	PSU	1	0
1	1A	745	1MG	2	0
1	1A	747	5MU	2	0
1	1A	955	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
59	EVN	1A	3001	1	116,123,123	2.00	21 (18%)	154,191,191	1.91	36 (23%)

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
59	EVN	1A	3001	1	-	0/50/234/234	1/13/13/13

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	3001	EVN	CDN-CAC	-6.67	1.38	1.51
59	1A	3001	EVN	CEG-CDI	-5.79	1.39	1.51
59	1A	3001	EVN	CDD-CDB	-4.35	1.39	1.50
59	1A	3001	EVN	CAD-CAJ	-4.12	1.40	1.50
59	1A	3001	EVN	CCT-CCS	-2.79	1.48	1.53
59	1A	3001	EVN	CAY-NDQ	-2.14	1.48	1.52
59	1A	3001	EVN	CBI-CBJ	-2.01	1.48	1.54
59	1A	3001	EVN	CAZ-CAU	2.00	1.56	1.51
59	1A	3001	EVN	OAL-CAJ	2.02	1.38	1.34
59	1A	3001	EVN	O1-C1	2.02	1.47	1.41
59	1A	3001	EVN	OBV-CBV	2.04	1.46	1.41
59	1A	3001	EVN	OCN-CCI	2.05	1.46	1.41
59	1A	3001	EVN	OBE-CBD	2.05	1.43	1.41
59	1A	3001	EVN	OBQ-CBM	2.23	1.47	1.41
59	1A	3001	EVN	OBX-CBW	2.45	1.48	1.43
59	1A	3001	EVN	OCN-CCM	2.69	1.48	1.43
59	1A	3001	EVN	OCX-CCY	3.38	1.47	1.41
59	1A	3001	EVN	OCZ-CCY	3.42	1.47	1.41
59	1A	3001	EVN	ODT-CAX	3.50	1.49	1.42
59	1A	3001	EVN	OCW-CCQ	5.58	1.45	1.40
59	1A	3001	EVN	ODS-NDQ	12.19	1.45	1.21

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1A	3001	EVN	OCX-CCS-CCT	-9.43	99.01	106.55
59	1A	3001	EVN	OCZ-CCT-CCS	-5.91	98.47	106.36
59	1A	3001	EVN	OCR-CCL-CCK	-5.28	94.64	103.45
59	1A	3001	EVN	CAP-OAQ-CAR	-4.05	104.28	114.19
59	1A	3001	EVN	OBK-CBJ-CBI	-3.93	96.90	103.98
59	1A	3001	EVN	CBD-OBE-CBF	-3.36	109.09	112.11
59	1A	3001	EVN	OCF-CCK-CCL	-3.17	98.90	103.49
59	1A	3001	EVN	CCY-OCZ-CCT	-3.16	101.27	106.22
59	1A	3001	EVN	CDW-CBF-CBA	-2.86	108.95	113.36
59	1A	3001	EVN	CAA-CAF-CAE	-2.69	115.65	120.64
59	1A	3001	EVN	ODL-CAE-CAD	-2.60	113.95	120.12
59	1A	3001	EVN	CBV-O4-C4	-2.52	111.85	118.00
59	1A	3001	EVN	CEF-O2-C2	-2.51	107.68	114.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1A	3001	EVN	CBD-CBC-CBB	-2.49	107.48	113.03
59	1A	3001	EVN	CCM-CCL-CCK	-2.48	107.47	112.57
59	1A	3001	EVN	ODJ-CDE-CDD	-2.45	116.47	121.14
59	1A	3001	EVN	CAP-OAS-CBA	-2.37	109.80	114.68
59	1A	3001	EVN	CDX-CBO-CBJ	-2.17	109.23	113.58
59	1A	3001	EVN	CDY-CBI-CBJ	-2.15	108.55	114.85
59	1A	3001	EVN	O2-C2-C3	-2.06	105.31	110.25
59	1A	3001	EVN	CDP-CAW-CAX	-2.05	109.47	113.58
59	1A	3001	EVN	CAU-OAT-CAN	-2.03	111.90	116.31
59	1A	3001	EVN	OAL-CAM-CAN	2.03	112.27	108.20
59	1A	3001	EVN	OAS-CAP-CAO	2.12	112.22	108.47
59	1A	3001	EVN	ODL-CAE-CAF	2.14	123.33	120.07
59	1A	3001	EVN	OAV-CAW-CDP	2.14	111.21	106.69
59	1A	3001	EVN	O1-C1-C2	2.15	113.50	109.07
59	1A	3001	EVN	O4-C4-C3	2.29	112.71	107.19
59	1A	3001	EVN	OAL-CAM-CAR	2.36	112.53	107.77
59	1A	3001	EVN	OCW-CCQ-OCR	2.36	114.32	109.91
59	1A	3001	EVN	OBQ-CBR-CBW	2.42	113.01	107.19
59	1A	3001	EVN	OBE-CBF-CDW	3.25	109.92	105.81
59	1A	3001	EVN	CDM-ODL-CAE	3.41	124.15	114.81
59	1A	3001	EVN	O1-CCI-OCN	4.32	117.83	108.98
59	1A	3001	EVN	CAE-CAF-CLAG	5.62	128.17	118.88
59	1A	3001	EVN	CAF-CAA-CAB	5.74	123.19	117.71

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	3001	EVN	CAU-CAW-CAX-CAY-CAZ-OAV

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.